



wwPDB EM Validation Summary Report ⓘ

Dec 9, 2025 – 11:23 AM EST

PDB ID : 9Y6S / pdb_00009y6s
EMDB ID : EMD-72629
Title : 96-nm repeat of the Leishmania tarentolae doublet microtubule
Authors : Doran, M.H.; Brown, A.
Deposited on : 2025-09-09
Resolution : 3.70 Å (reported)
Based on initial model : .

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev129
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) : 2.47

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.70 Å.

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

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

2 Entry composition

There are 168 unique types of molecules in this entry. The entry contains 3422719 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	AB	419	Total	C	N	O	S	0	0
			3283	2056	560	636	31		
1	AD	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	AF	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	AH	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	AJ	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	AL	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	AN	419	Total	C	N	O	S	0	0
			3283	2056	560	636	31		
1	B	418	Total	C	N	O	S	0	0
			3270	2039	564	637	30		
1	BD	430	Total	C	N	O	S	0	0
			3370	2106	579	653	32		
1	BF	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	BH	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	BJ	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	BL	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	BN	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	CA	424	Total	C	N	O	S	0	0
			3319	2076	568	643	32		
1	CC	430	Total	C	N	O	S	0	0
			3370	2106	579	653	32		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	CE	430	Total	C	N	O	S	0	0
			3370	2106	579	653	32		
1	CG	430	Total	C	N	O	S	0	0
			3370	2106	579	653	32		
1	CI	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	CK	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	CM	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	DA	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	DC	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	DE	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	DG	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	DI	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	DK	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	DM	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	E	430	Total	C	N	O	S	0	0
			3370	2106	579	653	32		
1	EB	430	Total	C	N	O	S	0	0
			3370	2106	579	653	32		
1	ED	430	Total	C	N	O	S	0	0
			3370	2106	579	653	32		
1	EF	430	Total	C	N	O	S	0	0
			3370	2106	579	653	32		
1	EH	430	Total	C	N	O	S	0	0
			3370	2106	579	653	32		
1	EJ	430	Total	C	N	O	S	0	0
			3370	2106	579	653	32		
1	EL	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	F	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	FB	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	FD	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	FF	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	FH	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	FJ	429	Total	C	N	O	S	0	0
			3361	2100	578	652	31		
1	FL	426	Total	C	N	O	S	0	0
			3343	2089	575	648	31		
1	G	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	GB	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	GD	426	Total	C	N	O	S	0	0
			3343	2089	575	648	31		
1	GF	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	GH	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	GJ	425	Total	C	N	O	S	0	0
			3335	2085	574	645	31		
1	GL	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	H	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	HB	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	HD	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	HF	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	HH	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	HJ	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	HL	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	I	430	Total	C	N	O	S	0	0
			3370	2106	579	653	32		
1	IB	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	ID	429	Total 3362	C 2101	N 578	O 652	S 31	0	0
1	IF	429	Total 3362	C 2101	N 578	O 652	S 31	0	0
1	IH	429	Total 3362	C 2101	N 578	O 652	S 31	0	0
1	IJ	429	Total 3362	C 2101	N 578	O 652	S 31	0	0
1	IL	429	Total 3362	C 2101	N 578	O 652	S 31	0	0
1	JA	429	Total 3362	C 2101	N 578	O 652	S 31	0	0
1	JC	429	Total 3362	C 2101	N 578	O 652	S 31	0	0
1	JE	429	Total 3362	C 2101	N 578	O 652	S 31	0	0
1	JG	429	Total 3362	C 2101	N 578	O 652	S 31	0	0
1	JI	429	Total 3362	C 2101	N 578	O 652	S 31	0	0
1	JK	429	Total 3362	C 2101	N 578	O 652	S 31	0	0
1	JM	426	Total 3343	C 2089	N 575	O 648	S 31	0	0
1	KA	430	Total 3370	C 2106	N 579	O 653	S 32	0	0
1	KC	429	Total 3362	C 2101	N 578	O 652	S 31	0	0
1	KE	429	Total 3362	C 2101	N 578	O 652	S 31	0	0
1	KG	429	Total 3362	C 2101	N 578	O 652	S 31	0	0
1	KI	429	Total 3362	C 2101	N 578	O 652	S 31	0	0
1	KK	429	Total 3362	C 2101	N 578	O 652	S 31	0	0
1	KM	429	Total 3362	C 2101	N 578	O 652	S 31	0	0
1	LA	429	Total 3362	C 2101	N 578	O 652	S 31	0	0
1	LC	429	Total 3362	C 2101	N 578	O 652	S 31	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	LE	429	Total 3362	C 2101	N 578	O 652	S 31	0	0
1	LG	429	Total 3362	C 2101	N 578	O 652	S 31	0	0
1	LI	429	Total 3362	C 2101	N 578	O 652	S 31	0	0
1	LK	429	Total 3362	C 2101	N 578	O 652	S 31	0	0
1	LM	429	Total 3362	C 2101	N 578	O 652	S 31	0	0
1	LO	429	Total 3362	C 2101	N 578	O 652	S 31	0	0
1	M	429	Total 3362	C 2101	N 578	O 652	S 31	0	0
1	MB	429	Total 3362	C 2101	N 578	O 652	S 31	0	0
1	MD	429	Total 3362	C 2101	N 578	O 652	S 31	0	0
1	MF	429	Total 3362	C 2101	N 578	O 652	S 31	0	0
1	MH	429	Total 3362	C 2101	N 578	O 652	S 31	0	0
1	MJ	429	Total 3362	C 2101	N 578	O 652	S 31	0	0
1	ML	429	Total 3362	C 2101	N 578	O 652	S 31	0	0
1	MN	429	Total 3362	C 2101	N 578	O 652	S 31	0	0
1	N	420	Total 3290	C 2060	N 561	O 638	S 31	0	0
1	NB	420	Total 3290	C 2060	N 561	O 638	S 31	0	0
1	ND	427	Total 3348	C 2092	N 576	O 649	S 31	0	0
1	NF	427	Total 3348	C 2092	N 576	O 649	S 31	0	0
1	NH	426	Total 3343	C 2089	N 575	O 648	S 31	0	0
1	NJ	429	Total 3362	C 2101	N 578	O 652	S 31	0	0
1	NL	426	Total 3343	C 2089	N 575	O 648	S 31	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	O	426	Total 3343	C 2089	N 575	O 648	S 31	0	0
1	OB	425	Total 3335	C 2085	N 574	O 645	S 31	0	0
1	OD	426	Total 3343	C 2089	N 575	O 648	S 31	0	0
1	OF	426	Total 3343	C 2089	N 575	O 648	S 31	0	0
1	OH	426	Total 3343	C 2089	N 575	O 648	S 31	0	0
1	OJ	426	Total 3343	C 2089	N 575	O 648	S 31	0	0
1	OL	426	Total 3343	C 2089	N 575	O 648	S 31	0	0
1	P	401	Total 3123	C 1946	N 540	O 609	S 28	0	0
1	PB	429	Total 3362	C 2101	N 578	O 652	S 31	0	0
1	PD	429	Total 3362	C 2101	N 578	O 652	S 31	0	0
1	PF	429	Total 3362	C 2101	N 578	O 652	S 31	0	0
1	PH	426	Total 3342	C 2089	N 575	O 647	S 31	0	0
1	PJ	429	Total 3362	C 2101	N 578	O 652	S 31	0	0
1	PL	429	Total 3362	C 2101	N 578	O 652	S 31	0	0
1	QA	427	Total 3348	C 2092	N 576	O 649	S 31	0	0
1	QC	427	Total 3348	C 2092	N 576	O 649	S 31	0	0
1	QE	426	Total 3343	C 2089	N 575	O 648	S 31	0	0
1	QG	427	Total 3348	C 2092	N 576	O 649	S 31	0	0
1	QI	427	Total 3348	C 2092	N 576	O 649	S 31	0	0
1	QK	427	Total 3348	C 2092	N 576	O 649	S 31	0	0
1	RA	426	Total 3343	C 2089	N 575	O 648	S 31	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	RC	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	RE	426	Total	C	N	O	S	0	0
			3343	2089	575	648	31		
1	RG	426	Total	C	N	O	S	0	0
			3343	2089	575	648	31		
1	RI	426	Total	C	N	O	S	0	0
			3342	2088	575	648	31		
1	RK	428	Total	C	N	O	S	0	0
			3355	2096	577	651	31		
1	S	425	Total	C	N	O	S	0	0
			3335	2085	574	645	31		
1	SB	425	Total	C	N	O	S	0	0
			3335	2085	574	645	31		
1	SD	425	Total	C	N	O	S	0	0
			3335	2085	574	645	31		
1	SF	425	Total	C	N	O	S	0	0
			3335	2085	574	645	31		
1	SH	428	Total	C	N	O	S	0	0
			3355	2096	577	651	31		
1	SJ	427	Total	C	N	O	S	0	0
			3348	2092	576	649	31		
1	T	427	Total	C	N	O	S	0	0
			3348	2092	576	649	31		
1	TB	428	Total	C	N	O	S	0	0
			3355	2096	577	651	31		
1	TD	426	Total	C	N	O	S	0	0
			3343	2089	575	648	31		
1	TF	427	Total	C	N	O	S	0	0
			3348	2092	576	649	31		
1	TH	426	Total	C	N	O	S	0	0
			3343	2089	575	648	31		
1	TJ	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	TL	427	Total	C	N	O	S	0	0
			3348	2092	576	649	31		
1	U	425	Total	C	N	O	S	0	0
			3335	2085	574	645	31		
1	UB	425	Total	C	N	O	S	0	0
			3335	2085	574	645	31		
1	UD	425	Total	C	N	O	S	0	0
			3335	2085	574	645	31		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	UF	425	Total 3335	C 2085	N 574	O 645	S 31	0	0
1	UH	425	Total 3335	C 2085	N 574	O 645	S 31	0	0
1	UJ	427	Total 3348	C 2092	N 576	O 649	S 31	0	0
1	UL	426	Total 3343	C 2089	N 575	O 648	S 31	0	0
1	V	428	Total 3355	C 2096	N 577	O 651	S 31	0	0
1	VB	426	Total 3343	C 2089	N 575	O 648	S 31	0	0
1	VD	427	Total 3348	C 2092	N 576	O 649	S 31	0	0
1	VF	428	Total 3355	C 2096	N 577	O 651	S 31	0	0
1	VH	425	Total 3335	C 2085	N 574	O 645	S 31	0	0
1	VJ	429	Total 3362	C 2101	N 578	O 652	S 31	0	0
1	VL	429	Total 3362	C 2101	N 578	O 652	S 31	0	0
1	W	425	Total 3335	C 2085	N 574	O 645	S 31	0	0
1	WB	425	Total 3335	C 2085	N 574	O 645	S 31	0	0
1	WD	425	Total 3335	C 2085	N 574	O 645	S 31	0	0
1	WF	427	Total 3348	C 2092	N 576	O 649	S 31	0	0
1	WH	425	Total 3335	C 2085	N 574	O 645	S 31	0	0
1	WJ	425	Total 3335	C 2085	N 574	O 645	S 31	0	0
1	WL	426	Total 3343	C 2089	N 575	O 648	S 31	0	0
1	AP	429	Total 3362	C 2101	N 578	O 652	S 31	0	0
1	AR	429	Total 3362	C 2101	N 578	O 652	S 31	0	0
1	AT	429	Total 3362	C 2101	N 578	O 652	S 31	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	AV	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	AX	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	AZ	419	Total	C	N	O	S	0	0
			3283	2056	560	636	31		
1	BP	430	Total	C	N	O	S	0	0
			3370	2106	579	653	32		
1	BR	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	BT	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	BV	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	BX	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	CO	430	Total	C	N	O	S	0	0
			3370	2106	579	653	32		
1	CQ	430	Total	C	N	O	S	0	0
			3370	2106	579	653	32		
1	CS	430	Total	C	N	O	S	0	0
			3370	2106	579	653	32		
1	CU	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	CW	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	CY	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	DO	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	DQ	426	Total	C	N	O	S	0	0
			3343	2089	575	648	31		
1	DS	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	DU	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	DW	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	DY	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	EN	430	Total	C	N	O	S	0	0
			3370	2106	579	653	32		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	EP	430	Total	C	N	O	S	0	0
			3370	2106	579	653	32		
1	ER	430	Total	C	N	O	S	0	0
			3370	2106	579	653	32		
1	ET	430	Total	C	N	O	S	0	0
			3370	2106	579	653	32		
1	EV	430	Total	C	N	O	S	0	0
			3370	2106	579	653	32		
1	EX	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	FN	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	FP	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	FR	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	FT	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	FV	429	Total	C	N	O	S	0	0
			3361	2100	578	652	31		
1	FX	426	Total	C	N	O	S	0	0
			3343	2089	575	648	31		
1	GN	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	GP	426	Total	C	N	O	S	0	0
			3343	2089	575	648	31		
1	GR	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	GT	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	GV	425	Total	C	N	O	S	0	0
			3335	2085	574	645	31		
1	GX	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	HN	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	HP	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	HR	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	HT	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	HV	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	HX	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	IN	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	IP	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	IR	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	IT	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	IV	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	IX	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	JO	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	JQ	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	JS	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	JU	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	JW	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	JY	426	Total	C	N	O	S	0	0
			3343	2089	575	648	31		
1	KO	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	KQ	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	KS	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	KU	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	KW	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	KY	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	LQ	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	LS	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	LU	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	LW	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	LY	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	MP	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	MR	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	MT	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	MV	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	MX	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	MZ	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	PN	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	PP	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	PR	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	PT	426	Total	C	N	O	S	0	0
			3342	2089	575	647	31		
1	PV	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	PX	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	QM	427	Total	C	N	O	S	0	0
			3348	2092	576	649	31		
1	QO	427	Total	C	N	O	S	0	0
			3348	2092	576	649	31		
1	QQ	426	Total	C	N	O	S	0	0
			3343	2089	575	648	31		
1	QS	427	Total	C	N	O	S	0	0
			3348	2092	576	649	31		
1	QU	427	Total	C	N	O	S	0	0
			3348	2092	576	649	31		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	QW	427	Total	C	N	O	S	0	0
			3348	2092	576	649	31		
1	RM	426	Total	C	N	O	S	0	0
			3343	2089	575	648	31		
1	RO	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	RQ	426	Total	C	N	O	S	0	0
			3343	2089	575	648	31		
1	RS	426	Total	C	N	O	S	0	0
			3343	2089	575	648	31		
1	RU	426	Total	C	N	O	S	0	0
			3342	2088	575	648	31		
1	RW	428	Total	C	N	O	S	0	0
			3355	2096	577	651	31		
1	SL	425	Total	C	N	O	S	0	0
			3335	2085	574	645	31		
1	SN	425	Total	C	N	O	S	0	0
			3335	2085	574	645	31		
1	SP	425	Total	C	N	O	S	0	0
			3335	2085	574	645	31		
1	SR	425	Total	C	N	O	S	0	0
			3335	2085	574	645	31		
1	ST	428	Total	C	N	O	S	0	0
			3355	2096	577	651	31		
1	SV	427	Total	C	N	O	S	0	0
			3348	2092	576	649	31		
1	TN	428	Total	C	N	O	S	0	0
			3355	2096	577	651	31		
1	TP	426	Total	C	N	O	S	0	0
			3343	2089	575	648	31		
1	TR	427	Total	C	N	O	S	0	0
			3348	2092	576	649	31		
1	TT	426	Total	C	N	O	S	0	0
			3343	2089	575	648	31		
1	TV	429	Total	C	N	O	S	0	0
			3362	2101	578	652	31		
1	TX	427	Total	C	N	O	S	0	0
			3348	2092	576	649	31		
1	UN	425	Total	C	N	O	S	0	0
			3335	2085	574	645	31		
1	UP	425	Total	C	N	O	S	0	0
			3335	2085	574	645	31		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	UR	425	Total 3335	C 2085	N 574	O 645	S 31	0	0
1	UT	425	Total 3335	C 2085	N 574	O 645	S 31	0	0
1	UV	427	Total 3348	C 2092	N 576	O 649	S 31	0	0
1	UX	426	Total 3343	C 2089	N 575	O 648	S 31	0	0
1	VN	426	Total 3343	C 2089	N 575	O 648	S 31	0	0
1	VP	427	Total 3348	C 2092	N 576	O 649	S 31	0	0
1	VR	428	Total 3355	C 2096	N 577	O 651	S 31	0	0
1	VT	425	Total 3335	C 2085	N 574	O 645	S 31	0	0
1	VV	429	Total 3362	C 2101	N 578	O 652	S 31	0	0
1	VX	429	Total 3362	C 2101	N 578	O 652	S 31	0	0
1	WN	425	Total 3335	C 2085	N 574	O 645	S 31	0	0
1	WP	425	Total 3335	C 2085	N 574	O 645	S 31	0	0
1	WR	427	Total 3348	C 2092	N 576	O 649	S 31	0	0
1	WT	425	Total 3335	C 2085	N 574	O 645	S 31	0	0
1	WV	425	Total 3335	C 2085	N 574	O 645	S 31	0	0
1	WX	426	Total 3343	C 2089	N 575	O 648	S 31	0	0
1	NN	420	Total 3290	C 2060	N 561	O 638	S 31	0	0
1	NP	427	Total 3348	C 2092	N 576	O 649	S 31	0	0
1	NR	427	Total 3348	C 2092	N 576	O 649	S 31	0	0
1	NT	426	Total 3343	C 2089	N 575	O 648	S 31	0	0
1	NV	429	Total 3362	C 2101	N 578	O 652	S 31	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	NX	426	Total	C	N	O	S	0	0
			3343	2089	575	648	31		
1	ON	425	Total	C	N	O	S	0	0
			3335	2085	574	645	31		
1	OP	426	Total	C	N	O	S	0	0
			3343	2089	575	648	31		
1	OR	426	Total	C	N	O	S	0	0
			3343	2089	575	648	31		
1	OT	426	Total	C	N	O	S	0	0
			3343	2089	575	648	31		
1	OV	426	Total	C	N	O	S	0	0
			3343	2089	575	648	31		
1	OX	426	Total	C	N	O	S	0	0
			3343	2089	575	648	31		

- Molecule 2 is a protein called Tubulin alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	AA	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	AC	433	Total	C	N	O	S	0	0
			3353	2117	570	643	23		
2	AE	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	AG	433	Total	C	N	O	S	0	0
			3352	2116	571	642	23		
2	AI	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	AK	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	AM	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	BA	429	Total	C	N	O	S	0	0
			3322	2098	566	635	23		
2	BE	429	Total	C	N	O	S	0	0
			3322	2098	566	635	23		
2	BG	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	BI	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	BK	429	Total	C	N	O	S	0	0
			3322	2098	566	635	23		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	BM	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	C	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	CB	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	CD	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	CF	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	CH	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	CJ	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	CL	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	D	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	DB	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	DD	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	DF	431	Total	C	N	O	S	0	0
			3337	2107	568	639	23		
2	DH	430	Total	C	N	O	S	0	0
			3328	2102	567	636	23		
2	DJ	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	DL	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	EA	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	EC	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	EE	432	Total	C	N	O	S	0	0
			3346	2112	569	642	23		
2	EG	433	Total	C	N	O	S	0	0
			3351	2114	570	644	23		
2	EI	431	Total	C	N	O	S	0	0
			3337	2107	568	639	23		
2	EK	431	Total	C	N	O	S	0	0
			3337	2107	568	639	23		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	FA	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	FC	434	Total	C	N	O	S	0	0
			3360	2119	571	647	23		
2	FE	432	Total	C	N	O	S	0	0
			3343	2110	569	641	23		
2	FG	431	Total	C	N	O	S	0	0
			3337	2107	568	639	23		
2	FI	429	Total	C	N	O	S	0	0
			3322	2098	566	635	23		
2	FK	431	Total	C	N	O	S	0	0
			3337	2107	568	639	23		
2	GA	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	GC	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	GE	431	Total	C	N	O	S	0	0
			3337	2107	568	639	23		
2	GG	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	GI	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	GK	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	HA	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	HC	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	HE	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	HG	432	Total	C	N	O	S	0	0
			3343	2110	569	641	23		
2	HI	431	Total	C	N	O	S	0	0
			3336	2106	568	639	23		
2	HK	432	Total	C	N	O	S	0	0
			3343	2110	569	641	23		
2	HM	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	IA	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	IC	432	Total	C	N	O	S	0	0
			3343	2110	569	641	23		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	IE	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	IG	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	II	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	IK	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	IM	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	J	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	JB	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	JD	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	JF	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	JH	432	Total	C	N	O	S	0	0
			3342	2110	569	640	23		
2	JJ	432	Total	C	N	O	S	0	0
			3343	2110	569	641	23		
2	JL	432	Total	C	N	O	S	0	0
			3343	2110	569	641	23		
2	JN	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	K	434	Total	C	N	O	S	0	0
			3358	2119	572	643	24		
2	KB	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	KD	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	KF	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	KH	431	Total	C	N	O	S	0	0
			3335	2106	568	638	23		
2	KJ	432	Total	C	N	O	S	0	0
			3346	2112	569	642	23		
2	KL	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	KN	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	L	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	LB	432	Total	C	N	O	S	0	0
			3346	2112	569	642	23		
2	LD	429	Total	C	N	O	S	0	0
			3322	2097	566	637	22		
2	LF	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	LH	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	LJ	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	LL	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	LN	432	Total	C	N	O	S	0	0
			3346	2112	569	642	23		
2	MA	431	Total	C	N	O	S	0	0
			3335	2106	568	638	23		
2	MC	437	Total	C	N	O	S	0	0
			3379	2133	575	647	24		
2	ME	436	Total	C	N	O	S	0	0
			3368	2124	573	647	24		
2	MG	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	MI	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	MK	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	MM	431	Total	C	N	O	S	0	0
			3335	2106	568	638	23		
2	NA	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	NC	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	NE	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	NG	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	NI	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	NK	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	NM	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	OA	432	Total	C	N	O	S	0	0
			3343	2110	569	641	23		
2	OC	431	Total	C	N	O	S	0	0
			3337	2107	568	639	23		
2	OE	431	Total	C	N	O	S	0	0
			3337	2107	568	639	23		
2	OG	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	OI	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	OK	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	OM	433	Total	C	N	O	S	0	0
			3352	2115	570	644	23		
2	PA	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	PC	431	Total	C	N	O	S	0	0
			3337	2107	568	639	23		
2	PE	431	Total	C	N	O	S	0	0
			3337	2107	568	639	23		
2	PG	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	PI	431	Total	C	N	O	S	0	0
			3337	2107	568	639	23		
2	PK	432	Total	C	N	O	S	0	0
			3343	2110	569	641	23		
2	PM	432	Total	C	N	O	S	0	0
			3343	2110	569	641	23		
2	Q	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	QB	429	Total	C	N	O	S	0	0
			3323	2100	566	634	23		
2	QD	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	QF	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	QH	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	QJ	431	Total	C	N	O	S	0	0
			3337	2107	568	639	23		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	QL	432	Total	C	N	O	S	0	0
			3343	2110	569	641	23		
2	R	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	RB	431	Total	C	N	O	S	0	0
			3337	2107	568	639	23		
2	RD	431	Total	C	N	O	S	0	0
			3337	2107	568	639	23		
2	RF	431	Total	C	N	O	S	0	0
			3337	2107	568	639	23		
2	RH	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	RJ	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	RL	431	Total	C	N	O	S	0	0
			3335	2106	568	638	23		
2	SA	431	Total	C	N	O	S	0	0
			3337	2107	568	639	23		
2	SC	431	Total	C	N	O	S	0	0
			3335	2106	568	638	23		
2	SE	431	Total	C	N	O	S	0	0
			3335	2106	568	638	23		
2	SG	431	Total	C	N	O	S	0	0
			3337	2107	568	639	23		
2	SI	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	SK	432	Total	C	N	O	S	0	0
			3343	2110	569	641	23		
2	TA	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	TC	428	Total	C	N	O	S	0	0
			3314	2093	565	634	22		
2	TE	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	TG	431	Total	C	N	O	S	0	0
			3337	2107	568	639	23		
2	TI	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	TK	433	Total	C	N	O	S	0	0
			3353	2117	570	643	23		
2	UA	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	UC	429	Total	C	N	O	S	0	0
			3322	2097	566	637	22		
2	UE	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	UG	431	Total	C	N	O	S	0	0
			3337	2107	568	639	23		
2	UI	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	UK	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	VA	431	Total	C	N	O	S	0	0
			3337	2107	568	639	23		
2	VC	431	Total	C	N	O	S	0	0
			3337	2107	568	639	23		
2	VE	431	Total	C	N	O	S	0	0
			3337	2107	568	639	23		
2	VG	431	Total	C	N	O	S	0	0
			3337	2107	568	639	23		
2	VI	432	Total	C	N	O	S	0	0
			3342	2109	569	641	23		
2	VK	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	VM	434	Total	C	N	O	S	0	0
			3360	2119	571	647	23		
2	WA	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	WC	431	Total	C	N	O	S	0	0
			3337	2107	568	639	23		
2	WE	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	WG	431	Total	C	N	O	S	0	0
			3337	2107	568	639	23		
2	WI	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	WK	431	Total	C	N	O	S	0	0
			3337	2107	568	639	23		
2	WM	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	AO	433	Total	C	N	O	S	0	0
			3353	2117	570	643	23		
2	AQ	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	AS	433	Total	C	N	O	S	0	0
			3352	2116	571	642	23		
2	AU	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	AW	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	AY	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	BO	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	BQ	429	Total	C	N	O	S	0	0
			3322	2098	566	635	23		
2	BS	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	BU	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	BW	429	Total	C	N	O	S	0	0
			3322	2098	566	635	23		
2	BY	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	CN	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	CP	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	CR	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	CT	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	CV	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	CX	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	DN	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	DP	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	DR	431	Total	C	N	O	S	0	0
			3337	2107	568	639	23		
2	DT	430	Total	C	N	O	S	0	0
			3328	2102	567	636	23		
2	DV	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	DX	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	EM	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	EO	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	EQ	432	Total	C	N	O	S	0	0
			3346	2112	569	642	23		
2	ES	433	Total	C	N	O	S	0	0
			3351	2114	570	644	23		
2	EU	431	Total	C	N	O	S	0	0
			3337	2107	568	639	23		
2	EW	431	Total	C	N	O	S	0	0
			3337	2107	568	639	23		
2	FM	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	FO	434	Total	C	N	O	S	0	0
			3360	2119	571	647	23		
2	FQ	432	Total	C	N	O	S	0	0
			3343	2110	569	641	23		
2	FS	431	Total	C	N	O	S	0	0
			3337	2107	568	639	23		
2	FU	429	Total	C	N	O	S	0	0
			3322	2098	566	635	23		
2	FW	431	Total	C	N	O	S	0	0
			3337	2107	568	639	23		
2	GM	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	GO	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	GQ	431	Total	C	N	O	S	0	0
			3337	2107	568	639	23		
2	GS	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	GU	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	GW	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	HO	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	HQ	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	HS	432	Total	C	N	O	S	0	0
			3343	2110	569	641	23		
2	HU	431	Total	C	N	O	S	0	0
			3336	2106	568	639	23		
2	HW	432	Total	C	N	O	S	0	0
			3343	2110	569	641	23		
2	HY	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	IO	432	Total	C	N	O	S	0	0
			3343	2110	569	641	23		
2	IQ	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	IS	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	IU	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	IW	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	IY	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	JP	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	JR	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	JT	432	Total	C	N	O	S	0	0
			3342	2110	569	640	23		
2	JV	432	Total	C	N	O	S	0	0
			3343	2110	569	641	23		
2	JX	432	Total	C	N	O	S	0	0
			3343	2110	569	641	23		
2	JZ	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	KP	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	KR	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	KT	431	Total	C	N	O	S	0	0
			3335	2106	568	638	23		
2	KV	432	Total	C	N	O	S	0	0
			3346	2112	569	642	23		
2	KX	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	KZ	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	LP	429	Total	C	N	O	S	0	0
			3322	2097	566	637	22		
2	LR	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	LT	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	LV	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	LX	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	LZ	432	Total	C	N	O	S	0	0
			3346	2112	569	642	23		
2	MO	437	Total	C	N	O	S	0	0
			3379	2133	575	647	24		
2	MQ	436	Total	C	N	O	S	0	0
			3368	2124	573	647	24		
2	MS	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	MU	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	MW	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	MY	431	Total	C	N	O	S	0	0
			3335	2106	568	638	23		
2	PO	431	Total	C	N	O	S	0	0
			3337	2107	568	639	23		
2	PQ	431	Total	C	N	O	S	0	0
			3337	2107	568	639	23		
2	PS	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	PU	431	Total	C	N	O	S	0	0
			3337	2107	568	639	23		
2	PW	432	Total	C	N	O	S	0	0
			3343	2110	569	641	23		
2	PY	432	Total	C	N	O	S	0	0
			3343	2110	569	641	23		
2	QN	429	Total	C	N	O	S	0	0
			3323	2100	566	634	23		
2	QP	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	QR	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	QT	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	QV	431	Total	C	N	O	S	0	0
			3337	2107	568	639	23		
2	QX	432	Total	C	N	O	S	0	0
			3343	2110	569	641	23		
2	RN	431	Total	C	N	O	S	0	0
			3337	2107	568	639	23		
2	RP	431	Total	C	N	O	S	0	0
			3337	2107	568	639	23		
2	RR	431	Total	C	N	O	S	0	0
			3337	2107	568	639	23		
2	RT	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	RV	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	RX	431	Total	C	N	O	S	0	0
			3335	2106	568	638	23		
2	SM	431	Total	C	N	O	S	0	0
			3337	2107	568	639	23		
2	SO	431	Total	C	N	O	S	0	0
			3335	2106	568	638	23		
2	SQ	431	Total	C	N	O	S	0	0
			3335	2106	568	638	23		
2	SS	431	Total	C	N	O	S	0	0
			3337	2107	568	639	23		
2	SU	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	SW	432	Total	C	N	O	S	0	0
			3343	2110	569	641	23		
2	TM	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	TO	428	Total	C	N	O	S	0	0
			3314	2093	565	634	22		
2	TQ	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	TS	431	Total	C	N	O	S	0	0
			3337	2107	568	639	23		
2	TU	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	TW	433	Total	C	N	O	S	0	0
			3353	2117	570	643	23		
2	UM	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	UO	429	Total	C	N	O	S	0	0
			3322	2097	566	637	22		
2	UQ	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	US	431	Total	C	N	O	S	0	0
			3337	2107	568	639	23		
2	UU	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	UW	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	VO	431	Total	C	N	O	S	0	0
			3337	2107	568	639	23		
2	VQ	431	Total	C	N	O	S	0	0
			3337	2107	568	639	23		
2	VS	431	Total	C	N	O	S	0	0
			3337	2107	568	639	23		
2	VU	432	Total	C	N	O	S	0	0
			3342	2109	569	641	23		
2	VW	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	VY	434	Total	C	N	O	S	0	0
			3360	2119	571	647	23		
2	WO	431	Total	C	N	O	S	0	0
			3337	2107	568	639	23		
2	WQ	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	WS	431	Total	C	N	O	S	0	0
			3337	2107	568	639	23		
2	WU	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	WW	431	Total	C	N	O	S	0	0
			3337	2107	568	639	23		
2	WY	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	NO	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	NQ	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	NS	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	NU	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	NW	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	NY	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	OO	431	Total	C	N	O	S	0	0
			3337	2107	568	639	23		
2	OQ	431	Total	C	N	O	S	0	0
			3337	2107	568	639	23		
2	OS	439	Total	C	N	O	S	0	0
			3394	2141	577	652	24		
2	OU	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	OW	430	Total	C	N	O	S	0	0
			3329	2103	567	636	23		
2	OY	433	Total	C	N	O	S	0	0
			3352	2115	570	644	23		

- Molecule 3 is a protein called CFAP20.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	X	183	Total	C	N	O	S	0	0
			1510	965	264	270	11		
3	XA	183	Total	C	N	O	S	0	0
			1510	965	264	270	11		
3	XB	183	Total	C	N	O	S	0	0
			1510	965	264	270	11		
3	XC	183	Total	C	N	O	S	0	0
			1510	965	264	270	11		
3	XD	183	Total	C	N	O	S	0	0
			1510	965	264	270	11		
3	XE	183	Total	C	N	O	S	0	0
			1510	965	264	270	11		
3	XF	183	Total	C	N	O	S	0	0
			1510	965	264	270	11		
3	XG	183	Total	C	N	O	S	0	0
			1510	965	264	270	11		
3	XH	183	Total	C	N	O	S	0	0
			1510	965	264	270	11		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	XI	183	Total	C	N	O	S	0	0
			1510	965	264	270	11		
3	XJ	183	Total	C	N	O	S	0	0
			1510	965	264	270	11		
3	XK	183	Total	C	N	O	S	0	0
			1510	965	264	270	11		
3	XL	183	Total	C	N	O	S	0	0
			1510	965	264	270	11		

- Molecule 4 is a protein called PACRGA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	XM	259	Total	C	N	O	S	0	0
			2045	1307	360	370	8		
4	XO	260	Total	C	N	O	S	0	0
			2053	1311	361	373	8		
4	XQ	260	Total	C	N	O	S	0	0
			2053	1311	361	373	8		
4	XR	260	Total	C	N	O	S	0	0
			2056	1313	364	371	8		
4	XT	260	Total	C	N	O	S	0	0
			2053	1311	361	373	8		
4	XV	260	Total	C	N	O	S	0	0
			2053	1311	361	373	8		
4	XW	260	Total	C	N	O	S	0	0
			2056	1313	364	371	8		

- Molecule 5 is a protein called PACRGB.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	XN	269	Total	C	N	O	S	0	0
			2116	1359	366	384	7		
5	XP	269	Total	C	N	O	S	0	0
			2116	1359	366	384	7		
5	XS	269	Total	C	N	O	S	0	0
			2116	1359	366	384	7		
5	XU	269	Total	C	N	O	S	0	0
			2116	1359	366	384	7		

- Molecule 6 is a protein called CCDC81.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	0A	257	Total	C	N	O	S	0	0
			2004	1261	359	371	13		
6	0	257	Total	C	N	O	S	0	0
			2004	1261	359	371	13		
6	0B	257	Total	C	N	O	S	0	0
			2004	1261	359	371	13		

- Molecule 7 is a protein called CFAP21.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	0C	121	Total	C	N	O	S	0	0
			935	584	159	188	4		
7	0D	354	Total	C	N	O	S	0	0
			2723	1683	492	537	11		
7	0E	354	Total	C	N	O	S	0	0
			2723	1683	492	537	11		

- Molecule 8 is a protein called CFAP45.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	0F	176	Total	C	N	O	S	0	0
			1439	859	288	280	12		
8	0I	285	Total	C	N	O	S	0	0
			2369	1421	471	459	18		
8	0H	349	Total	C	N	O	S	0	0
			2955	1772	596	570	17		
8	0K	28	Total	C	N	O		0	0
			229	146	41	42			
8	9A	226	Total	C	N	O	S	0	0
			1906	1147	379	373	7		
8	0G	444	Total	C	N	O	S	0	0
			3711	2221	751	718	21		
8	0J	449	Total	C	N	O	S	0	0
			3757	2255	754	727	21		

- Molecule 9 is a protein called CFAP52.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	0L	624	Total	C	N	O	S	0	0
			4757	2973	844	908	32		
9	0M	624	Total	C	N	O	S	0	0
			4757	2973	844	908	32		

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Mol	Chain	Residues	Atoms					AltConf	Trace
9	0N	624	Total	C	N	O	S	0	0
			4757	2973	844	908	32		
9	0O	624	Total	C	N	O	S	0	0
			4757	2973	844	908	32		
9	0P	624	Total	C	N	O	S	0	0
			4757	2973	844	908	32		
9	0Q	624	Total	C	N	O	S	0	0
			4757	2973	844	908	32		
9	9B	310	Total	C	N	O	S	0	0
			2357	1482	416	445	14		

- Molecule 10 is a protein called CFAP53.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	0R	309	Total	C	N	O	S	0	0
			2628	1579	535	501	13		
10	0T	221	Total	C	N	O	S	0	0
			1874	1148	360	359	7		
10	0S	460	Total	C	N	O	S	0	0
			3908	2370	779	743	16		

- Molecule 11 is a protein called CFAP67A.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	0U	333	Total	C	N	O	S	0	0
			2570	1621	437	495	17		
11	0V	333	Total	C	N	O	S	0	0
			2570	1621	437	495	17		

- Molecule 12 is a protein called CFAP67B.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	0W	339	Total	C	N	O	S	0	0
			2595	1647	427	501	20		
12	0X	339	Total	C	N	O	S	0	0
			2595	1647	427	501	20		

- Molecule 13 is a protein called CFAP106A.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	0Y	233	Total	C	N	O	S	0	0
			1836	1152	334	345	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
13	0Z	235	Total	C	N	O	S	0	0
			1849	1160	337	347	5		
13	0a	233	Total	C	N	O	S	0	0
			1836	1152	334	345	5		
13	0b	235	Total	C	N	O	S	0	0
			1849	1160	337	347	5		

- Molecule 14 is a protein called CFAP106B.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	0c	237	Total	C	N	O	S	0	0
			1929	1221	337	362	9		
14	0d	265	Total	C	N	O	S	0	0
			2150	1359	378	404	9		
14	0e	265	Total	C	N	O	S	0	0
			2150	1359	378	404	9		

- Molecule 15 is a protein called CFAP107.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	0f	160	Total	C	N	O	S	0	0
			1257	783	222	241	11		
15	0g	160	Total	C	N	O	S	0	0
			1257	783	222	241	11		
15	0h	30	Total	C	N	O	S	0	0
			218	137	34	46	1		

- Molecule 16 is a protein called CFAP115.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	0i	180	Total	C	N	O	S	0	0
			1463	930	264	263	6		
16	0j	688	Total	C	N	O	S	0	0
			5411	3423	987	975	26		
16	0l	640	Total	C	N	O	S	0	0
			5045	3192	918	914	21		
16	0k	710	Total	C	N	O	S	0	0
			5599	3537	1026	1009	27		

- Molecule 17 is a protein called CFAP127.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	0m	142	Total	C	N	O	S	0	0
			1155	704	220	227	4		
17	0n	406	Total	C	N	O	S	0	0
			3388	2054	668	654	12		
17	0o	406	Total	C	N	O	S	0	0
			3388	2054	668	654	12		
17	9C	20	Total	C	N	O		0	0
			171	107	35	29			

- Molecule 18 is a protein called CFAP141.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	0p	108	Total	C	N	O	S	0	0
			906	557	177	169	3		
18	0q	108	Total	C	N	O	S	0	0
			906	557	177	169	3		

- Molecule 19 is a protein called CFAP143.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	0r	254	Total	C	N	O	S	0	0
			2033	1246	376	396	15		
19	0s	254	Total	C	N	O	S	0	0
			2033	1246	376	396	15		

- Molecule 20 is a protein called CFAP161.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	0t	262	Total	C	N	O	S	0	0
			2062	1298	358	388	18		
20	0u	227	Total	C	N	O	S	0	0
			1769	1117	306	330	16		
20	9D	227	Total	C	N	O	S	0	0
			1769	1117	306	330	16		

- Molecule 21 is a protein called CFAP210.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	0w	449	Total	C	N	O	S	0	0
			3715	2242	741	724	8		
21	0v	73	Total	C	N	O		0	0
			582	351	115	116			

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Mol	Chain	Residues	Atoms					AltConf	Trace
21	0y	111	Total	C	N	O	S	0	0
			906	556	175	172	3		
21	0x	490	Total	C	N	O	S	0	0
			4059	2455	802	792	10		

- Molecule 22 is a protein called DMIP5.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	0z	143	Total	C	N	O	S	0	0
			1160	716	220	219	5		
22	1w	180	Total	C	N	O	S	0	0
			1481	915	278	281	7		
22	1x	206	Total	C	N	O	S	0	0
			1680	1031	322	315	12		
22	2A	143	Total	C	N	O	S	0	0
			1157	715	220	217	5		
22	1y	180	Total	C	N	O	S	0	0
			1481	915	278	281	7		
22	1z	206	Total	C	N	O	S	0	0
			1680	1031	322	315	12		

- Molecule 23 is a protein called RIB43.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	1A	270	Total	C	N	O	S	0	0
			2286	1390	449	436	11		
23	1D	54	Total	C	N	O	S	0	0
			464	285	91	85	3		
23	1E	362	Total	C	N	O	S	0	0
			3050	1855	590	590	15		
23	1C	195	Total	C	N	O	S	0	0
			1667	1015	321	322	9		
23	1G	74	Total	C	N	O	S	0	0
			635	387	120	124	4		
23	1F	362	Total	C	N	O	S	0	0
			3050	1855	590	590	15		
23	1B	348	Total	C	N	O	S	0	0
			2953	1796	574	568	15		

- Molecule 24 is a protein called RIB72A.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	1H	588	Total	C	N	O	S	0	0
			4698	2967	812	900	19		
24	1I	659	Total	C	N	O	S	0	0
			5276	3326	920	1003	27		
24	1J	670	Total	C	N	O	S	0	0
			5356	3372	940	1018	26		
24	1K	588	Total	C	N	O	S	0	0
			4697	2966	812	900	19		
24	1L	659	Total	C	N	O	S	0	0
			5276	3326	920	1003	27		
24	1M	670	Total	C	N	O	S	0	0
			5356	3372	940	1018	26		
24	1N	588	Total	C	N	O	S	0	0
			4697	2966	812	900	19		

- Molecule 25 is a protein called RIB72B.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	1O	710	Total	C	N	O	S	0	0
			5751	3614	1021	1096	20		
25	1P	710	Total	C	N	O	S	0	0
			5751	3614	1021	1096	20		

- Molecule 26 is a protein called RIB72C.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	1Q	655	Total	C	N	O	S	0	0
			5263	3323	927	988	25		
26	1R	655	Total	C	N	O	S	0	0
			5263	3323	927	988	25		

- Molecule 27 is a protein called RIB72D.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	1S	726	Total	C	N	O	S	0	0
			5834	3696	1029	1076	33		
27	1T	726	Total	C	N	O	S	0	0
			5834	3696	1029	1076	33		
27	9E	222	Total	C	N	O	S	0	0
			1787	1125	315	335	12		

- Molecule 28 is a protein called STOP family protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	1U	120	Total	C	N	O	S	0	0
			942	594	162	181	5		
28	1V	168	Total	C	N	O	S	0	0
			1313	823	230	250	10		
28	1X	120	Total	C	N	O	S	0	0
			942	594	162	181	5		
28	1a	57	Total	C	N	O	S	0	0
			446	279	80	84	3		
28	1b	168	Total	C	N	O	S	0	0
			1313	823	230	250	10		
28	1d	120	Total	C	N	O	S	0	0
			942	594	162	181	5		
28	1e	168	Total	C	N	O	S	0	0
			1313	823	230	250	10		
28	1g	120	Total	C	N	O	S	0	0
			942	594	162	181	5		
28	4V	62	Total	C	N	O	S	0	0
			486	305	86	91	4		
28	1W	48	Total	C	N	O	S	0	0
			371	229	68	69	5		
28	1Z	169	Total	C	N	O	S	0	0
			1325	829	237	252	7		
28	1c	168	Total	C	N	O	S	0	0
			1313	823	230	250	10		
28	9F	35	Total	C	N	O	S	0	0
			263	162	50	46	5		
28	1f	48	Total	C	N	O	S	0	0
			371	229	68	69	5		
28	1i	155	Total	C	N	O	S	0	0
			1218	767	214	230	7		
28	4X	188	Total	C	N	O	S	0	0
			1474	927	255	283	9		
28	4W	222	Total	C	N	O	S	0	0
			1742	1095	304	332	11		
28	1Y	241	Total	C	N	O	S	0	0
			1893	1188	334	360	11		
28	1h	229	Total	C	N	O	S	0	0
			1798	1132	313	342	11		

There are 342 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1U	52	LEU	ILE	conflict	UNP A0A504XB09
1U	83	GLU	ASP	conflict	UNP A0A504XB09

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Chain	Residue	Modelled	Actual	Comment	Reference
1U	86	GLN	LYS	conflict	UNP A0A504XB09
1U	128	ALA	THR	conflict	UNP A0A504XB09
1U	139	ARG	PRO	conflict	UNP A0A504XB09
1U	171	THR	ALA	conflict	UNP A0A504XB09
1U	186	ASN	SER	conflict	UNP A0A504XB09
1U	192	PRO	GLN	conflict	UNP A0A504XB09
1U	206	THR	VAL	conflict	UNP A0A504XB09
1U	207	LYS	GLN	conflict	UNP A0A504XB09
1U	209	ILE	VAL	conflict	UNP A0A504XB09
1U	220	ALA	THR	conflict	UNP A0A504XB09
1U	221	SER	VAL	conflict	UNP A0A504XB09
1U	223	SER	GLU	conflict	UNP A0A504XB09
1U	230	VAL	MET	conflict	UNP A0A504XB09
1U	239	THR	ALA	conflict	UNP A0A504XB09
1U	243	ILE	THR	conflict	UNP A0A504XB09
1U	252	ILE	LEU	conflict	UNP A0A504XB09
1V	52	LEU	ILE	conflict	UNP A0A504XB09
1V	83	GLU	ASP	conflict	UNP A0A504XB09
1V	86	GLN	LYS	conflict	UNP A0A504XB09
1V	128	ALA	THR	conflict	UNP A0A504XB09
1V	139	ARG	PRO	conflict	UNP A0A504XB09
1V	171	THR	ALA	conflict	UNP A0A504XB09
1V	186	ASN	SER	conflict	UNP A0A504XB09
1V	192	PRO	GLN	conflict	UNP A0A504XB09
1V	206	THR	VAL	conflict	UNP A0A504XB09
1V	207	LYS	GLN	conflict	UNP A0A504XB09
1V	209	ILE	VAL	conflict	UNP A0A504XB09
1V	220	ALA	THR	conflict	UNP A0A504XB09
1V	221	SER	VAL	conflict	UNP A0A504XB09
1V	223	SER	GLU	conflict	UNP A0A504XB09
1V	230	VAL	MET	conflict	UNP A0A504XB09
1V	239	THR	ALA	conflict	UNP A0A504XB09
1V	243	ILE	THR	conflict	UNP A0A504XB09
1V	252	ILE	LEU	conflict	UNP A0A504XB09
1X	52	LEU	ILE	conflict	UNP A0A504XB09
1X	83	GLU	ASP	conflict	UNP A0A504XB09
1X	86	GLN	LYS	conflict	UNP A0A504XB09
1X	128	ALA	THR	conflict	UNP A0A504XB09
1X	139	ARG	PRO	conflict	UNP A0A504XB09
1X	171	THR	ALA	conflict	UNP A0A504XB09
1X	186	ASN	SER	conflict	UNP A0A504XB09
1X	192	PRO	GLN	conflict	UNP A0A504XB09

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Chain	Residue	Modelled	Actual	Comment	Reference
1X	206	THR	VAL	conflict	UNP A0A504XB09
1X	207	LYS	GLN	conflict	UNP A0A504XB09
1X	209	ILE	VAL	conflict	UNP A0A504XB09
1X	220	ALA	THR	conflict	UNP A0A504XB09
1X	221	SER	VAL	conflict	UNP A0A504XB09
1X	223	SER	GLU	conflict	UNP A0A504XB09
1X	230	VAL	MET	conflict	UNP A0A504XB09
1X	239	THR	ALA	conflict	UNP A0A504XB09
1X	243	ILE	THR	conflict	UNP A0A504XB09
1X	252	ILE	LEU	conflict	UNP A0A504XB09
1a	52	LEU	ILE	conflict	UNP A0A504XB09
1a	83	GLU	ASP	conflict	UNP A0A504XB09
1a	86	GLN	LYS	conflict	UNP A0A504XB09
1a	128	ALA	THR	conflict	UNP A0A504XB09
1a	139	ARG	PRO	conflict	UNP A0A504XB09
1a	171	THR	ALA	conflict	UNP A0A504XB09
1a	186	ASN	SER	conflict	UNP A0A504XB09
1a	192	PRO	GLN	conflict	UNP A0A504XB09
1a	206	THR	VAL	conflict	UNP A0A504XB09
1a	207	LYS	GLN	conflict	UNP A0A504XB09
1a	209	ILE	VAL	conflict	UNP A0A504XB09
1a	220	ALA	THR	conflict	UNP A0A504XB09
1a	221	SER	VAL	conflict	UNP A0A504XB09
1a	223	SER	GLU	conflict	UNP A0A504XB09
1a	230	VAL	MET	conflict	UNP A0A504XB09
1a	239	THR	ALA	conflict	UNP A0A504XB09
1a	243	ILE	THR	conflict	UNP A0A504XB09
1a	252	ILE	LEU	conflict	UNP A0A504XB09
1b	52	LEU	ILE	conflict	UNP A0A504XB09
1b	83	GLU	ASP	conflict	UNP A0A504XB09
1b	86	GLN	LYS	conflict	UNP A0A504XB09
1b	128	ALA	THR	conflict	UNP A0A504XB09
1b	139	ARG	PRO	conflict	UNP A0A504XB09
1b	171	THR	ALA	conflict	UNP A0A504XB09
1b	186	ASN	SER	conflict	UNP A0A504XB09
1b	192	PRO	GLN	conflict	UNP A0A504XB09
1b	206	THR	VAL	conflict	UNP A0A504XB09
1b	207	LYS	GLN	conflict	UNP A0A504XB09
1b	209	ILE	VAL	conflict	UNP A0A504XB09
1b	220	ALA	THR	conflict	UNP A0A504XB09
1b	221	SER	VAL	conflict	UNP A0A504XB09
1b	223	SER	GLU	conflict	UNP A0A504XB09

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Chain	Residue	Modelled	Actual	Comment	Reference
1b	230	VAL	MET	conflict	UNP A0A504XB09
1b	239	THR	ALA	conflict	UNP A0A504XB09
1b	243	ILE	THR	conflict	UNP A0A504XB09
1b	252	ILE	LEU	conflict	UNP A0A504XB09
1d	52	LEU	ILE	conflict	UNP A0A504XB09
1d	83	GLU	ASP	conflict	UNP A0A504XB09
1d	86	GLN	LYS	conflict	UNP A0A504XB09
1d	128	ALA	THR	conflict	UNP A0A504XB09
1d	139	ARG	PRO	conflict	UNP A0A504XB09
1d	171	THR	ALA	conflict	UNP A0A504XB09
1d	186	ASN	SER	conflict	UNP A0A504XB09
1d	192	PRO	GLN	conflict	UNP A0A504XB09
1d	206	THR	VAL	conflict	UNP A0A504XB09
1d	207	LYS	GLN	conflict	UNP A0A504XB09
1d	209	ILE	VAL	conflict	UNP A0A504XB09
1d	220	ALA	THR	conflict	UNP A0A504XB09
1d	221	SER	VAL	conflict	UNP A0A504XB09
1d	223	SER	GLU	conflict	UNP A0A504XB09
1d	230	VAL	MET	conflict	UNP A0A504XB09
1d	239	THR	ALA	conflict	UNP A0A504XB09
1d	243	ILE	THR	conflict	UNP A0A504XB09
1d	252	ILE	LEU	conflict	UNP A0A504XB09
1e	52	LEU	ILE	conflict	UNP A0A504XB09
1e	83	GLU	ASP	conflict	UNP A0A504XB09
1e	86	GLN	LYS	conflict	UNP A0A504XB09
1e	128	ALA	THR	conflict	UNP A0A504XB09
1e	139	ARG	PRO	conflict	UNP A0A504XB09
1e	171	THR	ALA	conflict	UNP A0A504XB09
1e	186	ASN	SER	conflict	UNP A0A504XB09
1e	192	PRO	GLN	conflict	UNP A0A504XB09
1e	206	THR	VAL	conflict	UNP A0A504XB09
1e	207	LYS	GLN	conflict	UNP A0A504XB09
1e	209	ILE	VAL	conflict	UNP A0A504XB09
1e	220	ALA	THR	conflict	UNP A0A504XB09
1e	221	SER	VAL	conflict	UNP A0A504XB09
1e	223	SER	GLU	conflict	UNP A0A504XB09
1e	230	VAL	MET	conflict	UNP A0A504XB09
1e	239	THR	ALA	conflict	UNP A0A504XB09
1e	243	ILE	THR	conflict	UNP A0A504XB09
1e	252	ILE	LEU	conflict	UNP A0A504XB09
1g	52	LEU	ILE	conflict	UNP A0A504XB09
1g	83	GLU	ASP	conflict	UNP A0A504XB09

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Chain	Residue	Modelled	Actual	Comment	Reference
1g	86	GLN	LYS	conflict	UNP A0A504XB09
1g	128	ALA	THR	conflict	UNP A0A504XB09
1g	139	ARG	PRO	conflict	UNP A0A504XB09
1g	171	THR	ALA	conflict	UNP A0A504XB09
1g	186	ASN	SER	conflict	UNP A0A504XB09
1g	192	PRO	GLN	conflict	UNP A0A504XB09
1g	206	THR	VAL	conflict	UNP A0A504XB09
1g	207	LYS	GLN	conflict	UNP A0A504XB09
1g	209	ILE	VAL	conflict	UNP A0A504XB09
1g	220	ALA	THR	conflict	UNP A0A504XB09
1g	221	SER	VAL	conflict	UNP A0A504XB09
1g	223	SER	GLU	conflict	UNP A0A504XB09
1g	230	VAL	MET	conflict	UNP A0A504XB09
1g	239	THR	ALA	conflict	UNP A0A504XB09
1g	243	ILE	THR	conflict	UNP A0A504XB09
1g	252	ILE	LEU	conflict	UNP A0A504XB09
4V	52	LEU	ILE	conflict	UNP A0A504XB09
4V	83	GLU	ASP	conflict	UNP A0A504XB09
4V	86	GLN	LYS	conflict	UNP A0A504XB09
4V	128	ALA	THR	conflict	UNP A0A504XB09
4V	139	ARG	PRO	conflict	UNP A0A504XB09
4V	171	THR	ALA	conflict	UNP A0A504XB09
4V	186	ASN	SER	conflict	UNP A0A504XB09
4V	192	PRO	GLN	conflict	UNP A0A504XB09
4V	206	THR	VAL	conflict	UNP A0A504XB09
4V	207	LYS	GLN	conflict	UNP A0A504XB09
4V	209	ILE	VAL	conflict	UNP A0A504XB09
4V	220	ALA	THR	conflict	UNP A0A504XB09
4V	221	SER	VAL	conflict	UNP A0A504XB09
4V	223	SER	GLU	conflict	UNP A0A504XB09
4V	230	VAL	MET	conflict	UNP A0A504XB09
4V	239	THR	ALA	conflict	UNP A0A504XB09
4V	243	ILE	THR	conflict	UNP A0A504XB09
4V	252	ILE	LEU	conflict	UNP A0A504XB09
1W	52	LEU	ILE	conflict	UNP A0A504XB09
1W	83	GLU	ASP	conflict	UNP A0A504XB09
1W	86	GLN	LYS	conflict	UNP A0A504XB09
1W	128	ALA	THR	conflict	UNP A0A504XB09
1W	139	ARG	PRO	conflict	UNP A0A504XB09
1W	171	THR	ALA	conflict	UNP A0A504XB09
1W	186	ASN	SER	conflict	UNP A0A504XB09
1W	192	PRO	GLN	conflict	UNP A0A504XB09

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Chain	Residue	Modelled	Actual	Comment	Reference
1W	206	THR	VAL	conflict	UNP A0A504XB09
1W	207	LYS	GLN	conflict	UNP A0A504XB09
1W	209	ILE	VAL	conflict	UNP A0A504XB09
1W	220	ALA	THR	conflict	UNP A0A504XB09
1W	221	SER	VAL	conflict	UNP A0A504XB09
1W	223	SER	GLU	conflict	UNP A0A504XB09
1W	230	VAL	MET	conflict	UNP A0A504XB09
1W	239	THR	ALA	conflict	UNP A0A504XB09
1W	243	ILE	THR	conflict	UNP A0A504XB09
1W	252	ILE	LEU	conflict	UNP A0A504XB09
1Z	52	LEU	ILE	conflict	UNP A0A504XB09
1Z	83	GLU	ASP	conflict	UNP A0A504XB09
1Z	86	GLN	LYS	conflict	UNP A0A504XB09
1Z	128	ALA	THR	conflict	UNP A0A504XB09
1Z	139	ARG	PRO	conflict	UNP A0A504XB09
1Z	171	THR	ALA	conflict	UNP A0A504XB09
1Z	186	ASN	SER	conflict	UNP A0A504XB09
1Z	192	PRO	GLN	conflict	UNP A0A504XB09
1Z	206	THR	VAL	conflict	UNP A0A504XB09
1Z	207	LYS	GLN	conflict	UNP A0A504XB09
1Z	209	ILE	VAL	conflict	UNP A0A504XB09
1Z	220	ALA	THR	conflict	UNP A0A504XB09
1Z	221	SER	VAL	conflict	UNP A0A504XB09
1Z	223	SER	GLU	conflict	UNP A0A504XB09
1Z	230	VAL	MET	conflict	UNP A0A504XB09
1Z	239	THR	ALA	conflict	UNP A0A504XB09
1Z	243	ILE	THR	conflict	UNP A0A504XB09
1Z	252	ILE	LEU	conflict	UNP A0A504XB09
1c	52	LEU	ILE	conflict	UNP A0A504XB09
1c	83	GLU	ASP	conflict	UNP A0A504XB09
1c	86	GLN	LYS	conflict	UNP A0A504XB09
1c	128	ALA	THR	conflict	UNP A0A504XB09
1c	139	ARG	PRO	conflict	UNP A0A504XB09
1c	171	THR	ALA	conflict	UNP A0A504XB09
1c	186	ASN	SER	conflict	UNP A0A504XB09
1c	192	PRO	GLN	conflict	UNP A0A504XB09
1c	206	THR	VAL	conflict	UNP A0A504XB09
1c	207	LYS	GLN	conflict	UNP A0A504XB09
1c	209	ILE	VAL	conflict	UNP A0A504XB09
1c	220	ALA	THR	conflict	UNP A0A504XB09
1c	221	SER	VAL	conflict	UNP A0A504XB09
1c	223	SER	GLU	conflict	UNP A0A504XB09

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Chain	Residue	Modelled	Actual	Comment	Reference
1c	230	VAL	MET	conflict	UNP A0A504XB09
1c	239	THR	ALA	conflict	UNP A0A504XB09
1c	243	ILE	THR	conflict	UNP A0A504XB09
1c	252	ILE	LEU	conflict	UNP A0A504XB09
9F	52	LEU	ILE	conflict	UNP A0A504XB09
9F	83	GLU	ASP	conflict	UNP A0A504XB09
9F	86	GLN	LYS	conflict	UNP A0A504XB09
9F	128	ALA	THR	conflict	UNP A0A504XB09
9F	139	ARG	PRO	conflict	UNP A0A504XB09
9F	171	THR	ALA	conflict	UNP A0A504XB09
9F	186	ASN	SER	conflict	UNP A0A504XB09
9F	192	PRO	GLN	conflict	UNP A0A504XB09
9F	206	THR	VAL	conflict	UNP A0A504XB09
9F	207	LYS	GLN	conflict	UNP A0A504XB09
9F	209	ILE	VAL	conflict	UNP A0A504XB09
9F	220	ALA	THR	conflict	UNP A0A504XB09
9F	221	SER	VAL	conflict	UNP A0A504XB09
9F	223	SER	GLU	conflict	UNP A0A504XB09
9F	230	VAL	MET	conflict	UNP A0A504XB09
9F	239	THR	ALA	conflict	UNP A0A504XB09
9F	243	ILE	THR	conflict	UNP A0A504XB09
9F	252	ILE	LEU	conflict	UNP A0A504XB09
1f	52	LEU	ILE	conflict	UNP A0A504XB09
1f	83	GLU	ASP	conflict	UNP A0A504XB09
1f	86	GLN	LYS	conflict	UNP A0A504XB09
1f	128	ALA	THR	conflict	UNP A0A504XB09
1f	139	ARG	PRO	conflict	UNP A0A504XB09
1f	171	THR	ALA	conflict	UNP A0A504XB09
1f	186	ASN	SER	conflict	UNP A0A504XB09
1f	192	PRO	GLN	conflict	UNP A0A504XB09
1f	206	THR	VAL	conflict	UNP A0A504XB09
1f	207	LYS	GLN	conflict	UNP A0A504XB09
1f	209	ILE	VAL	conflict	UNP A0A504XB09
1f	220	ALA	THR	conflict	UNP A0A504XB09
1f	221	SER	VAL	conflict	UNP A0A504XB09
1f	223	SER	GLU	conflict	UNP A0A504XB09
1f	230	VAL	MET	conflict	UNP A0A504XB09
1f	239	THR	ALA	conflict	UNP A0A504XB09
1f	243	ILE	THR	conflict	UNP A0A504XB09
1f	252	ILE	LEU	conflict	UNP A0A504XB09
1i	52	LEU	ILE	conflict	UNP A0A504XB09
1i	83	GLU	ASP	conflict	UNP A0A504XB09

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Chain	Residue	Modelled	Actual	Comment	Reference
1i	86	GLN	LYS	conflict	UNP A0A504XB09
1i	128	ALA	THR	conflict	UNP A0A504XB09
1i	139	ARG	PRO	conflict	UNP A0A504XB09
1i	171	THR	ALA	conflict	UNP A0A504XB09
1i	186	ASN	SER	conflict	UNP A0A504XB09
1i	192	PRO	GLN	conflict	UNP A0A504XB09
1i	206	THR	VAL	conflict	UNP A0A504XB09
1i	207	LYS	GLN	conflict	UNP A0A504XB09
1i	209	ILE	VAL	conflict	UNP A0A504XB09
1i	220	ALA	THR	conflict	UNP A0A504XB09
1i	221	SER	VAL	conflict	UNP A0A504XB09
1i	223	SER	GLU	conflict	UNP A0A504XB09
1i	230	VAL	MET	conflict	UNP A0A504XB09
1i	239	THR	ALA	conflict	UNP A0A504XB09
1i	243	ILE	THR	conflict	UNP A0A504XB09
1i	252	ILE	LEU	conflict	UNP A0A504XB09
4X	52	LEU	ILE	conflict	UNP A0A504XB09
4X	83	GLU	ASP	conflict	UNP A0A504XB09
4X	86	GLN	LYS	conflict	UNP A0A504XB09
4X	128	ALA	THR	conflict	UNP A0A504XB09
4X	139	ARG	PRO	conflict	UNP A0A504XB09
4X	171	THR	ALA	conflict	UNP A0A504XB09
4X	186	ASN	SER	conflict	UNP A0A504XB09
4X	192	PRO	GLN	conflict	UNP A0A504XB09
4X	206	THR	VAL	conflict	UNP A0A504XB09
4X	207	LYS	GLN	conflict	UNP A0A504XB09
4X	209	ILE	VAL	conflict	UNP A0A504XB09
4X	220	ALA	THR	conflict	UNP A0A504XB09
4X	221	SER	VAL	conflict	UNP A0A504XB09
4X	223	SER	GLU	conflict	UNP A0A504XB09
4X	230	VAL	MET	conflict	UNP A0A504XB09
4X	239	THR	ALA	conflict	UNP A0A504XB09
4X	243	ILE	THR	conflict	UNP A0A504XB09
4X	252	ILE	LEU	conflict	UNP A0A504XB09
4W	52	LEU	ILE	conflict	UNP A0A504XB09
4W	83	GLU	ASP	conflict	UNP A0A504XB09
4W	86	GLN	LYS	conflict	UNP A0A504XB09
4W	128	ALA	THR	conflict	UNP A0A504XB09
4W	139	ARG	PRO	conflict	UNP A0A504XB09
4W	171	THR	ALA	conflict	UNP A0A504XB09
4W	186	ASN	SER	conflict	UNP A0A504XB09
4W	192	PRO	GLN	conflict	UNP A0A504XB09

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Chain	Residue	Modelled	Actual	Comment	Reference
4W	206	THR	VAL	conflict	UNP A0A504XB09
4W	207	LYS	GLN	conflict	UNP A0A504XB09
4W	209	ILE	VAL	conflict	UNP A0A504XB09
4W	220	ALA	THR	conflict	UNP A0A504XB09
4W	221	SER	VAL	conflict	UNP A0A504XB09
4W	223	SER	GLU	conflict	UNP A0A504XB09
4W	230	VAL	MET	conflict	UNP A0A504XB09
4W	239	THR	ALA	conflict	UNP A0A504XB09
4W	243	ILE	THR	conflict	UNP A0A504XB09
4W	252	ILE	LEU	conflict	UNP A0A504XB09
1Y	52	LEU	ILE	conflict	UNP A0A504XB09
1Y	83	GLU	ASP	conflict	UNP A0A504XB09
1Y	86	GLN	LYS	conflict	UNP A0A504XB09
1Y	128	ALA	THR	conflict	UNP A0A504XB09
1Y	139	ARG	PRO	conflict	UNP A0A504XB09
1Y	171	THR	ALA	conflict	UNP A0A504XB09
1Y	186	ASN	SER	conflict	UNP A0A504XB09
1Y	192	PRO	GLN	conflict	UNP A0A504XB09
1Y	206	THR	VAL	conflict	UNP A0A504XB09
1Y	207	LYS	GLN	conflict	UNP A0A504XB09
1Y	209	ILE	VAL	conflict	UNP A0A504XB09
1Y	220	ALA	THR	conflict	UNP A0A504XB09
1Y	221	SER	VAL	conflict	UNP A0A504XB09
1Y	223	SER	GLU	conflict	UNP A0A504XB09
1Y	230	VAL	MET	conflict	UNP A0A504XB09
1Y	239	THR	ALA	conflict	UNP A0A504XB09
1Y	243	ILE	THR	conflict	UNP A0A504XB09
1Y	252	ILE	LEU	conflict	UNP A0A504XB09
1h	52	LEU	ILE	conflict	UNP A0A504XB09
1h	83	GLU	ASP	conflict	UNP A0A504XB09
1h	86	GLN	LYS	conflict	UNP A0A504XB09
1h	128	ALA	THR	conflict	UNP A0A504XB09
1h	139	ARG	PRO	conflict	UNP A0A504XB09
1h	171	THR	ALA	conflict	UNP A0A504XB09
1h	186	ASN	SER	conflict	UNP A0A504XB09
1h	192	PRO	GLN	conflict	UNP A0A504XB09
1h	206	THR	VAL	conflict	UNP A0A504XB09
1h	207	LYS	GLN	conflict	UNP A0A504XB09
1h	209	ILE	VAL	conflict	UNP A0A504XB09
1h	220	ALA	THR	conflict	UNP A0A504XB09
1h	221	SER	VAL	conflict	UNP A0A504XB09
1h	223	SER	GLU	conflict	UNP A0A504XB09

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Chain	Residue	Modelled	Actual	Comment	Reference
1h	230	VAL	MET	conflict	UNP A0A504XB09
1h	239	THR	ALA	conflict	UNP A0A504XB09
1h	243	ILE	THR	conflict	UNP A0A504XB09
1h	252	ILE	LEU	conflict	UNP A0A504XB09

- Molecule 29 is a protein called DMIP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	1j	113	Total	C	N	O	S	0	0
			909	584	153	168	4		
29	1k	103	Total	C	N	O	S	0	0
			801	502	140	157	2		
29	1l	113	Total	C	N	O	S	0	0
			909	584	153	168	4		
29	1m	103	Total	C	N	O	S	0	0
			801	502	140	157	2		
29	1n	113	Total	C	N	O	S	0	0
			909	584	153	168	4		
29	9G	53	Total	C	N	O	S	0	0
			420	268	72	78	2		

- Molecule 30 is a protein called DMIP3.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	1o	128	Total	C	N	O	S	0	0
			1035	645	193	192	5		
30	1p	128	Total	C	N	O	S	0	0
			1035	645	193	192	5		

- Molecule 31 is a protein called DMIP4.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	1q	214	Total	C	N	O	S	0	0
			1679	1025	322	321	11		
31	1r	106	Total	C	N	O	S	0	0
			868	532	166	165	5		
31	1s	183	Total	C	N	O	S	0	0
			1446	884	273	277	12		
31	1t	214	Total	C	N	O	S	0	0
			1679	1025	322	321	11		
31	1u	106	Total	C	N	O	S	0	0
			868	532	166	165	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
31	1v	183	Total	C	N	O	S	0	0
			1446	884	273	277	12		
31	9H	75	Total	C	N	O	S	0	0
			618	372	125	116	5		

- Molecule 32 is a protein called DMIP6.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	2B	251	Total	C	N	O	S	0	0
			1977	1231	357	377	12		
32	2C	230	Total	C	N	O	S	0	0
			1814	1130	329	344	11		
32	2D	251	Total	C	N	O	S	0	0
			1977	1231	357	377	12		
32	2E	230	Total	C	N	O	S	0	0
			1814	1130	329	344	11		

- Molecule 33 is a protein called DMIP7.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	2F	284	Total	C	N	O	S	0	0
			2253	1411	411	418	13		
33	2G	283	Total	C	N	O	S	0	0
			2245	1407	409	416	13		
33	2H	288	Total	C	N	O	S	0	0
			2281	1428	416	424	13		
33	2I	243	Total	C	N	O	S	0	0
			1937	1208	355	363	11		
33	2J	283	Total	C	N	O	S	0	0
			2245	1407	409	416	13		
33	2K	288	Total	C	N	O	S	0	0
			2281	1428	416	424	13		
33	9I	243	Total	C	N	O	S	0	0
			1937	1208	355	363	11		

- Molecule 34 is a protein called DMIP8.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	2L	172	Total	C	N	O	S	0	0
			1433	904	254	269	6		
34	2M	172	Total	C	N	O	S	0	0
			1433	904	254	269	6		

- Molecule 35 is a protein called DMIP9.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	2N	135	Total	C	N	O	S	0	0
			1103	698	208	194	3		
35	2P	161	Total	C	N	O	S	0	0
			1324	827	251	240	6		
35	2O	274	Total	C	N	O	S	0	0
			2235	1404	420	402	9		

- Molecule 36 is a protein called DMIP10.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	2Q	291	Total	C	N	O	S	0	0
			2320	1483	394	429	14		
36	2R	291	Total	C	N	O	S	0	0
			2320	1483	394	429	14		

- Molecule 37 is a protein called DMIP11.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	2S	237	Total	C	N	O	S	0	0
			1798	1126	317	340	15		

- Molecule 38 is a protein called DMIP12.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	2U	229	Total	C	N	O	S	0	0
			1807	1111	329	355	12		
38	2V	109	Total	C	N	O	S	0	0
			870	530	167	169	4		
38	2W	109	Total	C	N	O	S	0	0
			870	530	167	169	4		

- Molecule 39 is a protein called DMIP13.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	2X	227	Total	C	N	O	S	0	0
			1774	1081	355	328	10		
39	2Y	227	Total	C	N	O	S	0	0
			1774	1081	355	328	10		

- Molecule 40 is a protein called DMIP14.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	2Z	283	Total	C	N	O	S	0	0
			2258	1427	412	414	5		
40	2a	283	Total	C	N	O	S	0	0
			2258	1427	412	414	5		

- Molecule 41 is a protein called DMIP15.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	2b	121	Total	C	N	O	S	0	0
			1006	613	195	194	4		
41	2e	325	Total	C	N	O	S	0	0
			2735	1649	546	526	14		
41	2h	237	Total	C	N	O	S	0	0
			1978	1187	396	385	10		
41	2k	167	Total	C	N	O	S	0	0
			1369	834	266	262	7		
41	2n	42	Total	C	N	O		0	0
			361	219	72	70			
41	2o	287	Total	C	N	O	S	0	0
			2453	1473	490	478	12		
41	2d	245	Total	C	N	O	S	0	0
			2092	1254	418	408	12		
41	2f	325	Total	C	N	O	S	0	0
			2735	1649	546	526	14		
41	2g	52	Total	C	N	O	S	0	0
			454	275	89	88	2		
41	2j	149	Total	C	N	O	S	0	0
			1301	776	266	252	7		
41	2m	264	Total	C	N	O	S	0	0
			2228	1338	445	432	13		
41	2p	287	Total	C	N	O	S	0	0
			2453	1473	490	478	12		
41	2q	49	Total	C	N	O	S	0	0
			425	257	86	80	2		
41	2c	306	Total	C	N	O	S	0	0
			2599	1565	519	502	13		
41	2i	309	Total	C	N	O	S	0	0
			2615	1574	523	505	13		
41	2l	325	Total	C	N	O	S	0	0
			2735	1649	546	526	14		

- Molecule 42 is a protein called DMIP16.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	2r	315	Total	C	N	O	S	0	0
			2473	1564	439	460	10		
42	2s	315	Total	C	N	O	S	0	0
			2473	1564	439	460	10		

- Molecule 43 is a protein called DMIP17.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	2t	214	Total	C	N	O	S	0	0
			1713	1075	302	324	12		
43	2u	214	Total	C	N	O	S	0	0
			1713	1075	302	324	12		

- Molecule 44 is a protein called DMIP18.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	2v	280	Total	C	N	O	S	0	0
			2264	1438	391	425	10		
44	2w	412	Total	C	N	O	S	0	0
			3291	2082	565	629	15		
44	2x	412	Total	C	N	O	S	0	0
			3291	2082	565	629	15		

- Molecule 45 is a protein called DMIP19.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	2y	287	Total	C	N	O	S	0	0
			2316	1424	424	460	8		
45	3A	187	Total	C	N	O	S	0	0
			1435	890	257	287	1		
45	2z	409	Total	C	N	O	S	0	0
			3258	2010	596	644	8		

- Molecule 46 is a protein called DMIP20.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	3B	418	Total	C	N	O	S	0	0
			3308	2069	596	631	12		
46	3C	418	Total	C	N	O	S	0	0
			3308	2069	596	631	12		

- Molecule 47 is a protein called DMIP21.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	3D	412	Total	C	N	O	S	0	0
			3212	1986	586	628	12		
47	3E	412	Total	C	N	O	S	0	0
			3212	1986	586	628	12		

- Molecule 48 is a protein called DMIP22.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	3I	80	Total	C	N	O	S	0	0
			640	400	114	122	4		
48	3F	155	Total	C	N	O	S	0	0
			1254	777	240	230	7		
48	3G	90	Total	C	N	O	S	0	0
			733	456	139	134	4		
48	3H	103	Total	C	N	O	S	0	0
			832	516	161	151	4		
48	3M	29	Total	C	N	O	S	0	0
			247	155	44	45	3		
48	3L	29	Total	C	N	O	S	0	0
			247	155	44	45	3		
48	9J	80	Total	C	N	O	S	0	0
			640	400	114	122	4		
48	3J	90	Total	C	N	O	S	0	0
			733	456	139	134	4		
48	3K	103	Total	C	N	O	S	0	0
			832	516	161	151	4		
48	3O	29	Total	C	N	O	S	0	0
			247	155	44	45	3		
48	3N	29	Total	C	N	O	S	0	0
			247	155	44	45	3		

- Molecule 49 is a protein called DMIP23.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	3P	256	Total	C	N	O	S	0	0
			2002	1260	351	380	11		
49	3Q	490	Total	C	N	O	S	0	0
			3825	2406	666	735	18		
49	3R	490	Total	C	N	O	S	0	0
			3825	2406	666	735	18		

- Molecule 50 is a protein called DMIP24.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	3S	25	Total	C	N	O	S	0	0
			182	109	36	33	4		
50	X1	39	Total	C	N	O	S	0	0
			304	183	58	63			
50	3T	64	Total	C	N	O	S	0	0
			486	292	94	96	4		

- Molecule 51 is a protein called DMIP25.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	3U	140	Total	C	N	O	S	0	0
			1074	681	186	203	4		
51	3V	140	Total	C	N	O	S	0	0
			1074	681	186	203	4		

- Molecule 52 is a protein called DMIP26.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	3X	202	Total	C	N	O	S	0	0
			1650	1025	305	309	11		
52	3W	153	Total	C	N	O	S	0	0
			1264	786	231	239	8		
52	3Y	49	Total	C	N	O	S	0	0
			386	239	74	70	3		

- Molecule 53 is a protein called DMIP27.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	3Z	181	Total	C	N	O	S	0	0
			1405	862	264	271	8		
53	3a	87	Total	C	N	O	S	0	0
			712	442	130	136	4		
53	4Y	181	Total	C	N	O	S	0	0
			1403	860	264	271	8		

- Molecule 54 is a protein called ArcMAP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	3b	136	Total	C	N	O	S	0	0
			1126	695	204	223	4		
54	3c	136	Total	C	N	O	S	0	0
			1126	695	204	223	4		

- Molecule 55 is a protein called ArcMAP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	3d	148	Total	C	N	O	S	0	0
			1240	765	229	240	6		
55	3e	148	Total	C	N	O	S	0	0
			1240	765	229	240	6		

- Molecule 56 is a protein called ArcMAP4.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	3f	165	Total	C	N	O	S	0	0
			1408	857	263	280	8		
56	3g	165	Total	C	N	O	S	0	0
			1408	857	263	280	8		
56	3h	165	Total	C	N	O	S	0	0
			1408	857	263	280	8		
56	3i	165	Total	C	N	O	S	0	0
			1408	857	263	280	8		
56	3j	165	Total	C	N	O	S	0	0
			1408	857	263	280	8		
56	3k	165	Total	C	N	O	S	0	0
			1408	857	263	280	8		
56	3l	165	Total	C	N	O	S	0	0
			1408	857	263	280	8		

- Molecule 57 is a protein called ArcMAP3.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	3m	144	Total	C	N	O	S	0	0
			1216	745	236	231	4		
57	3n	144	Total	C	N	O	S	0	0
			1216	745	236	231	4		

- Molecule 58 is a protein called CFAP96.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	3o	55	Total	C	N	O	S	0	0
			459	293	79	85	2		
58	3p	161	Total	C	N	O	S	0	0
			1276	821	220	233	2		
58	4O	175	Total	C	N	O	S	0	0
			1399	899	245	253	2		
58	4a	154	Total	C	N	O	S	0	0
			1233	796	213	223	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
58	3q	148	Total	C	N	O	S	0	0
			1159	744	201	212	2		
58	4Q	69	Total	C	N	O	S	0	0
			529	346	84	98	1		
58	4c	69	Total	C	N	O	S	0	0
			529	346	84	98	1		
58	4P	215	Total	C	N	O	S	0	0
			1707	1103	290	311	3		
58	4b	194	Total	C	N	O	S	0	0
			1541	1000	258	281	2		

- Molecule 59 is a protein called CFAP97.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	3r	130	Total	C	N	O	S	0	0
			1098	668	221	205	4		
59	3s	130	Total	C	N	O	S	0	0
			1098	668	221	205	4		
59	3t	130	Total	C	N	O	S	0	0
			1098	668	221	205	4		
59	3u	130	Total	C	N	O	S	0	0
			1098	668	221	205	4		
59	3v	63	Total	C	N	O	S	0	0
			533	326	105	98	4		

- Molecule 60 is a protein called DMAP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	3w	166	Total	C	N	O	S	0	0
			1362	872	235	249	6		
60	3y	126	Total	C	N	O	S	0	0
			985	625	178	181	1		
60	3x	267	Total	C	N	O	S	0	0
			2165	1380	381	397	7		

- Molecule 61 is a protein called DMAP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	4A	29	Total	C	N	O	S	0	0
			229	142	43	43	1		
61	4B	201	Total	C	N	O	S	0	0
			1584	1003	275	302	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
61	4C	201	Total	C	N	O	S	0	0
			1584	1003	275	302	4		

- Molecule 62 is a protein called distal DC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	5B	393	Total	C	N	O	S	0	0
			3140	1922	594	613	11		
62	5C	393	Total	C	N	O	S	0	0
			3140	1922	594	613	11		
62	5D	393	Total	C	N	O	S	0	0
			3140	1922	594	613	11		
62	5E	168	Total	C	N	O	S	0	0
			1348	828	258	257	5		
62	5A	225	Total	C	N	O	S	0	0
			1792	1094	336	356	6		

- Molecule 63 is a protein called ODAD1 central coiled coil region domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	5G	444	Total	C	N	O	S	0	0
			3594	2191	674	710	19		
63	5H	444	Total	C	N	O	S	0	0
			3594	2191	674	710	19		
63	5I	444	Total	C	N	O	S	0	0
			3594	2191	674	710	19		
63	5J	185	Total	C	N	O	S	0	0
			1541	942	295	296	8		
63	5F	259	Total	C	N	O	S	0	0
			2053	1249	379	414	11		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
5G	273	PHE	SER	conflict	UNP A0A640KPU2
5H	273	PHE	SER	conflict	UNP A0A640KPU2
5I	273	PHE	SER	conflict	UNP A0A640KPU2
5J	273	PHE	SER	conflict	UNP A0A640KPU2
5F	273	PHE	SER	conflict	UNP A0A640KPU2

- Molecule 64 is a protein called ODA dDC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	5K	384	Total	C	N	O	S	0	0
			3128	1989	546	572	21		
64	5L	384	Total	C	N	O	S	0	0
			3128	1989	546	572	21		
64	5M	384	Total	C	N	O	S	0	0
			3128	1989	546	572	21		
64	5N	384	Total	C	N	O	S	0	0
			3128	1989	546	572	21		

- Molecule 65 is a protein called DC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	5O	107	Total	C	N	O	S	0	0
			809	523	130	152	4		
65	5P	107	Total	C	N	O	S	0	0
			809	523	130	152	4		
65	5Q	107	Total	C	N	O	S	0	0
			809	523	130	152	4		
65	5R	107	Total	C	N	O	S	0	0
			809	523	130	152	4		

- Molecule 66 is a protein called DC6.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	5S	92	Total	C	N	O	S	0	0
			749	470	137	133	9		
66	5T	92	Total	C	N	O	S	0	0
			749	470	137	133	9		
66	5U	92	Total	C	N	O	S	0	0
			749	470	137	133	9		
66	5V	92	Total	C	N	O	S	0	0
			749	470	137	133	9		

- Molecule 67 is a protein called Dynein heavy chain, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	5X	4565	Total	C	N	O	S	0	0
			36792	23377	6358	6859	198		
67	5W	3144	Total	C	N	O	S	0	0
			25199	16022	4339	4693	145		
67	5Y	4565	Total	C	N	O	S	0	0
			36794	23378	6359	6859	198		

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Mol	Chain	Residues	Atoms					AltConf	Trace
67	5Z	4565	Total	C	N	O	S	0	0
			36793	23378	6358	6859	198		
67	5a	1201	Total	C	N	O	S	0	0
			9781	6190	1721	1827	43		

- Molecule 68 is a protein called Dynein heavy chain, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	5c	4178	Total	C	N	O	S	0	0
			33422	21212	5674	6353	183		
68	5b	2730	Total	C	N	O	S	0	0
			21827	13877	3716	4102	132		
68	5d	4178	Total	C	N	O	S	0	0
			33422	21212	5674	6353	183		
68	5e	4178	Total	C	N	O	S	0	0
			33422	21212	5674	6353	183		
68	5f	1240	Total	C	N	O	S	0	0
			9901	6257	1666	1934	44		

- Molecule 69 is a protein called Dynein intermediate-chain-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	5g	565	Total	C	N	O	S	0	0
			4413	2802	751	830	30		
69	5h	565	Total	C	N	O	S	0	0
			4413	2802	751	830	30		
69	5i	565	Total	C	N	O	S	0	0
			4413	2802	751	830	30		
69	5j	565	Total	C	N	O	S	0	0
			4413	2802	751	830	30		

- Molecule 70 is a protein called Dynein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	5k	596	Total	C	N	O	S	0	0
			4766	2990	832	918	26		
70	5l	596	Total	C	N	O	S	0	0
			4766	2990	832	918	26		
70	5m	596	Total	C	N	O	S	0	0
			4766	2990	832	918	26		
70	5n	596	Total	C	N	O	S	0	0
			4766	2990	832	918	26		

- Molecule 71 is a protein called Dynein axonemal light chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	5o	208	Total	C	N	O	S	0	0
			1661	1047	292	312	10		
71	5p	208	Total	C	N	O	S	0	0
			1661	1047	292	312	10		
71	5q	208	Total	C	N	O	S	0	0
			1661	1047	292	312	10		
71	5r	208	Total	C	N	O	S	0	0
			1661	1047	292	312	10		

- Molecule 72 is a protein called EF-hand domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	5s	202	Total	C	N	O	S	0	0
			1576	1004	271	292	9		
72	5t	202	Total	C	N	O	S	0	0
			1576	1004	271	292	9		
72	5u	202	Total	C	N	O	S	0	0
			1576	1004	271	292	9		
72	5v	202	Total	C	N	O	S	0	0
			1576	1004	271	292	9		

- Molecule 73 is a protein called Dynein light chain roadblock.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	5w	112	Total	C	N	O	S	0	0
			867	544	152	166	5		
73	5x	112	Total	C	N	O	S	0	0
			867	544	152	166	5		
73	5y	112	Total	C	N	O	S	0	0
			867	544	152	166	5		
73	5z	112	Total	C	N	O	S	0	0
			867	544	152	166	5		

- Molecule 74 is a protein called Dynein light chain roadblock.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	6A	97	Total	C	N	O	S	0	0
			771	481	137	148	5		
74	6B	97	Total	C	N	O	S	0	0
			771	481	137	148	5		
74	6C	97	Total	C	N	O	S	0	0
			771	481	137	148	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
74	6D	97	Total	C	N	O	S	0	0
			771	481	137	148	5		

- Molecule 75 is a protein called Dynein light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	6E	99	Total	C	N	O	S	0	0
			824	532	133	151	8		
75	6F	99	Total	C	N	O	S	0	0
			824	532	133	151	8		
75	6G	99	Total	C	N	O	S	0	0
			824	532	133	151	8		
75	6H	99	Total	C	N	O	S	0	0
			824	532	133	151	8		

- Molecule 76 is a protein called Dynein light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	6I	90	Total	C	N	O	S	0	0
			721	466	117	133	5		
76	6J	90	Total	C	N	O	S	0	0
			721	466	117	133	5		
76	6K	90	Total	C	N	O	S	0	0
			721	466	117	133	5		
76	6L	90	Total	C	N	O	S	0	0
			721	466	117	133	5		

- Molecule 77 is a protein called Dynein light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	6M	91	Total	C	N	O	S	0	0
			745	481	121	136	7		
77	6N	91	Total	C	N	O	S	0	0
			745	481	121	136	7		
77	6O	91	Total	C	N	O	S	0	0
			745	481	121	136	7		
77	6P	91	Total	C	N	O	S	0	0
			745	481	121	136	7		
77	7U	88	Total	C	N	O	S	0	0
			717	463	117	131	6		
77	7V	88	Total	C	N	O	S	0	0
			717	463	117	131	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
77	7W	83	Total 677	C 440	N 108	O 123	S 6	0	0
77	7X	83	Total 677	C 440	N 108	O 123	S 6	0	0
77	7S	87	Total 709	C 459	N 115	O 129	S 6	0	0
77	7T	77	Total 632	C 413	N 100	O 113	S 6	0	0
77	9k	88	Total 717	C 463	N 117	O 131	S 6	0	0
77	9l	88	Total 717	C 463	N 117	O 131	S 6	0	0
77	9m	83	Total 677	C 440	N 108	O 123	S 6	0	0
77	9n	83	Total 677	C 440	N 108	O 123	S 6	0	0
77	9i	87	Total 709	C 459	N 115	O 129	S 6	0	0
77	9j	77	Total 632	C 413	N 100	O 113	S 6	0	0
77	8s	91	Total 745	C 481	N 121	O 136	S 7	0	0
77	8t	91	Total 745	C 481	N 121	O 136	S 7	0	0
77	8c	91	Total 745	C 481	N 121	O 136	S 7	0	0
77	8d	91	Total 745	C 481	N 121	O 136	S 7	0	0
77	8e	91	Total 745	C 481	N 121	O 136	S 7	0	0
77	8f	91	Total 745	C 481	N 121	O 136	S 7	0	0
77	8g	83	Total 677	C 440	N 108	O 123	S 6	0	0
77	8h	91	Total 745	C 481	N 121	O 136	S 7	0	0
77	8i	91	Total 745	C 481	N 121	O 136	S 7	0	0
77	8j	91	Total 745	C 481	N 121	O 136	S 7	0	0
77	8k	91	Total 745	C 481	N 121	O 136	S 7	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
77	8l	91	Total	C	N	O	S	0	0
			745	481	121	136	7		
77	8m	91	Total	C	N	O	S	0	0
			745	481	121	136	7		
77	8n	91	Total	C	N	O	S	0	0
			745	481	121	136	7		

- Molecule 78 is a protein called Dynein light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	6Q	89	Total	C	N	O	S	0	0
			733	470	126	133	4		
78	6R	89	Total	C	N	O	S	0	0
			733	470	126	133	4		
78	6S	89	Total	C	N	O	S	0	0
			733	470	126	133	4		
78	6T	89	Total	C	N	O	S	0	0
			733	470	126	133	4		

- Molecule 79 is a protein called Dynein light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	6U	91	Total	C	N	O	S	0	0
			749	489	119	134	7		
79	6V	91	Total	C	N	O	S	0	0
			749	489	119	134	7		
79	6W	91	Total	C	N	O	S	0	0
			749	489	119	134	7		
79	6X	91	Total	C	N	O	S	0	0
			749	489	119	134	7		

- Molecule 80 is a protein called Dynein light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	6Y	96	Total	C	N	O	S	0	0
			767	483	134	146	4		
80	6Z	96	Total	C	N	O	S	0	0
			767	483	134	146	4		
80	6a	96	Total	C	N	O	S	0	0
			767	483	134	146	4		
80	6b	96	Total	C	N	O	S	0	0
			767	483	134	146	4		

- Molecule 81 is a protein called Outer arm dynein-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	6c	100	Total	C	N	O	S	0	0
			795	515	126	150	4		
81	6d	100	Total	C	N	O	S	0	0
			795	515	126	150	4		
81	6e	100	Total	C	N	O	S	0	0
			795	515	126	150	4		
81	6f	100	Total	C	N	O	S	0	0
			795	515	126	150	4		

- Molecule 82 is a protein called Dynein light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	6g	113	Total	C	N	O	S	0	0
			913	580	156	171	6		
82	6h	113	Total	C	N	O	S	0	0
			913	580	156	171	6		
82	6i	113	Total	C	N	O	S	0	0
			913	580	156	171	6		
82	6j	113	Total	C	N	O	S	0	0
			913	580	156	171	6		

- Molecule 83 is a protein called IDAa heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	6k	3972	Total	C	N	O	S	0	0
			31758	20128	5481	5984	165		

- Molecule 84 is a protein called Actin.

Mol	Chain	Residues	Atoms					AltConf	Trace
84	6l	371	Total	C	N	O	S	0	0
			2911	1836	495	556	24		
84	7A	361	Total	C	N	O	S	0	0
			2835	1789	480	544	22		

- Molecule 85 is a protein called DLP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
85	6m	410	Total	C	N	O	S	0	0
			3265	2032	592	633	8		

- Molecule 86 is a protein called Dynein arm light chain, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
86	6n	207	Total	C	N	O	S	0	0
			1701	1060	306	330	5		
86	6r	211	Total	C	N	O	S	0	0
			1725	1070	311	338	6		

- Molecule 87 is a protein called Putative dynein heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
87	6o	3797	Total	C	N	O	S	0	0
			30354	19276	5261	5630	187		

- Molecule 88 is a protein called Actin-like protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
88	6p	407	Total	C	N	O	S	0	0
			3087	1937	529	608	13		

- Molecule 89 is a protein called 33 kDa inner dynein arm light chain, axonemal, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
89	6q	226	Total	C	N	O	S	0	0
			1812	1131	340	337	4		

- Molecule 90 is a protein called Anaphase-promoting complex subunit 5 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
90	6s	245	Total	C	N	O	S	0	0
			1886	1182	344	345	15		

- Molecule 91 is a protein called Actin-like protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
91	9R	302	Total	C	N	O	S	0	0
			2382	1509	413	448	12		

- Molecule 92 is a protein called Centrin, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
92	9S	129	Total	C	N	O	S	0	0
			1052	652	181	213	6		

- Molecule 93 is a protein called Dynein heavy chain, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
93	9Q	3918	Total	C	N	O	S	0	0
			30600	19344	5306	5780	170		

- Molecule 94 is a protein called ARM1.

Mol	Chain	Residues	Atoms					AltConf	Trace
94	9T	381	Total	C	N	O	S	0	0
			2975	1859	557	548	11		

- Molecule 95 is a protein called Dynein heavy chain, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
95	6t	4062	Total	C	N	O	S	0	0
			32279	20527	5507	6050	195		

- Molecule 96 is a protein called Actin-like protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
96	6u	392	Total	C	N	O	S	0	0
			3067	1935	536	580	16		

- Molecule 97 is a protein called DLP4.

Mol	Chain	Residues	Atoms					AltConf	Trace
97	6v	312	Total	C	N	O	S	0	0
			2471	1523	461	475	12		

- Molecule 98 is a protein called Dynein arm light chain, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
98	6w	274	Total	C	N	O	S	0	0
			2183	1354	416	409	4		

- Molecule 99 is a protein called TAX-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
99	6x	326	Total	C	N	O	S	0	0
			2613	1656	458	486	13		

- Molecule 100 is a protein called Tetratricopeptide repeat protein 29.

Mol	Chain	Residues	Atoms					AltConf	Trace
100	6y	383	Total	C	N	O	S	0	0
			3020	1880	539	583	18		

- Molecule 101 is a protein called Roadblock/LAMTOR2 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
101	7Q	96	Total	C	N	O	S	0	0
			734	460	126	144	4		
101	9g	96	Total	C	N	O	S	0	0
			734	460	126	144	4		

- Molecule 102 is a protein called Dynein-associated protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
102	7R	109	Total	C	N	O	S	0	0
			867	546	153	164	4		
102	9h	109	Total	C	N	O	S	0	0
			867	546	153	164	4		

- Molecule 103 is a protein called IC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
103	7N	325	Total	C	N	O	S	0	0
			2566	1645	445	462	14		
103	9c	325	Total	C	N	O	S	0	0
			2566	1645	445	462	14		

- Molecule 104 is a protein called Dynein axonemal intermediate chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
104	7O	233	Total	C	N	O	S	0	0
			1828	1167	315	337	9		
104	9d	392	Total	C	N	O	S	0	0
			3092	1954	531	590	17		

- Molecule 105 is a protein called Dynein light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
105	9M	103	Total	C	N	O	S	0	0
			845	535	144	161	5		
105	9p	103	Total	C	N	O	S	0	0
			845	535	144	161	5		

- Molecule 106 is a protein called Dynein-light chain-protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
106	9L	103	Total	C	N	O	S	0	0
			791	498	134	153	6		
106	9o	103	Total	C	N	O	S	0	0
			791	498	134	153	6		

- Molecule 107 is a protein called Ankyrin/TPR repeat protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
107	7F	296	Total	C	N	O	S	0	0
			2252	1376	409	452	15		
107	9e	296	Total	C	N	O	S	0	0
			2252	1376	409	452	15		

- Molecule 108 is a protein called IC97/Casc1 N-terminal domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
108	9K	565	Total	C	N	O	S	0	0
			4601	2917	798	866	20		
108	9f	565	Total	C	N	O	S	0	0
			4601	2917	798	866	20		

- Molecule 109 is a protein called Dynein heavy chain, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
109	7G	3724	Total	C	N	O	S	0	0
			29867	18977	5125	5599	166		
109	9a	1431	Total	C	N	O	S	0	0
			11631	7372	2038	2172	49		

- Molecule 110 is a protein called Dynein heavy chain, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
110	7I	3788	Total	C	N	O	S	0	0
			30637	19418	5331	5707	181		
110	9b	1106	Total	C	N	O	S	0	0
			9051	5738	1585	1677	51		

- Molecule 111 is a protein called DUF4200 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
111	9U	81	Total	C	N	O	S	0	0
			616	373	115	122	6		
111	9r	286	Total	C	N	O	S	0	0
			2334	1425	442	451	16		

- Molecule 112 is a protein called DUF4200 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
112	9V	83	Total	C	N	O	S	0	0
			692	428	134	126	4		
112	9s	298	Total	C	N	O	S	0	0
			2453	1506	457	478	12		

- Molecule 113 is a protein called Leucine-rich repeat-containing protein 51.

Mol	Chain	Residues	Atoms					AltConf	Trace
113	9q	442	Total	C	N	O	S	0	0
			3509	2209	633	652	15		

- Molecule 114 is a protein called Dynein heavy chain, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
114	6z	3680	Total	C	N	O	S	0	0
			29150	18419	5041	5528	162		

- Molecule 115 is a protein called Centrin, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
115	7B	152	Total	C	N	O	S	0	0
			1202	758	200	237	7		

- Molecule 116 is a protein called Dynein heavy chain, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
116	7C	3636	Total	C	N	O	S	0	0
			28996	18416	4982	5443	155		

- Molecule 117 is a protein called Actin-like protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
117	7D	419	Total	C	N	O	S	0	0
			3190	1998	563	609	20		

- Molecule 118 is a protein called Centrin, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
118	7E	150	Total	C	N	O	S	0	0
			1210	750	209	247	4		

- Molecule 119 is a protein called Dynein regulatory complex protein 1 C-terminal domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
119	8A	452	Total	C	N	O	S	0	0
			3770	2334	704	721	11		

- Molecule 120 is a protein called Cilia- and flagella-associated protein 91.

Mol	Chain	Residues	Atoms					AltConf	Trace
120	8K	214	Total	C	N	O	S	0	0
			1728	1060	340	322	6		

- Molecule 121 is a protein called T-lymphocyte triggering factor, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
121	8E	431	Total	C	N	O	S	0	0
			3596	2204	671	704	17		

- Molecule 122 is a protein called T-lymphocyte triggering factor, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
122	8D	400	Total	C	N	O	S	0	0
			3394	2103	619	662	10		

- Molecule 123 is a protein called Dynein regulatory complex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
123	8B	372	Total	C	N	O	S	0	0
			3062	1883	550	609	20		

- Molecule 124 is a protein called AAA+ ATPase domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
124	8J	778	Total	C	N	O	S	0	0
			6100	3823	1111	1137	29		

- Molecule 125 is a protein called Leucine-rich repeat protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
125	8F	456	Total	C	N	O	S	0	0
			3580	2241	648	668	23		

- Molecule 126 is a protein called Calmodulin.

Mol	Chain	Residues	Atoms					AltConf	Trace
126	8M	148	Total	C	N	O	S	0	0
			1163	713	186	254	10		
126	8L	148	Total	C	N	O	S	0	0
			1163	713	186	254	10		
126	9N	149	Total	C	N	O	S	0	0
			1173	719	188	256	10		
126	9O	149	Total	C	N	O	S	0	0
			1173	719	188	256	10		

- Molecule 127 is a protein called Leucine-rich repeat protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
127	8N	323	Total	C	N	O	S	0	0
			2458	1543	438	462	15		

- Molecule 128 is a protein called Leucine-rich repeat protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
128	8O	387	Total	C	N	O	S	0	0
			2870	1778	522	556	14		

- Molecule 129 is a protein called Ubiquitin-like domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
129	8P	99	Total	C	N	O	S	0	0
			814	519	135	157	3		
129	4f	73	Total	C	N	O	S	0	0
			621	396	106	117	2		

- Molecule 130 is a protein called Leucine-rich repeat protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
130	8R	337	Total	C	N	O	S	0	0
			2445	1514	433	488	10		

- Molecule 131 is a protein called Transglutaminase-like domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
131	8G	606	Total	C	N	O	S	0	0
			4902	3115	848	917	22		

- Molecule 132 is a protein called Dynein regulatory complex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
132	8C	546	Total	C	N	O	S	0	0
			4418	2757	806	840	15		

- Molecule 133 is a protein called Dynein regulatory complex protein 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
133	8H	120	Total	C	N	O	S	0	0
			935	565	177	189	4		

- Molecule 134 is a protein called Dynein regulatory complex protein 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
134	8I	174	Total	C	N	O	S	0	0
			1433	873	278	277	5		

- Molecule 135 is a protein called Cilia- and flagella-associated protein 43.

Mol	Chain	Residues	Atoms					AltConf	Trace
135	7K	1298	Total	C	N	O	S	0	0
			10069	6250	1827	1919	73		

- Molecule 136 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
136	7L	1476	Total	C	N	O	S	0	0
			11521	7199	2068	2189	65		

- Molecule 137 is a protein called Tudor domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
137	7M	252	Total	C	N	O	S	0	0
			1985	1261	325	387	12		

- Molecule 138 is a protein called CFAP253.

Mol	Chain	Residues	Atoms					AltConf	Trace
138	8r	197	Total	C	N	O	S	0	0
			1627	1014	313	297	3		

- Molecule 139 is a protein called Radial spoke protein 3, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
139	8u	44	Total	C	N	O	S	0	0
			354	211	74	66	3		
139	8v	40	Total	C	N	O	S	0	0
			330	200	66	60	4		
139	8o	59	Total	C	N	O	S	0	0
			483	299	79	104	1		
139	8p	99	Total	C	N	O	S	0	0
			803	499	136	163	5		

- Molecule 140 is a protein called Kinesin-MORN.

Mol	Chain	Residues	Atoms					AltConf	Trace
140	8a	620	Total	C	N	O	S	0	0
			5006	3129	913	936	28		

- Molecule 141 is a protein called Leucine-rich repeat protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
141	8b	366	Total	C	N	O	S	0	0
			2764	1713	496	535	20		

- Molecule 142 is a protein called Cilia- and flagella-associated protein 206.

Mol	Chain	Residues	Atoms					AltConf	Trace
142	8q	560	Total	C	N	O	S	0	0
			4277	2684	757	807	29		

- Molecule 143 is a protein called Cilia- and flagella-associated protein 251.

Mol	Chain	Residues	Atoms					AltConf	Trace
143	8w	1005	Total	C	N	O	S	0	0
			7768	4918	1350	1452	48		

- Molecule 144 is a protein called Coiled-coil domain-containing protein 39.

Mol	Chain	Residues	Atoms					AltConf	Trace
144	4R	359	Total	C	N	O	S	0	0
			2942	1806	541	587	8		
144	4S	282	Total	C	N	O	S	0	0
			2339	1419	439	473	8		

- Molecule 145 is a protein called Coiled-coil domain-containing protein 40.

Mol	Chain	Residues	Atoms					AltConf	Trace
145	4T	430	Total	C	N	O	S	0	0
			3493	2145	643	684	21		
145	4U	276	Total	C	N	O	S	0	0
			2260	1372	421	458	9		

- Molecule 146 is a protein called CCDC113/CCDC96 coiled-coil domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
146	9t	255	Total	C	N	O	S	0	0
			2109	1292	421	388	8		

- Molecule 147 is a protein called Cilia- and flagella-associated protein 263.

Mol	Chain	Residues	Atoms					AltConf	Trace
147	9u	283	Total	C	N	O	S	0	0
			2270	1377	438	444	11		

- Molecule 148 is a protein called Enkurin domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
148	4D	105	Total	C	N	O	S	0	0
			836	517	167	150	2		

- Molecule 149 is a protein called C2HC/C3H-type domain-containing protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
149	4E	27	Total	C	N	O	0	0
			216	134	44	38		

- Molecule 150 is a protein called Sperm-tail PG-rich repeat.

Mol	Chain	Residues	Atoms					AltConf	Trace
150	4F	254	Total	C	N	O	S	0	0
			1945	1226	351	361	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
150	4G	83	Total	C	N	O	S	0	0
			661	420	111	127	3		

- Molecule 151 is a protein called DMAP6.

Mol	Chain	Residues	Atoms					AltConf	Trace
151	4H	45	Total	C	N	O	S	0	0
			359	223	67	68	1		

- Molecule 152 is a protein called DMAP7.

Mol	Chain	Residues	Atoms					AltConf	Trace
152	4I	120	Total	C	N	O	S	0	0
			959	595	194	168	2		
152	4J	57	Total	C	N	O	S	0	0
			456	279	78	94	5		

- Molecule 153 is a protein called IJAP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
153	4K	50	Total	C	N	O	S	0	0
			400	245	82	68	5		

- Molecule 154 is a protein called LIM zinc-binding domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
154	4L	128	Total	C	N	O	S	0	0
			998	614	187	184	13		

- Molecule 155 is a protein called IJAP3.

Mol	Chain	Residues	Atoms					AltConf	Trace
155	4M	75	Total	C	N	O	S	0	0
			581	362	105	112	2		
155	4N	177	Total	C	N	O	S	0	0
			1437	893	277	263	4		

- Molecule 156 is a protein called Leucine-rich repeat protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
156	4d	491	Total	C	N	O	S	0	0
			3737	2317	683	711	26		

- Molecule 157 is a protein called Ribonuclease inhibitor-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
157	4e	507	Total	C	N	O	S	0	0
			3833	2362	721	729	21		

- Molecule 158 is a protein called Leucine-rich repeat protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
158	4g	84	Total	C	N	O	S	0	0
			660	408	128	121	3		

- Molecule 159 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
159	9W	919	Total	C	N	O	S	0	0
			7288	4584	1287	1377	40		

- Molecule 160 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
160	9X	971	Total	C	N	O	S	0	0
			7686	4789	1396	1462	39		

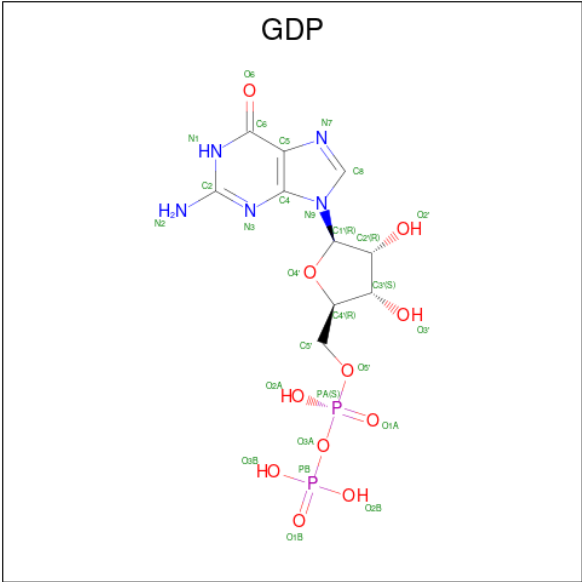
- Molecule 161 is a protein called Cilia- and flagella-associated protein 58 central coiled coil domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
161	9Y	539	Total	C	N	O	S	0	0
			4412	2692	835	860	25		

- Molecule 162 is a protein called Cilia- and flagella-associated protein 58 central coiled coil domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
162	9Z	534	Total	C	N	O	S	0	0
			4339	2668	838	820	13		

- Molecule 163 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



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

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Mol	Chain	Residues	Atoms					AltConf
163	CA	1	Total 28	C 10	N 5	O 11	P 2	0
163	CC	1	Total 28	C 10	N 5	O 11	P 2	0
163	CE	1	Total 28	C 10	N 5	O 11	P 2	0
163	CG	1	Total 28	C 10	N 5	O 11	P 2	0
163	CI	1	Total 28	C 10	N 5	O 11	P 2	0
163	CK	1	Total 28	C 10	N 5	O 11	P 2	0
163	CM	1	Total 28	C 10	N 5	O 11	P 2	0
163	DA	1	Total 28	C 10	N 5	O 11	P 2	0
163	DC	1	Total 28	C 10	N 5	O 11	P 2	0
163	DE	1	Total 28	C 10	N 5	O 11	P 2	0
163	DG	1	Total 28	C 10	N 5	O 11	P 2	0
163	DI	1	Total 28	C 10	N 5	O 11	P 2	0
163	DK	1	Total 28	C 10	N 5	O 11	P 2	0
163	DM	1	Total 28	C 10	N 5	O 11	P 2	0
163	E	1	Total 28	C 10	N 5	O 11	P 2	0
163	EB	1	Total 28	C 10	N 5	O 11	P 2	0
163	ED	1	Total 28	C 10	N 5	O 11	P 2	0
163	EF	1	Total 28	C 10	N 5	O 11	P 2	0
163	EH	1	Total 28	C 10	N 5	O 11	P 2	0
163	EJ	1	Total 28	C 10	N 5	O 11	P 2	0
163	EL	1	Total 28	C 10	N 5	O 11	P 2	0

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

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Mol	Chain	Residues	Atoms					AltConf
163	I	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	IB	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	ID	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	IF	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	IH	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	IJ	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	IL	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	JA	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	JC	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	JE	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	JG	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	JI	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	JK	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	JM	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	KA	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	KC	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	KE	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	KG	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	KI	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	KK	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	KM	1	Total	C	N	O	P	0
			28	10	5	11	2	

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Mol	Chain	Residues	Atoms					AltConf
163	LA	1	Total 28	C 10	N 5	O 11	P 2	0
163	LC	1	Total 28	C 10	N 5	O 11	P 2	0
163	LE	1	Total 28	C 10	N 5	O 11	P 2	0
163	LG	1	Total 28	C 10	N 5	O 11	P 2	0
163	LI	1	Total 28	C 10	N 5	O 11	P 2	0
163	LK	1	Total 28	C 10	N 5	O 11	P 2	0
163	LM	1	Total 28	C 10	N 5	O 11	P 2	0
163	LO	1	Total 28	C 10	N 5	O 11	P 2	0
163	M	1	Total 28	C 10	N 5	O 11	P 2	0
163	MB	1	Total 28	C 10	N 5	O 11	P 2	0
163	MD	1	Total 28	C 10	N 5	O 11	P 2	0
163	MF	1	Total 28	C 10	N 5	O 11	P 2	0
163	MH	1	Total 28	C 10	N 5	O 11	P 2	0
163	MJ	1	Total 28	C 10	N 5	O 11	P 2	0
163	ML	1	Total 28	C 10	N 5	O 11	P 2	0
163	MN	1	Total 28	C 10	N 5	O 11	P 2	0
163	N	1	Total 28	C 10	N 5	O 11	P 2	0
163	NB	1	Total 28	C 10	N 5	O 11	P 2	0
163	ND	1	Total 28	C 10	N 5	O 11	P 2	0
163	NF	1	Total 28	C 10	N 5	O 11	P 2	0
163	NH	1	Total 28	C 10	N 5	O 11	P 2	0

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Mol	Chain	Residues	Atoms					AltConf
163	NJ	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	NL	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	O	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	OB	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	OD	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	OF	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	OH	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	OJ	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	OL	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	P	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	PB	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	PD	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	PF	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	PH	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	PJ	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	PL	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	QA	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	QC	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	QE	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	QG	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	QI	1	Total	C	N	O	P	0
			28	10	5	11	2	

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Mol	Chain	Residues	Atoms					AltConf
163	QK	1	Total 28	C 10	N 5	O 11	P 2	0
163	RA	1	Total 28	C 10	N 5	O 11	P 2	0
163	RC	1	Total 28	C 10	N 5	O 11	P 2	0
163	RE	1	Total 28	C 10	N 5	O 11	P 2	0
163	RG	1	Total 28	C 10	N 5	O 11	P 2	0
163	RI	1	Total 28	C 10	N 5	O 11	P 2	0
163	RK	1	Total 28	C 10	N 5	O 11	P 2	0
163	S	1	Total 28	C 10	N 5	O 11	P 2	0
163	SB	1	Total 28	C 10	N 5	O 11	P 2	0
163	SD	1	Total 28	C 10	N 5	O 11	P 2	0
163	SF	1	Total 28	C 10	N 5	O 11	P 2	0
163	SH	1	Total 28	C 10	N 5	O 11	P 2	0
163	SJ	1	Total 28	C 10	N 5	O 11	P 2	0
163	T	1	Total 28	C 10	N 5	O 11	P 2	0
163	TB	1	Total 28	C 10	N 5	O 11	P 2	0
163	TD	1	Total 28	C 10	N 5	O 11	P 2	0
163	TF	1	Total 28	C 10	N 5	O 11	P 2	0
163	TH	1	Total 28	C 10	N 5	O 11	P 2	0
163	TJ	1	Total 28	C 10	N 5	O 11	P 2	0
163	TL	1	Total 28	C 10	N 5	O 11	P 2	0
163	U	1	Total 28	C 10	N 5	O 11	P 2	0

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

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Mol	Chain	Residues	Atoms					AltConf
163	AR	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	AT	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	AV	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	AX	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	AZ	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	BP	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	BR	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	BT	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	BV	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	BX	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	CO	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	CQ	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	CS	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	CU	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	CW	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	CY	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	DO	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	DQ	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	DS	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	DU	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	DW	1	Total	C	N	O	P	0
			28	10	5	11	2	

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Mol	Chain	Residues	Atoms					AltConf
163	DY	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	EN	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	EP	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	ER	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	ET	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	EV	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	EX	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	FN	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	FP	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	FR	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	FT	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	FV	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	FX	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	GN	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	GP	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	GR	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	GT	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	GV	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	GX	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	HN	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	HP	1	Total	C	N	O	P	0
			28	10	5	11	2	

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Mol	Chain	Residues	Atoms					AltConf
163	HR	1	Total 28	C 10	N 5	O 11	P 2	0
163	HT	1	Total 28	C 10	N 5	O 11	P 2	0
163	HV	1	Total 28	C 10	N 5	O 11	P 2	0
163	HX	1	Total 28	C 10	N 5	O 11	P 2	0
163	IN	1	Total 28	C 10	N 5	O 11	P 2	0
163	IP	1	Total 28	C 10	N 5	O 11	P 2	0
163	IR	1	Total 28	C 10	N 5	O 11	P 2	0
163	IT	1	Total 28	C 10	N 5	O 11	P 2	0
163	IV	1	Total 28	C 10	N 5	O 11	P 2	0
163	IX	1	Total 28	C 10	N 5	O 11	P 2	0
163	JO	1	Total 28	C 10	N 5	O 11	P 2	0
163	JQ	1	Total 28	C 10	N 5	O 11	P 2	0
163	JS	1	Total 28	C 10	N 5	O 11	P 2	0
163	JU	1	Total 28	C 10	N 5	O 11	P 2	0
163	JW	1	Total 28	C 10	N 5	O 11	P 2	0
163	JY	1	Total 28	C 10	N 5	O 11	P 2	0
163	KO	1	Total 28	C 10	N 5	O 11	P 2	0
163	KQ	1	Total 28	C 10	N 5	O 11	P 2	0
163	KS	1	Total 28	C 10	N 5	O 11	P 2	0
163	KU	1	Total 28	C 10	N 5	O 11	P 2	0
163	KW	1	Total 28	C 10	N 5	O 11	P 2	0

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Mol	Chain	Residues	Atoms					AltConf
163	KY	1	Total 28	C 10	N 5	O 11	P 2	0
163	LQ	1	Total 28	C 10	N 5	O 11	P 2	0
163	LS	1	Total 28	C 10	N 5	O 11	P 2	0
163	LU	1	Total 28	C 10	N 5	O 11	P 2	0
163	LW	1	Total 28	C 10	N 5	O 11	P 2	0
163	LY	1	Total 28	C 10	N 5	O 11	P 2	0
163	MP	1	Total 28	C 10	N 5	O 11	P 2	0
163	MR	1	Total 28	C 10	N 5	O 11	P 2	0
163	MT	1	Total 28	C 10	N 5	O 11	P 2	0
163	MV	1	Total 28	C 10	N 5	O 11	P 2	0
163	MX	1	Total 28	C 10	N 5	O 11	P 2	0
163	MZ	1	Total 28	C 10	N 5	O 11	P 2	0
163	PN	1	Total 28	C 10	N 5	O 11	P 2	0
163	PP	1	Total 28	C 10	N 5	O 11	P 2	0
163	PR	1	Total 28	C 10	N 5	O 11	P 2	0
163	PT	1	Total 28	C 10	N 5	O 11	P 2	0
163	PV	1	Total 28	C 10	N 5	O 11	P 2	0
163	PX	1	Total 28	C 10	N 5	O 11	P 2	0
163	QM	1	Total 28	C 10	N 5	O 11	P 2	0
163	QO	1	Total 28	C 10	N 5	O 11	P 2	0
163	QQ	1	Total 28	C 10	N 5	O 11	P 2	0

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Mol	Chain	Residues	Atoms					AltConf
163	QS	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	QU	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	QW	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	RM	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	RO	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	RQ	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	RS	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	RU	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	RW	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	SL	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	SN	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	SP	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	SR	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	ST	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	SV	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	TN	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	TP	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	TR	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	TT	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	TV	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	TX	1	Total	C	N	O	P	0
			28	10	5	11	2	

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Mol	Chain	Residues	Atoms					AltConf
163	UN	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	UP	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	UR	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	UT	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	UV	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	UX	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	VN	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	VP	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	VR	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	VT	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	VV	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	VX	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	WN	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	WP	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	WR	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	WT	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	WV	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	WX	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	NN	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	NP	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	NR	1	Total	C	N	O	P	0
			28	10	5	11	2	

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Mol	Chain	Residues	Atoms					AltConf
163	NT	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	NV	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	NX	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	ON	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	OP	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	OR	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	OT	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	OV	1	Total	C	N	O	P	0
			28	10	5	11	2	
163	OX	1	Total	C	N	O	P	0
			28	10	5	11	2	

- Molecule 164 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
164	A	1	Total	Mg	0
			1	1	
164	AC	1	Total	Mg	0
			1	1	
164	AE	1	Total	Mg	0
			1	1	
164	AG	1	Total	Mg	0
			1	1	
164	AI	1	Total	Mg	0
			1	1	
164	AK	1	Total	Mg	0
			1	1	
164	AM	1	Total	Mg	0
			1	1	
164	BA	1	Total	Mg	0
			1	1	
164	BE	1	Total	Mg	0
			1	1	
164	BG	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
164	BI	1	Total 1	Mg 1	0
164	BK	1	Total 1	Mg 1	0
164	BM	1	Total 1	Mg 1	0
164	C	1	Total 1	Mg 1	0
164	CB	1	Total 1	Mg 1	0
164	CD	1	Total 1	Mg 1	0
164	CF	1	Total 1	Mg 1	0
164	CH	1	Total 1	Mg 1	0
164	CJ	1	Total 1	Mg 1	0
164	CK	1	Total 1	Mg 1	0
164	D	1	Total 1	Mg 1	0
164	DB	1	Total 1	Mg 1	0
164	DD	1	Total 1	Mg 1	0
164	DF	1	Total 1	Mg 1	0
164	DH	1	Total 1	Mg 1	0
164	DJ	1	Total 1	Mg 1	0
164	DK	1	Total 1	Mg 1	0
164	EA	1	Total 1	Mg 1	0
164	EC	1	Total 1	Mg 1	0
164	EE	1	Total 1	Mg 1	0
164	EG	1	Total 1	Mg 1	0

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Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
164	EI	1	1	1	0
164	EK	1	1	1	0
164	FA	1	1	1	0
164	FC	1	1	1	0
164	FE	1	1	1	0
164	FG	1	1	1	0
164	FI	1	1	1	0
164	FJ	1	1	1	0
164	GA	1	1	1	0
164	GC	1	1	1	0
164	GE	1	1	1	0
164	GG	1	1	1	0
164	GI	1	1	1	0
164	GK	1	1	1	0
164	HA	1	1	1	0
164	HB	1	1	1	0
164	HD	1	1	1	0
164	HG	1	1	1	0
164	HH	1	1	1	0
164	HK	1	1	1	0
164	HL	1	1	1	0

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Mol	Chain	Residues	Atoms		AltConf
164	I	1	Total 1	Mg 1	0
164	IC	1	Total 1	Mg 1	0
164	IE	1	Total 1	Mg 1	0
164	IG	1	Total 1	Mg 1	0
164	II	1	Total 1	Mg 1	0
164	IK	1	Total 1	Mg 1	0
164	IL	1	Total 1	Mg 1	0
164	J	1	Total 1	Mg 1	0
164	JB	1	Total 1	Mg 1	0
164	JD	1	Total 1	Mg 1	0
164	JF	1	Total 1	Mg 1	0
164	JH	1	Total 1	Mg 1	0
164	JJ	1	Total 1	Mg 1	0
164	JL	1	Total 1	Mg 1	0
164	JM	1	Total 1	Mg 1	0
164	K	1	Total 1	Mg 1	0
164	KB	1	Total 1	Mg 1	0
164	KD	1	Total 1	Mg 1	0
164	KF	1	Total 1	Mg 1	0
164	KH	1	Total 1	Mg 1	0
164	KJ	1	Total 1	Mg 1	0

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Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
164	KL	1	1	1	0
164	KN	1	1	1	0
164	L	1	1	1	0
164	LB	1	1	1	0
164	LD	1	1	1	0
164	LF	1	1	1	0
164	LG	1	1	1	0
164	LJ	1	1	1	0
164	LL	1	1	1	0
164	LN	1	1	1	0
164	MA	1	1	1	0
164	MC	1	1	1	0
164	ME	1	1	1	0
164	MG	1	1	1	0
164	MI	1	1	1	0
164	MK	1	1	1	0
164	MM	1	1	1	0
164	NA	1	1	1	0
164	NC	1	1	1	0
164	NE	1	1	1	0
164	NG	1	1	1	0

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Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
164	NI	1	1	1	0
164	NJ	1	1	1	0
164	NM	1	1	1	0
164	OA	1	1	1	0
164	OC	1	1	1	0
164	OD	1	1	1	0
164	OG	1	1	1	0
164	OI	1	1	1	0
164	OK	1	1	1	0
164	OM	1	1	1	0
164	PA	1	1	1	0
164	PC	1	1	1	0
164	PE	1	1	1	0
164	PF	1	1	1	0
164	PI	1	1	1	0
164	PK	1	1	1	0
164	PL	1	1	1	0
164	Q	1	1	1	0
164	QB	1	1	1	0
164	QD	1	1	1	0
164	QF	1	1	1	0

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Mol	Chain	Residues	Atoms		AltConf
164	QH	1	Total 1	Mg 1	0
164	QJ	1	Total 1	Mg 1	0
164	QL	1	Total 1	Mg 1	0
164	R	1	Total 1	Mg 1	0
164	RB	1	Total 1	Mg 1	0
164	RD	1	Total 1	Mg 1	0
164	RF	1	Total 1	Mg 1	0
164	RH	1	Total 1	Mg 1	0
164	RJ	1	Total 1	Mg 1	0
164	RL	1	Total 1	Mg 1	0
164	SA	1	Total 1	Mg 1	0
164	SB	1	Total 1	Mg 1	0
164	SE	1	Total 1	Mg 1	0
164	SG	1	Total 1	Mg 1	0
164	SI	1	Total 1	Mg 1	0
164	SJ	1	Total 1	Mg 1	0
164	T	1	Total 1	Mg 1	0
164	TC	1	Total 1	Mg 1	0
164	TE	1	Total 1	Mg 1	0
164	TG	1	Total 1	Mg 1	0
164	TI	1	Total 1	Mg 1	0

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Mol	Chain	Residues	Atoms		AltConf
164	TK	1	Total 1	Mg 1	0
164	TL	1	Total 1	Mg 1	0
164	UA	1	Total 1	Mg 1	0
164	UC	1	Total 1	Mg 1	0
164	UE	1	Total 1	Mg 1	0
164	UG	1	Total 1	Mg 1	0
164	UI	1	Total 1	Mg 1	0
164	UK	1	Total 1	Mg 1	0
164	VA	1	Total 1	Mg 1	0
164	VC	1	Total 1	Mg 1	0
164	VE	1	Total 1	Mg 1	0
164	VG	1	Total 1	Mg 1	0
164	VI	1	Total 1	Mg 1	0
164	VK	1	Total 1	Mg 1	0
164	VM	1	Total 1	Mg 1	0
164	WA	1	Total 1	Mg 1	0
164	WC	1	Total 1	Mg 1	0
164	WE	1	Total 1	Mg 1	0
164	WF	1	Total 1	Mg 1	0
164	WI	1	Total 1	Mg 1	0
164	WK	1	Total 1	Mg 1	0

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Mol	Chain	Residues	Atoms		AltConf
164	WM	1	Total 1	Mg 1	0
164	AO	1	Total 1	Mg 1	0
164	AQ	1	Total 1	Mg 1	0
164	AS	1	Total 1	Mg 1	0
164	AU	1	Total 1	Mg 1	0
164	AW	1	Total 1	Mg 1	0
164	AY	1	Total 1	Mg 1	0
164	BO	1	Total 1	Mg 1	0
164	BQ	1	Total 1	Mg 1	0
164	BS	1	Total 1	Mg 1	0
164	BU	1	Total 1	Mg 1	0
164	BW	1	Total 1	Mg 1	0
164	BY	1	Total 1	Mg 1	0
164	CN	1	Total 1	Mg 1	0
164	CP	1	Total 1	Mg 1	0
164	CR	1	Total 1	Mg 1	0
164	CT	1	Total 1	Mg 1	0
164	CV	1	Total 1	Mg 1	0
164	CX	1	Total 1	Mg 1	0
164	DN	1	Total 1	Mg 1	0
164	DP	1	Total 1	Mg 1	0

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Mol	Chain	Residues	Atoms		AltConf
164	DR	1	Total 1	Mg 1	0
164	DT	1	Total 1	Mg 1	0
164	DV	1	Total 1	Mg 1	0
164	DW	1	Total 1	Mg 1	0
164	EM	1	Total 1	Mg 1	0
164	EO	1	Total 1	Mg 1	0
164	EQ	1	Total 1	Mg 1	0
164	ES	1	Total 1	Mg 1	0
164	EU	1	Total 1	Mg 1	0
164	EW	1	Total 1	Mg 1	0
164	FM	1	Total 1	Mg 1	0
164	FO	1	Total 1	Mg 1	0
164	FQ	1	Total 1	Mg 1	0
164	FR	1	Total 1	Mg 1	0
164	FT	1	Total 1	Mg 1	0
164	FV	1	Total 1	Mg 1	0
164	GM	1	Total 1	Mg 1	0
164	GO	1	Total 1	Mg 1	0
164	GQ	1	Total 1	Mg 1	0
164	GS	1	Total 1	Mg 1	0
164	GT	1	Total 1	Mg 1	0

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Mol	Chain	Residues	Atoms		AltConf
164	GV	1	Total 1	Mg 1	0
164	HN	1	Total 1	Mg 1	0
164	HP	1	Total 1	Mg 1	0
164	HS	1	Total 1	Mg 1	0
164	HT	1	Total 1	Mg 1	0
164	HW	1	Total 1	Mg 1	0
164	HX	1	Total 1	Mg 1	0
164	IO	1	Total 1	Mg 1	0
164	IQ	1	Total 1	Mg 1	0
164	IS	1	Total 1	Mg 1	0
164	IT	1	Total 1	Mg 1	0
164	IW	1	Total 1	Mg 1	0
164	IX	1	Total 1	Mg 1	0
164	JP	1	Total 1	Mg 1	0
164	JR	1	Total 1	Mg 1	0
164	JT	1	Total 1	Mg 1	0
164	JV	1	Total 1	Mg 1	0
164	JX	1	Total 1	Mg 1	0
164	JY	1	Total 1	Mg 1	0
164	KP	1	Total 1	Mg 1	0
164	KR	1	Total 1	Mg 1	0

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Mol	Chain	Residues	Atoms		AltConf
164	KT	1	Total 1	Mg 1	0
164	KV	1	Total 1	Mg 1	0
164	KX	1	Total 1	Mg 1	0
164	KZ	1	Total 1	Mg 1	0
164	LP	1	Total 1	Mg 1	0
164	LR	1	Total 1	Mg 1	0
164	LT	1	Total 1	Mg 1	0
164	LV	1	Total 1	Mg 1	0
164	LX	1	Total 1	Mg 1	0
164	LZ	1	Total 1	Mg 1	0
164	MO	1	Total 1	Mg 1	0
164	MQ	1	Total 1	Mg 1	0
164	MS	1	Total 1	Mg 1	0
164	MU	1	Total 1	Mg 1	0
164	MW	1	Total 1	Mg 1	0
164	MY	1	Total 1	Mg 1	0
164	PO	1	Total 1	Mg 1	0
164	PQ	1	Total 1	Mg 1	0
164	PR	1	Total 1	Mg 1	0
164	PU	1	Total 1	Mg 1	0
164	PW	1	Total 1	Mg 1	0

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Mol	Chain	Residues	Atoms		AltConf
164	PX	1	Total 1	Mg 1	0
164	QN	1	Total 1	Mg 1	0
164	QP	1	Total 1	Mg 1	0
164	QR	1	Total 1	Mg 1	0
164	QT	1	Total 1	Mg 1	0
164	QV	1	Total 1	Mg 1	0
164	QX	1	Total 1	Mg 1	0
164	RN	1	Total 1	Mg 1	0
164	RP	1	Total 1	Mg 1	0
164	RR	1	Total 1	Mg 1	0
164	RT	1	Total 1	Mg 1	0
164	RV	1	Total 1	Mg 1	0
164	RX	1	Total 1	Mg 1	0
164	SM	1	Total 1	Mg 1	0
164	SN	1	Total 1	Mg 1	0
164	SQ	1	Total 1	Mg 1	0
164	SS	1	Total 1	Mg 1	0
164	SU	1	Total 1	Mg 1	0
164	SV	1	Total 1	Mg 1	0
164	TO	1	Total 1	Mg 1	0
164	TQ	1	Total 1	Mg 1	0

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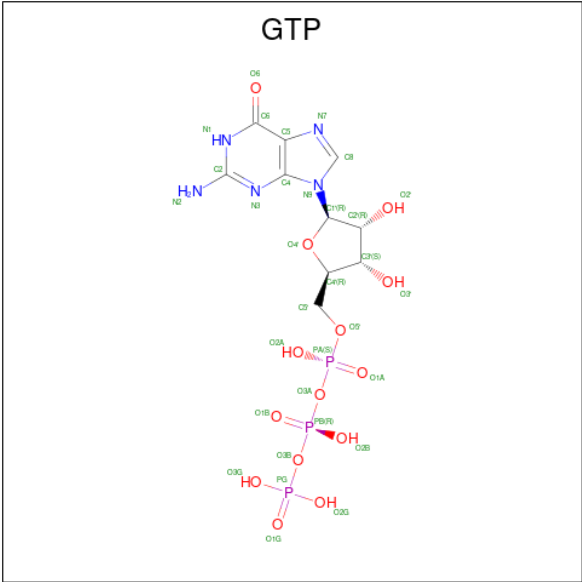
Mol	Chain	Residues	Atoms		AltConf
164	TS	1	Total 1	Mg 1	0
164	TU	1	Total 1	Mg 1	0
164	TW	1	Total 1	Mg 1	0
164	UM	1	Total 1	Mg 1	0
164	UO	1	Total 1	Mg 1	0
164	UQ	1	Total 1	Mg 1	0
164	US	1	Total 1	Mg 1	0
164	UU	1	Total 1	Mg 1	0
164	UW	1	Total 1	Mg 1	0
164	VO	1	Total 1	Mg 1	0
164	VQ	1	Total 1	Mg 1	0
164	VS	1	Total 1	Mg 1	0
164	VU	1	Total 1	Mg 1	0
164	VW	1	Total 1	Mg 1	0
164	VY	1	Total 1	Mg 1	0
164	WO	1	Total 1	Mg 1	0
164	WQ	1	Total 1	Mg 1	0
164	WR	1	Total 1	Mg 1	0
164	WU	1	Total 1	Mg 1	0
164	WW	1	Total 1	Mg 1	0
164	WY	1	Total 1	Mg 1	0

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Mol	Chain	Residues	Atoms		AltConf
164	NO	1	Total 1	Mg 1	0
164	NQ	1	Total 1	Mg 1	0
164	NS	1	Total 1	Mg 1	0
164	NU	1	Total 1	Mg 1	0
164	NV	1	Total 1	Mg 1	0
164	NY	1	Total 1	Mg 1	0
164	OO	1	Total 1	Mg 1	0
164	OP	1	Total 1	Mg 1	0
164	OS	1	Total 1	Mg 1	0
164	OU	1	Total 1	Mg 1	0
164	OW	1	Total 1	Mg 1	0
164	OY	1	Total 1	Mg 1	0
164	6l	1	Total 1	Mg 1	0
164	6p	1	Total 1	Mg 1	0
164	9R	1	Total 1	Mg 1	0
164	7A	1	Total 1	Mg 1	0
164	7D	1	Total 1	Mg 1	0

- Molecule 165 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



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

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Mol	Chain	Residues	Atoms					AltConf
165	CB	1	Total 32	C 10	N 5	O 14	P 3	0
165	CC	1	Total 32	C 10	N 5	O 14	P 3	0
165	CE	1	Total 32	C 10	N 5	O 14	P 3	0
165	CH	1	Total 32	C 10	N 5	O 14	P 3	0
165	CJ	1	Total 32	C 10	N 5	O 14	P 3	0
165	CK	1	Total 32	C 10	N 5	O 14	P 3	0
165	D	1	Total 32	C 10	N 5	O 14	P 3	0
165	DB	1	Total 32	C 10	N 5	O 14	P 3	0
165	DD	1	Total 32	C 10	N 5	O 14	P 3	0
165	DE	1	Total 32	C 10	N 5	O 14	P 3	0
165	DH	1	Total 32	C 10	N 5	O 14	P 3	0
165	DJ	1	Total 32	C 10	N 5	O 14	P 3	0
165	DL	1	Total 32	C 10	N 5	O 14	P 3	0
165	EA	1	Total 32	C 10	N 5	O 14	P 3	0
165	EC	1	Total 32	C 10	N 5	O 14	P 3	0
165	ED	1	Total 32	C 10	N 5	O 14	P 3	0
165	EG	1	Total 32	C 10	N 5	O 14	P 3	0
165	EI	1	Total 32	C 10	N 5	O 14	P 3	0
165	EJ	1	Total 32	C 10	N 5	O 14	P 3	0
165	FA	1	Total 32	C 10	N 5	O 14	P 3	0
165	FC	1	Total 32	C 10	N 5	O 14	P 3	0

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Mol	Chain	Residues	Atoms					AltConf
165	FE	1	Total 32	C 10	N 5	O 14	P 3	0
165	FG	1	Total 32	C 10	N 5	O 14	P 3	0
165	FI	1	Total 32	C 10	N 5	O 14	P 3	0
165	FJ	1	Total 32	C 10	N 5	O 14	P 3	0
165	G	1	Total 32	C 10	N 5	O 14	P 3	0
165	GC	1	Total 32	C 10	N 5	O 14	P 3	0
165	GE	1	Total 32	C 10	N 5	O 14	P 3	0
165	GG	1	Total 32	C 10	N 5	O 14	P 3	0
165	GI	1	Total 32	C 10	N 5	O 14	P 3	0
165	GK	1	Total 32	C 10	N 5	O 14	P 3	0
165	GL	1	Total 32	C 10	N 5	O 14	P 3	0
165	HA	1	Total 32	C 10	N 5	O 14	P 3	0
165	HB	1	Total 32	C 10	N 5	O 14	P 3	0
165	HE	1	Total 32	C 10	N 5	O 14	P 3	0
165	HG	1	Total 32	C 10	N 5	O 14	P 3	0
165	HI	1	Total 32	C 10	N 5	O 14	P 3	0
165	HK	1	Total 32	C 10	N 5	O 14	P 3	0
165	HM	1	Total 32	C 10	N 5	O 14	P 3	0
165	IA	1	Total 32	C 10	N 5	O 14	P 3	0
165	IC	1	Total 32	C 10	N 5	O 14	P 3	0
165	IE	1	Total 32	C 10	N 5	O 14	P 3	0

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Mol	Chain	Residues	Atoms					AltConf
165	IG	1	Total 32	C 10	N 5	O 14	P 3	0
165	II	1	Total 32	C 10	N 5	O 14	P 3	0
165	IK	1	Total 32	C 10	N 5	O 14	P 3	0
165	IM	1	Total 32	C 10	N 5	O 14	P 3	0
165	J	1	Total 32	C 10	N 5	O 14	P 3	0
165	JB	1	Total 32	C 10	N 5	O 14	P 3	0
165	JD	1	Total 32	C 10	N 5	O 14	P 3	0
165	JF	1	Total 32	C 10	N 5	O 14	P 3	0
165	JH	1	Total 32	C 10	N 5	O 14	P 3	0
165	JJ	1	Total 32	C 10	N 5	O 14	P 3	0
165	JK	1	Total 32	C 10	N 5	O 14	P 3	0
165	JN	1	Total 32	C 10	N 5	O 14	P 3	0
165	K	1	Total 32	C 10	N 5	O 14	P 3	0
165	KB	1	Total 32	C 10	N 5	O 14	P 3	0
165	KD	1	Total 32	C 10	N 5	O 14	P 3	0
165	KF	1	Total 32	C 10	N 5	O 14	P 3	0
165	KH	1	Total 32	C 10	N 5	O 14	P 3	0
165	KJ	1	Total 32	C 10	N 5	O 14	P 3	0
165	KL	1	Total 32	C 10	N 5	O 14	P 3	0
165	KN	1	Total 32	C 10	N 5	O 14	P 3	0
165	L	1	Total 32	C 10	N 5	O 14	P 3	0

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Mol	Chain	Residues	Atoms					AltConf
165	LB	1	Total 32	C 10	N 5	O 14	P 3	0
165	LD	1	Total 32	C 10	N 5	O 14	P 3	0
165	LF	1	Total 32	C 10	N 5	O 14	P 3	0
165	LH	1	Total 32	C 10	N 5	O 14	P 3	0
165	LJ	1	Total 32	C 10	N 5	O 14	P 3	0
165	LL	1	Total 32	C 10	N 5	O 14	P 3	0
165	LN	1	Total 32	C 10	N 5	O 14	P 3	0
165	MA	1	Total 32	C 10	N 5	O 14	P 3	0
165	MC	1	Total 32	C 10	N 5	O 14	P 3	0
165	ME	1	Total 32	C 10	N 5	O 14	P 3	0
165	MG	1	Total 32	C 10	N 5	O 14	P 3	0
165	MI	1	Total 32	C 10	N 5	O 14	P 3	0
165	MJ	1	Total 32	C 10	N 5	O 14	P 3	0
165	MM	1	Total 32	C 10	N 5	O 14	P 3	0
165	NA	1	Total 32	C 10	N 5	O 14	P 3	0
165	NC	1	Total 32	C 10	N 5	O 14	P 3	0
165	NE	1	Total 32	C 10	N 5	O 14	P 3	0
165	NF	1	Total 32	C 10	N 5	O 14	P 3	0
165	NI	1	Total 32	C 10	N 5	O 14	P 3	0
165	NK	1	Total 32	C 10	N 5	O 14	P 3	0
165	NM	1	Total 32	C 10	N 5	O 14	P 3	0

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Mol	Chain	Residues	Atoms					AltConf
165	OA	1	Total 32	C 10	N 5	O 14	P 3	0
165	OC	1	Total 32	C 10	N 5	O 14	P 3	0
165	OD	1	Total 32	C 10	N 5	O 14	P 3	0
165	OG	1	Total 32	C 10	N 5	O 14	P 3	0
165	OI	1	Total 32	C 10	N 5	O 14	P 3	0
165	OK	1	Total 32	C 10	N 5	O 14	P 3	0
165	OM	1	Total 32	C 10	N 5	O 14	P 3	0
165	PA	1	Total 32	C 10	N 5	O 14	P 3	0
165	PC	1	Total 32	C 10	N 5	O 14	P 3	0
165	PE	1	Total 32	C 10	N 5	O 14	P 3	0
165	PG	1	Total 32	C 10	N 5	O 14	P 3	0
165	PI	1	Total 32	C 10	N 5	O 14	P 3	0
165	PK	1	Total 32	C 10	N 5	O 14	P 3	0
165	PM	1	Total 32	C 10	N 5	O 14	P 3	0
165	Q	1	Total 32	C 10	N 5	O 14	P 3	0
165	QB	1	Total 32	C 10	N 5	O 14	P 3	0
165	QC	1	Total 32	C 10	N 5	O 14	P 3	0
165	QF	1	Total 32	C 10	N 5	O 14	P 3	0
165	QH	1	Total 32	C 10	N 5	O 14	P 3	0
165	QI	1	Total 32	C 10	N 5	O 14	P 3	0
165	QL	1	Total 32	C 10	N 5	O 14	P 3	0

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Mol	Chain	Residues	Atoms					AltConf
165	R	1	Total 32	C 10	N 5	O 14	P 3	0
165	RB	1	Total 32	C 10	N 5	O 14	P 3	0
165	RC	1	Total 32	C 10	N 5	O 14	P 3	0
165	RF	1	Total 32	C 10	N 5	O 14	P 3	0
165	RH	1	Total 32	C 10	N 5	O 14	P 3	0
165	RJ	1	Total 32	C 10	N 5	O 14	P 3	0
165	RL	1	Total 32	C 10	N 5	O 14	P 3	0
165	SA	1	Total 32	C 10	N 5	O 14	P 3	0
165	SC	1	Total 32	C 10	N 5	O 14	P 3	0
165	SE	1	Total 32	C 10	N 5	O 14	P 3	0
165	SG	1	Total 32	C 10	N 5	O 14	P 3	0
165	SI	1	Total 32	C 10	N 5	O 14	P 3	0
165	SK	1	Total 32	C 10	N 5	O 14	P 3	0
165	T	1	Total 32	C 10	N 5	O 14	P 3	0
165	TC	1	Total 32	C 10	N 5	O 14	P 3	0
165	TE	1	Total 32	C 10	N 5	O 14	P 3	0
165	TG	1	Total 32	C 10	N 5	O 14	P 3	0
165	TI	1	Total 32	C 10	N 5	O 14	P 3	0
165	TK	1	Total 32	C 10	N 5	O 14	P 3	0
165	UA	1	Total 32	C 10	N 5	O 14	P 3	0
165	UC	1	Total 32	C 10	N 5	O 14	P 3	0

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Mol	Chain	Residues	Atoms					AltConf
165	UE	1	Total 32	C 10	N 5	O 14	P 3	0
165	UG	1	Total 32	C 10	N 5	O 14	P 3	0
165	UI	1	Total 32	C 10	N 5	O 14	P 3	0
165	UK	1	Total 32	C 10	N 5	O 14	P 3	0
165	VA	1	Total 32	C 10	N 5	O 14	P 3	0
165	VC	1	Total 32	C 10	N 5	O 14	P 3	0
165	VE	1	Total 32	C 10	N 5	O 14	P 3	0
165	VG	1	Total 32	C 10	N 5	O 14	P 3	0
165	VH	1	Total 32	C 10	N 5	O 14	P 3	0
165	VK	1	Total 32	C 10	N 5	O 14	P 3	0
165	VM	1	Total 32	C 10	N 5	O 14	P 3	0
165	WA	1	Total 32	C 10	N 5	O 14	P 3	0
165	WC	1	Total 32	C 10	N 5	O 14	P 3	0
165	WE	1	Total 32	C 10	N 5	O 14	P 3	0
165	WG	1	Total 32	C 10	N 5	O 14	P 3	0
165	WI	1	Total 32	C 10	N 5	O 14	P 3	0
165	WK	1	Total 32	C 10	N 5	O 14	P 3	0
165	WM	1	Total 32	C 10	N 5	O 14	P 3	0
165	AO	1	Total 32	C 10	N 5	O 14	P 3	0
165	AP	1	Total 32	C 10	N 5	O 14	P 3	0
165	AS	1	Total 32	C 10	N 5	O 14	P 3	0

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Mol	Chain	Residues	Atoms					AltConf
165	AU	1	Total 32	C 10	N 5	O 14	P 3	0
165	AW	1	Total 32	C 10	N 5	O 14	P 3	0
165	AY	1	Total 32	C 10	N 5	O 14	P 3	0
165	BO	1	Total 32	C 10	N 5	O 14	P 3	0
165	BQ	1	Total 32	C 10	N 5	O 14	P 3	0
165	BS	1	Total 32	C 10	N 5	O 14	P 3	0
165	BU	1	Total 32	C 10	N 5	O 14	P 3	0
165	BW	1	Total 32	C 10	N 5	O 14	P 3	0
165	BY	1	Total 32	C 10	N 5	O 14	P 3	0
165	CN	1	Total 32	C 10	N 5	O 14	P 3	0
165	CO	1	Total 32	C 10	N 5	O 14	P 3	0
165	CQ	1	Total 32	C 10	N 5	O 14	P 3	0
165	CT	1	Total 32	C 10	N 5	O 14	P 3	0
165	CV	1	Total 32	C 10	N 5	O 14	P 3	0
165	CW	1	Total 32	C 10	N 5	O 14	P 3	0
165	DN	1	Total 32	C 10	N 5	O 14	P 3	0
165	DP	1	Total 32	C 10	N 5	O 14	P 3	0
165	DQ	1	Total 32	C 10	N 5	O 14	P 3	0
165	DT	1	Total 32	C 10	N 5	O 14	P 3	0
165	DV	1	Total 32	C 10	N 5	O 14	P 3	0
165	DX	1	Total 32	C 10	N 5	O 14	P 3	0

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Mol	Chain	Residues	Atoms					AltConf
165	EM	1	Total 32	C 10	N 5	O 14	P 3	0
165	EO	1	Total 32	C 10	N 5	O 14	P 3	0
165	EP	1	Total 32	C 10	N 5	O 14	P 3	0
165	ES	1	Total 32	C 10	N 5	O 14	P 3	0
165	EU	1	Total 32	C 10	N 5	O 14	P 3	0
165	EV	1	Total 32	C 10	N 5	O 14	P 3	0
165	FM	1	Total 32	C 10	N 5	O 14	P 3	0
165	FO	1	Total 32	C 10	N 5	O 14	P 3	0
165	FQ	1	Total 32	C 10	N 5	O 14	P 3	0
165	FS	1	Total 32	C 10	N 5	O 14	P 3	0
165	FT	1	Total 32	C 10	N 5	O 14	P 3	0
165	FV	1	Total 32	C 10	N 5	O 14	P 3	0
165	GO	1	Total 32	C 10	N 5	O 14	P 3	0
165	GQ	1	Total 32	C 10	N 5	O 14	P 3	0
165	GS	1	Total 32	C 10	N 5	O 14	P 3	0
165	GU	1	Total 32	C 10	N 5	O 14	P 3	0
165	GW	1	Total 32	C 10	N 5	O 14	P 3	0
165	HN	1	Total 32	C 10	N 5	O 14	P 3	0
165	HQ	1	Total 32	C 10	N 5	O 14	P 3	0
165	HS	1	Total 32	C 10	N 5	O 14	P 3	0
165	HU	1	Total 32	C 10	N 5	O 14	P 3	0

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Mol	Chain	Residues	Atoms					AltConf
165	HW	1	Total 32	C 10	N 5	O 14	P 3	0
165	HY	1	Total 32	C 10	N 5	O 14	P 3	0
165	IO	1	Total 32	C 10	N 5	O 14	P 3	0
165	IQ	1	Total 32	C 10	N 5	O 14	P 3	0
165	IS	1	Total 32	C 10	N 5	O 14	P 3	0
165	IU	1	Total 32	C 10	N 5	O 14	P 3	0
165	IW	1	Total 32	C 10	N 5	O 14	P 3	0
165	IY	1	Total 32	C 10	N 5	O 14	P 3	0
165	JP	1	Total 32	C 10	N 5	O 14	P 3	0
165	JR	1	Total 32	C 10	N 5	O 14	P 3	0
165	JT	1	Total 32	C 10	N 5	O 14	P 3	0
165	JV	1	Total 32	C 10	N 5	O 14	P 3	0
165	JW	1	Total 32	C 10	N 5	O 14	P 3	0
165	JZ	1	Total 32	C 10	N 5	O 14	P 3	0
165	KP	1	Total 32	C 10	N 5	O 14	P 3	0
165	KR	1	Total 32	C 10	N 5	O 14	P 3	0
165	KT	1	Total 32	C 10	N 5	O 14	P 3	0
165	KV	1	Total 32	C 10	N 5	O 14	P 3	0
165	KX	1	Total 32	C 10	N 5	O 14	P 3	0
165	KZ	1	Total 32	C 10	N 5	O 14	P 3	0
165	LP	1	Total 32	C 10	N 5	O 14	P 3	0

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Mol	Chain	Residues	Atoms					AltConf
165	LR	1	Total 32	C 10	N 5	O 14	P 3	0
165	LT	1	Total 32	C 10	N 5	O 14	P 3	0
165	LV	1	Total 32	C 10	N 5	O 14	P 3	0
165	LX	1	Total 32	C 10	N 5	O 14	P 3	0
165	LZ	1	Total 32	C 10	N 5	O 14	P 3	0
165	MO	1	Total 32	C 10	N 5	O 14	P 3	0
165	MQ	1	Total 32	C 10	N 5	O 14	P 3	0
165	MS	1	Total 32	C 10	N 5	O 14	P 3	0
165	MU	1	Total 32	C 10	N 5	O 14	P 3	0
165	MV	1	Total 32	C 10	N 5	O 14	P 3	0
165	MY	1	Total 32	C 10	N 5	O 14	P 3	0
165	PO	1	Total 32	C 10	N 5	O 14	P 3	0
165	PQ	1	Total 32	C 10	N 5	O 14	P 3	0
165	PS	1	Total 32	C 10	N 5	O 14	P 3	0
165	PU	1	Total 32	C 10	N 5	O 14	P 3	0
165	PW	1	Total 32	C 10	N 5	O 14	P 3	0
165	PY	1	Total 32	C 10	N 5	O 14	P 3	0
165	QN	1	Total 32	C 10	N 5	O 14	P 3	0
165	QO	1	Total 32	C 10	N 5	O 14	P 3	0
165	QR	1	Total 32	C 10	N 5	O 14	P 3	0
165	QT	1	Total 32	C 10	N 5	O 14	P 3	0

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Mol	Chain	Residues	Atoms					AltConf
165	QU	1	Total 32	C 10	N 5	O 14	P 3	0
165	QX	1	Total 32	C 10	N 5	O 14	P 3	0
165	RN	1	Total 32	C 10	N 5	O 14	P 3	0
165	RO	1	Total 32	C 10	N 5	O 14	P 3	0
165	RR	1	Total 32	C 10	N 5	O 14	P 3	0
165	RT	1	Total 32	C 10	N 5	O 14	P 3	0
165	RV	1	Total 32	C 10	N 5	O 14	P 3	0
165	RX	1	Total 32	C 10	N 5	O 14	P 3	0
165	SM	1	Total 32	C 10	N 5	O 14	P 3	0
165	SO	1	Total 32	C 10	N 5	O 14	P 3	0
165	SQ	1	Total 32	C 10	N 5	O 14	P 3	0
165	SS	1	Total 32	C 10	N 5	O 14	P 3	0
165	SU	1	Total 32	C 10	N 5	O 14	P 3	0
165	SW	1	Total 32	C 10	N 5	O 14	P 3	0
165	TM	1	Total 32	C 10	N 5	O 14	P 3	0
165	TO	1	Total 32	C 10	N 5	O 14	P 3	0
165	TQ	1	Total 32	C 10	N 5	O 14	P 3	0
165	TS	1	Total 32	C 10	N 5	O 14	P 3	0
165	TU	1	Total 32	C 10	N 5	O 14	P 3	0
165	TW	1	Total 32	C 10	N 5	O 14	P 3	0
165	UM	1	Total 32	C 10	N 5	O 14	P 3	0

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Mol	Chain	Residues	Atoms					AltConf
165	UO	1	Total 32	C 10	N 5	O 14	P 3	0
165	UQ	1	Total 32	C 10	N 5	O 14	P 3	0
165	US	1	Total 32	C 10	N 5	O 14	P 3	0
165	UU	1	Total 32	C 10	N 5	O 14	P 3	0
165	UW	1	Total 32	C 10	N 5	O 14	P 3	0
165	VO	1	Total 32	C 10	N 5	O 14	P 3	0
165	VQ	1	Total 32	C 10	N 5	O 14	P 3	0
165	VS	1	Total 32	C 10	N 5	O 14	P 3	0
165	VT	1	Total 32	C 10	N 5	O 14	P 3	0
165	VW	1	Total 32	C 10	N 5	O 14	P 3	0
165	VY	1	Total 32	C 10	N 5	O 14	P 3	0
165	WO	1	Total 32	C 10	N 5	O 14	P 3	0
165	WQ	1	Total 32	C 10	N 5	O 14	P 3	0
165	WS	1	Total 32	C 10	N 5	O 14	P 3	0
165	WU	1	Total 32	C 10	N 5	O 14	P 3	0
165	WW	1	Total 32	C 10	N 5	O 14	P 3	0
165	WY	1	Total 32	C 10	N 5	O 14	P 3	0
165	NO	1	Total 32	C 10	N 5	O 14	P 3	0
165	NQ	1	Total 32	C 10	N 5	O 14	P 3	0
165	NR	1	Total 32	C 10	N 5	O 14	P 3	0
165	NU	1	Total 32	C 10	N 5	O 14	P 3	0

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Mol	Chain	Residues	Atoms					AltConf
165	NW	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	NY	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	OO	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	OP	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	OS	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	OU	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	OW	1	Total	C	N	O	P	0
			32	10	5	14	3	
165	OY	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 166 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
166	KB	1	Total	Zn	0
			1	1	
166	KD	1	Total	Zn	0
			1	1	
166	KN	1	Total	Zn	0
			1	1	
166	LD	1	Total	Zn	0
			1	1	
166	LF	1	Total	Zn	0
			1	1	
166	LN	1	Total	Zn	0
			1	1	
166	KP	1	Total	Zn	0
			1	1	
166	LP	1	Total	Zn	0
			1	1	
166	LR	1	Total	Zn	0
			1	1	
166	LZ	1	Total	Zn	0
			1	1	
166	0A	1	Total	Zn	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
166	0	1	Total 1	Zn 1	0
166	0z	1	Total 1	Zn 1	0
166	1V	2	Total 2	Zn 2	0
166	1b	2	Total 2	Zn 2	0
166	1e	2	Total 2	Zn 2	0
166	1q	1	Total 1	Zn 1	0
166	1s	1	Total 1	Zn 1	0
166	1w	1	Total 1	Zn 1	0
166	1x	1	Total 1	Zn 1	0
166	3S	1	Total 1	Zn 1	0
166	0B	1	Total 1	Zn 1	0
166	2A	1	Total 1	Zn 1	0
166	1W	2	Total 2	Zn 2	0
166	1Z	1	Total 1	Zn 1	0
166	1c	2	Total 2	Zn 2	0
166	9F	2	Total 2	Zn 2	0
166	1f	2	Total 2	Zn 2	0
166	1i	2	Total 2	Zn 2	0
166	1t	1	Total 1	Zn 1	0
166	1v	1	Total 1	Zn 1	0
166	1z	1	Total 1	Zn 1	0

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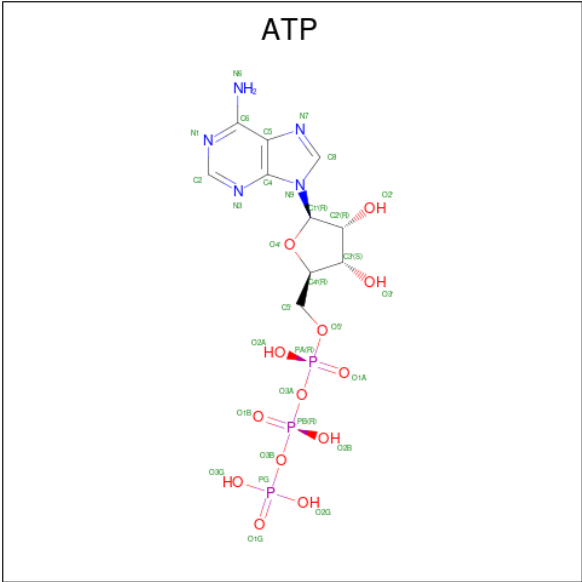
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Mol	Chain	Residues	Atoms		AltConf
166	3T	1	Total 1	Zn 1	0
166	4X	2	Total 2	Zn 2	0
166	1Y	1	Total 1	Zn 1	0
166	5S	1	Total 1	Zn 1	0
166	5T	1	Total 1	Zn 1	0
166	5U	1	Total 1	Zn 1	0
166	5V	1	Total 1	Zn 1	0
166	4L	2	Total 2	Zn 2	0

- Molecule 167 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
167	1S	1	Total 1	Ca 1	0
167	2v	1	Total 1	Ca 1	0
167	2w	1	Total 1	Ca 1	0
167	1T	1	Total 1	Ca 1	0
167	2x	1	Total 1	Ca 1	0

- Molecule 168 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



Mol	Chain	Residues	Atoms					AltConf
168	2v	1	Total	C	N	O	P	0
			31	10	5	13	3	
168	2w	1	Total	C	N	O	P	0
			31	10	5	13	3	
168	2x	1	Total	C	N	O	P	0
			31	10	5	13	3	
168	6l	1	Total	C	N	O	P	0
			31	10	5	13	3	
168	6p	1	Total	C	N	O	P	0
			31	10	5	13	3	
168	9R	1	Total	C	N	O	P	0
			31	10	5	13	3	
168	6u	1	Total	C	N	O	P	0
			31	10	5	13	3	
168	7A	1	Total	C	N	O	P	0
			31	10	5	13	3	
168	7D	1	Total	C	N	O	P	0
			31	10	5	13	3	
168	8a	1	Total	C	N	O	P	0
			31	10	5	13	3	

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

3 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	281984	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 ($e^-/\text{\AA}^2$)	62.6	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.144	Depositor
Minimum map value	0.000	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.00285	Depositor
Map size (Å)	860.51, 778.05005, 1200.99	wwPDB
Map dimensions	647, 585, 903	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.33, 1.33, 1.33	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 956 ligands modelled in this entry, 355 are monoatomic - leaving 601 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
163	GDP	DQ	500	-	25,30,30	0.93	1 (4%)	30,47,47	1.09	2 (6%)
165	GTP	GC	501	164	29,34,34	1.20	1 (3%)	35,54,54	1.45	7 (20%)
163	GDP	TB	500	-	25,30,30	0.94	1 (4%)	30,47,47	1.08	2 (6%)
165	GTP	NQ	501	164	29,34,34	1.29	3 (10%)	35,54,54	1.25	4 (11%)
165	GTP	IS	501	164	29,34,34	1.21	2 (6%)	35,54,54	1.25	4 (11%)
163	GDP	CY	500	-	25,30,30	1.01	1 (4%)	30,47,47	1.13	2 (6%)
165	GTP	HI	501	164	29,34,34	1.19	2 (6%)	35,54,54	1.26	4 (11%)
163	GDP	IT	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.06	2 (6%)
163	GDP	UT	500	-	25,30,30	0.96	1 (4%)	30,47,47	1.08	2 (6%)
165	GTP	QN	501	164	29,34,34	1.26	3 (10%)	35,54,54	1.30	4 (11%)
163	GDP	QQ	500	-	25,30,30	0.94	1 (4%)	30,47,47	1.08	2 (6%)
163	GDP	OJ	500	-	25,30,30	0.95	1 (4%)	30,47,47	1.07	2 (6%)
165	GTP	RB	501	164	29,34,34	1.28	3 (10%)	35,54,54	1.27	4 (11%)
163	GDP	AL	500	-	25,30,30	0.94	1 (4%)	30,47,47	1.12	3 (10%)
163	GDP	CI	500	-	25,30,30	0.93	1 (4%)	30,47,47	1.10	2 (6%)
165	GTP	KZ	501	164	29,34,34	1.20	2 (6%)	35,54,54	1.29	4 (11%)
163	GDP	RE	500	-	25,30,30	0.97	1 (4%)	30,47,47	1.18	4 (13%)
163	GDP	AZ	500	-	25,30,30	0.94	1 (4%)	30,47,47	1.10	2 (6%)
165	GTP	BS	501	164	29,34,34	1.23	2 (6%)	35,54,54	1.26	4 (11%)
163	GDP	MD	500	-	25,30,30	0.95	1 (4%)	30,47,47	1.09	2 (6%)
163	GDP	JQ	500	-	25,30,30	0.95	1 (4%)	30,47,47	1.07	2 (6%)
165	GTP	IU	501	164	29,34,34	1.20	2 (6%)	35,54,54	1.30	4 (11%)
165	GTP	FO	501	164	29,34,34	1.22	1 (3%)	35,54,54	1.25	4 (11%)
165	GTP	DQ	501	164	29,34,34	1.26	3 (10%)	35,54,54	1.32	4 (11%)
168	ATP	2v	501	-	28,33,33	0.65	0	34,52,52	0.59	1 (2%)
165	GTP	RL	501	164	29,34,34	1.25	2 (6%)	35,54,54	1.32	4 (11%)
163	GDP	MP	500	-	25,30,30	0.95	1 (4%)	30,47,47	1.09	2 (6%)
163	GDP	A	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.12	2 (6%)
163	GDP	GL	500	-	25,30,30	0.91	1 (4%)	30,47,47	1.10	2 (6%)
165	GTP	RO	501	164	29,34,34	1.27	3 (10%)	35,54,54	1.27	4 (11%)
163	GDP	PH	500	-	25,30,30	0.94	1 (4%)	30,47,47	1.07	2 (6%)
165	GTP	VQ	501	164	29,34,34	1.22	2 (6%)	35,54,54	1.34	5 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
163	GDP	JK	500	-	25,30,30	0.95	1 (4%)	30,47,47	1.04	2 (6%)
163	GDP	CQ	500	-	25,30,30	0.96	1 (4%)	30,47,47	1.11	2 (6%)
163	GDP	RM	500	-	25,30,30	0.95	1 (4%)	30,47,47	1.07	2 (6%)
163	GDP	IH	500	-	25,30,30	0.95	1 (4%)	30,47,47	1.06	2 (6%)
163	GDP	AP	500	-	25,30,30	0.93	1 (4%)	30,47,47	1.07	2 (6%)
163	GDP	GH	500	-	25,30,30	0.95	1 (4%)	30,47,47	1.08	2 (6%)
165	GTP	HS	501	164	29,34,34	1.21	2 (6%)	35,54,54	1.33	5 (14%)
163	GDP	OD	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.08	2 (6%)
163	GDP	MB	500	-	25,30,30	0.96	1 (4%)	30,47,47	1.06	2 (6%)
163	GDP	EX	500	-	25,30,30	1.07	2 (8%)	30,47,47	1.08	2 (6%)
163	GDP	DY	500	-	25,30,30	0.96	1 (4%)	30,47,47	1.07	2 (6%)
165	GTP	VO	501	164	29,34,34	1.28	3 (10%)	35,54,54	1.24	4 (11%)
163	GDP	OT	500	-	25,30,30	0.95	1 (4%)	30,47,47	1.06	2 (6%)
163	GDP	MH	500	-	25,30,30	0.97	1 (4%)	30,47,47	1.09	2 (6%)
163	GDP	NF	500	-	25,30,30	0.95	1 (4%)	30,47,47	1.06	1 (3%)
165	GTP	TU	501	164	29,34,34	1.27	2 (6%)	35,54,54	1.26	4 (11%)
163	GDP	GF	500	-	25,30,30	0.92	1 (4%)	30,47,47	1.11	2 (6%)
165	GTP	IE	501	164	29,34,34	1.27	2 (6%)	35,54,54	1.41	5 (14%)
163	GDP	RS	500	-	25,30,30	0.94	1 (4%)	30,47,47	1.05	2 (6%)
165	GTP	FT	503	164	29,34,34	1.19	2 (6%)	35,54,54	1.41	7 (20%)
165	GTP	RX	501	164	29,34,34	1.25	2 (6%)	35,54,54	1.32	4 (11%)
165	GTP	DX	501	-	29,34,34	1.25	2 (6%)	35,54,54	1.50	8 (22%)
163	GDP	UR	500	-	25,30,30	0.94	1 (4%)	30,47,47	1.09	2 (6%)
165	GTP	FV	503	-	29,34,34	1.22	2 (6%)	35,54,54	1.40	5 (14%)
165	GTP	WO	501	164	29,34,34	1.26	2 (6%)	35,54,54	1.25	4 (11%)
163	GDP	LC	500	-	25,30,30	0.95	1 (4%)	30,47,47	1.08	2 (6%)
165	GTP	SC	501	164	29,34,34	1.20	2 (6%)	35,54,54	1.27	4 (11%)
165	GTP	WC	501	164	29,34,34	1.26	2 (6%)	35,54,54	1.25	4 (11%)
163	GDP	LY	500	-	25,30,30	0.95	1 (4%)	30,47,47	1.06	2 (6%)
163	GDP	RI	500	-	25,30,30	0.95	1 (4%)	30,47,47	1.06	1 (3%)
165	GTP	FE	501	164	29,34,34	1.20	2 (6%)	35,54,54	1.23	3 (8%)
163	GDP	PX	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.08	2 (6%)
163	GDP	LK	500	-	25,30,30	0.97	1 (4%)	30,47,47	1.08	2 (6%)
165	GTP	PQ	501	164	29,34,34	1.25	2 (6%)	35,54,54	1.31	4 (11%)
163	GDP	DK	501	-	25,30,30	0.94	1 (4%)	30,47,47	1.09	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
165	GTP	WE	501	164	29,34,34	1.25	2 (6%)	35,54,54	1.31	5 (14%)
165	GTP	NW	501	-	29,34,34	1.18	2 (6%)	35,54,54	1.37	5 (14%)
163	GDP	TN	500	-	25,30,30	0.95	1 (4%)	30,47,47	1.08	2 (6%)
163	GDP	IN	500	-	25,30,30	0.96	1 (4%)	30,47,47	1.06	1 (3%)
163	GDP	MT	500	-	25,30,30	0.97	1 (4%)	30,47,47	1.08	2 (6%)
163	GDP	KM	500	-	25,30,30	0.95	1 (4%)	30,47,47	1.06	2 (6%)
165	GTP	KV	501	164	29,34,34	1.24	2 (6%)	35,54,54	1.29	4 (11%)
163	GDP	HR	500	-	25,30,30	0.95	1 (4%)	30,47,47	1.03	1 (3%)
163	GDP	IP	500	-	25,30,30	0.95	1 (4%)	30,47,47	1.07	2 (6%)
163	GDP	VV	500	-	25,30,30	0.94	1 (4%)	30,47,47	1.08	3 (10%)
163	GDP	IF	500	-	25,30,30	0.95	1 (4%)	30,47,47	1.07	2 (6%)
163	GDP	LQ	500	-	25,30,30	0.94	1 (4%)	30,47,47	1.07	1 (3%)
165	GTP	OG	501	164	29,34,34	1.20	2 (6%)	35,54,54	1.38	5 (14%)
165	GTP	SG	501	164	29,34,34	1.23	2 (6%)	35,54,54	1.30	5 (14%)
165	GTP	VS	501	164	29,34,34	1.30	4 (13%)	35,54,54	1.26	4 (11%)
163	GDP	BJ	500	-	25,30,30	0.94	1 (4%)	30,47,47	1.10	2 (6%)
165	GTP	GS	501	164	29,34,34	1.21	2 (6%)	35,54,54	1.42	5 (14%)
165	GTP	TS	501	164	29,34,34	1.24	2 (6%)	35,54,54	1.25	4 (11%)
163	GDP	AN	500	-	25,30,30	0.93	1 (4%)	30,47,47	1.10	2 (6%)
165	GTP	FJ	503	164	29,34,34	1.26	2 (6%)	35,54,54	1.39	5 (14%)
163	GDP	OB	500	-	25,30,30	0.95	1 (4%)	30,47,47	1.11	2 (6%)
163	GDP	GN	500	-	25,30,30	0.97	1 (4%)	30,47,47	1.12	3 (10%)
165	GTP	AP	501	164	29,34,34	1.23	1 (3%)	35,54,54	1.30	4 (11%)
163	GDP	GP	500	-	25,30,30	0.93	1 (4%)	30,47,47	1.11	2 (6%)
165	GTP	OI	501	164	29,34,34	1.22	2 (6%)	35,54,54	1.29	4 (11%)
168	ATP	8a	801	-	28,33,33	0.78	1 (3%)	34,52,52	0.61	1 (2%)
163	GDP	DI	500	-	25,30,30	0.94	1 (4%)	30,47,47	1.12	3 (10%)
165	GTP	II	501	164	29,34,34	1.20	2 (6%)	35,54,54	1.30	4 (11%)
165	GTP	NA	501	-	29,34,34	1.23	2 (6%)	35,54,54	1.27	4 (11%)
163	GDP	PT	500	-	25,30,30	0.94	1 (4%)	30,47,47	1.06	2 (6%)
163	GDP	TV	500	-	25,30,30	0.94	1 (4%)	30,47,47	1.08	2 (6%)
165	GTP	LD	502	164	29,34,34	1.26	2 (6%)	35,54,54	1.26	4 (11%)
163	GDP	FB	500	-	25,30,30	0.96	1 (4%)	30,47,47	1.14	3 (10%)
163	GDP	ER	500	-	25,30,30	0.93	1 (4%)	30,47,47	1.08	2 (6%)
165	GTP	OD	503	164	29,34,34	1.25	3 (10%)	35,54,54	1.32	5 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
165	GTP	DV	501	164	29,34,34	1.24	1 (3%)	35,54,54	1.31	3 (8%)
163	GDP	NJ	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.07	2 (6%)
163	GDP	SD	500	-	25,30,30	0.94	1 (4%)	30,47,47	1.07	2 (6%)
165	GTP	UG	501	164	29,34,34	1.21	2 (6%)	35,54,54	1.28	4 (11%)
165	GTP	HW	501	164	29,34,34	1.21	2 (6%)	35,54,54	1.28	4 (11%)
165	GTP	IY	501	164	29,34,34	1.25	2 (6%)	35,54,54	1.25	4 (11%)
165	GTP	IQ	501	164	29,34,34	1.27	2 (6%)	35,54,54	1.41	5 (14%)
163	GDP	OH	500	-	25,30,30	0.95	1 (4%)	30,47,47	1.06	1 (3%)
163	GDP	VJ	500	-	25,30,30	0.94	1 (4%)	30,47,47	1.07	3 (10%)
165	GTP	SI	501	164	29,34,34	1.20	2 (6%)	35,54,54	1.29	4 (11%)
163	GDP	NN	500	-	25,30,30	0.96	1 (4%)	30,47,47	1.09	1 (3%)
165	GTP	HA	501	164	29,34,34	1.22	2 (6%)	35,54,54	1.24	4 (11%)
163	GDP	BL	500	-	25,30,30	0.93	1 (4%)	30,47,47	1.11	2 (6%)
165	GTP	JB	501	164	29,34,34	1.22	2 (6%)	35,54,54	1.27	4 (11%)
165	GTP	TG	501	164	29,34,34	1.24	2 (6%)	35,54,54	1.25	4 (11%)
163	GDP	BP	500	-	25,30,30	0.96	1 (4%)	30,47,47	1.09	3 (10%)
165	GTP	KB	502	164	29,34,34	1.23	2 (6%)	35,54,54	1.23	4 (11%)
165	GTP	BE	501	164	29,34,34	1.23	1 (3%)	35,54,54	1.29	5 (14%)
165	GTP	CB	501	164	29,34,34	1.25	2 (6%)	35,54,54	1.27	4 (11%)
165	GTP	CO	501	164	29,34,34	1.28	1 (3%)	35,54,54	1.31	3 (8%)
165	GTP	VE	501	164	29,34,34	1.22	2 (6%)	35,54,54	1.35	5 (14%)
165	GTP	JV	501	164	29,34,34	1.27	2 (6%)	35,54,54	1.26	4 (11%)
163	GDP	JU	500	-	25,30,30	0.98	1 (4%)	30,47,47	1.07	3 (10%)
165	GTP	GO	501	164	29,34,34	1.21	1 (3%)	35,54,54	1.37	5 (14%)
163	GDP	HL	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.03	1 (3%)
165	GTP	JR	501	164	29,34,34	1.20	2 (6%)	35,54,54	1.35	5 (14%)
165	GTP	T	503	164	29,34,34	1.26	3 (10%)	35,54,54	1.30	5 (14%)
168	ATP	7D	601	164	28,33,33	0.73	0	34,52,52	0.58	1 (2%)
163	GDP	NB	500	-	25,30,30	0.97	1 (4%)	30,47,47	1.09	1 (3%)
163	GDP	KI	500	-	25,30,30	0.96	1 (4%)	30,47,47	1.08	2 (6%)
163	GDP	GJ	500	-	25,30,30	0.92	1 (4%)	30,47,47	1.11	2 (6%)
163	GDP	UL	500	-	25,30,30	0.96	1 (4%)	30,47,47	1.07	2 (6%)
163	GDP	SB	501	-	25,30,30	0.94	1 (4%)	30,47,47	1.07	2 (6%)
165	GTP	BQ	501	164	29,34,34	1.19	2 (6%)	35,54,54	1.26	4 (11%)
163	GDP	UD	500	-	25,30,30	0.96	1 (4%)	30,47,47	1.07	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
163	GDP	FL	500	-	25,30,30	0.95	1 (4%)	30,47,47	1.13	2 (6%)
163	GDP	TD	500	-	25,30,30	0.95	1 (4%)	30,47,47	1.09	2 (6%)
163	GDP	VD	500	-	25,30,30	0.94	1 (4%)	30,47,47	1.07	2 (6%)
165	GTP	D	501	-	29,34,34	1.33	3 (10%)	35,54,54	1.39	5 (14%)
163	GDP	TH	500	-	25,30,30	0.96	1 (4%)	30,47,47	1.06	2 (6%)
163	GDP	U	500	-	25,30,30	0.95	1 (4%)	30,47,47	1.09	2 (6%)
165	GTP	NY	501	164	29,34,34	1.26	3 (10%)	35,54,54	1.25	4 (11%)
165	GTP	GQ	501	164	29,34,34	1.21	2 (6%)	35,54,54	1.53	6 (17%)
165	GTP	MI	501	164	29,34,34	1.26	2 (6%)	35,54,54	1.24	4 (11%)
163	GDP	V	500	-	25,30,30	0.95	1 (4%)	30,47,47	1.06	2 (6%)
165	GTP	FA	501	164	29,34,34	1.23	1 (3%)	35,54,54	1.22	4 (11%)
165	GTP	PY	501	164	29,34,34	1.25	2 (6%)	35,54,54	1.25	4 (11%)
163	GDP	LW	500	-	25,30,30	0.97	1 (4%)	30,47,47	1.09	2 (6%)
165	GTP	QU	501	164	29,34,34	1.24	3 (10%)	35,54,54	1.30	4 (11%)
163	GDP	NL	500	-	25,30,30	0.95	1 (4%)	30,47,47	1.05	1 (3%)
165	GTP	VW	501	164	29,34,34	1.26	2 (6%)	35,54,54	1.27	4 (11%)
165	GTP	OK	501	-	29,34,34	1.20	2 (6%)	35,54,54	1.32	4 (11%)
163	GDP	VT	500	-	25,30,30	0.96	1 (4%)	30,47,47	1.06	2 (6%)
163	GDP	SR	500	-	25,30,30	0.95	1 (4%)	30,47,47	1.06	1 (3%)
165	GTP	TW	501	164	29,34,34	1.22	2 (6%)	35,54,54	1.24	4 (11%)
165	GTP	KJ	501	164	29,34,34	1.23	2 (6%)	35,54,54	1.29	4 (11%)
163	GDP	DG	500	-	25,30,30	0.93	1 (4%)	30,47,47	1.08	2 (6%)
163	GDP	PL	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.08	2 (6%)
163	GDP	RW	500	-	25,30,30	0.96	1 (4%)	30,47,47	1.07	2 (6%)
165	GTP	JK	501	164	29,34,34	1.21	2 (6%)	35,54,54	1.33	4 (11%)
165	GTP	EU	501	164	29,34,34	1.21	1 (3%)	35,54,54	1.31	4 (11%)
165	GTP	MU	501	164	29,34,34	1.26	2 (6%)	35,54,54	1.23	4 (11%)
165	GTP	PO	501	164	29,34,34	1.25	2 (6%)	35,54,54	1.27	4 (11%)
165	GTP	TQ	501	164	29,34,34	1.21	2 (6%)	35,54,54	1.25	4 (11%)
163	GDP	DM	500	-	25,30,30	0.94	1 (4%)	30,47,47	1.08	2 (6%)
163	GDP	LA	500	-	25,30,30	0.95	1 (4%)	30,47,47	1.06	2 (6%)
165	GTP	LF	502	164	29,34,34	1.21	2 (6%)	35,54,54	1.35	5 (14%)
165	GTP	IG	501	164	29,34,34	1.21	2 (6%)	35,54,54	1.25	4 (11%)
163	GDP	JW	500	-	25,30,30	0.96	1 (4%)	30,47,47	1.04	2 (6%)
165	GTP	LT	501	164	29,34,34	1.24	2 (6%)	35,54,54	1.36	5 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
165	GTP	IM	501	164	29,34,34	1.24	2 (6%)	35,54,54	1.25	4 (11%)
165	GTP	RJ	501	-	29,34,34	1.26	2 (6%)	35,54,54	1.30	4 (11%)
163	GDP	HT	501	-	25,30,30	0.94	1 (4%)	30,47,47	1.07	2 (6%)
165	GTP	BA	501	164	29,34,34	1.27	2 (6%)	35,54,54	1.26	4 (11%)
163	GDP	WJ	500	-	25,30,30	0.94	1 (4%)	30,47,47	1.05	2 (6%)
165	GTP	GK	501	164	29,34,34	1.27	1 (3%)	35,54,54	1.39	6 (17%)
165	GTP	HG	501	164	29,34,34	1.22	2 (6%)	35,54,54	1.33	5 (14%)
165	GTP	BW	501	164	29,34,34	1.24	2 (6%)	35,54,54	1.29	3 (8%)
165	GTP	ED	501	164	29,34,34	1.27	1 (3%)	35,54,54	1.39	6 (17%)
163	GDP	MF	500	-	25,30,30	0.96	1 (4%)	30,47,47	1.06	2 (6%)
165	GTP	QC	501	164	29,34,34	1.27	2 (6%)	35,54,54	1.31	5 (14%)
163	GDP	O	500	-	25,30,30	0.98	1 (4%)	30,47,47	1.04	2 (6%)
165	GTP	KL	501	164	29,34,34	1.25	3 (10%)	35,54,54	1.28	4 (11%)
165	GTP	BI	501	164	29,34,34	1.27	3 (10%)	35,54,54	1.40	5 (14%)
163	GDP	KW	500	-	25,30,30	0.96	1 (4%)	30,47,47	1.06	2 (6%)
163	GDP	MN	500	-	25,30,30	0.97	1 (4%)	30,47,47	1.07	3 (10%)
163	GDP	QK	500	-	25,30,30	0.99	1 (4%)	30,47,47	1.01	1 (3%)
165	GTP	JD	501	164	29,34,34	1.23	2 (6%)	35,54,54	1.26	4 (11%)
165	GTP	SK	501	164	29,34,34	1.26	2 (6%)	35,54,54	1.27	4 (11%)
163	GDP	DE	500	-	25,30,30	0.95	1 (4%)	30,47,47	1.12	2 (6%)
165	GTP	HM	501	164	29,34,34	1.21	2 (6%)	35,54,54	1.22	4 (11%)
165	GTP	EP	501	164	29,34,34	1.27	2 (6%)	35,54,54	1.31	5 (14%)
163	GDP	VH	500	-	25,30,30	0.96	1 (4%)	30,47,47	1.07	2 (6%)
163	GDP	LG	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.09	2 (6%)
165	GTP	NF	501	-	29,34,34	1.31	4 (13%)	35,54,54	1.31	4 (11%)
163	GDP	KQ	500	-	25,30,30	0.99	1 (4%)	30,47,47	1.07	2 (6%)
165	GTP	QO	501	164	29,34,34	1.27	3 (10%)	35,54,54	1.31	5 (14%)
163	GDP	HF	500	-	25,30,30	0.95	1 (4%)	30,47,47	1.03	1 (3%)
165	GTP	SO	501	164	29,34,34	1.21	2 (6%)	35,54,54	1.27	4 (11%)
163	GDP	TJ	500	-	25,30,30	0.96	1 (4%)	30,47,47	1.08	2 (6%)
165	GTP	AA	501	164	29,34,34	1.24	1 (3%)	35,54,54	1.26	4 (11%)
163	GDP	FX	500	-	25,30,30	0.95	1 (4%)	30,47,47	1.12	2 (6%)
163	GDP	KK	500	-	25,30,30	0.96	1 (4%)	30,47,47	1.06	2 (6%)
165	GTP	OA	501	164	29,34,34	1.24	2 (6%)	35,54,54	1.26	4 (11%)
165	GTP	DB	501	164	29,34,34	1.22	2 (6%)	35,54,54	1.67	5 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
165	GTP	PA	501	164	29,34,34	1.28	2 (6%)	35,54,54	1.27	4 (11%)
163	GDP	ED	500	-	25,30,30	0.95	1 (4%)	30,47,47	1.11	2 (6%)
163	GDP	FP	500	-	25,30,30	0.95	1 (4%)	30,47,47	1.07	2 (6%)
163	GDP	EH	500	-	25,30,30	0.96	1 (4%)	30,47,47	1.10	2 (6%)
163	GDP	KU	500	-	25,30,30	0.96	1 (4%)	30,47,47	1.07	2 (6%)
165	GTP	HQ	501	164	29,34,34	1.22	2 (6%)	35,54,54	1.23	4 (11%)
165	GTP	WI	501	164	29,34,34	1.27	2 (6%)	35,54,54	1.27	4 (11%)
163	GDP	HN	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.06	1 (3%)
163	GDP	OL	500	-	25,30,30	0.96	1 (4%)	30,47,47	1.06	2 (6%)
163	GDP	UP	500	-	25,30,30	0.95	1 (4%)	30,47,47	1.07	1 (3%)
165	GTP	MO	501	164	29,34,34	1.22	2 (6%)	35,54,54	1.28	4 (11%)
163	GDP	PP	500	-	25,30,30	0.96	1 (4%)	30,47,47	1.06	2 (6%)
165	GTP	UA	501	164	29,34,34	1.25	2 (6%)	35,54,54	1.22	4 (11%)
165	GTP	AY	501	164	29,34,34	1.22	1 (3%)	35,54,54	1.24	4 (11%)
163	GDP	LE	500	-	25,30,30	0.95	1 (4%)	30,47,47	1.08	1 (3%)
165	GTP	JF	501	164	29,34,34	1.20	2 (6%)	35,54,54	1.35	5 (14%)
163	GDP	GR	500	-	25,30,30	0.92	1 (4%)	30,47,47	1.13	2 (6%)
165	GTP	FI	501	164	29,34,34	1.22	1 (3%)	35,54,54	1.32	5 (14%)
163	GDP	VL	500	-	25,30,30	0.97	1 (4%)	30,47,47	1.06	2 (6%)
165	GTP	QT	501	164	29,34,34	1.25	2 (6%)	35,54,54	1.38	6 (17%)
163	GDP	UH	500	-	25,30,30	0.96	1 (4%)	30,47,47	1.07	2 (6%)
163	GDP	NX	500	-	25,30,30	0.95	1 (4%)	30,47,47	1.05	2 (6%)
165	GTP	WQ	501	164	29,34,34	1.26	2 (6%)	35,54,54	1.31	5 (14%)
165	GTP	QX	501	-	29,34,34	1.26	2 (6%)	35,54,54	1.26	4 (11%)
163	GDP	DW	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.05	2 (6%)
165	GTP	EC	501	164	29,34,34	1.24	1 (3%)	35,54,54	1.23	4 (11%)
163	GDP	SV	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.06	2 (6%)
165	GTP	WY	501	164	29,34,34	1.27	2 (6%)	35,54,54	1.25	4 (11%)
165	GTP	AK	501	164	29,34,34	1.28	2 (6%)	35,54,54	1.29	4 (11%)
163	GDP	GV	501	-	25,30,30	0.91	1 (4%)	30,47,47	1.12	2 (6%)
165	GTP	J	501	164	29,34,34	1.24	2 (6%)	35,54,54	1.23	4 (11%)
168	ATP	2x	501	-	28,33,33	0.67	0	34,52,52	0.59	1 (2%)
163	GDP	SJ	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.06	2 (6%)
163	GDP	MR	500	-	25,30,30	0.96	1 (4%)	30,47,47	1.07	2 (6%)
165	GTP	MG	501	164	29,34,34	1.19	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
163	GDP	CK	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.11	2 (6%)
165	GTP	AG	501	164	29,34,34	1.20	1 (3%)	35,54,54	1.23	4 (11%)
165	GTP	CV	501	164	29,34,34	1.27	2 (6%)	35,54,54	1.37	5 (14%)
163	GDP	WD	500	-	25,30,30	0.95	1 (4%)	30,47,47	1.08	2 (6%)
163	GDP	E	500	-	25,30,30	1.10	3 (12%)	30,47,47	1.22	4 (13%)
163	GDP	RG	500	-	25,30,30	0.95	1 (4%)	30,47,47	1.06	2 (6%)
163	GDP	SP	500	-	25,30,30	0.94	1 (4%)	30,47,47	1.07	2 (6%)
163	GDP	GT	501	-	25,30,30	0.94	1 (4%)	30,47,47	1.08	2 (6%)
163	GDP	QS	500	-	25,30,30	0.94	1 (4%)	30,47,47	1.10	2 (6%)
165	GTP	NR	501	-	29,34,34	1.29	4 (13%)	35,54,54	1.30	4 (11%)
165	GTP	QI	501	164	29,34,34	1.25	3 (10%)	35,54,54	1.30	5 (14%)
163	GDP	VF	500	-	25,30,30	0.97	1 (4%)	30,47,47	1.09	2 (6%)
168	ATP	2w	501	-	28,33,33	0.67	0	34,52,52	0.58	1 (2%)
163	GDP	PR	501	-	25,30,30	0.94	1 (4%)	30,47,47	1.05	2 (6%)
165	GTP	NE	501	164	29,34,34	1.28	3 (10%)	35,54,54	1.24	4 (11%)
165	GTP	PG	501	-	29,34,34	1.21	2 (6%)	35,54,54	1.30	4 (11%)
163	GDP	KO	500	-	25,30,30	0.96	1 (4%)	30,47,47	1.07	1 (3%)
165	GTP	UK	501	164	29,34,34	1.26	2 (6%)	35,54,54	1.26	4 (11%)
165	GTP	LN	502	164	29,34,34	1.26	2 (6%)	35,54,54	1.25	4 (11%)
165	GTP	UE	501	164	29,34,34	1.21	2 (6%)	35,54,54	1.24	4 (11%)
163	GDP	CW	500	-	25,30,30	0.98	1 (4%)	30,47,47	1.16	2 (6%)
165	GTP	AO	501	164	29,34,34	1.21	1 (3%)	35,54,54	1.25	4 (11%)
163	GDP	JI	500	-	25,30,30	0.97	1 (4%)	30,47,47	1.07	3 (10%)
165	GTP	BK	501	164	29,34,34	1.24	1 (3%)	35,54,54	1.28	4 (11%)
163	GDP	CO	500	-	25,30,30	0.96	1 (4%)	30,47,47	1.07	2 (6%)
165	GTP	NU	501	164	29,34,34	1.22	2 (6%)	35,54,54	1.28	4 (11%)
165	GTP	HB	503	164	29,34,34	1.26	3 (10%)	35,54,54	1.28	5 (14%)
163	GDP	QO	500	-	25,30,30	0.93	1 (4%)	30,47,47	1.09	2 (6%)
165	GTP	ME	501	164	29,34,34	1.29	3 (10%)	35,54,54	1.32	4 (11%)
163	GDP	GX	500	-	25,30,30	0.93	1 (4%)	30,47,47	1.09	2 (6%)
163	GDP	PJ	500	-	25,30,30	0.93	1 (4%)	30,47,47	1.04	2 (6%)
165	GTP	VH	501	164	29,34,34	1.24	2 (6%)	35,54,54	1.30	4 (11%)
163	GDP	RC	500	-	25,30,30	0.95	1 (4%)	30,47,47	1.07	2 (6%)
163	GDP	AF	500	-	25,30,30	0.95	1 (4%)	30,47,47	1.07	2 (6%)
163	GDP	AV	500	-	25,30,30	0.94	1 (4%)	30,47,47	1.11	3 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
165	GTP	NM	501	164	29,34,34	1.25	2 (6%)	35,54,54	1.25	4 (11%)
163	GDP	PN	500	-	25,30,30	0.95	1 (4%)	30,47,47	1.07	2 (6%)
165	GTP	BY	501	164	29,34,34	1.26	1 (3%)	35,54,54	1.28	4 (11%)
165	GTP	DN	501	164	29,34,34	1.23	1 (3%)	35,54,54	1.52	5 (14%)
163	GDP	UJ	500	-	25,30,30	0.94	1 (4%)	30,47,47	1.07	2 (6%)
165	GTP	UI	501	164	29,34,34	1.25	2 (6%)	35,54,54	1.31	4 (11%)
163	GDP	RA	500	-	25,30,30	0.95	1 (4%)	30,47,47	1.07	2 (6%)
163	GDP	BD	500	-	25,30,30	0.96	1 (4%)	30,47,47	1.09	3 (10%)
163	GDP	AD	500	-	25,30,30	0.93	1 (4%)	30,47,47	1.10	3 (10%)
165	GTP	CH	501	164	29,34,34	1.21	2 (6%)	35,54,54	1.40	5 (14%)
163	GDP	JC	500	-	25,30,30	0.95	1 (4%)	30,47,47	1.06	2 (6%)
163	GDP	CA	500	-	25,30,30	0.97	1 (4%)	30,47,47	1.12	3 (10%)
163	GDP	QI	500	-	25,30,30	0.94	1 (4%)	30,47,47	1.08	2 (6%)
163	GDP	SH	500	-	25,30,30	0.96	1 (4%)	30,47,47	1.08	2 (6%)
165	GTP	OY	501	164	29,34,34	1.22	2 (6%)	35,54,54	1.26	4 (11%)
165	GTP	OP	503	164	29,34,34	1.24	3 (10%)	35,54,54	1.31	5 (14%)
163	GDP	IR	500	-	25,30,30	0.96	1 (4%)	30,47,47	1.07	2 (6%)
165	GTP	JN	501	164	29,34,34	1.23	2 (6%)	35,54,54	1.25	4 (11%)
165	GTP	JT	501	164	29,34,34	1.22	2 (6%)	35,54,54	1.26	4 (11%)
165	GTP	GL	501	164	29,34,34	1.27	1 (3%)	35,54,54	1.40	6 (17%)
165	GTP	TK	501	164	29,34,34	1.22	2 (6%)	35,54,54	1.24	4 (11%)
163	GDP	RQ	500	-	25,30,30	0.96	1 (4%)	30,47,47	1.17	4 (13%)
163	GDP	NP	500	-	25,30,30	0.98	1 (4%)	30,47,47	1.10	2 (6%)
165	GTP	SQ	501	164	29,34,34	1.22	2 (6%)	35,54,54	1.32	5 (14%)
165	GTP	WM	501	164	29,34,34	1.28	2 (6%)	35,54,54	1.25	4 (11%)
163	GDP	CU	500	-	25,30,30	0.94	1 (4%)	30,47,47	1.09	3 (10%)
165	GTP	DP	501	164	29,34,34	1.23	2 (6%)	35,54,54	1.63	7 (20%)
165	GTP	IO	501	164	29,34,34	1.28	3 (10%)	35,54,54	1.32	4 (11%)
165	GTP	K	501	164	29,34,34	1.26	3 (10%)	35,54,54	1.30	4 (11%)
165	GTP	RT	501	164	29,34,34	1.23	2 (6%)	35,54,54	1.31	4 (11%)
163	GDP	AB	500	-	25,30,30	0.94	1 (4%)	30,47,47	1.09	2 (6%)
168	ATP	9R	500	164	28,33,33	0.68	0	34,52,52	0.59	1 (2%)
163	GDP	KG	500	-	25,30,30	0.98	1 (4%)	30,47,47	1.08	2 (6%)
165	GTP	JH	501	164	29,34,34	1.21	2 (6%)	35,54,54	1.26	4 (11%)
165	GTP	QF	501	164	29,34,34	1.18	2 (6%)	35,54,54	1.31	4 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
165	GTP	UM	501	164	29,34,34	1.25	2 (6%)	35,54,54	1.21	4 (11%)
165	GTP	OW	501	-	29,34,34	1.21	2 (6%)	35,54,54	1.32	4 (11%)
163	GDP	IV	500	-	25,30,30	0.95	1 (4%)	30,47,47	1.07	2 (6%)
163	GDP	CC	500	-	25,30,30	0.94	1 (4%)	30,47,47	1.09	3 (10%)
165	GTP	JW	501	164	29,34,34	1.21	2 (6%)	35,54,54	1.33	4 (11%)
163	GDP	BV	500	-	25,30,30	0.95	1 (4%)	30,47,47	1.05	2 (6%)
165	GTP	KF	501	164	29,34,34	1.27	3 (10%)	35,54,54	1.24	4 (11%)
163	GDP	BF	500	-	25,30,30	0.95	1 (4%)	30,47,47	1.06	2 (6%)
165	GTP	QB	501	164	29,34,34	1.25	2 (6%)	35,54,54	1.29	4 (11%)
165	GTP	VY	501	164	29,34,34	1.25	2 (6%)	35,54,54	1.24	4 (11%)
165	GTP	TM	501	164	29,34,34	1.26	3 (10%)	35,54,54	1.30	5 (14%)
165	GTP	AB	501	164	29,34,34	1.24	1 (3%)	35,54,54	1.22	4 (11%)
163	GDP	QU	500	-	25,30,30	0.95	1 (4%)	30,47,47	1.09	2 (6%)
163	GDP	VP	500	-	25,30,30	0.93	1 (4%)	30,47,47	1.08	2 (6%)
163	GDP	WV	500	-	25,30,30	0.94	1 (4%)	30,47,47	1.06	2 (6%)
165	GTP	WK	501	164	29,34,34	1.24	2 (6%)	35,54,54	1.25	4 (11%)
163	GDP	CM	500	-	25,30,30	0.98	2 (8%)	30,47,47	1.20	3 (10%)
165	GTP	CC	501	164	29,34,34	1.29	1 (3%)	35,54,54	1.32	4 (11%)
165	GTP	DH	501	164	29,34,34	1.21	2 (6%)	35,54,54	1.28	4 (11%)
163	GDP	HJ	500	-	25,30,30	0.95	1 (4%)	30,47,47	1.07	2 (6%)
163	GDP	IB	500	-	25,30,30	0.96	1 (4%)	30,47,47	1.06	1 (3%)
163	GDP	JM	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.04	2 (6%)
163	GDP	M	500	-	25,30,30	0.97	1 (4%)	30,47,47	1.07	2 (6%)
163	GDP	EN	500	-	25,30,30	0.96	1 (4%)	30,47,47	1.09	2 (6%)
163	GDP	NT	500	-	25,30,30	0.97	1 (4%)	30,47,47	1.08	2 (6%)
165	GTP	NI	501	164	29,34,34	1.23	2 (6%)	35,54,54	1.28	4 (11%)
165	GTP	L	501	164	29,34,34	1.24	2 (6%)	35,54,54	1.26	4 (11%)
165	GTP	CQ	501	164	29,34,34	1.26	3 (10%)	35,54,54	1.37	6 (17%)
165	GTP	NO	501	164	29,34,34	1.25	2 (6%)	35,54,54	1.26	4 (11%)
165	GTP	MC	501	164	29,34,34	1.22	2 (6%)	35,54,54	1.28	4 (11%)
163	GDP	RU	500	-	25,30,30	0.95	1 (4%)	30,47,47	1.06	1 (3%)
165	GTP	VK	501	164	29,34,34	1.25	2 (6%)	35,54,54	1.27	4 (11%)
165	GTP	AD	501	164	29,34,34	1.19	2 (6%)	35,54,54	1.32	5 (14%)
165	GTP	CT	501	164	29,34,34	1.23	2 (6%)	35,54,54	1.43	6 (17%)
163	GDP	KE	500	-	25,30,30	0.98	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
163	GDP	ML	500	-	25,30,30	0.97	1 (4%)	30,47,47	1.07	2 (6%)
165	GTP	MM	501	164	29,34,34	1.26	2 (6%)	35,54,54	1.28	4 (11%)
163	GDP	HP	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.08	2 (6%)
168	ATP	6u	700	-	28,33,33	0.71	0	34,52,52	0.59	1 (2%)
163	GDP	DO	500	-	25,30,30	0.94	1 (4%)	30,47,47	1.12	2 (6%)
165	GTP	HY	501	164	29,34,34	1.21	2 (6%)	35,54,54	1.21	4 (11%)
165	GTP	WU	501	164	29,34,34	1.26	2 (6%)	35,54,54	1.27	4 (11%)
163	GDP	NH	500	-	25,30,30	0.97	1 (4%)	30,47,47	1.07	2 (6%)
163	GDP	OF	500	-	25,30,30	0.95	1 (4%)	30,47,47	1.09	2 (6%)
163	GDP	FT	501	-	25,30,30	0.94	1 (4%)	30,47,47	1.09	2 (6%)
165	GTP	KN	502	164	29,34,34	1.21	2 (6%)	35,54,54	1.29	4 (11%)
165	GTP	KX	501	164	29,34,34	1.24	3 (10%)	35,54,54	1.28	4 (11%)
163	GDP	AJ	500	-	25,30,30	0.93	1 (4%)	30,47,47	1.09	2 (6%)
165	GTP	RR	501	164	29,34,34	1.21	2 (6%)	35,54,54	1.33	4 (11%)
163	GDP	CS	500	-	25,30,30	0.93	1 (4%)	30,47,47	1.07	2 (6%)
163	GDP	WL	500	-	25,30,30	0.94	1 (4%)	30,47,47	1.08	2 (6%)
163	GDP	AH	500	-	25,30,30	0.92	1 (4%)	30,47,47	1.08	3 (10%)
165	GTP	SA	501	164	29,34,34	1.24	2 (6%)	35,54,54	1.25	4 (11%)
163	GDP	QG	500	-	25,30,30	0.95	1 (4%)	30,47,47	1.10	2 (6%)
165	GTP	KT	501	164	29,34,34	1.23	2 (6%)	35,54,54	1.36	5 (14%)
165	GTP	EM	501	164	29,34,34	1.27	1 (3%)	35,54,54	1.28	4 (11%)
165	GTP	OM	501	164	29,34,34	1.22	2 (6%)	35,54,54	1.25	4 (11%)
165	GTP	CN	501	164	29,34,34	1.28	1 (3%)	35,54,54	1.26	4 (11%)
163	GDP	IJ	500	-	25,30,30	0.95	1 (4%)	30,47,47	1.07	2 (6%)
165	GTP	IW	501	164	29,34,34	1.48	6 (20%)	35,54,54	1.35	5 (14%)
163	GDP	TR	500	-	25,30,30	0.94	1 (4%)	30,47,47	1.07	2 (6%)
163	GDP	QE	500	-	25,30,30	0.93	1 (4%)	30,47,47	1.09	2 (6%)
165	GTP	LR	502	164	29,34,34	1.21	2 (6%)	35,54,54	1.35	5 (14%)
163	GDP	F	500	-	25,30,30	0.93	1 (4%)	30,47,47	1.10	2 (6%)
163	GDP	GB	500	-	25,30,30	0.96	1 (4%)	30,47,47	1.05	2 (6%)
165	GTP	NK	501	-	29,34,34	1.20	2 (6%)	35,54,54	1.36	5 (14%)
165	GTP	TO	501	164	29,34,34	1.20	2 (6%)	35,54,54	1.32	4 (11%)
163	GDP	ST	500	-	25,30,30	0.96	1 (4%)	30,47,47	1.08	2 (6%)
163	GDP	LS	500	-	25,30,30	0.97	1 (4%)	30,47,47	1.08	2 (6%)
163	GDP	WB	500	-	25,30,30	0.93	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
163	GDP	MJ	500	-	25,30,30	0.97	1 (4%)	30,47,47	1.17	3 (10%)
163	GDP	FN	500	-	25,30,30	0.98	1 (4%)	30,47,47	1.20	3 (10%)
165	GTP	PW	501	164	29,34,34	1.23	2 (6%)	35,54,54	1.30	4 (11%)
165	GTP	MQ	501	164	29,34,34	1.28	2 (6%)	35,54,54	1.31	4 (11%)
165	GTP	NC	501	164	29,34,34	1.25	2 (6%)	35,54,54	1.26	4 (11%)
163	GDP	G	500	-	25,30,30	0.97	1 (4%)	30,47,47	1.07	2 (6%)
163	GDP	OX	500	-	25,30,30	0.94	1 (4%)	30,47,47	1.05	2 (6%)
168	ATP	6p	500	164	28,33,33	0.77	0	34,52,52	0.60	1 (2%)
165	GTP	RV	501	-	29,34,34	1.25	2 (6%)	35,54,54	1.30	4 (11%)
163	GDP	FH	500	-	25,30,30	0.93	1 (4%)	30,47,47	1.06	2 (6%)
163	GDP	BX	500	-	25,30,30	0.96	1 (4%)	30,47,47	1.08	1 (3%)
165	GTP	CK	503	164	29,34,34	1.24	2 (6%)	35,54,54	1.27	4 (11%)
165	GTP	AW	501	164	29,34,34	1.26	2 (6%)	35,54,54	1.27	4 (11%)
163	GDP	NR	500	-	25,30,30	0.95	1 (4%)	30,47,47	1.06	1 (3%)
165	GTP	UW	501	164	29,34,34	1.25	2 (6%)	35,54,54	1.26	4 (11%)
165	GTP	CE	501	164	29,34,34	1.27	3 (10%)	35,54,54	1.31	4 (11%)
165	GTP	BG	501	164	29,34,34	1.23	2 (6%)	35,54,54	1.28	4 (11%)
165	GTP	PC	501	164	29,34,34	1.25	2 (6%)	35,54,54	1.27	4 (11%)
163	GDP	LU	500	-	25,30,30	0.96	1 (4%)	30,47,47	1.06	2 (6%)
165	GTP	RH	501	164	29,34,34	1.22	2 (6%)	35,54,54	1.31	4 (11%)
165	GTP	KD	502	164	29,34,34	1.26	2 (6%)	35,54,54	1.26	4 (11%)
163	GDP	HH	501	-	25,30,30	0.94	1 (4%)	30,47,47	1.08	2 (6%)
163	GDP	MV	500	-	25,30,30	0.98	1 (4%)	30,47,47	1.18	3 (10%)
163	GDP	P	500	-	25,30,30	0.97	1 (4%)	30,47,47	1.16	3 (10%)
163	GDP	TX	500	-	25,30,30	0.98	1 (4%)	30,47,47	1.05	2 (6%)
165	GTP	RN	501	164	29,34,34	1.28	2 (6%)	35,54,54	1.27	4 (11%)
163	GDP	S	500	-	25,30,30	0.93	1 (4%)	30,47,47	1.08	2 (6%)
163	GDP	DS	500	-	25,30,30	0.94	1 (4%)	30,47,47	1.09	2 (6%)
163	GDP	WH	500	-	25,30,30	0.96	1 (4%)	30,47,47	1.08	2 (6%)
165	GTP	KH	501	164	29,34,34	1.23	2 (6%)	35,54,54	1.35	5 (14%)
163	GDP	ID	500	-	25,30,30	0.95	1 (4%)	30,47,47	1.06	2 (6%)
165	GTP	SW	501	164	29,34,34	1.24	2 (6%)	35,54,54	1.27	4 (11%)
163	GDP	NV	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.07	2 (6%)
165	GTP	FQ	501	164	29,34,34	1.21	2 (6%)	35,54,54	1.26	4 (11%)
165	GTP	LJ	501	164	29,34,34	1.21	2 (6%)	35,54,54	1.31	4 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
163	GDP	SL	500	-	25,30,30	0.93	1 (4%)	30,47,47	1.08	2 (6%)
165	GTP	OS	501	164	29,34,34	1.21	2 (6%)	35,54,54	1.37	5 (14%)
163	GDP	SN	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.06	2 (6%)
165	GTP	VC	501	164	29,34,34	1.28	3 (10%)	35,54,54	1.23	4 (11%)
163	GDP	EP	500	-	25,30,30	0.96	1 (4%)	30,47,47	1.09	2 (6%)
163	GDP	JY	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.05	2 (6%)
163	GDP	KA	500	-	25,30,30	0.95	1 (4%)	30,47,47	1.07	1 (3%)
163	GDP	SF	500	-	25,30,30	0.95	1 (4%)	30,47,47	1.05	1 (3%)
163	GDP	IX	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.09	2 (6%)
163	GDP	AX	500	-	25,30,30	0.94	1 (4%)	30,47,47	1.09	3 (10%)
163	GDP	PV	500	-	25,30,30	0.93	1 (4%)	30,47,47	1.04	2 (6%)
163	GDP	UN	500	-	25,30,30	0.97	1 (4%)	30,47,47	1.10	2 (6%)
168	ATP	7A	402	-	28,33,33	0.77	0	34,52,52	0.60	1 (2%)
163	GDP	JG	500	-	25,30,30	0.96	1 (4%)	30,47,47	1.05	2 (6%)
165	GTP	HU	501	164	29,34,34	1.19	2 (6%)	35,54,54	1.26	4 (11%)
163	GDP	CG	500	-	25,30,30	0.94	1 (4%)	30,47,47	1.10	3 (10%)
165	GTP	AS	501	164	29,34,34	1.21	2 (6%)	35,54,54	1.24	4 (11%)
165	GTP	RF	501	164	29,34,34	1.20	2 (6%)	35,54,54	1.33	4 (11%)
163	GDP	OR	500	-	25,30,30	0.95	1 (4%)	30,47,47	1.08	2 (6%)
165	GTP	LZ	502	164	29,34,34	1.26	2 (6%)	35,54,54	1.25	4 (11%)
163	GDP	TF	500	-	25,30,30	0.94	1 (4%)	30,47,47	1.07	2 (6%)
165	GTP	VG	501	164	29,34,34	1.29	3 (10%)	35,54,54	1.26	4 (11%)
163	GDP	WX	500	-	25,30,30	0.95	1 (4%)	30,47,47	1.08	2 (6%)
165	GTP	JJ	501	164	29,34,34	1.26	2 (6%)	35,54,54	1.26	3 (8%)
163	GDP	HX	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.03	1 (3%)
163	GDP	JO	500	-	25,30,30	0.96	1 (4%)	30,47,47	1.06	2 (6%)
165	GTP	C	501	164	29,34,34	1.27	2 (6%)	35,54,54	1.31	4 (11%)
163	GDP	QW	500	-	25,30,30	1.00	1 (4%)	30,47,47	1.01	2 (6%)
163	GDP	WF	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.07	2 (6%)
163	GDP	HD	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.08	2 (6%)
163	GDP	H	500	-	25,30,30	0.98	1 (4%)	30,47,47	1.05	2 (6%)
163	GDP	KC	500	-	25,30,30	0.96	1 (4%)	30,47,47	1.07	2 (6%)
165	GTP	AI	501	164	29,34,34	1.19	2 (6%)	35,54,54	1.26	4 (11%)
165	GTP	AM	501	164	29,34,34	1.23	1 (3%)	35,54,54	1.34	4 (11%)
165	GTP	IA	501	164	29,34,34	1.22	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
165	GTP	WW	501	164	29,34,34	1.25	2 (6%)	35,54,54	1.25	4 (11%)
165	GTP	FG	501	164	29,34,34	1.22	2 (6%)	35,54,54	1.27	4 (11%)
168	ATP	6l	400	164	28,33,33	0.68	0	34,52,52	0.67	1 (2%)
165	GTP	PS	501	-	29,34,34	1.21	2 (6%)	35,54,54	1.30	4 (11%)
165	GTP	R	501	164	29,34,34	1.24	2 (6%)	35,54,54	1.28	4 (11%)
165	GTP	KR	501	164	29,34,34	1.28	3 (10%)	35,54,54	1.24	4 (11%)
163	GDP	JE	500	-	25,30,30	0.95	1 (4%)	30,47,47	1.07	2 (6%)
165	GTP	CJ	501	164	29,34,34	1.26	2 (6%)	35,54,54	1.28	4 (11%)
163	GDP	I	501	-	25,30,30	0.94	1 (4%)	30,47,47	1.10	2 (6%)
165	GTP	SU	501	164	29,34,34	1.20	2 (6%)	35,54,54	1.30	4 (11%)
163	GDP	HV	500	-	25,30,30	0.95	1 (4%)	30,47,47	1.06	2 (6%)
163	GDP	EL	500	-	25,30,30	1.02	1 (4%)	30,47,47	1.03	2 (6%)
163	GDP	QM	500	-	25,30,30	0.96	1 (4%)	30,47,47	1.07	1 (3%)
163	GDP	N	500	-	25,30,30	0.98	1 (4%)	30,47,47	1.07	2 (6%)
165	GTP	LB	501	164	29,34,34	1.27	3 (10%)	35,54,54	1.25	4 (11%)
163	GDP	CE	500	-	25,30,30	0.95	1 (4%)	30,47,47	1.10	2 (6%)
165	GTP	VT	501	164	29,34,34	1.23	2 (6%)	35,54,54	1.30	4 (11%)
165	GTP	LL	501	164	29,34,34	1.24	2 (6%)	35,54,54	1.24	4 (11%)
165	GTP	PE	501	164	29,34,34	1.24	2 (6%)	35,54,54	1.31	4 (11%)
163	GDP	TP	500	-	25,30,30	0.96	1 (4%)	30,47,47	1.10	2 (6%)
165	GTP	GU	501	164	29,34,34	1.21	2 (6%)	35,54,54	1.26	4 (11%)
163	GDP	FR	501	-	25,30,30	0.94	1 (4%)	30,47,47	1.07	1 (3%)
163	GDP	ET	500	-	25,30,30	0.95	1 (4%)	30,47,47	1.02	1 (3%)
163	GDP	ON	500	-	25,30,30	0.95	1 (4%)	30,47,47	1.10	3 (10%)
165	GTP	Q	501	164	29,34,34	1.24	2 (6%)	35,54,54	1.26	4 (11%)
165	GTP	SS	501	164	29,34,34	1.22	2 (6%)	35,54,54	1.30	5 (14%)
165	GTP	TC	501	164	29,34,34	1.21	2 (6%)	35,54,54	1.32	4 (11%)
163	GDP	IL	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.09	2 (6%)
163	GDP	UX	500	-	25,30,30	0.96	1 (4%)	30,47,47	1.08	2 (6%)
163	GDP	FJ	501	-	25,30,30	0.93	1 (4%)	30,47,47	1.07	2 (6%)
165	GTP	KP	502	164	29,34,34	1.26	2 (6%)	35,54,54	1.26	4 (11%)
163	GDP	T	501	-	25,30,30	0.92	1 (4%)	30,47,47	1.04	2 (6%)
163	GDP	BR	500	-	25,30,30	0.94	1 (4%)	30,47,47	1.13	3 (10%)
165	GTP	SM	501	164	29,34,34	1.23	2 (6%)	35,54,54	1.25	4 (11%)
165	GTP	FC	501	164	29,34,34	1.23	1 (3%)	35,54,54	1.27	4 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
165	GTP	DJ	501	164	29,34,34	1.27	1 (3%)	35,54,54	1.34	5 (14%)
163	GDP	WR	501	-	25,30,30	0.94	1 (4%)	30,47,47	1.07	2 (6%)
165	GTP	UO	501	164	29,34,34	1.25	2 (6%)	35,54,54	1.27	4 (11%)
165	GTP	EI	501	164	29,34,34	1.21	2 (6%)	35,54,54	1.28	4 (11%)
163	GDP	FV	501	-	25,30,30	0.94	1 (4%)	30,47,47	1.06	2 (6%)
165	GTP	UU	501	164	29,34,34	1.26	2 (6%)	35,54,54	1.30	4 (11%)
165	GTP	WS	501	164	29,34,34	1.18	2 (6%)	35,54,54	1.30	4 (11%)
165	GTP	LH	501	164	29,34,34	1.23	2 (6%)	35,54,54	1.37	5 (14%)
165	GTP	US	501	164	29,34,34	1.20	2 (6%)	35,54,54	1.28	4 (11%)
163	GDP	EF	500	-	25,30,30	0.94	1 (4%)	30,47,47	1.09	2 (6%)
163	GDP	VX	500	-	25,30,30	0.96	1 (4%)	30,47,47	1.06	2 (6%)
165	GTP	FM	501	164	29,34,34	1.22	1 (3%)	35,54,54	1.25	4 (11%)
163	GDP	GD	500	-	25,30,30	0.92	1 (4%)	30,47,47	1.07	2 (6%)
163	GDP	W	500	-	25,30,30	0.95	1 (4%)	30,47,47	1.07	2 (6%)
165	GTP	EA	501	164	29,34,34	1.27	2 (6%)	35,54,54	1.31	4 (11%)
165	GTP	MS	501	164	29,34,34	1.19	2 (6%)	35,54,54	1.28	4 (11%)
165	GTP	UC	501	164	29,34,34	1.24	2 (6%)	35,54,54	1.27	4 (11%)
165	GTP	JZ	501	164	29,34,34	1.22	2 (6%)	35,54,54	1.24	4 (11%)
163	GDP	LI	500	-	25,30,30	0.96	1 (4%)	30,47,47	1.05	1 (3%)
165	GTP	MY	501	164	29,34,34	1.27	2 (6%)	35,54,54	1.28	4 (11%)
163	GDP	KS	500	-	25,30,30	0.96	1 (4%)	30,47,47	1.08	1 (3%)
163	GDP	WT	500	-	25,30,30	0.96	1 (4%)	30,47,47	1.08	2 (6%)
165	GTP	TE	501	164	29,34,34	1.21	2 (6%)	35,54,54	1.25	4 (11%)
165	GTP	PI	501	164	29,34,34	1.23	2 (6%)	35,54,54	1.27	4 (11%)
165	GTP	WA	501	164	29,34,34	1.26	2 (6%)	35,54,54	1.24	4 (11%)
165	GTP	AU	501	164	29,34,34	1.19	2 (6%)	35,54,54	1.30	4 (11%)
163	GDP	EB	500	-	25,30,30	0.95	1 (4%)	30,47,47	1.07	1 (3%)
163	GDP	RK	500	-	25,30,30	0.96	1 (4%)	30,47,47	1.07	2 (6%)
165	GTP	BM	501	164	29,34,34	1.27	1 (3%)	35,54,54	1.41	6 (17%)
163	GDP	BH	500	-	25,30,30	0.94	1 (4%)	30,47,47	1.10	3 (10%)
165	GTP	OU	501	164	29,34,34	1.22	2 (6%)	35,54,54	1.28	4 (11%)
165	GTP	QH	501	164	29,34,34	1.24	2 (6%)	35,54,54	1.37	6 (17%)
163	GDP	ND	500	-	25,30,30	0.99	1 (4%)	30,47,47	1.11	3 (10%)
163	GDP	UF	500	-	25,30,30	0.95	1 (4%)	30,47,47	1.08	2 (6%)
165	GTP	DD	501	164	29,34,34	1.24	1 (3%)	35,54,54	1.48	7 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
165	GTP	LX	501	164	29,34,34	1.24	2 (6%)	35,54,54	1.24	4 (11%)
163	GDP	VN	500	-	25,30,30	0.94	1 (4%)	30,47,47	1.09	2 (6%)
163	GDP	LO	500	-	25,30,30	0.95	1 (4%)	30,47,47	1.08	2 (6%)
163	GDP	JS	500	-	25,30,30	0.97	1 (4%)	30,47,47	1.05	2 (6%)
165	GTP	IC	501	164	29,34,34	1.28	3 (10%)	35,54,54	1.31	4 (11%)
163	GDP	AT	500	-	25,30,30	0.93	1 (4%)	30,47,47	1.09	3 (10%)
163	GDP	UV	500	-	25,30,30	0.95	1 (4%)	30,47,47	1.06	2 (6%)
165	GTP	UQ	501	164	29,34,34	1.22	2 (6%)	35,54,54	1.24	4 (11%)
163	GDP	OV	500	-	25,30,30	0.94	1 (4%)	30,47,47	1.06	2 (6%)
165	GTP	GI	501	164	29,34,34	1.24	2 (6%)	35,54,54	1.30	6 (17%)
163	GDP	UB	500	-	25,30,30	0.97	1 (4%)	30,47,47	1.09	2 (6%)
163	GDP	VR	500	-	25,30,30	0.96	1 (4%)	30,47,47	1.09	2 (6%)
163	GDP	TT	500	-	25,30,30	0.96	1 (4%)	30,47,47	1.05	2 (6%)
163	GDP	WN	500	-	25,30,30	0.94	1 (4%)	30,47,47	1.07	2 (6%)
163	GDP	MZ	500	-	25,30,30	0.96	1 (4%)	30,47,47	1.07	3 (10%)
165	GTP	GE	501	164	29,34,34	1.25	1 (3%)	35,54,54	1.42	6 (17%)
163	GDP	KY	500	-	25,30,30	0.95	1 (4%)	30,47,47	1.07	2 (6%)
165	GTP	LV	501	164	29,34,34	1.22	2 (6%)	35,54,54	1.32	4 (11%)
163	GDP	VB	500	-	25,30,30	0.95	1 (4%)	30,47,47	1.09	2 (6%)
165	GTP	QR	501	164	29,34,34	1.19	2 (6%)	35,54,54	1.30	4 (11%)
163	GDP	BN	500	-	25,30,30	0.95	1 (4%)	30,47,47	1.12	3 (10%)
163	GDP	AR	500	-	25,30,30	0.95	1 (4%)	30,47,47	1.09	2 (6%)
163	GDP	DC	500	-	25,30,30	0.94	1 (4%)	30,47,47	1.05	2 (6%)
163	GDP	OP	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.08	2 (6%)
165	GTP	JP	501	164	29,34,34	1.24	2 (6%)	35,54,54	1.26	4 (11%)
165	GTP	VM	501	164	29,34,34	1.25	2 (6%)	35,54,54	1.23	4 (11%)
165	GTP	EJ	501	164	29,34,34	1.31	3 (10%)	35,54,54	1.28	5 (14%)
163	GDP	FD	500	-	25,30,30	0.92	1 (4%)	30,47,47	1.11	2 (6%)
165	GTP	OO	501	164	29,34,34	1.26	2 (6%)	35,54,54	1.28	4 (11%)
165	GTP	GG	501	164	29,34,34	1.18	1 (3%)	35,54,54	1.42	6 (17%)
165	GTP	PU	501	164	29,34,34	1.22	2 (6%)	35,54,54	1.27	4 (11%)
165	GTP	DL	501	-	29,34,34	1.22	1 (3%)	35,54,54	1.35	5 (14%)
165	GTP	MA	501	164	29,34,34	1.27	2 (6%)	35,54,54	1.25	4 (11%)
163	GDP	DA	500	-	25,30,30	0.92	1 (4%)	30,47,47	1.07	2 (6%)
165	GTP	PM	501	164	29,34,34	1.25	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
165	GTP	QL	501	-	29,34,34	1.25	2 (6%)	35,54,54	1.26	4 (11%)
165	GTP	RC	501	164	29,34,34	1.27	3 (10%)	35,54,54	1.27	4 (11%)
165	GTP	FS	501	164	29,34,34	1.20	1 (3%)	35,54,54	1.44	5 (14%)
165	GTP	HE	501	164	29,34,34	1.21	2 (6%)	35,54,54	1.24	4 (11%)
163	GDP	EJ	500	-	25,30,30	0.95	1 (4%)	30,47,47	1.08	2 (6%)
165	GTP	CW	501	164	29,34,34	1.26	1 (3%)	35,54,54	1.27	4 (11%)
165	GTP	VA	501	164	29,34,34	1.24	2 (6%)	35,54,54	1.24	4 (11%)
163	GDP	QC	500	-	25,30,30	0.93	1 (4%)	30,47,47	1.09	2 (6%)
163	GDP	BT	500	-	25,30,30	0.94	1 (4%)	30,47,47	1.13	2 (6%)
163	GDP	EV	500	-	25,30,30	0.94	1 (4%)	30,47,47	1.11	3 (10%)
165	GTP	OC	501	164	29,34,34	1.25	2 (6%)	35,54,54	1.27	4 (11%)
165	GTP	ES	501	164	29,34,34	1.24	1 (3%)	35,54,54	1.42	6 (17%)
165	GTP	BU	501	164	29,34,34	1.27	2 (6%)	35,54,54	1.39	6 (17%)
163	GDP	PD	500	-	25,30,30	0.94	1 (4%)	30,47,47	1.07	2 (6%)
163	GDP	RO	500	-	25,30,30	0.94	1 (4%)	30,47,47	1.07	2 (6%)
165	GTP	WG	501	164	29,34,34	1.18	2 (6%)	35,54,54	1.30	4 (11%)
163	GDP	JA	500	-	25,30,30	0.97	1 (4%)	30,47,47	1.07	2 (6%)
163	GDP	QA	500	-	25,30,30	0.97	1 (4%)	30,47,47	1.06	1 (3%)
163	GDP	DU	500	-	25,30,30	0.94	1 (4%)	30,47,47	1.08	2 (6%)
163	GDP	PF	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.04	2 (6%)
163	GDP	LM	500	-	25,30,30	0.95	1 (4%)	30,47,47	1.06	2 (6%)
163	GDP	FF	500	-	25,30,30	0.94	1 (4%)	30,47,47	1.10	2 (6%)
165	GTP	LP	502	164	29,34,34	1.25	2 (6%)	35,54,54	1.25	4 (11%)
165	GTP	HK	501	164	29,34,34	1.21	2 (6%)	35,54,54	1.27	4 (11%)
165	GTP	EV	501	164	29,34,34	1.26	1 (3%)	35,54,54	1.37	6 (17%)
165	GTP	MJ	501	164	29,34,34	1.25	2 (6%)	35,54,54	1.29	4 (11%)
163	GDP	MX	500	-	25,30,30	0.98	1 (4%)	30,47,47	1.07	2 (6%)
165	GTP	G	501	164	29,34,34	1.24	1 (3%)	35,54,54	1.36	6 (17%)
165	GTP	EG	501	164	29,34,34	1.23	1 (3%)	35,54,54	1.42	6 (17%)
165	GTP	BO	501	164	29,34,34	1.27	1 (3%)	35,54,54	1.34	5 (14%)
163	GDP	HB	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.07	2 (6%)
163	GDP	WP	500	-	25,30,30	0.95	1 (4%)	30,47,47	1.08	2 (6%)
165	GTP	DT	501	164	29,34,34	1.18	2 (6%)	35,54,54	1.30	4 (11%)
165	GTP	MV	501	164	29,34,34	1.26	2 (6%)	35,54,54	1.29	4 (11%)
165	GTP	EO	501	164	29,34,34	1.24	1 (3%)	35,54,54	1.25	4 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
165	GTP	TI	501	164	29,34,34	1.27	2 (6%)	35,54,54	1.26	4 (11%)
165	GTP	HN	503	164	29,34,34	1.25	3 (10%)	35,54,54	1.28	4 (11%)
165	GTP	GW	501	164	29,34,34	1.25	1 (3%)	35,54,54	1.35	6 (17%)
165	GTP	PK	501	164	29,34,34	1.23	2 (6%)	35,54,54	1.30	4 (11%)
163	GDP	TL	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.05	2 (6%)
165	GTP	IK	501	164	29,34,34	1.49	6 (20%)	35,54,54	1.36	5 (14%)
163	GDP	PB	500	-	25,30,30	0.95	1 (4%)	30,47,47	1.07	1 (3%)
165	GTP	SE	501	164	29,34,34	1.20	1 (3%)	35,54,54	1.32	5 (14%)
165	GTP	DE	501	164	29,34,34	1.23	2 (6%)	35,54,54	1.32	5 (14%)

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
163	GDP	DQ	500	-	-	3/12/32/32	0/3/3/3
165	GTP	GC	501	164	-	5/18/38/38	0/3/3/3
163	GDP	TB	500	-	-	3/12/32/32	0/3/3/3
165	GTP	NQ	501	164	-	4/18/38/38	0/3/3/3
165	GTP	IS	501	164	-	7/18/38/38	0/3/3/3
163	GDP	CY	500	-	-	5/12/32/32	0/3/3/3
165	GTP	HI	501	164	-	2/18/38/38	0/3/3/3
163	GDP	IT	501	-	-	2/12/32/32	0/3/3/3
163	GDP	UT	500	-	-	1/12/32/32	0/3/3/3
165	GTP	QN	501	164	-	2/18/38/38	0/3/3/3
163	GDP	QQ	500	-	-	2/12/32/32	0/3/3/3
163	GDP	OJ	500	-	-	3/12/32/32	0/3/3/3
165	GTP	RB	501	164	-	3/18/38/38	0/3/3/3
163	GDP	AL	500	-	-	3/12/32/32	0/3/3/3
163	GDP	CI	500	-	-	4/12/32/32	0/3/3/3
165	GTP	KZ	501	164	-	3/18/38/38	0/3/3/3
163	GDP	RE	500	-	-	0/12/32/32	0/3/3/3
163	GDP	AZ	500	-	-	2/12/32/32	0/3/3/3
165	GTP	BS	501	164	-	1/18/38/38	0/3/3/3
163	GDP	MD	500	-	-	1/12/32/32	0/3/3/3
163	GDP	JQ	500	-	-	1/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
165	GTP	IU	501	164	-	3/18/38/38	0/3/3/3
165	GTP	FO	501	164	-	3/18/38/38	0/3/3/3
165	GTP	DQ	501	164	-	6/18/38/38	0/3/3/3
168	ATP	2v	501	-	-	2/18/38/38	0/3/3/3
165	GTP	RL	501	164	-	9/18/38/38	0/3/3/3
163	GDP	MP	500	-	-	1/12/32/32	0/3/3/3
163	GDP	A	501	-	-	2/12/32/32	0/3/3/3
163	GDP	GL	500	-	-	3/12/32/32	0/3/3/3
165	GTP	RO	501	164	-	7/18/38/38	0/3/3/3
163	GDP	PH	500	-	-	1/12/32/32	0/3/3/3
165	GTP	VQ	501	164	-	1/18/38/38	0/3/3/3
163	GDP	JK	500	-	-	3/12/32/32	0/3/3/3
163	GDP	CQ	500	-	-	3/12/32/32	0/3/3/3
163	GDP	RM	500	-	-	1/12/32/32	0/3/3/3
163	GDP	IH	500	-	-	2/12/32/32	0/3/3/3
163	GDP	AP	500	-	-	1/12/32/32	0/3/3/3
163	GDP	GH	500	-	-	3/12/32/32	0/3/3/3
165	GTP	HS	501	164	-	3/18/38/38	0/3/3/3
163	GDP	OD	501	-	-	2/12/32/32	0/3/3/3
163	GDP	MB	500	-	-	2/12/32/32	0/3/3/3
163	GDP	EX	500	-	-	2/12/32/32	0/3/3/3
163	GDP	DY	500	-	-	1/12/32/32	0/3/3/3
165	GTP	VO	501	164	-	6/18/38/38	0/3/3/3
163	GDP	OT	500	-	-	3/12/32/32	0/3/3/3
163	GDP	MH	500	-	-	1/12/32/32	0/3/3/3
163	GDP	NF	500	-	-	3/12/32/32	0/3/3/3
165	GTP	TU	501	164	-	4/18/38/38	0/3/3/3
163	GDP	GF	500	-	-	4/12/32/32	0/3/3/3
165	GTP	IE	501	164	-	2/18/38/38	0/3/3/3
163	GDP	RS	500	-	-	1/12/32/32	0/3/3/3
165	GTP	FT	503	164	-	5/18/38/38	0/3/3/3
165	GTP	RX	501	164	-	9/18/38/38	0/3/3/3
165	GTP	DX	501	-	-	9/18/38/38	0/3/3/3
163	GDP	UR	500	-	-	1/12/32/32	0/3/3/3
165	GTP	FV	503	-	-	3/18/38/38	0/3/3/3
165	GTP	WO	501	164	-	2/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
163	GDP	LC	500	-	-	2/12/32/32	0/3/3/3
165	GTP	SC	501	164	-	6/18/38/38	0/3/3/3
165	GTP	WC	501	164	-	2/18/38/38	0/3/3/3
163	GDP	LY	500	-	-	1/12/32/32	0/3/3/3
163	GDP	RI	500	-	-	0/12/32/32	0/3/3/3
165	GTP	FE	501	164	-	6/18/38/38	0/3/3/3
163	GDP	PX	501	-	-	1/12/32/32	0/3/3/3
163	GDP	LK	500	-	-	1/12/32/32	0/3/3/3
165	GTP	PQ	501	164	-	0/18/38/38	0/3/3/3
163	GDP	DK	501	-	-	2/12/32/32	0/3/3/3
165	GTP	WE	501	164	-	8/18/38/38	0/3/3/3
165	GTP	NW	501	-	-	3/18/38/38	0/3/3/3
163	GDP	TN	500	-	-	3/12/32/32	0/3/3/3
163	GDP	IN	500	-	-	3/12/32/32	0/3/3/3
163	GDP	MT	500	-	-	1/12/32/32	0/3/3/3
163	GDP	KM	500	-	-	2/12/32/32	0/3/3/3
165	GTP	KV	501	164	-	3/18/38/38	0/3/3/3
163	GDP	HR	500	-	-	2/12/32/32	0/3/3/3
163	GDP	IP	500	-	-	1/12/32/32	0/3/3/3
163	GDP	VV	500	-	-	2/12/32/32	0/3/3/3
163	GDP	IF	500	-	-	3/12/32/32	0/3/3/3
163	GDP	LQ	500	-	-	2/12/32/32	0/3/3/3
165	GTP	OG	501	164	-	3/18/38/38	0/3/3/3
165	GTP	SG	501	164	-	8/18/38/38	0/3/3/3
165	GTP	VS	501	164	-	4/18/38/38	0/3/3/3
163	GDP	BJ	500	-	-	3/12/32/32	0/3/3/3
165	GTP	GS	501	164	-	4/18/38/38	0/3/3/3
165	GTP	TS	501	164	-	1/18/38/38	0/3/3/3
163	GDP	AN	500	-	-	2/12/32/32	0/3/3/3
165	GTP	FJ	503	164	-	5/18/38/38	0/3/3/3
163	GDP	OB	500	-	-	5/12/32/32	0/3/3/3
163	GDP	GN	500	-	-	1/12/32/32	0/3/3/3
165	GTP	AP	501	164	-	4/18/38/38	0/3/3/3
163	GDP	GP	500	-	-	4/12/32/32	0/3/3/3
165	GTP	OI	501	164	-	6/18/38/38	0/3/3/3
168	ATP	8a	801	-	-	1/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
163	GDP	DI	500	-	-	2/12/32/32	0/3/3/3
165	GTP	II	501	164	-	3/18/38/38	0/3/3/3
165	GTP	NA	501	-	-	7/18/38/38	0/3/3/3
163	GDP	PT	500	-	-	1/12/32/32	0/3/3/3
163	GDP	TV	500	-	-	2/12/32/32	0/3/3/3
165	GTP	LD	502	164	-	6/18/38/38	0/3/3/3
163	GDP	FB	500	-	-	0/12/32/32	0/3/3/3
163	GDP	ER	500	-	-	2/12/32/32	0/3/3/3
165	GTP	OD	503	164	-	4/18/38/38	0/3/3/3
165	GTP	DV	501	164	-	3/18/38/38	0/3/3/3
163	GDP	NJ	501	-	-	1/12/32/32	0/3/3/3
163	GDP	SD	500	-	-	3/12/32/32	0/3/3/3
165	GTP	UG	501	164	-	5/18/38/38	0/3/3/3
165	GTP	HW	501	164	-	4/18/38/38	0/3/3/3
165	GTP	IY	501	164	-	4/18/38/38	0/3/3/3
165	GTP	IQ	501	164	-	2/18/38/38	0/3/3/3
163	GDP	OH	500	-	-	3/12/32/32	0/3/3/3
163	GDP	VJ	500	-	-	2/12/32/32	0/3/3/3
165	GTP	SI	501	164	-	3/18/38/38	0/3/3/3
163	GDP	NN	500	-	-	3/12/32/32	0/3/3/3
165	GTP	HA	501	164	-	3/18/38/38	0/3/3/3
163	GDP	BL	500	-	-	4/12/32/32	0/3/3/3
165	GTP	JB	501	164	-	2/18/38/38	0/3/3/3
165	GTP	TG	501	164	-	1/18/38/38	0/3/3/3
163	GDP	BP	500	-	-	2/12/32/32	0/3/3/3
165	GTP	KB	502	164	-	4/18/38/38	0/3/3/3
165	GTP	BE	501	164	-	7/18/38/38	0/3/3/3
165	GTP	CB	501	164	-	3/18/38/38	0/3/3/3
165	GTP	CO	501	164	-	4/18/38/38	0/3/3/3
165	GTP	VE	501	164	-	1/18/38/38	0/3/3/3
165	GTP	JV	501	164	-	3/18/38/38	0/3/3/3
163	GDP	JU	500	-	-	1/12/32/32	0/3/3/3
165	GTP	GO	501	164	-	4/18/38/38	0/3/3/3
163	GDP	HL	501	-	-	1/12/32/32	0/3/3/3
165	GTP	JR	501	164	-	3/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
165	GTP	T	503	164	-	7/18/38/38	0/3/3/3
168	ATP	7D	601	164	-	10/18/38/38	0/3/3/3
163	GDP	NB	500	-	-	3/12/32/32	0/3/3/3
163	GDP	KI	500	-	-	3/12/32/32	0/3/3/3
163	GDP	GJ	500	-	-	2/12/32/32	0/3/3/3
163	GDP	UL	500	-	-	1/12/32/32	0/3/3/3
163	GDP	SB	501	-	-	3/12/32/32	0/3/3/3
165	GTP	BQ	501	164	-	8/18/38/38	0/3/3/3
163	GDP	UD	500	-	-	3/12/32/32	0/3/3/3
163	GDP	FL	500	-	-	4/12/32/32	0/3/3/3
163	GDP	TD	500	-	-	1/12/32/32	0/3/3/3
163	GDP	VD	500	-	-	1/12/32/32	0/3/3/3
165	GTP	D	501	-	-	9/18/38/38	0/3/3/3
163	GDP	TH	500	-	-	1/12/32/32	0/3/3/3
163	GDP	U	500	-	-	2/12/32/32	0/3/3/3
165	GTP	NY	501	164	-	4/18/38/38	0/3/3/3
165	GTP	GQ	501	164	-	4/18/38/38	0/3/3/3
165	GTP	MI	501	164	-	5/18/38/38	0/3/3/3
163	GDP	V	500	-	-	1/12/32/32	0/3/3/3
165	GTP	FA	501	164	-	4/18/38/38	0/3/3/3
165	GTP	PY	501	164	-	3/18/38/38	0/3/3/3
163	GDP	LW	500	-	-	1/12/32/32	0/3/3/3
165	GTP	QU	501	164	-	4/18/38/38	0/3/3/3
163	GDP	NL	500	-	-	1/12/32/32	0/3/3/3
165	GTP	VW	501	164	-	5/18/38/38	0/3/3/3
165	GTP	OK	501	-	-	6/18/38/38	0/3/3/3
163	GDP	VT	500	-	-	1/12/32/32	0/3/3/3
163	GDP	SR	500	-	-	1/12/32/32	0/3/3/3
165	GTP	TW	501	164	-	5/18/38/38	0/3/3/3
165	GTP	KJ	501	164	-	3/18/38/38	0/3/3/3
163	GDP	DG	500	-	-	2/12/32/32	0/3/3/3
163	GDP	PL	501	-	-	1/12/32/32	0/3/3/3
163	GDP	RW	500	-	-	2/12/32/32	0/3/3/3
165	GTP	JK	501	164	-	3/18/38/38	0/3/3/3
165	GTP	EU	501	164	-	4/18/38/38	0/3/3/3
165	GTP	MU	501	164	-	5/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
165	GTP	PO	501	164	-	3/18/38/38	0/3/3/3
165	GTP	TQ	501	164	-	6/18/38/38	0/3/3/3
163	GDP	DM	500	-	-	2/12/32/32	0/3/3/3
163	GDP	LA	500	-	-	2/12/32/32	0/3/3/3
165	GTP	LF	502	164	-	2/18/38/38	0/3/3/3
165	GTP	IG	501	164	-	7/18/38/38	0/3/3/3
163	GDP	JW	500	-	-	3/12/32/32	0/3/3/3
165	GTP	LT	501	164	-	3/18/38/38	0/3/3/3
165	GTP	IM	501	164	-	4/18/38/38	0/3/3/3
165	GTP	RJ	501	-	-	1/18/38/38	0/3/3/3
163	GDP	HT	501	-	-	1/12/32/32	0/3/3/3
165	GTP	BA	501	164	-	3/18/38/38	0/3/3/3
163	GDP	WJ	500	-	-	1/12/32/32	0/3/3/3
165	GTP	GK	501	164	-	3/18/38/38	0/3/3/3
165	GTP	HG	501	164	-	3/18/38/38	0/3/3/3
165	GTP	BW	501	164	-	3/18/38/38	0/3/3/3
165	GTP	ED	501	164	-	4/18/38/38	0/3/3/3
163	GDP	MF	500	-	-	3/12/32/32	0/3/3/3
165	GTP	QC	501	164	-	5/18/38/38	0/3/3/3
163	GDP	O	500	-	-	2/12/32/32	0/3/3/3
165	GTP	KL	501	164	-	2/18/38/38	0/3/3/3
165	GTP	BI	501	164	-	5/18/38/38	0/3/3/3
163	GDP	KW	500	-	-	1/12/32/32	0/3/3/3
163	GDP	MN	500	-	-	2/12/32/32	0/3/3/3
163	GDP	QK	500	-	-	5/12/32/32	0/3/3/3
165	GTP	JD	501	164	-	5/18/38/38	0/3/3/3
165	GTP	SK	501	164	-	0/18/38/38	0/3/3/3
163	GDP	DE	500	-	-	4/12/32/32	0/3/3/3
165	GTP	HM	501	164	-	3/18/38/38	0/3/3/3
165	GTP	EP	501	164	-	5/18/38/38	0/3/3/3
163	GDP	VH	500	-	-	1/12/32/32	0/3/3/3
163	GDP	LG	501	-	-	2/12/32/32	0/3/3/3
165	GTP	NF	501	-	-	6/18/38/38	0/3/3/3
163	GDP	KQ	500	-	-	1/12/32/32	0/3/3/3
165	GTP	QO	501	164	-	5/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
163	GDP	HF	500	-	-	2/12/32/32	0/3/3/3
165	GTP	SO	501	164	-	6/18/38/38	0/3/3/3
163	GDP	TJ	500	-	-	2/12/32/32	0/3/3/3
165	GTP	AA	501	164	-	6/18/38/38	0/3/3/3
163	GDP	FX	500	-	-	4/12/32/32	0/3/3/3
163	GDP	KK	500	-	-	1/12/32/32	0/3/3/3
165	GTP	OA	501	164	-	4/18/38/38	0/3/3/3
165	GTP	DB	501	164	-	3/18/38/38	0/3/3/3
165	GTP	PA	501	164	-	0/18/38/38	0/3/3/3
163	GDP	ED	500	-	-	4/12/32/32	0/3/3/3
163	GDP	FP	500	-	-	1/12/32/32	0/3/3/3
163	GDP	EH	500	-	-	1/12/32/32	0/3/3/3
163	GDP	KU	500	-	-	3/12/32/32	0/3/3/3
165	GTP	HQ	501	164	-	4/18/38/38	0/3/3/3
165	GTP	WI	501	164	-	3/18/38/38	0/3/3/3
163	GDP	HN	501	-	-	3/12/32/32	0/3/3/3
163	GDP	OL	500	-	-	2/12/32/32	0/3/3/3
163	GDP	UP	500	-	-	3/12/32/32	0/3/3/3
165	GTP	MO	501	164	-	4/18/38/38	0/3/3/3
163	GDP	PP	500	-	-	4/12/32/32	0/3/3/3
165	GTP	UA	501	164	-	5/18/38/38	0/3/3/3
165	GTP	AY	501	164	-	5/18/38/38	0/3/3/3
163	GDP	LE	500	-	-	2/12/32/32	0/3/3/3
165	GTP	JF	501	164	-	3/18/38/38	0/3/3/3
163	GDP	GR	500	-	-	0/12/32/32	0/3/3/3
165	GTP	FI	501	164	-	5/18/38/38	0/3/3/3
163	GDP	VL	500	-	-	1/12/32/32	0/3/3/3
165	GTP	QT	501	164	-	10/18/38/38	0/3/3/3
163	GDP	UH	500	-	-	1/12/32/32	0/3/3/3
163	GDP	NX	500	-	-	1/12/32/32	0/3/3/3
165	GTP	WQ	501	164	-	8/18/38/38	0/3/3/3
165	GTP	QX	501	-	-	3/18/38/38	0/3/3/3
163	GDP	DW	501	-	-	1/12/32/32	0/3/3/3
165	GTP	EC	501	164	-	3/18/38/38	0/3/3/3
163	GDP	SV	501	-	-	2/12/32/32	0/3/3/3
165	GTP	WY	501	164	-	3/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
165	GTP	AK	501	164	-	3/18/38/38	0/3/3/3
163	GDP	GV	501	-	-	4/12/32/32	0/3/3/3
165	GTP	J	501	164	-	8/18/38/38	0/3/3/3
168	ATP	2x	501	-	-	5/18/38/38	0/3/3/3
163	GDP	SJ	501	-	-	2/12/32/32	0/3/3/3
163	GDP	MR	500	-	-	3/12/32/32	0/3/3/3
165	GTP	MG	501	164	-	5/18/38/38	0/3/3/3
163	GDP	CK	501	-	-	6/12/32/32	0/3/3/3
165	GTP	AG	501	164	-	6/18/38/38	0/3/3/3
165	GTP	CV	501	164	-	3/18/38/38	0/3/3/3
163	GDP	WD	500	-	-	2/12/32/32	0/3/3/3
163	GDP	E	500	-	-	3/12/32/32	0/3/3/3
163	GDP	RG	500	-	-	1/12/32/32	0/3/3/3
163	GDP	SP	500	-	-	3/12/32/32	0/3/3/3
163	GDP	GT	501	-	-	2/12/32/32	0/3/3/3
163	GDP	QS	500	-	-	1/12/32/32	0/3/3/3
165	GTP	NR	501	-	-	6/18/38/38	0/3/3/3
165	GTP	QI	501	164	-	4/18/38/38	0/3/3/3
163	GDP	VF	500	-	-	1/12/32/32	0/3/3/3
168	ATP	2w	501	-	-	5/18/38/38	0/3/3/3
163	GDP	PR	501	-	-	3/12/32/32	0/3/3/3
165	GTP	NE	501	164	-	4/18/38/38	0/3/3/3
165	GTP	PG	501	-	-	5/18/38/38	0/3/3/3
163	GDP	KO	500	-	-	1/12/32/32	0/3/3/3
165	GTP	UK	501	164	-	5/18/38/38	0/3/3/3
165	GTP	LN	502	164	-	3/18/38/38	0/3/3/3
165	GTP	UE	501	164	-	9/18/38/38	0/3/3/3
163	GDP	CW	500	-	-	5/12/32/32	0/3/3/3
165	GTP	AO	501	164	-	4/18/38/38	0/3/3/3
163	GDP	JI	500	-	-	1/12/32/32	0/3/3/3
165	GTP	BK	501	164	-	3/18/38/38	0/3/3/3
163	GDP	CO	500	-	-	0/12/32/32	0/3/3/3
165	GTP	NU	501	164	-	1/18/38/38	0/3/3/3
165	GTP	HB	503	164	-	7/18/38/38	0/3/3/3
163	GDP	QO	500	-	-	2/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
165	GTP	ME	501	164	-	5/18/38/38	0/3/3/3
163	GDP	GX	500	-	-	4/12/32/32	0/3/3/3
163	GDP	PJ	500	-	-	3/12/32/32	0/3/3/3
165	GTP	VH	501	164	-	4/18/38/38	0/3/3/3
163	GDP	RC	500	-	-	1/12/32/32	0/3/3/3
163	GDP	AF	500	-	-	1/12/32/32	0/3/3/3
163	GDP	AV	500	-	-	3/12/32/32	0/3/3/3
165	GTP	NM	501	164	-	4/18/38/38	0/3/3/3
163	GDP	PN	500	-	-	1/12/32/32	0/3/3/3
165	GTP	BY	501	164	-	4/18/38/38	0/3/3/3
165	GTP	DN	501	164	-	3/18/38/38	0/3/3/3
163	GDP	UJ	500	-	-	1/12/32/32	0/3/3/3
165	GTP	UI	501	164	-	3/18/38/38	0/3/3/3
163	GDP	RA	500	-	-	1/12/32/32	0/3/3/3
163	GDP	BD	500	-	-	2/12/32/32	0/3/3/3
163	GDP	AD	500	-	-	3/12/32/32	0/3/3/3
165	GTP	CH	501	164	-	5/18/38/38	0/3/3/3
163	GDP	JC	500	-	-	2/12/32/32	0/3/3/3
163	GDP	CA	500	-	-	3/12/32/32	0/3/3/3
163	GDP	QI	500	-	-	2/12/32/32	0/3/3/3
163	GDP	SH	500	-	-	2/12/32/32	0/3/3/3
165	GTP	OY	501	164	-	5/18/38/38	0/3/3/3
165	GTP	OP	503	164	-	4/18/38/38	0/3/3/3
163	GDP	IR	500	-	-	3/12/32/32	0/3/3/3
165	GTP	JN	501	164	-	3/18/38/38	0/3/3/3
165	GTP	JT	501	164	-	5/18/38/38	0/3/3/3
165	GTP	GL	501	164	-	9/18/38/38	0/3/3/3
165	GTP	TK	501	164	-	5/18/38/38	0/3/3/3
163	GDP	RQ	500	-	-	0/12/32/32	0/3/3/3
163	GDP	NP	500	-	-	0/12/32/32	0/3/3/3
165	GTP	SQ	501	164	-	5/18/38/38	0/3/3/3
165	GTP	WM	501	164	-	3/18/38/38	0/3/3/3
163	GDP	CU	500	-	-	0/12/32/32	0/3/3/3
165	GTP	DP	501	164	-	3/18/38/38	0/3/3/3
165	GTP	IO	501	164	-	4/18/38/38	0/3/3/3
165	GTP	K	501	164	-	2/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
165	GTP	RT	501	164	-	2/18/38/38	0/3/3/3
163	GDP	AB	500	-	-	3/12/32/32	0/3/3/3
168	ATP	9R	500	164	-	6/18/38/38	0/3/3/3
163	GDP	KG	500	-	-	2/12/32/32	0/3/3/3
165	GTP	JH	501	164	-	5/18/38/38	0/3/3/3
165	GTP	QF	501	164	-	2/18/38/38	0/3/3/3
165	GTP	UM	501	164	-	5/18/38/38	0/3/3/3
165	GTP	OW	501	-	-	6/18/38/38	0/3/3/3
163	GDP	IV	500	-	-	2/12/32/32	0/3/3/3
163	GDP	CC	500	-	-	3/12/32/32	0/3/3/3
165	GTP	JW	501	164	-	3/18/38/38	0/3/3/3
163	GDP	BV	500	-	-	2/12/32/32	0/3/3/3
165	GTP	KF	501	164	-	6/18/38/38	0/3/3/3
163	GDP	BF	500	-	-	1/12/32/32	0/3/3/3
165	GTP	QB	501	164	-	2/18/38/38	0/3/3/3
165	GTP	VY	501	164	-	5/18/38/38	0/3/3/3
165	GTP	TM	501	164	-	7/18/38/38	0/3/3/3
165	GTP	AB	501	164	-	5/18/38/38	0/3/3/3
163	GDP	QU	500	-	-	2/12/32/32	0/3/3/3
163	GDP	VP	500	-	-	1/12/32/32	0/3/3/3
163	GDP	WV	500	-	-	1/12/32/32	0/3/3/3
165	GTP	WK	501	164	-	5/18/38/38	0/3/3/3
163	GDP	CM	500	-	-	3/12/32/32	0/3/3/3
165	GTP	CC	501	164	-	4/18/38/38	0/3/3/3
165	GTP	DH	501	164	-	1/18/38/38	0/3/3/3
163	GDP	HJ	500	-	-	2/12/32/32	0/3/3/3
163	GDP	IB	500	-	-	3/12/32/32	0/3/3/3
163	GDP	JM	501	-	-	0/12/32/32	0/3/3/3
163	GDP	M	500	-	-	3/12/32/32	0/3/3/3
163	GDP	EN	500	-	-	3/12/32/32	0/3/3/3
163	GDP	NT	500	-	-	2/12/32/32	0/3/3/3
165	GTP	NI	501	164	-	1/18/38/38	0/3/3/3
165	GTP	L	501	164	-	4/18/38/38	0/3/3/3
165	GTP	CQ	501	164	-	6/18/38/38	0/3/3/3
165	GTP	NO	501	164	-	3/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
165	GTP	MC	501	164	-	4/18/38/38	0/3/3/3
163	GDP	RU	500	-	-	0/12/32/32	0/3/3/3
165	GTP	VK	501	164	-	5/18/38/38	0/3/3/3
165	GTP	AD	501	164	-	4/18/38/38	0/3/3/3
165	GTP	CT	501	164	-	6/18/38/38	0/3/3/3
163	GDP	KE	500	-	-	1/12/32/32	0/3/3/3
163	GDP	ML	500	-	-	1/12/32/32	0/3/3/3
165	GTP	MM	501	164	-	2/18/38/38	0/3/3/3
163	GDP	HP	501	-	-	3/12/32/32	0/3/3/3
168	ATP	6u	700	-	-	7/18/38/38	0/3/3/3
163	GDP	DO	500	-	-	1/12/32/32	0/3/3/3
165	GTP	HY	501	164	-	3/18/38/38	0/3/3/3
165	GTP	WU	501	164	-	3/18/38/38	0/3/3/3
163	GDP	NH	500	-	-	2/12/32/32	0/3/3/3
163	GDP	OF	500	-	-	1/12/32/32	0/3/3/3
163	GDP	FT	501	-	-	1/12/32/32	0/3/3/3
165	GTP	KN	502	164	-	3/18/38/38	0/3/3/3
165	GTP	KX	501	164	-	2/18/38/38	0/3/3/3
163	GDP	AJ	500	-	-	2/12/32/32	0/3/3/3
165	GTP	RR	501	164	-	1/18/38/38	0/3/3/3
163	GDP	CS	500	-	-	2/12/32/32	0/3/3/3
163	GDP	WL	500	-	-	1/12/32/32	0/3/3/3
163	GDP	AH	500	-	-	3/12/32/32	0/3/3/3
165	GTP	SA	501	164	-	3/18/38/38	0/3/3/3
163	GDP	QG	500	-	-	1/12/32/32	0/3/3/3
165	GTP	KT	501	164	-	5/18/38/38	0/3/3/3
165	GTP	EM	501	164	-	4/18/38/38	0/3/3/3
165	GTP	OM	501	164	-	5/18/38/38	0/3/3/3
165	GTP	CN	501	164	-	3/18/38/38	0/3/3/3
163	GDP	IJ	500	-	-	2/12/32/32	0/3/3/3
165	GTP	IW	501	164	-	3/18/38/38	0/3/3/3
163	GDP	TR	500	-	-	1/12/32/32	0/3/3/3
163	GDP	QE	500	-	-	2/12/32/32	0/3/3/3
165	GTP	LR	502	164	-	2/18/38/38	0/3/3/3
163	GDP	F	500	-	-	3/12/32/32	0/3/3/3
163	GDP	GB	500	-	-	2/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
165	GTP	NK	501	-	-	3/18/38/38	0/3/3/3
165	GTP	TO	501	164	-	5/18/38/38	0/3/3/3
163	GDP	ST	500	-	-	2/12/32/32	0/3/3/3
163	GDP	LS	500	-	-	2/12/32/32	0/3/3/3
163	GDP	WB	500	-	-	1/12/32/32	0/3/3/3
163	GDP	MJ	500	-	-	3/12/32/32	0/3/3/3
163	GDP	FN	500	-	-	0/12/32/32	0/3/3/3
165	GTP	PW	501	164	-	3/18/38/38	0/3/3/3
165	GTP	MQ	501	164	-	5/18/38/38	0/3/3/3
165	GTP	NC	501	164	-	3/18/38/38	0/3/3/3
163	GDP	G	500	-	-	2/12/32/32	0/3/3/3
163	GDP	OX	500	-	-	2/12/32/32	0/3/3/3
168	ATP	6p	500	164	-	9/18/38/38	0/3/3/3
165	GTP	RV	501	-	-	1/18/38/38	0/3/3/3
163	GDP	FH	500	-	-	0/12/32/32	0/3/3/3
163	GDP	BX	500	-	-	3/12/32/32	0/3/3/3
165	GTP	CK	503	164	-	3/18/38/38	0/3/3/3
165	GTP	AW	501	164	-	3/18/38/38	0/3/3/3
163	GDP	NR	500	-	-	3/12/32/32	0/3/3/3
165	GTP	UW	501	164	-	5/18/38/38	0/3/3/3
165	GTP	CE	501	164	-	6/18/38/38	0/3/3/3
165	GTP	BG	501	164	-	1/18/38/38	0/3/3/3
165	GTP	PC	501	164	-	3/18/38/38	0/3/3/3
163	GDP	LU	500	-	-	3/12/32/32	0/3/3/3
165	GTP	RH	501	164	-	2/18/38/38	0/3/3/3
165	GTP	KD	502	164	-	3/18/38/38	0/3/3/3
163	GDP	HH	501	-	-	1/12/32/32	0/3/3/3
163	GDP	MV	500	-	-	3/12/32/32	0/3/3/3
163	GDP	P	500	-	-	2/12/32/32	0/3/3/3
163	GDP	TX	500	-	-	0/12/32/32	0/3/3/3
165	GTP	RN	501	164	-	3/18/38/38	0/3/3/3
163	GDP	S	500	-	-	2/12/32/32	0/3/3/3
163	GDP	DS	500	-	-	2/12/32/32	0/3/3/3
163	GDP	WH	500	-	-	2/12/32/32	0/3/3/3
165	GTP	KH	501	164	-	5/18/38/38	0/3/3/3
163	GDP	ID	500	-	-	1/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
165	GTP	SW	501	164	-	0/18/38/38	0/3/3/3
163	GDP	NV	501	-	-	1/12/32/32	0/3/3/3
165	GTP	FQ	501	164	-	6/18/38/38	0/3/3/3
165	GTP	LJ	501	164	-	4/18/38/38	0/3/3/3
163	GDP	SL	500	-	-	2/12/32/32	0/3/3/3
165	GTP	OS	501	164	-	3/18/38/38	0/3/3/3
163	GDP	SN	501	-	-	3/12/32/32	0/3/3/3
165	GTP	VC	501	164	-	6/18/38/38	0/3/3/3
163	GDP	EP	500	-	-	1/12/32/32	0/3/3/3
163	GDP	JY	501	-	-	0/12/32/32	0/3/3/3
163	GDP	KA	500	-	-	3/12/32/32	0/3/3/3
163	GDP	SF	500	-	-	1/12/32/32	0/3/3/3
163	GDP	IX	501	-	-	0/12/32/32	0/3/3/3
163	GDP	AX	500	-	-	2/12/32/32	0/3/3/3
163	GDP	PV	500	-	-	3/12/32/32	0/3/3/3
163	GDP	UN	500	-	-	3/12/32/32	0/3/3/3
168	ATP	7A	402	-	-	6/18/38/38	0/3/3/3
163	GDP	JG	500	-	-	2/12/32/32	0/3/3/3
165	GTP	HU	501	164	-	2/18/38/38	0/3/3/3
163	GDP	CG	500	-	-	1/12/32/32	0/3/3/3
165	GTP	AS	501	164	-	8/18/38/38	0/3/3/3
165	GTP	RF	501	164	-	1/18/38/38	0/3/3/3
163	GDP	OR	500	-	-	1/12/32/32	0/3/3/3
165	GTP	LZ	502	164	-	3/18/38/38	0/3/3/3
163	GDP	TF	500	-	-	1/12/32/32	0/3/3/3
165	GTP	VG	501	164	-	4/18/38/38	0/3/3/3
163	GDP	WX	500	-	-	1/12/32/32	0/3/3/3
165	GTP	JJ	501	164	-	3/18/38/38	0/3/3/3
163	GDP	HX	501	-	-	1/12/32/32	0/3/3/3
163	GDP	JO	500	-	-	2/12/32/32	0/3/3/3
165	GTP	C	501	164	-	6/18/38/38	0/3/3/3
163	GDP	QW	500	-	-	5/12/32/32	0/3/3/3
163	GDP	WF	501	-	-	1/12/32/32	0/3/3/3
163	GDP	HD	501	-	-	3/12/32/32	0/3/3/3
163	GDP	H	500	-	-	1/12/32/32	0/3/3/3
163	GDP	KC	500	-	-	1/12/32/32	0/3/3/3
165	GTP	AI	501	164	-	3/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
165	GTP	AM	501	164	-	5/18/38/38	0/3/3/3
165	GTP	IA	501	164	-	6/18/38/38	0/3/3/3
165	GTP	WW	501	164	-	5/18/38/38	0/3/3/3
165	GTP	FG	501	164	-	8/18/38/38	0/3/3/3
168	ATP	6I	400	164	-	7/18/38/38	0/3/3/3
165	GTP	PS	501	-	-	5/18/38/38	0/3/3/3
165	GTP	R	501	164	-	6/18/38/38	0/3/3/3
165	GTP	KR	501	164	-	6/18/38/38	0/3/3/3
163	GDP	JE	500	-	-	1/12/32/32	0/3/3/3
165	GTP	CJ	501	164	-	3/18/38/38	0/3/3/3
163	GDP	I	501	-	-	0/12/32/32	0/3/3/3
165	GTP	SU	501	164	-	3/18/38/38	0/3/3/3
163	GDP	HV	500	-	-	2/12/32/32	0/3/3/3
163	GDP	EL	500	-	-	3/12/32/32	0/3/3/3
163	GDP	QM	500	-	-	2/12/32/32	0/3/3/3
163	GDP	N	500	-	-	1/12/32/32	0/3/3/3
165	GTP	LB	501	164	-	3/18/38/38	0/3/3/3
163	GDP	CE	500	-	-	3/12/32/32	0/3/3/3
165	GTP	VT	501	164	-	4/18/38/38	0/3/3/3
165	GTP	LL	501	164	-	4/18/38/38	0/3/3/3
165	GTP	PE	501	164	-	0/18/38/38	0/3/3/3
163	GDP	TP	500	-	-	1/12/32/32	0/3/3/3
165	GTP	GU	501	164	-	4/18/38/38	0/3/3/3
163	GDP	FR	501	-	-	3/12/32/32	0/3/3/3
163	GDP	ET	500	-	-	1/12/32/32	0/3/3/3
163	GDP	ON	500	-	-	5/12/32/32	0/3/3/3
165	GTP	Q	501	164	-	3/18/38/38	0/3/3/3
165	GTP	SS	501	164	-	8/18/38/38	0/3/3/3
165	GTP	TC	501	164	-	5/18/38/38	0/3/3/3
163	GDP	IL	501	-	-	0/12/32/32	0/3/3/3
163	GDP	UX	500	-	-	1/12/32/32	0/3/3/3
163	GDP	FJ	501	-	-	2/12/32/32	0/3/3/3
165	GTP	KP	502	164	-	3/18/38/38	0/3/3/3
163	GDP	T	501	-	-	1/12/32/32	0/3/3/3
163	GDP	BR	500	-	-	3/12/32/32	0/3/3/3
165	GTP	SM	501	164	-	3/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
165	GTP	FC	501	164	-	4/18/38/38	0/3/3/3
165	GTP	DJ	501	164	-	4/18/38/38	0/3/3/3
163	GDP	WR	501	-	-	1/12/32/32	0/3/3/3
165	GTP	UO	501	164	-	3/18/38/38	0/3/3/3
165	GTP	EI	501	164	-	5/18/38/38	0/3/3/3
163	GDP	FV	501	-	-	1/12/32/32	0/3/3/3
165	GTP	UU	501	164	-	3/18/38/38	0/3/3/3
165	GTP	WS	501	164	-	1/18/38/38	0/3/3/3
165	GTP	LH	501	164	-	3/18/38/38	0/3/3/3
165	GTP	US	501	164	-	5/18/38/38	0/3/3/3
163	GDP	EF	500	-	-	3/12/32/32	0/3/3/3
163	GDP	VX	500	-	-	1/12/32/32	0/3/3/3
165	GTP	FM	501	164	-	2/18/38/38	0/3/3/3
163	GDP	GD	500	-	-	4/12/32/32	0/3/3/3
163	GDP	W	500	-	-	1/12/32/32	0/3/3/3
165	GTP	EA	501	164	-	2/18/38/38	0/3/3/3
165	GTP	MS	501	164	-	5/18/38/38	0/3/3/3
165	GTP	UC	501	164	-	3/18/38/38	0/3/3/3
165	GTP	JZ	501	164	-	3/18/38/38	0/3/3/3
163	GDP	LI	500	-	-	3/12/32/32	0/3/3/3
165	GTP	MY	501	164	-	2/18/38/38	0/3/3/3
163	GDP	KS	500	-	-	2/12/32/32	0/3/3/3
163	GDP	WT	500	-	-	2/12/32/32	0/3/3/3
165	GTP	TE	501	164	-	6/18/38/38	0/3/3/3
165	GTP	PI	501	164	-	4/18/38/38	0/3/3/3
165	GTP	WA	501	164	-	2/18/38/38	0/3/3/3
165	GTP	AU	501	164	-	3/18/38/38	0/3/3/3
163	GDP	EB	500	-	-	4/12/32/32	0/3/3/3
163	GDP	RK	500	-	-	2/12/32/32	0/3/3/3
165	GTP	BM	501	164	-	3/18/38/38	0/3/3/3
163	GDP	BH	500	-	-	3/12/32/32	0/3/3/3
165	GTP	OU	501	164	-	6/18/38/38	0/3/3/3
165	GTP	QH	501	164	-	10/18/38/38	0/3/3/3
163	GDP	ND	500	-	-	0/12/32/32	0/3/3/3
163	GDP	UF	500	-	-	1/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
165	GTP	DD	501	164	-	3/18/38/38	0/3/3/3
165	GTP	LX	501	164	-	4/18/38/38	0/3/3/3
163	GDP	VN	500	-	-	1/12/32/32	0/3/3/3
163	GDP	LO	500	-	-	3/12/32/32	0/3/3/3
163	GDP	JS	500	-	-	2/12/32/32	0/3/3/3
165	GTP	IC	501	164	-	4/18/38/38	0/3/3/3
163	GDP	AT	500	-	-	4/12/32/32	0/3/3/3
163	GDP	UV	500	-	-	1/12/32/32	0/3/3/3
165	GTP	UQ	501	164	-	9/18/38/38	0/3/3/3
163	GDP	OV	500	-	-	3/12/32/32	0/3/3/3
165	GTP	GI	501	164	-	1/18/38/38	0/3/3/3
163	GDP	UB	500	-	-	3/12/32/32	0/3/3/3
163	GDP	VR	500	-	-	1/12/32/32	0/3/3/3
163	GDP	TT	500	-	-	1/12/32/32	0/3/3/3
163	GDP	WN	500	-	-	1/12/32/32	0/3/3/3
163	GDP	MZ	500	-	-	2/12/32/32	0/3/3/3
165	GTP	GE	501	164	-	5/18/38/38	0/3/3/3
163	GDP	KY	500	-	-	2/12/32/32	0/3/3/3
165	GTP	LV	501	164	-	5/18/38/38	0/3/3/3
163	GDP	VB	500	-	-	1/12/32/32	0/3/3/3
165	GTP	QR	501	164	-	2/18/38/38	0/3/3/3
163	GDP	BN	500	-	-	3/12/32/32	0/3/3/3
163	GDP	AR	500	-	-	1/12/32/32	0/3/3/3
163	GDP	DC	500	-	-	4/12/32/32	0/3/3/3
163	GDP	OP	501	-	-	2/12/32/32	0/3/3/3
165	GTP	JP	501	164	-	5/18/38/38	0/3/3/3
165	GTP	VM	501	164	-	5/18/38/38	0/3/3/3
165	GTP	EJ	501	164	-	5/18/38/38	0/3/3/3
163	GDP	FD	500	-	-	3/12/32/32	0/3/3/3
165	GTP	OO	501	164	-	1/18/38/38	0/3/3/3
165	GTP	GG	501	164	-	4/18/38/38	0/3/3/3
165	GTP	PU	501	164	-	4/18/38/38	0/3/3/3
165	GTP	DL	501	-	-	10/18/38/38	0/3/3/3
165	GTP	MA	501	164	-	0/18/38/38	0/3/3/3
163	GDP	DA	500	-	-	4/12/32/32	0/3/3/3
165	GTP	PM	501	164	-	3/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
165	GTP	QL	501	-	-	3/18/38/38	0/3/3/3
165	GTP	RC	501	164	-	7/18/38/38	0/3/3/3
165	GTP	FS	501	164	-	3/18/38/38	0/3/3/3
165	GTP	HE	501	164	-	4/18/38/38	0/3/3/3
163	GDP	EJ	500	-	-	1/12/32/32	0/3/3/3
165	GTP	CW	501	164	-	4/18/38/38	0/3/3/3
165	GTP	VA	501	164	-	4/18/38/38	0/3/3/3
163	GDP	QC	500	-	-	2/12/32/32	0/3/3/3
163	GDP	BT	500	-	-	3/12/32/32	0/3/3/3
163	GDP	EV	500	-	-	4/12/32/32	0/3/3/3
165	GTP	OC	501	164	-	1/18/38/38	0/3/3/3
165	GTP	ES	501	164	-	7/18/38/38	0/3/3/3
165	GTP	BU	501	164	-	4/18/38/38	0/3/3/3
163	GDP	PD	500	-	-	4/12/32/32	0/3/3/3
163	GDP	RO	500	-	-	1/12/32/32	0/3/3/3
165	GTP	WG	501	164	-	1/18/38/38	0/3/3/3
163	GDP	JA	500	-	-	1/12/32/32	0/3/3/3
163	GDP	QA	500	-	-	1/12/32/32	0/3/3/3
163	GDP	DU	500	-	-	2/12/32/32	0/3/3/3
163	GDP	PF	501	-	-	3/12/32/32	0/3/3/3
163	GDP	LM	500	-	-	1/12/32/32	0/3/3/3
163	GDP	FF	500	-	-	4/12/32/32	0/3/3/3
165	GTP	LP	502	164	-	6/18/38/38	0/3/3/3
165	GTP	HK	501	164	-	4/18/38/38	0/3/3/3
165	GTP	EV	501	164	-	4/18/38/38	0/3/3/3
165	GTP	MJ	501	164	-	5/18/38/38	0/3/3/3
163	GDP	MX	500	-	-	1/12/32/32	0/3/3/3
165	GTP	G	501	164	-	7/18/38/38	0/3/3/3
165	GTP	EG	501	164	-	7/18/38/38	0/3/3/3
165	GTP	BO	501	164	-	4/18/38/38	0/3/3/3
163	GDP	HB	501	-	-	3/12/32/32	0/3/3/3
163	GDP	WP	500	-	-	2/12/32/32	0/3/3/3
165	GTP	DT	501	164	-	3/18/38/38	0/3/3/3
165	GTP	MV	501	164	-	5/18/38/38	0/3/3/3
165	GTP	EO	501	164	-	4/18/38/38	0/3/3/3
165	GTP	TI	501	164	-	4/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
165	GTP	HN	503	164	-	7/18/38/38	0/3/3/3
165	GTP	GW	501	164	-	3/18/38/38	0/3/3/3
165	GTP	PK	501	164	-	3/18/38/38	0/3/3/3
163	GDP	TL	501	-	-	0/12/32/32	0/3/3/3
165	GTP	IK	501	164	-	3/18/38/38	0/3/3/3
163	GDP	PB	500	-	-	1/12/32/32	0/3/3/3
165	GTP	SE	501	164	-	5/18/38/38	0/3/3/3
165	GTP	DE	501	164	-	6/18/38/38	0/3/3/3

The worst 5 of 895 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
165	G	501	GTP	C5-C6	-4.66	1.38	1.47
165	DJ	501	GTP	C5-C6	-4.64	1.38	1.47
165	GQ	501	GTP	C5-C6	-4.55	1.38	1.47
165	EJ	501	GTP	C5-C6	-4.53	1.38	1.47
165	FI	501	GTP	C5-C6	-4.52	1.38	1.47

The worst 5 of 1887 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
165	DB	501	GTP	C4'-O4'-C1'	-4.64	105.68	109.92
165	DP	501	GTP	C4'-O4'-C1'	-4.19	106.09	109.92
165	DP	501	GTP	O4'-C1'-N9	4.02	114.07	108.75
165	DN	501	GTP	C4'-O4'-C1'	-4.00	106.26	109.92
165	DB	501	GTP	O4'-C1'-N9	3.98	114.03	108.75

There are no chirality outliers.

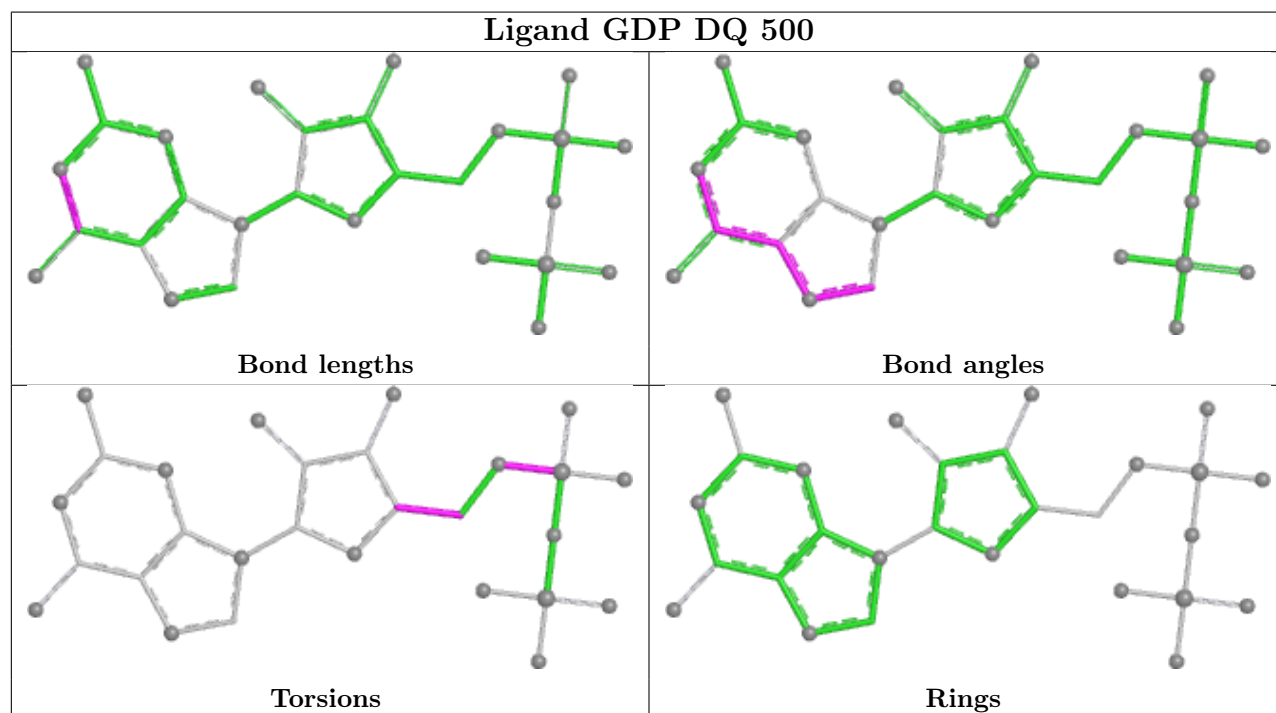
5 of 1844 torsion outliers are listed below:

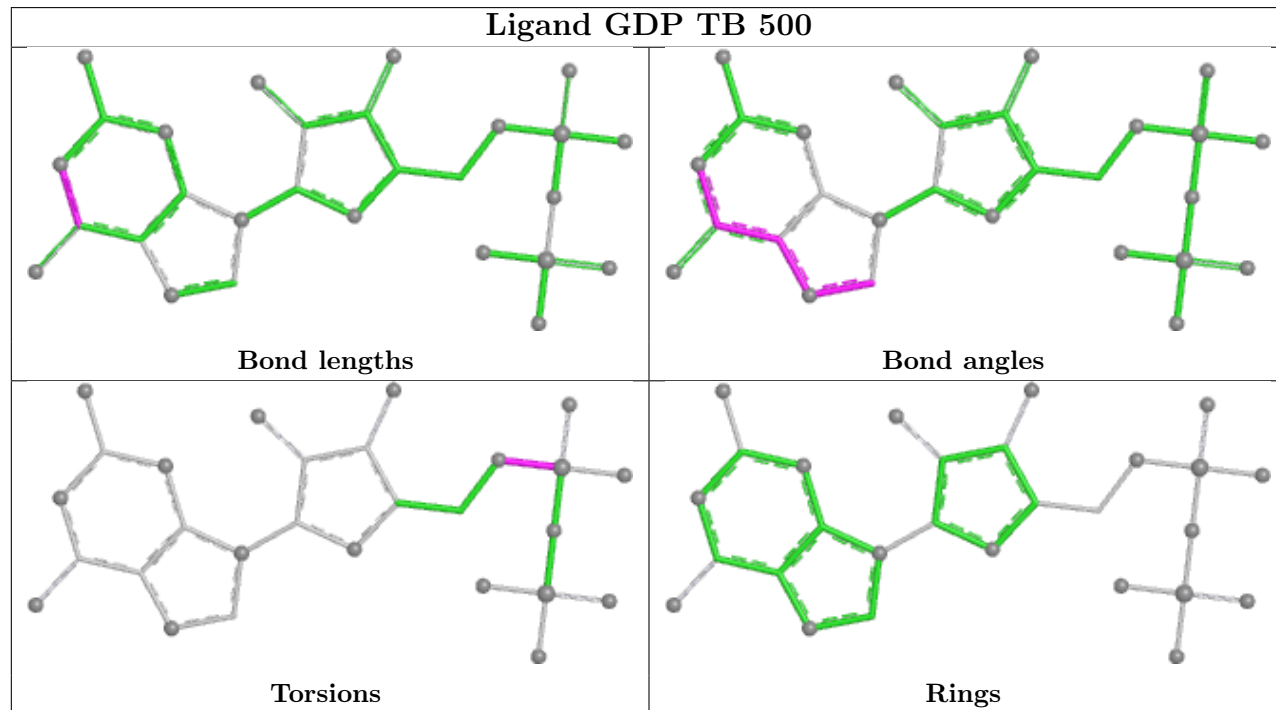
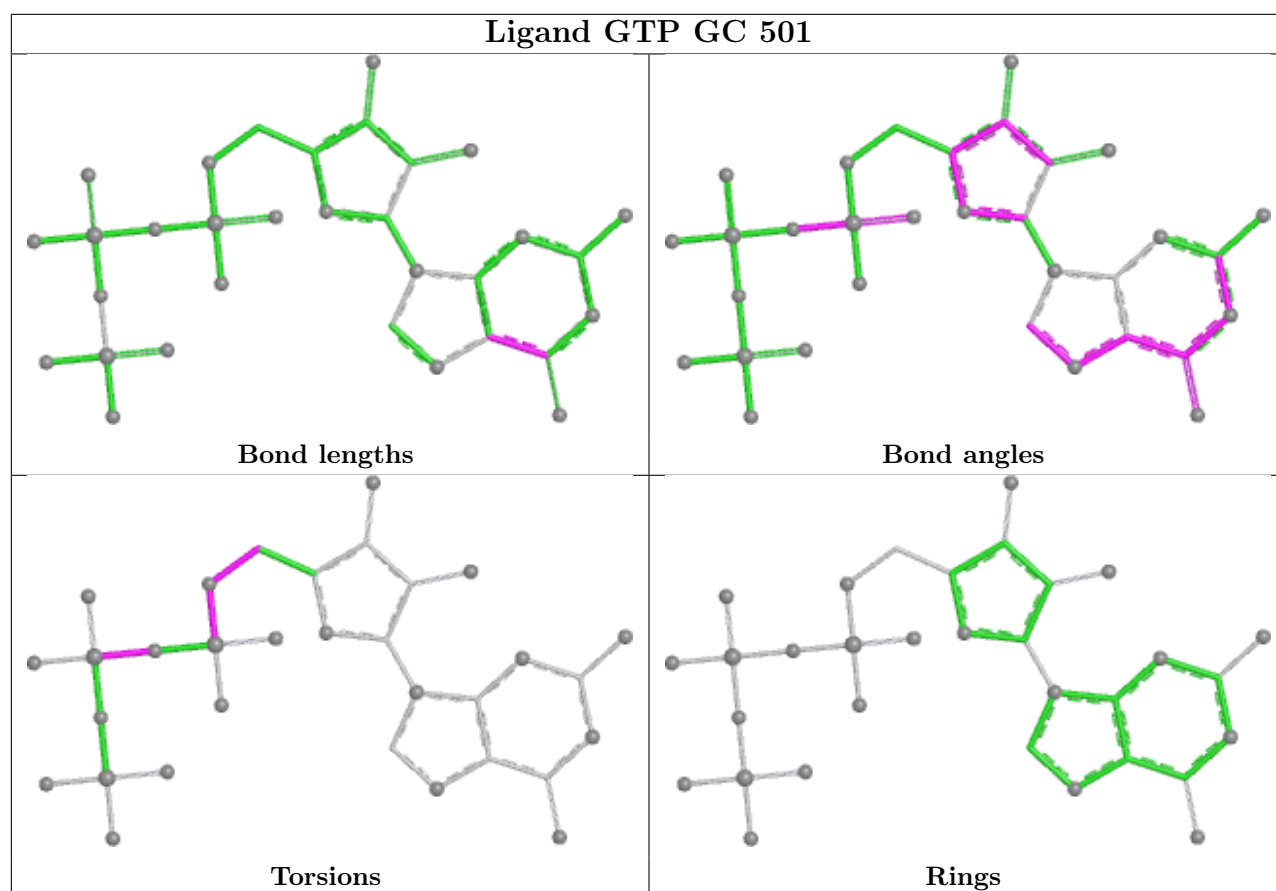
Mol	Chain	Res	Type	Atoms
163	AB	500	GDP	C5'-O5'-PA-O3A
163	AB	500	GDP	C5'-O5'-PA-O1A
163	AD	500	GDP	C5'-O5'-PA-O3A
163	AD	500	GDP	C5'-O5'-PA-O1A
163	AF	500	GDP	C5'-O5'-PA-O1A

There are no ring outliers.

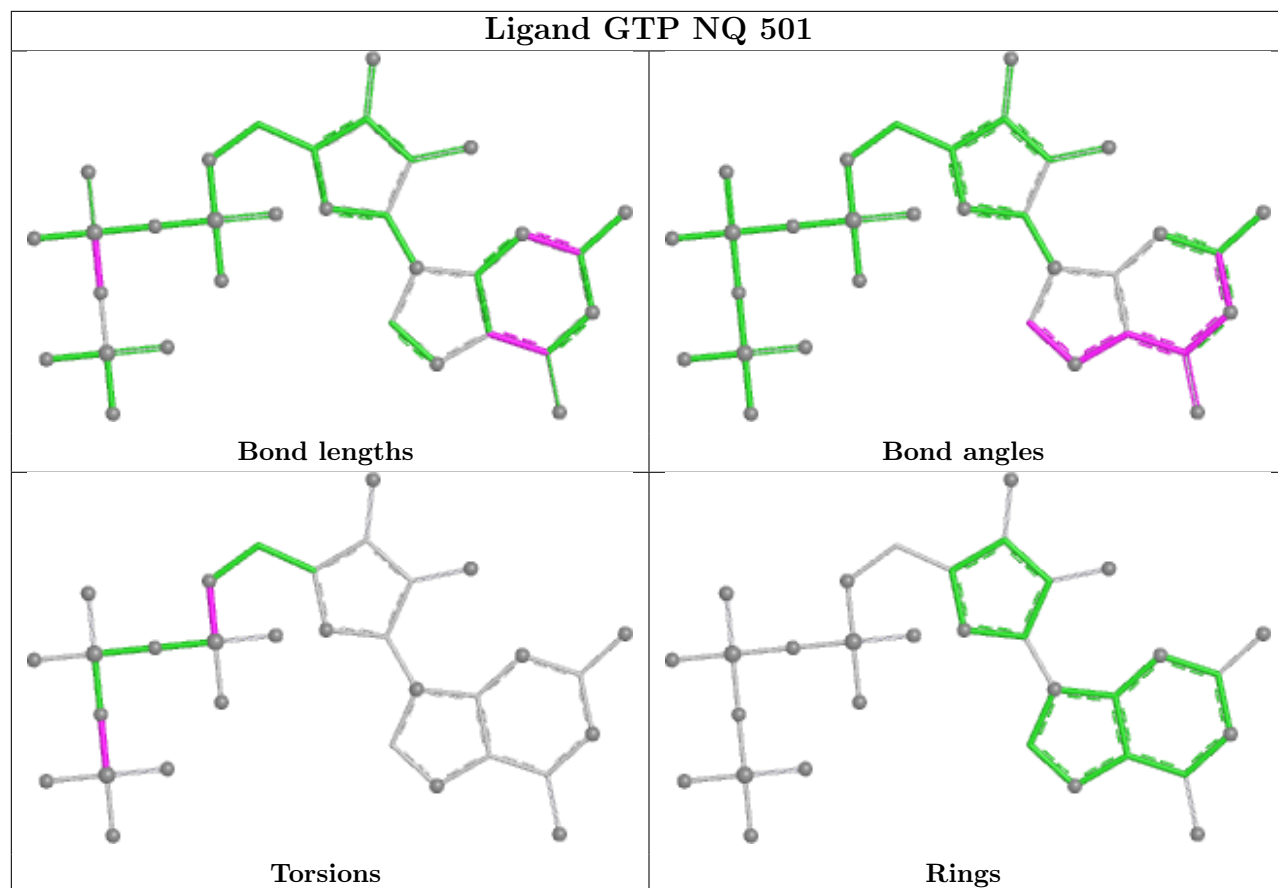
No monomer is involved in short contacts.

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

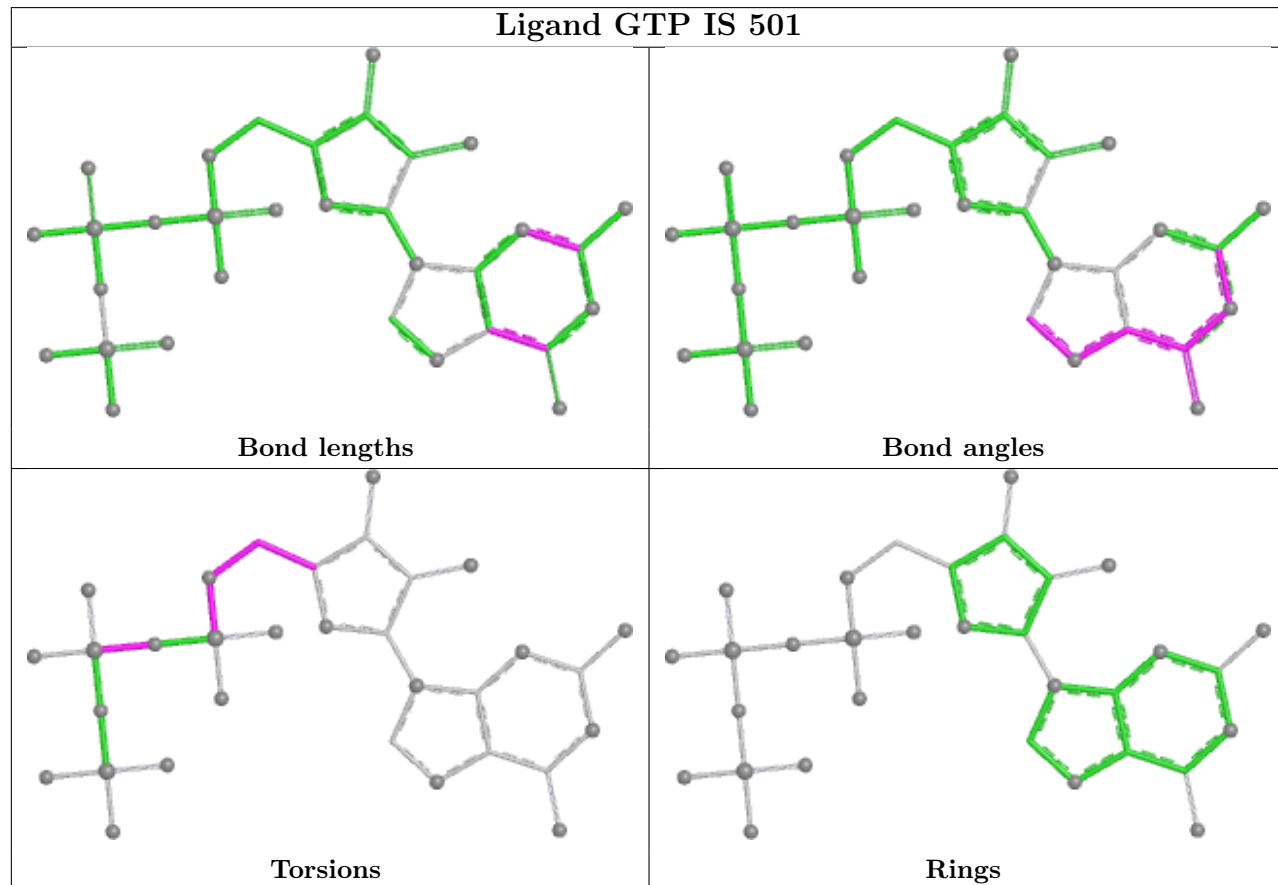


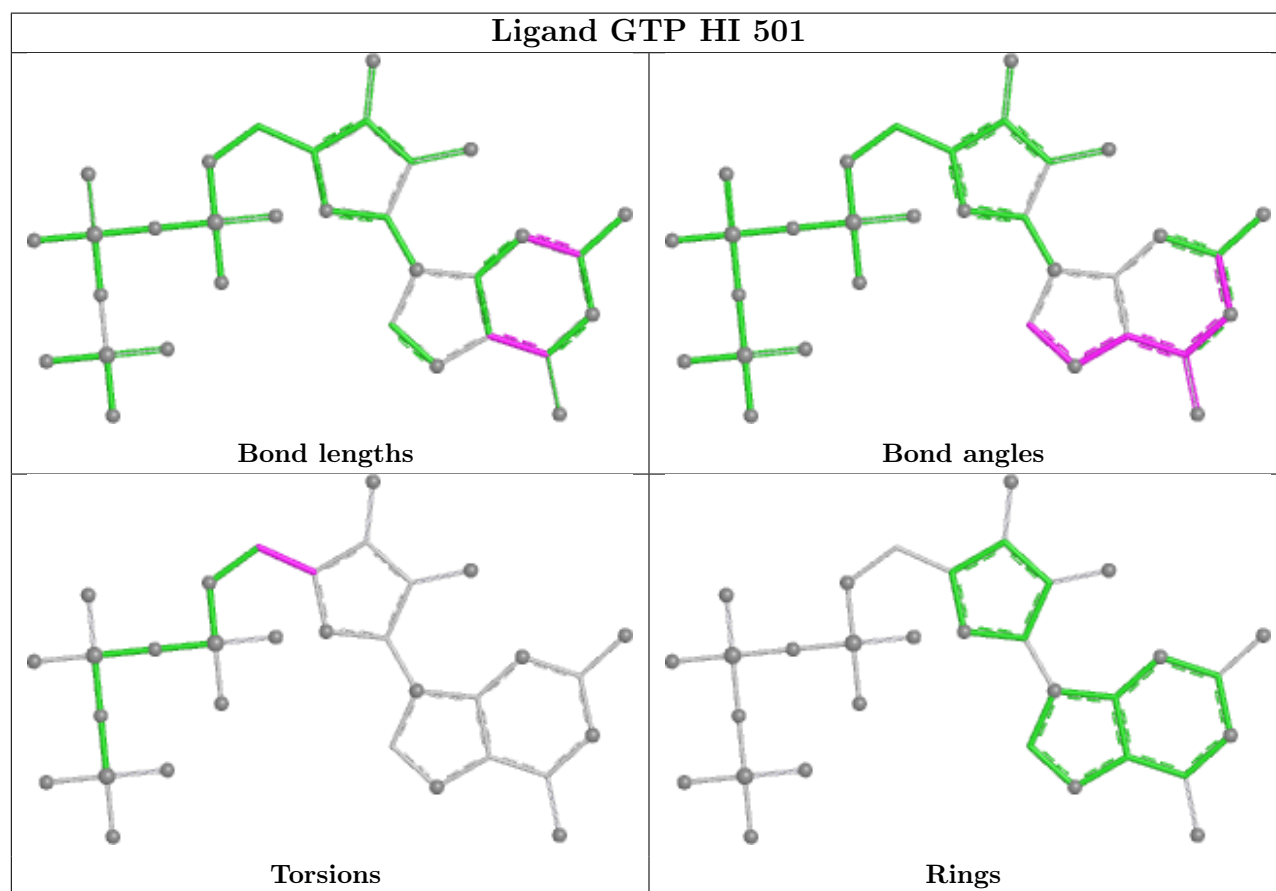
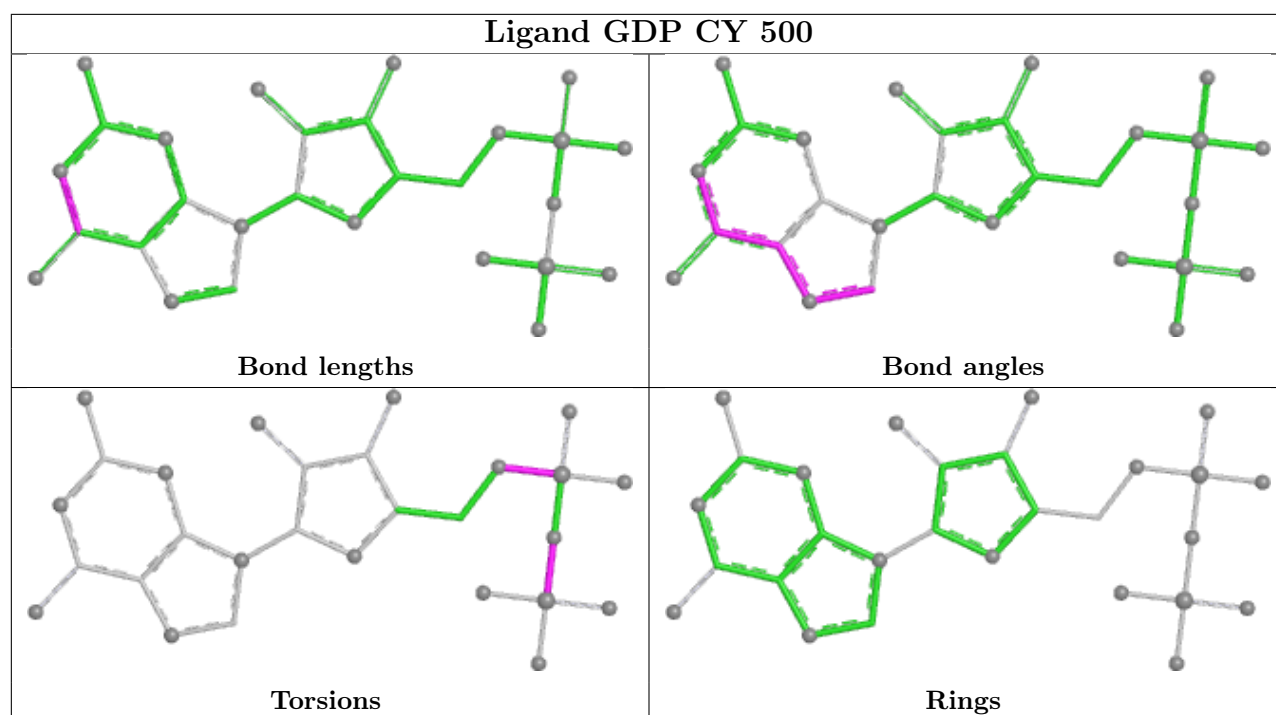


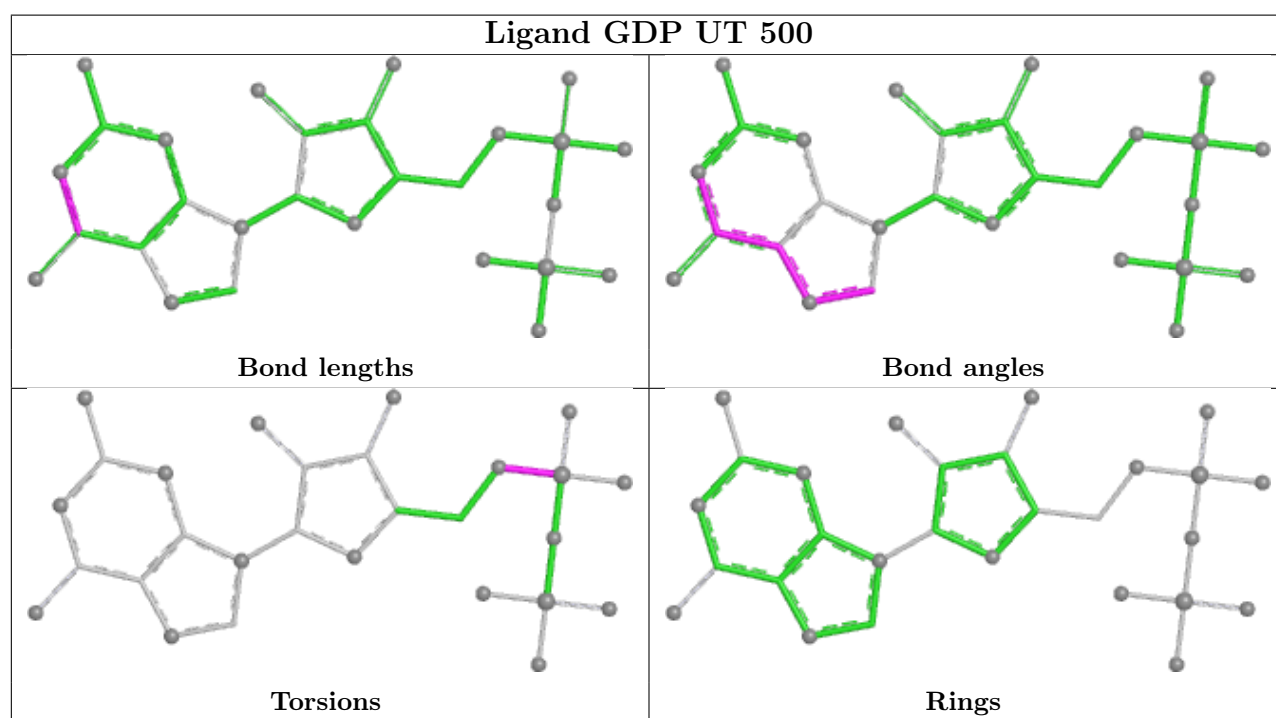
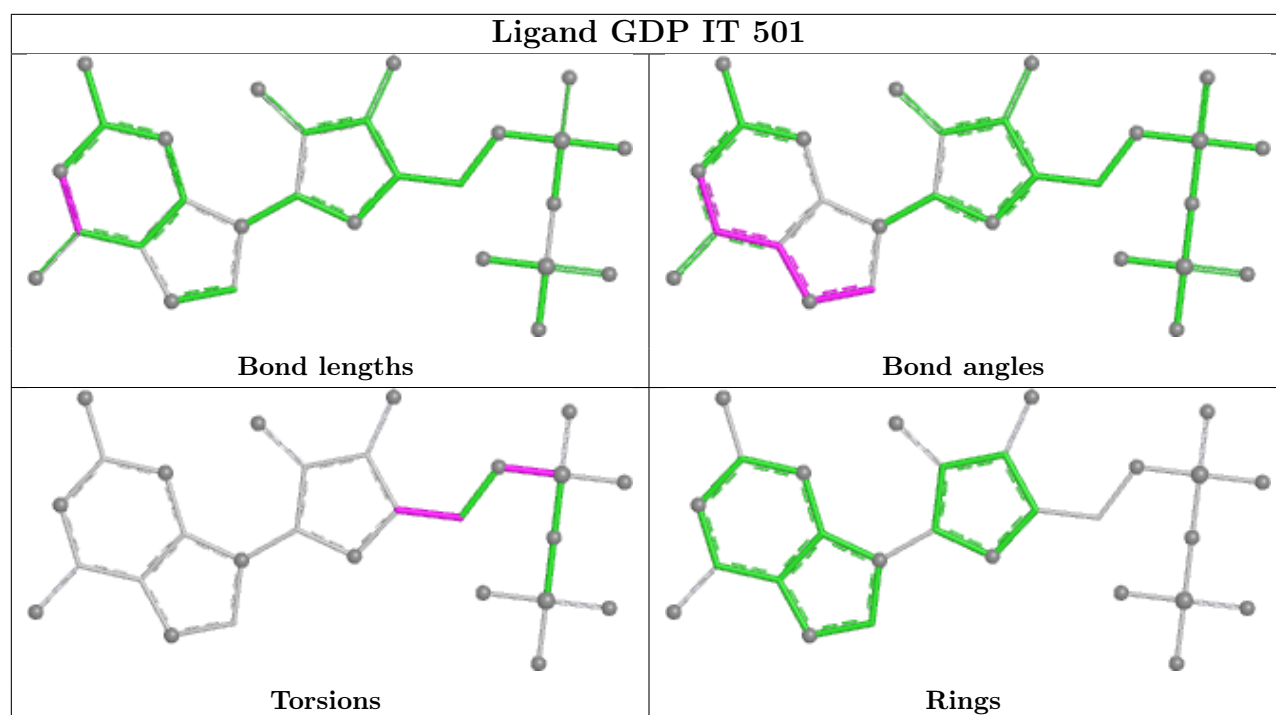
Ligand GTP NQ 501



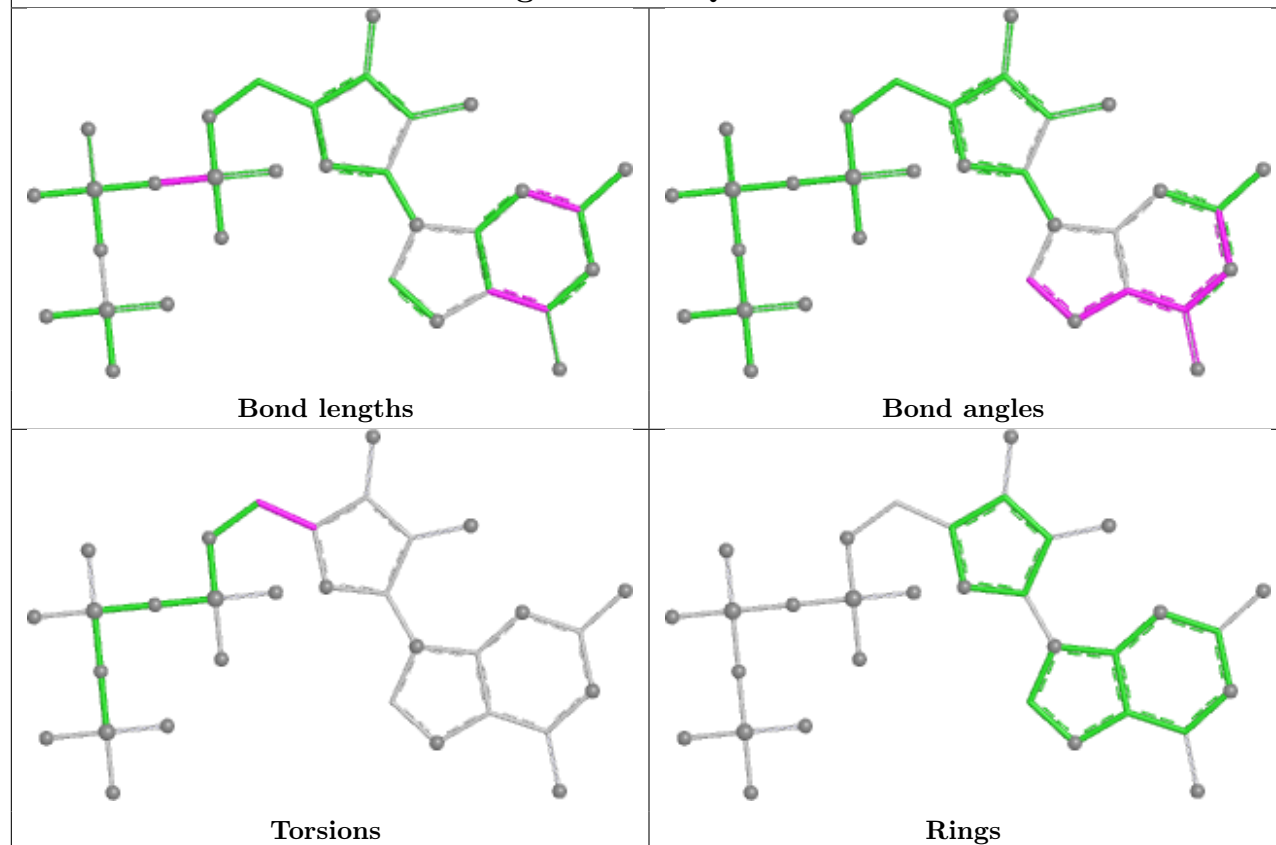
Ligand GTP IS 501



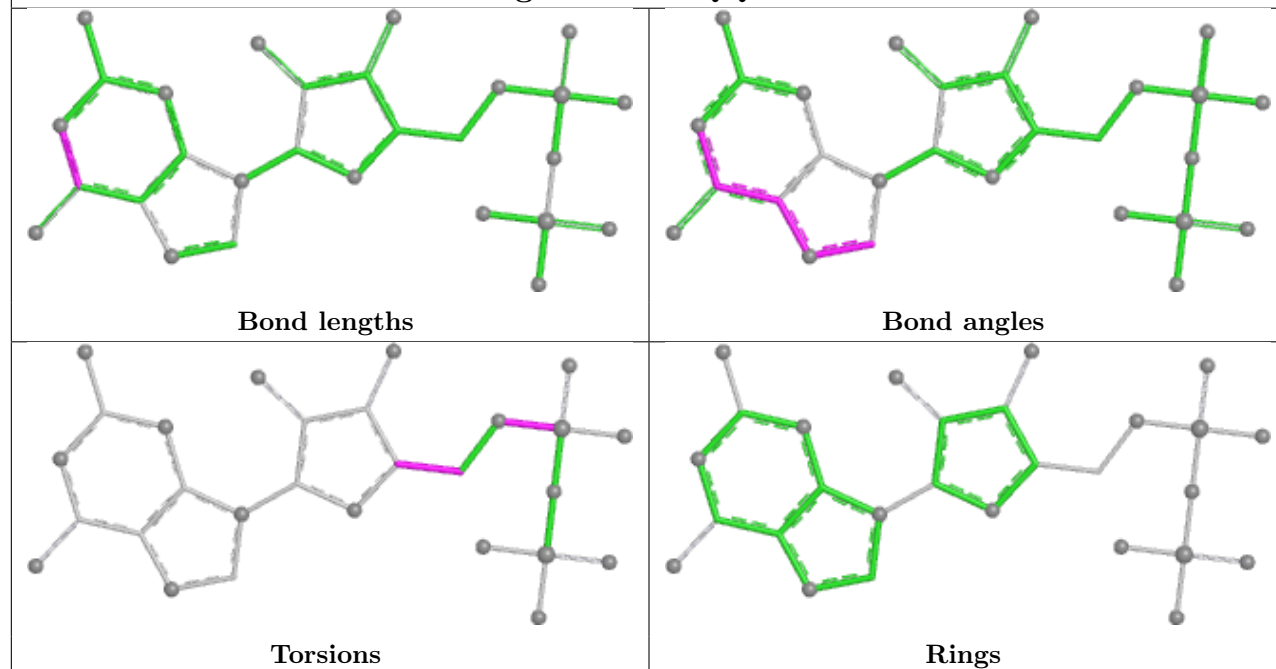


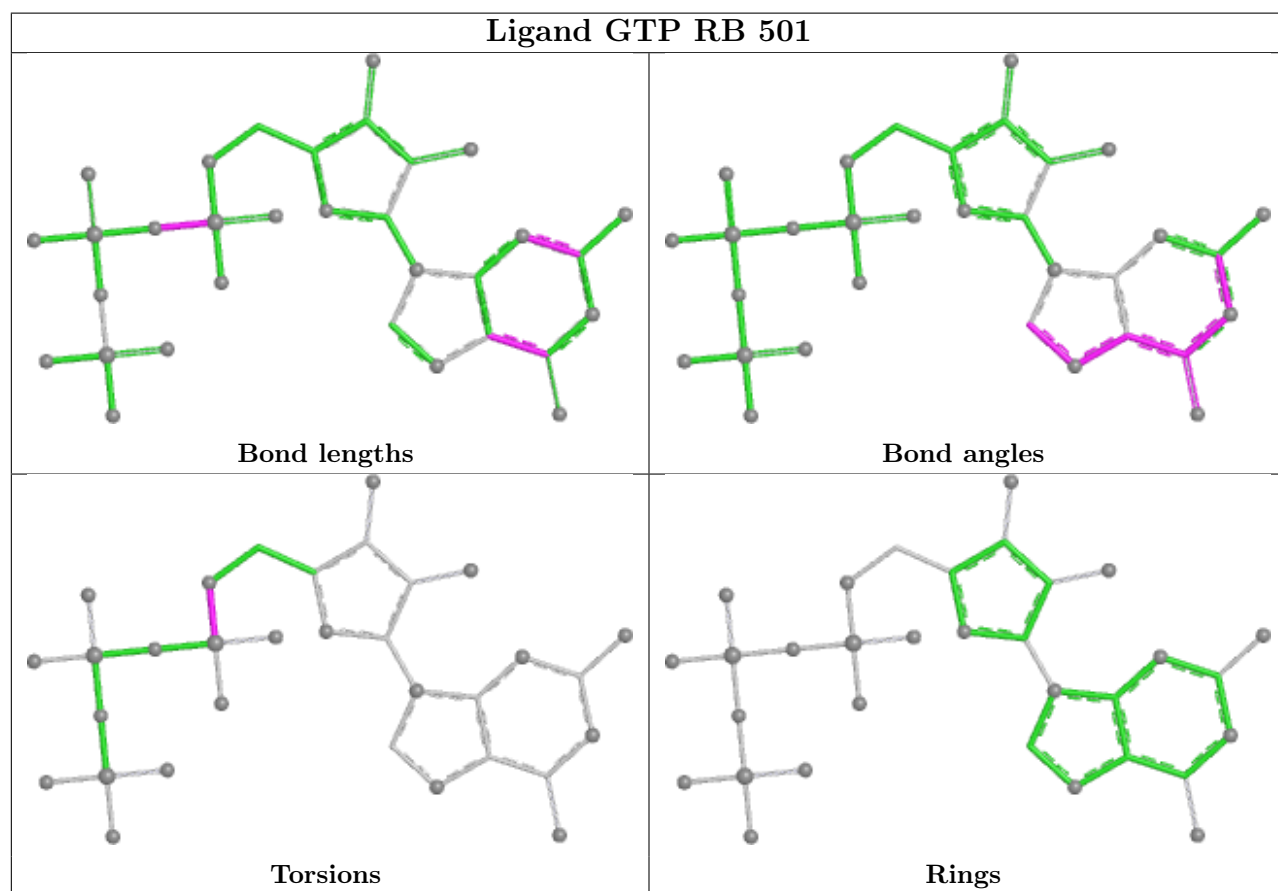
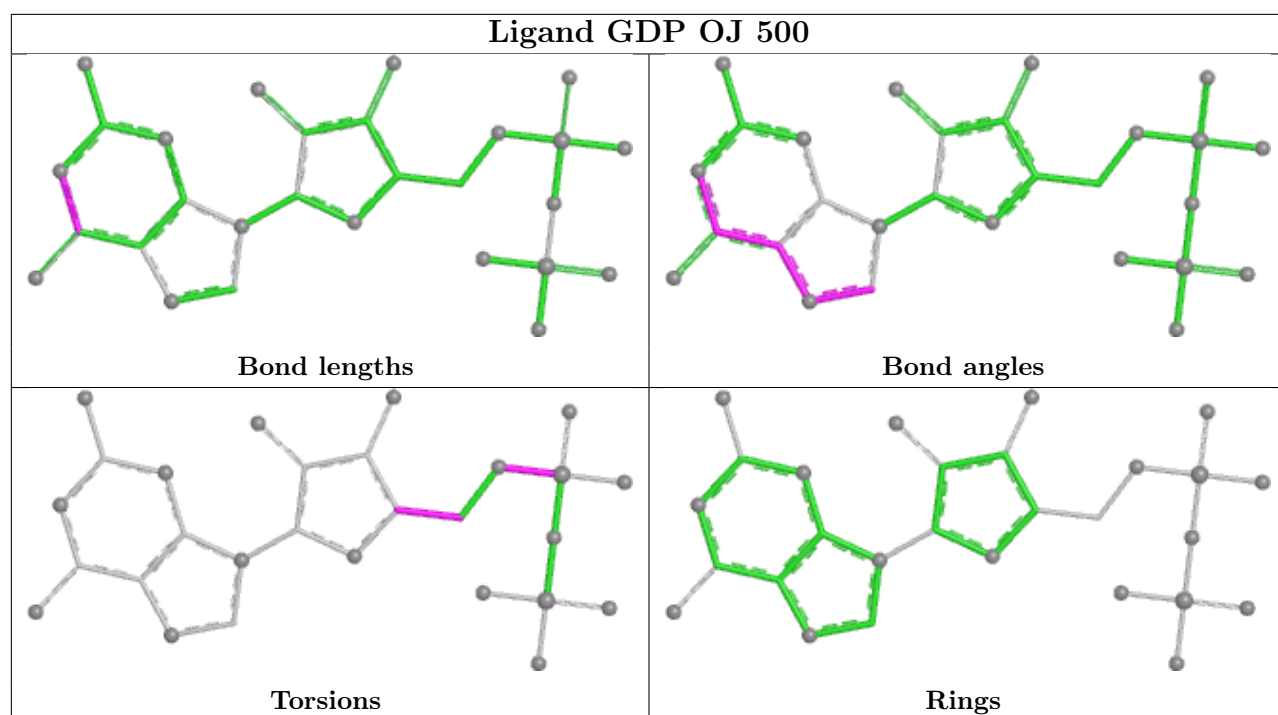


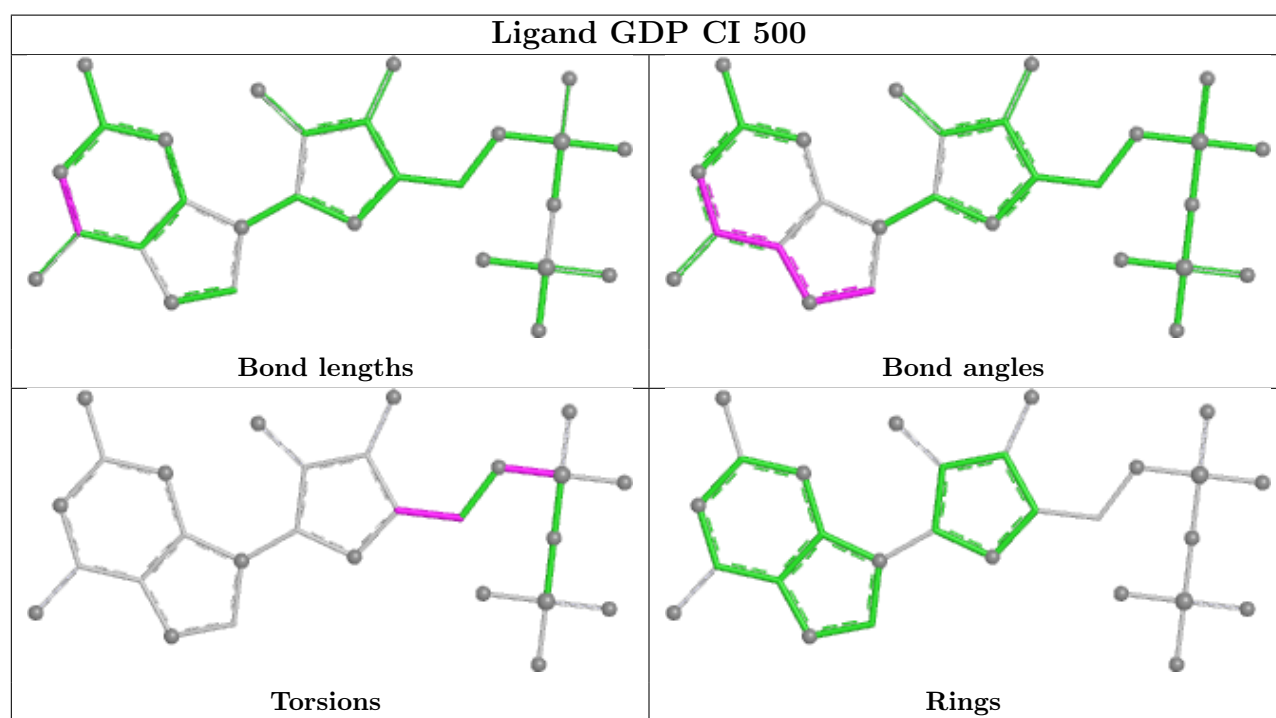
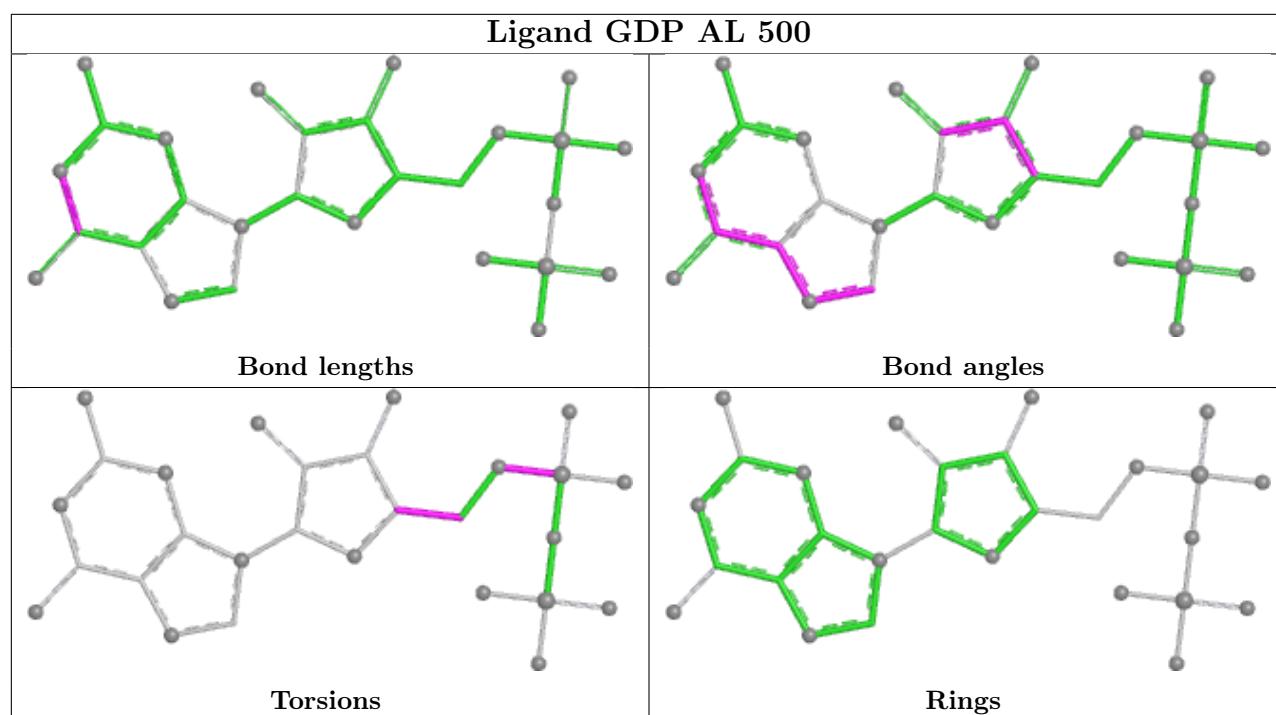
Ligand GTP QN 501

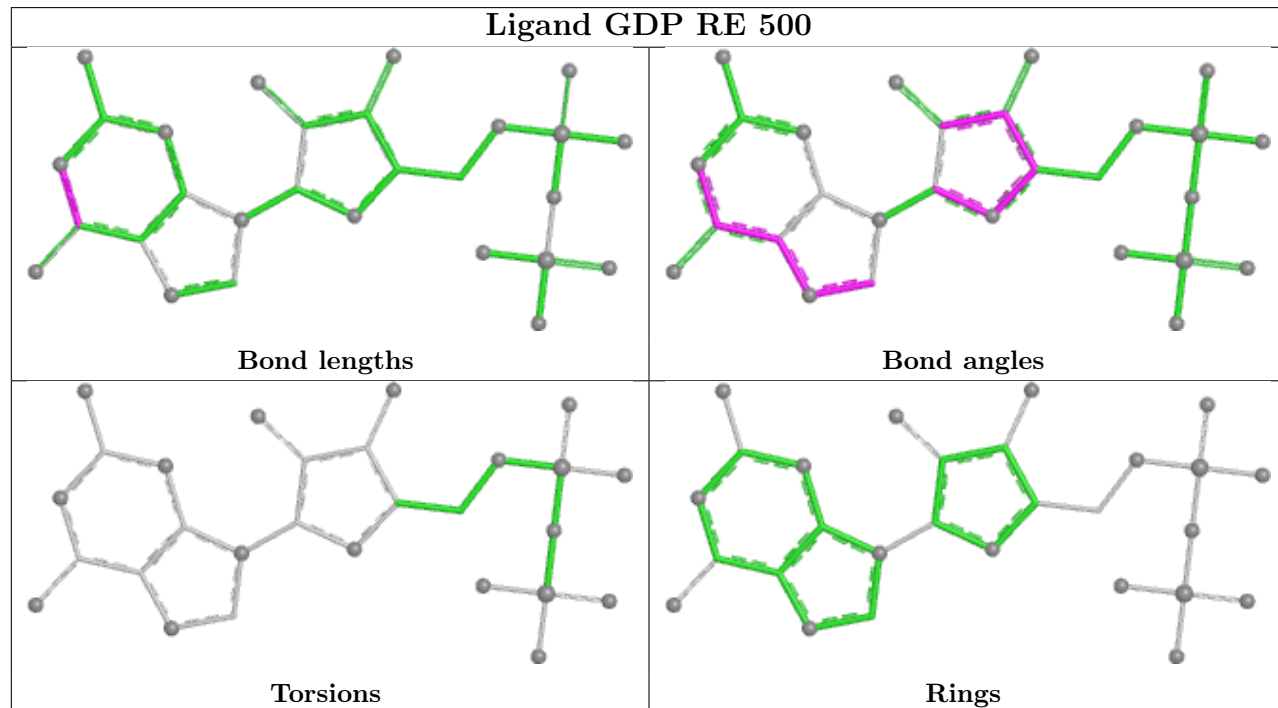
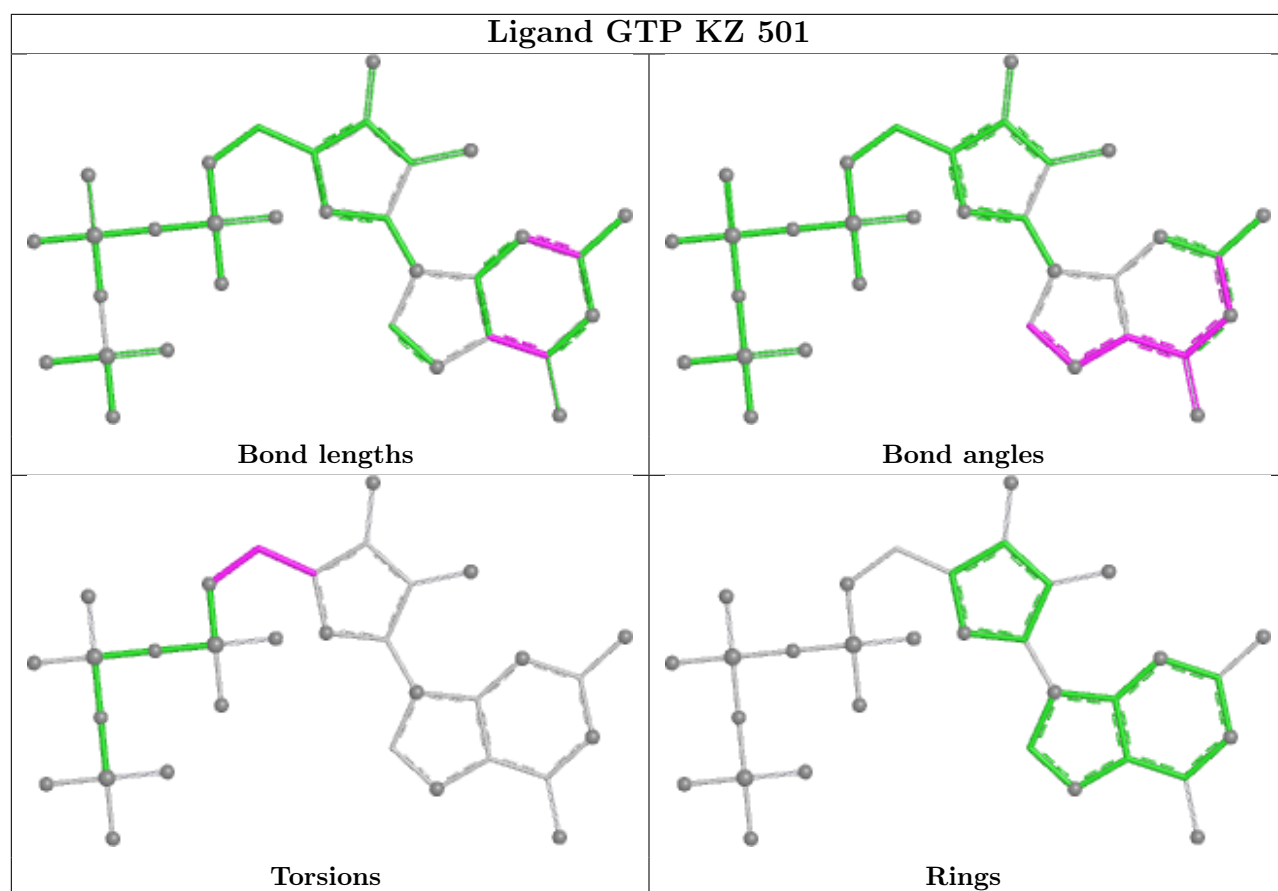


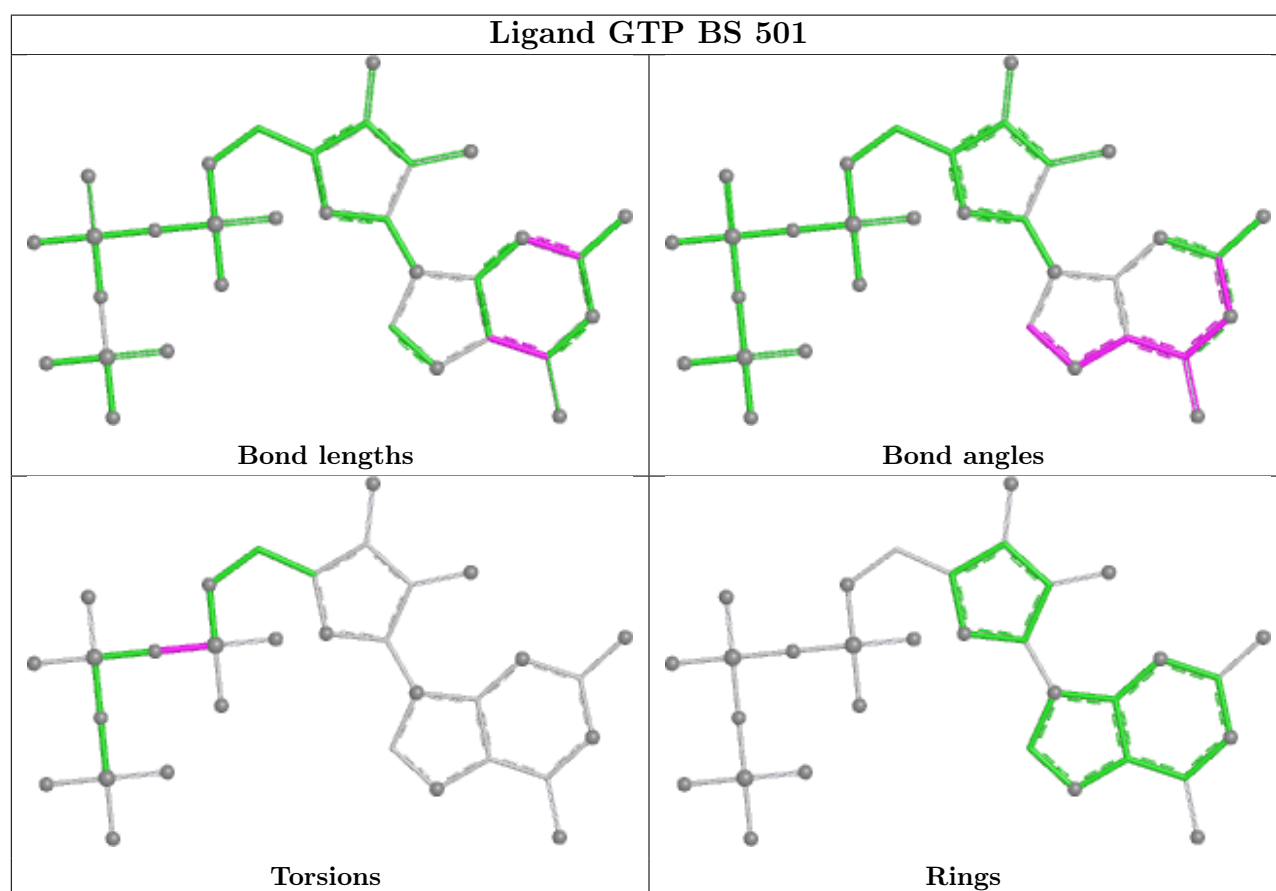
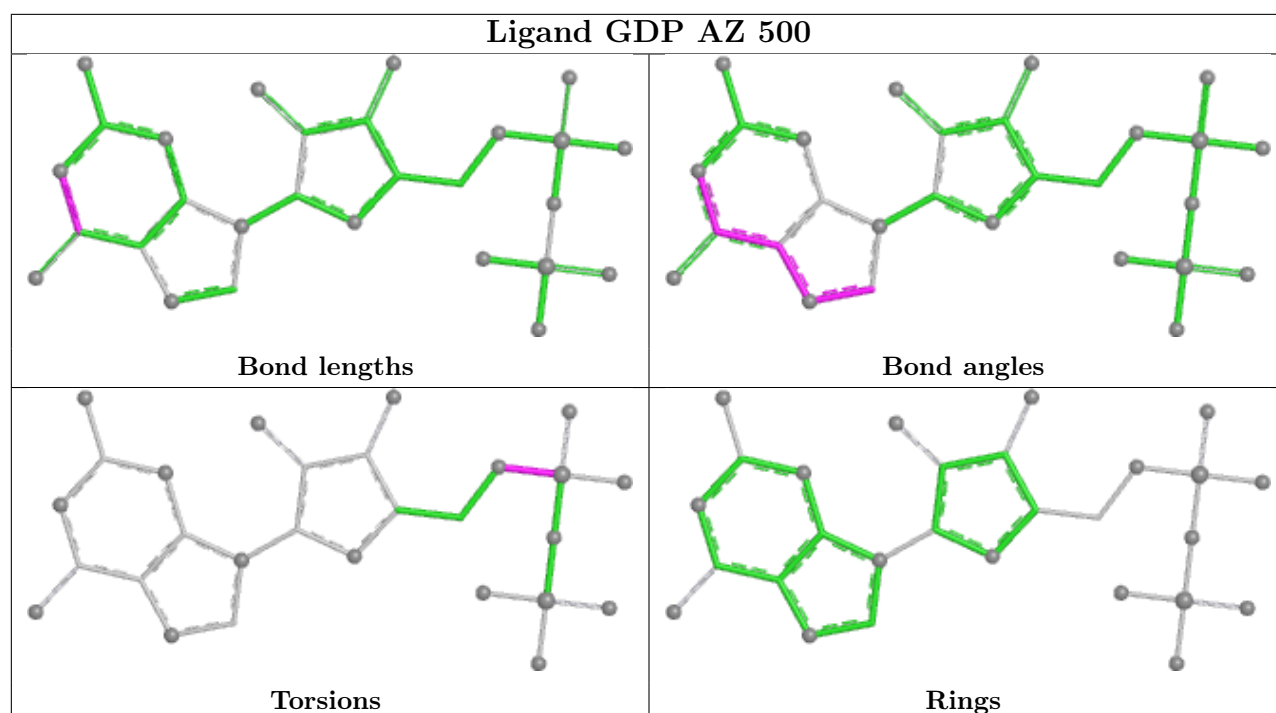
Ligand GDP QQ 500

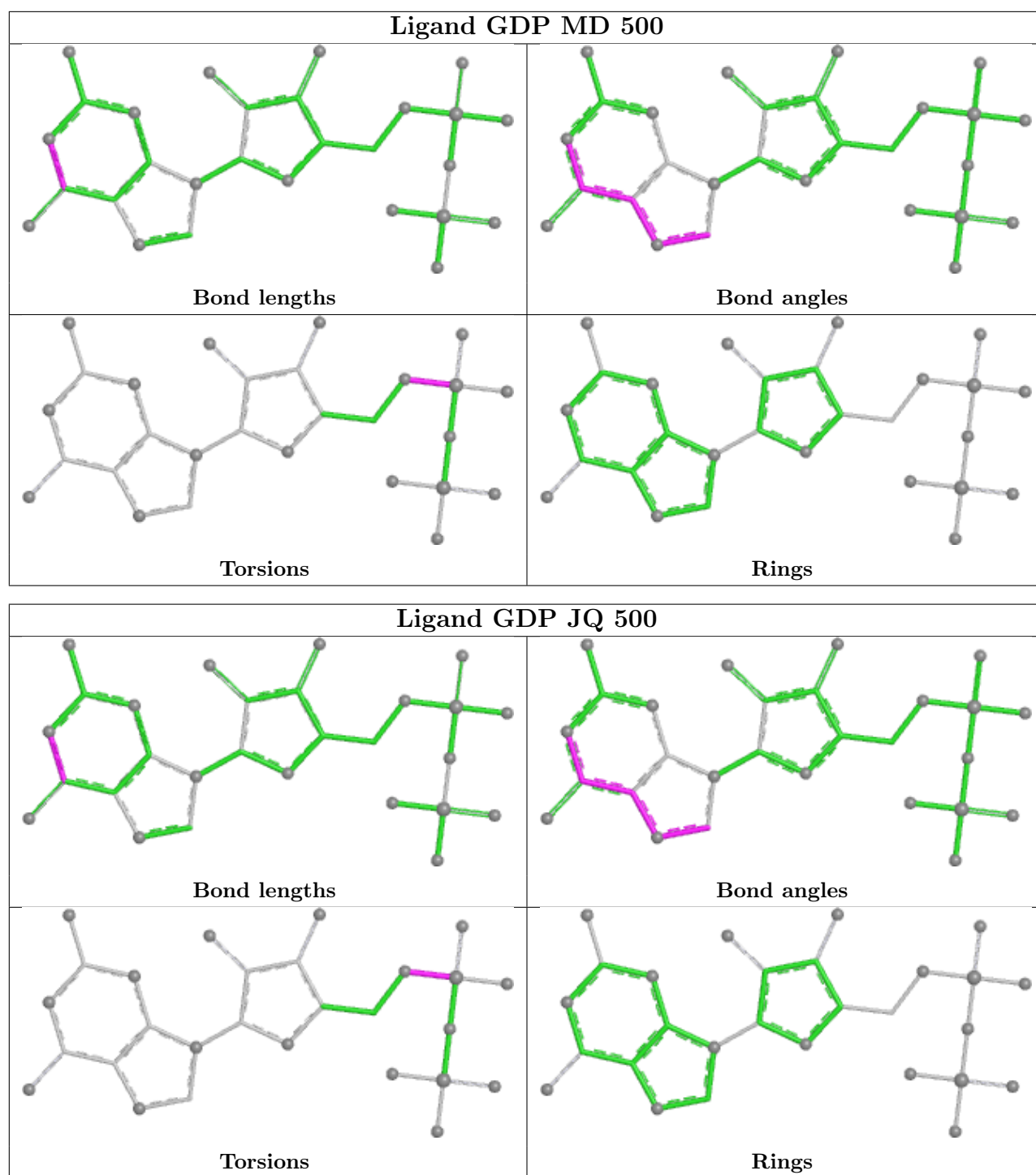




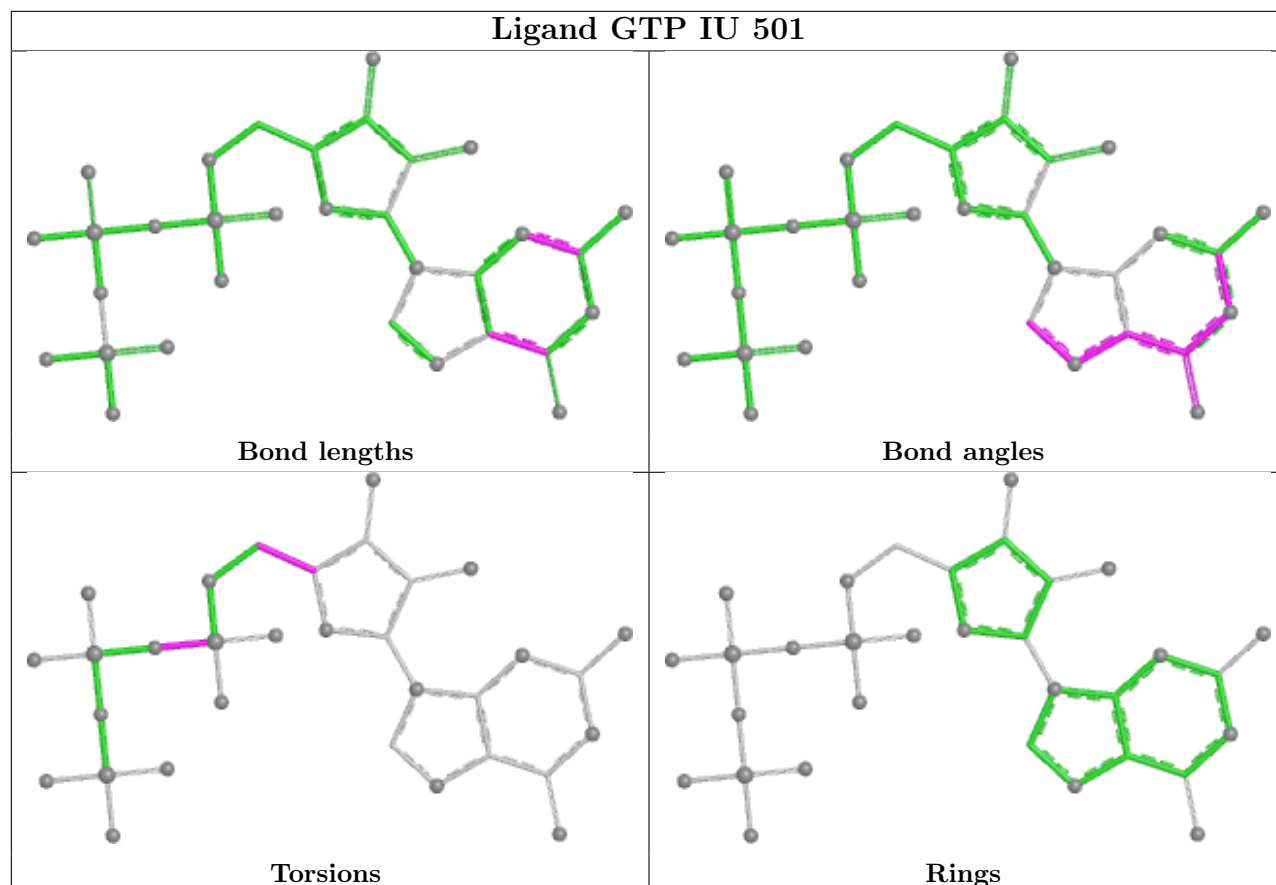




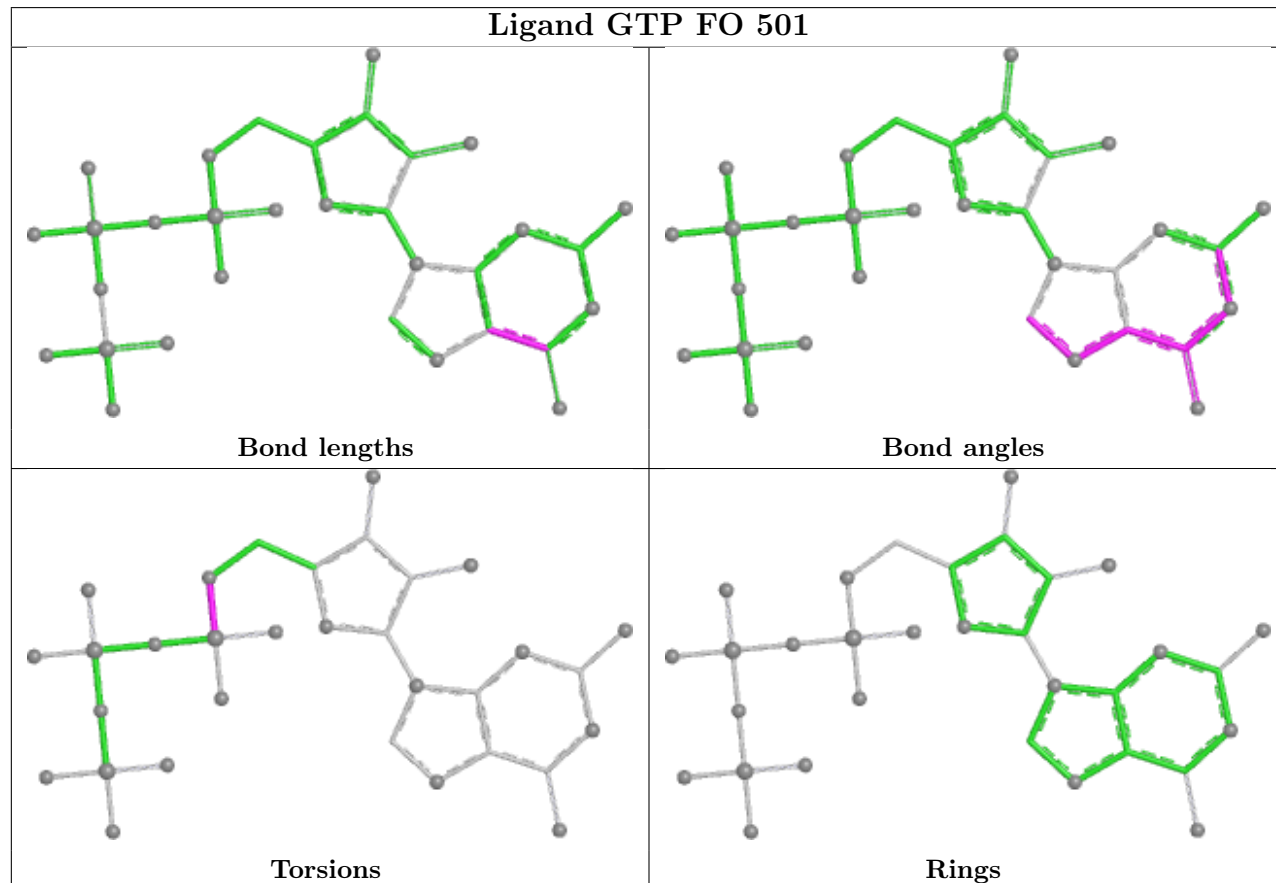


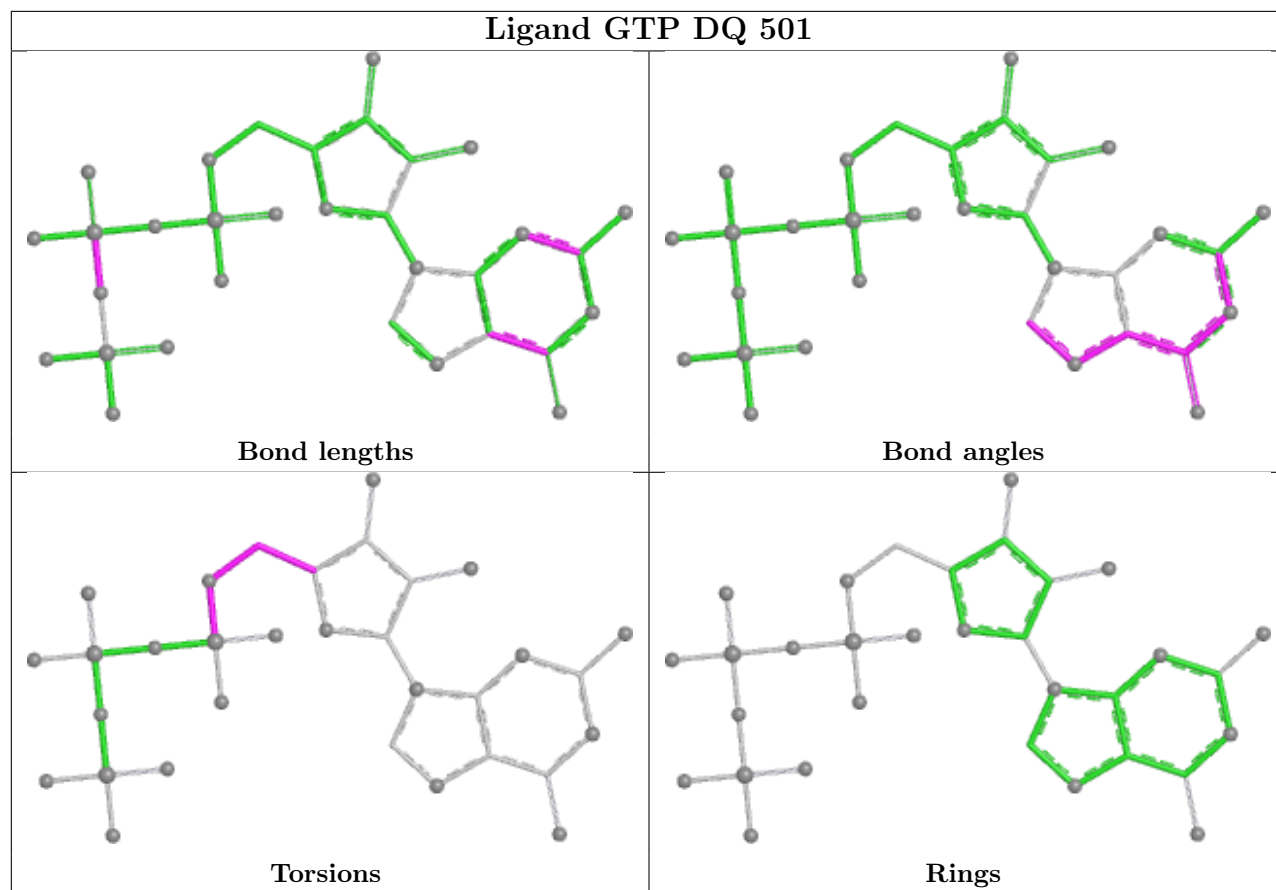


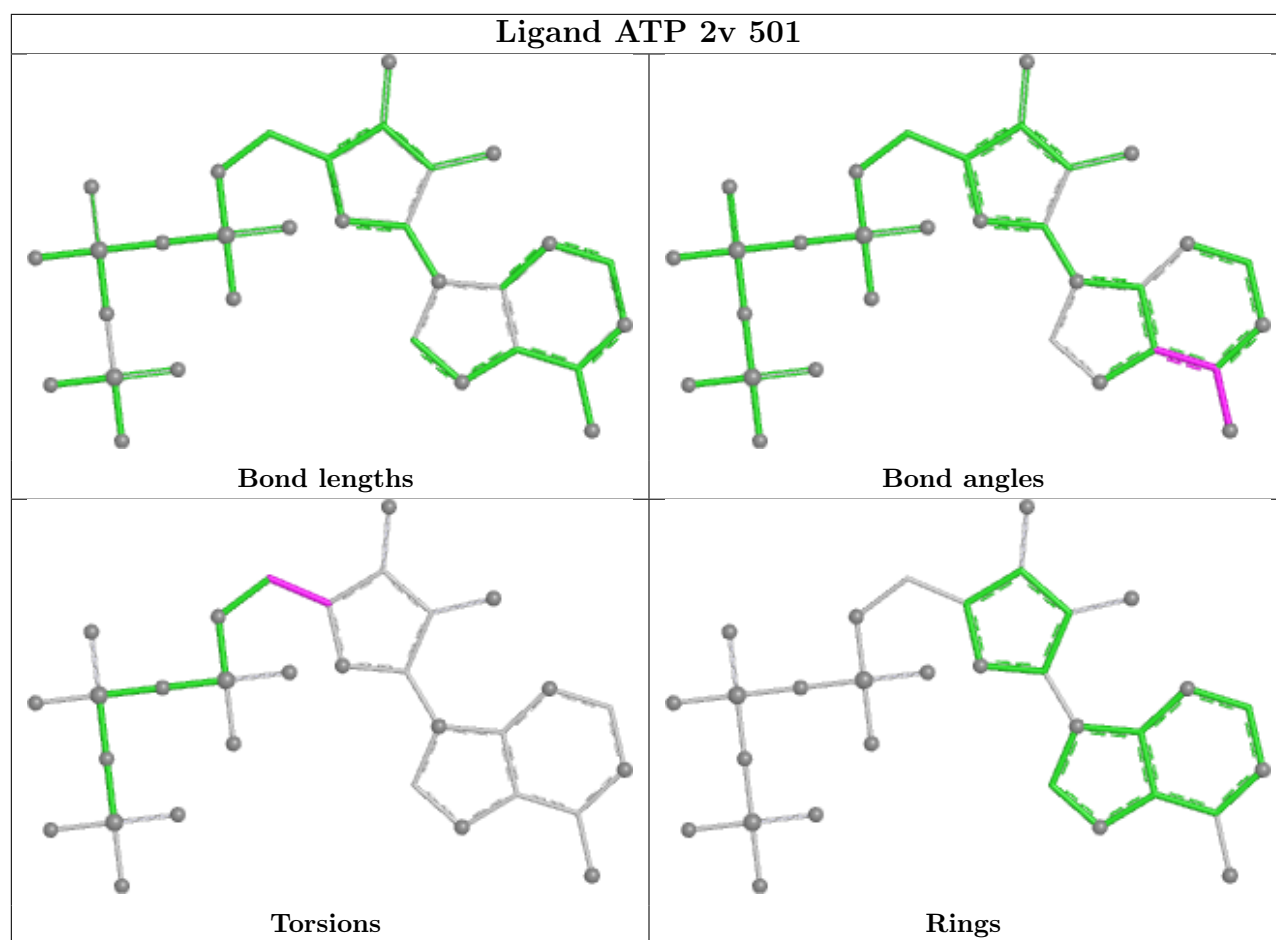
Ligand GTP IU 501

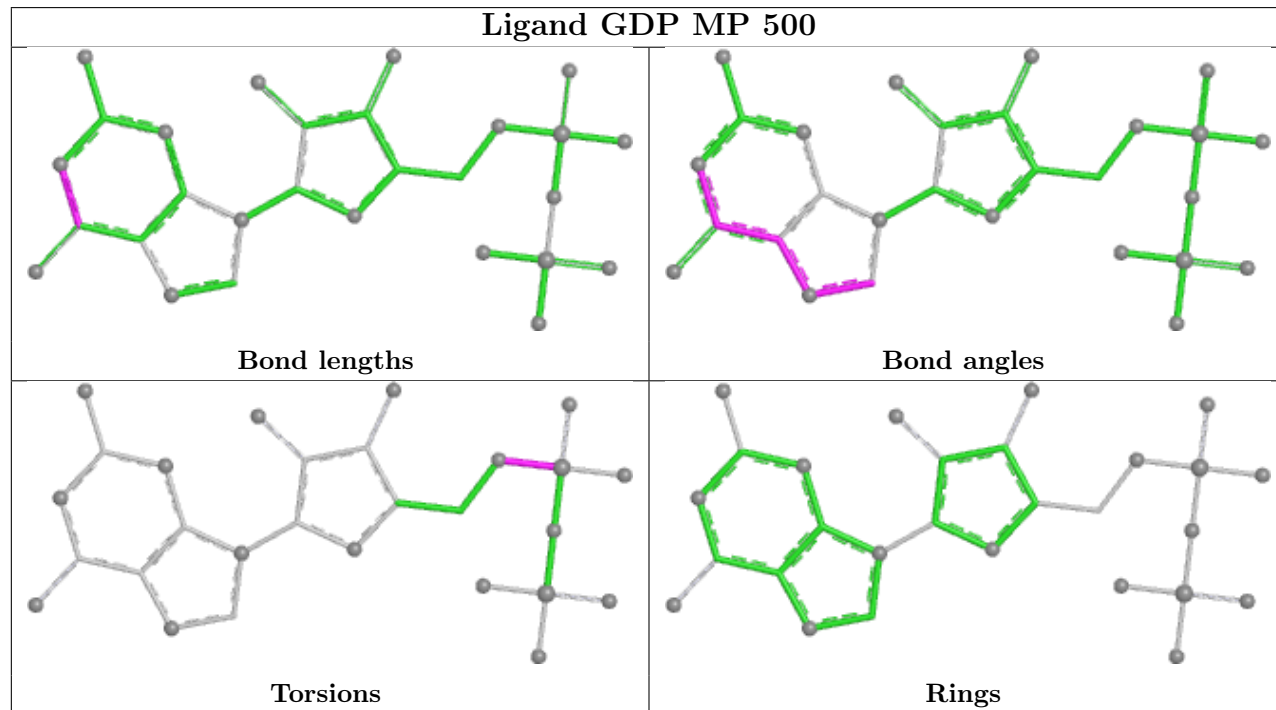
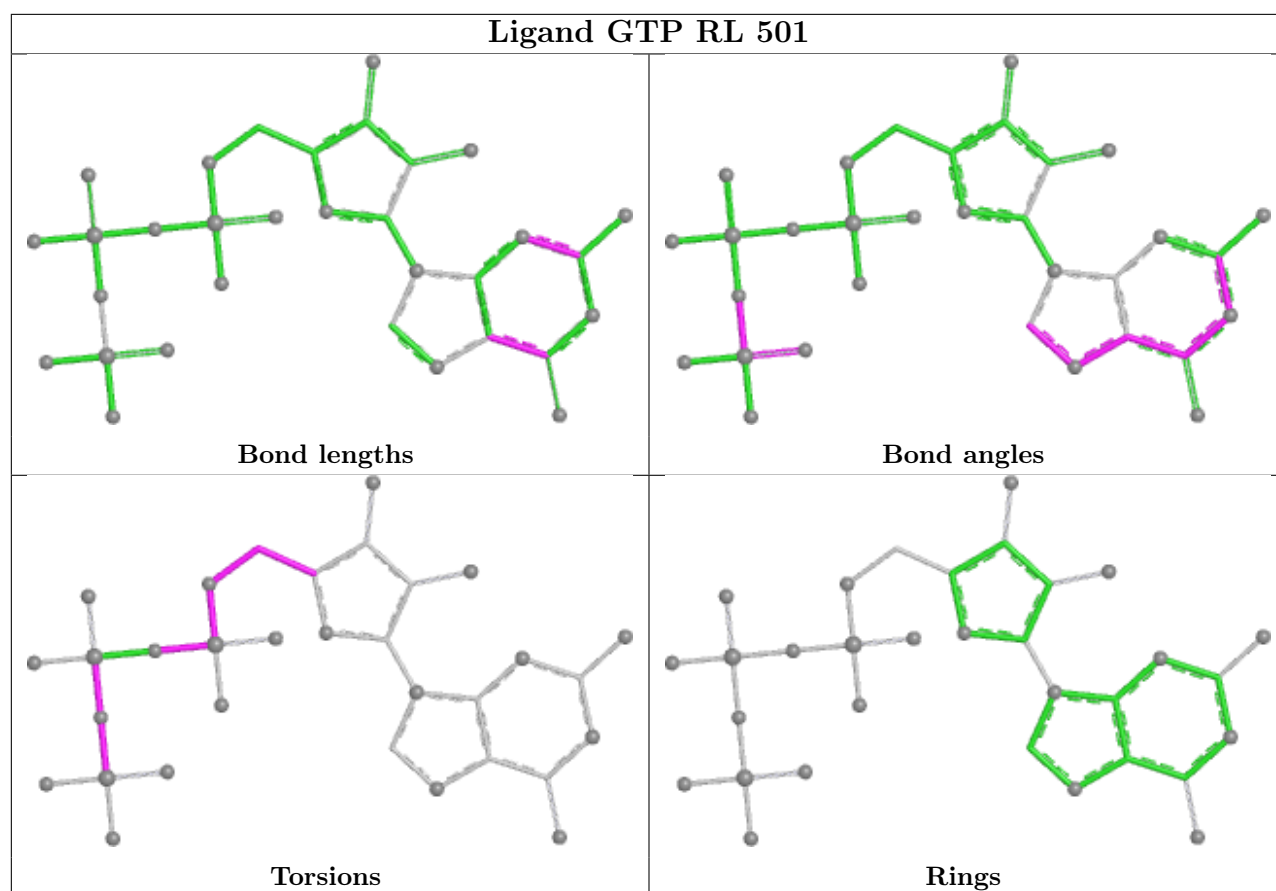


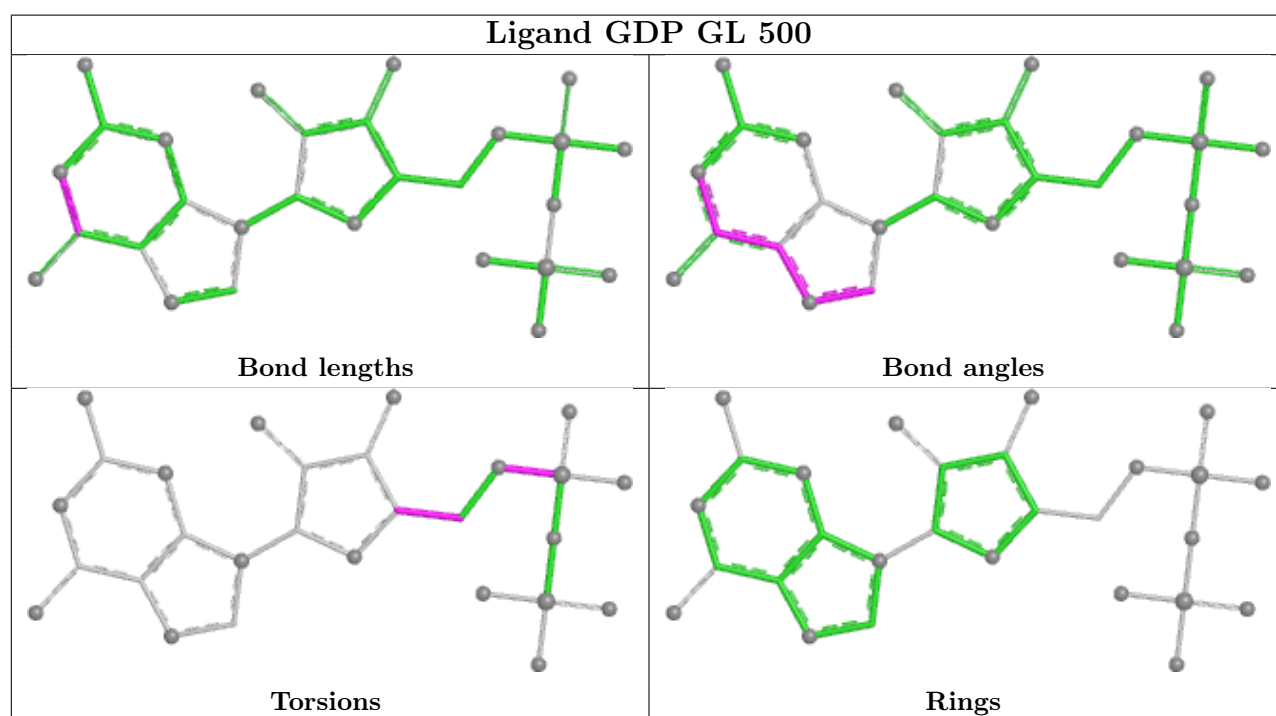
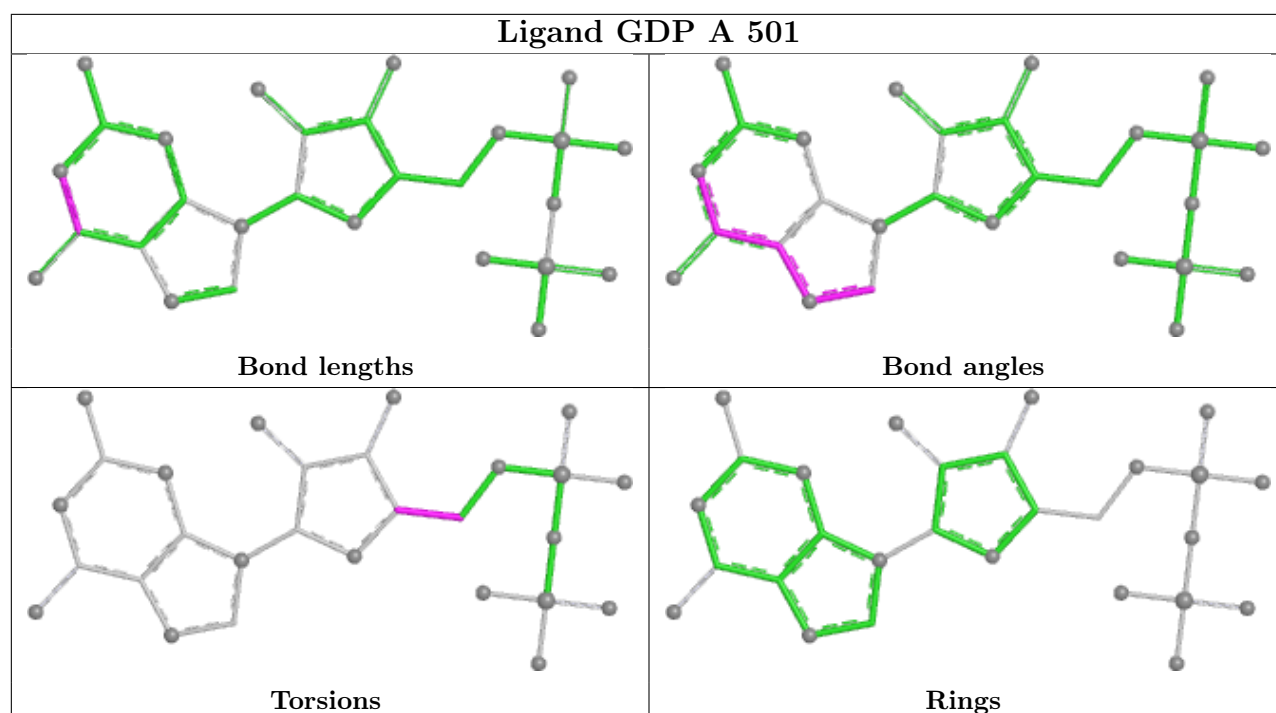
Ligand GTP FO 501

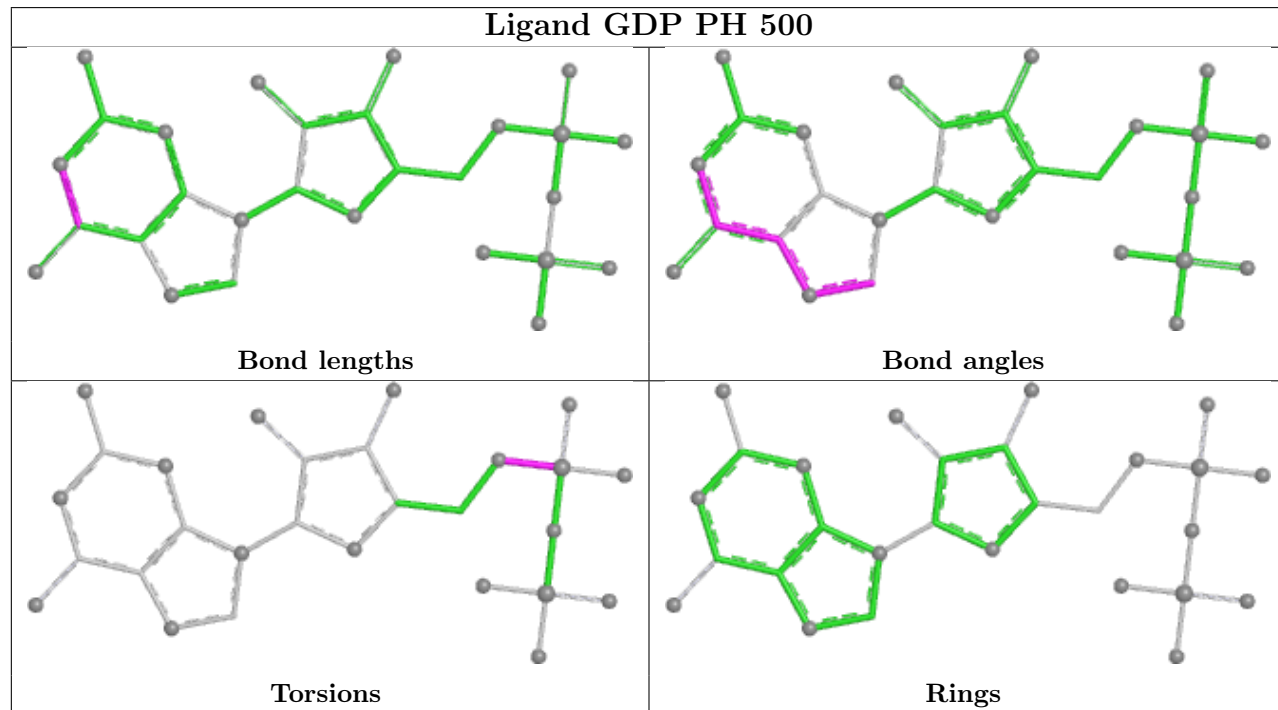
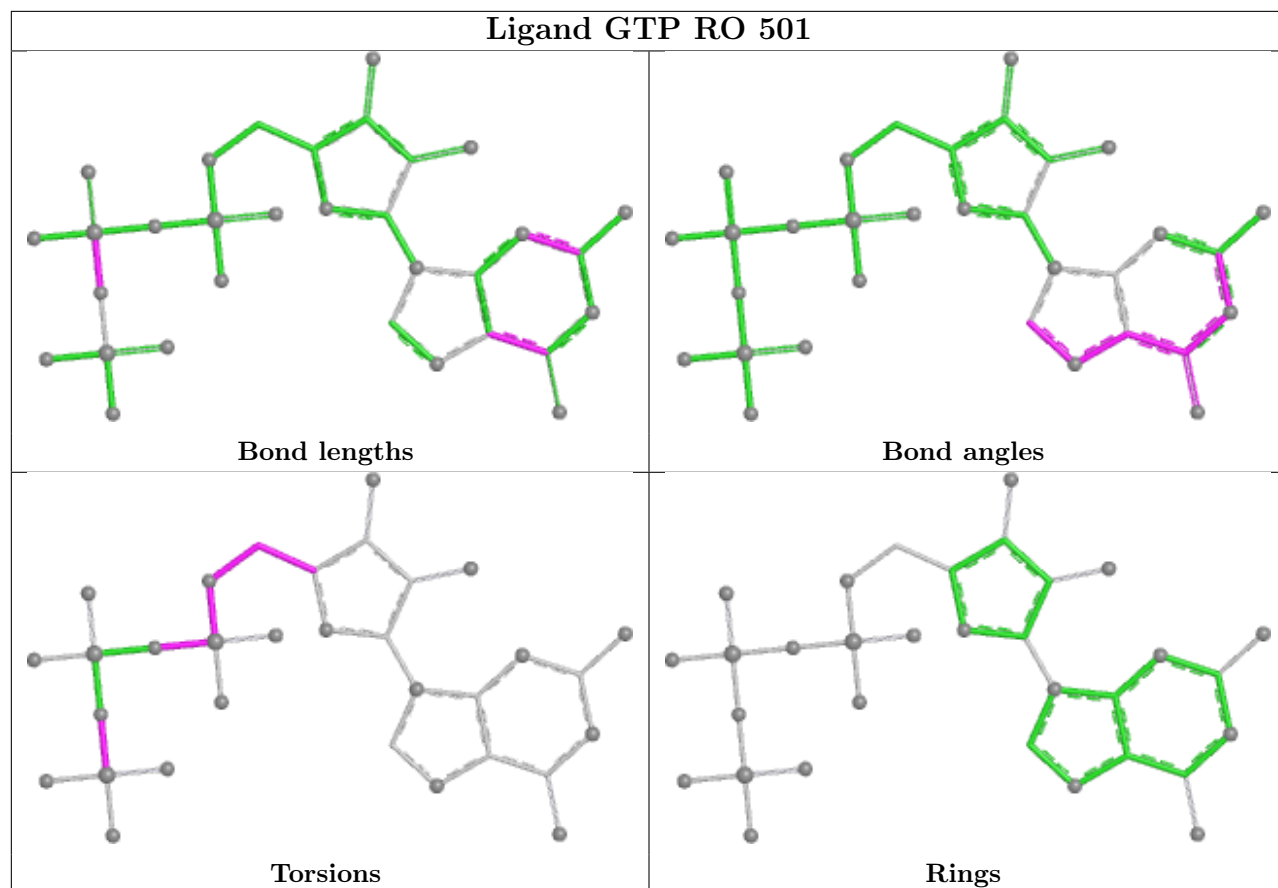


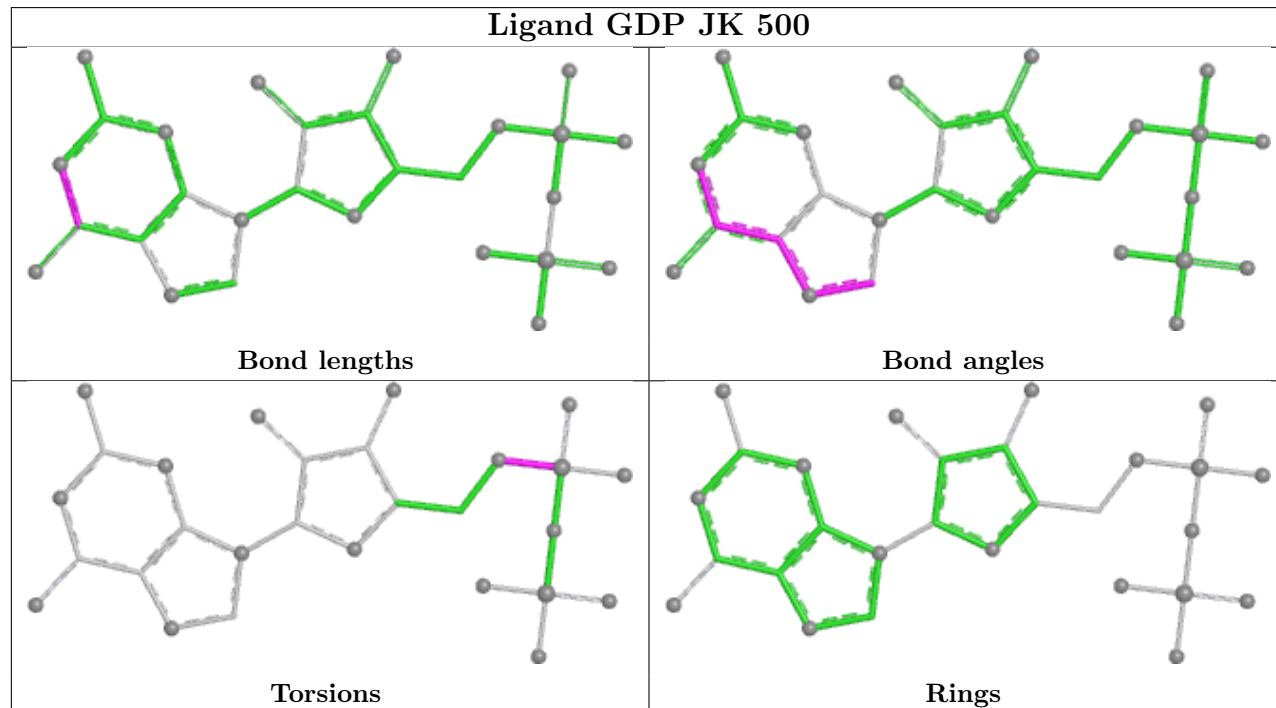
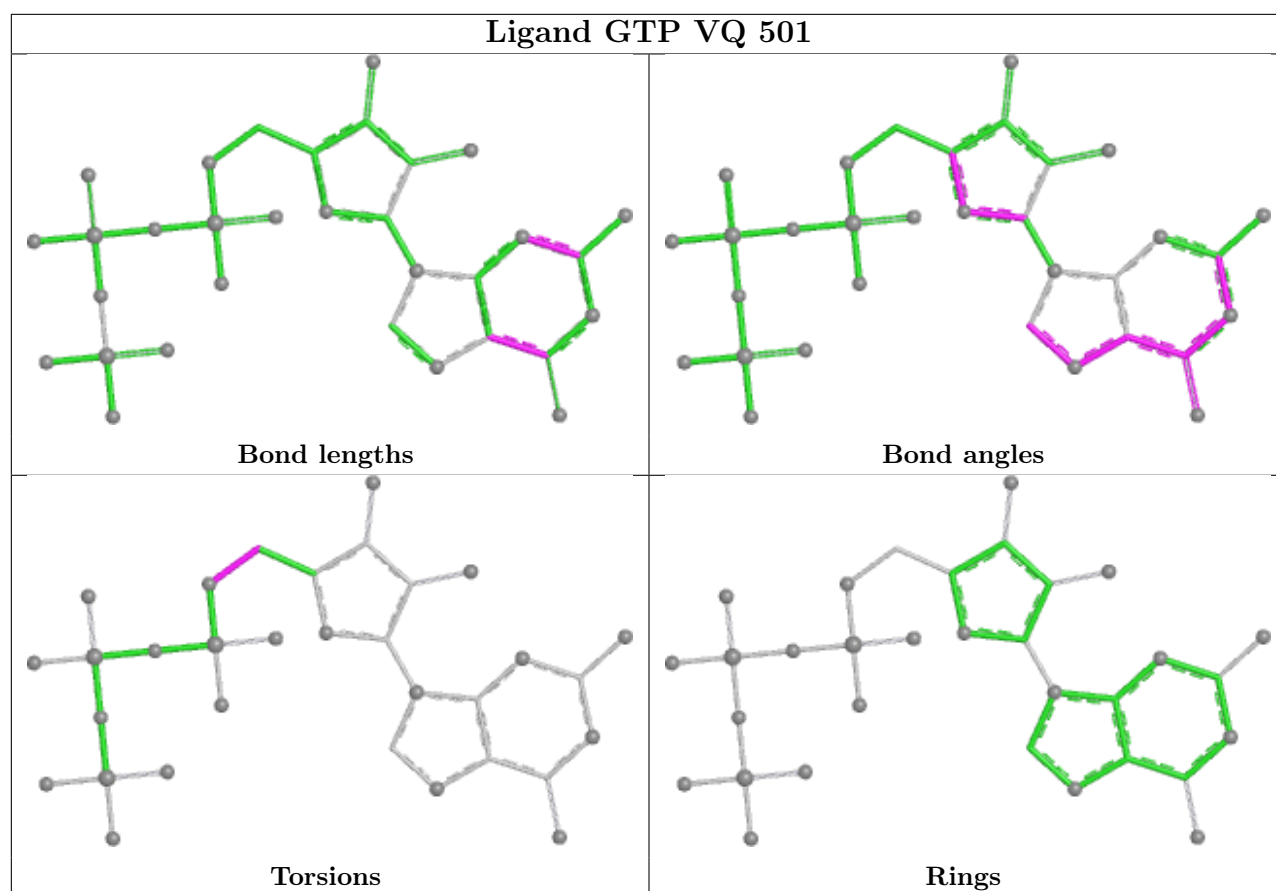


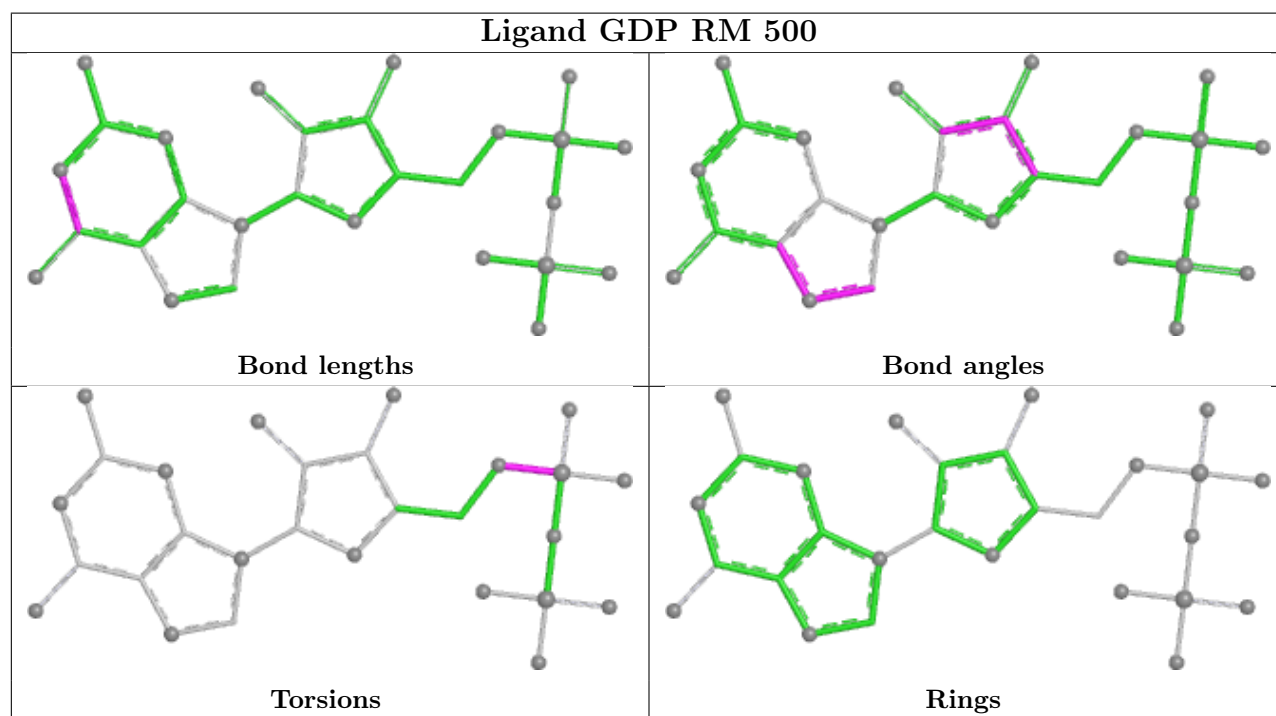
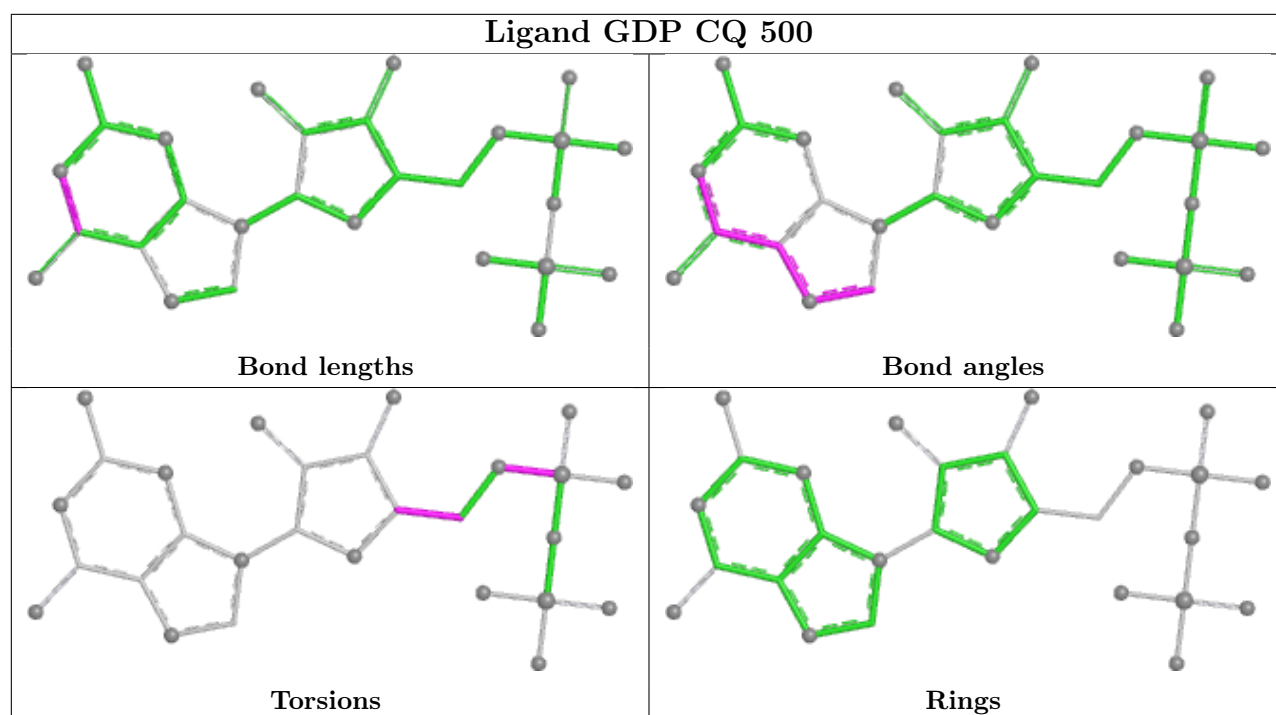


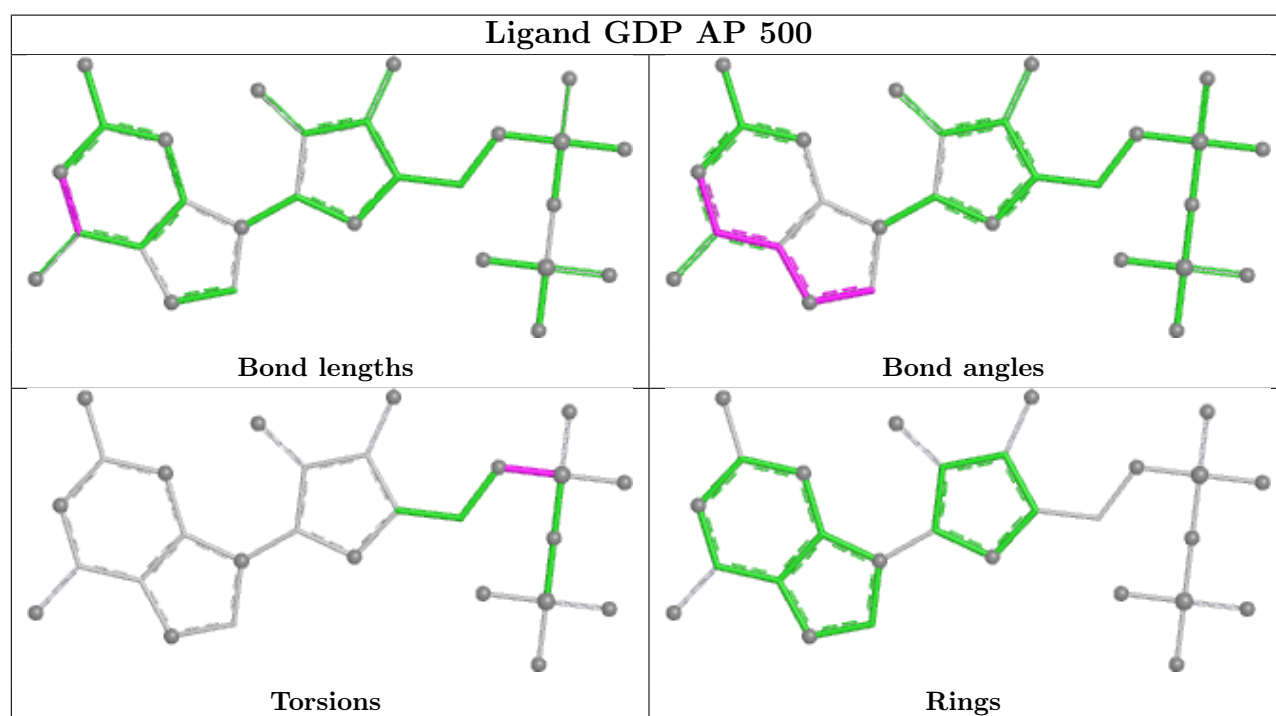
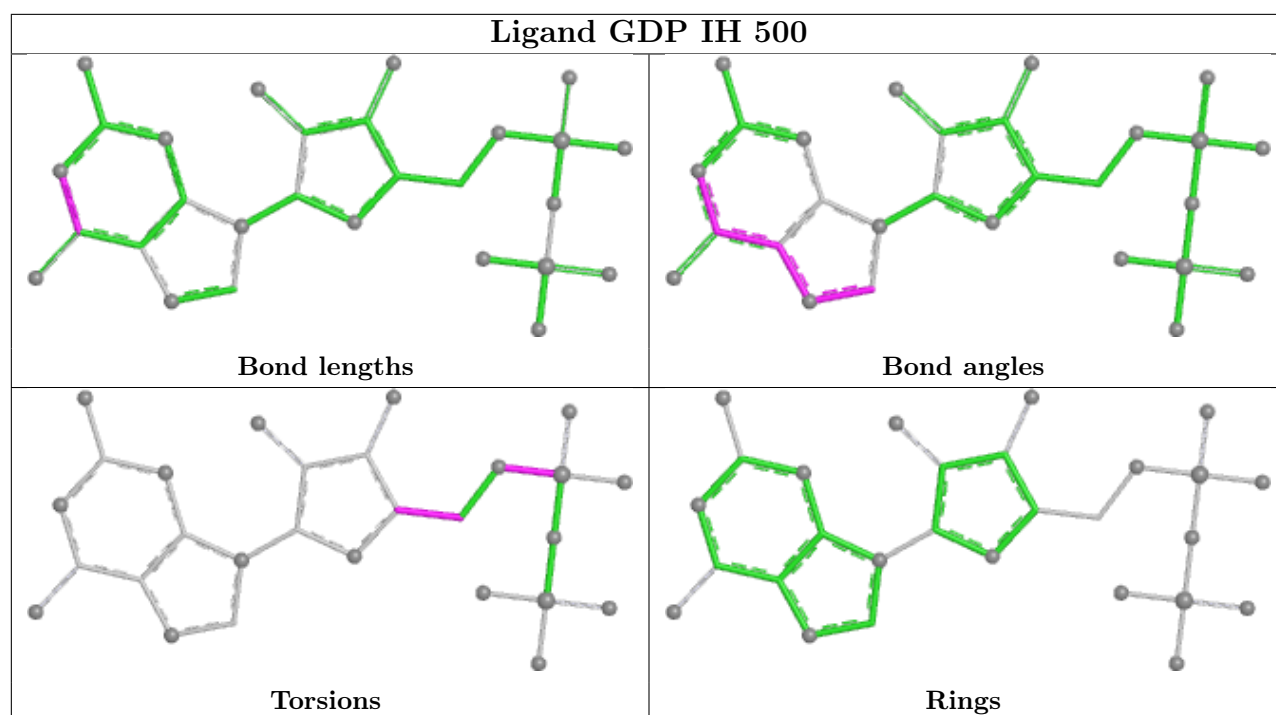


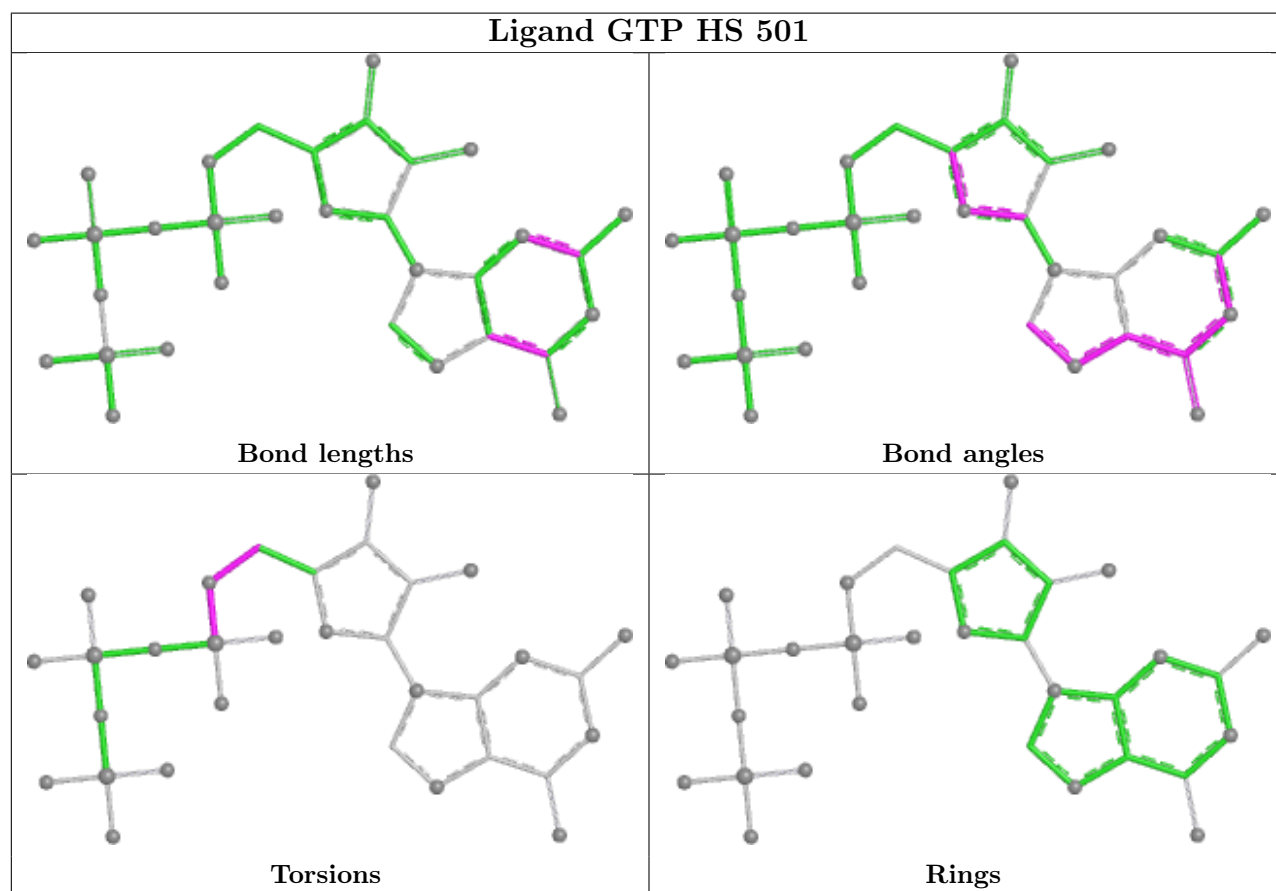
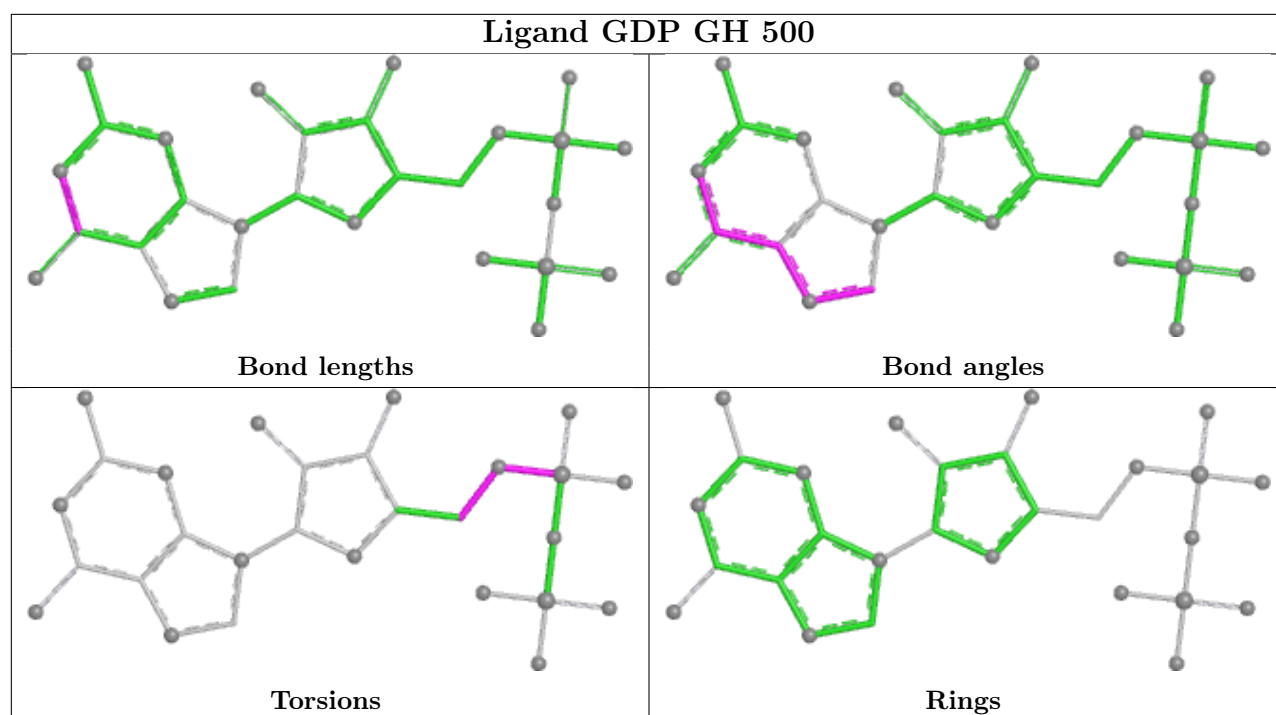


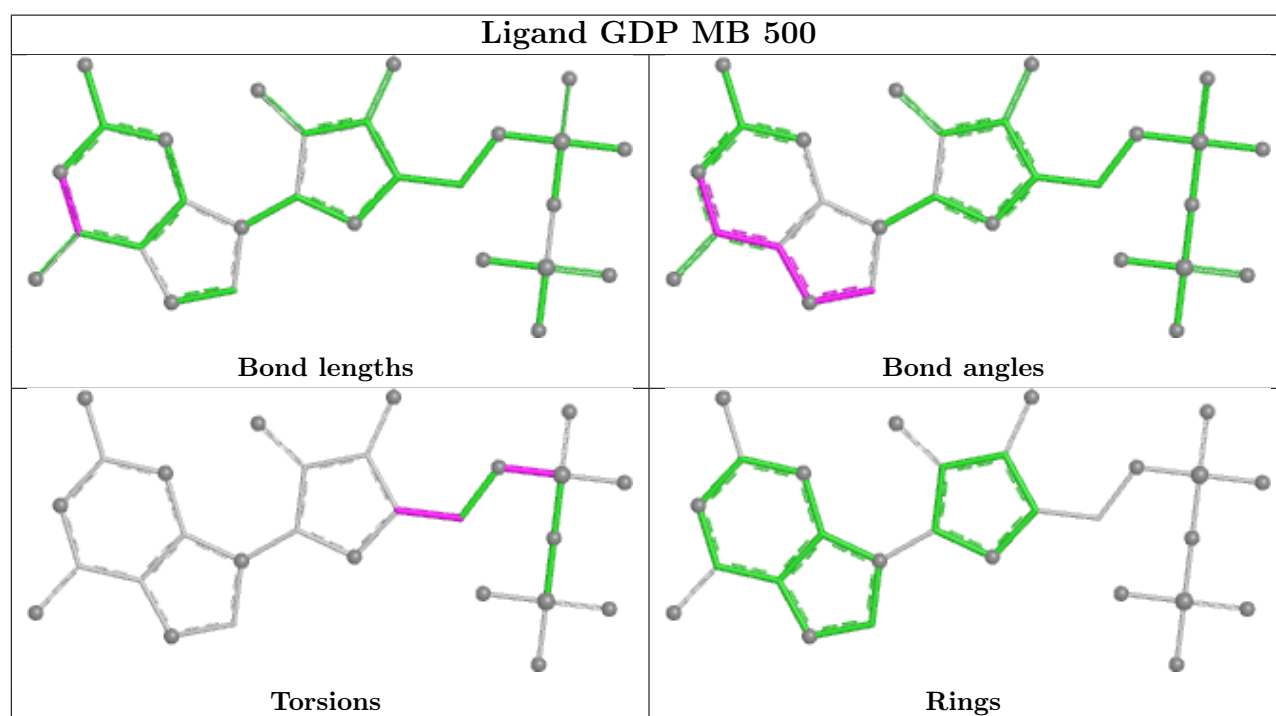
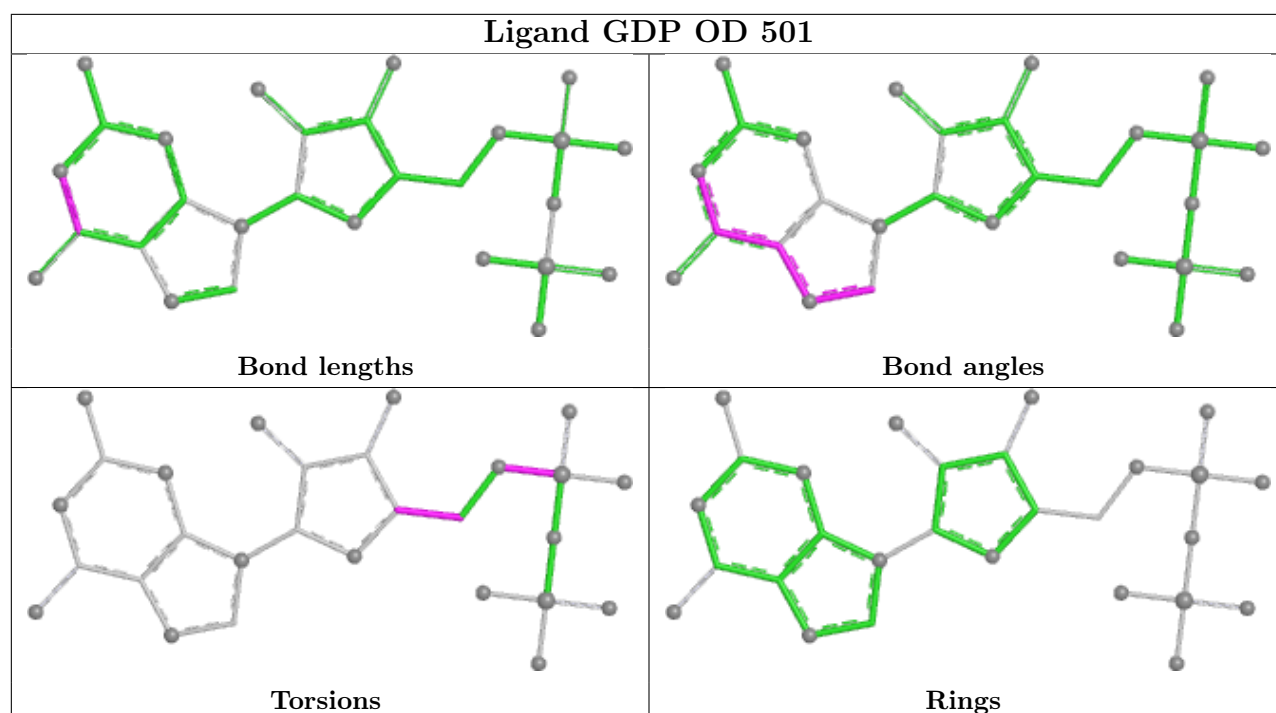


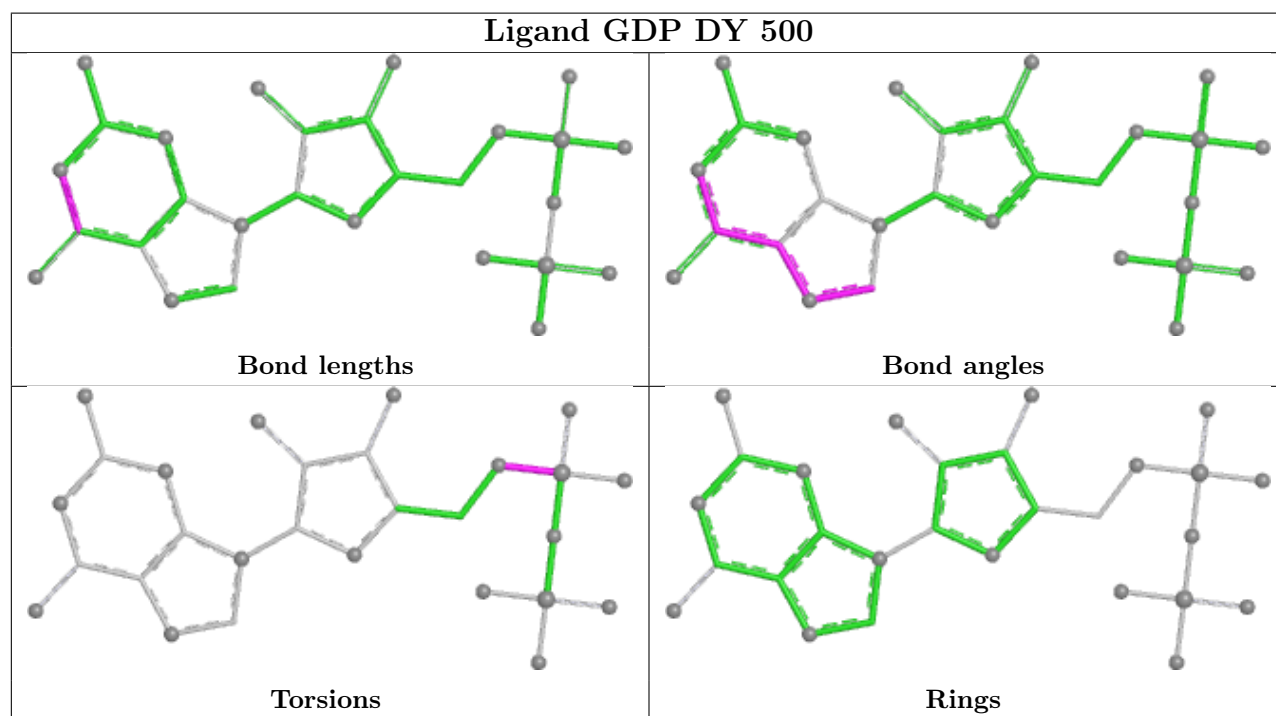
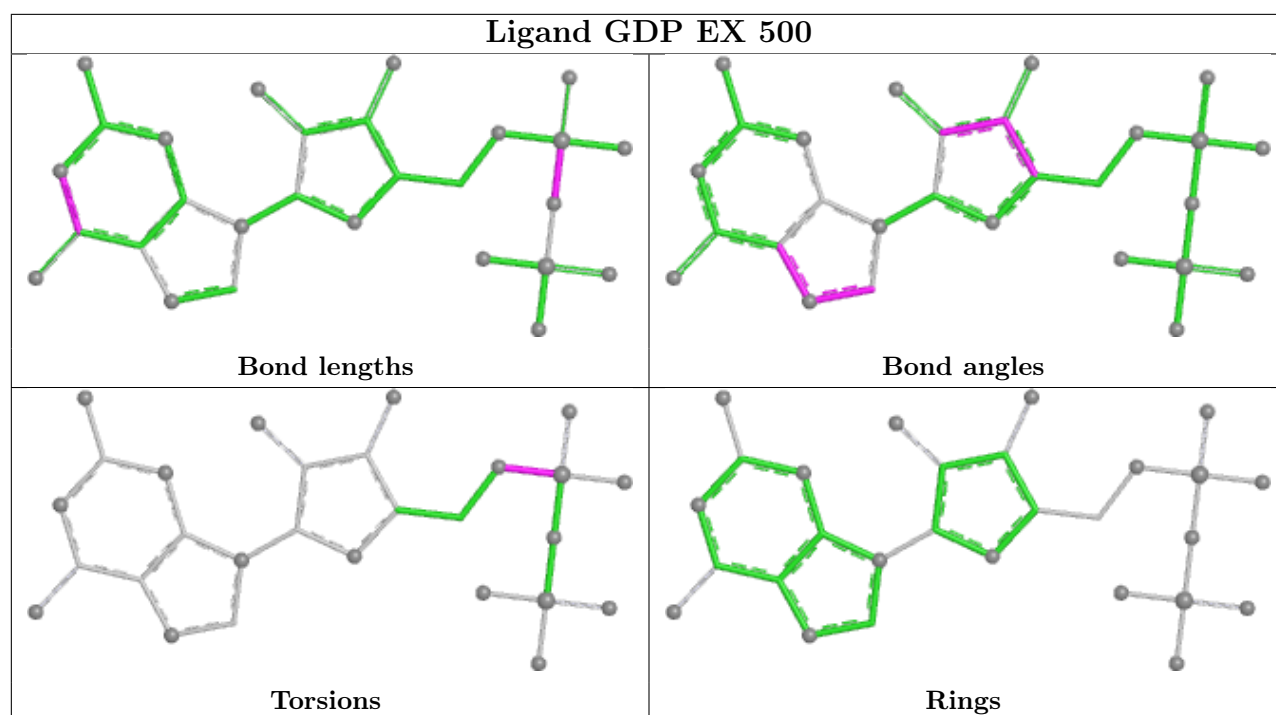


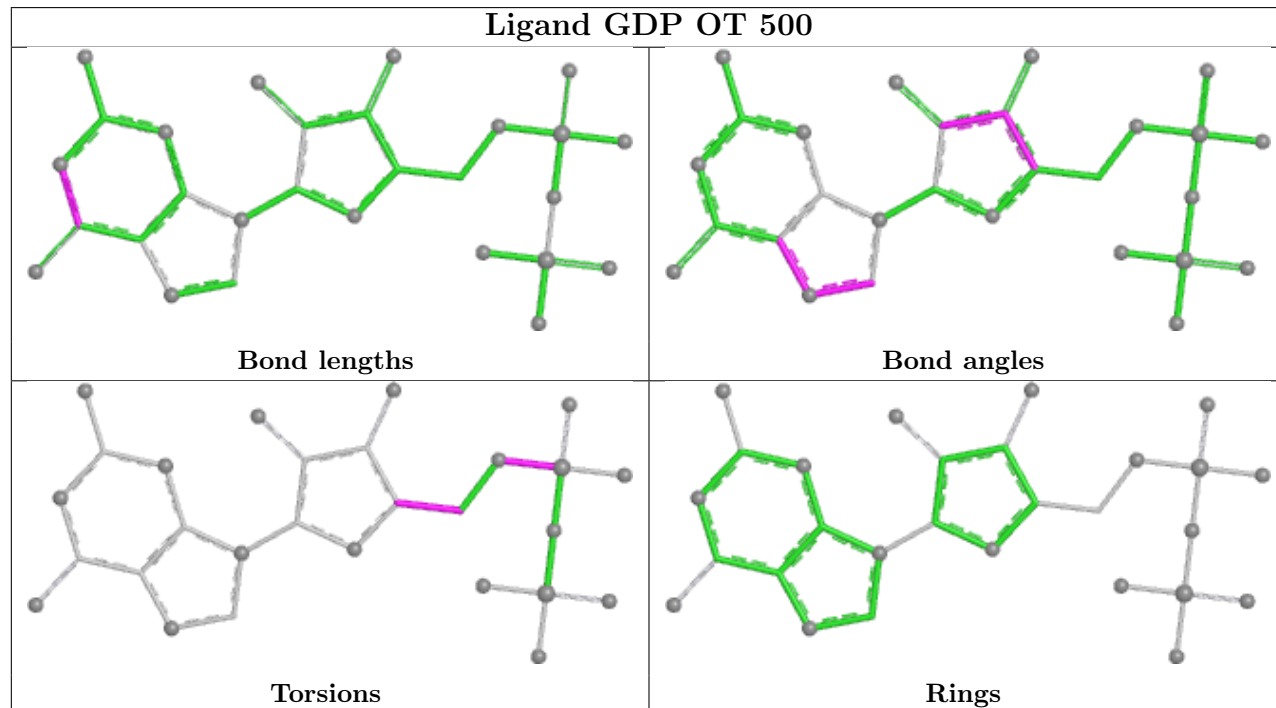
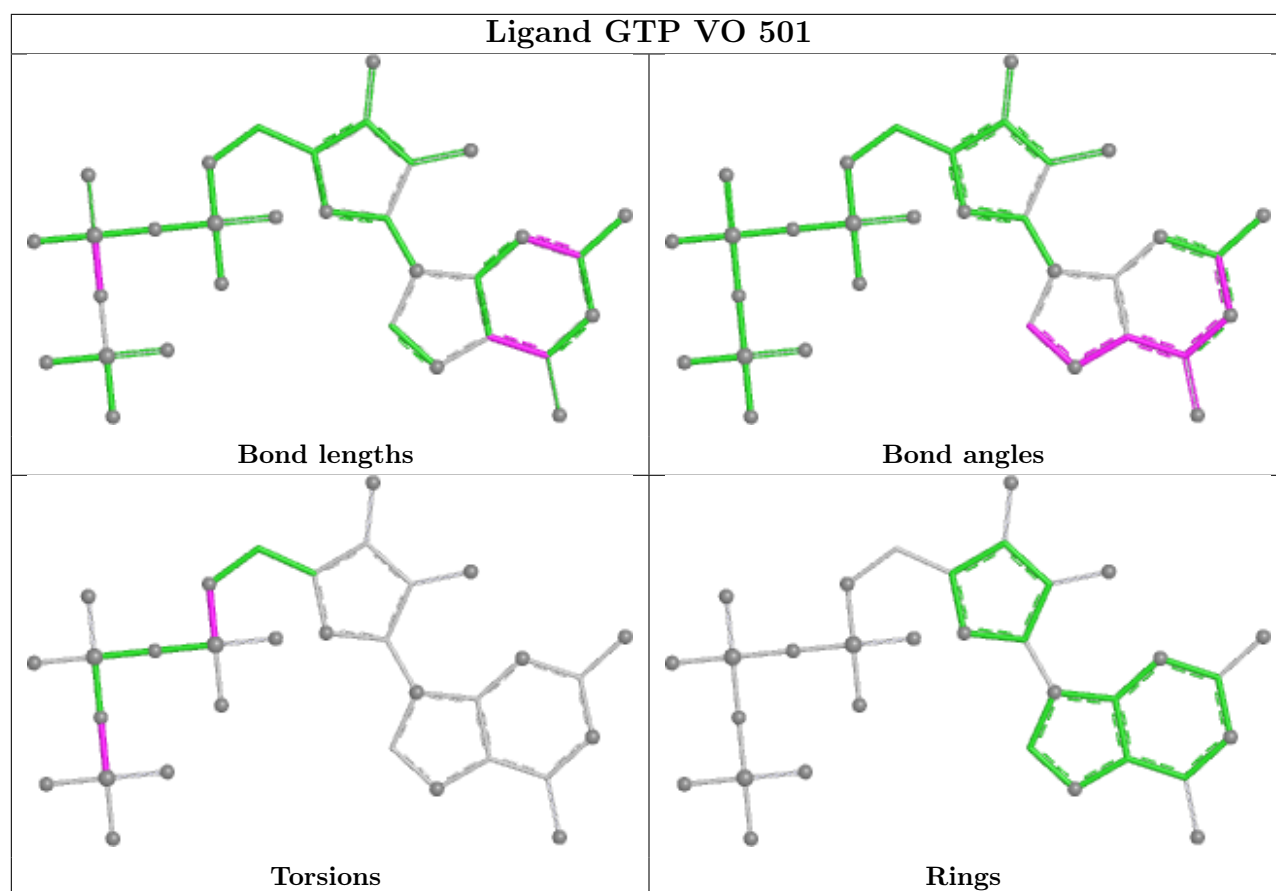


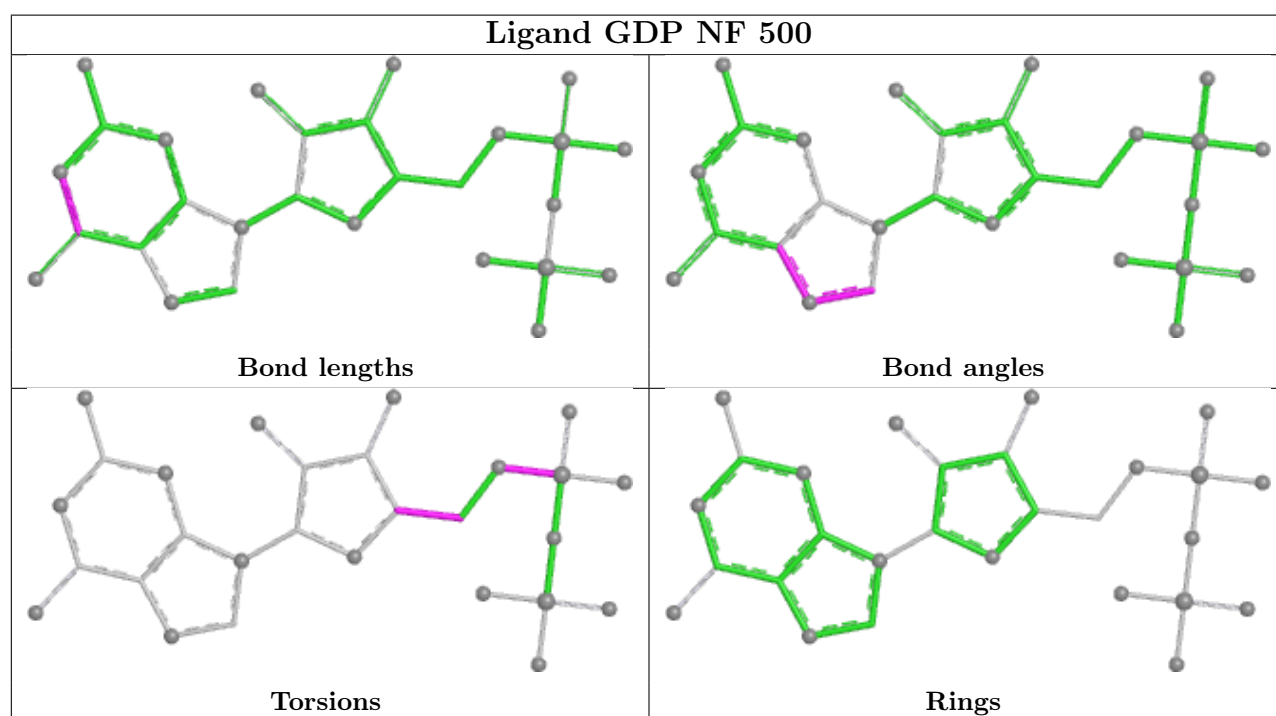
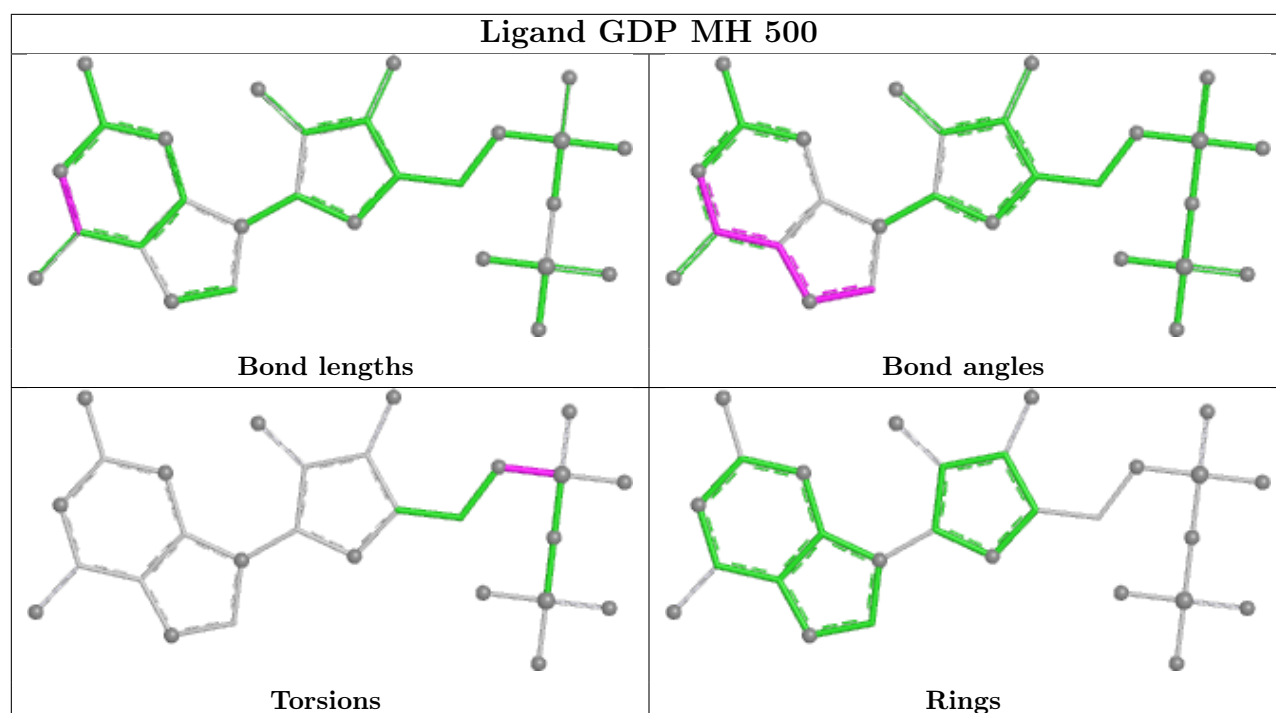


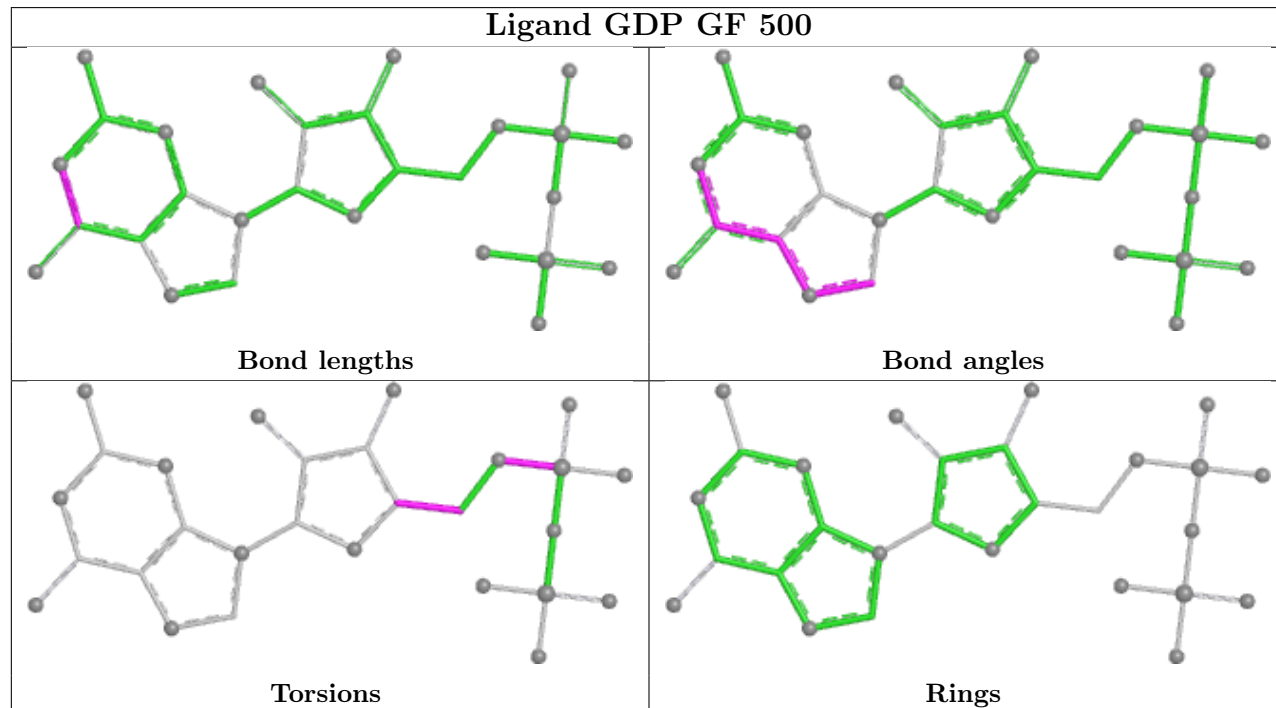
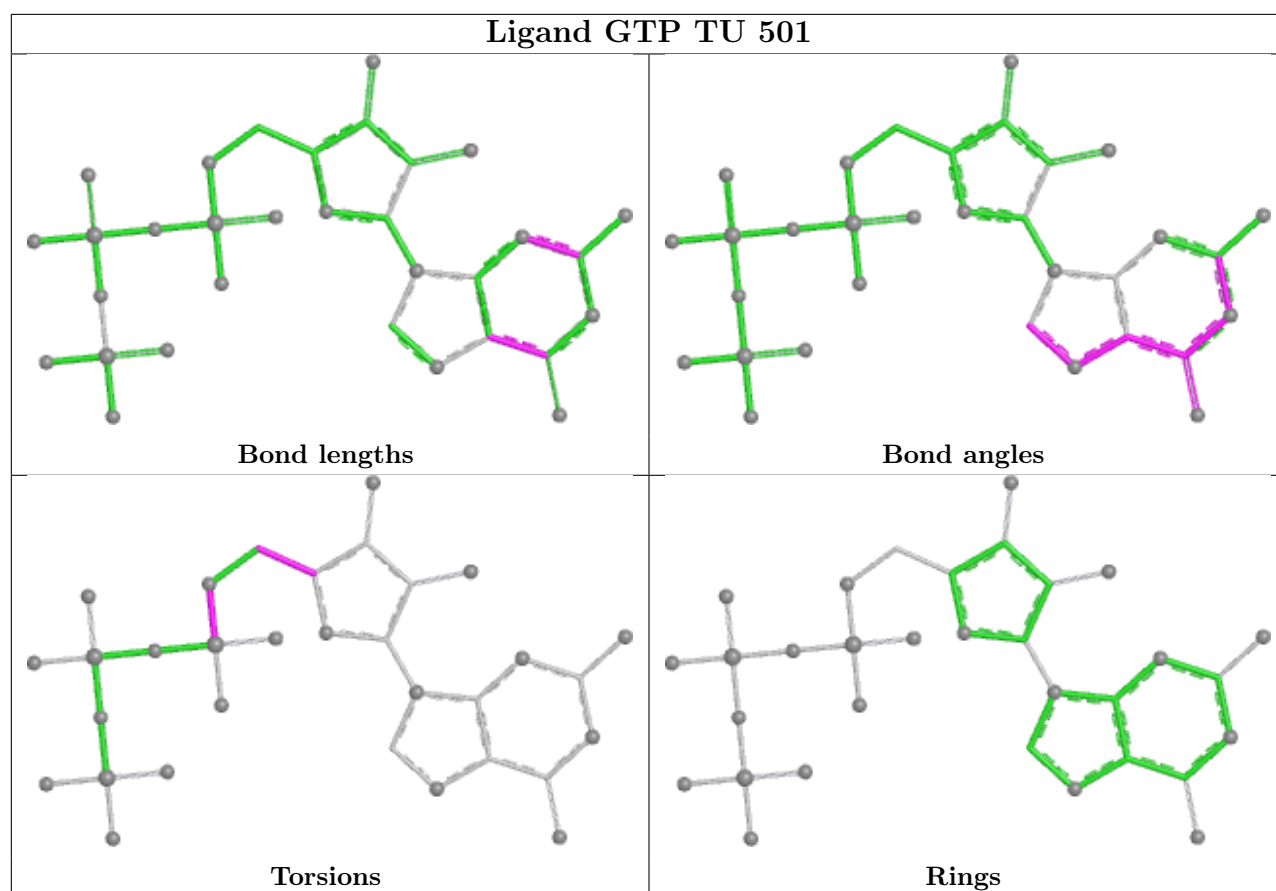


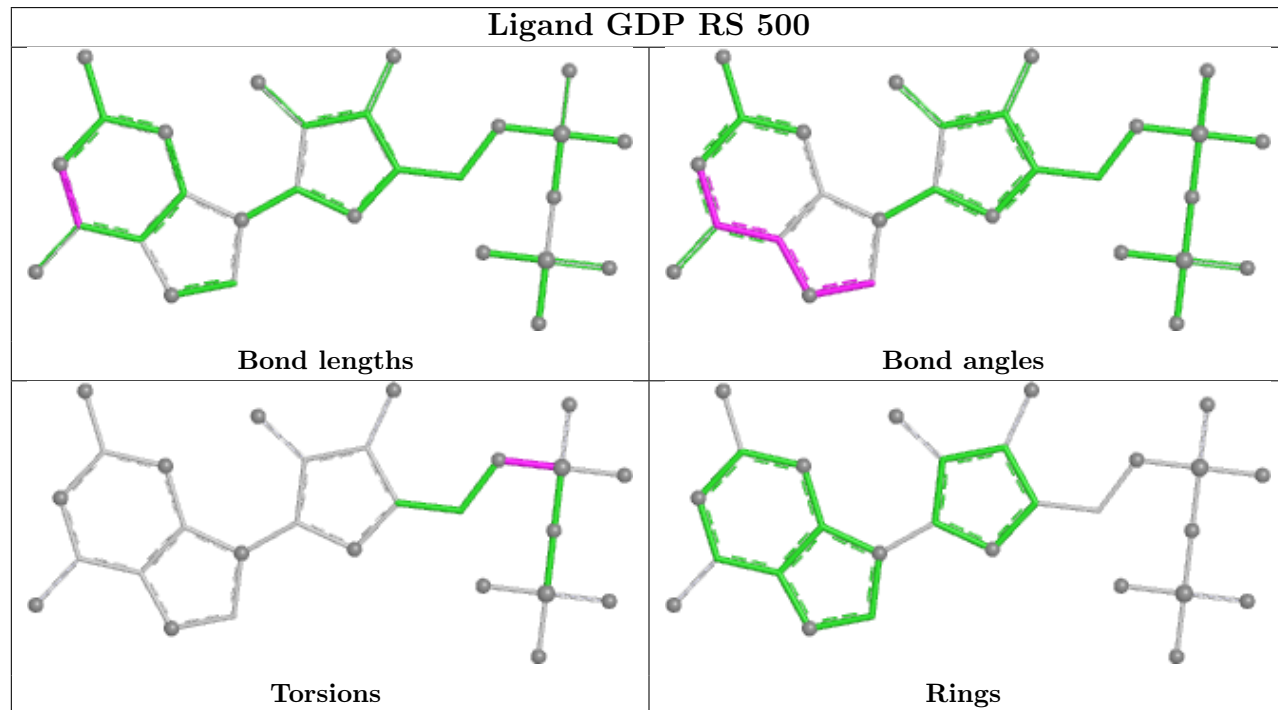
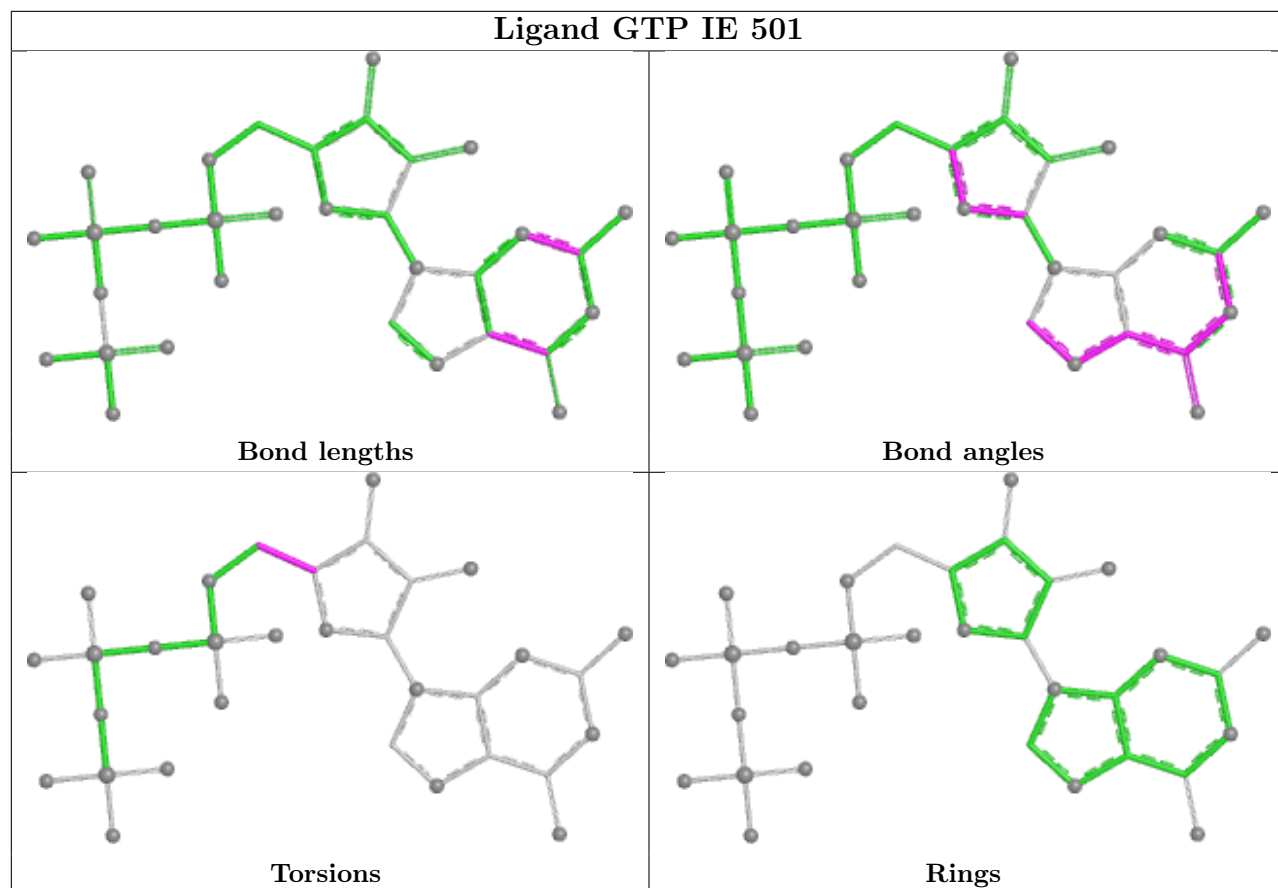




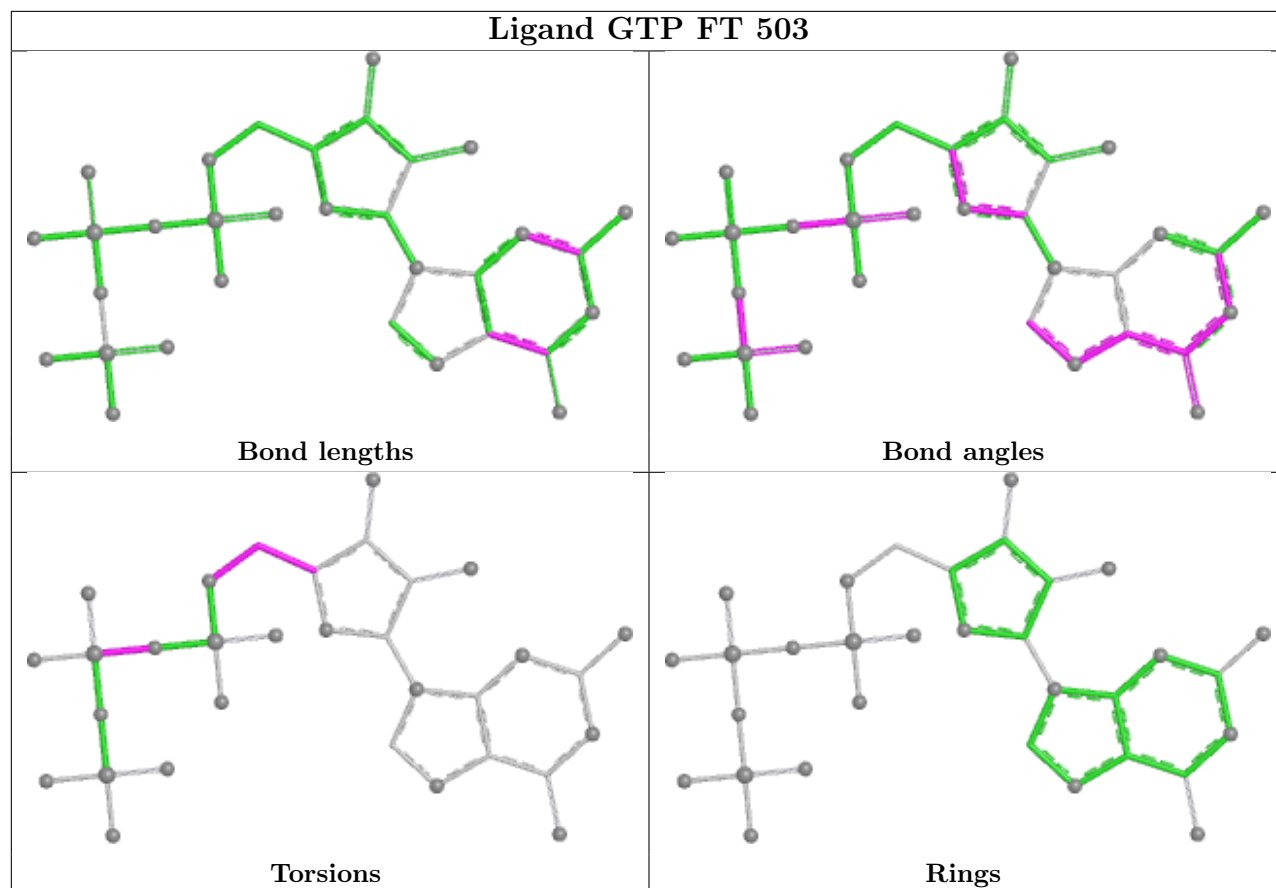




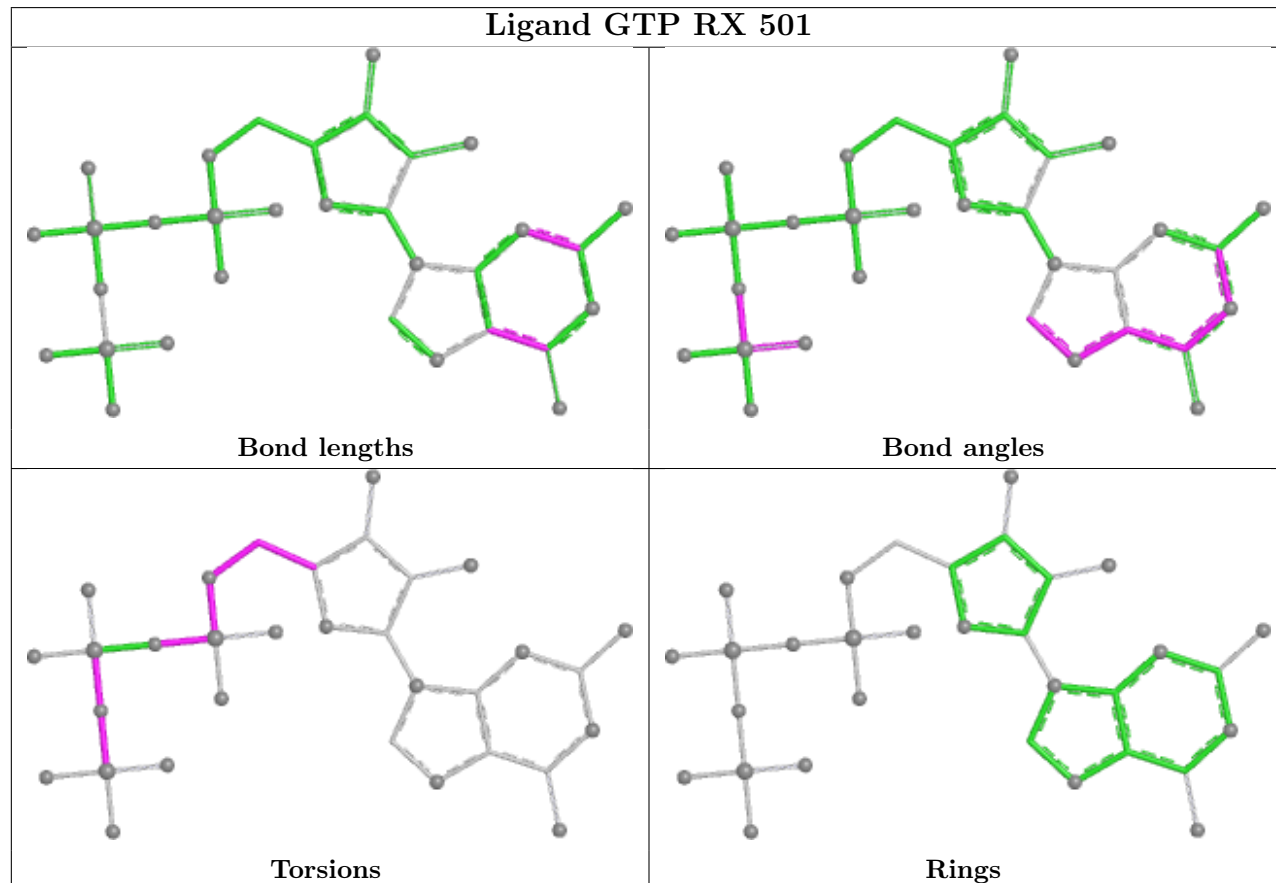


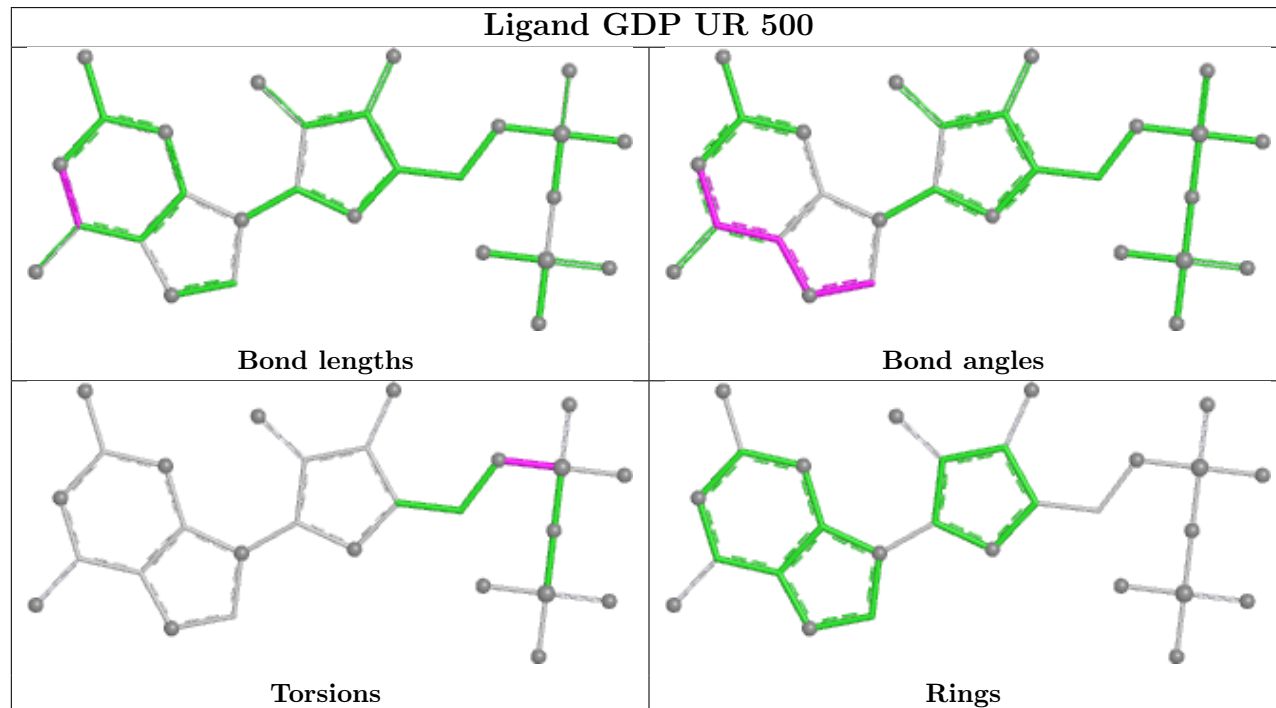
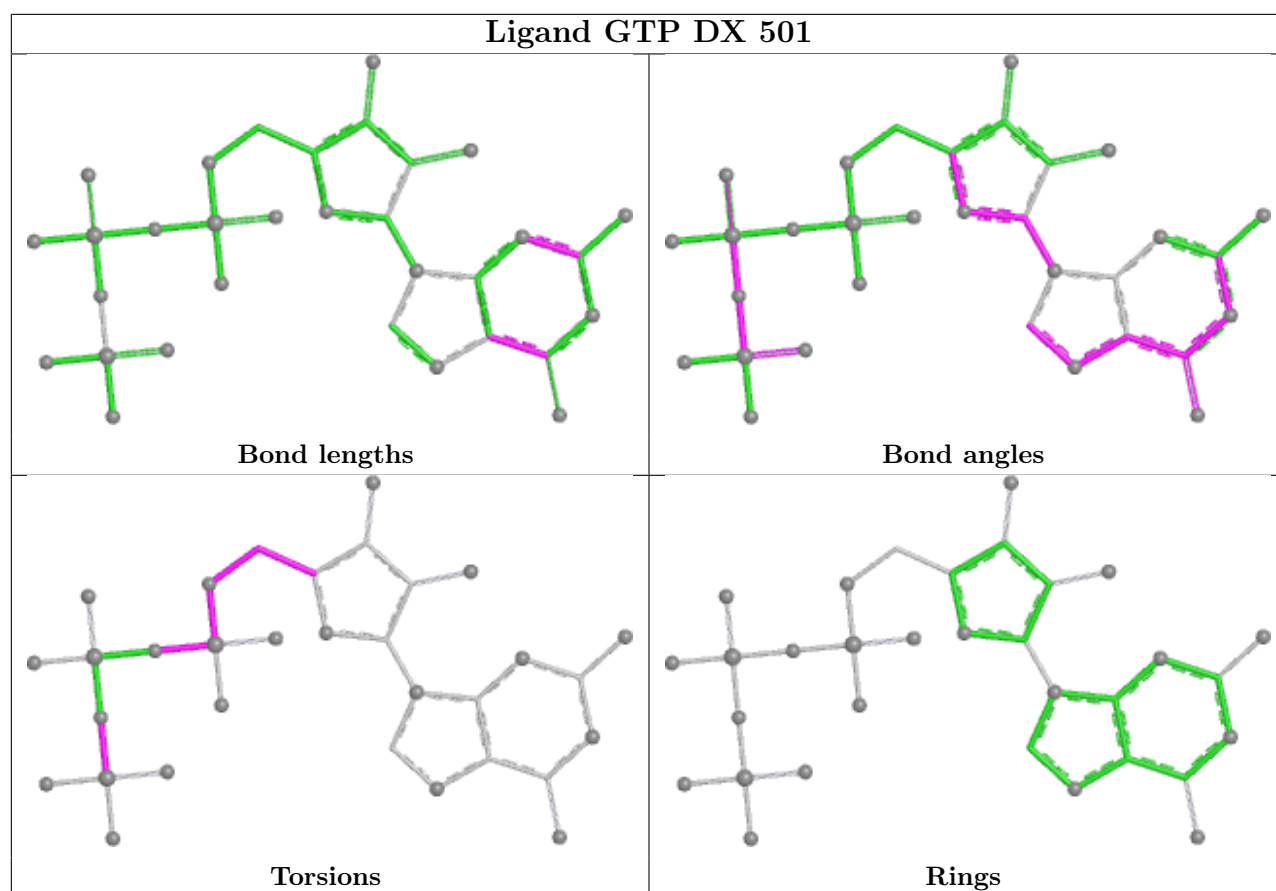


Ligand GTP FT 503

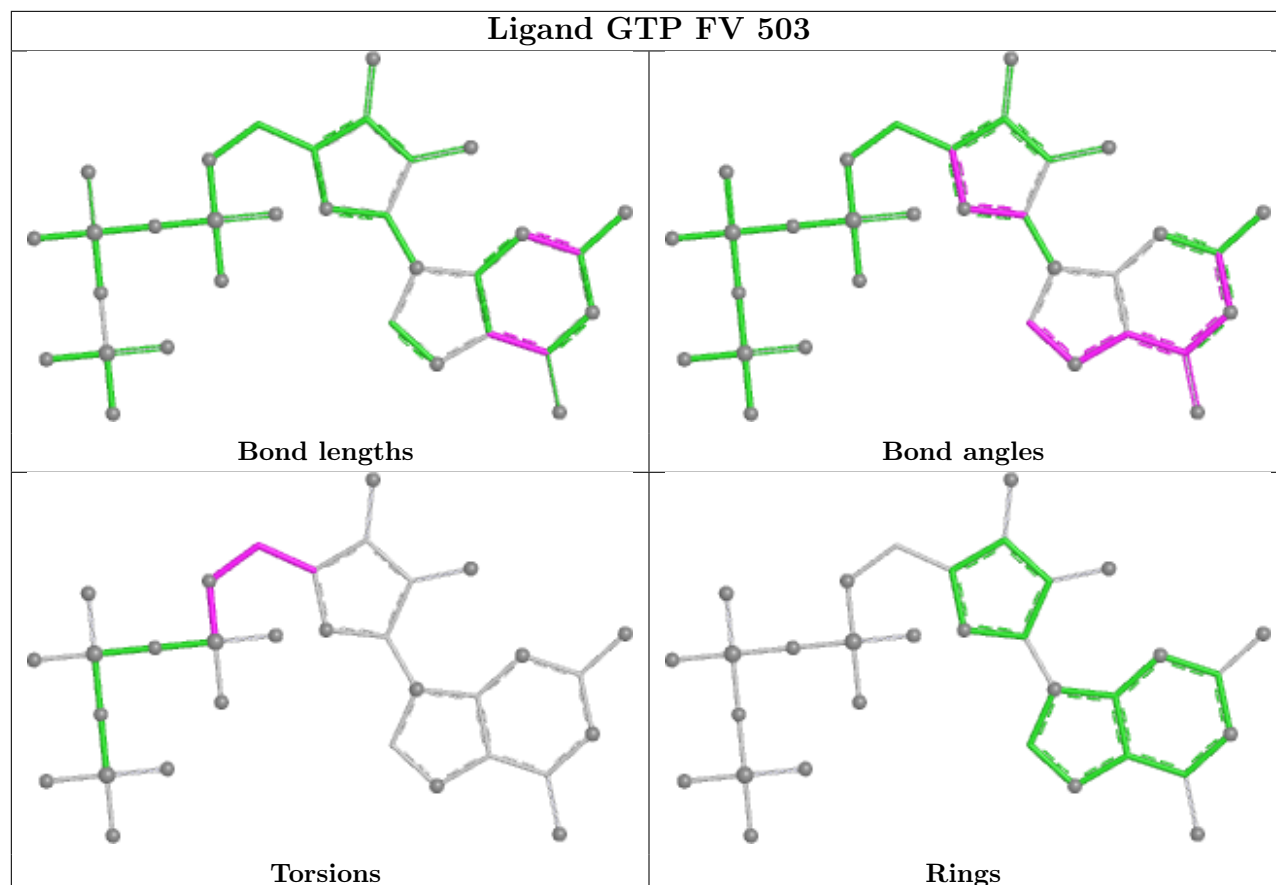


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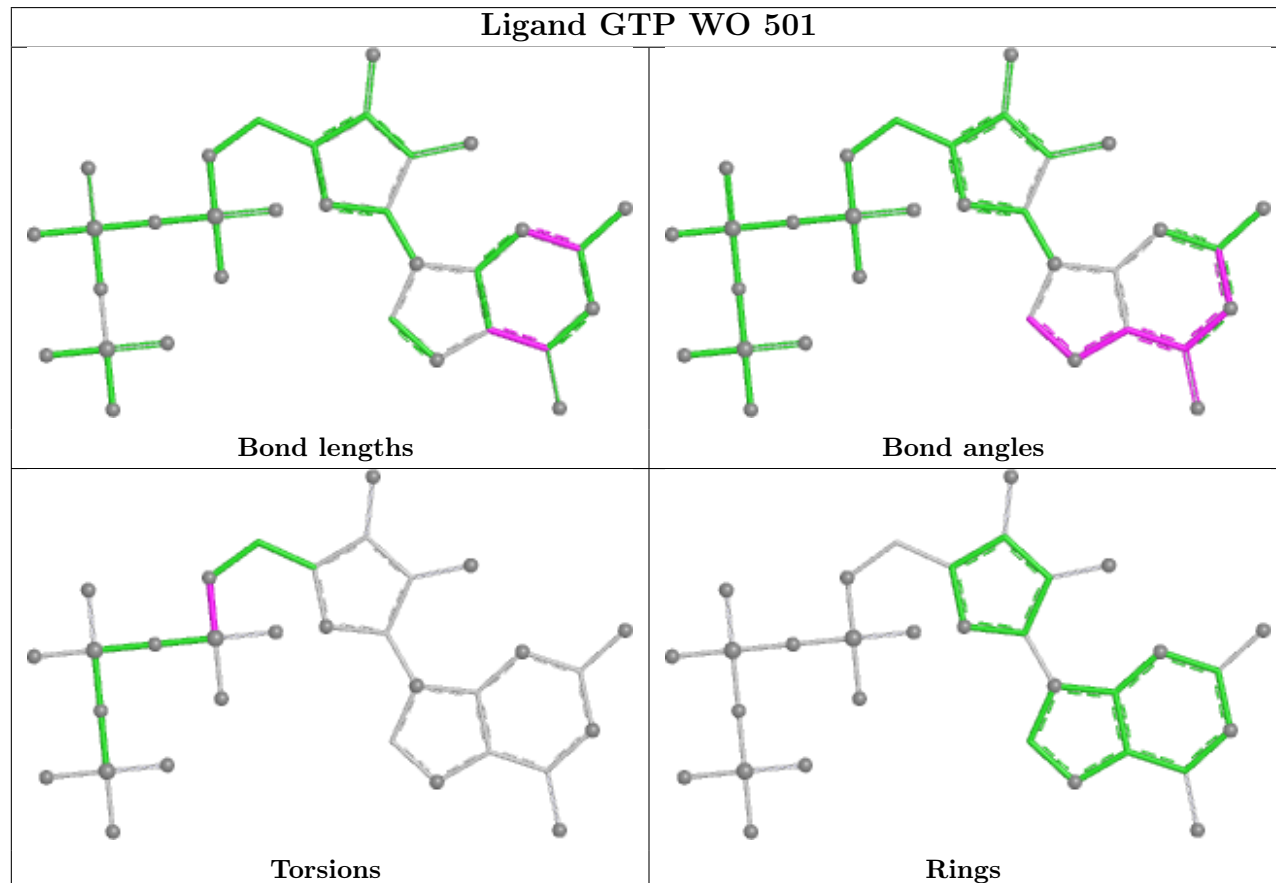


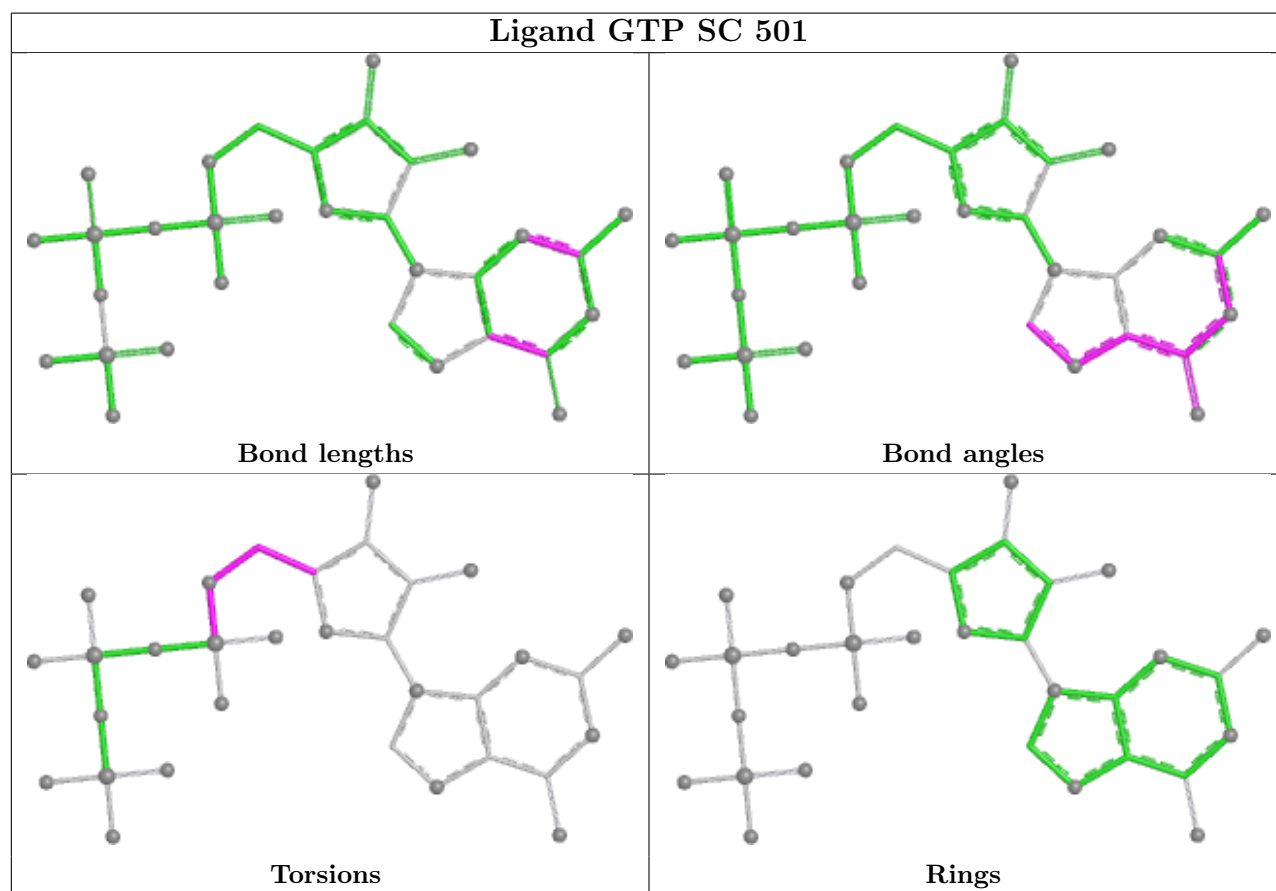
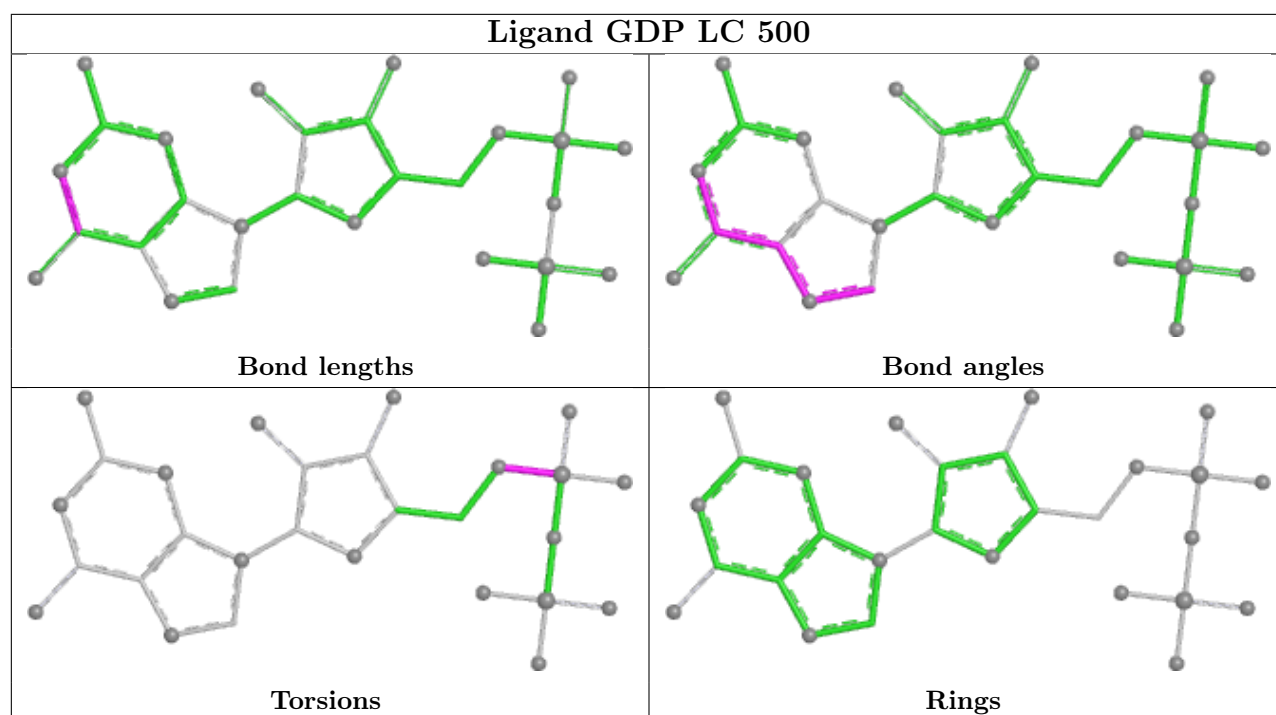


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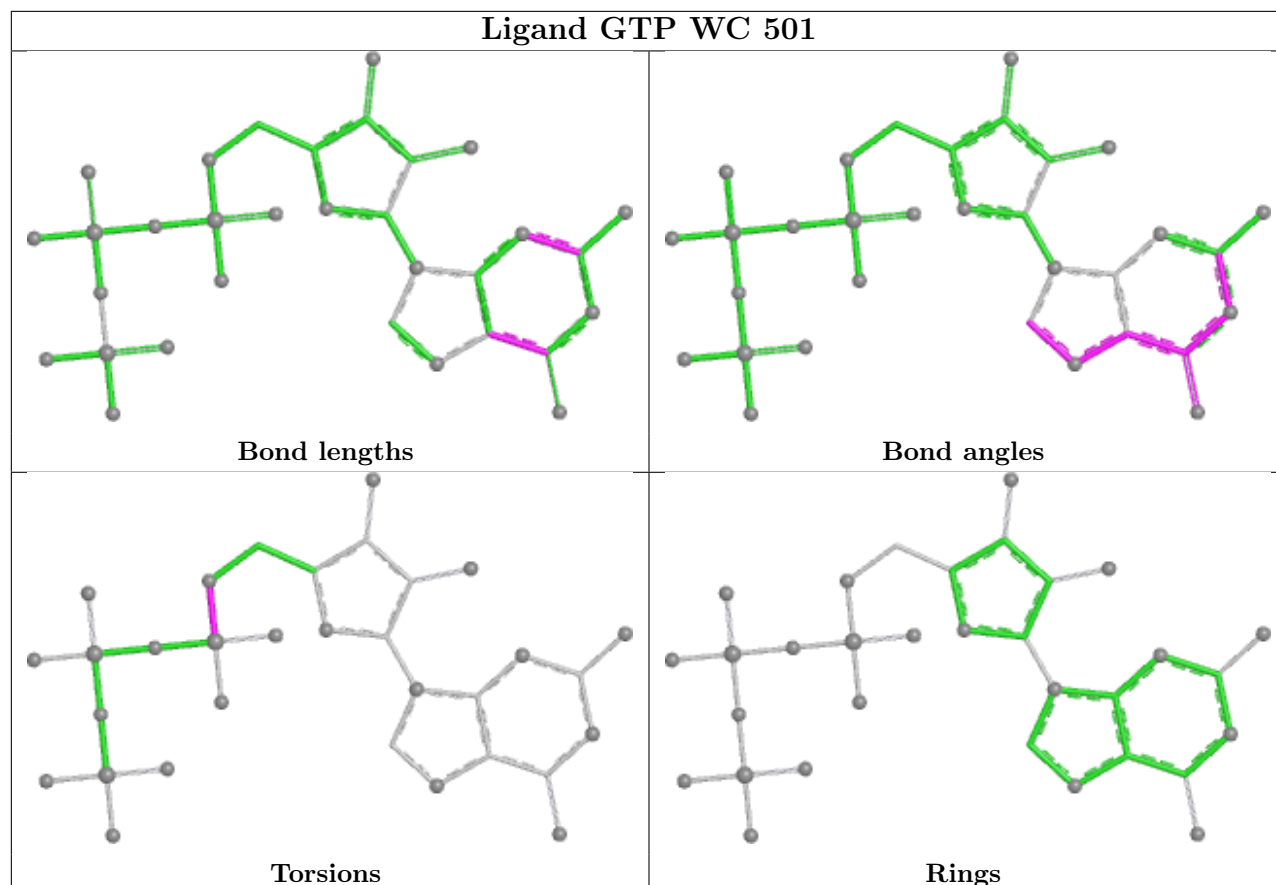


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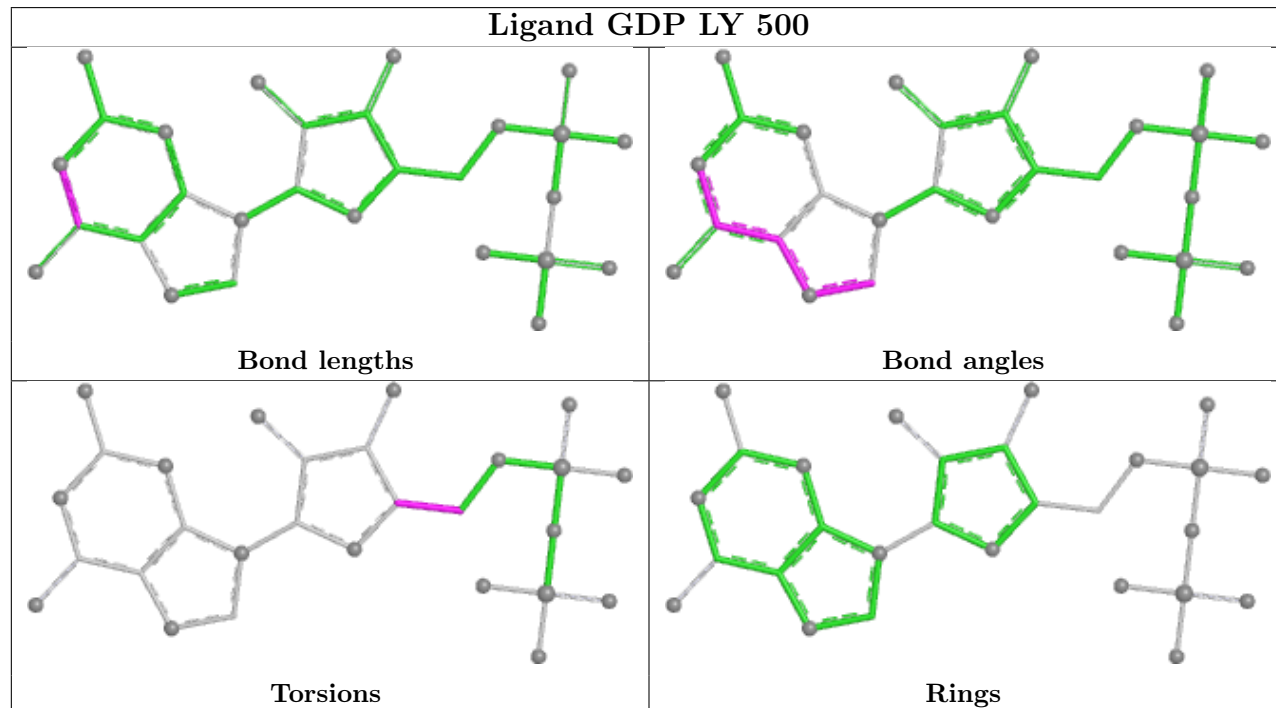


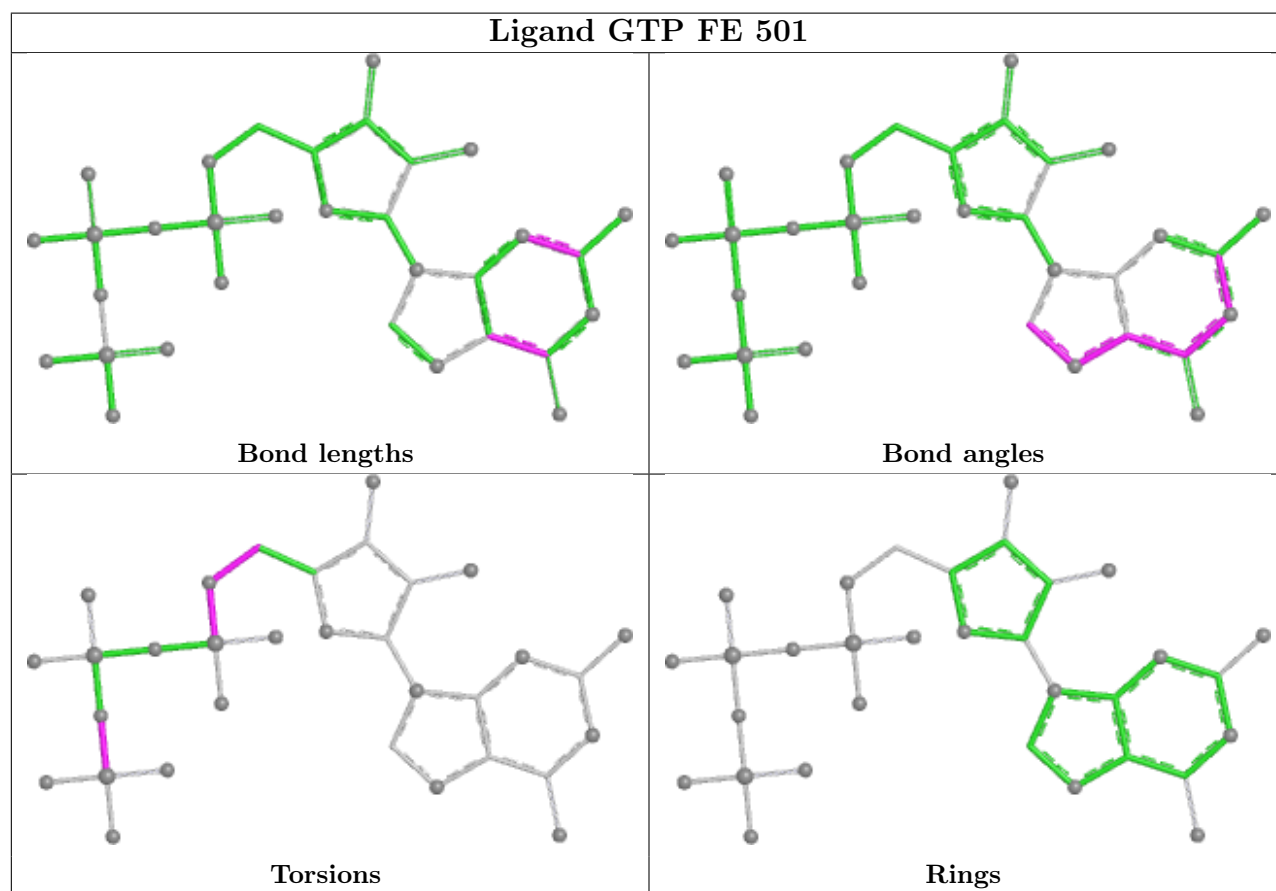
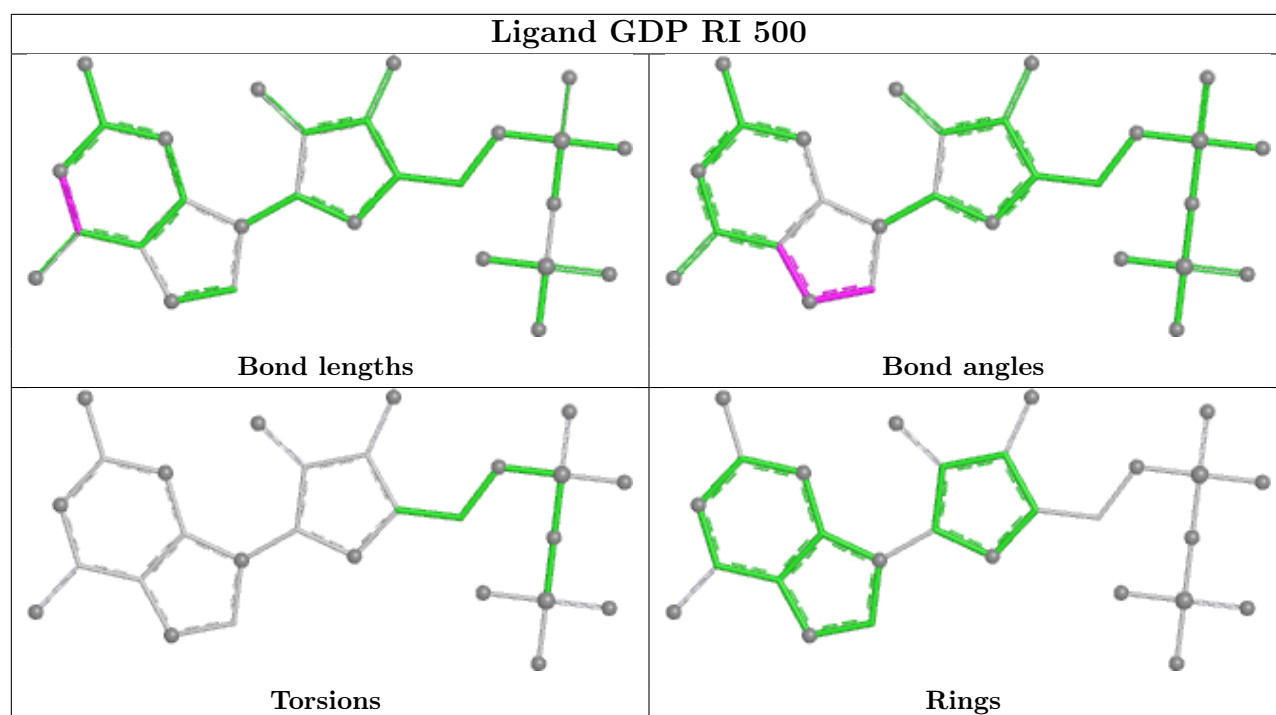


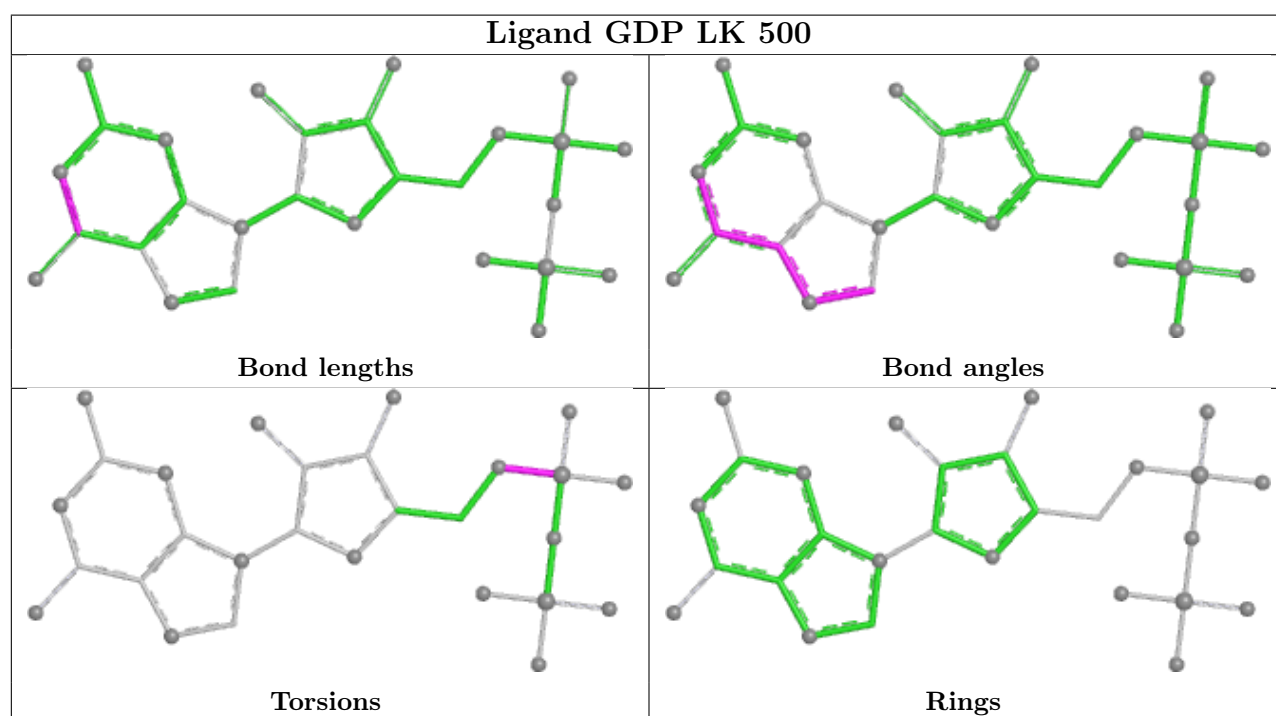
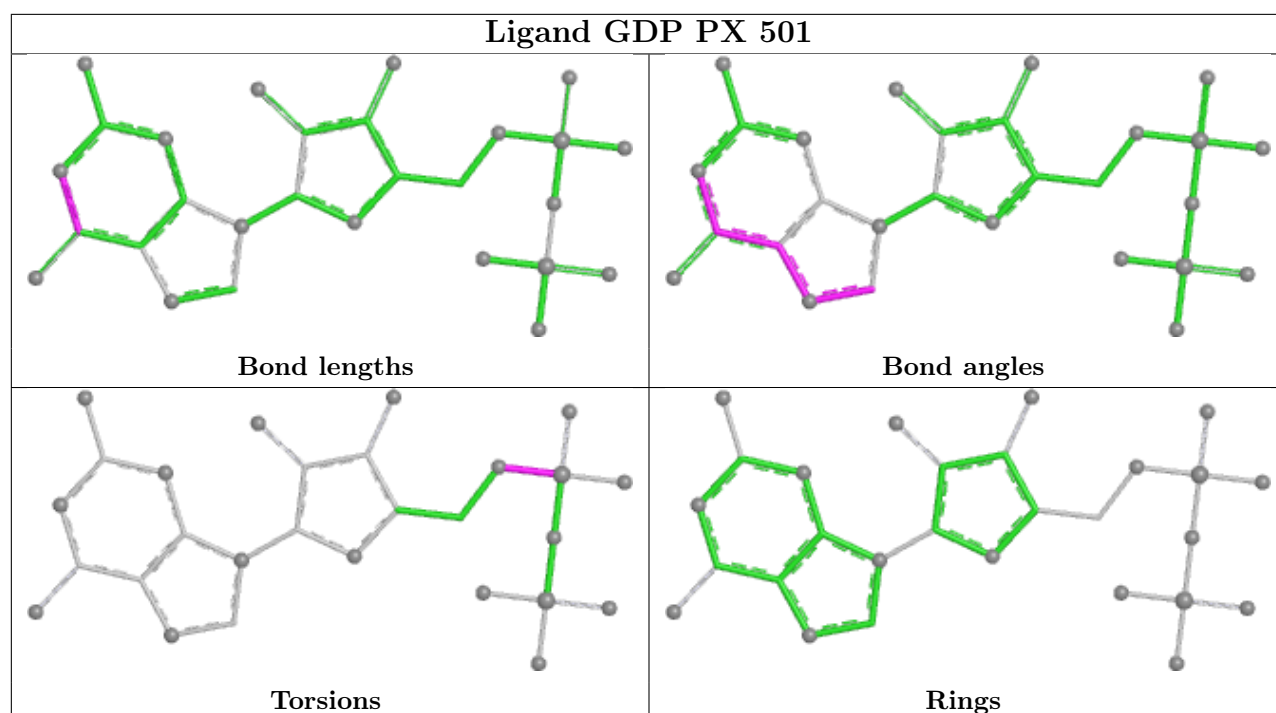
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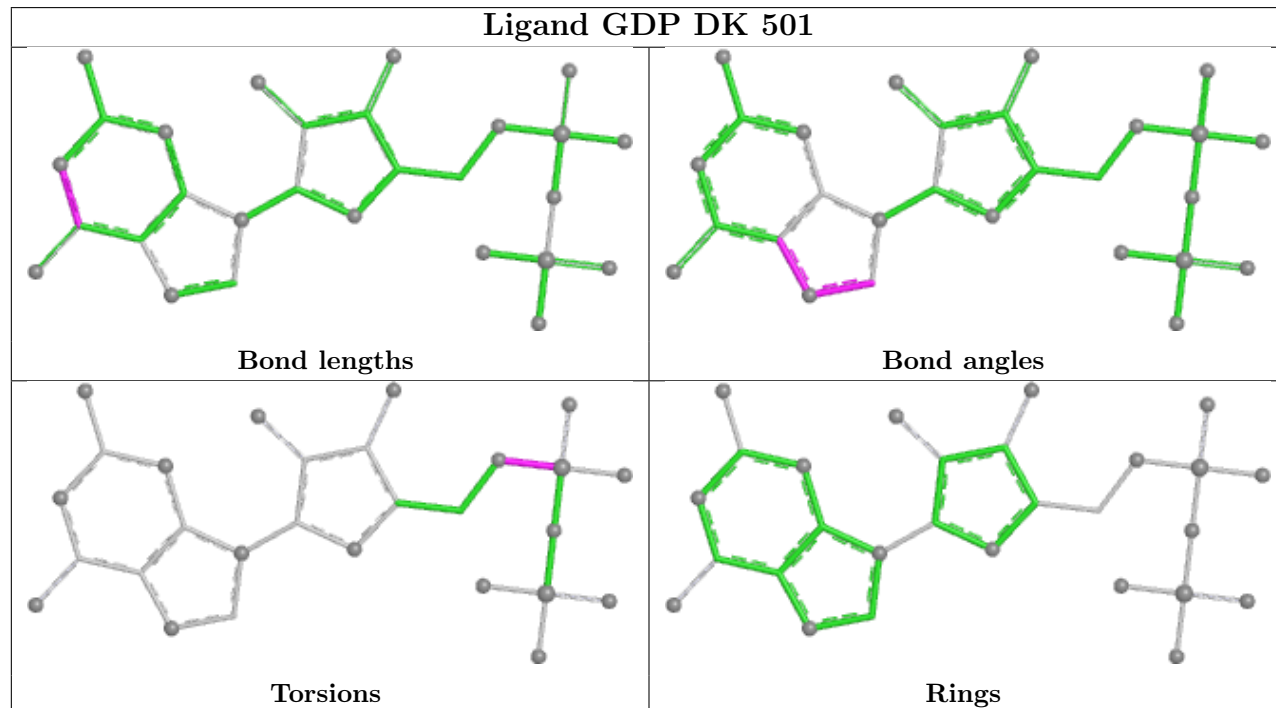
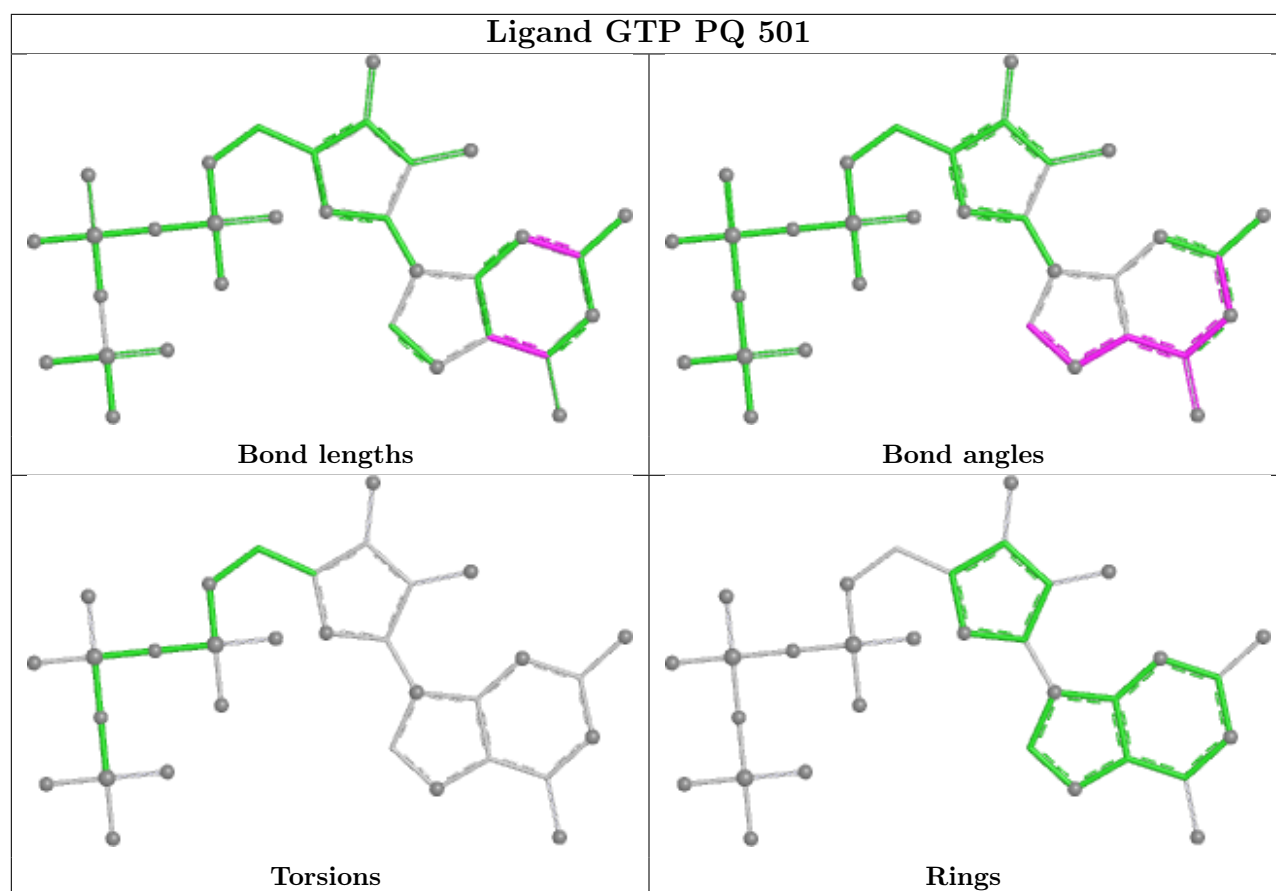


Ligand GDP LY 500

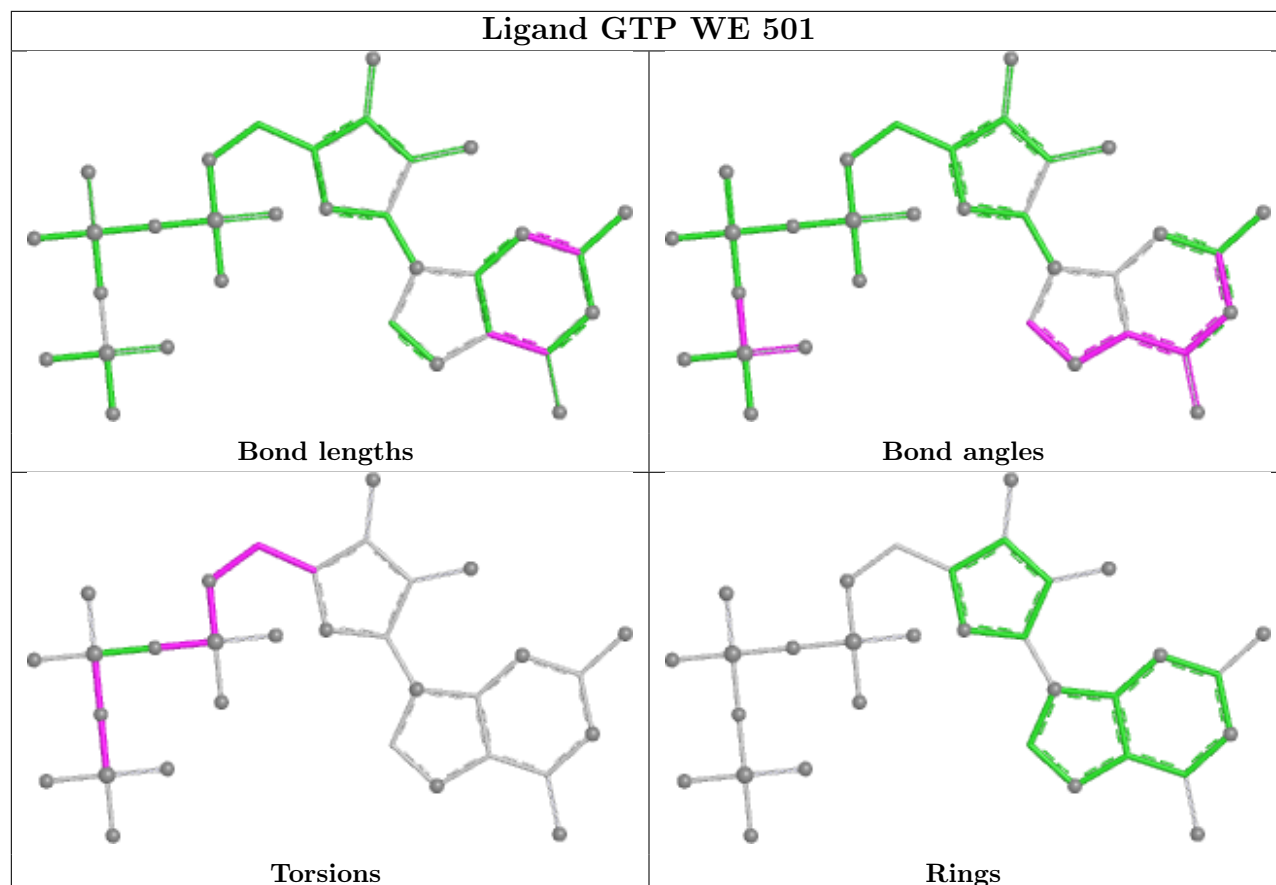




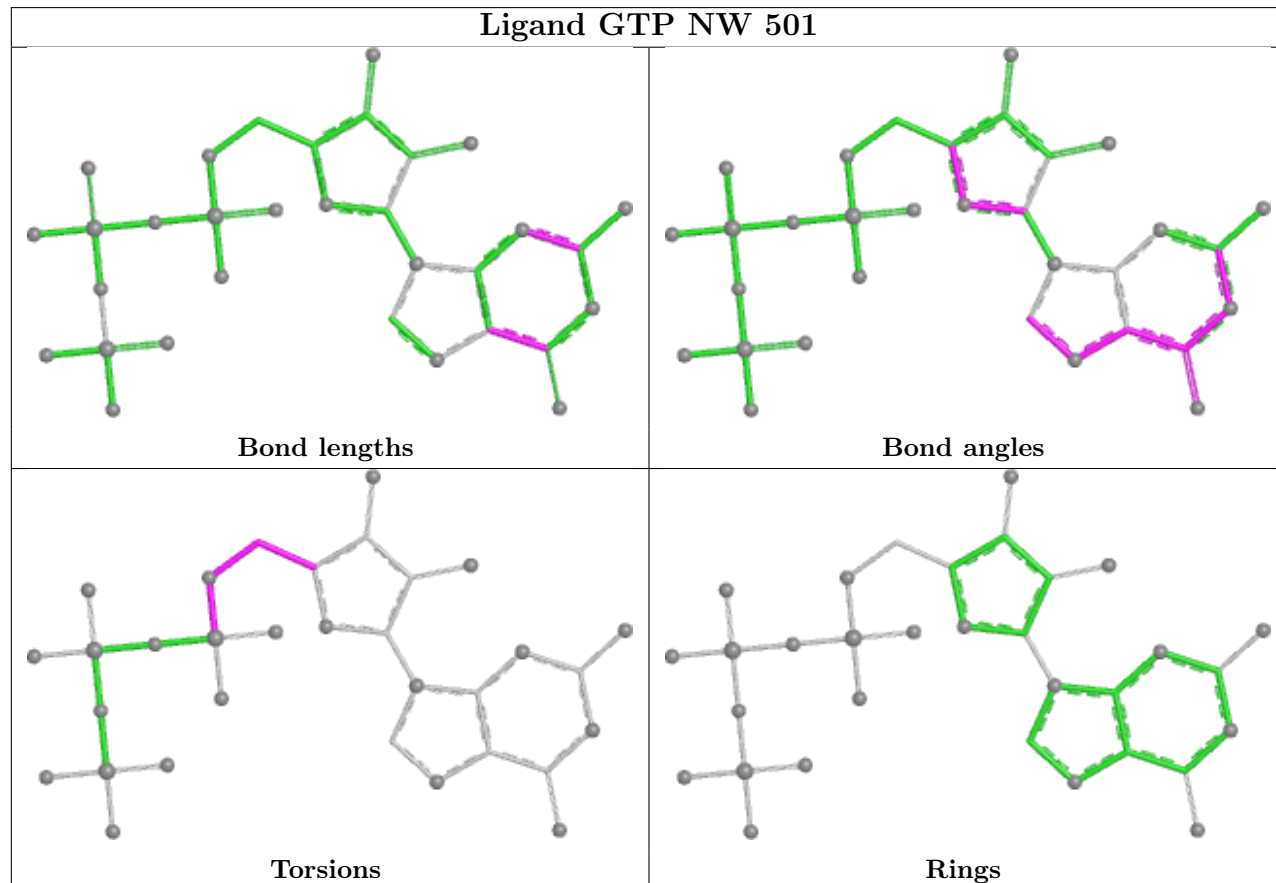


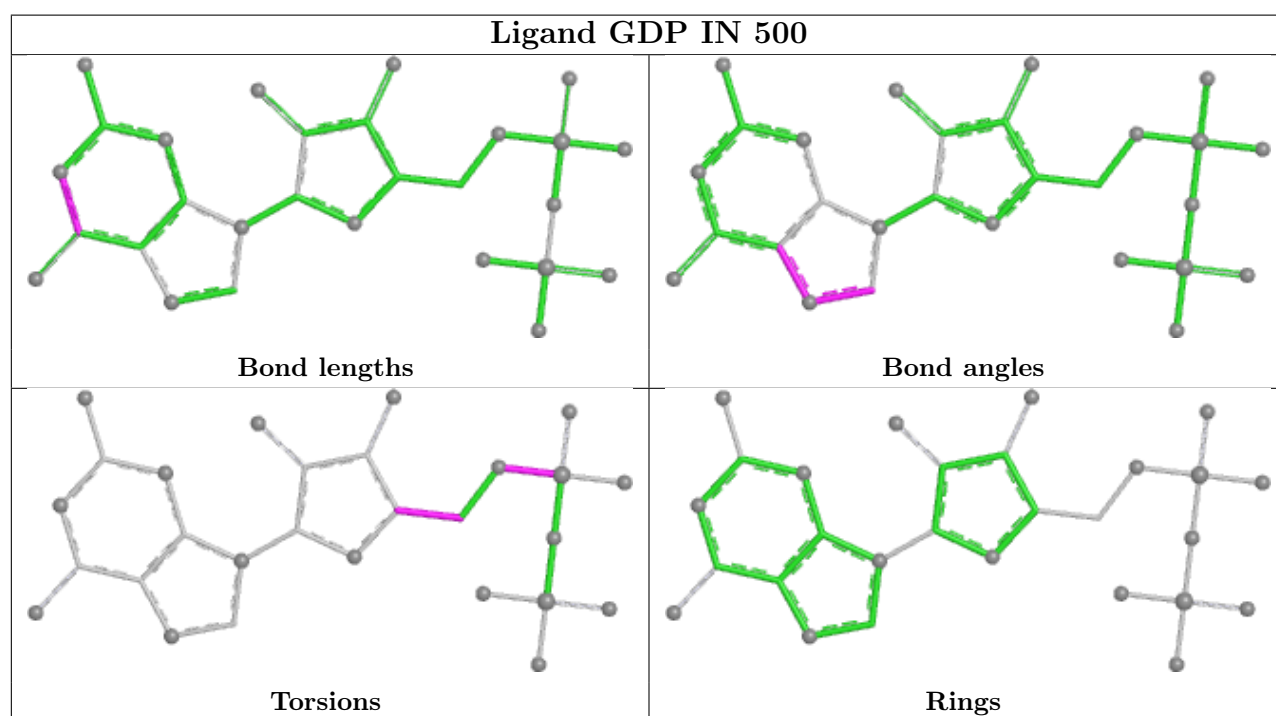
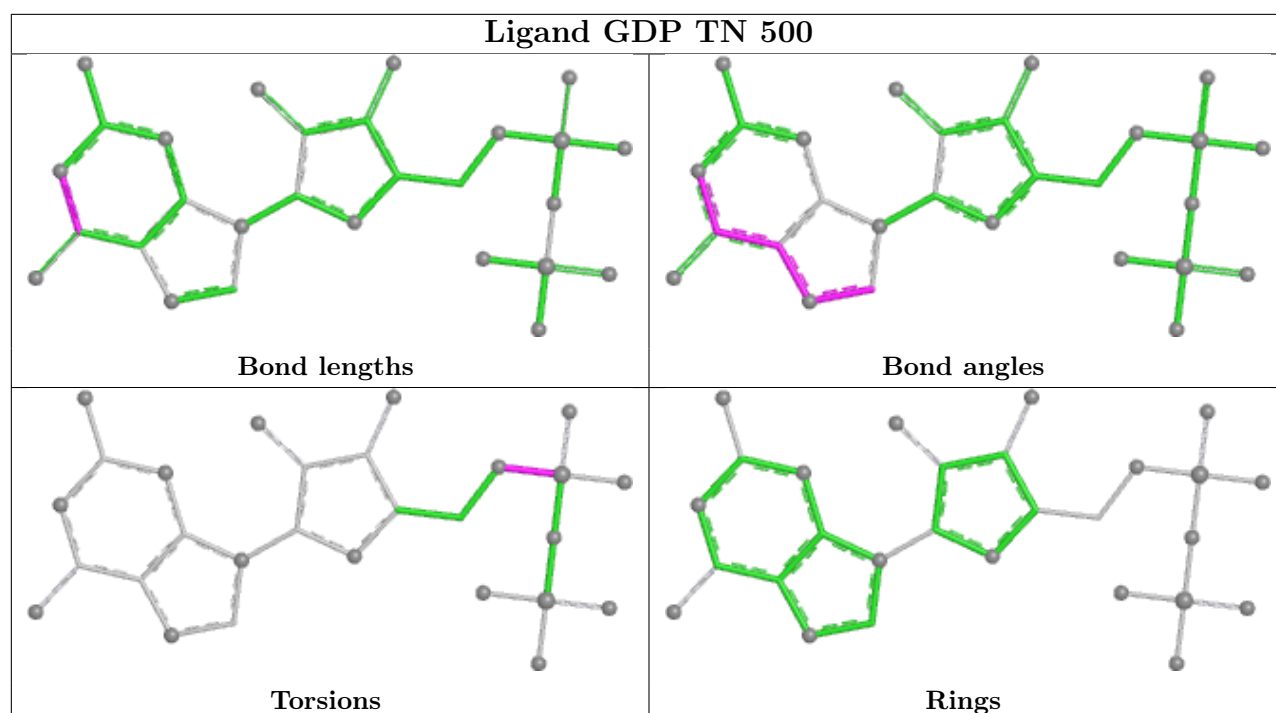


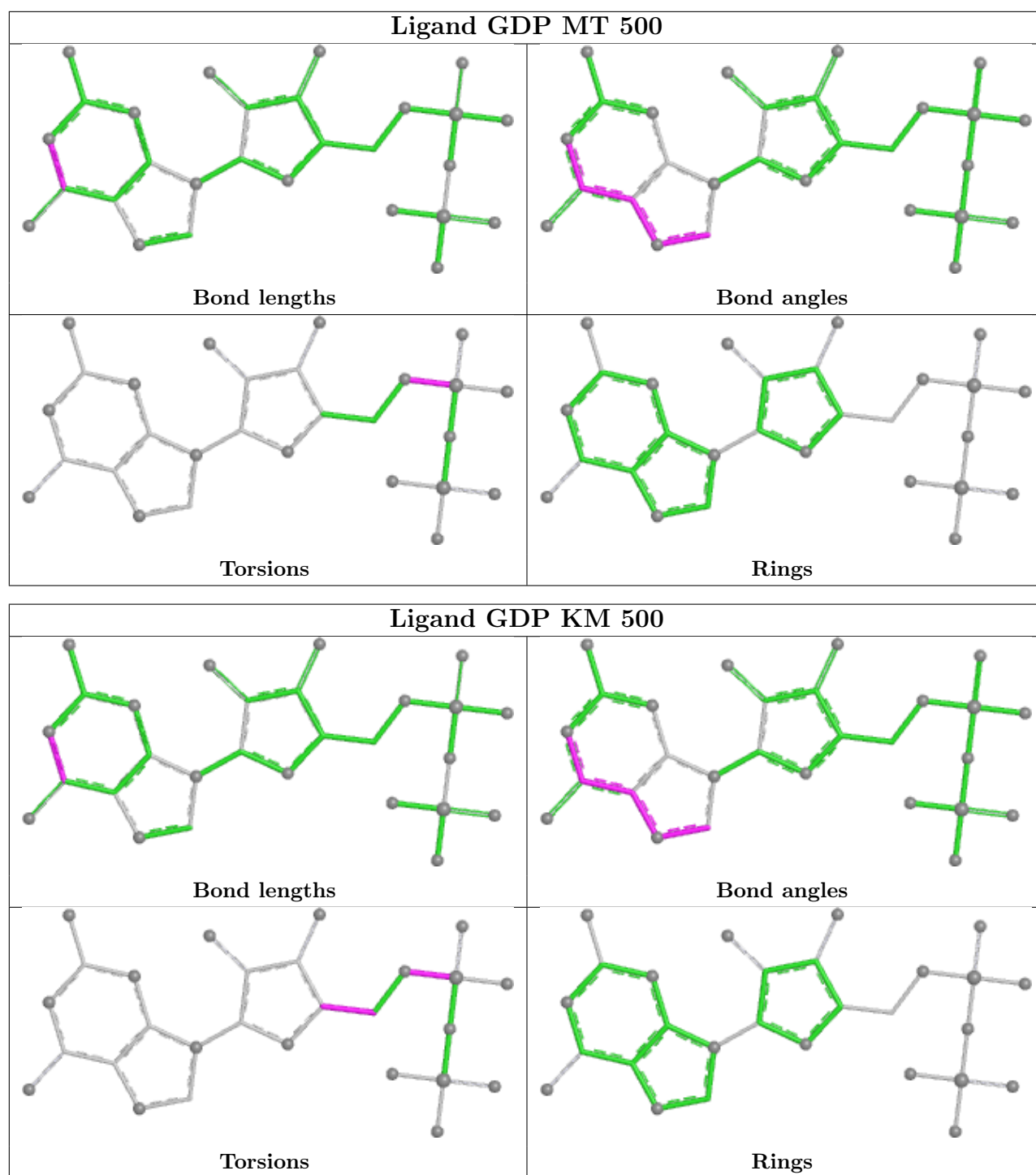
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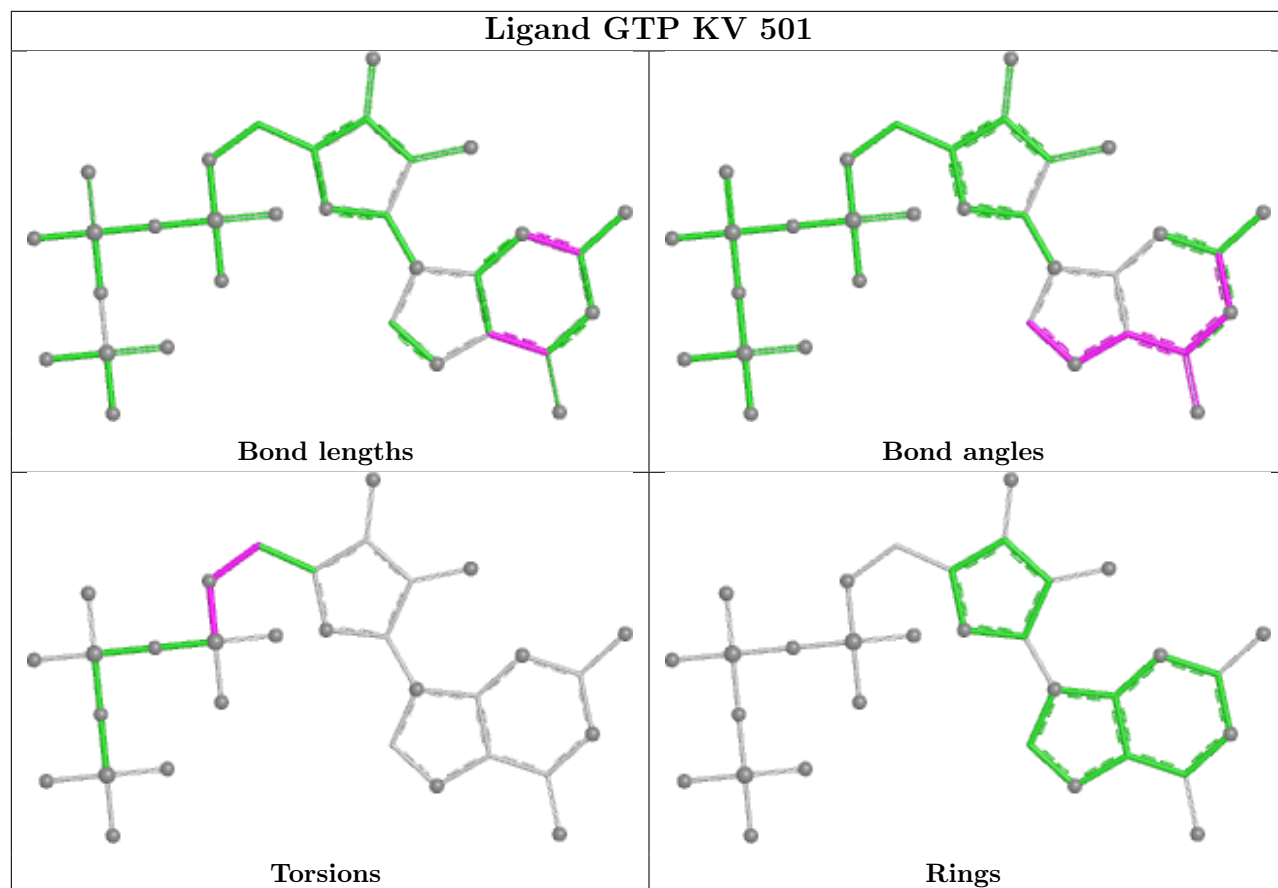
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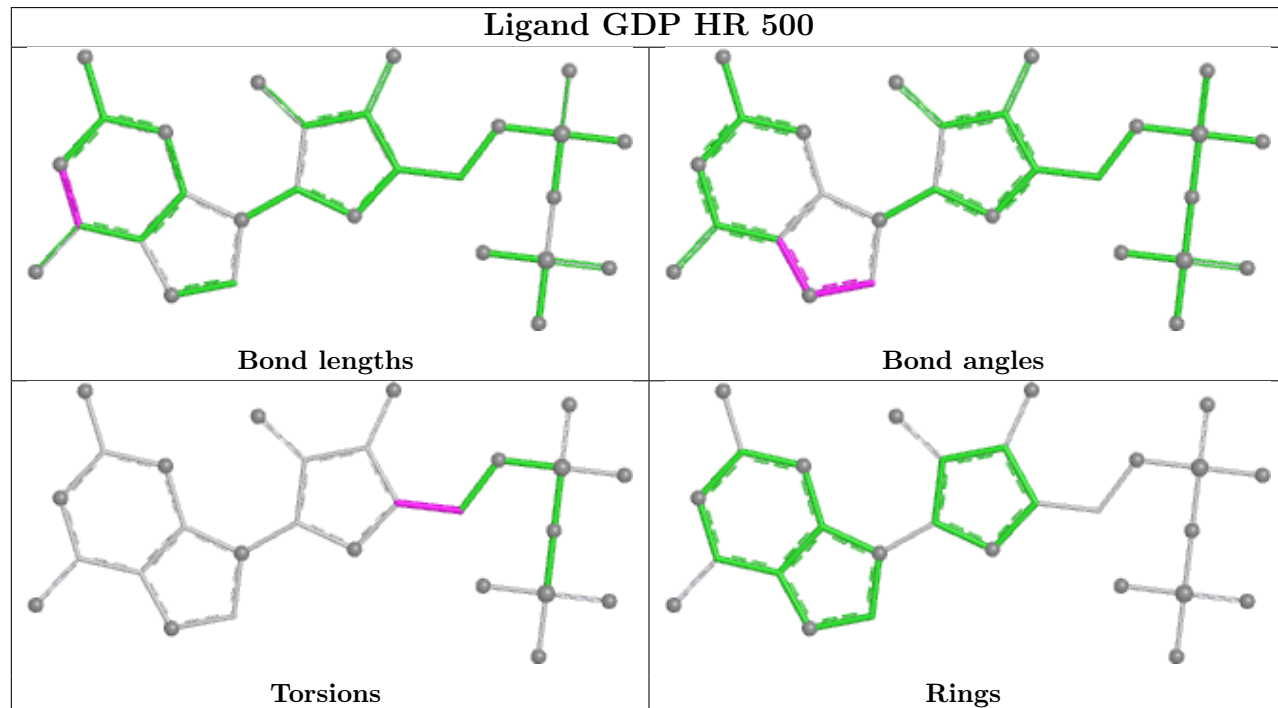


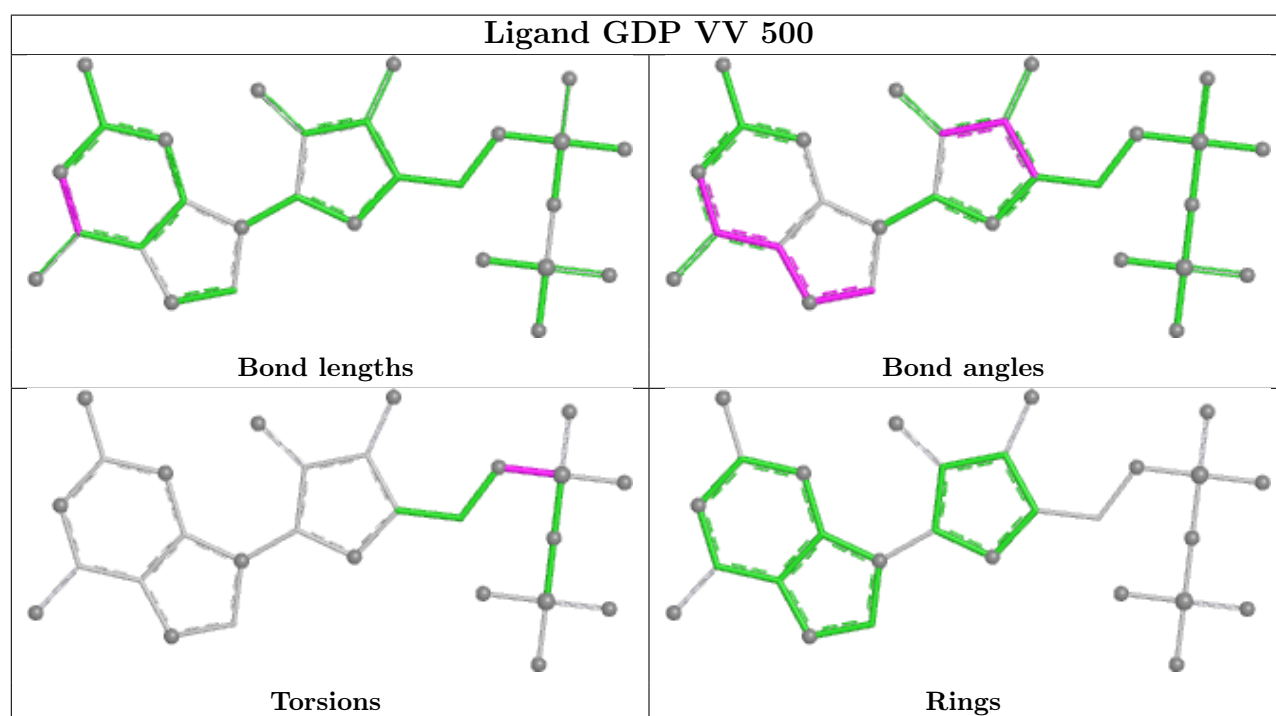
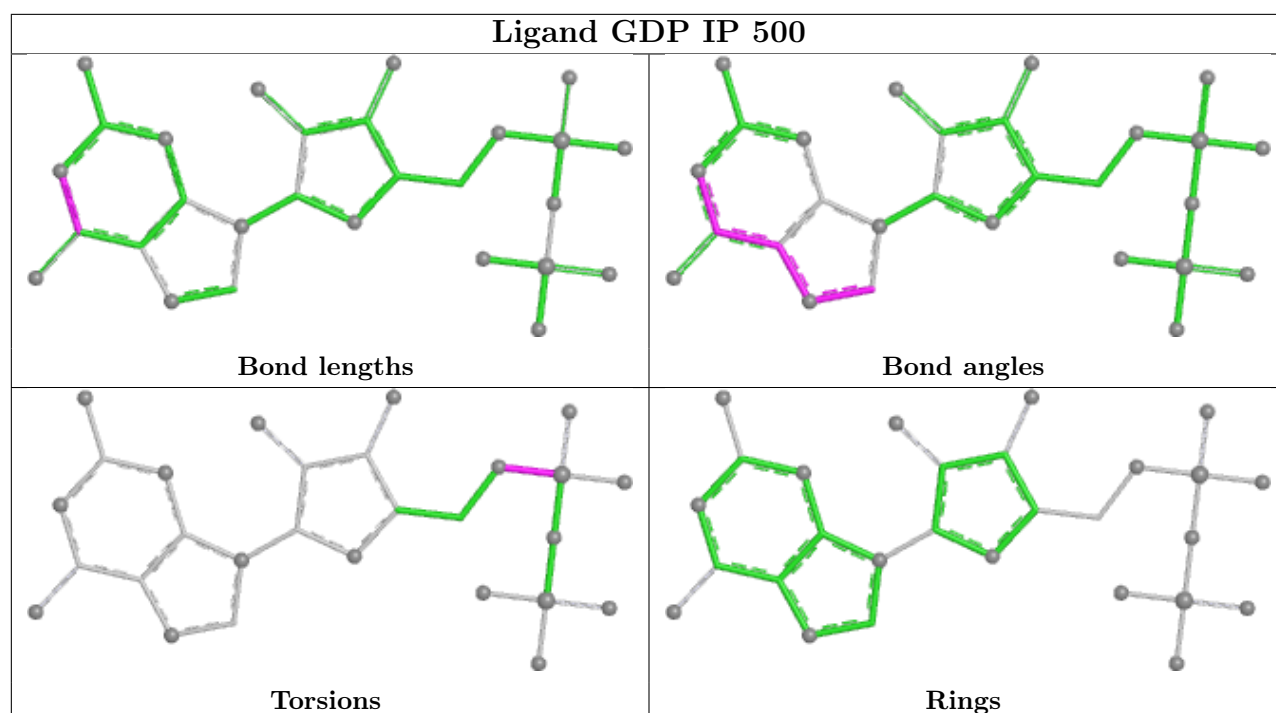


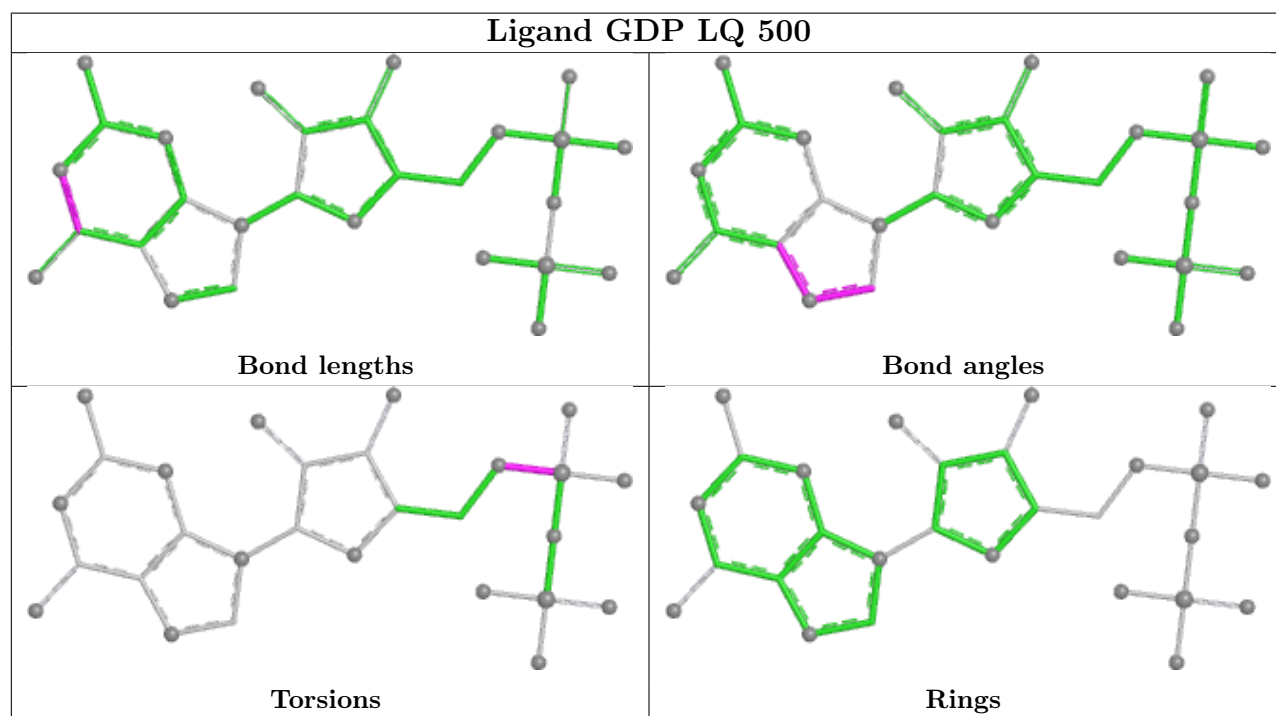
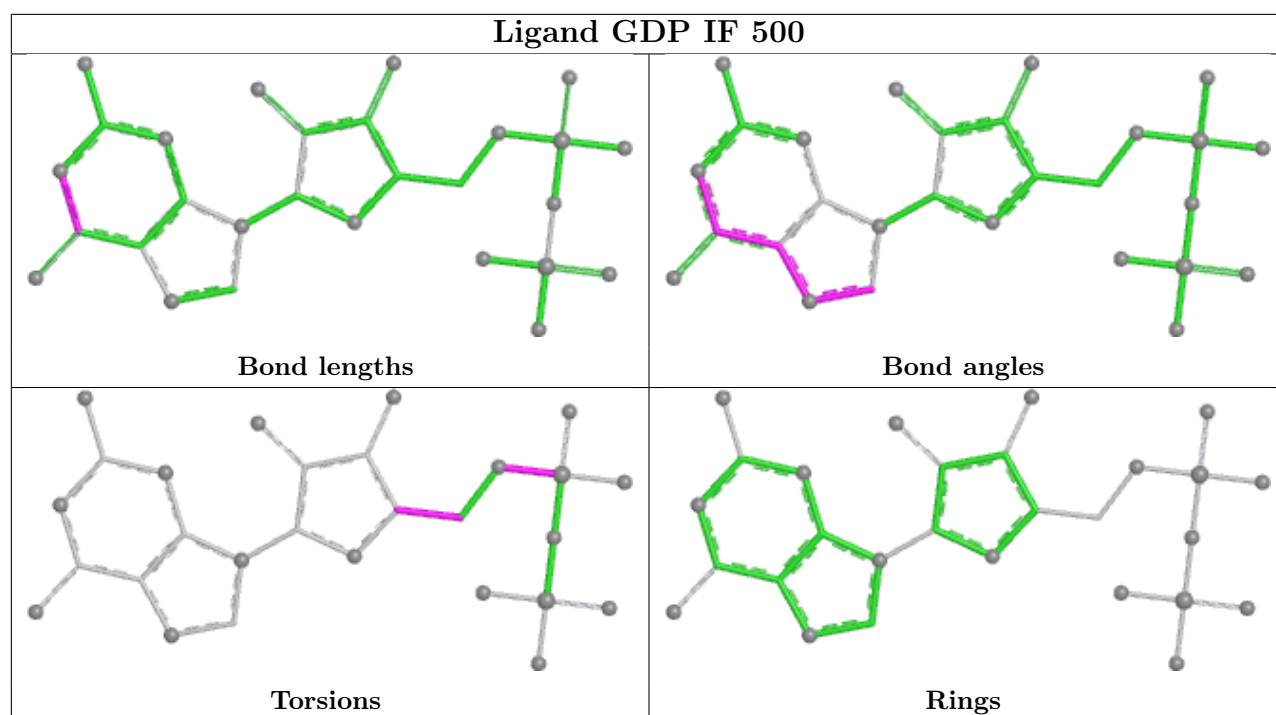
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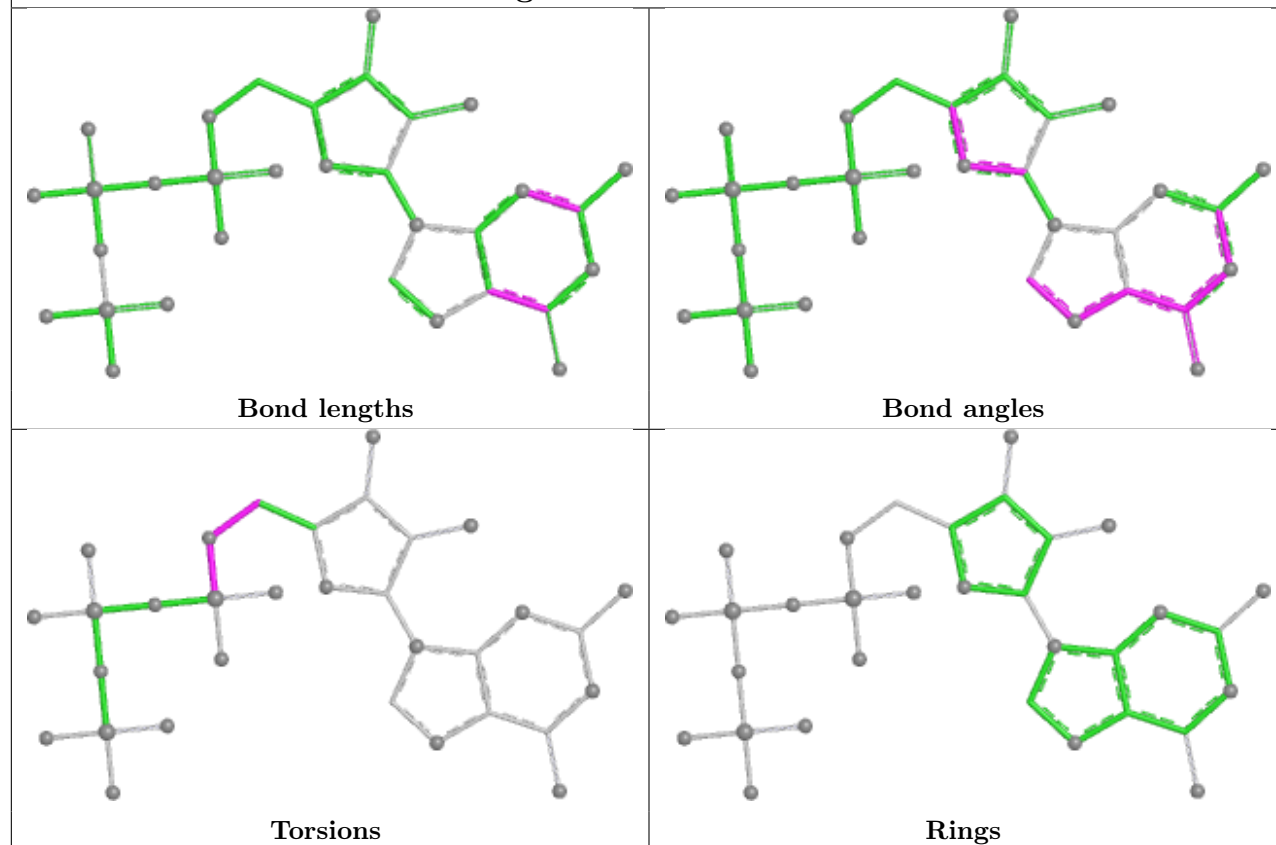
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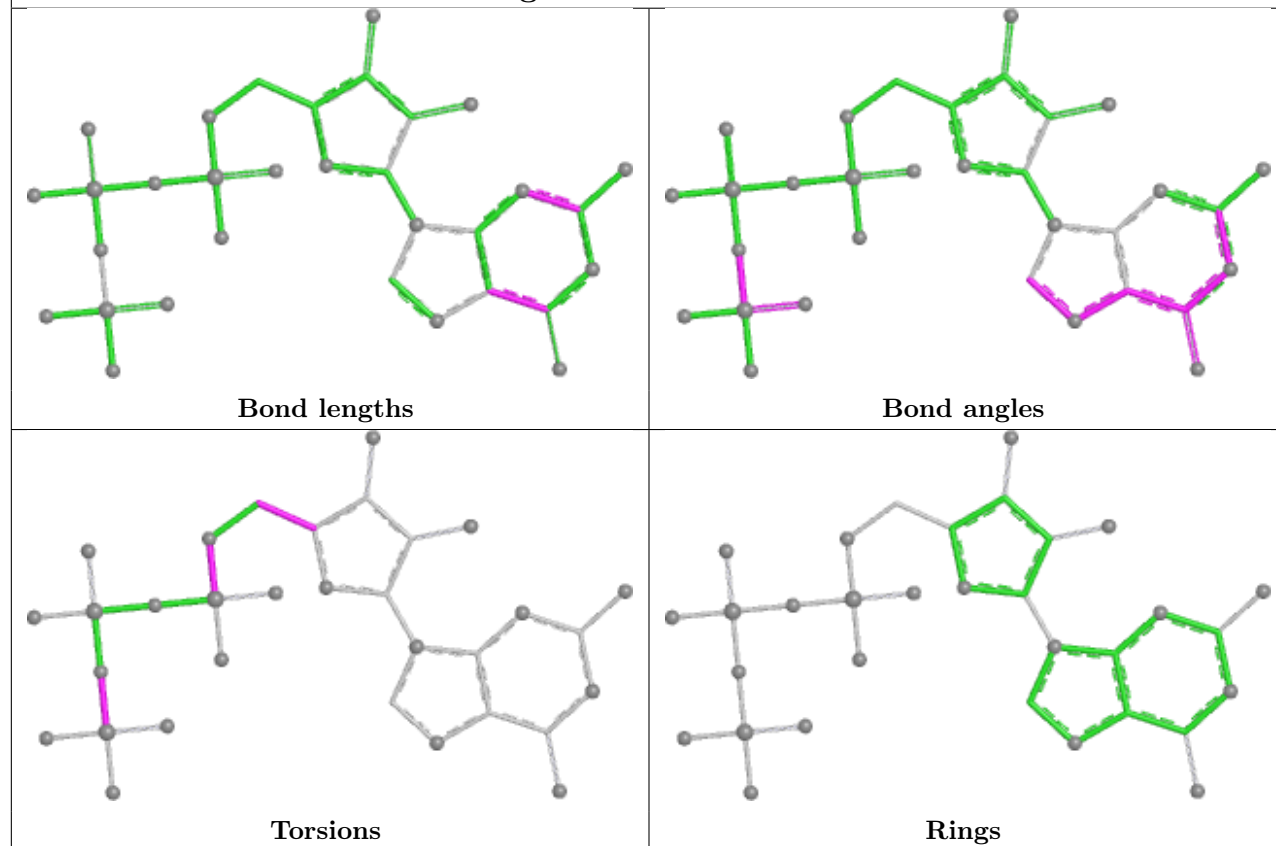


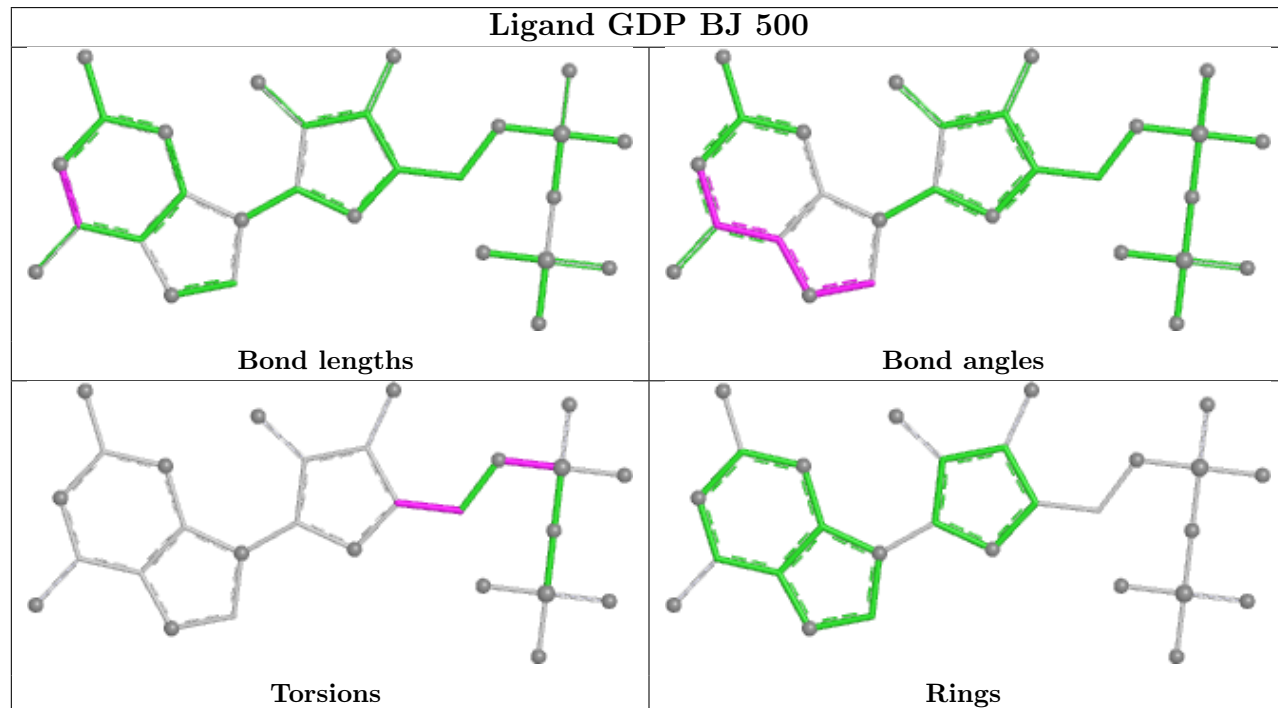
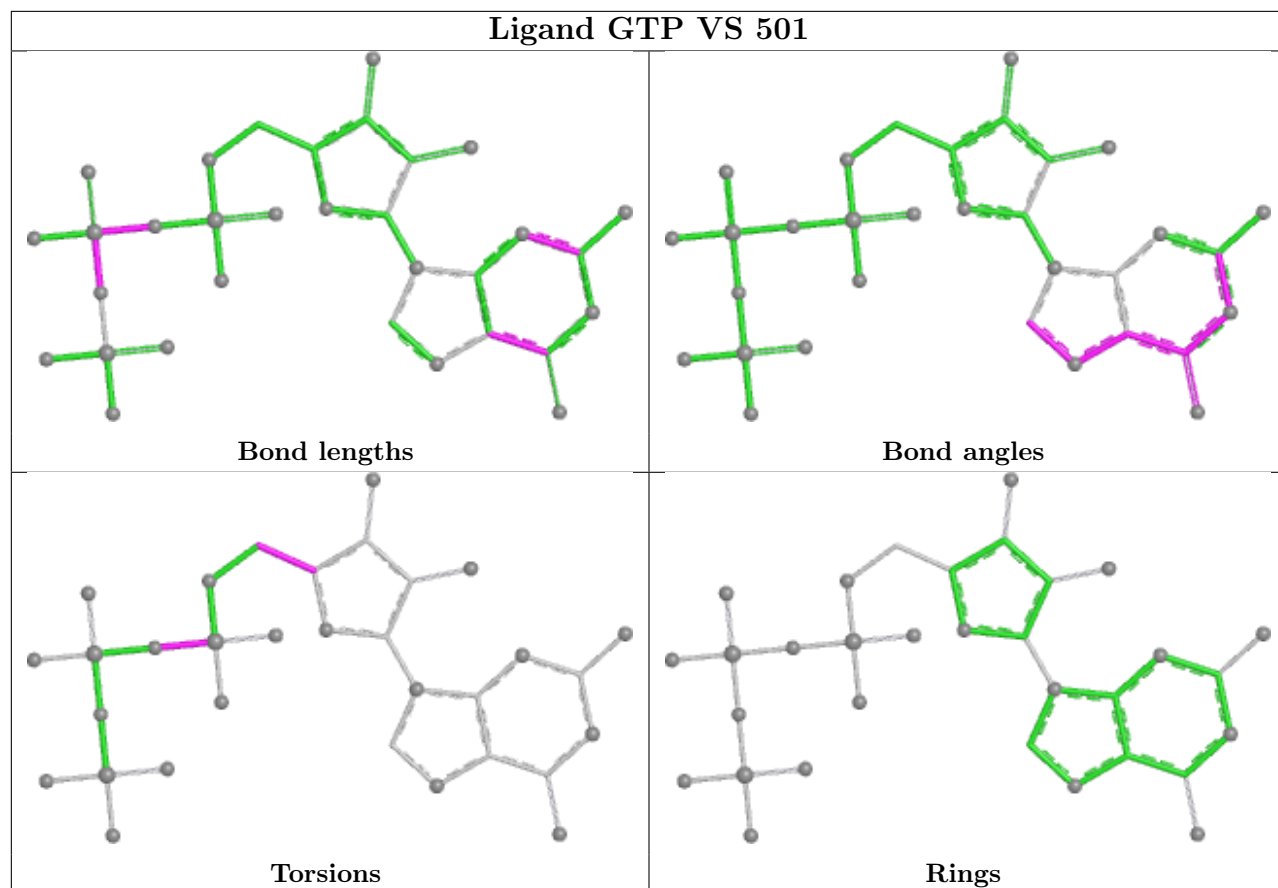


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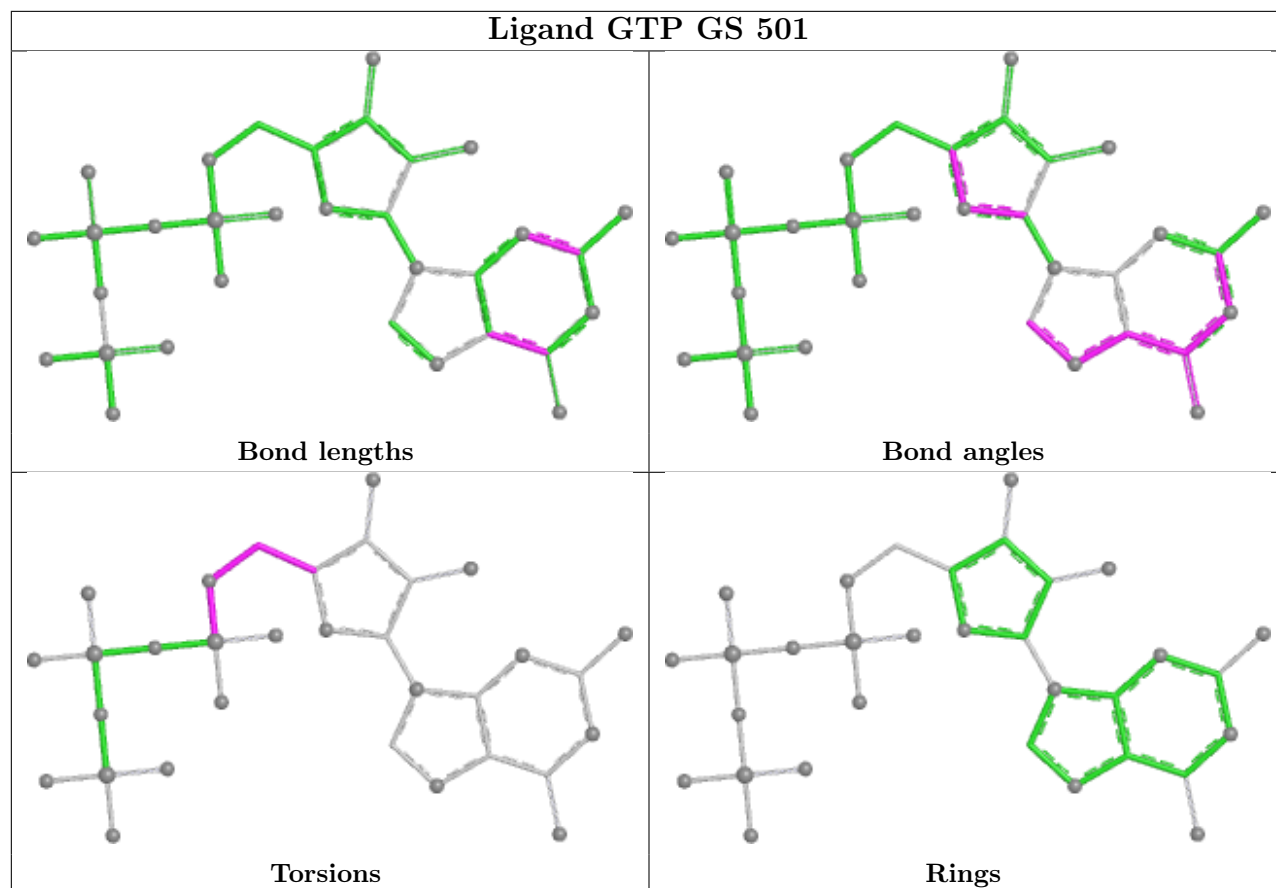


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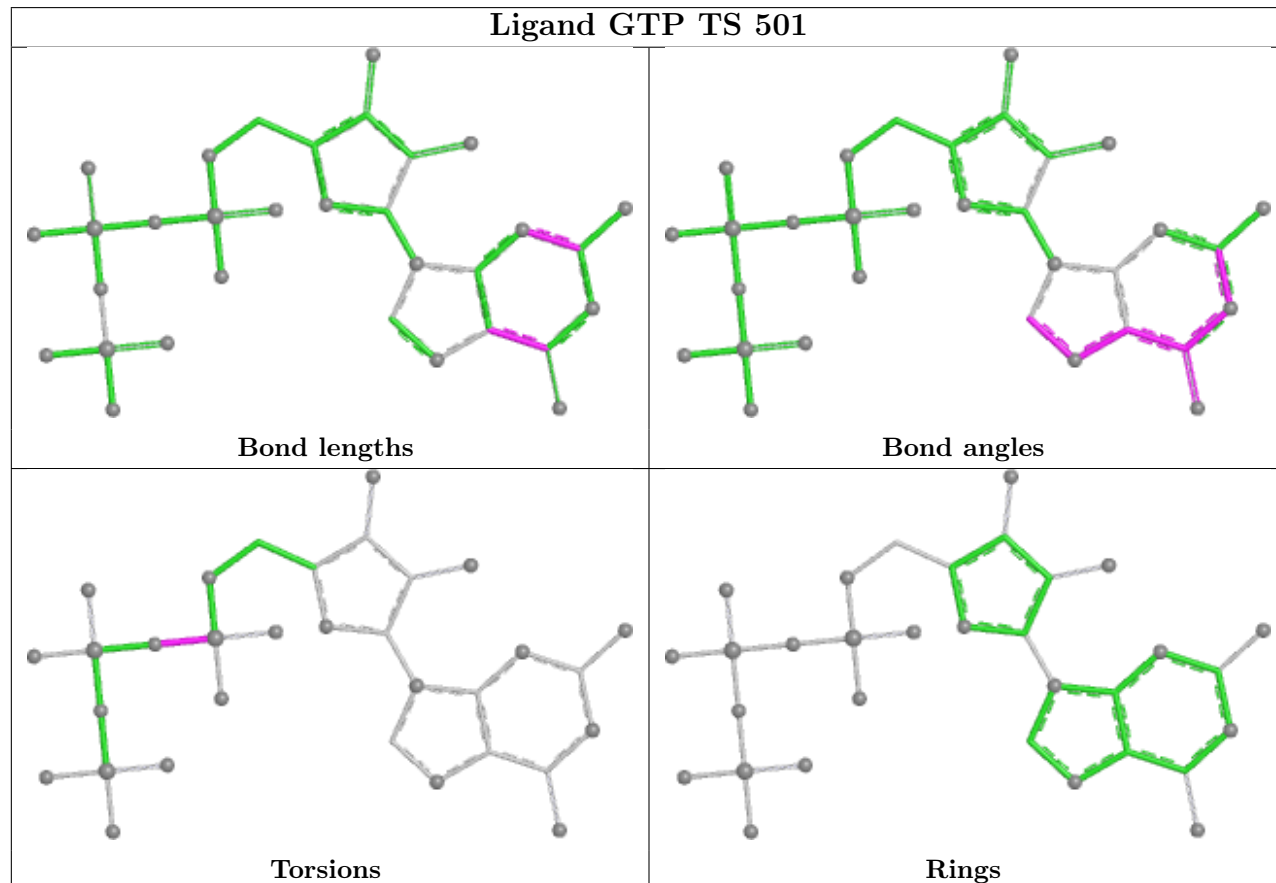


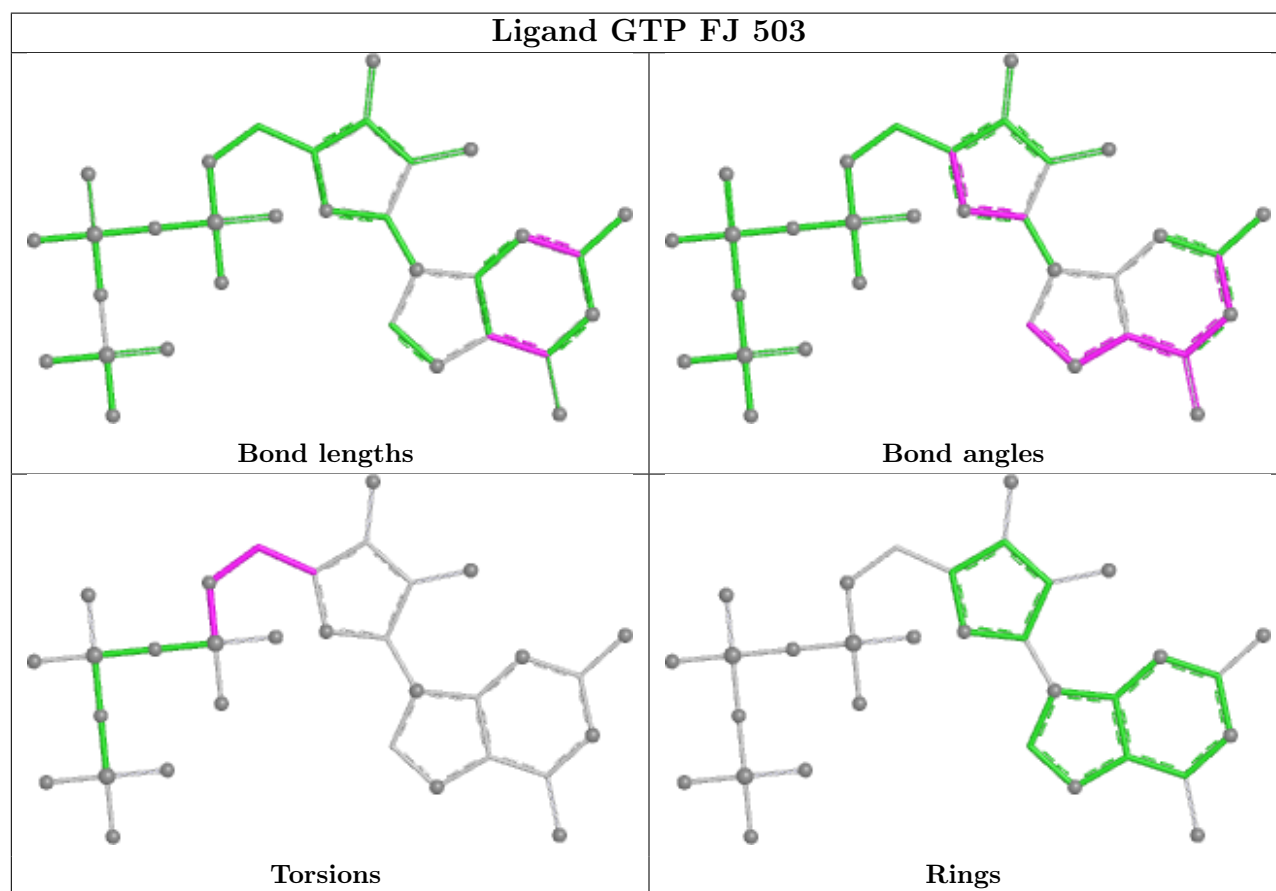
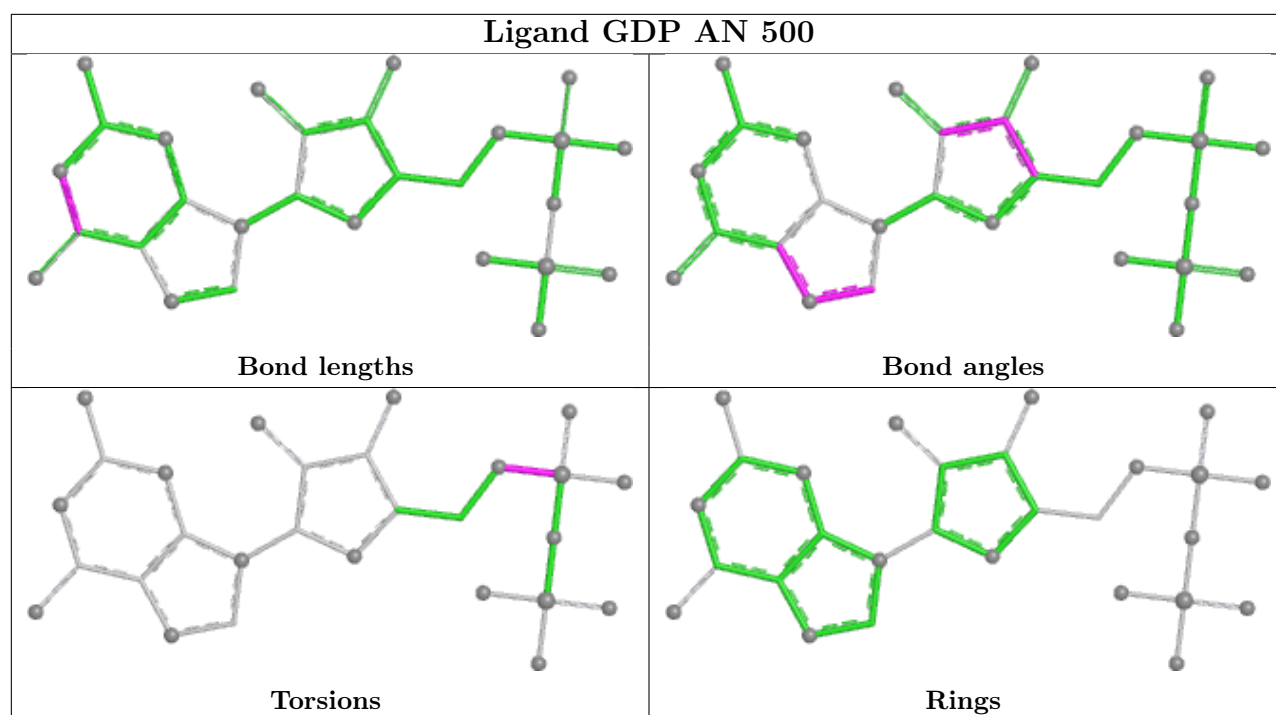


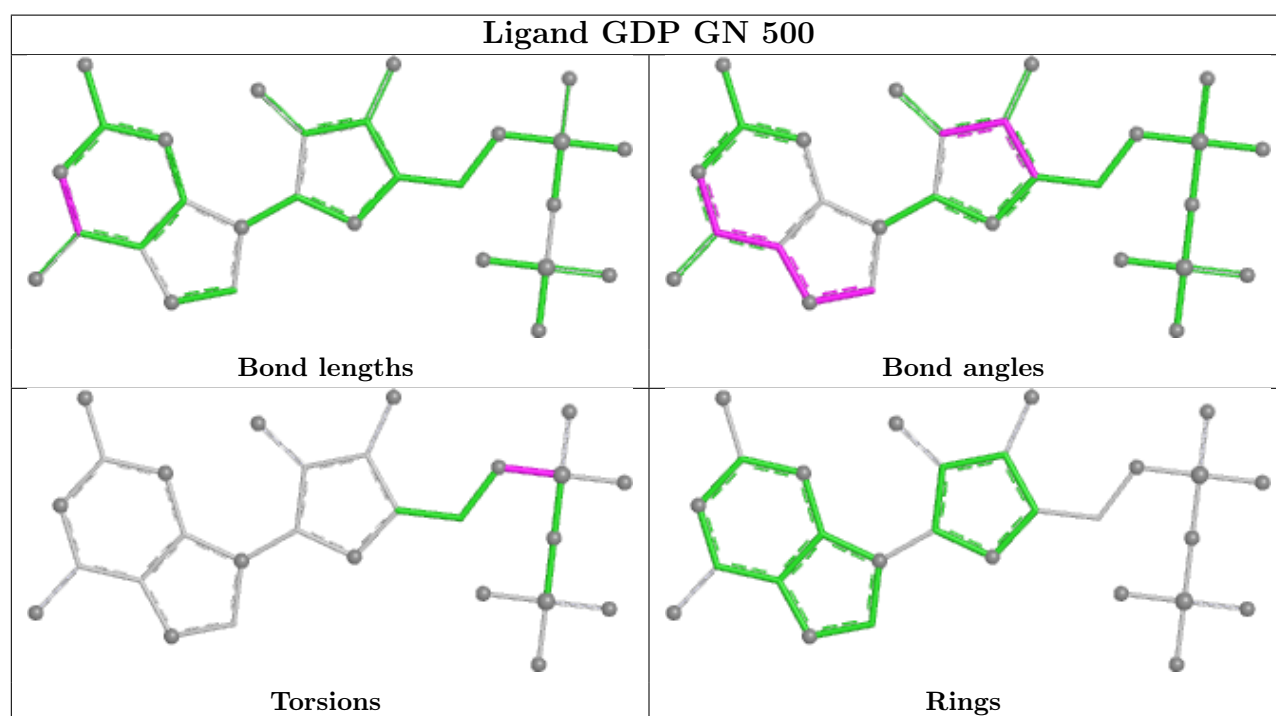
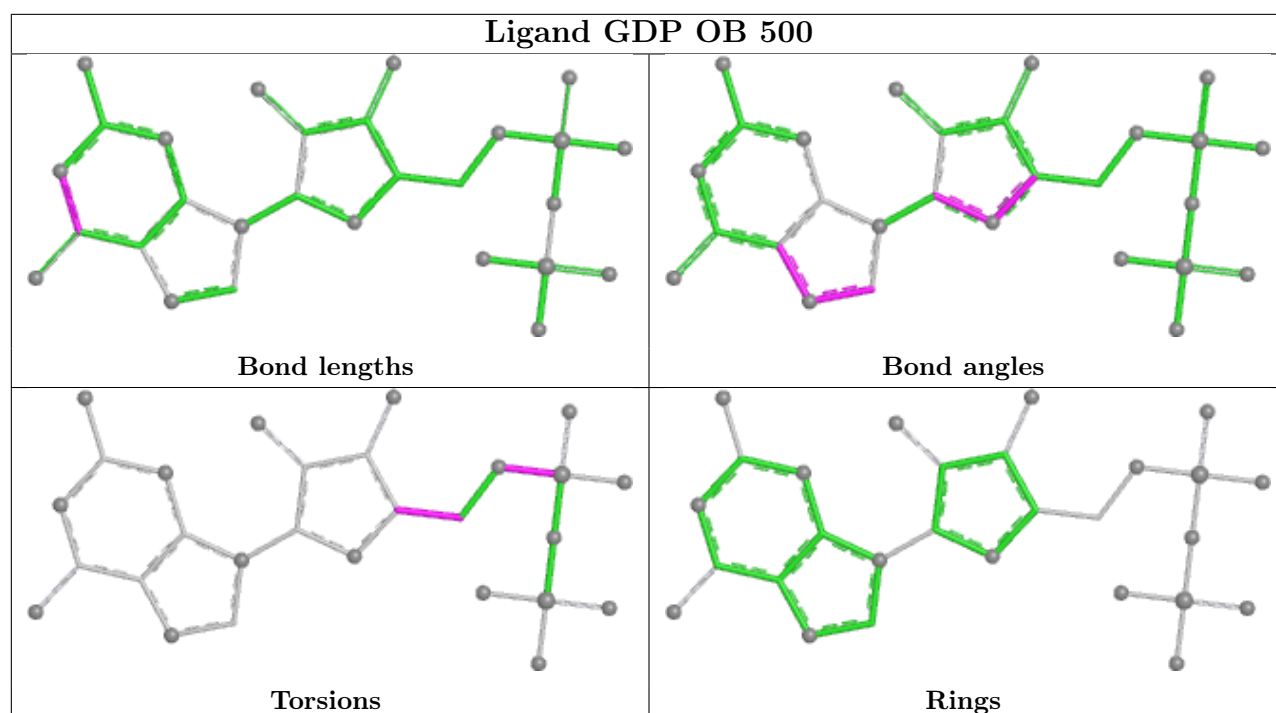
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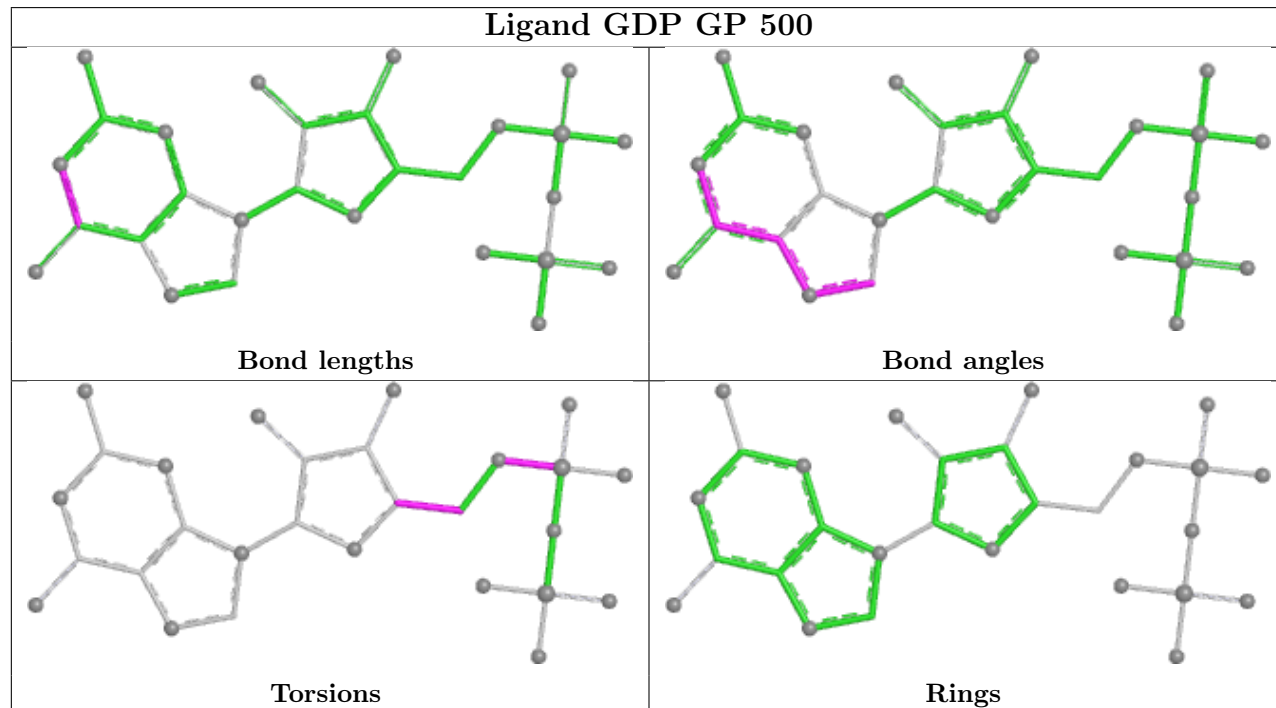
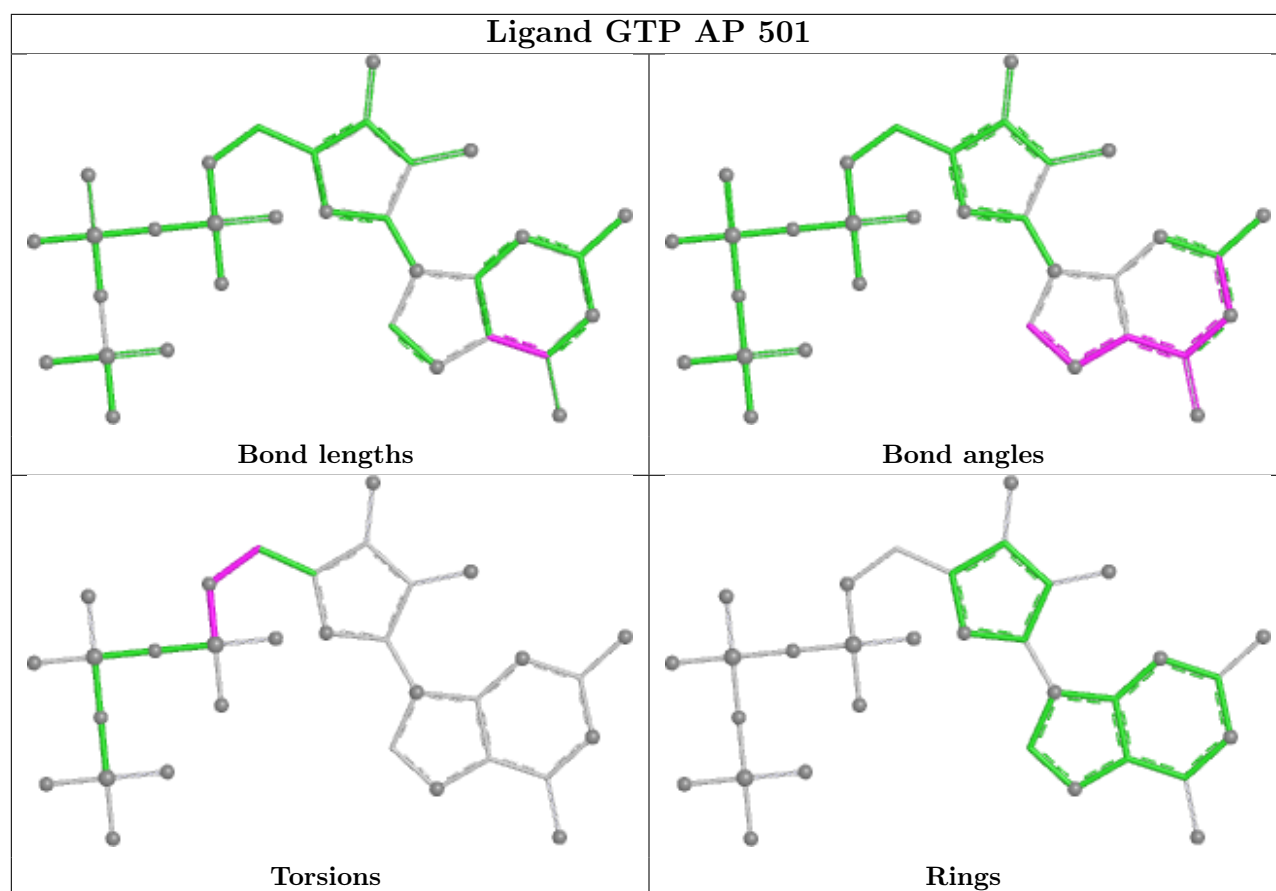


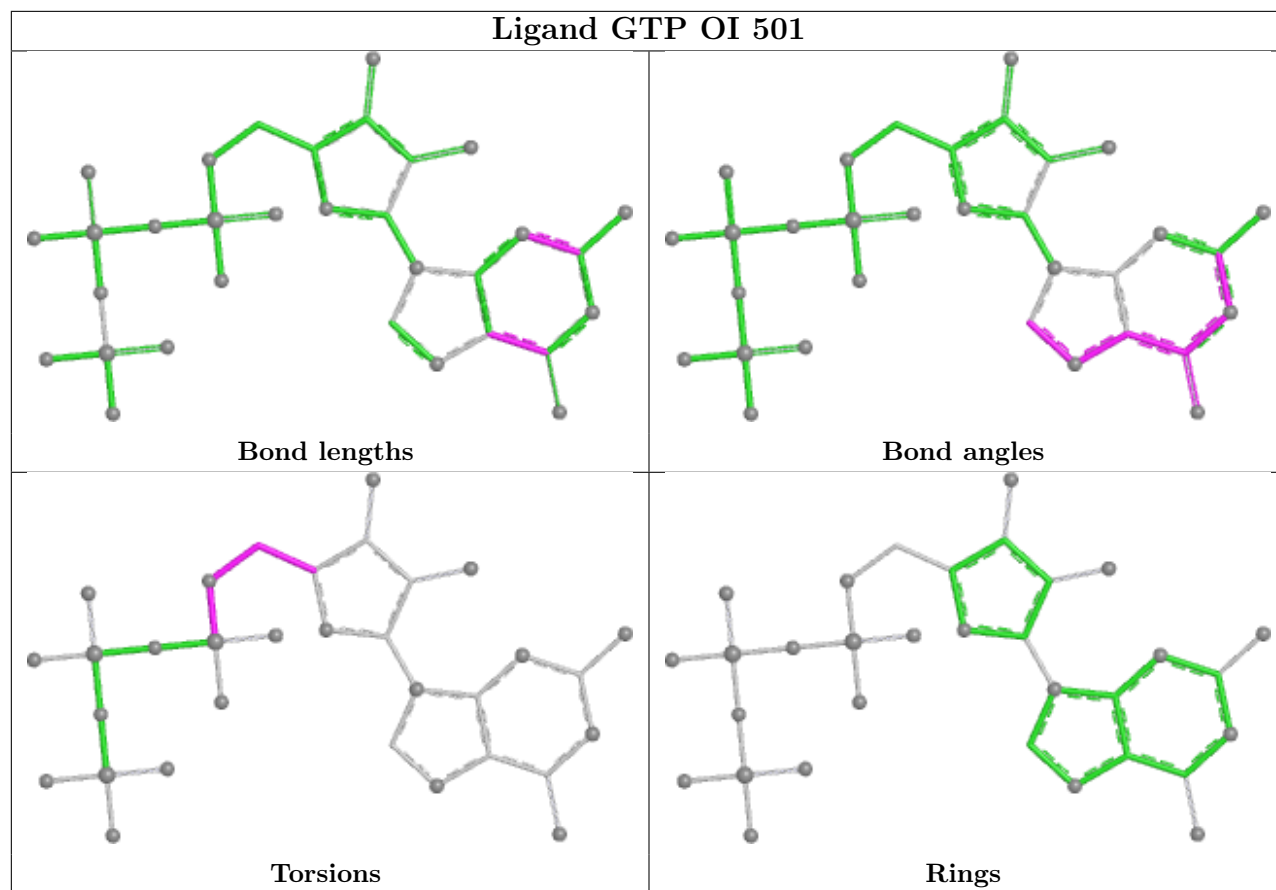
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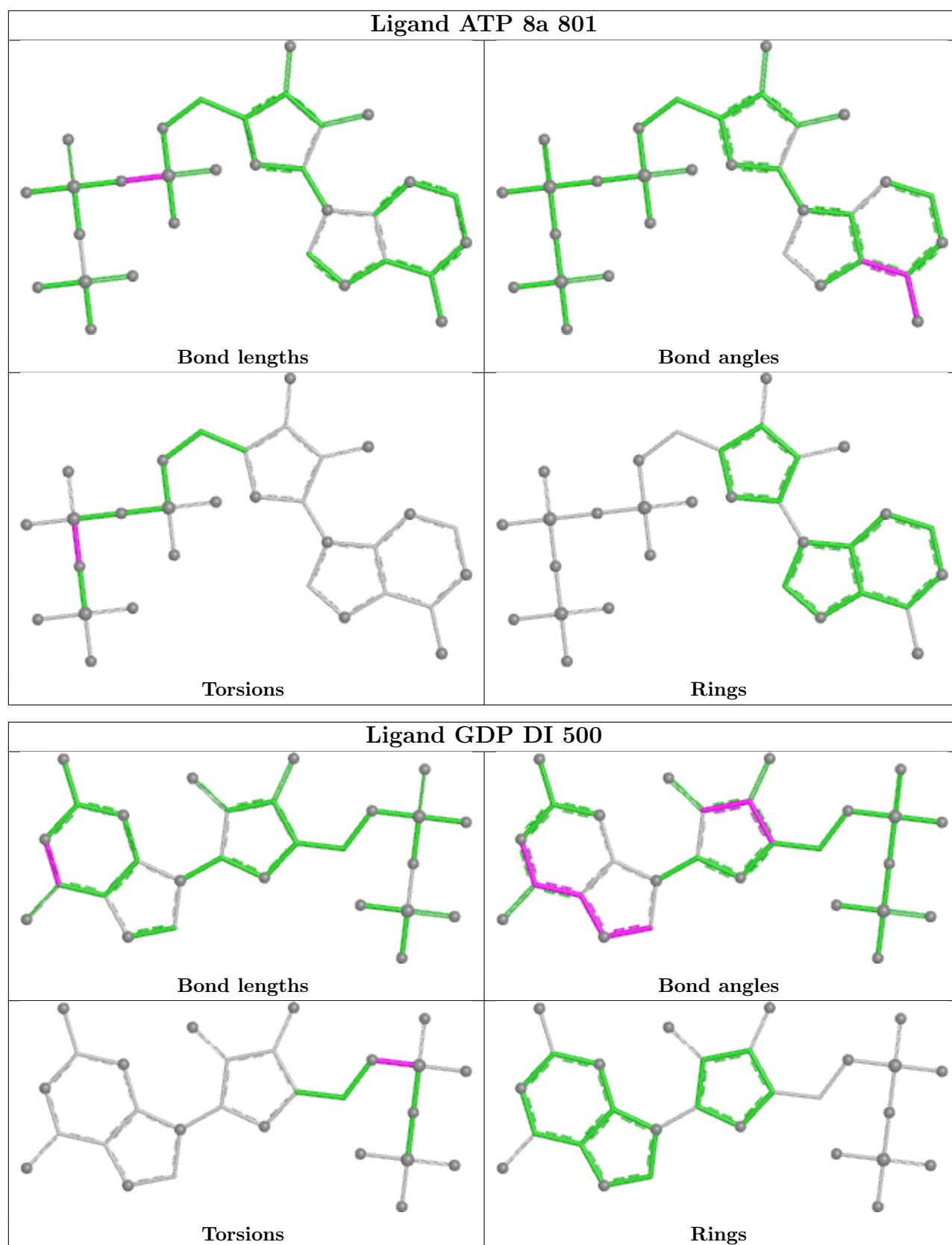


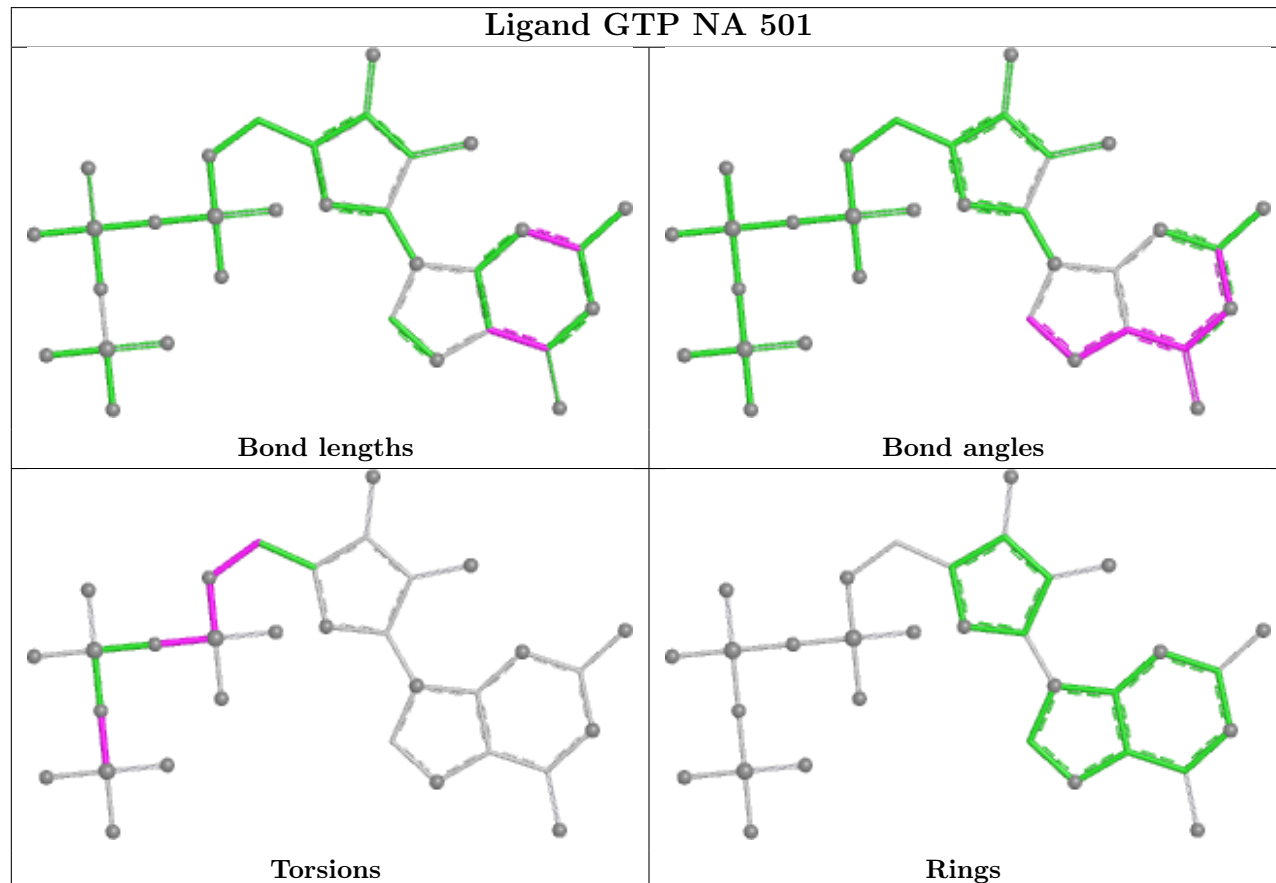
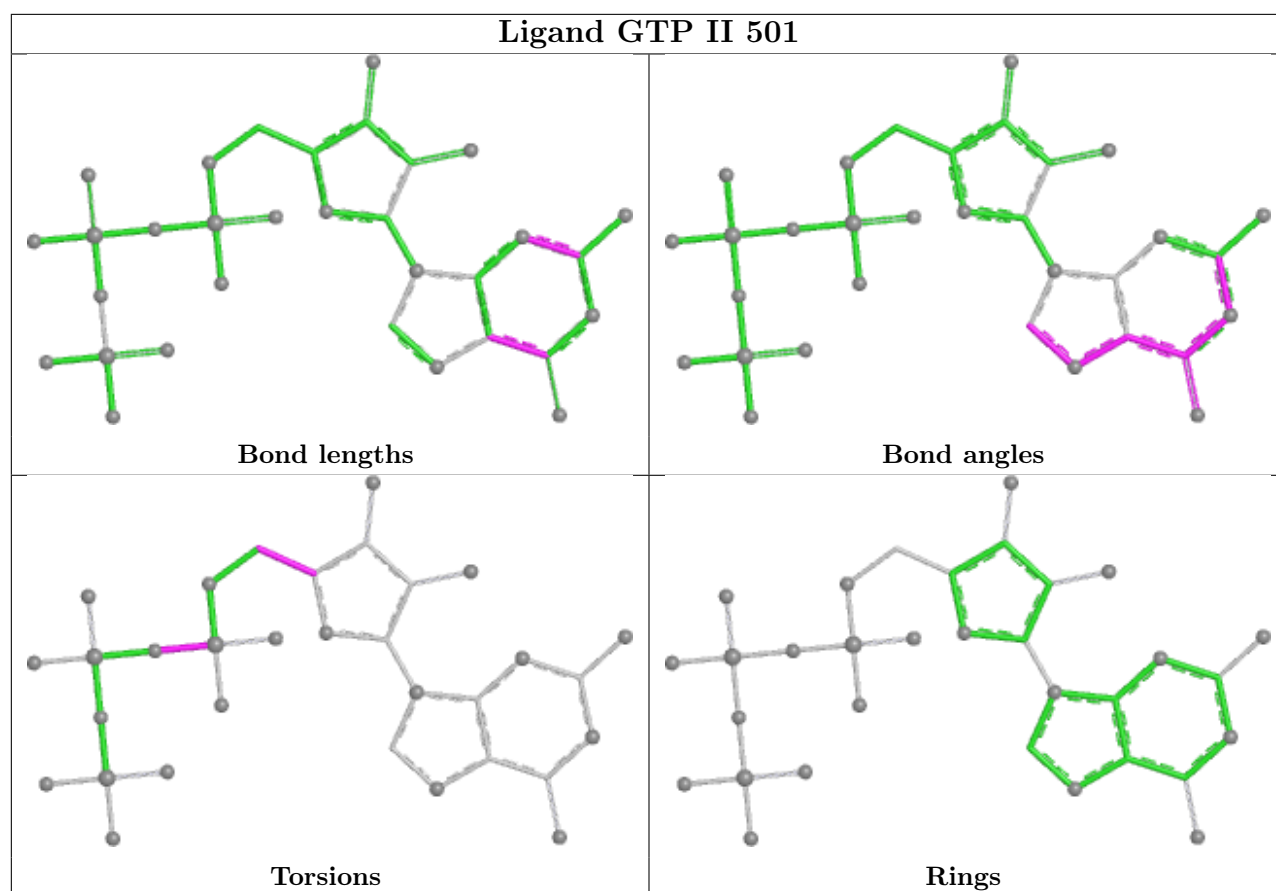


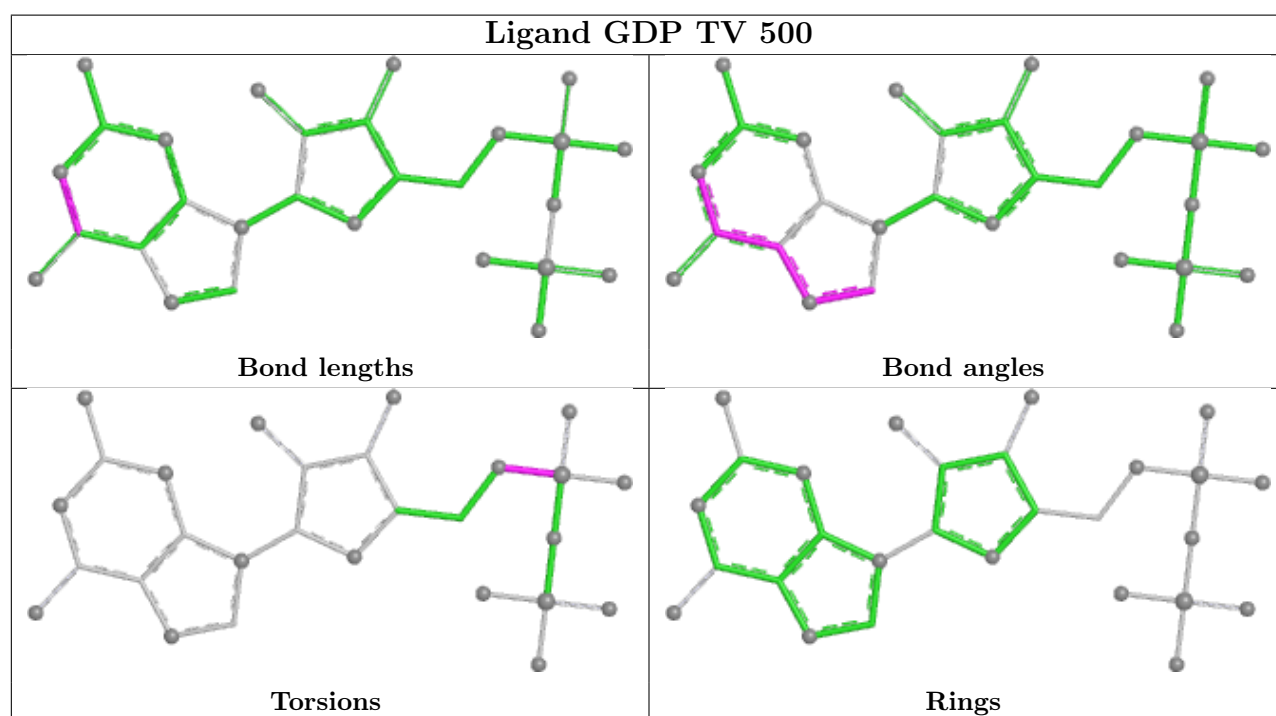
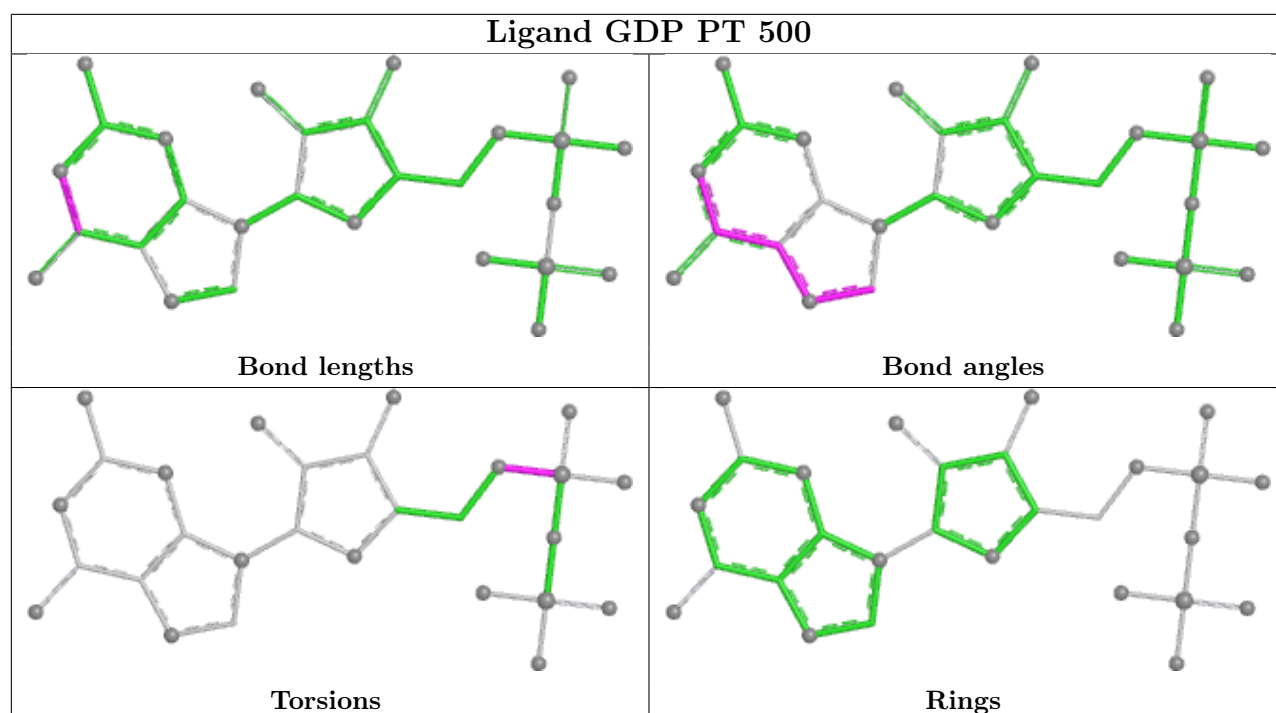


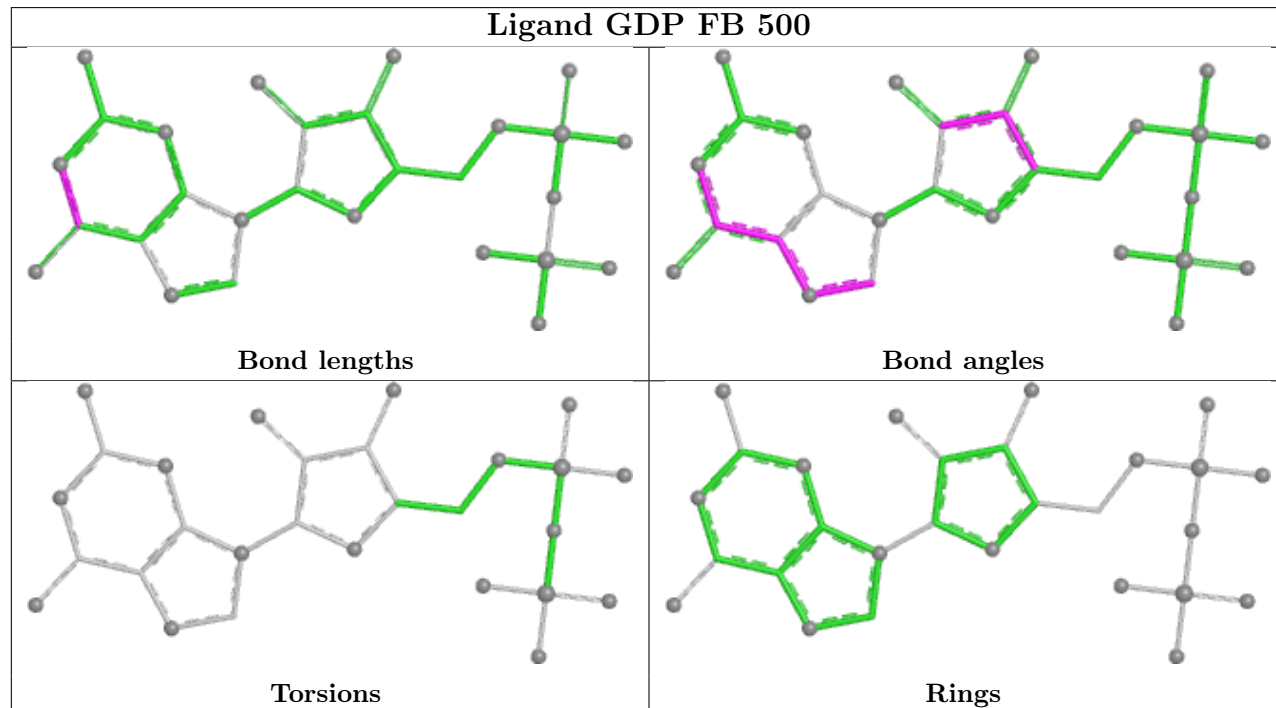
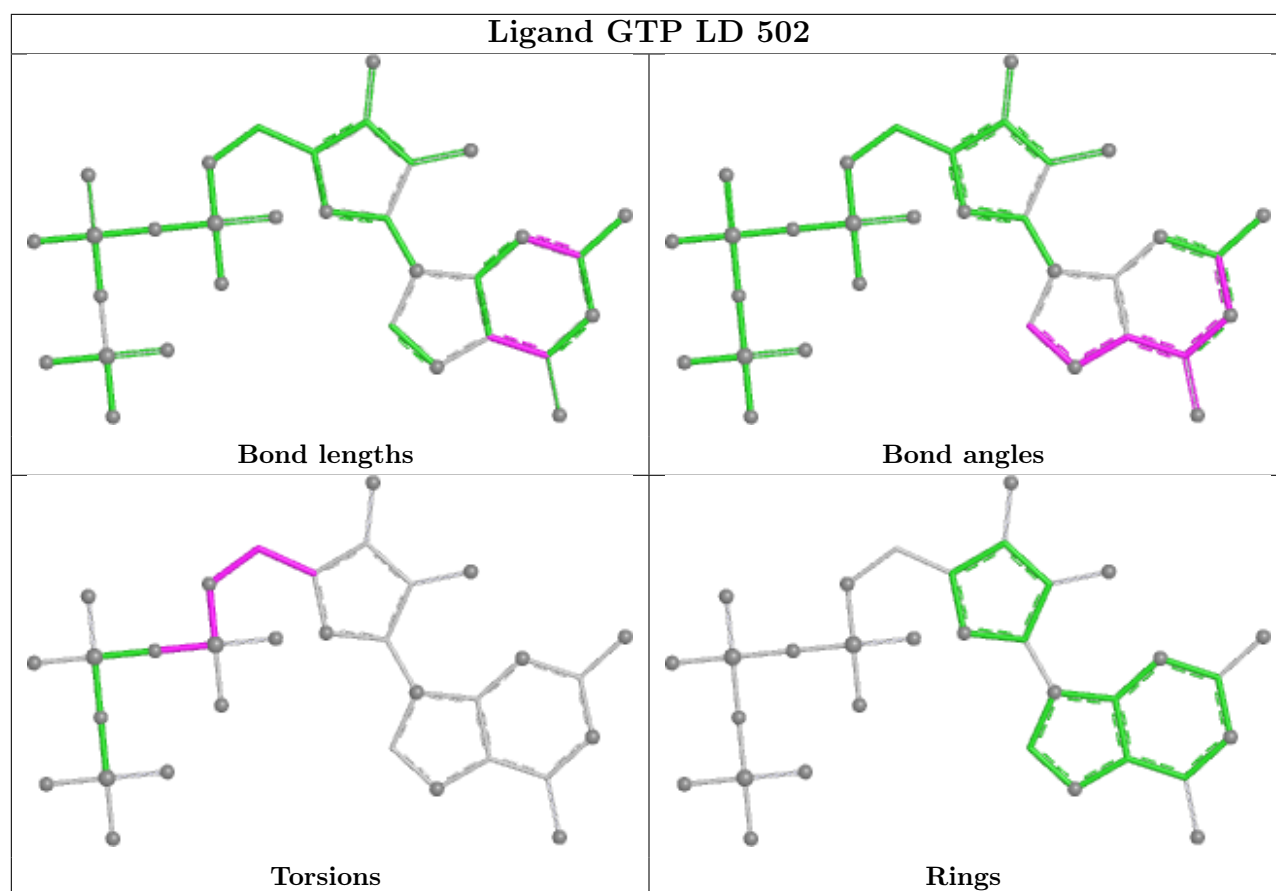


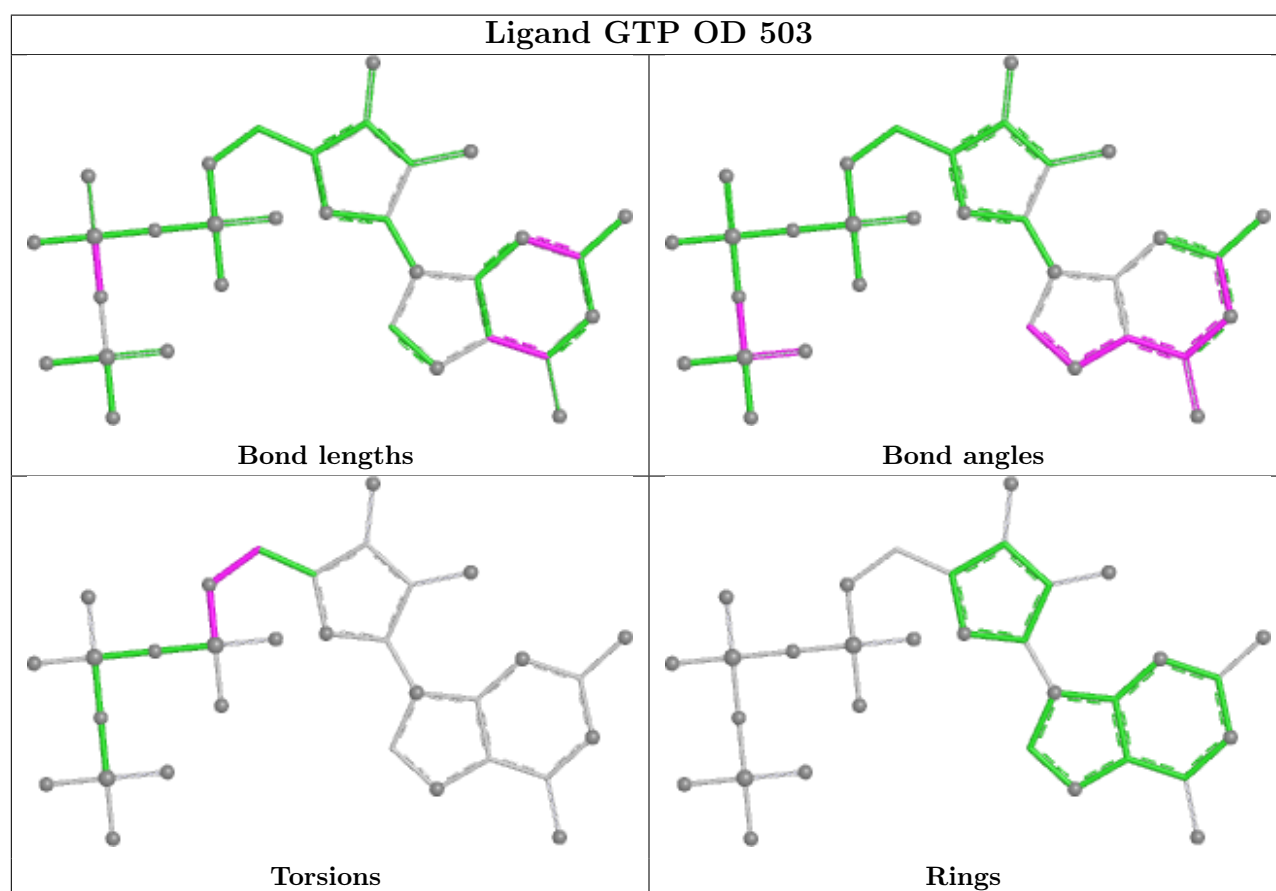
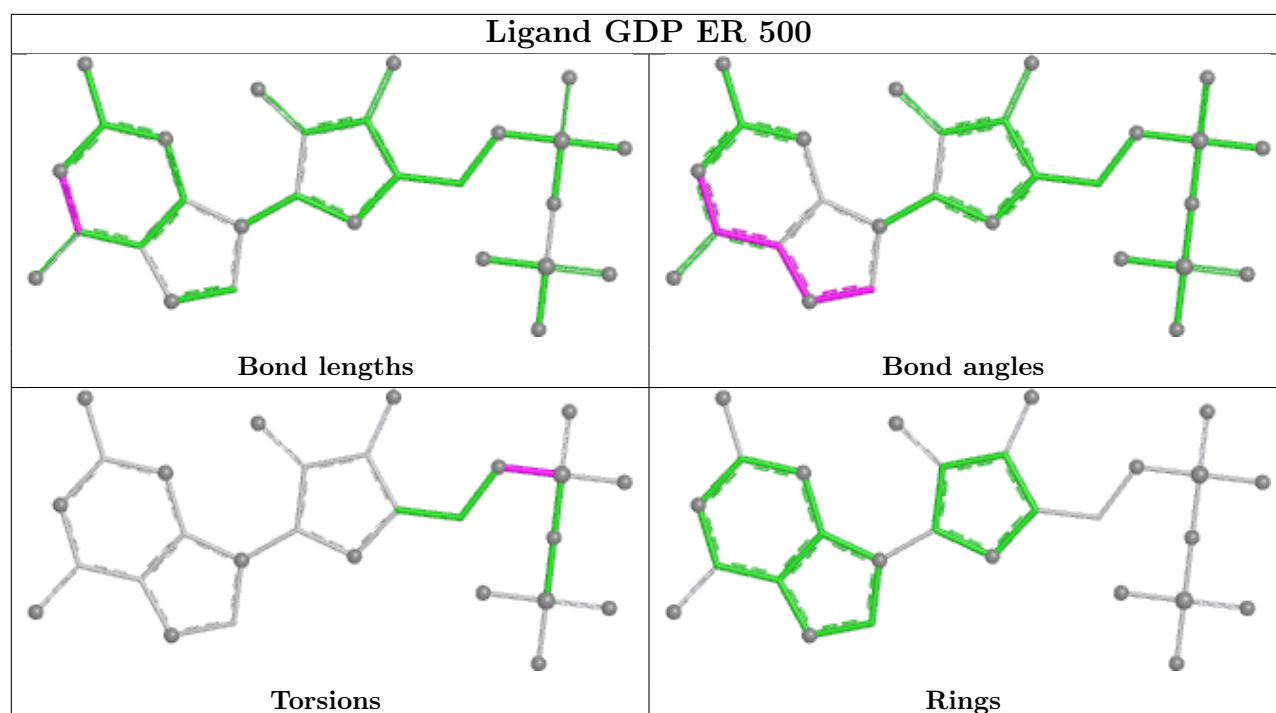




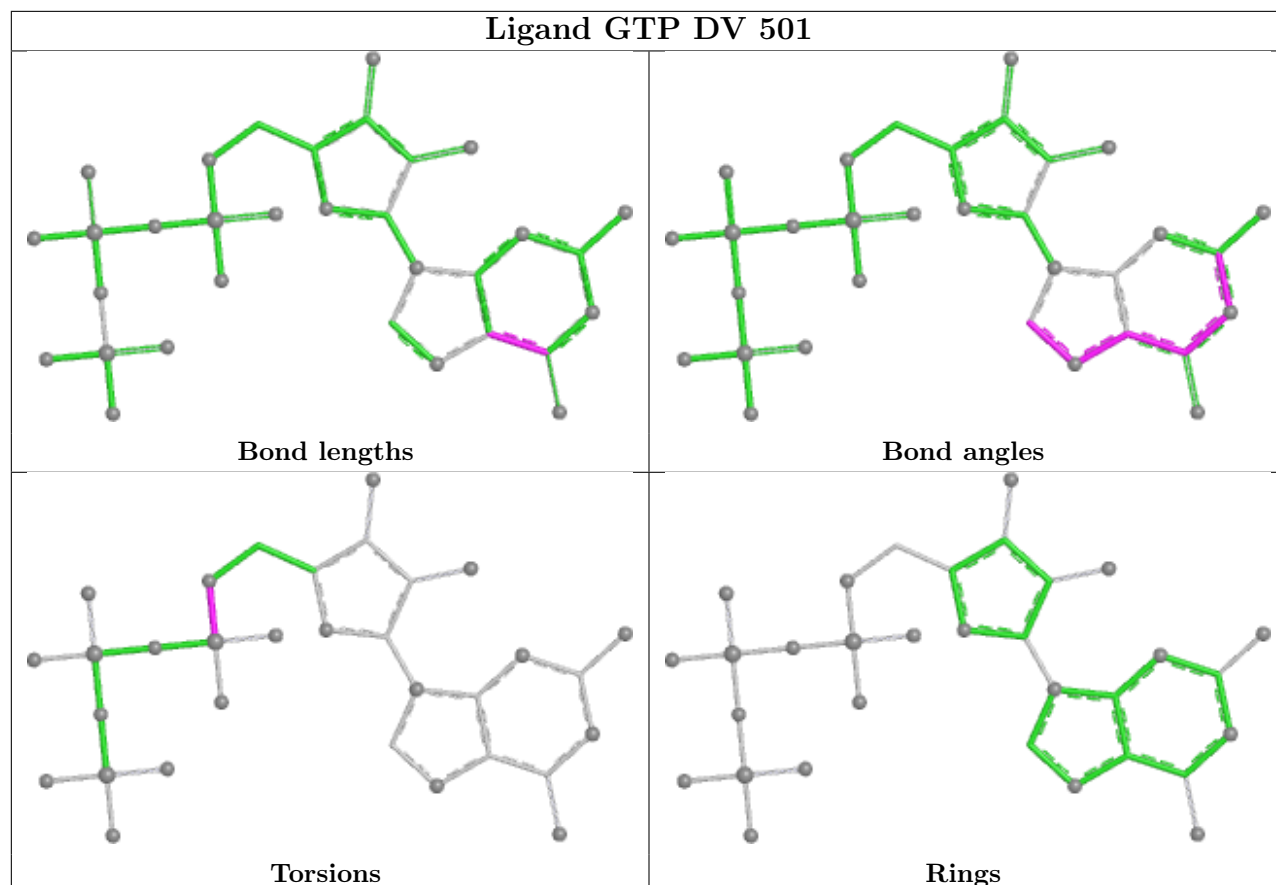




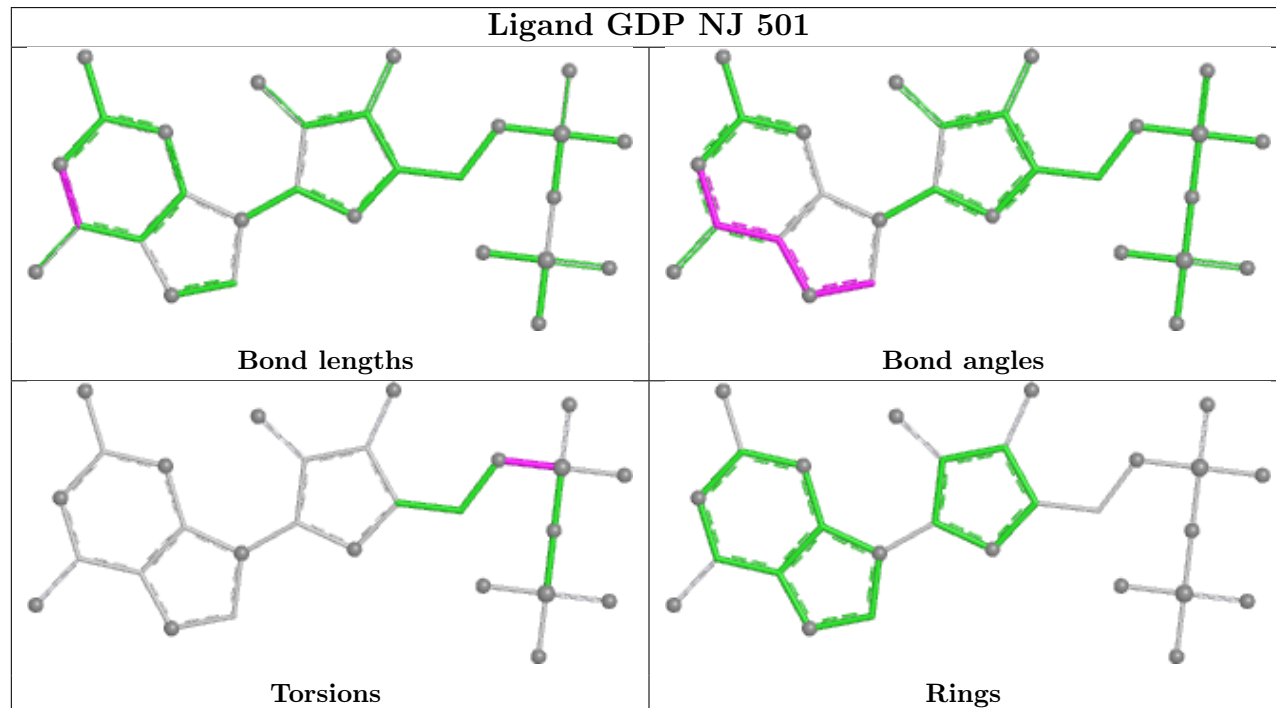


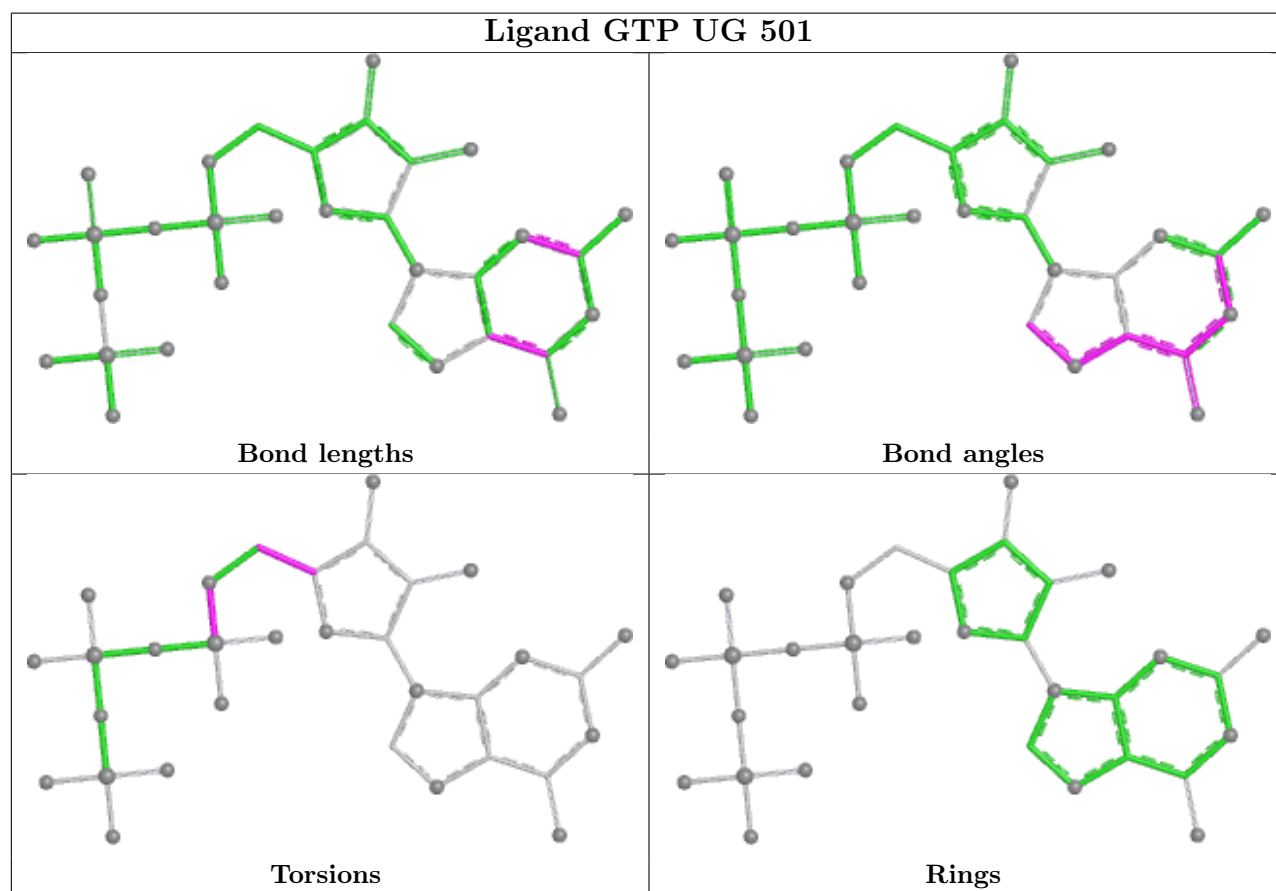
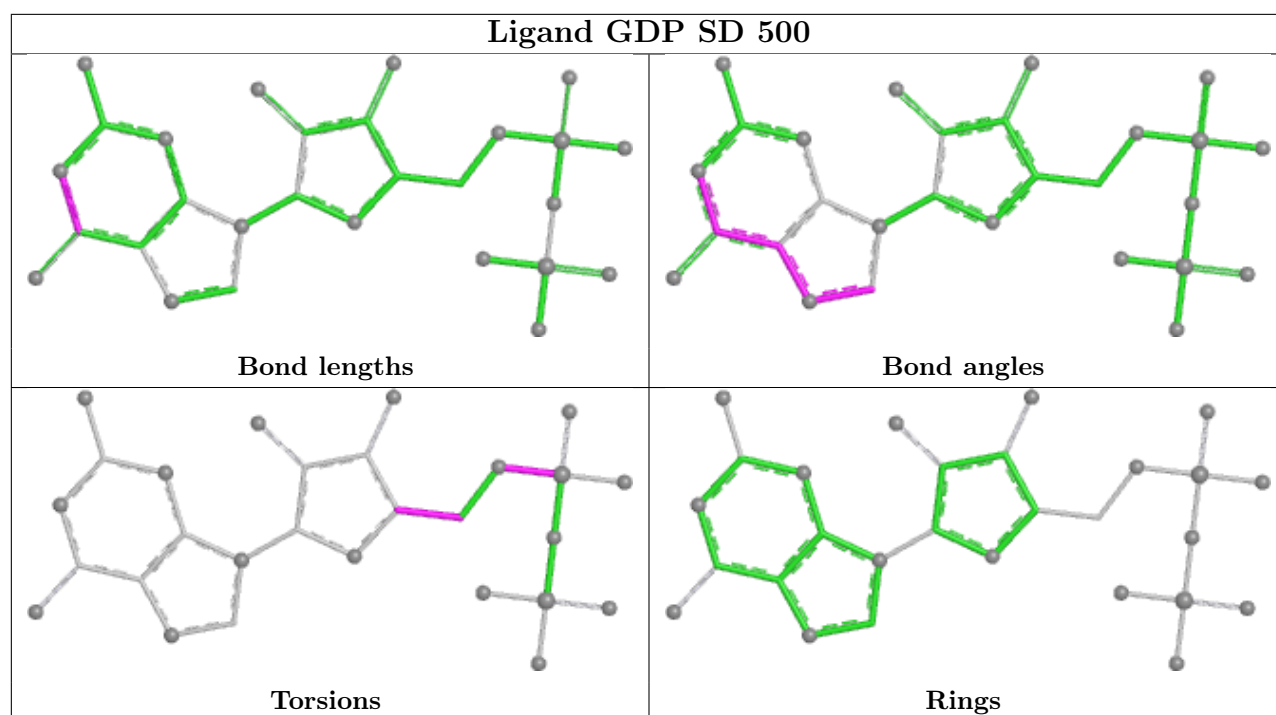


Ligand GTP DV 501

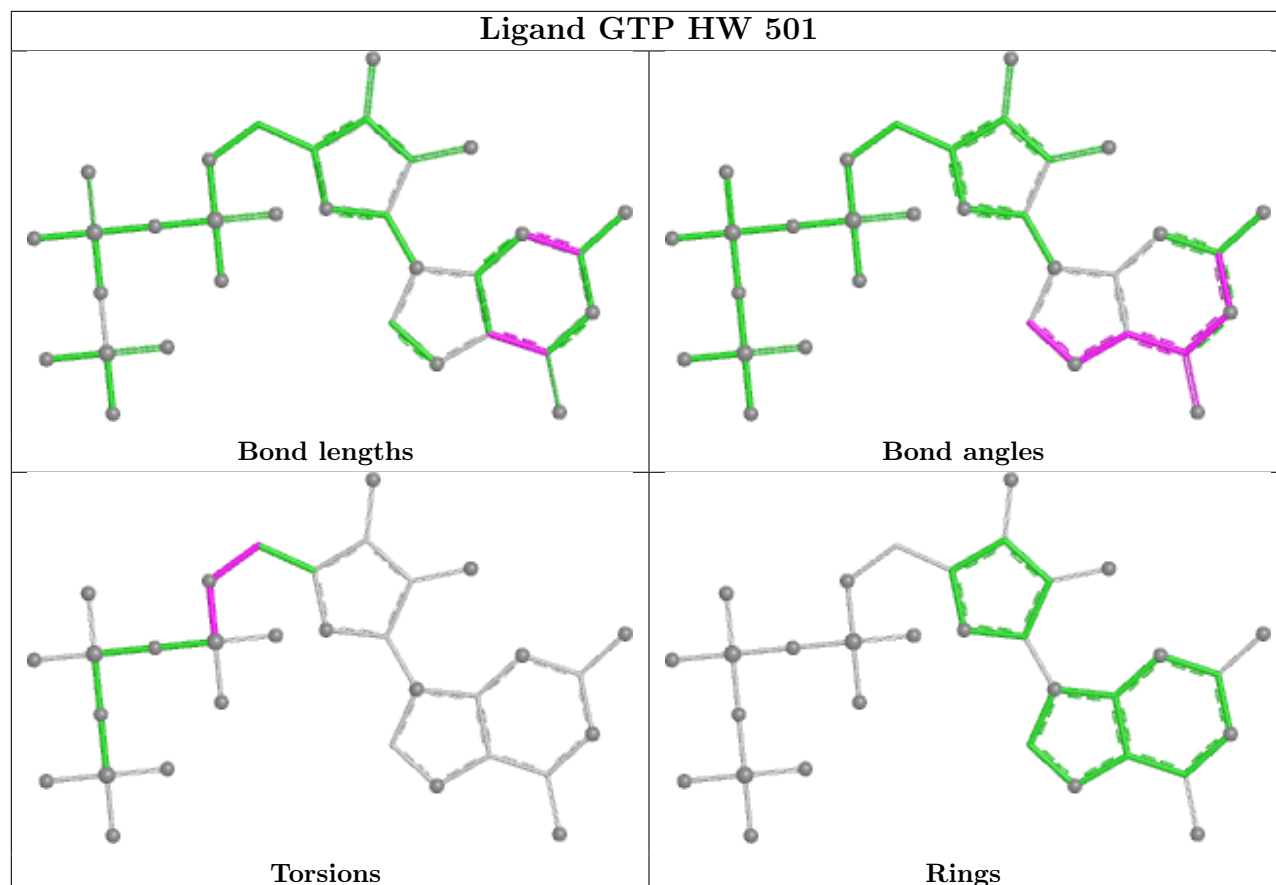


Ligand GDP NJ 501

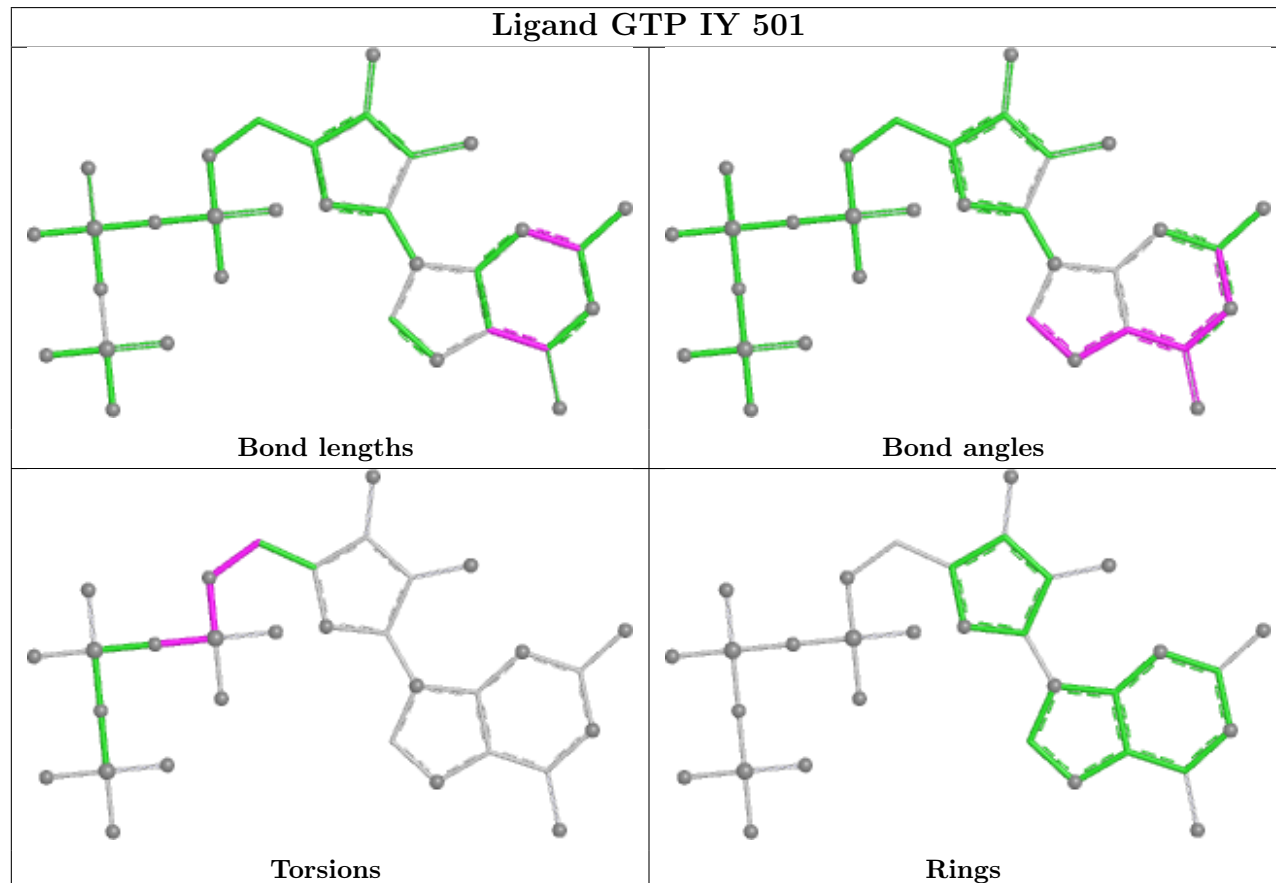


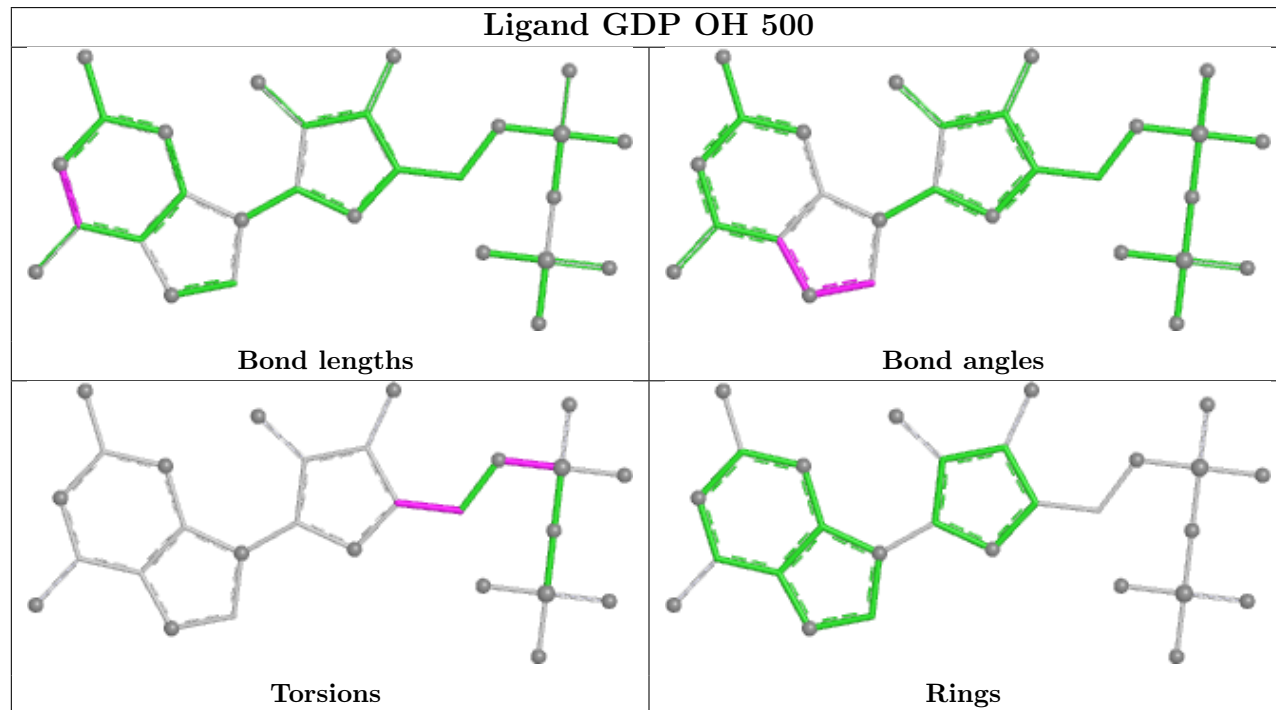
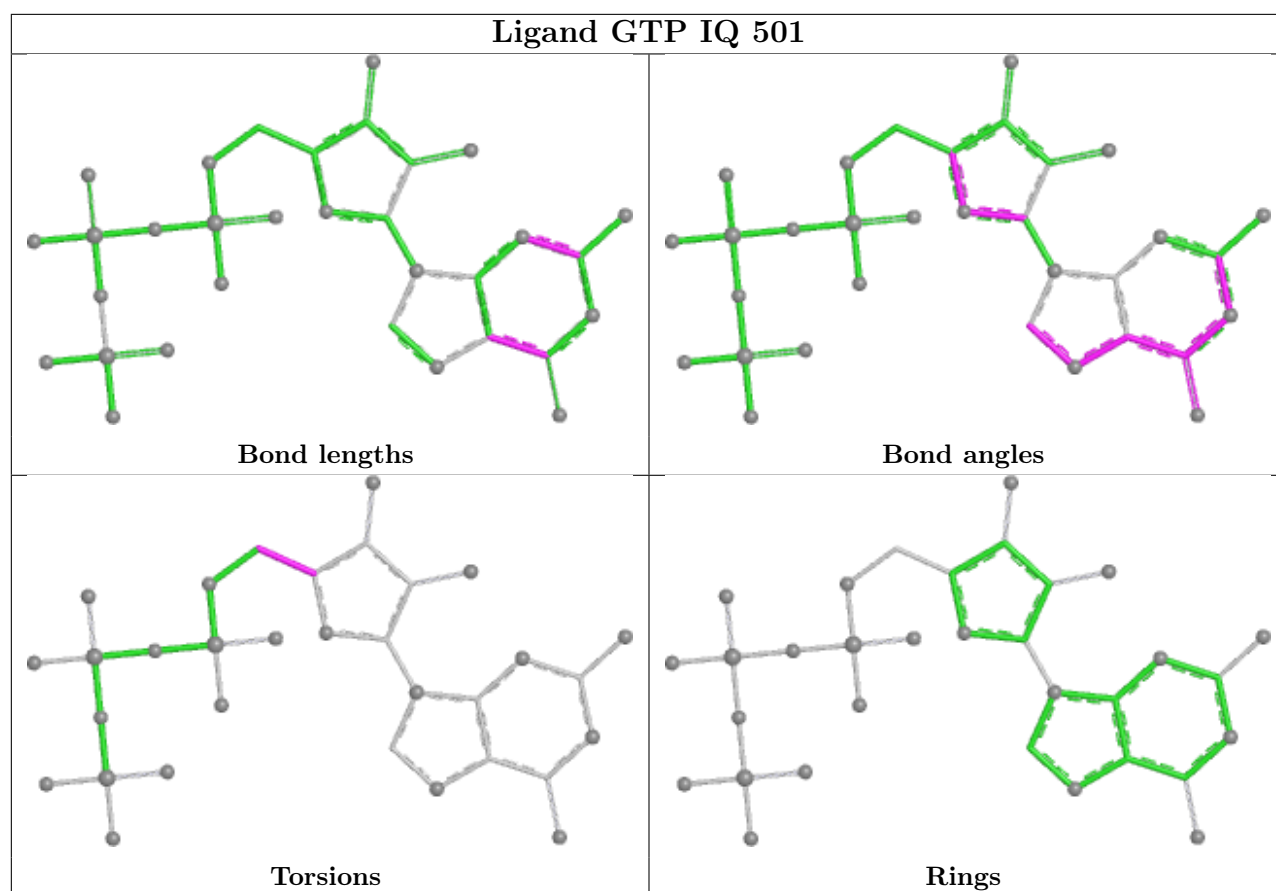


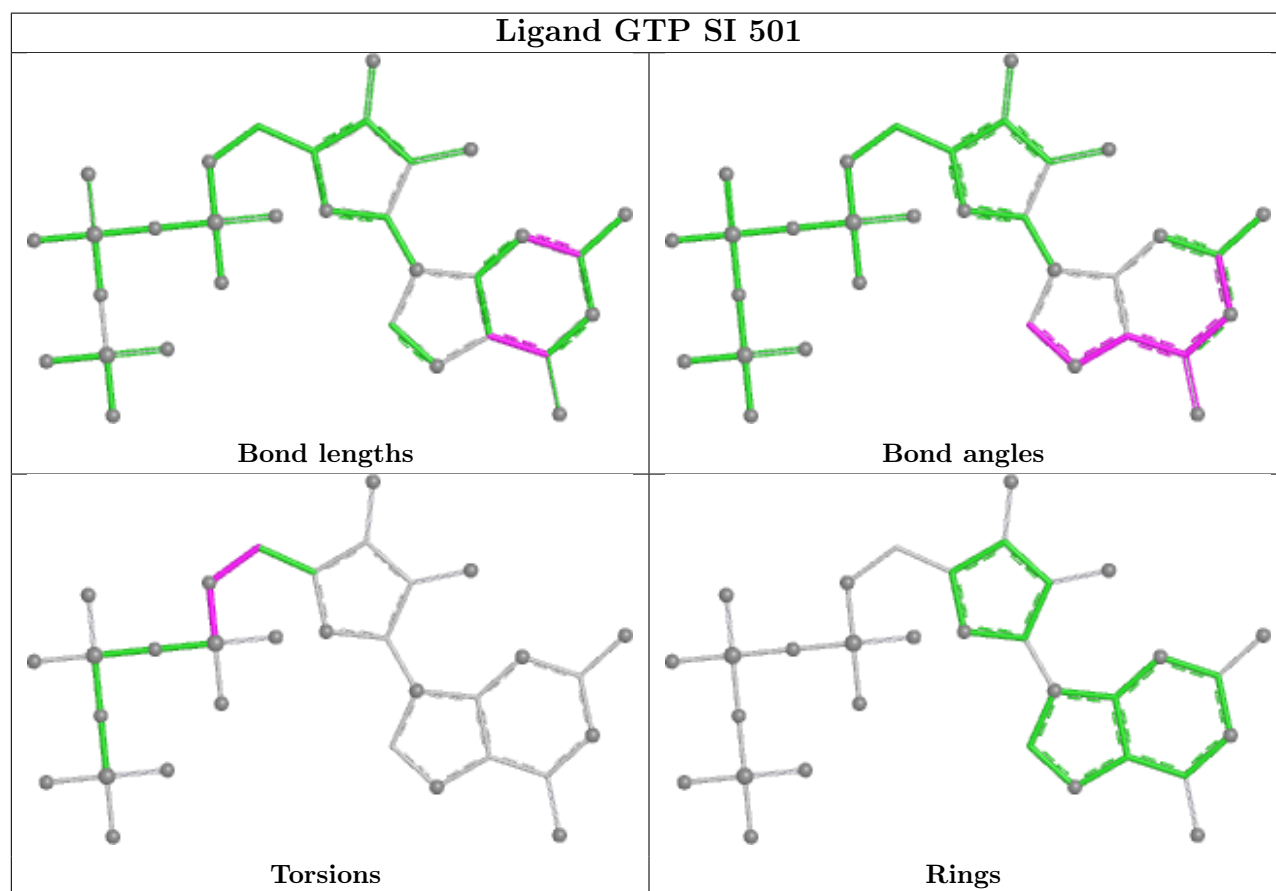
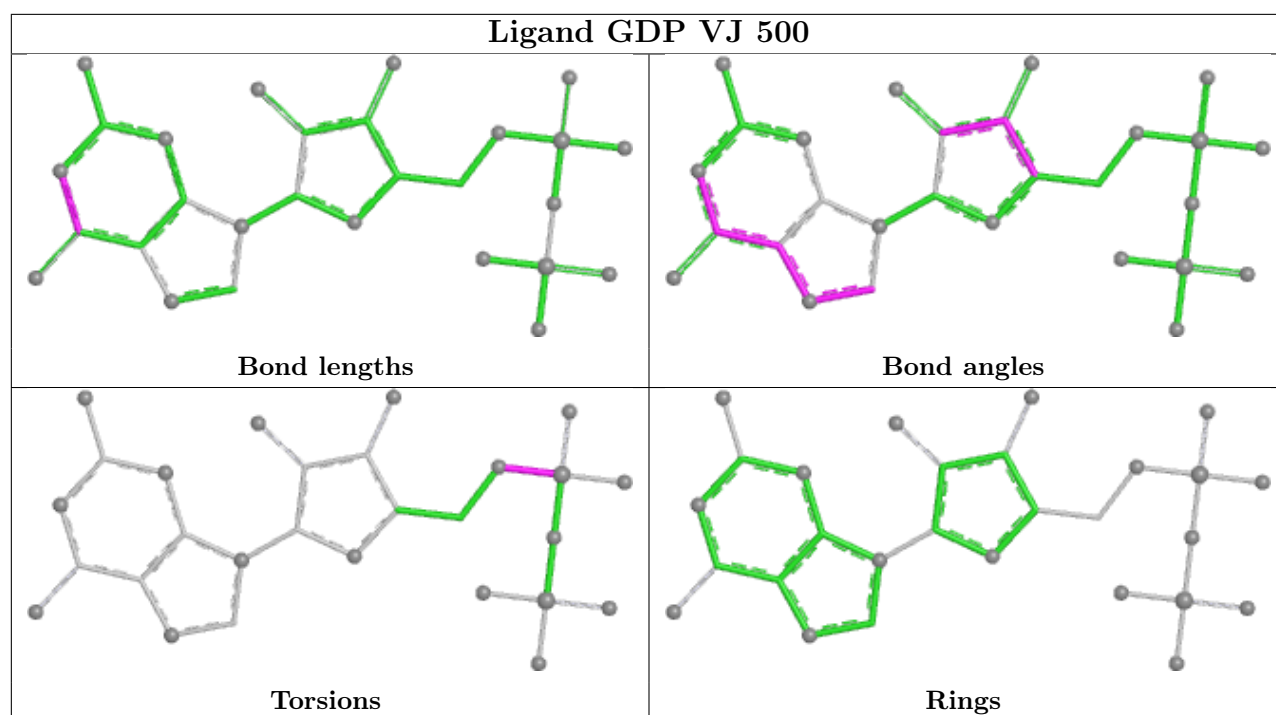
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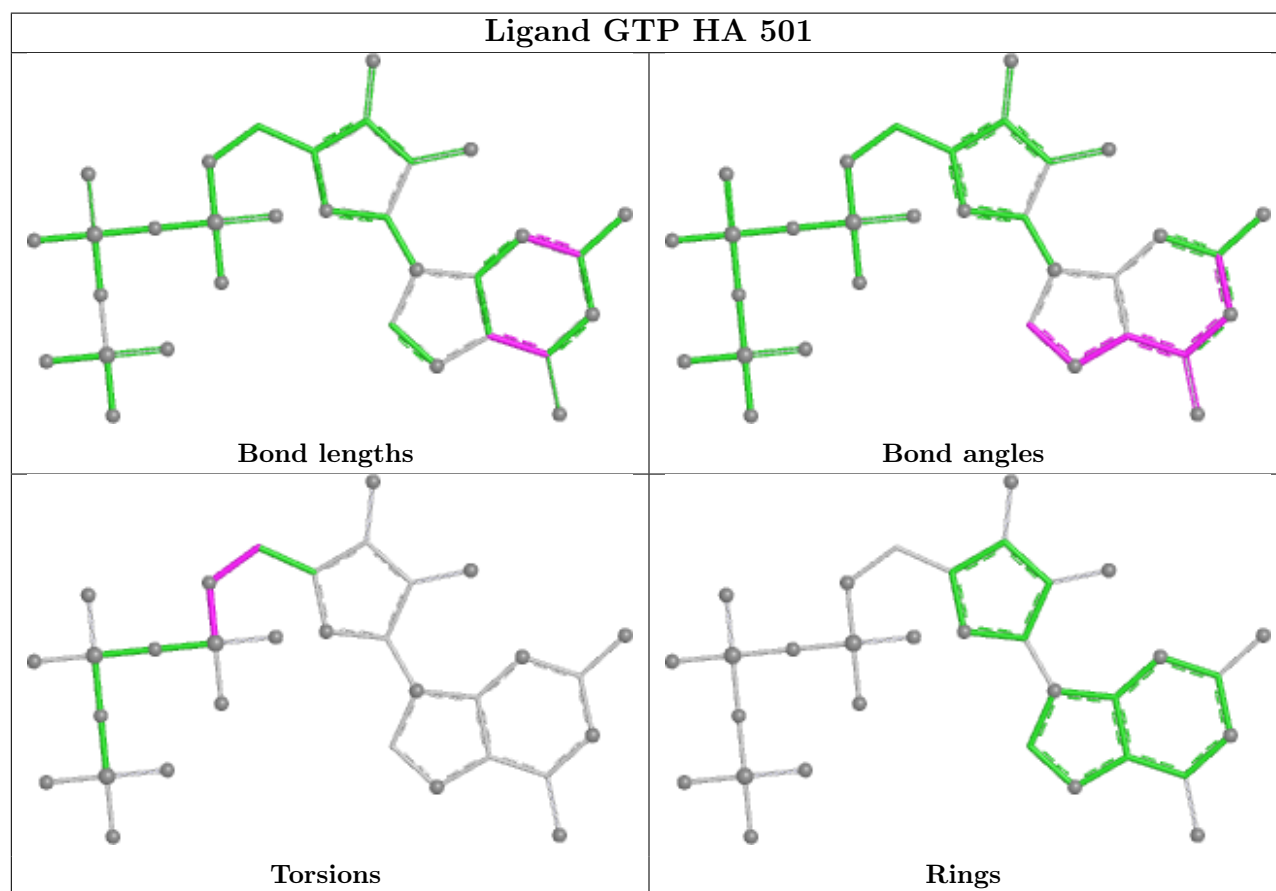
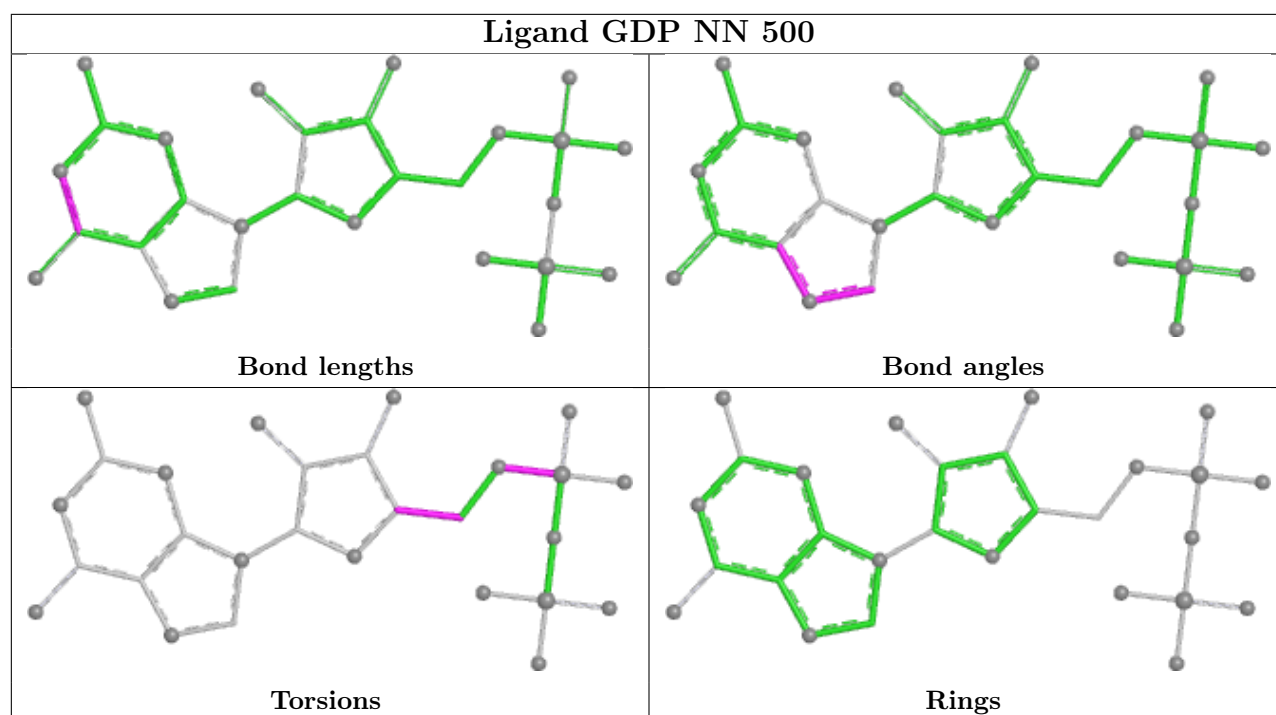


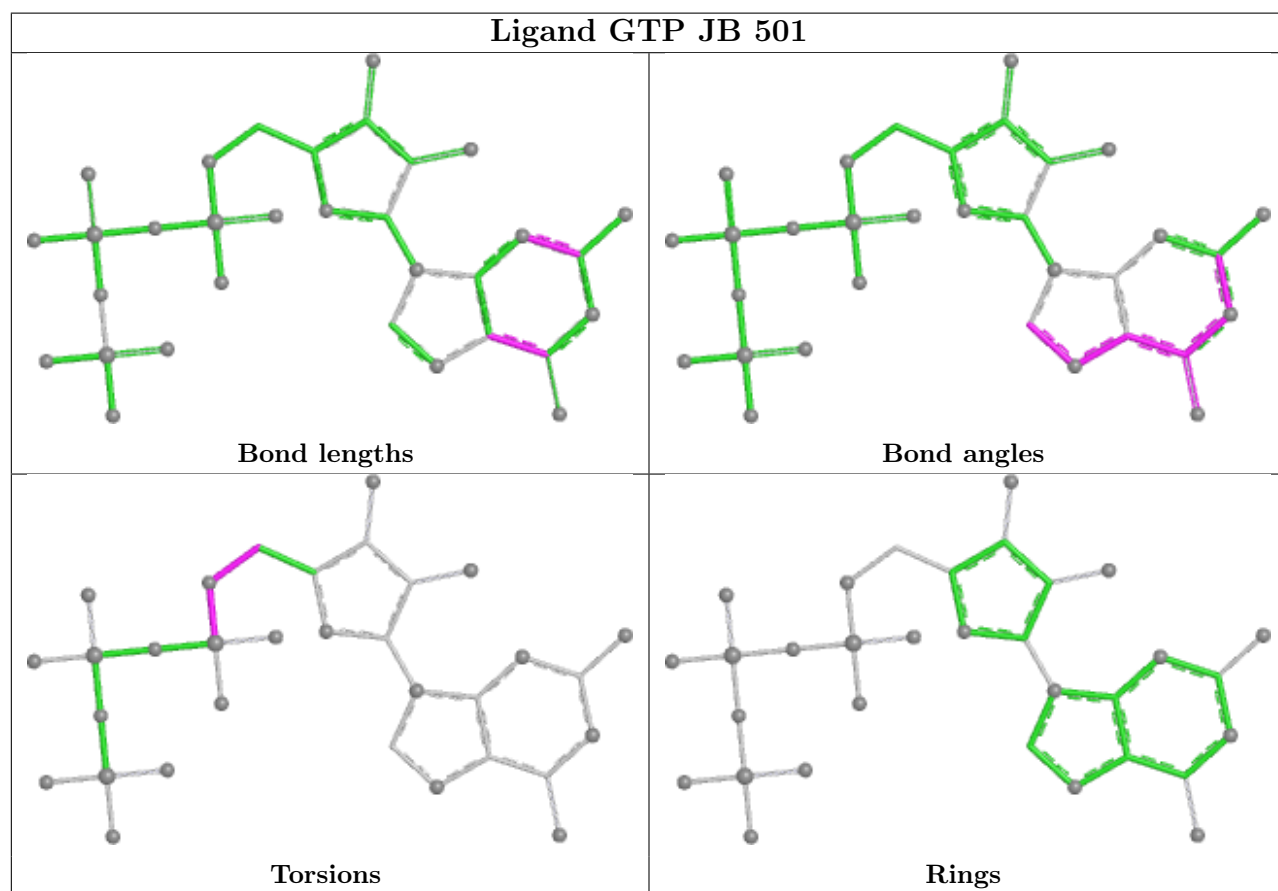
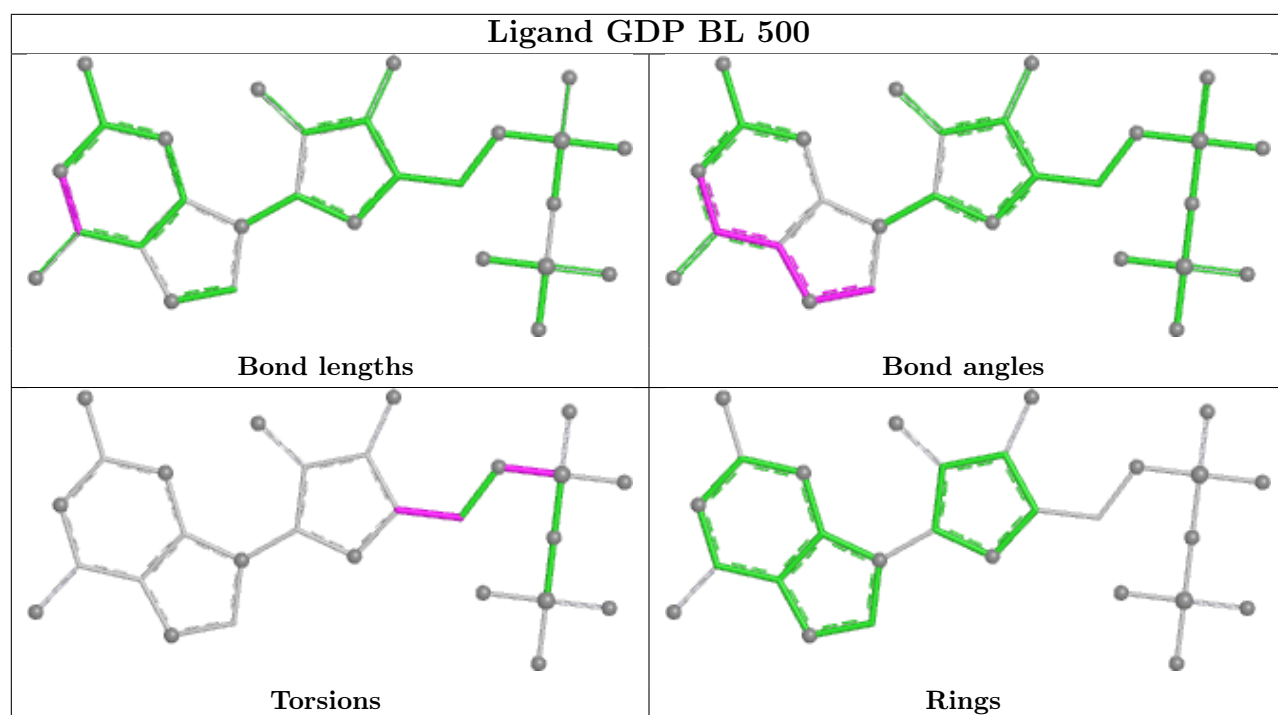
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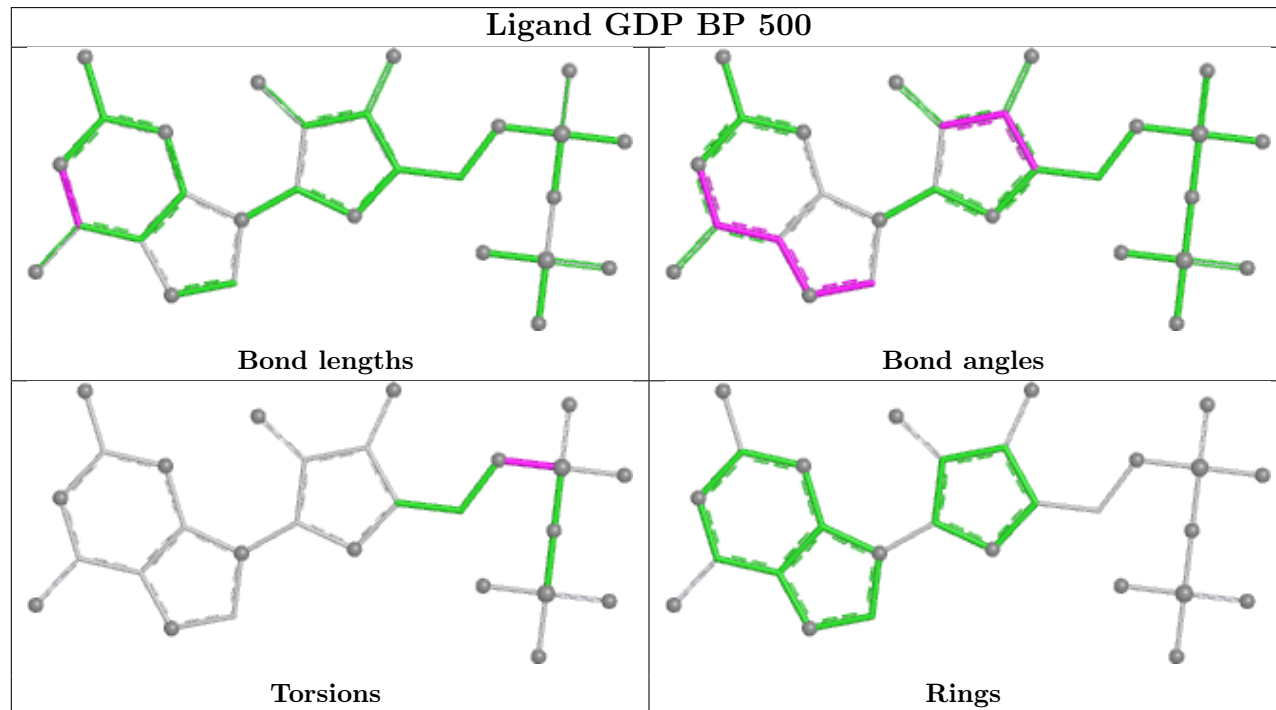
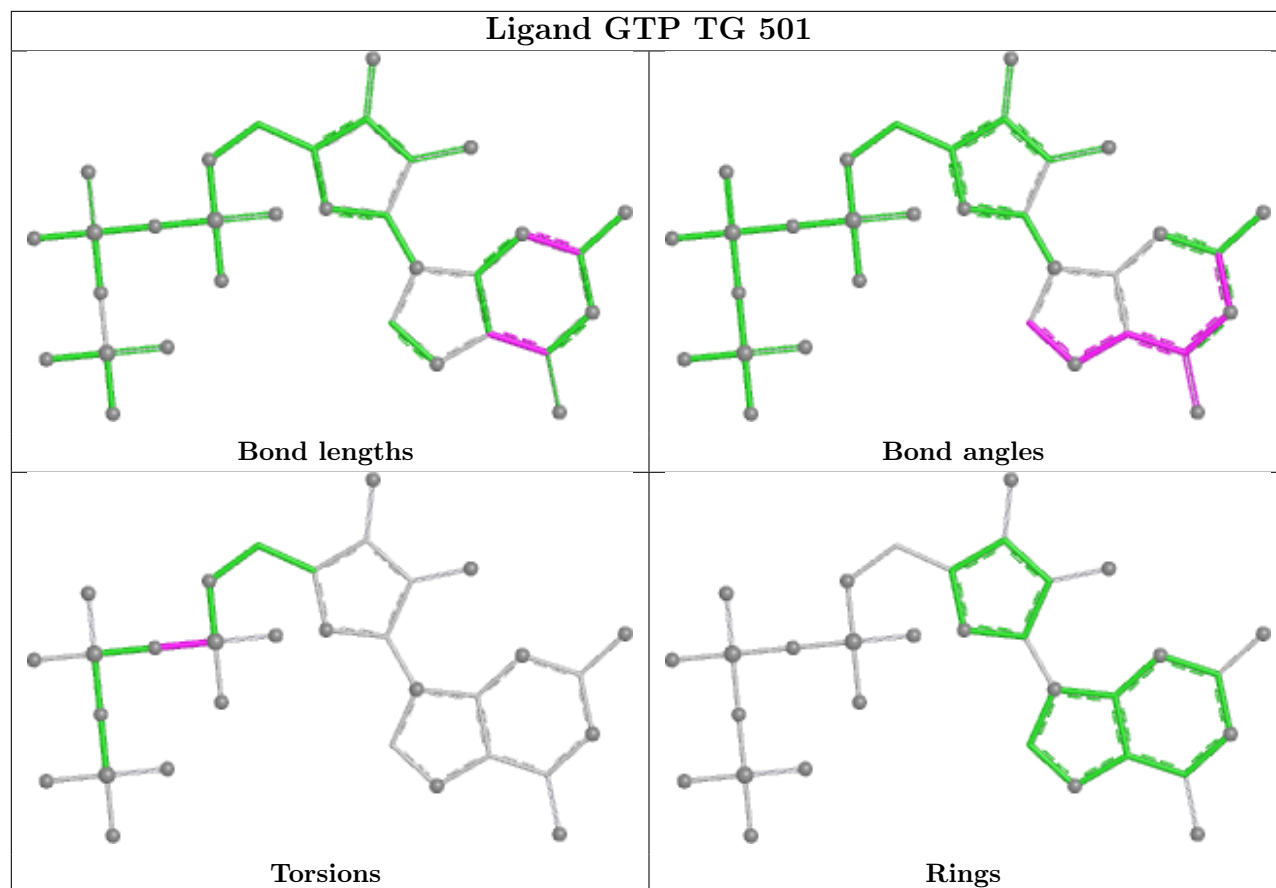




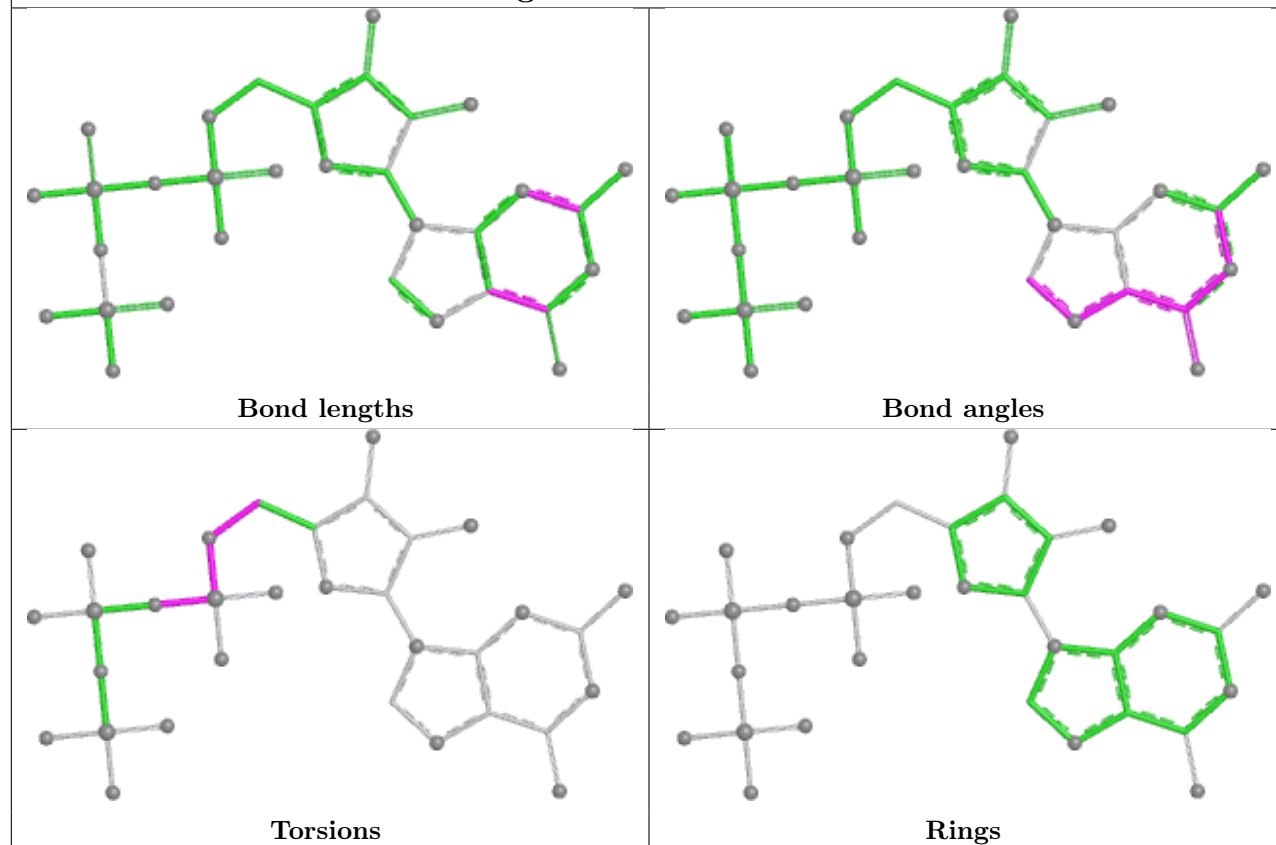




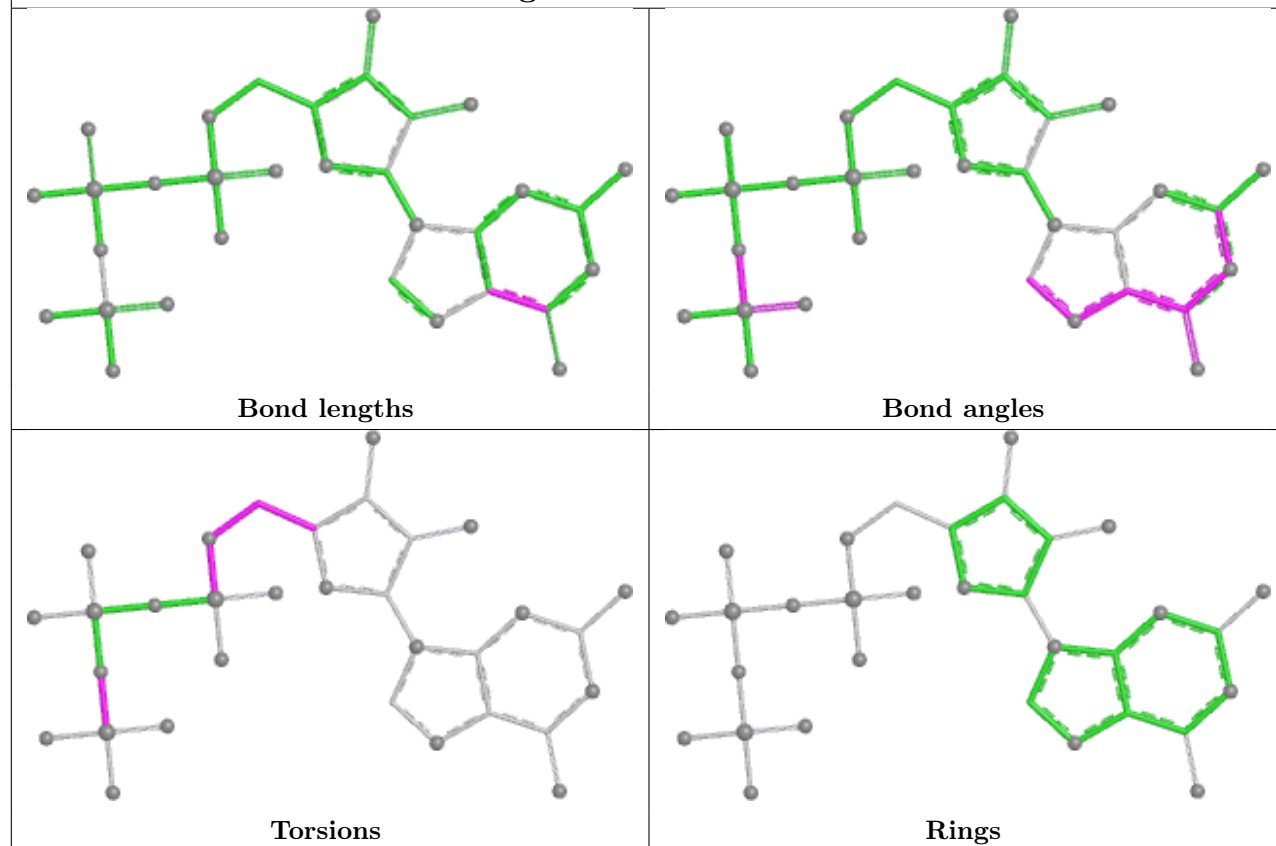




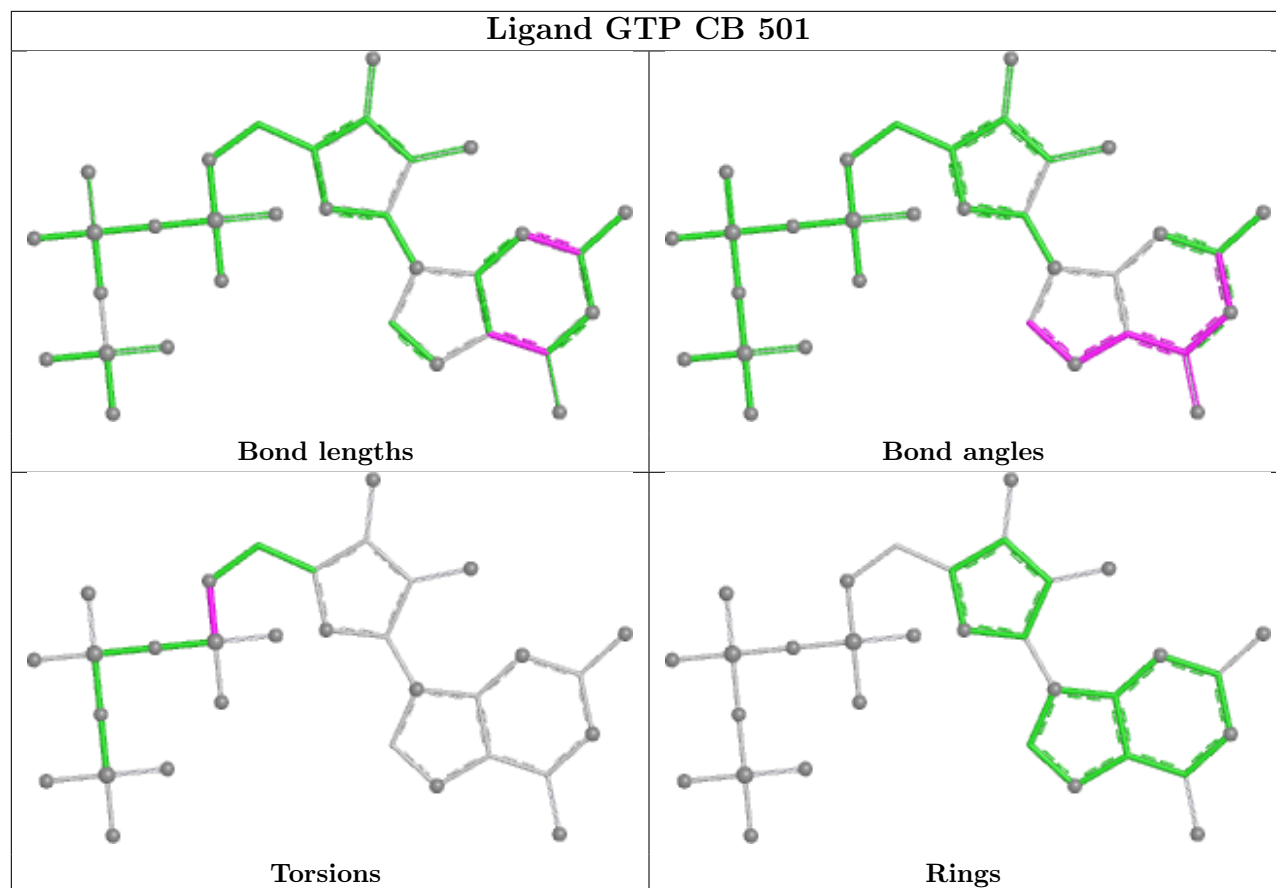
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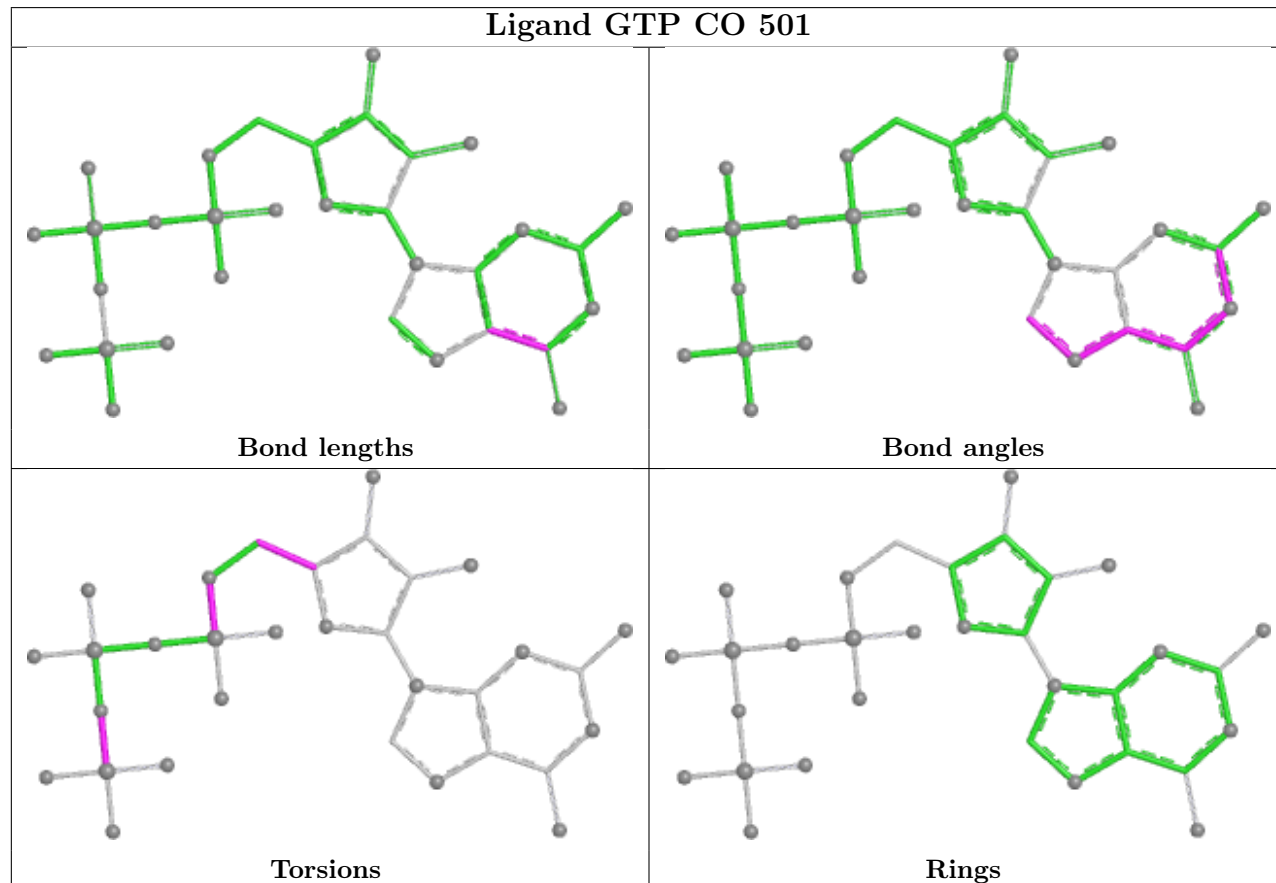
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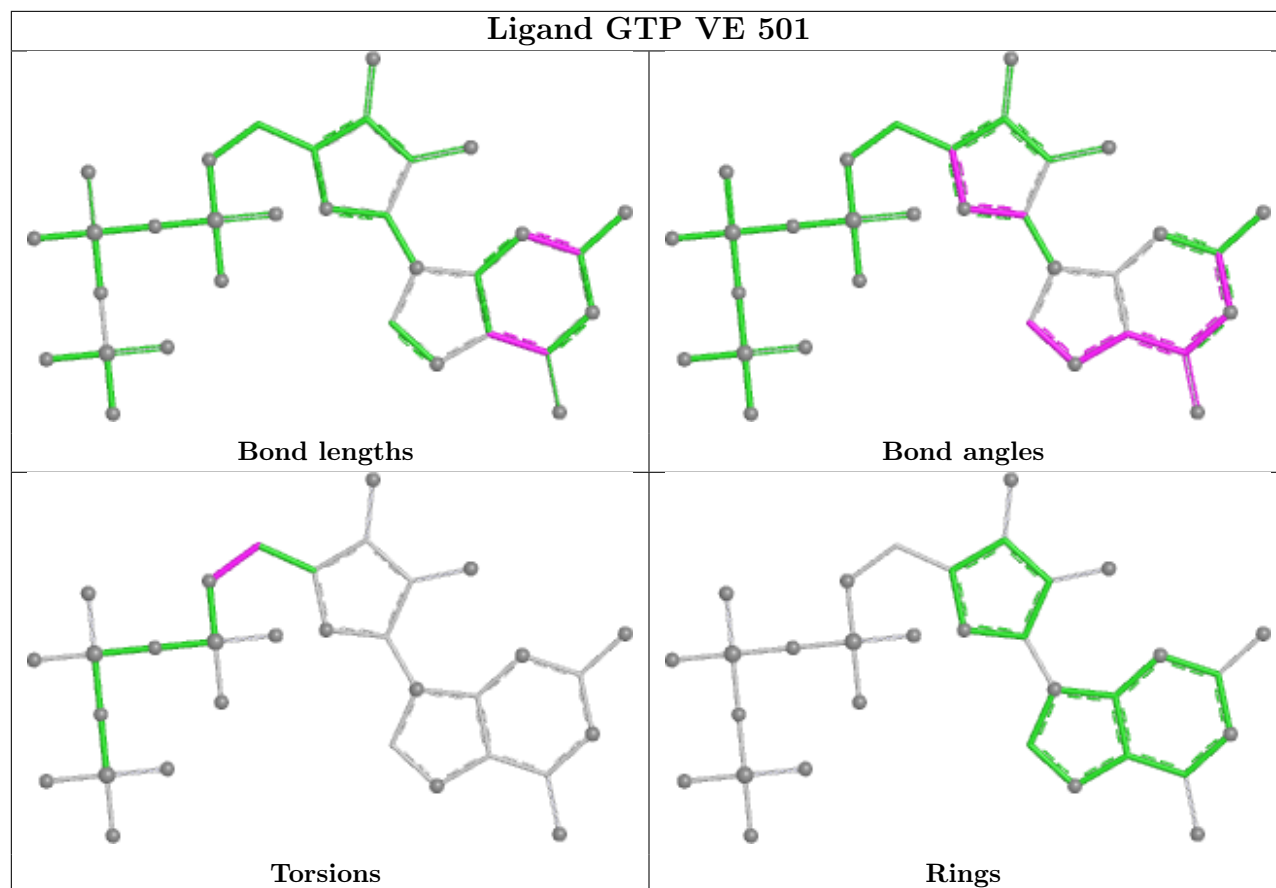
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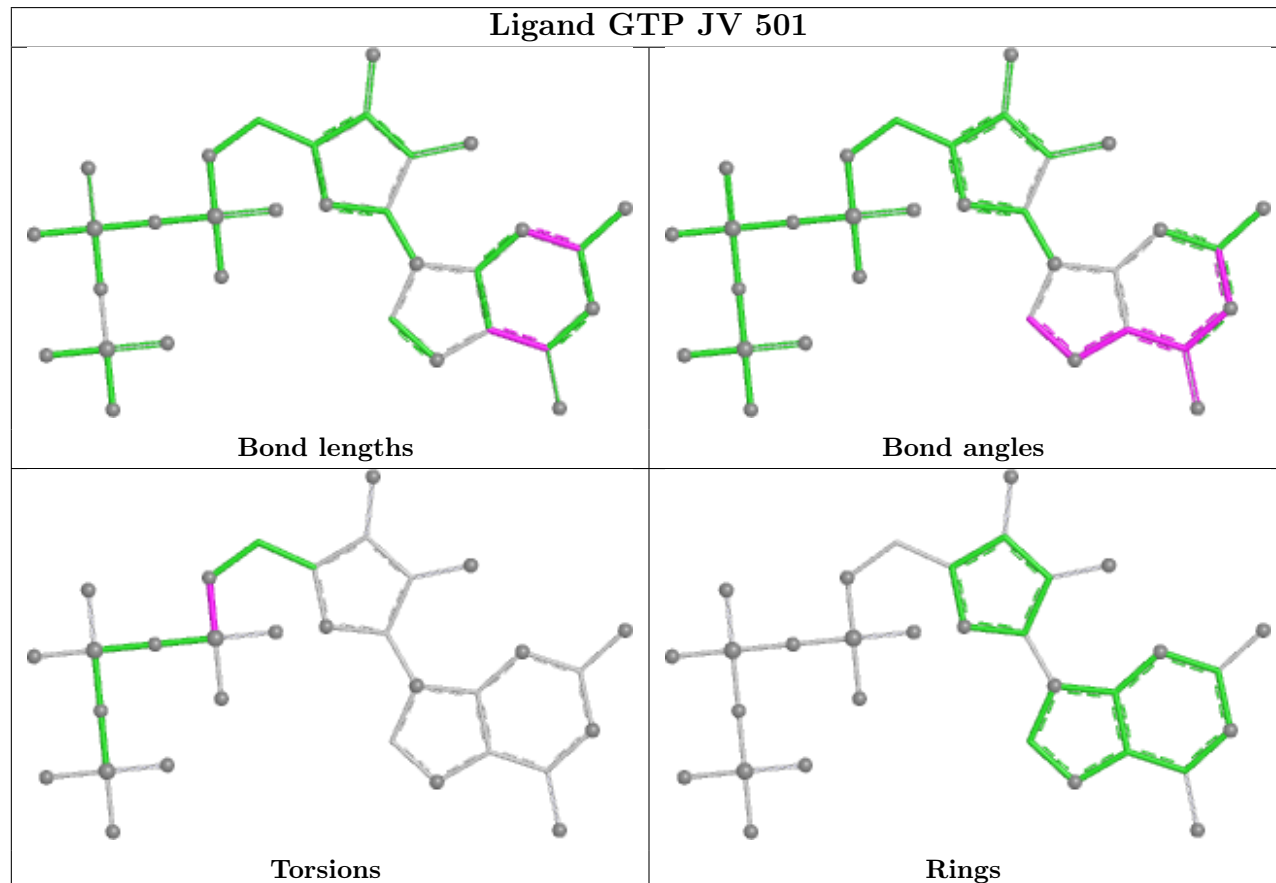
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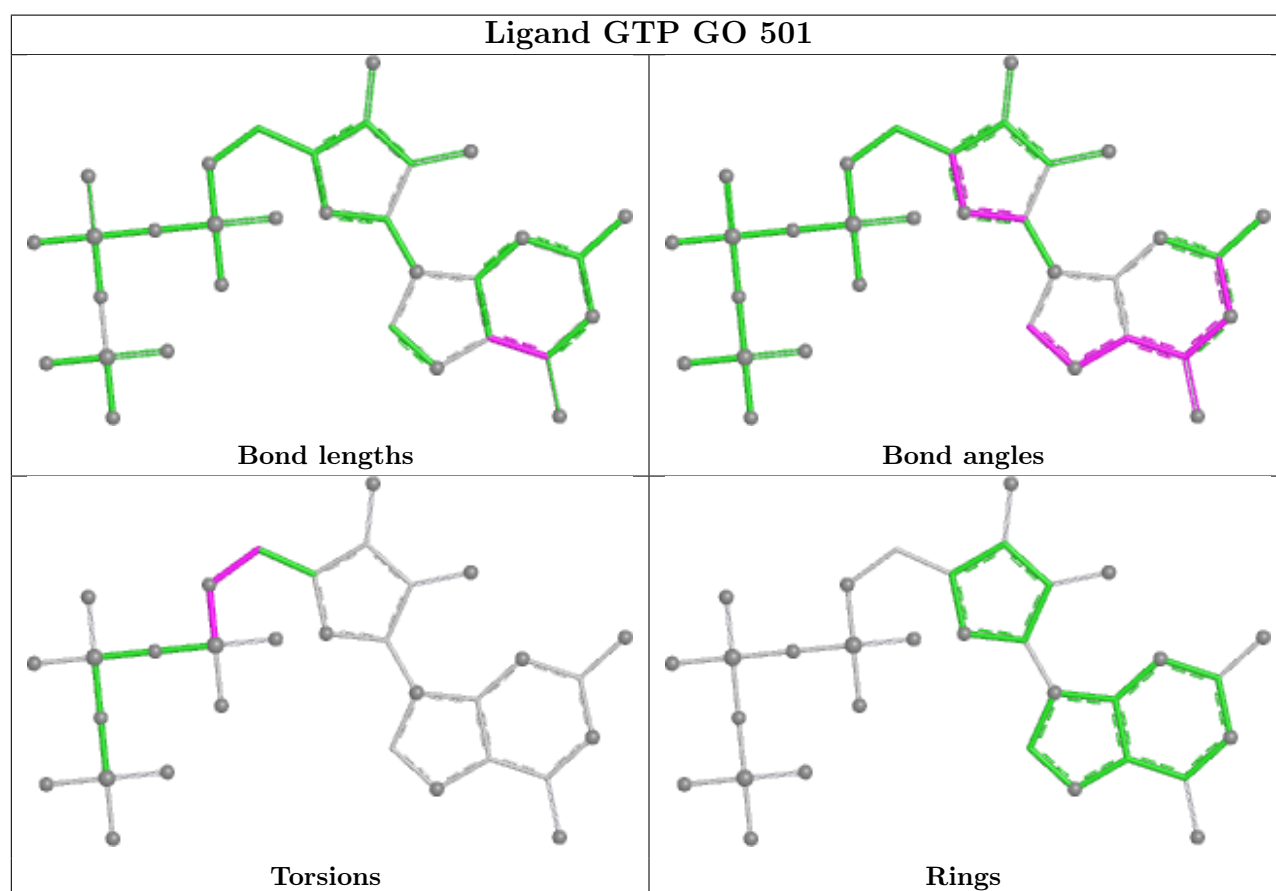
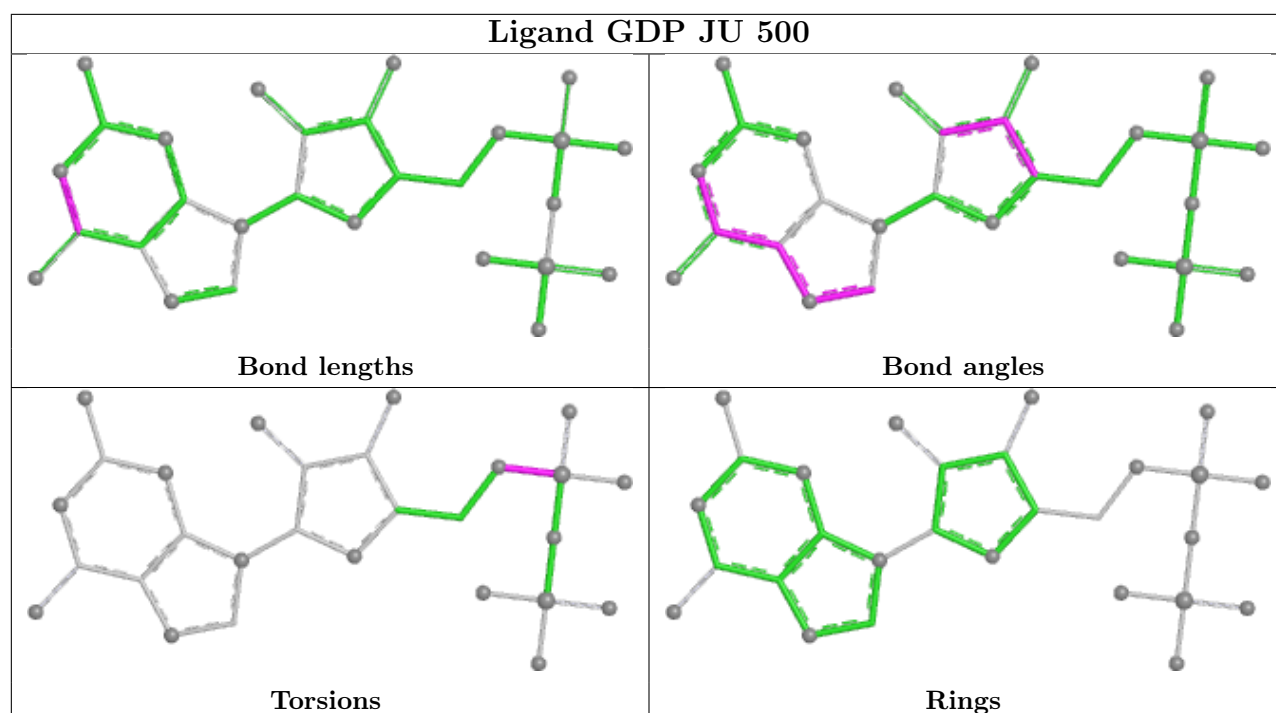


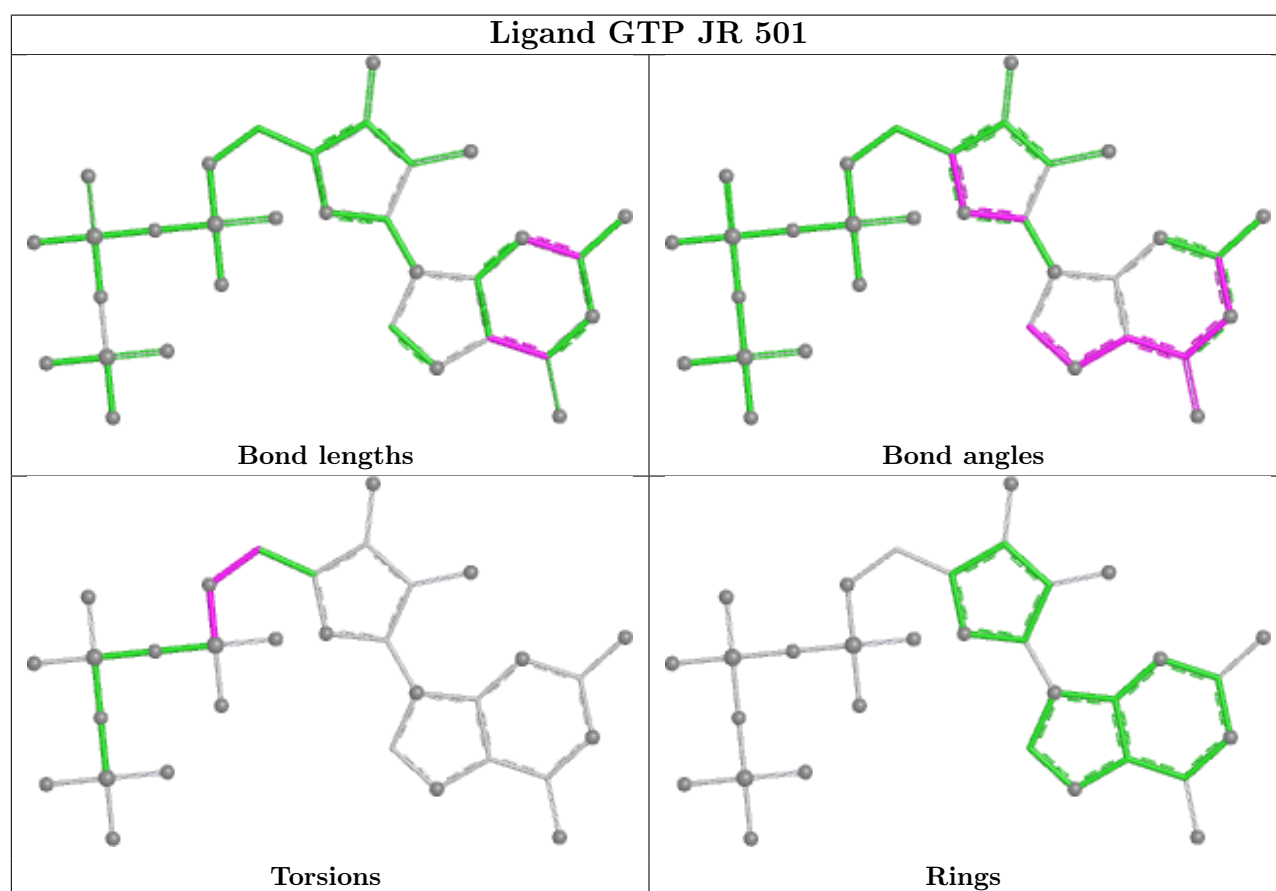
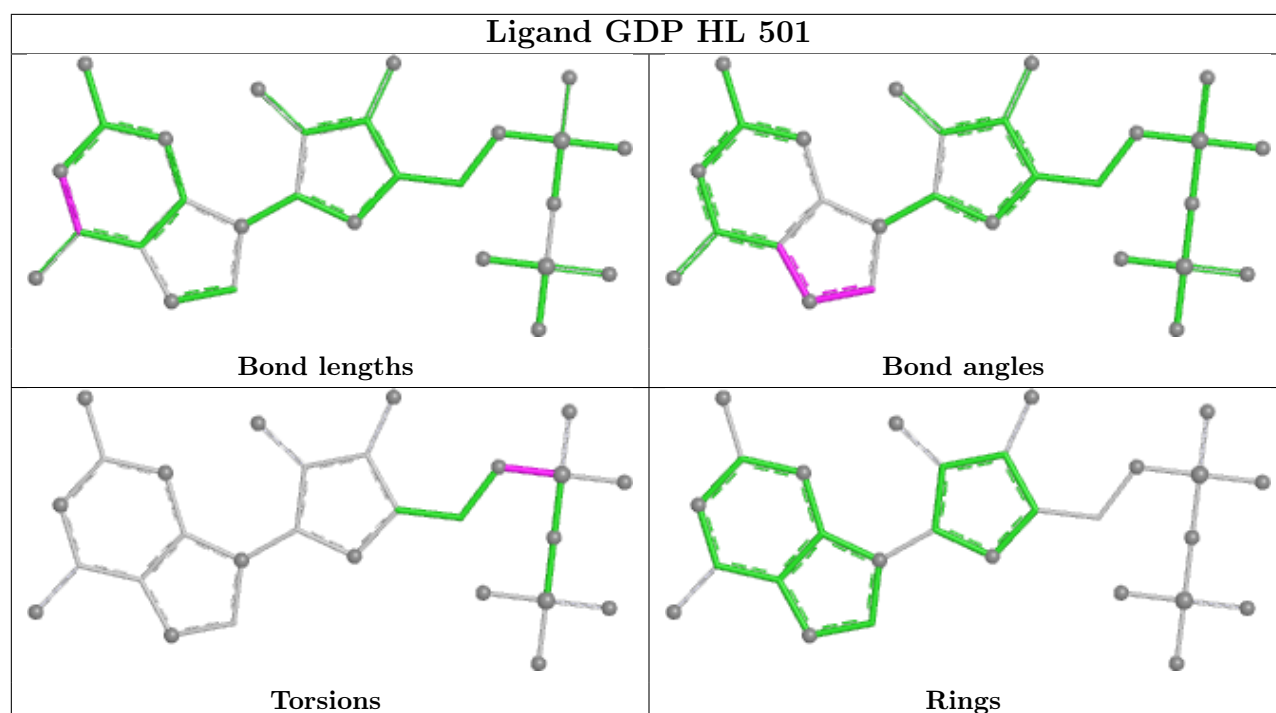
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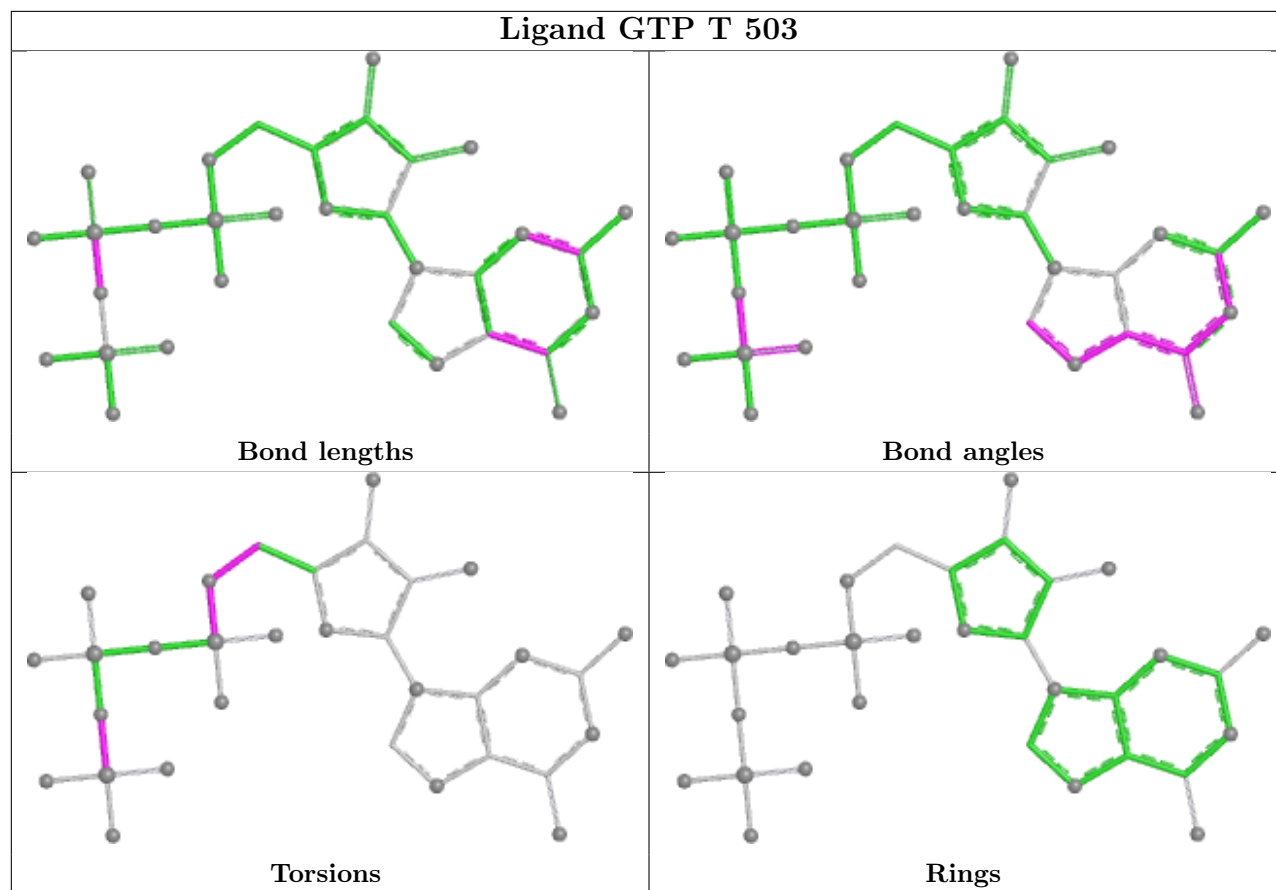


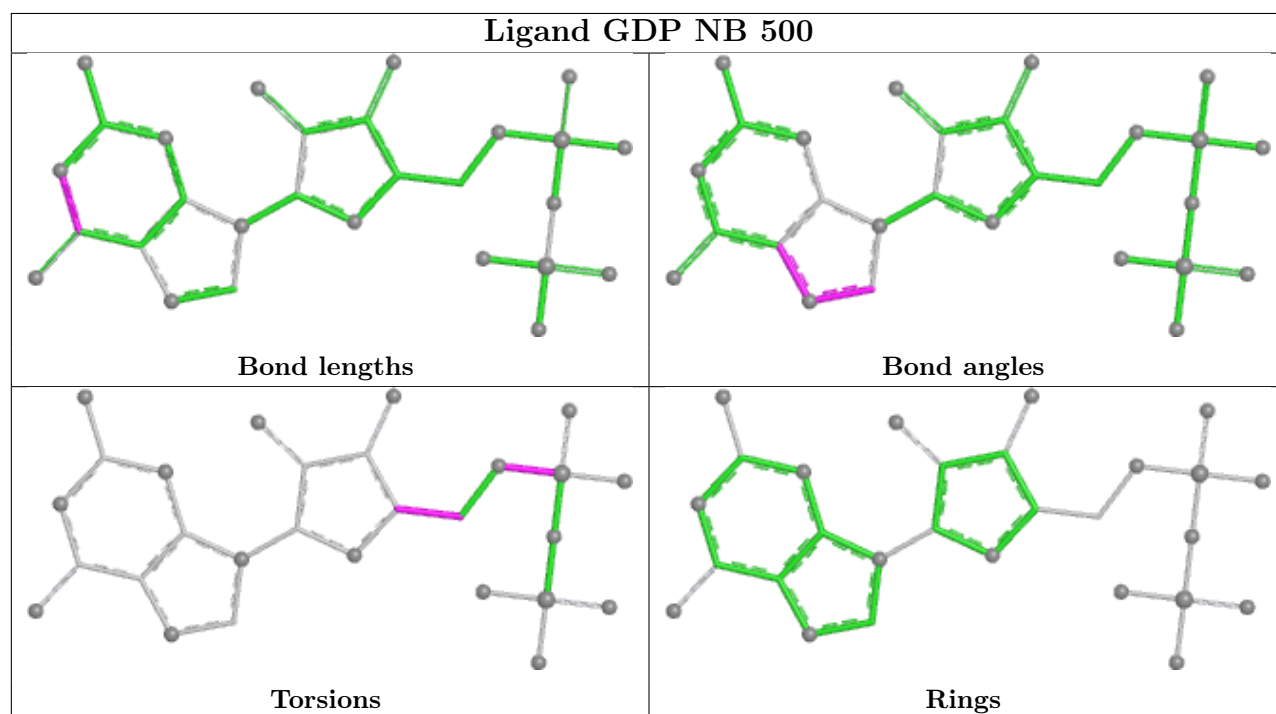
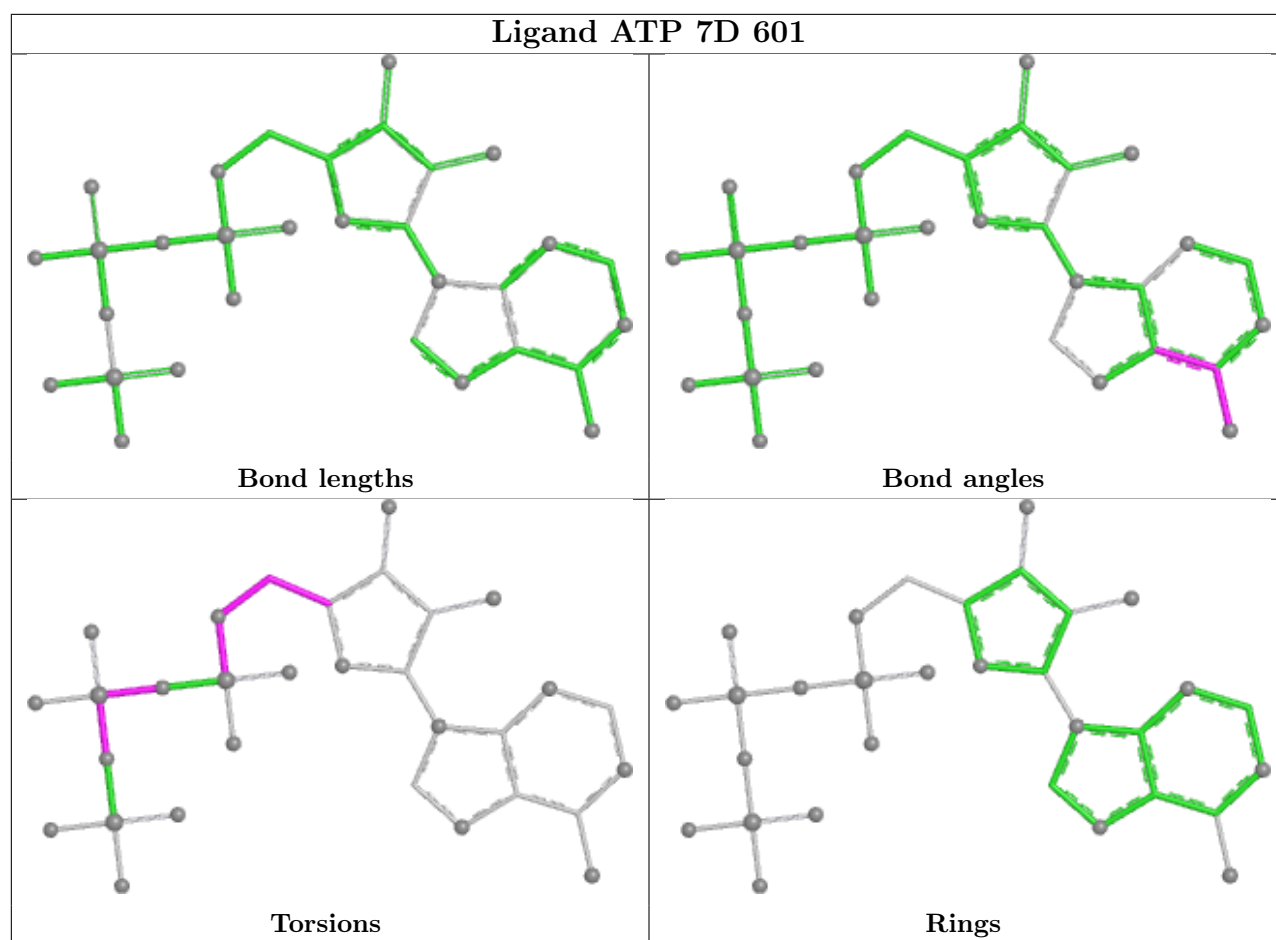
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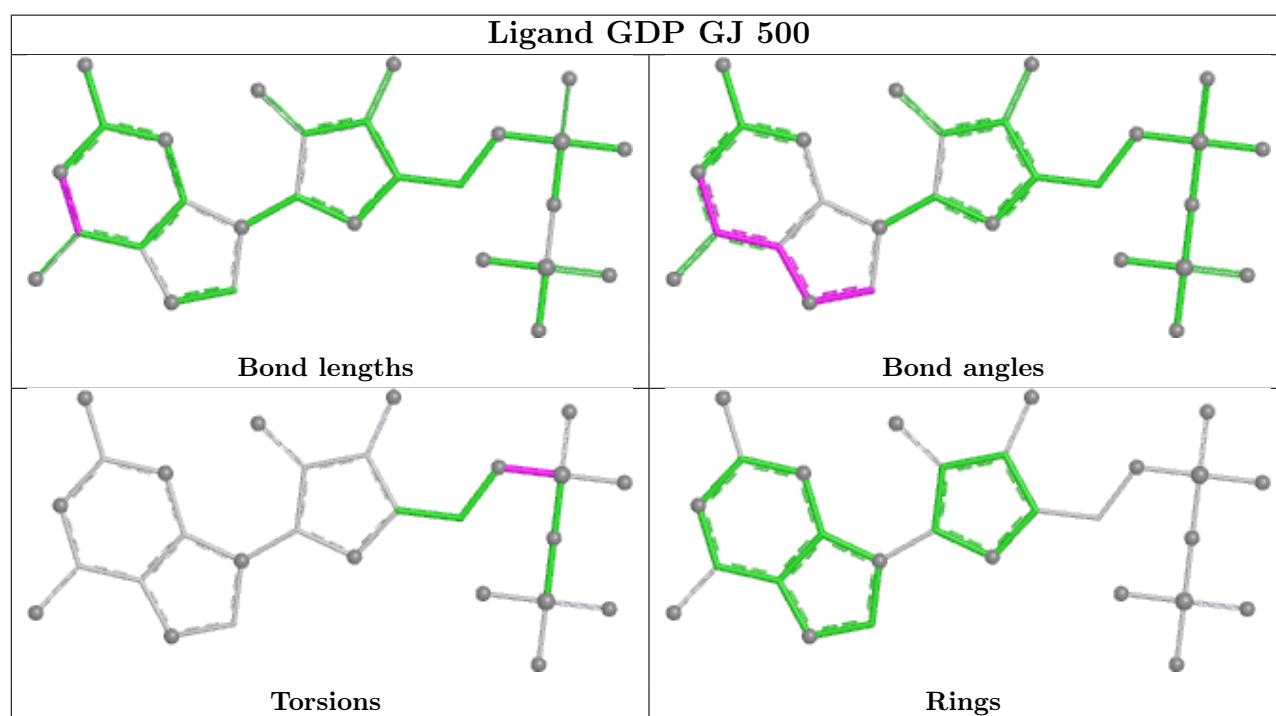
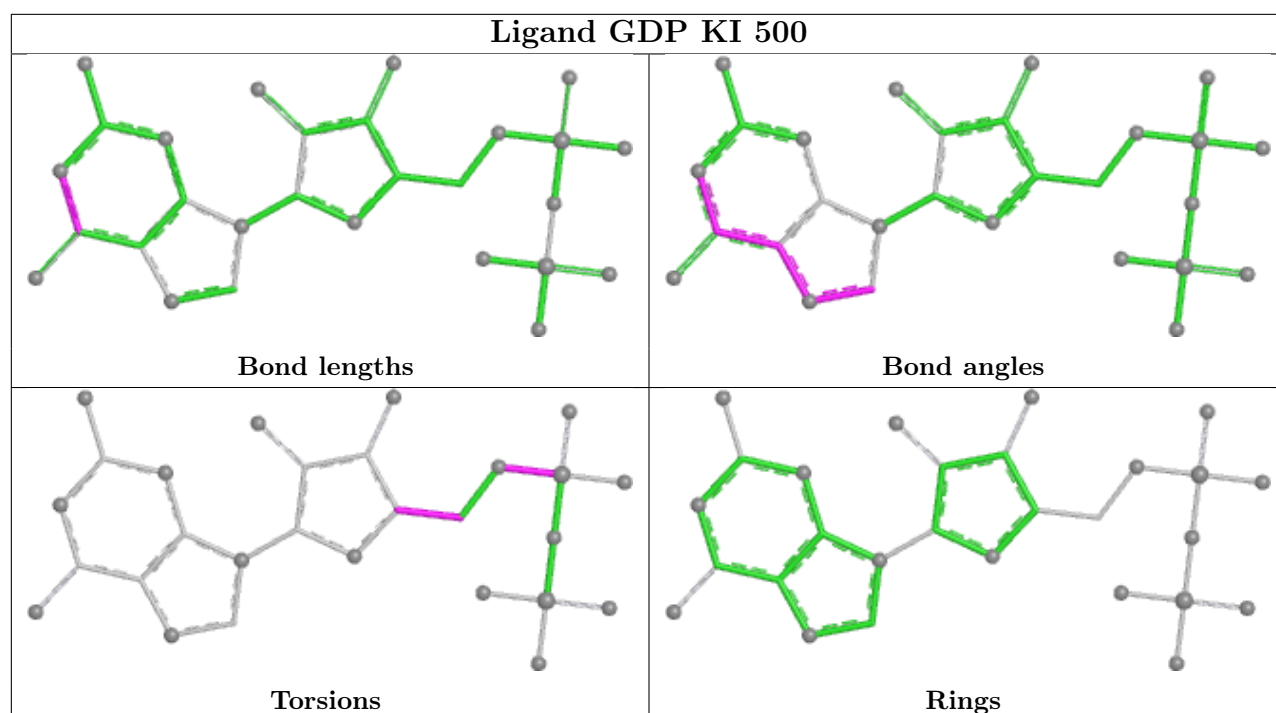


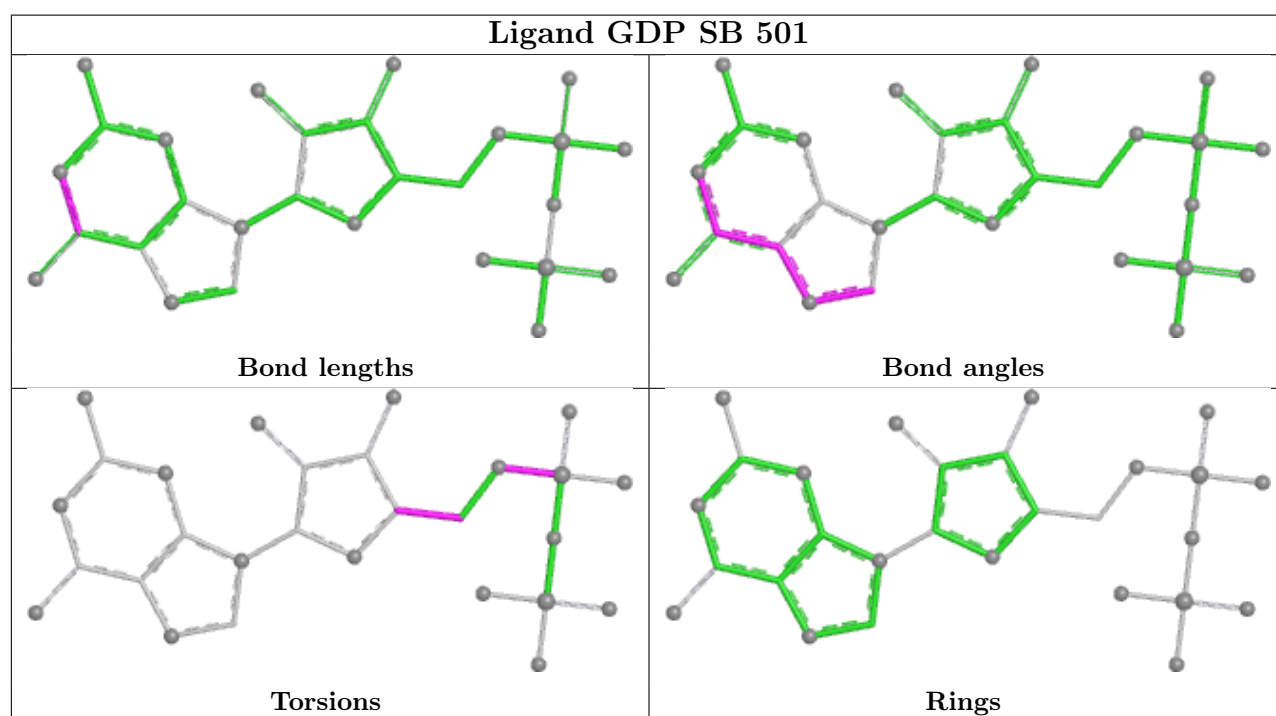
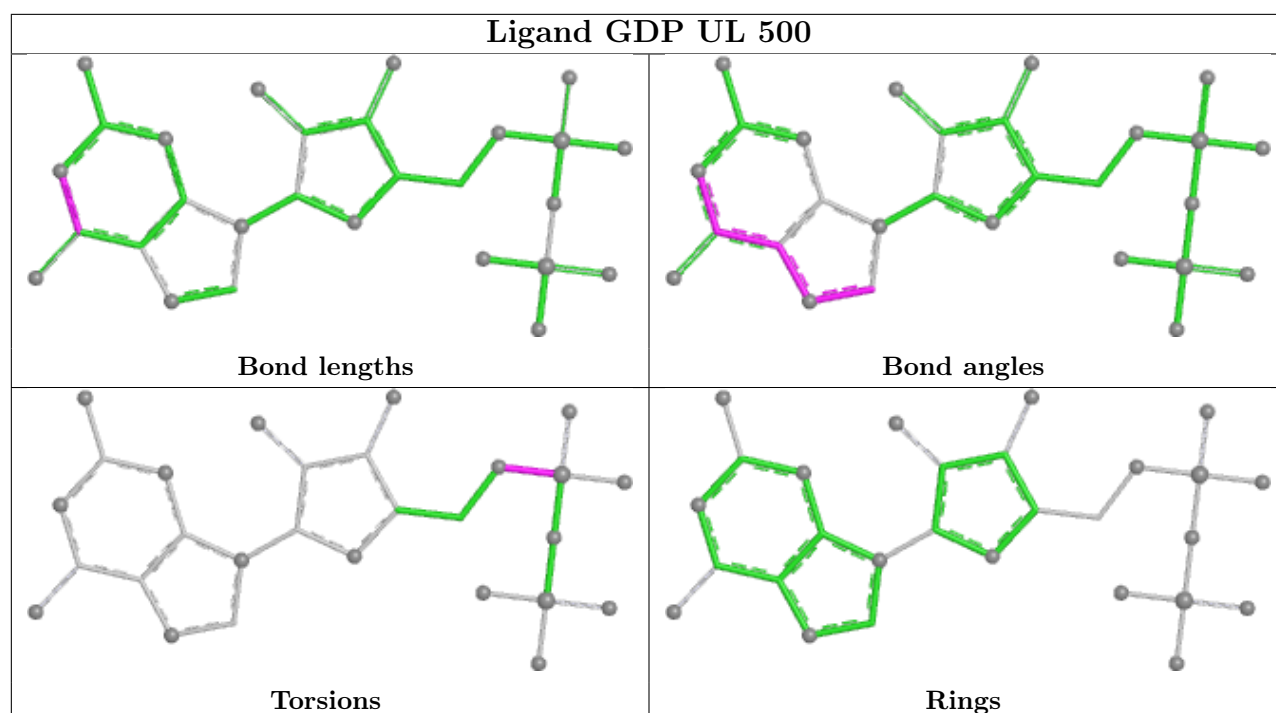


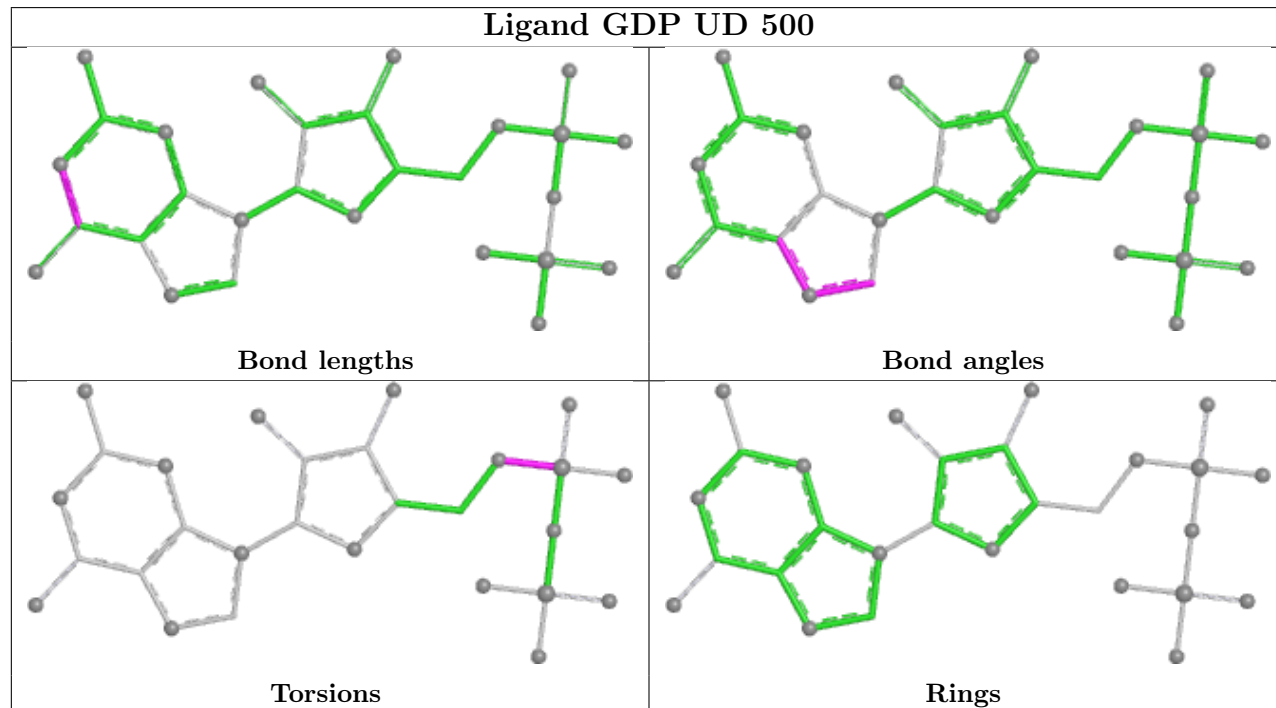
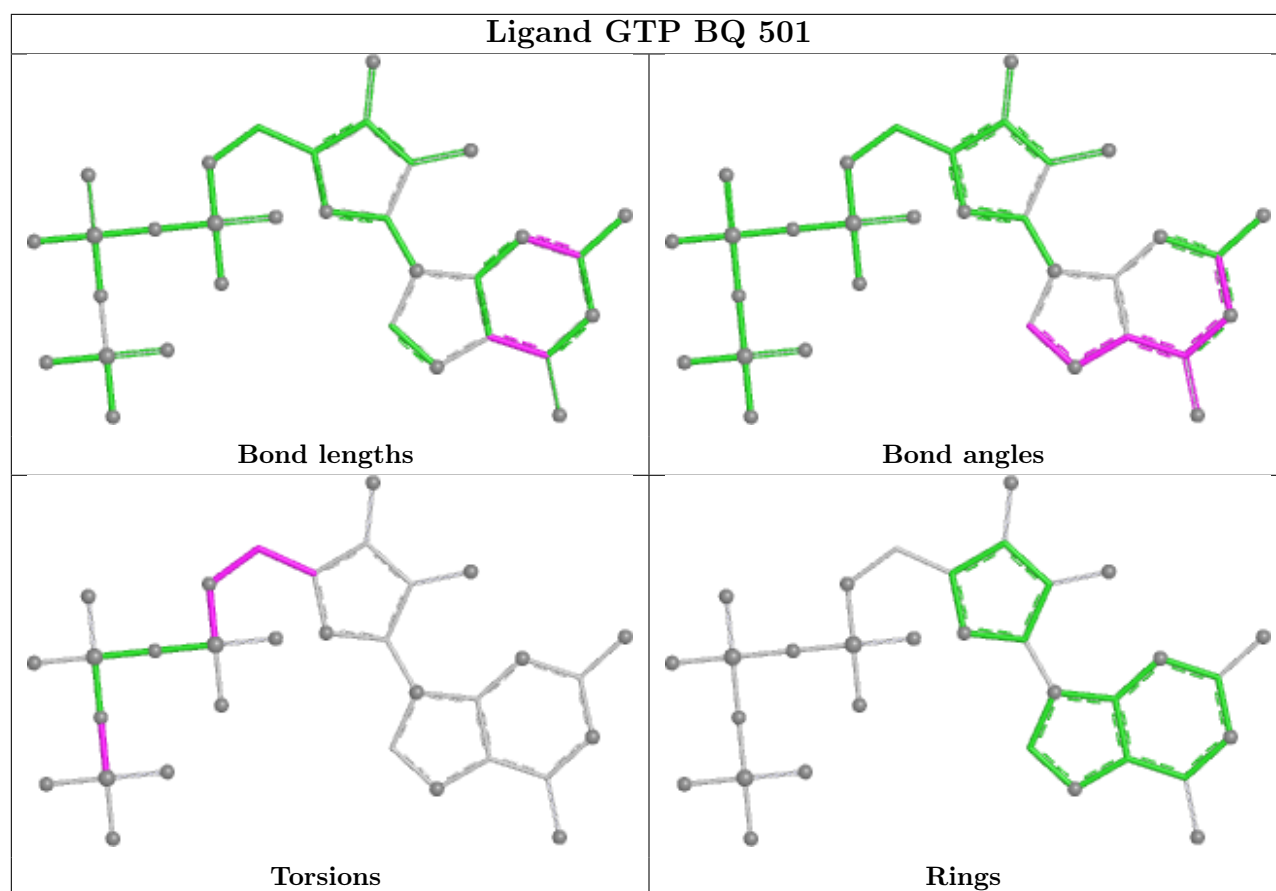


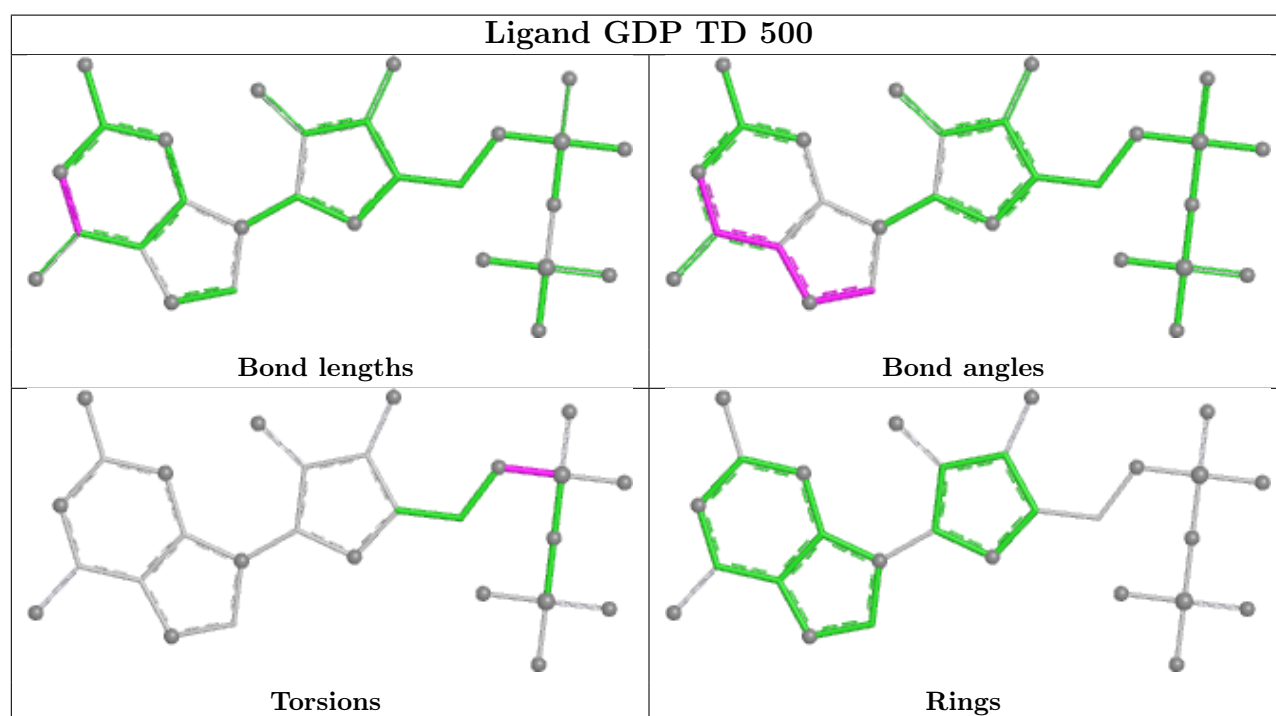
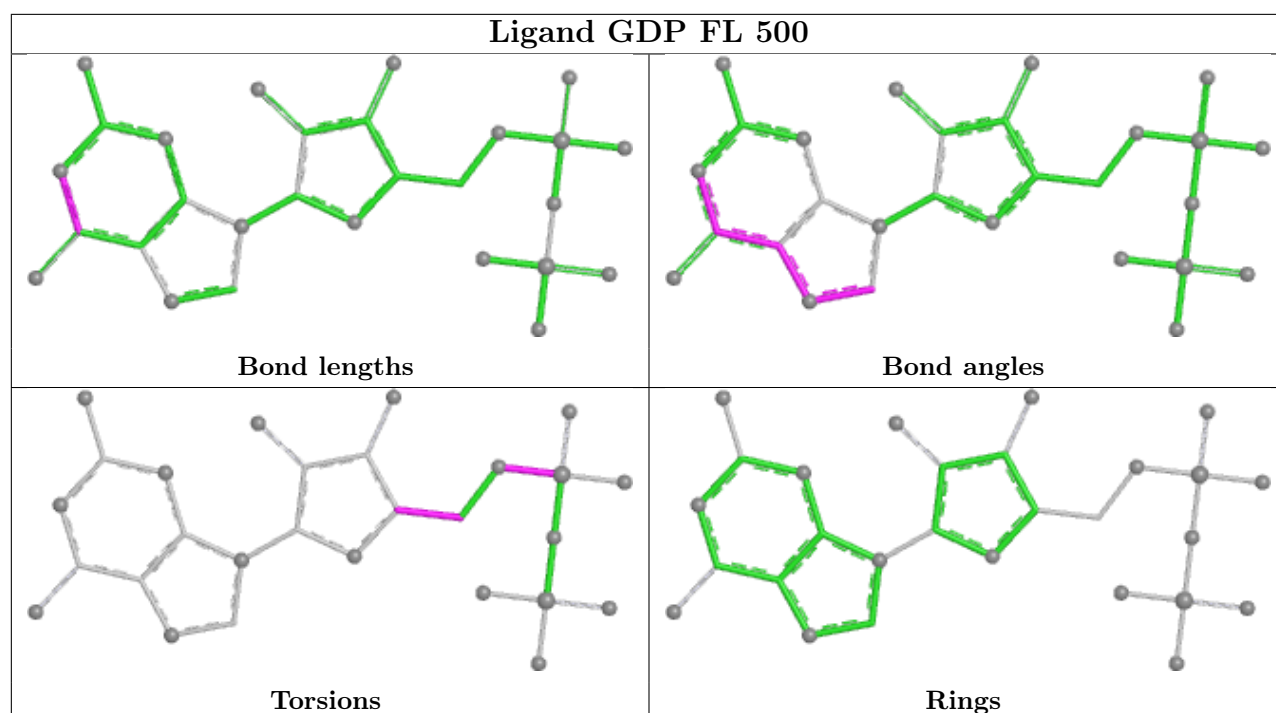


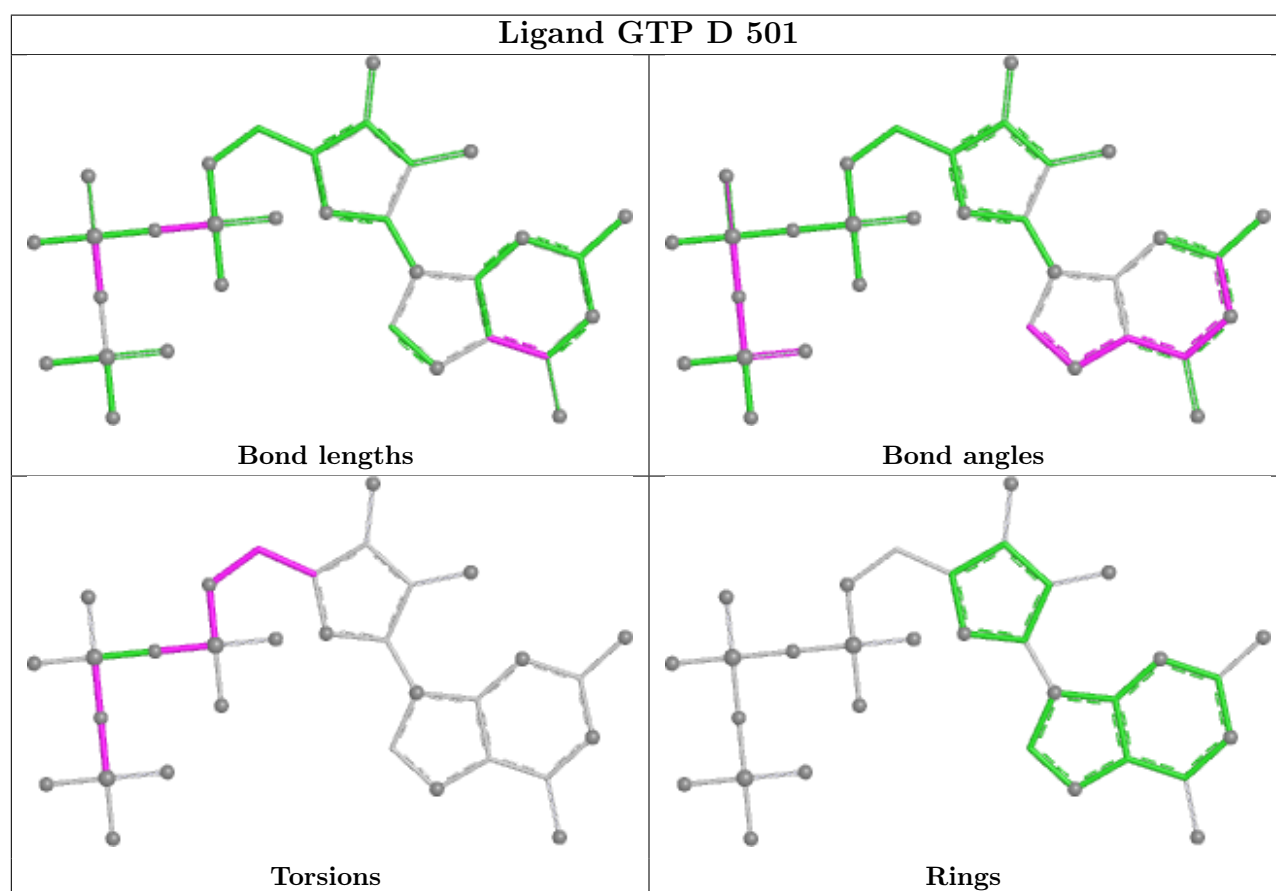
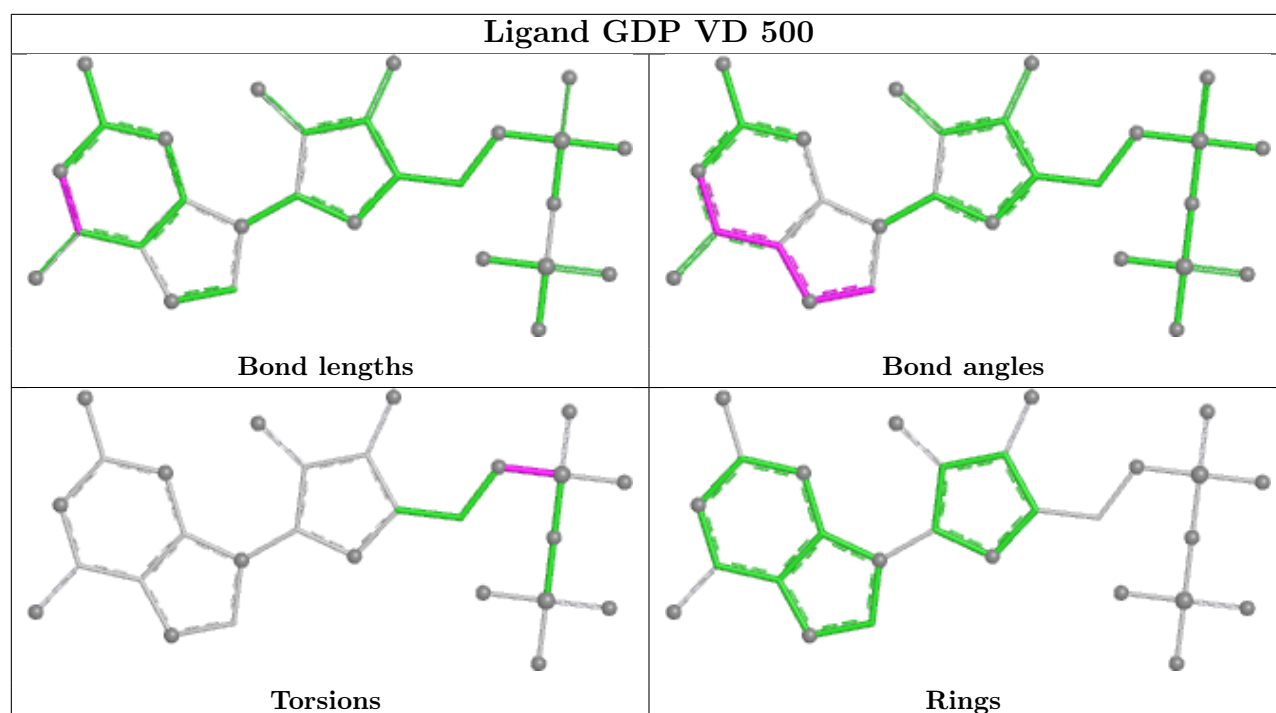


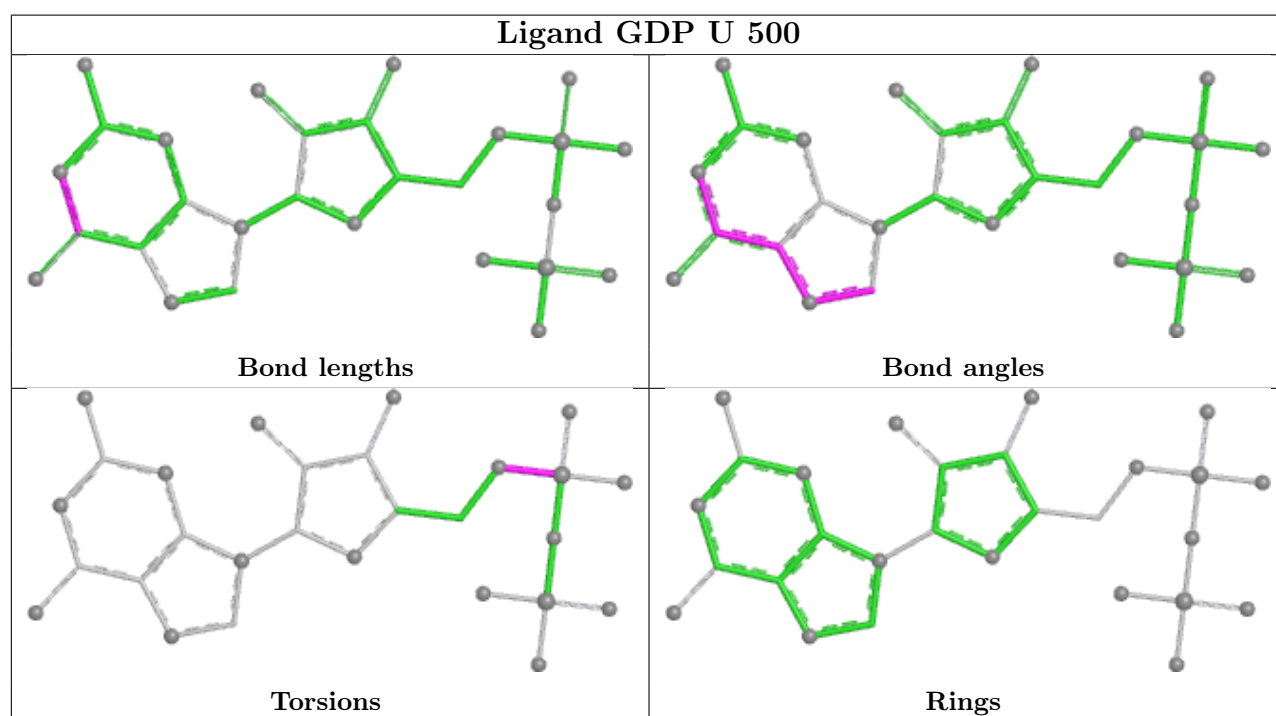
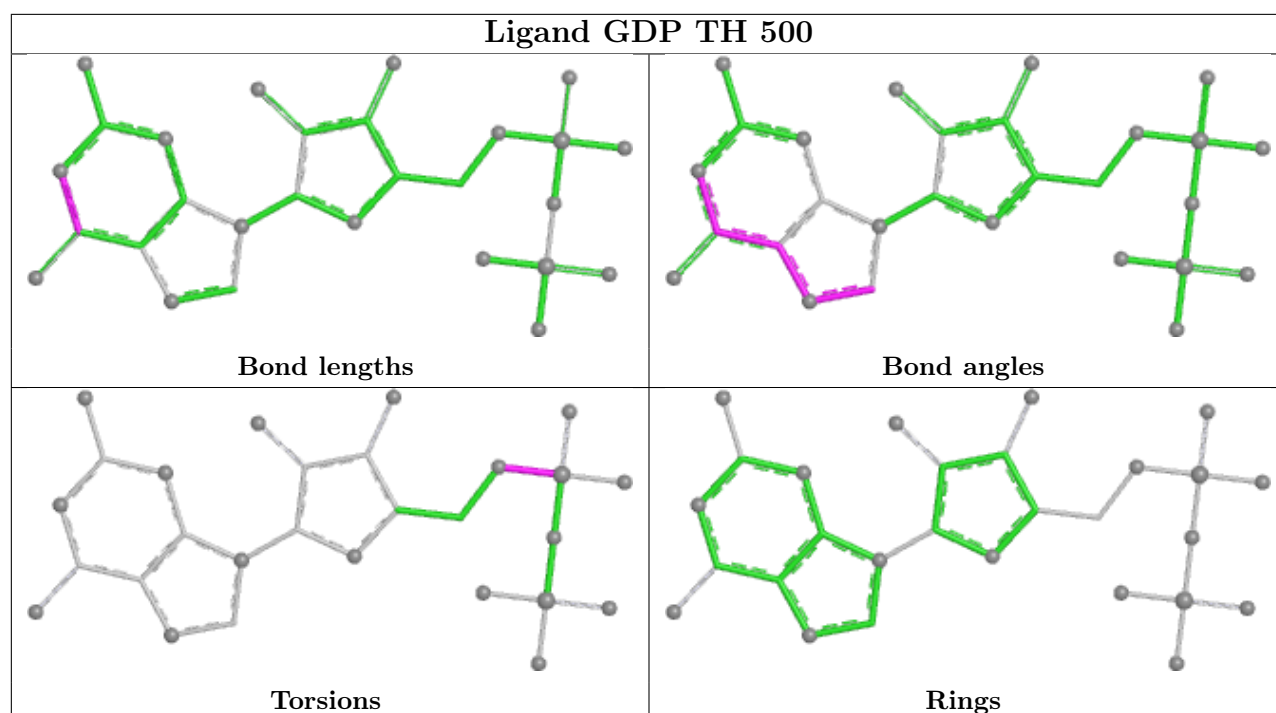




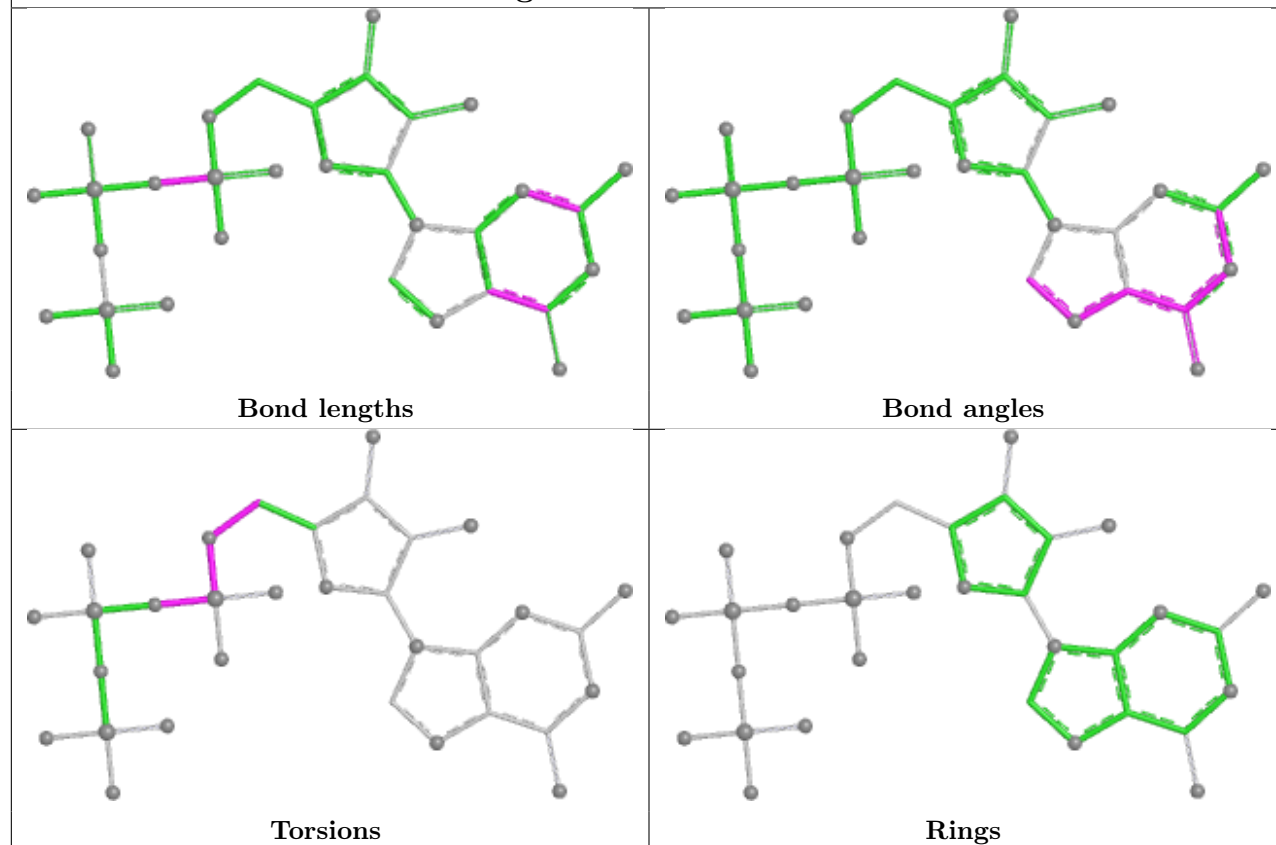




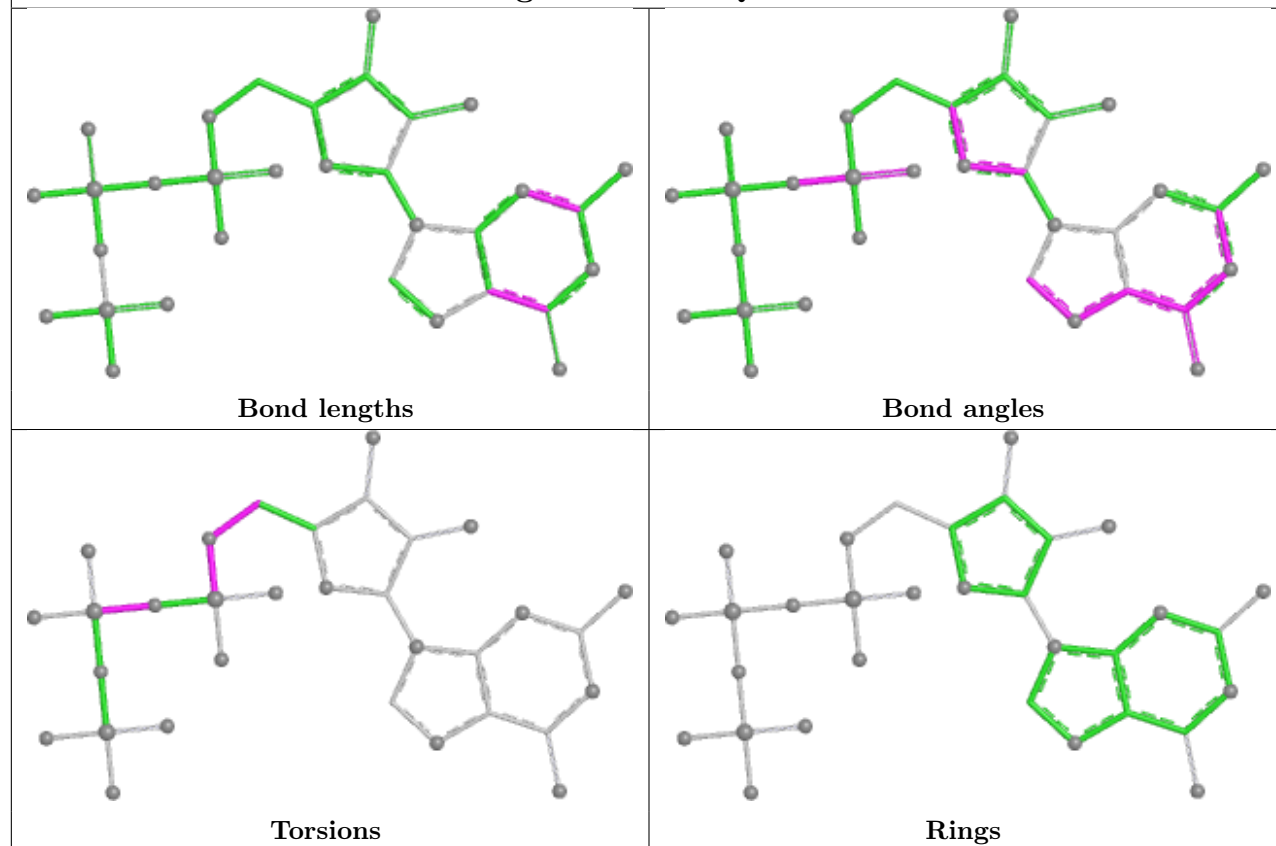


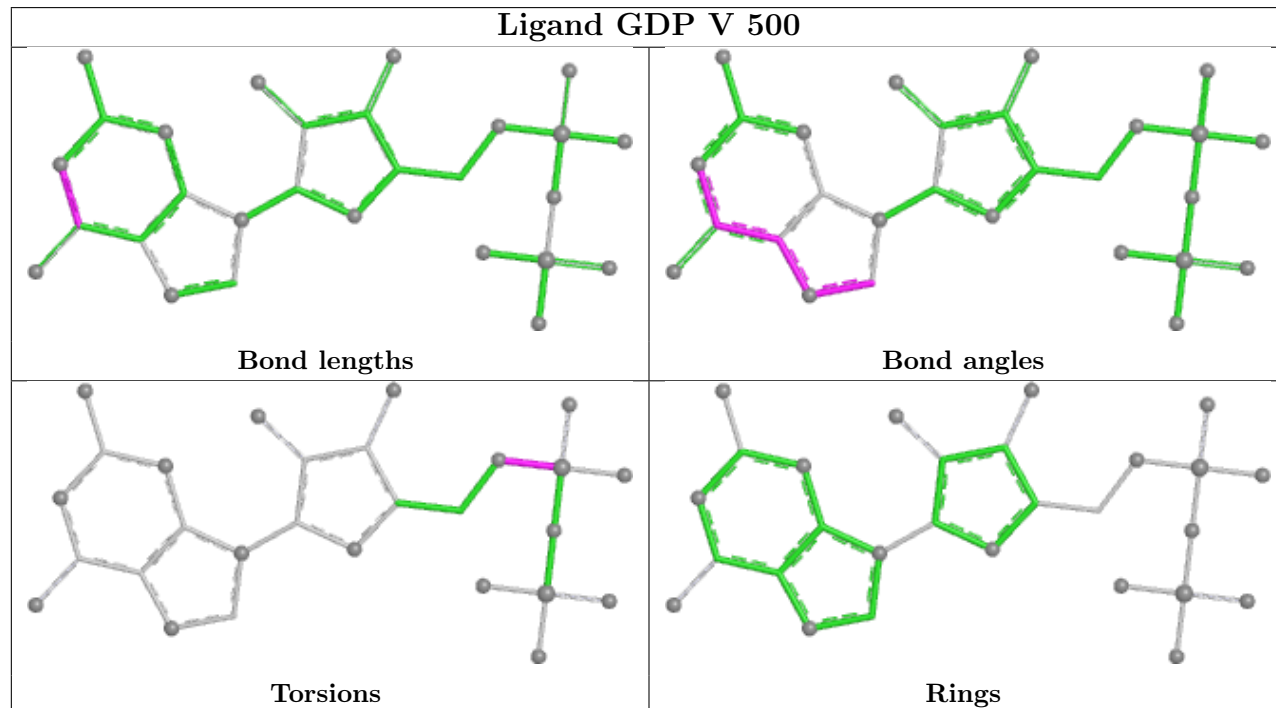
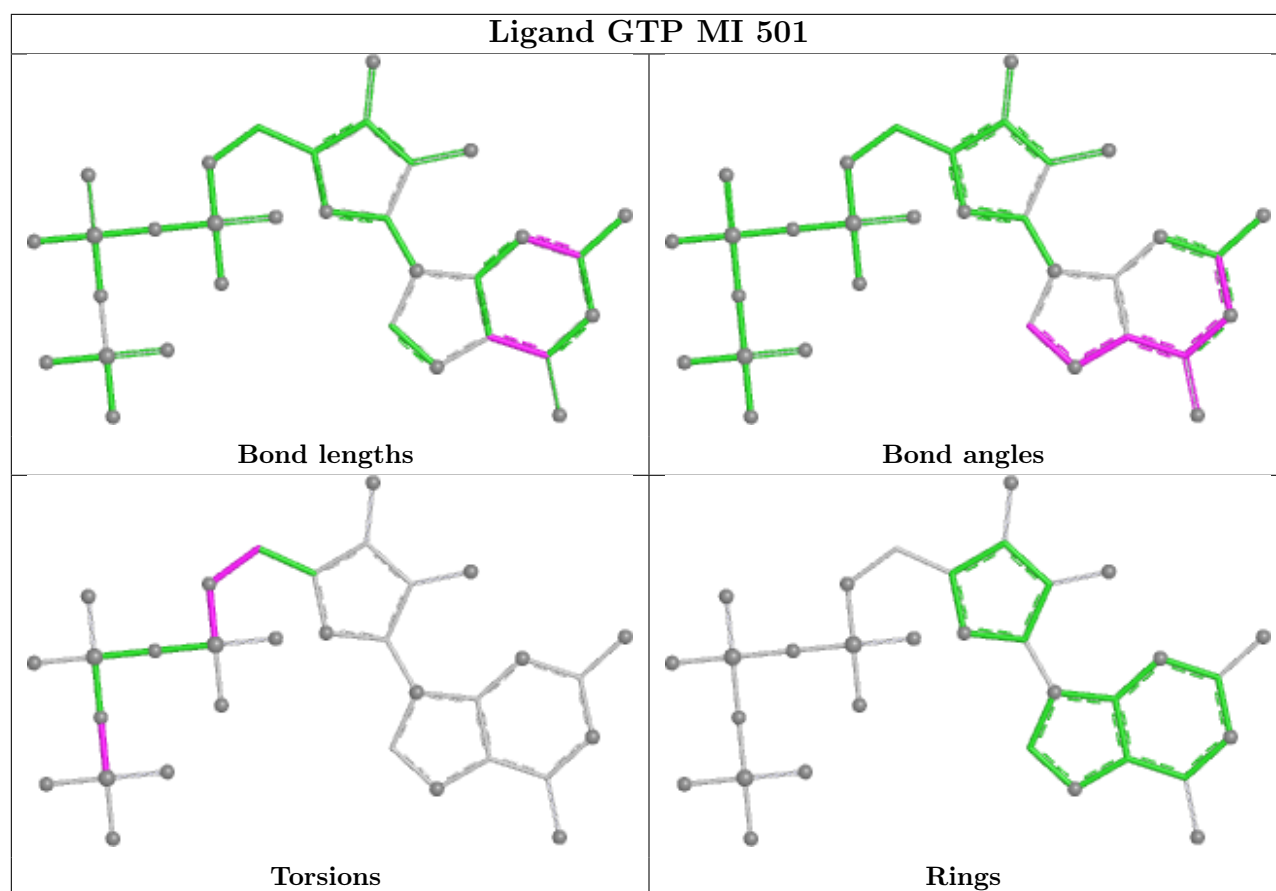


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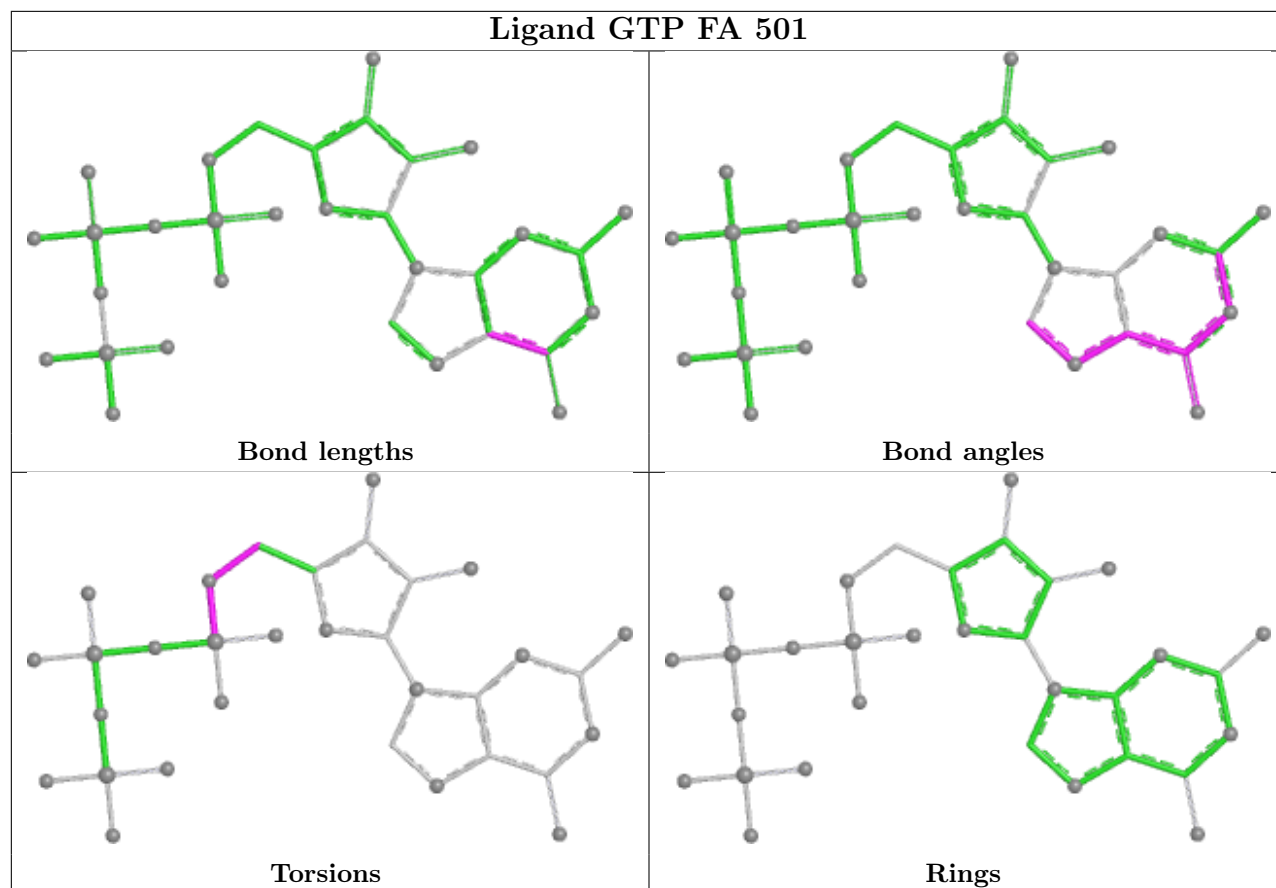


Ligand GTP GQ 501

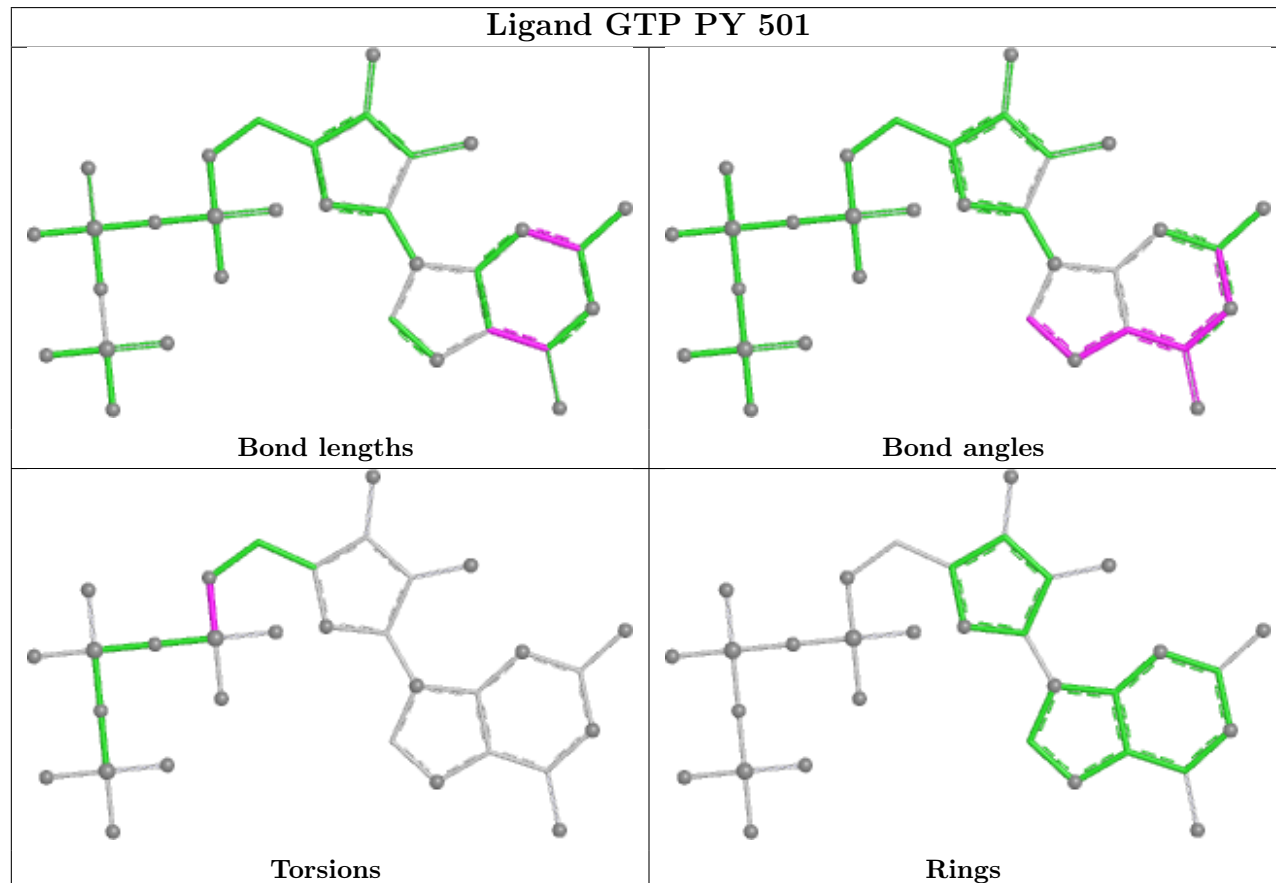


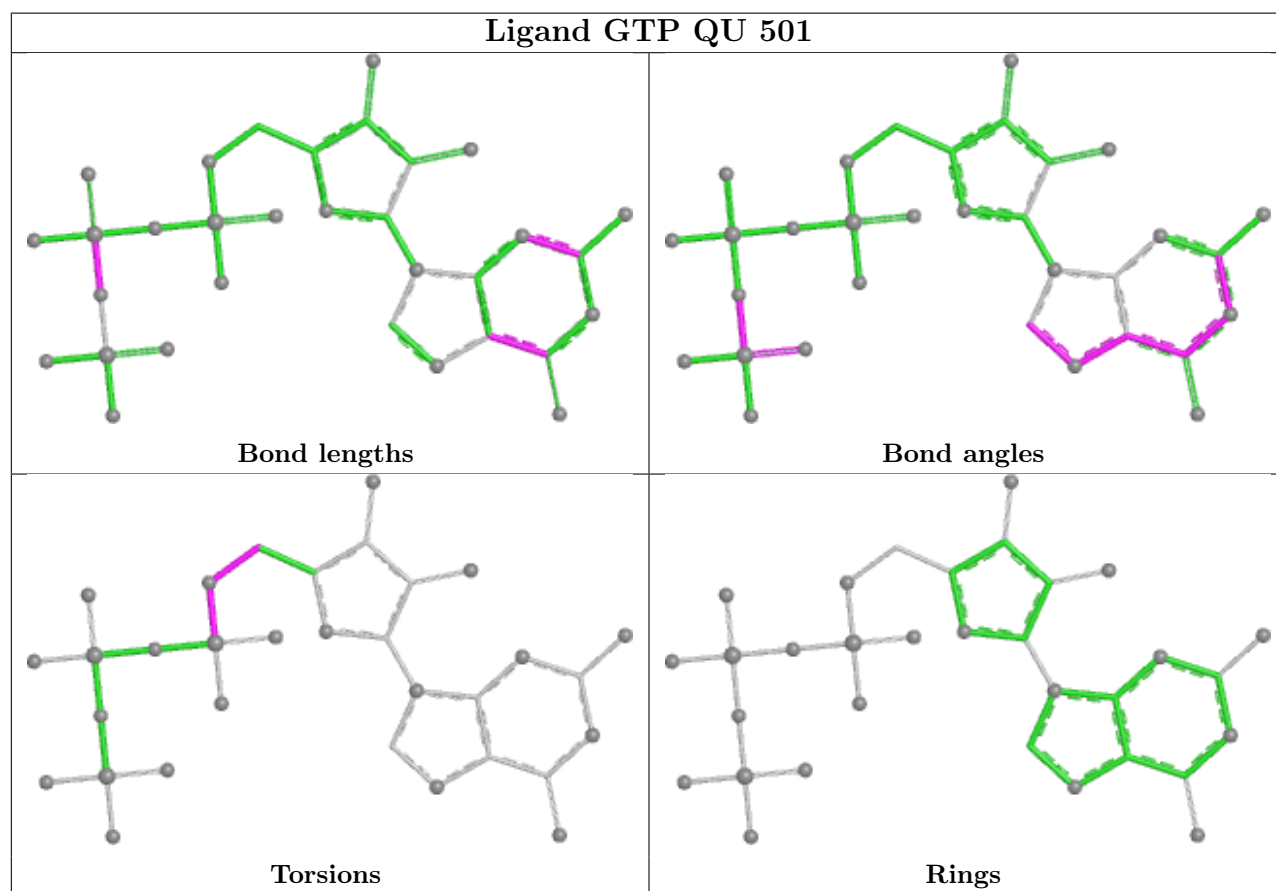
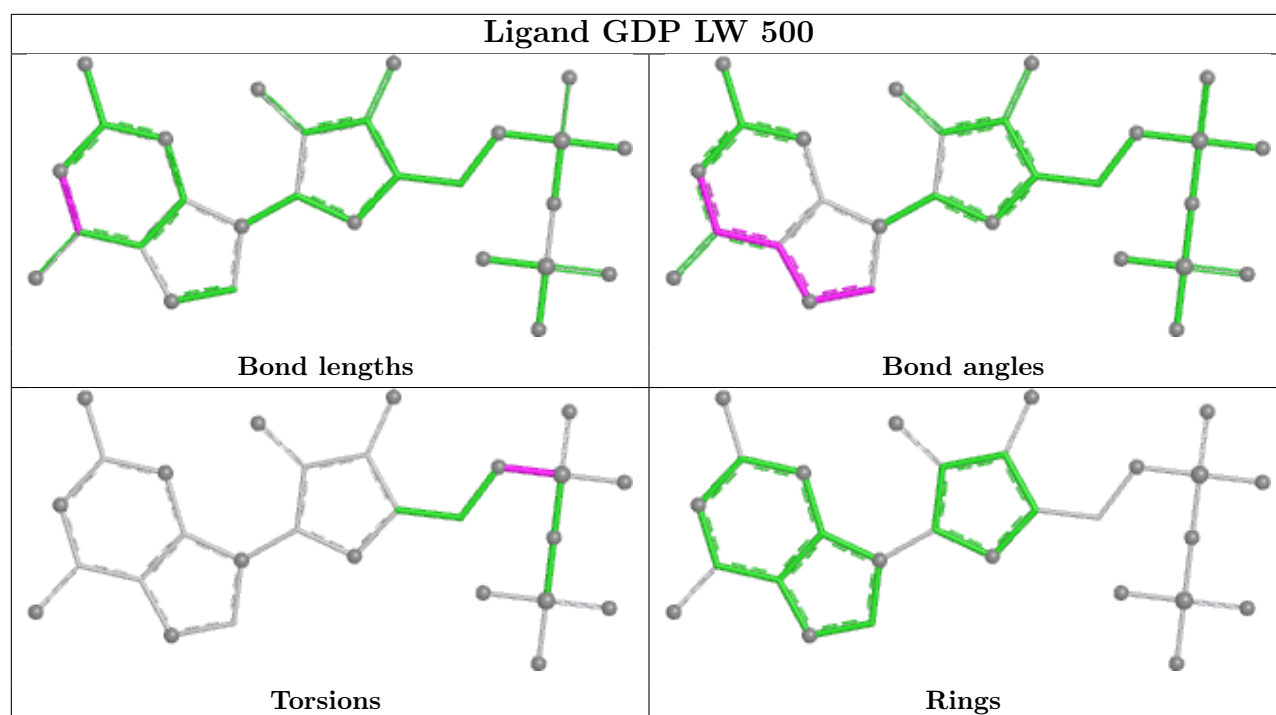


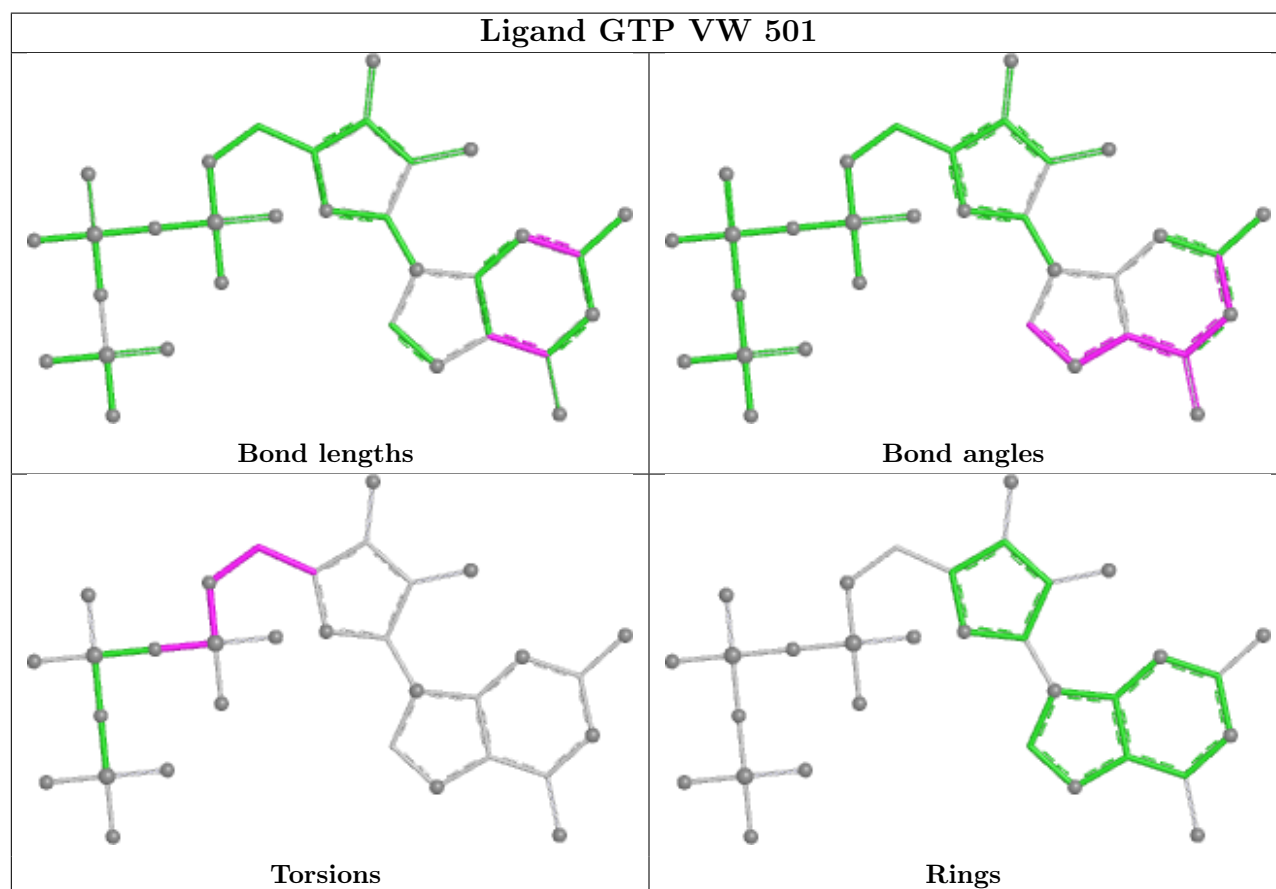
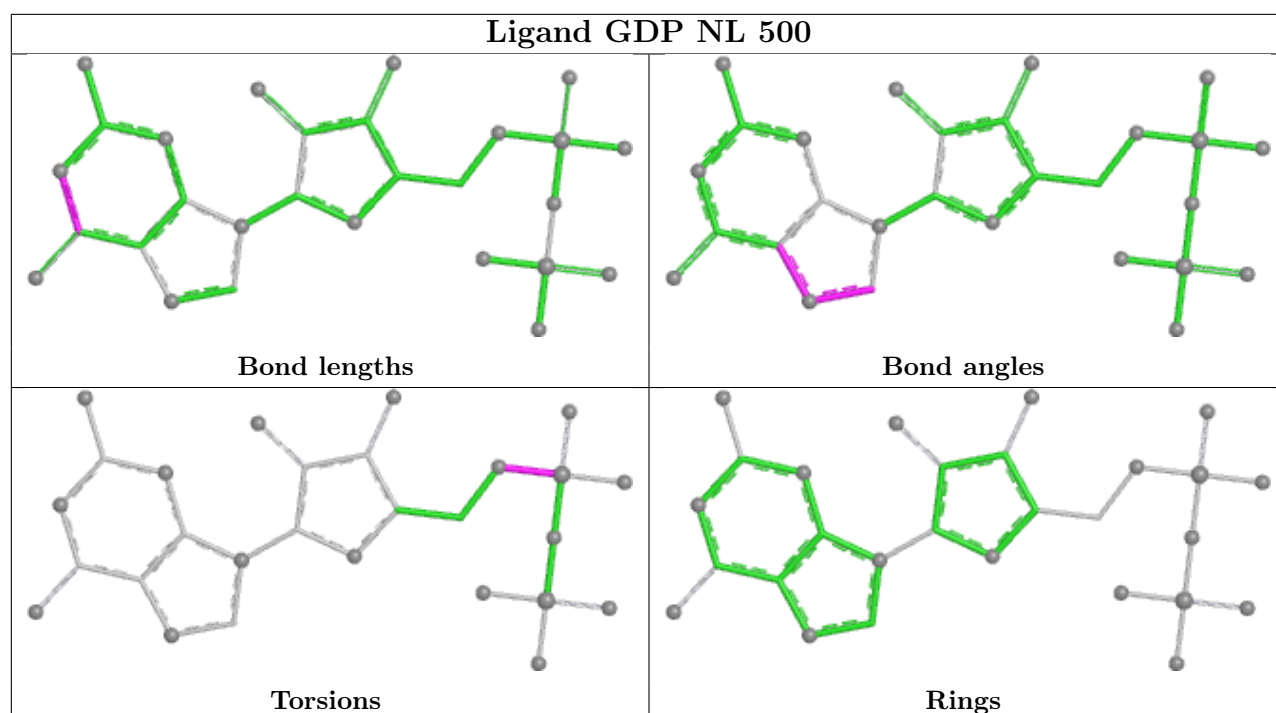
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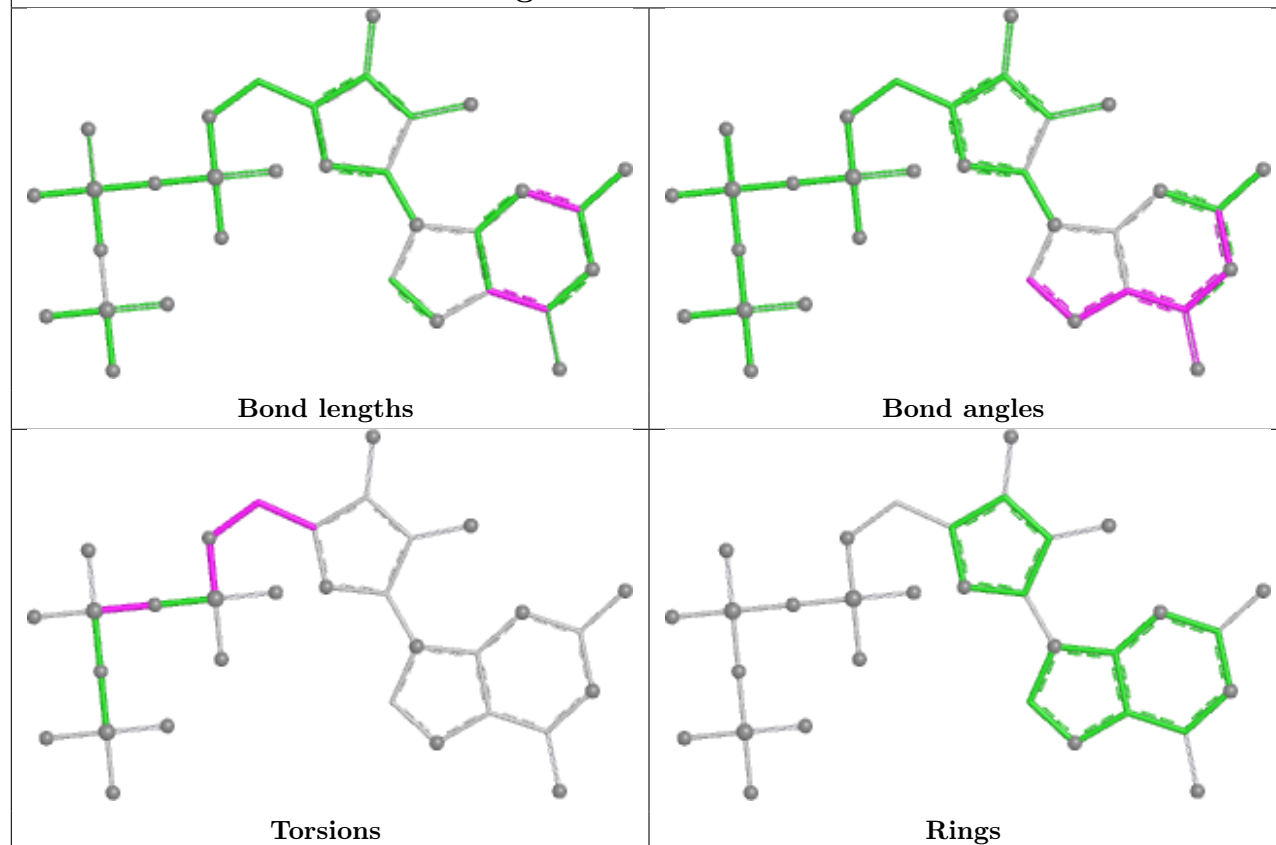
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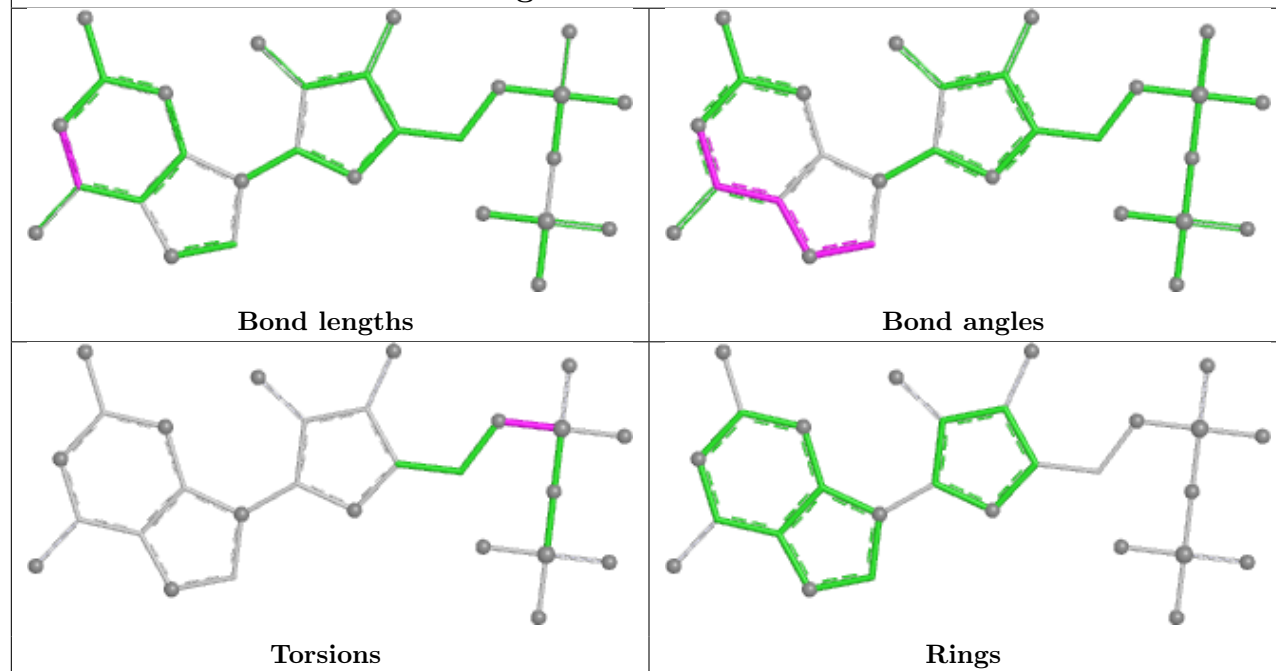


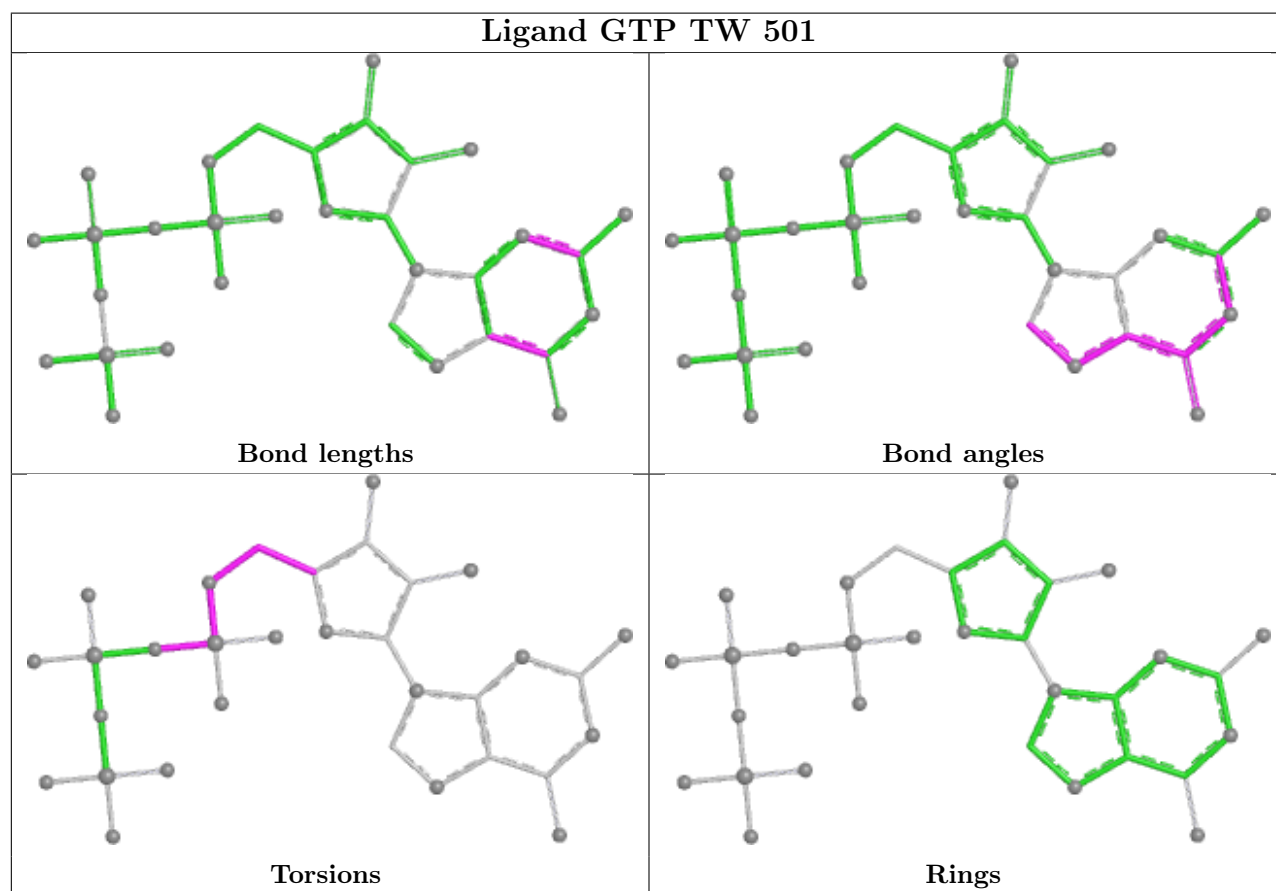
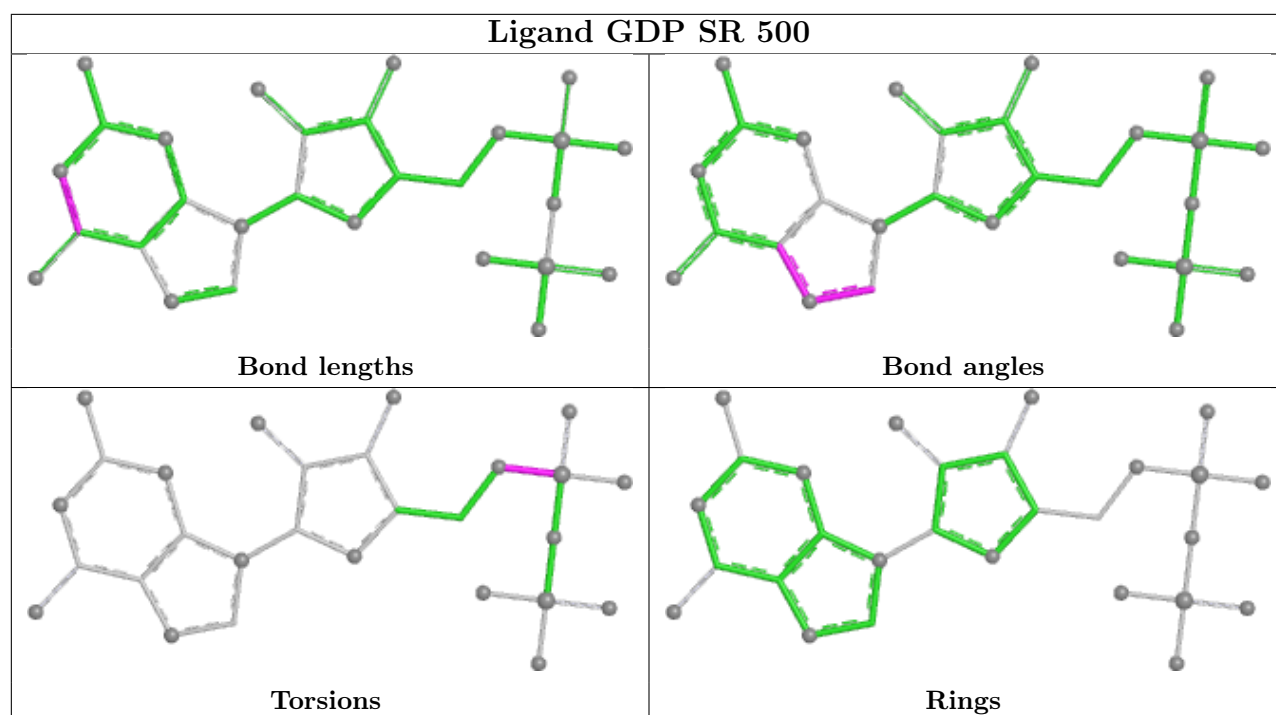


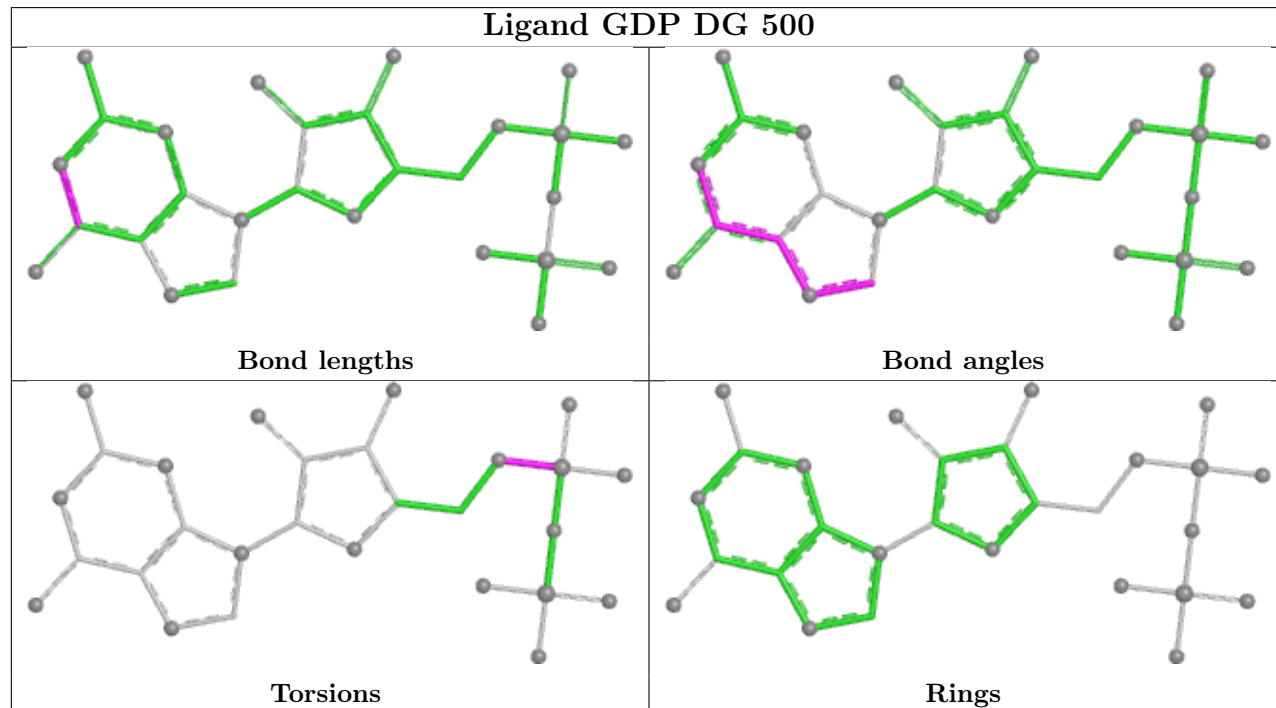
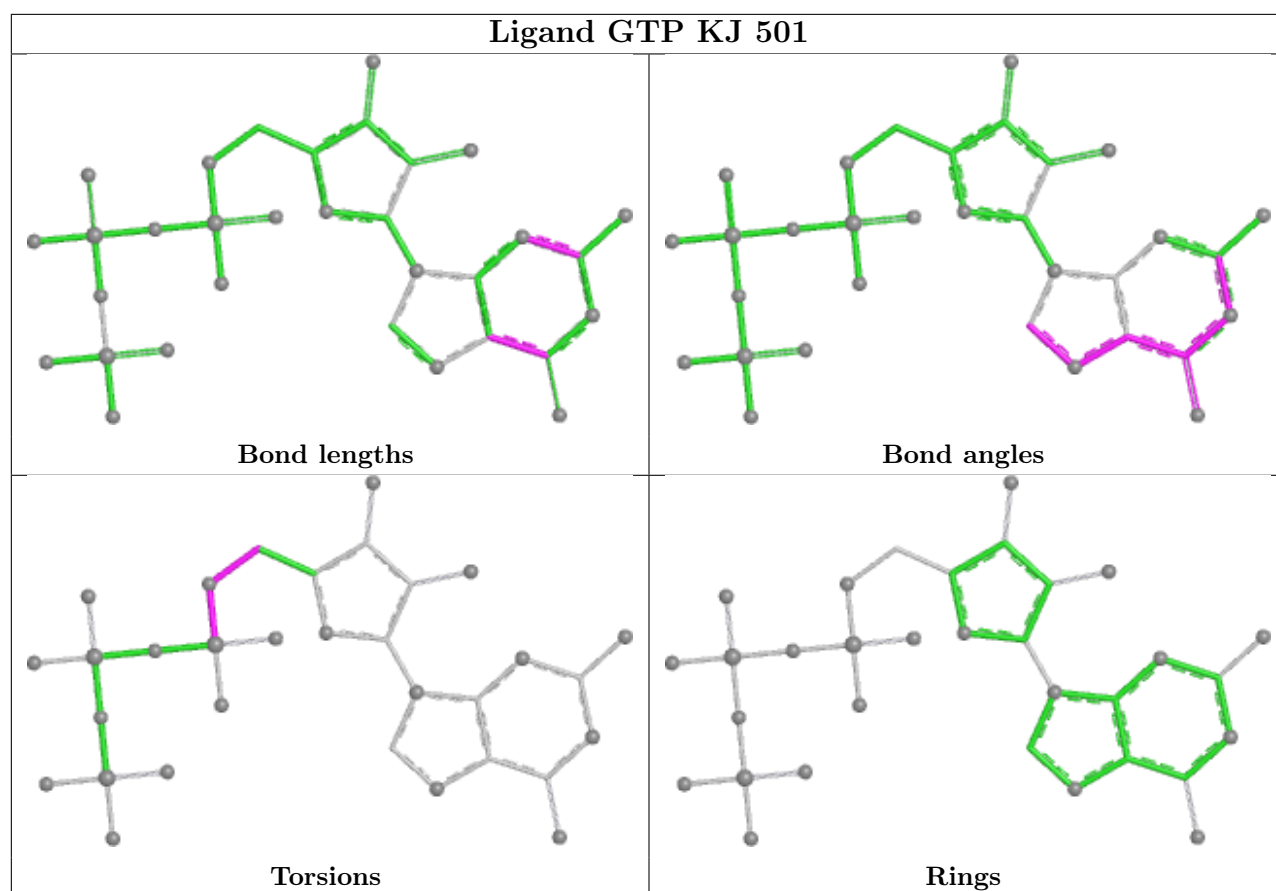
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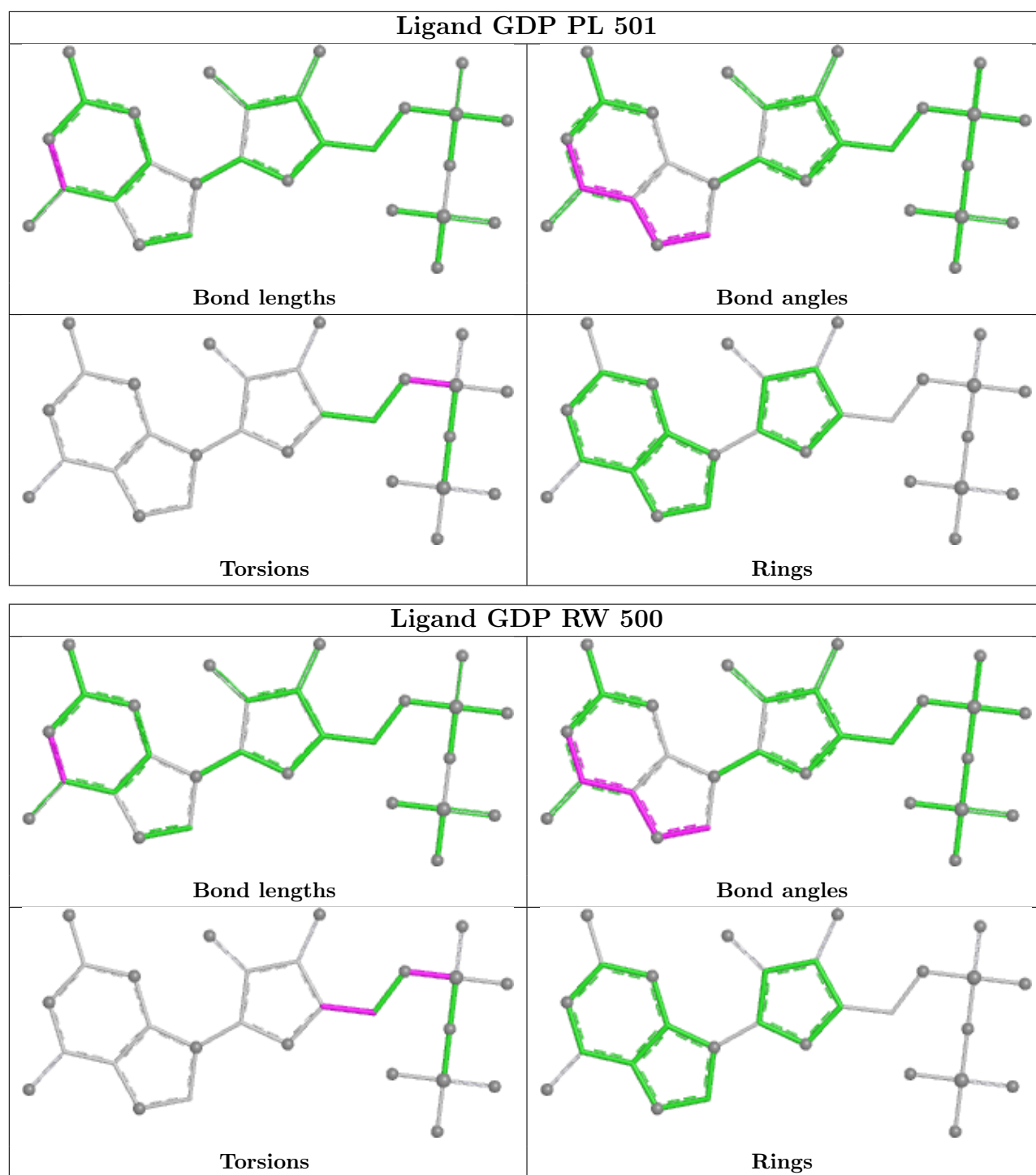


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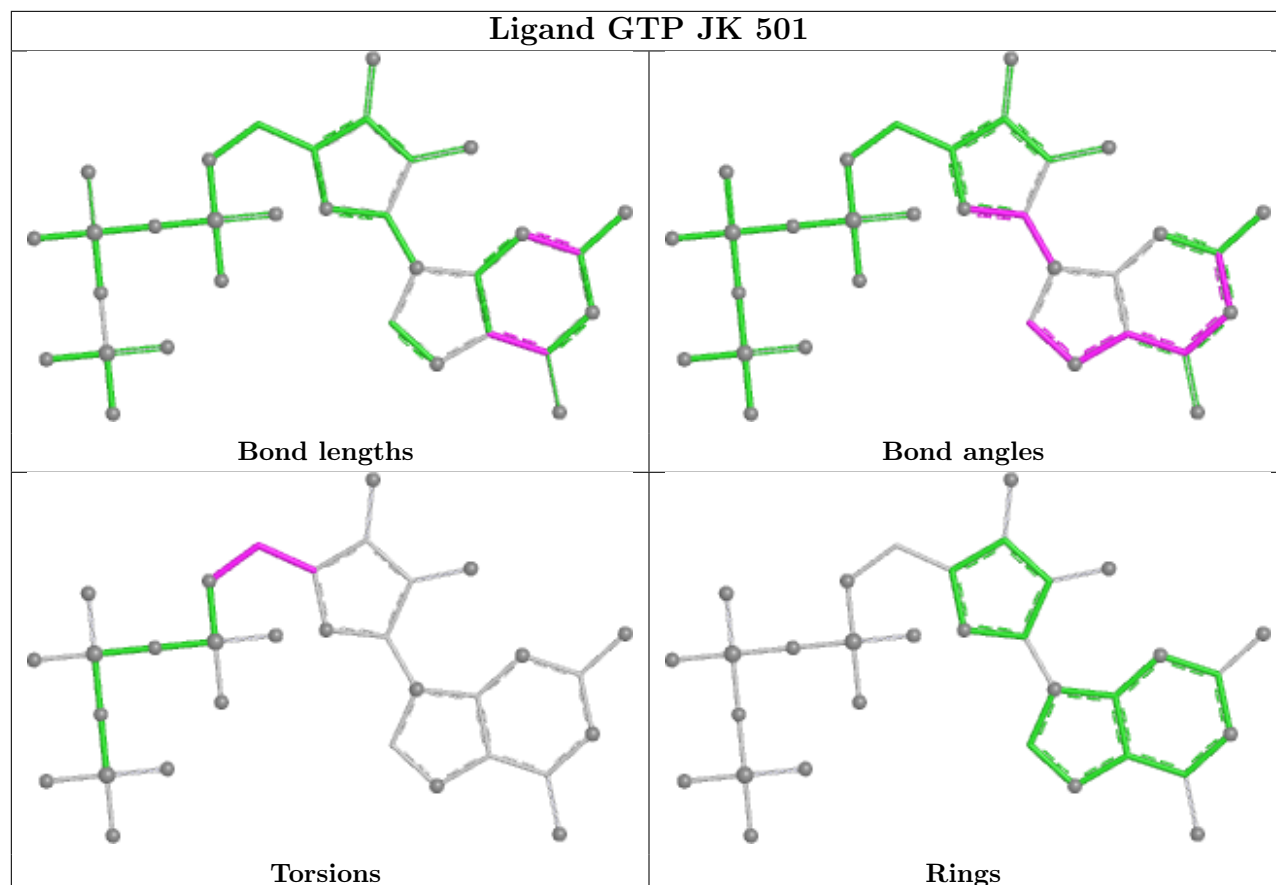




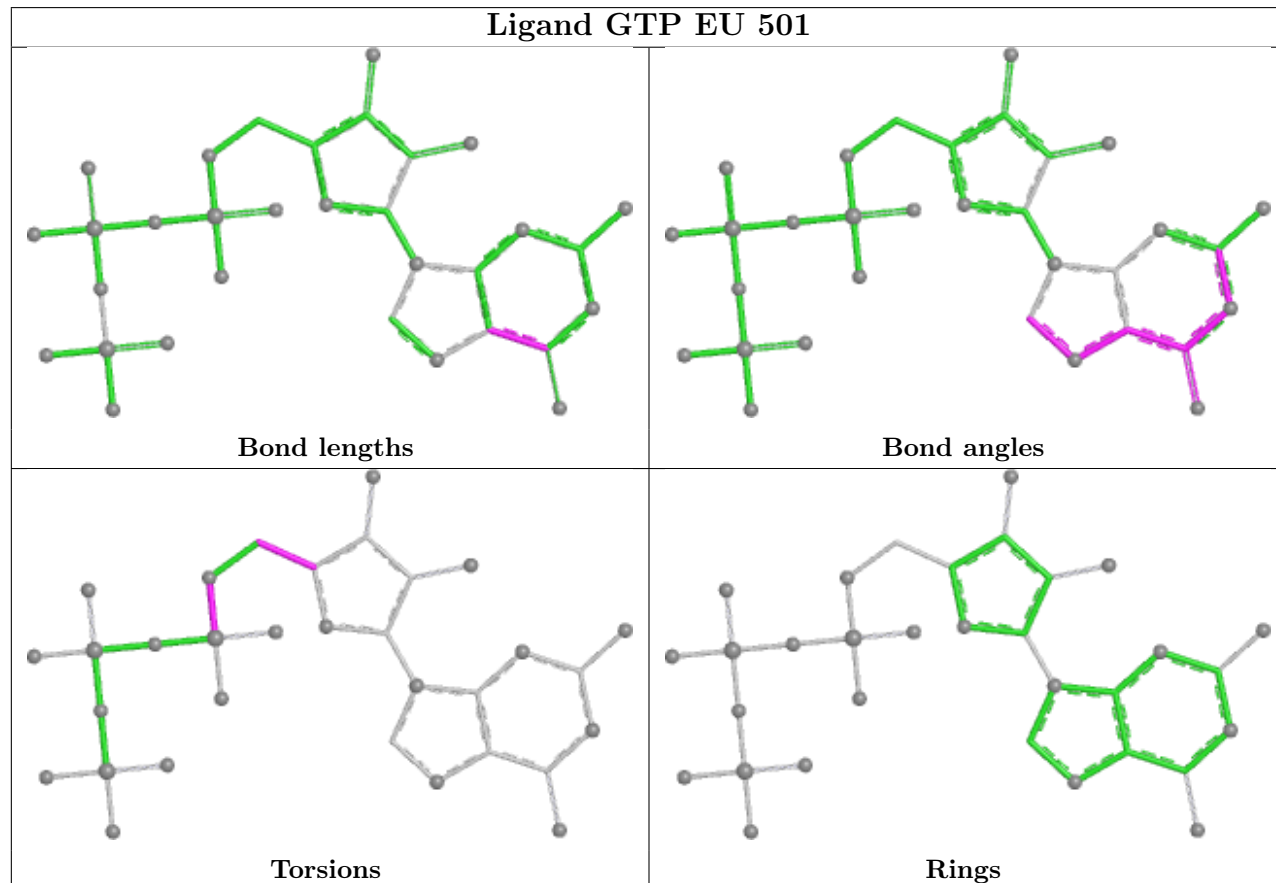




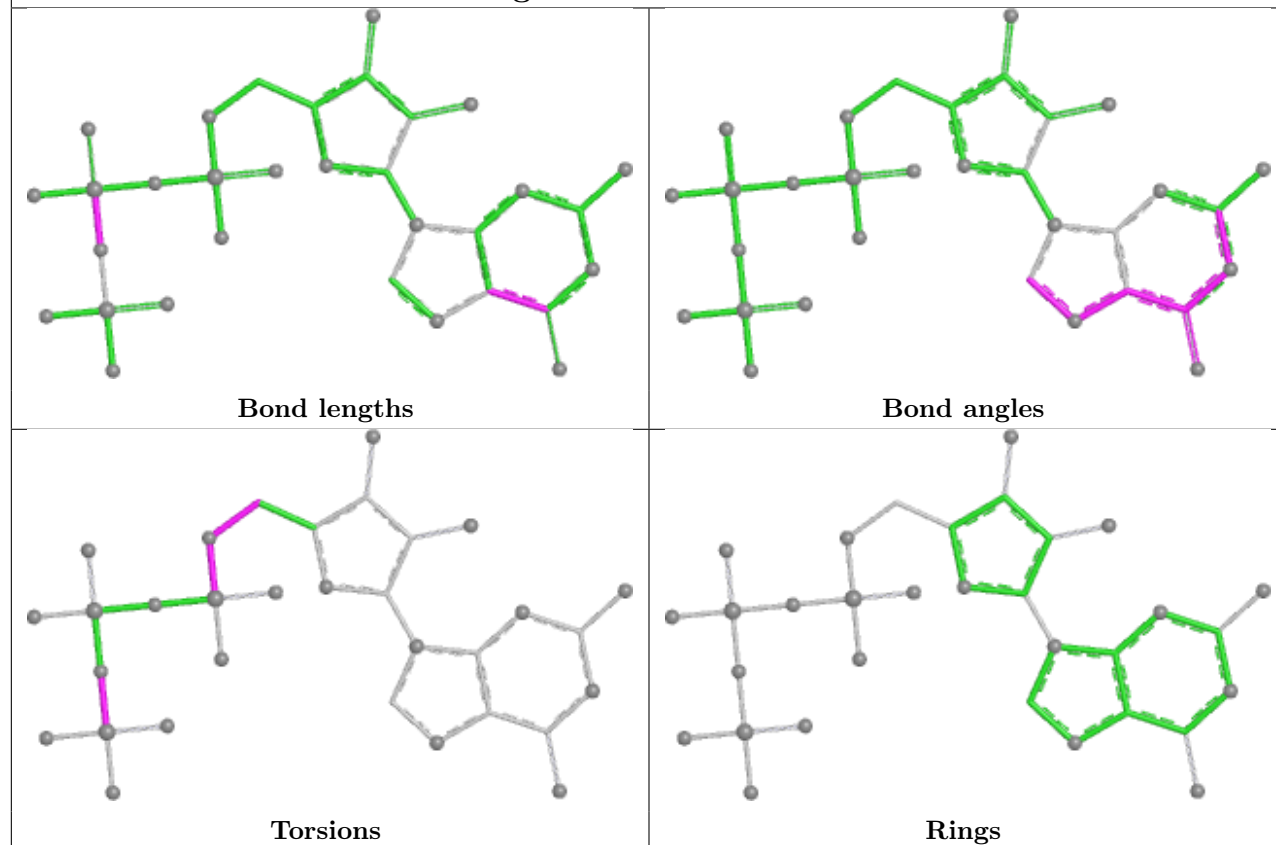
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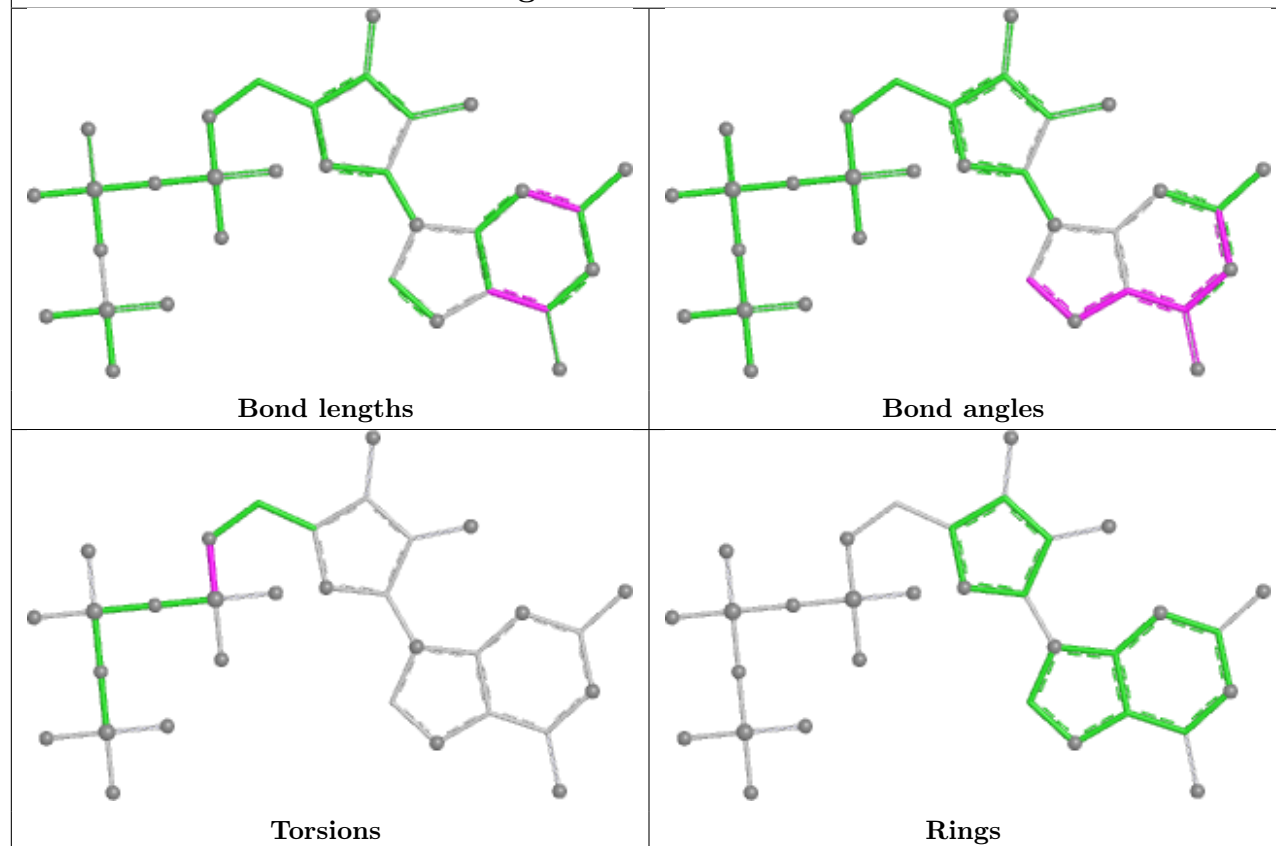
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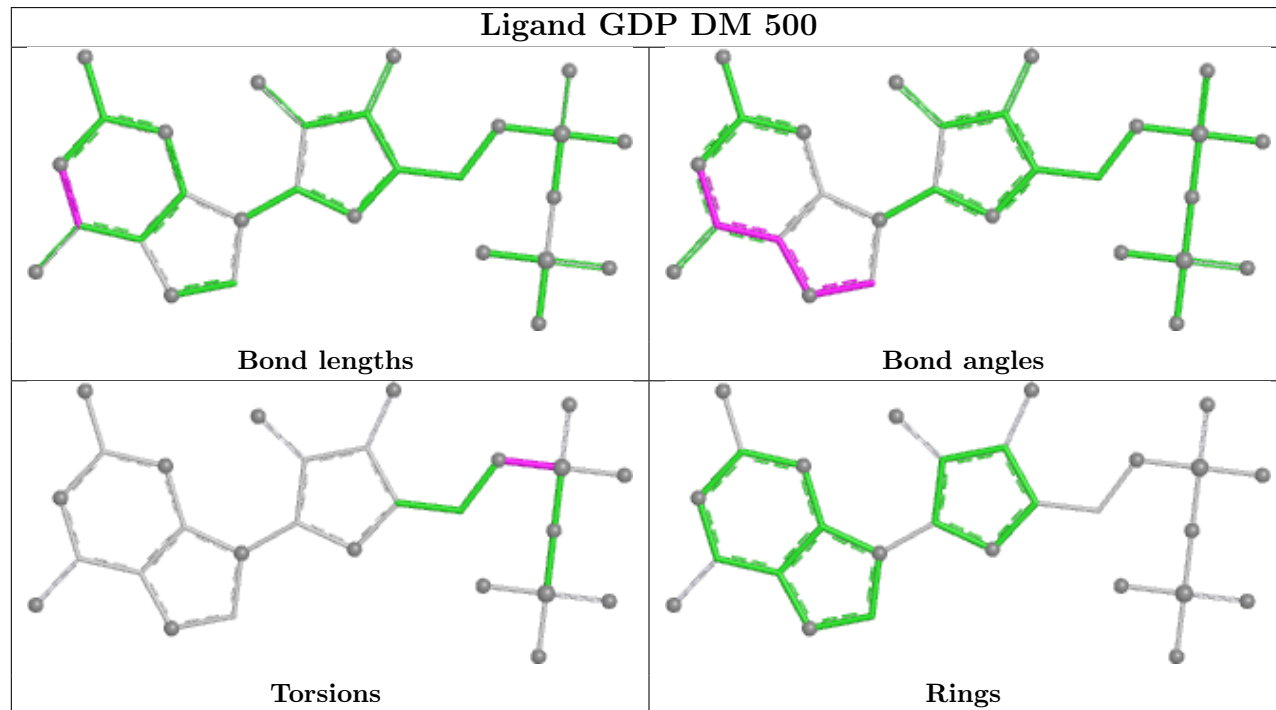
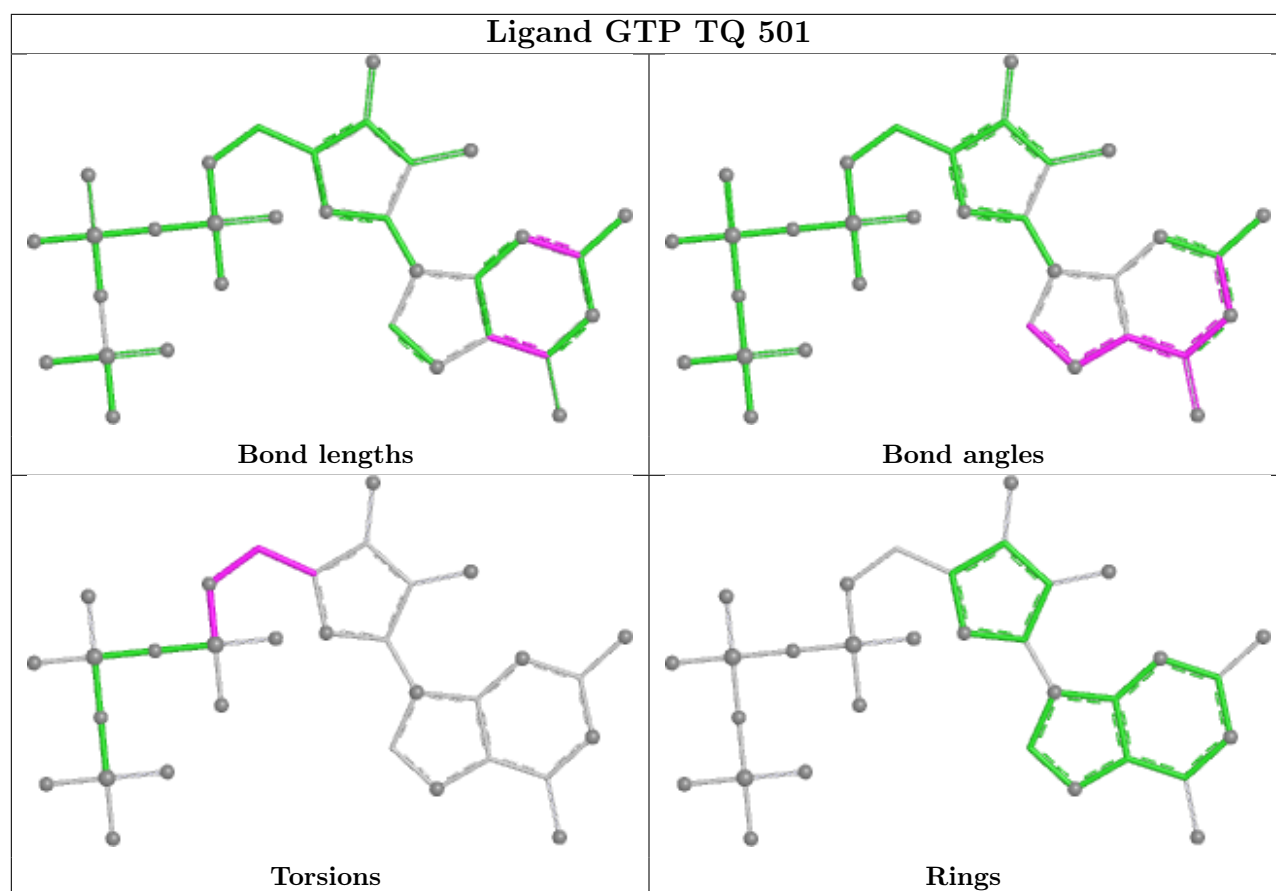


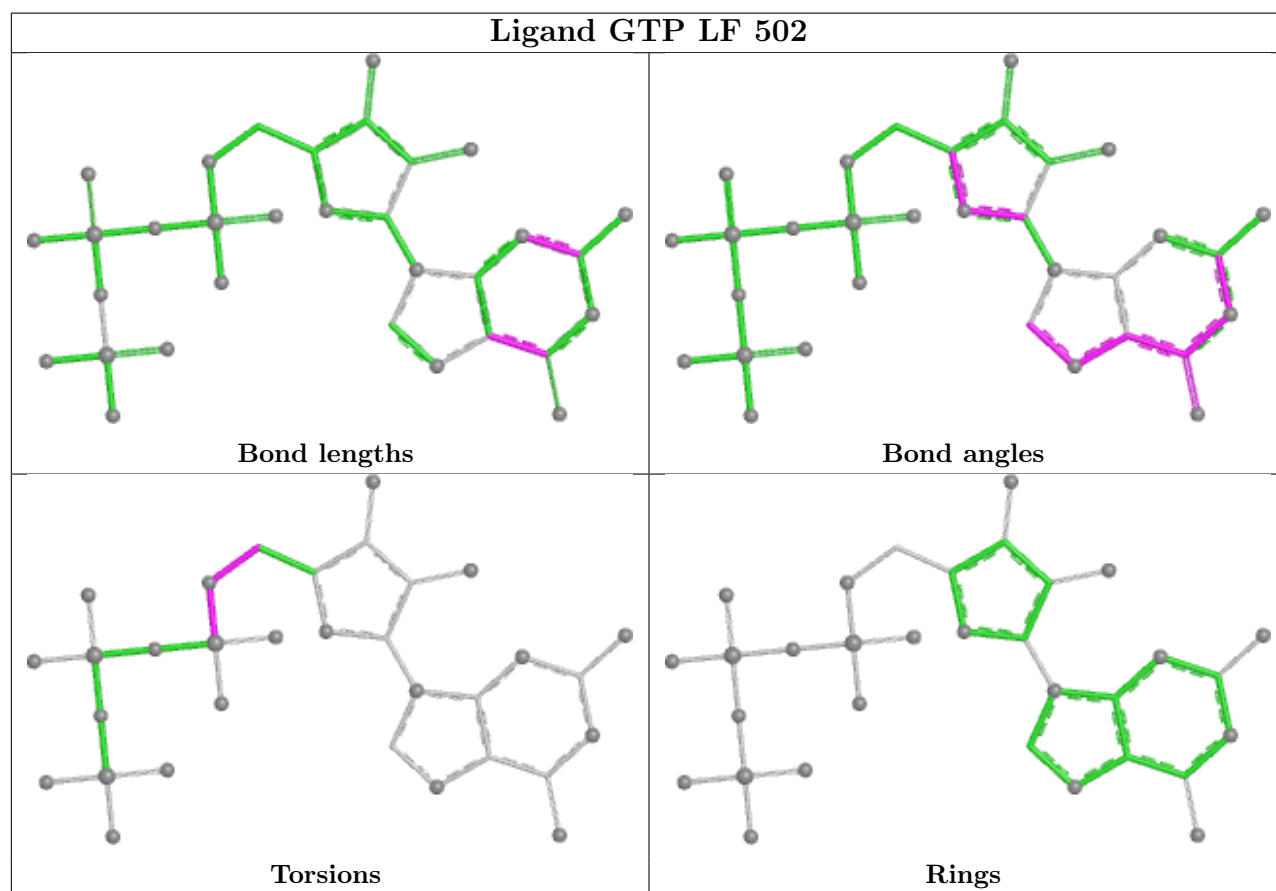
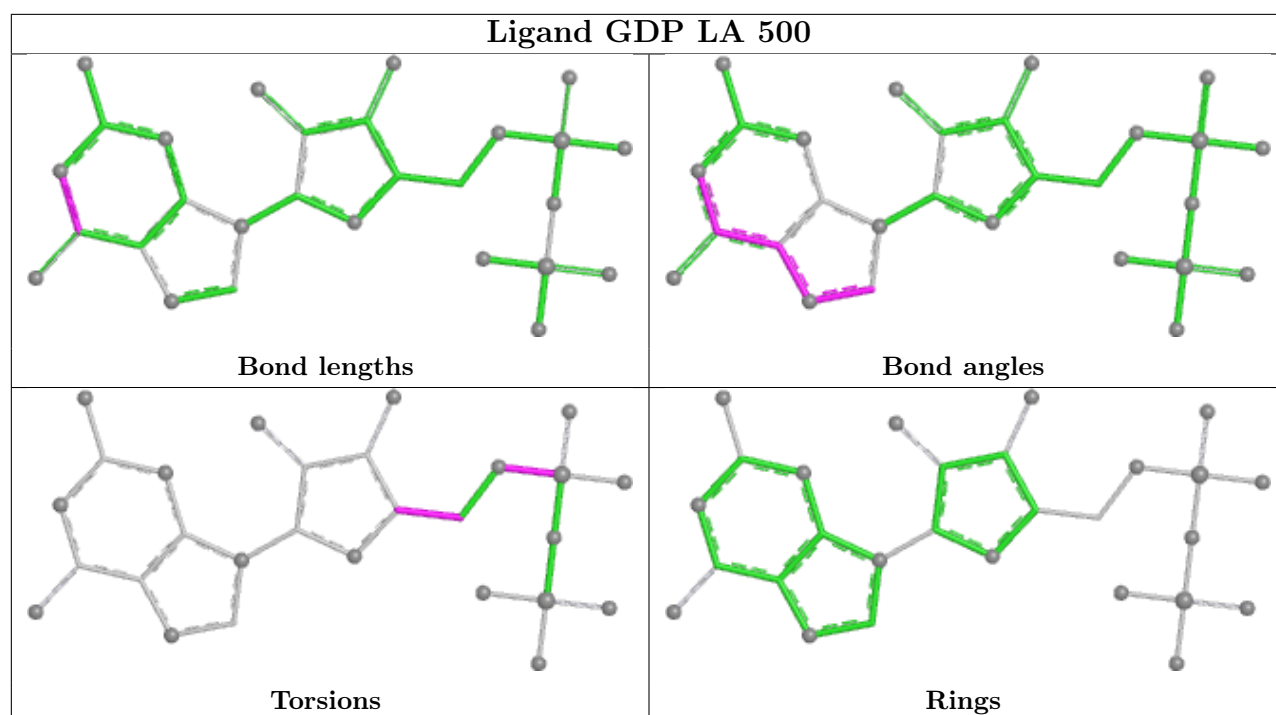
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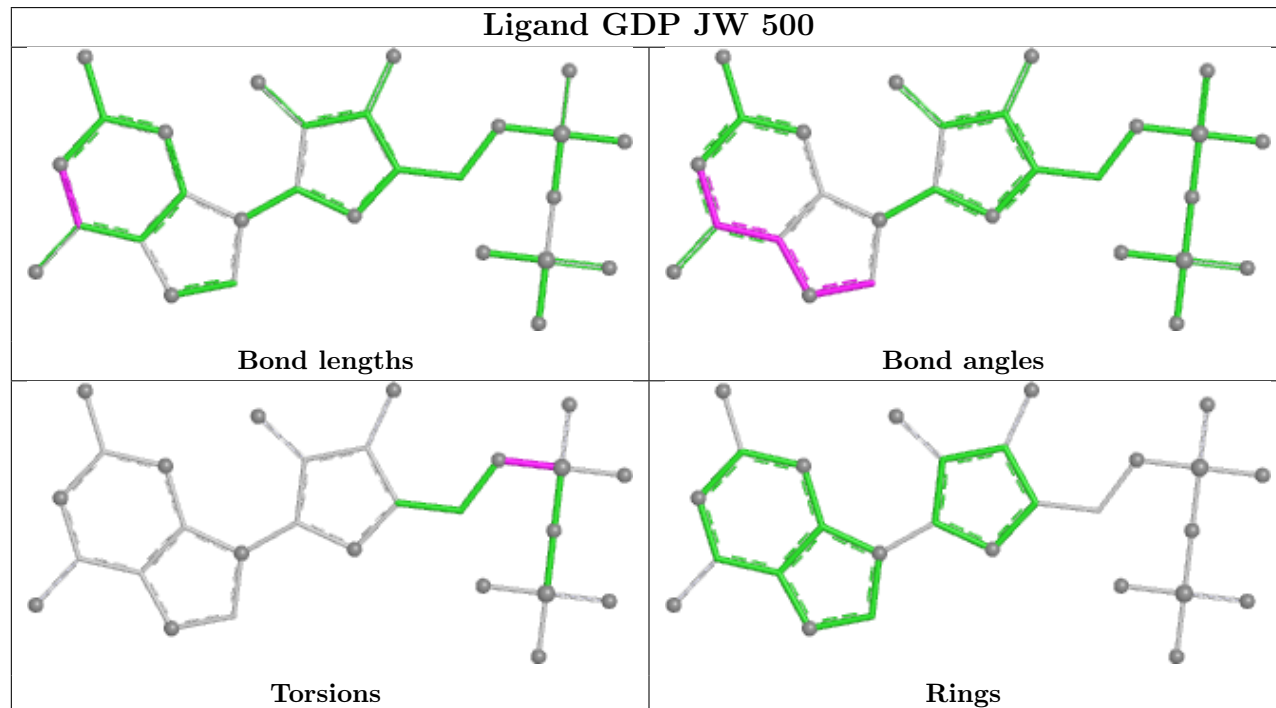
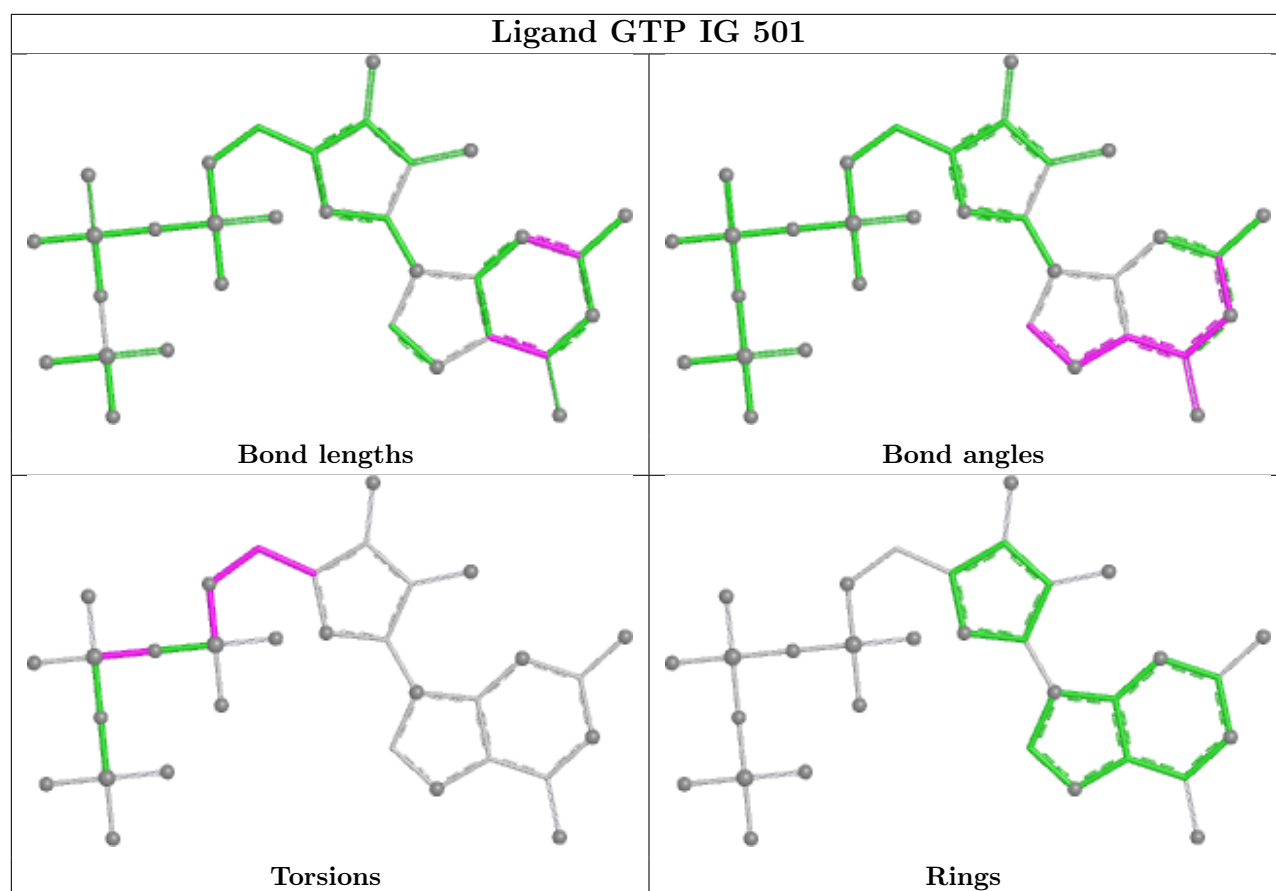


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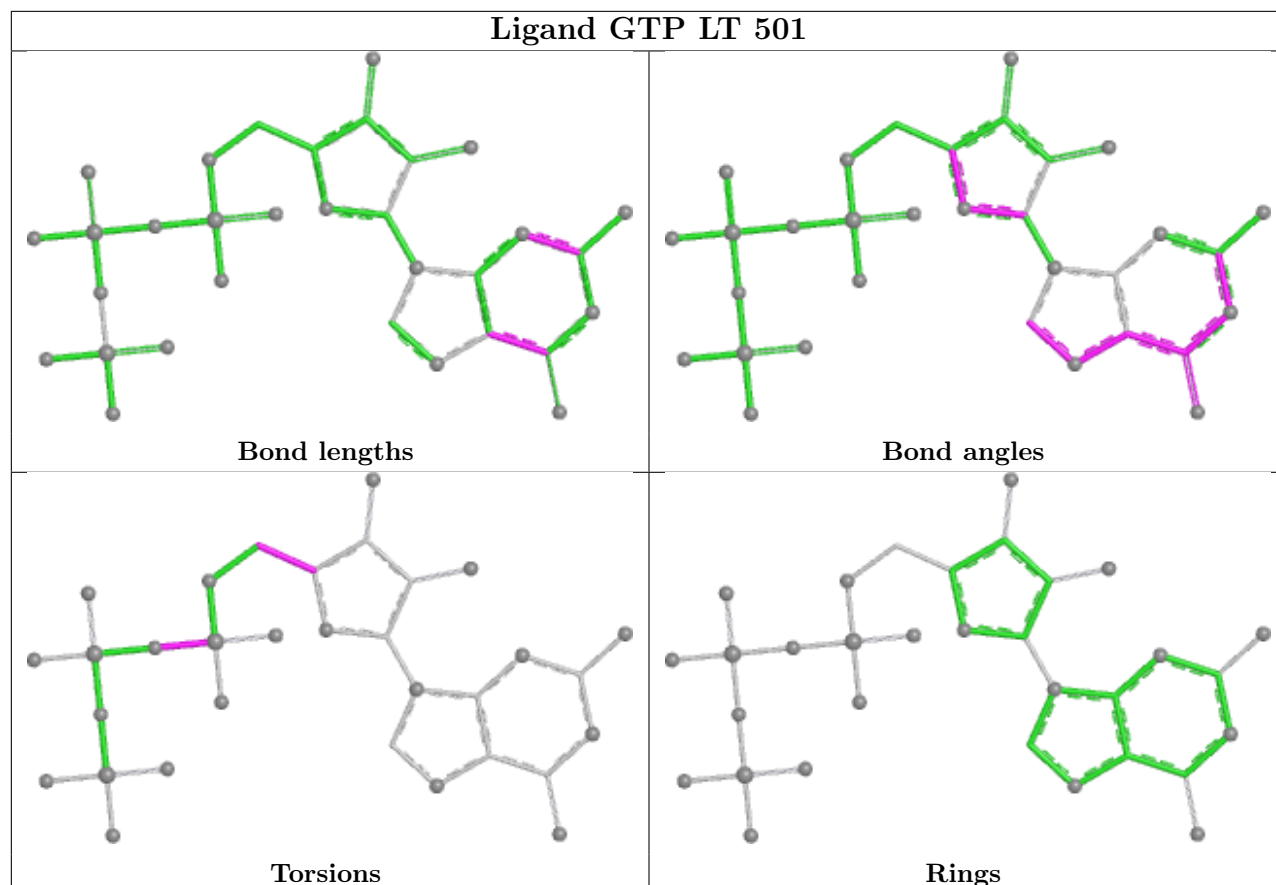




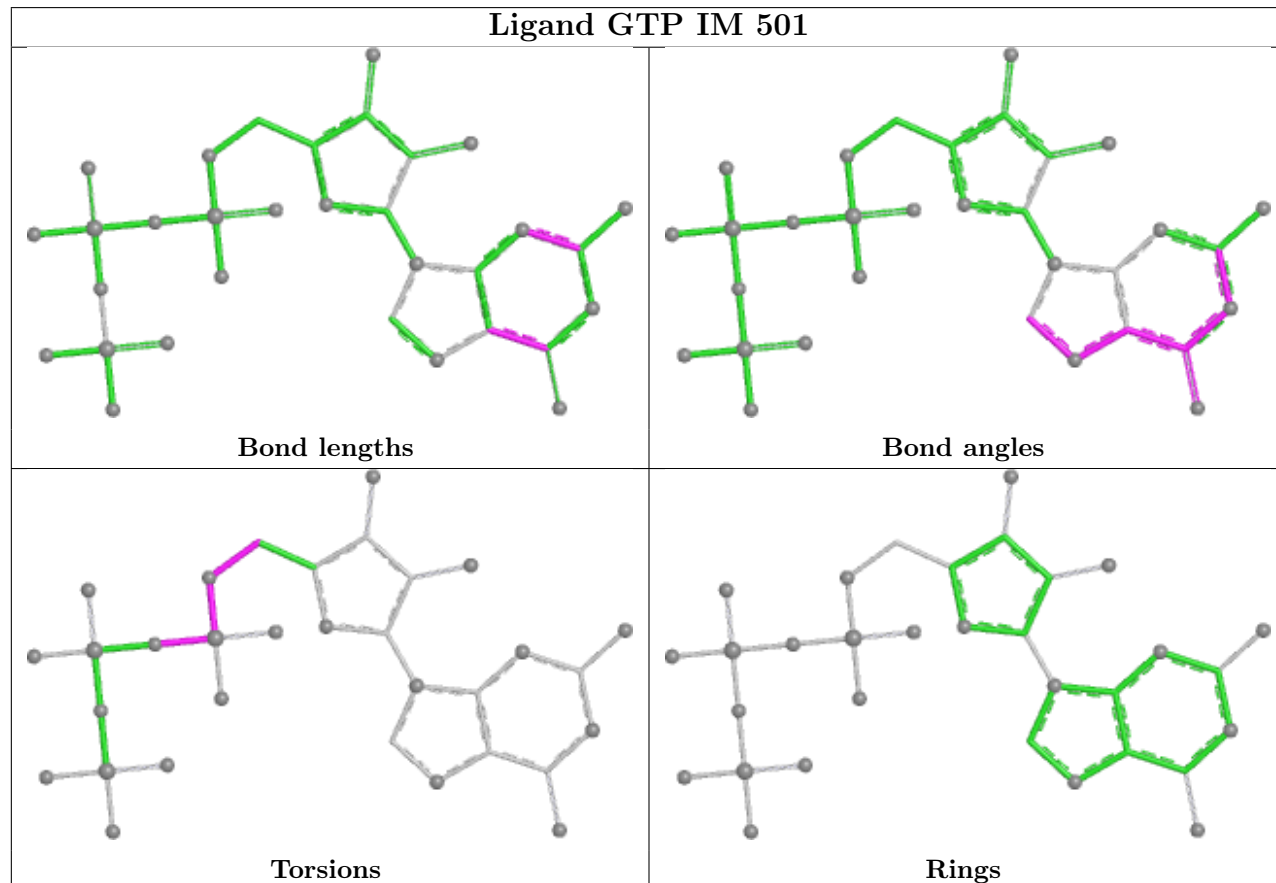


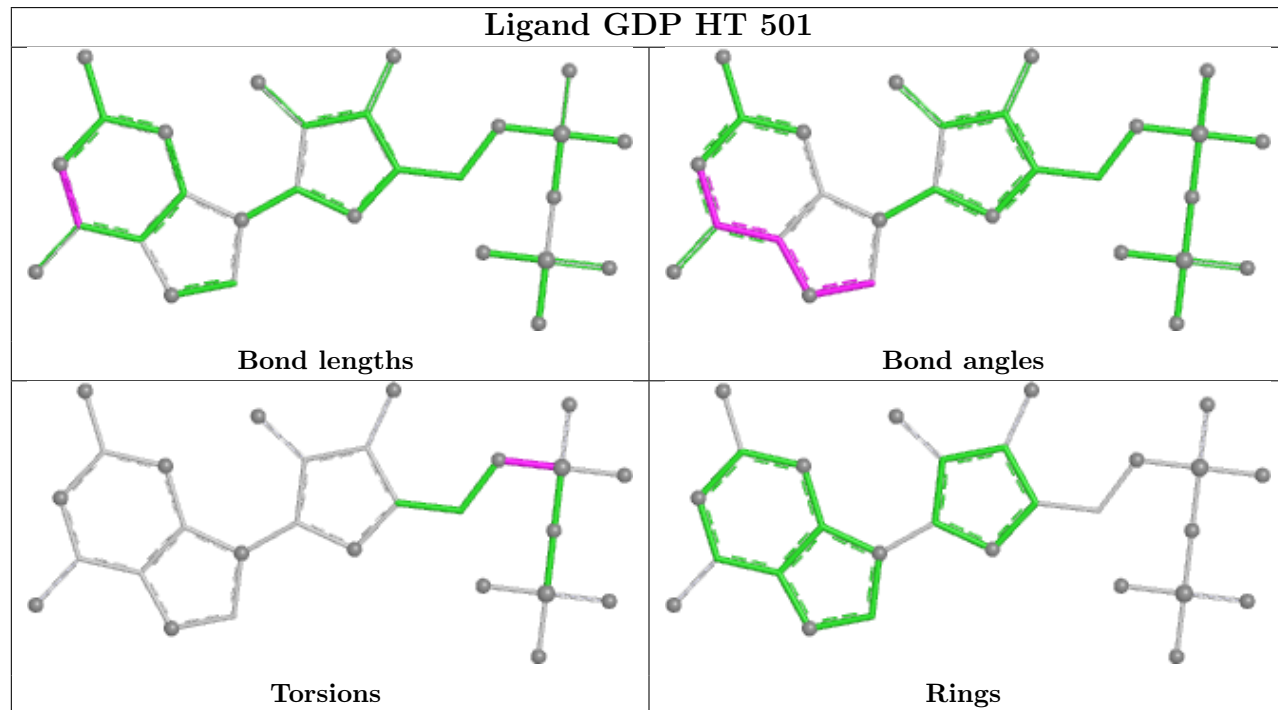
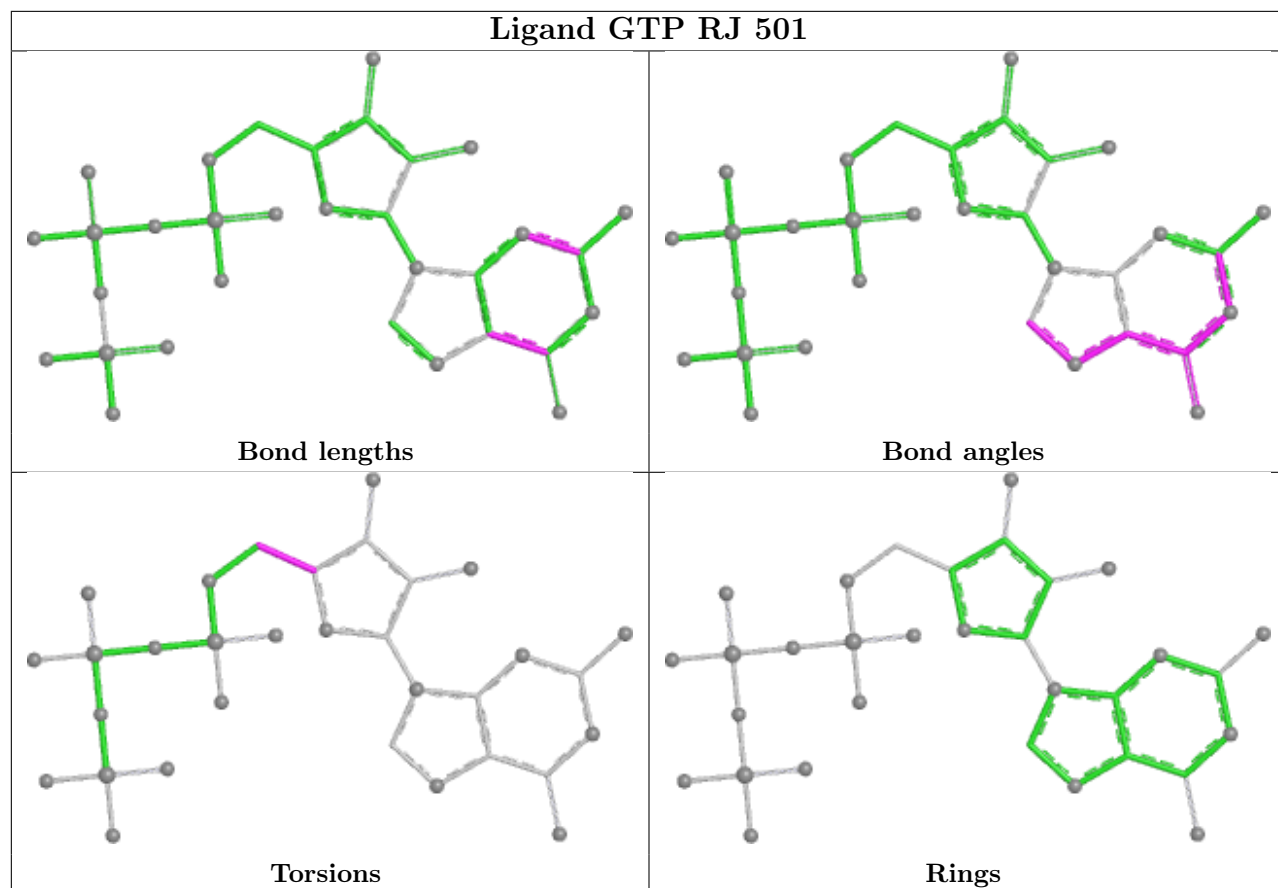


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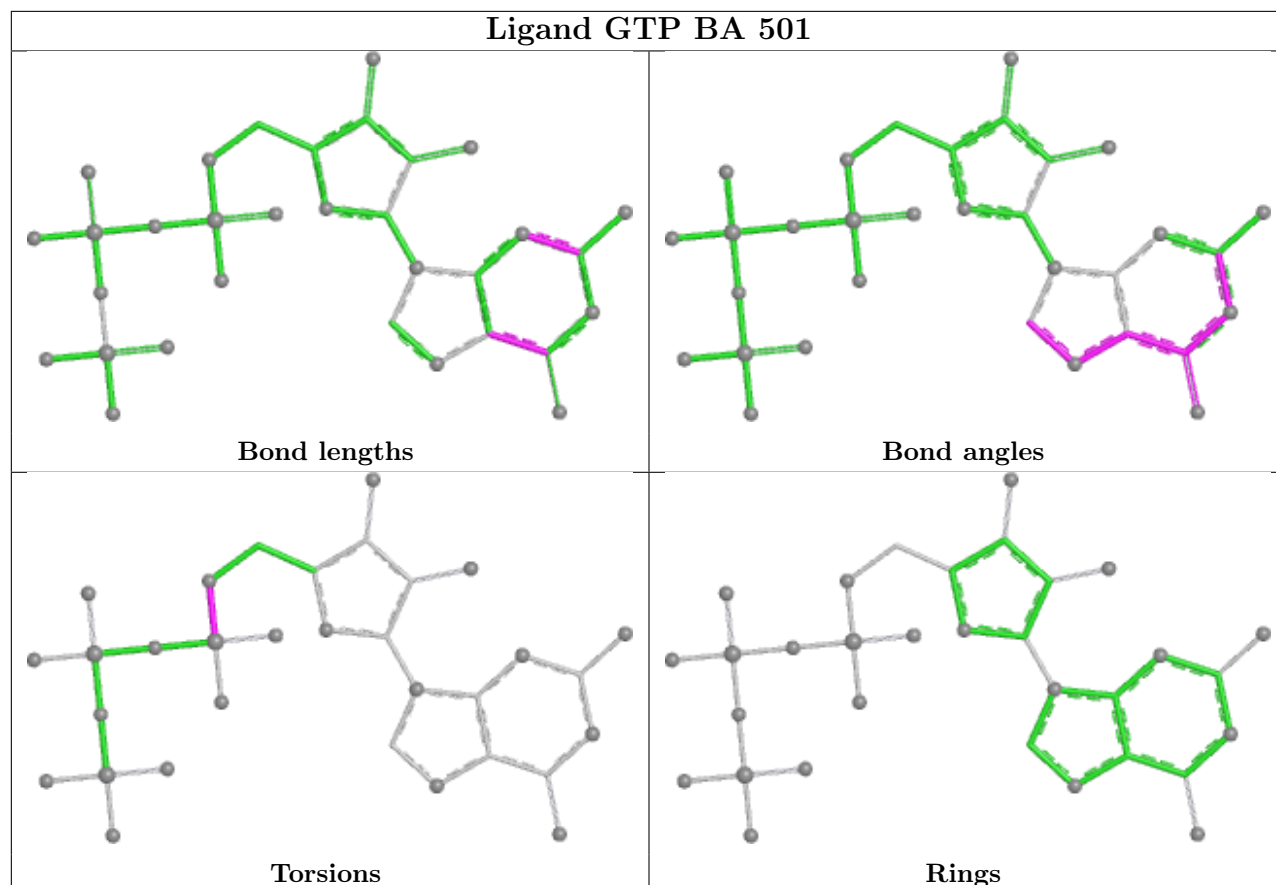


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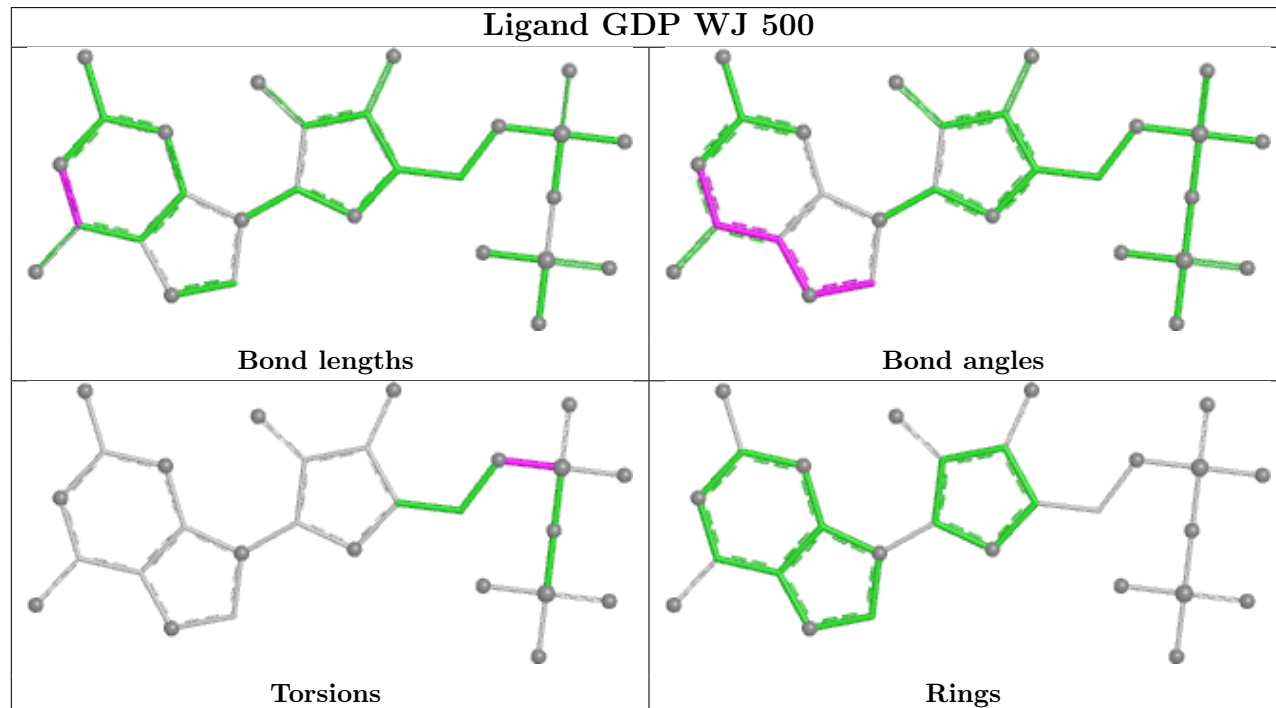




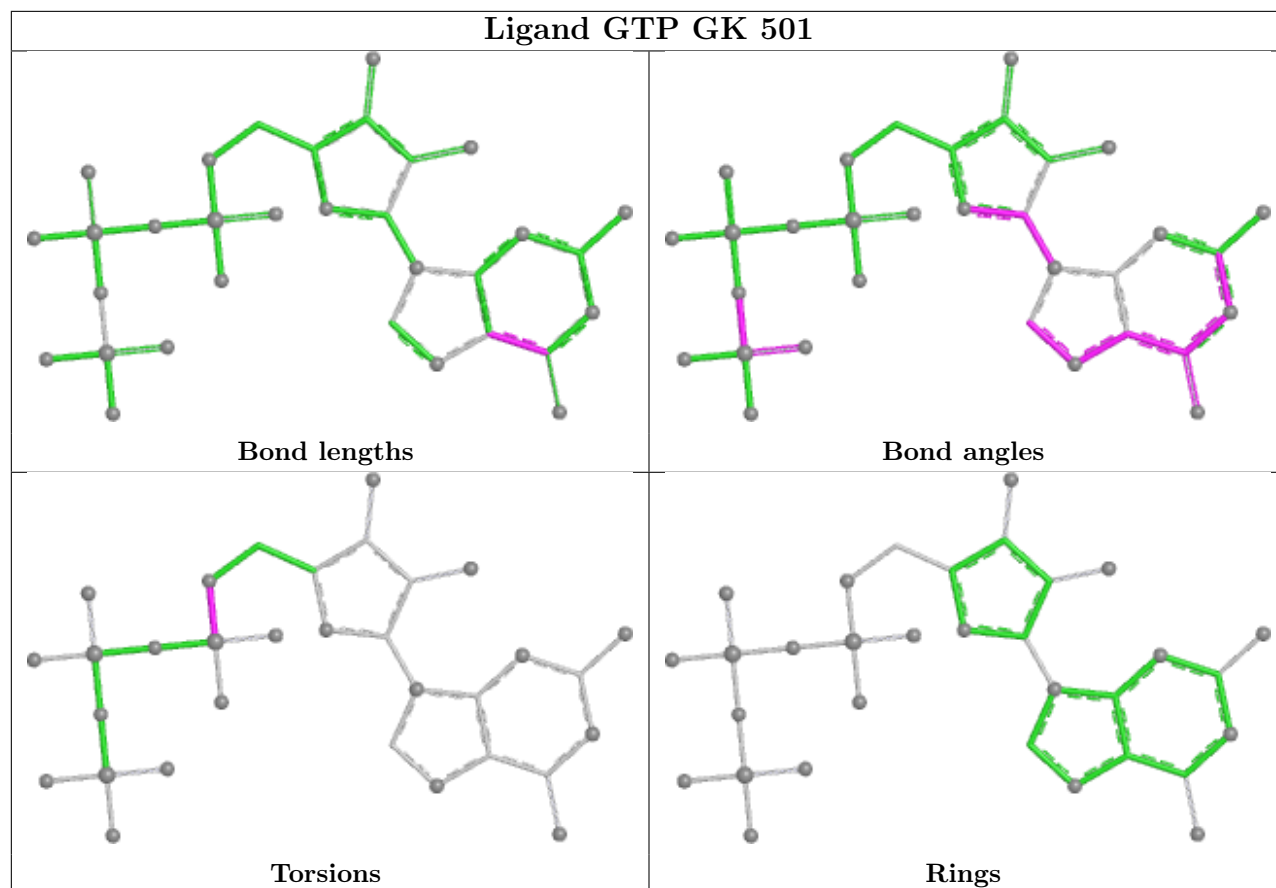
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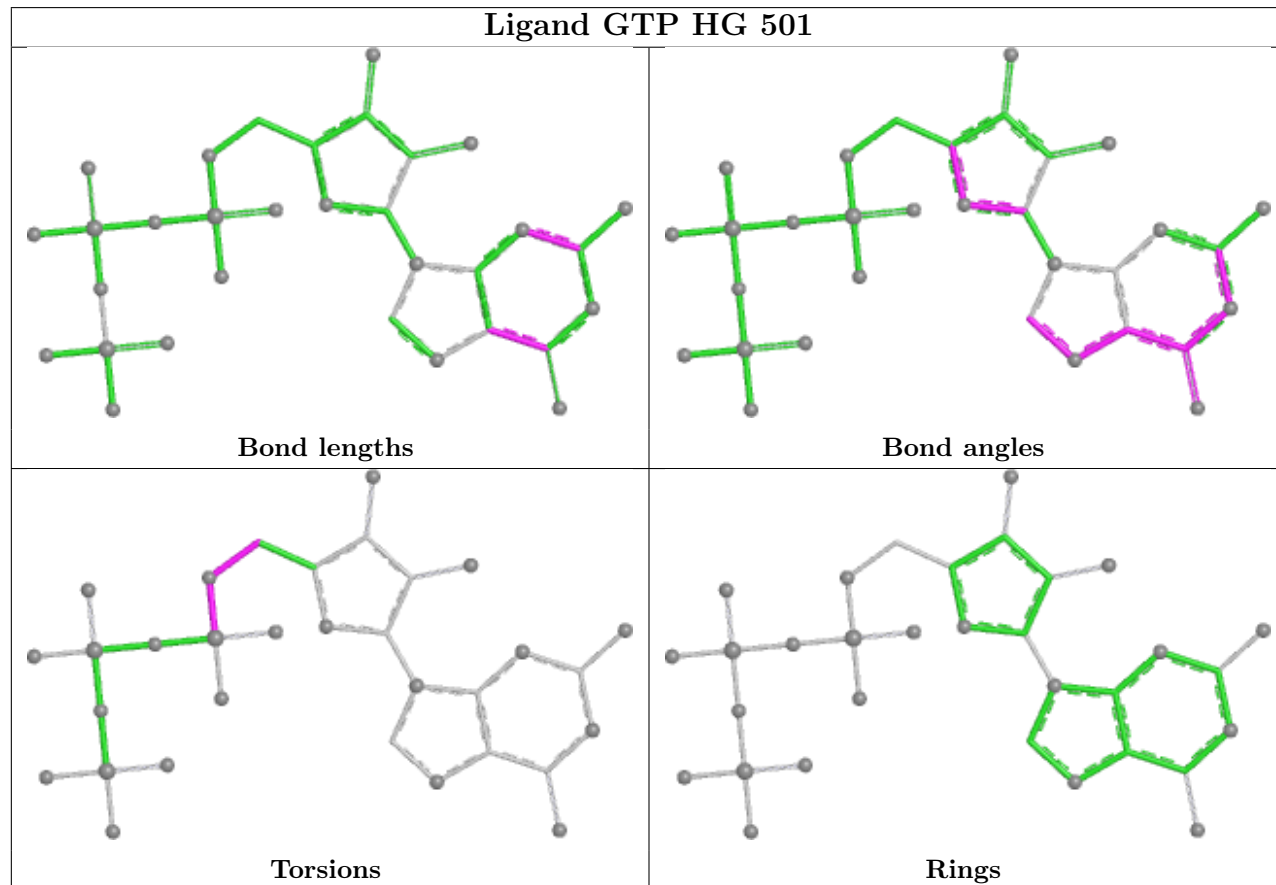
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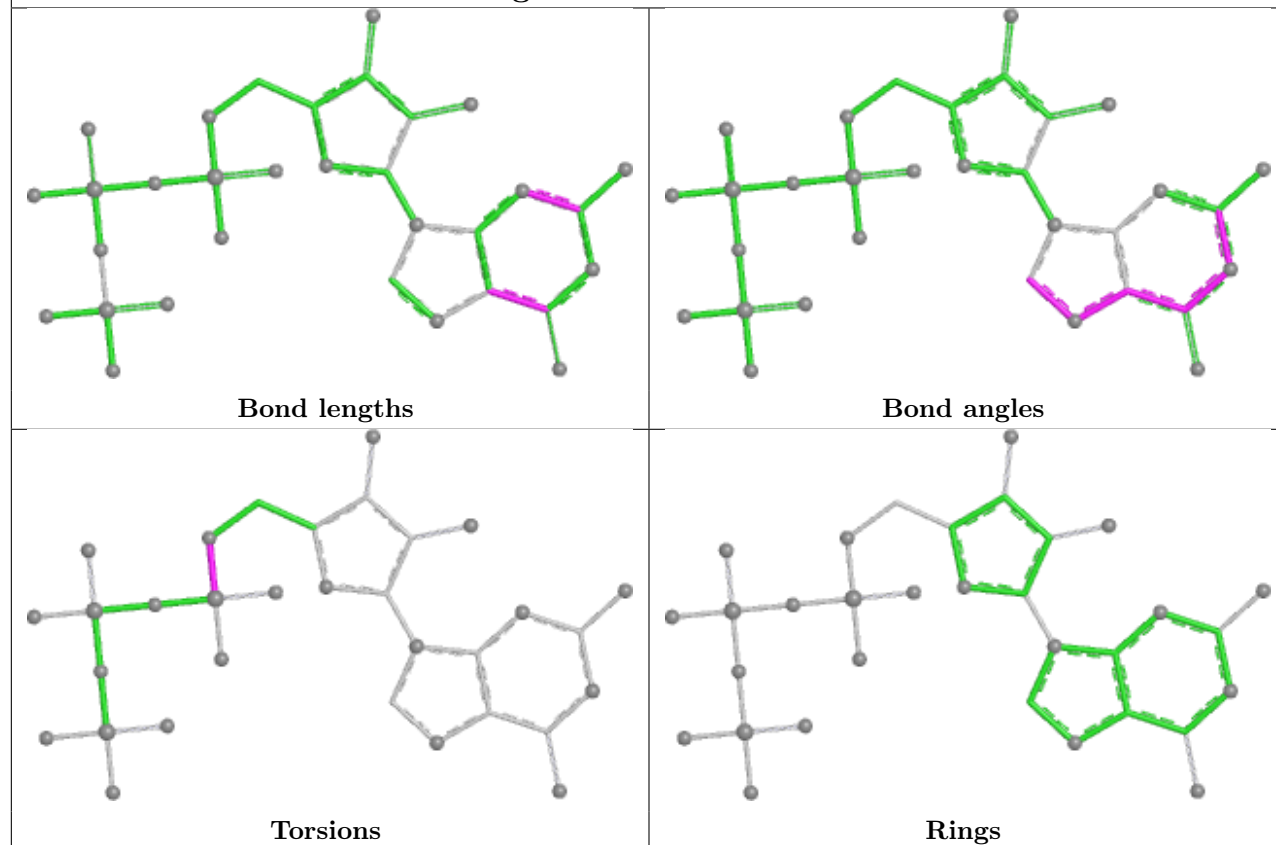
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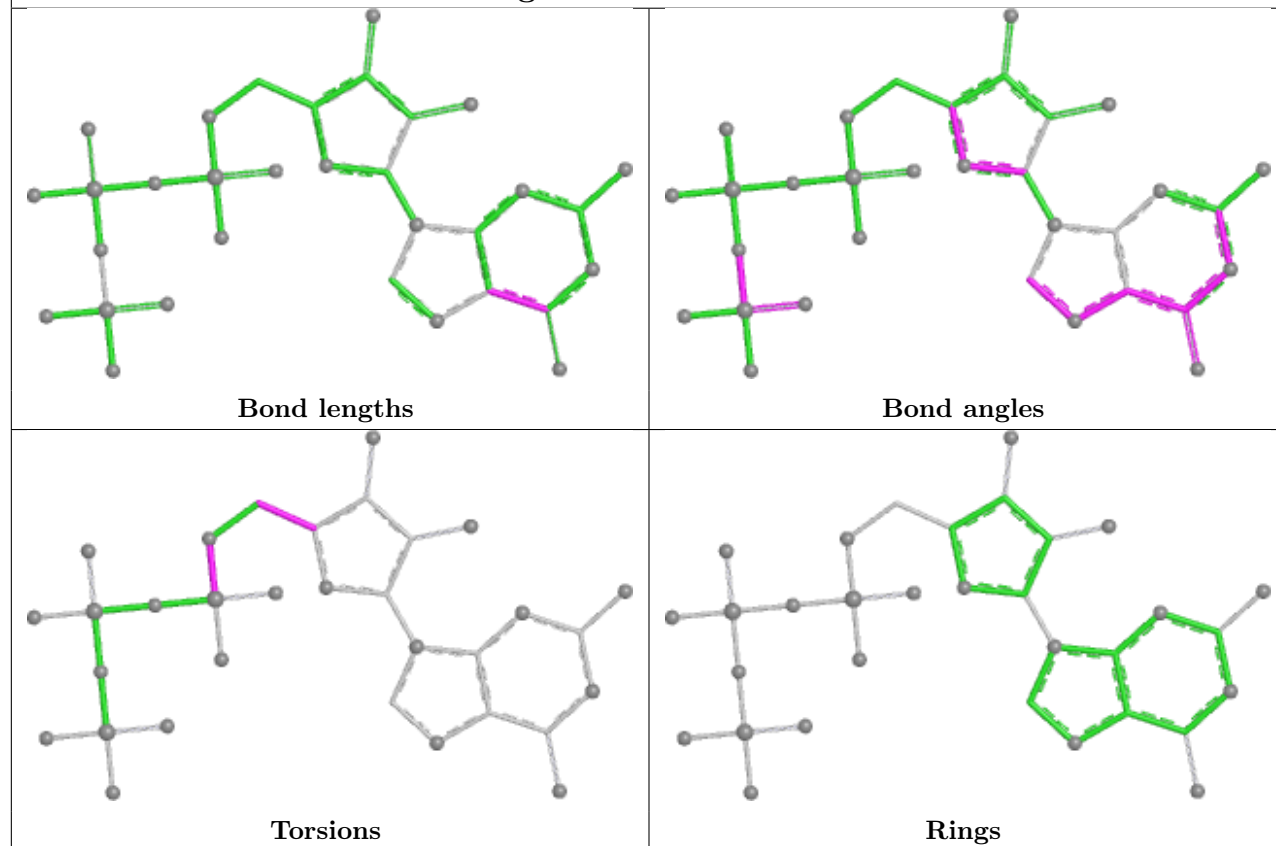
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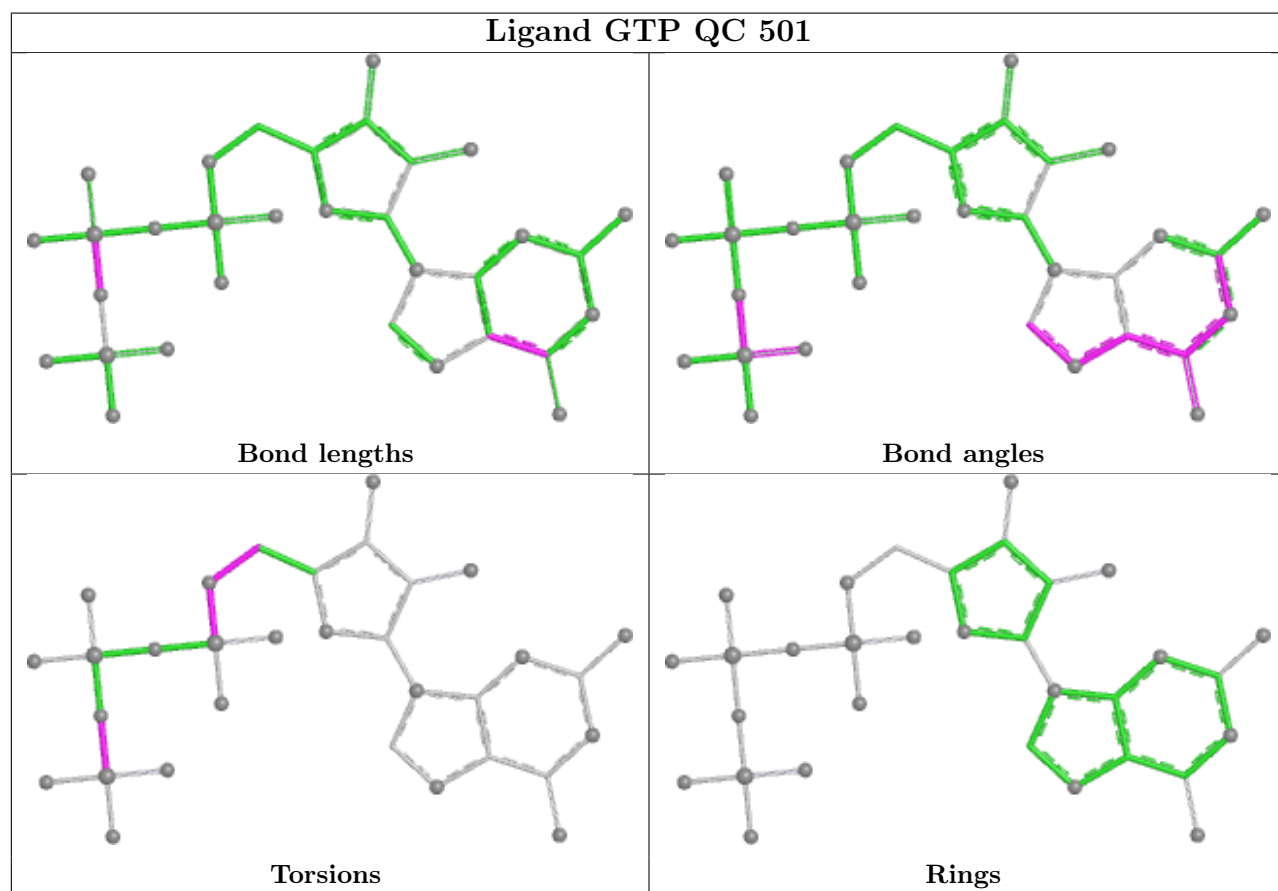
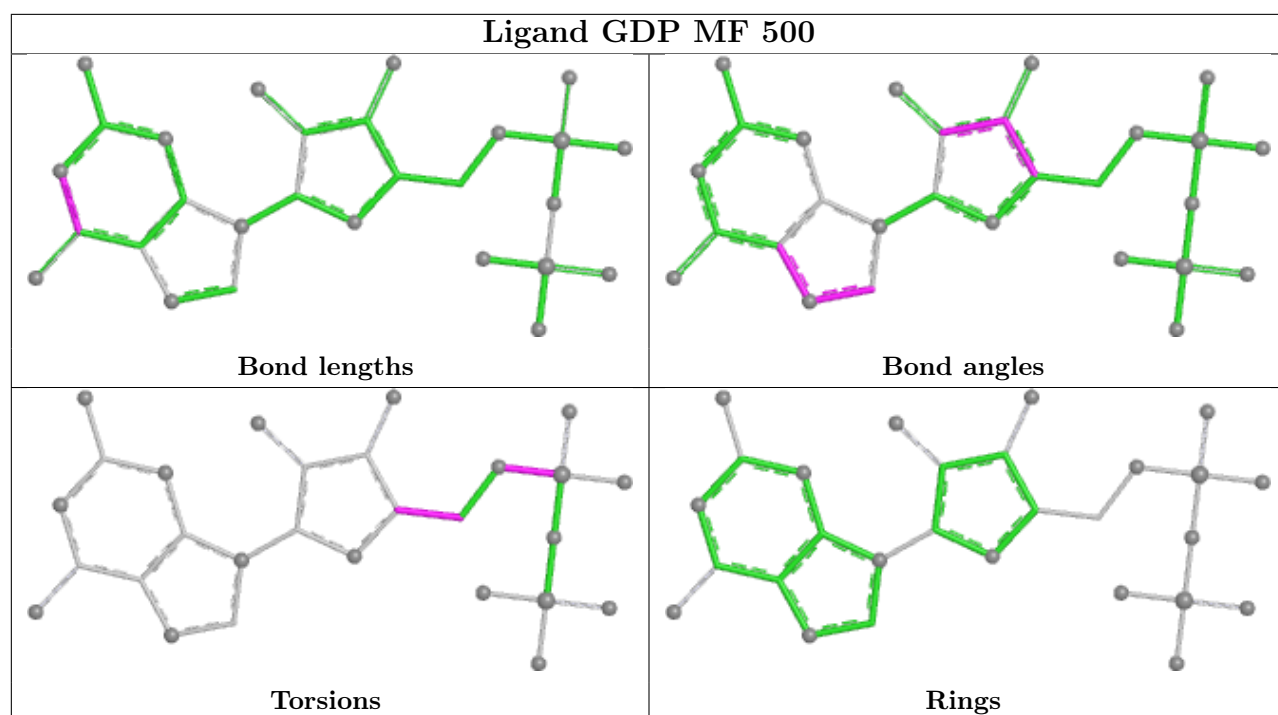


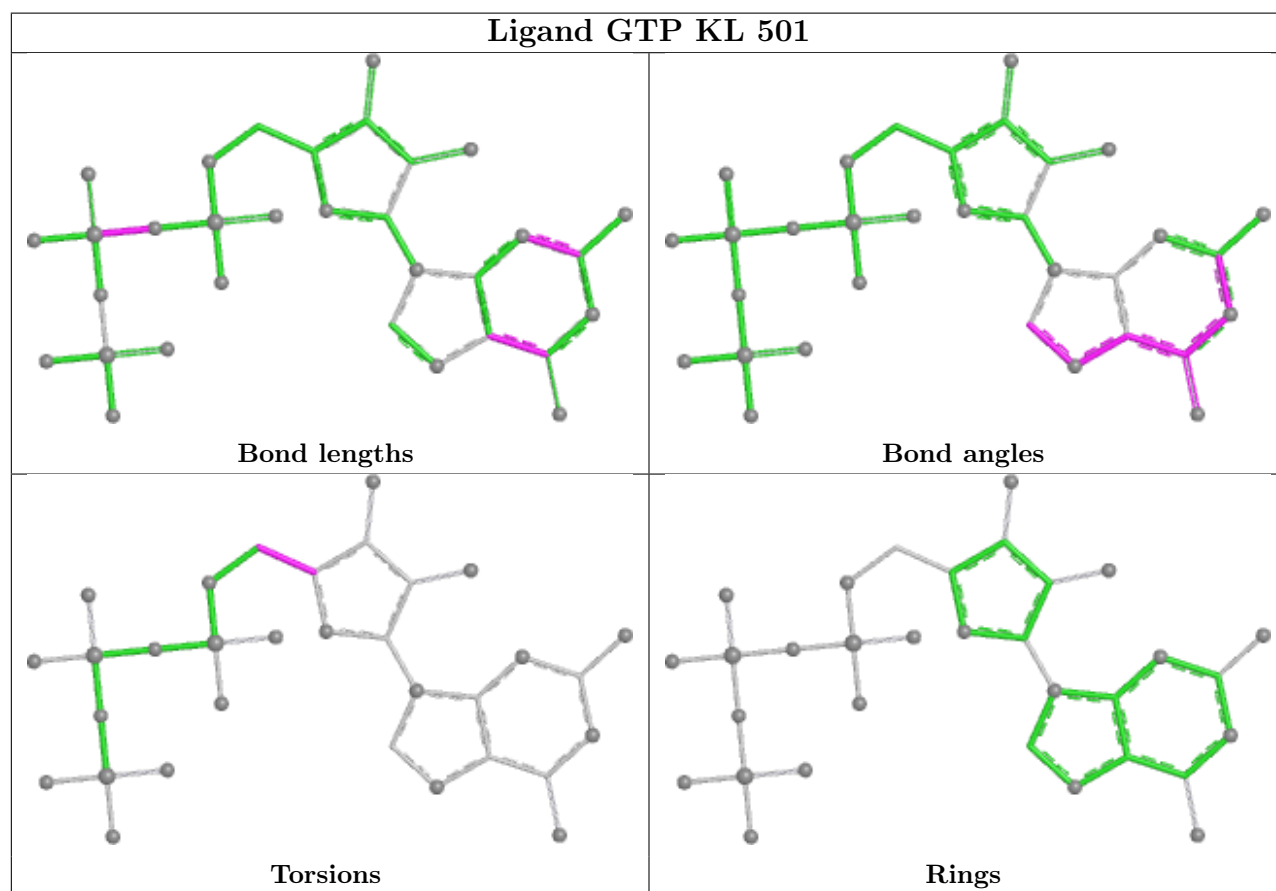
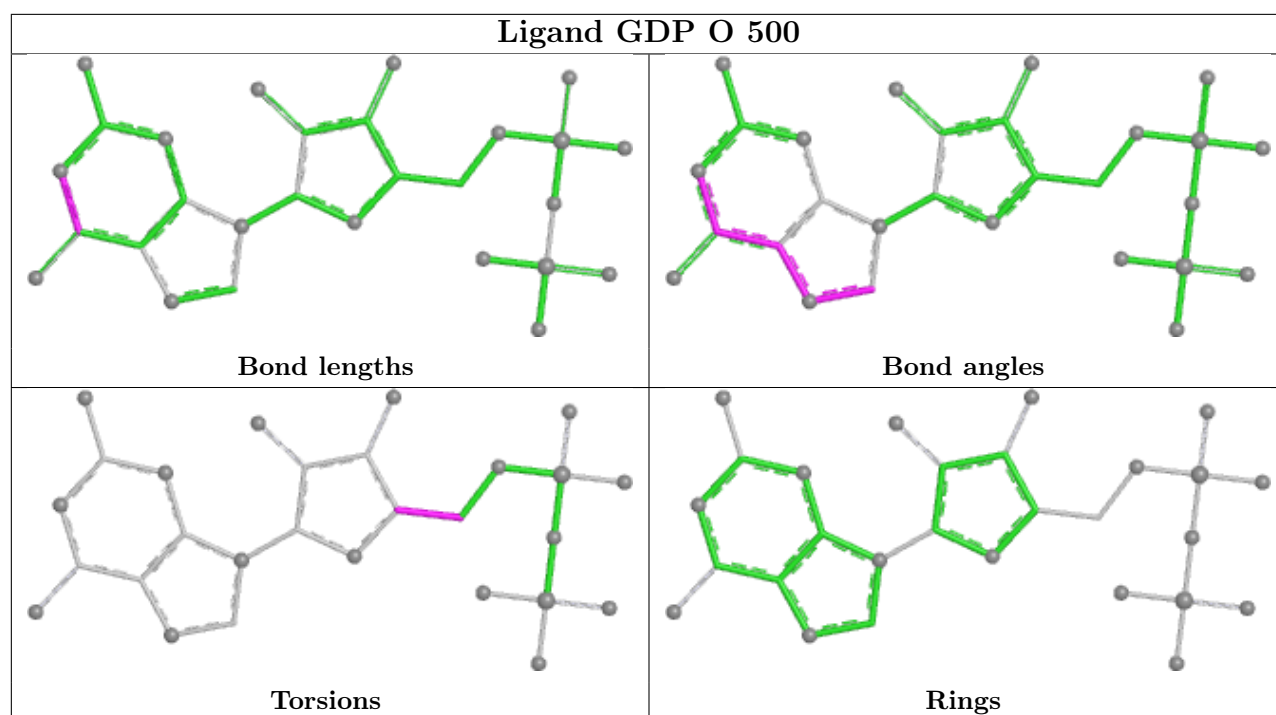
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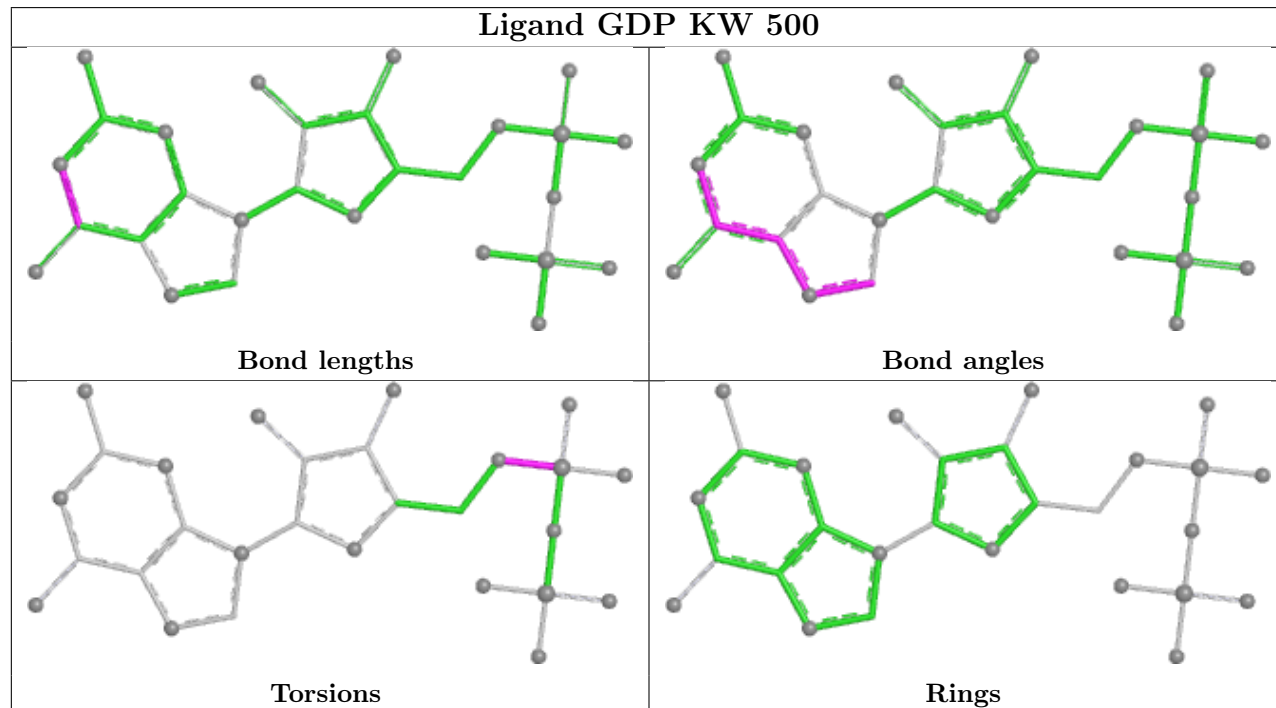
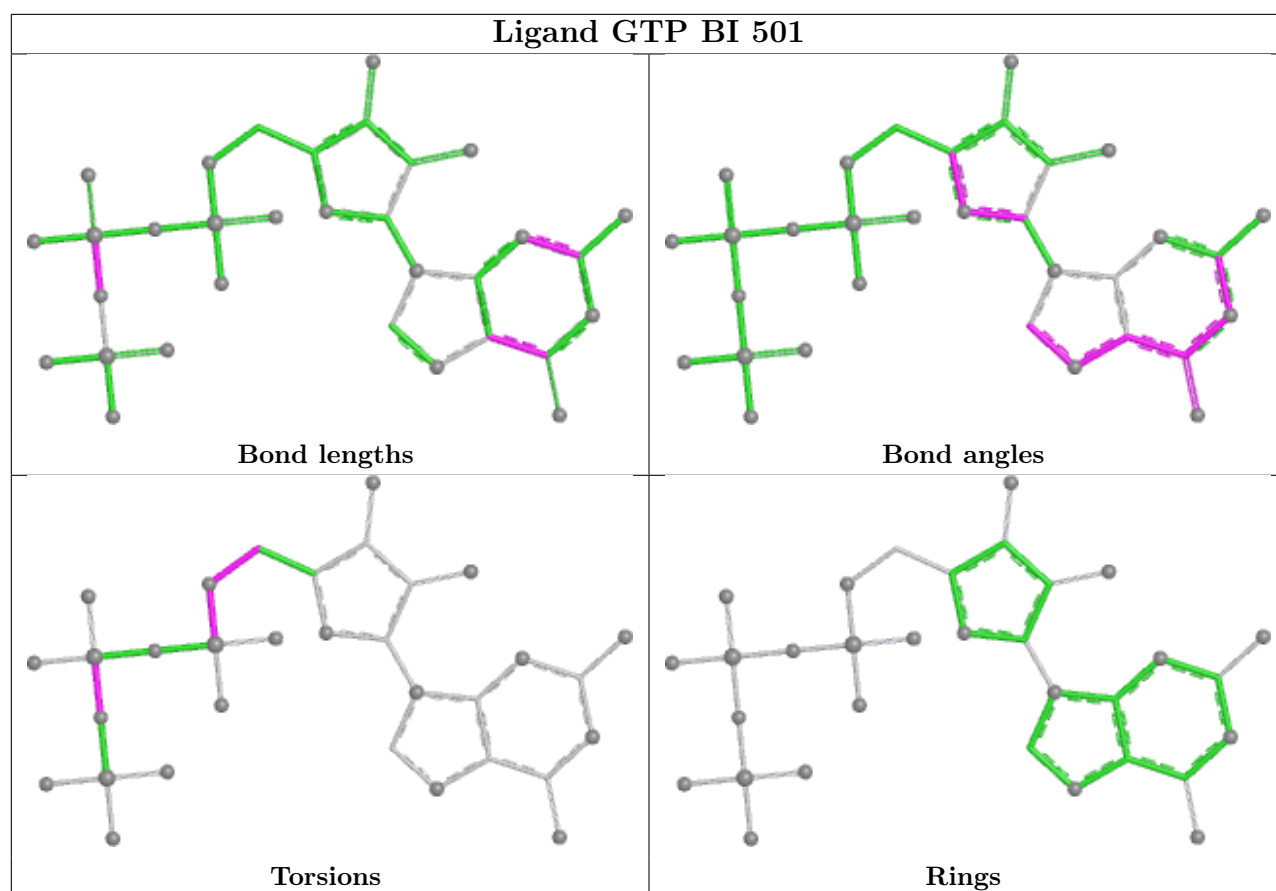


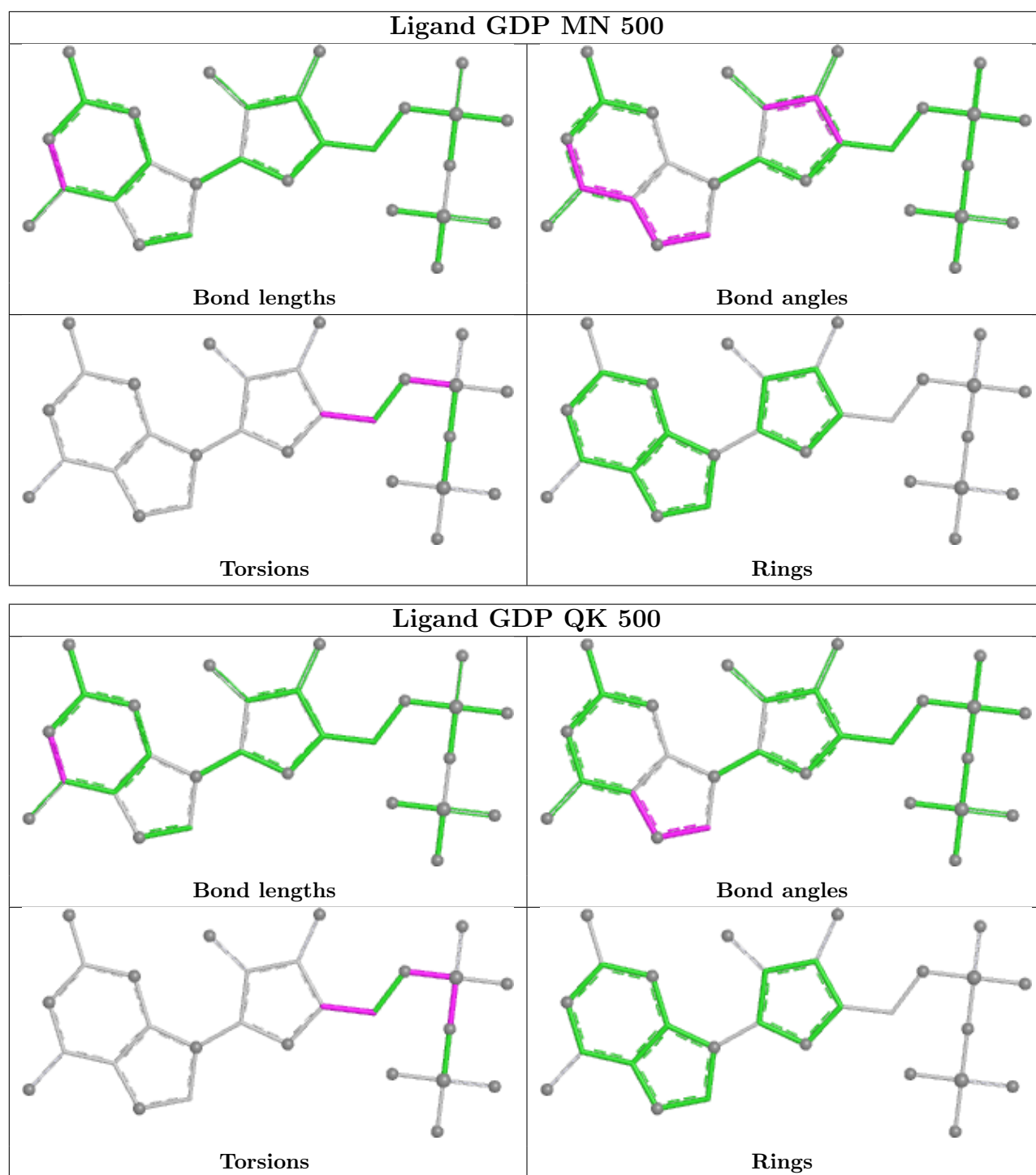
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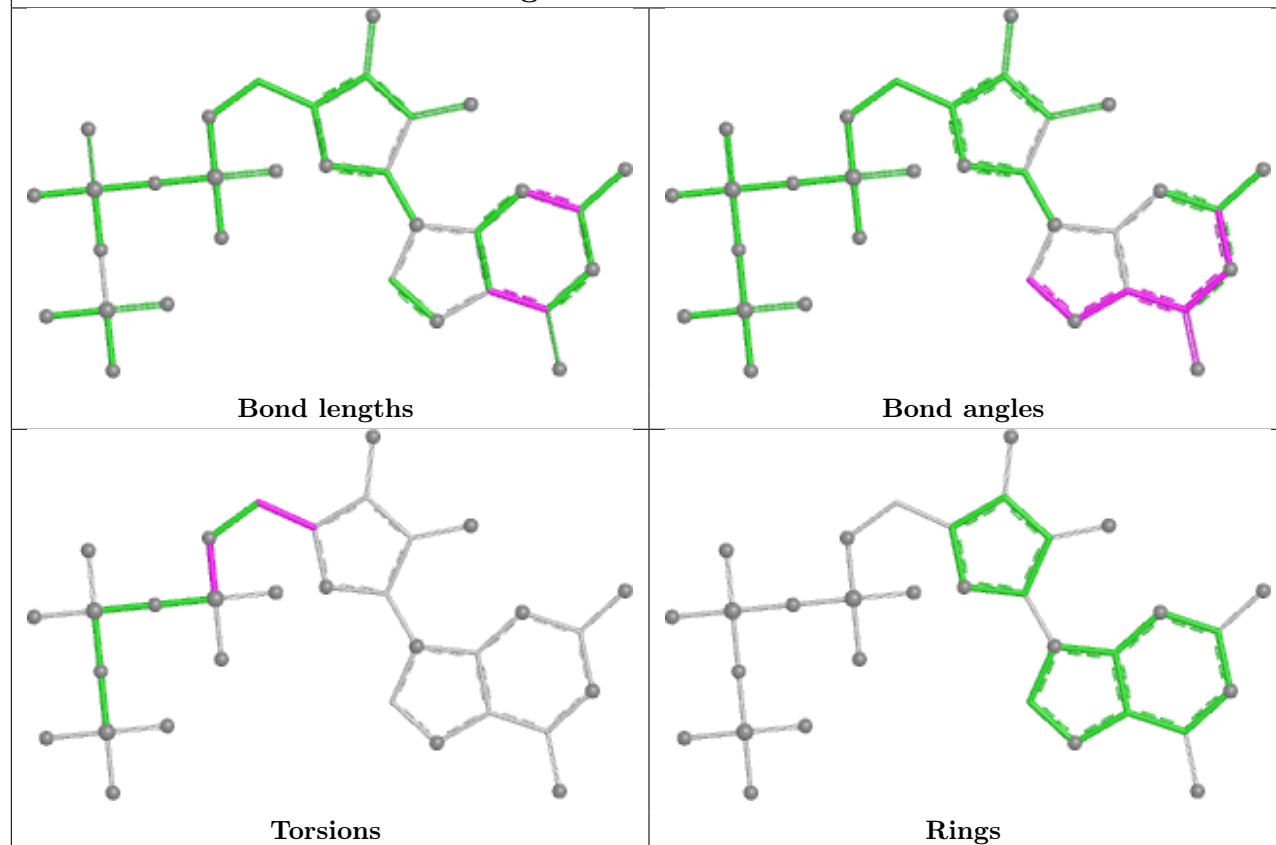




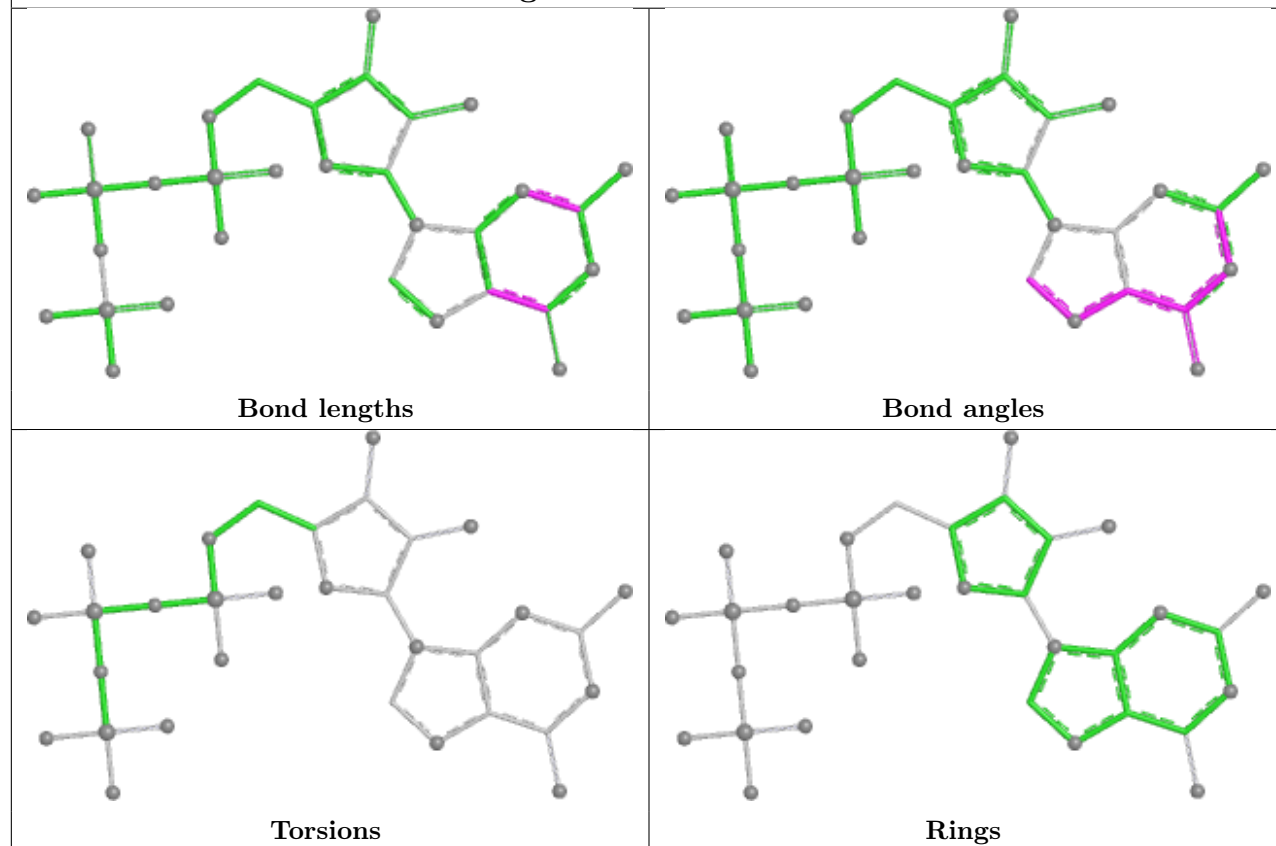


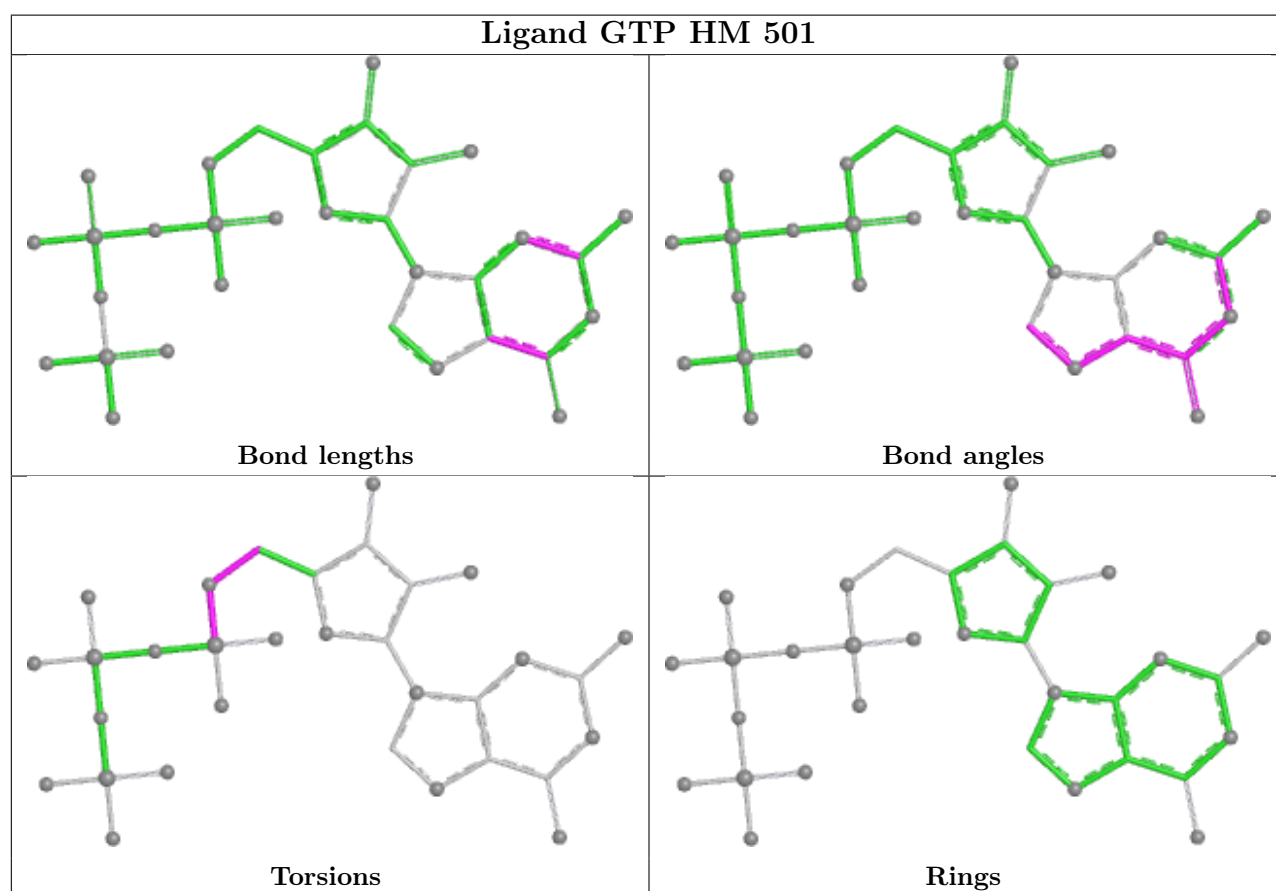
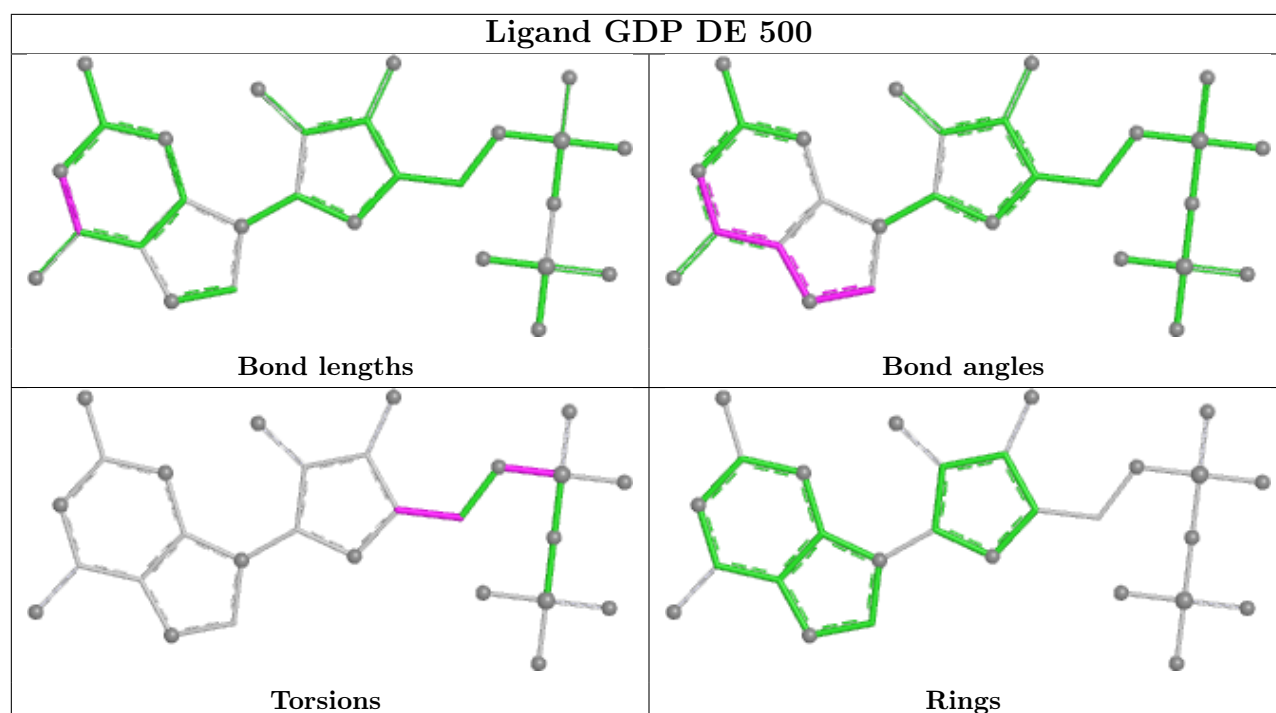


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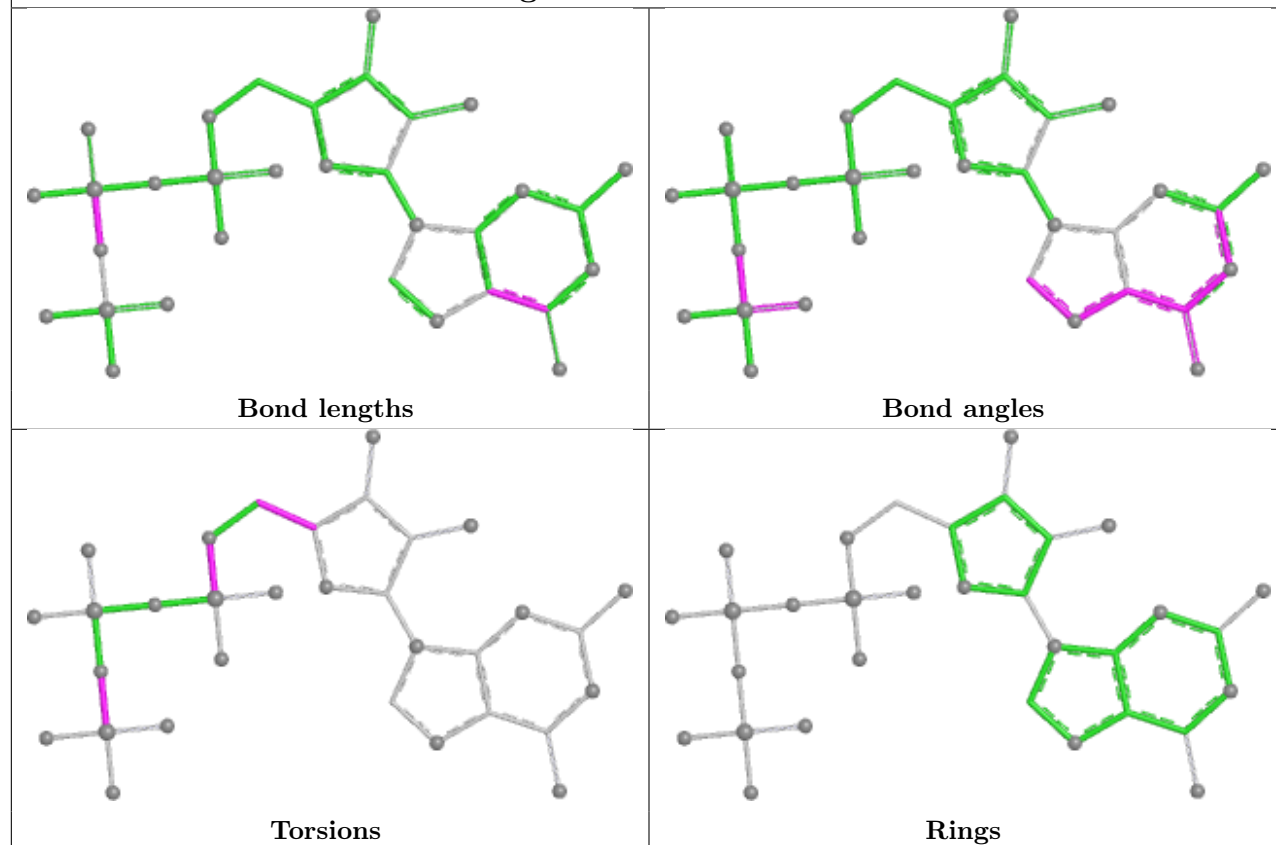


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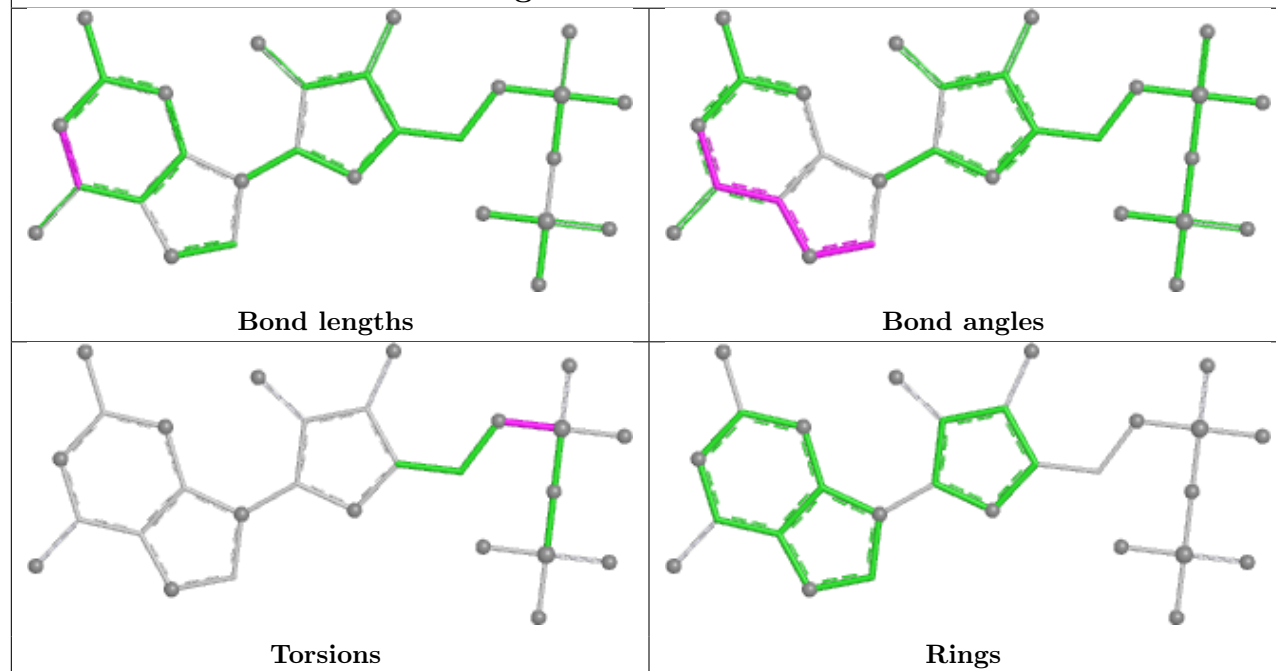


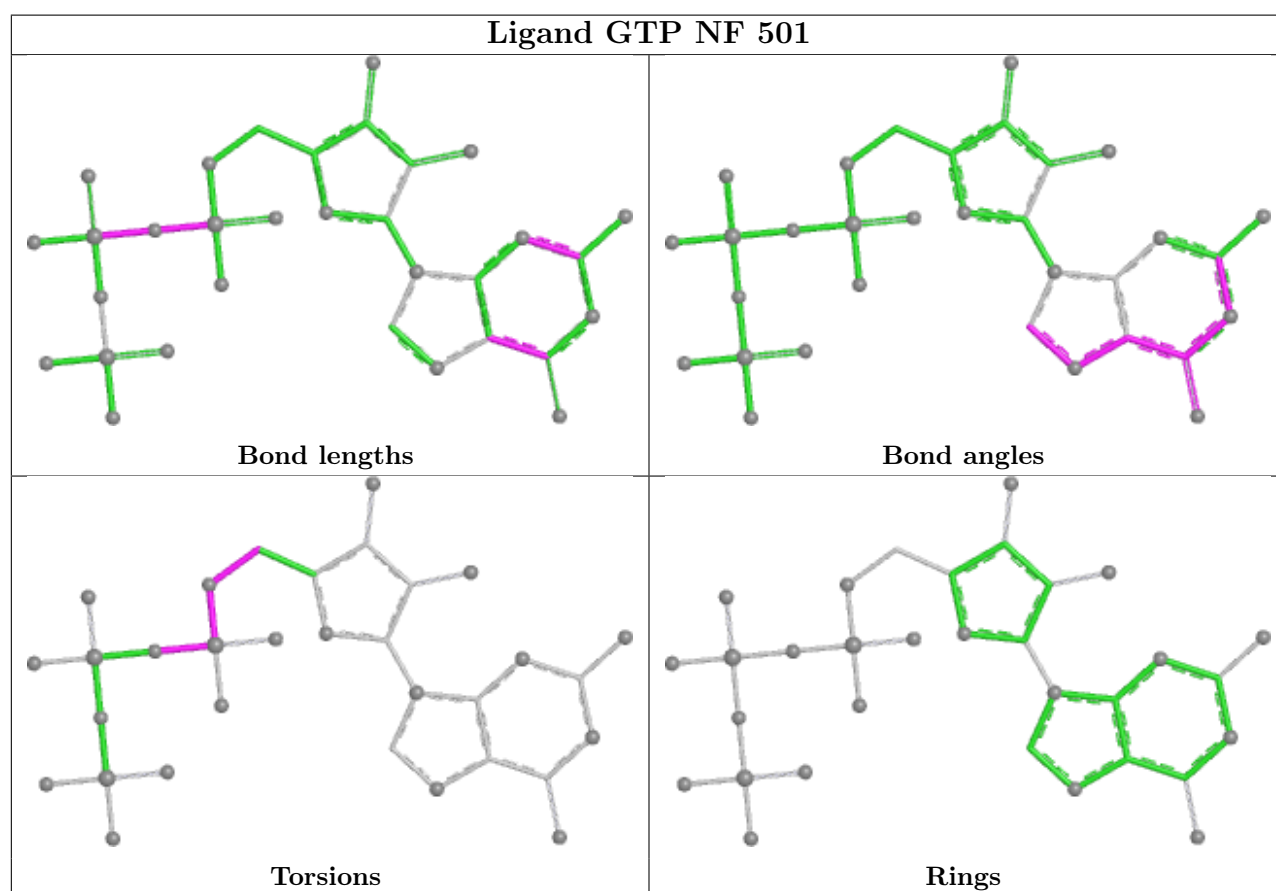
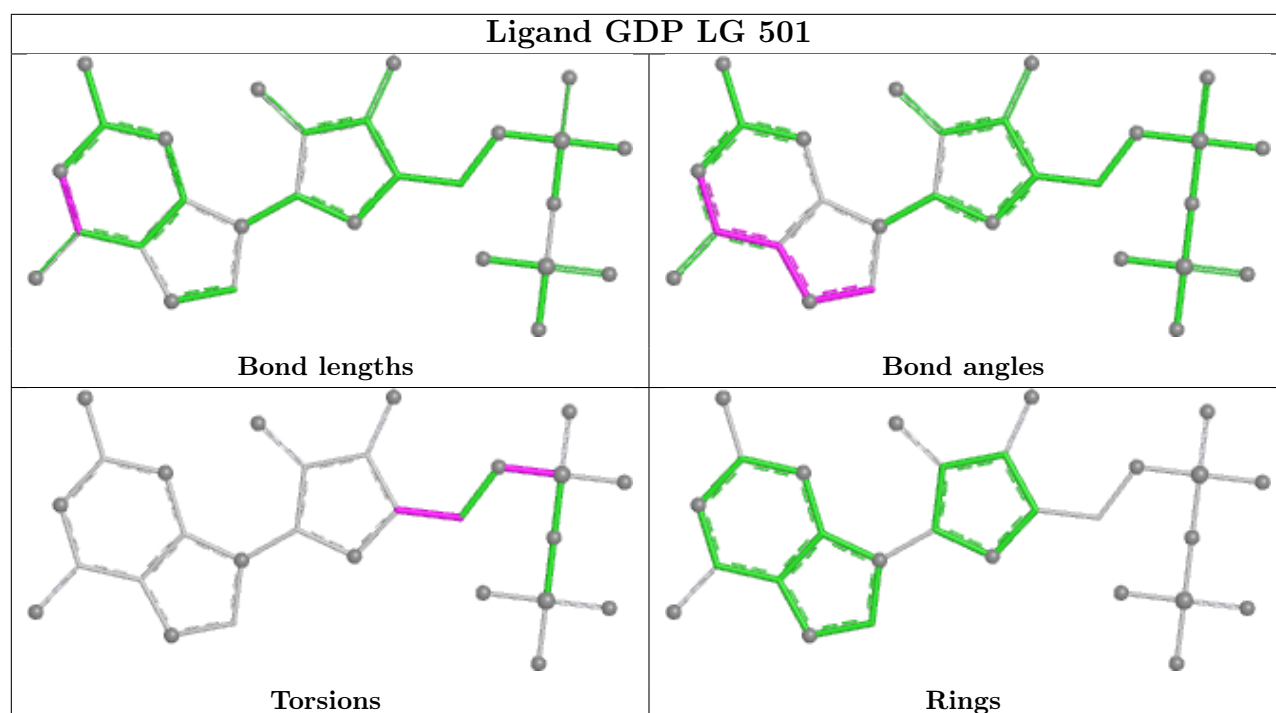


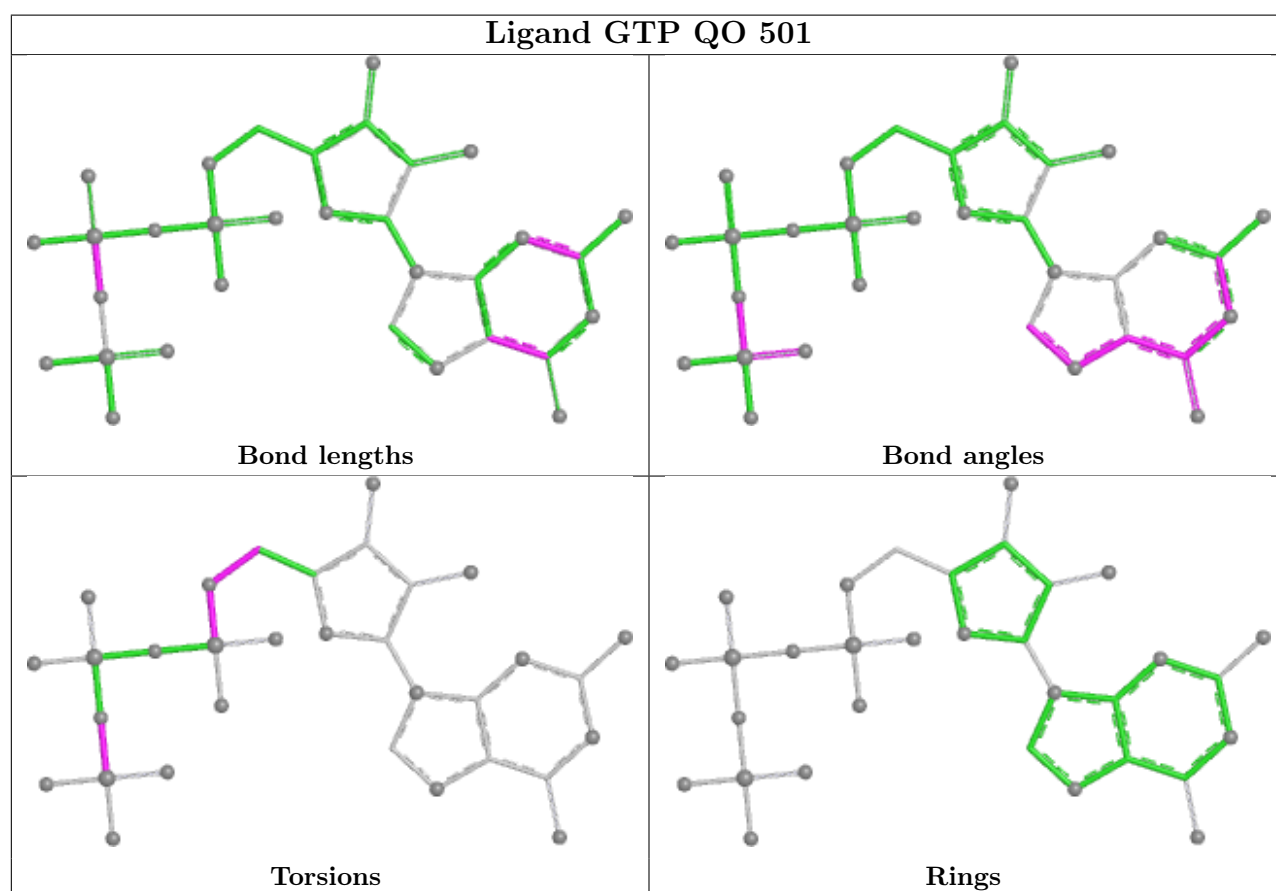
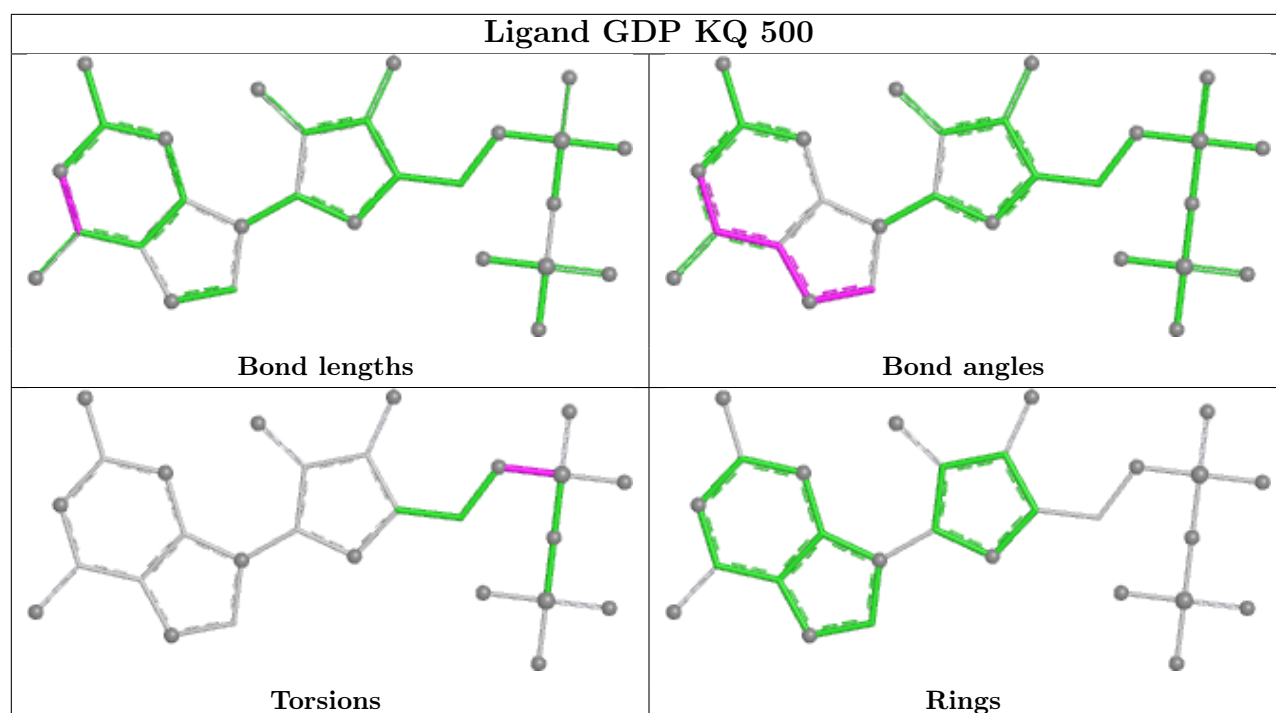
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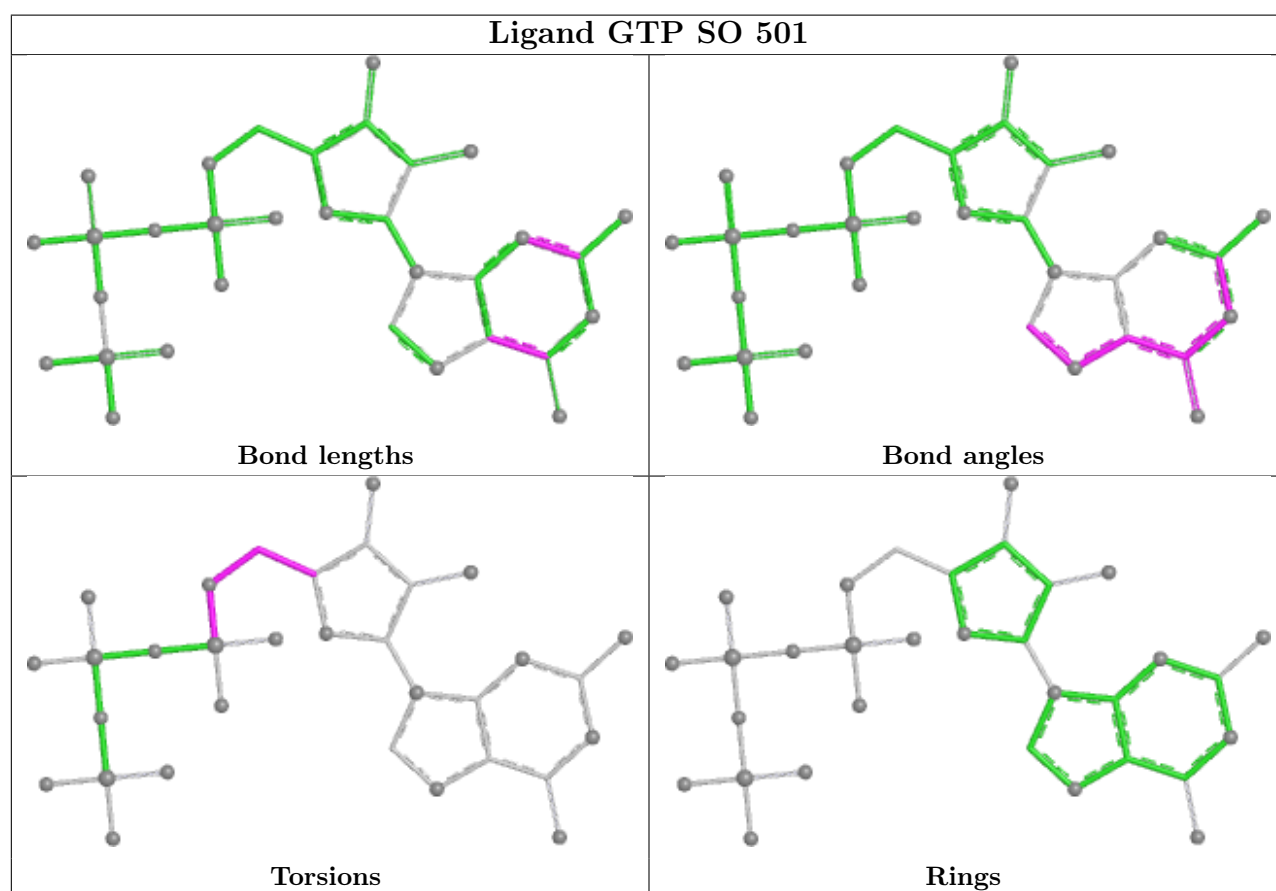
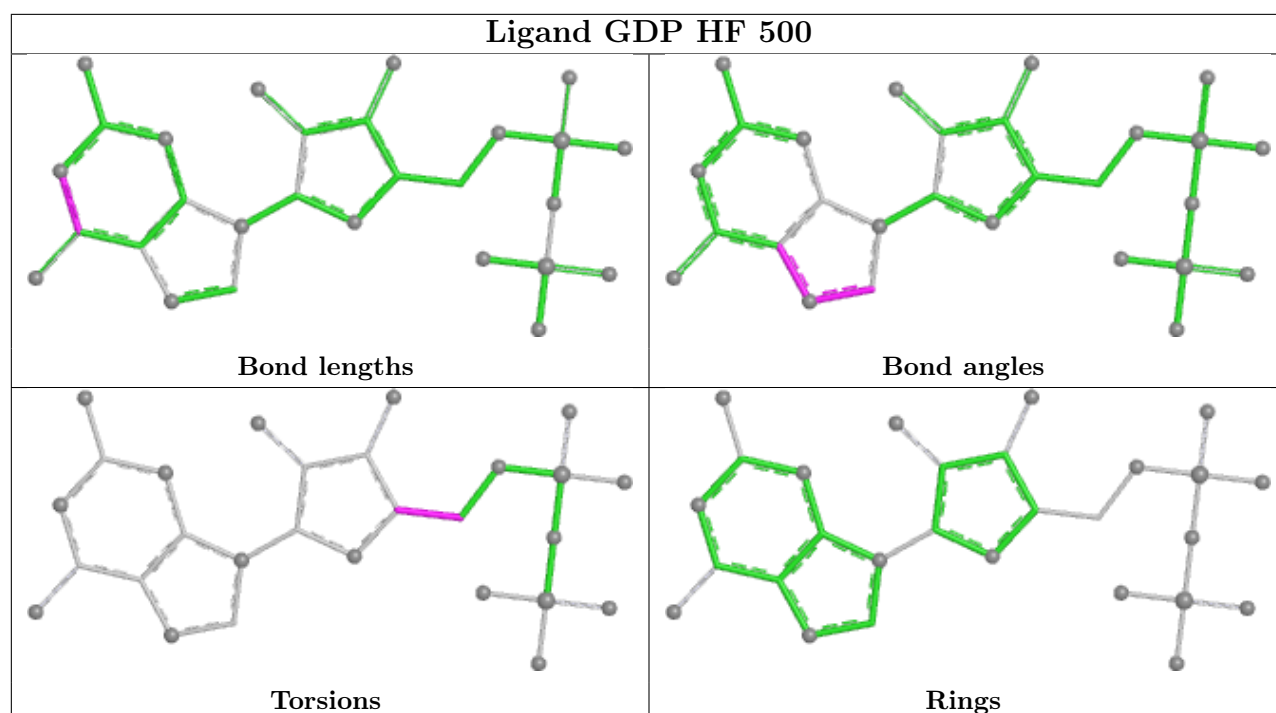


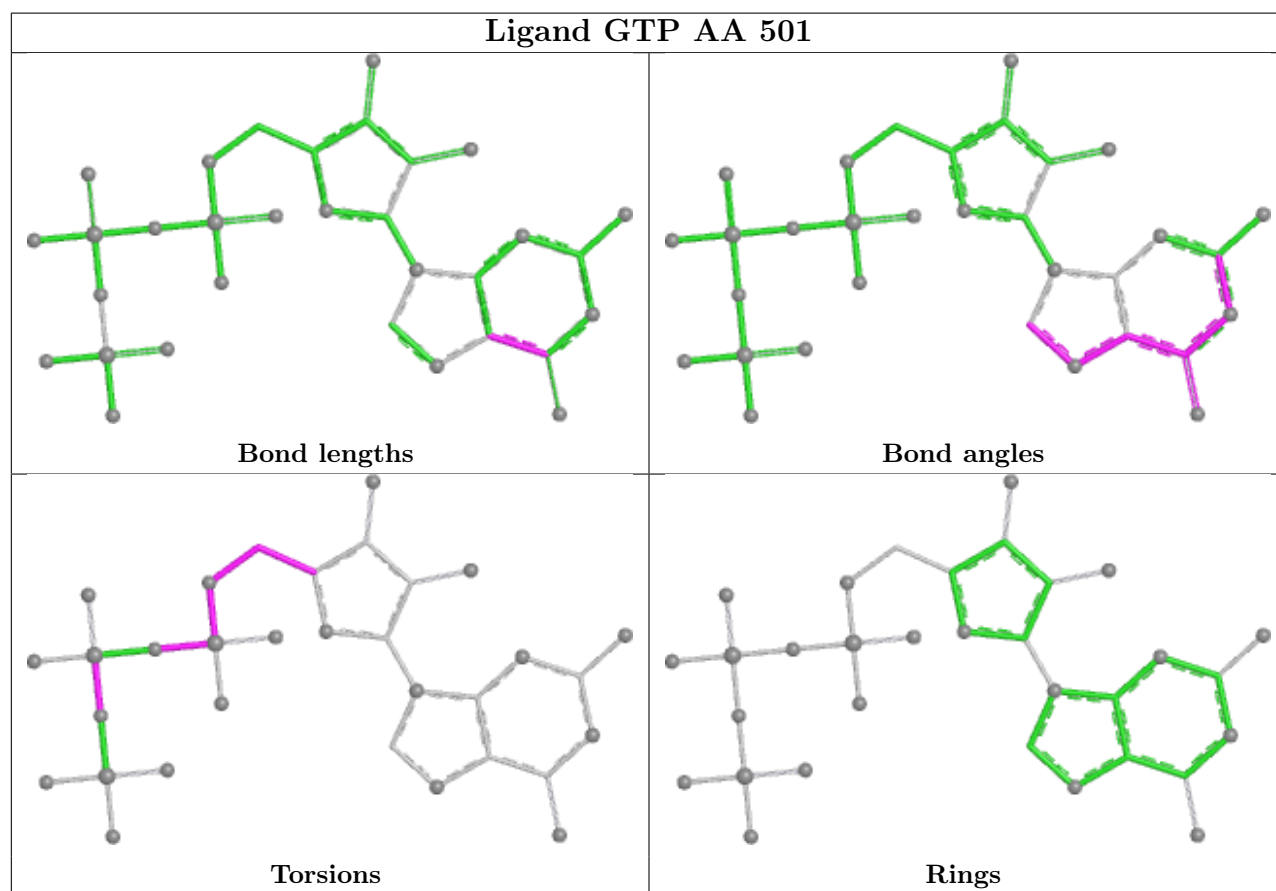
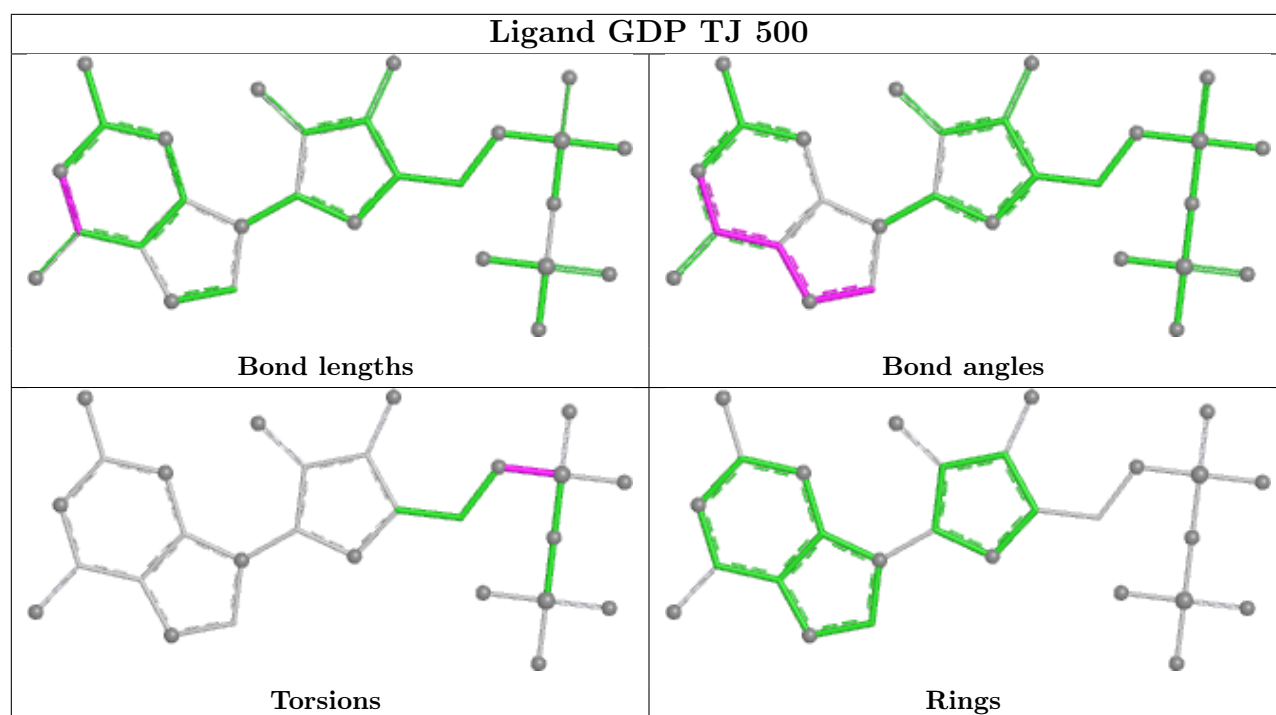
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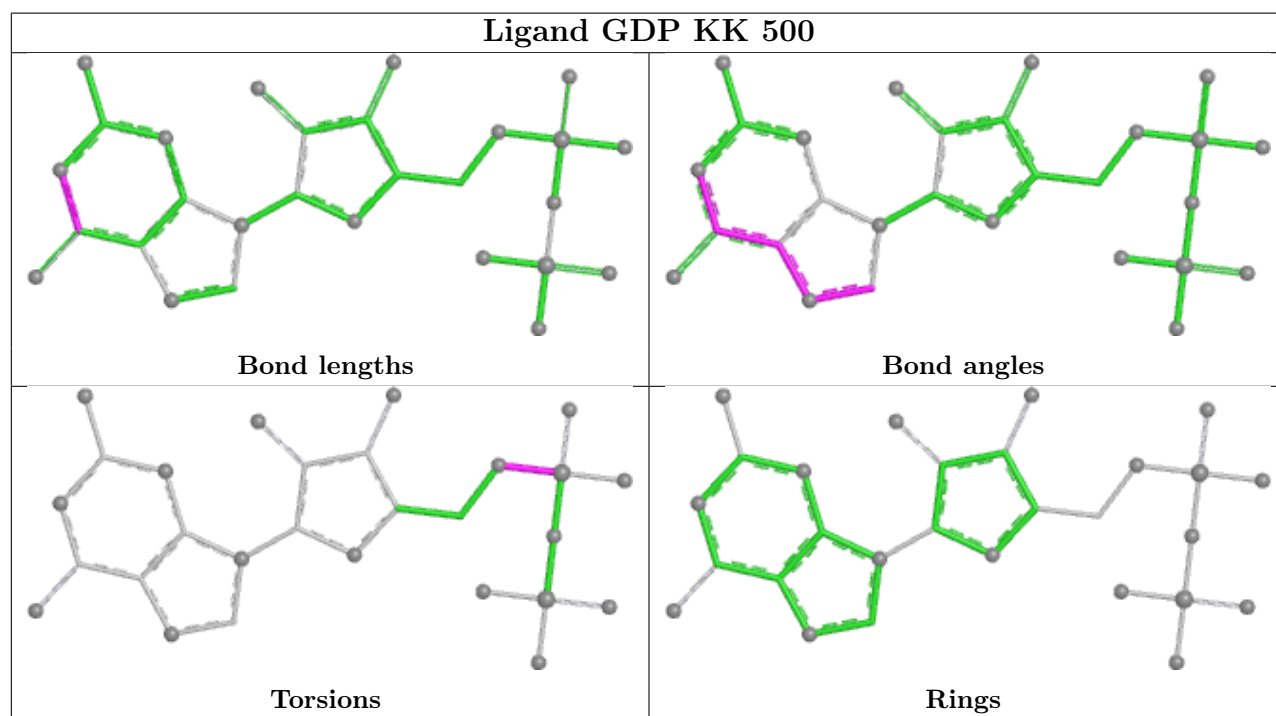
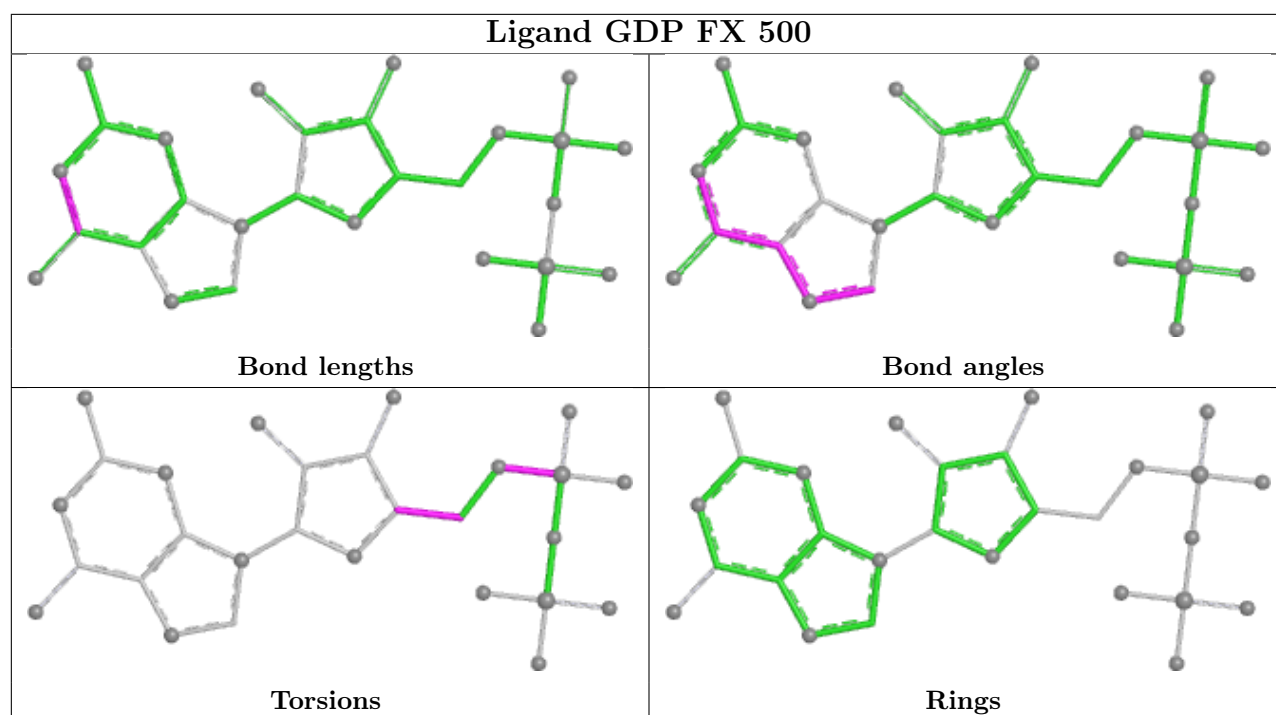




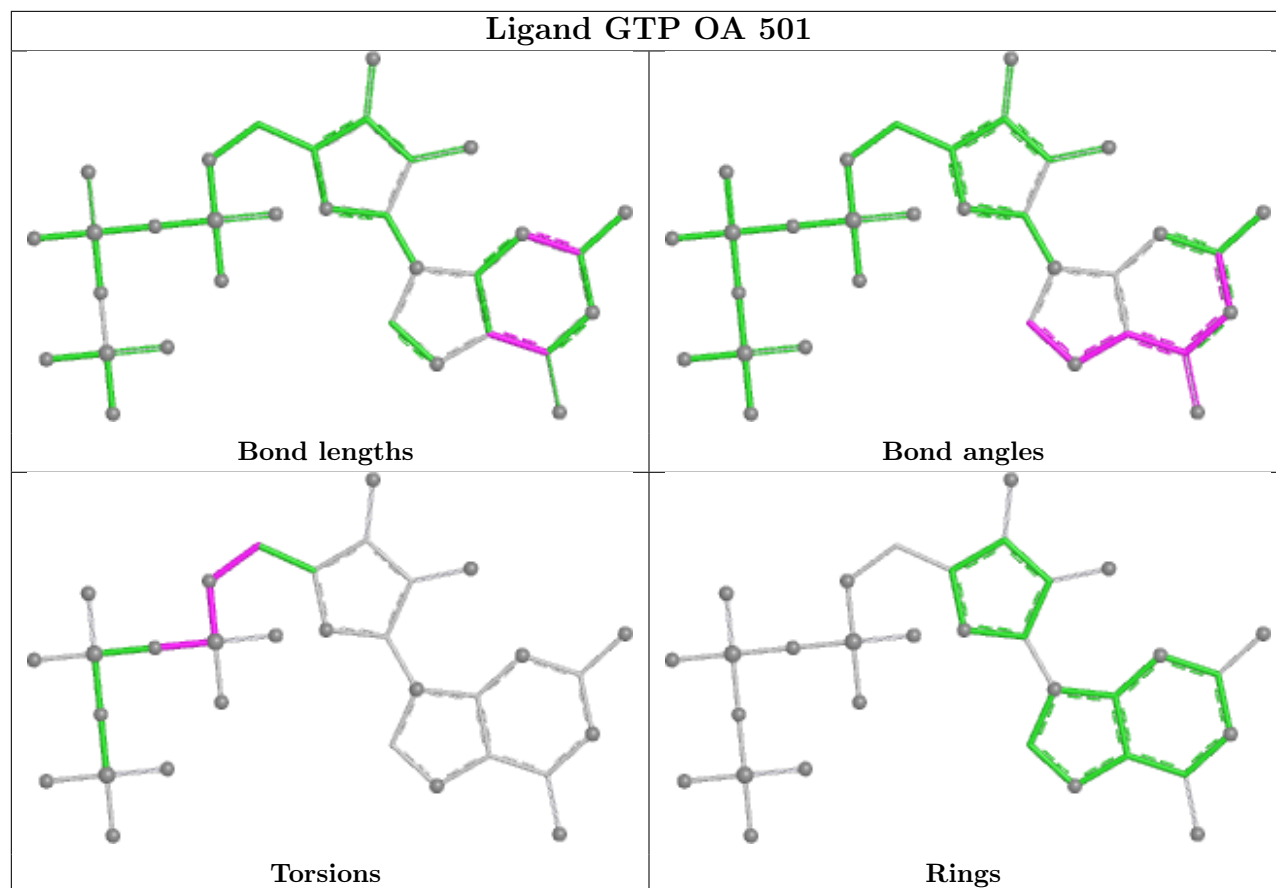




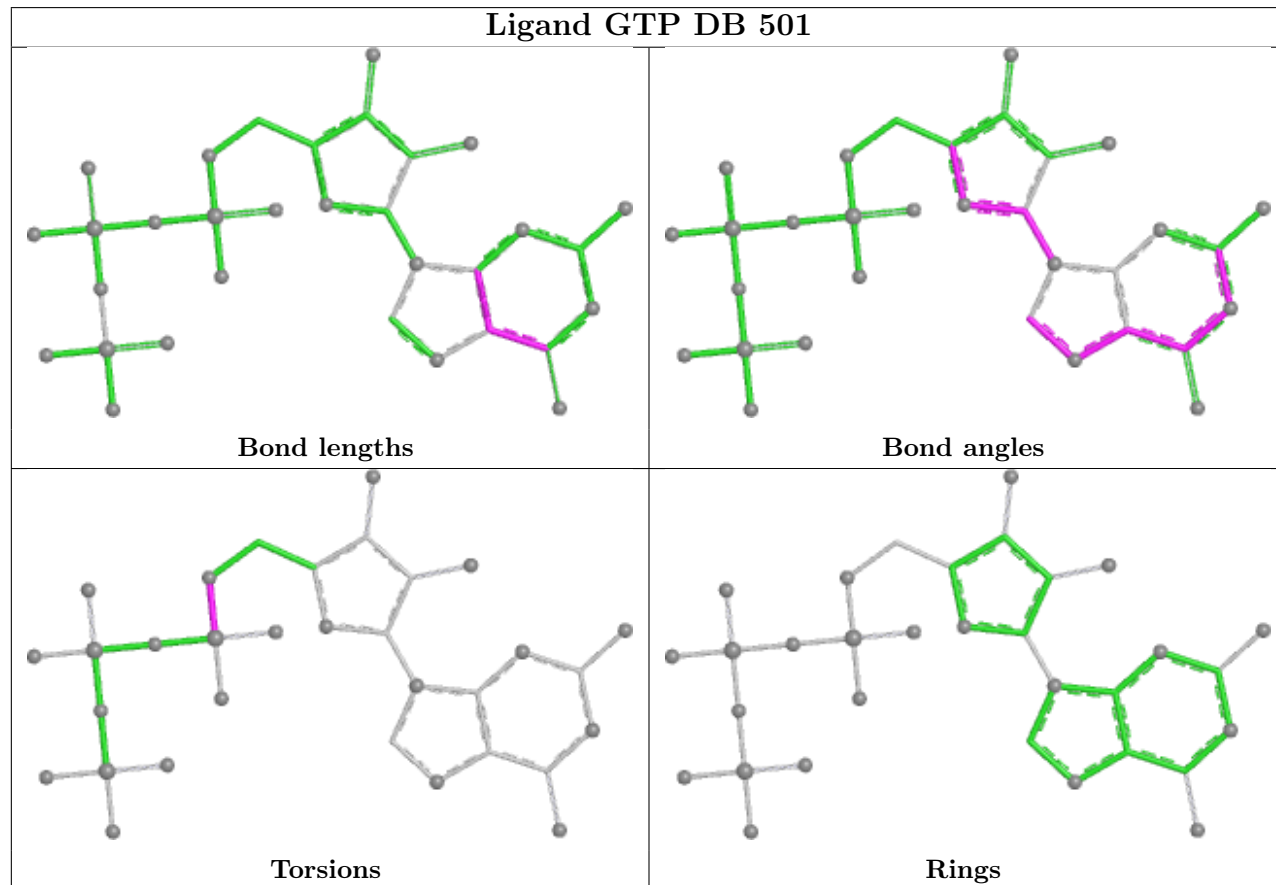


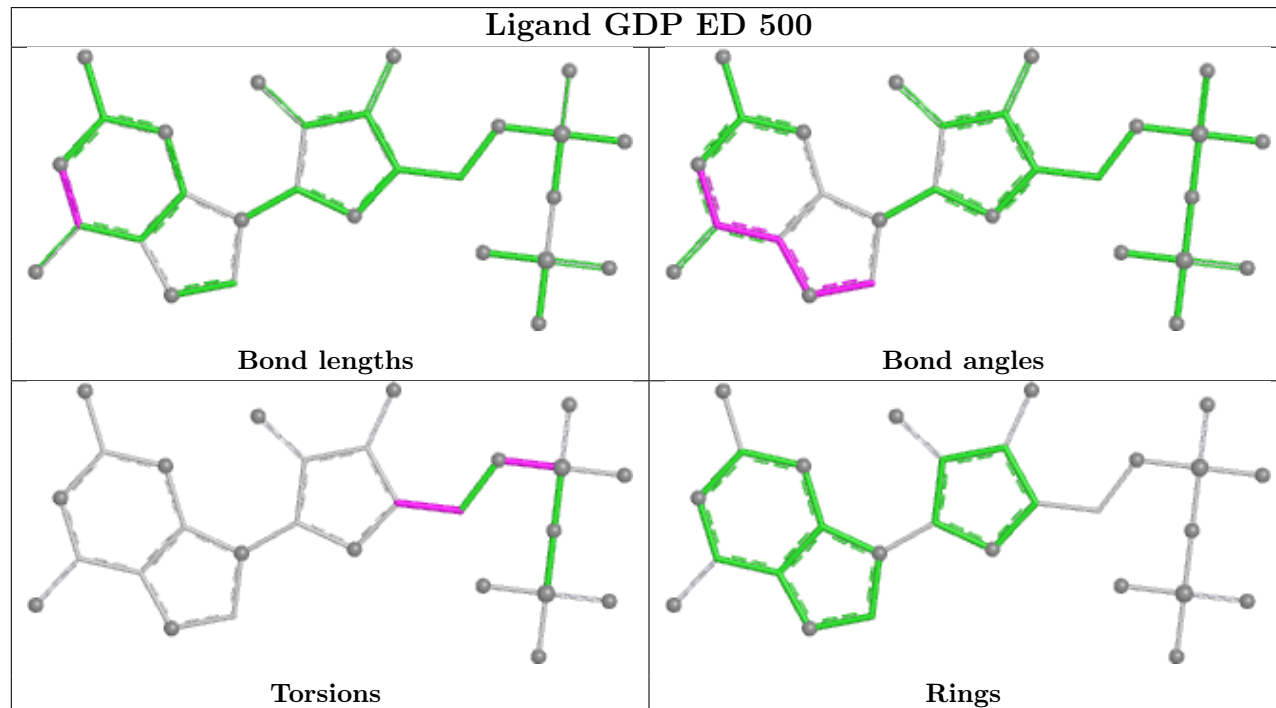
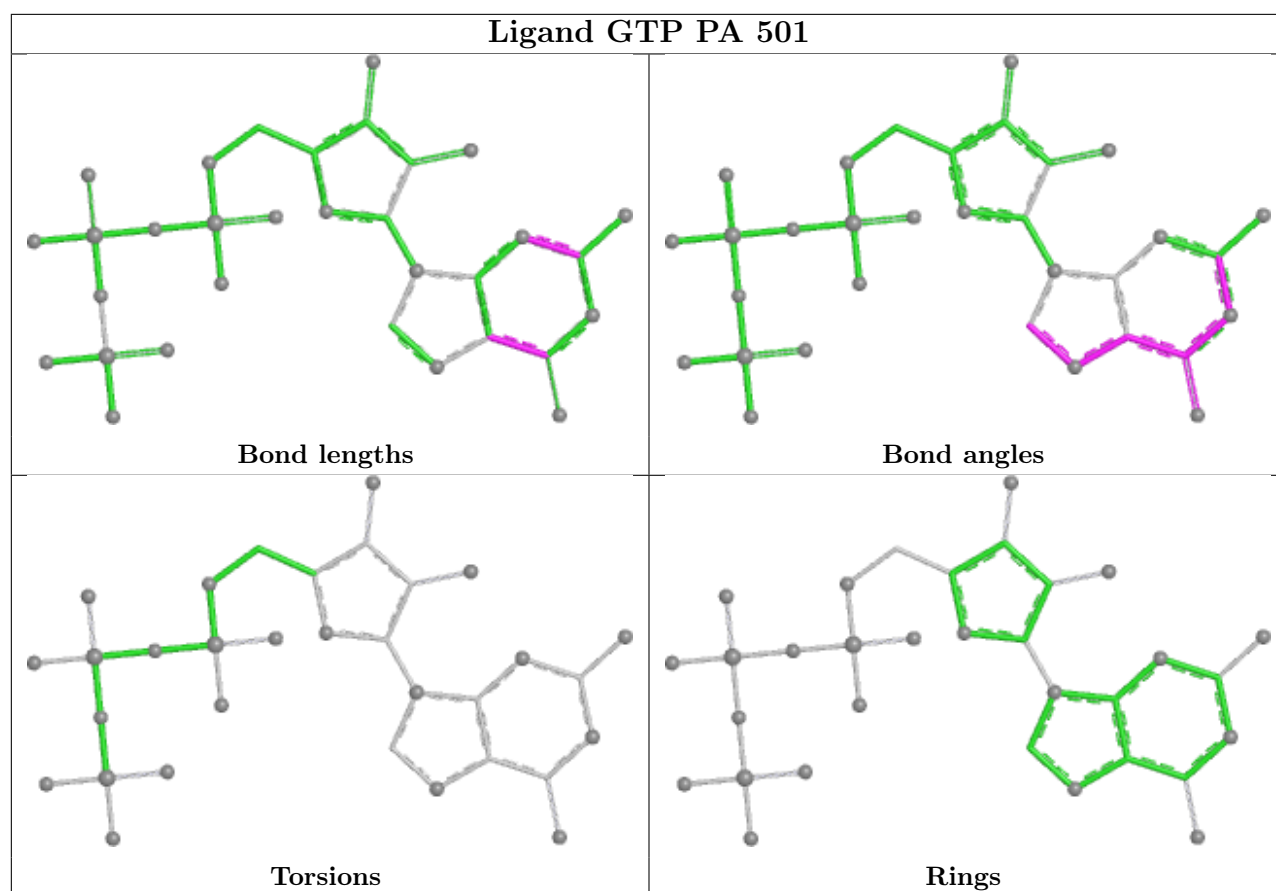


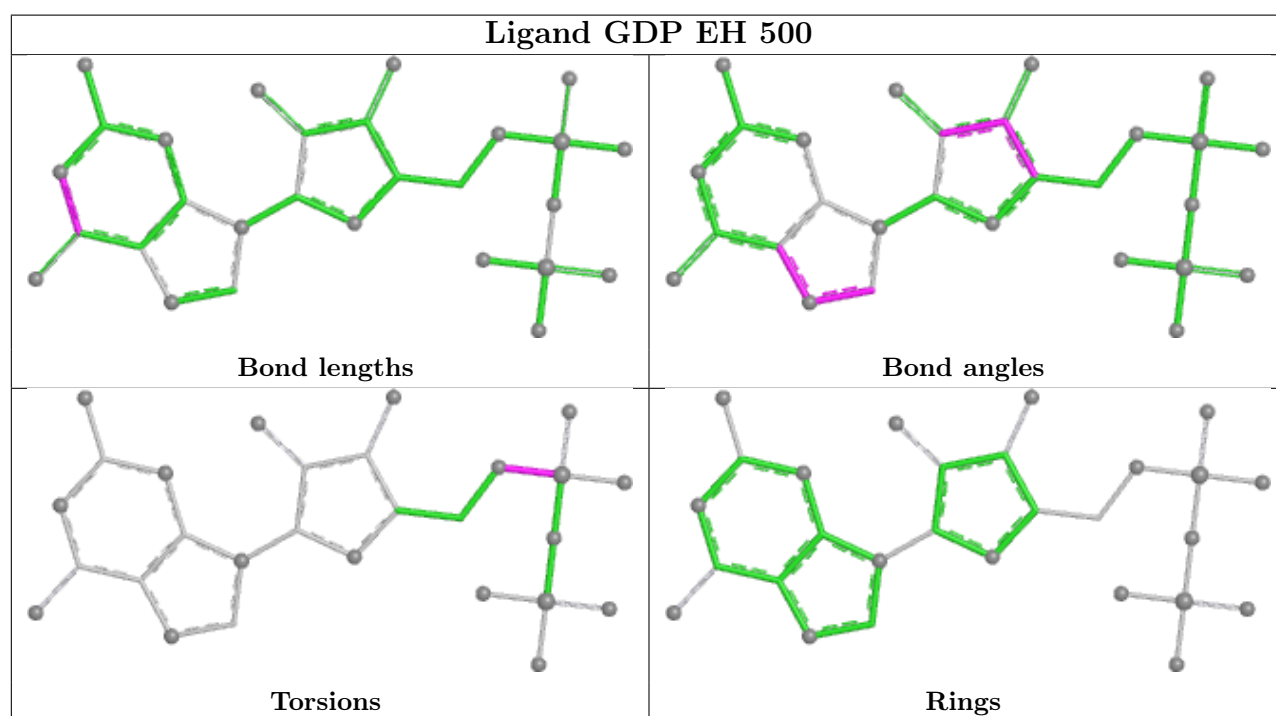
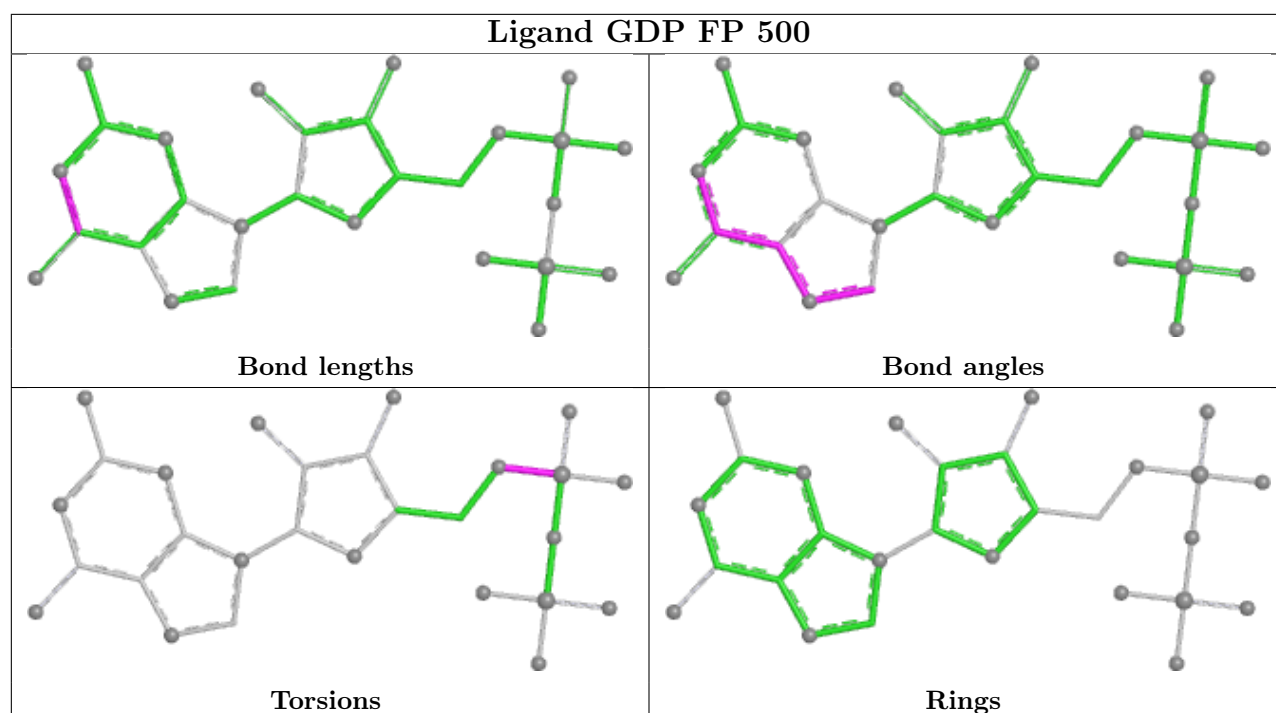
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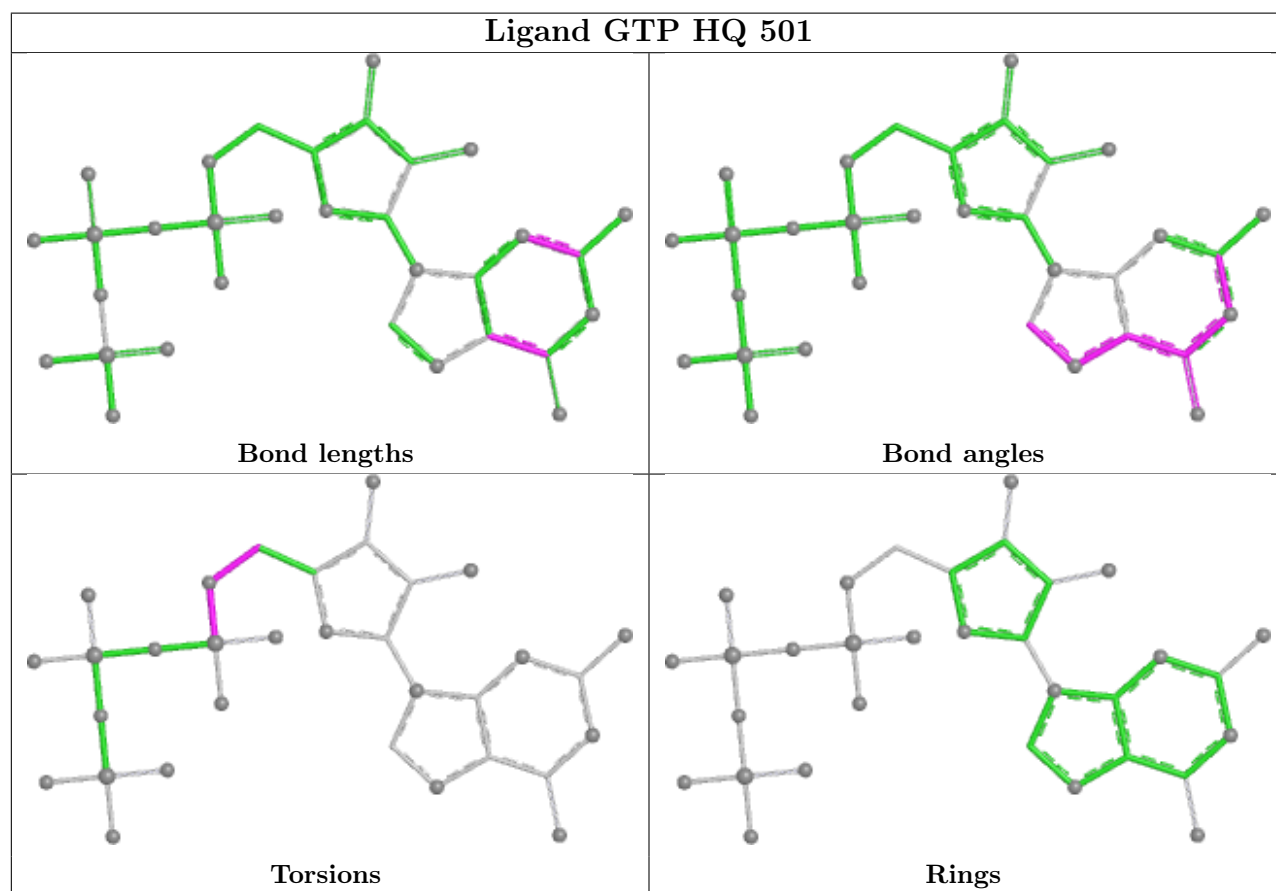
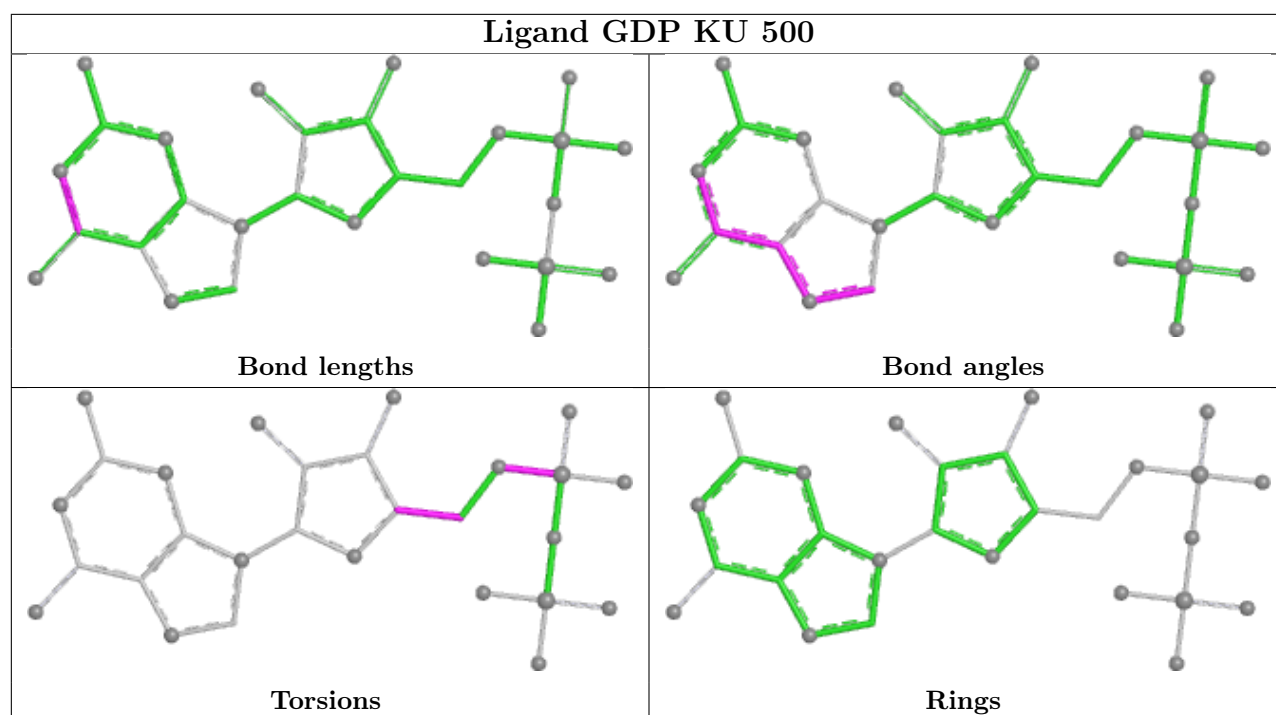


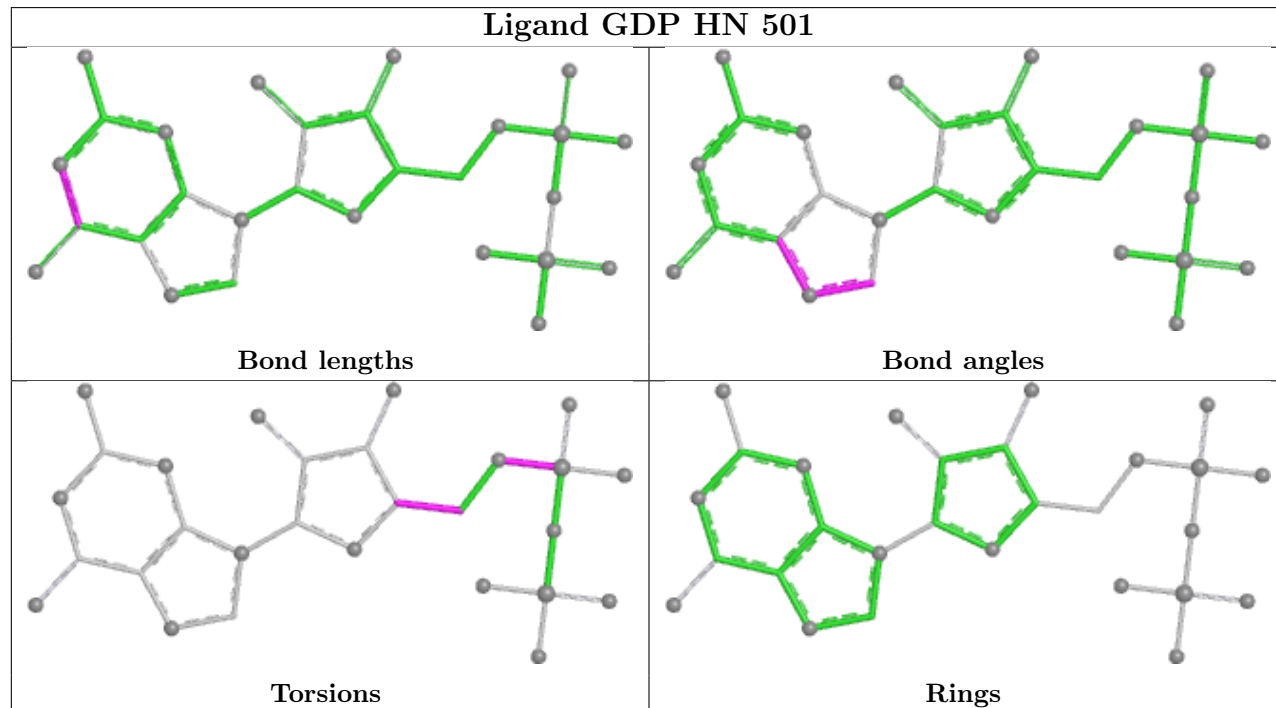
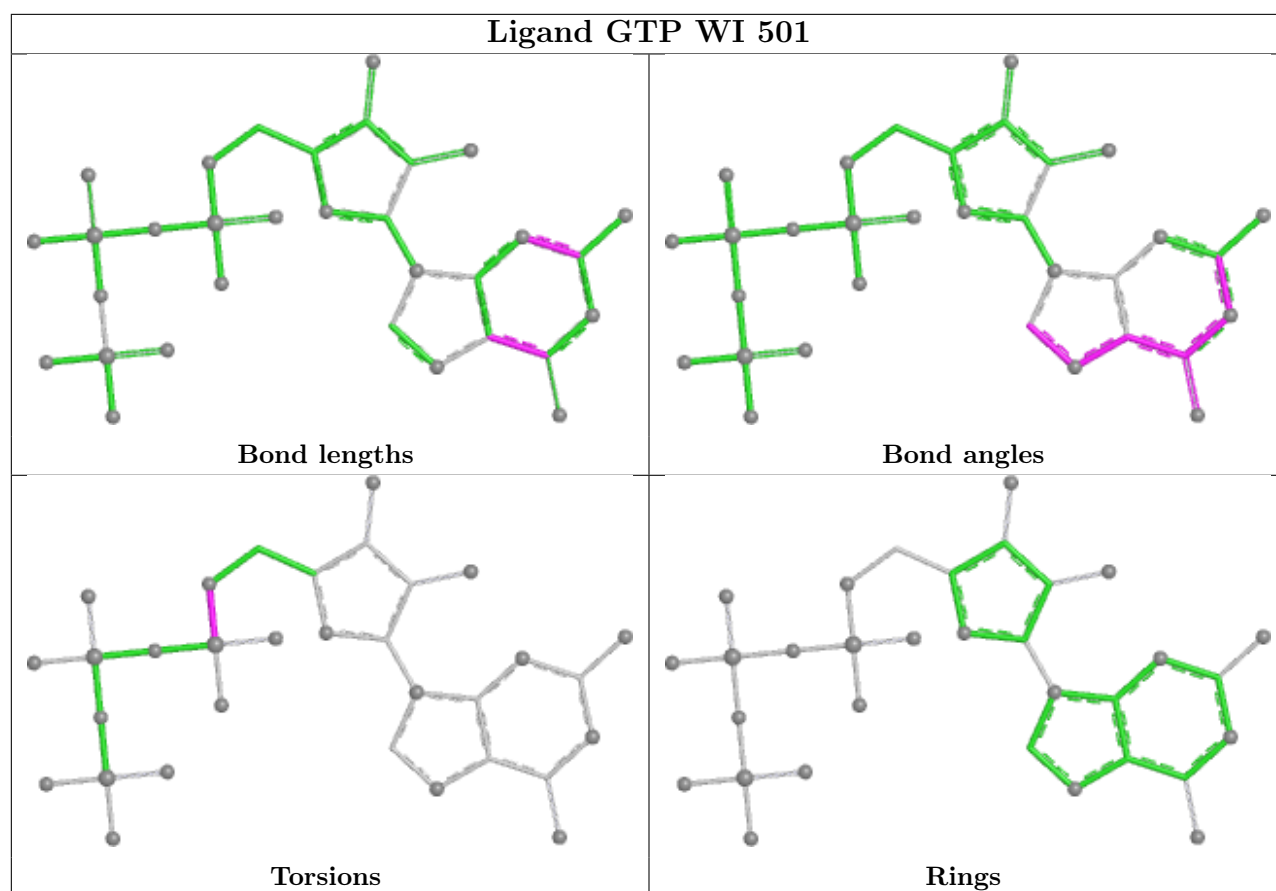
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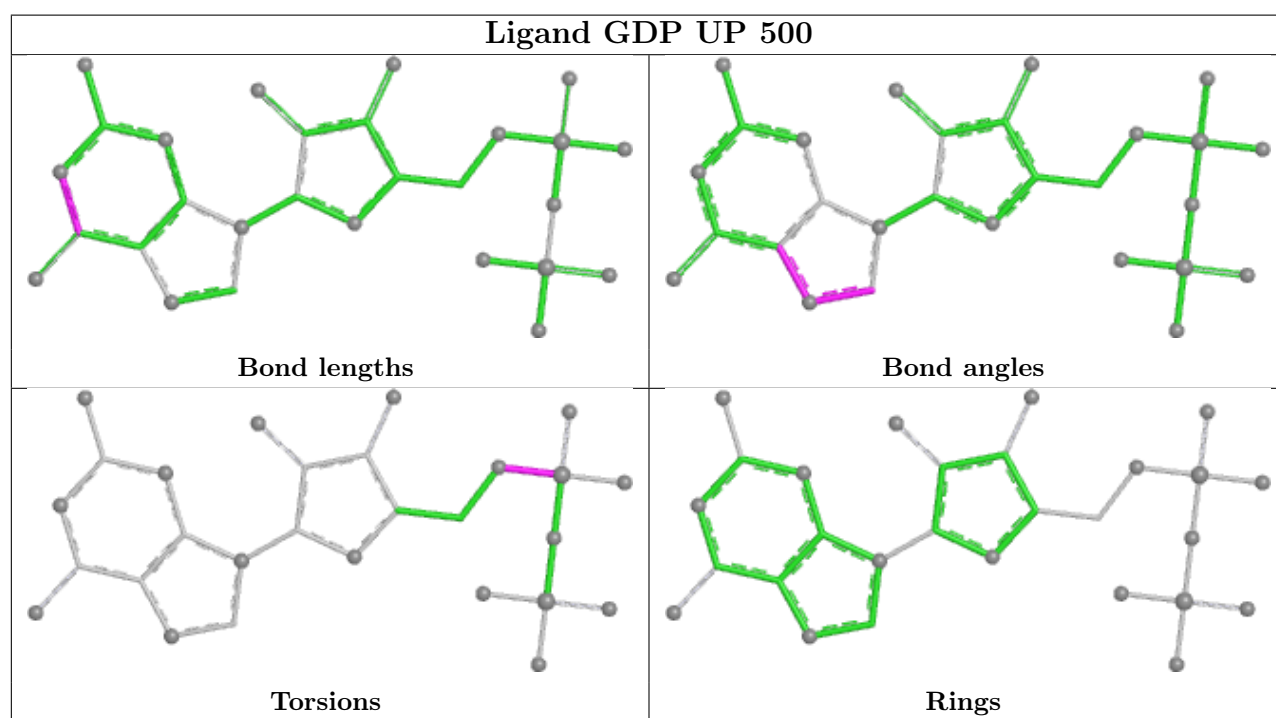
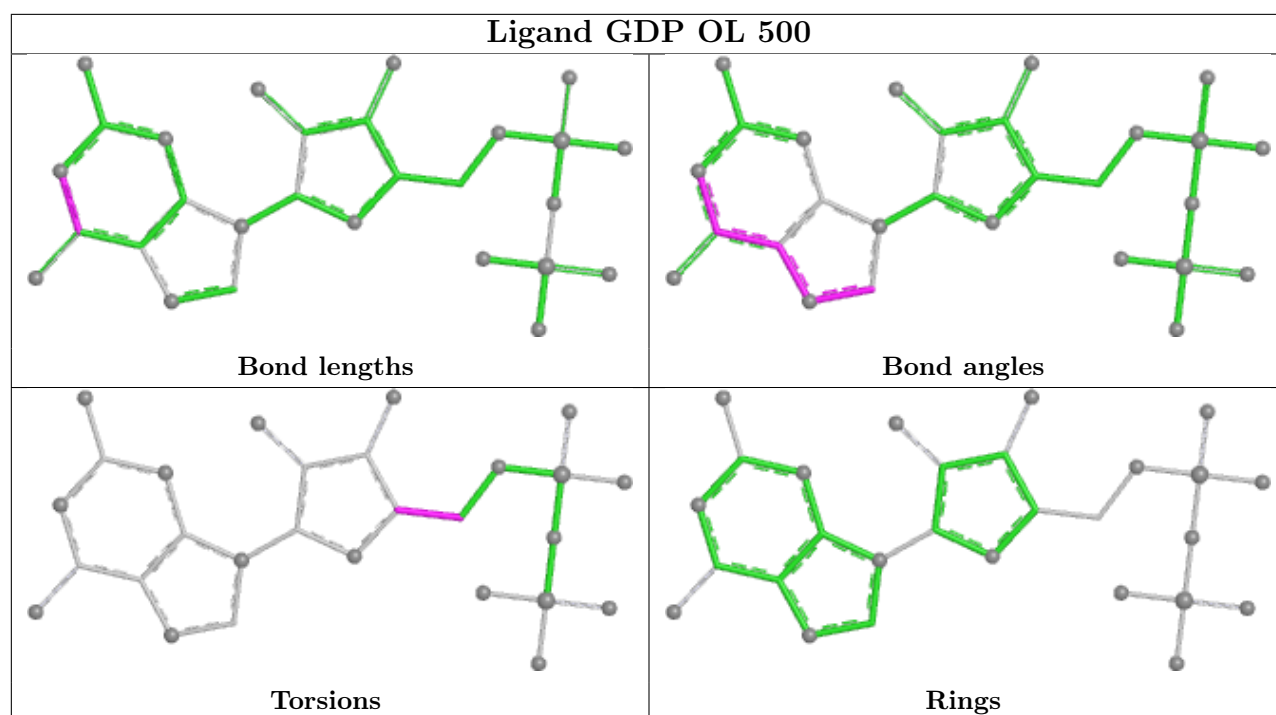


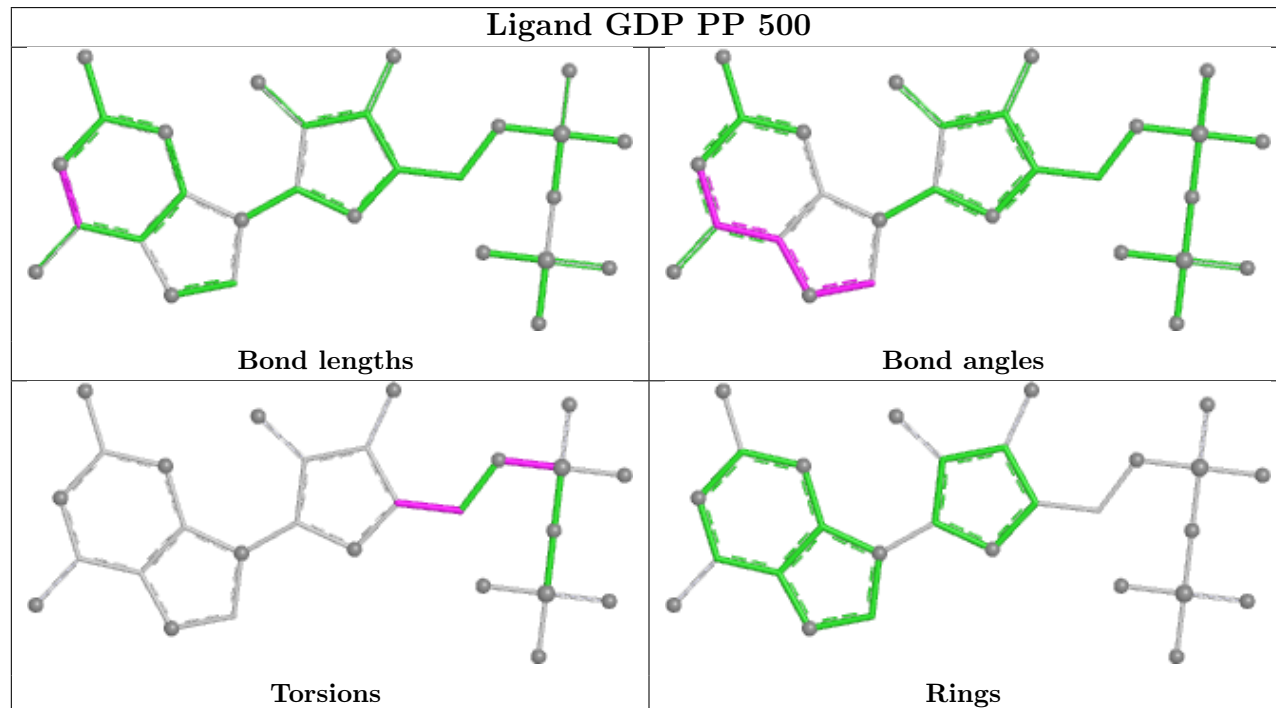
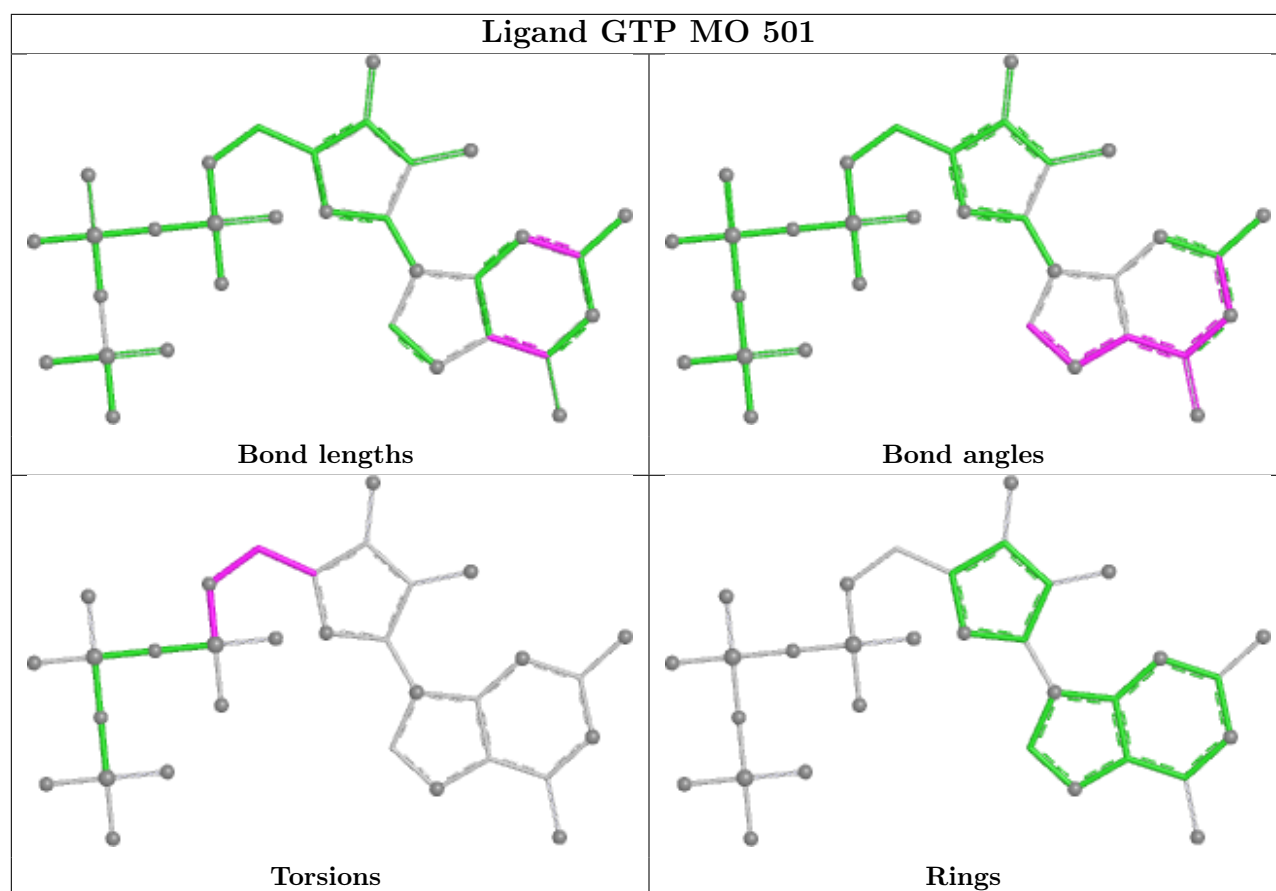




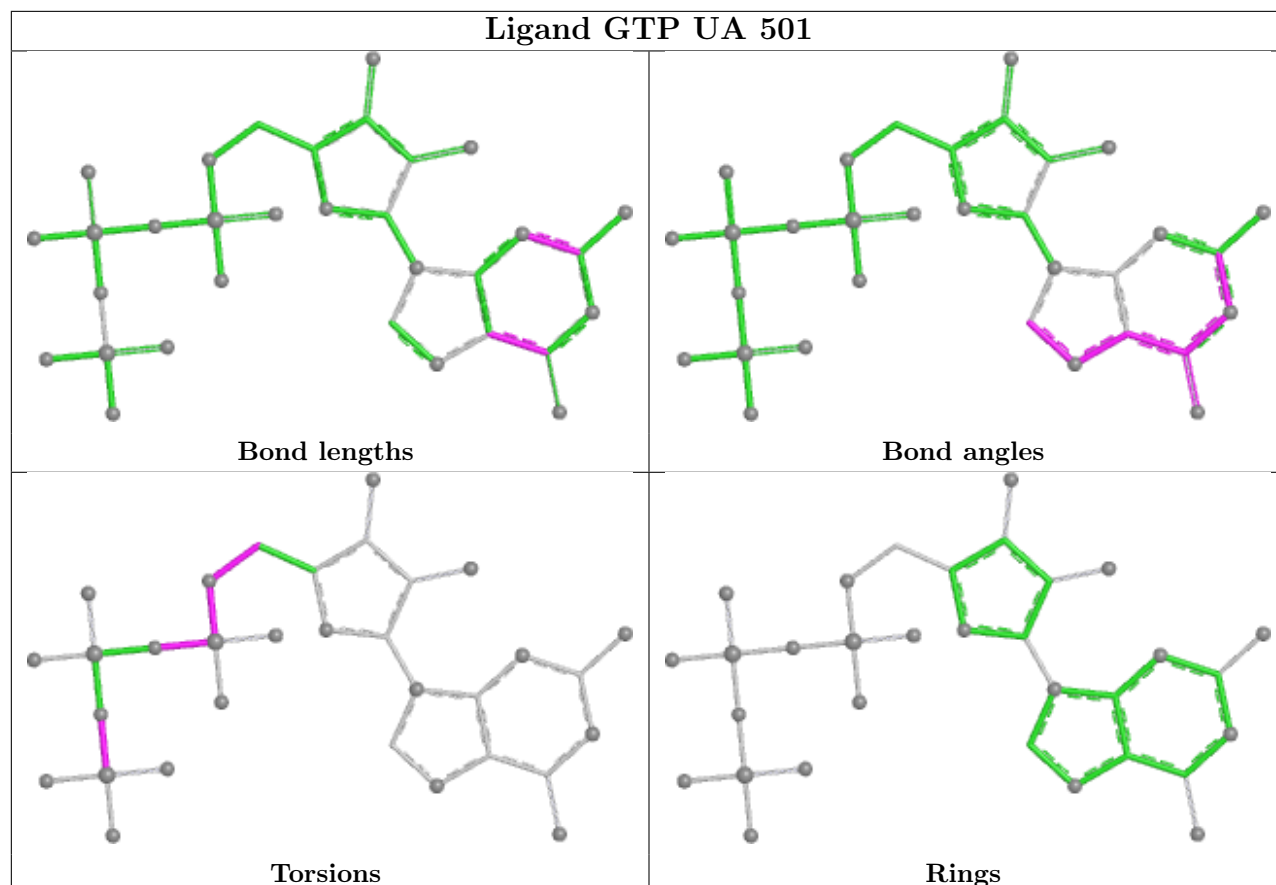




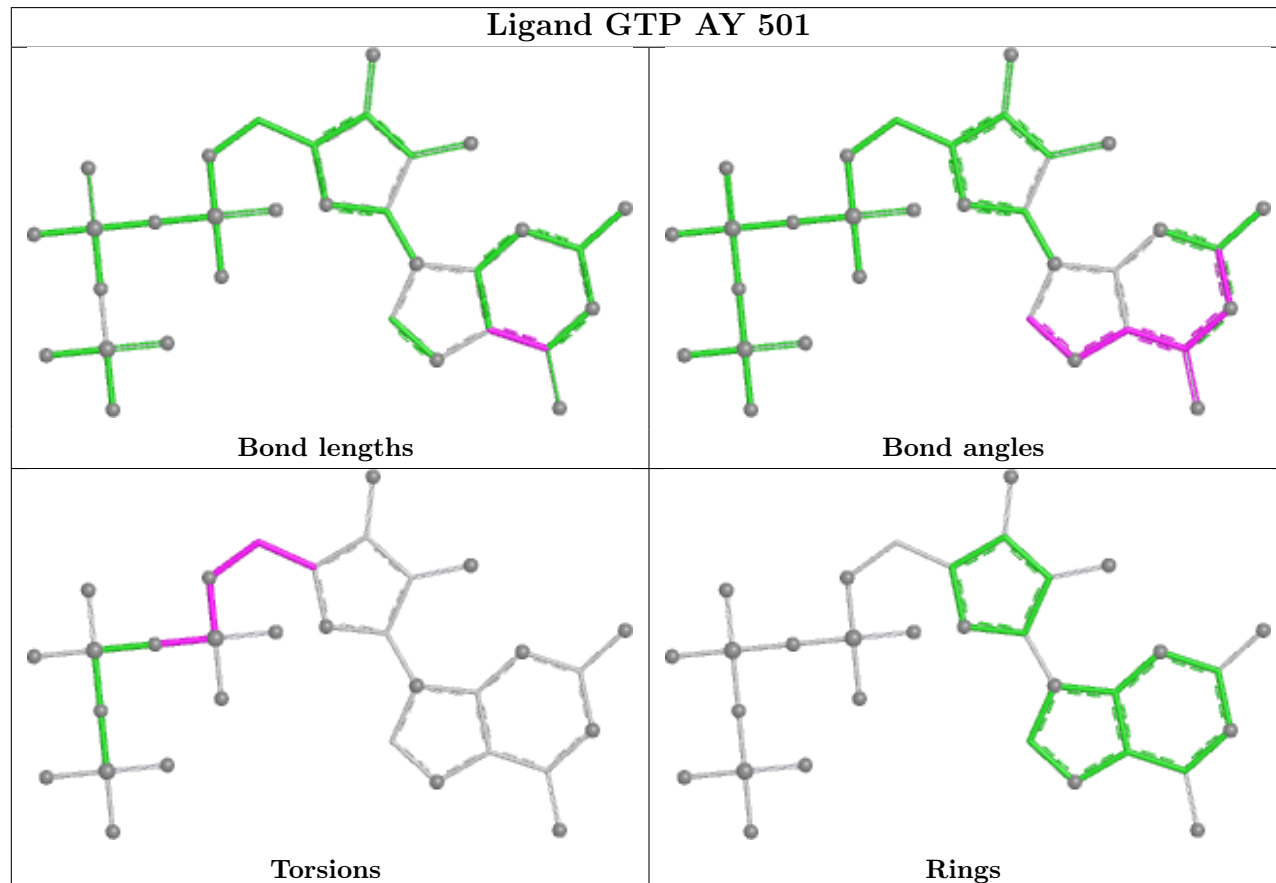


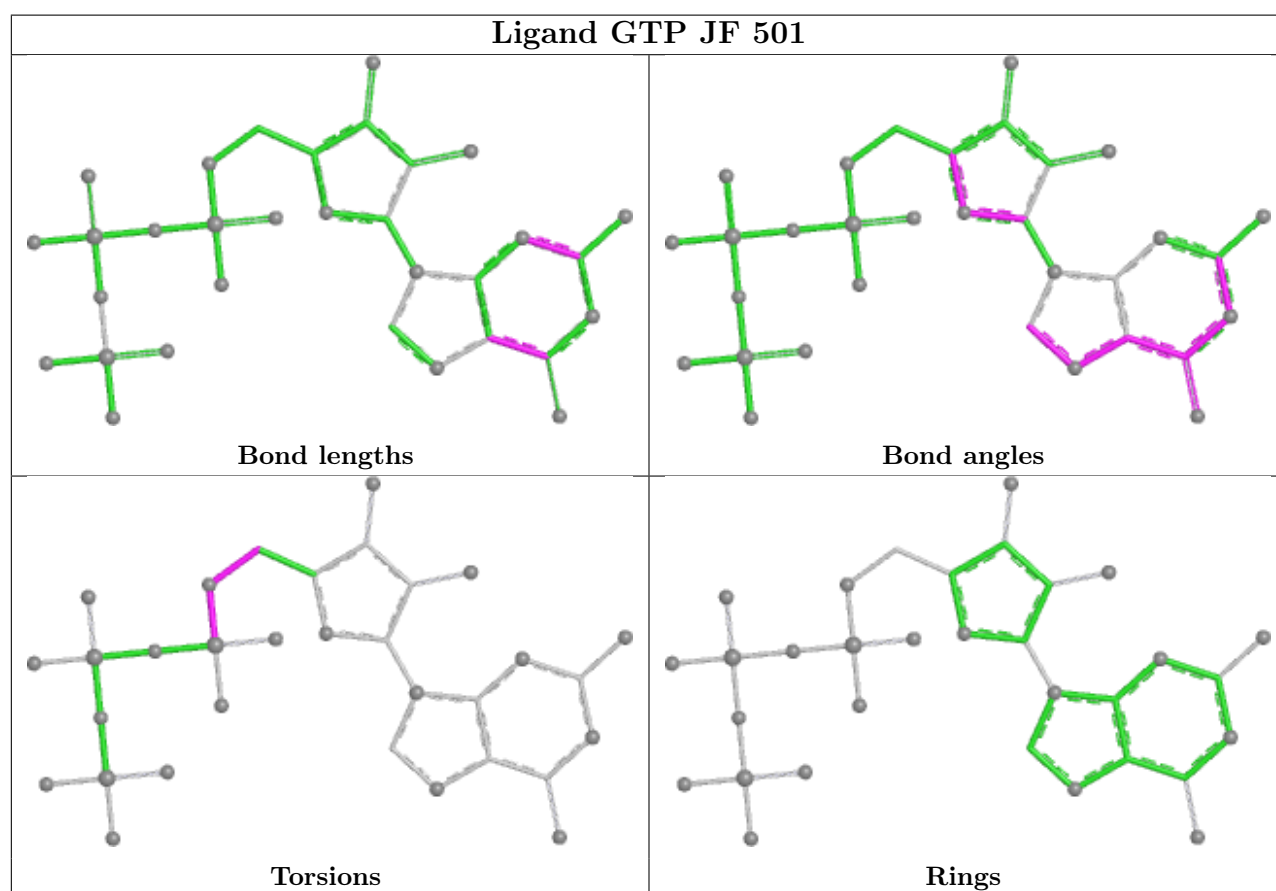
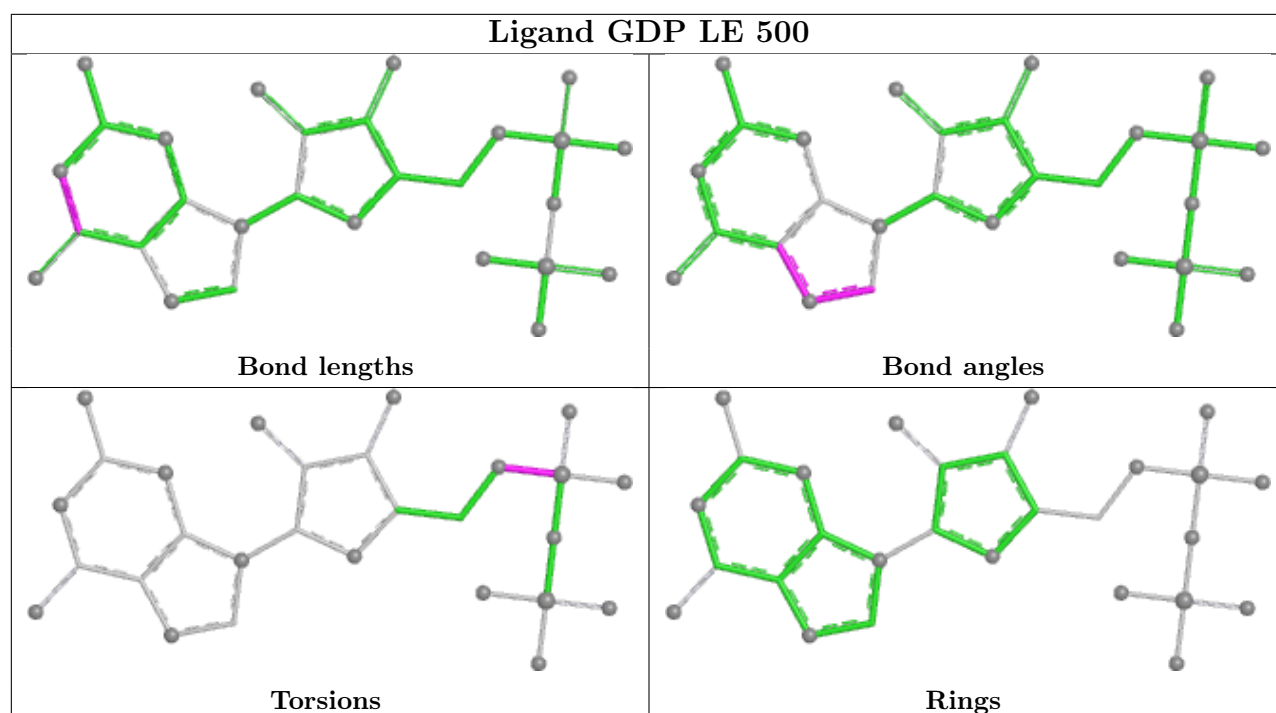


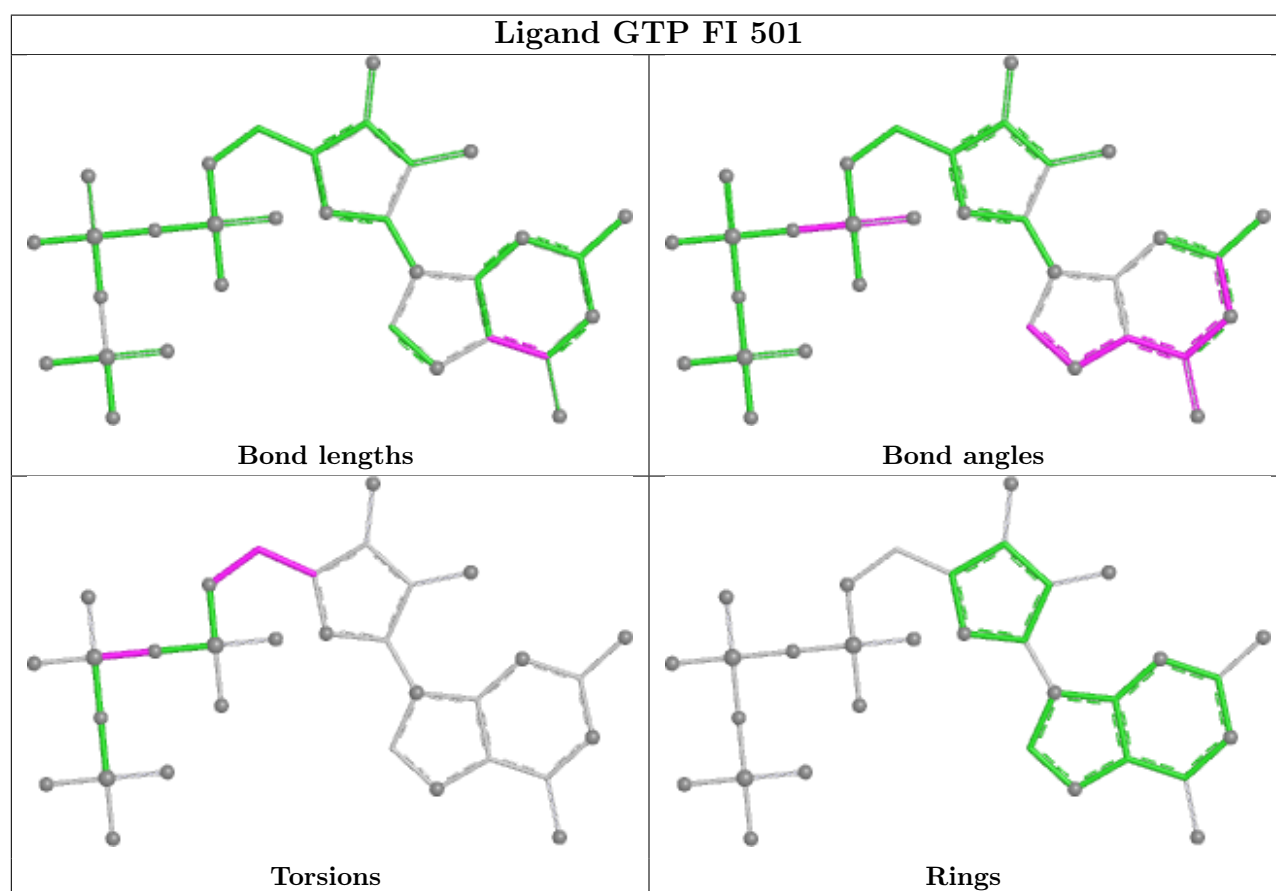
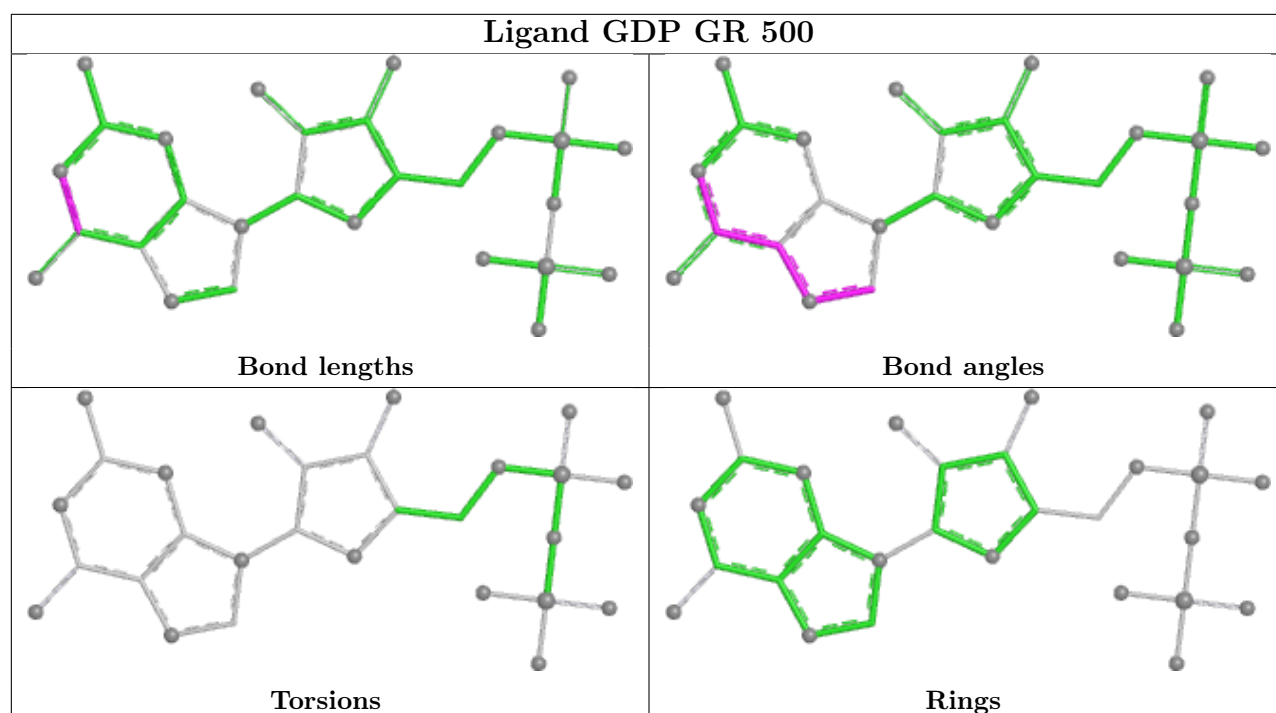
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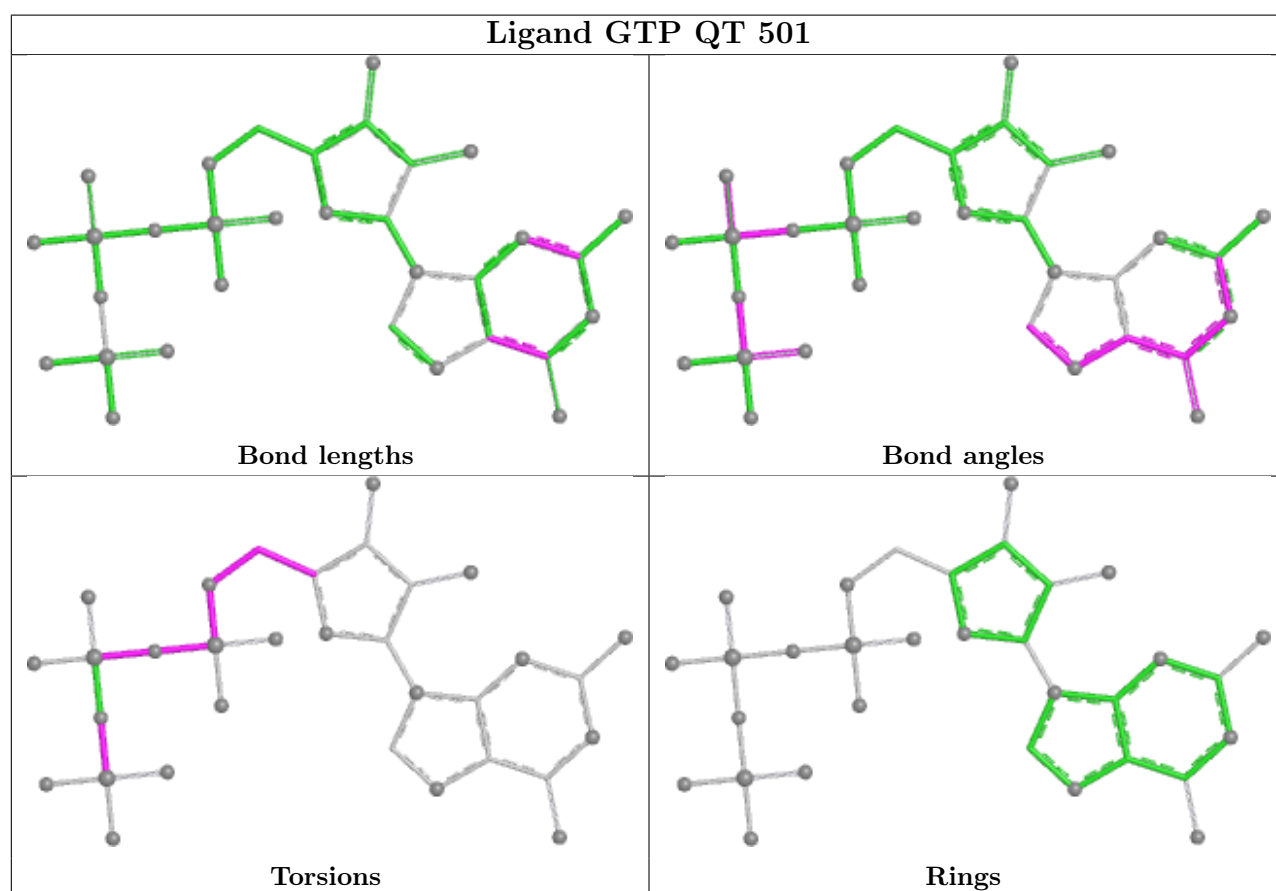
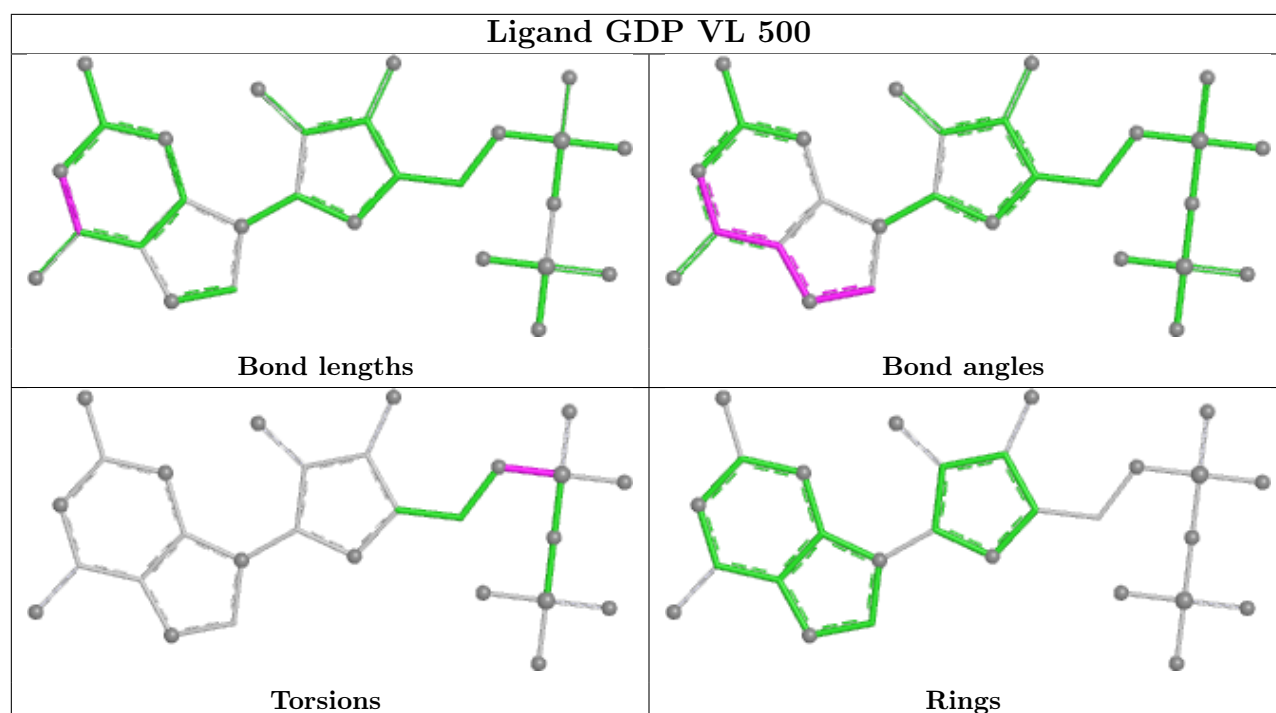


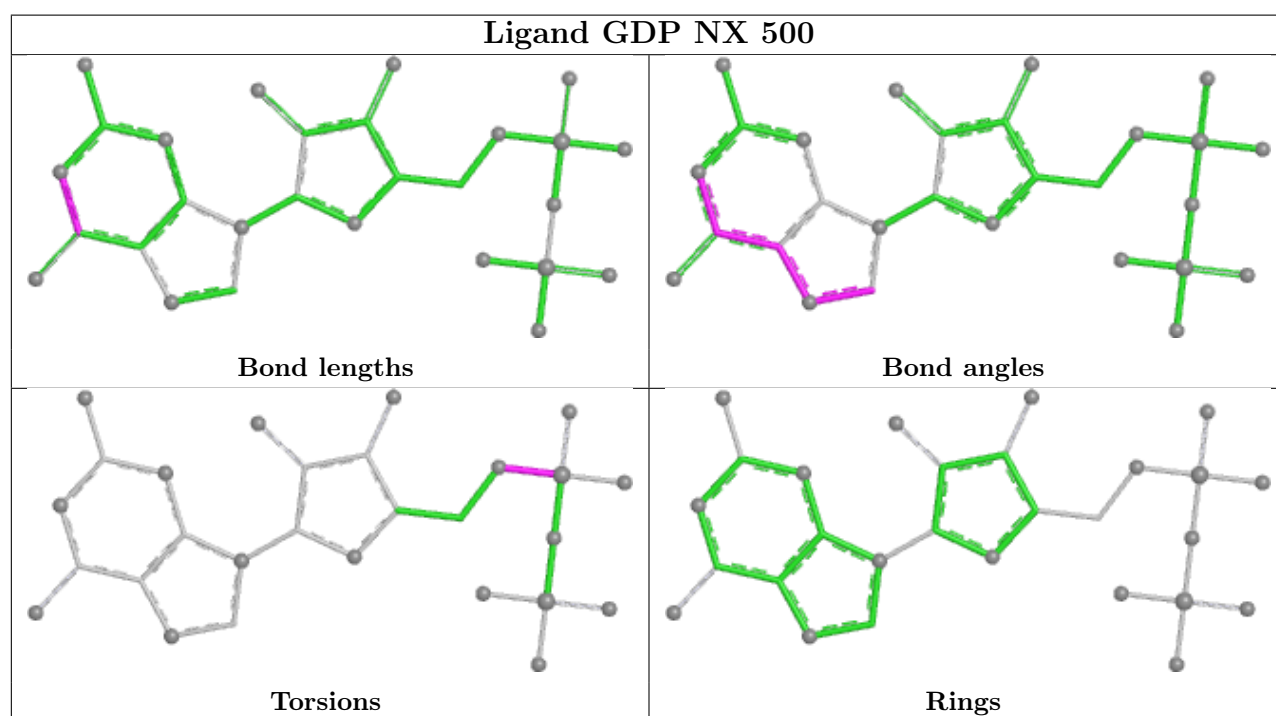
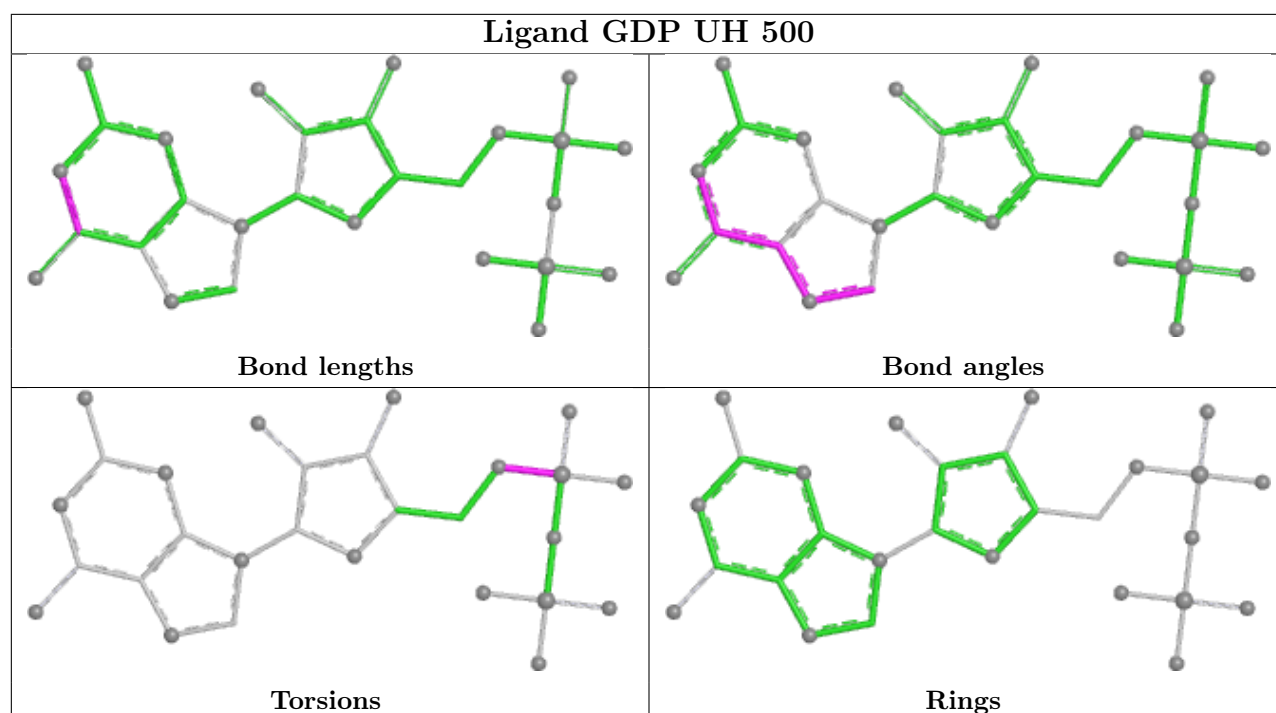
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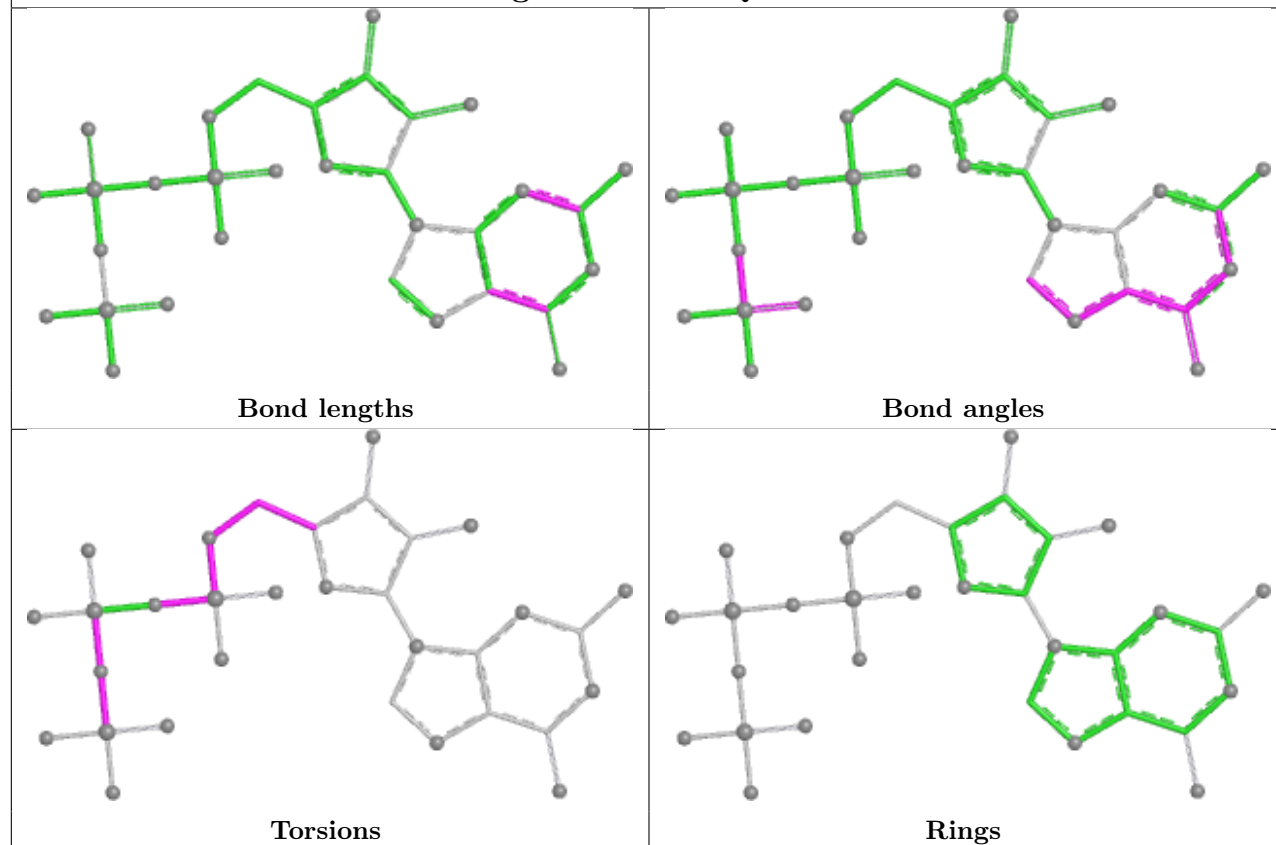




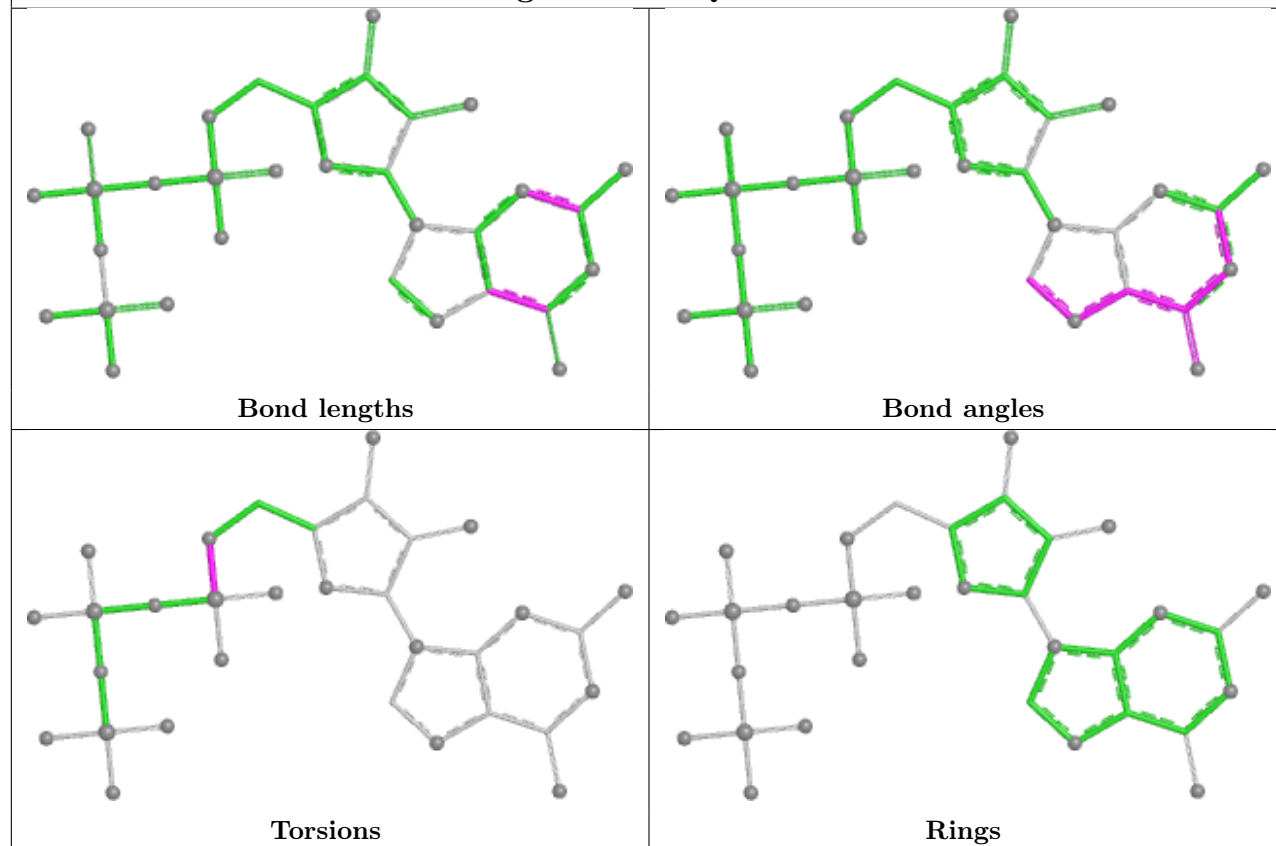


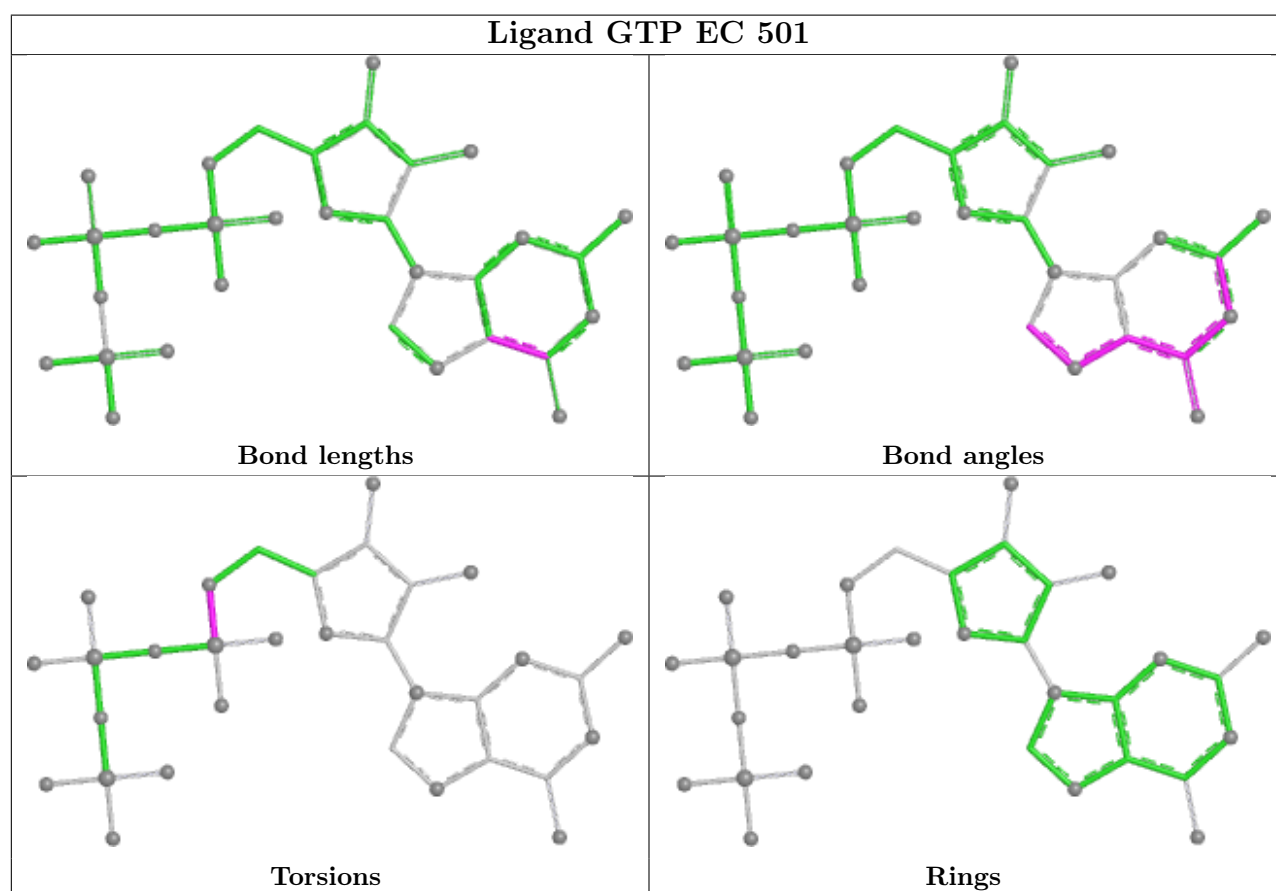
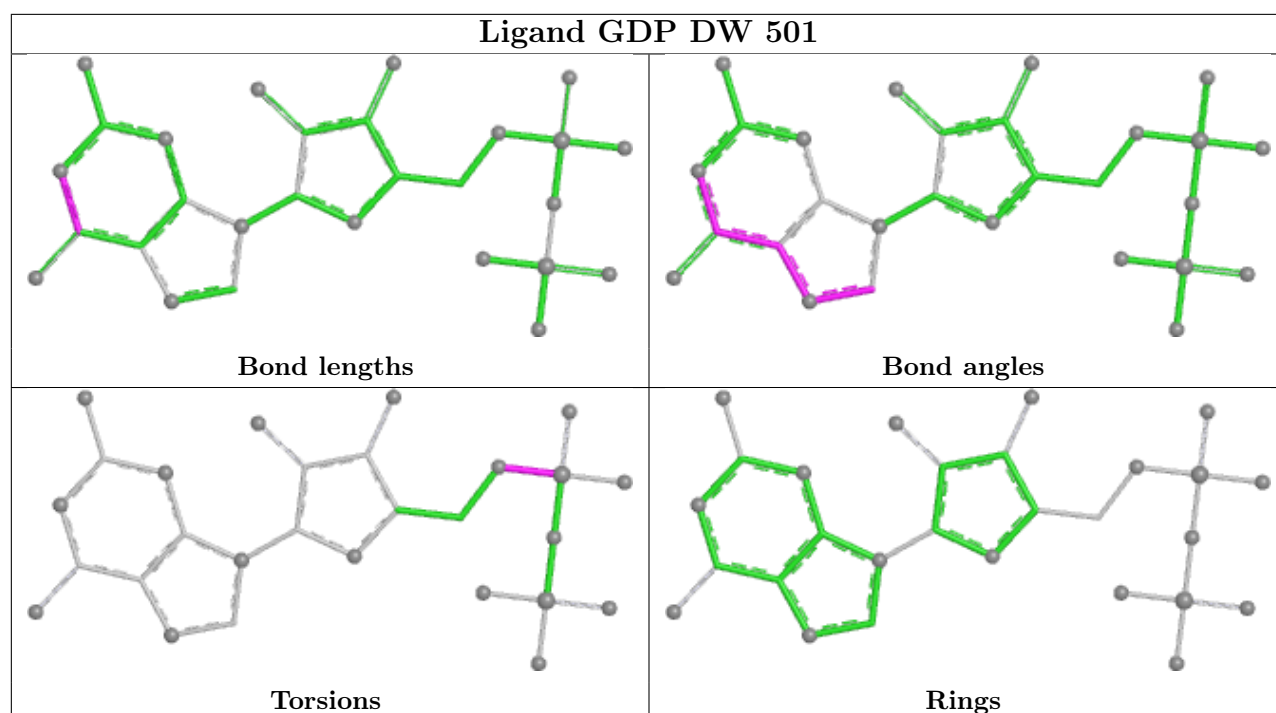


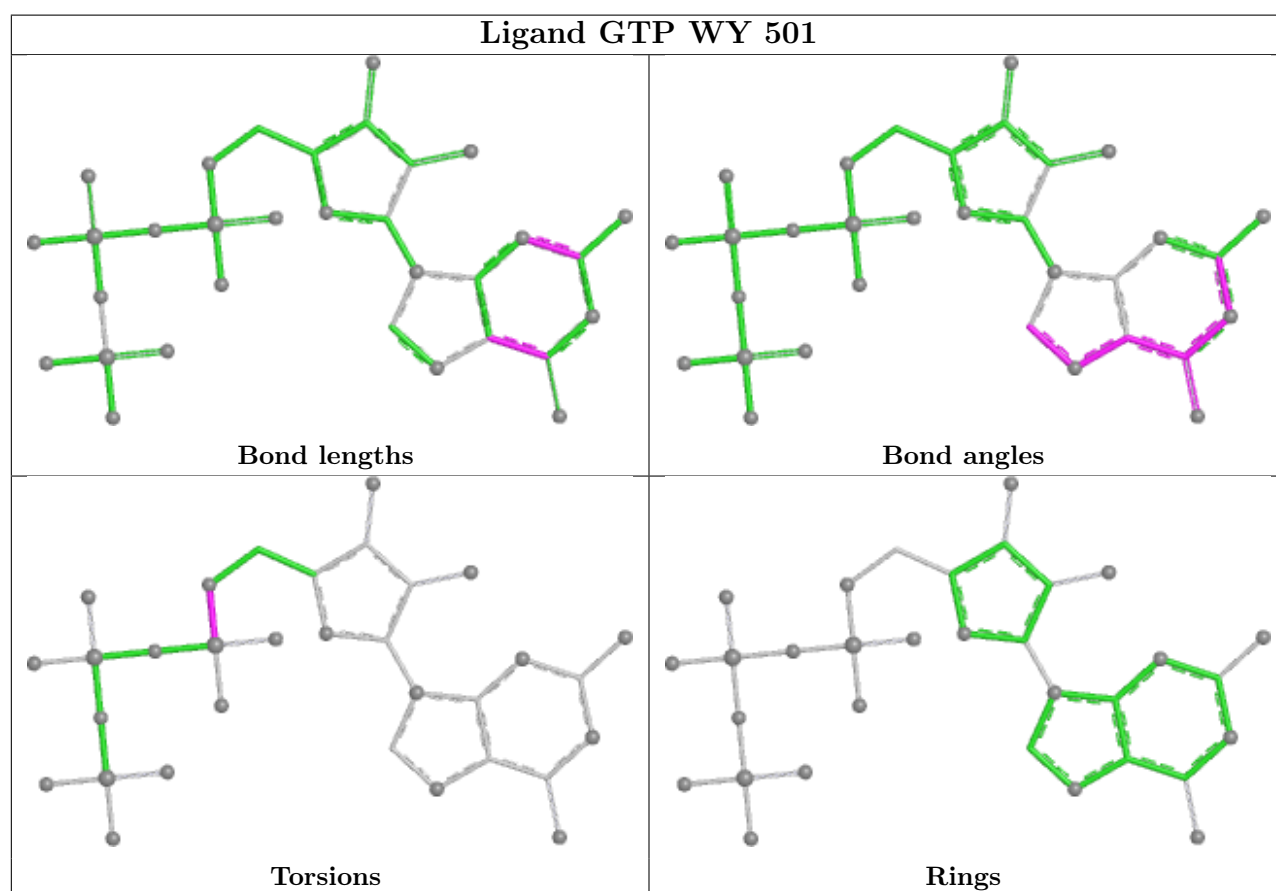
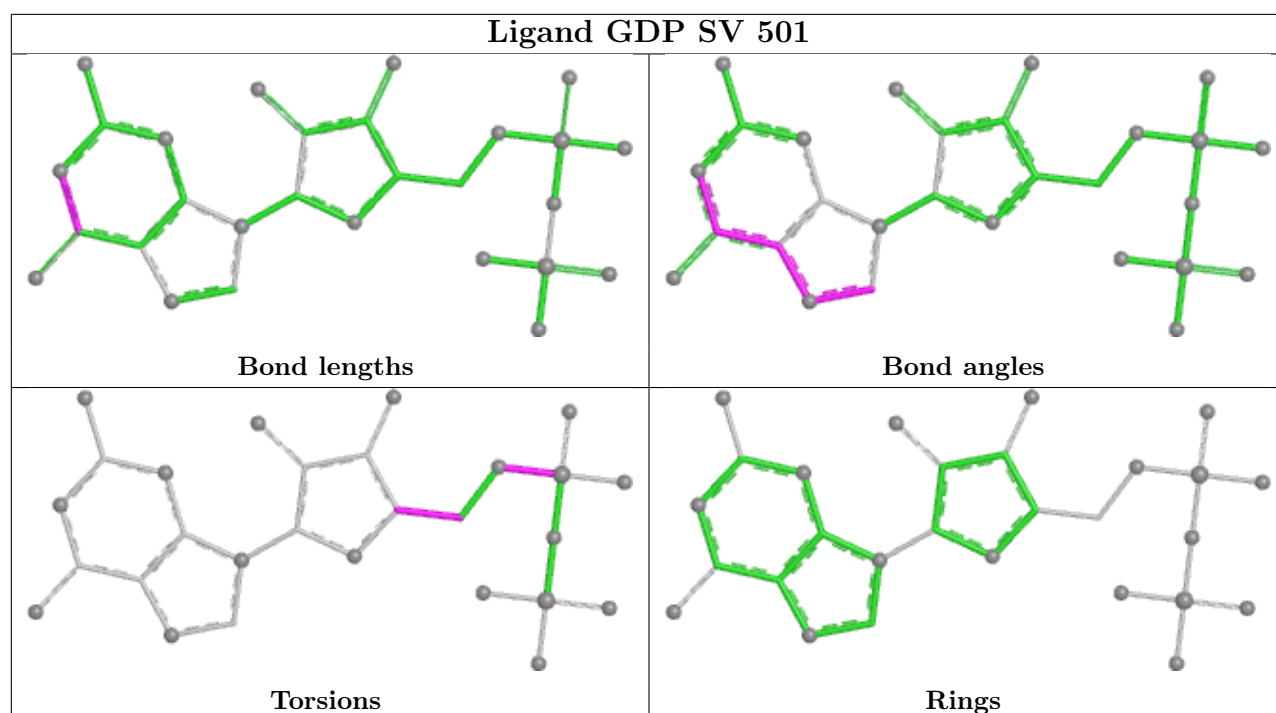
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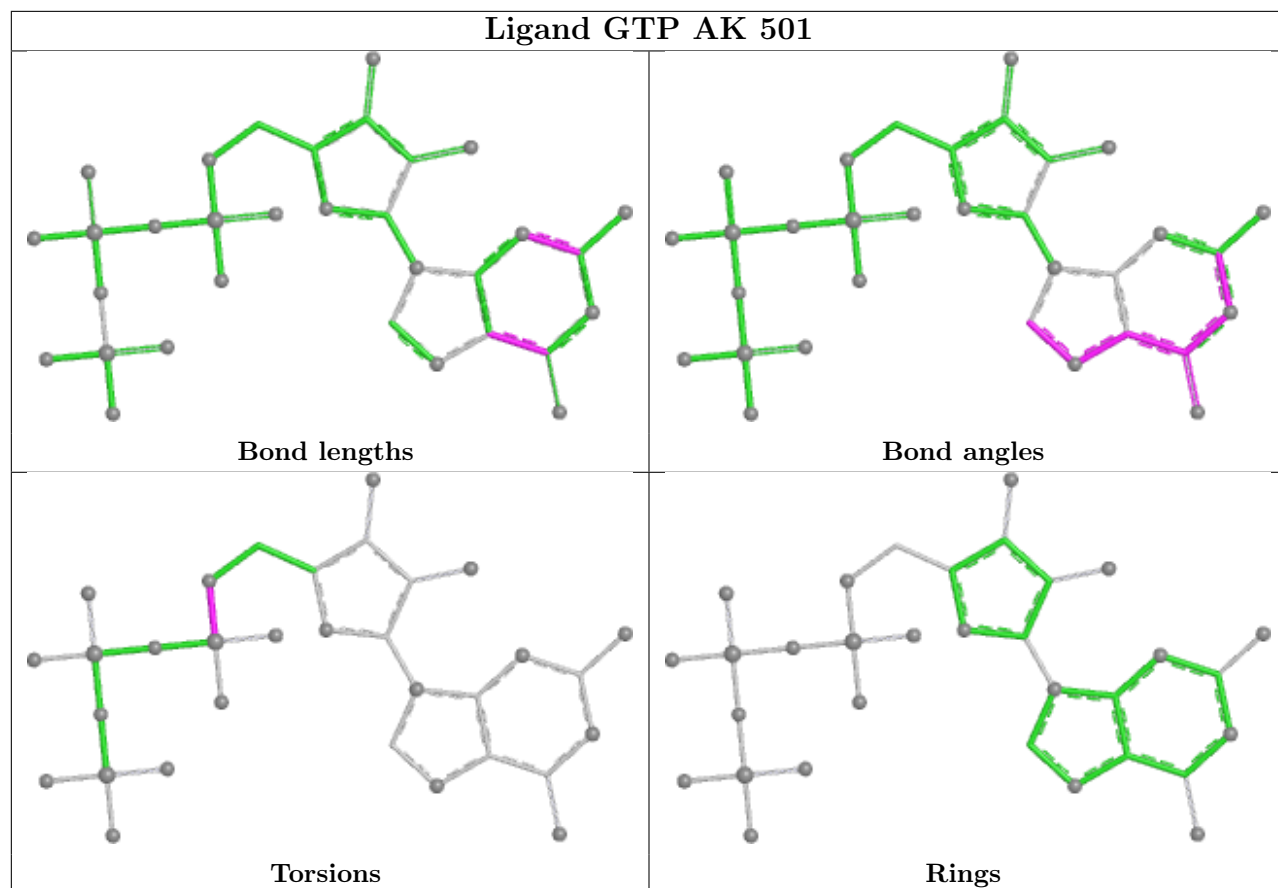
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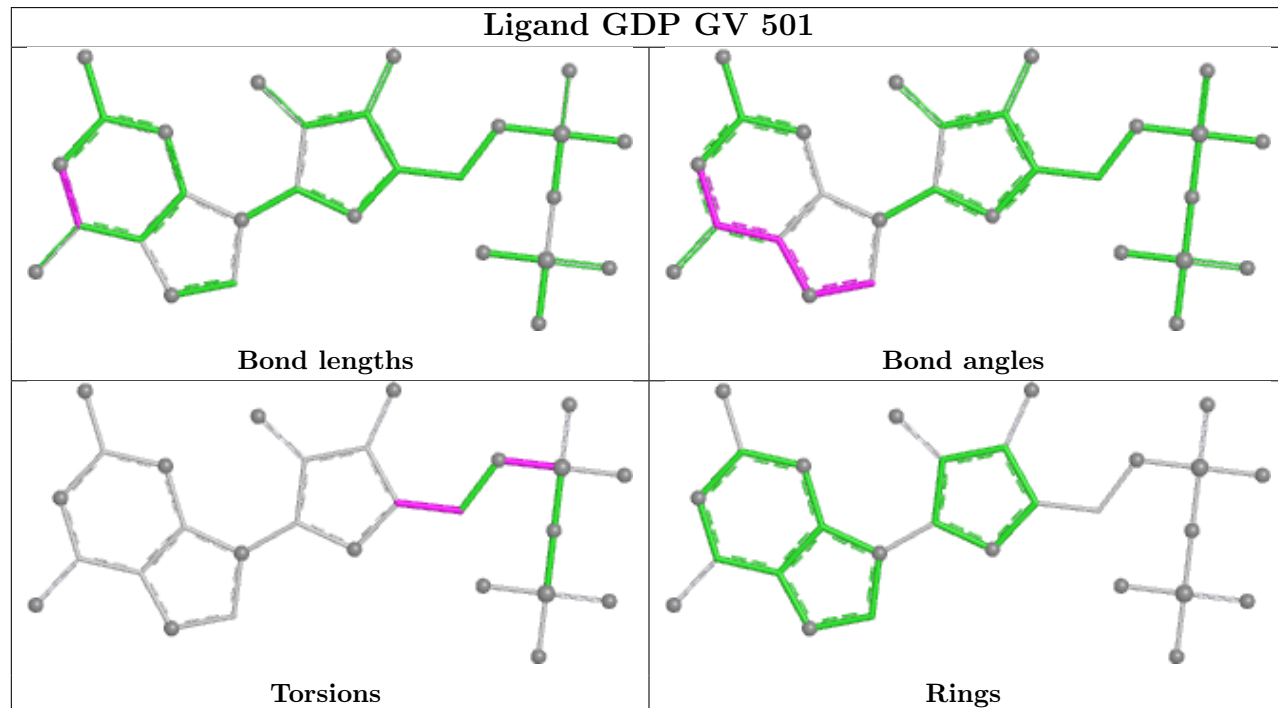


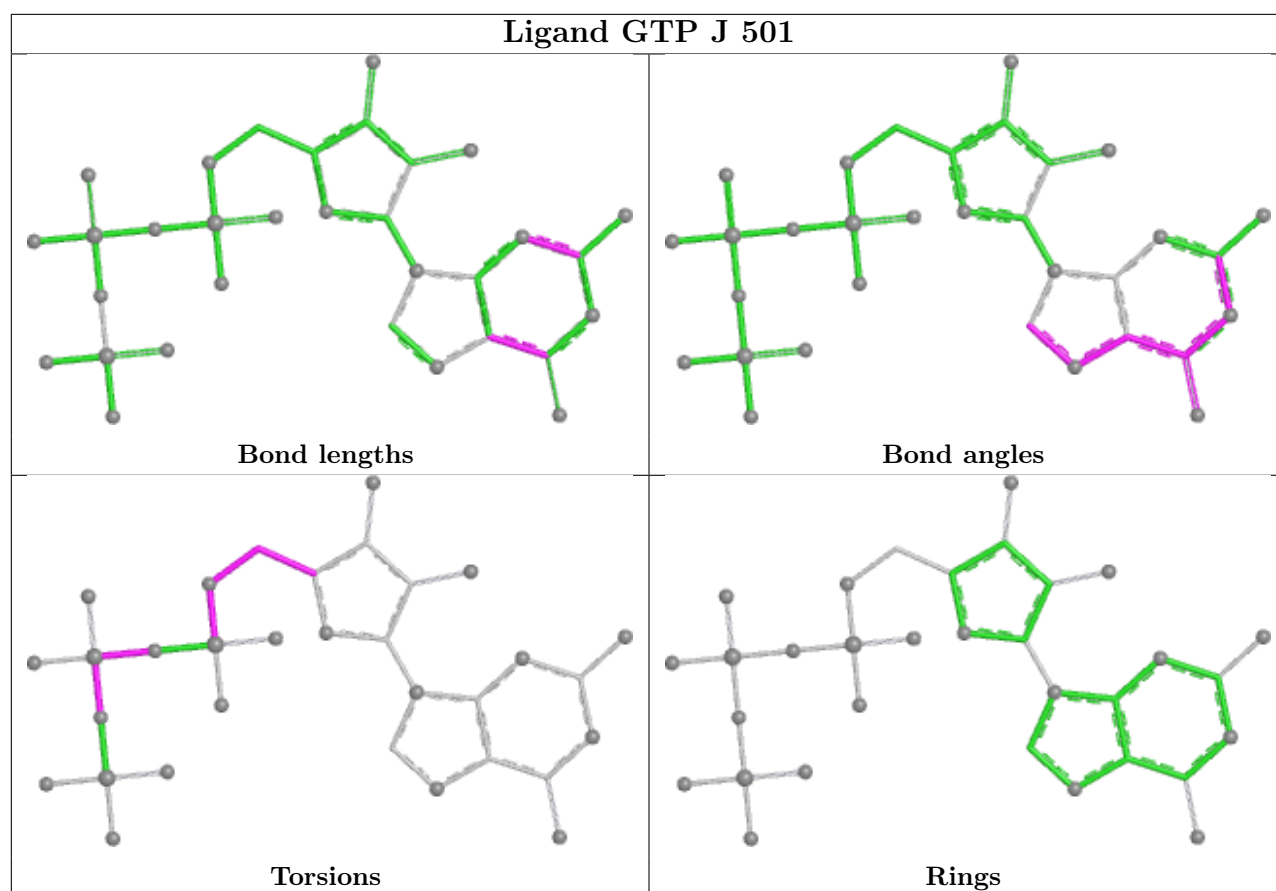


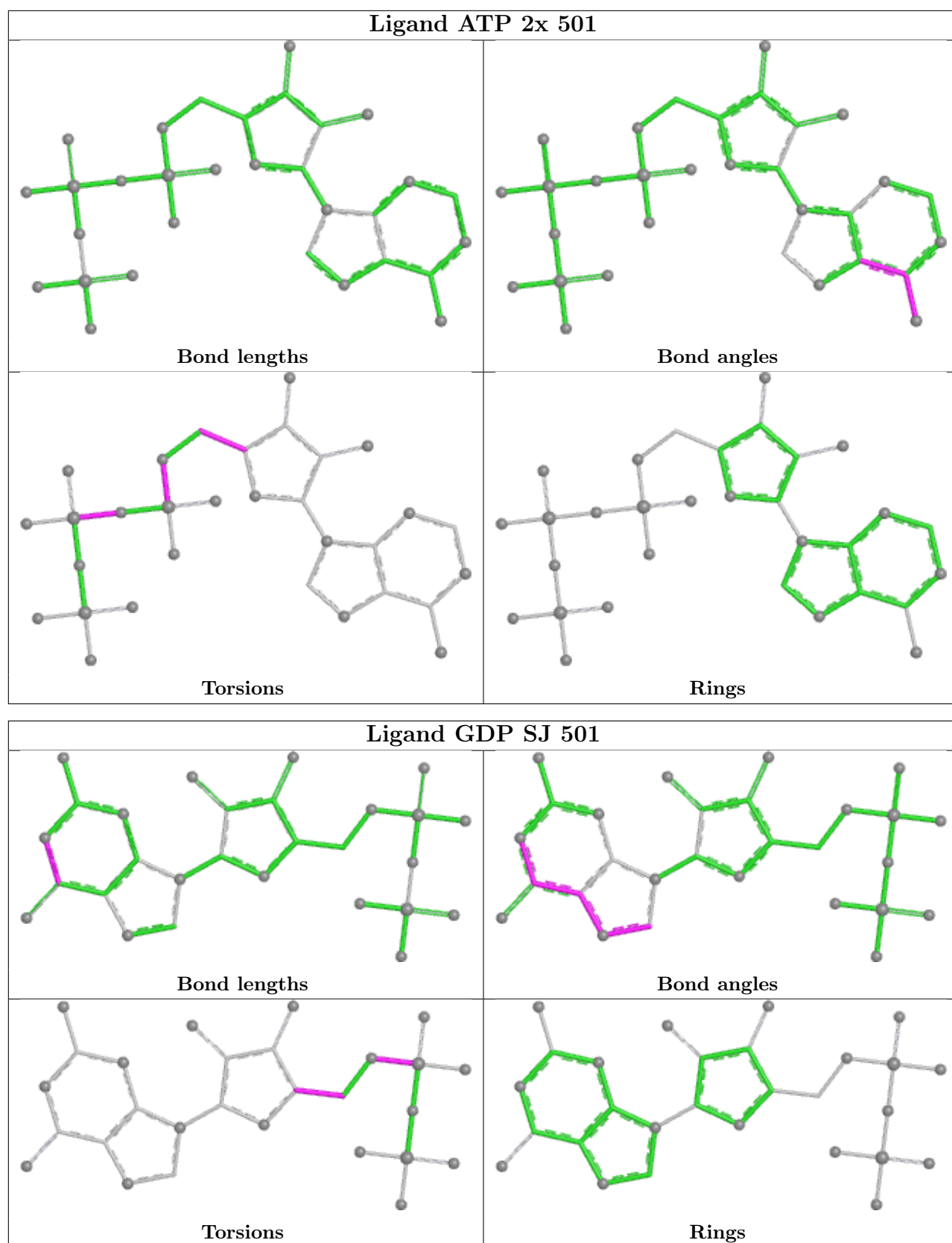
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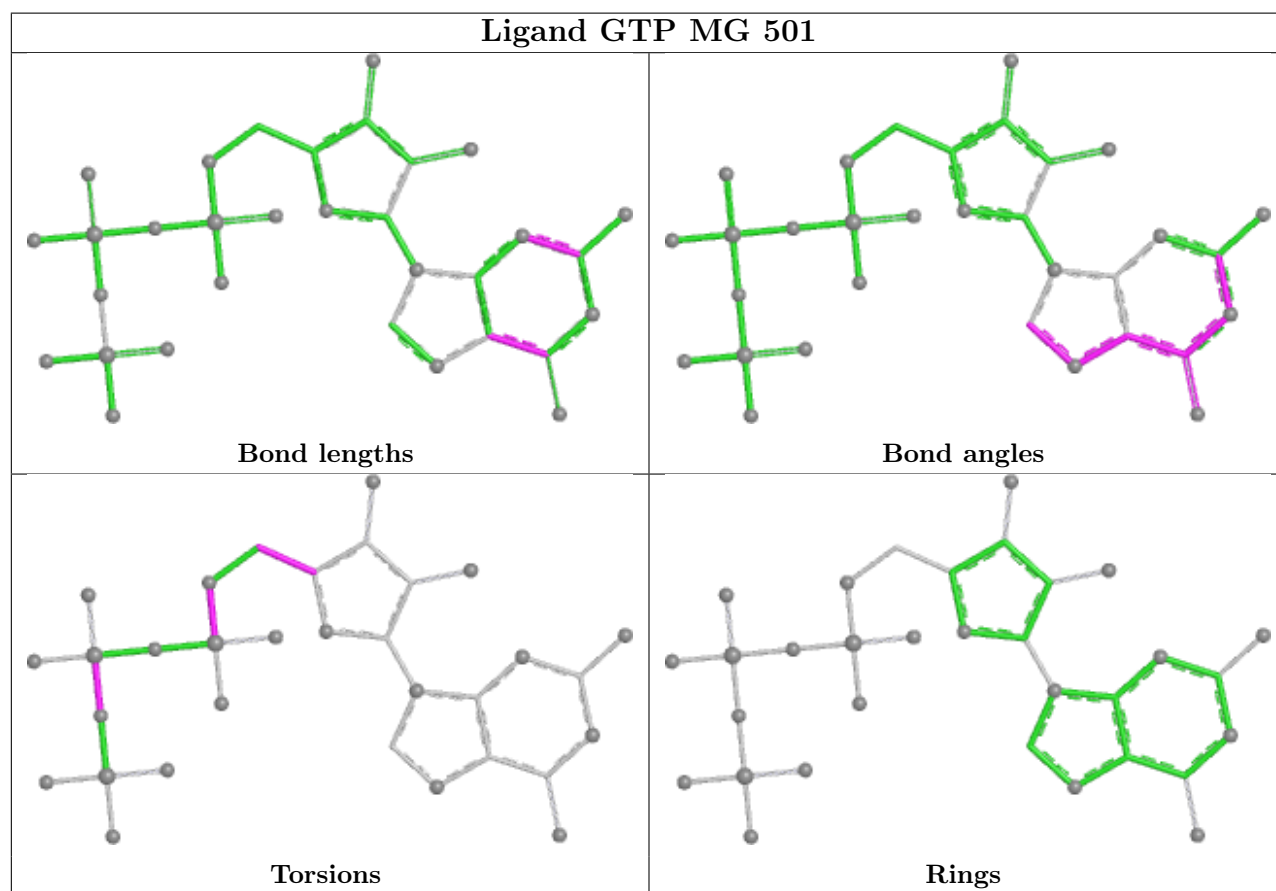
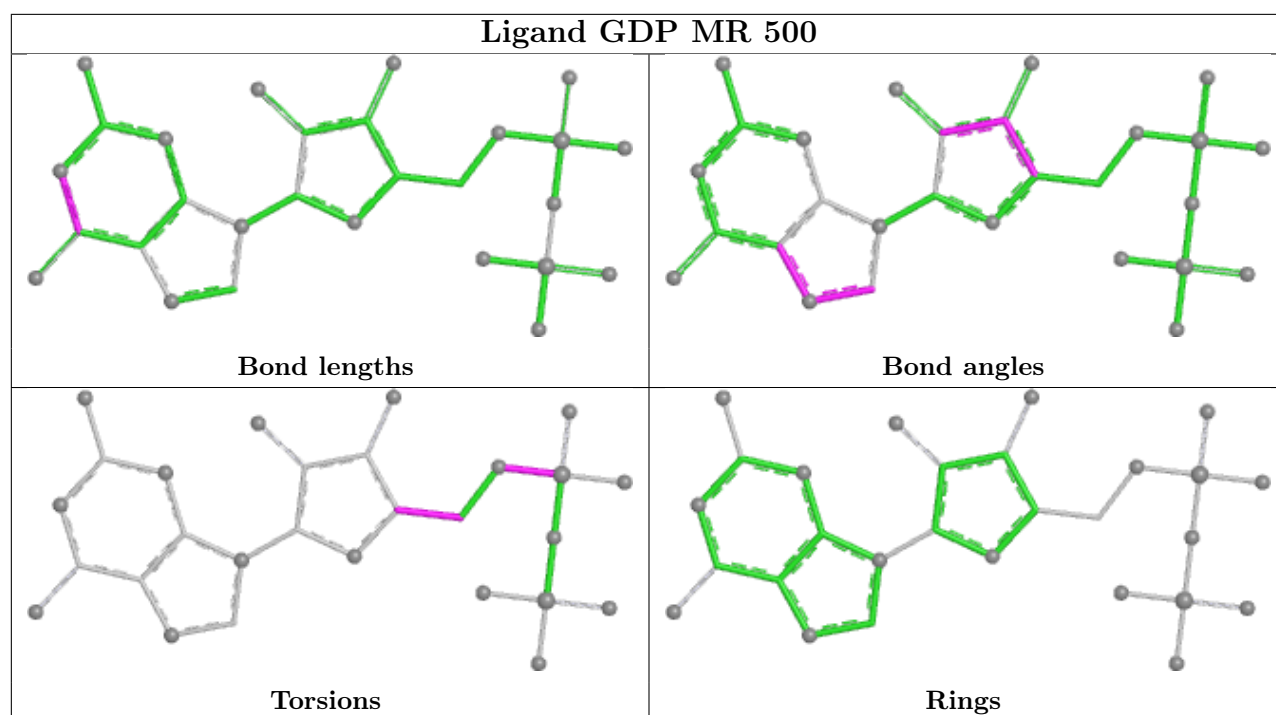


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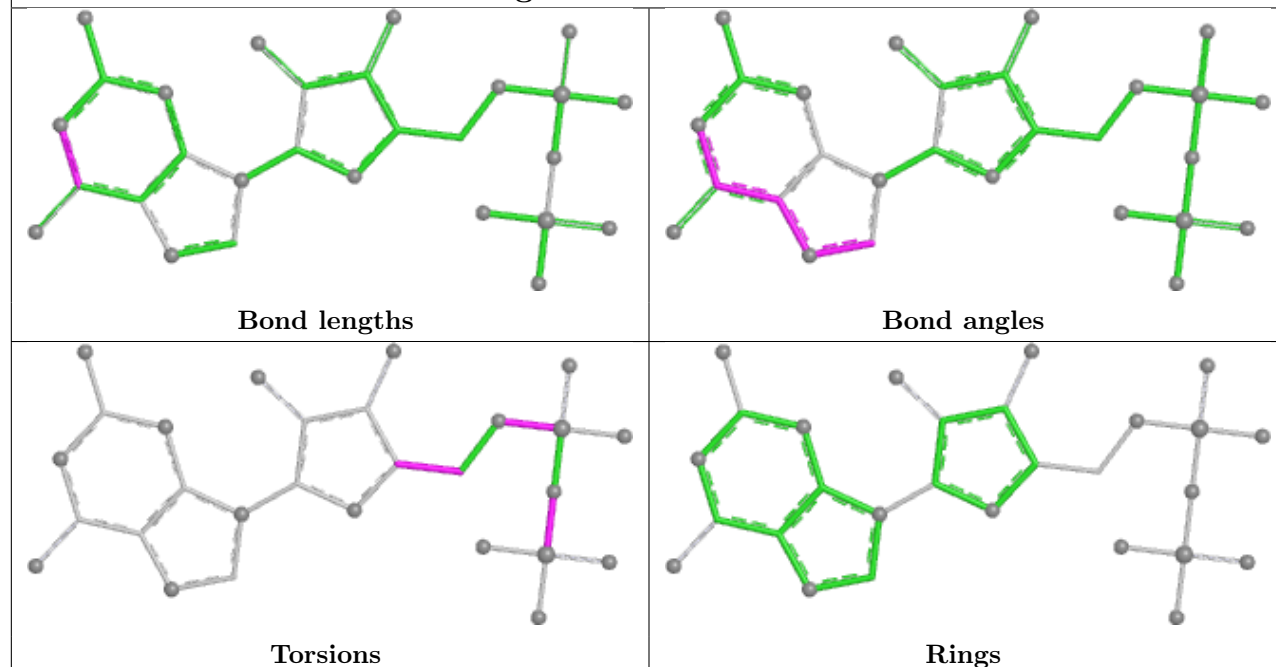




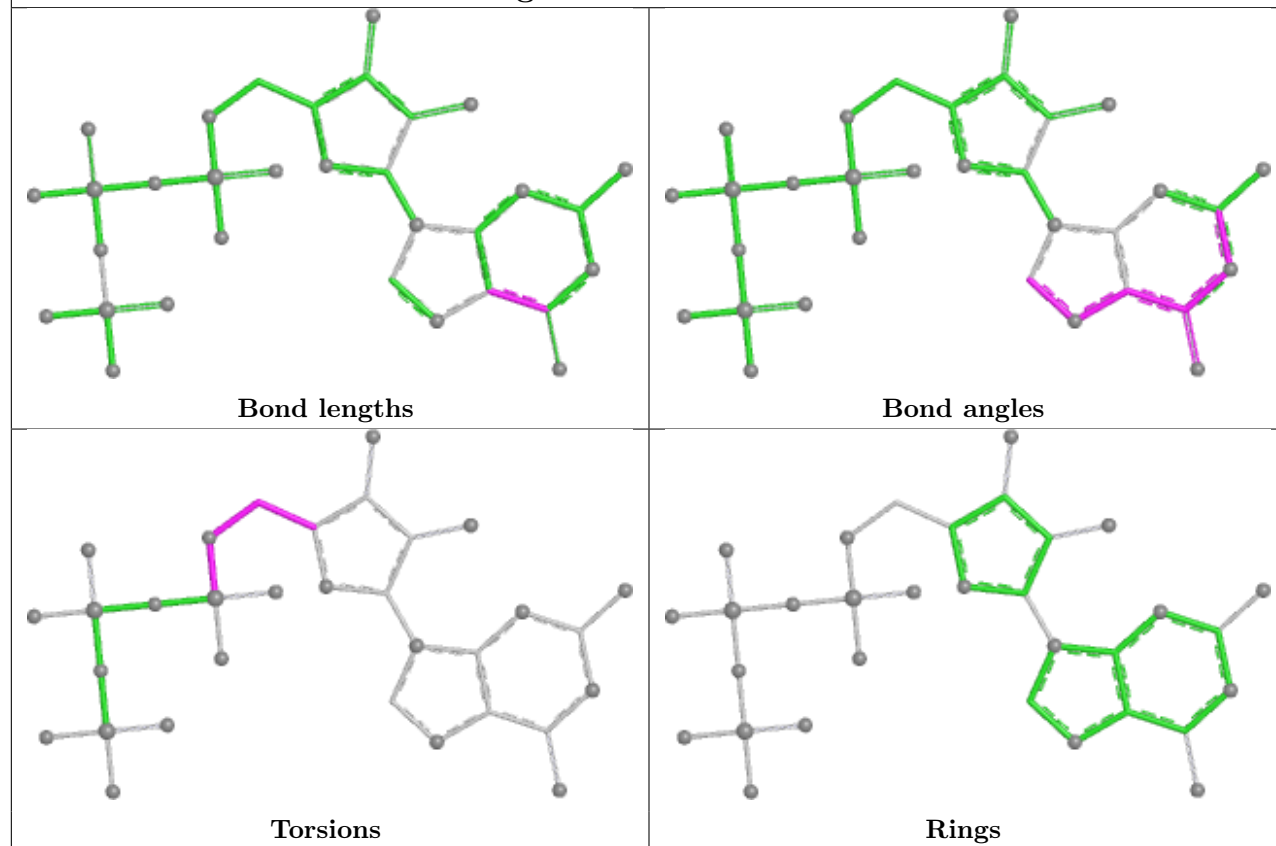


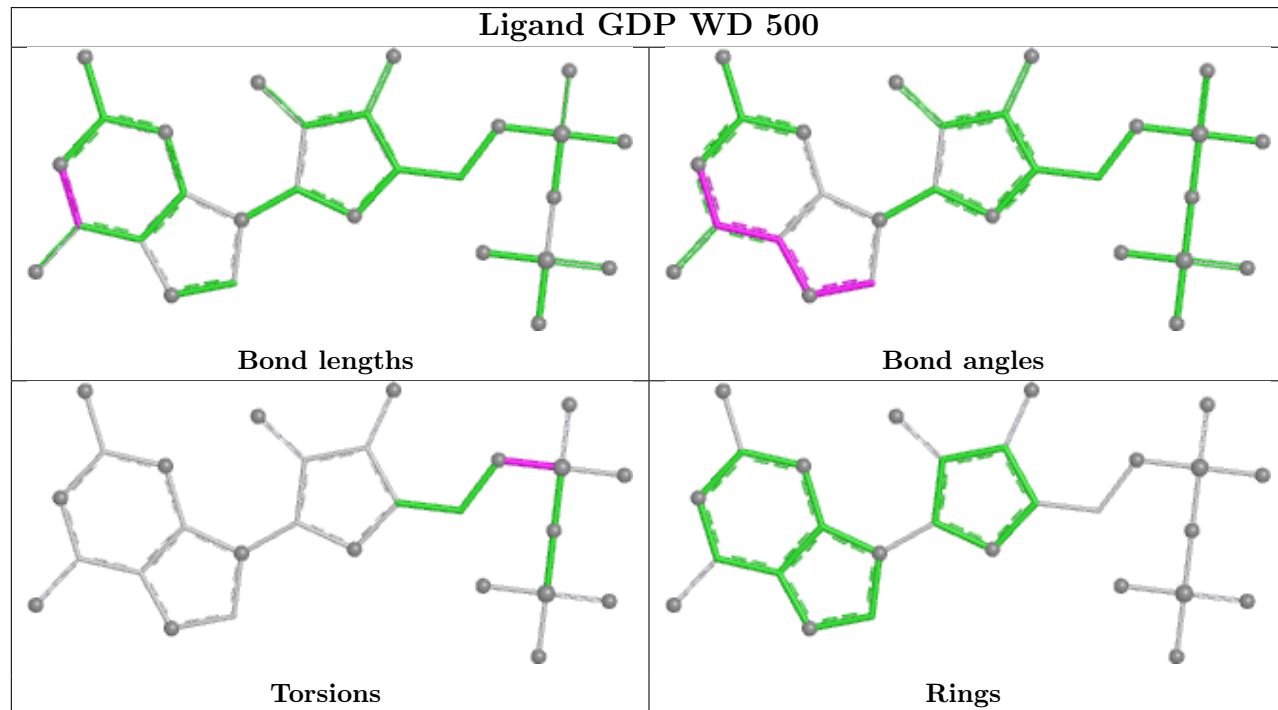
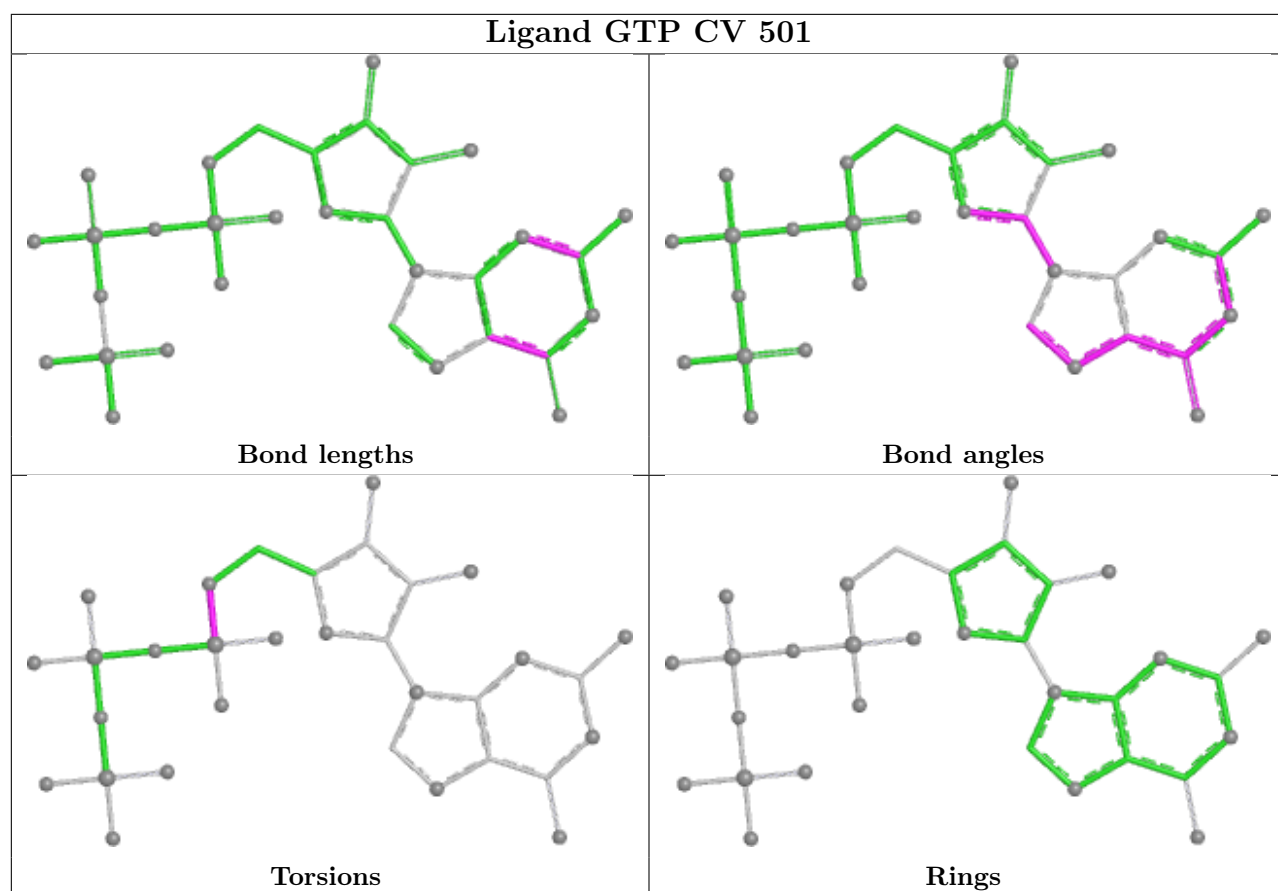


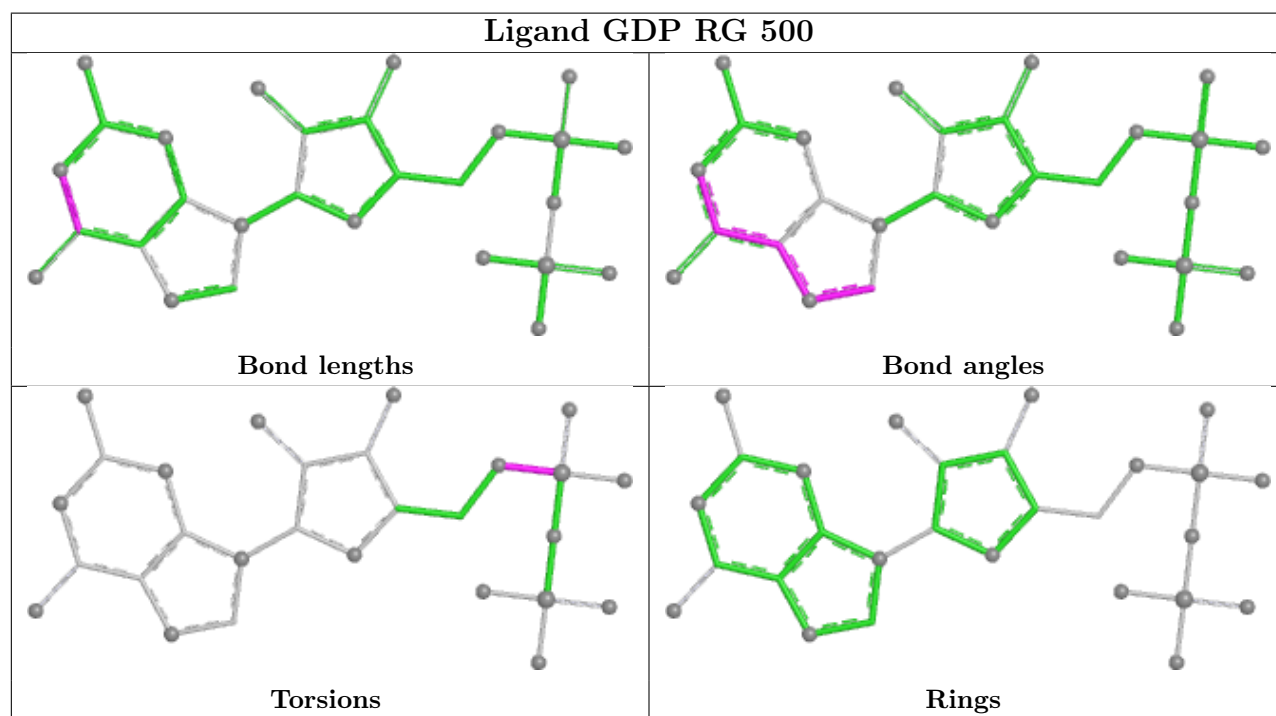
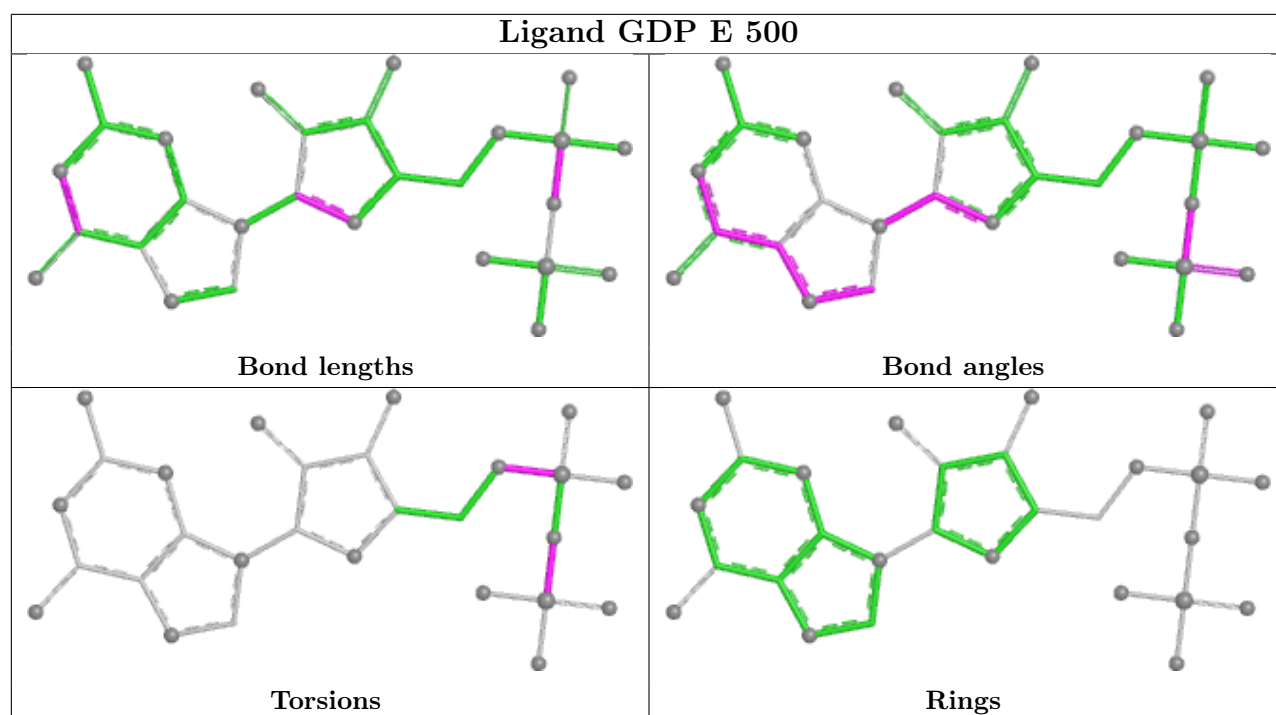
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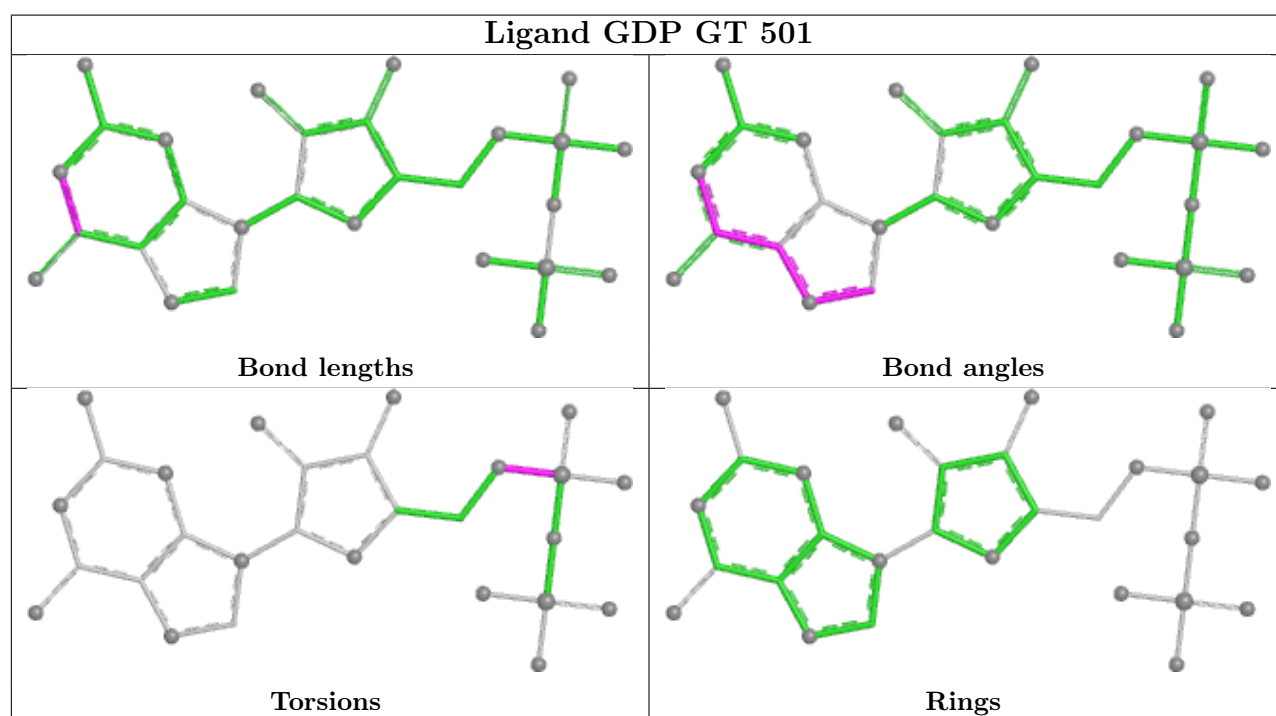
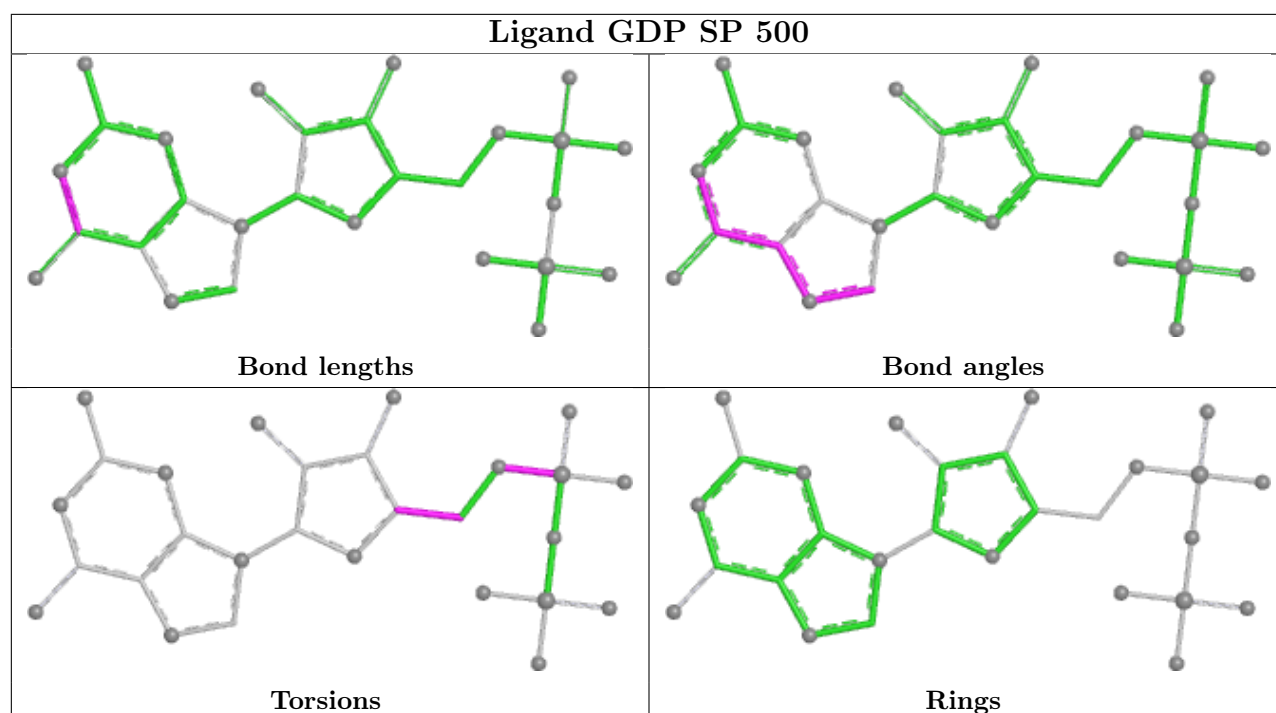


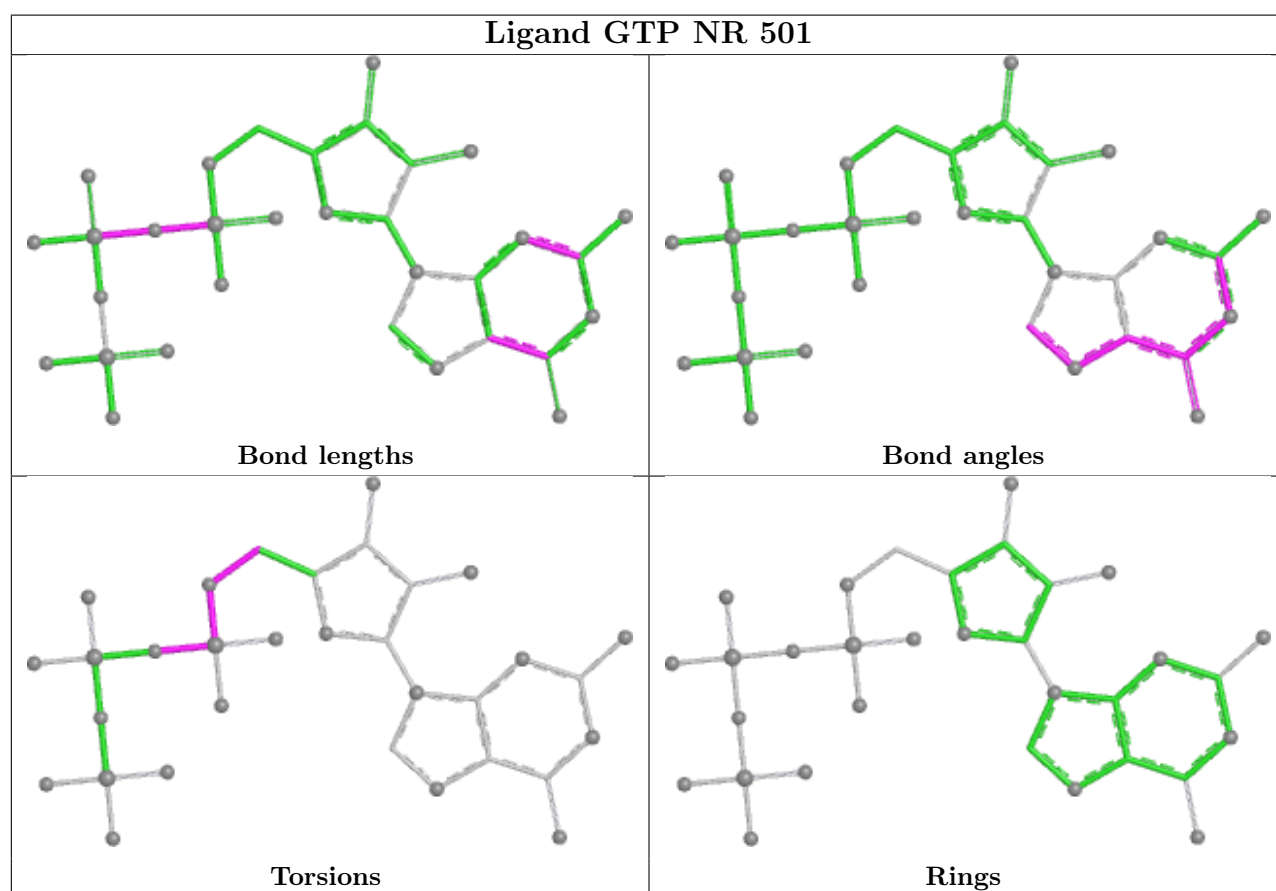
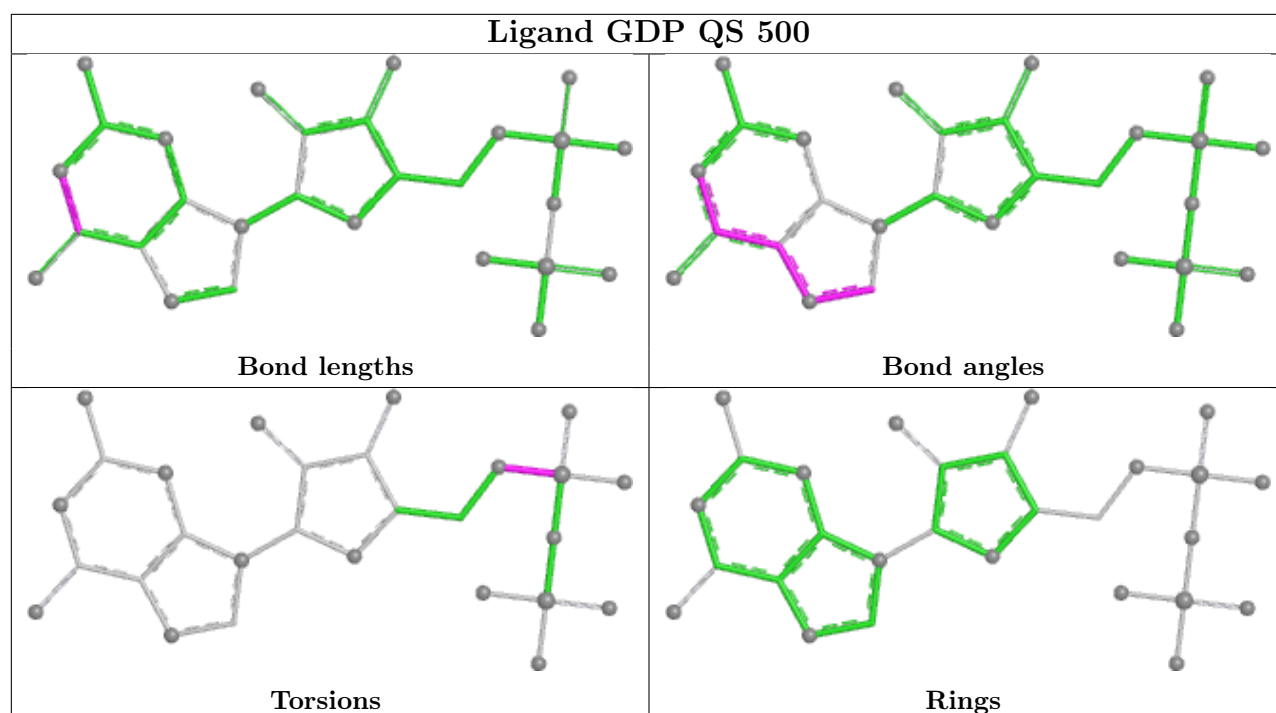
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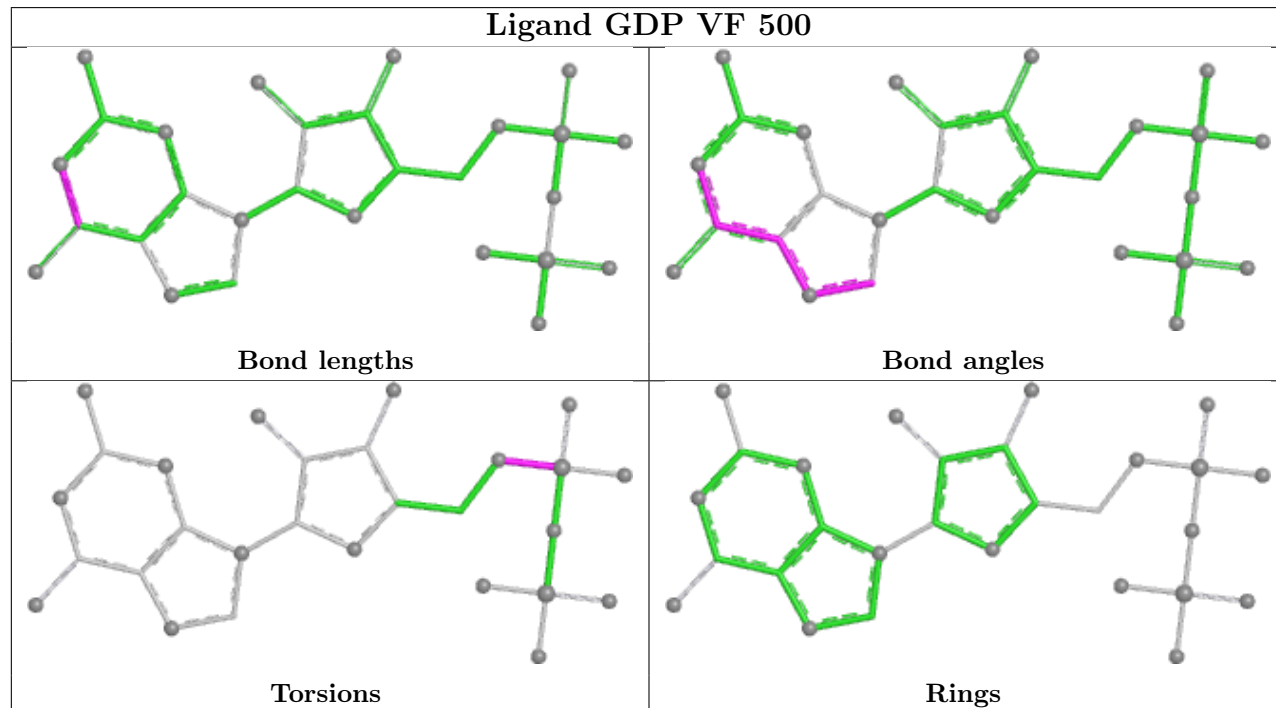
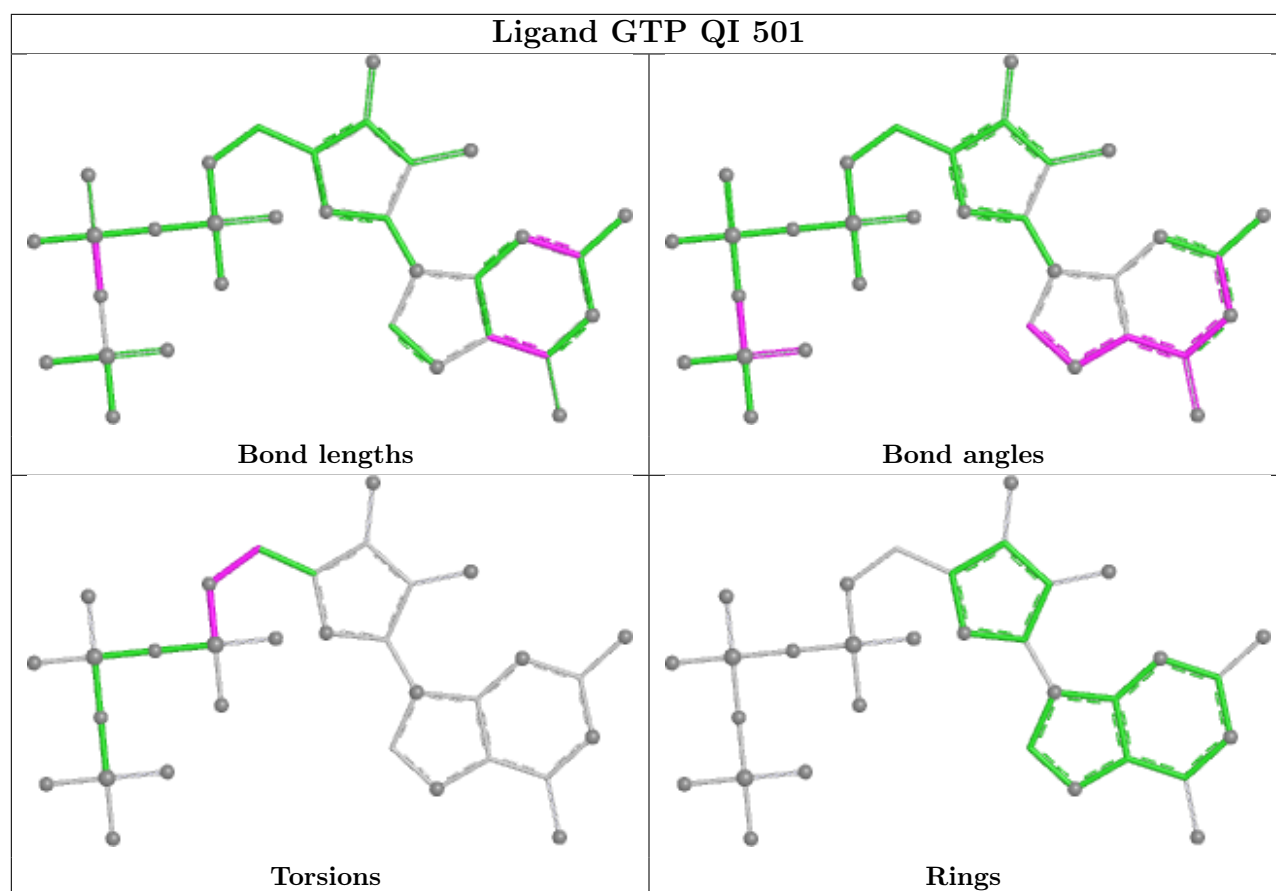


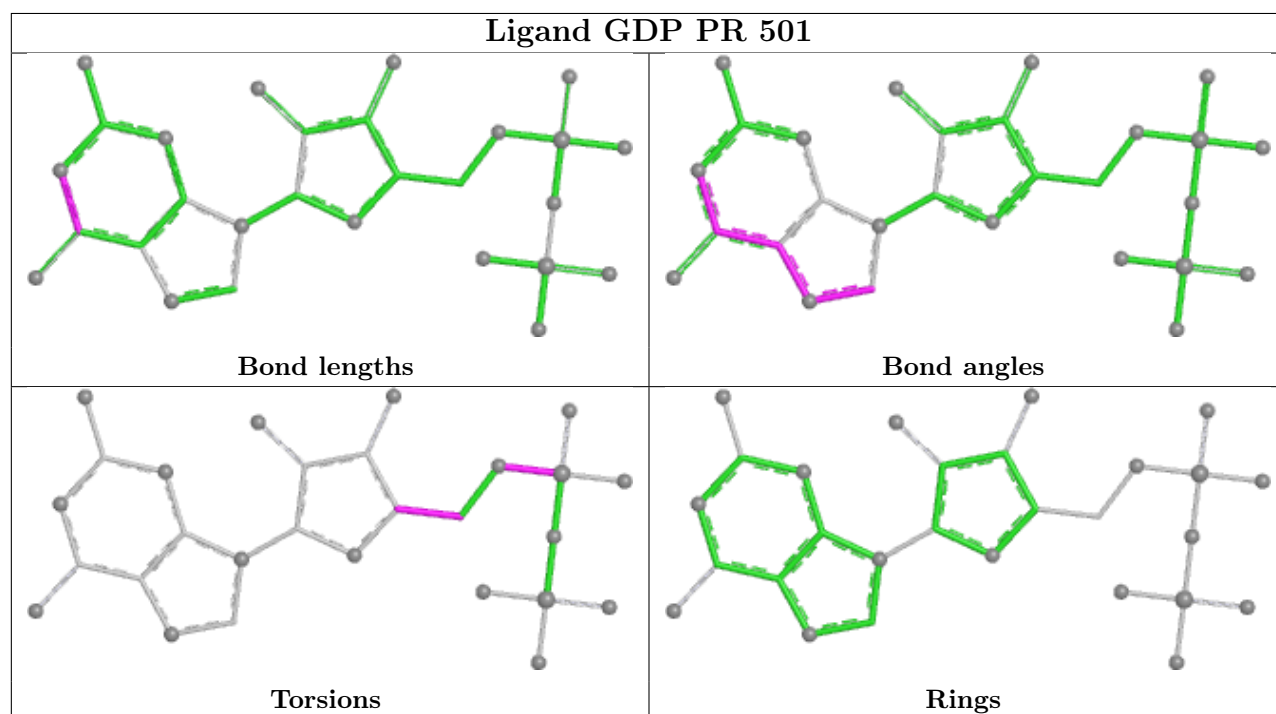
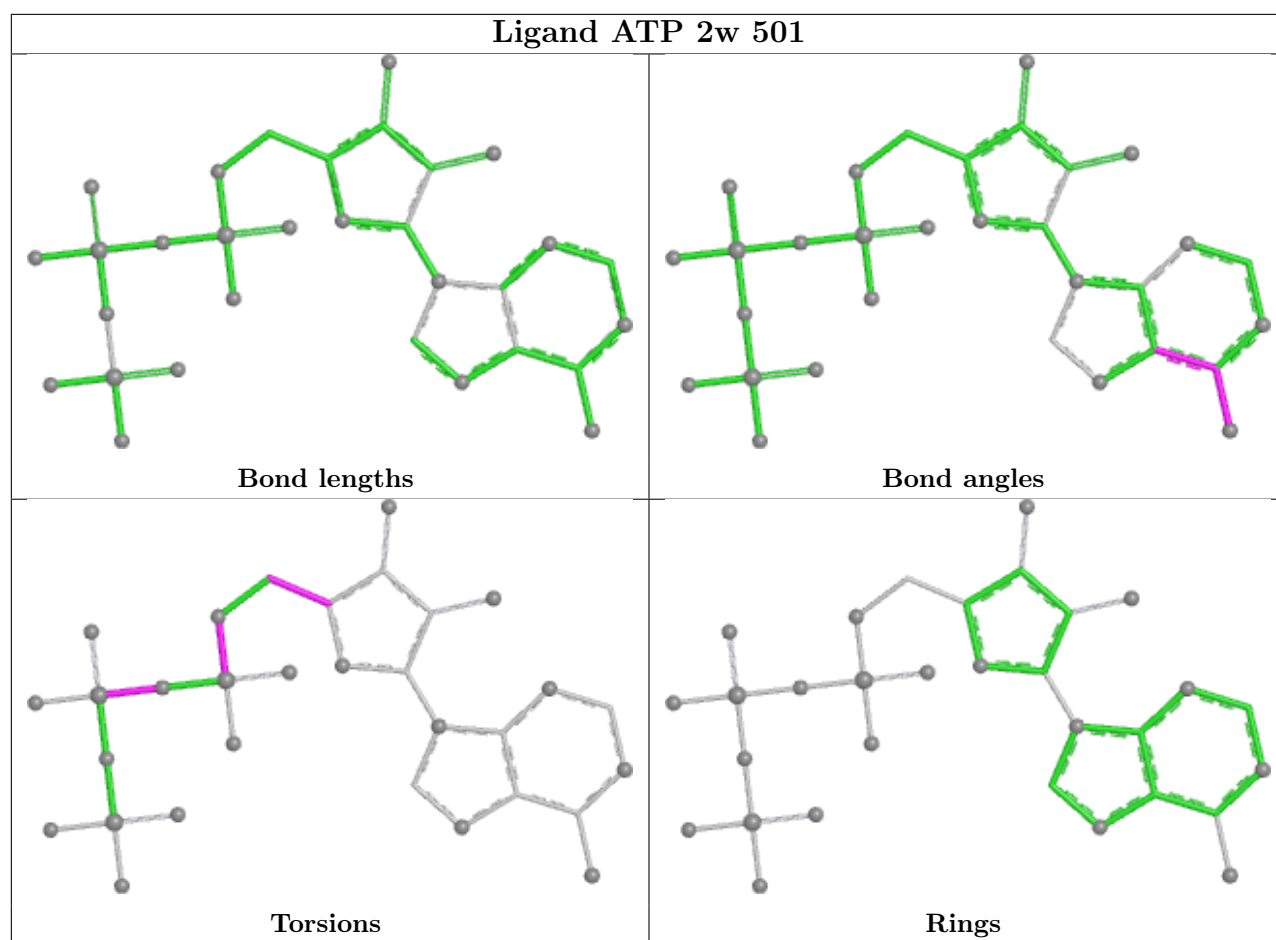




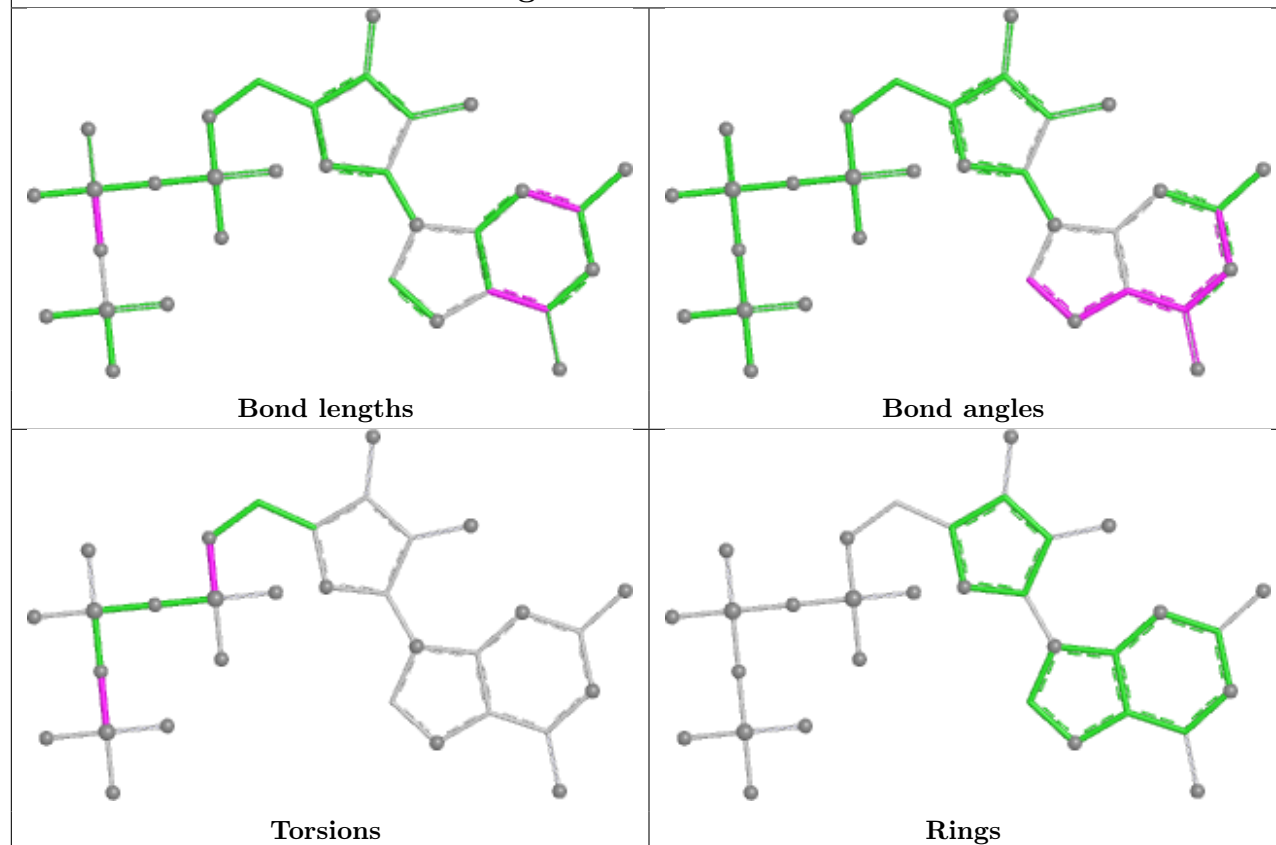




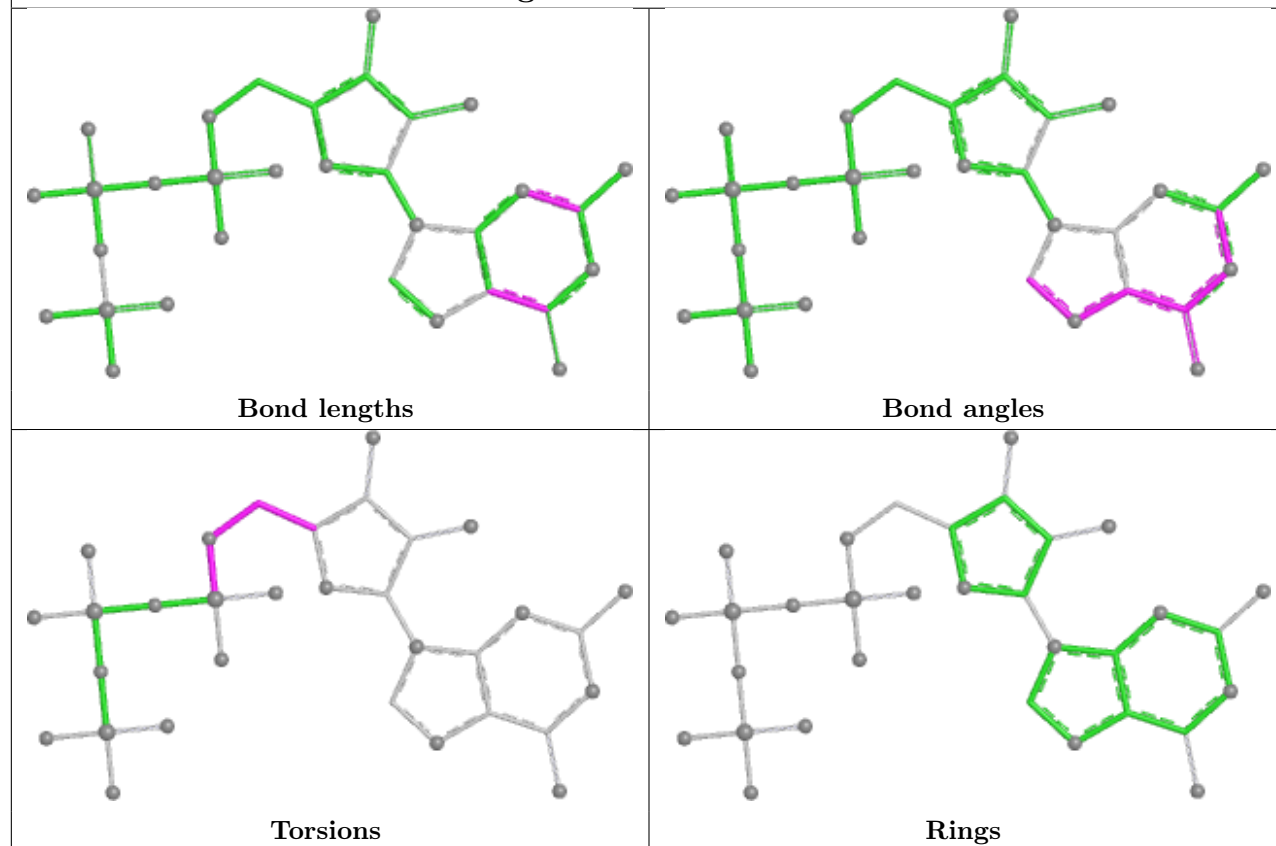


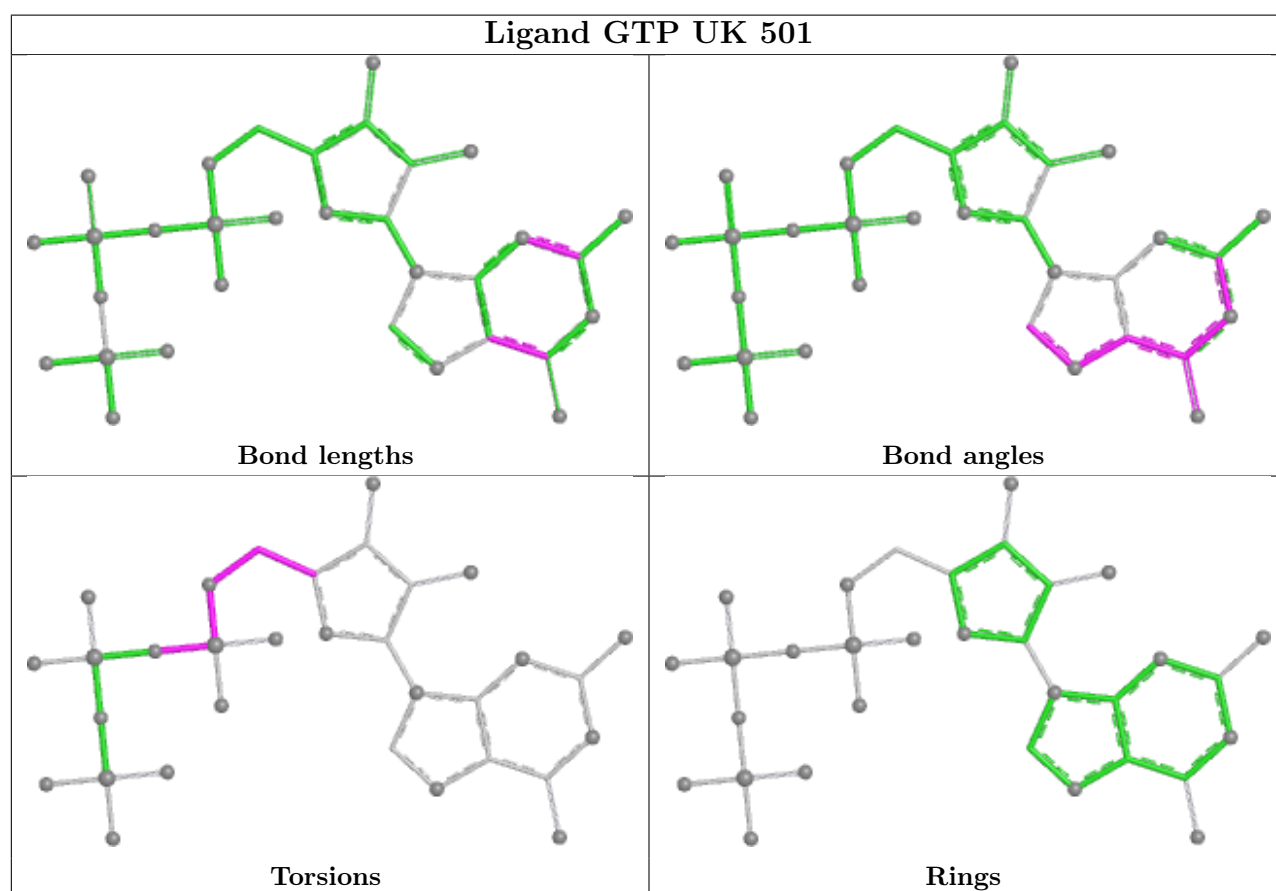
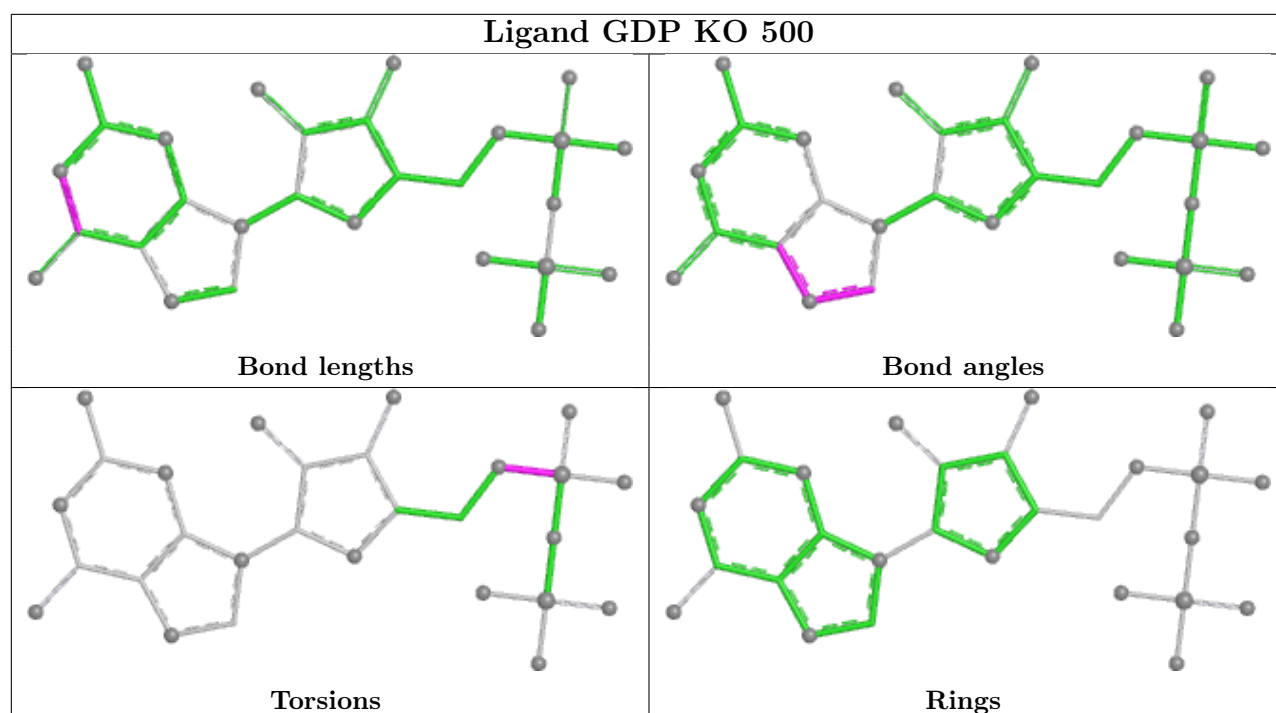


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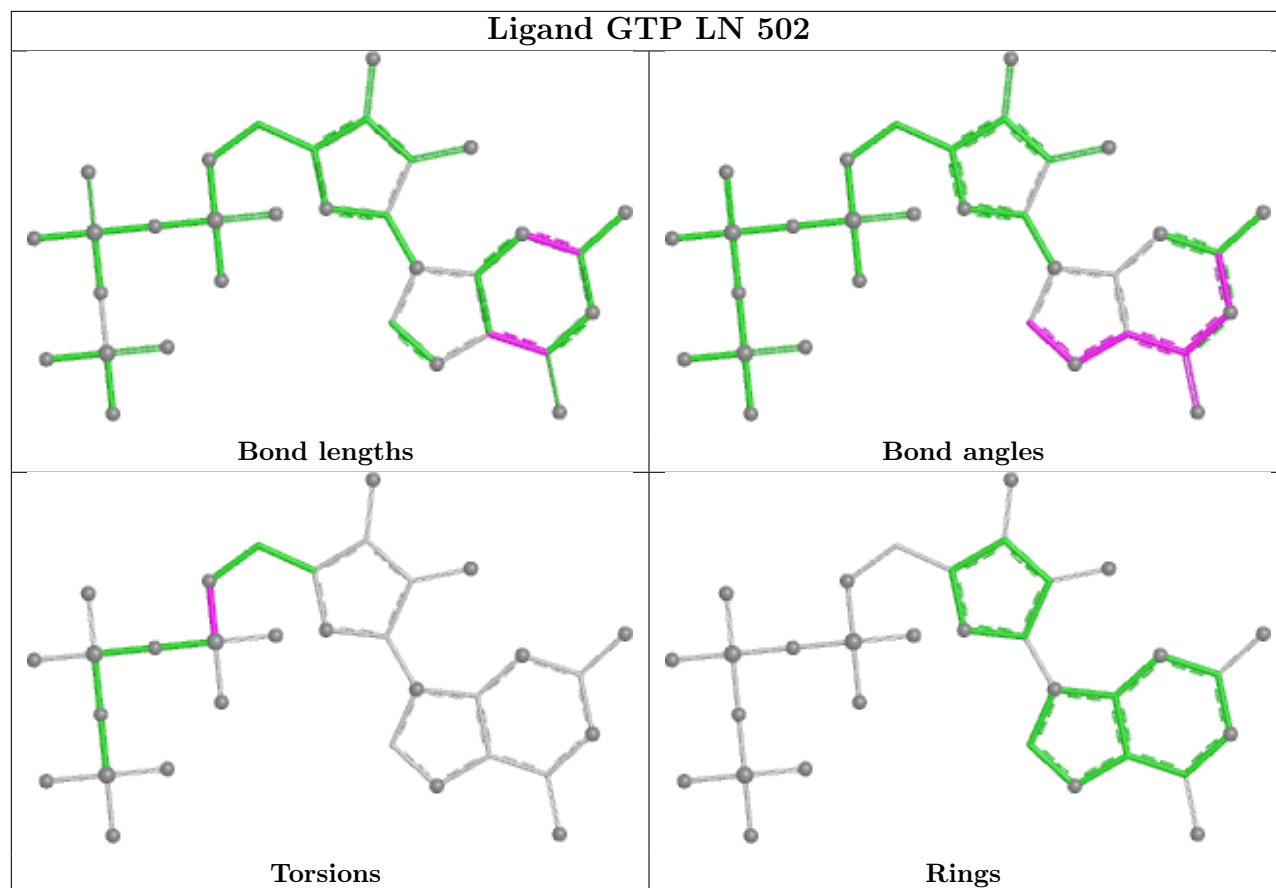


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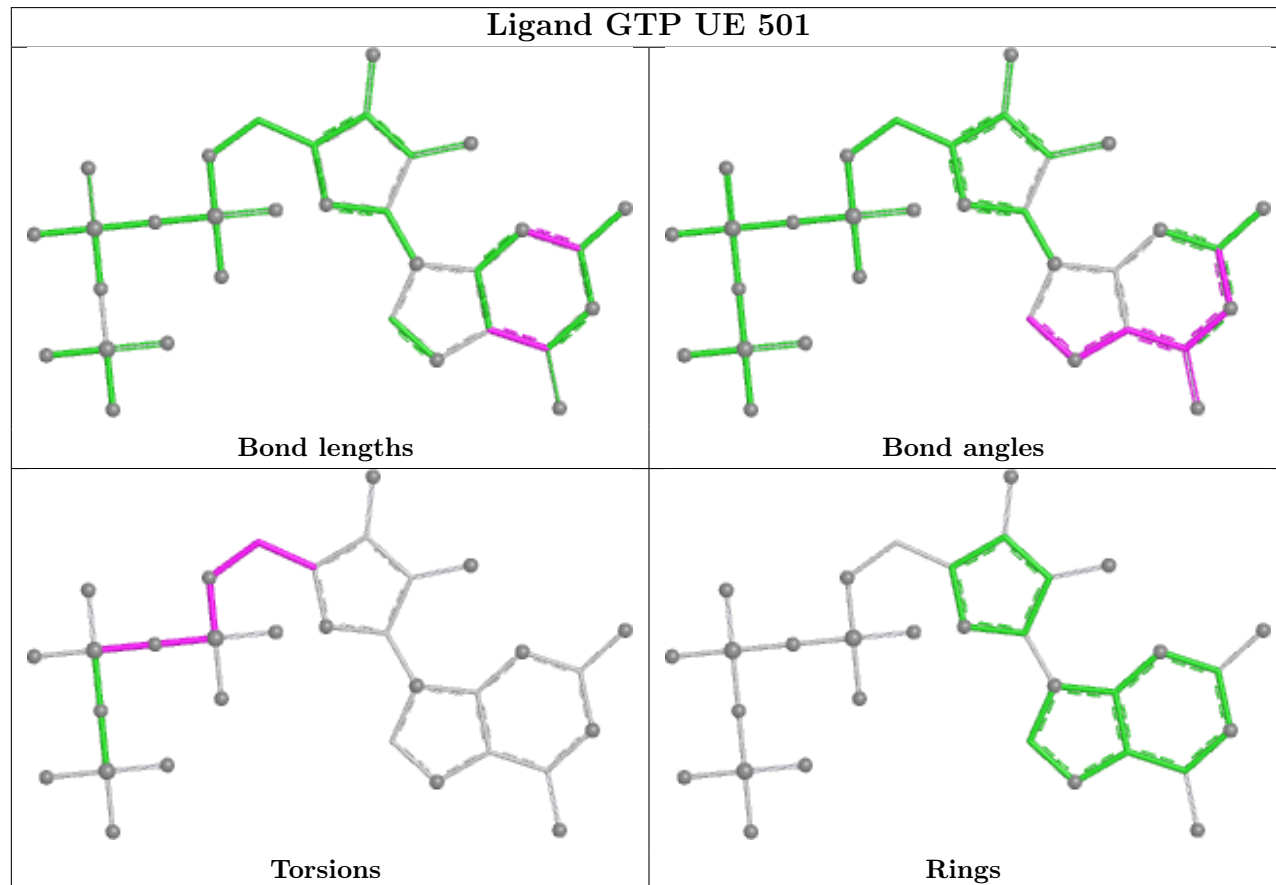


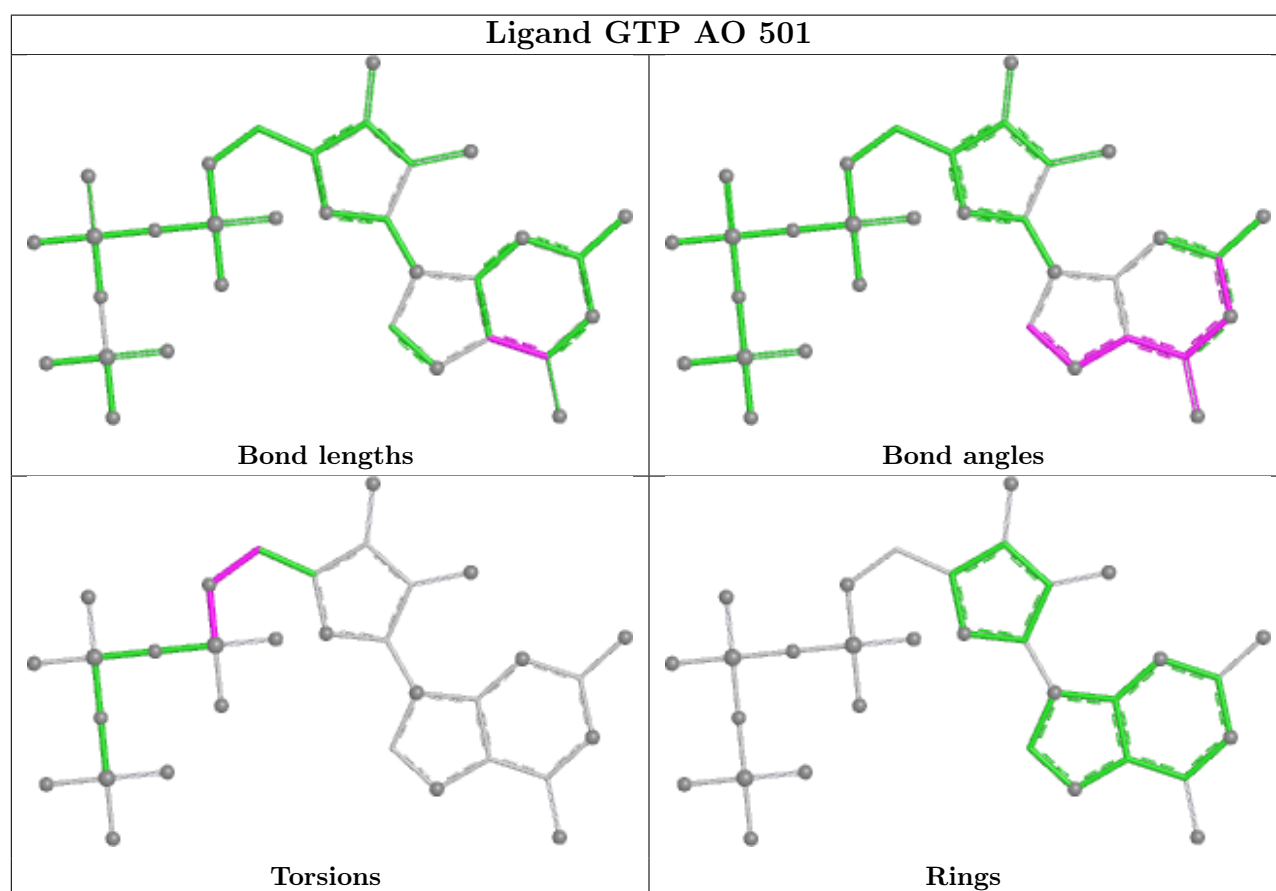
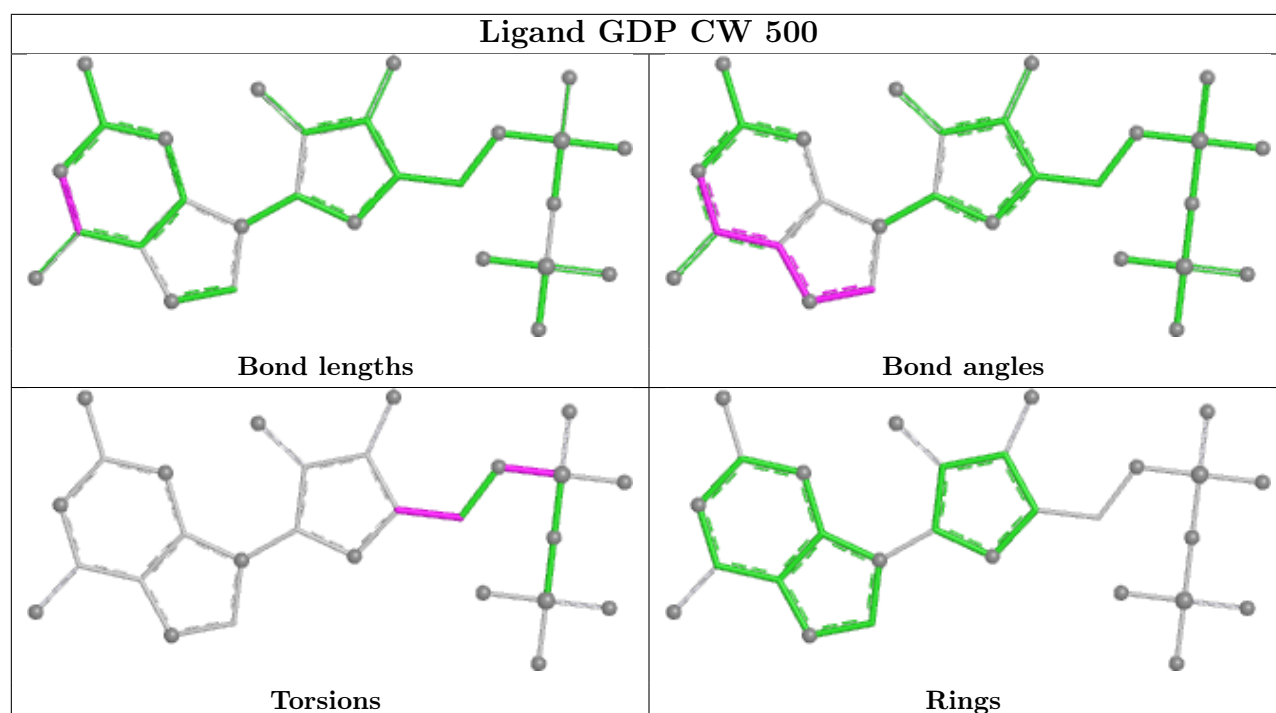


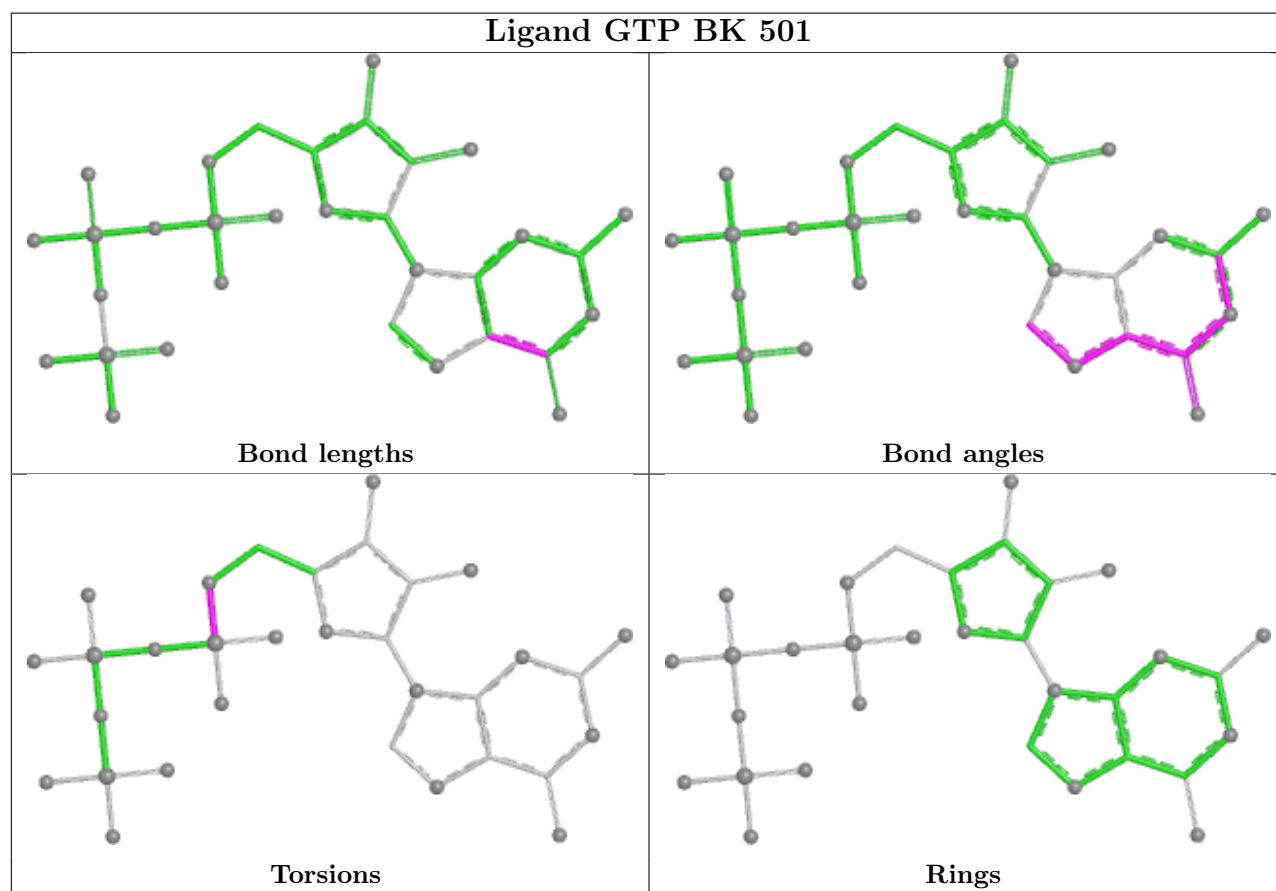
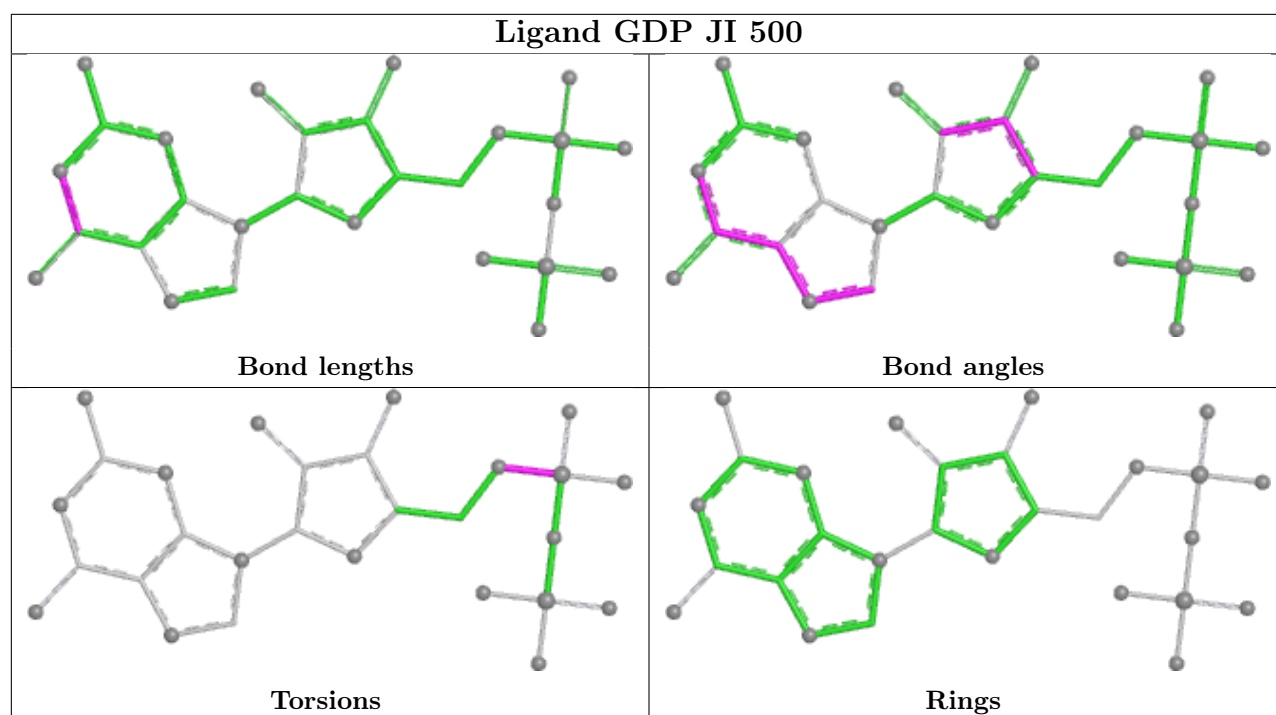
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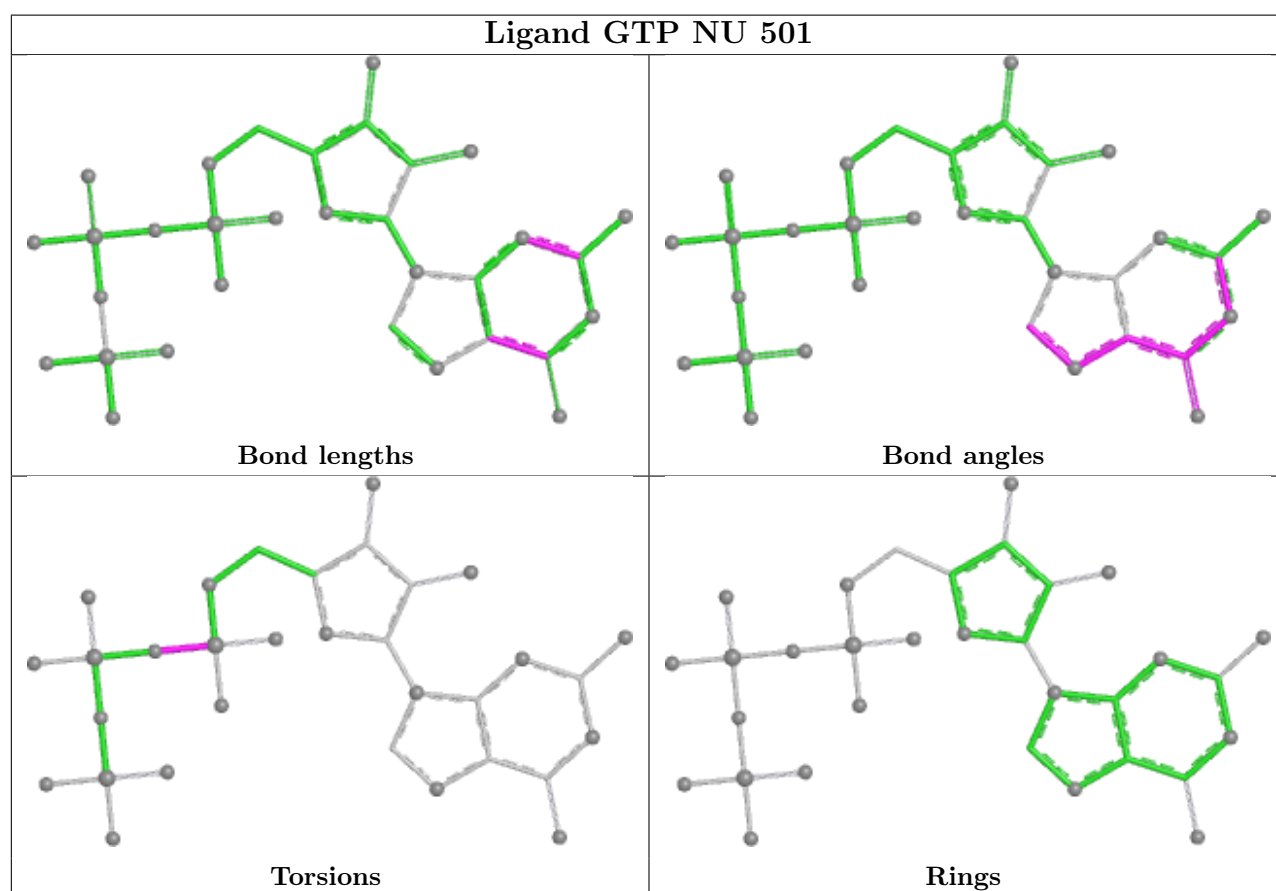
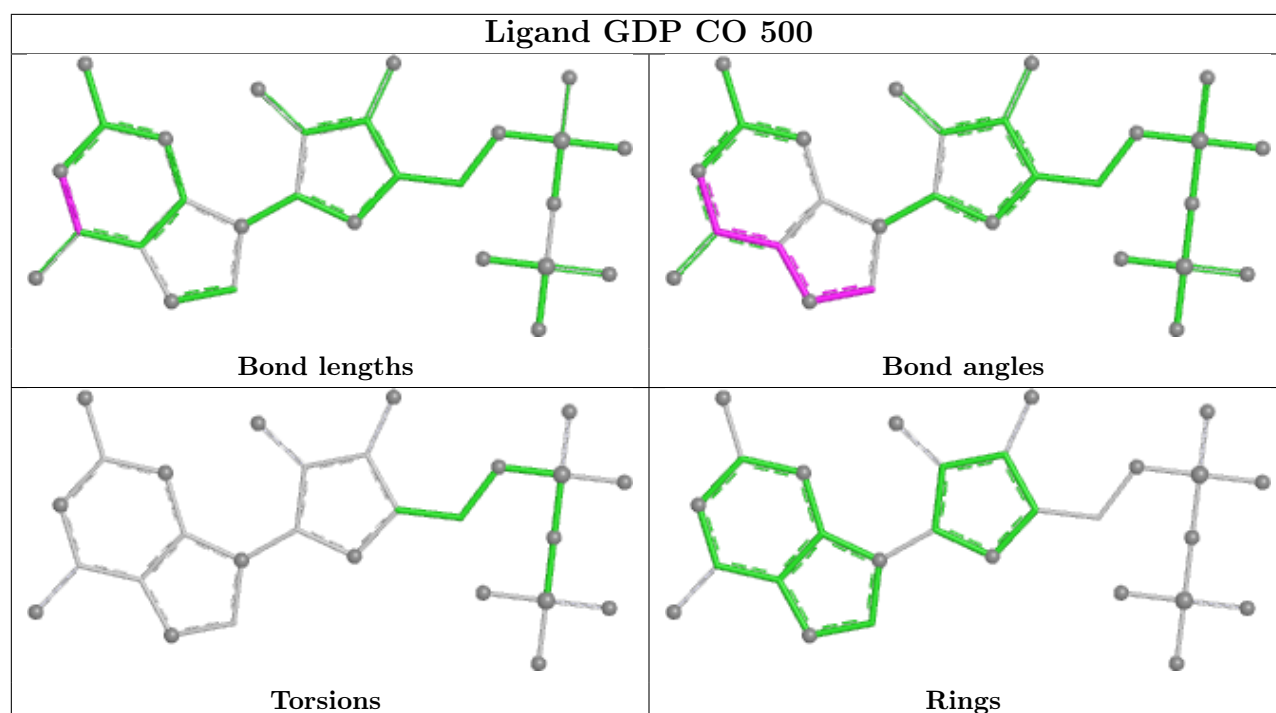


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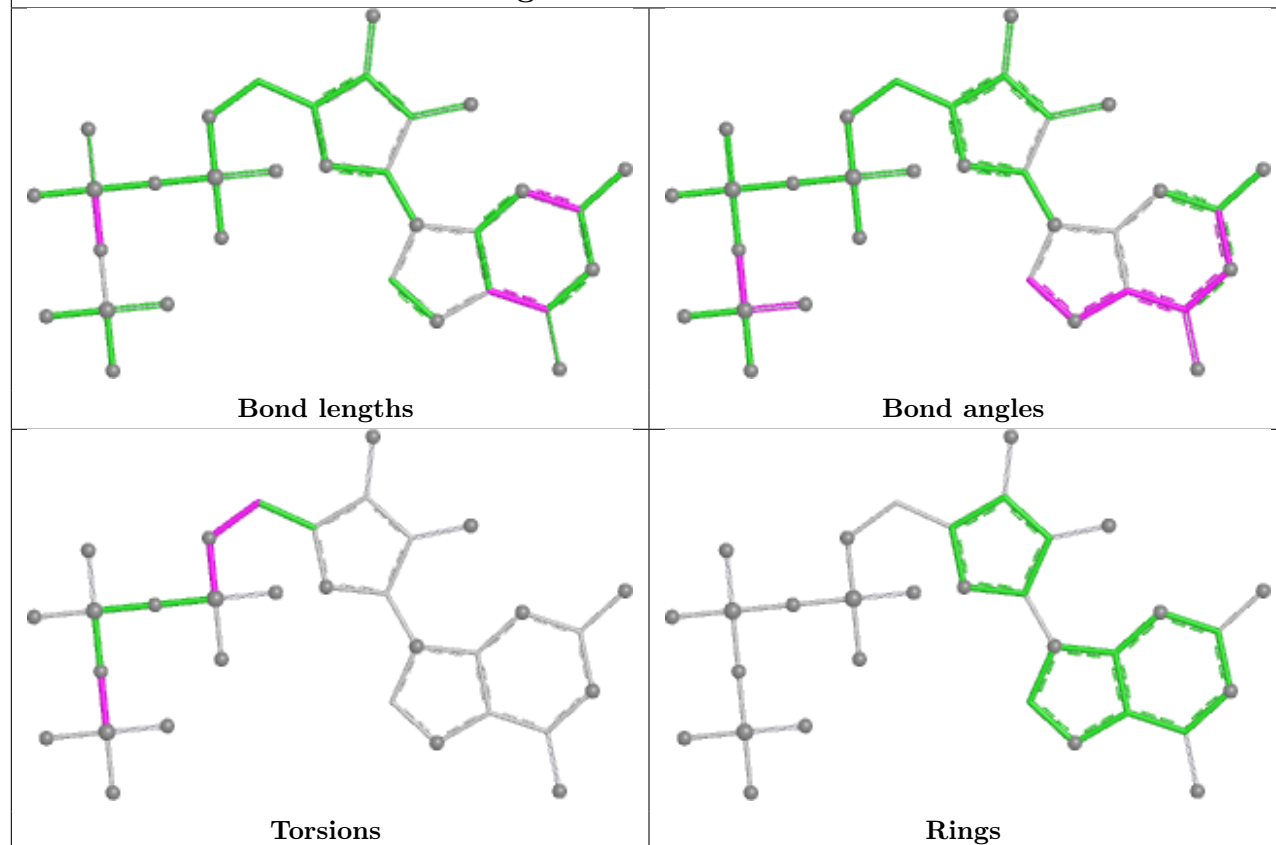




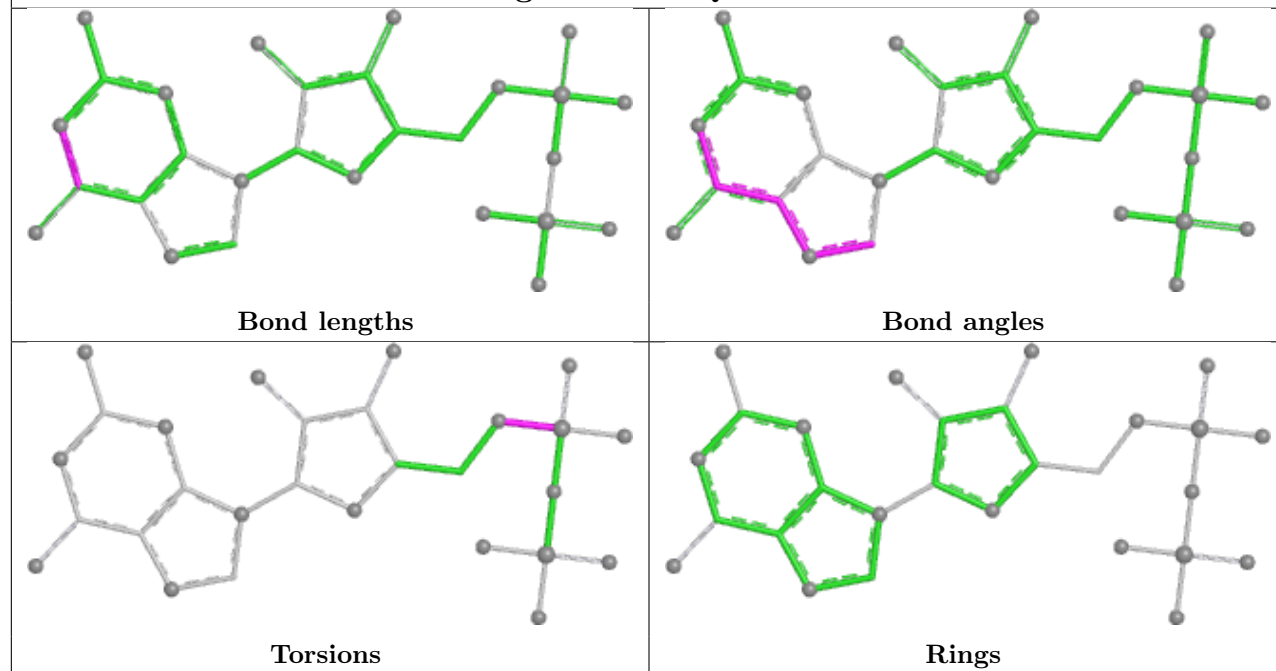




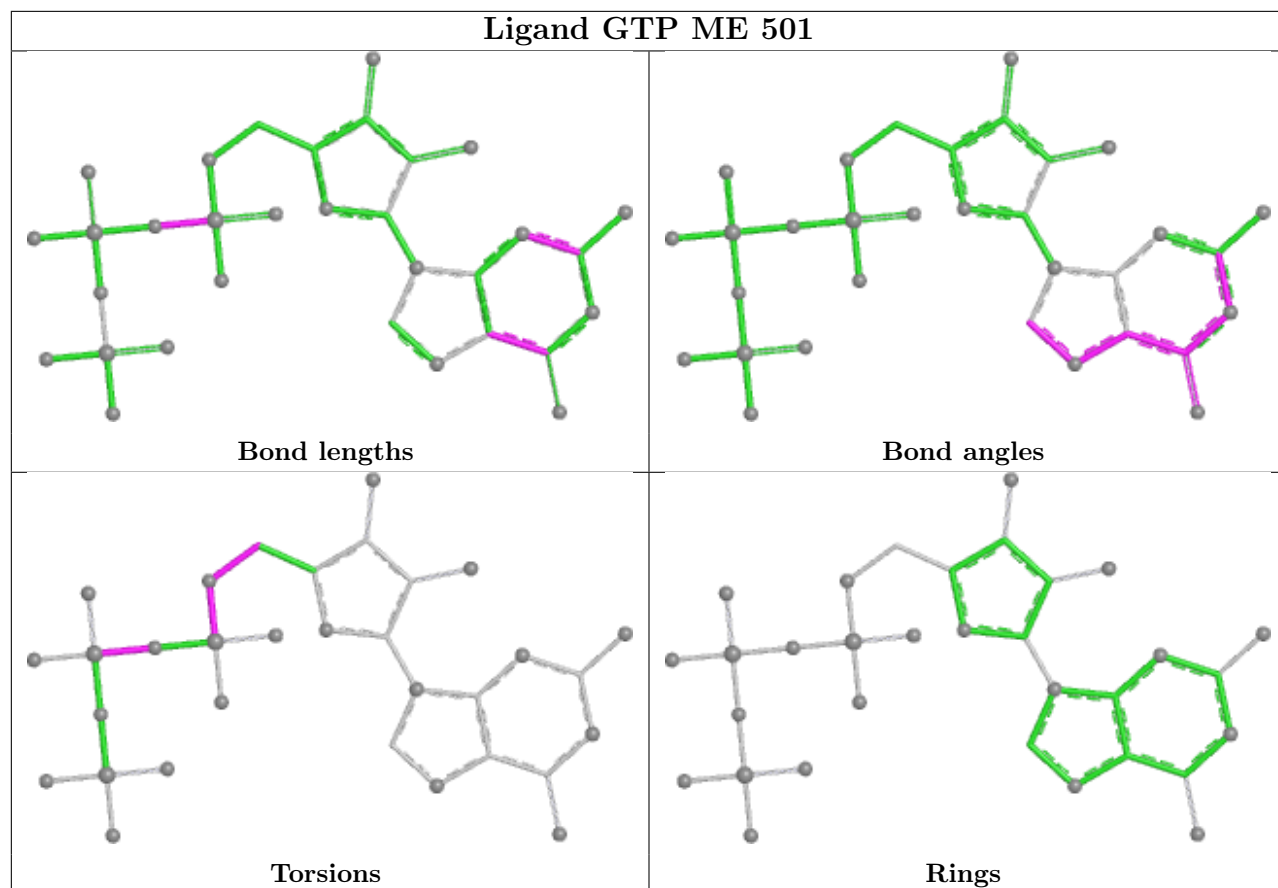
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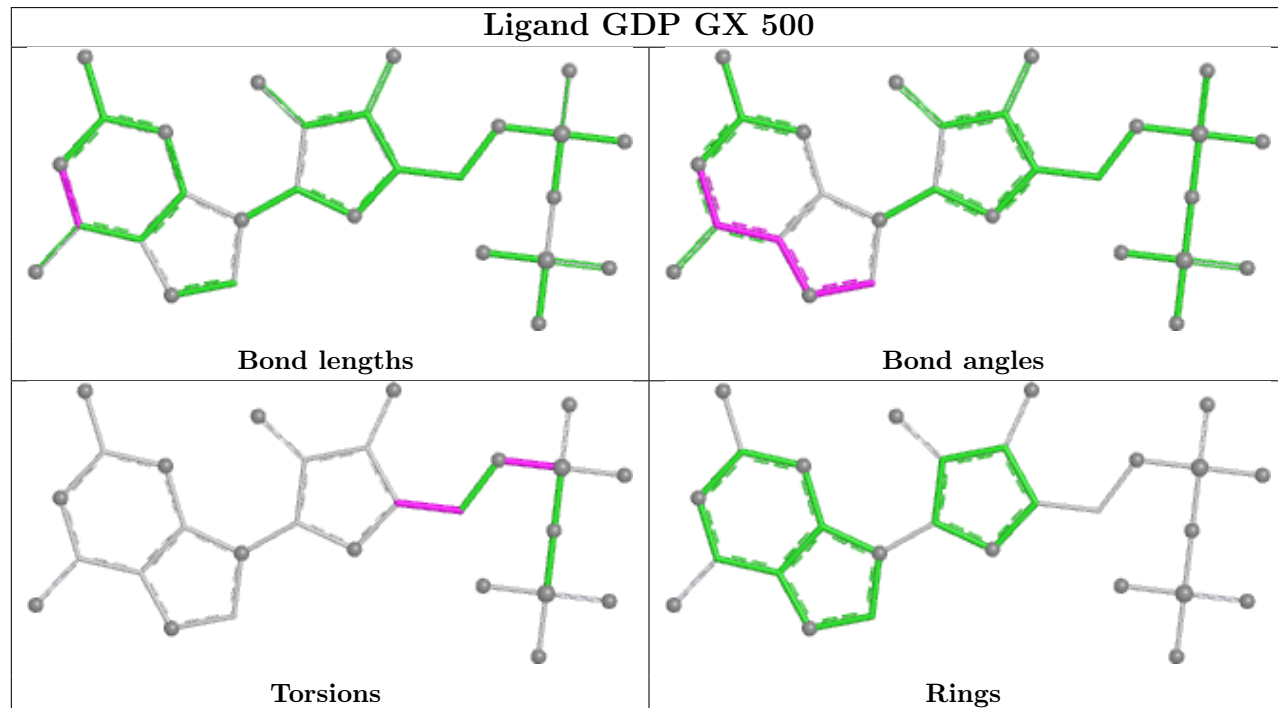
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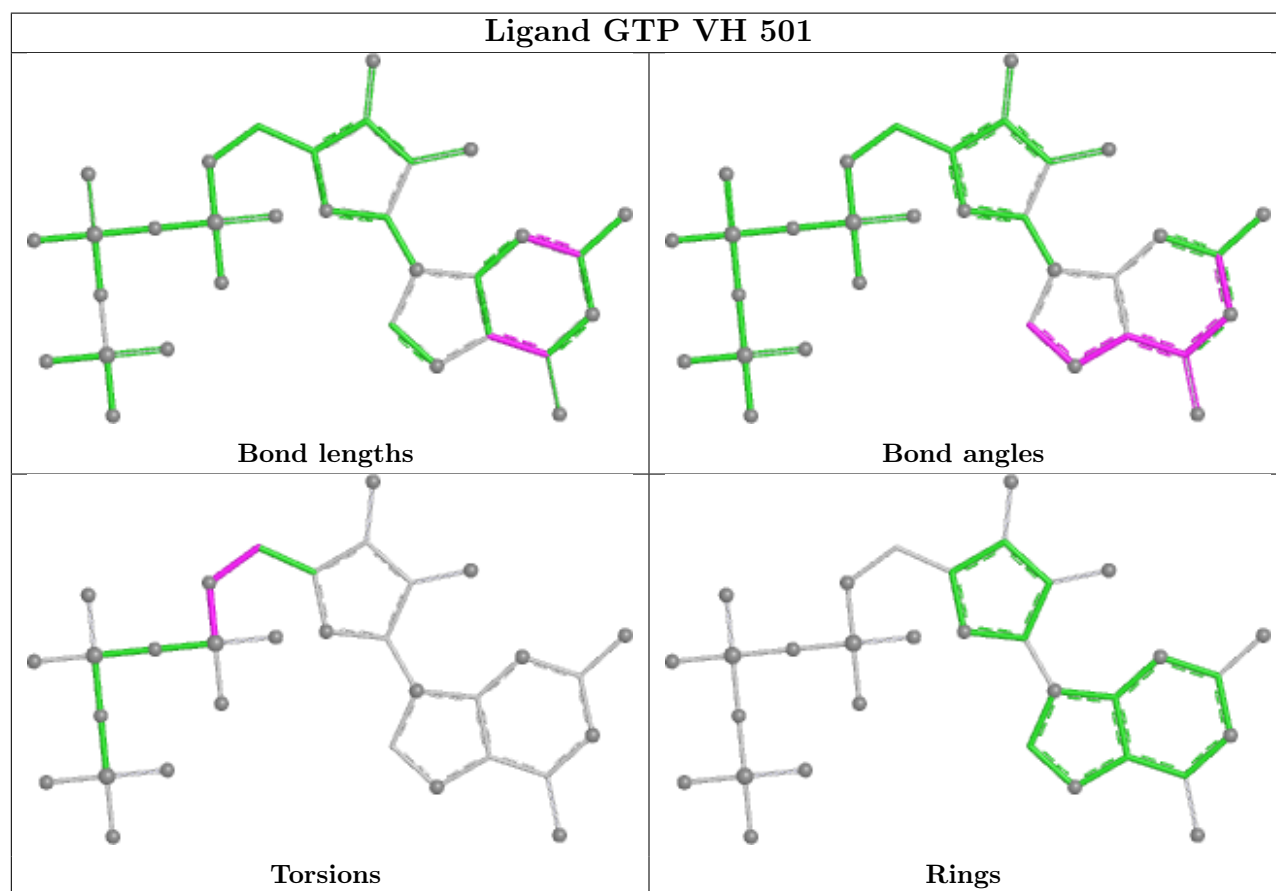
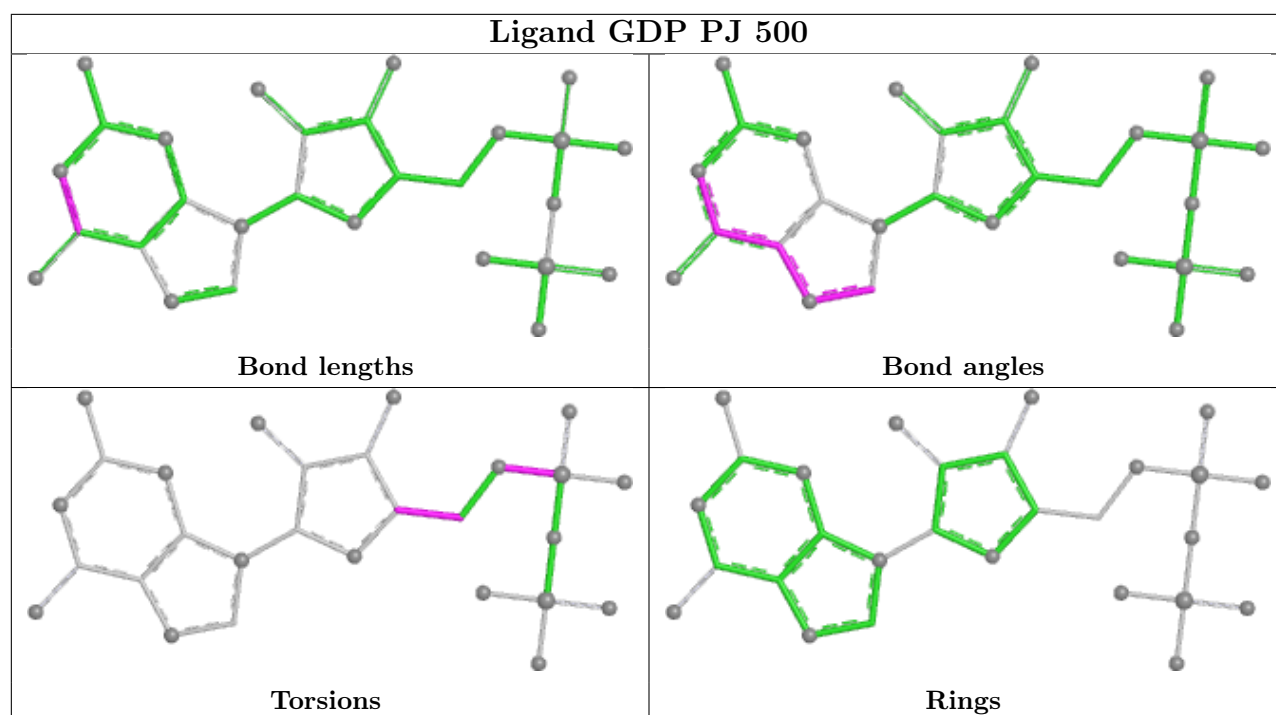


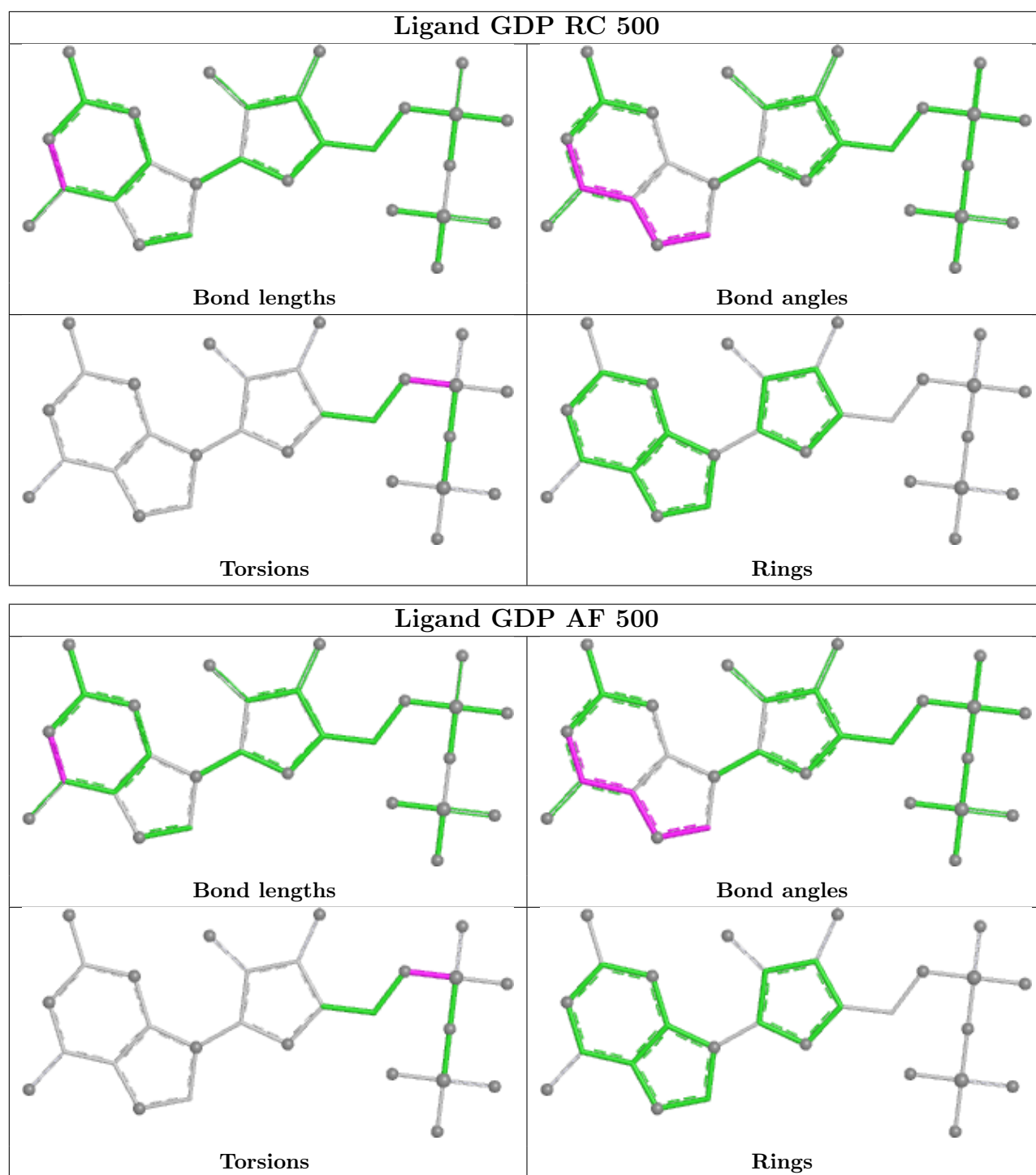
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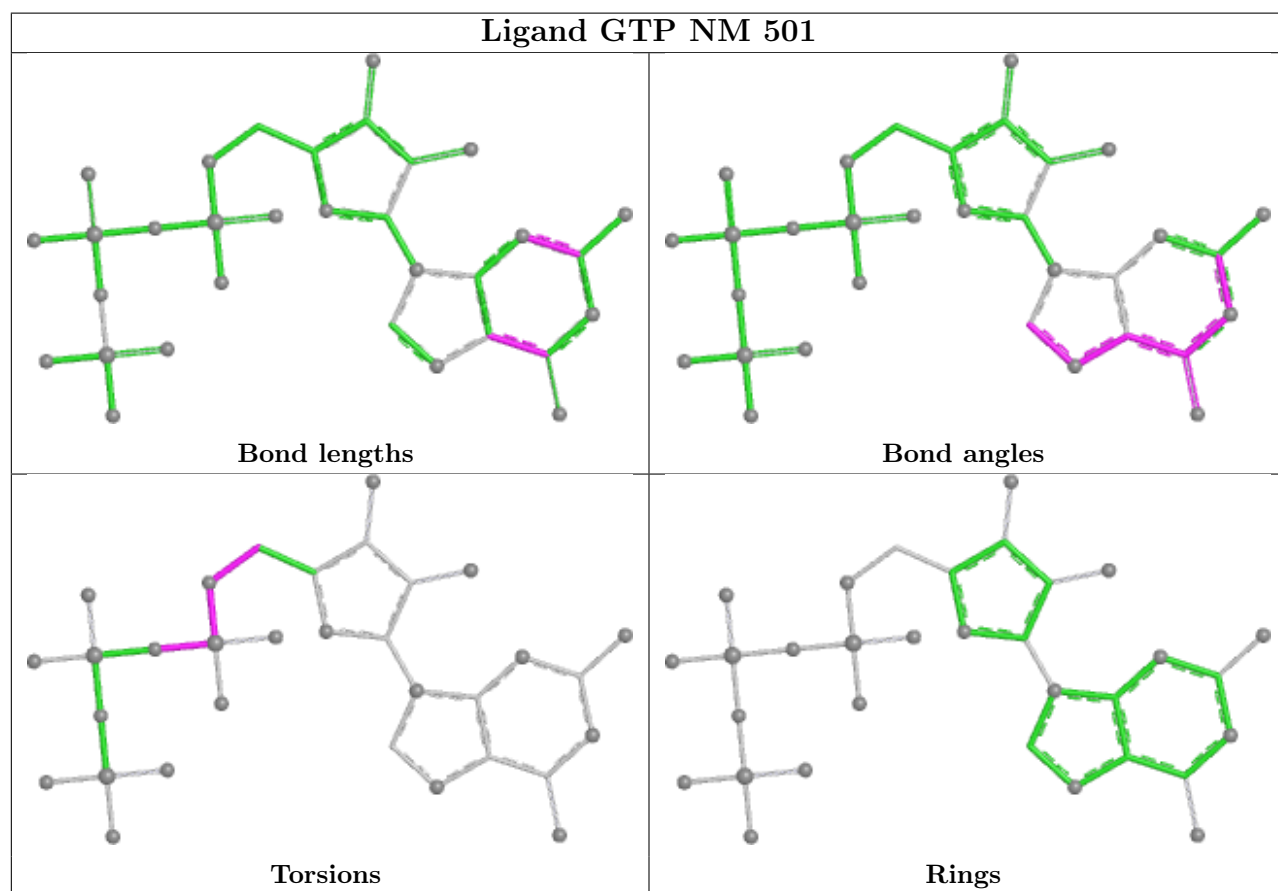
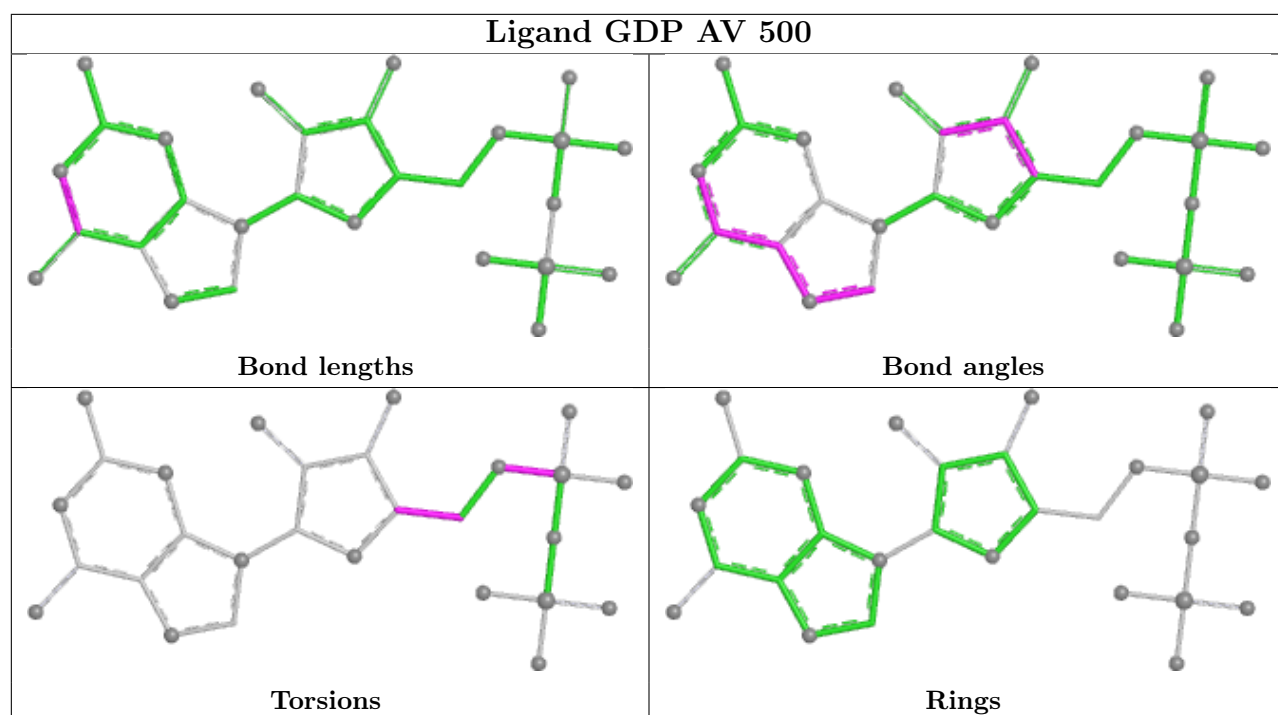


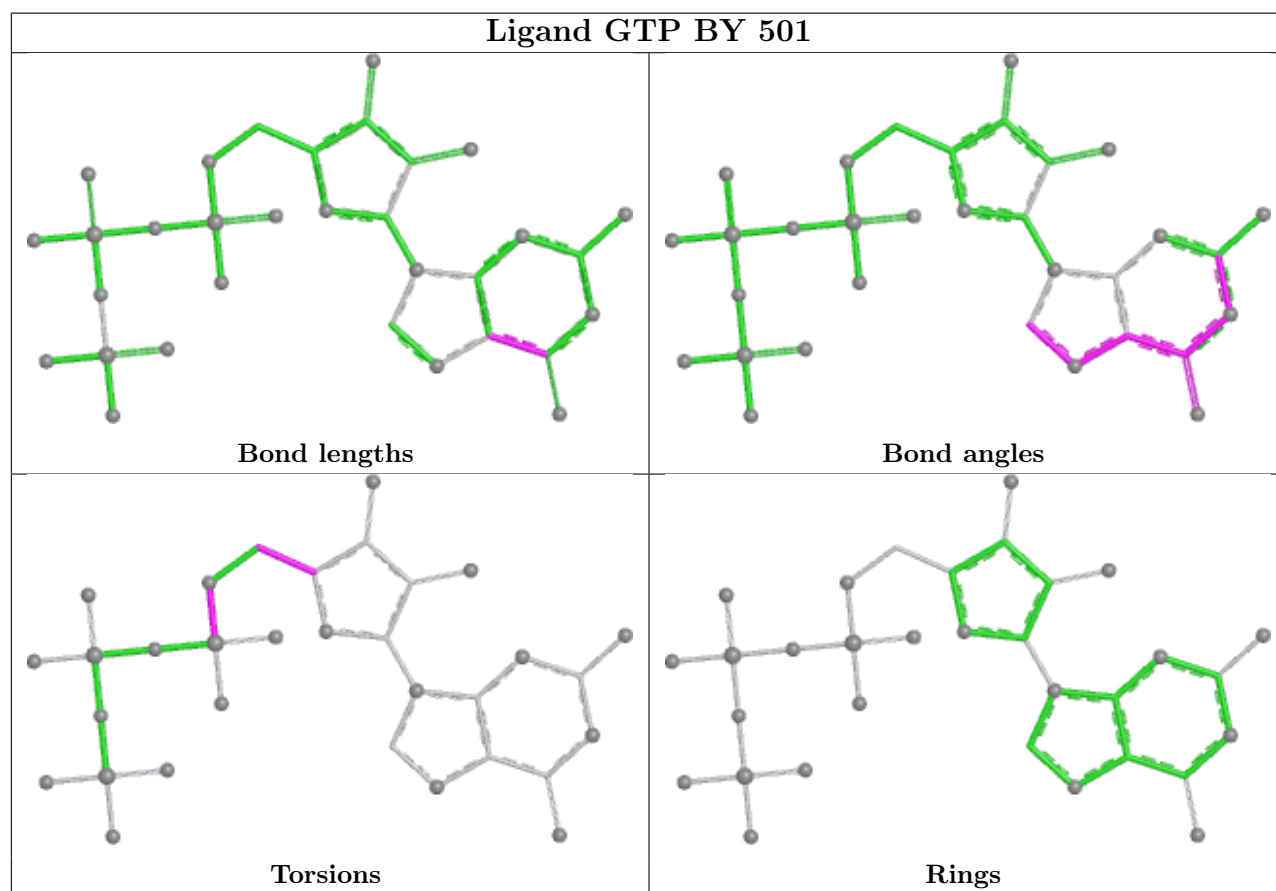
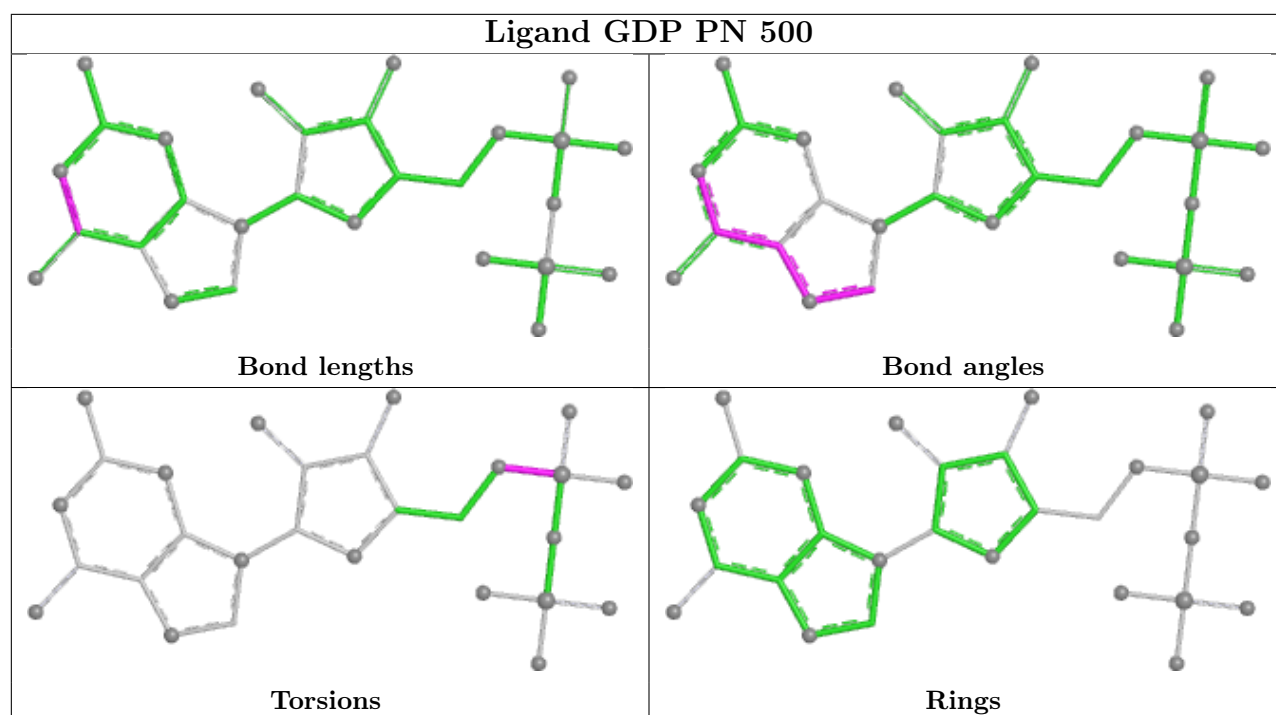
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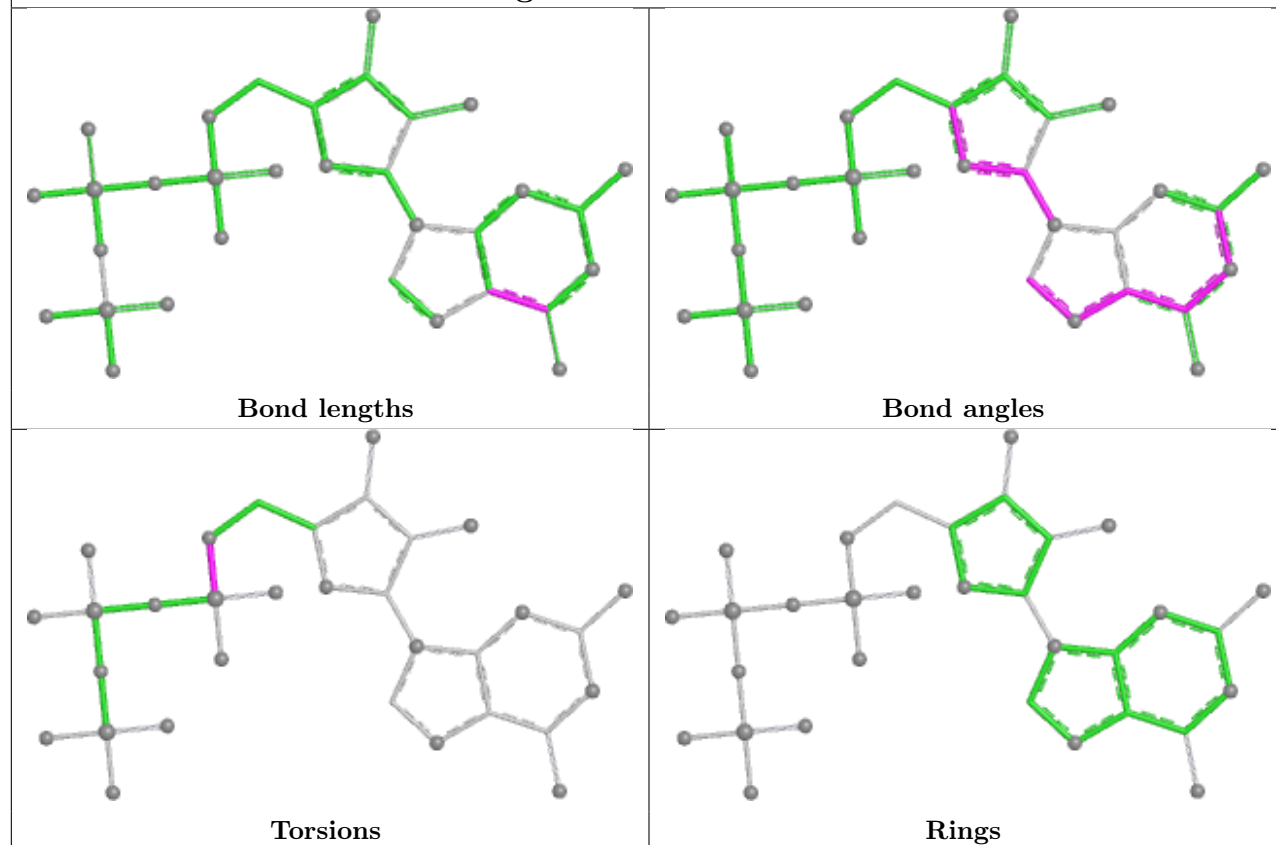




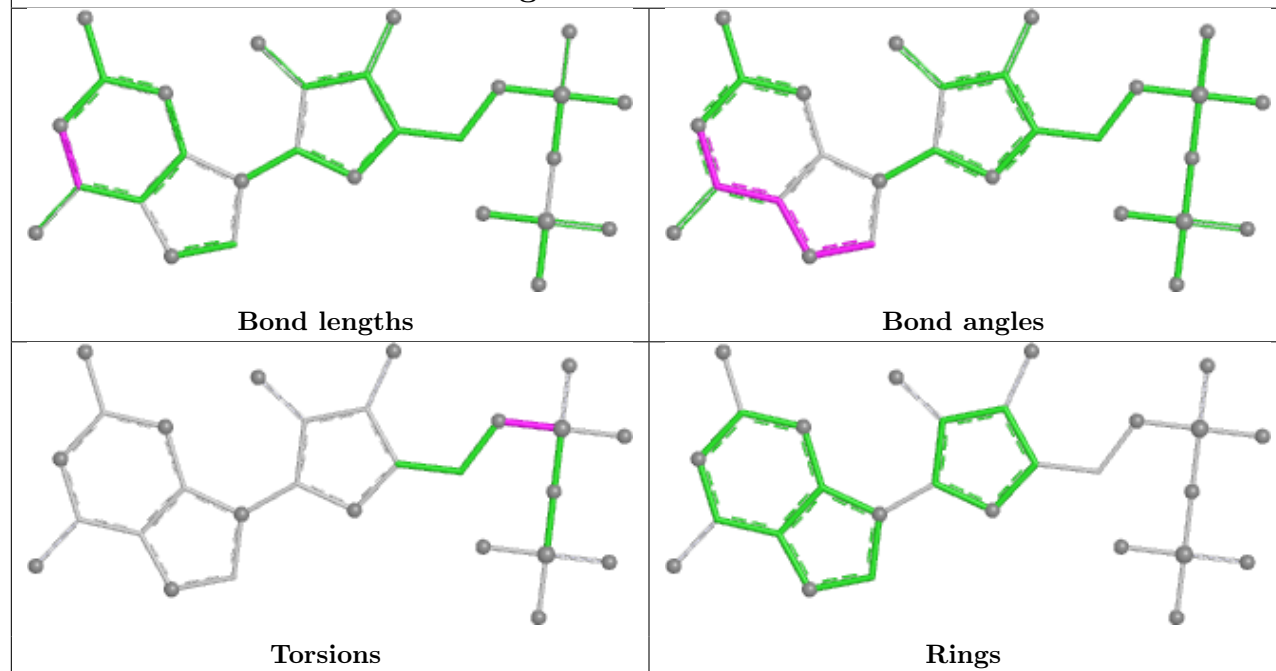


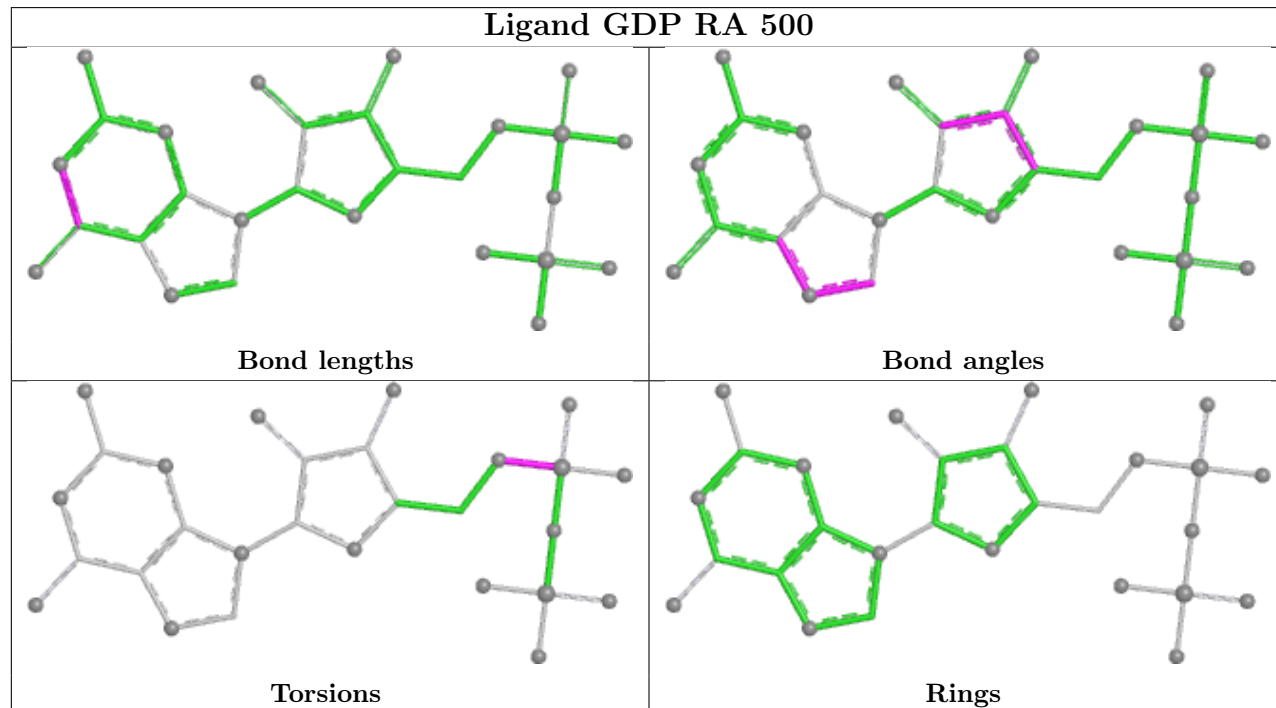
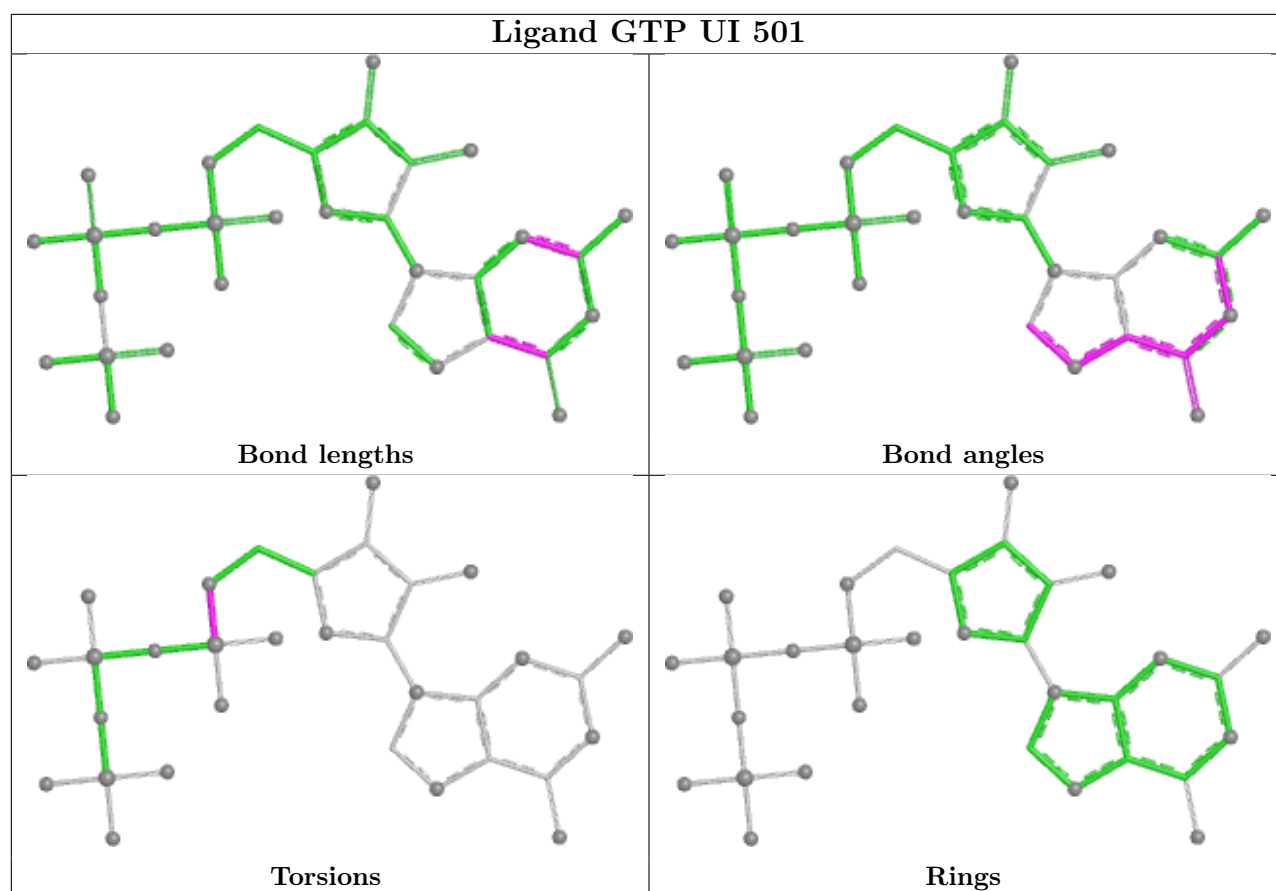


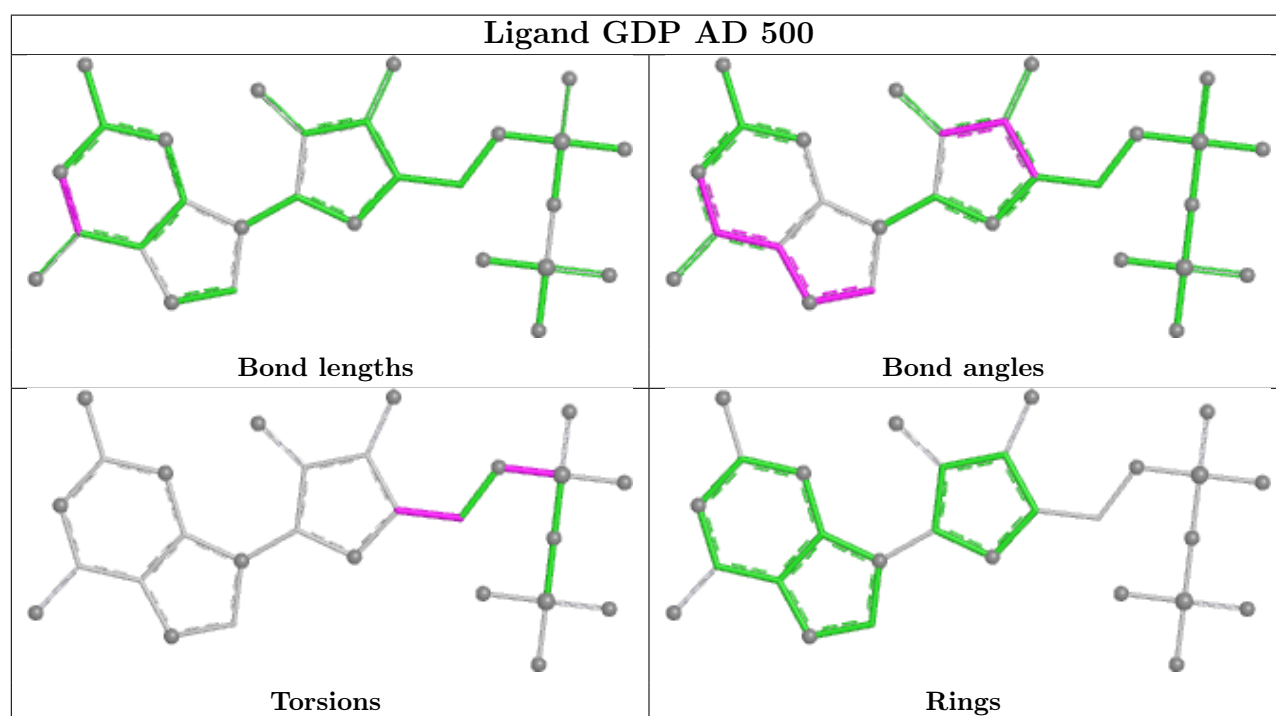
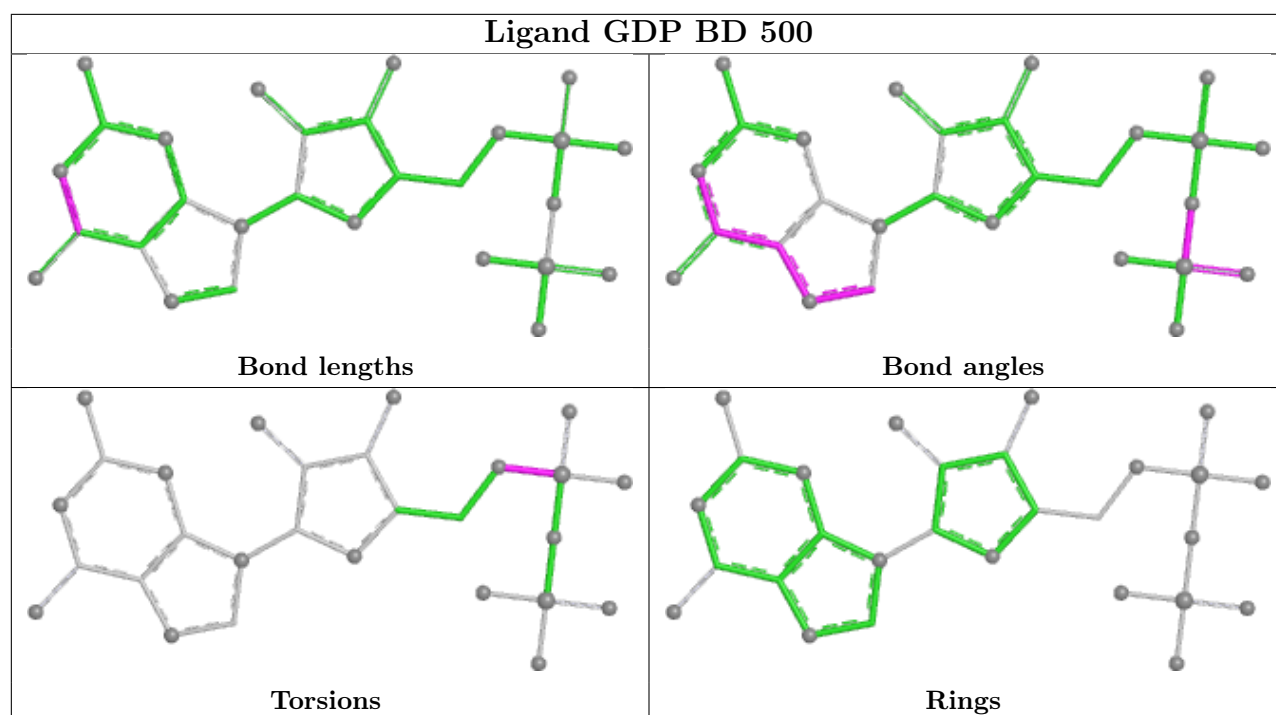
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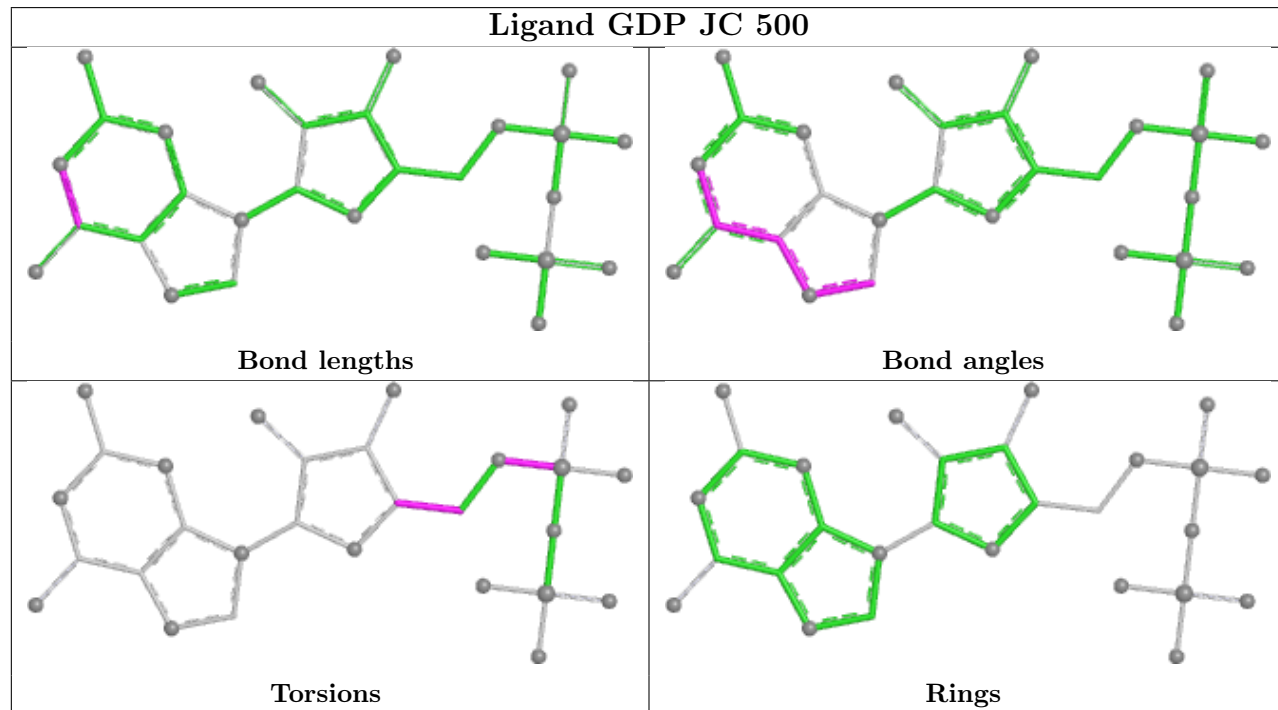
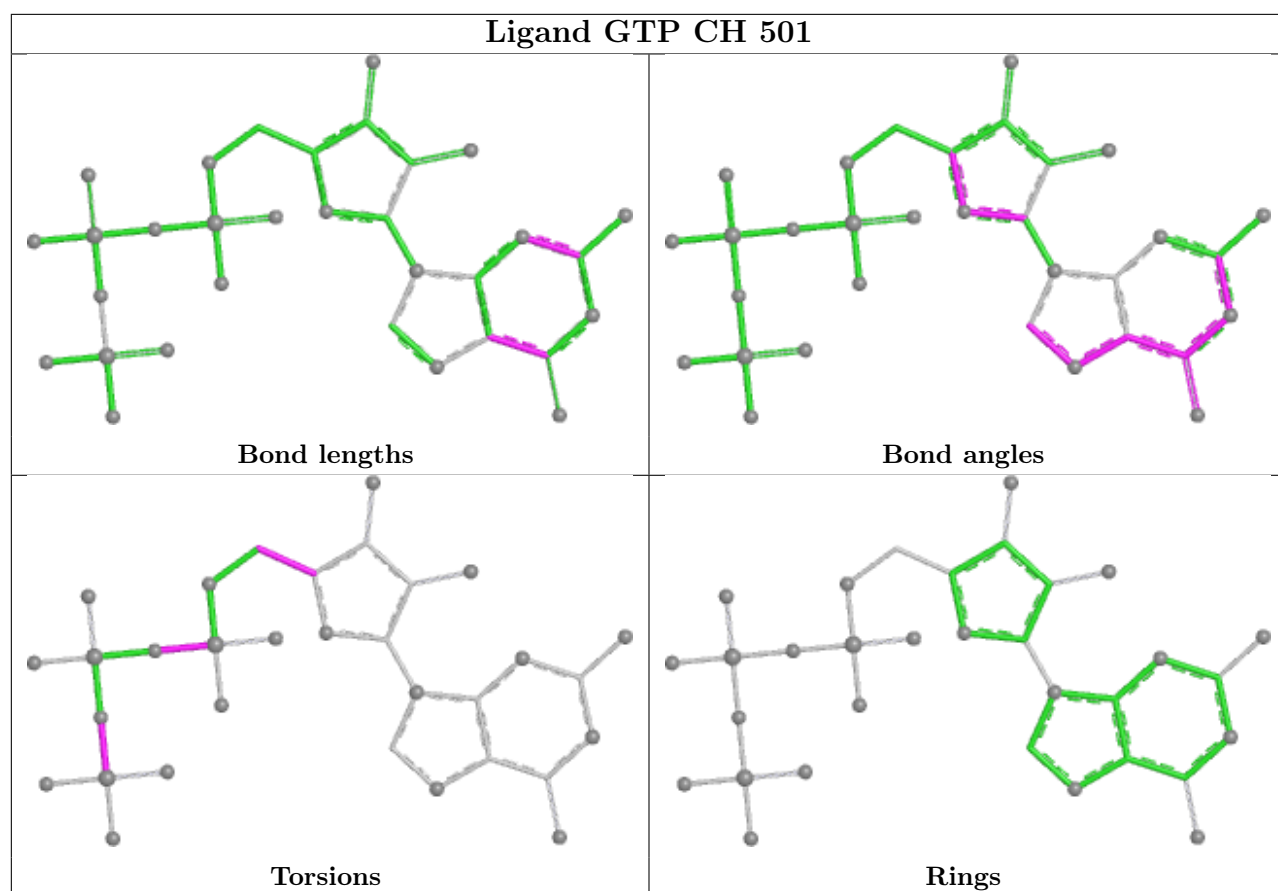


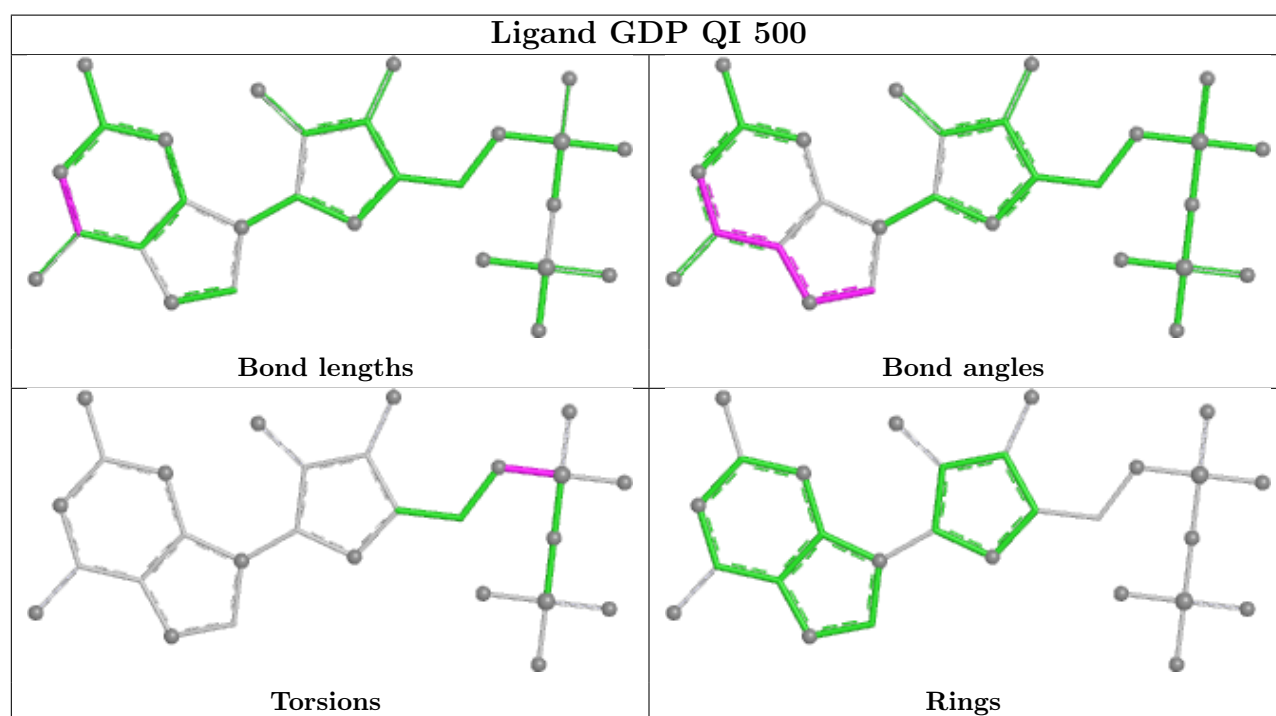
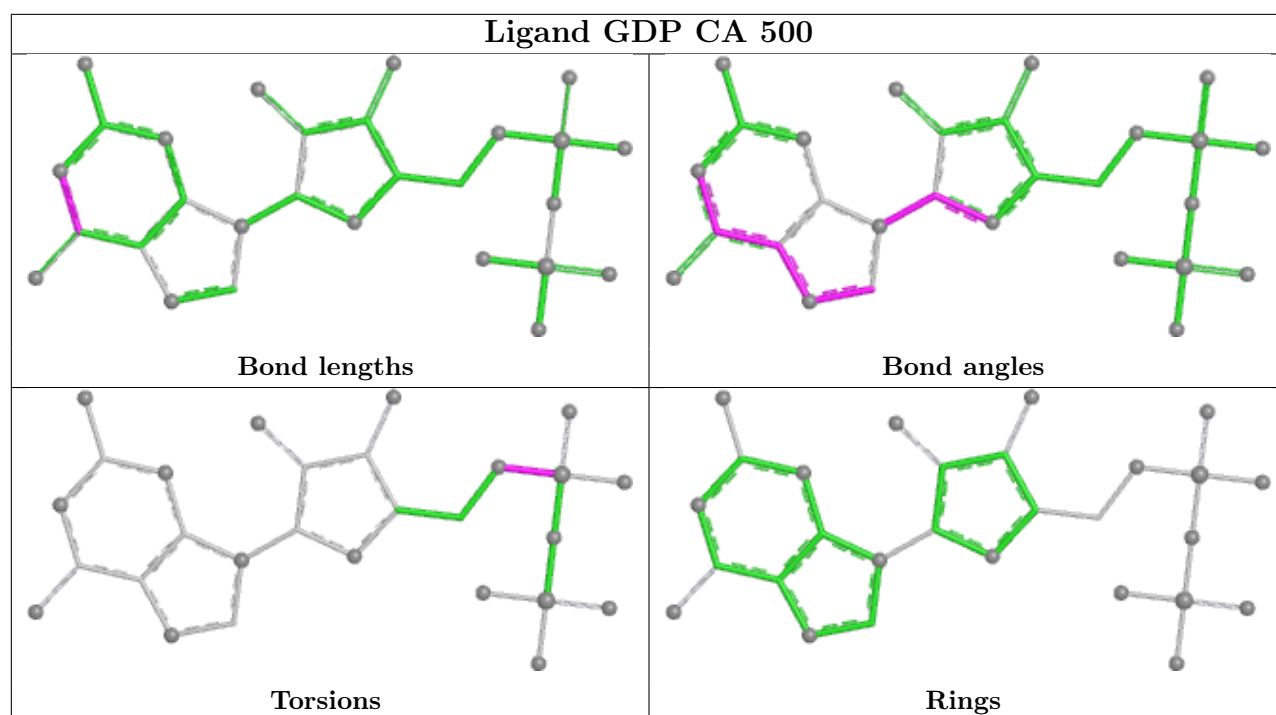
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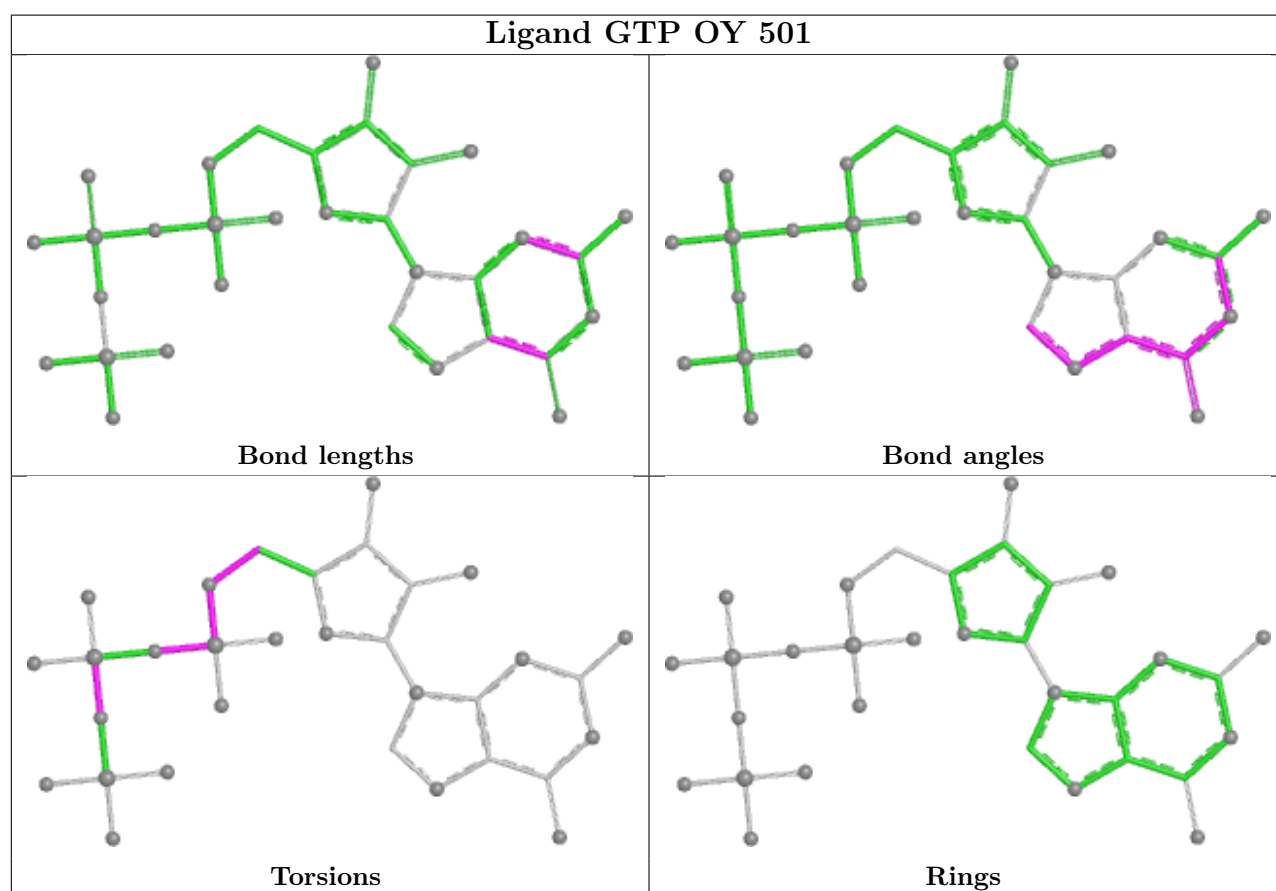
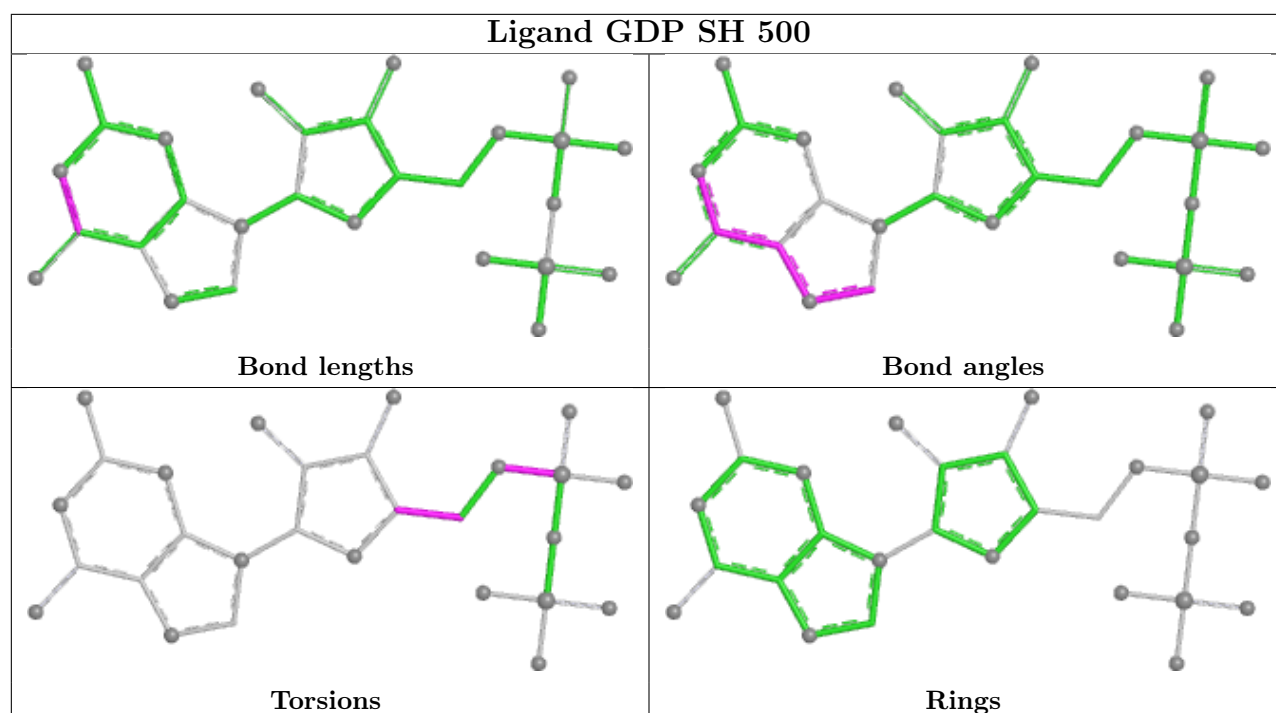


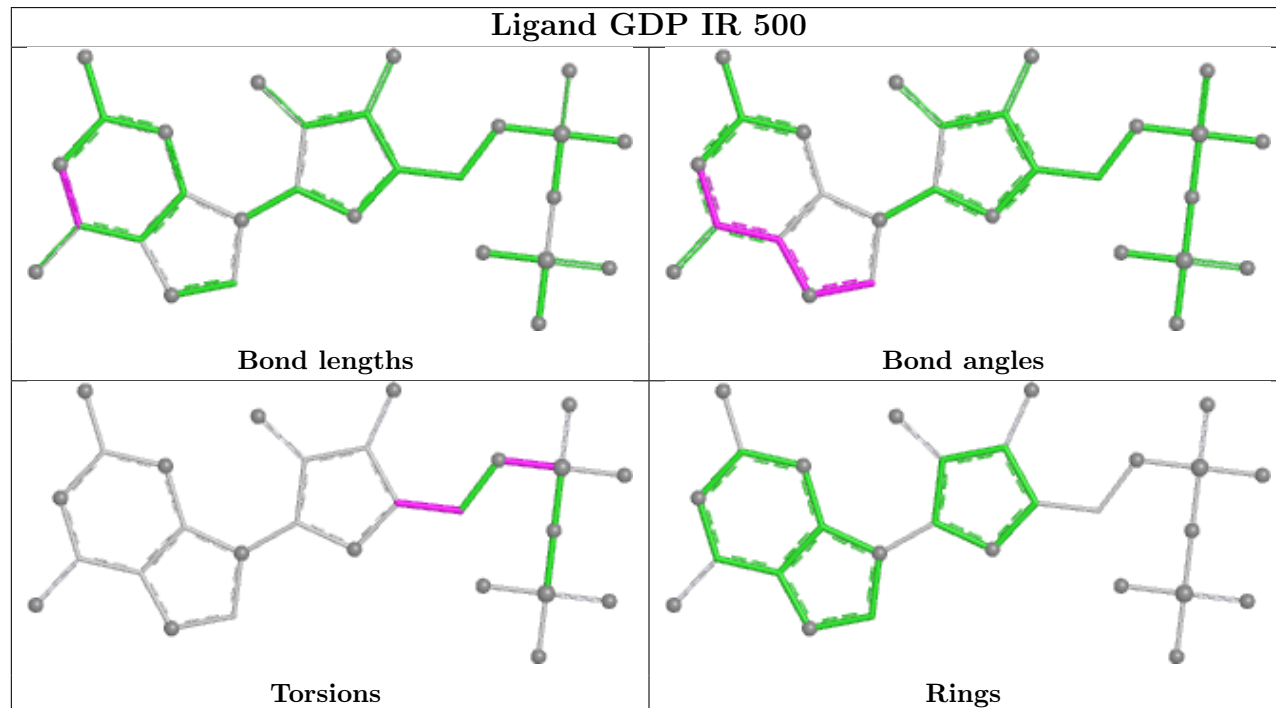
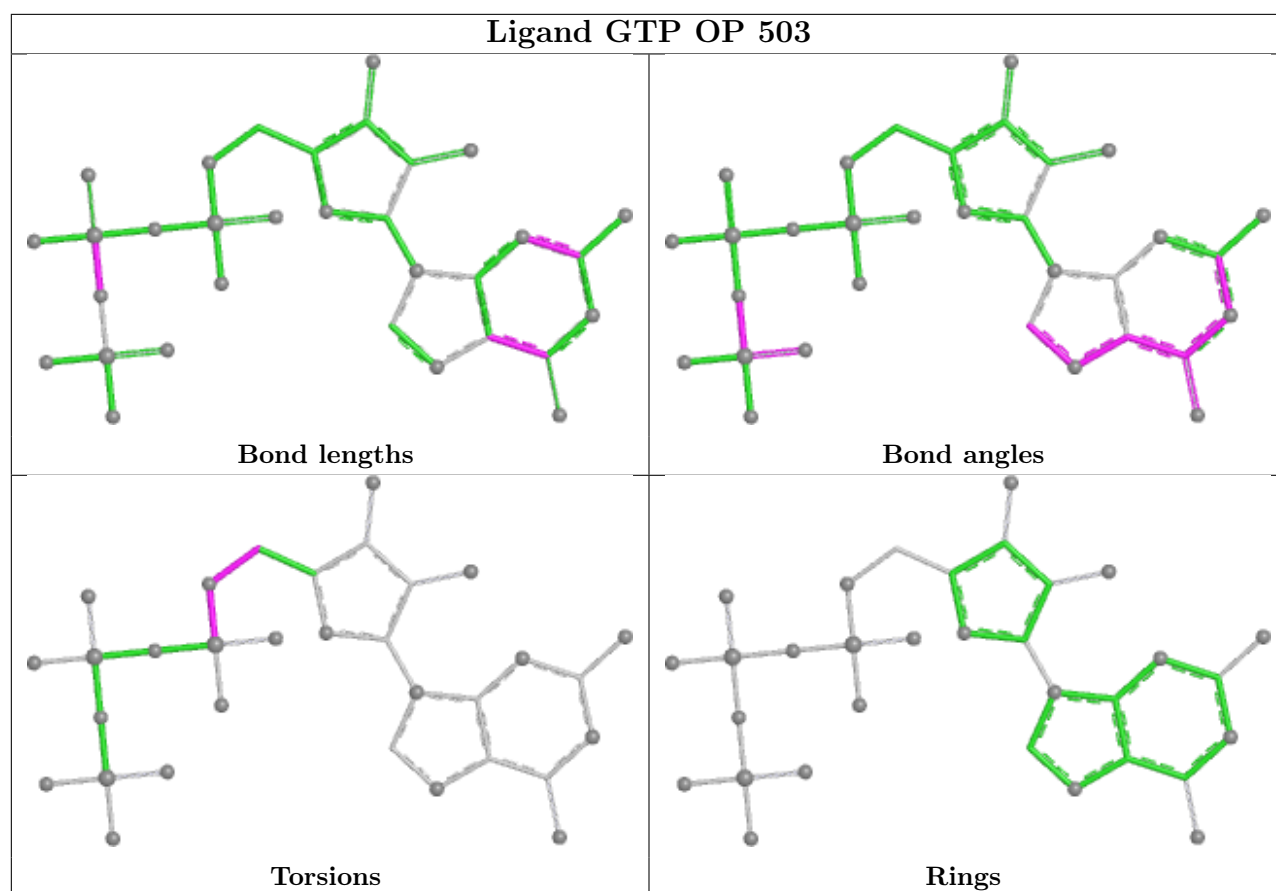




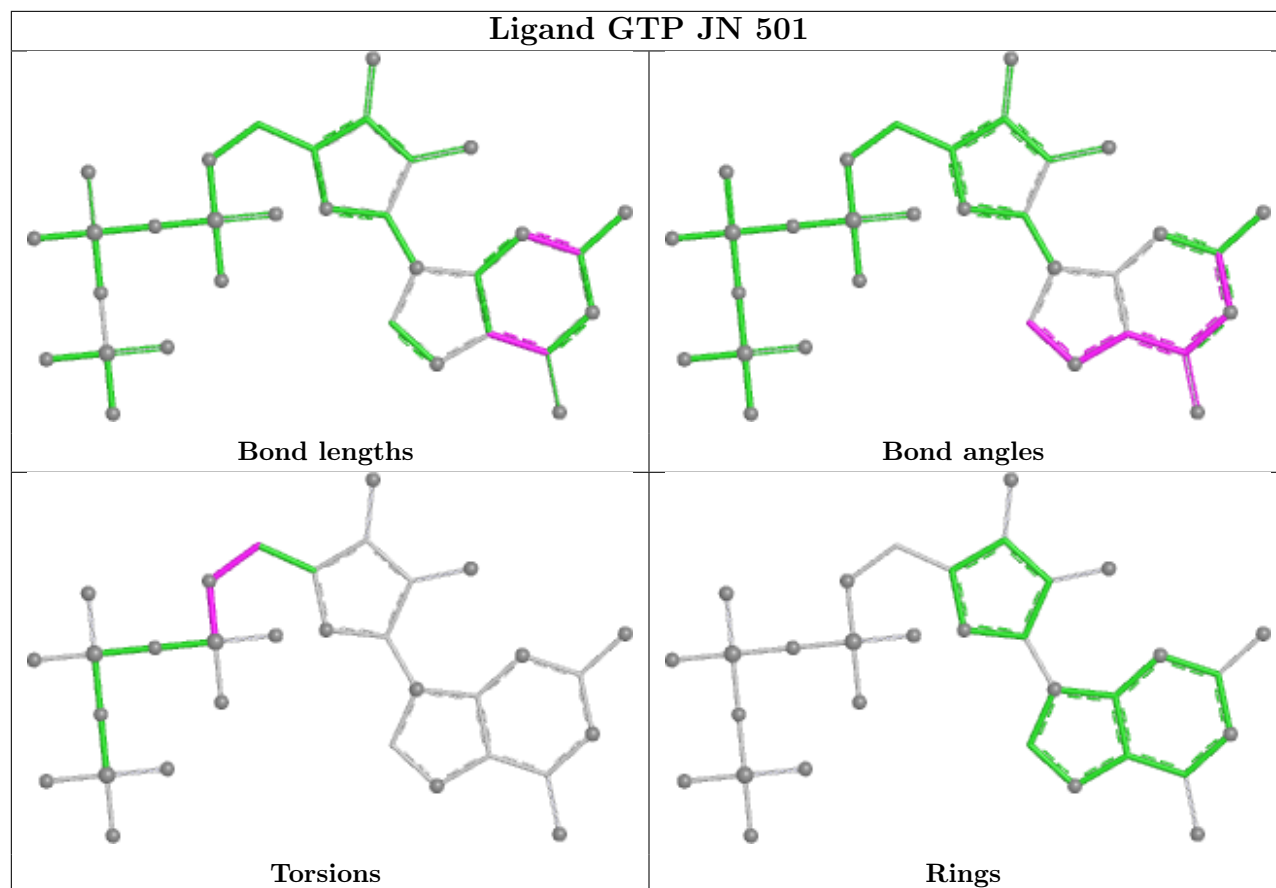




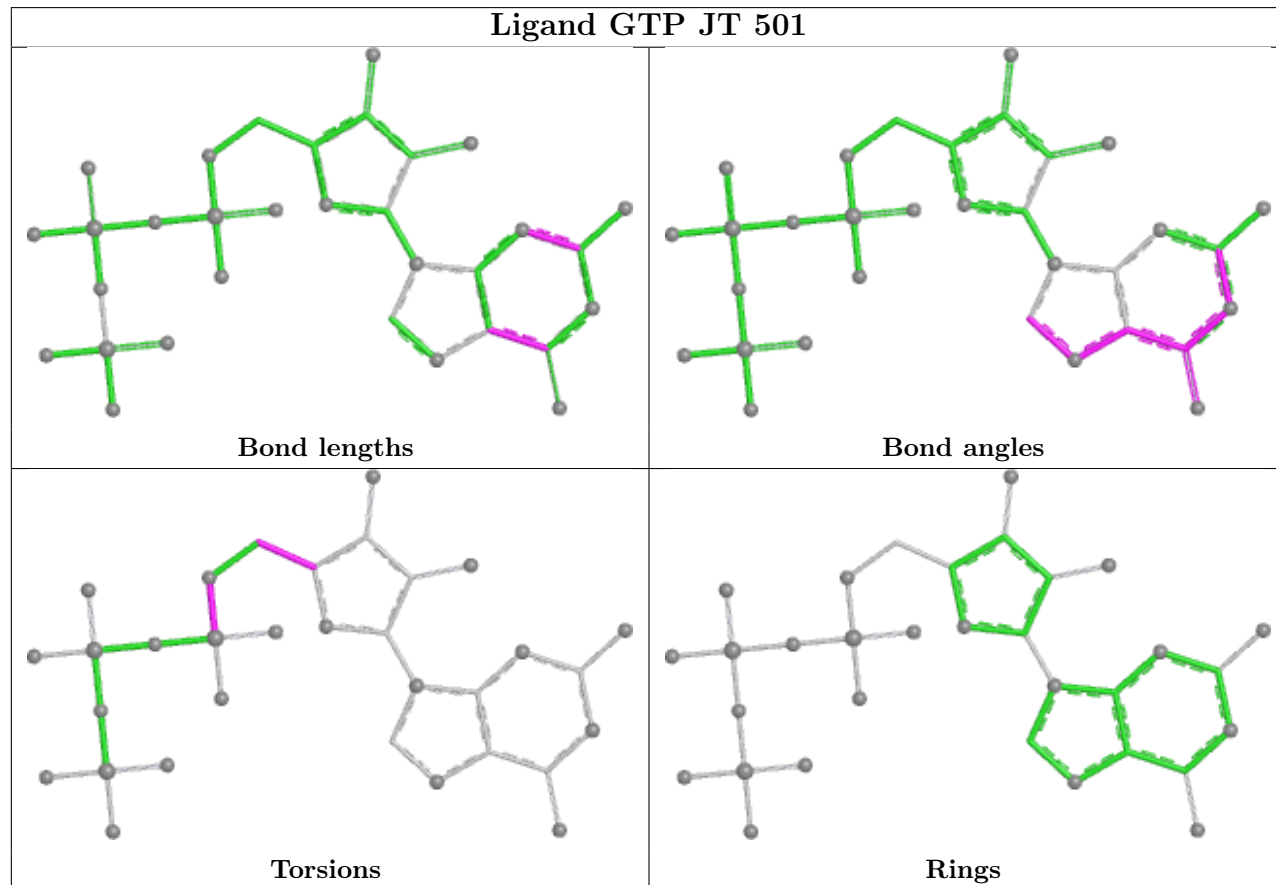




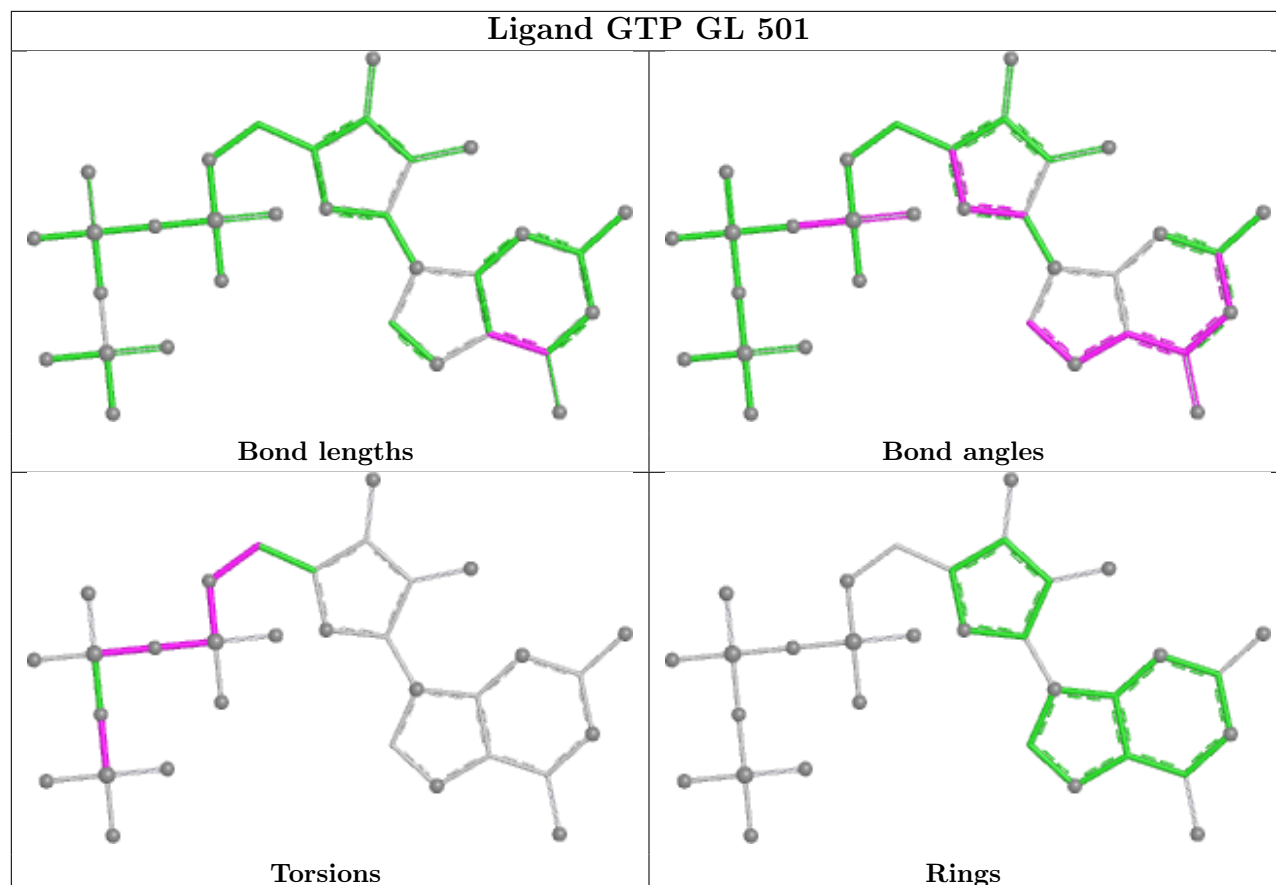
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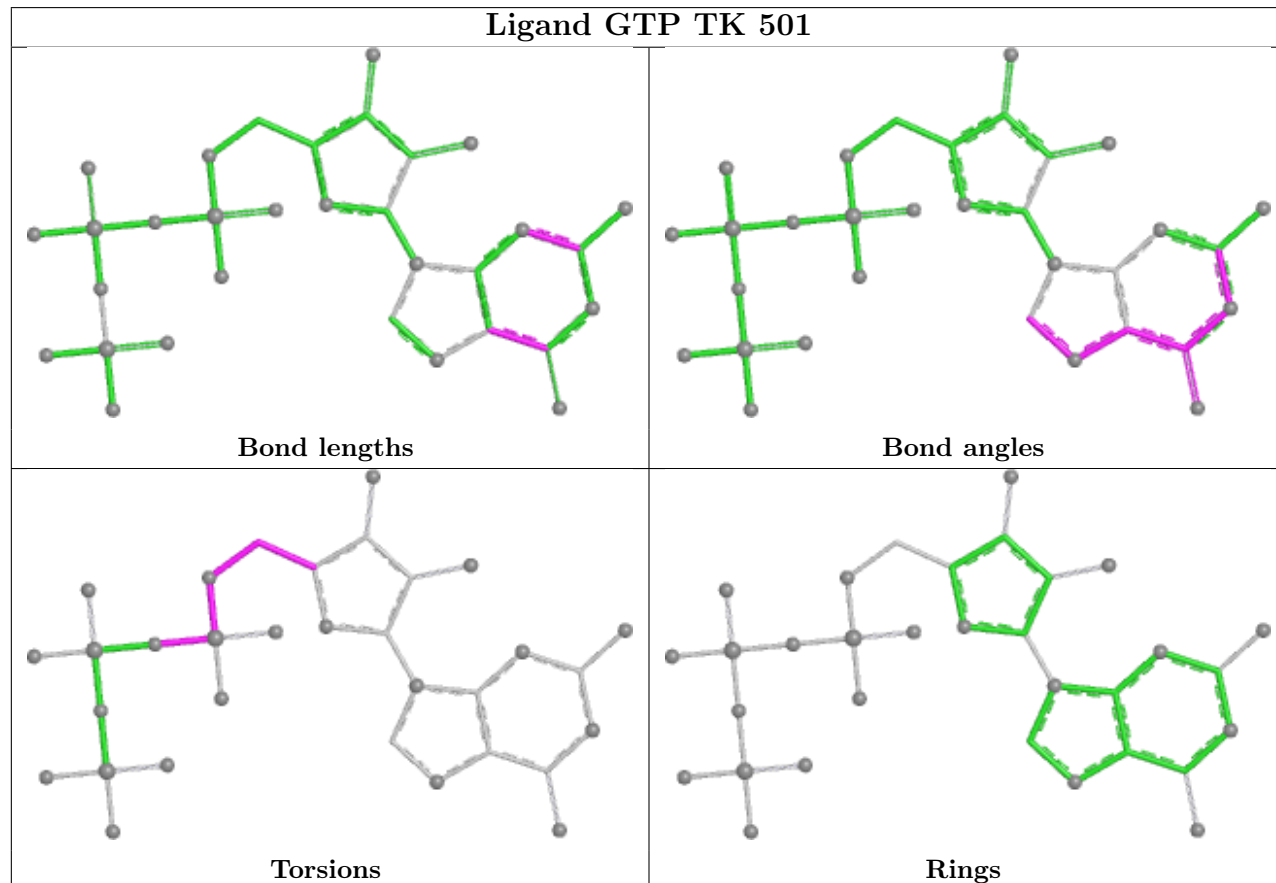
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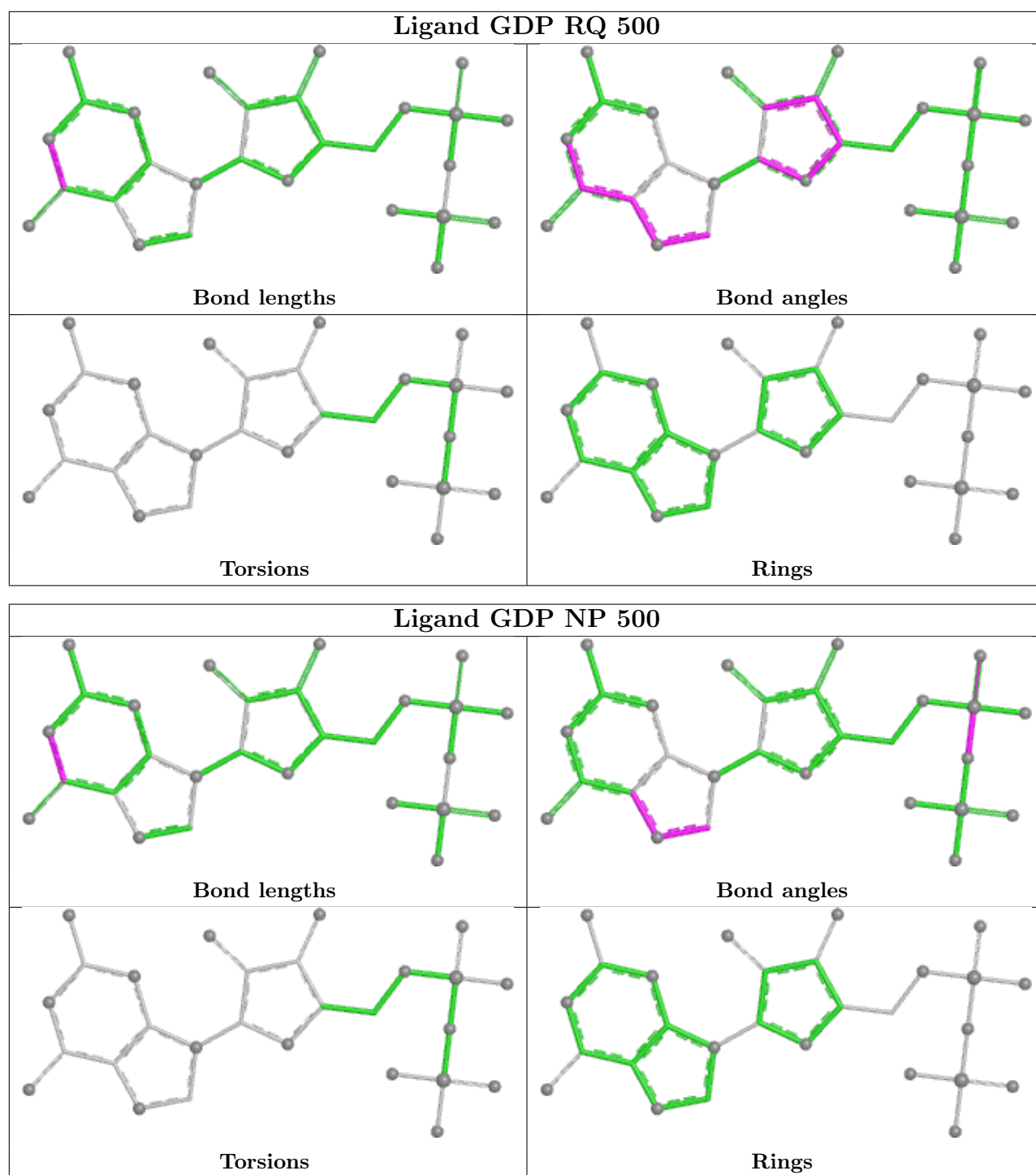


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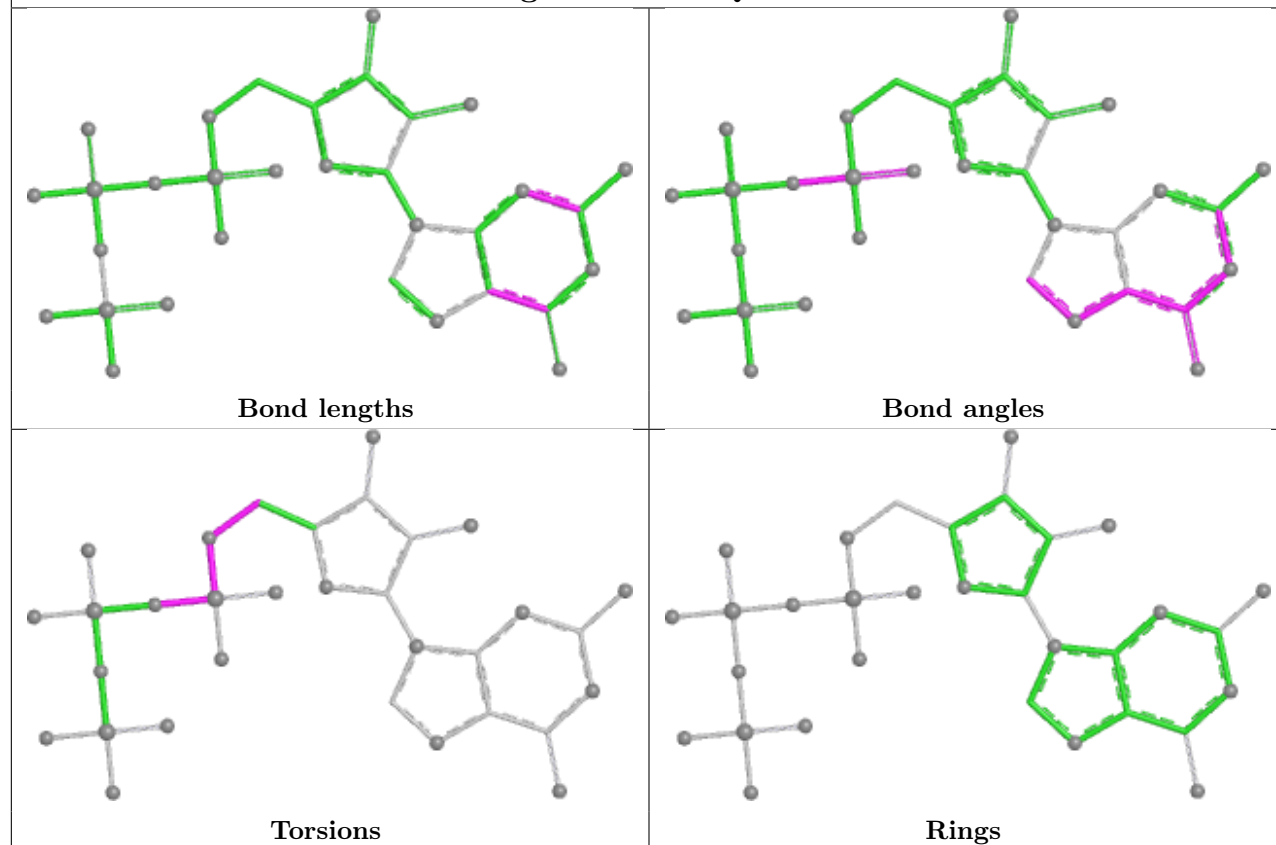


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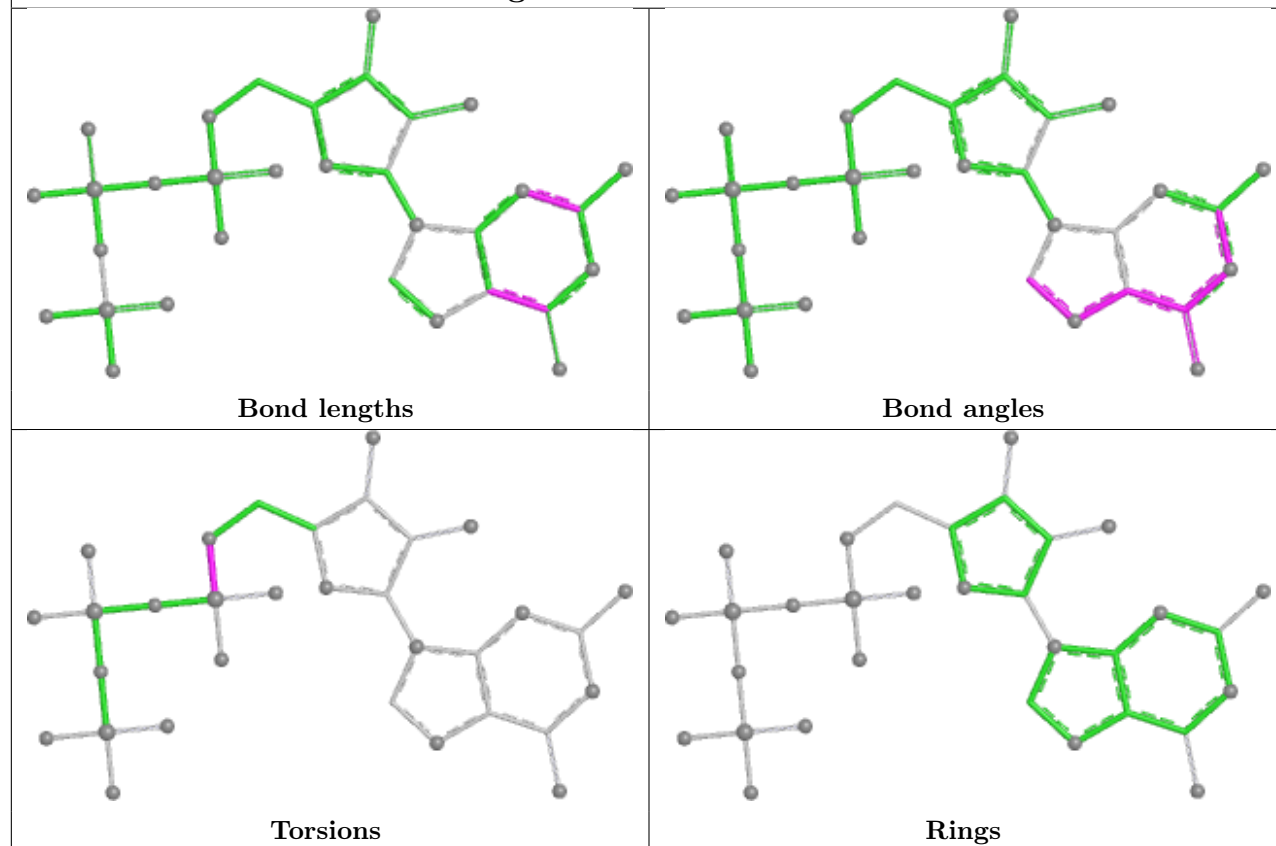


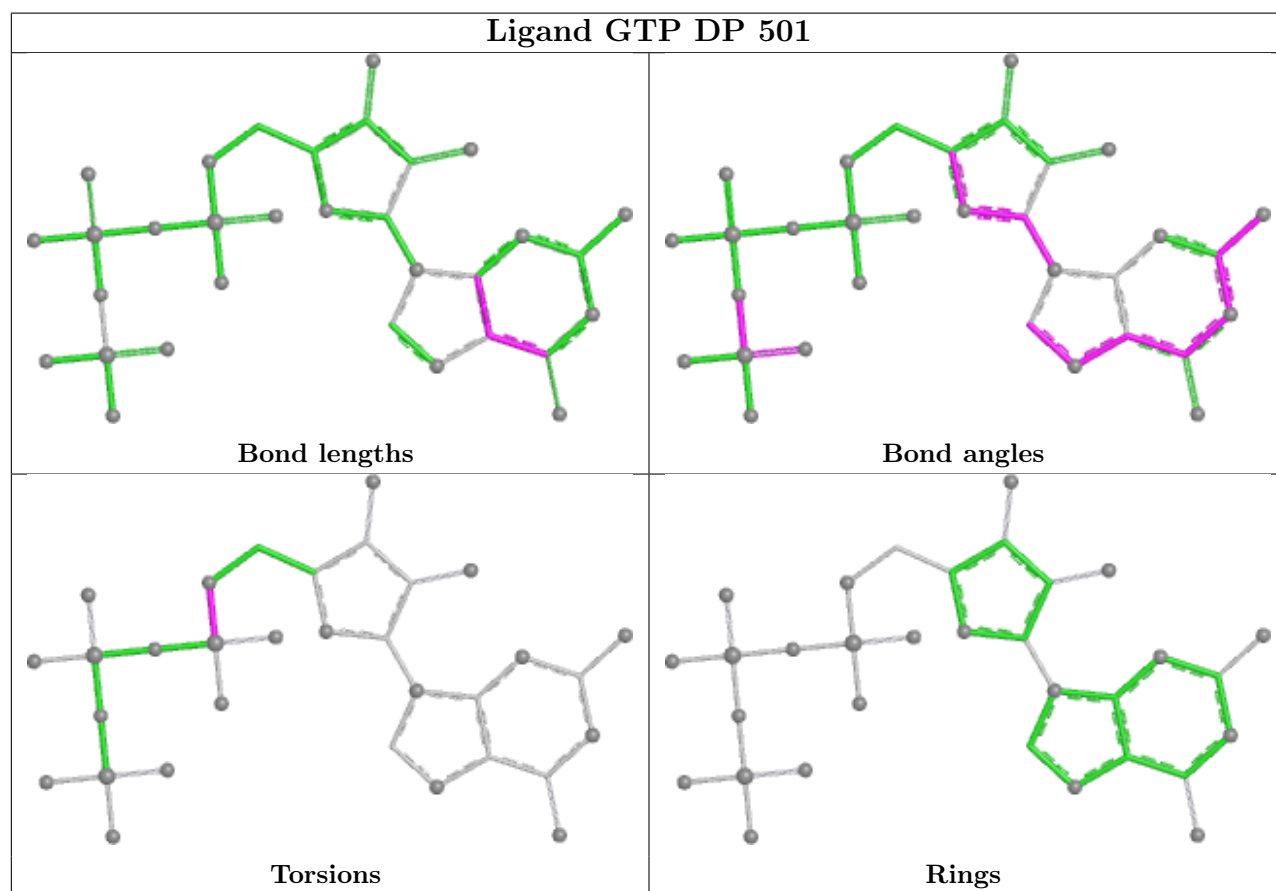
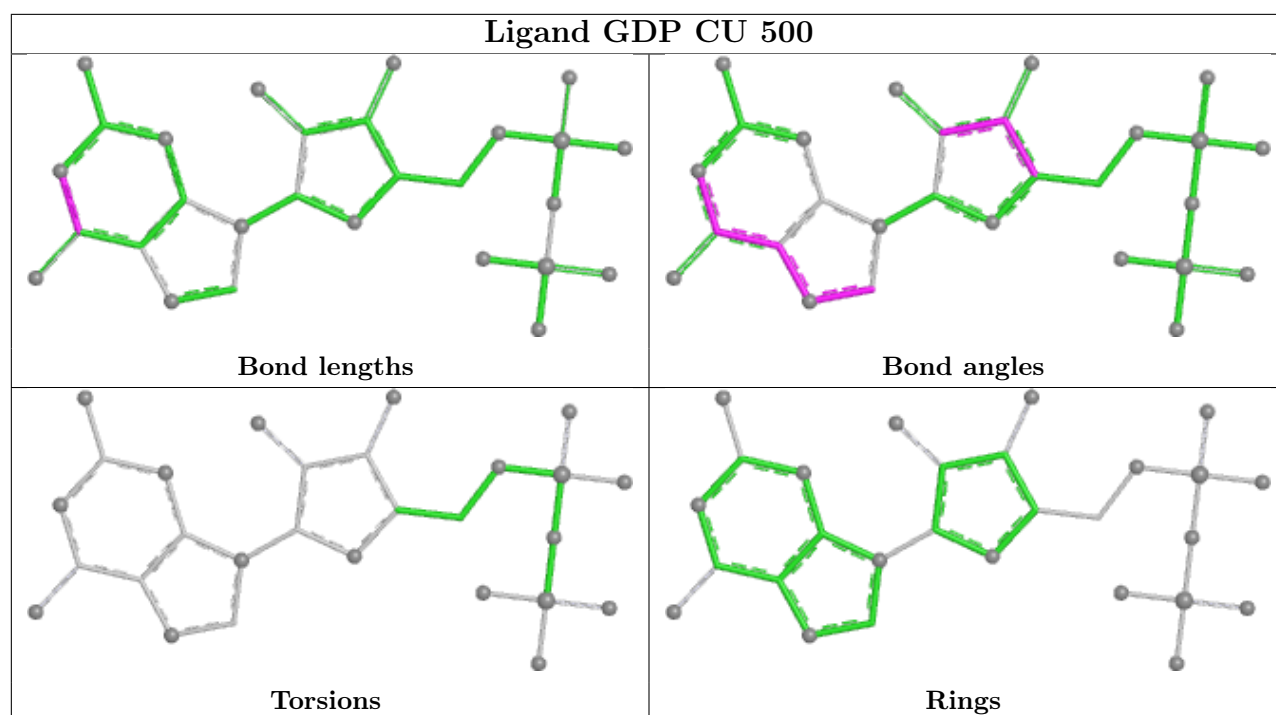


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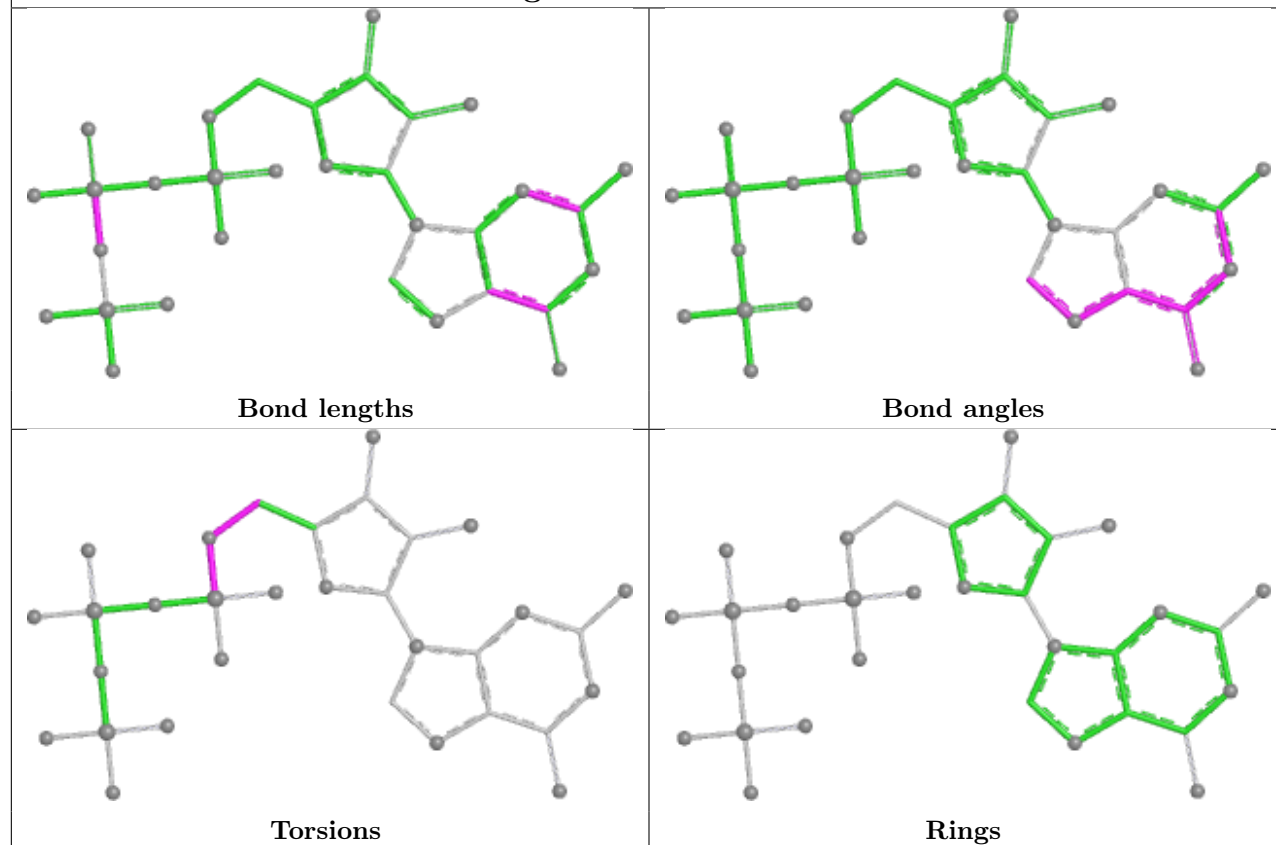


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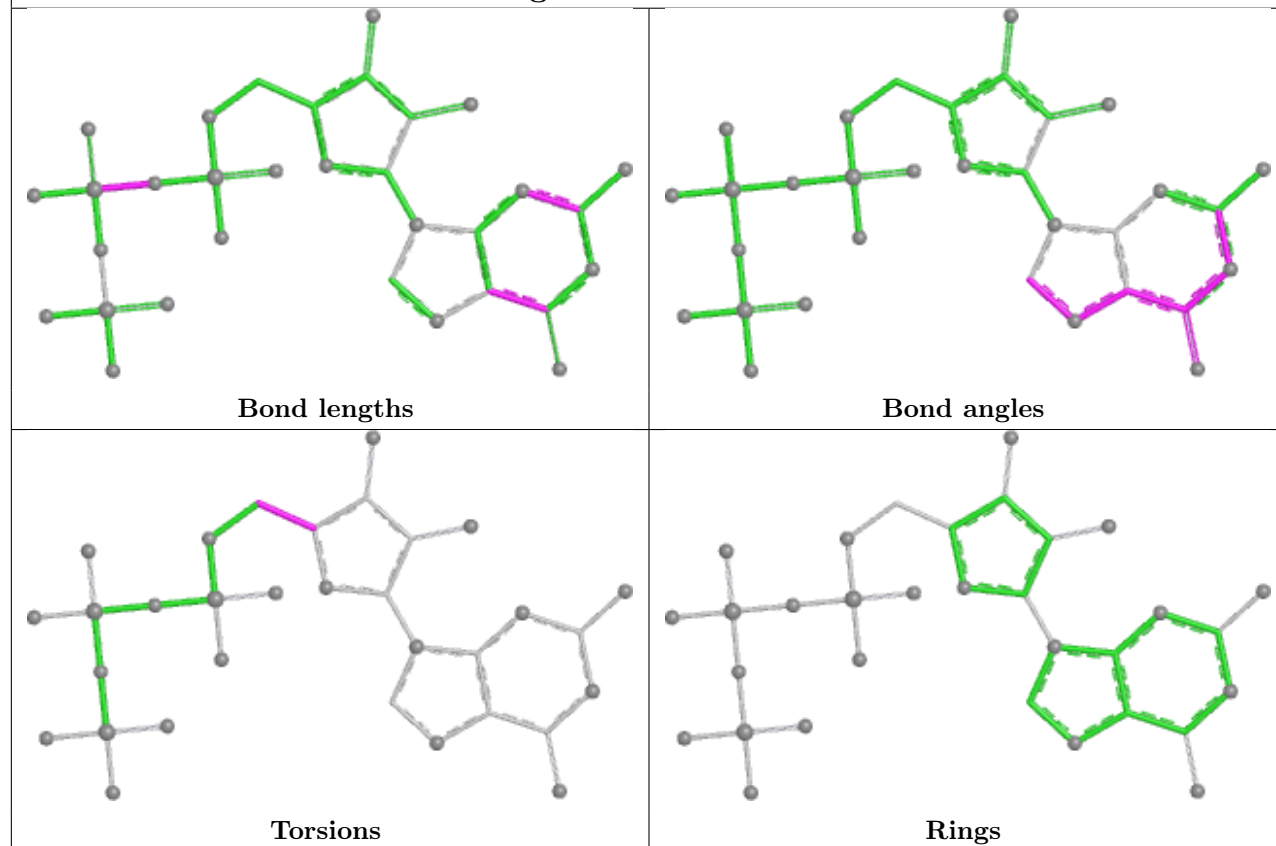


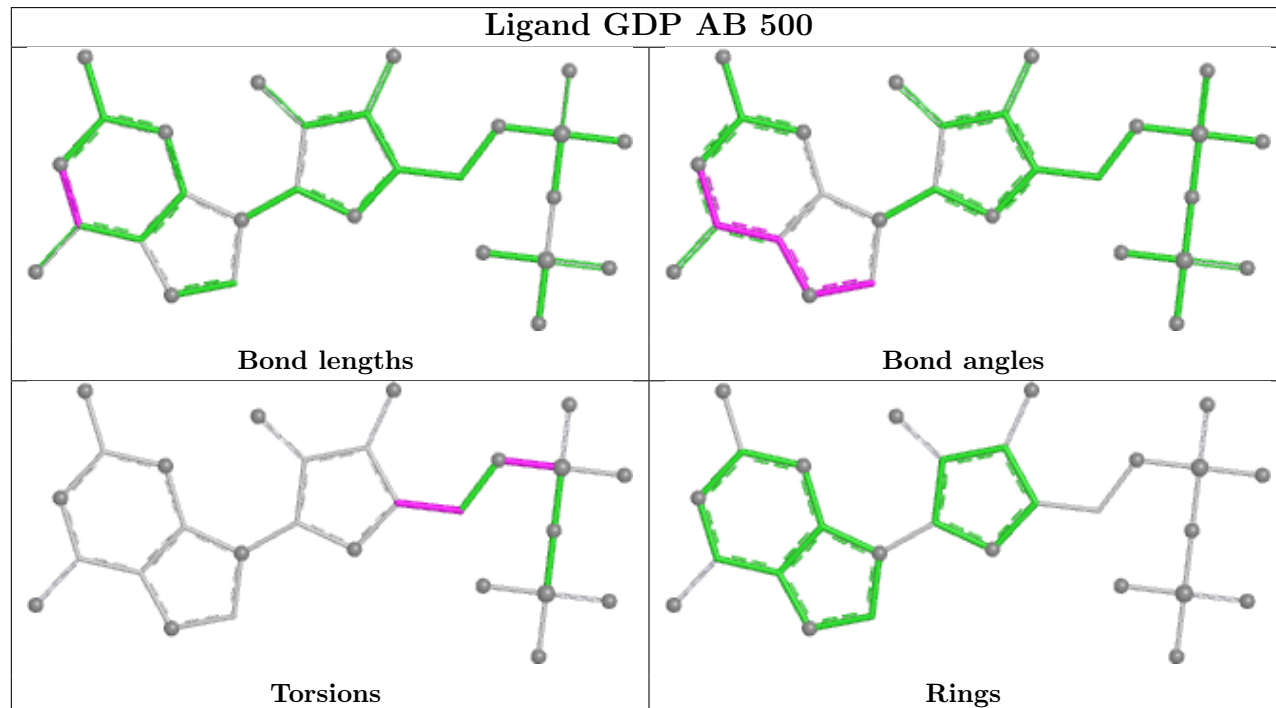
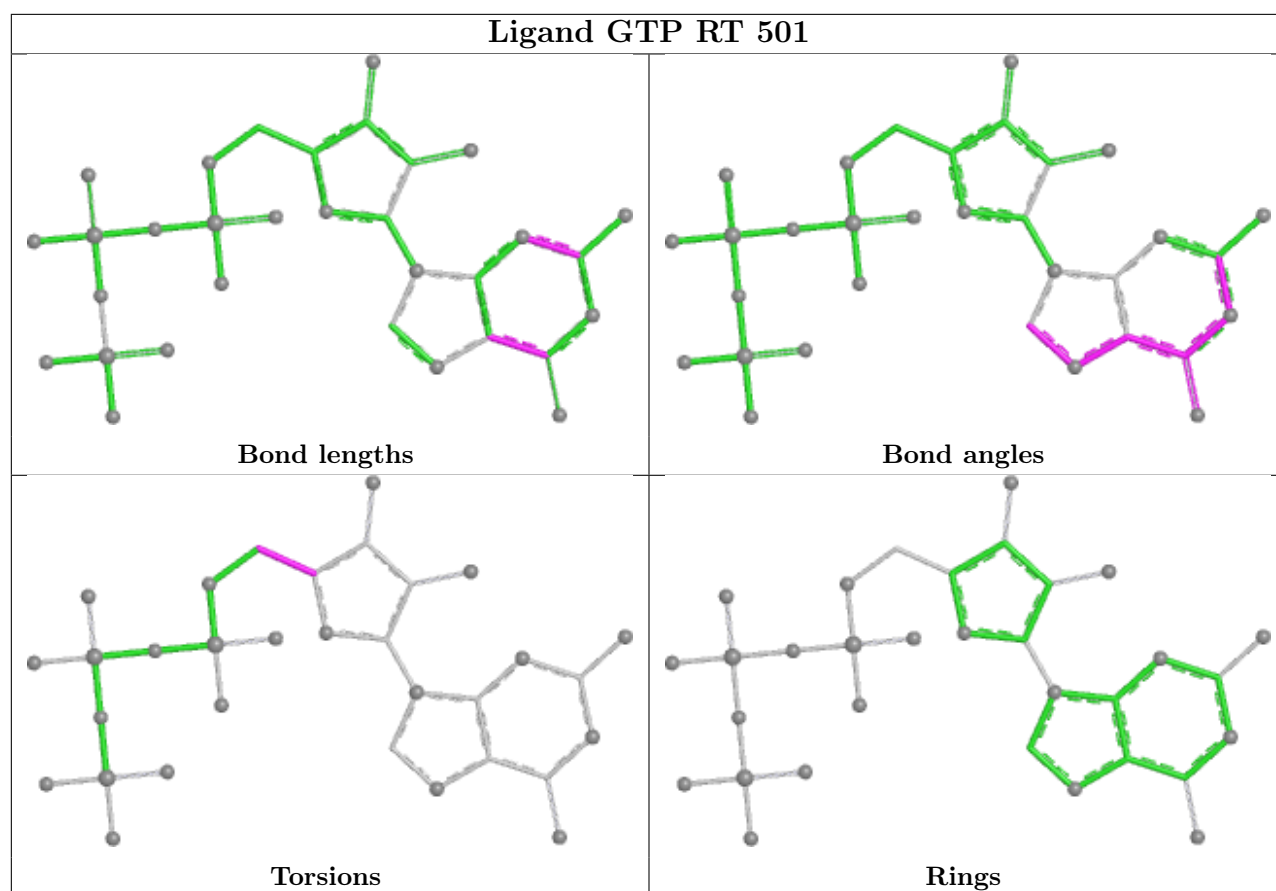


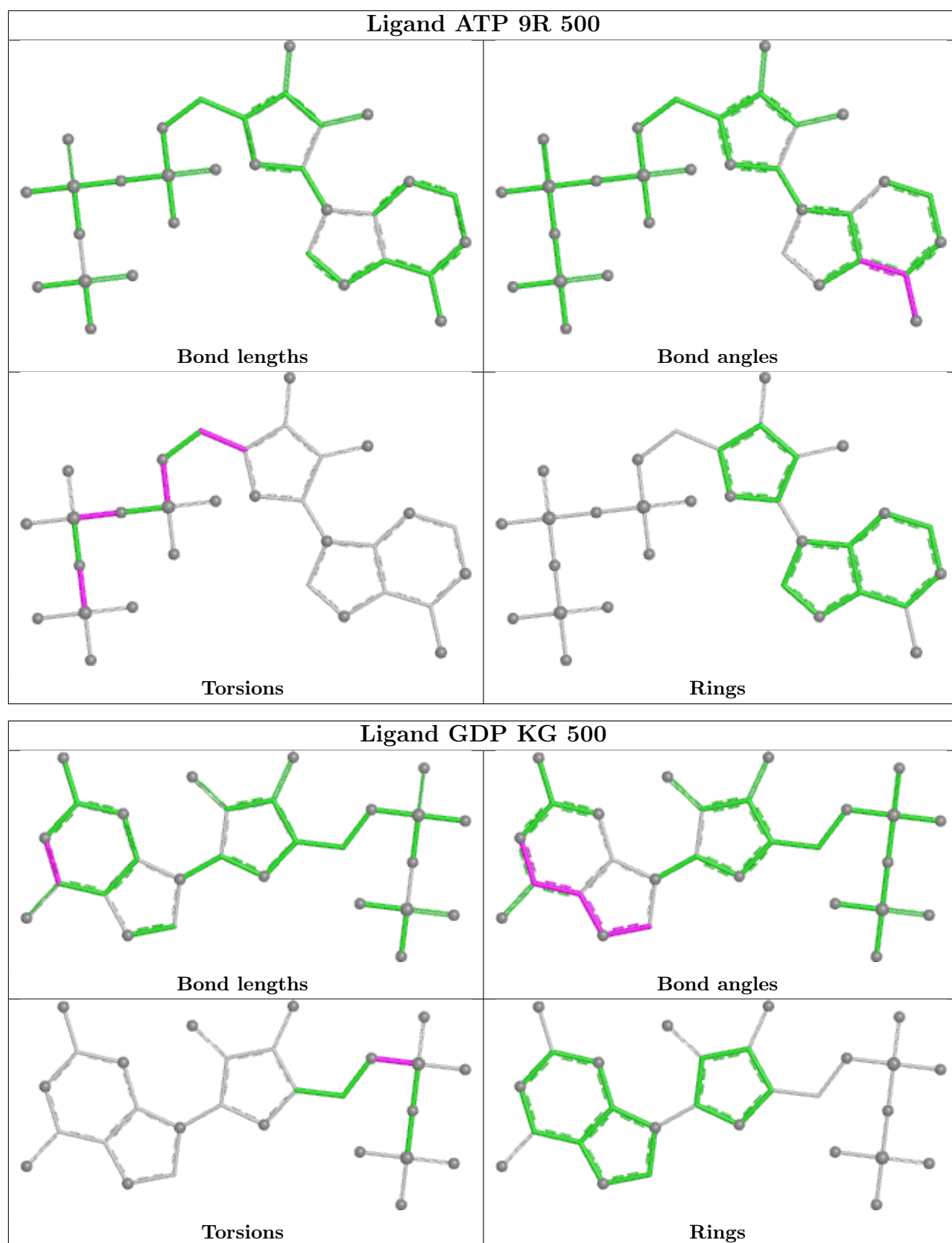
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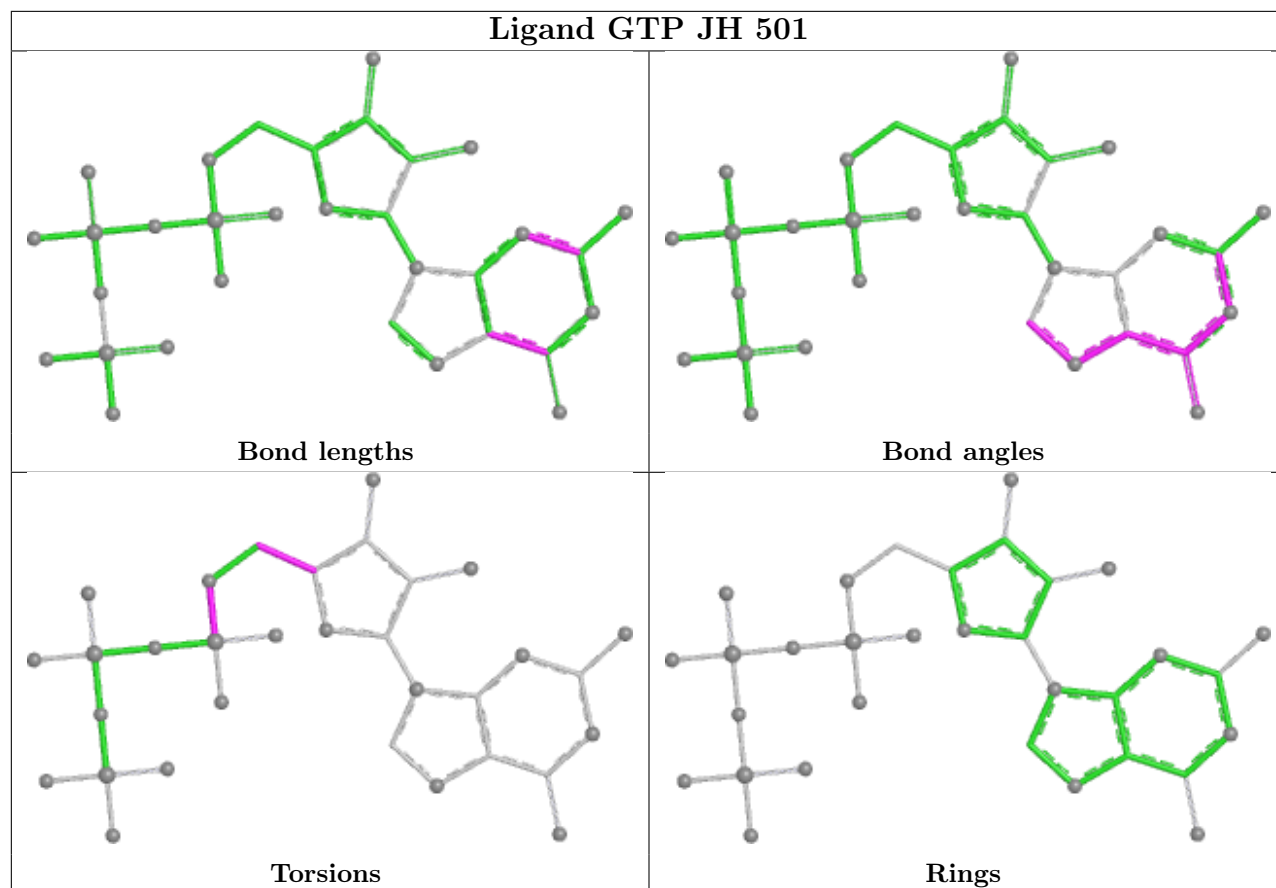
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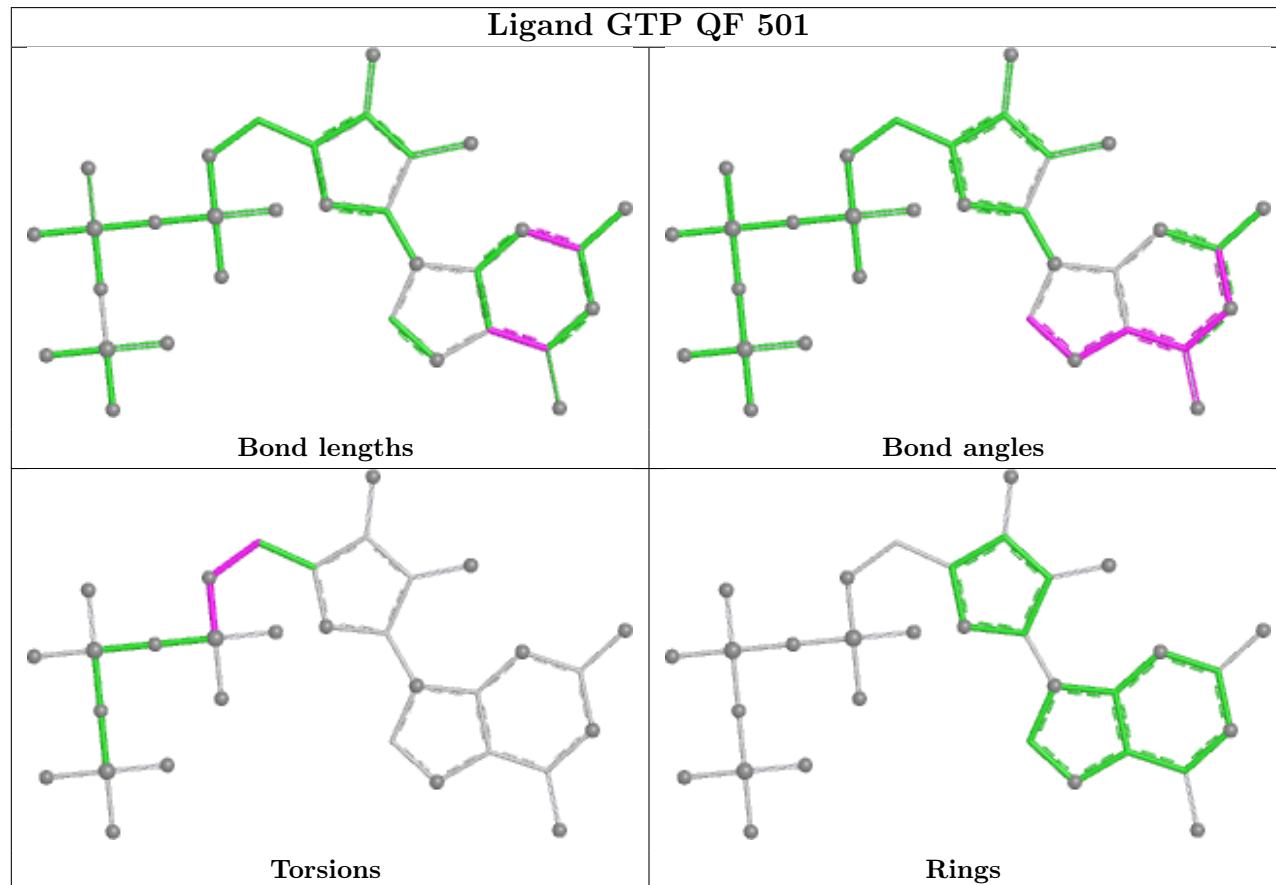




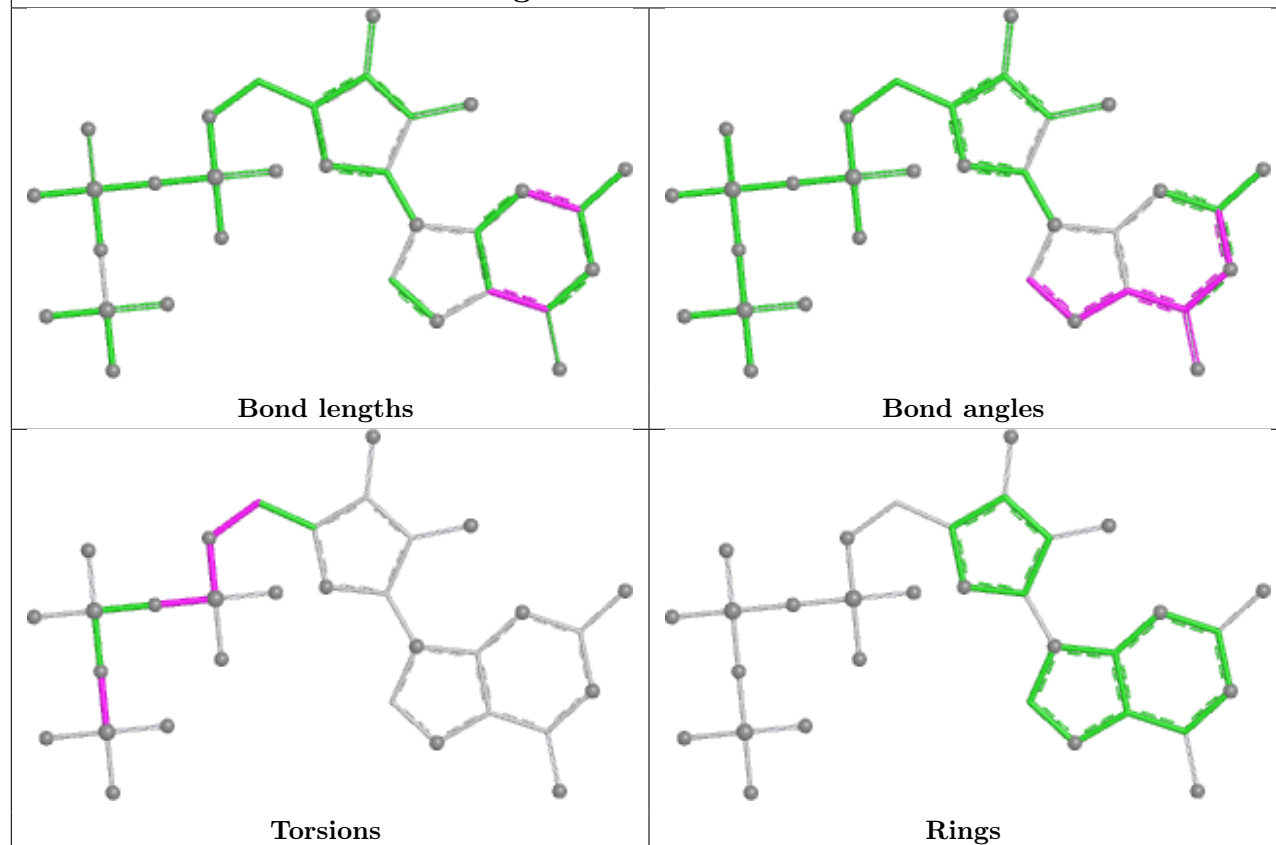
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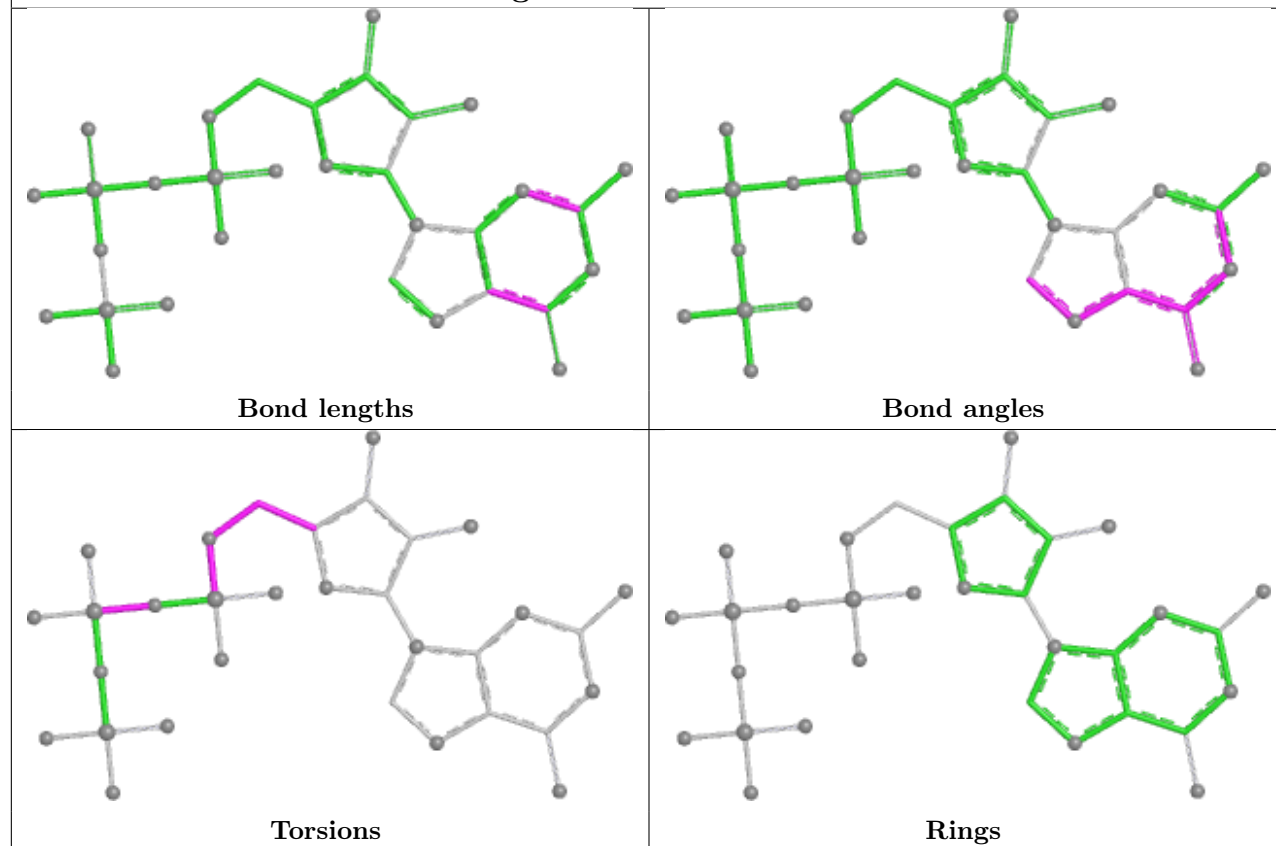
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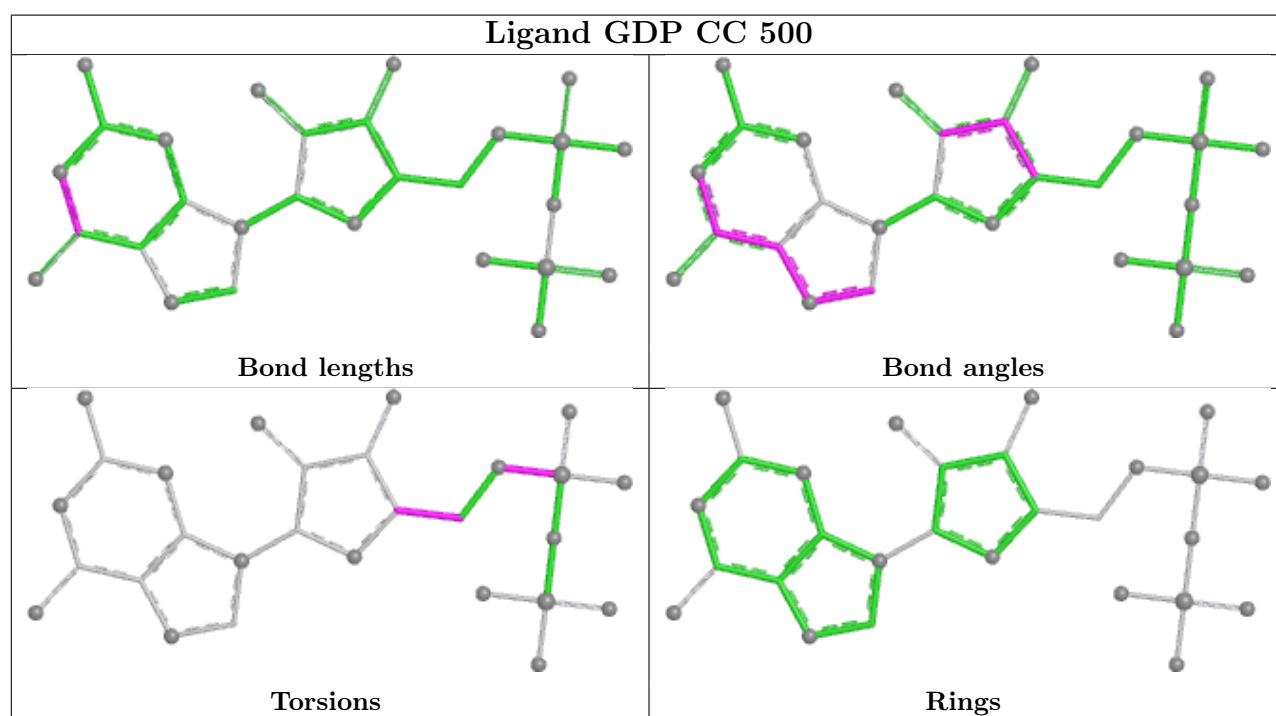
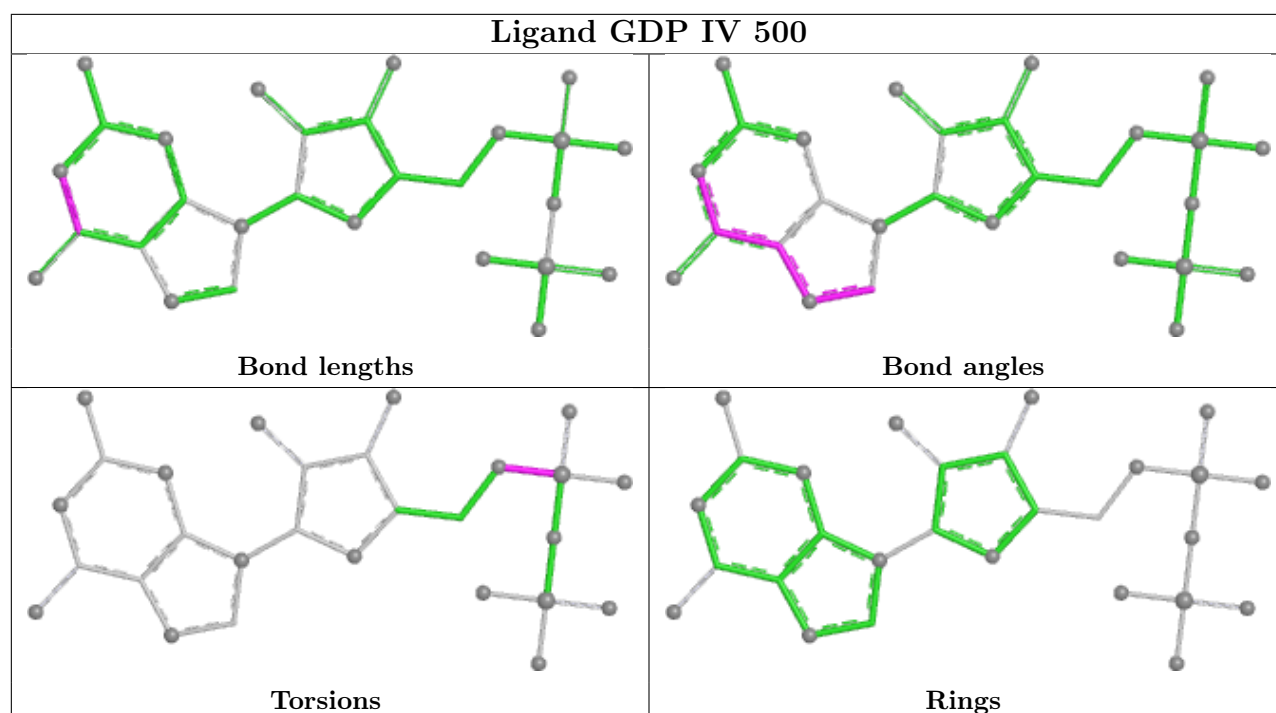


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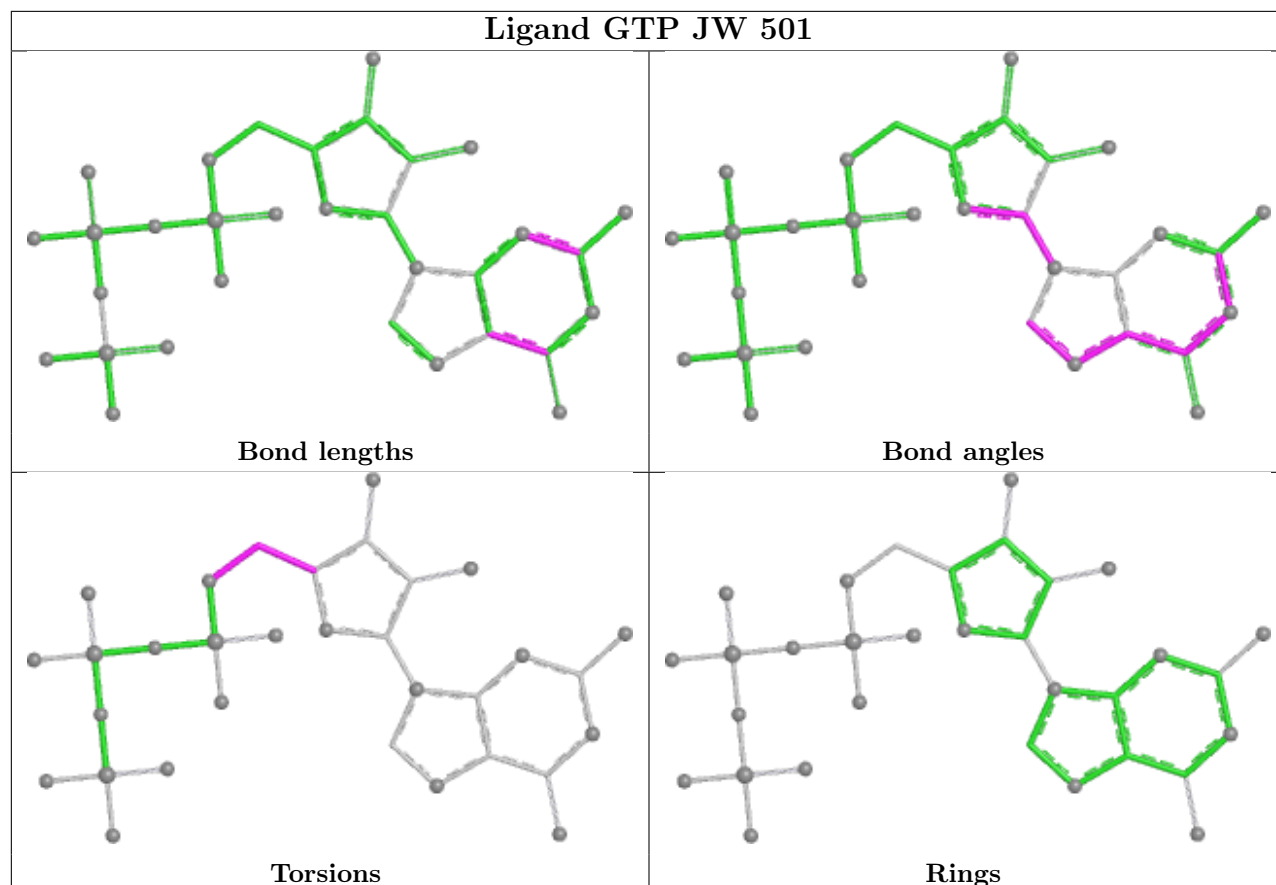


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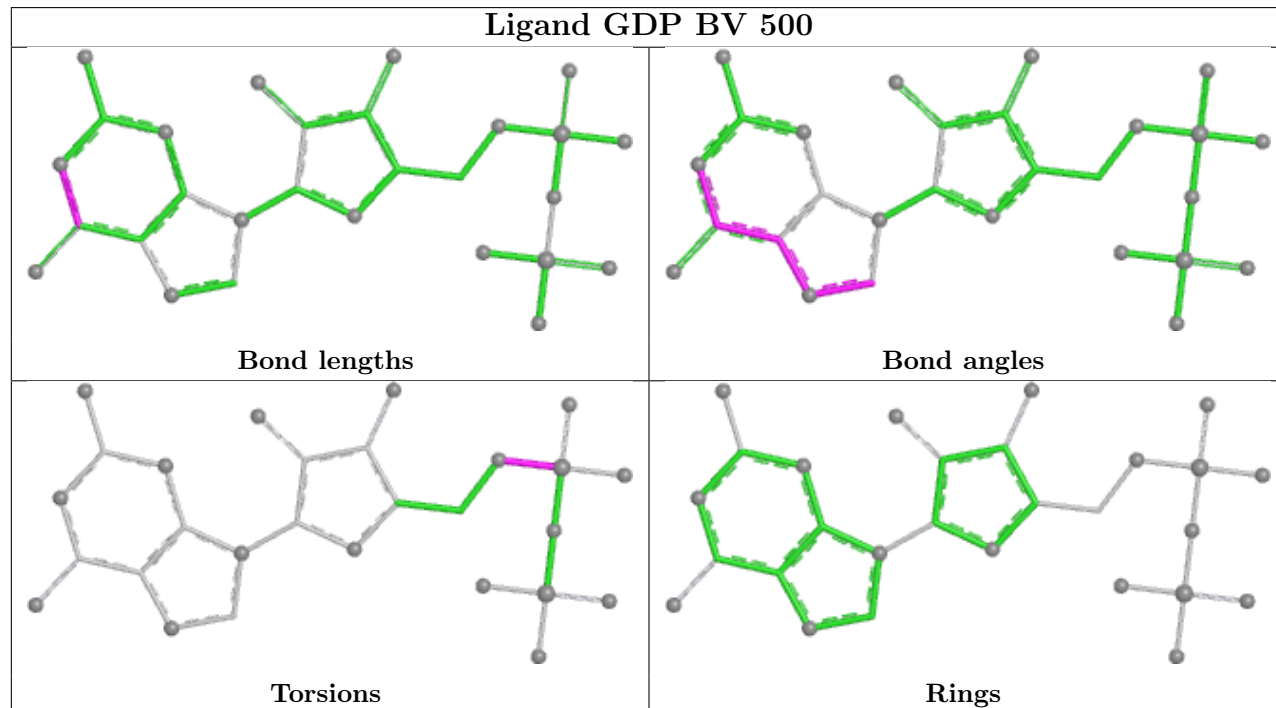


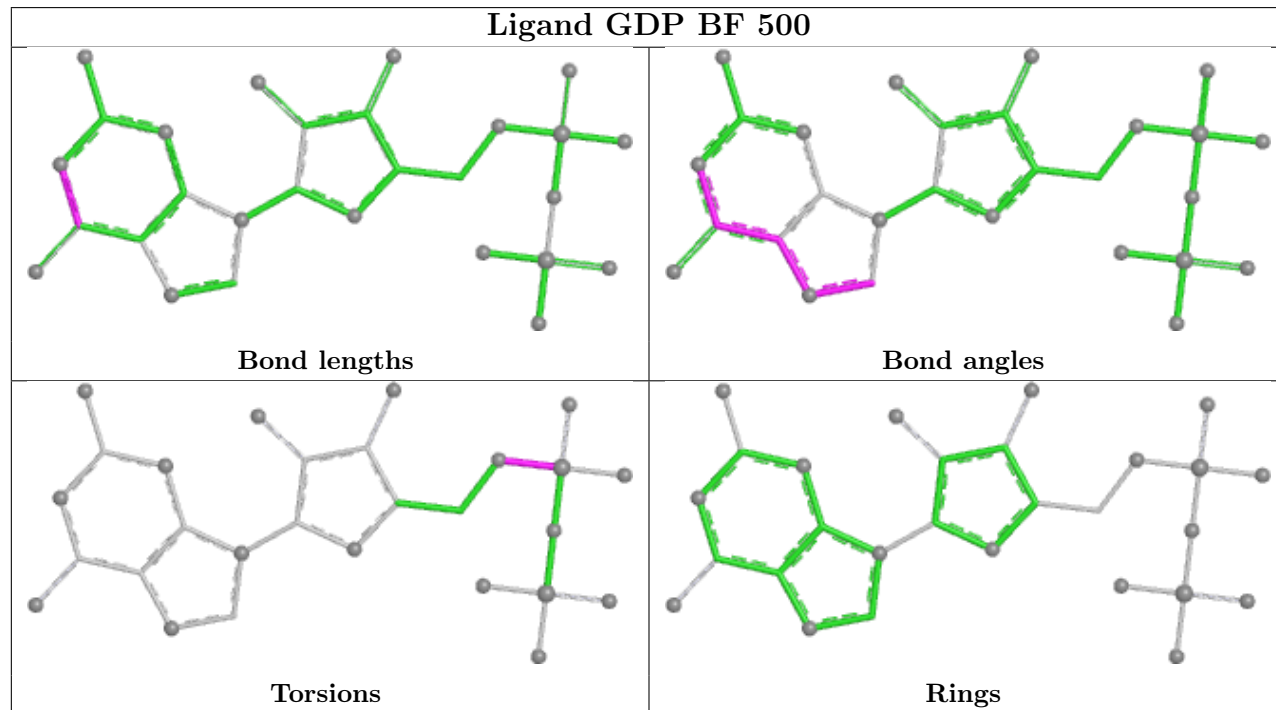
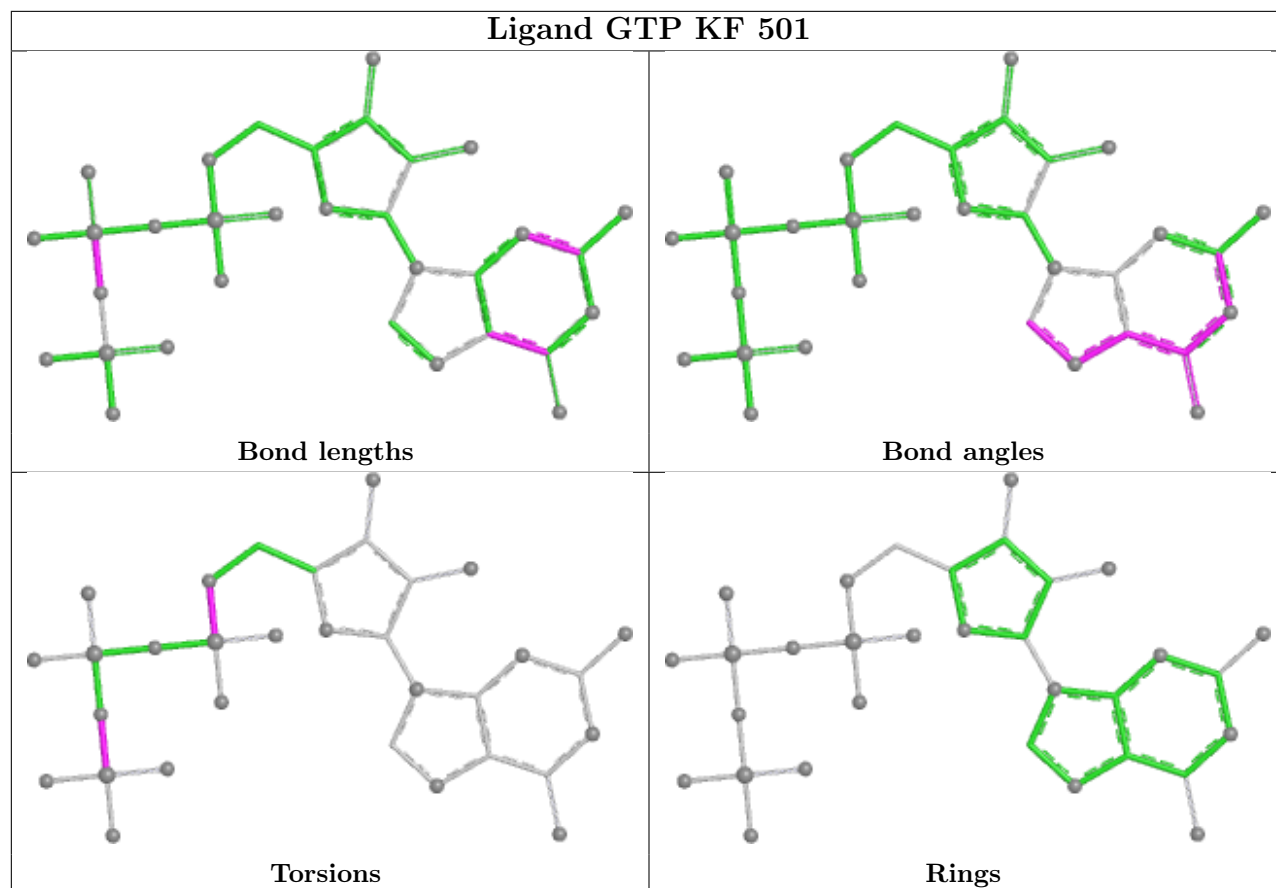


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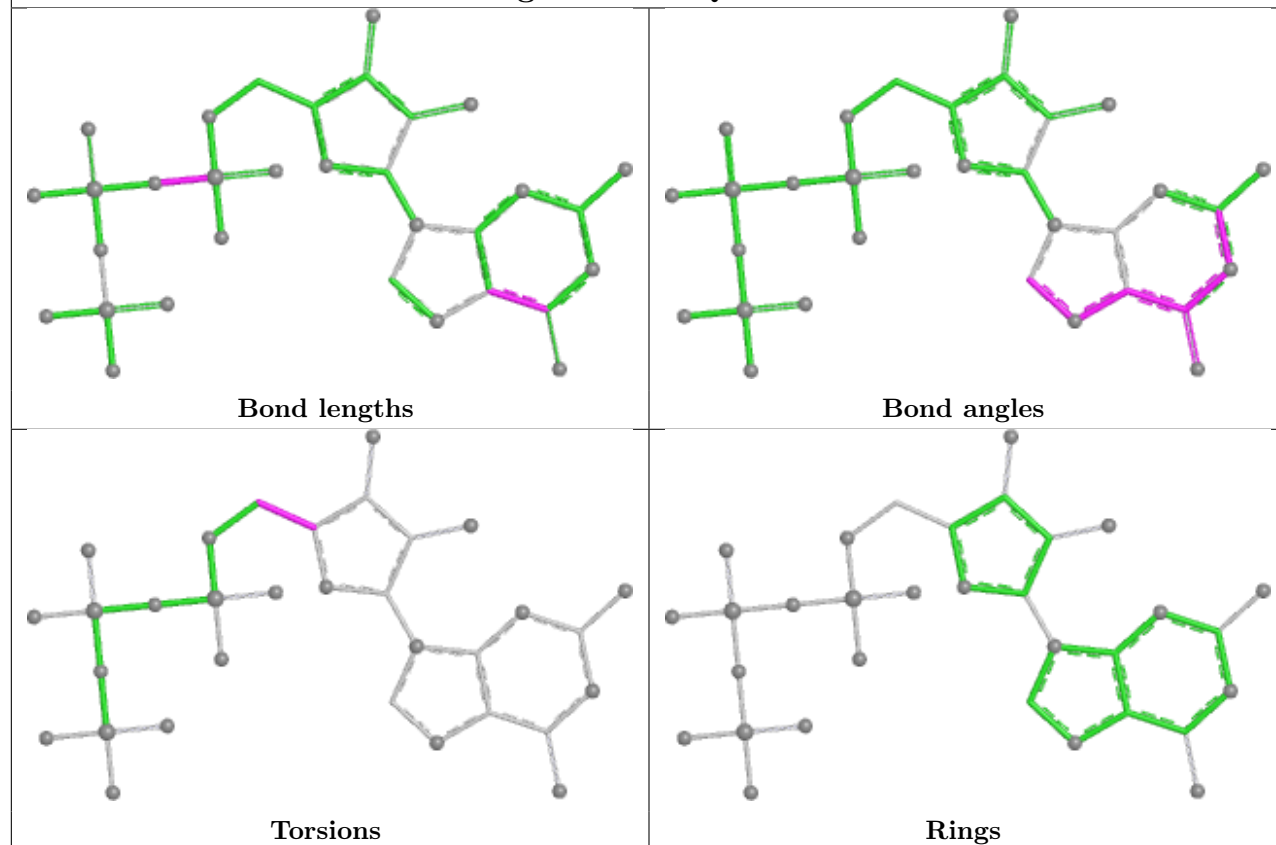


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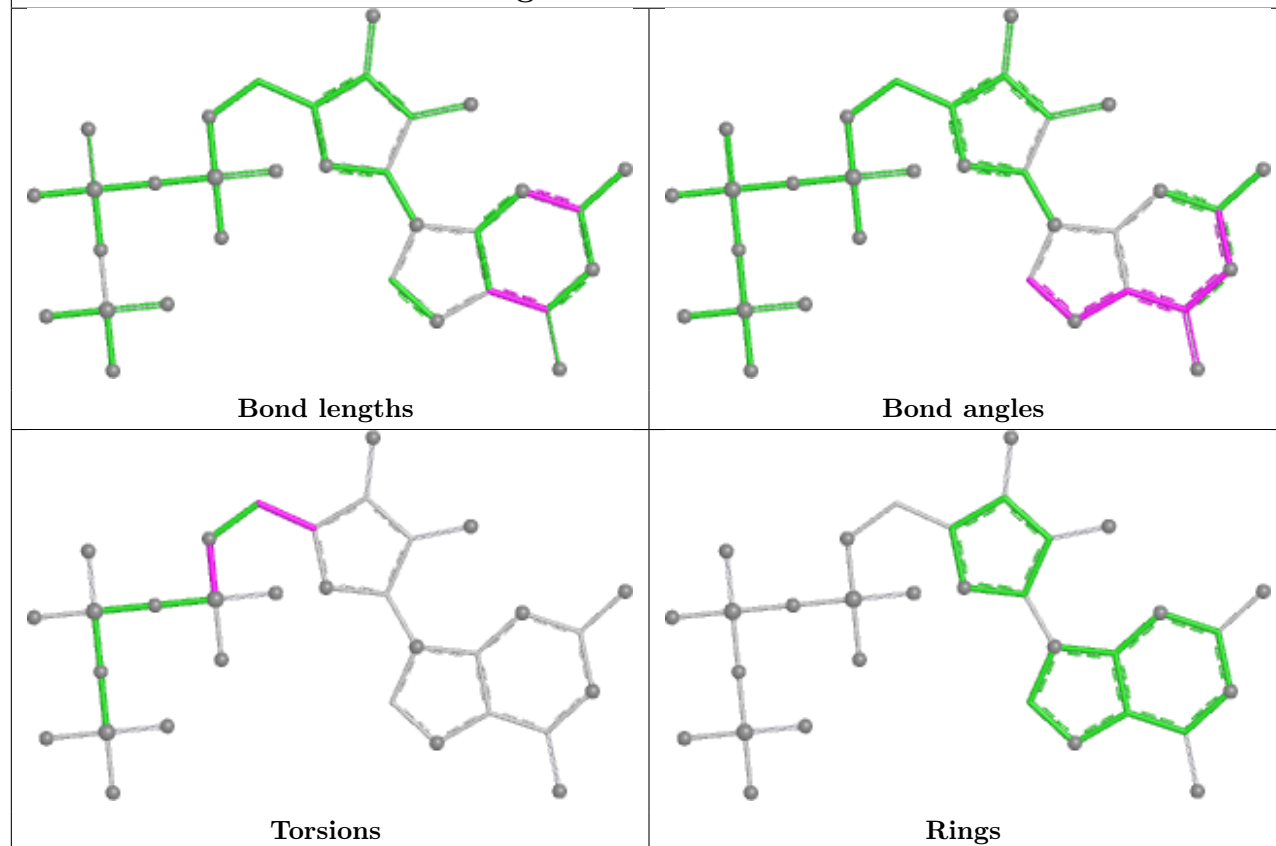




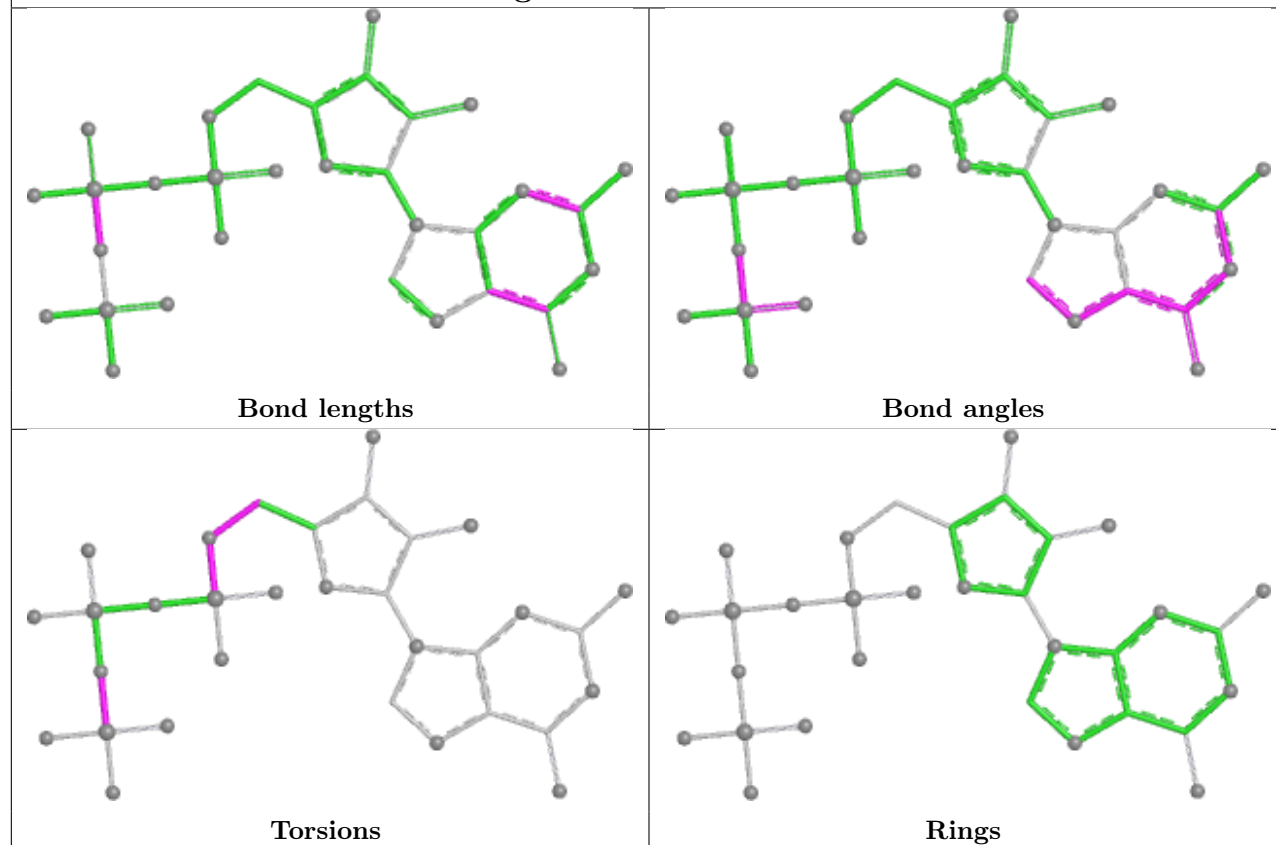
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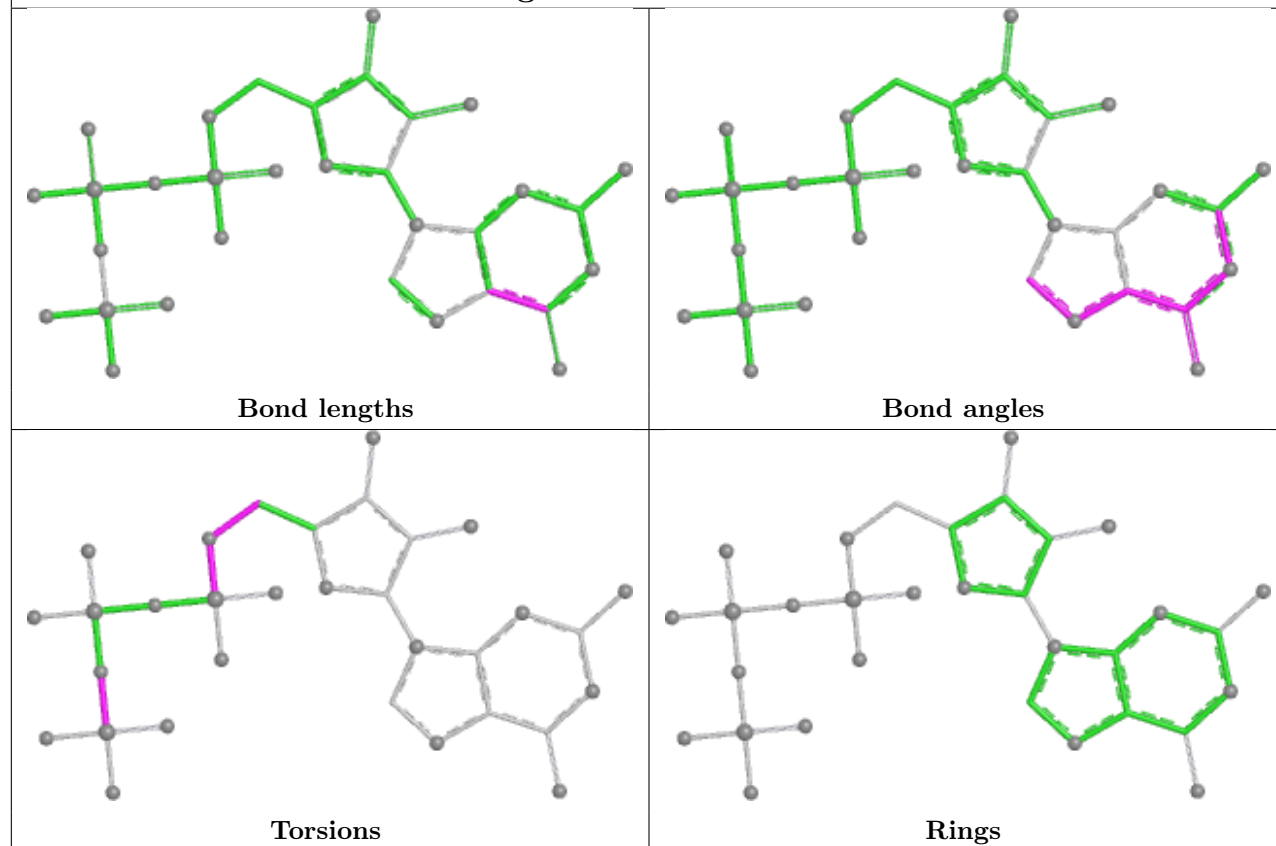
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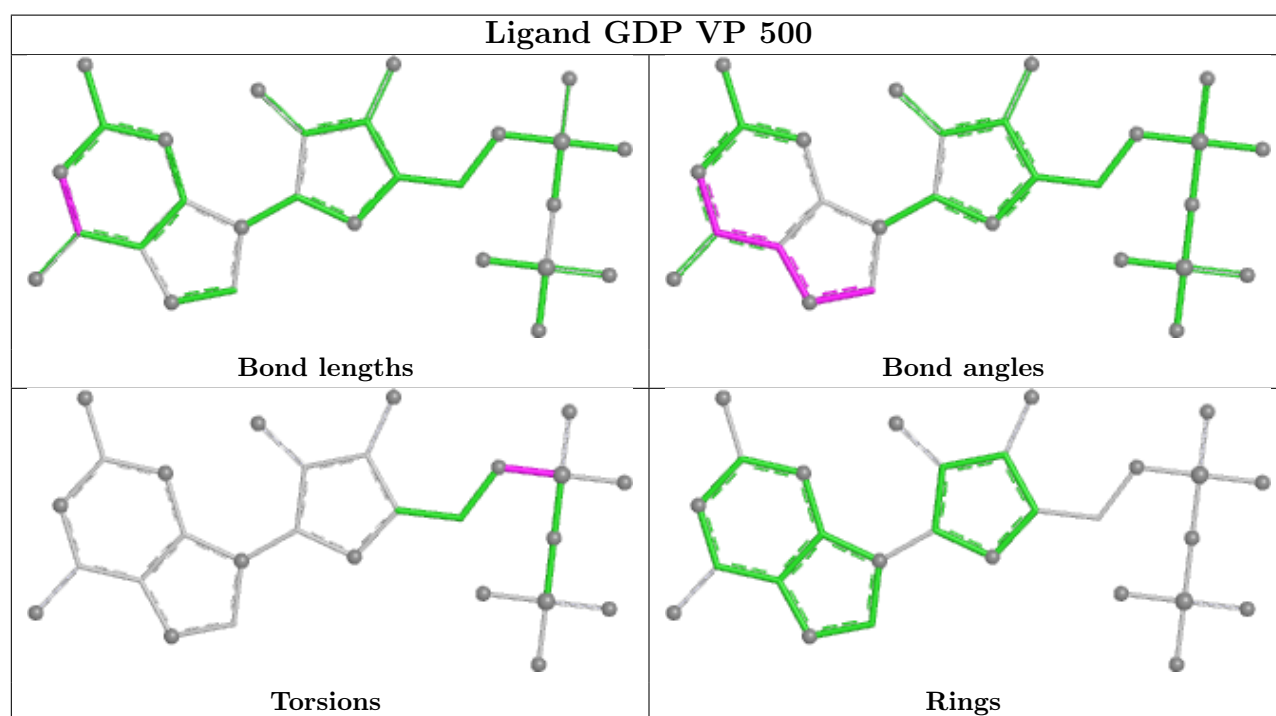
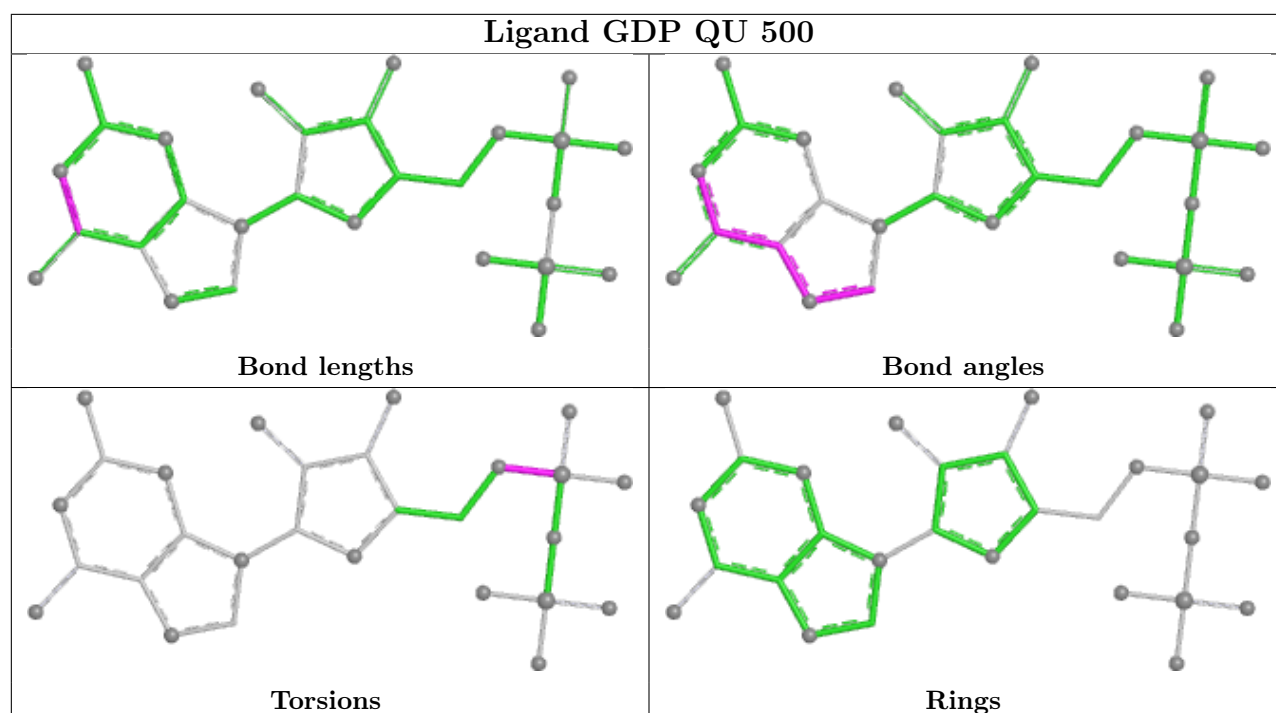


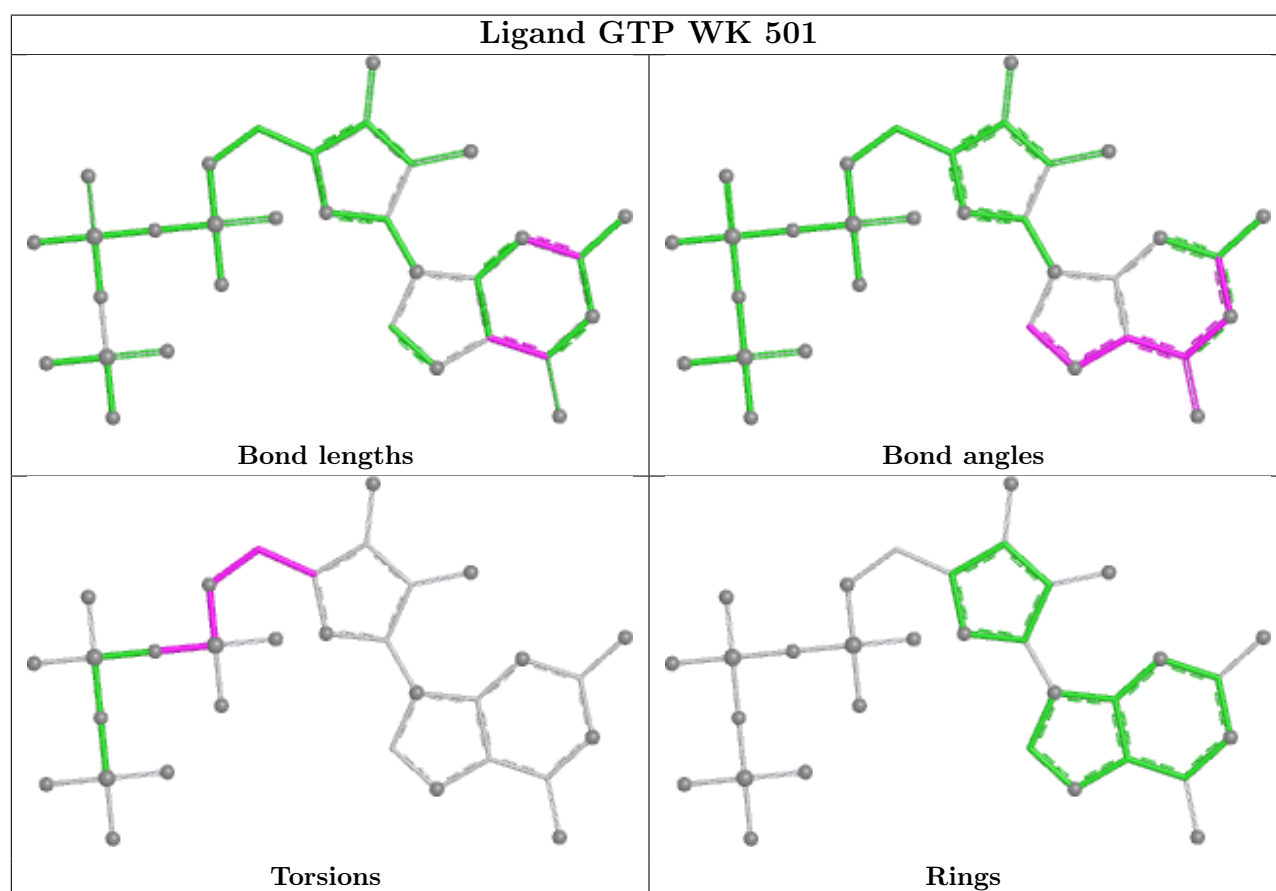
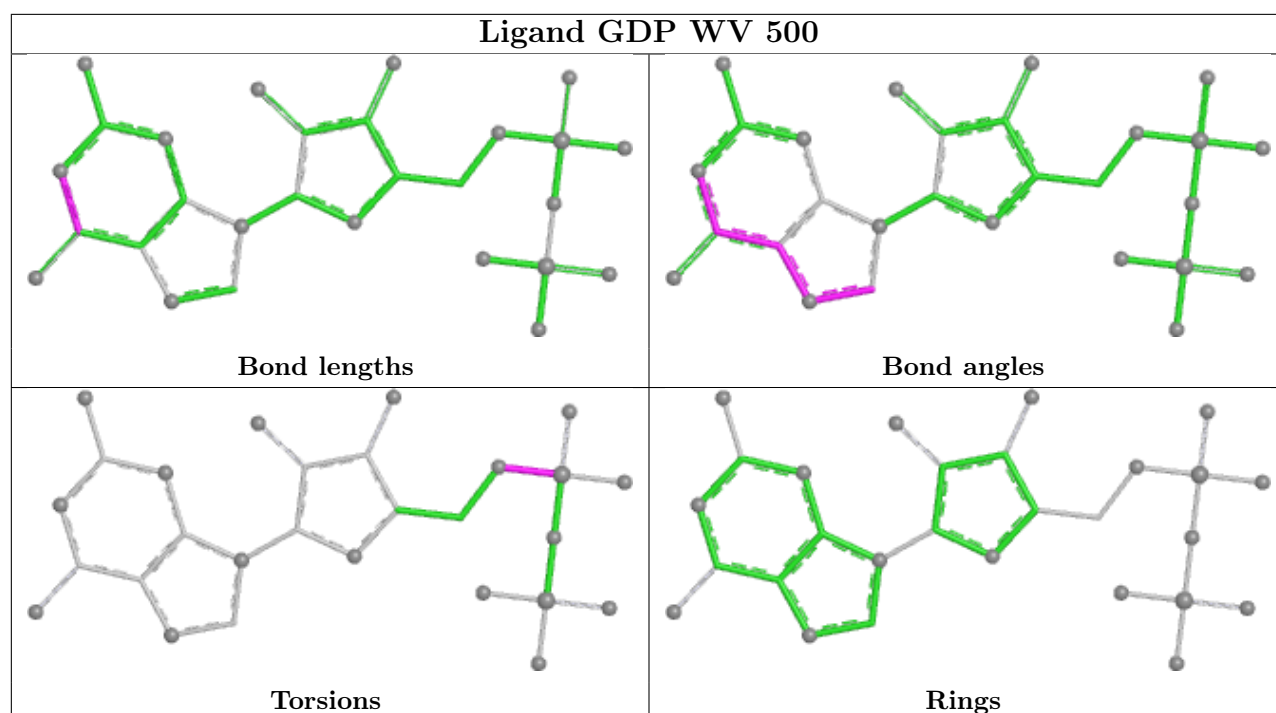
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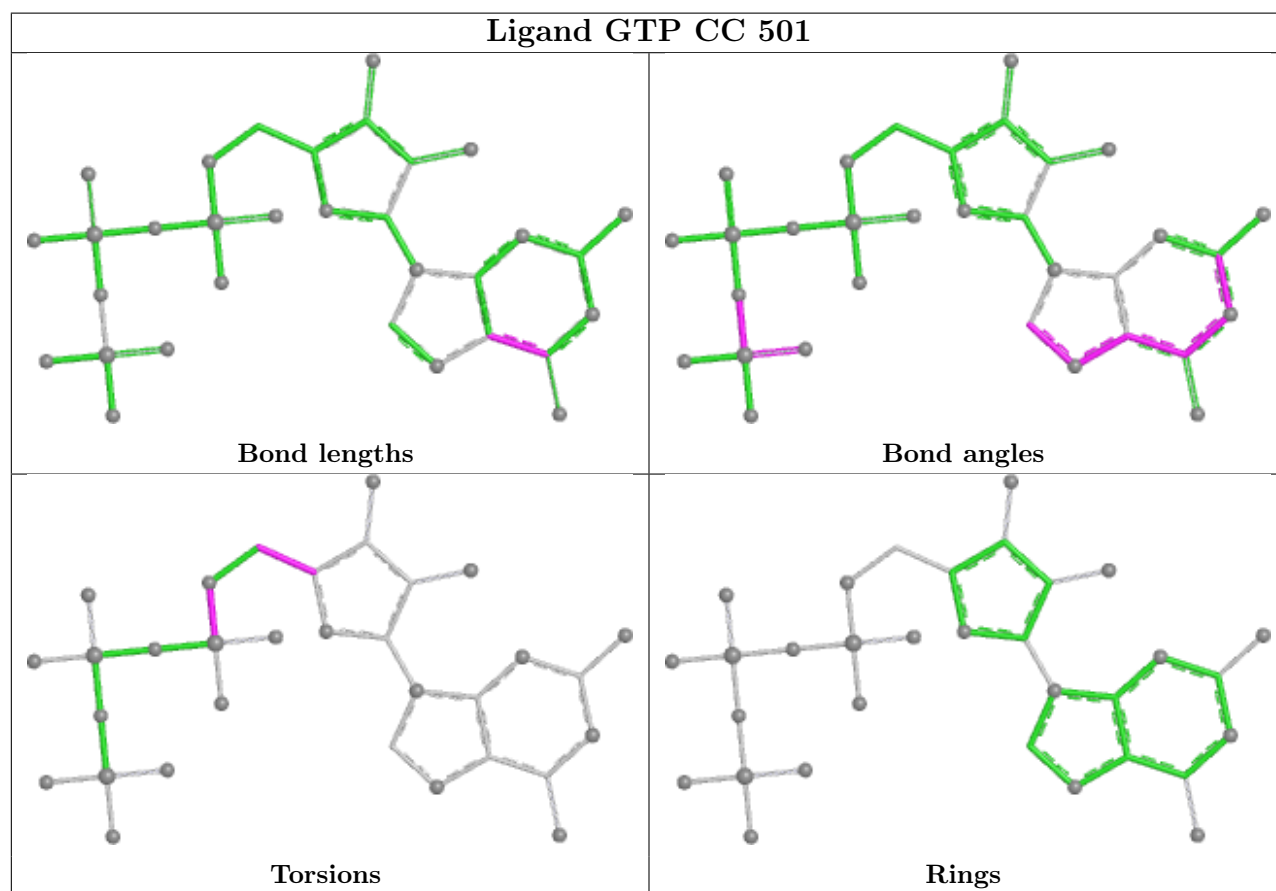
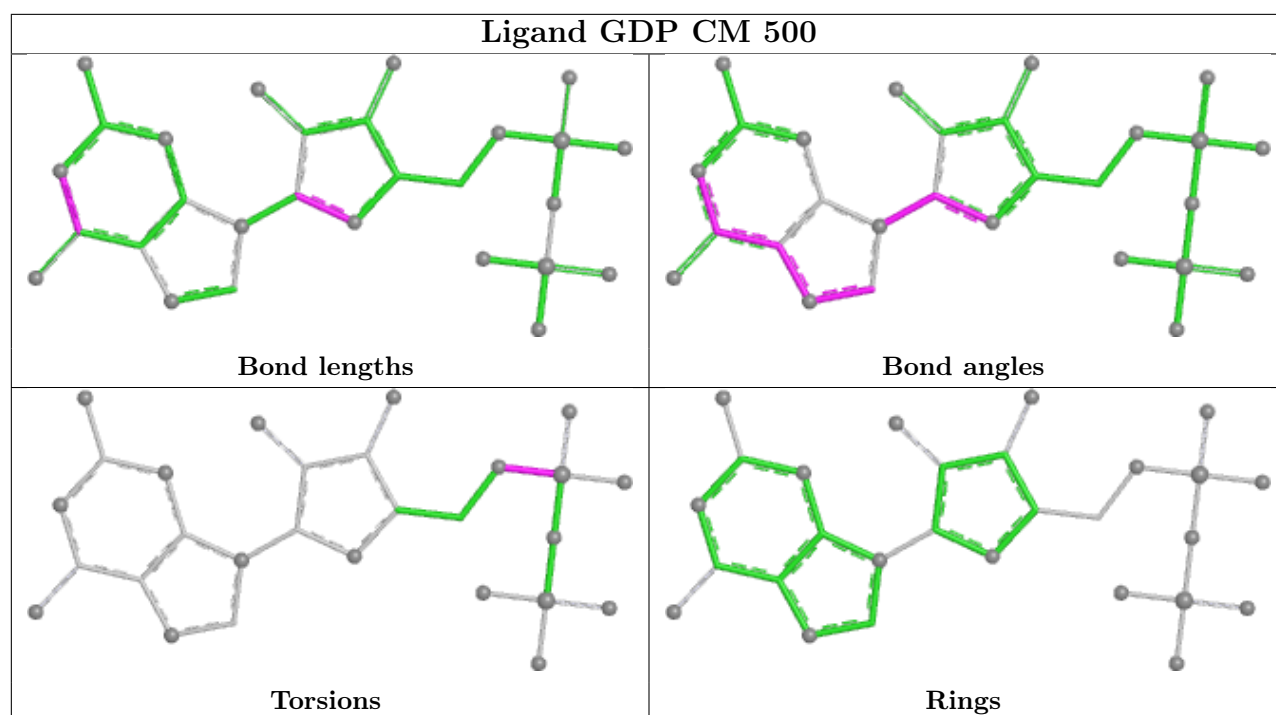


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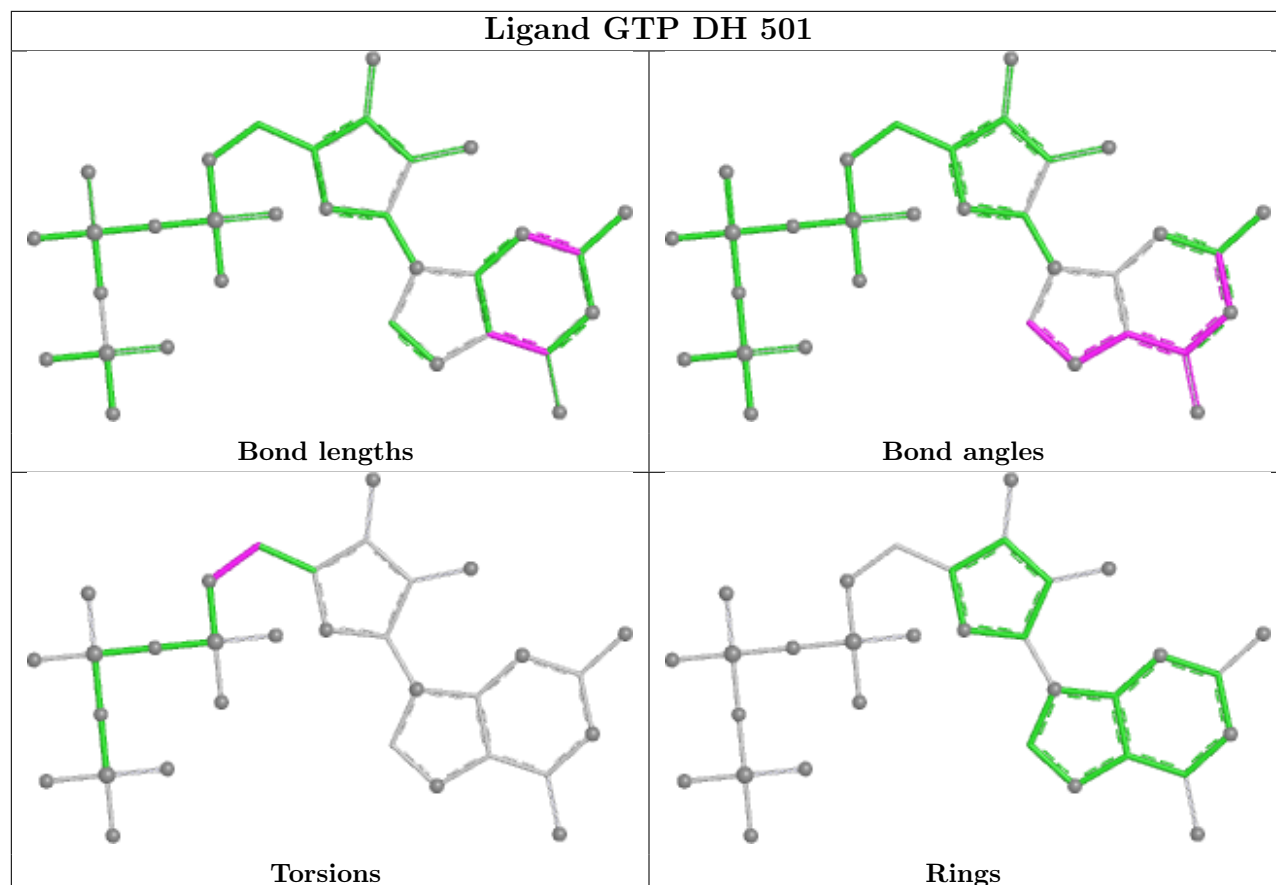




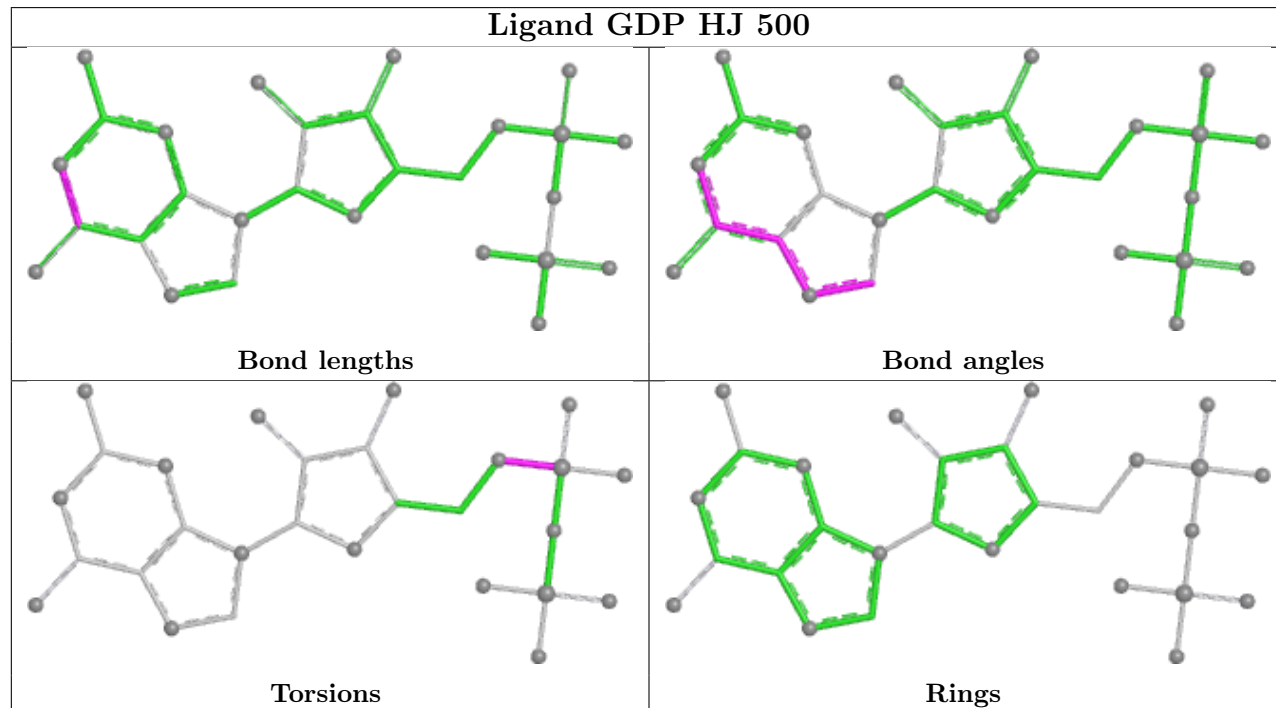


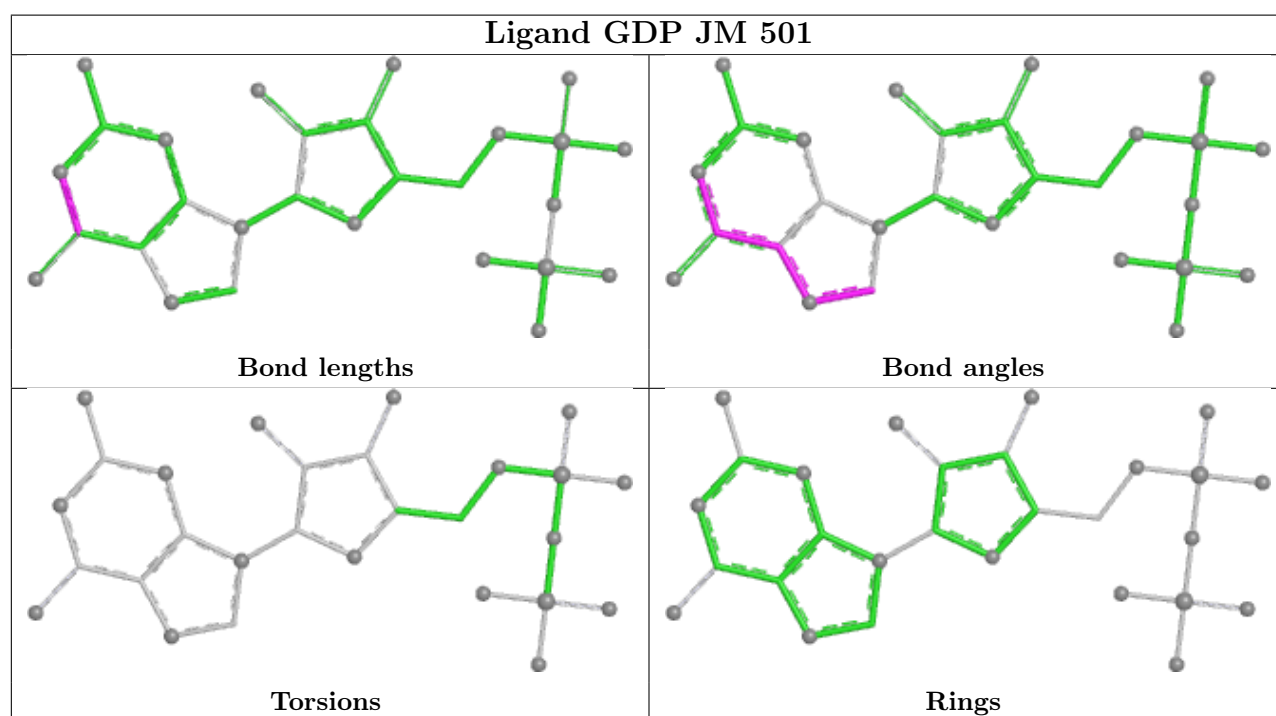
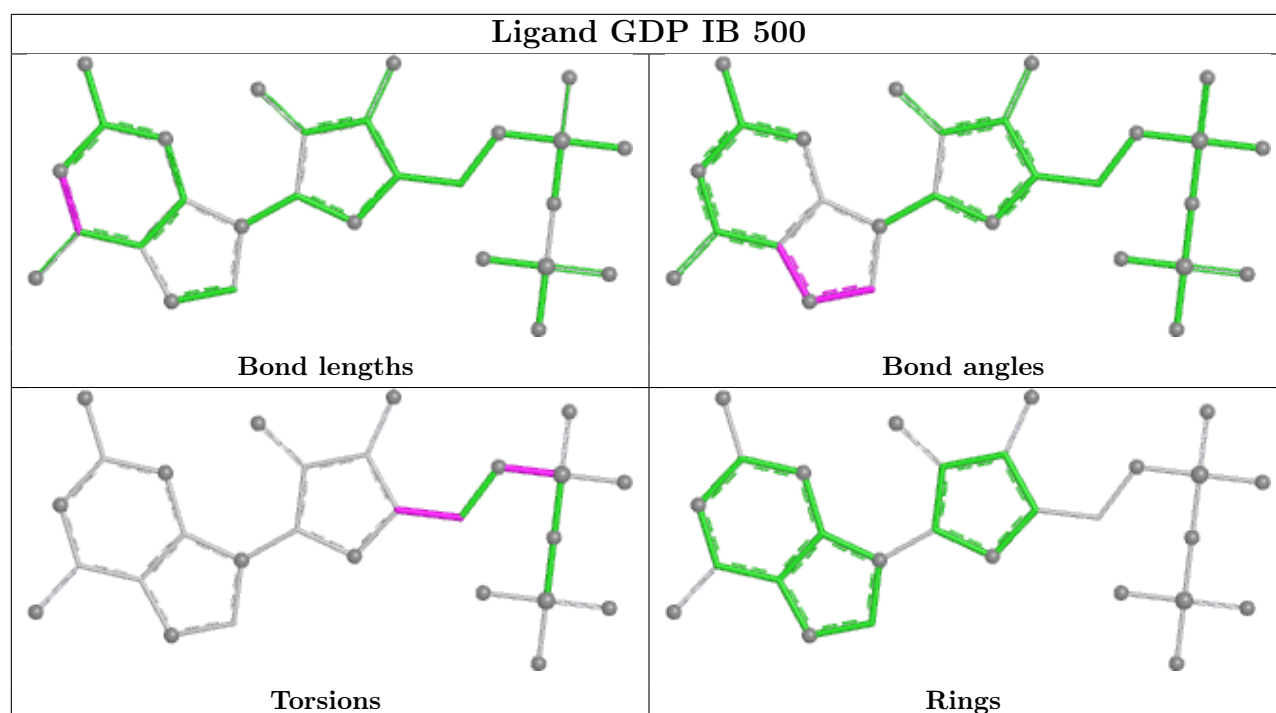


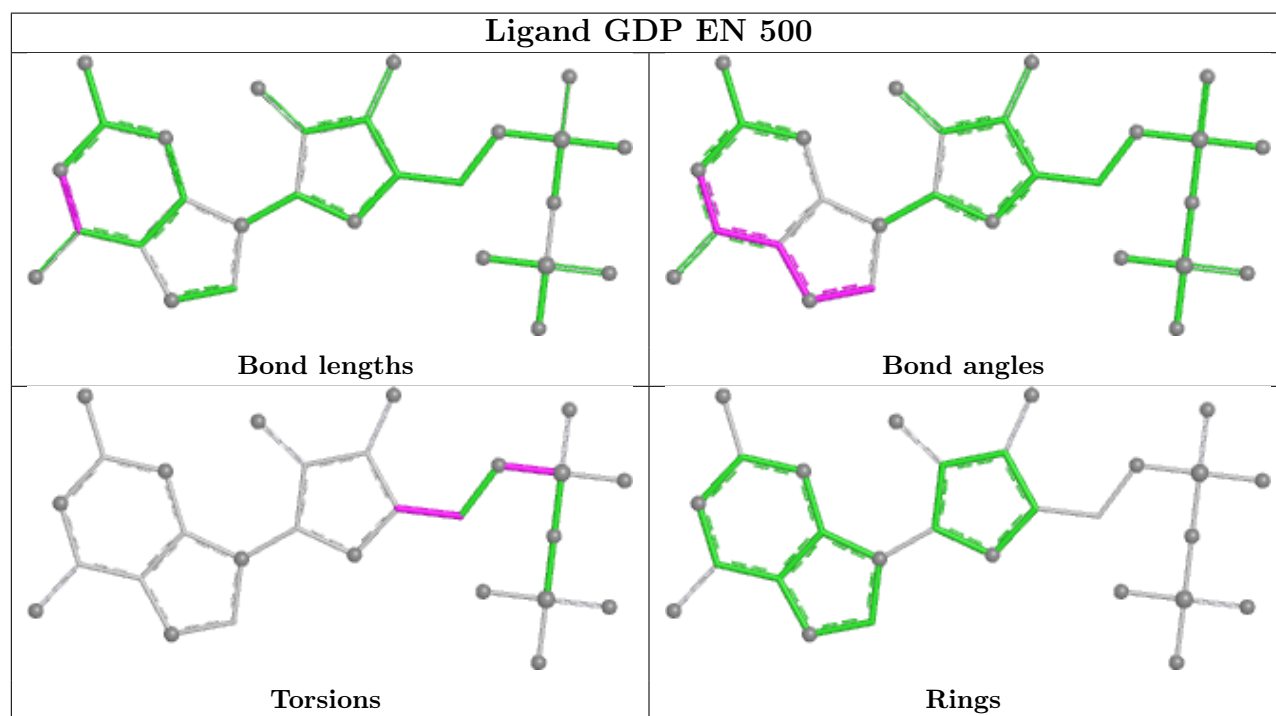
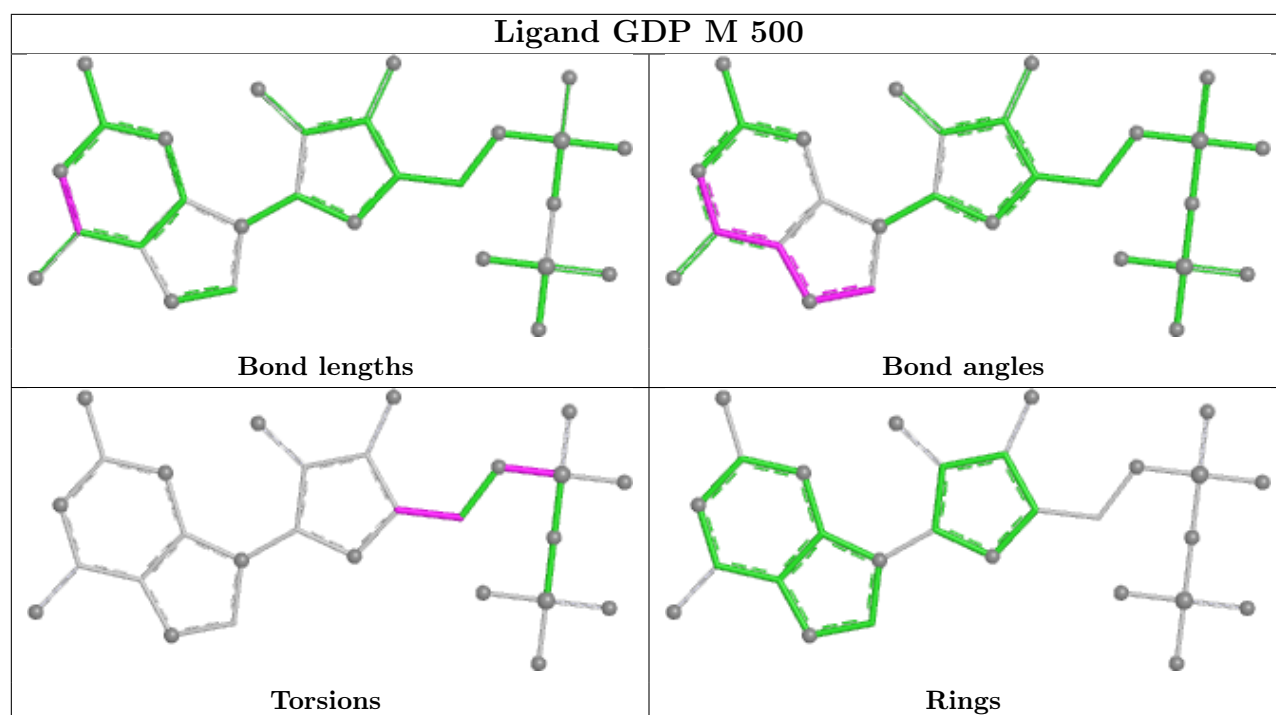
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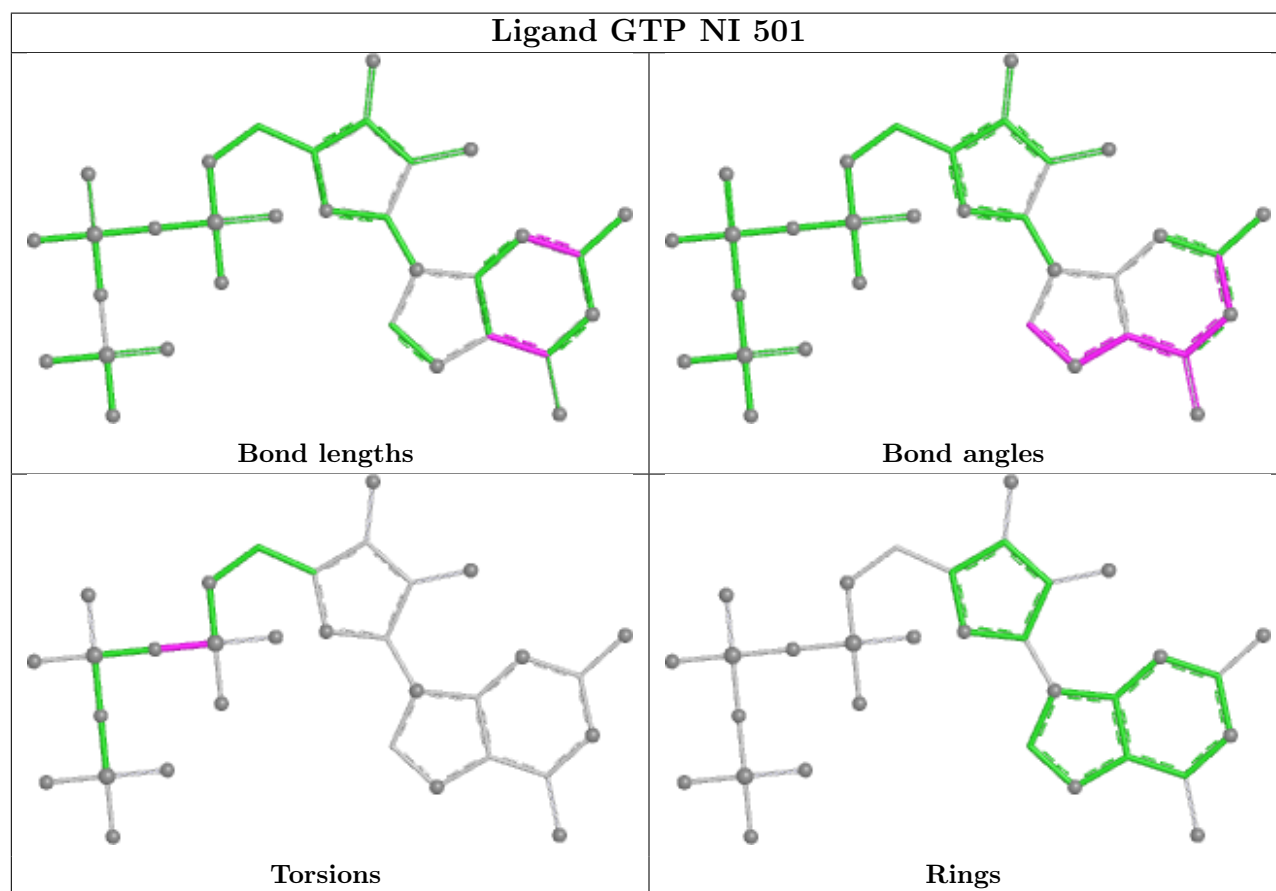
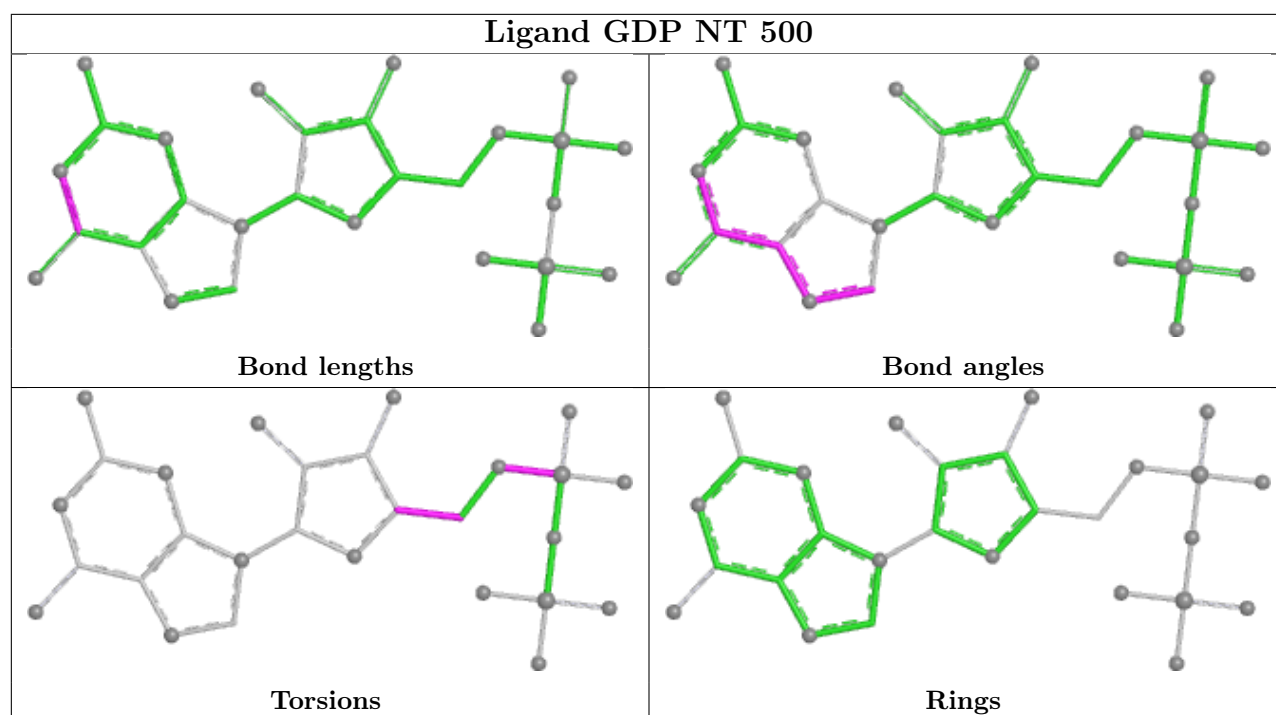


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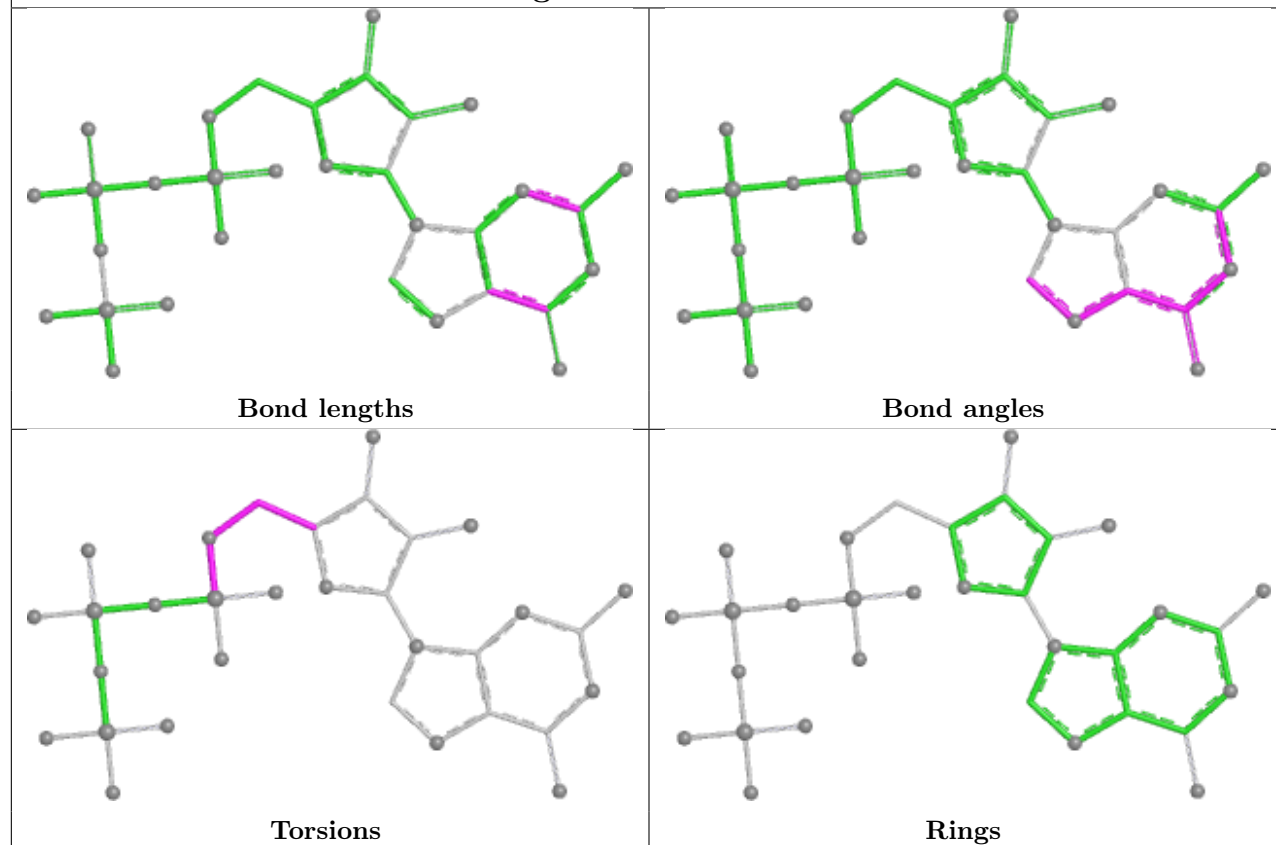




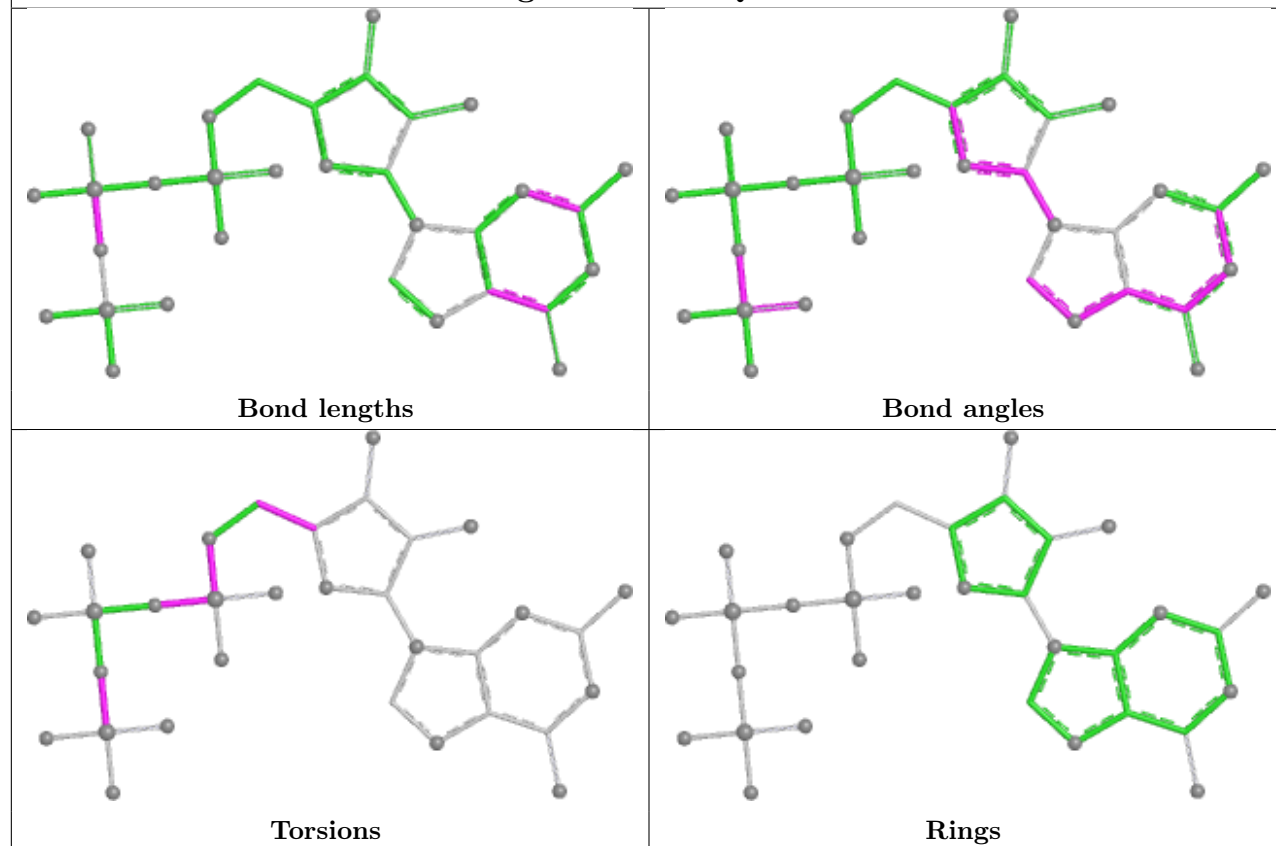




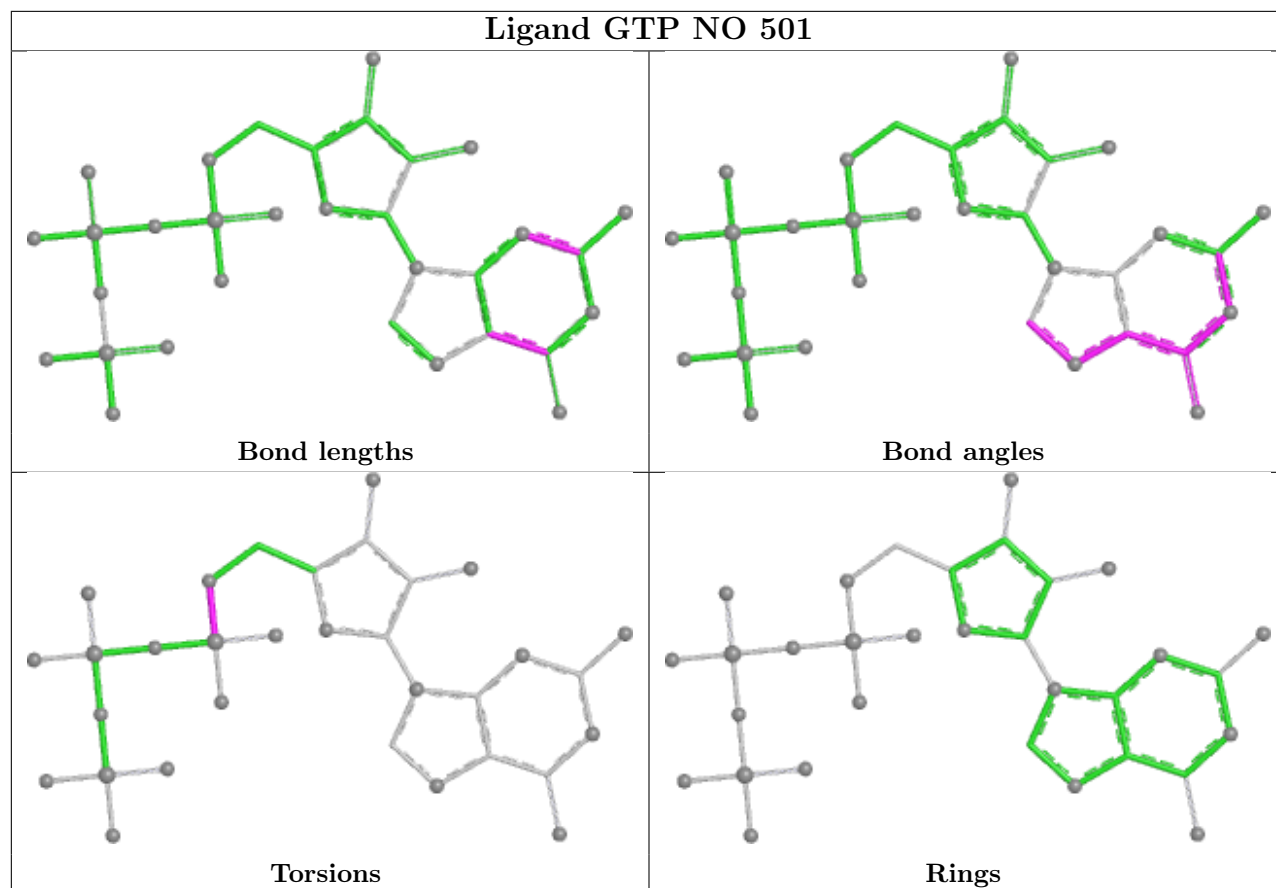
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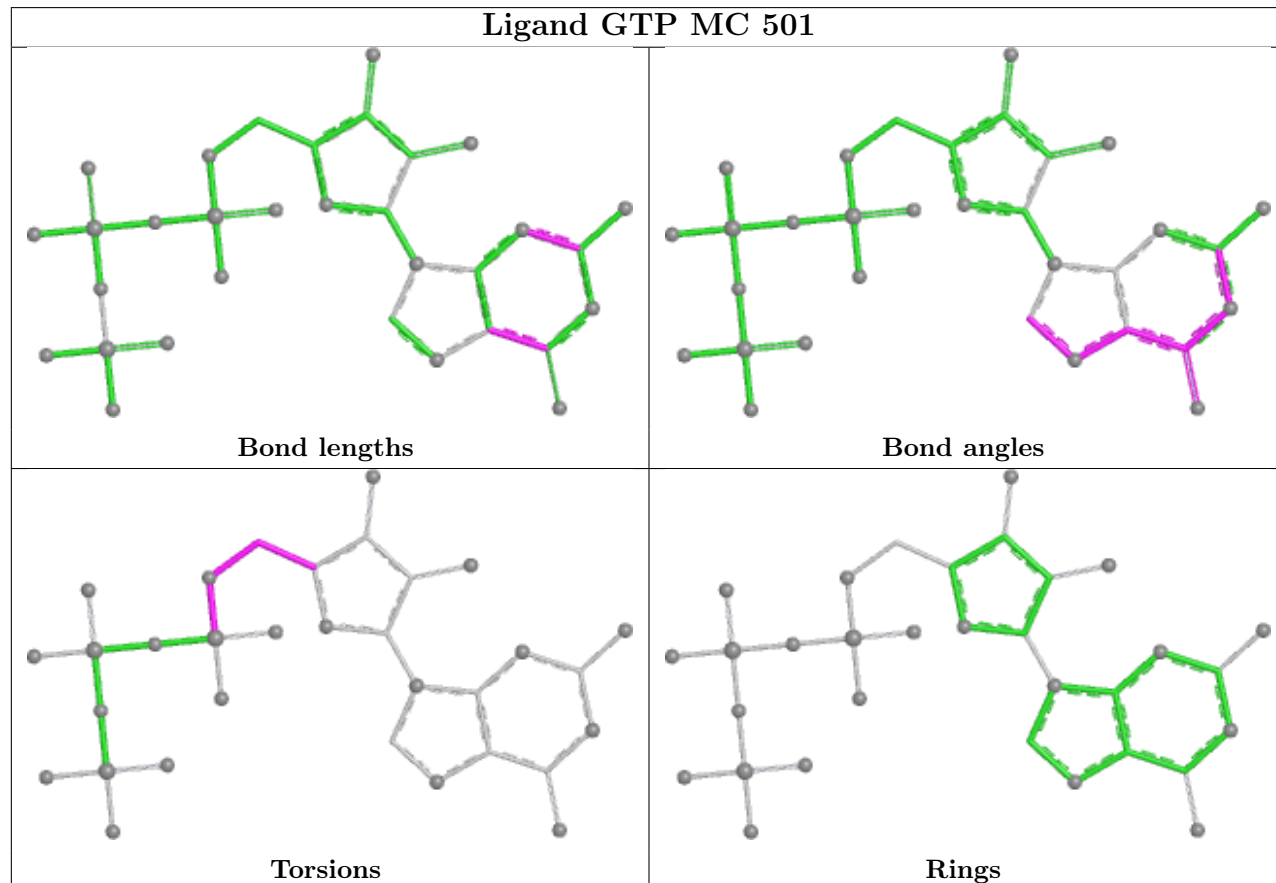
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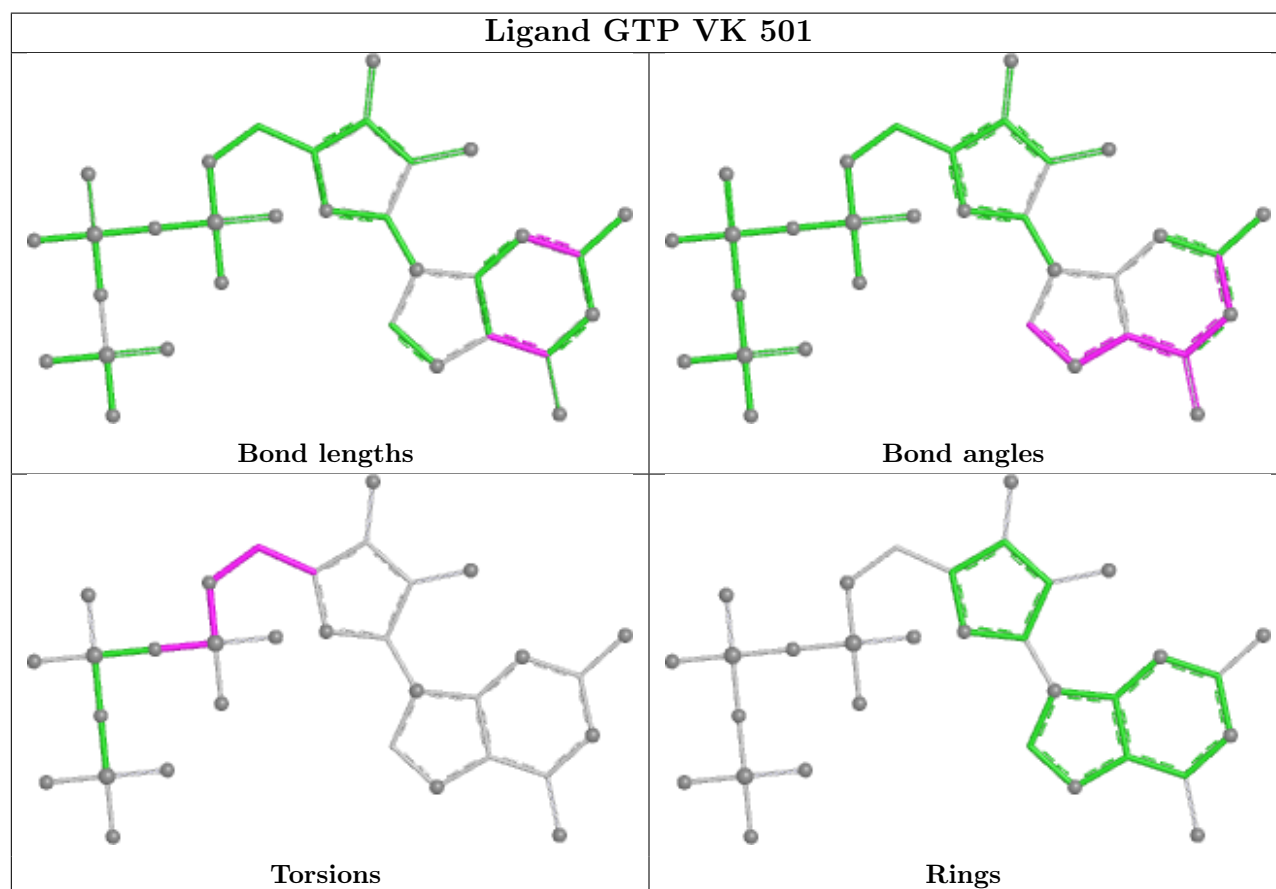
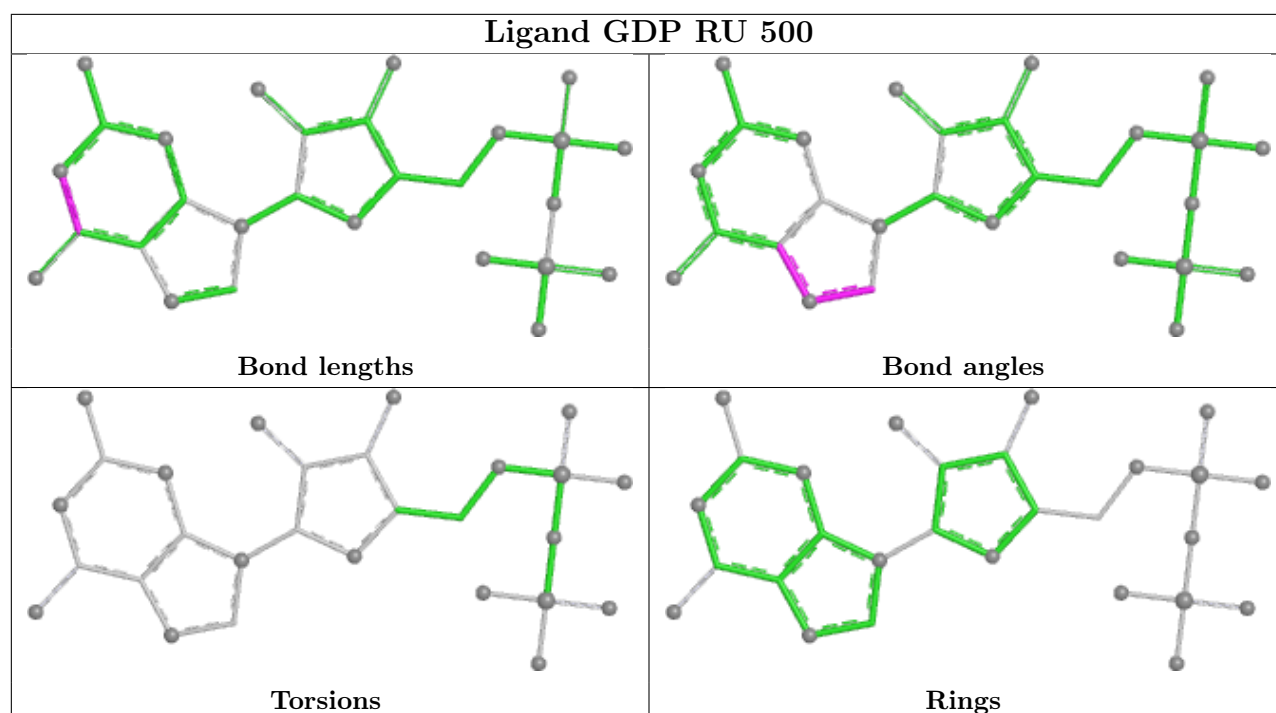


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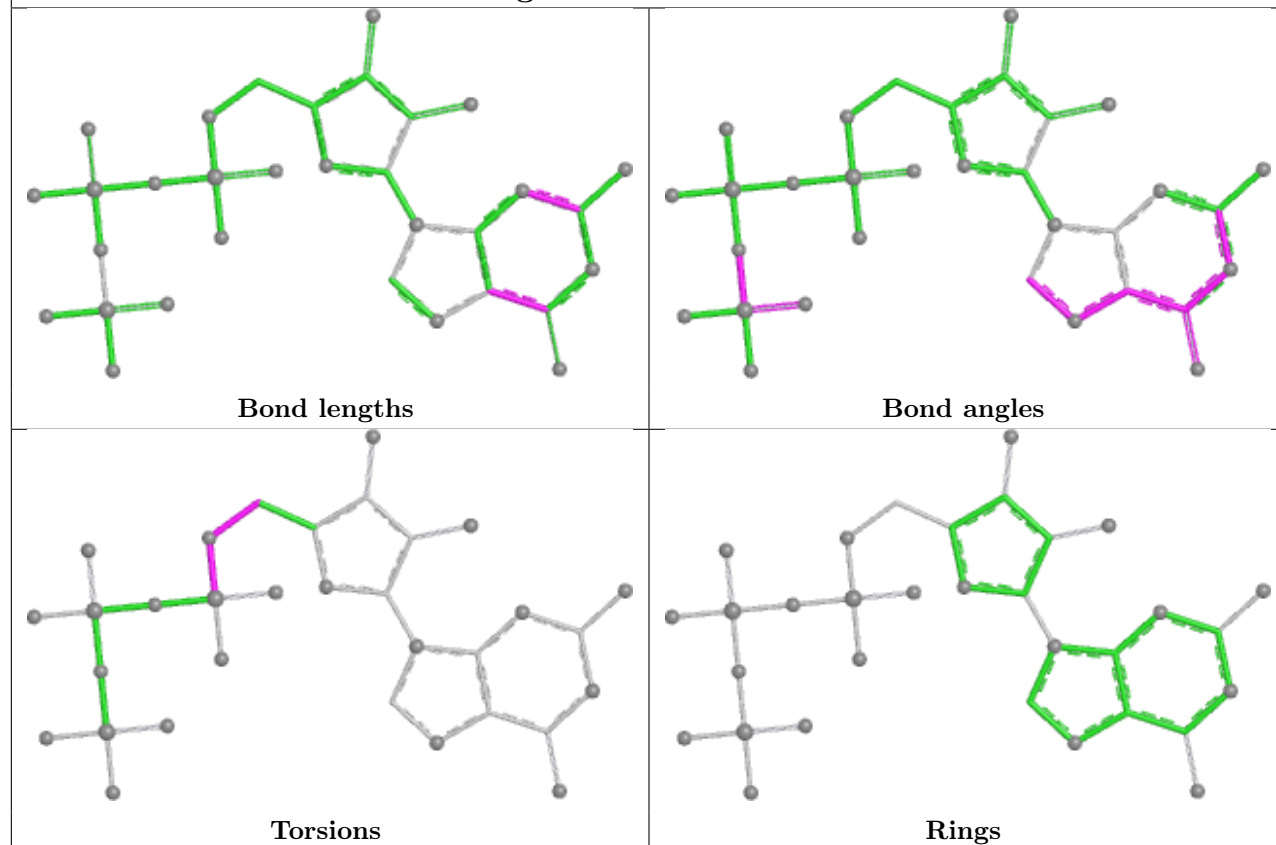


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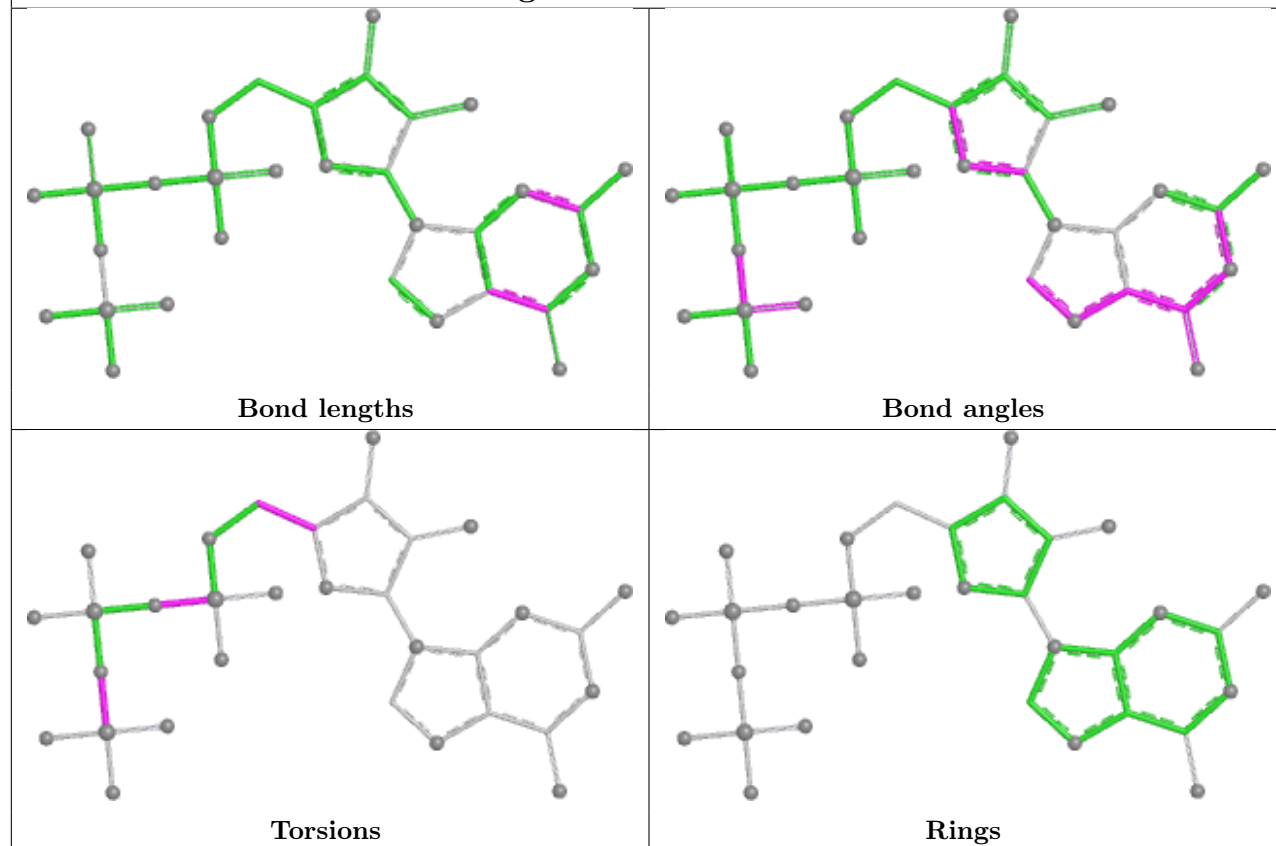


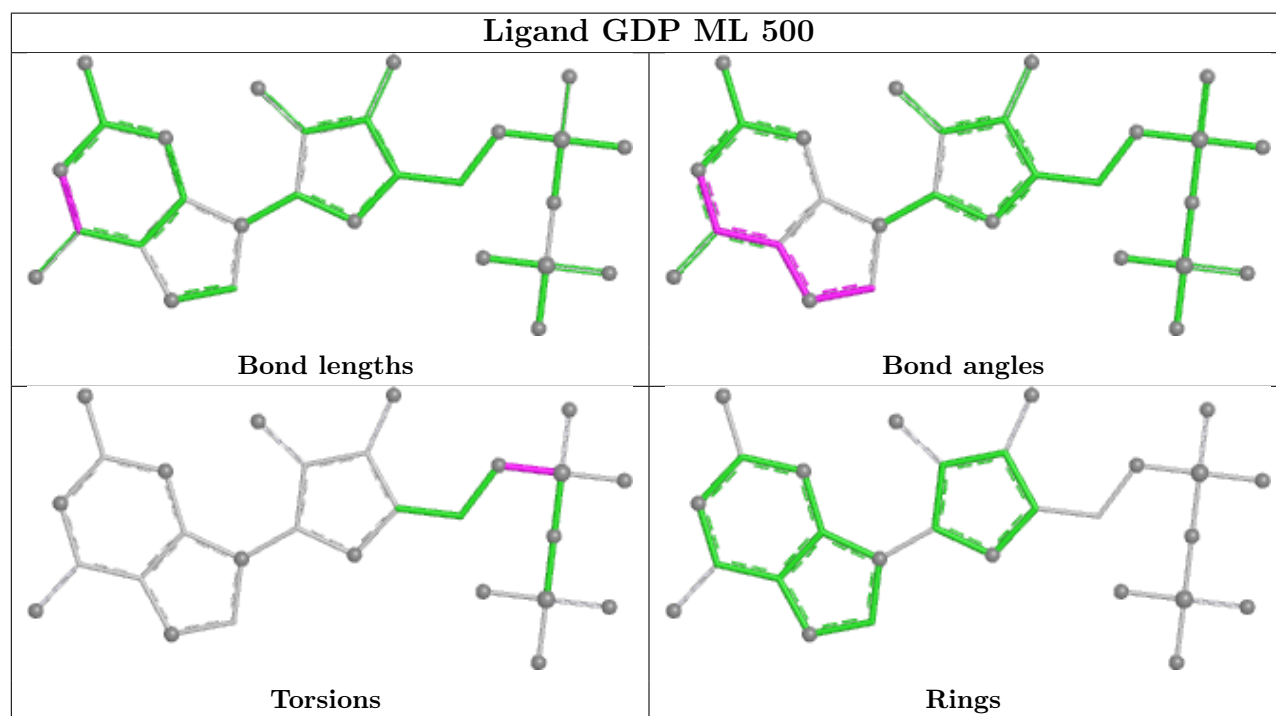
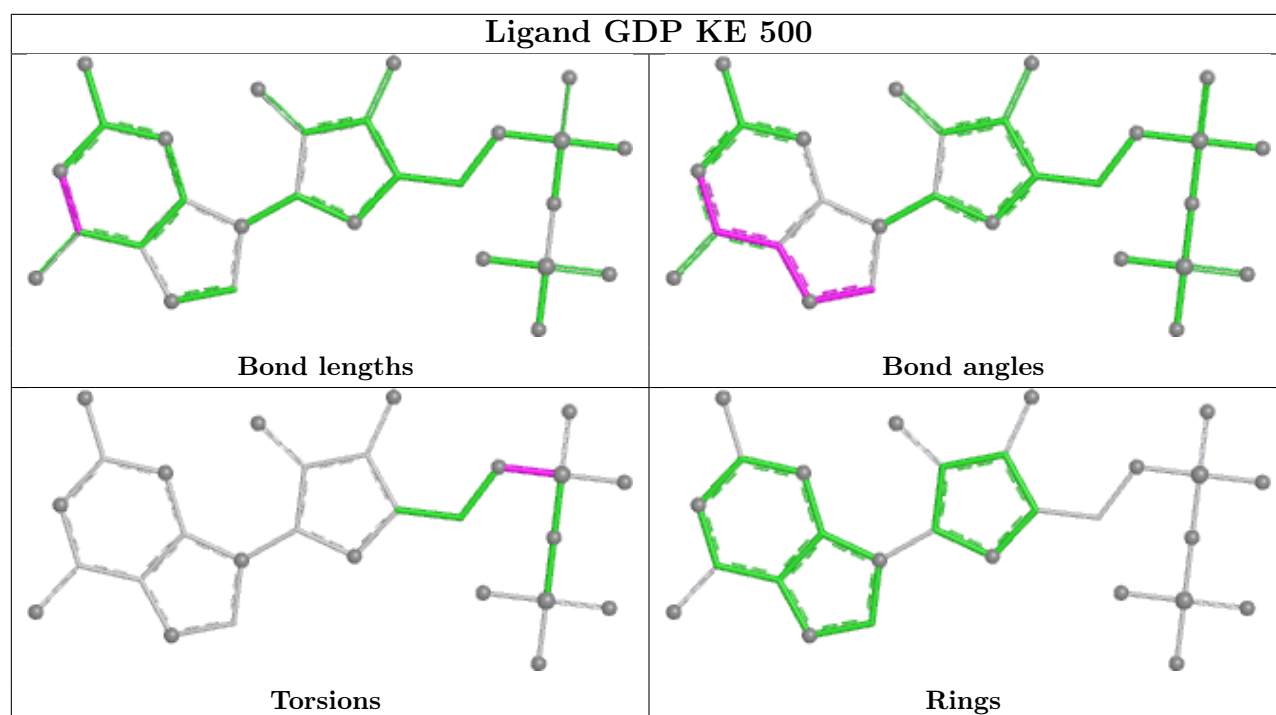


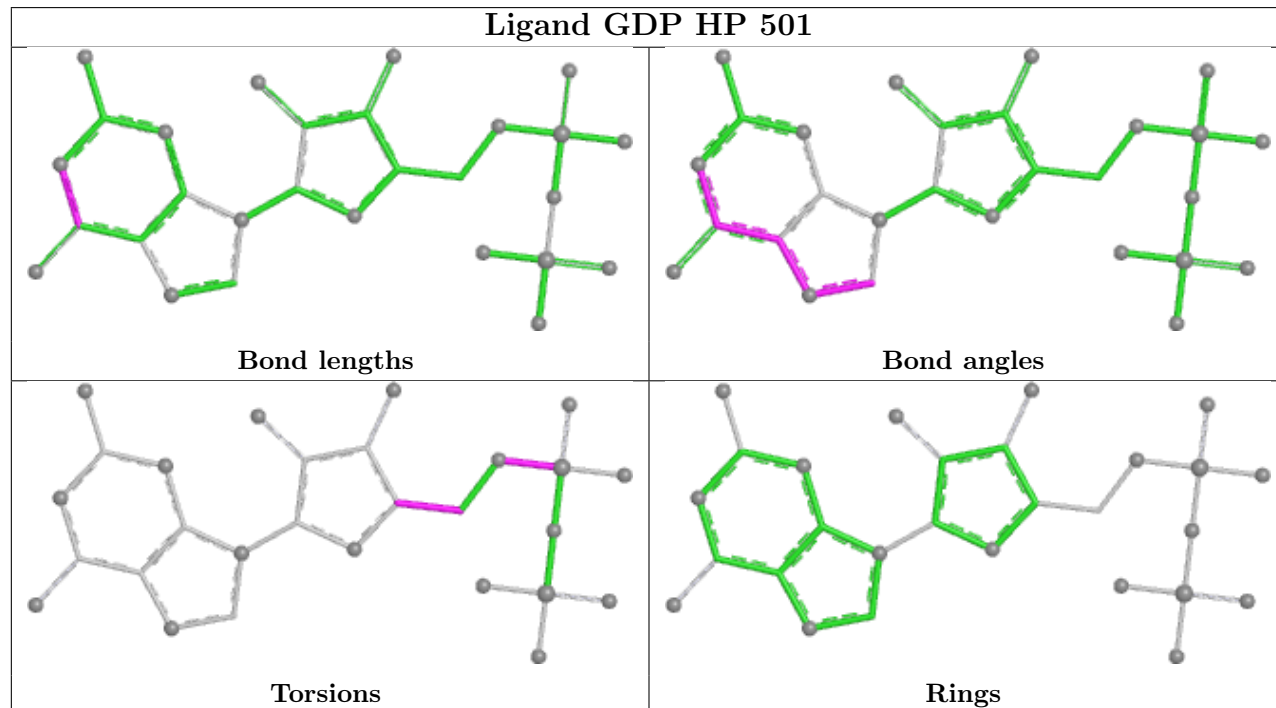
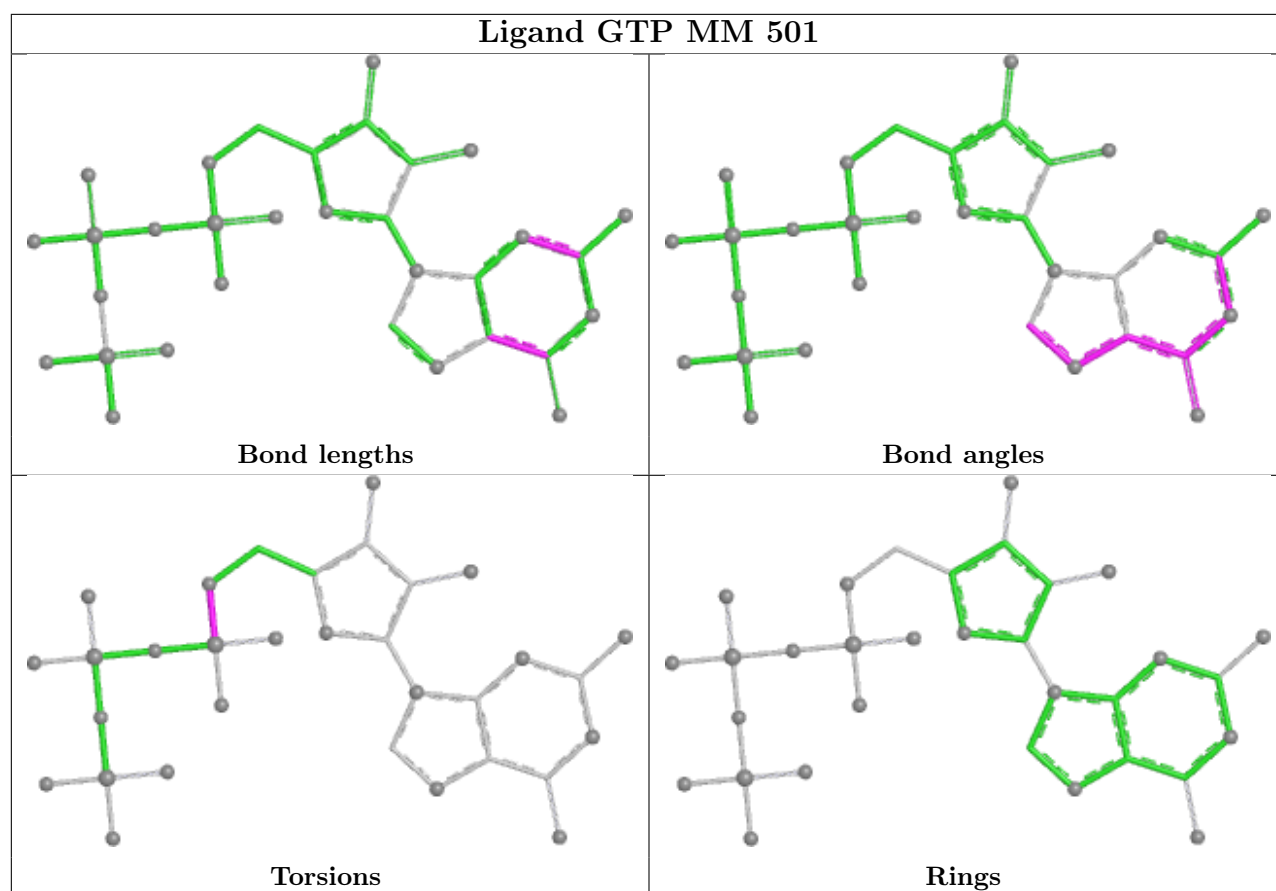
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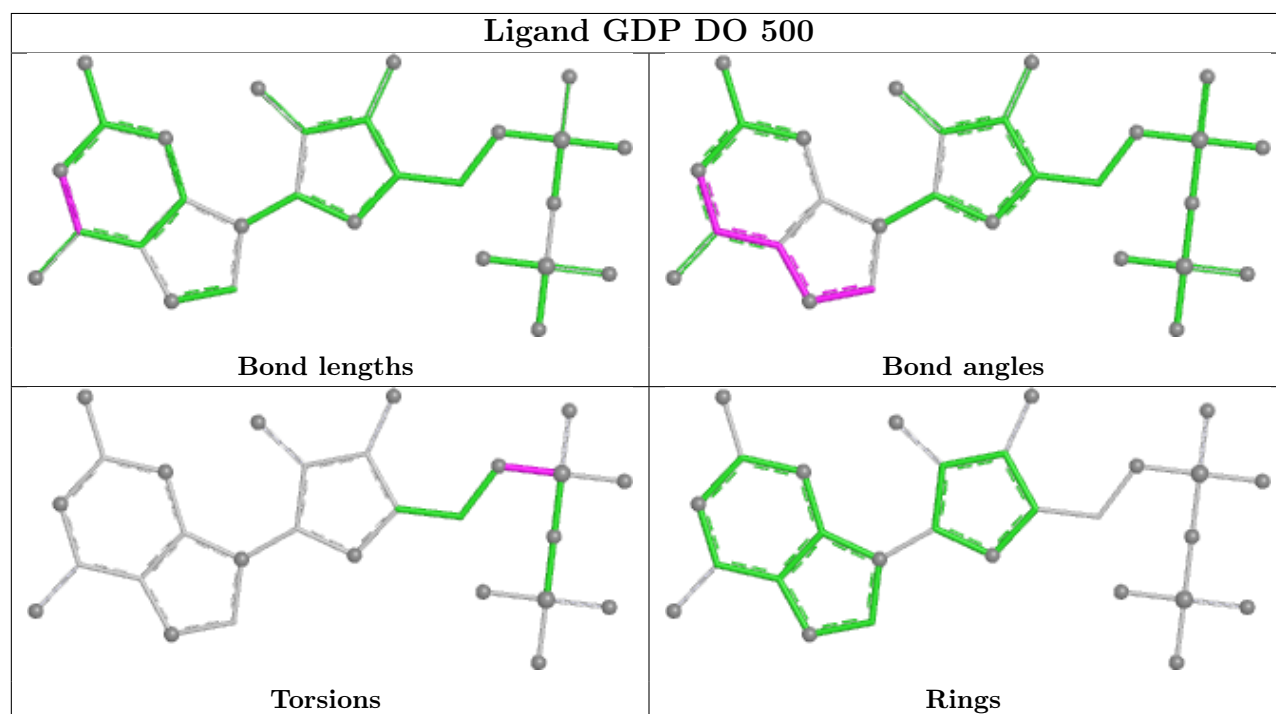
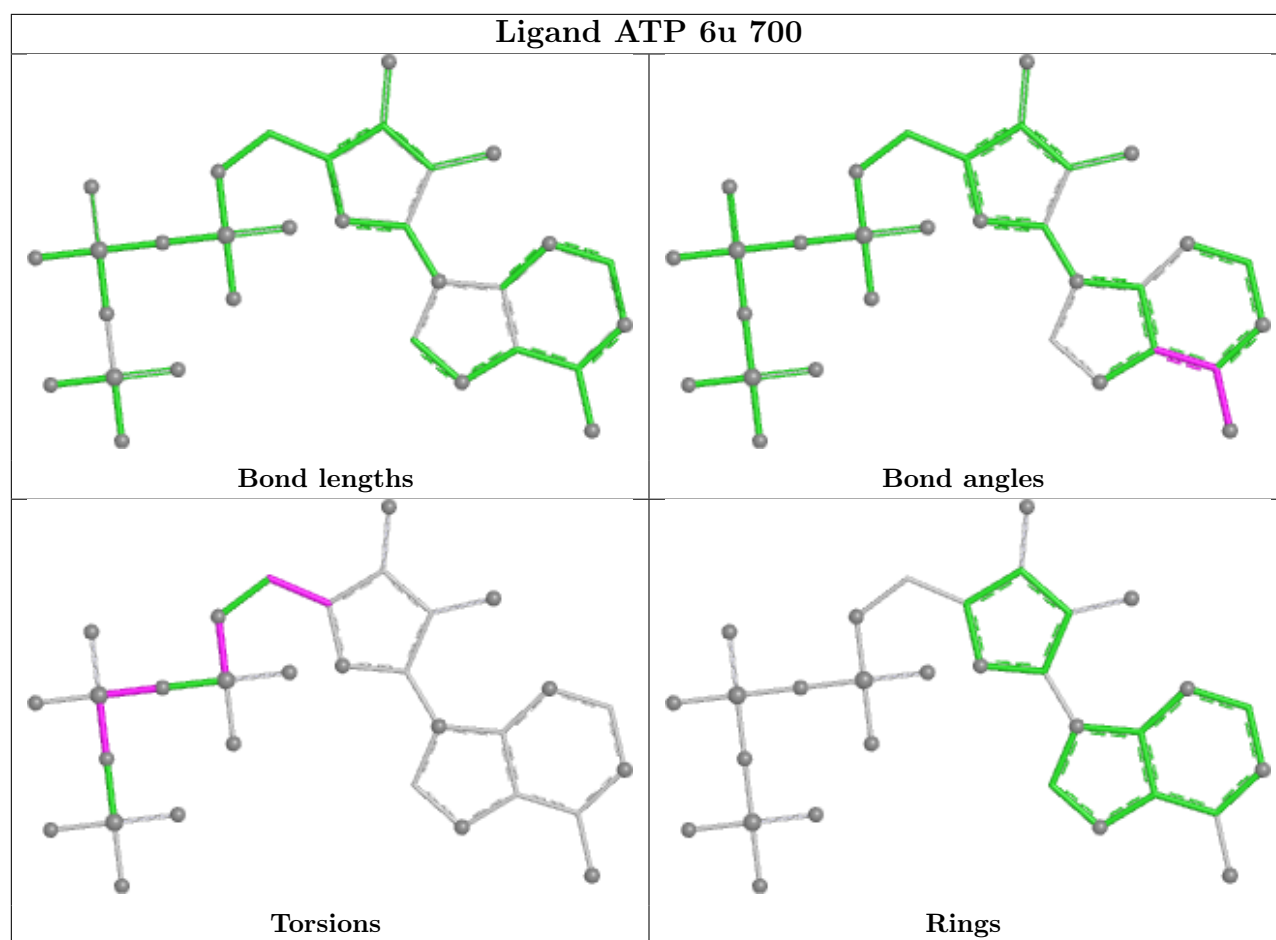


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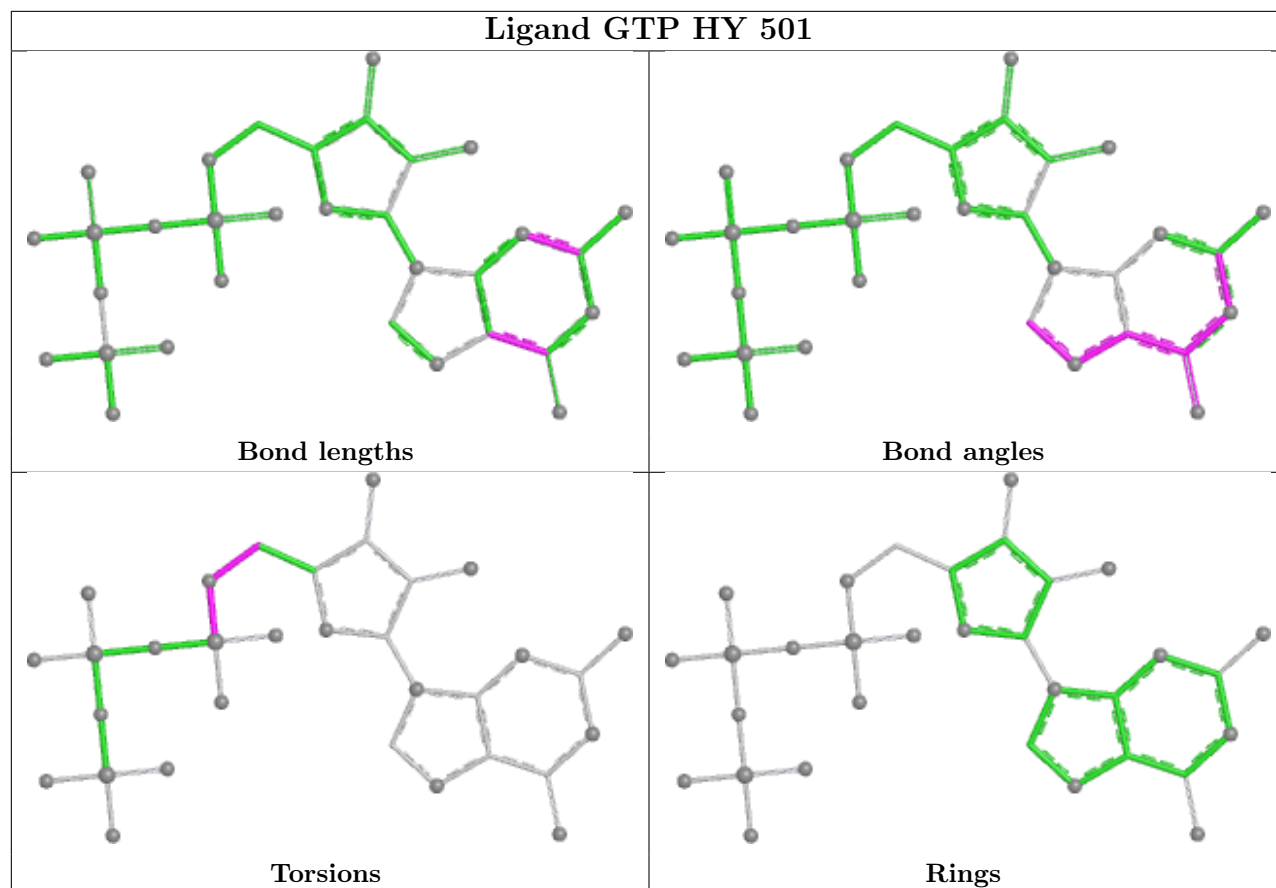




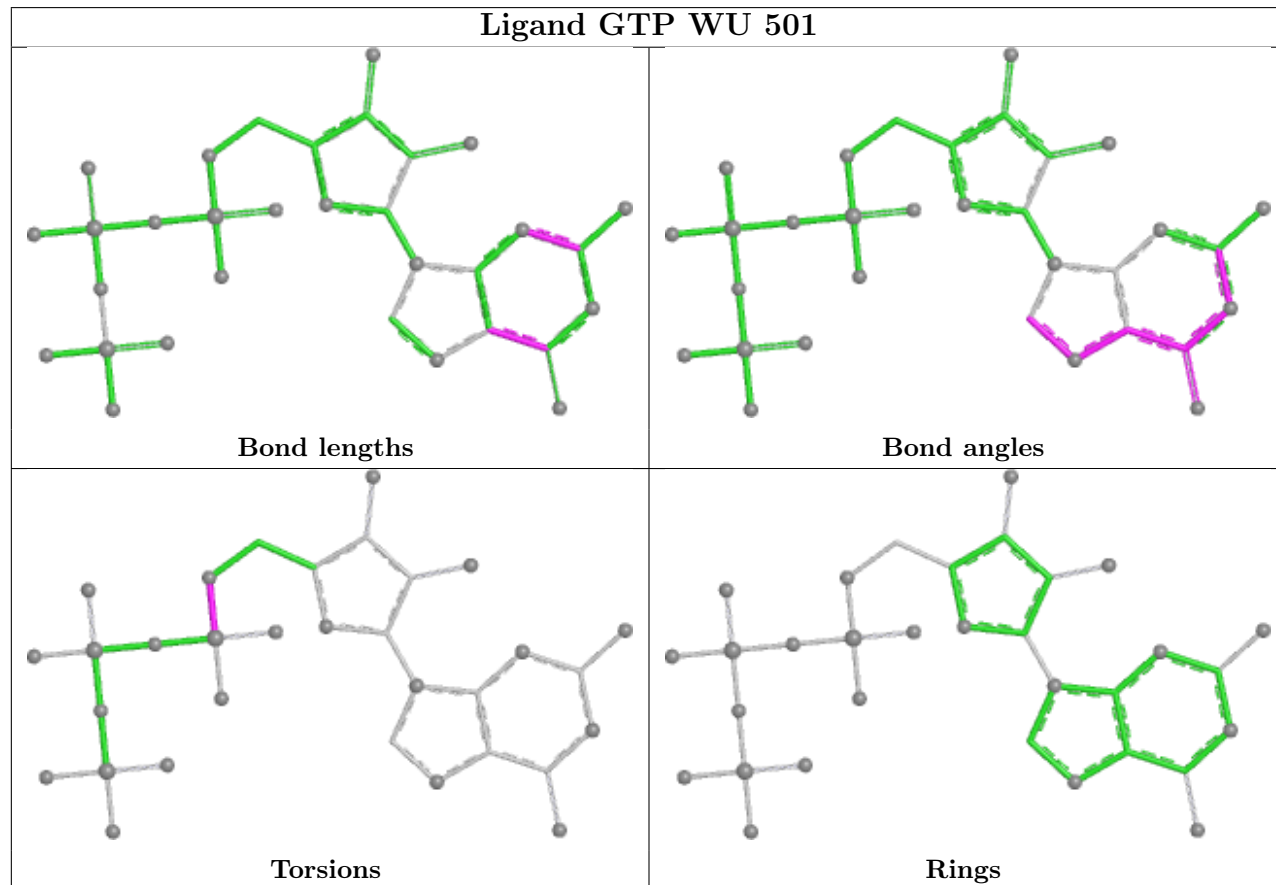


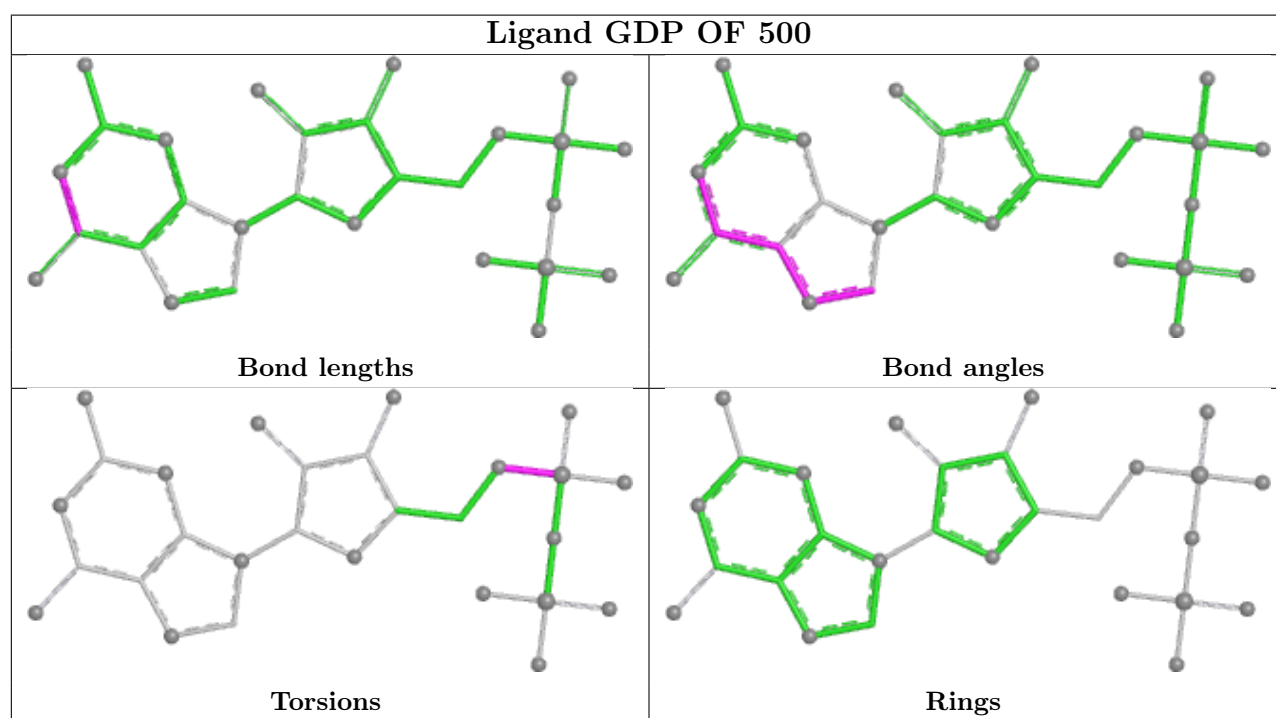
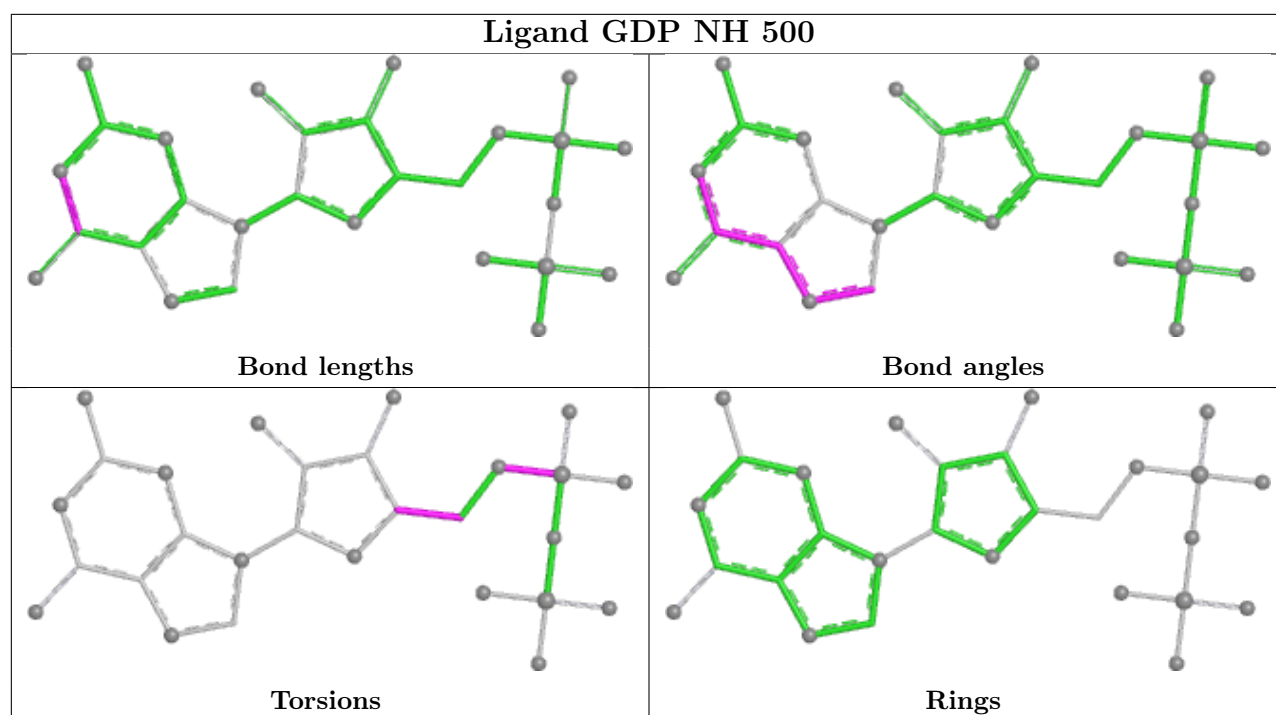


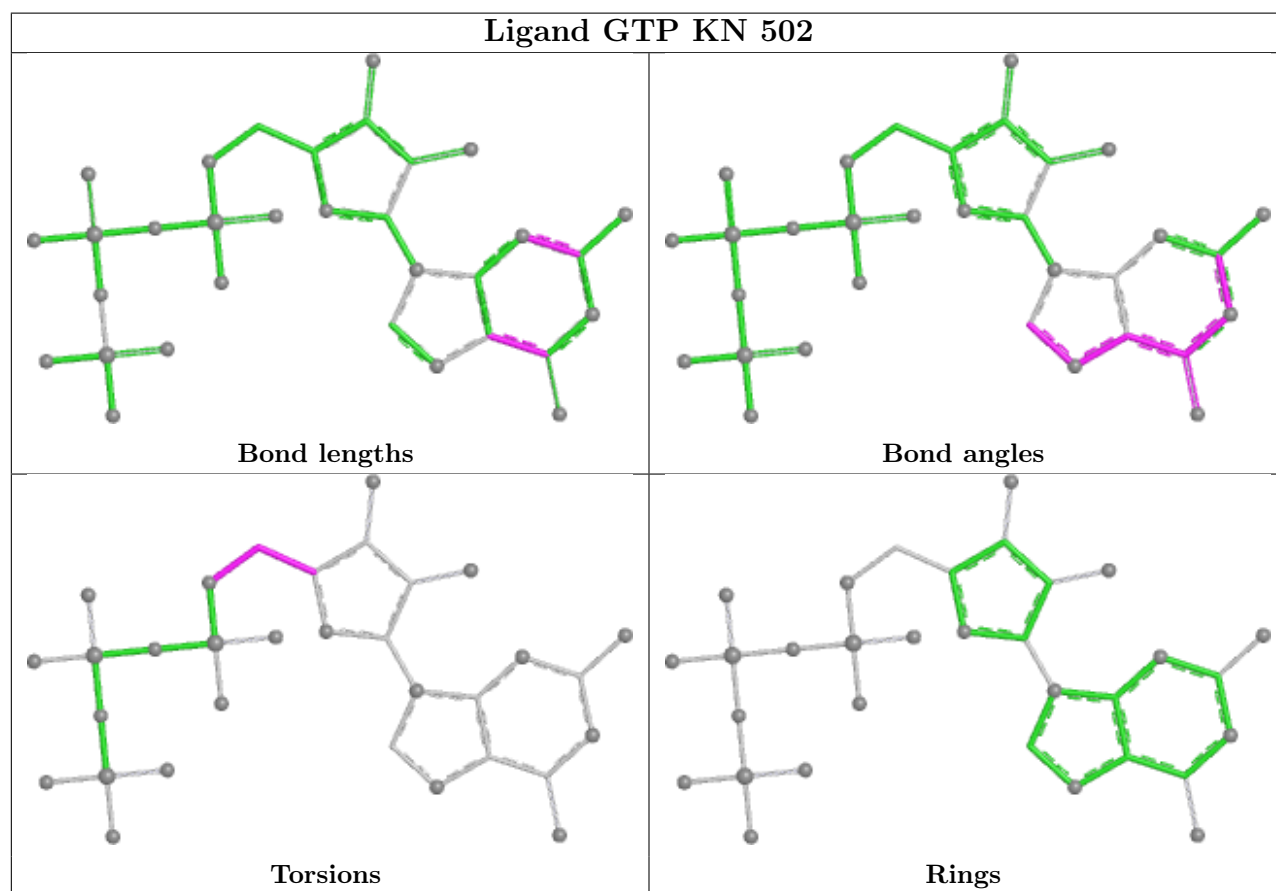
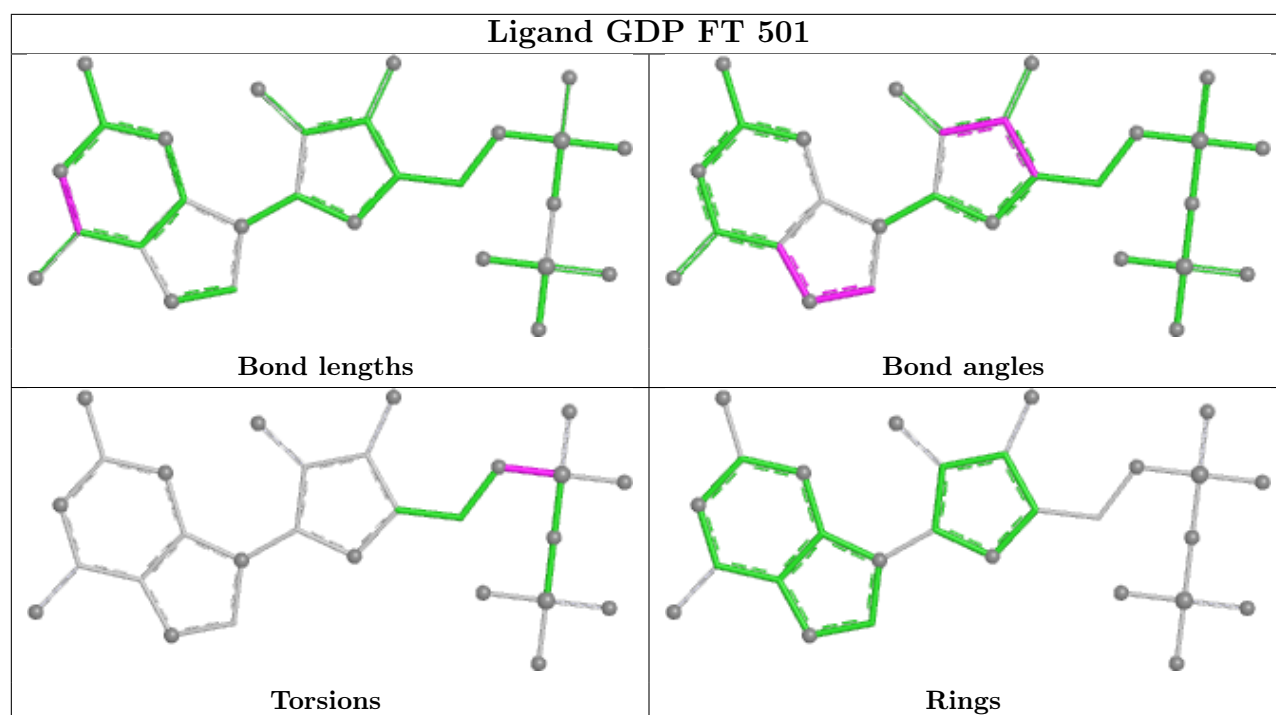
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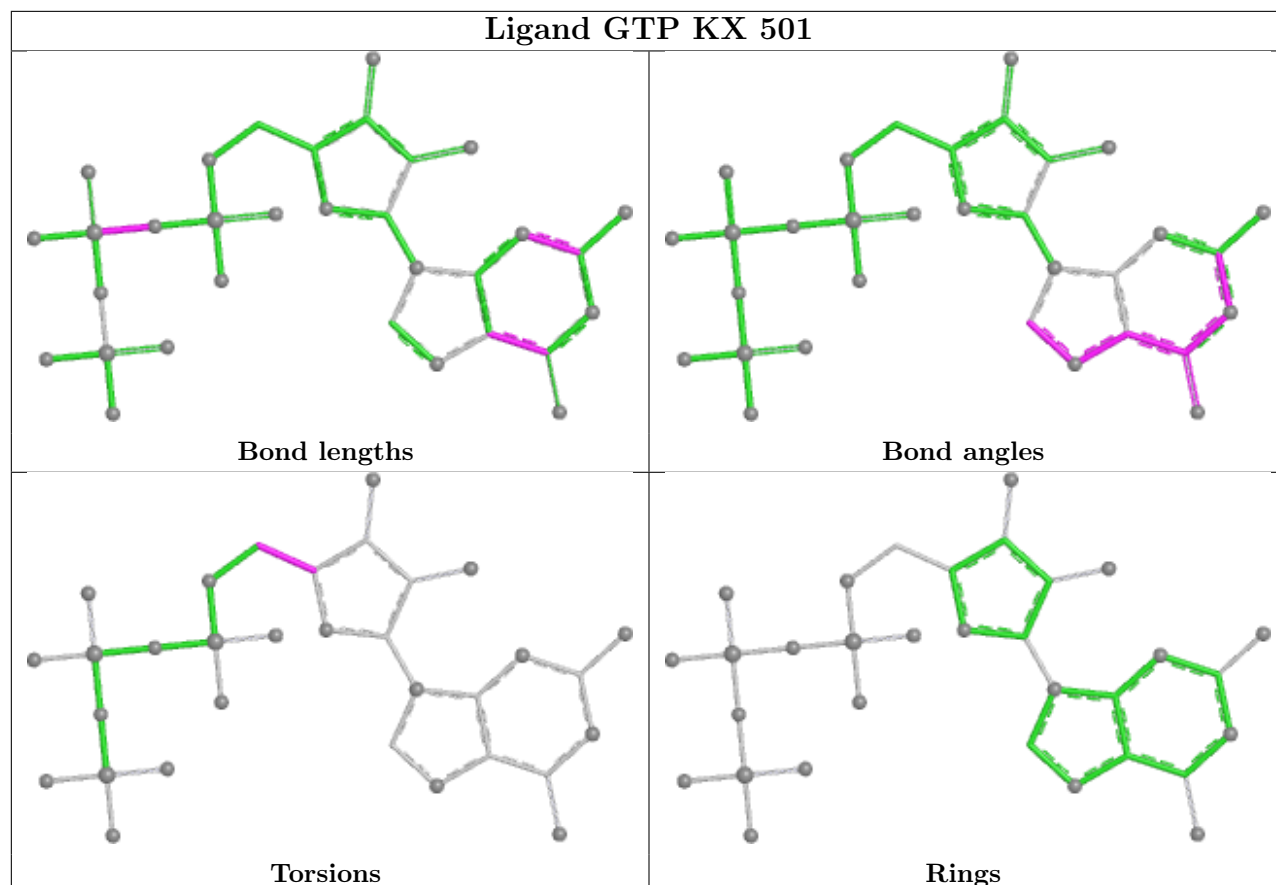
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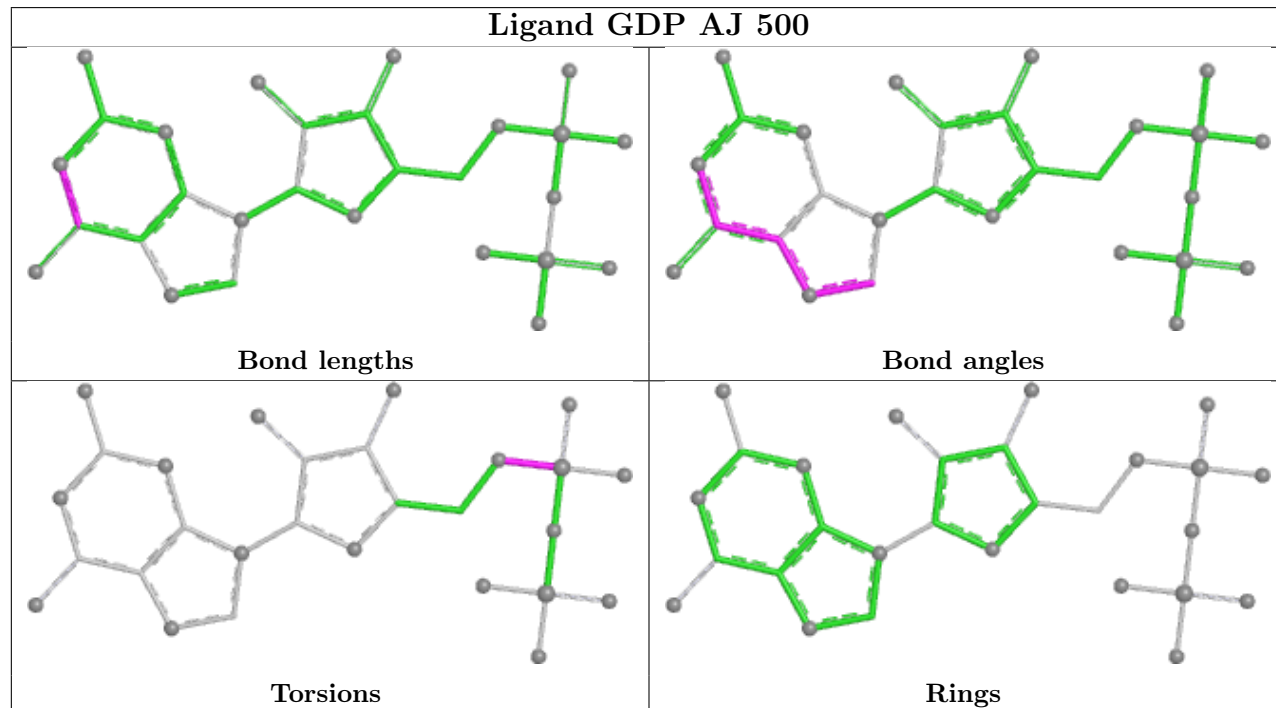


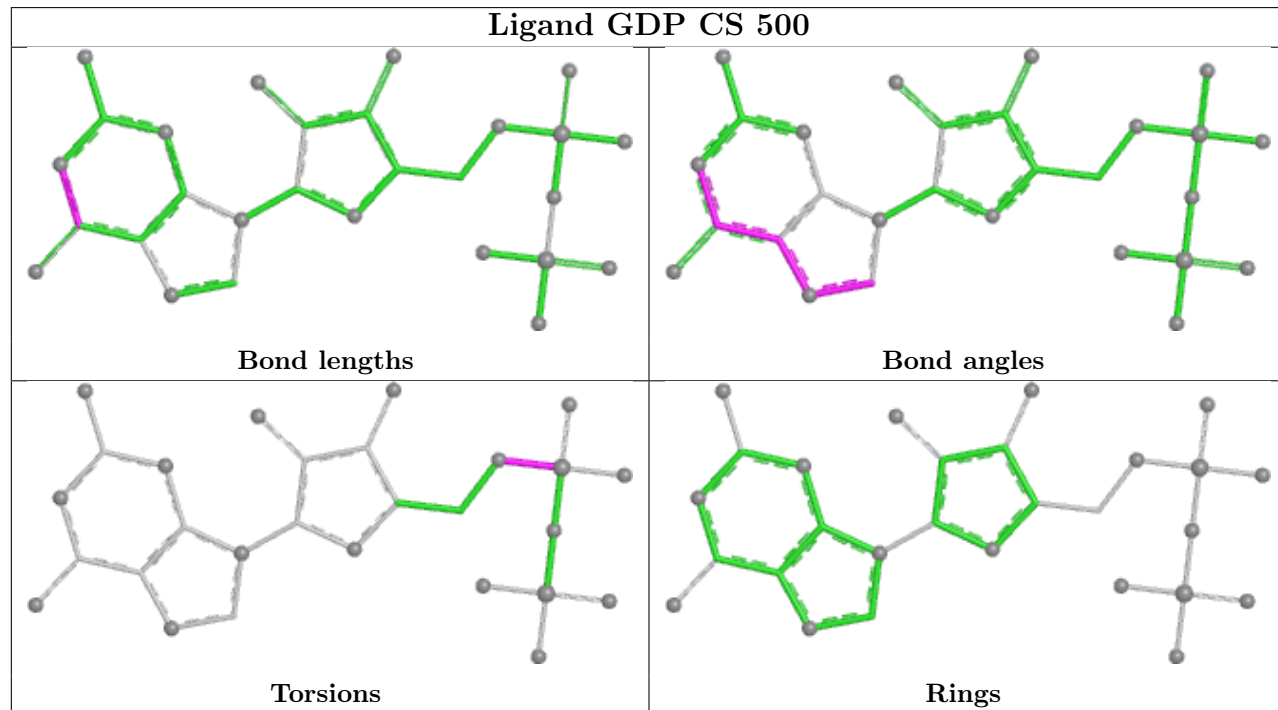
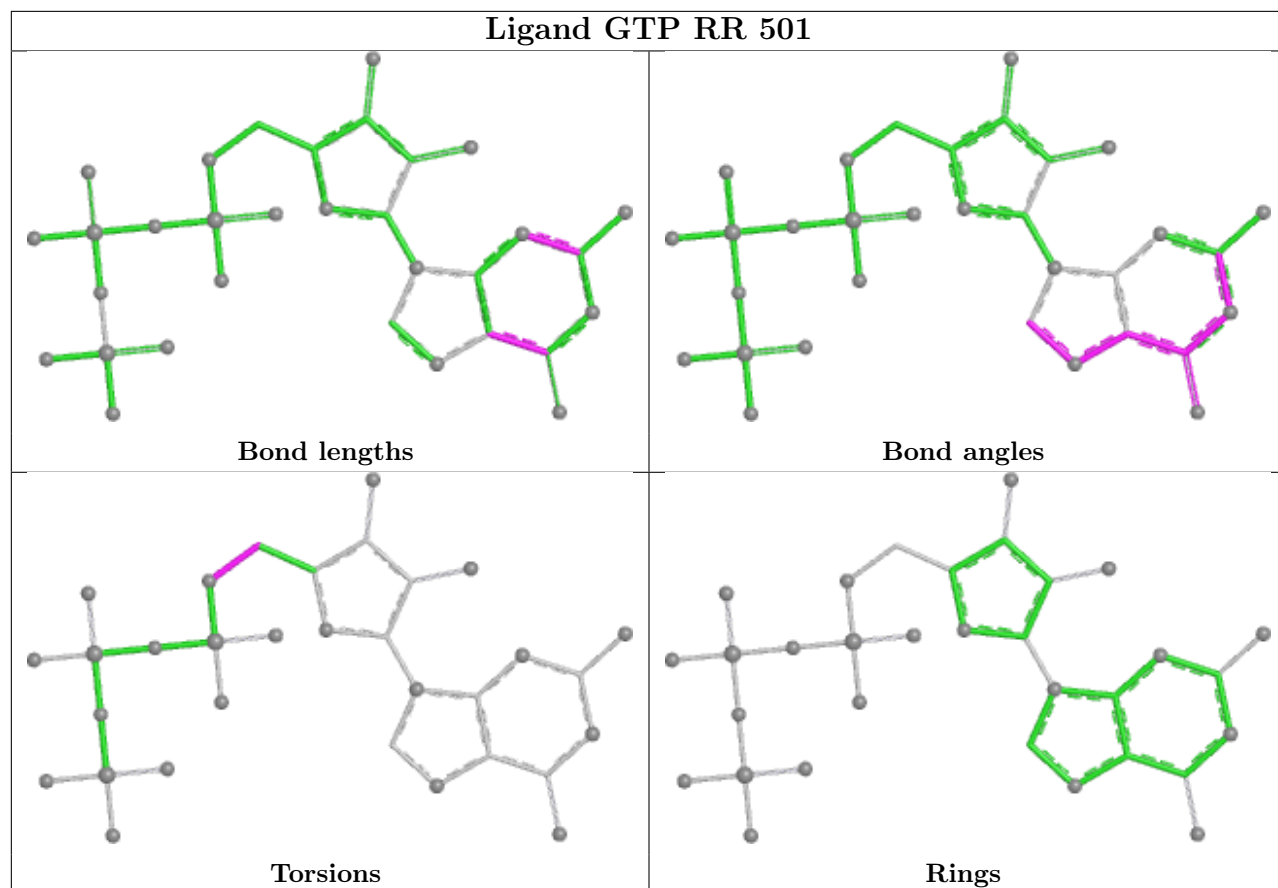


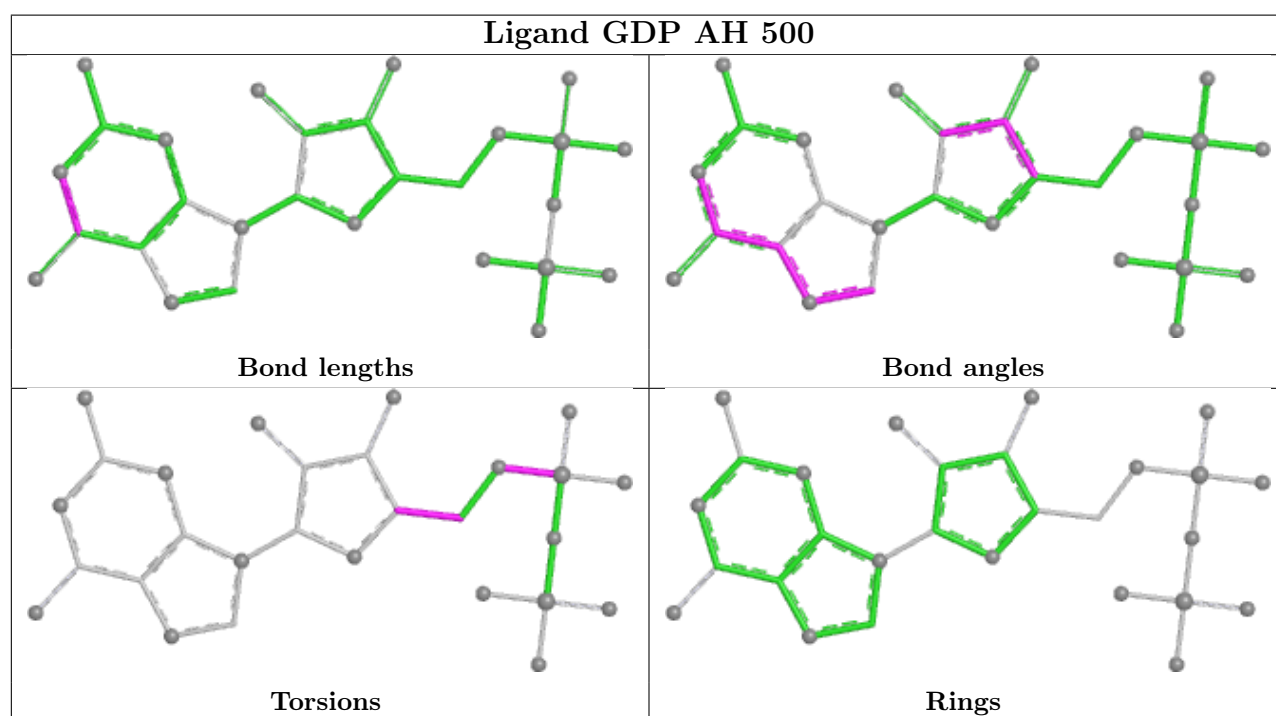
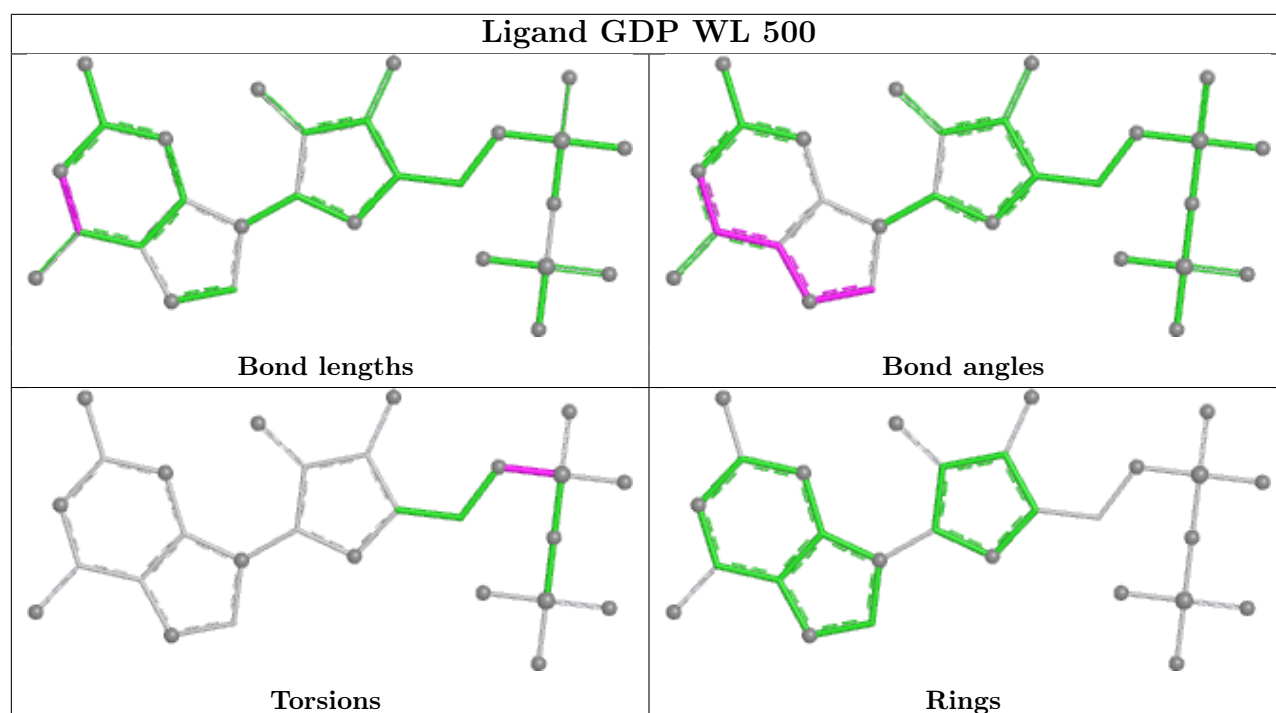
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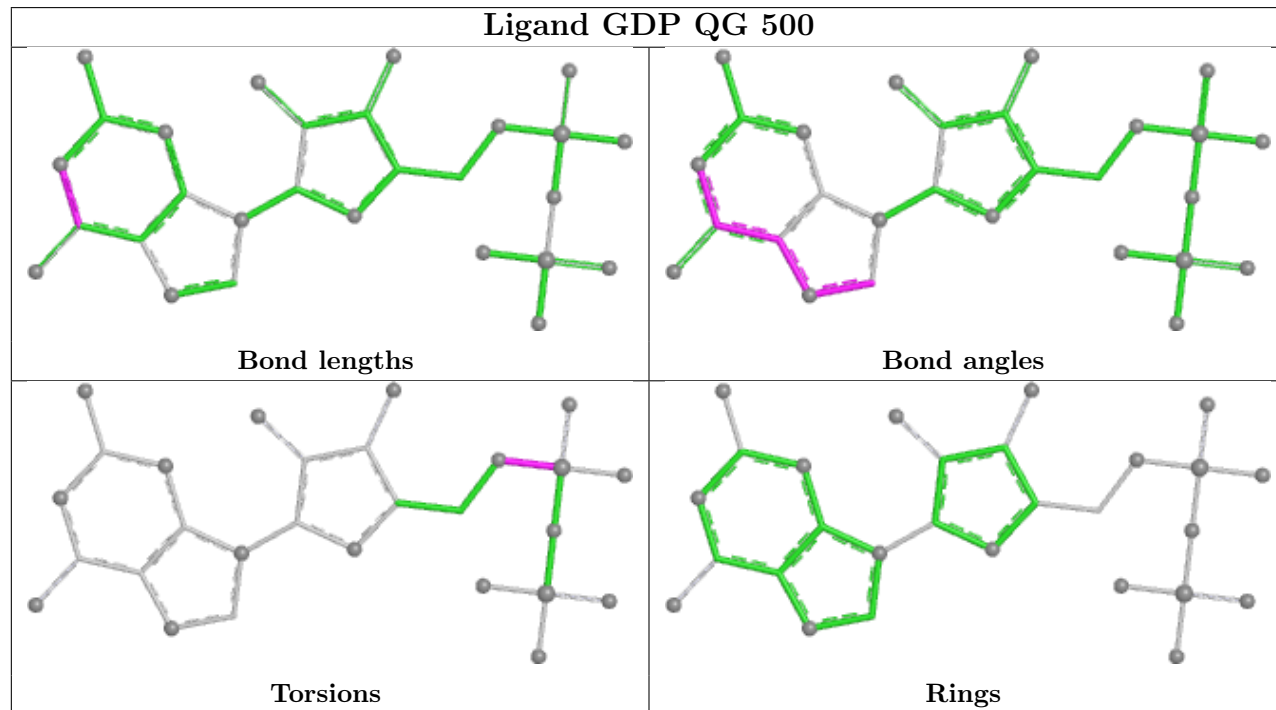
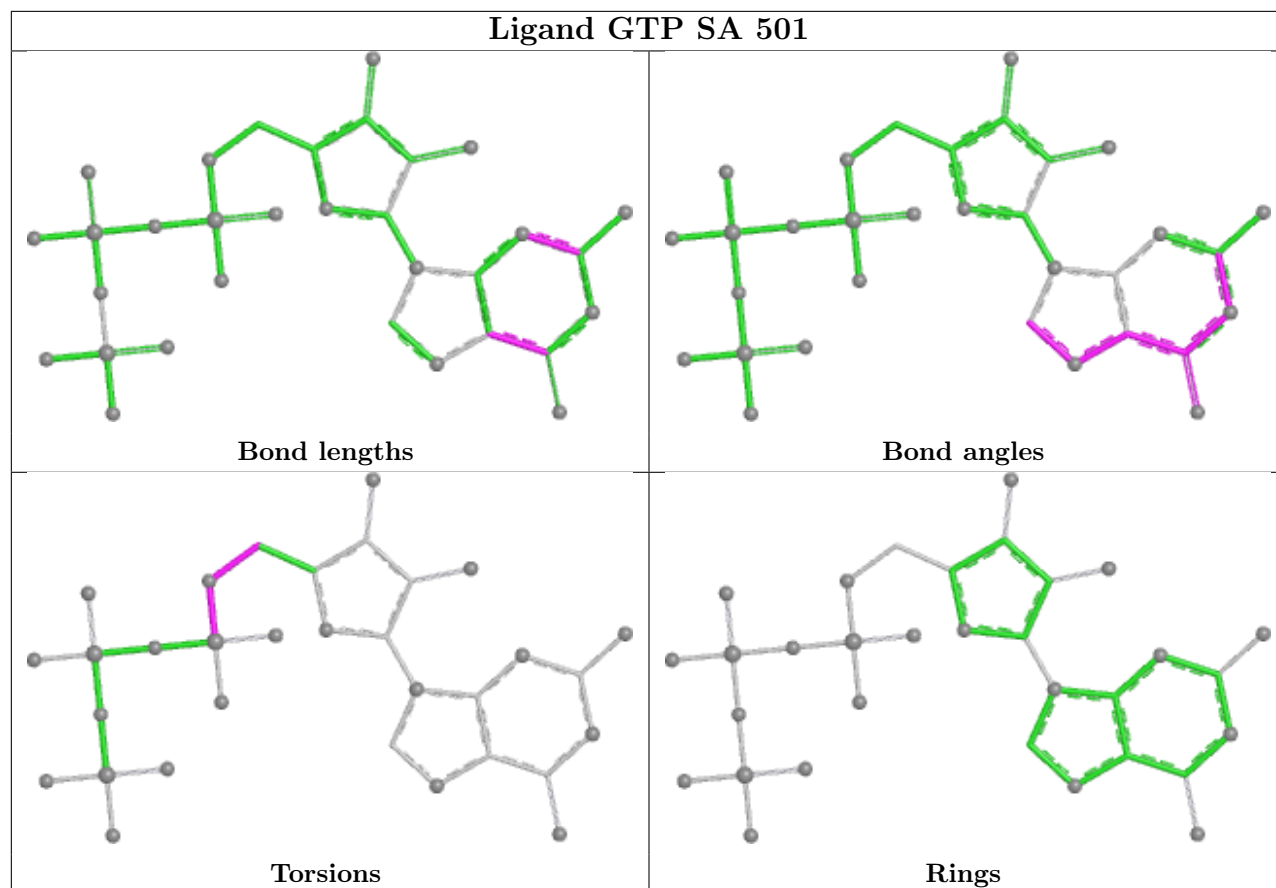


Ligand GDP AJ 500

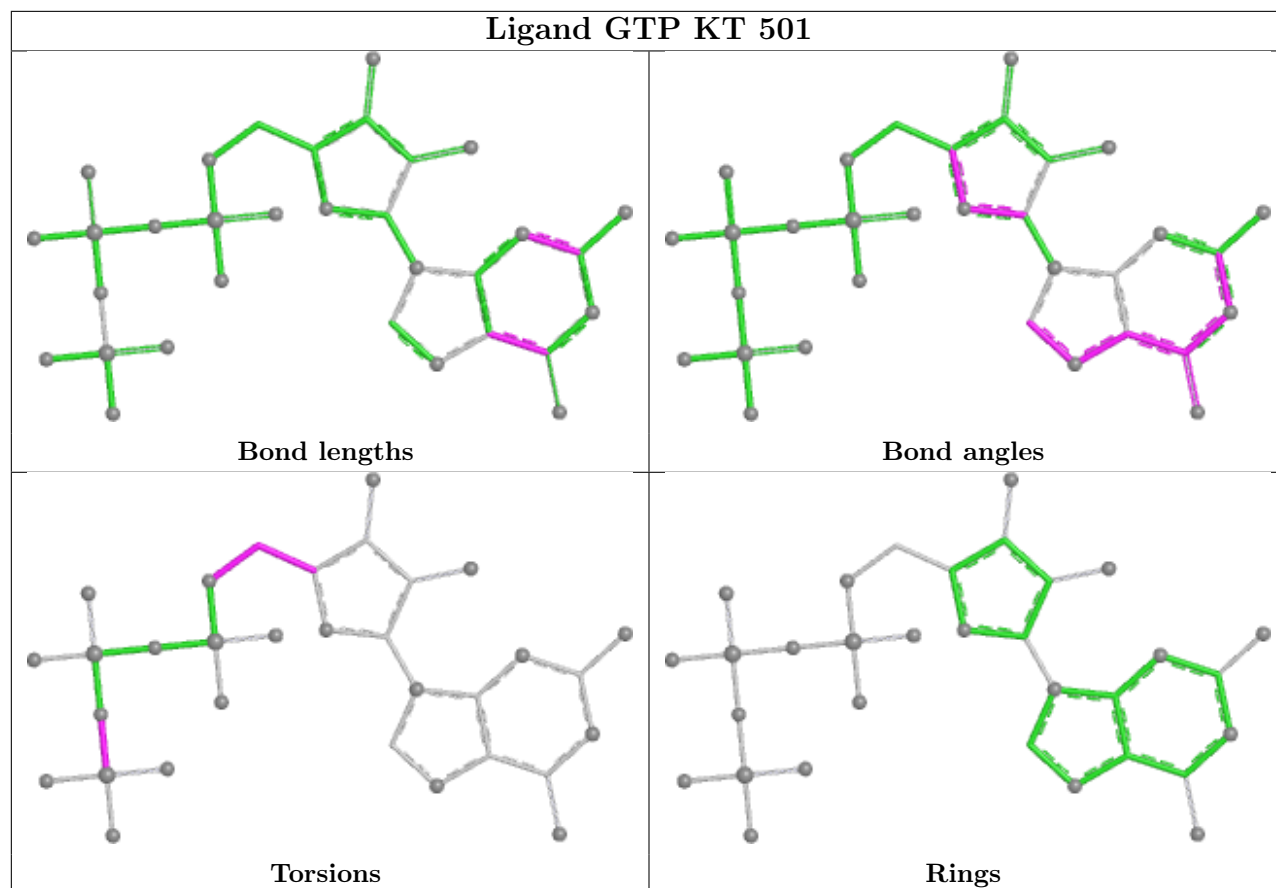




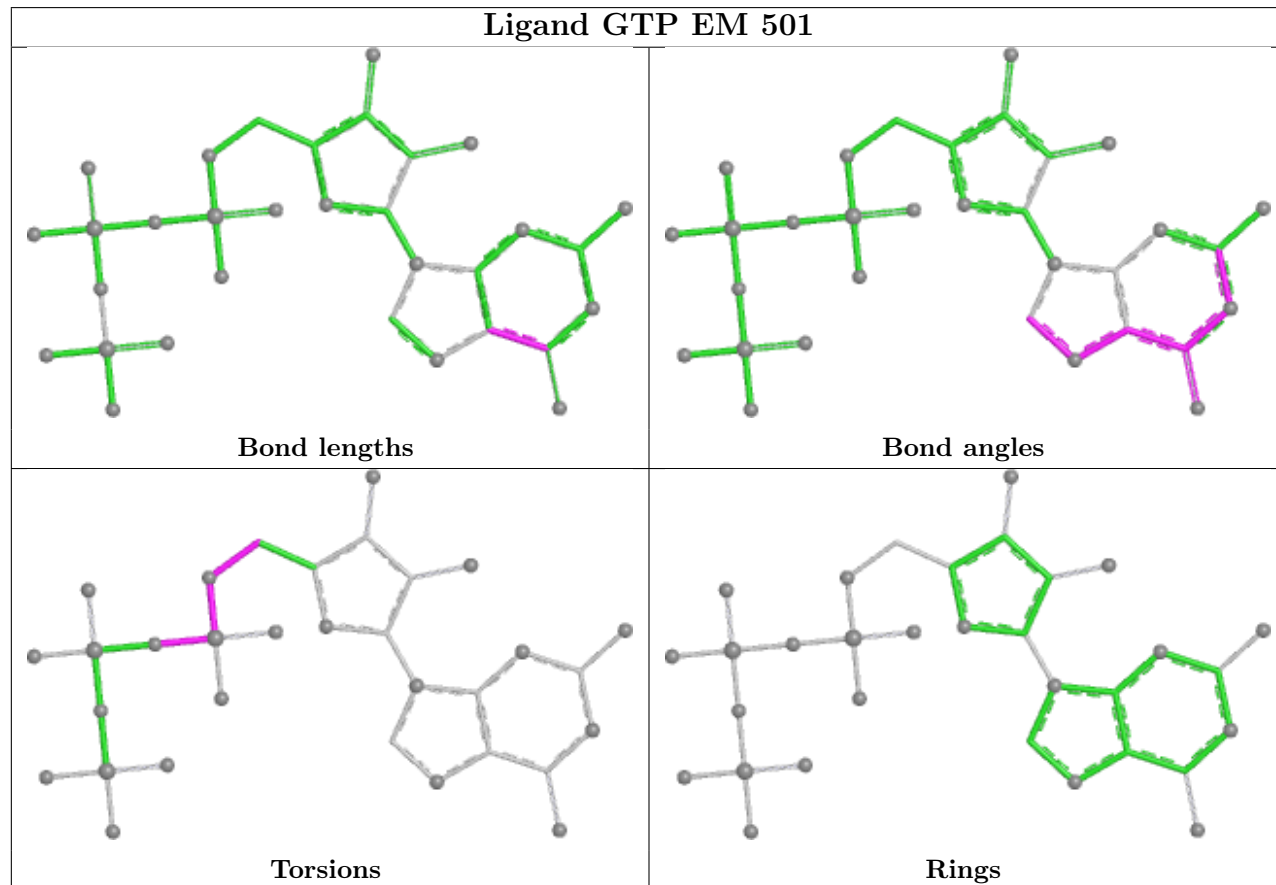




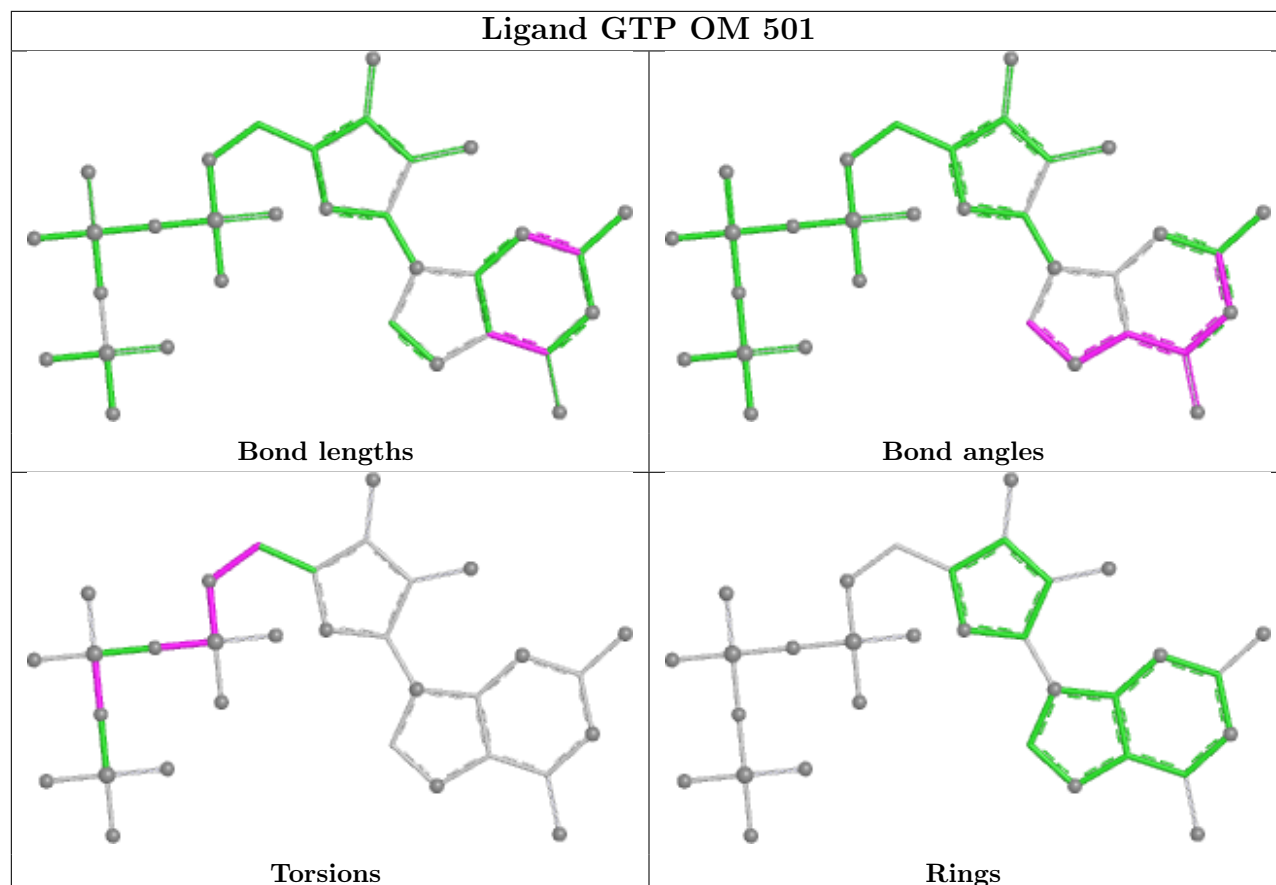
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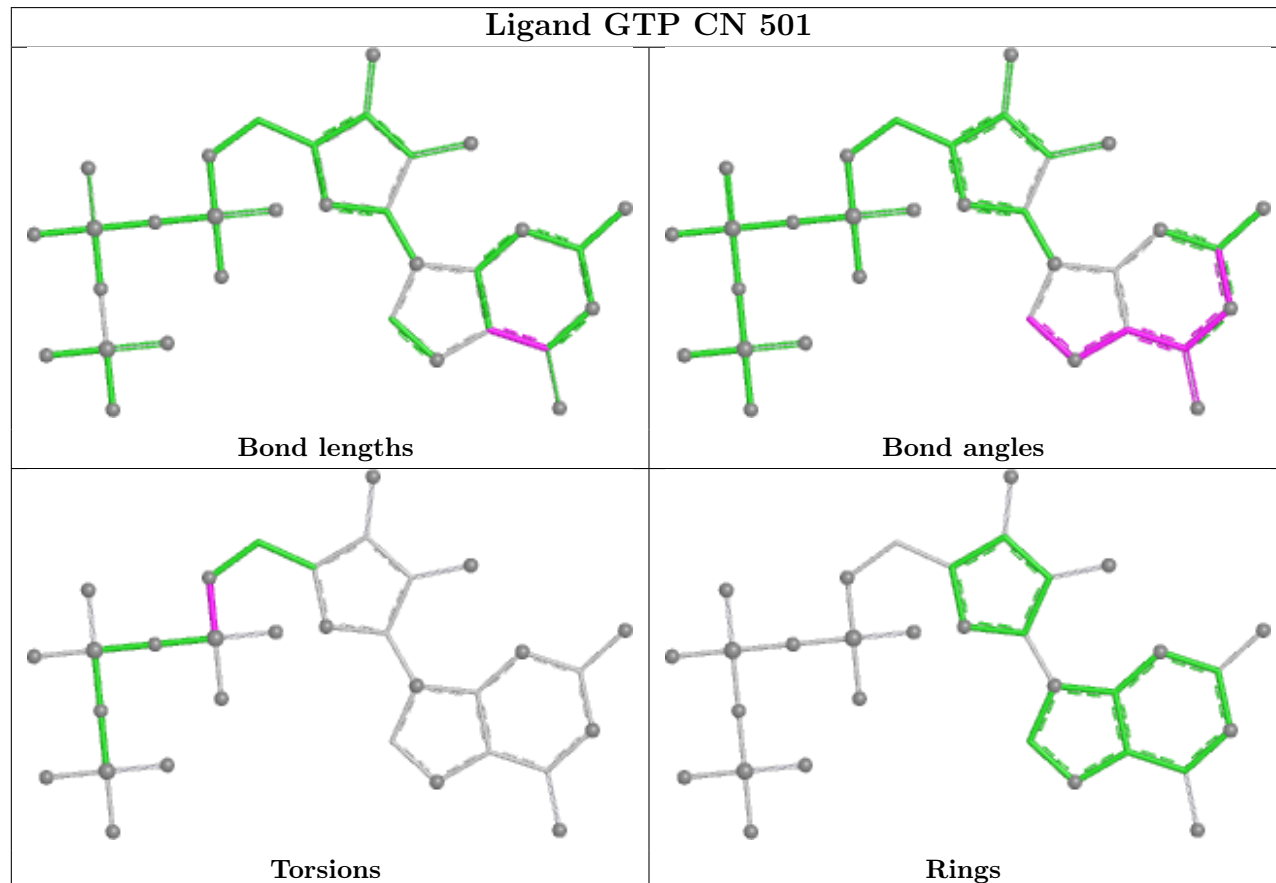
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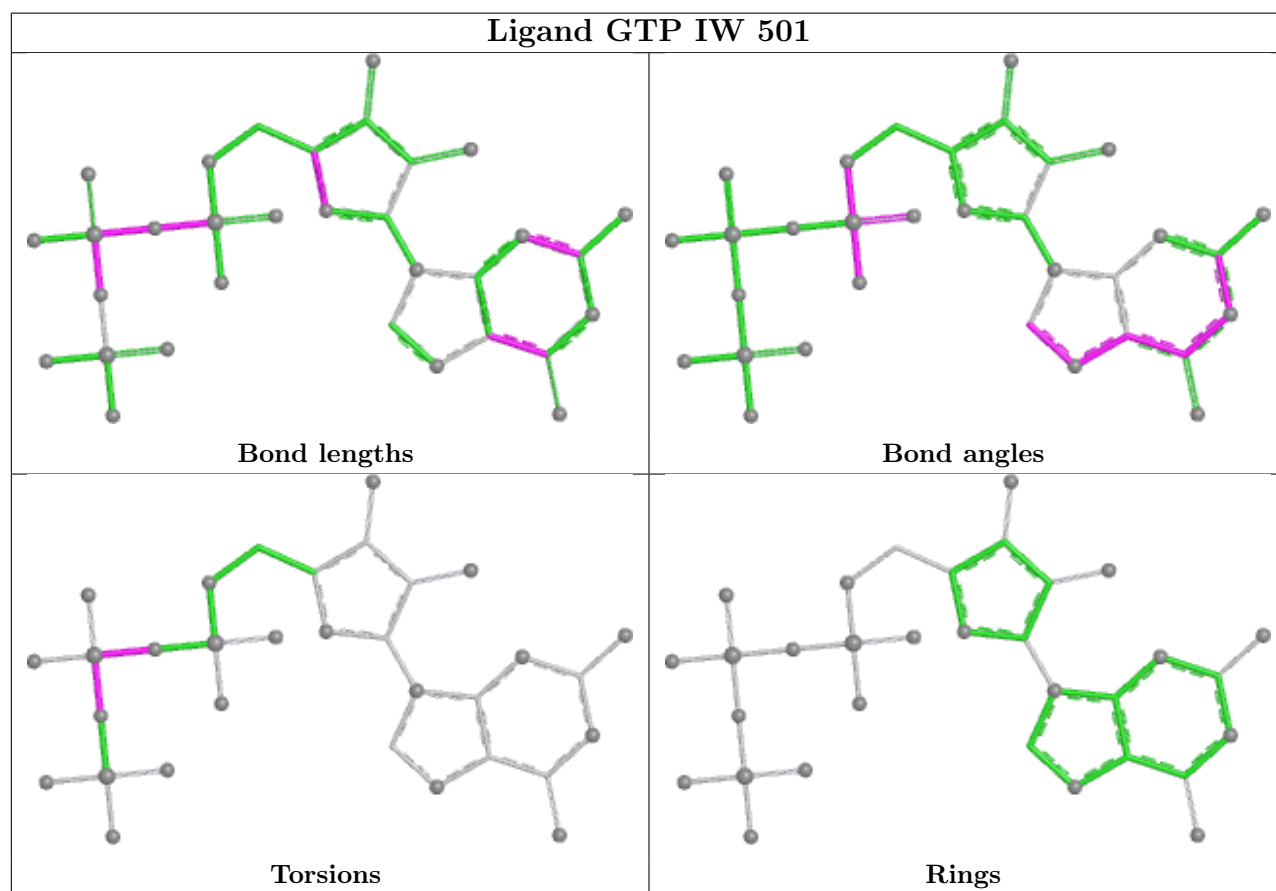
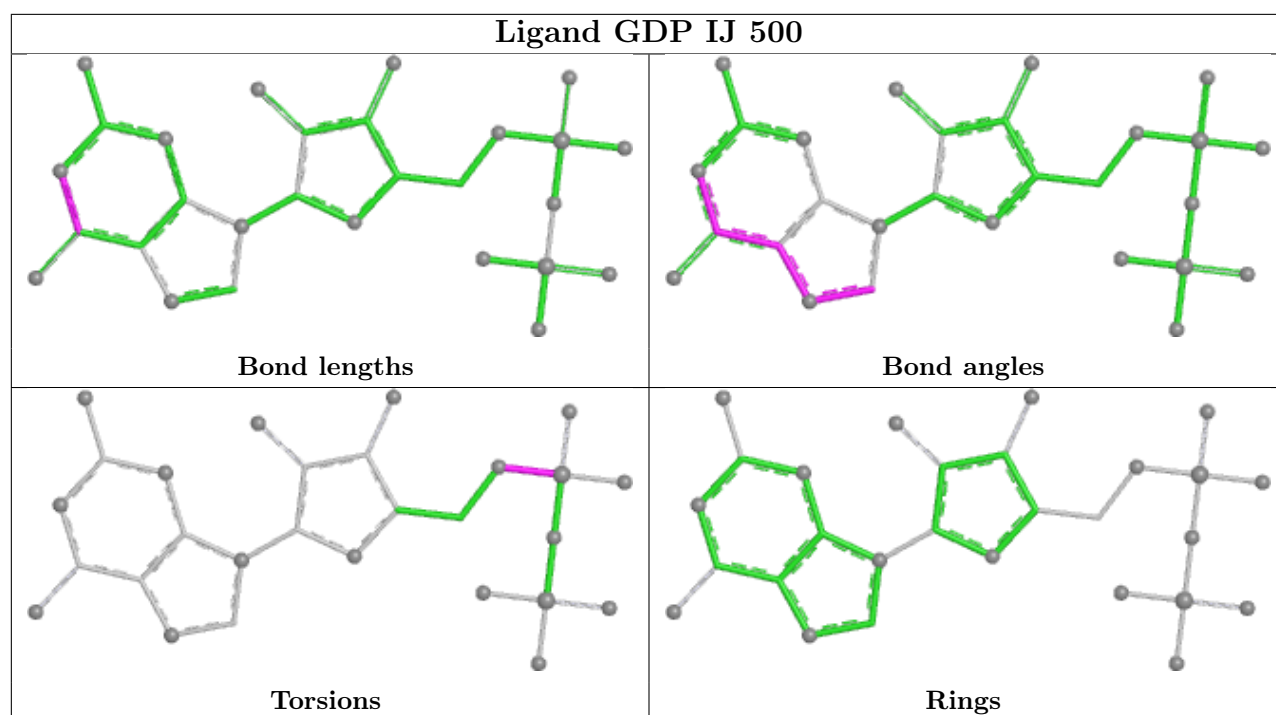


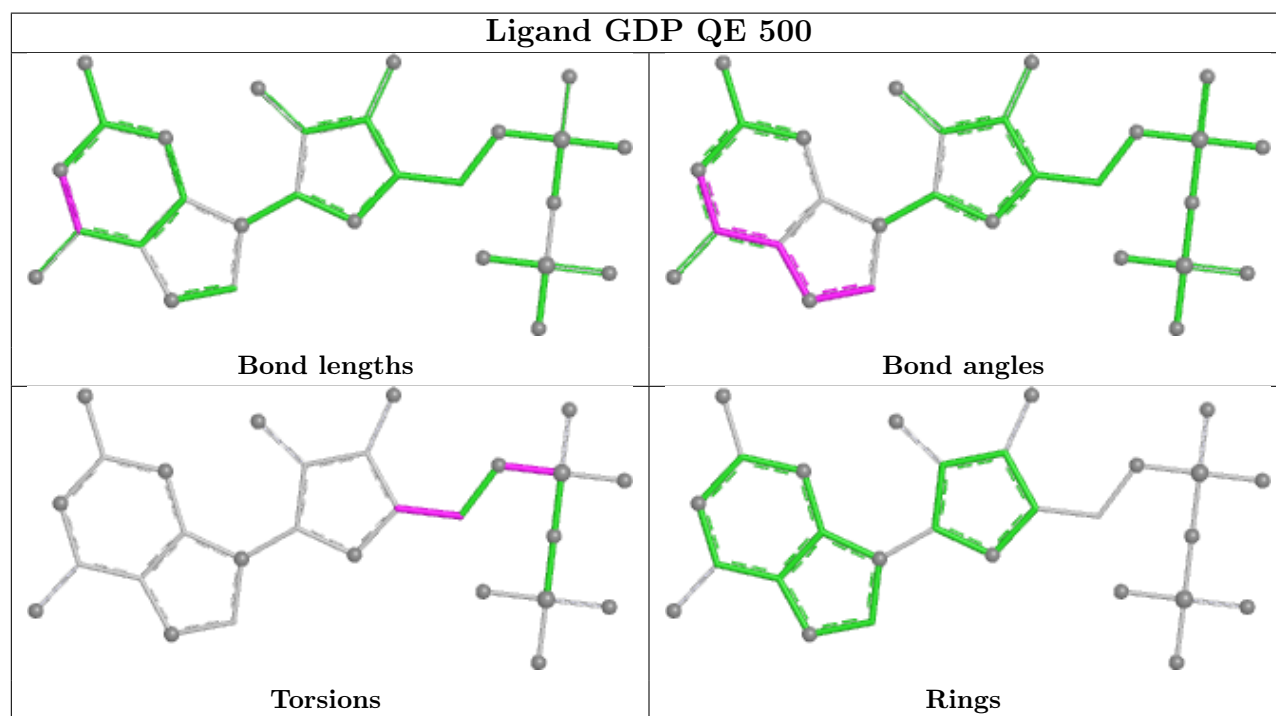
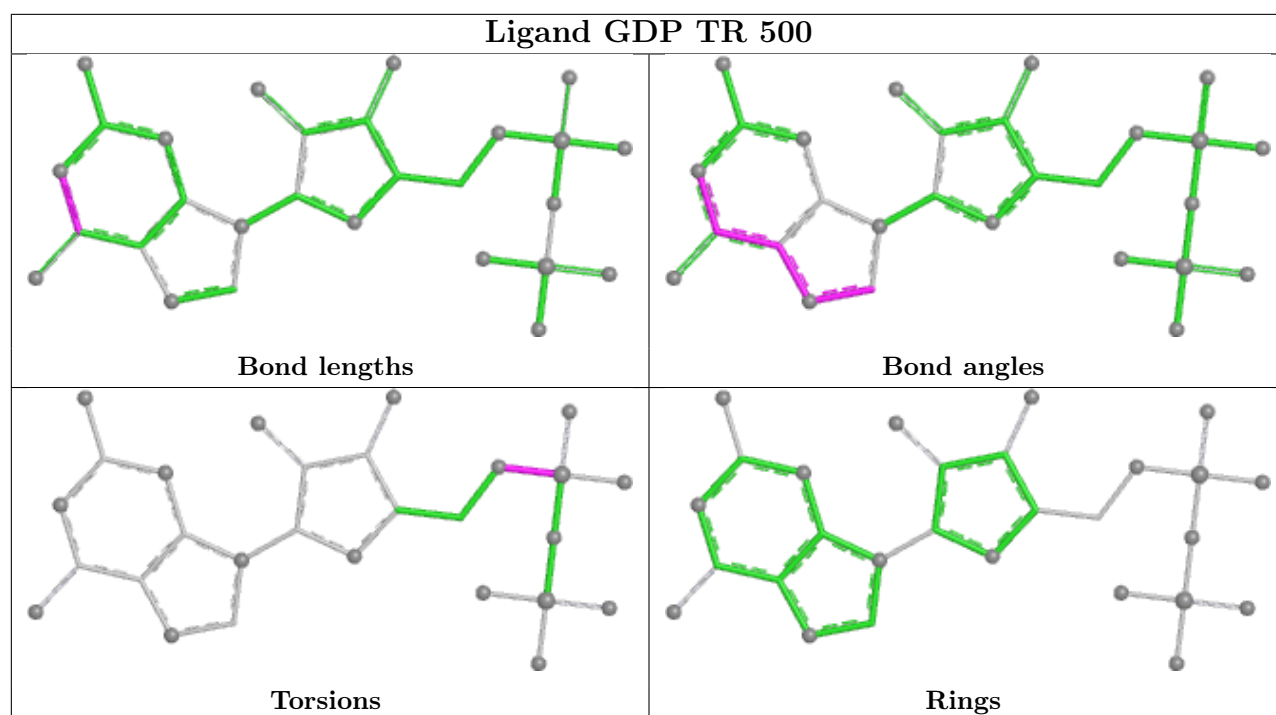
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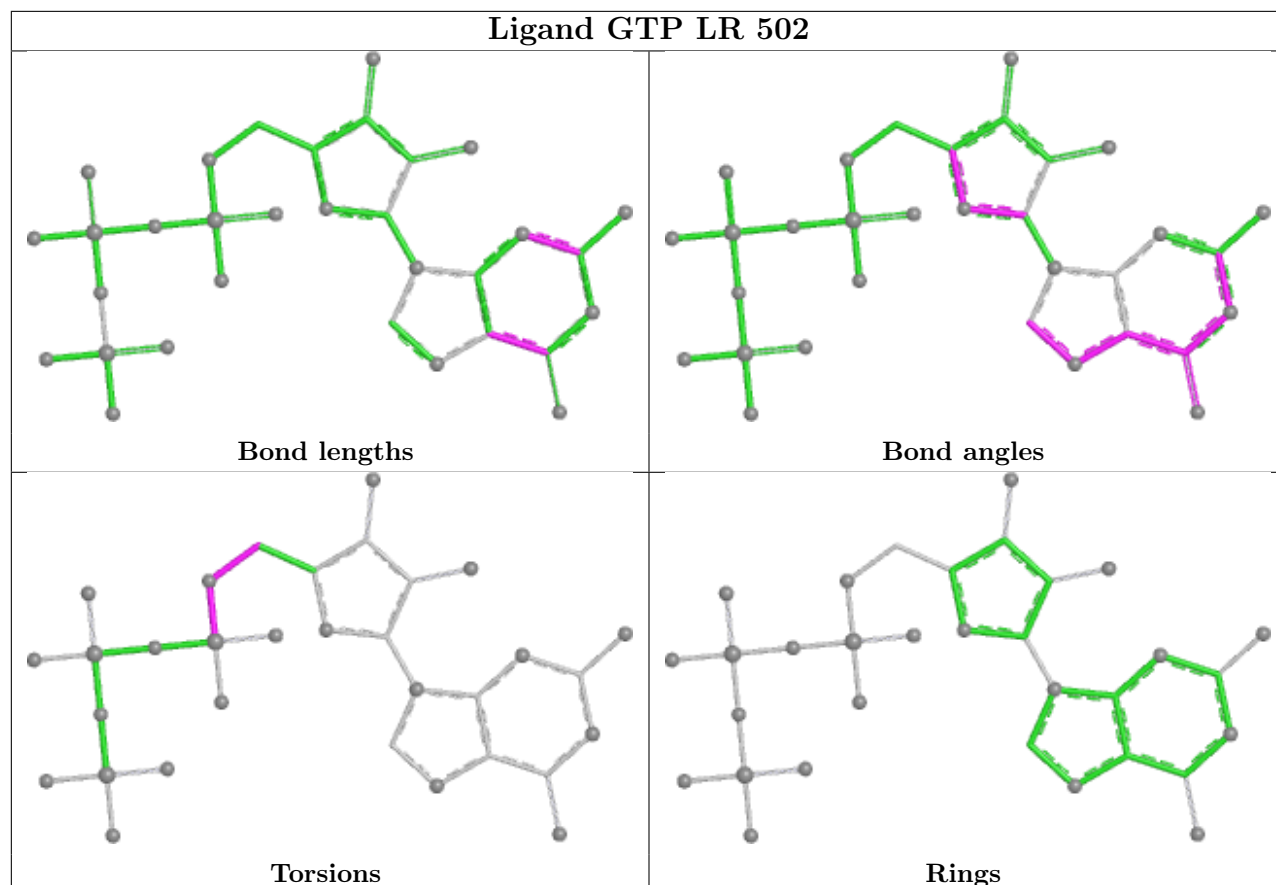
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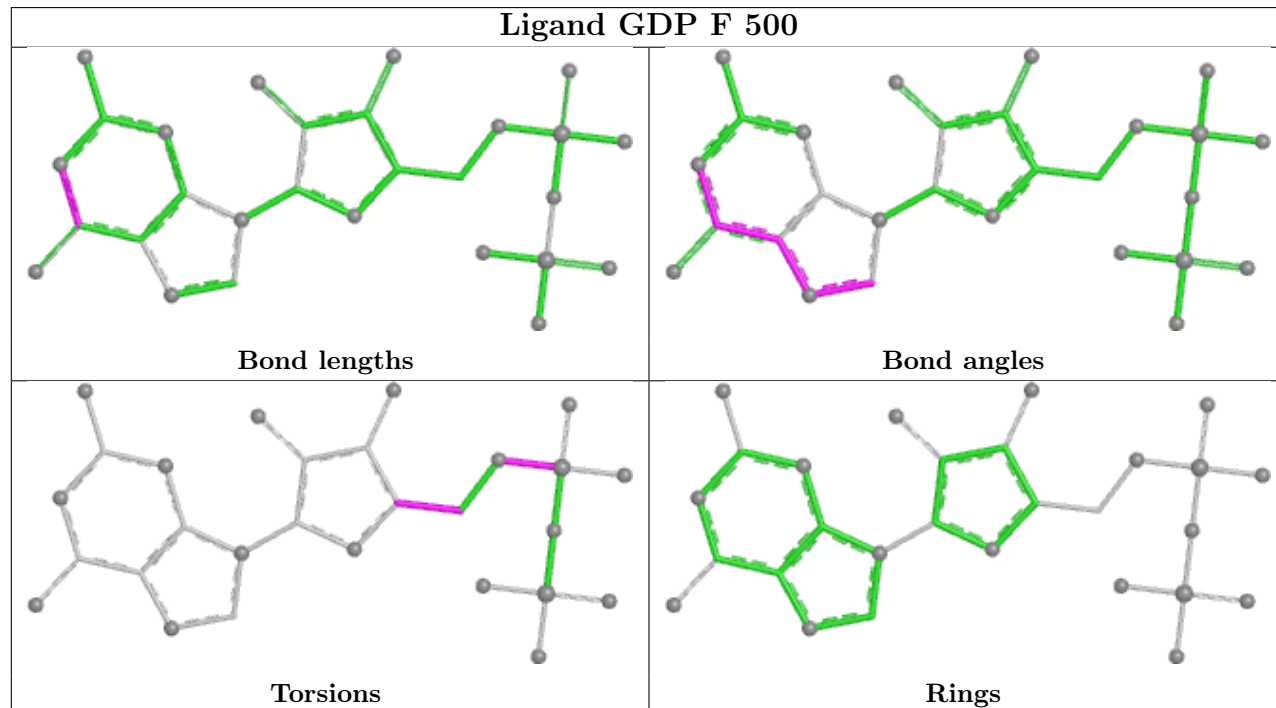


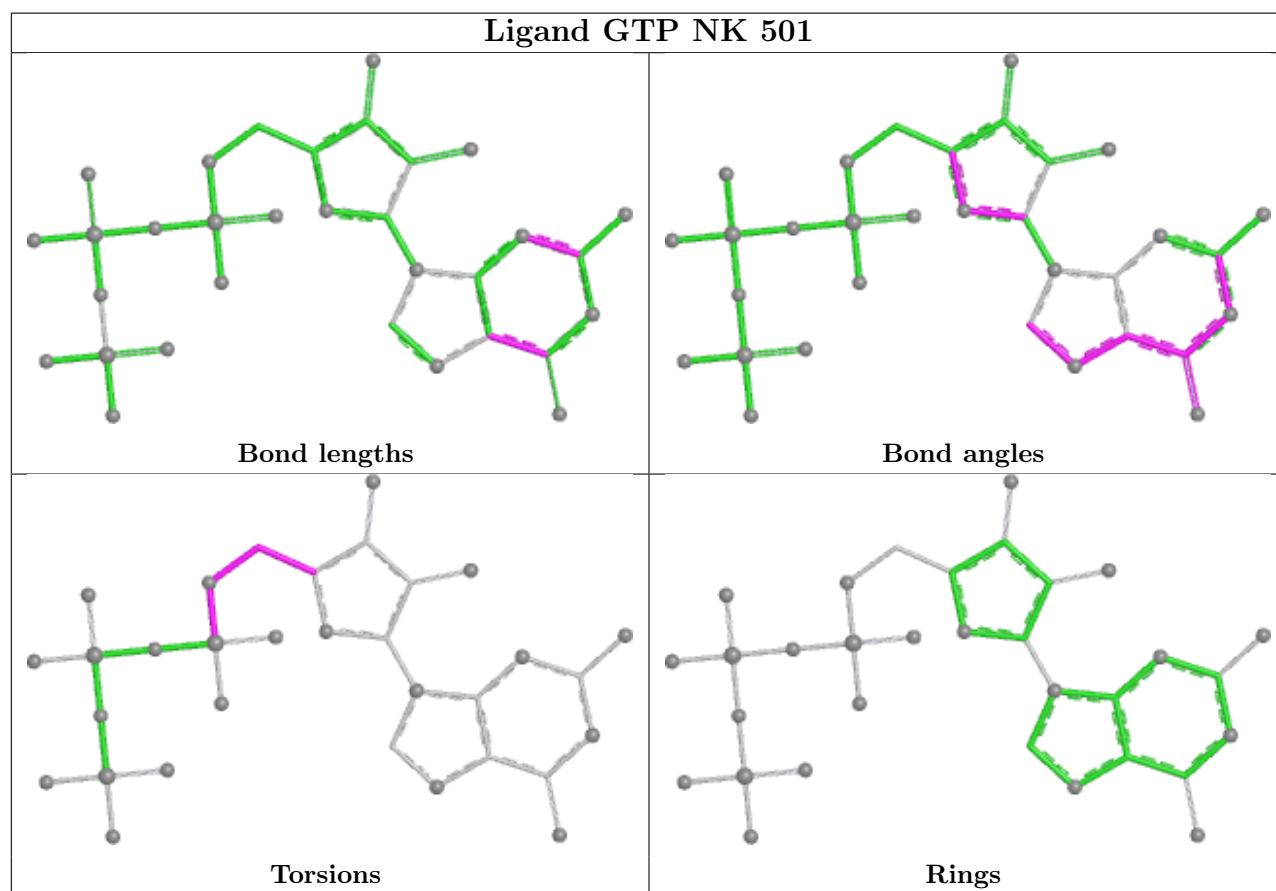
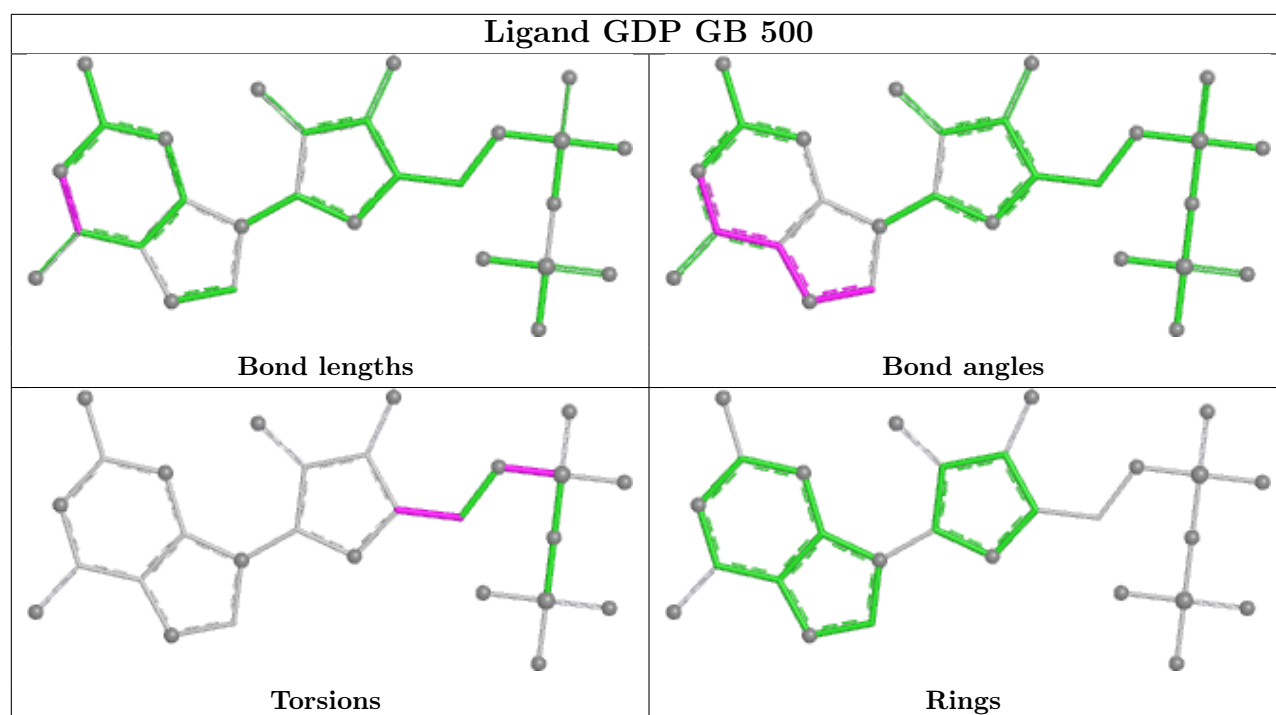


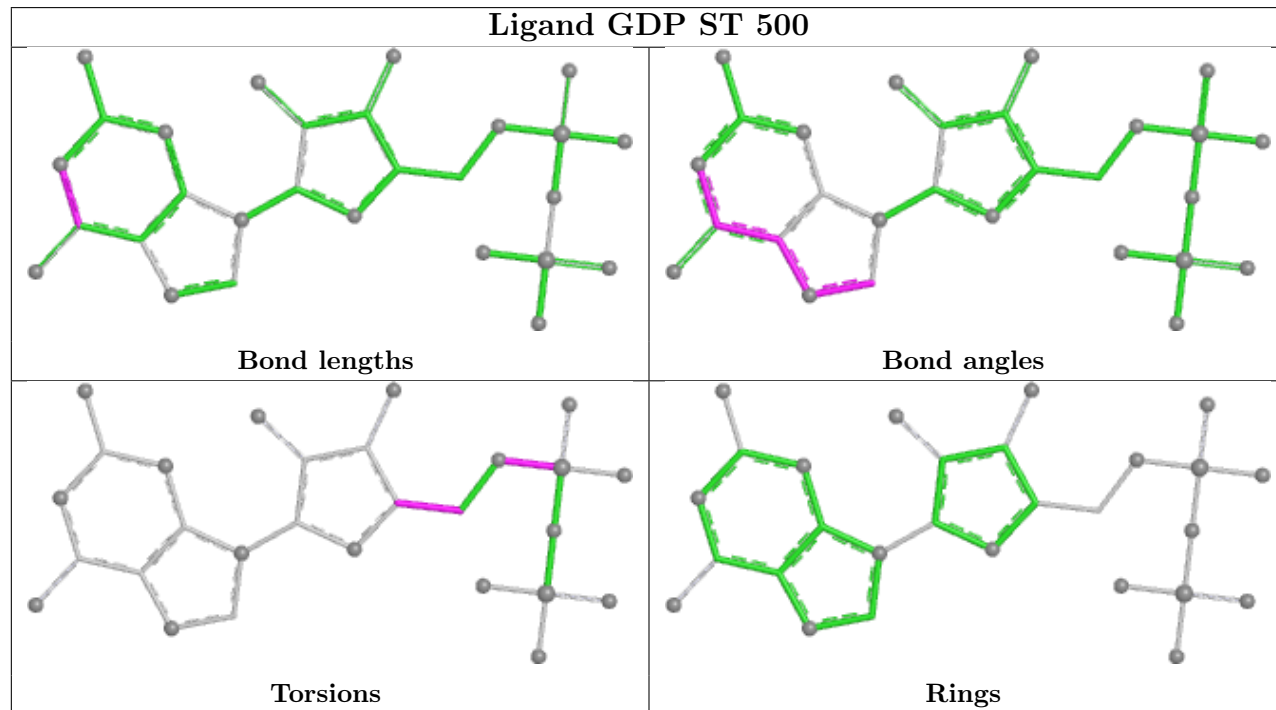
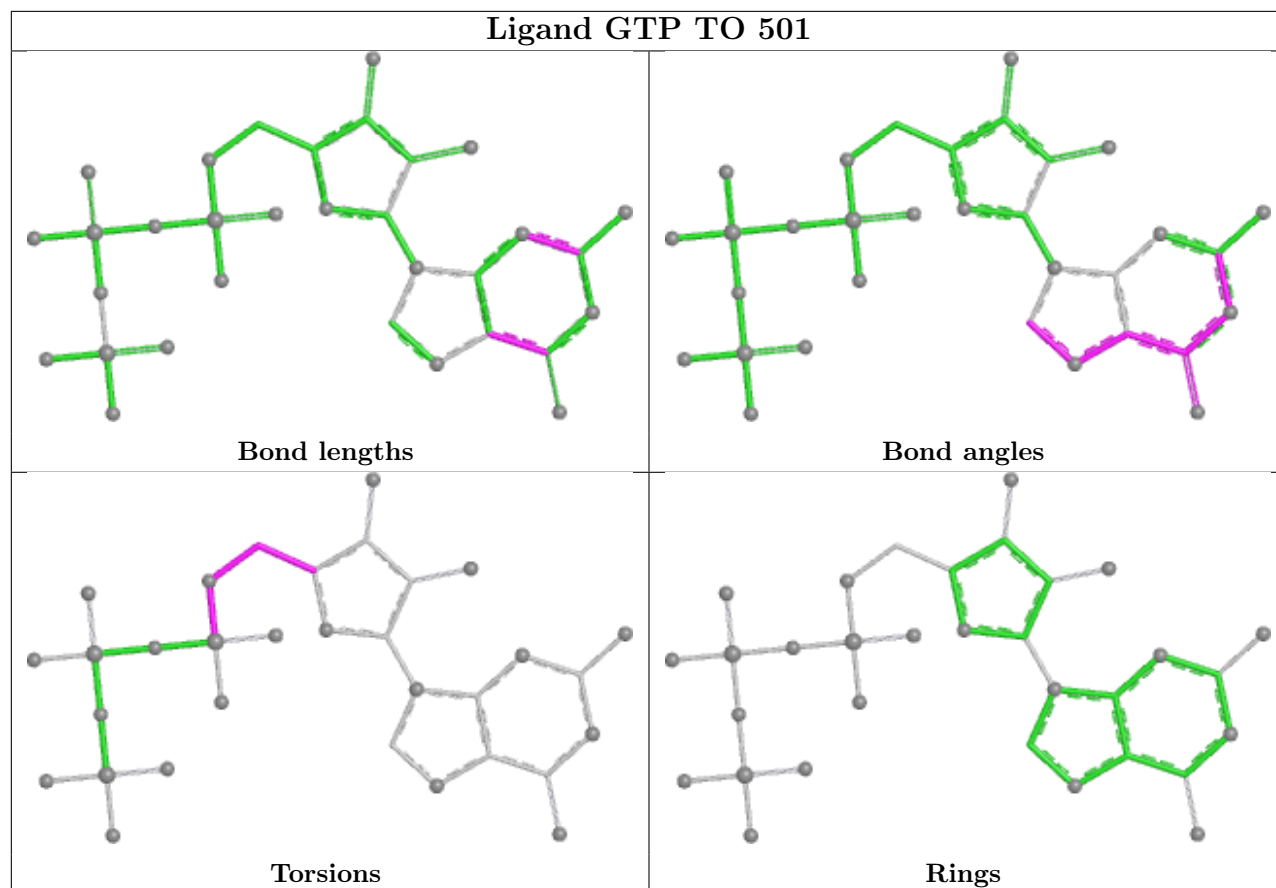
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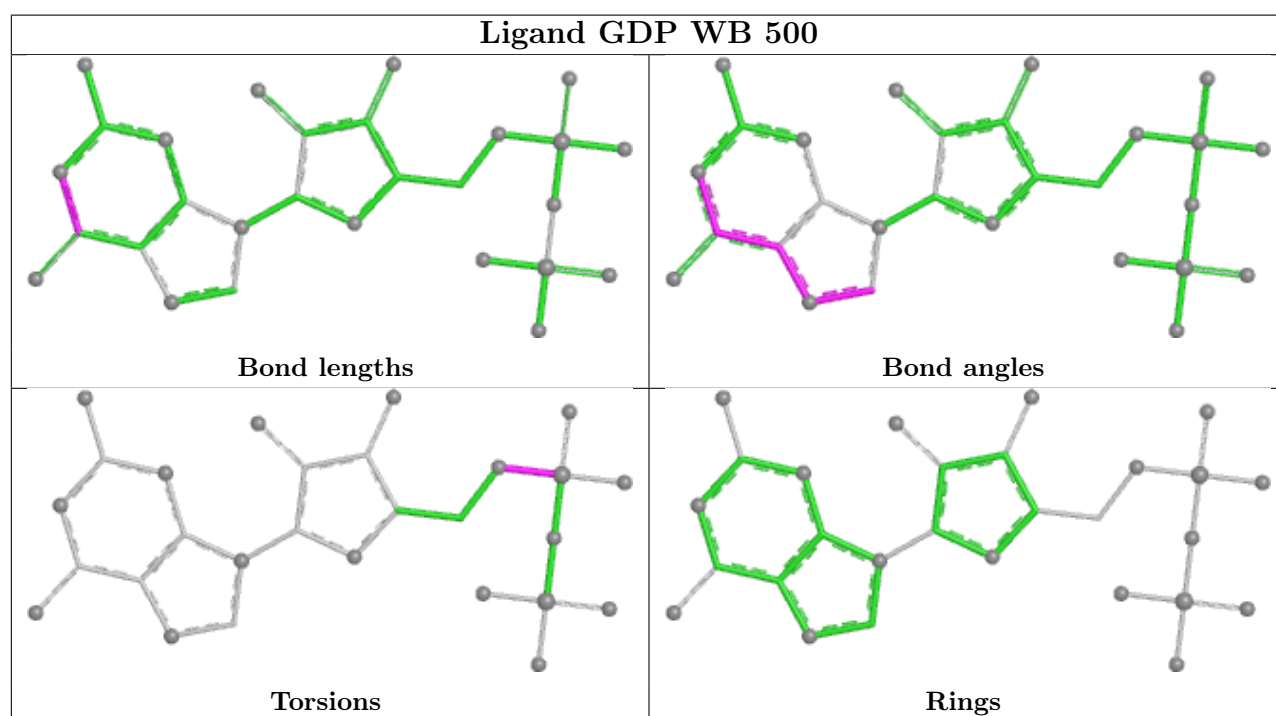
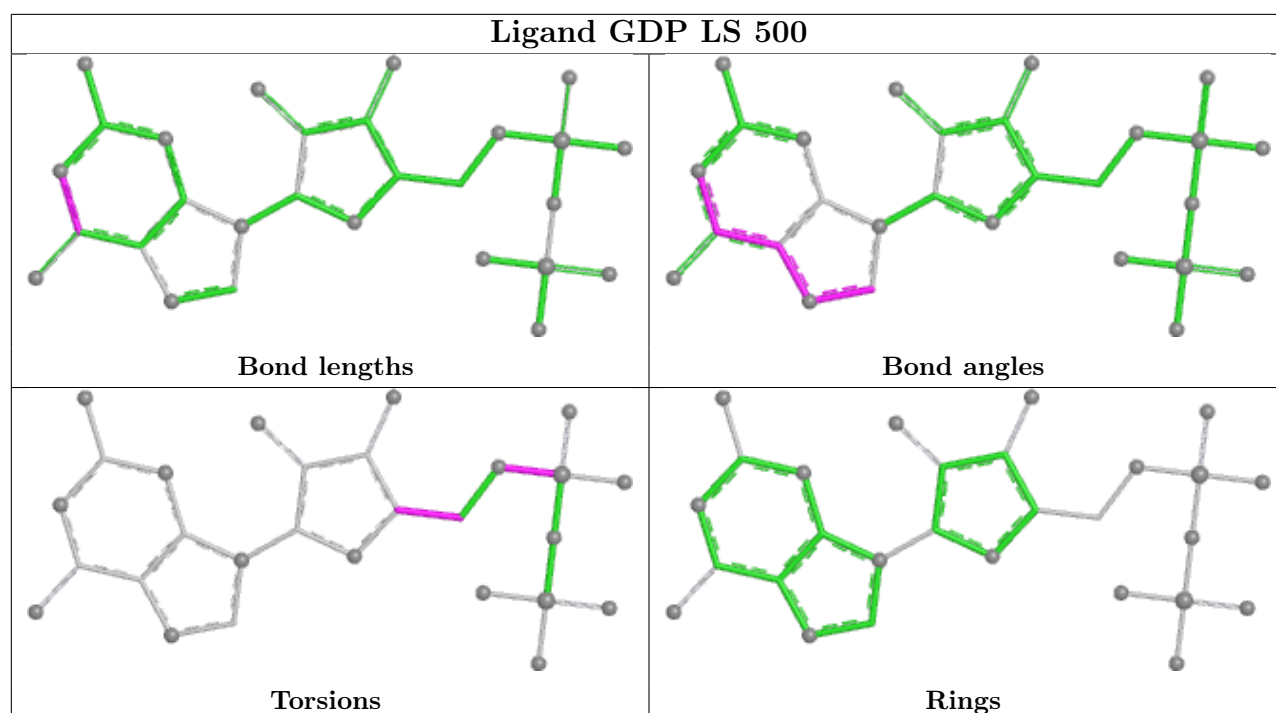


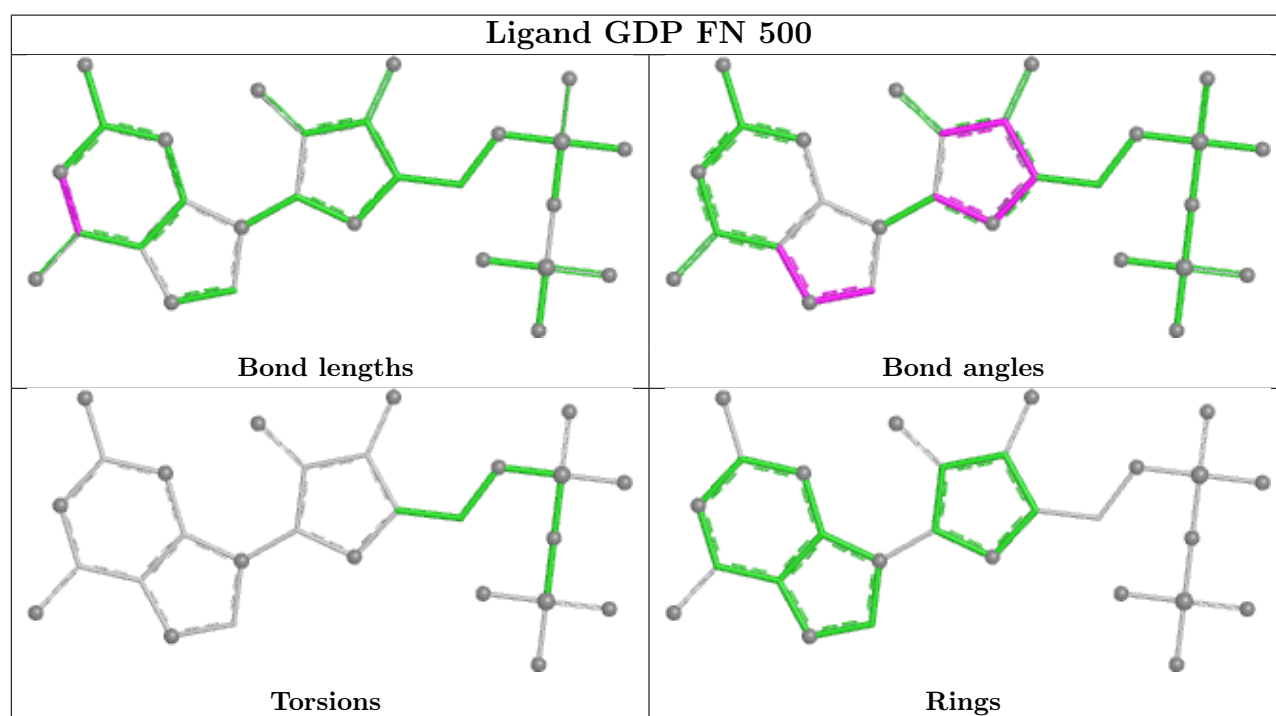
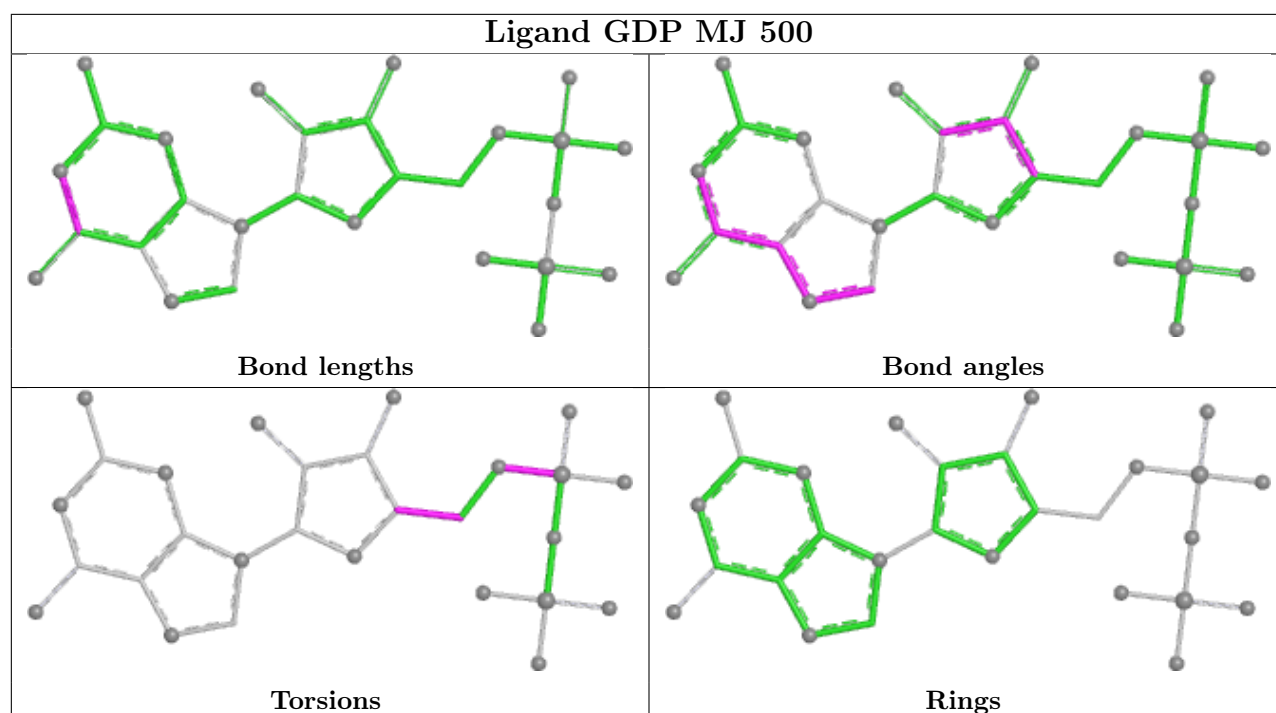
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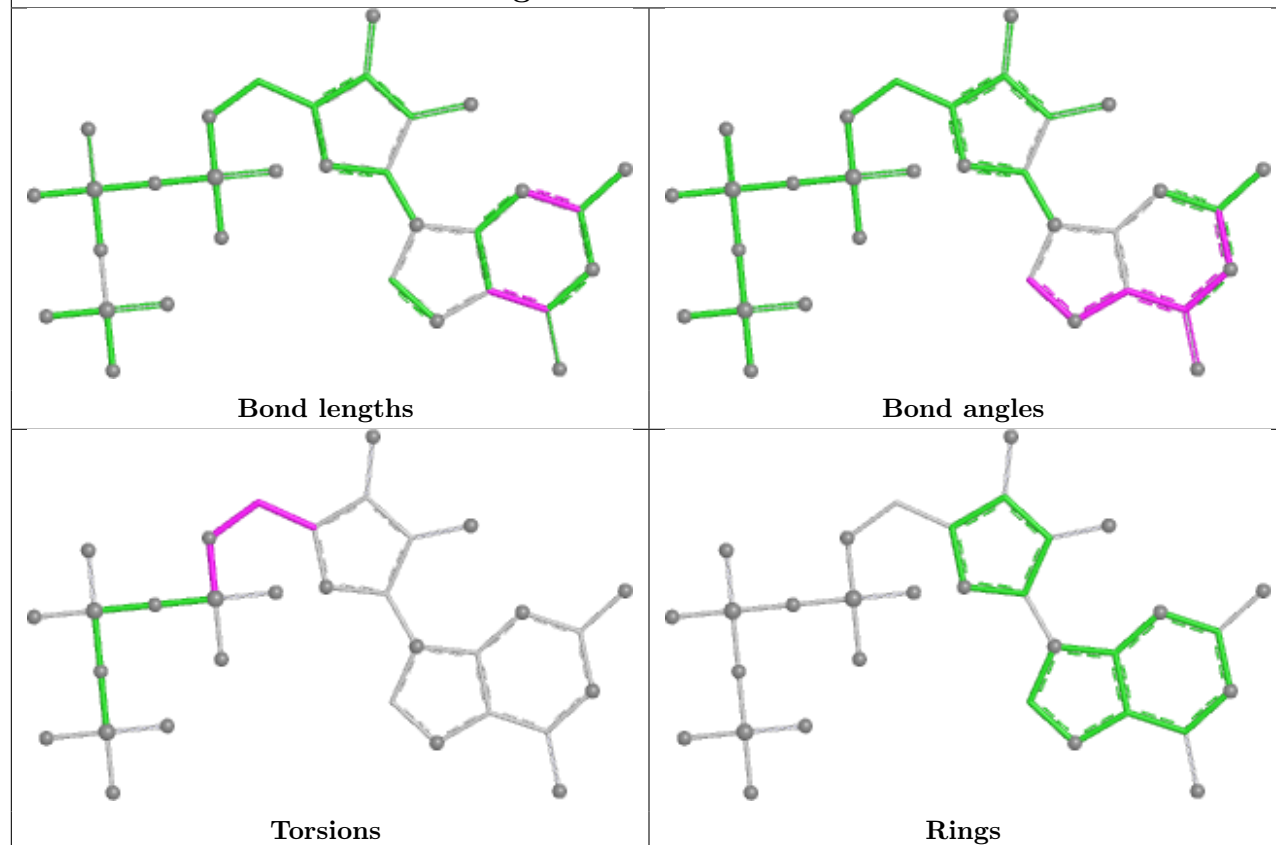




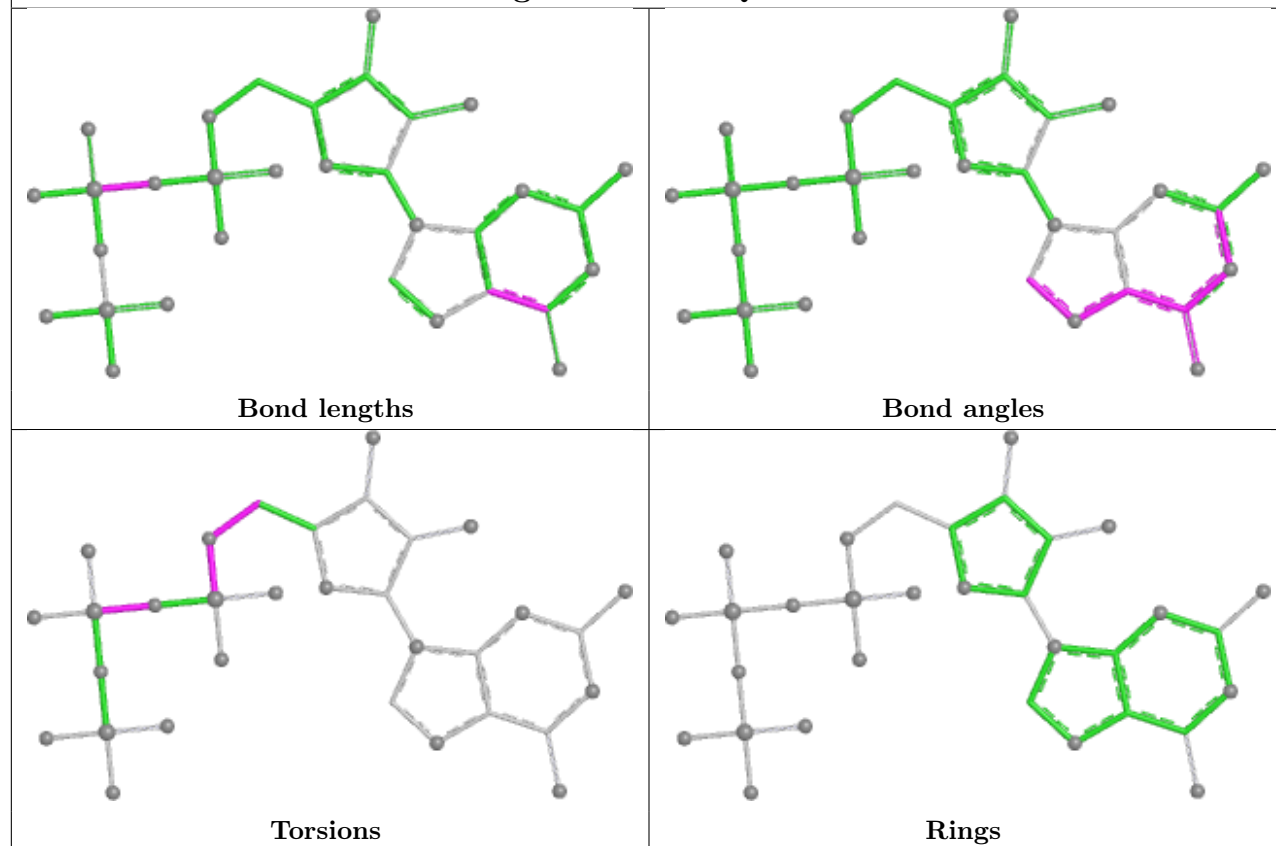


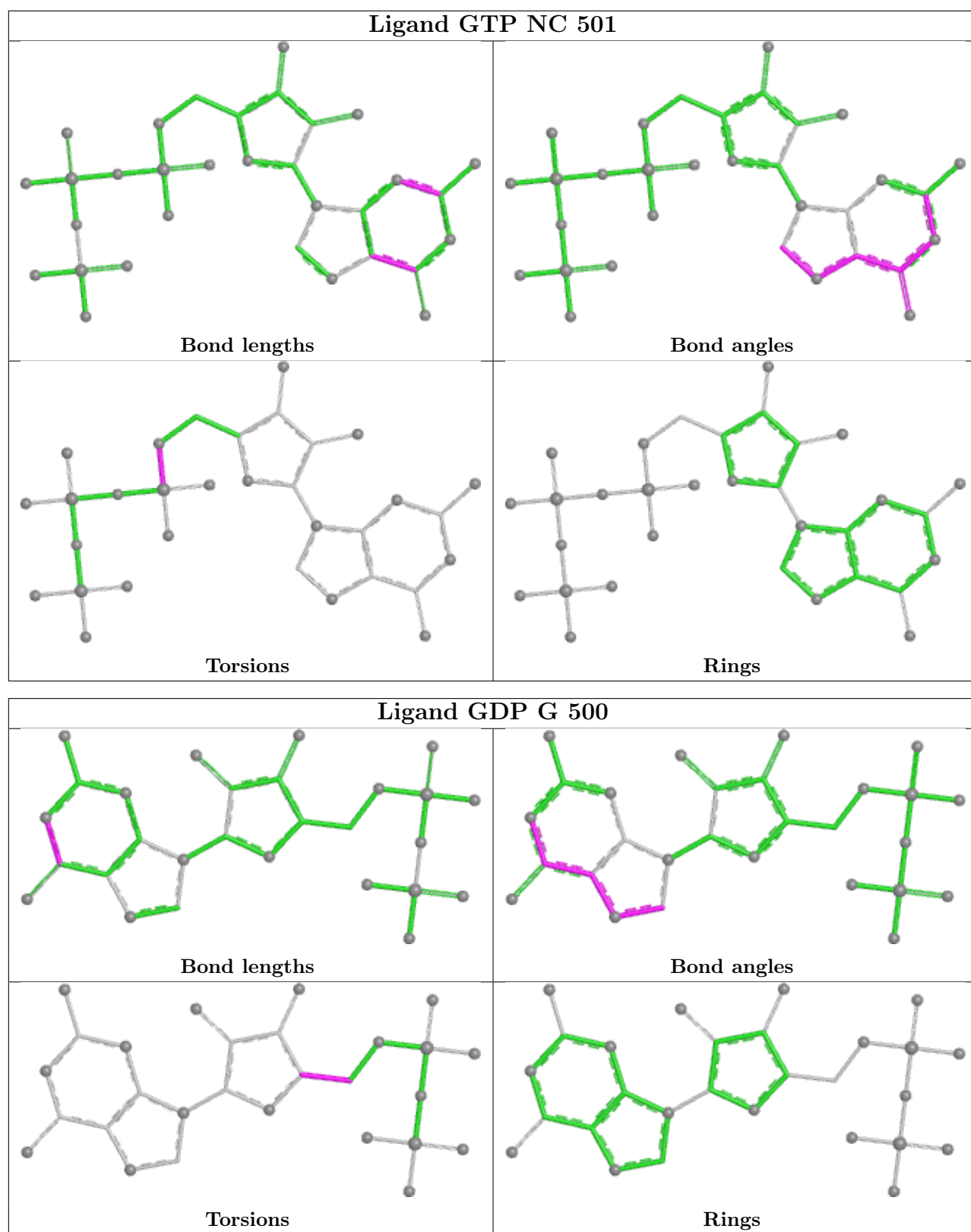


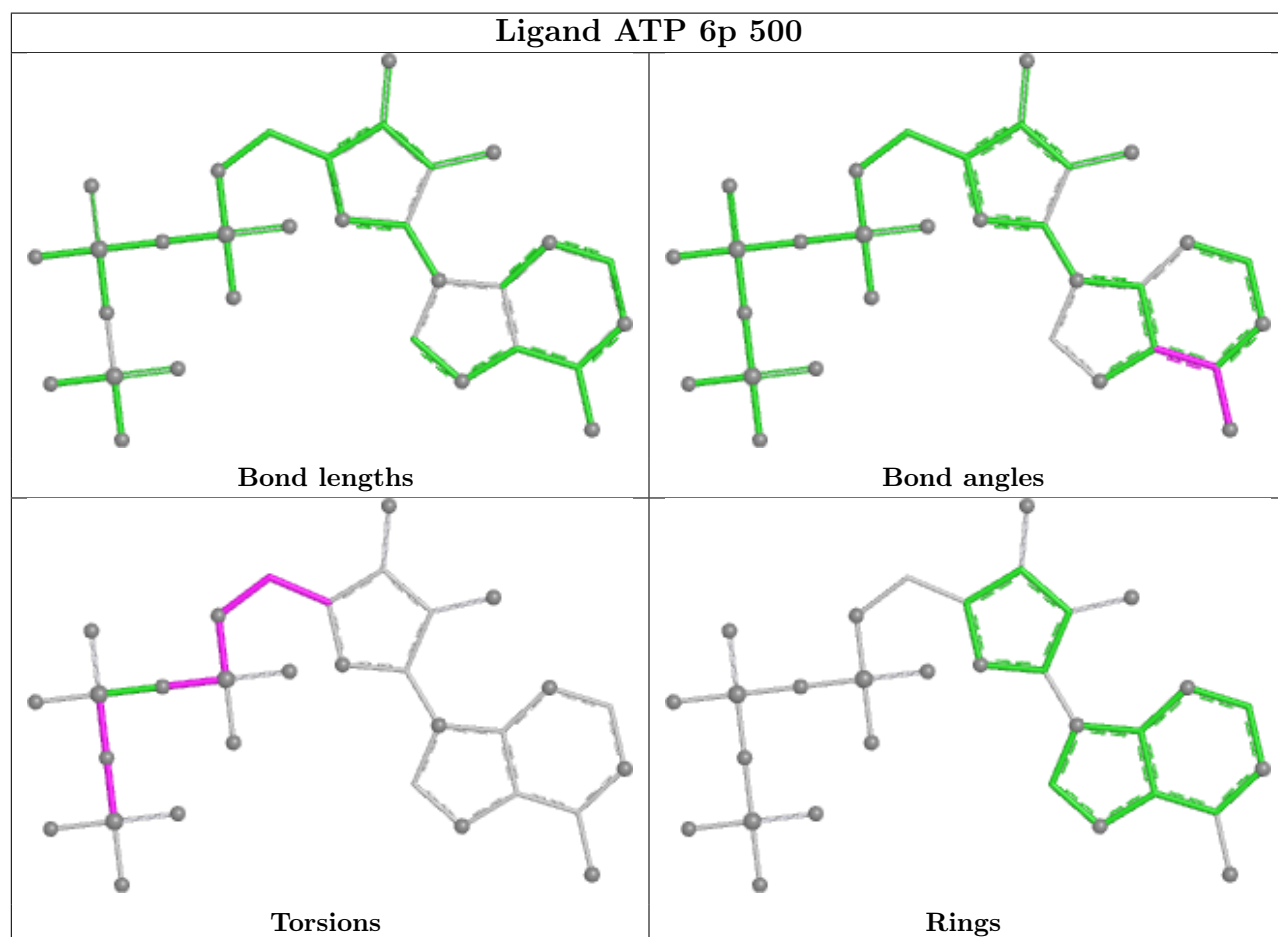
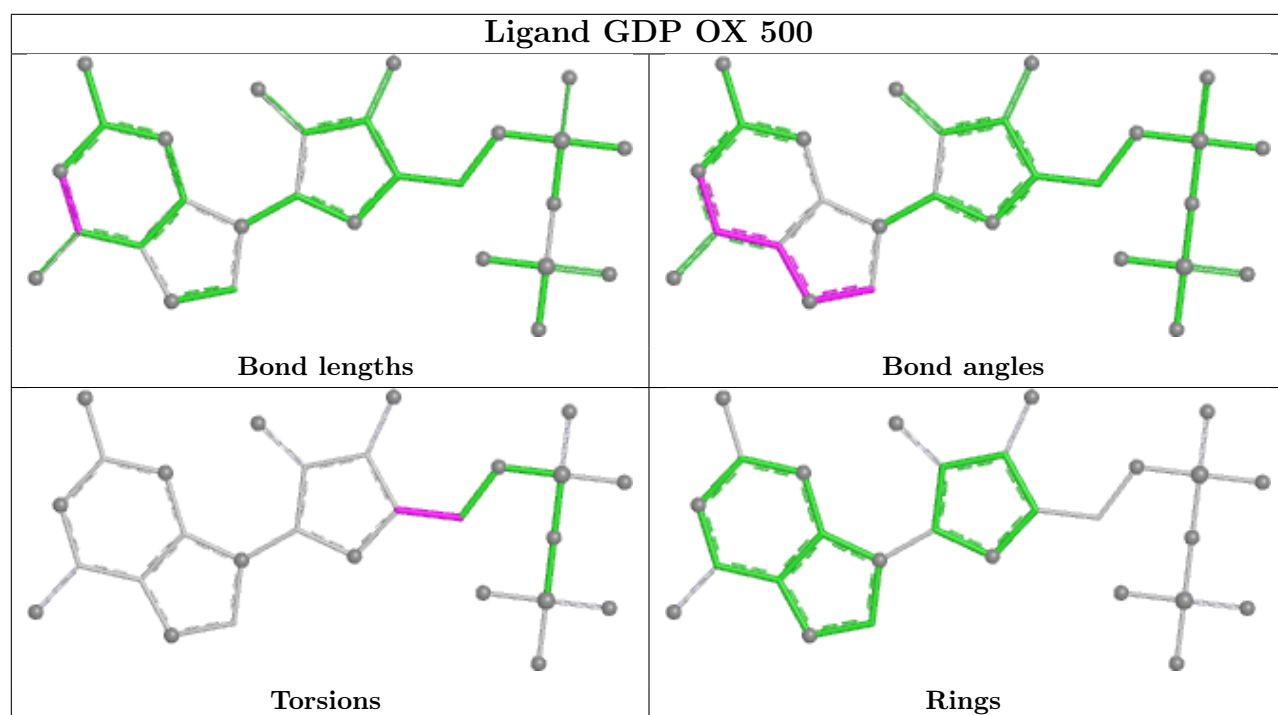
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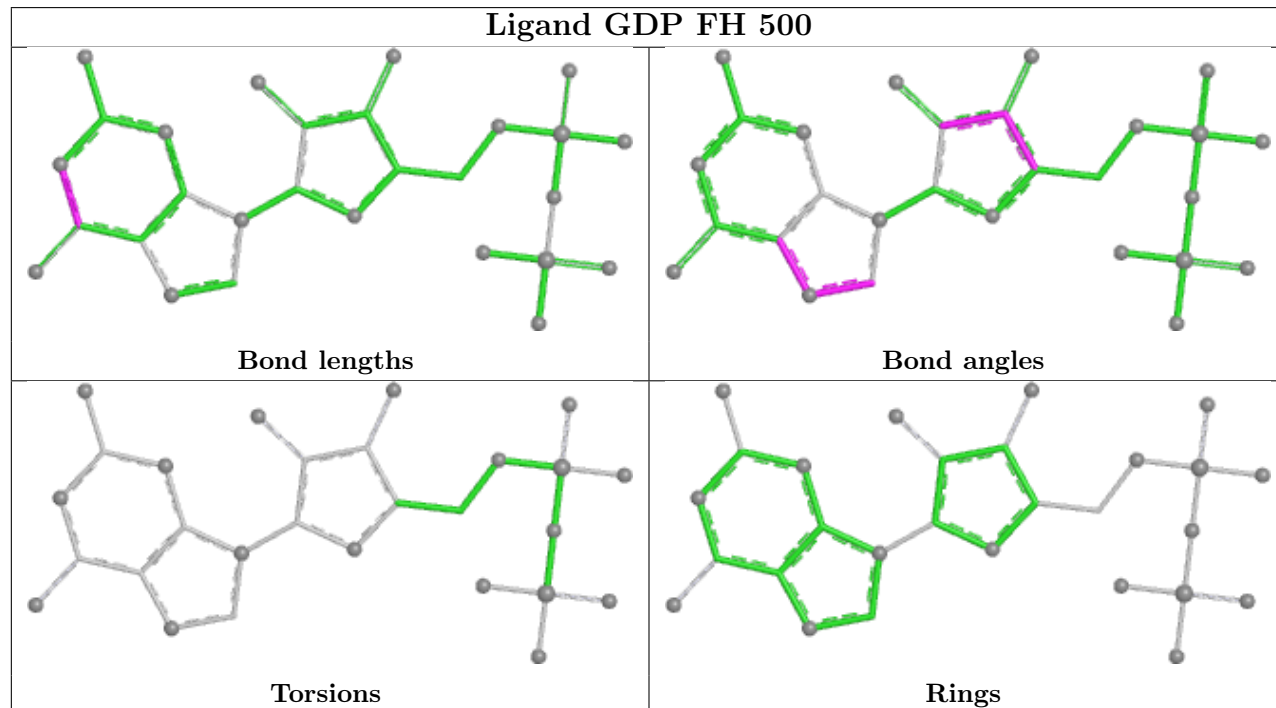
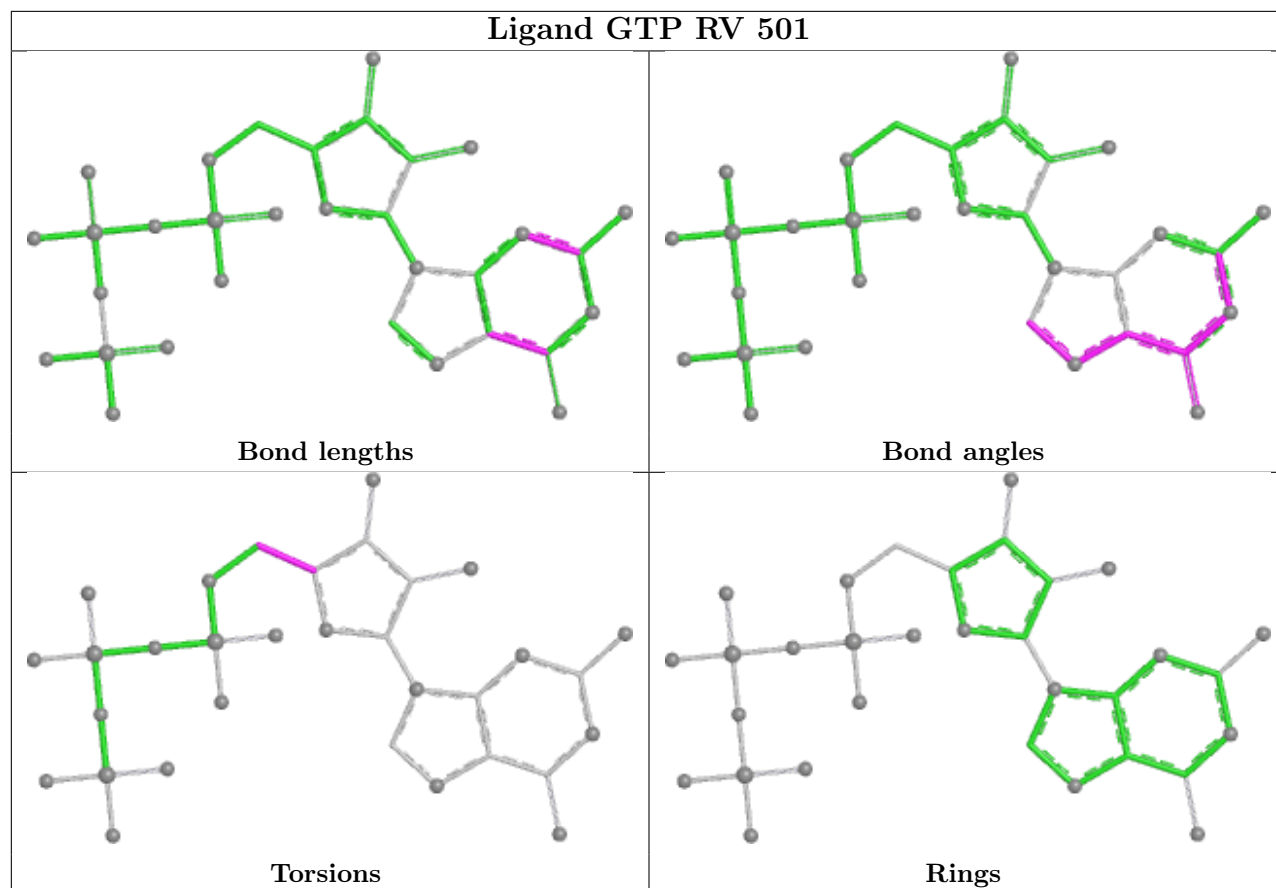


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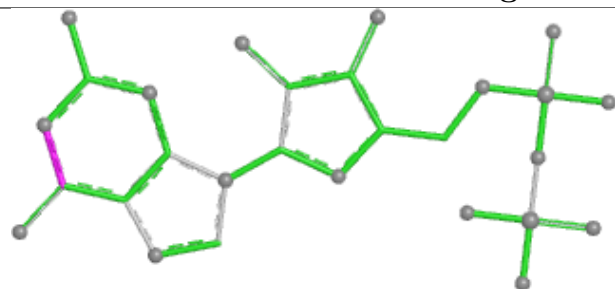




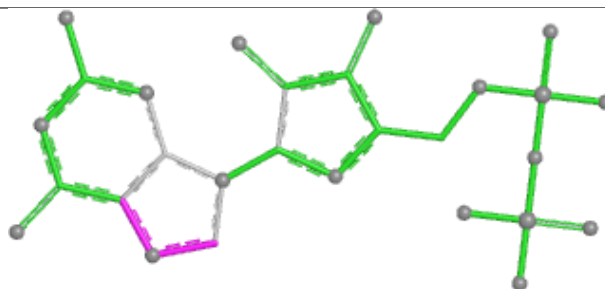




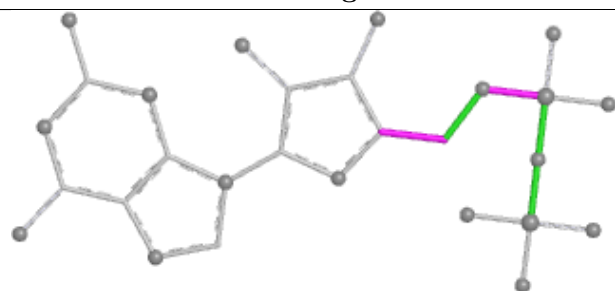
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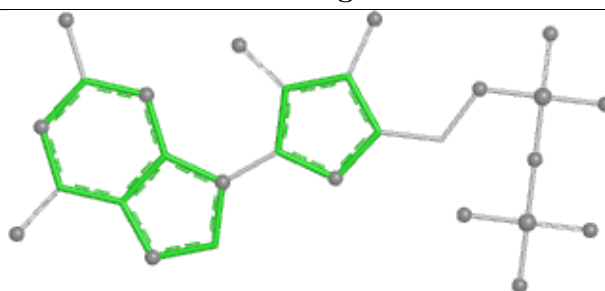
Bond lengths



Bond angles

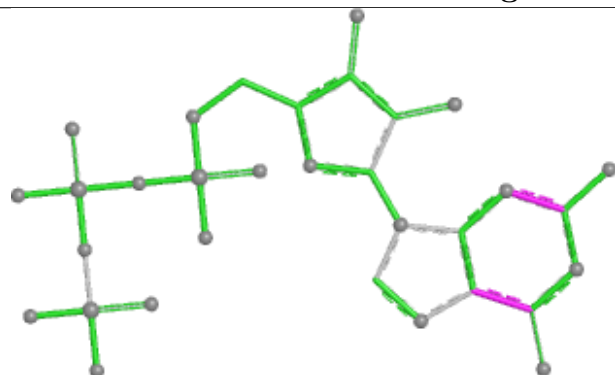


Torsions

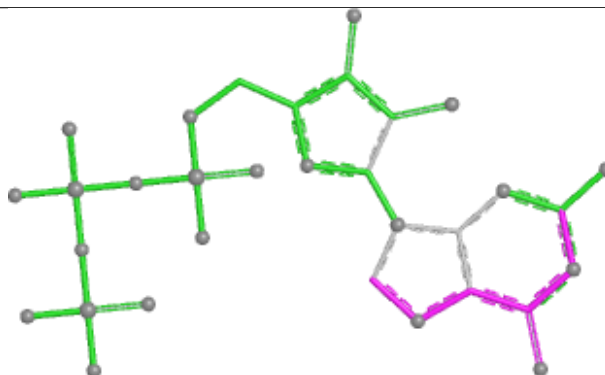


Rings

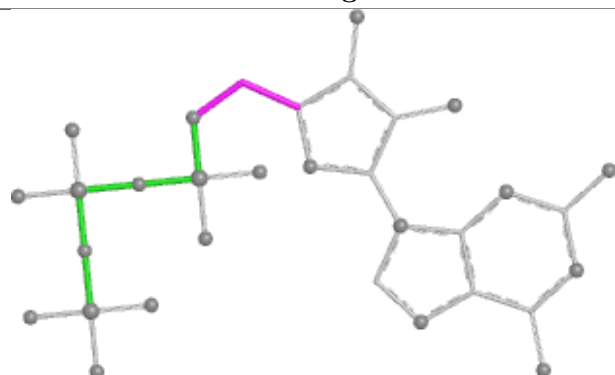
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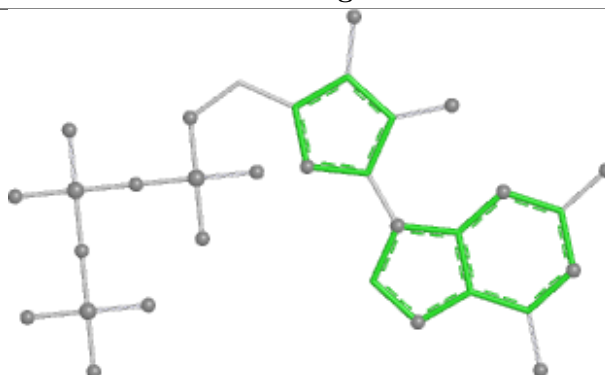
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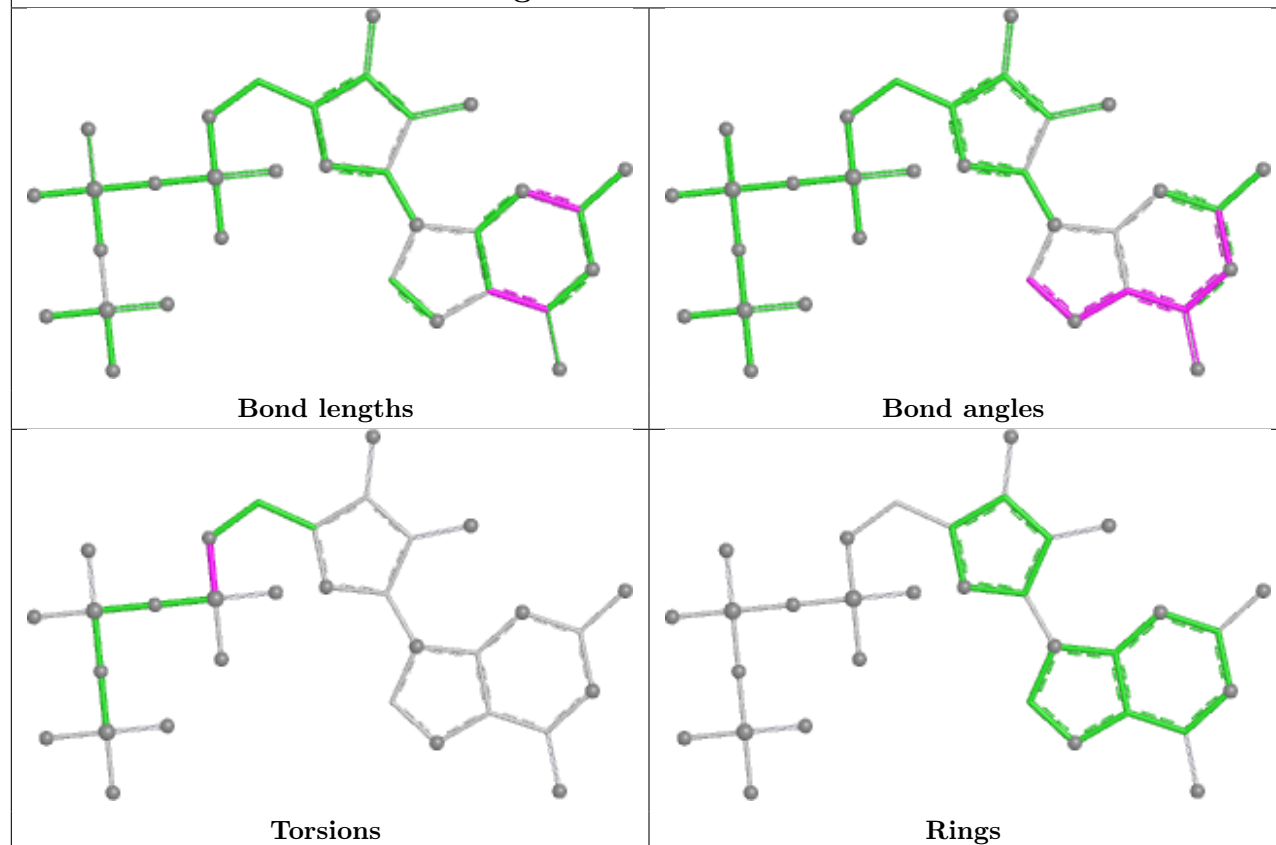


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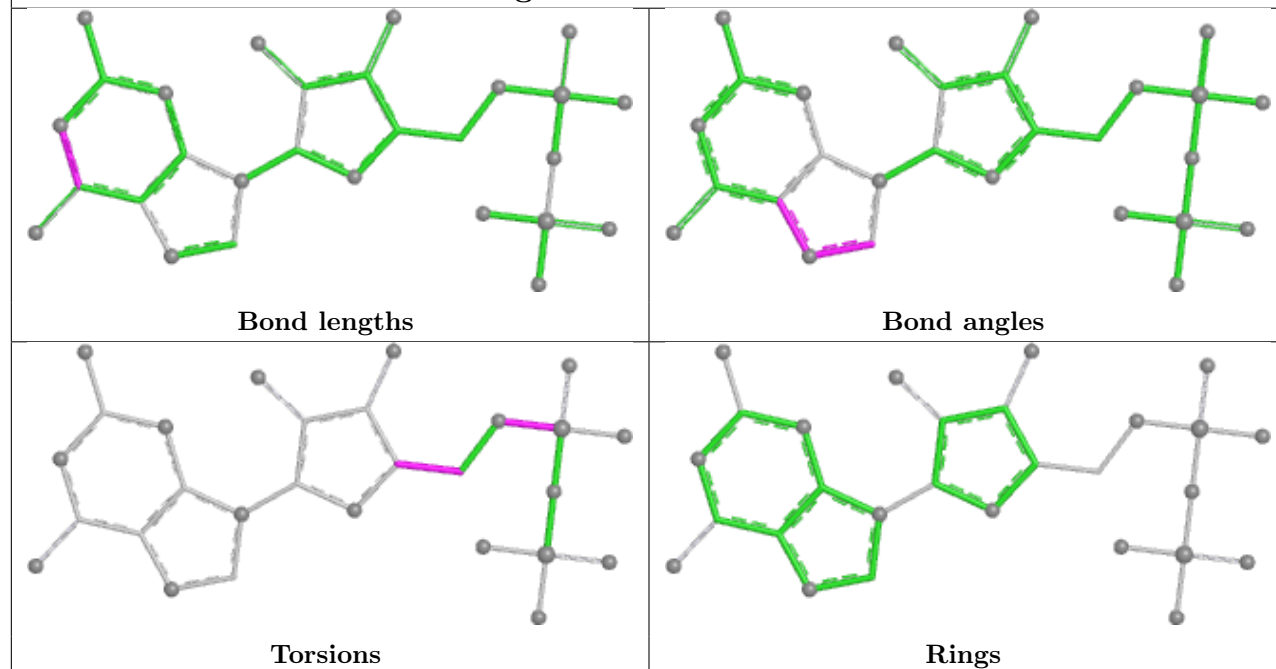


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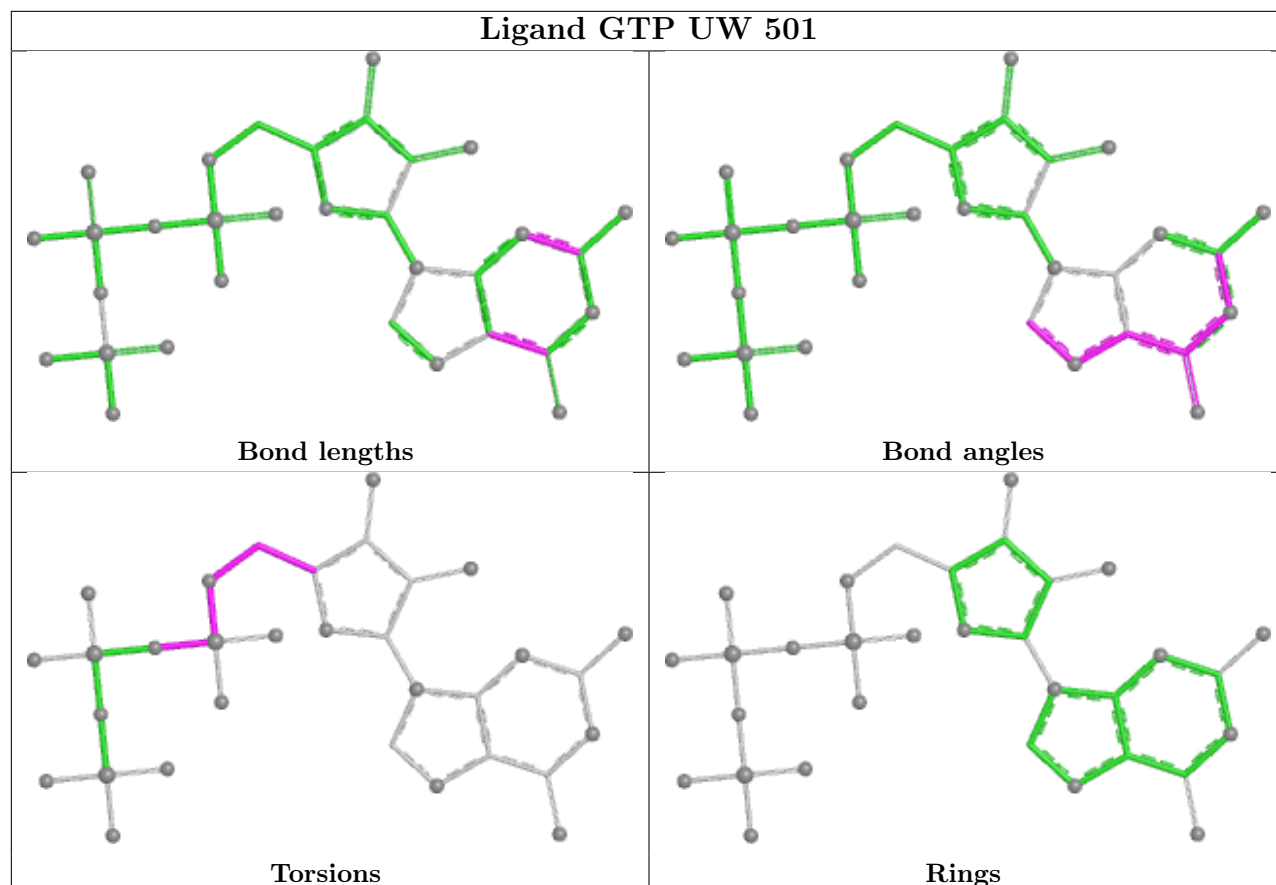
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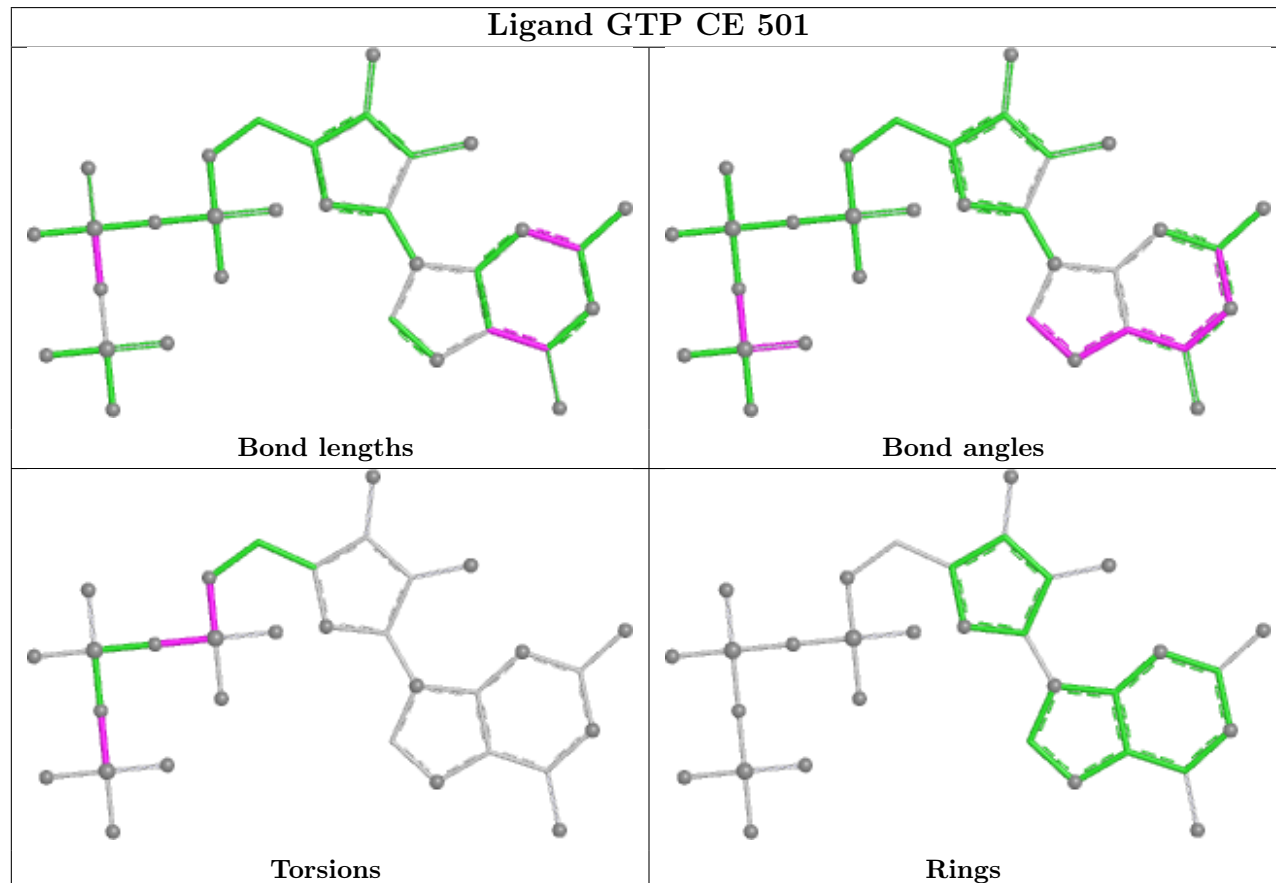
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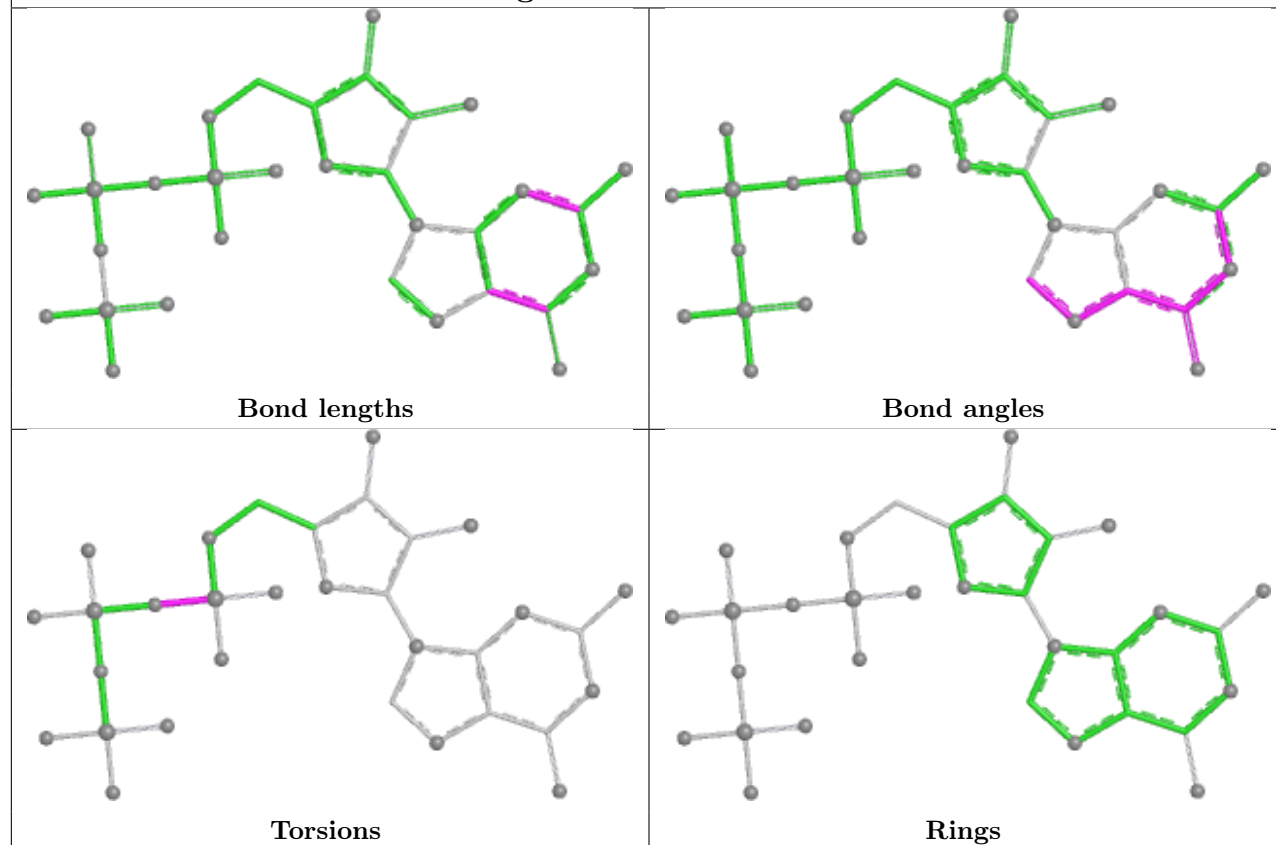
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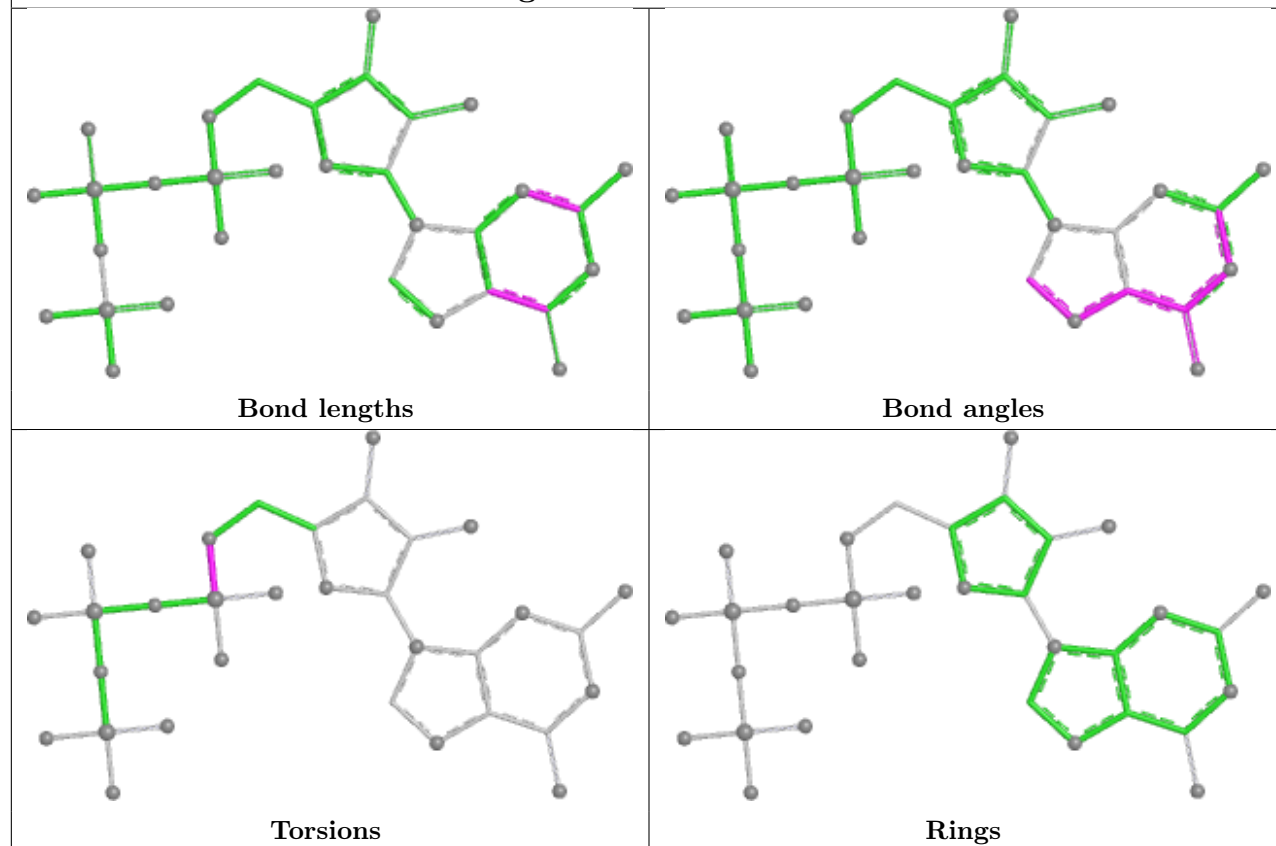
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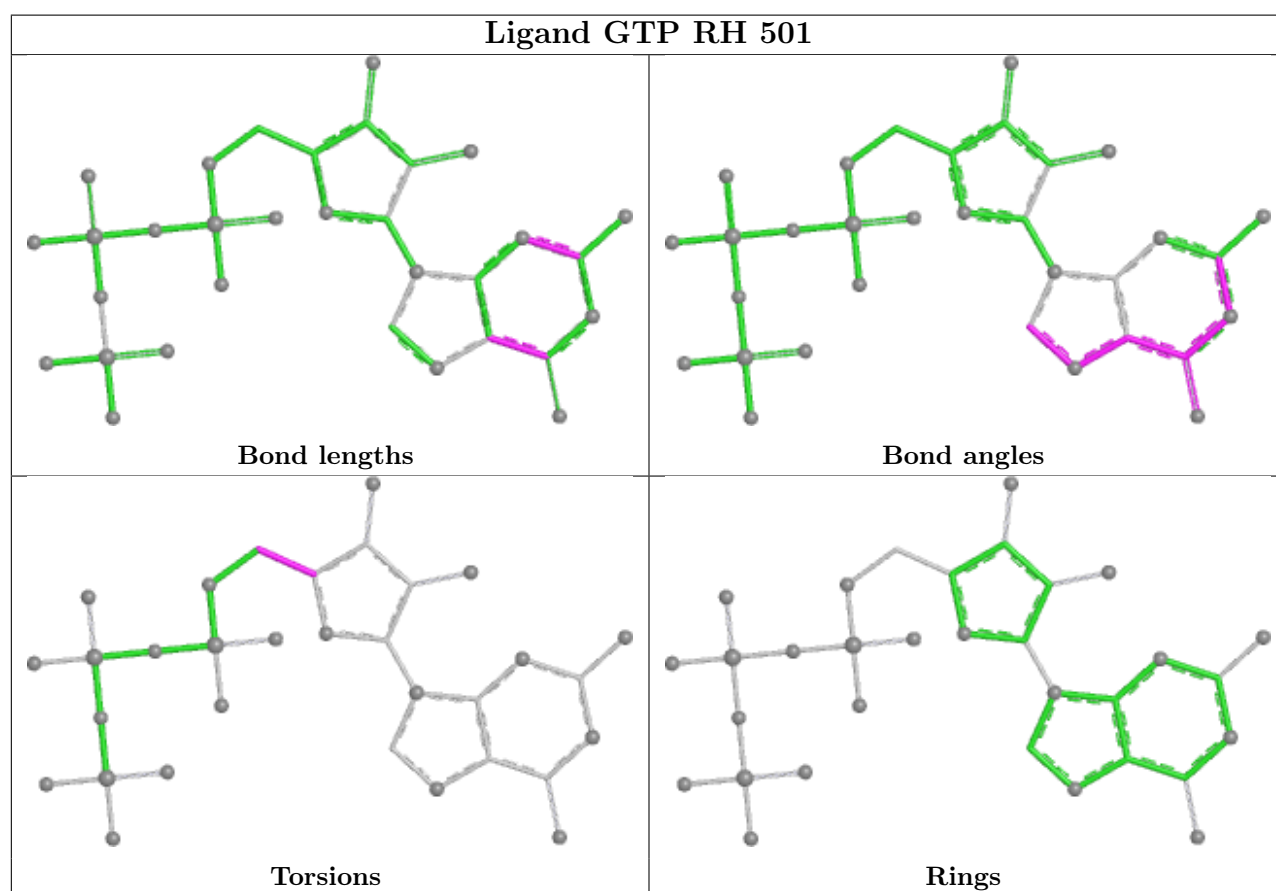
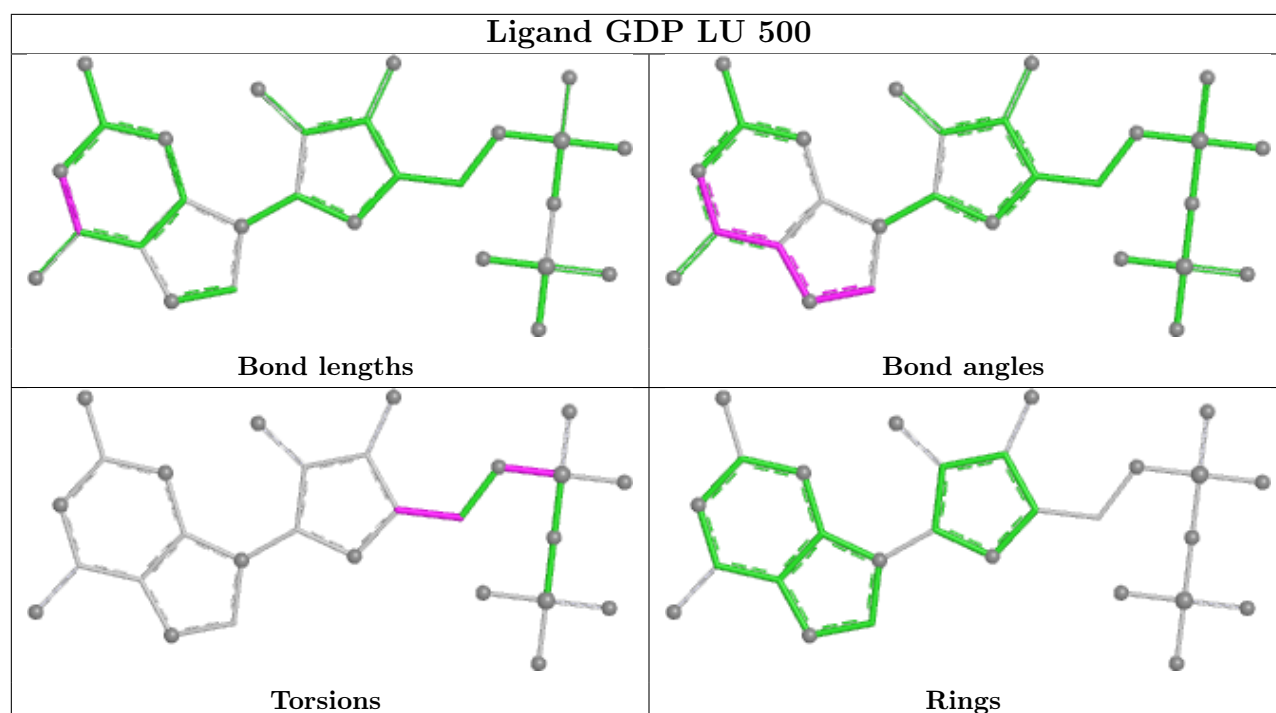


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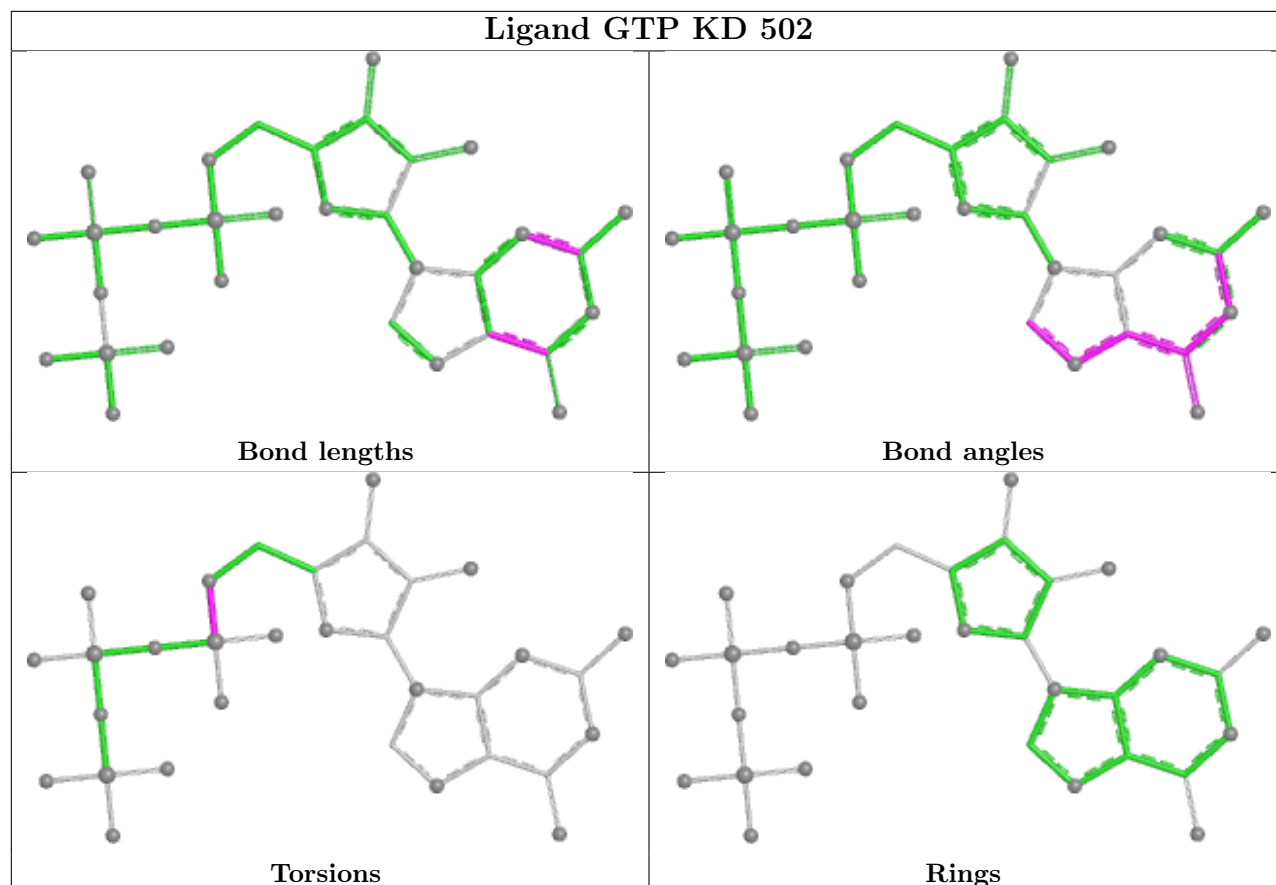


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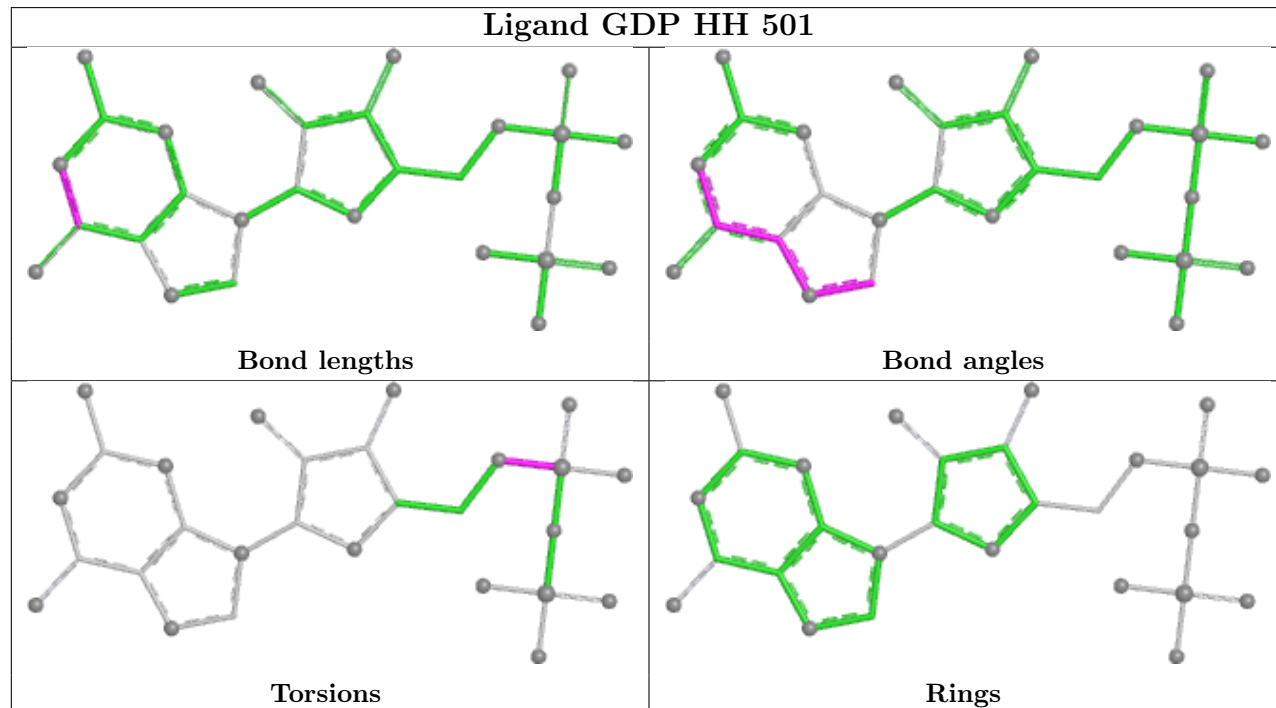


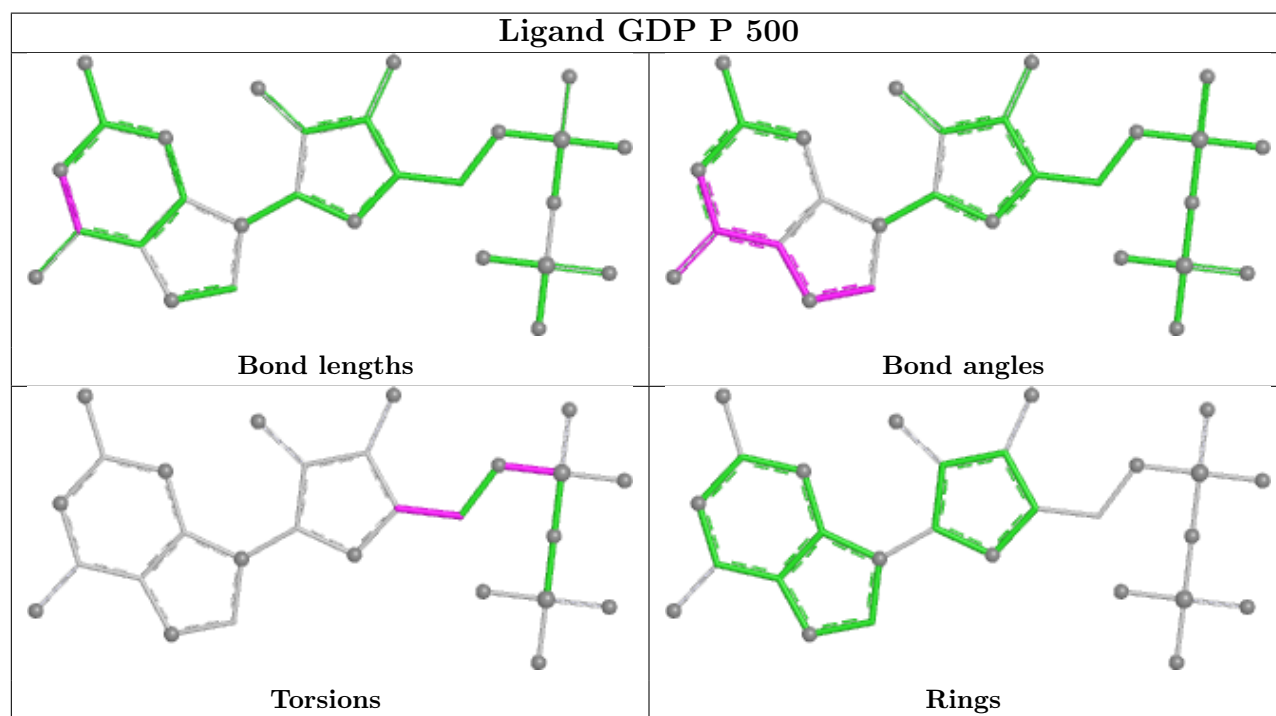
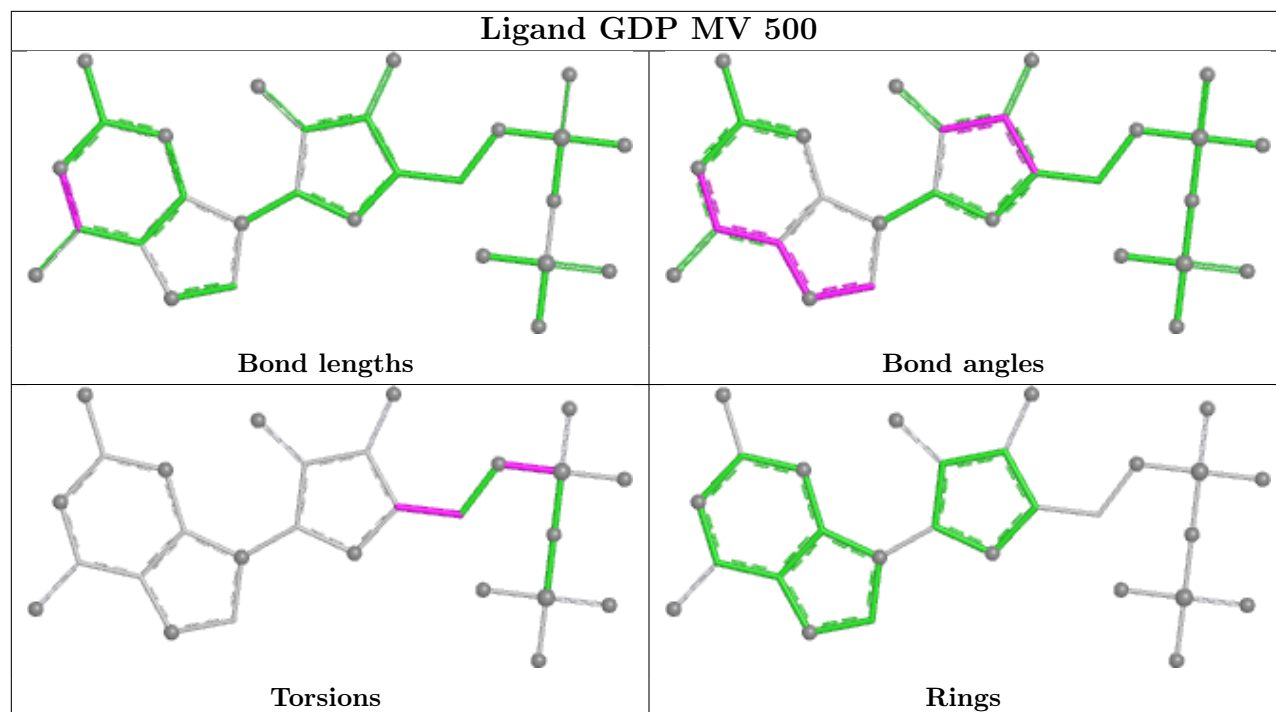


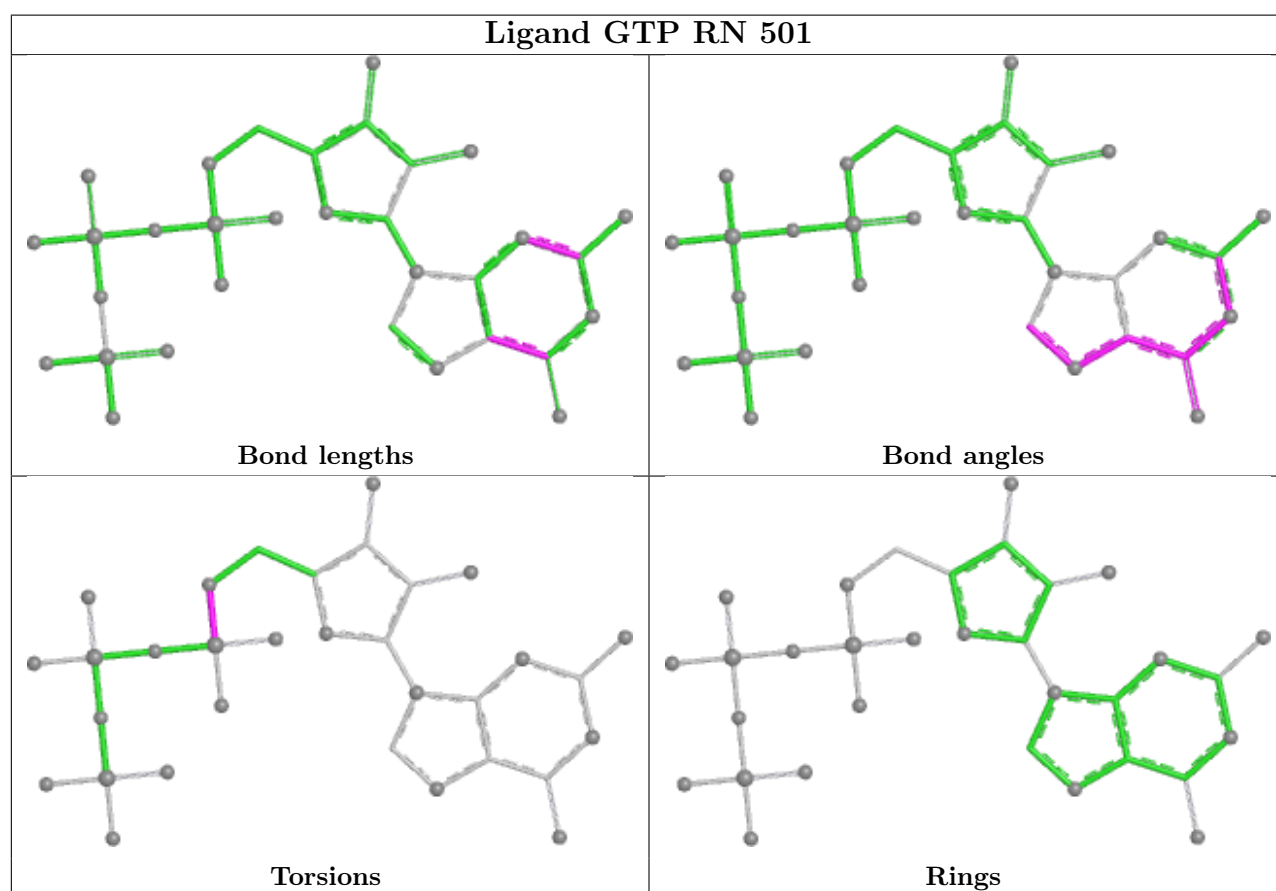
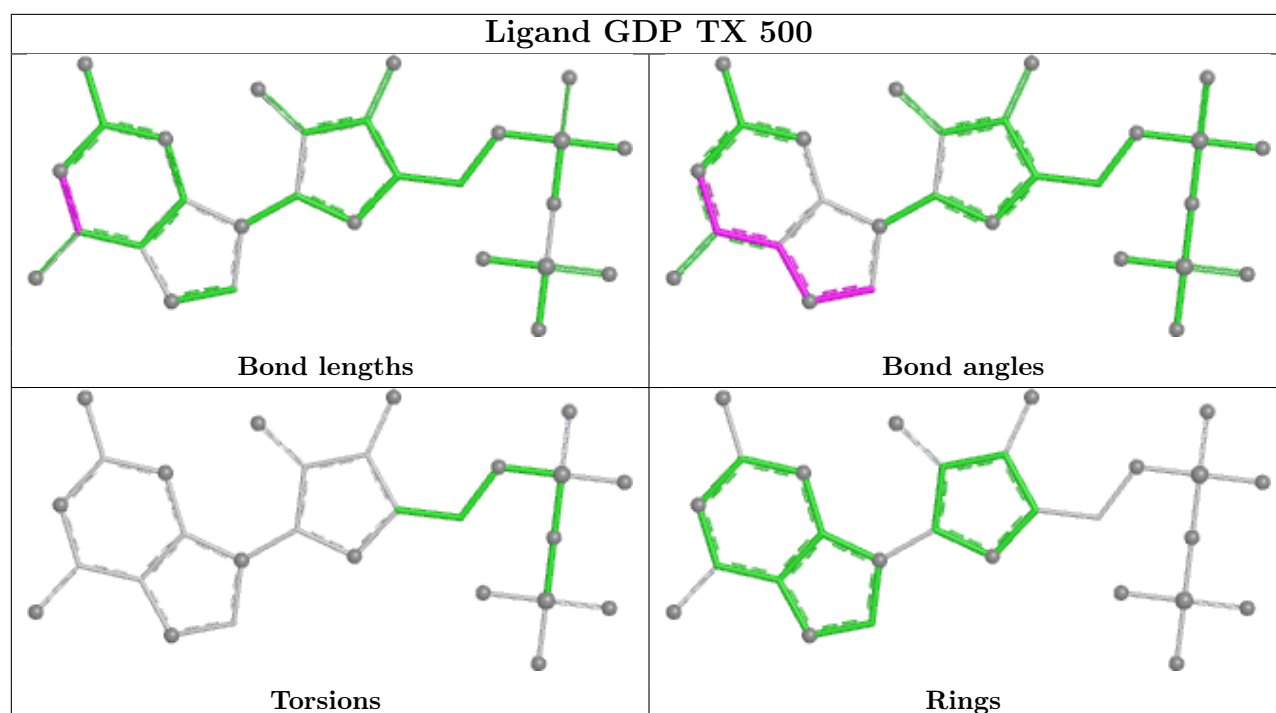
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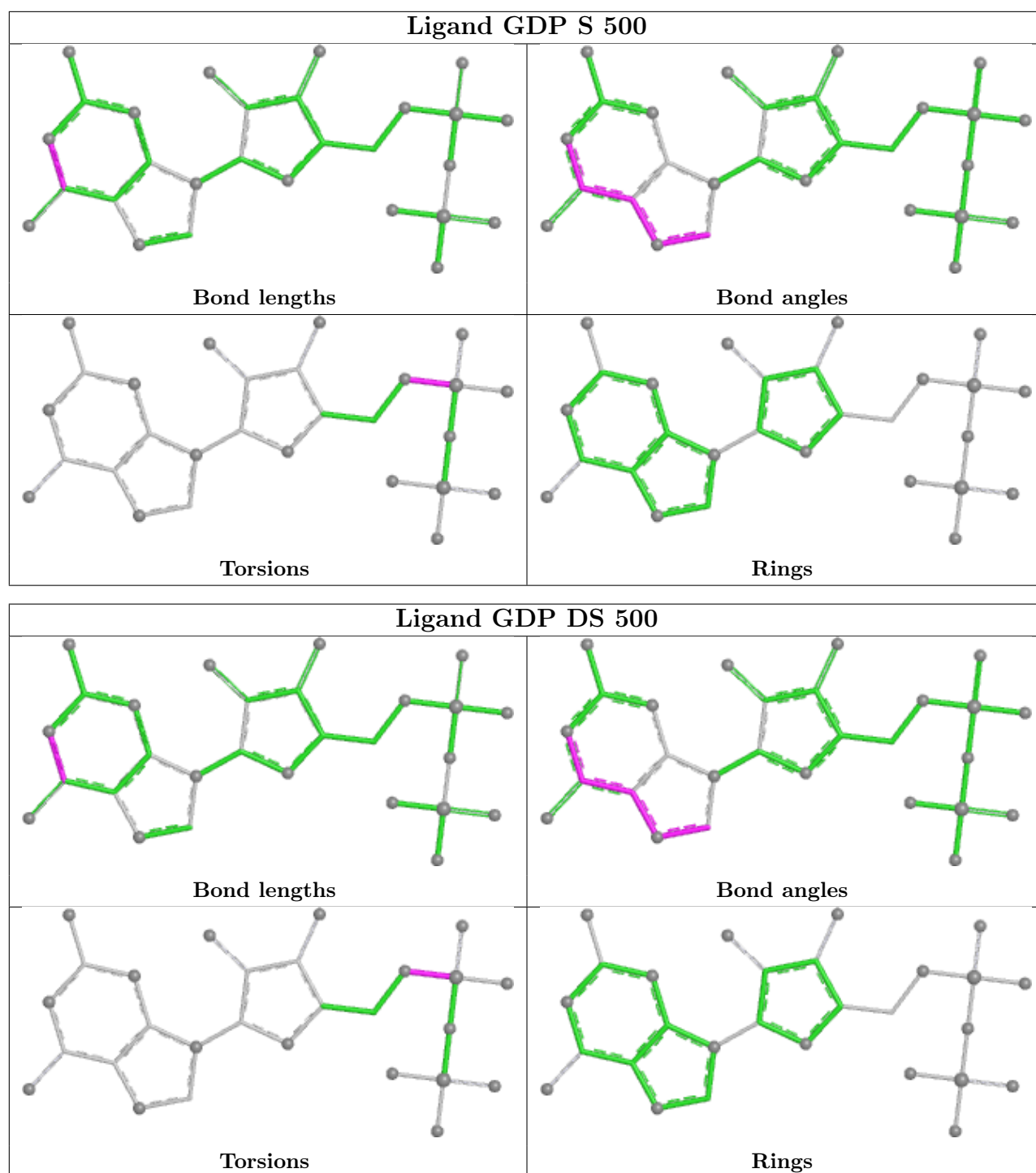


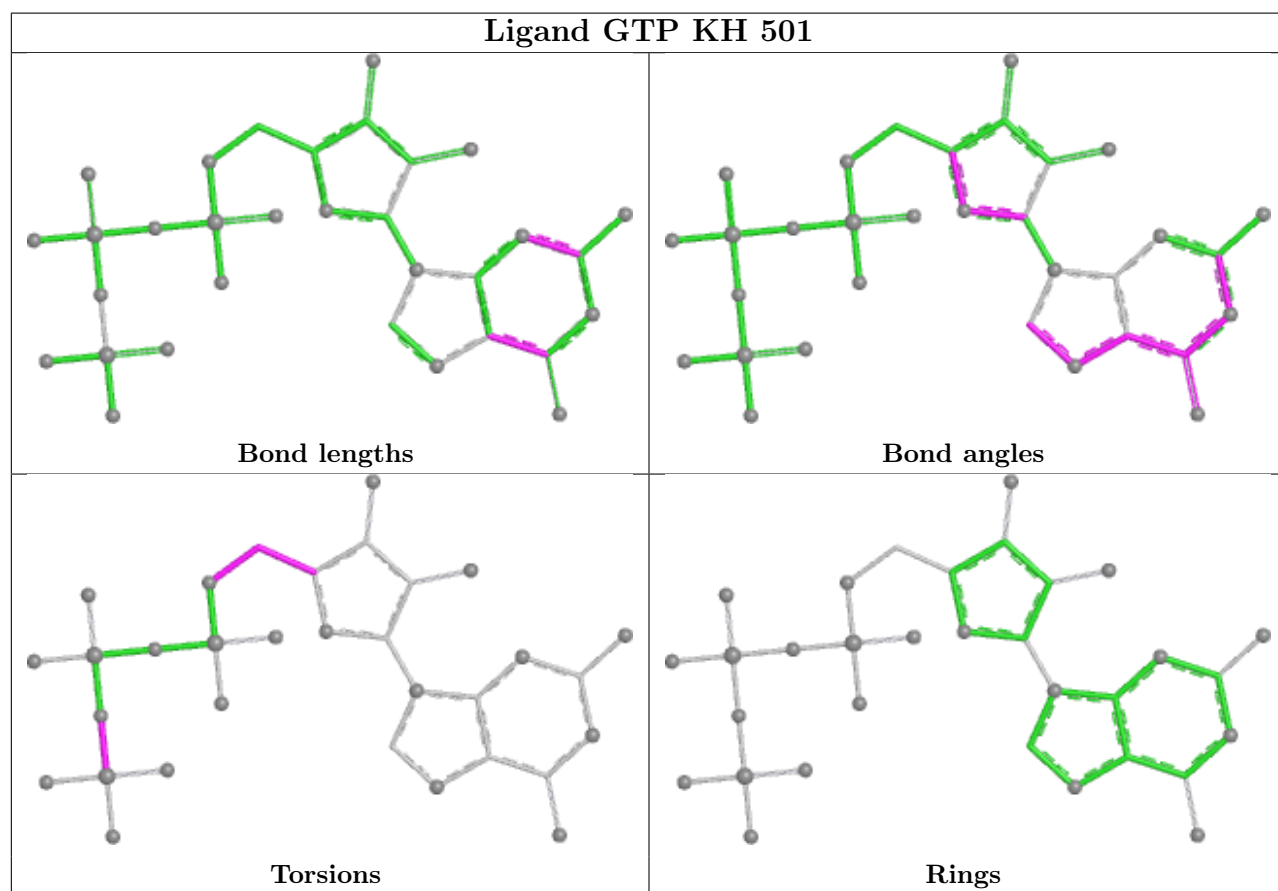
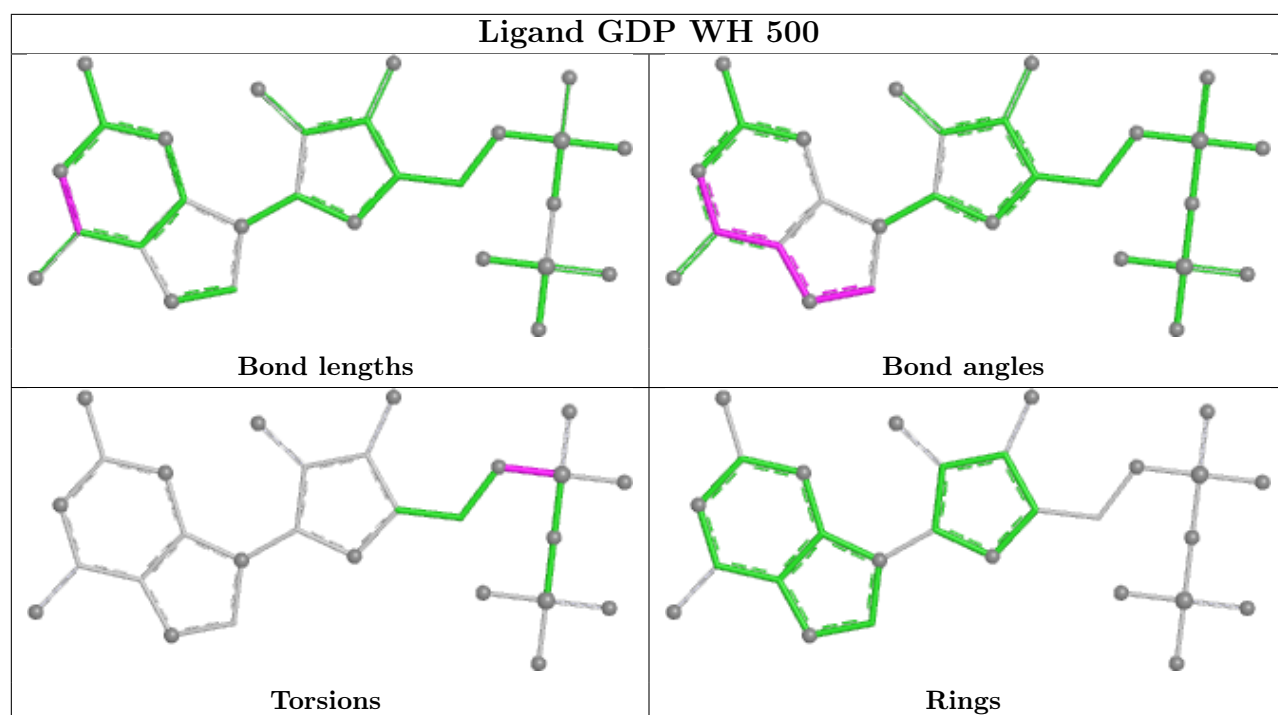
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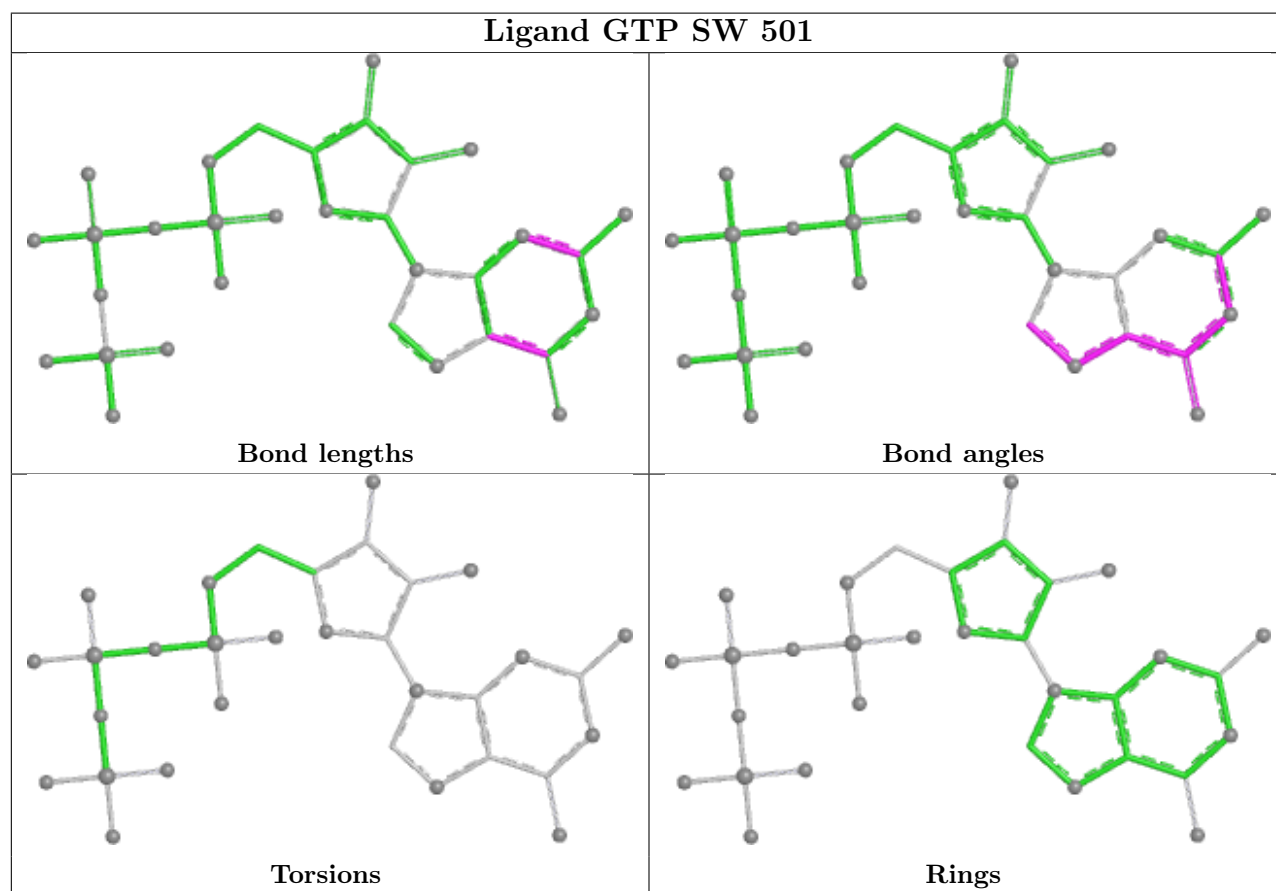
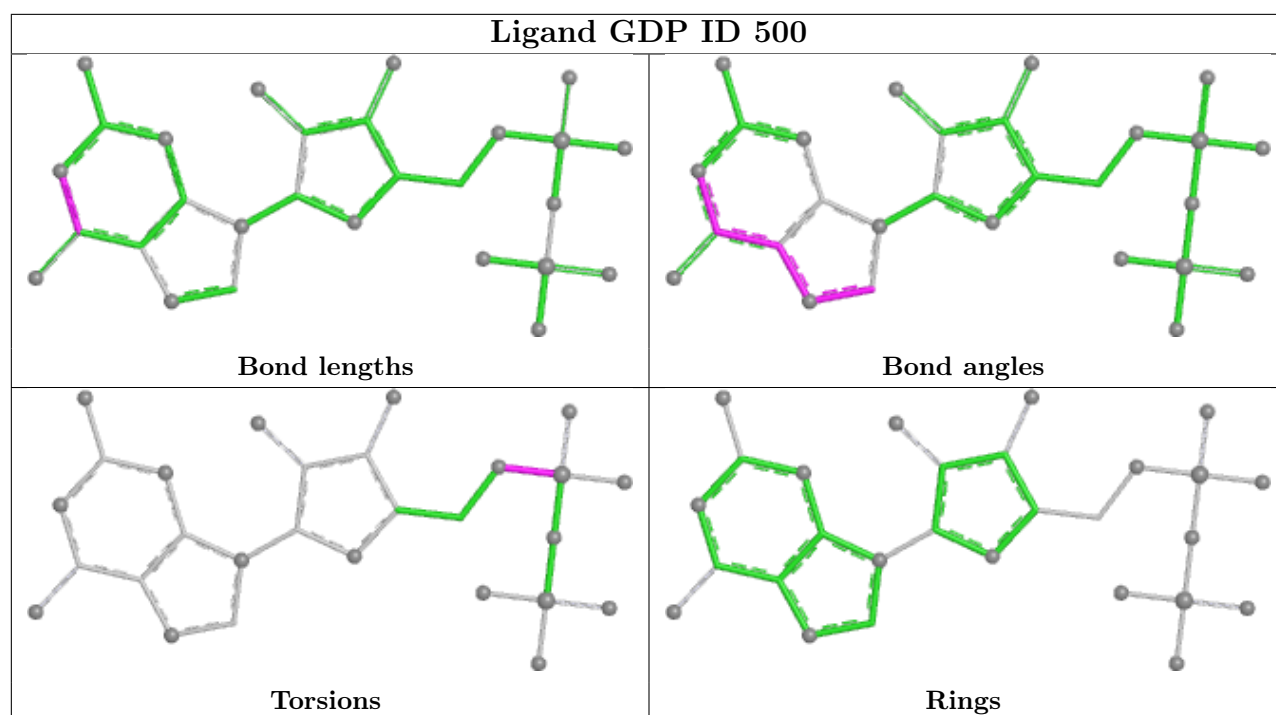


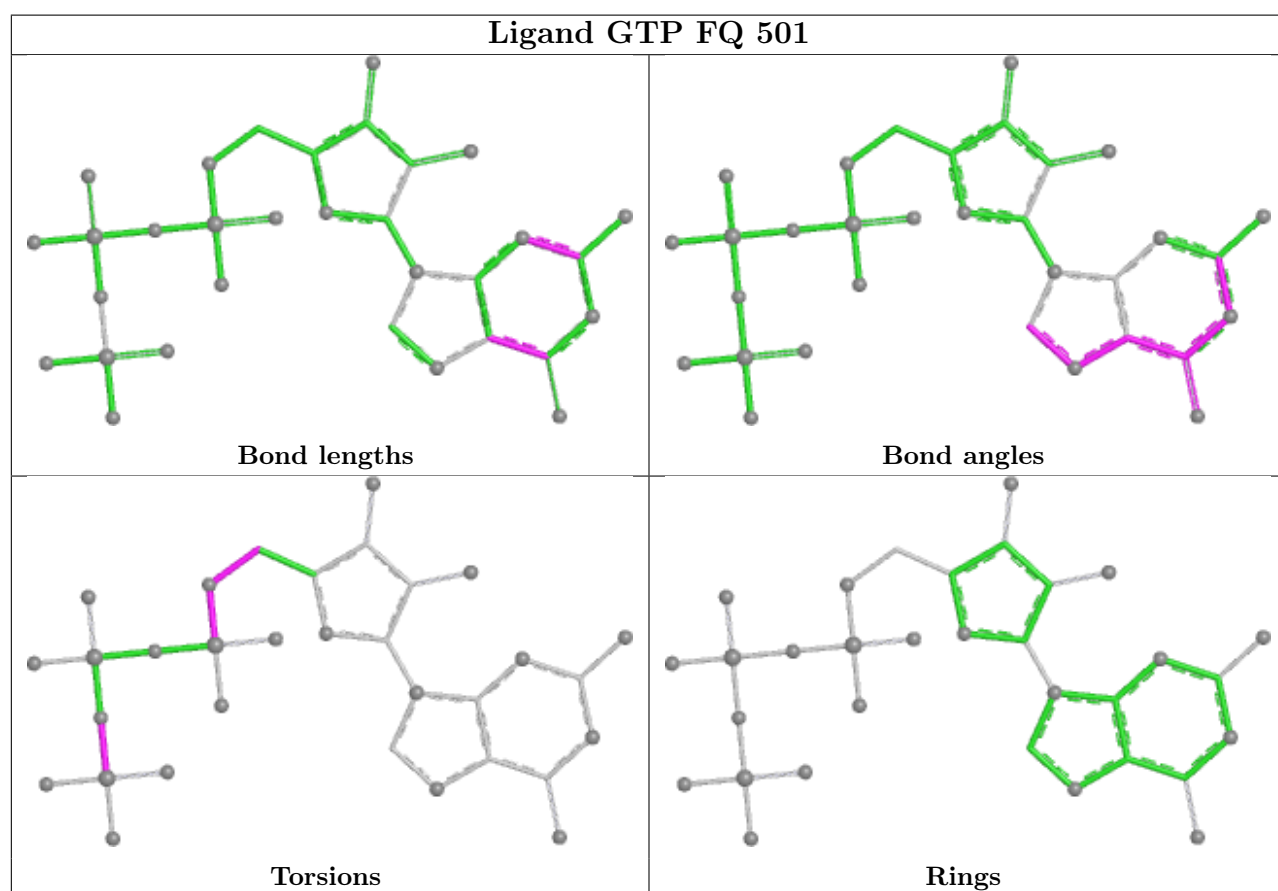
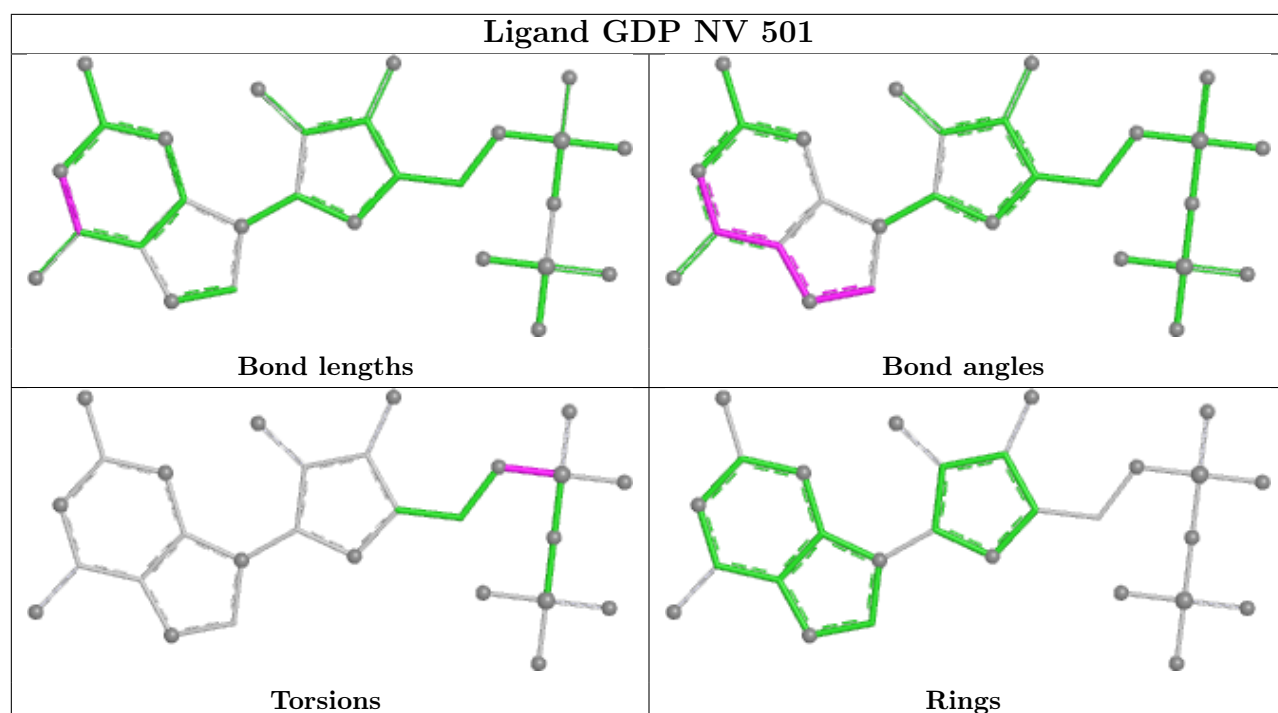


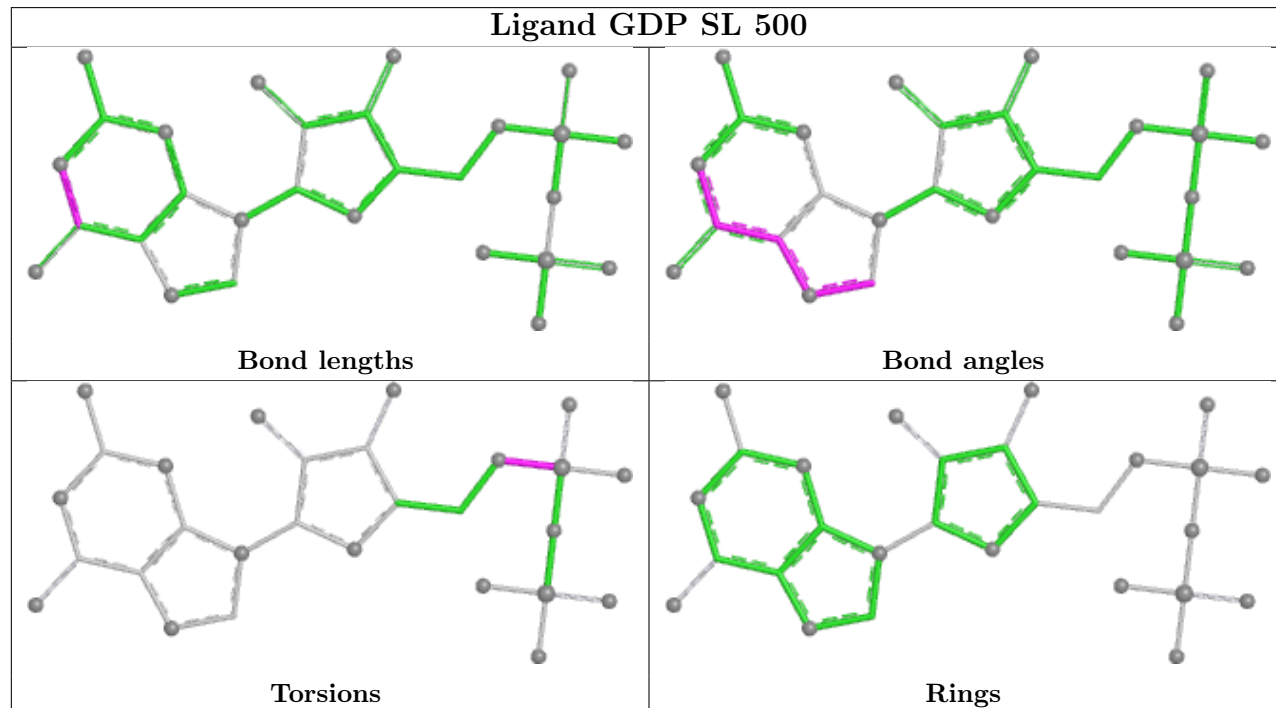
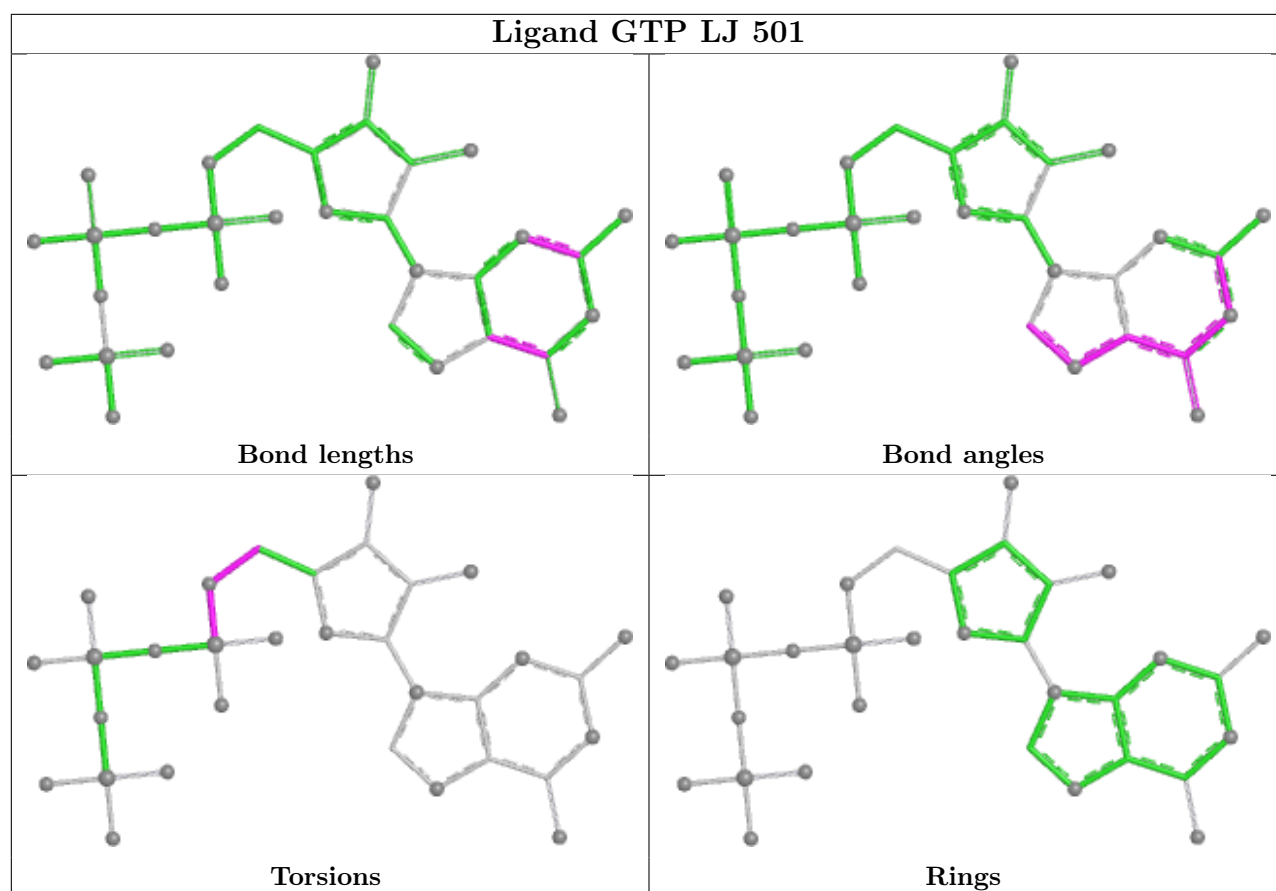


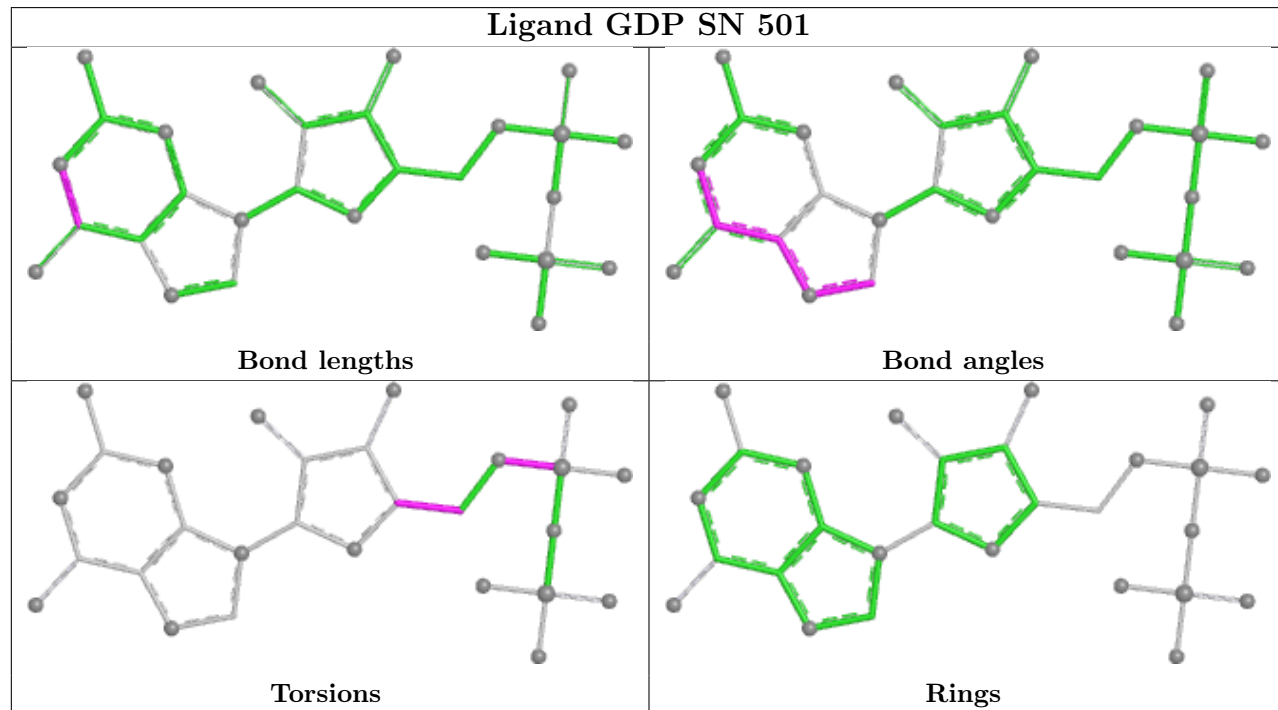
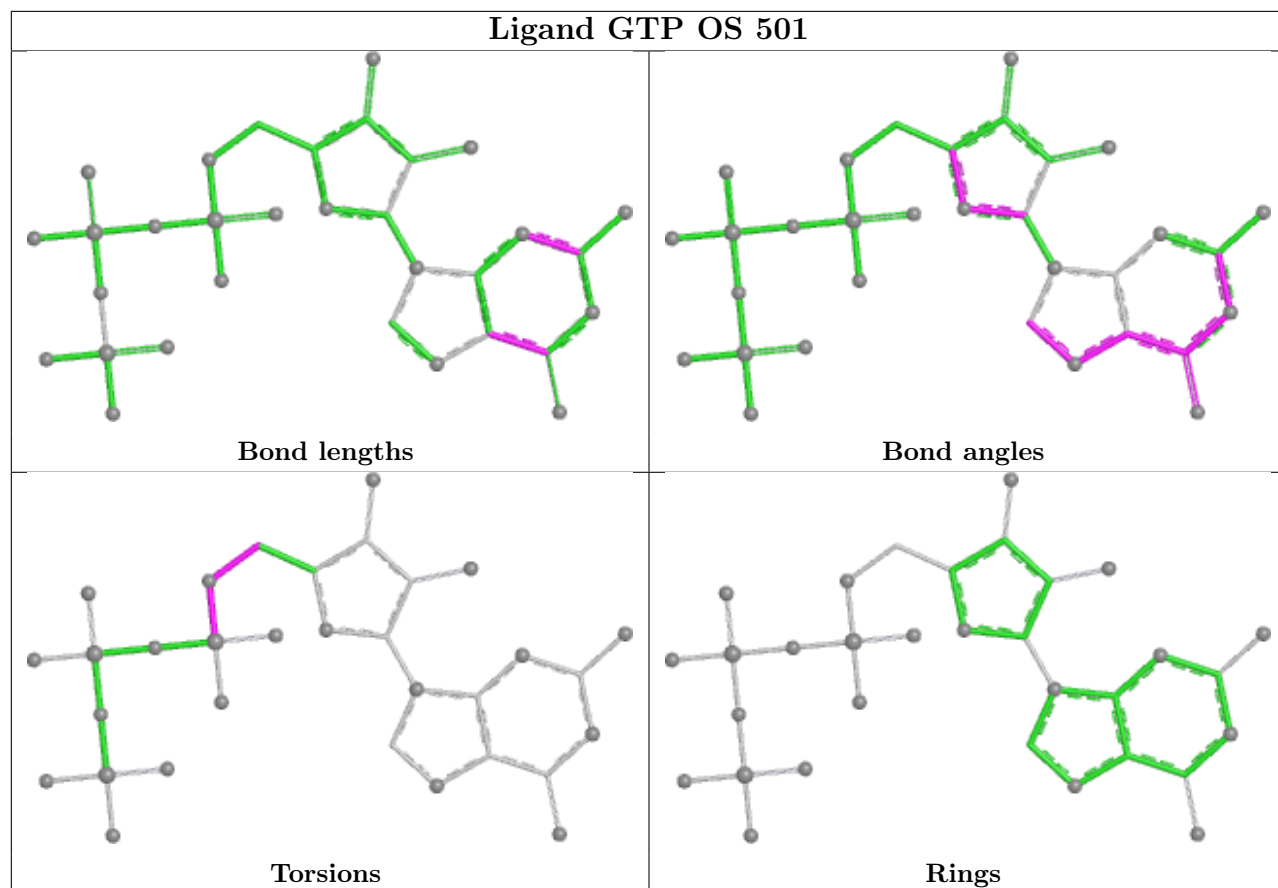


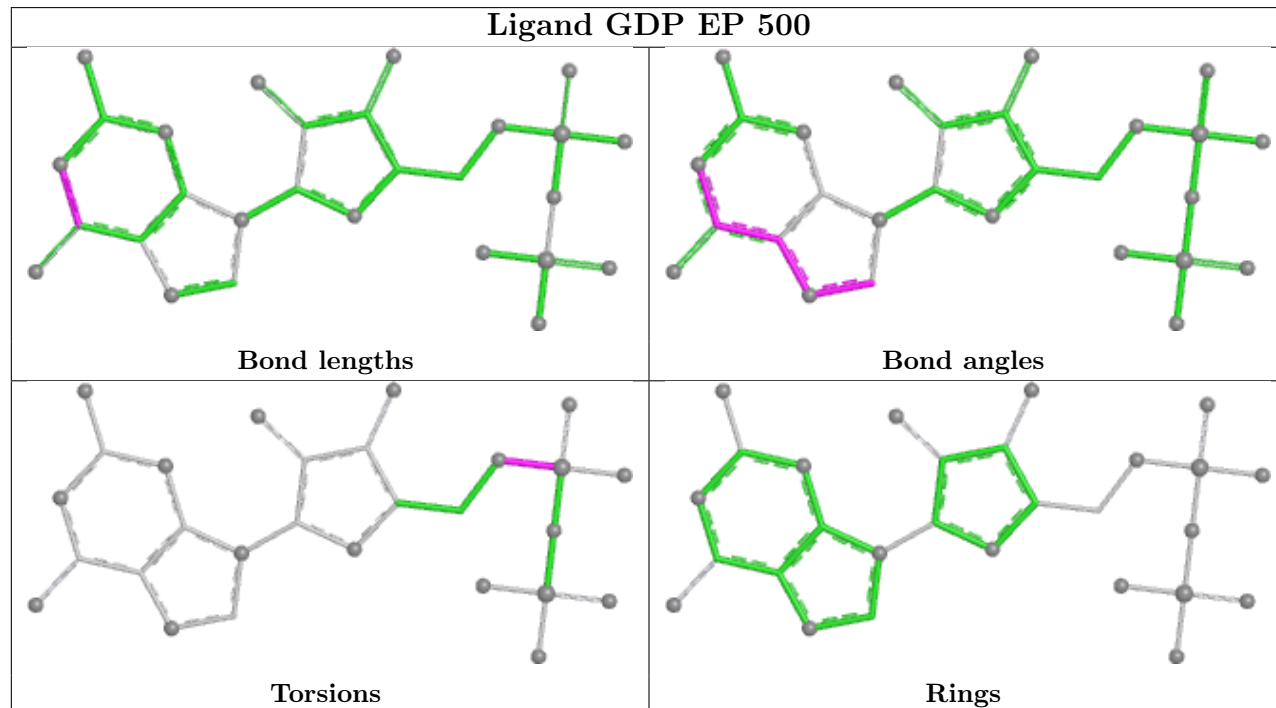
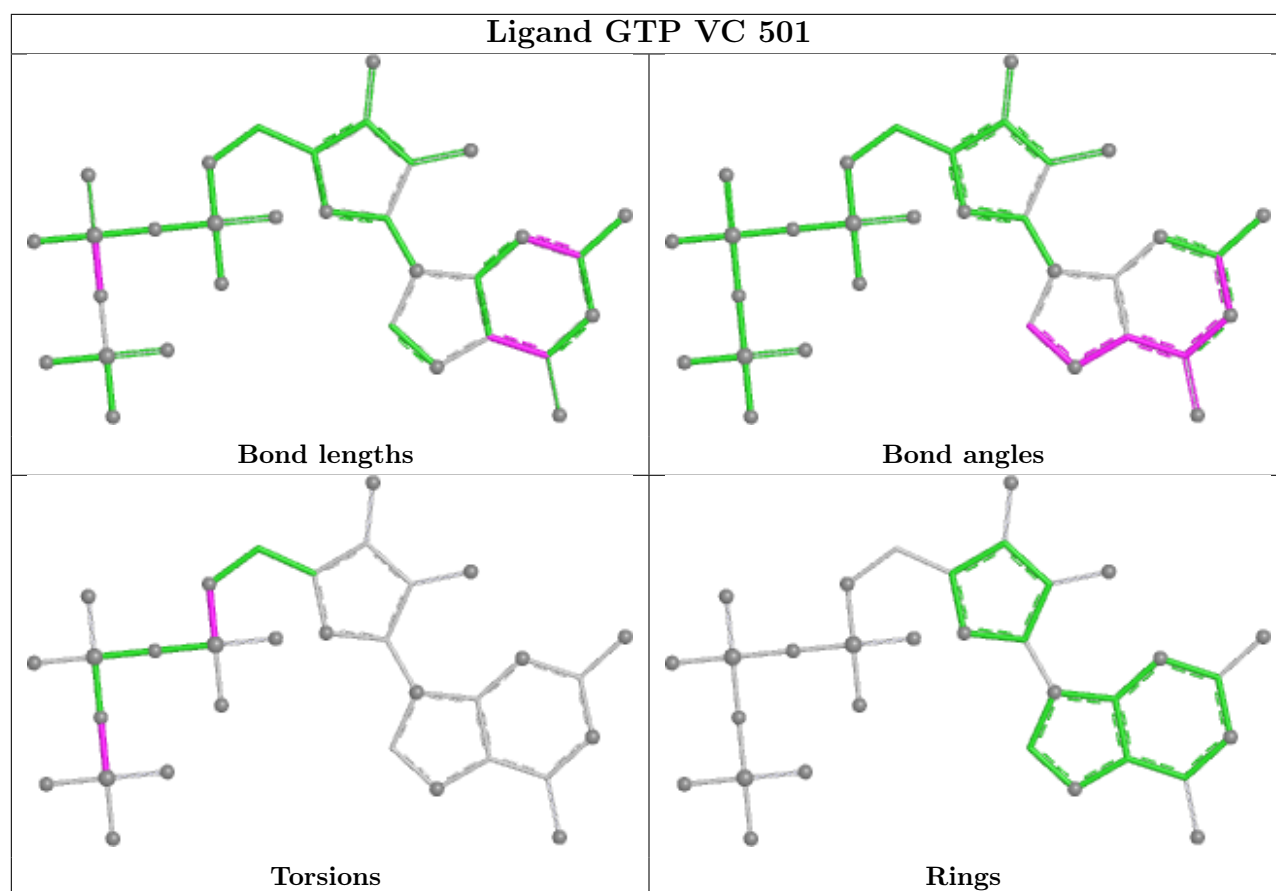


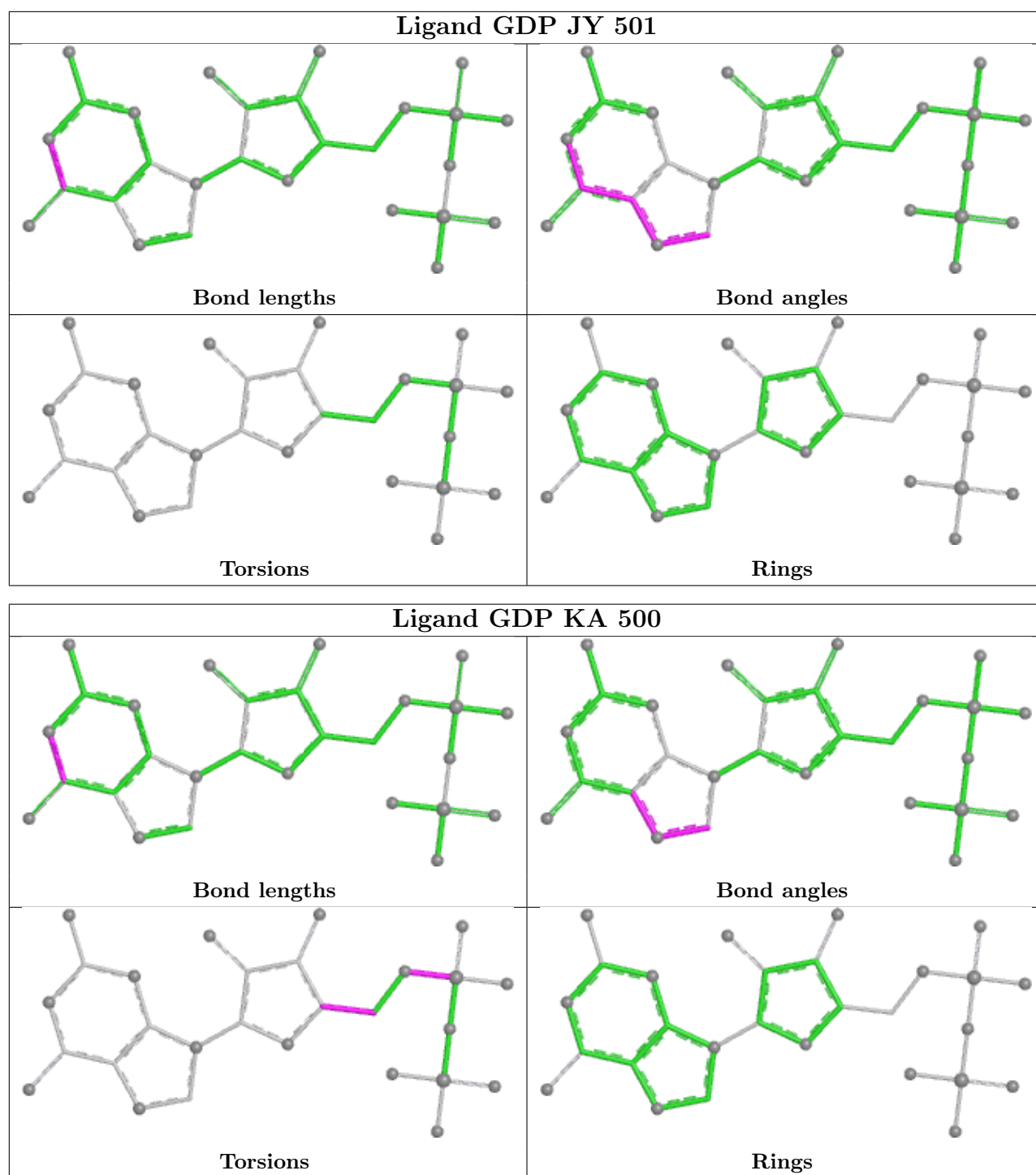


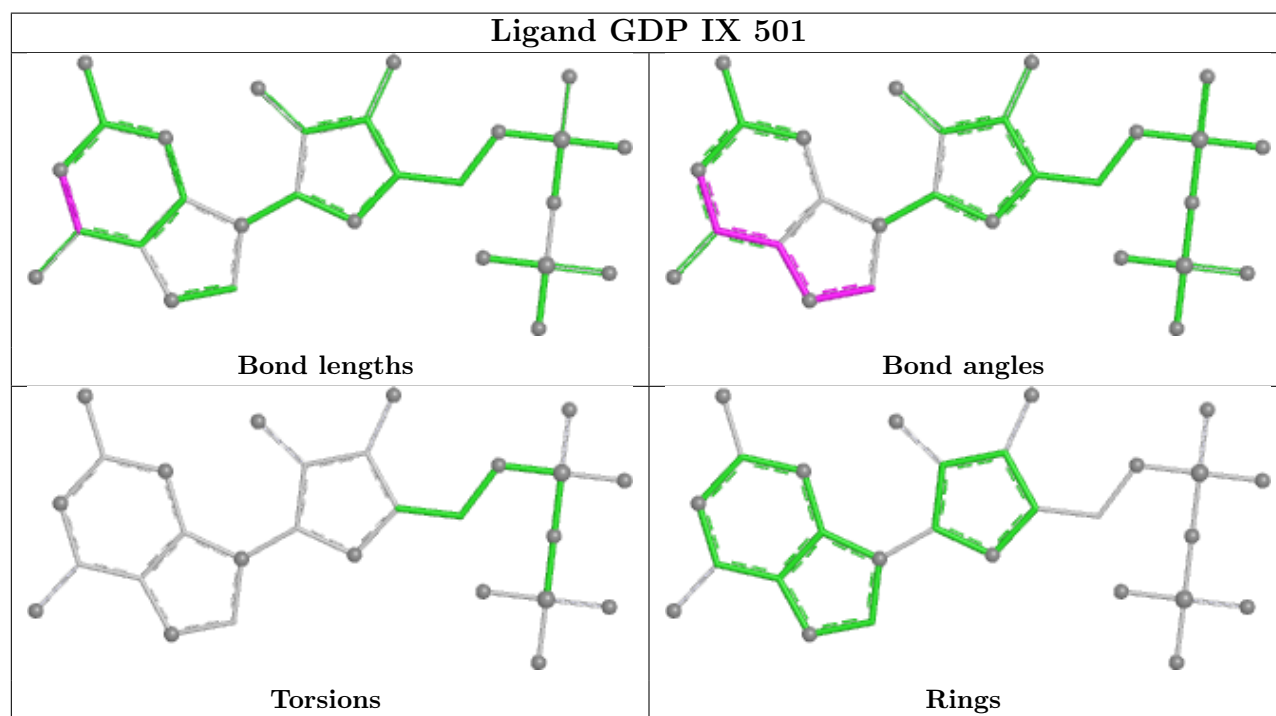
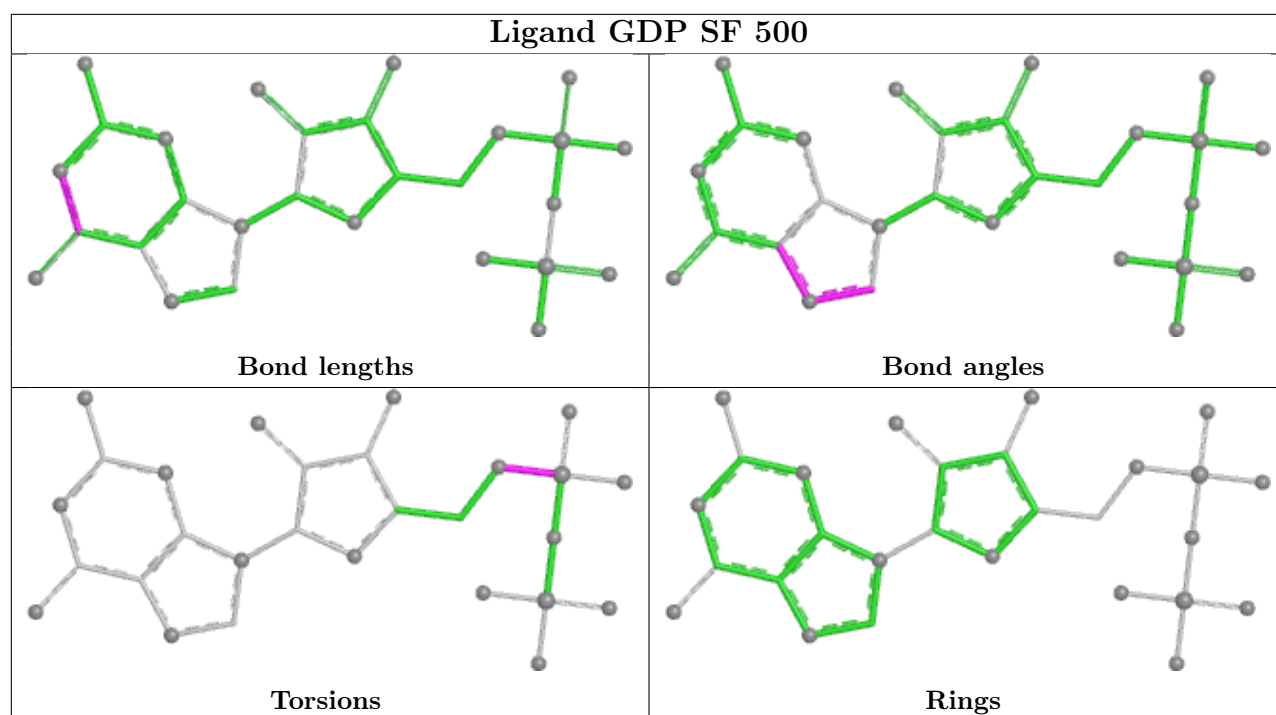


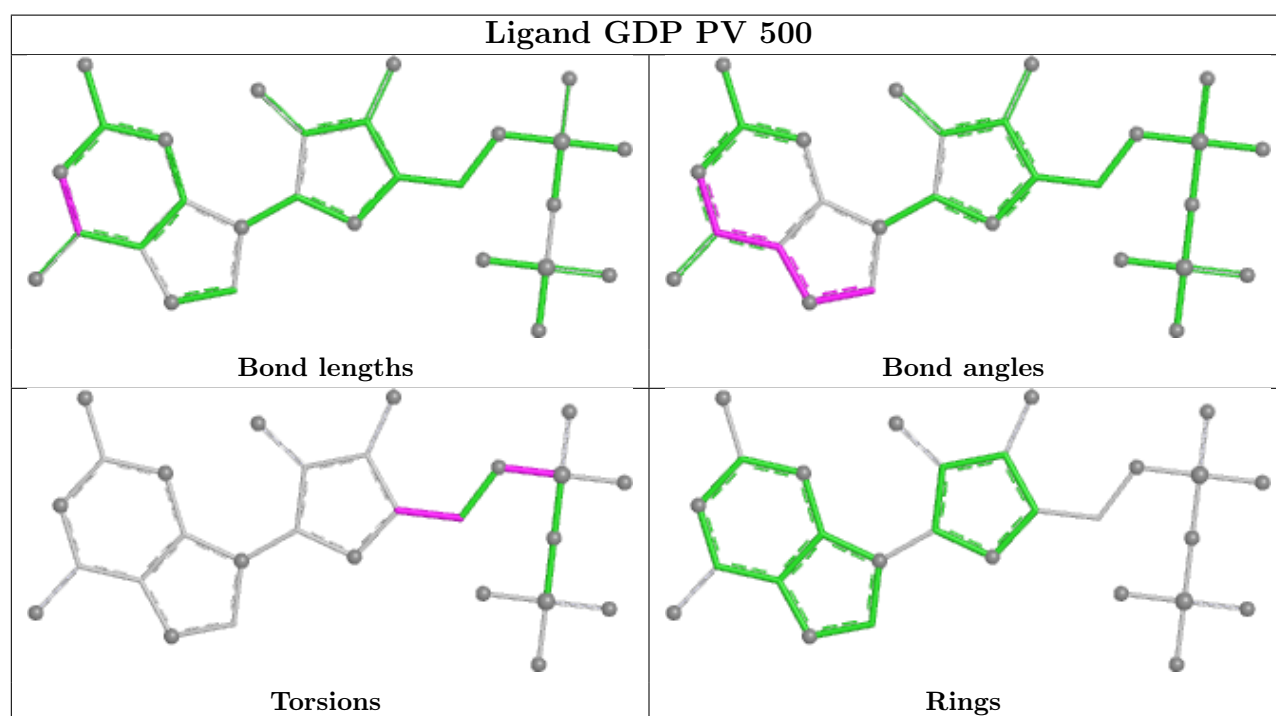
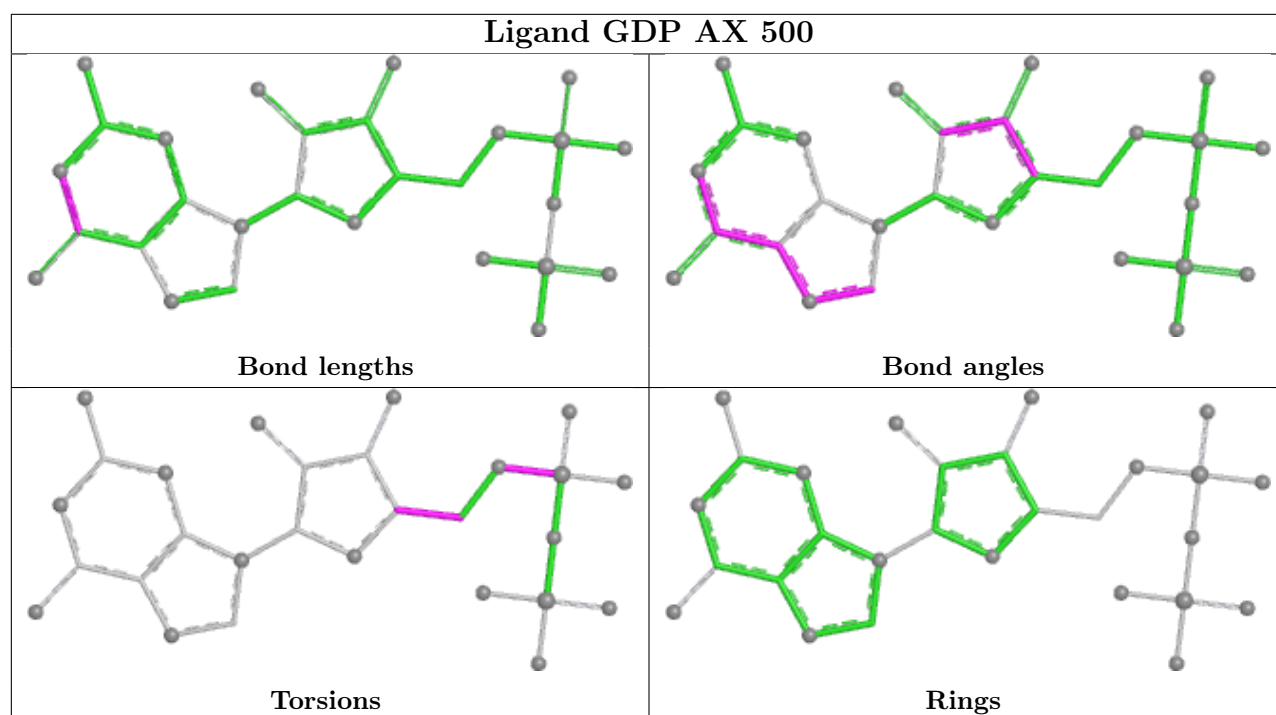


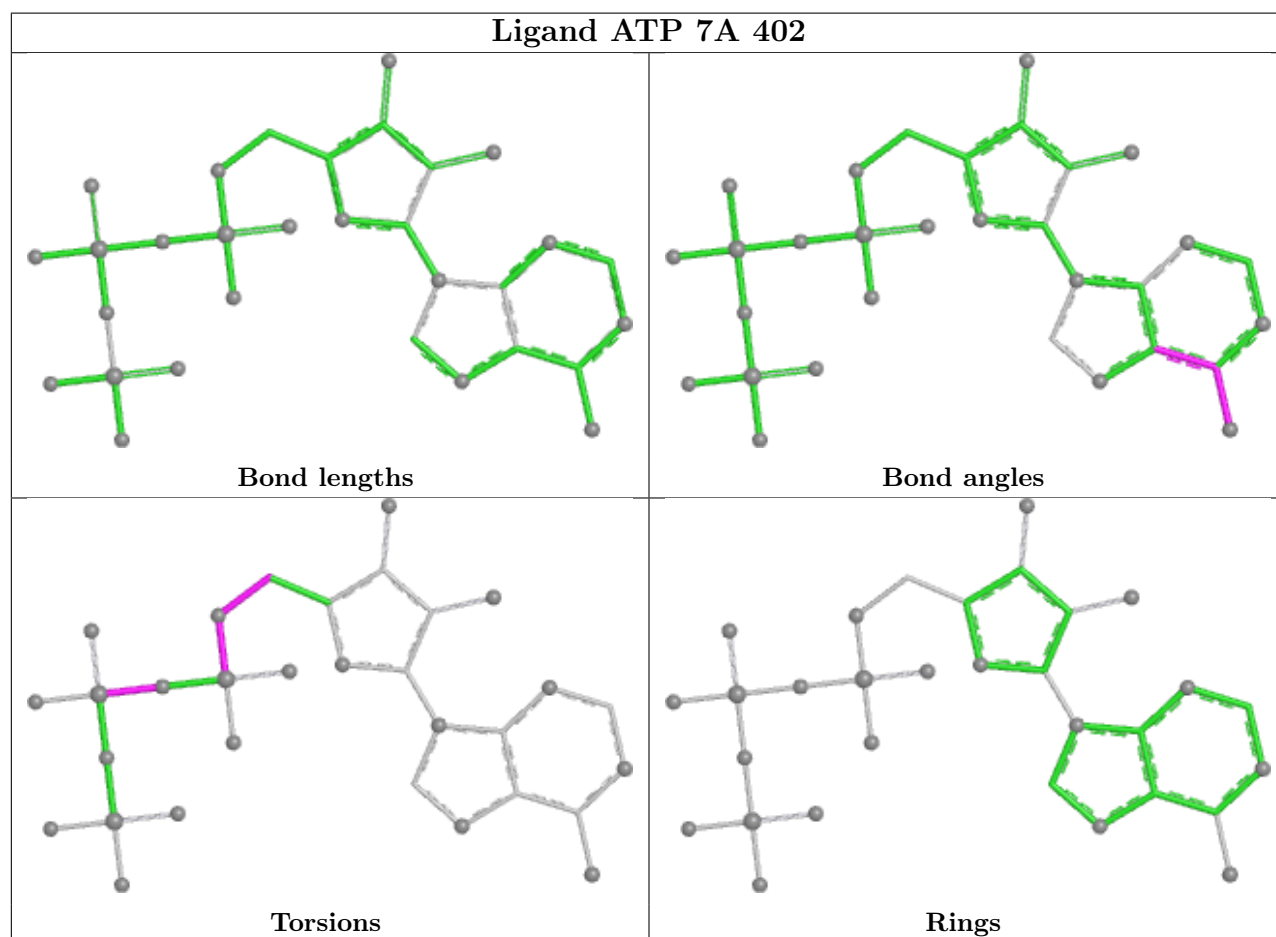
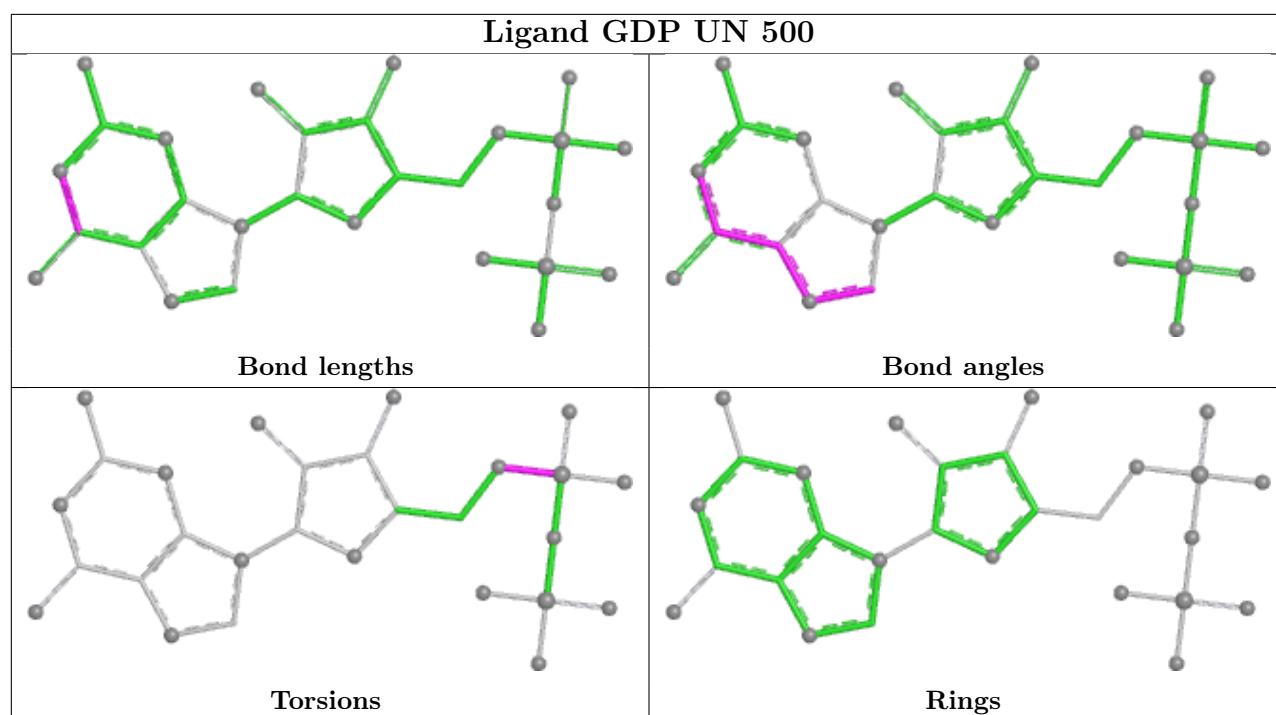


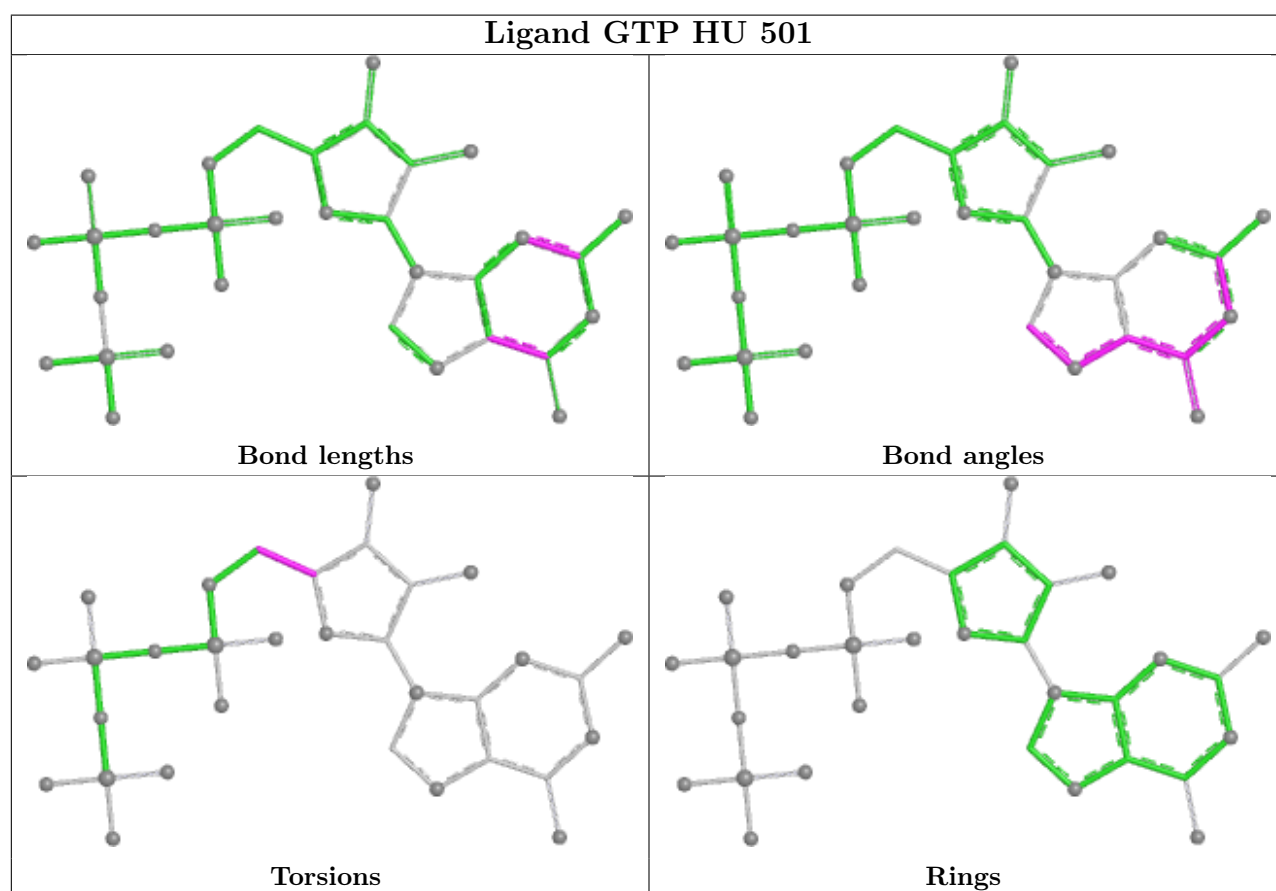
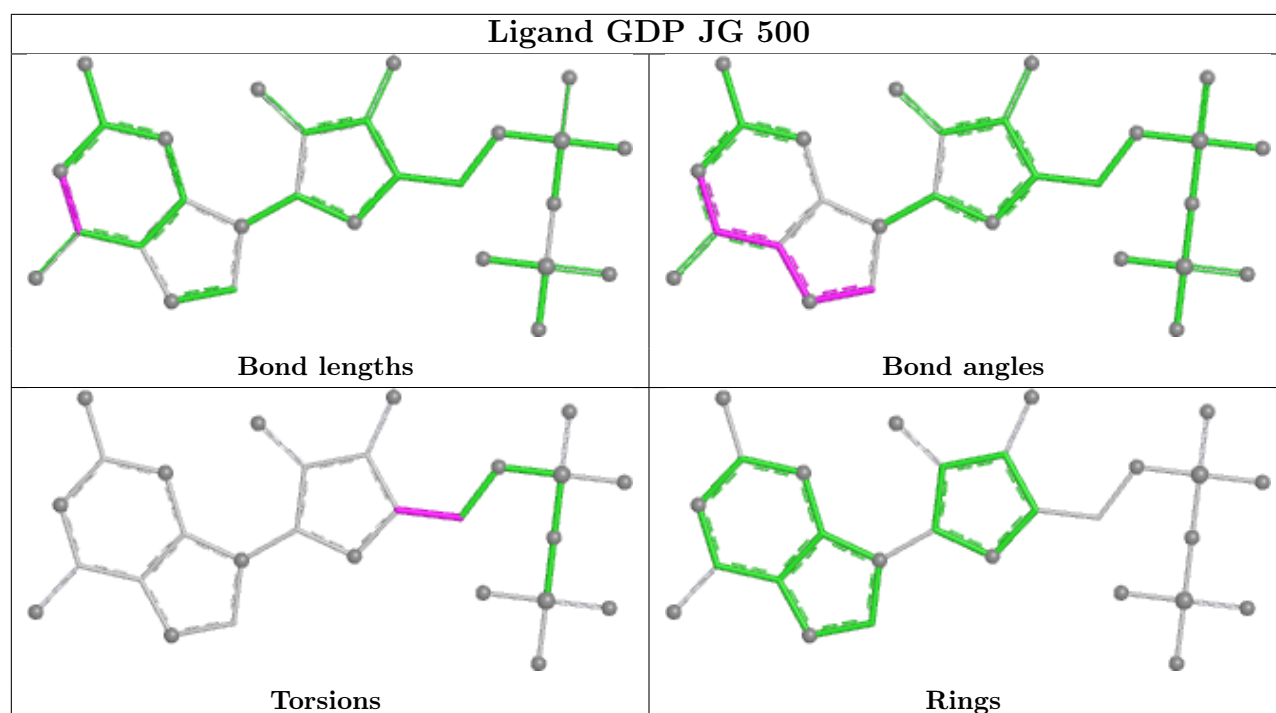


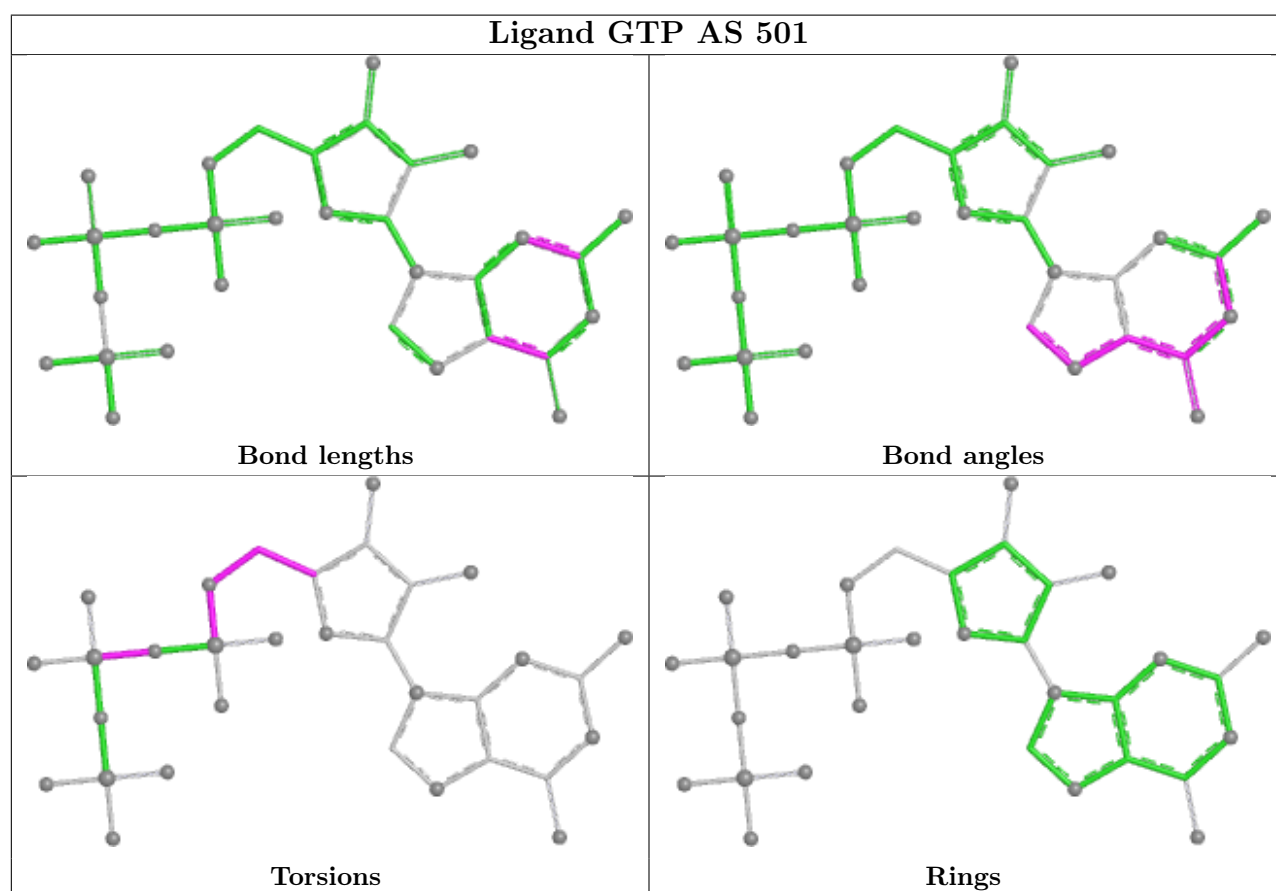
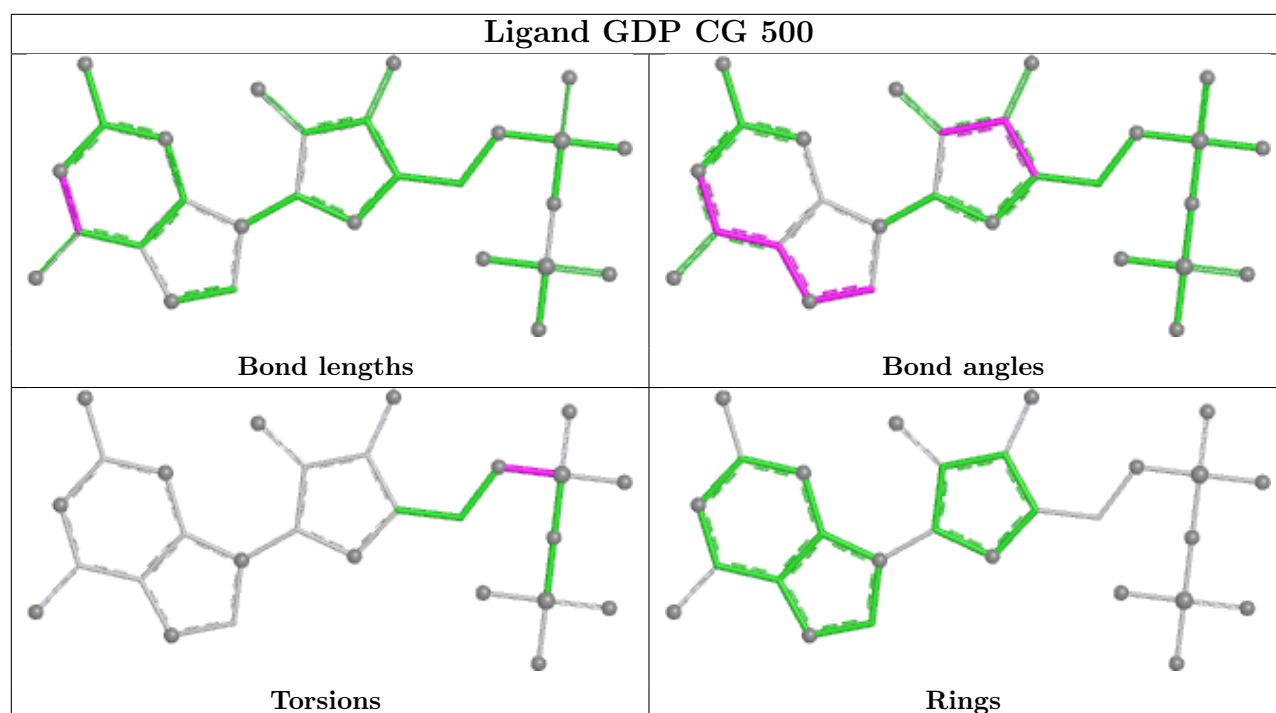


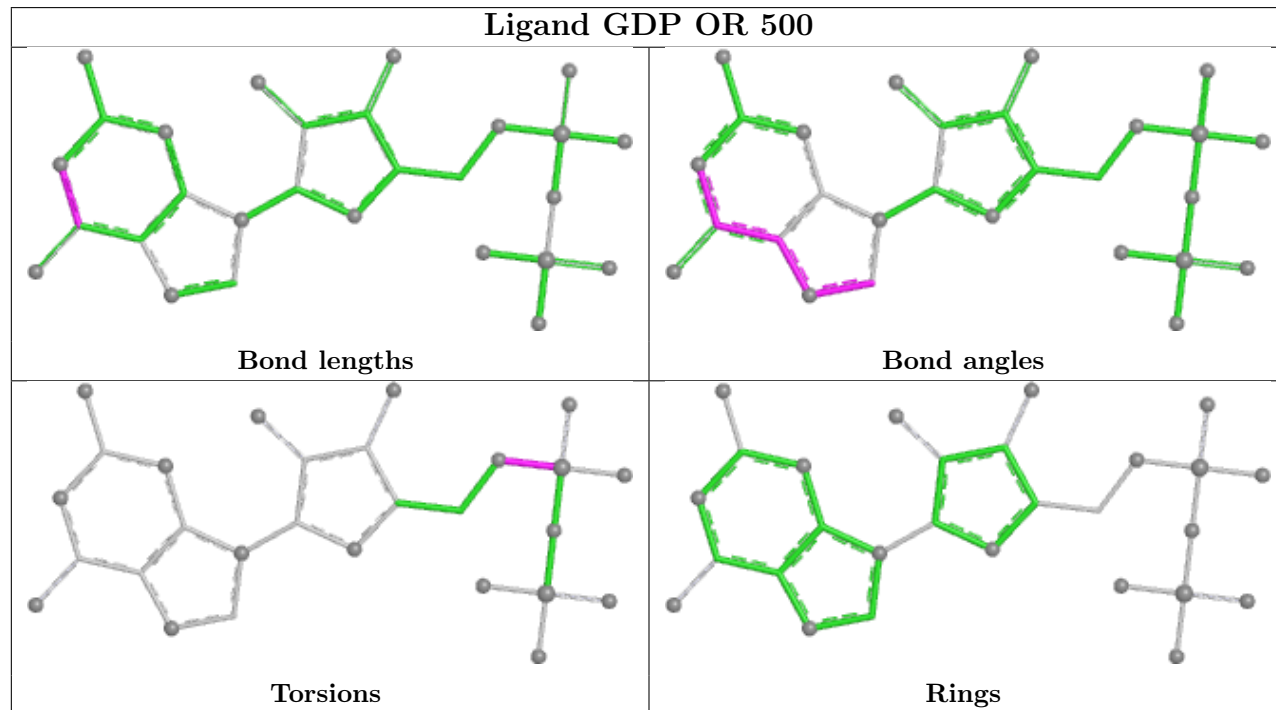
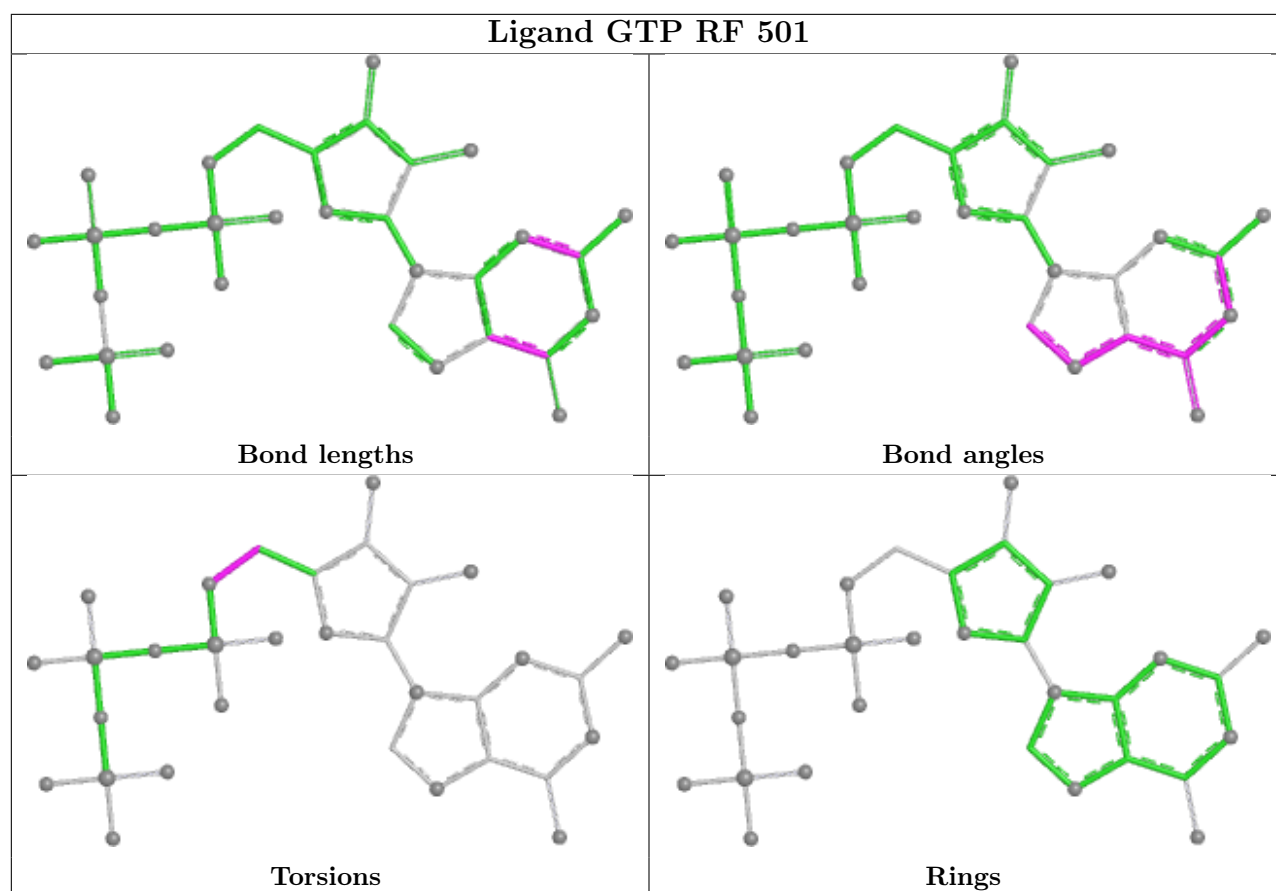


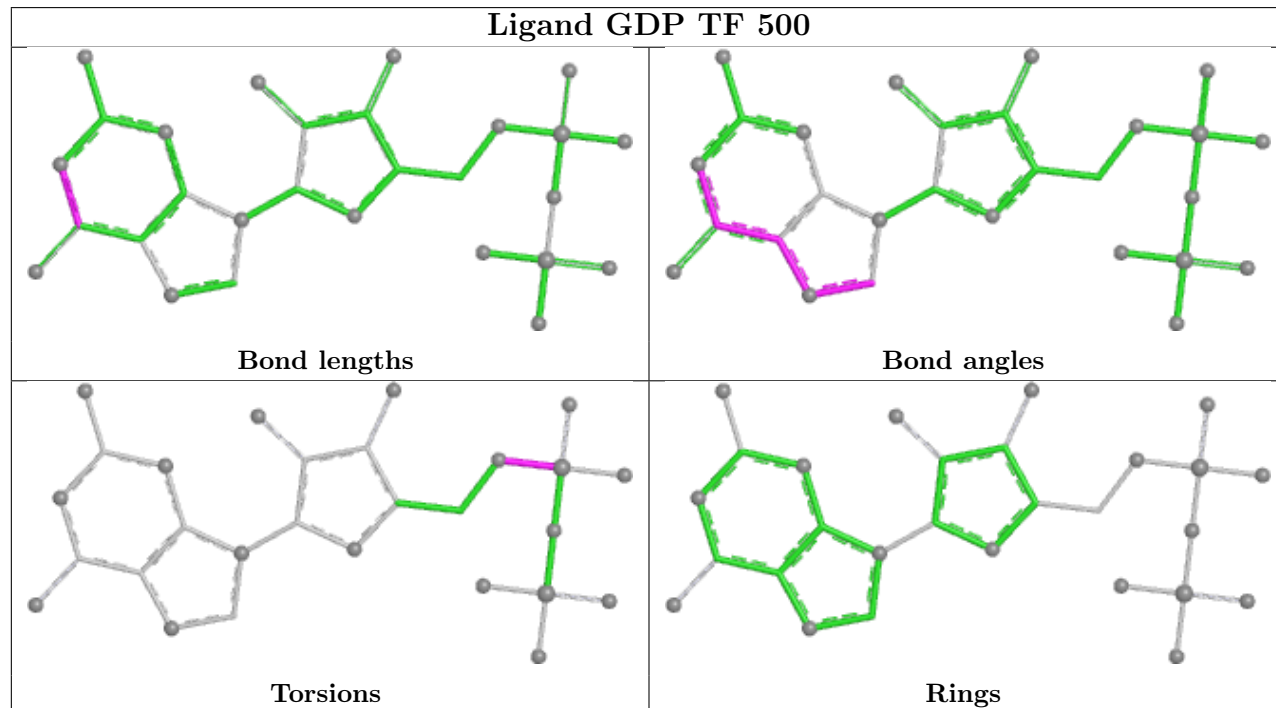
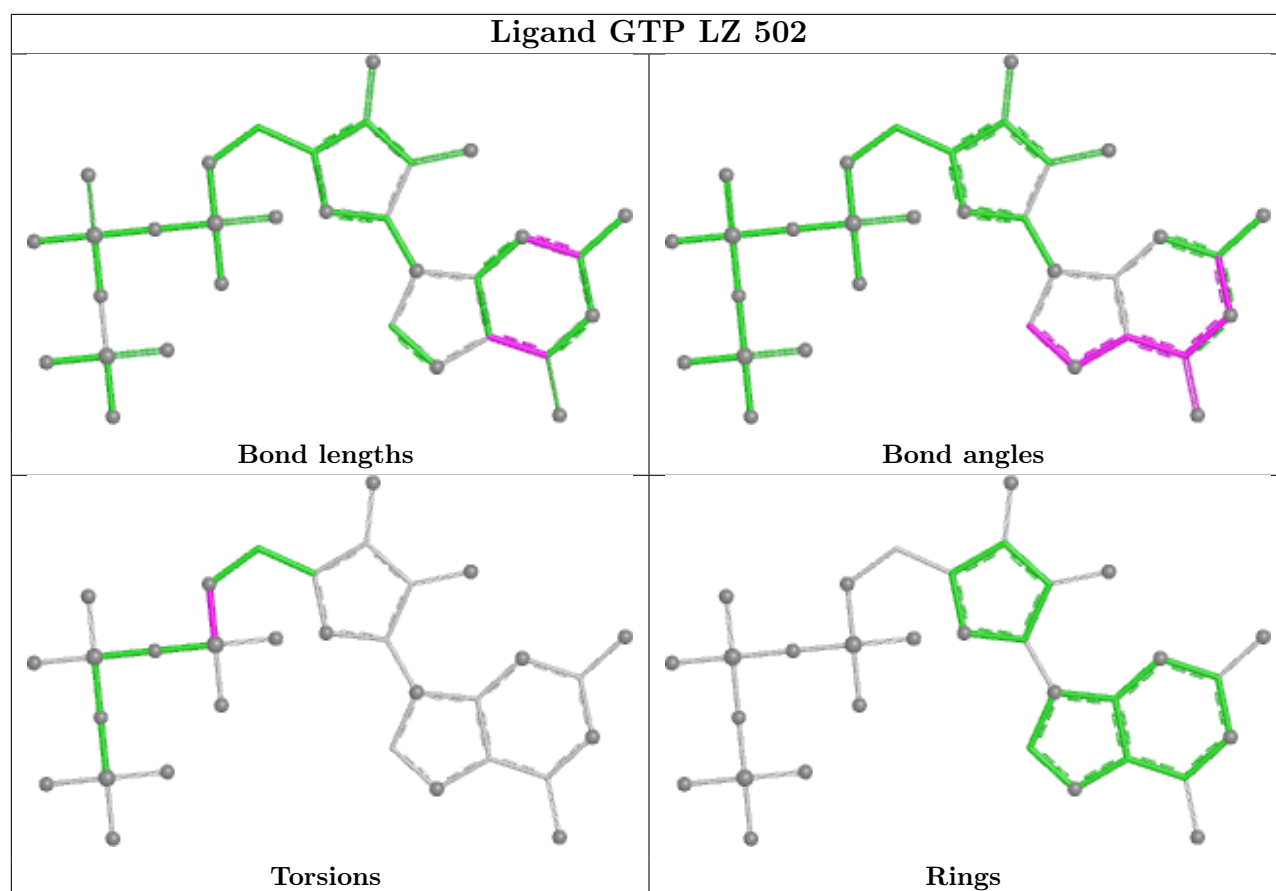




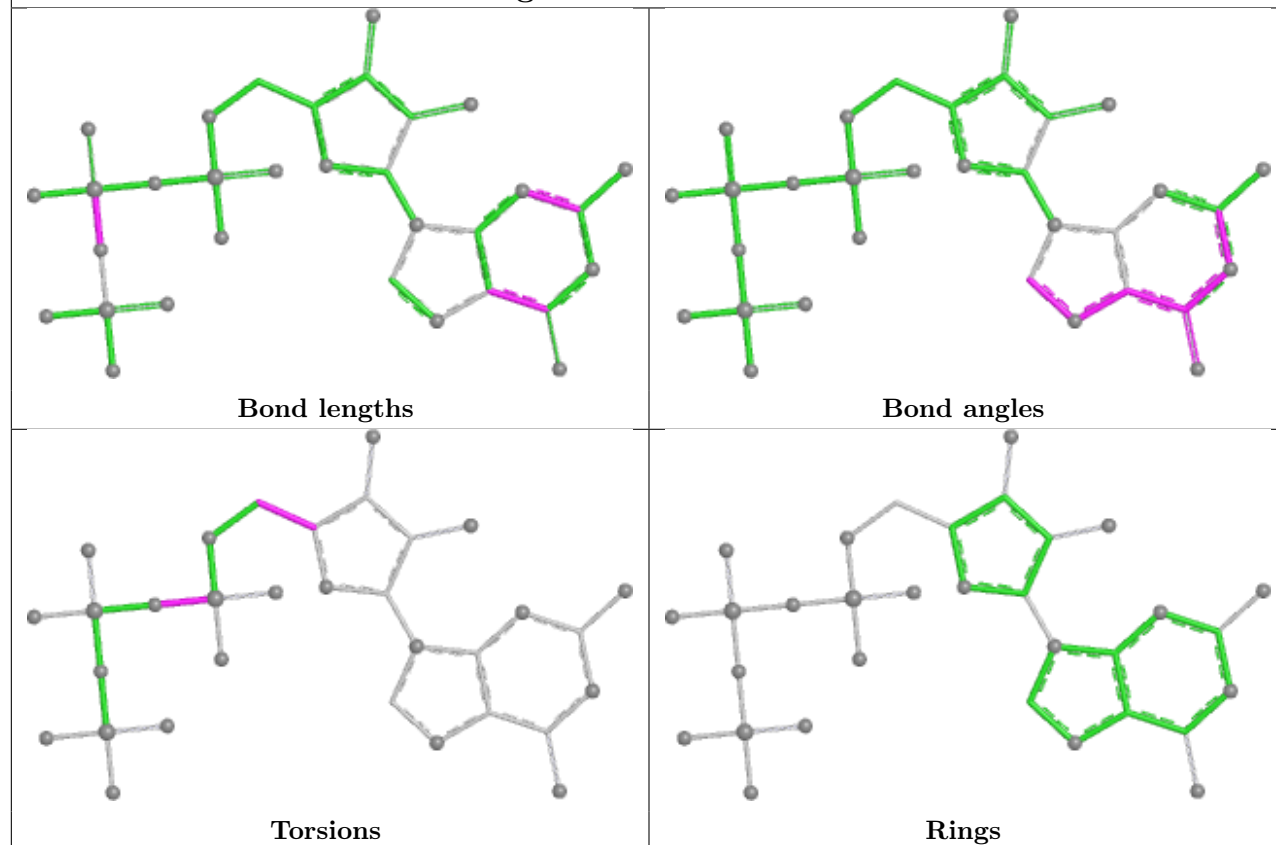




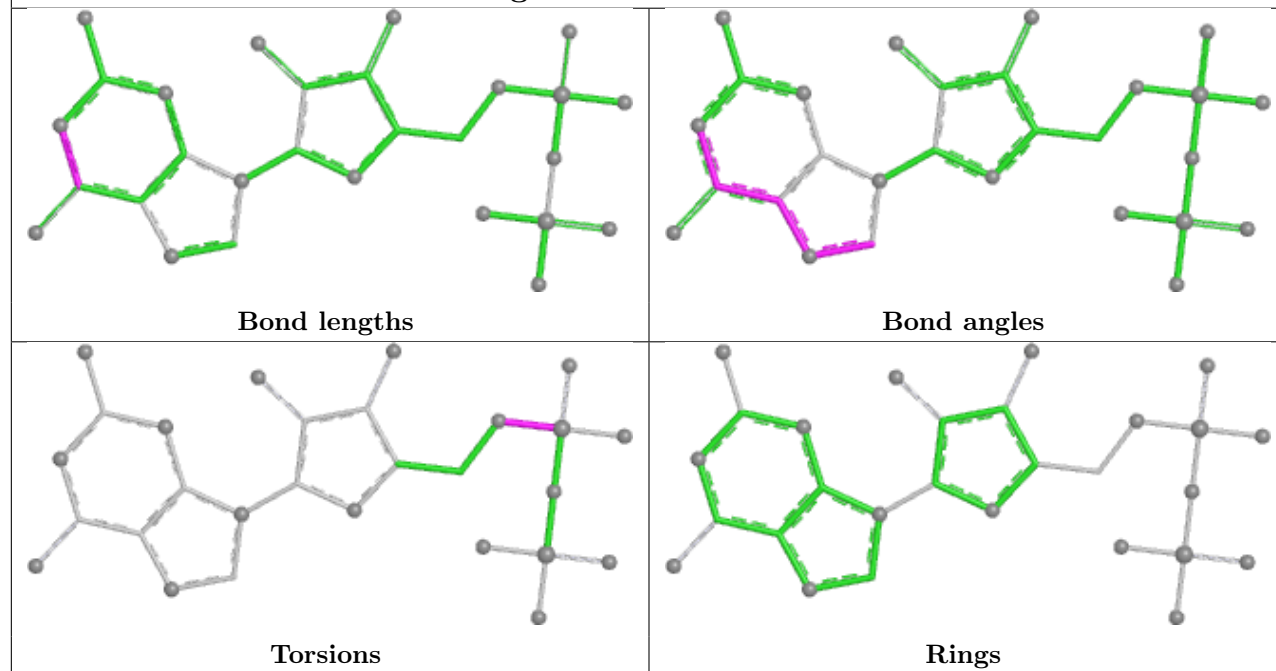


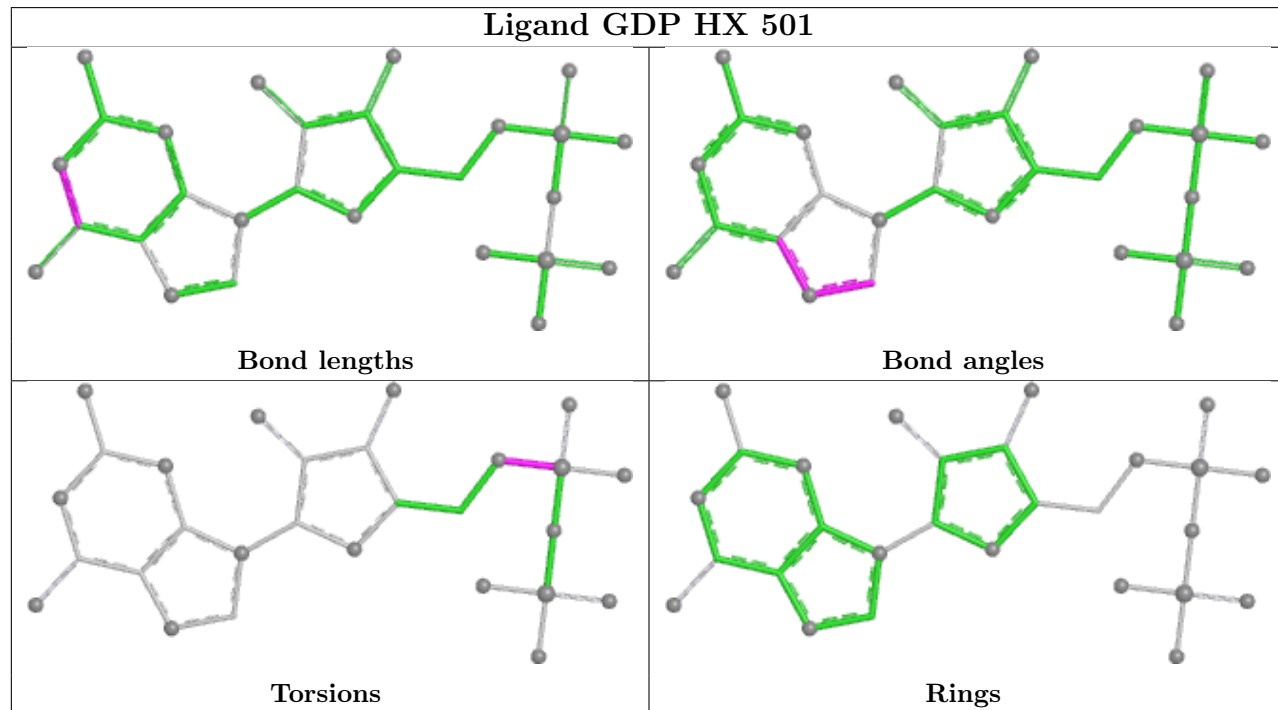
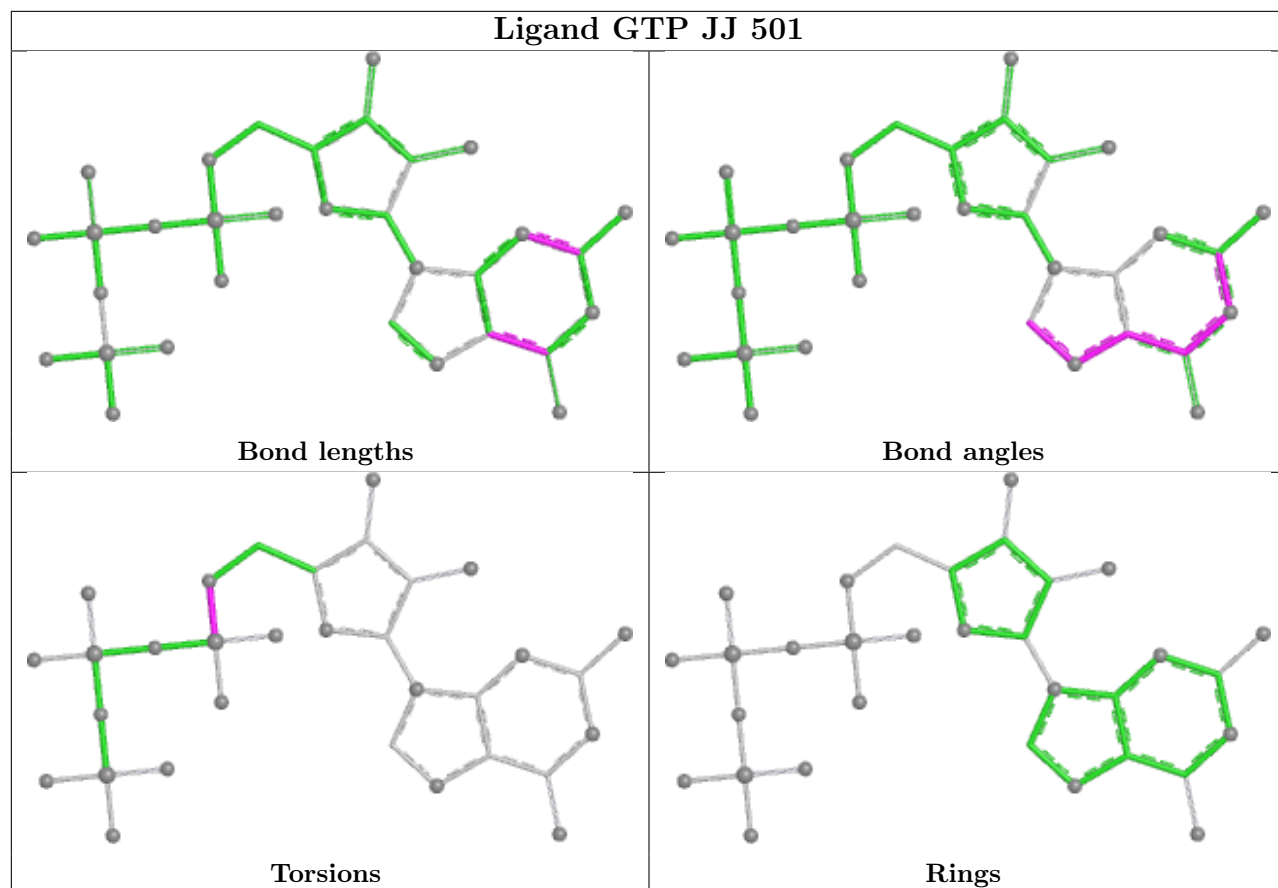


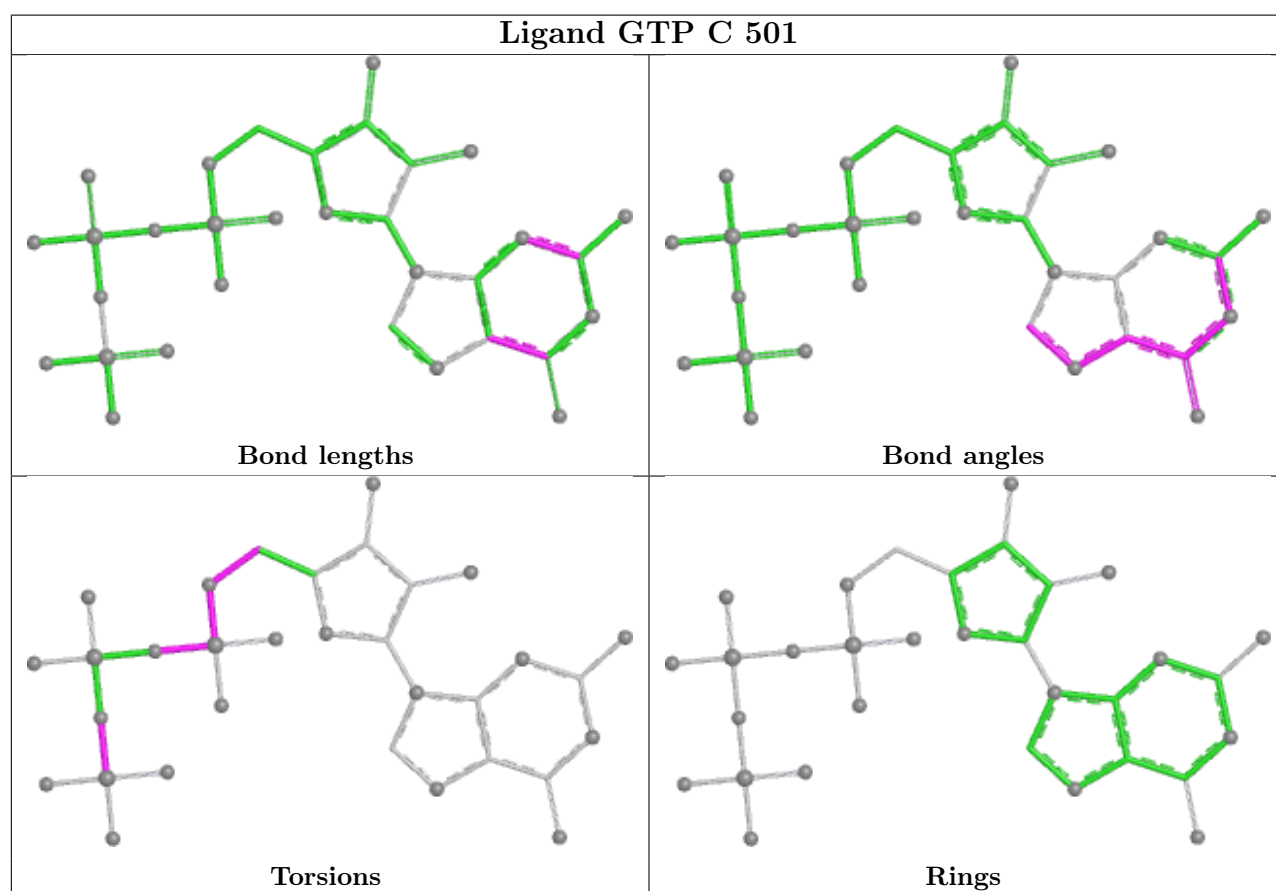
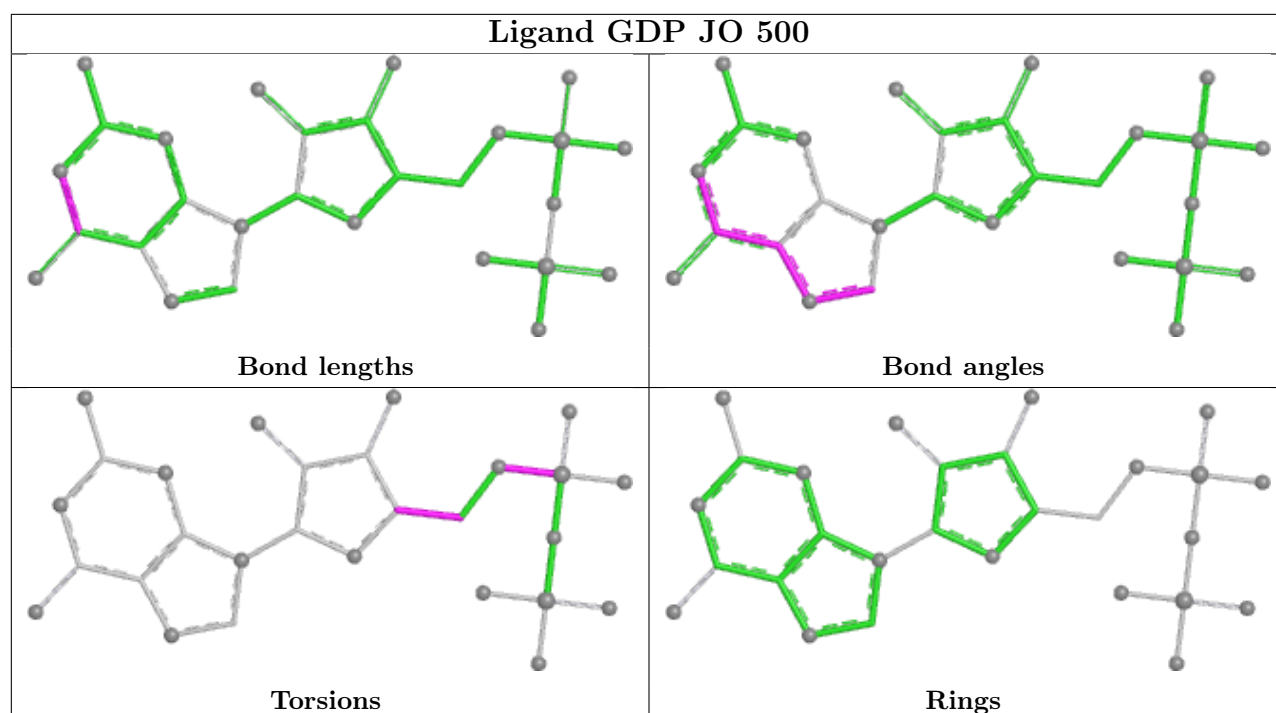
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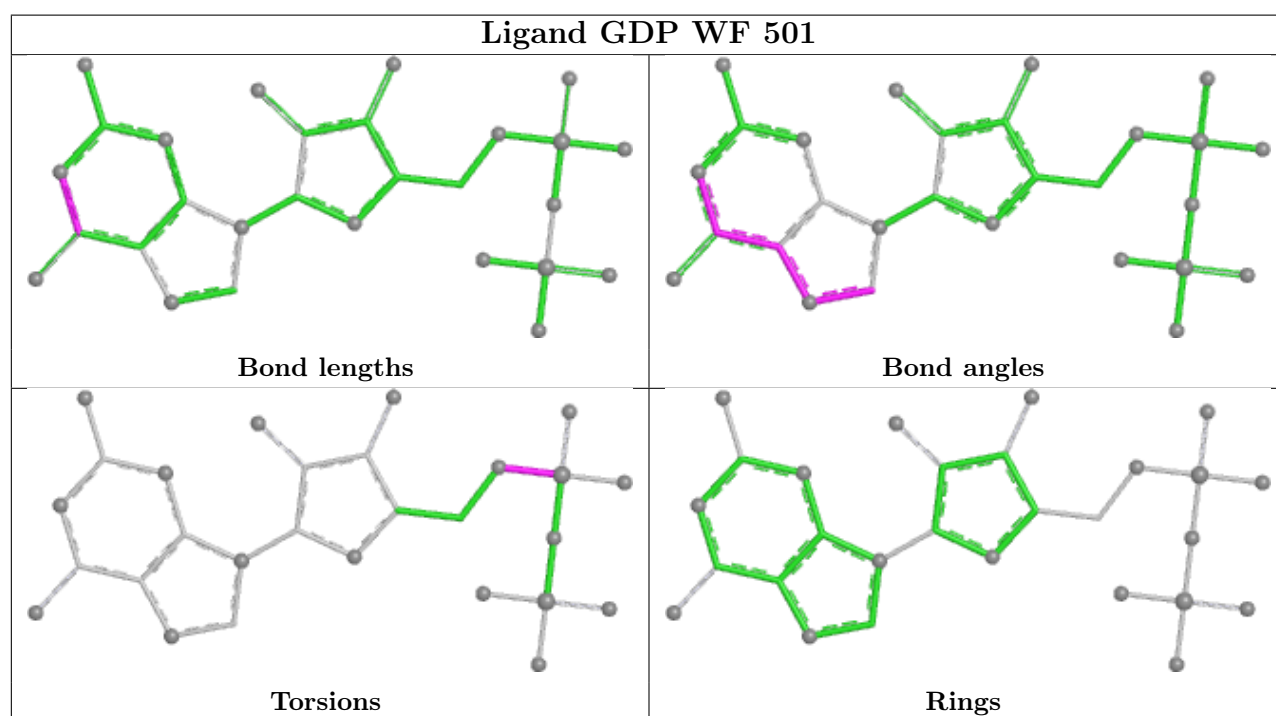
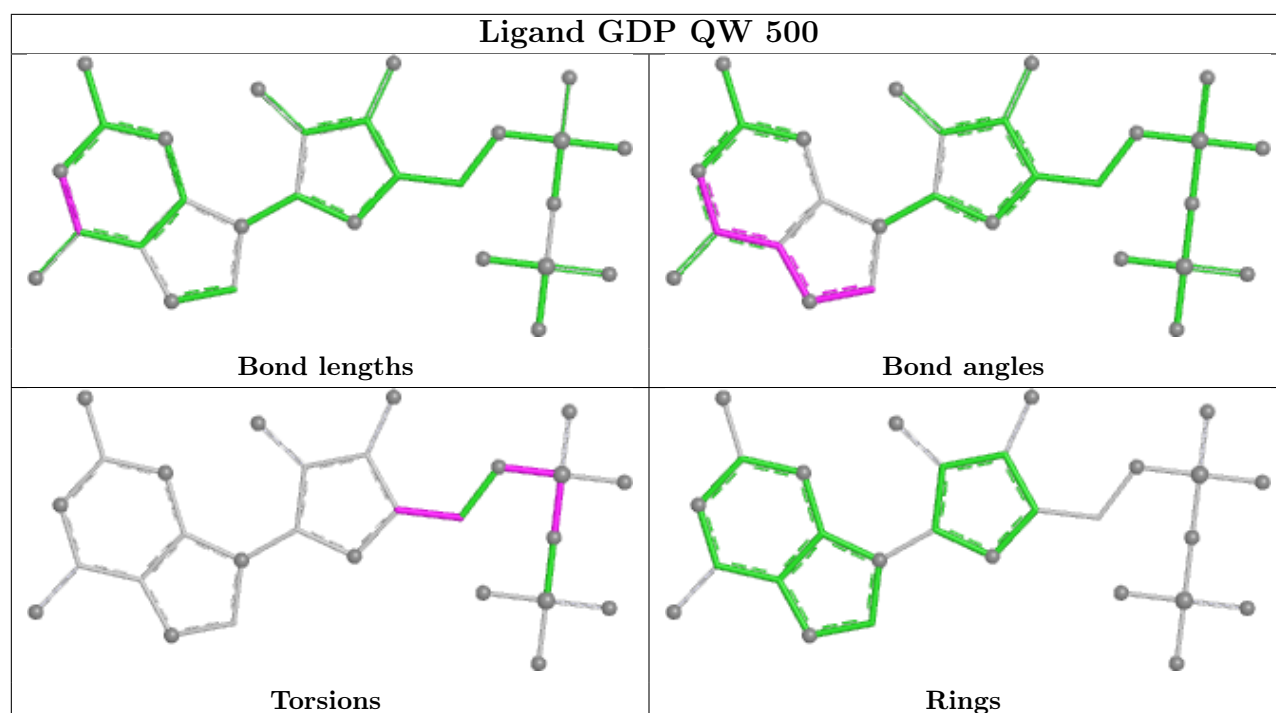


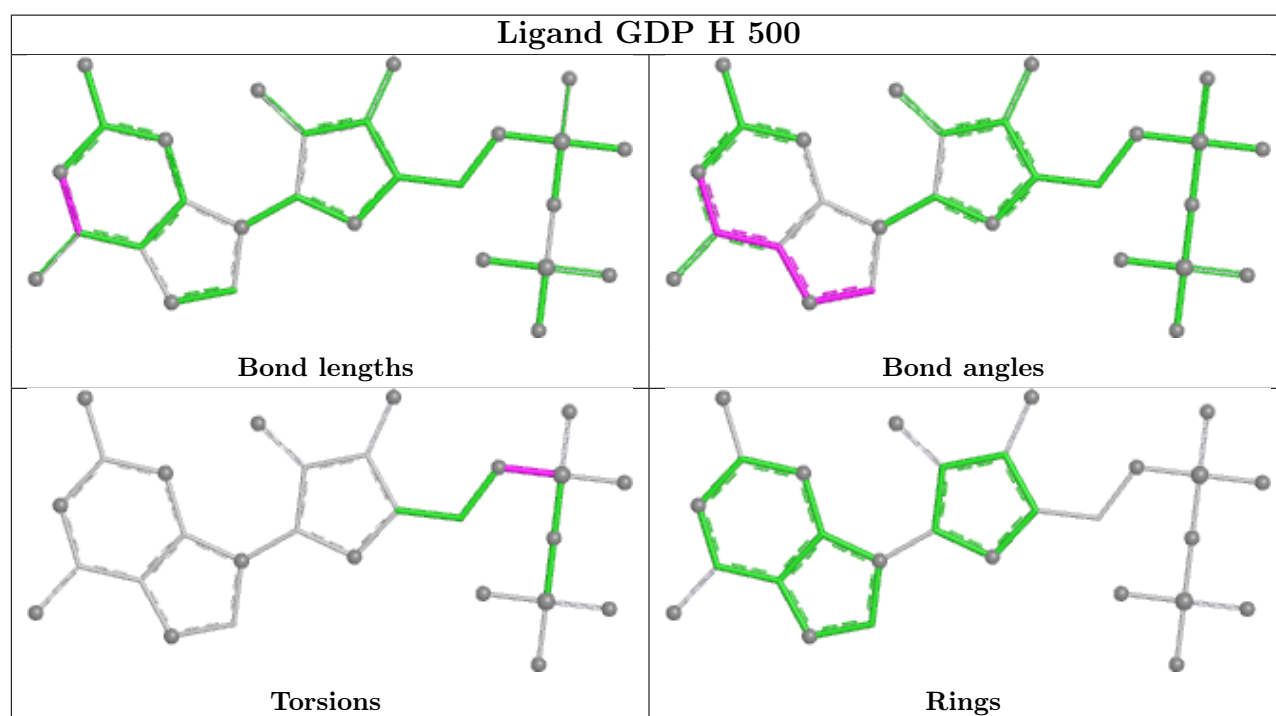
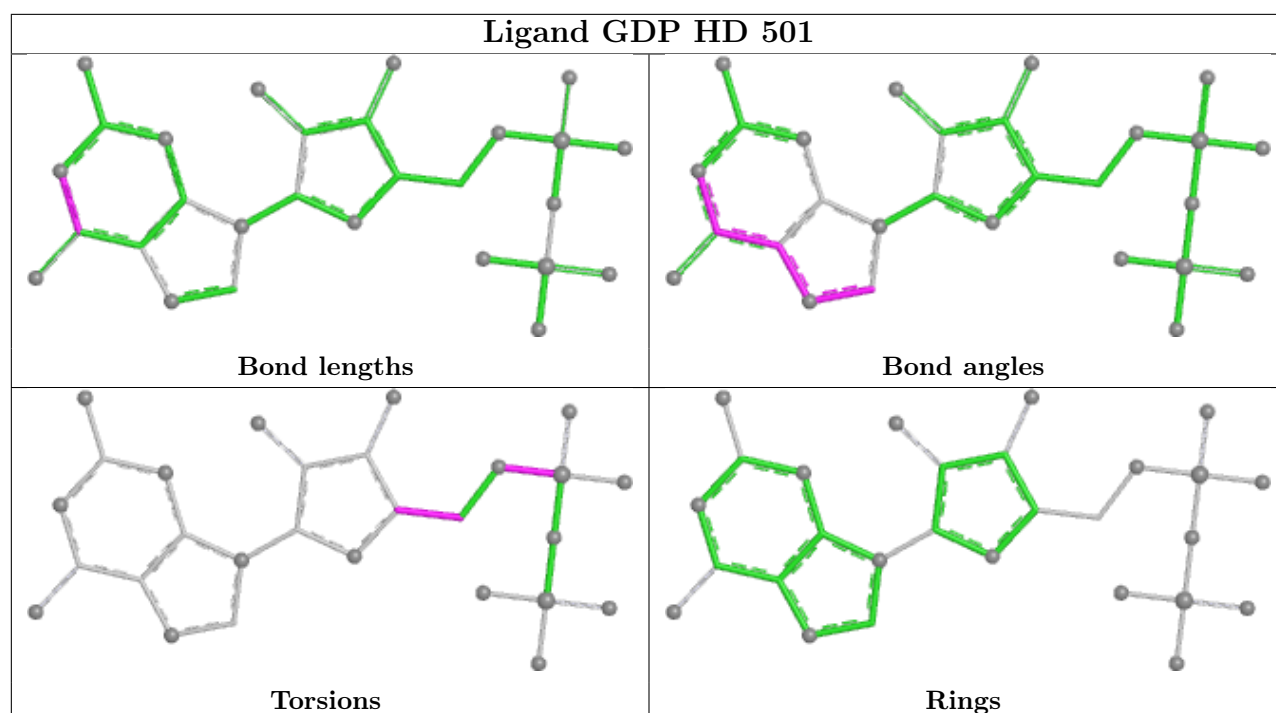
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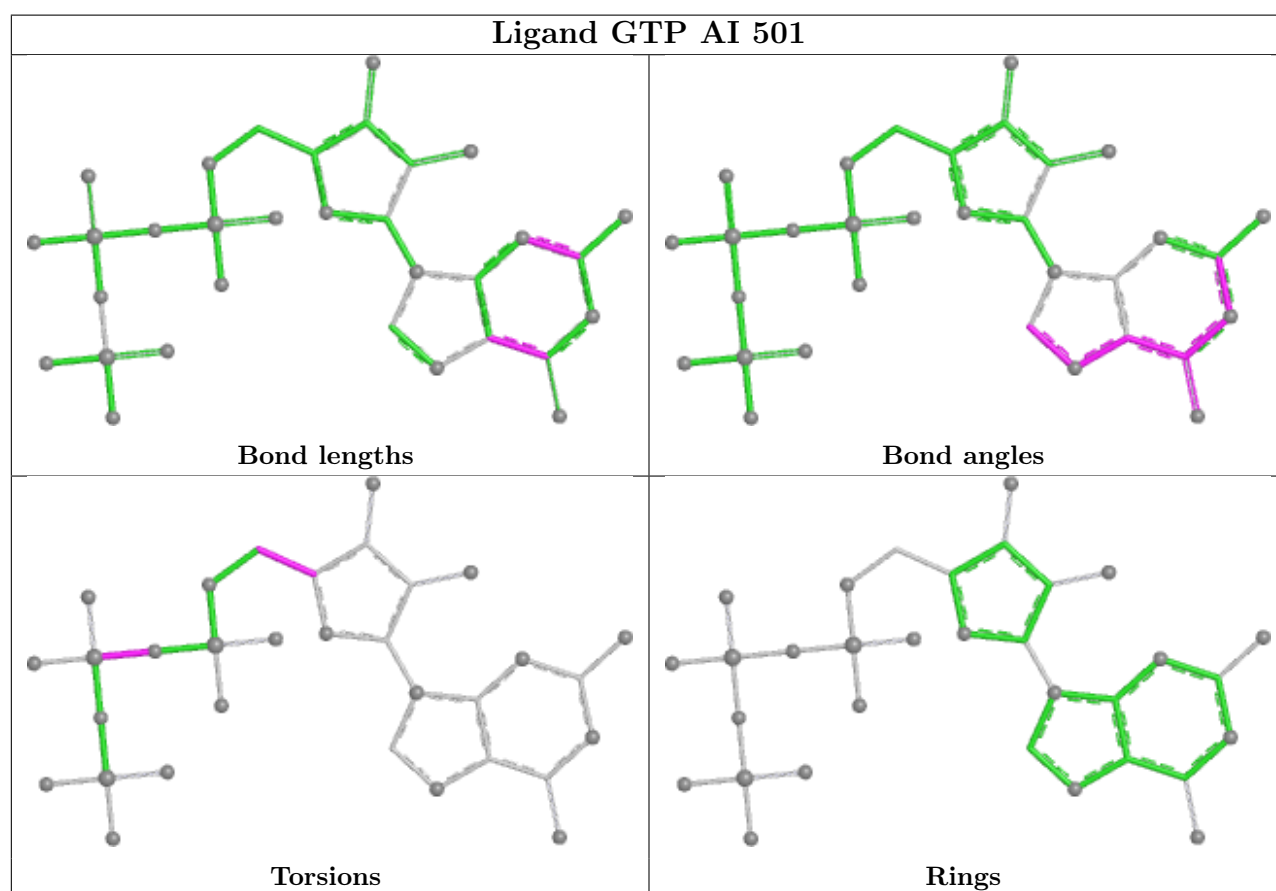
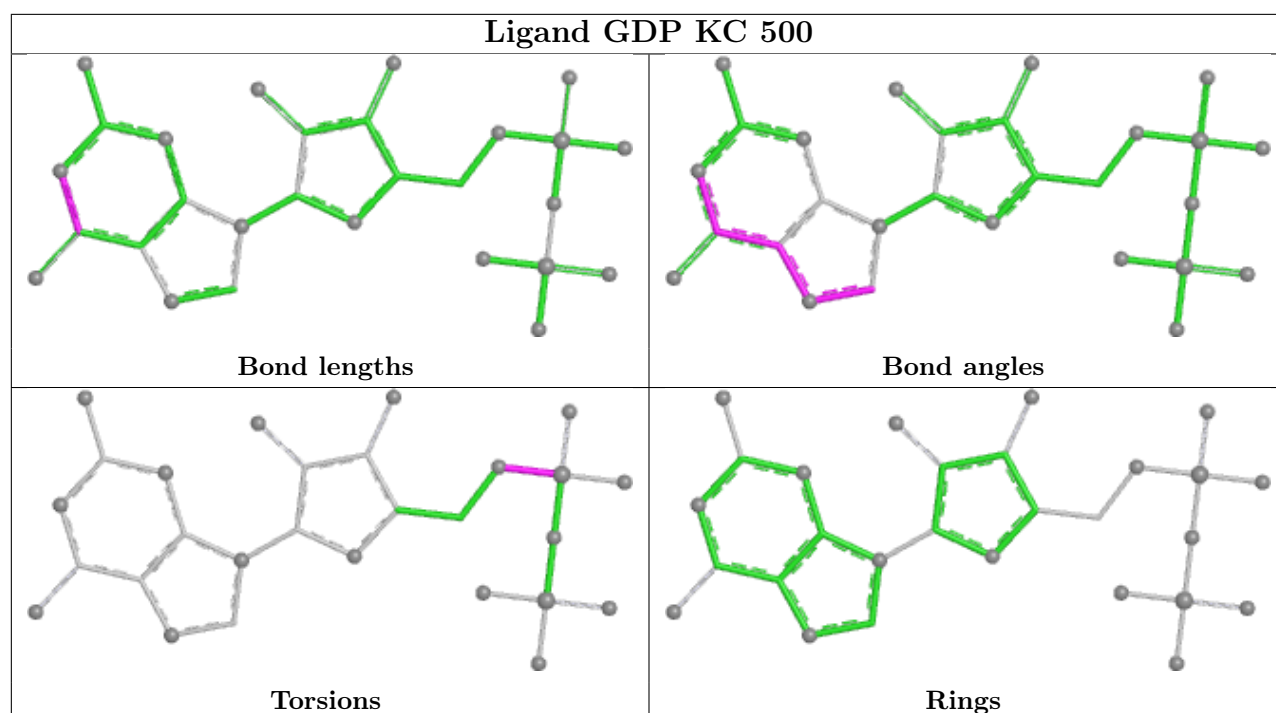




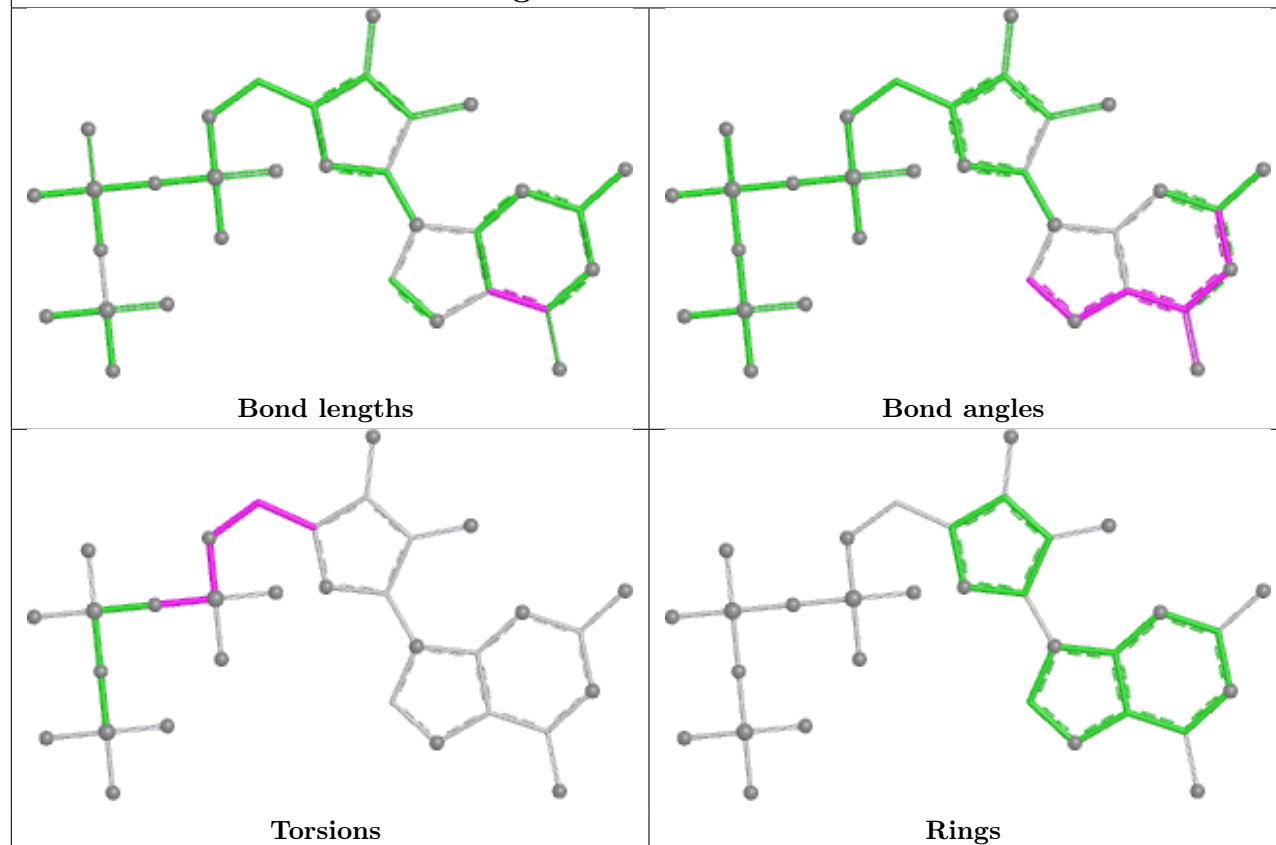




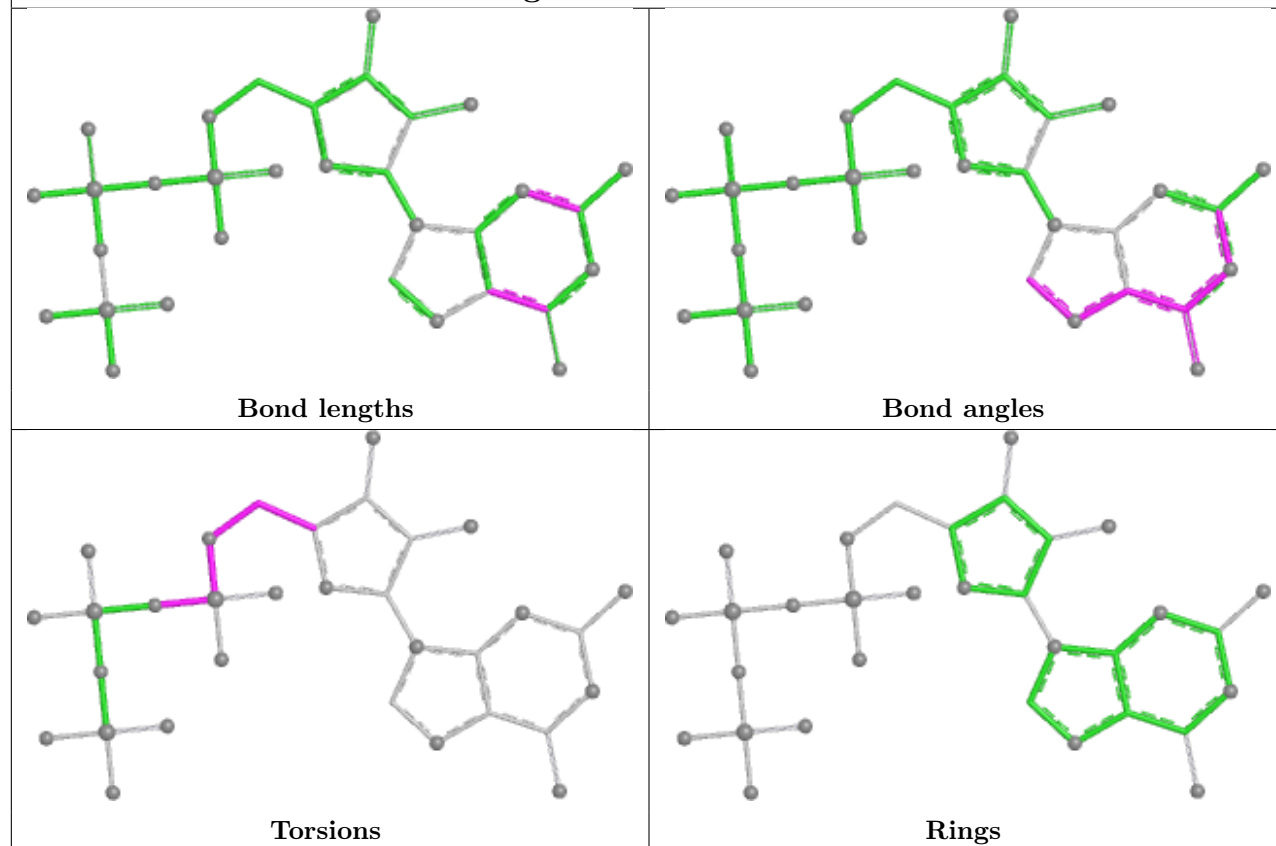




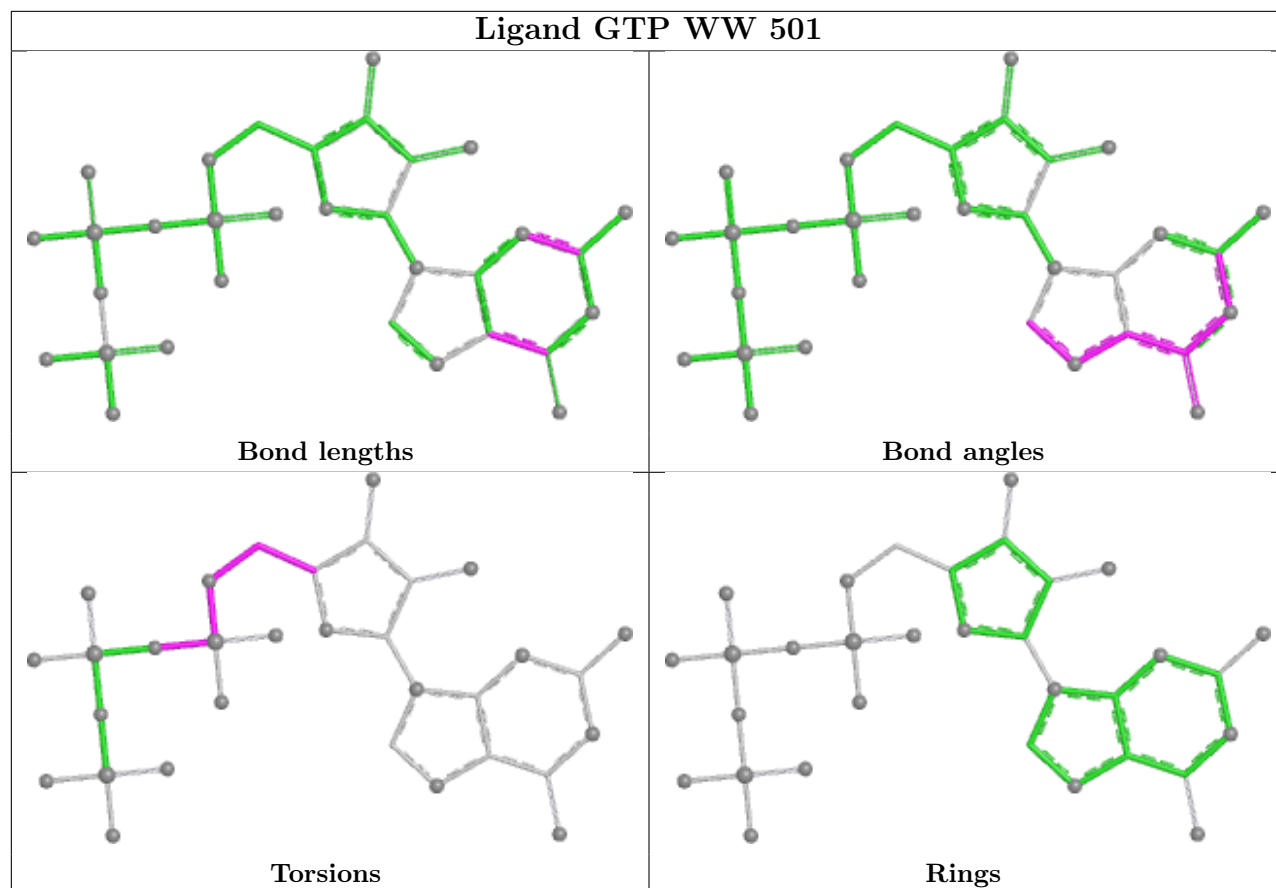
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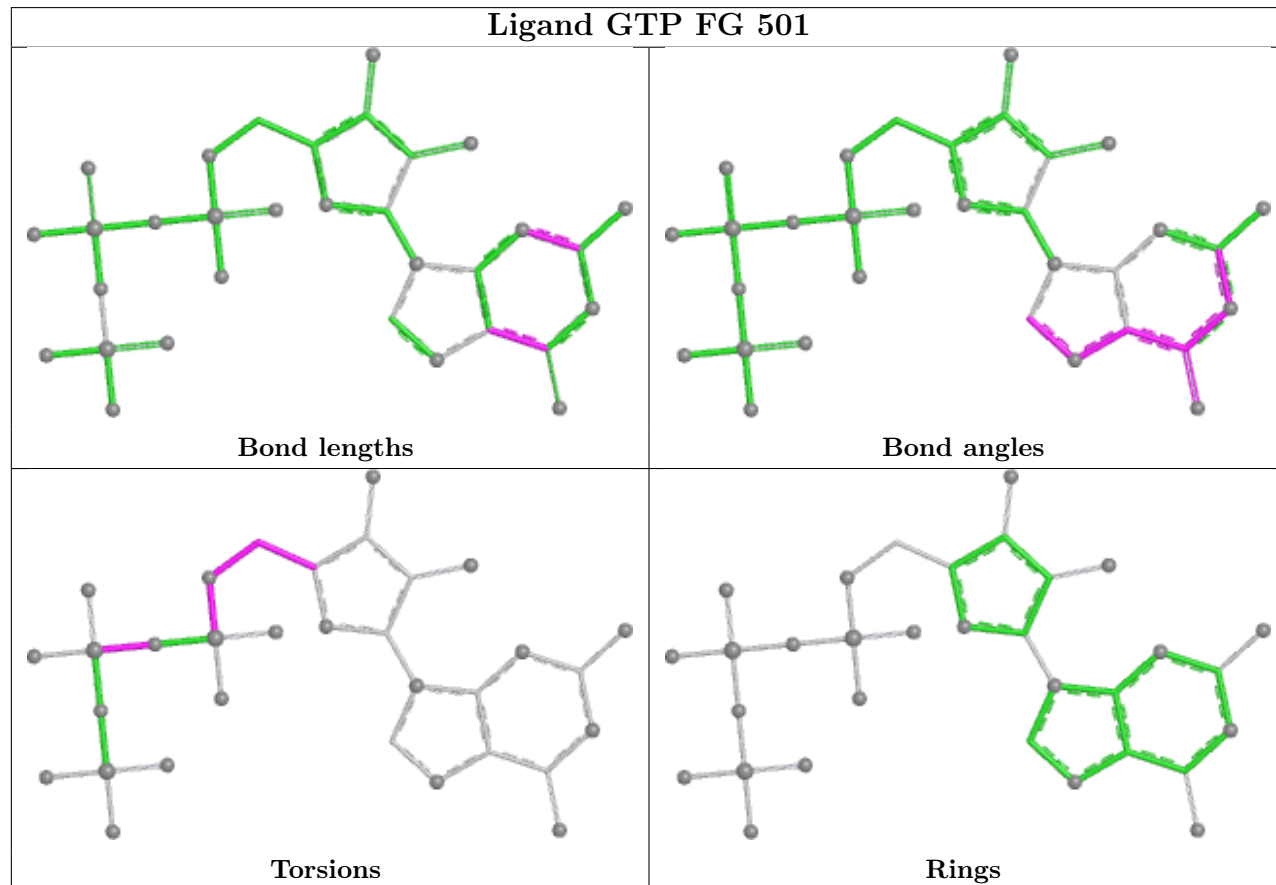
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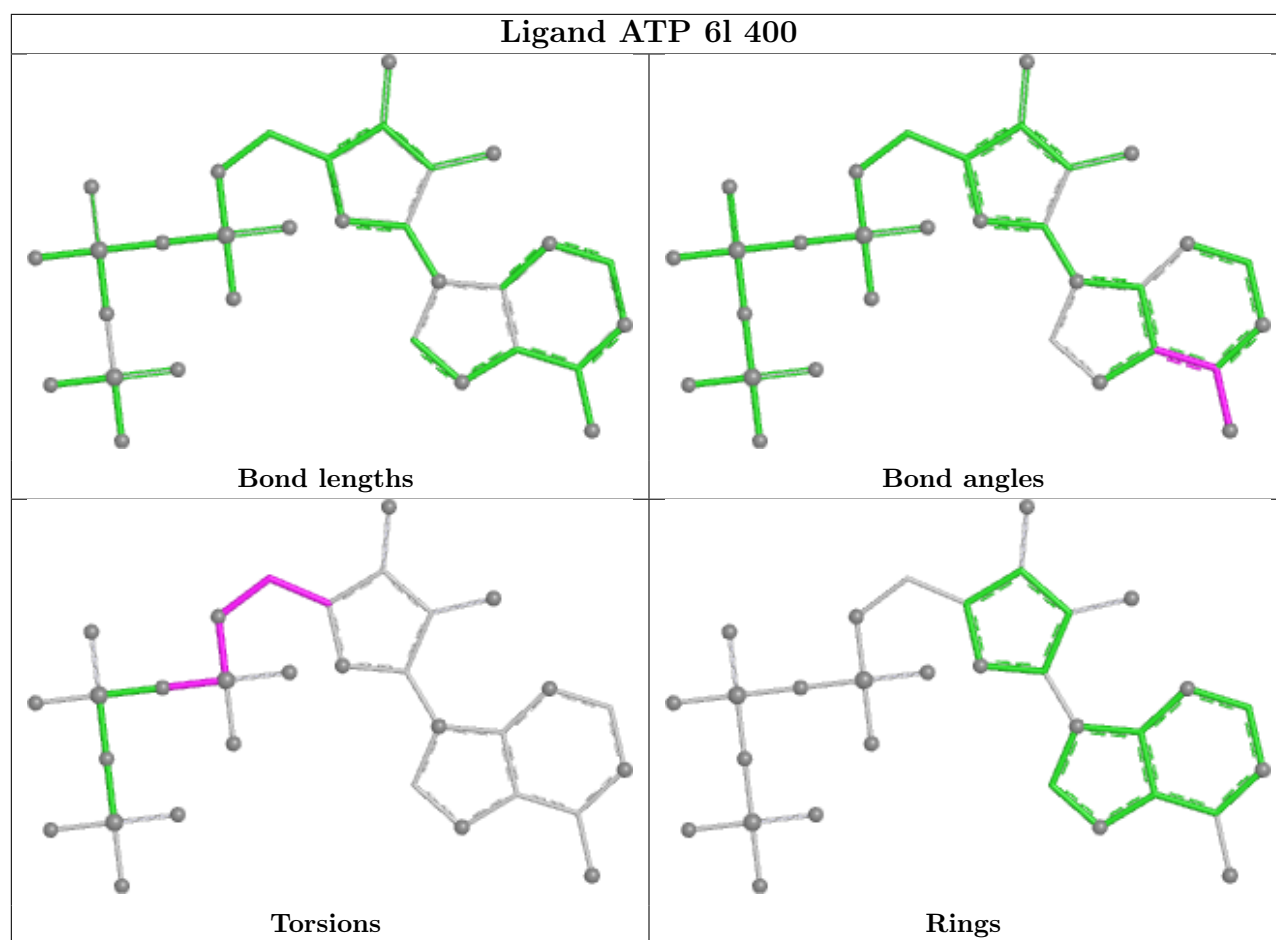


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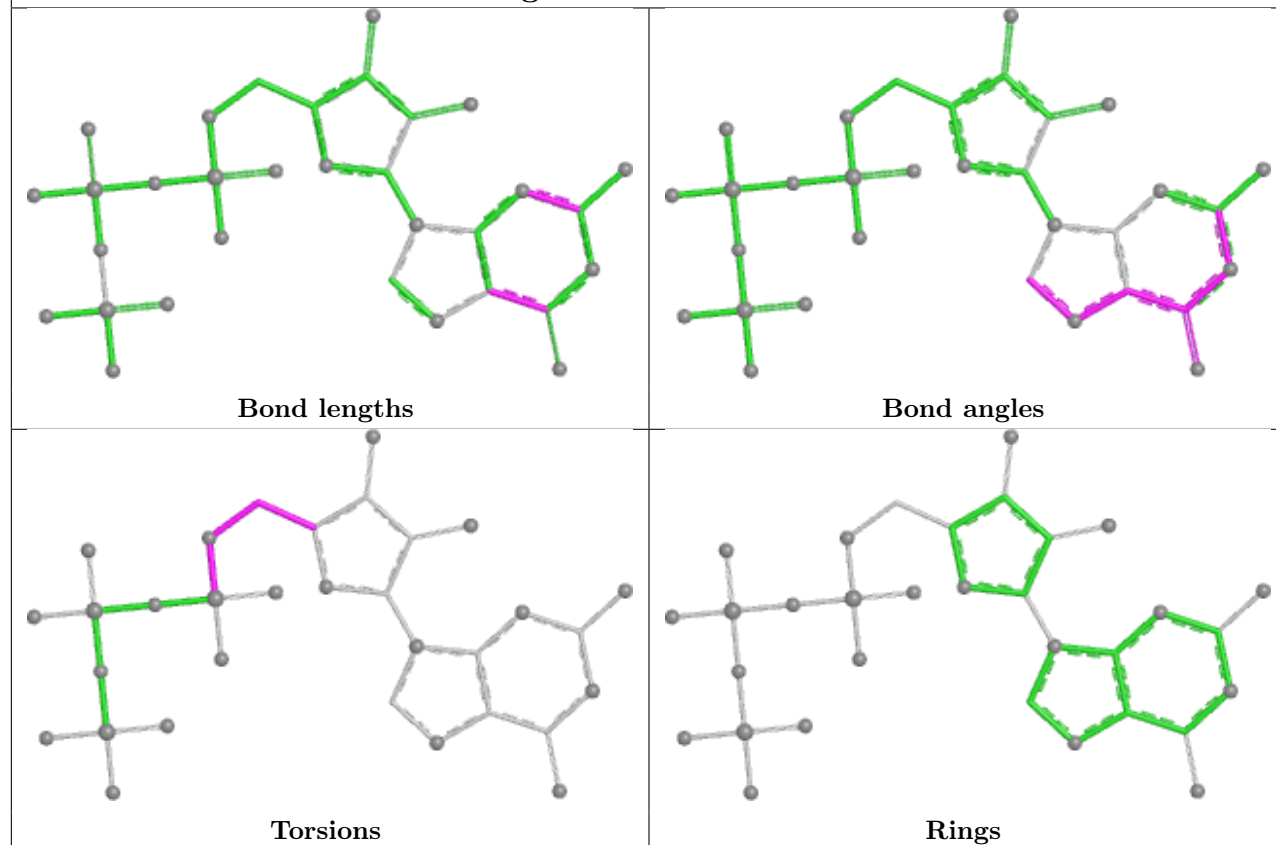


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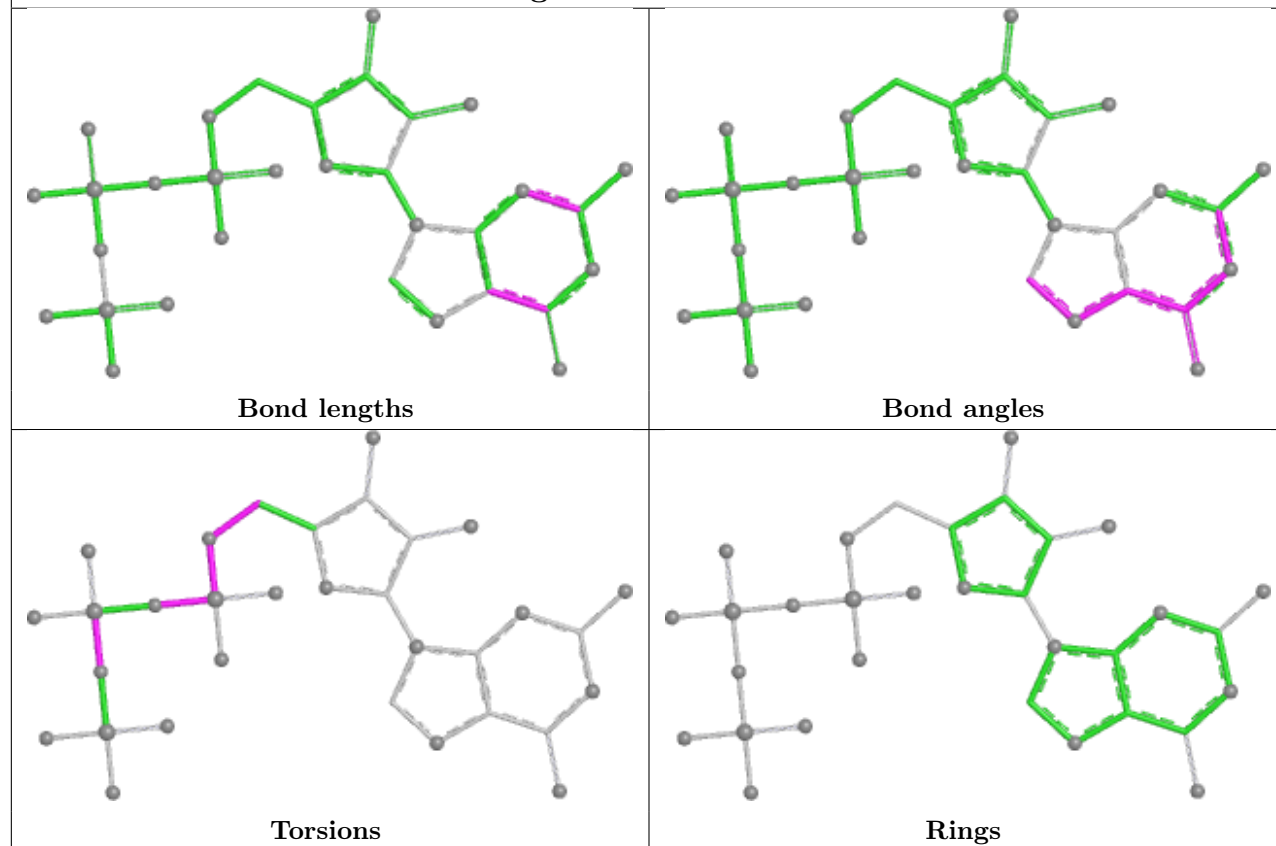




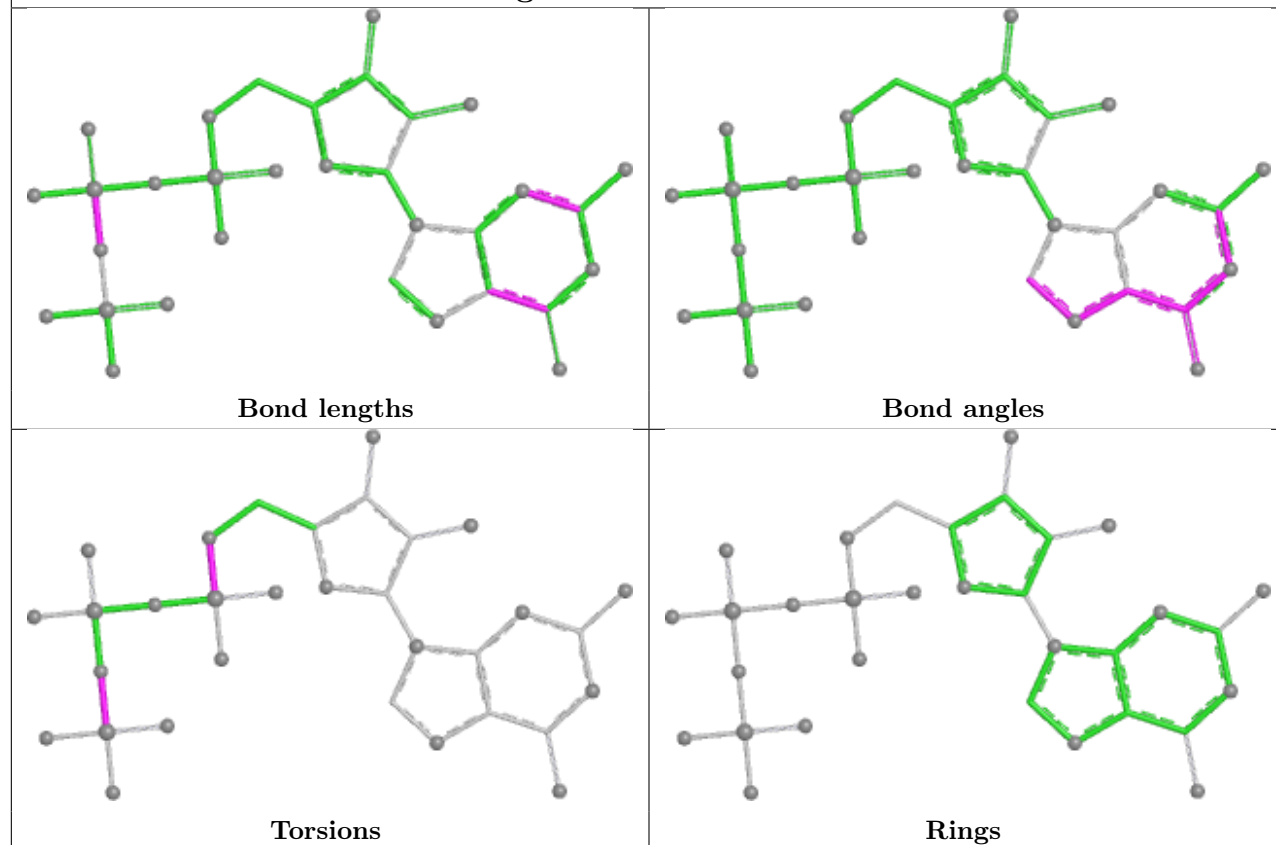
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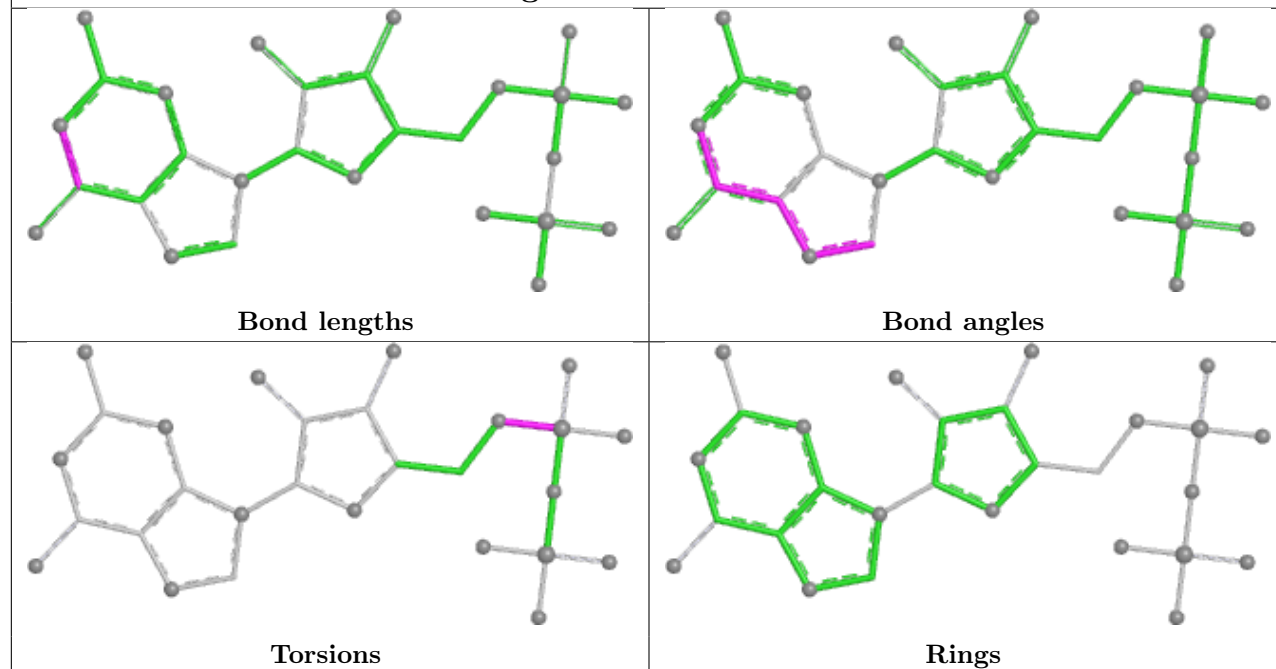
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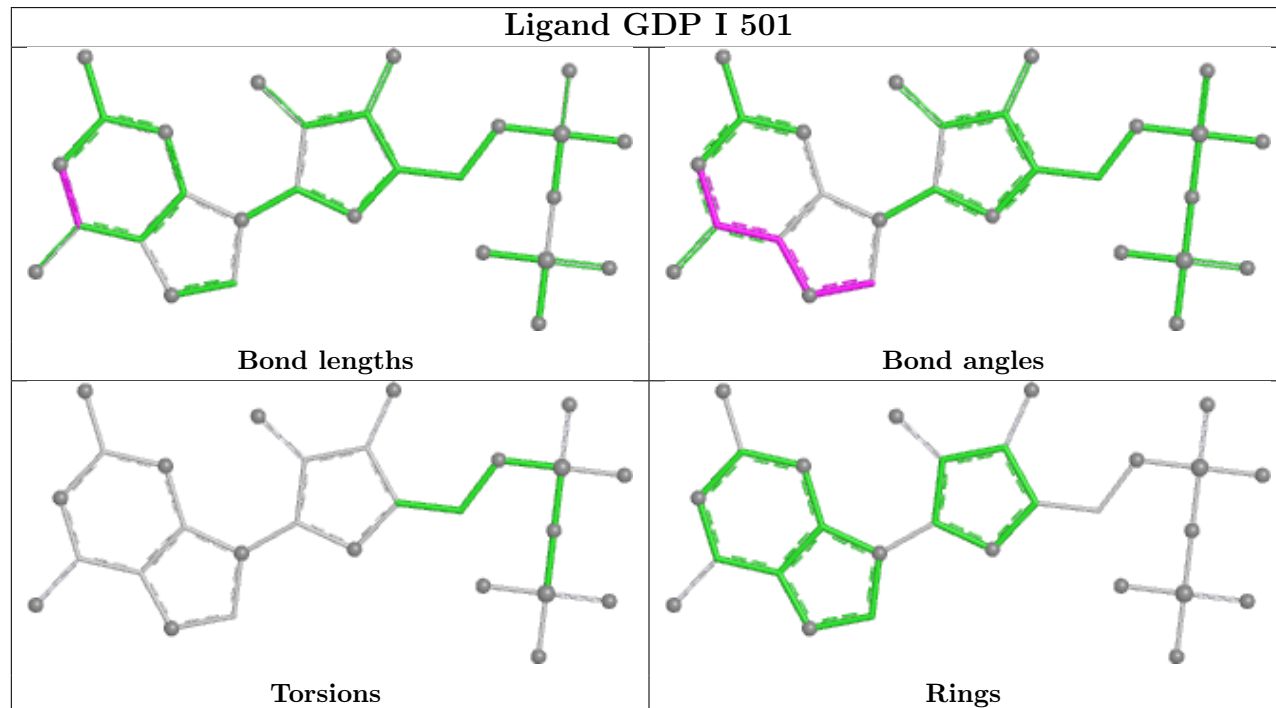
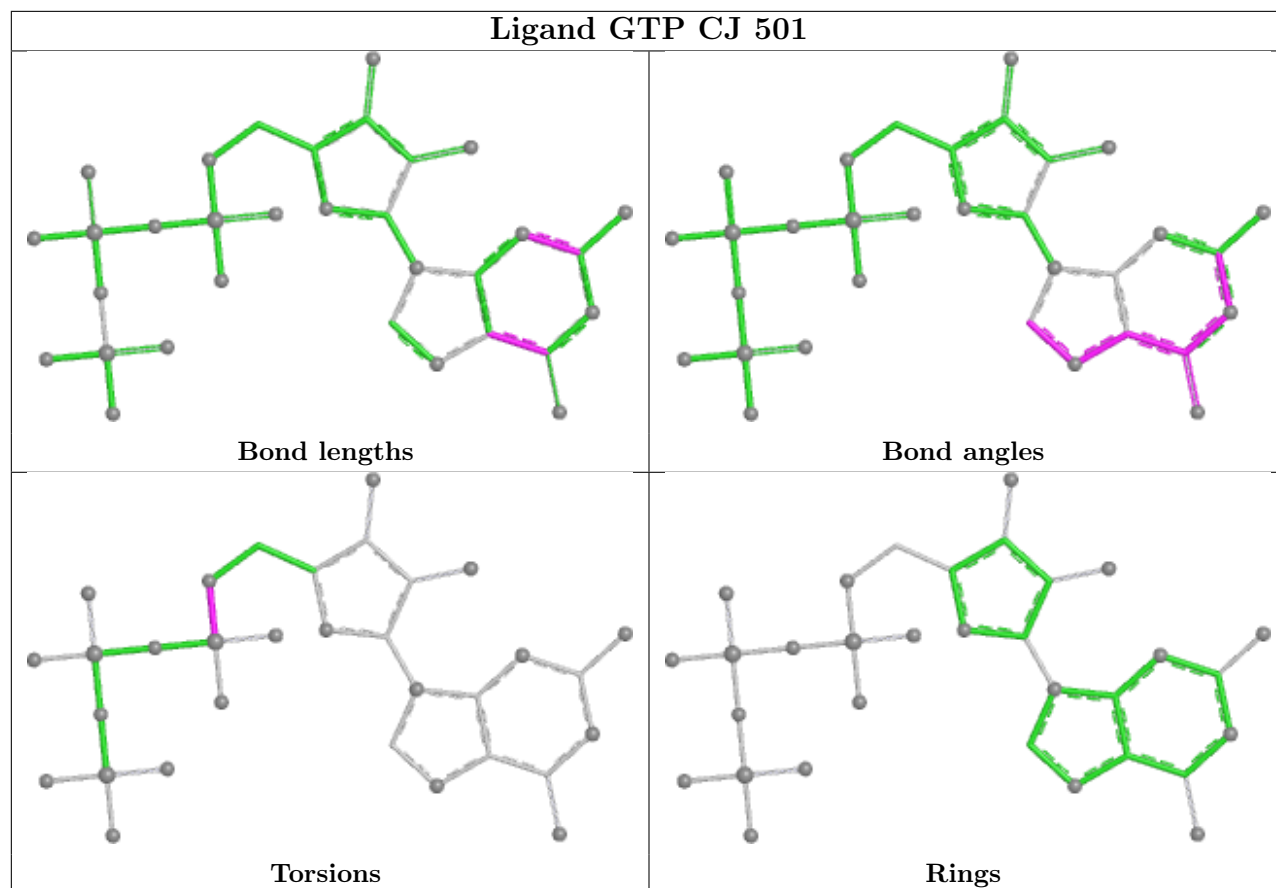


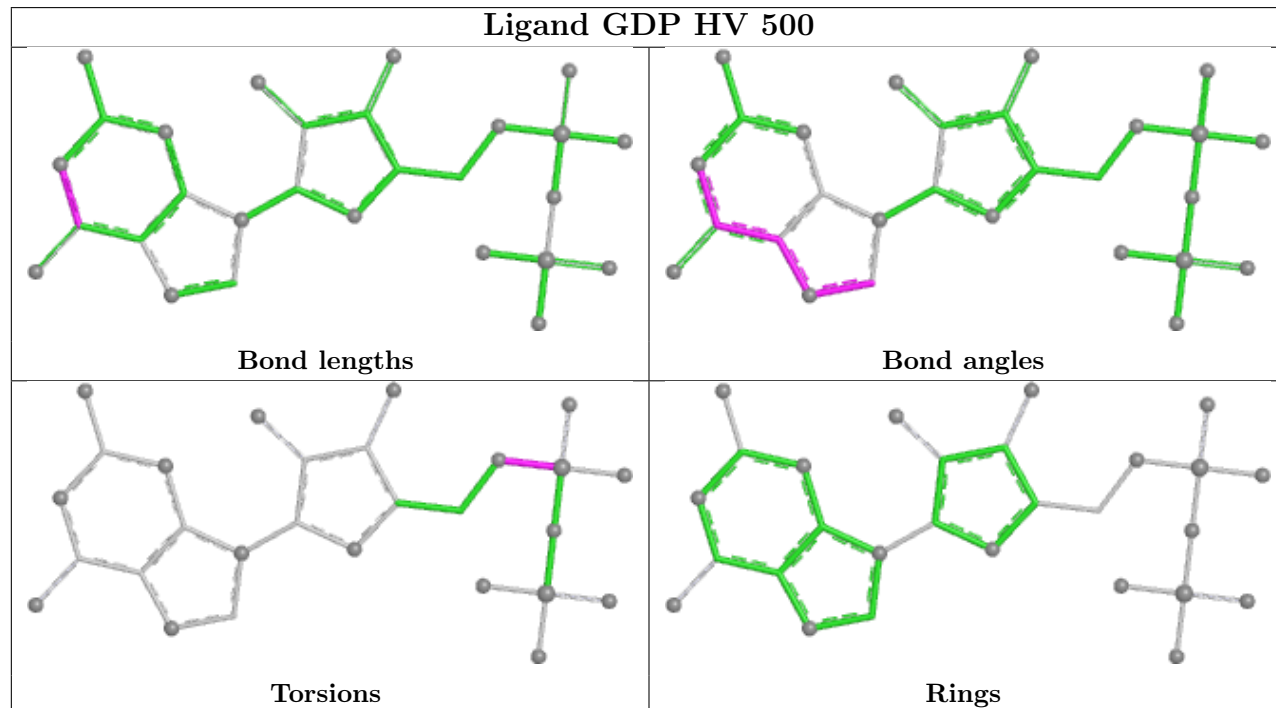
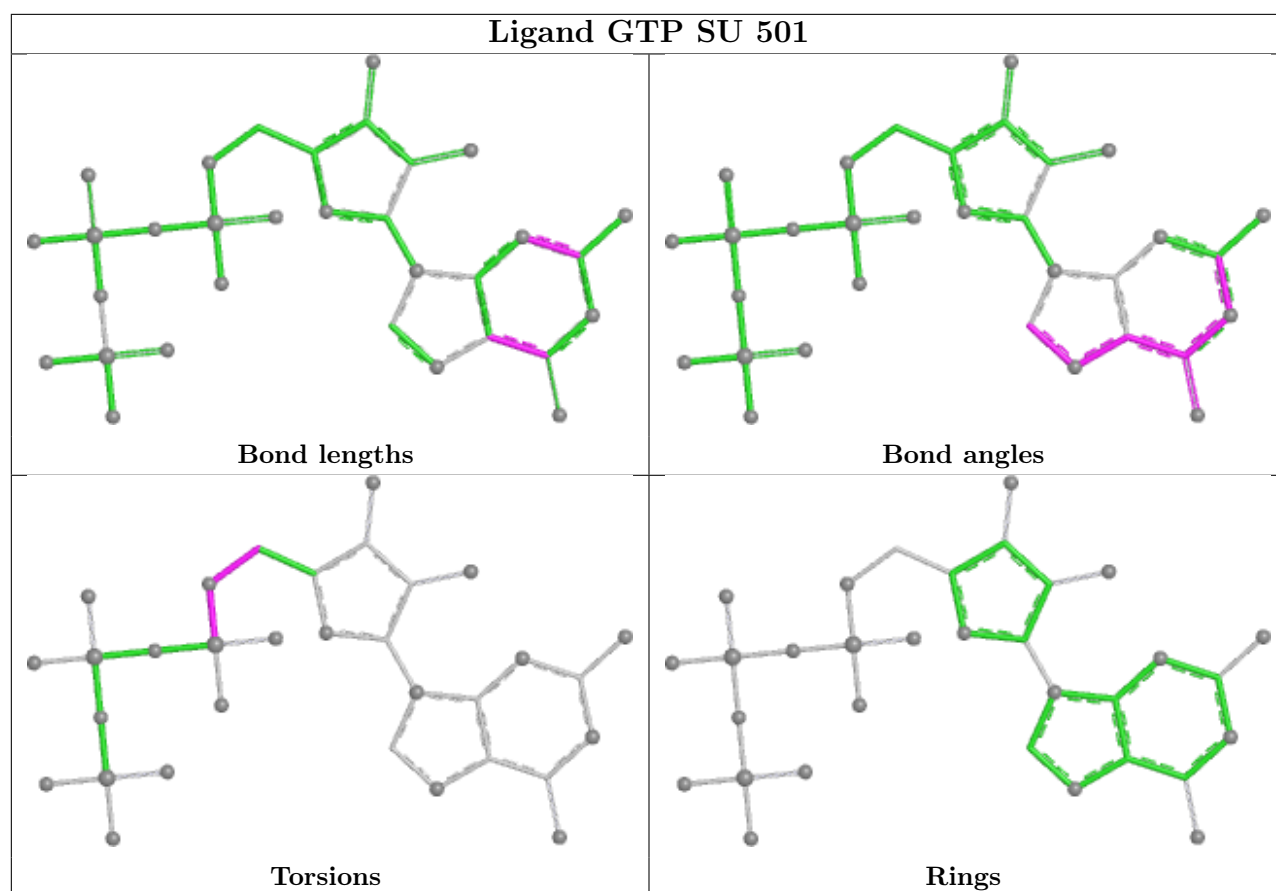
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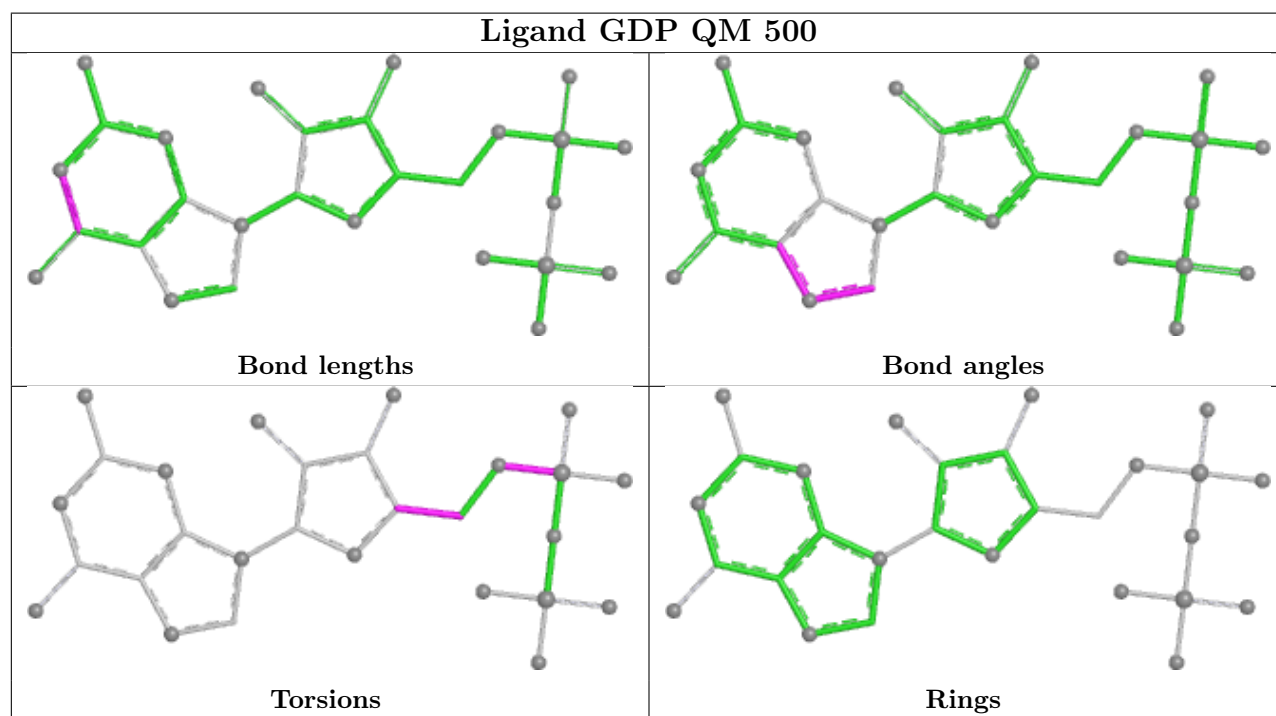
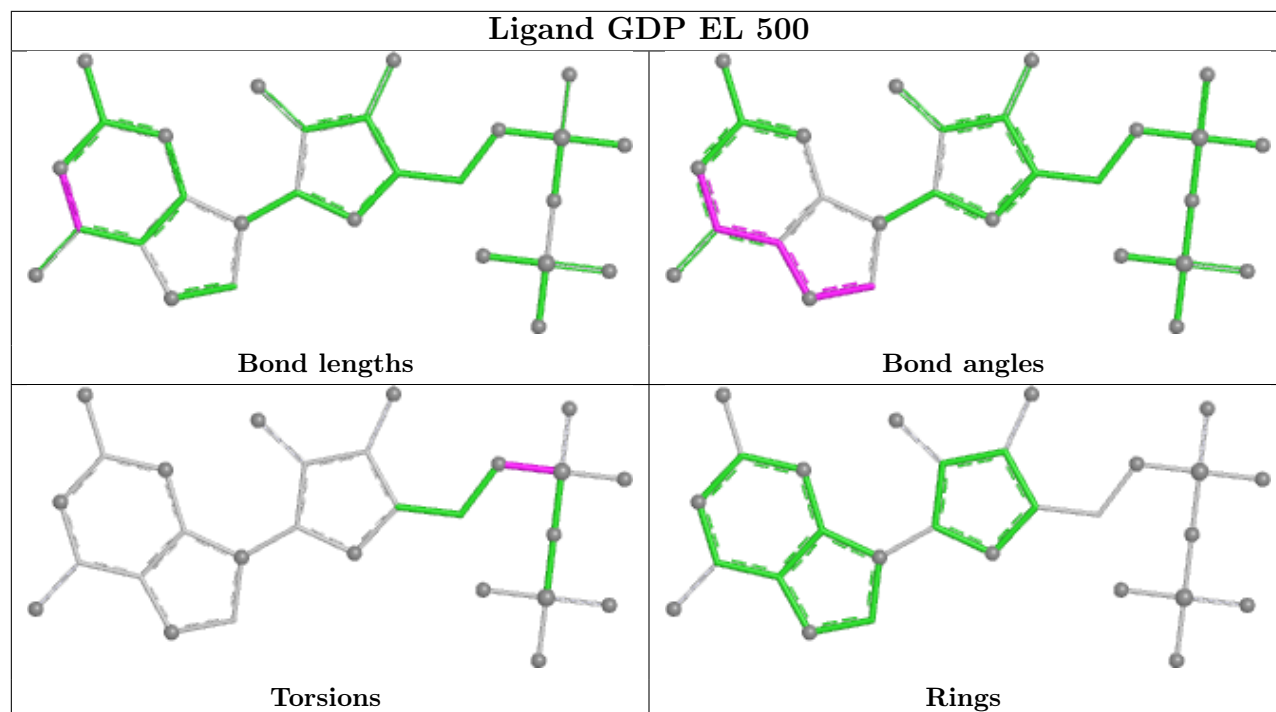


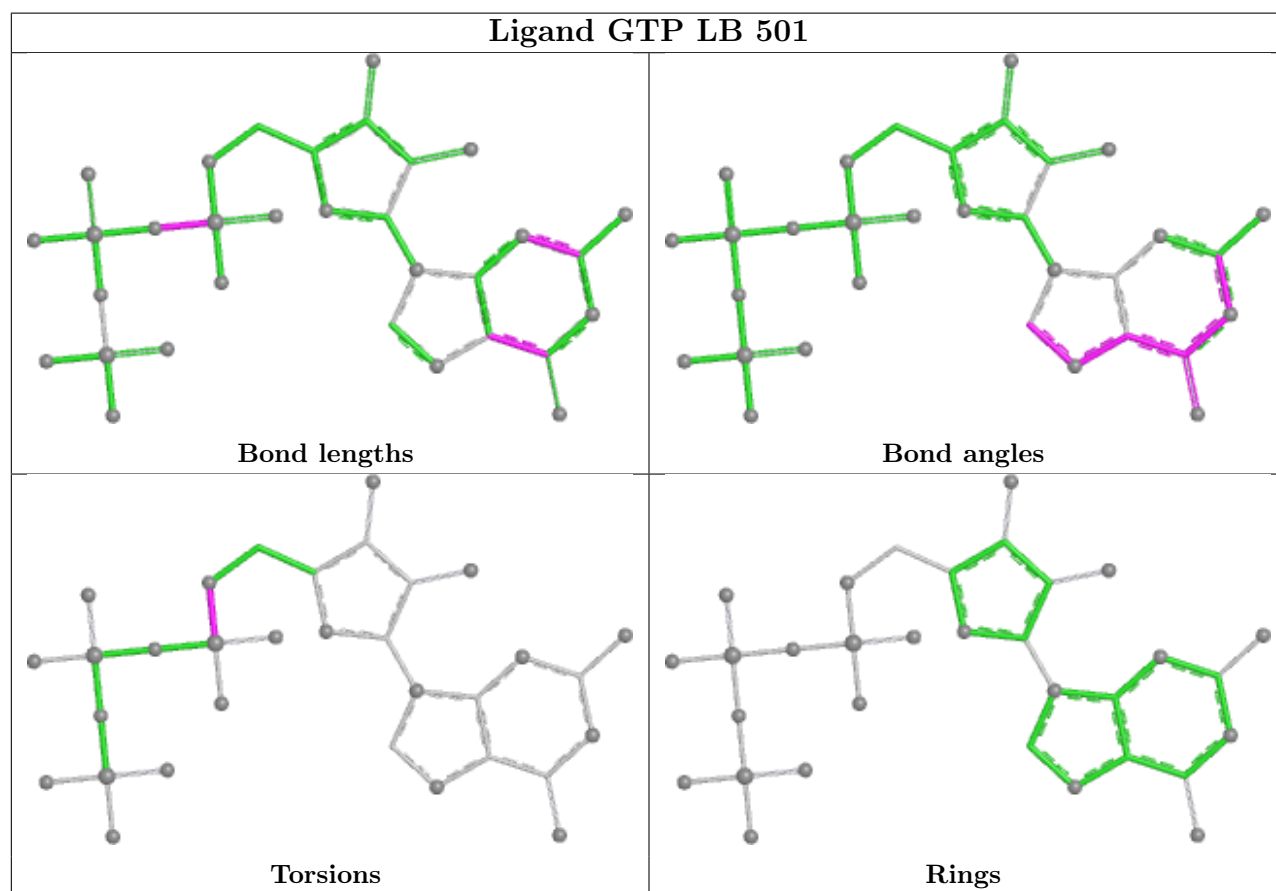
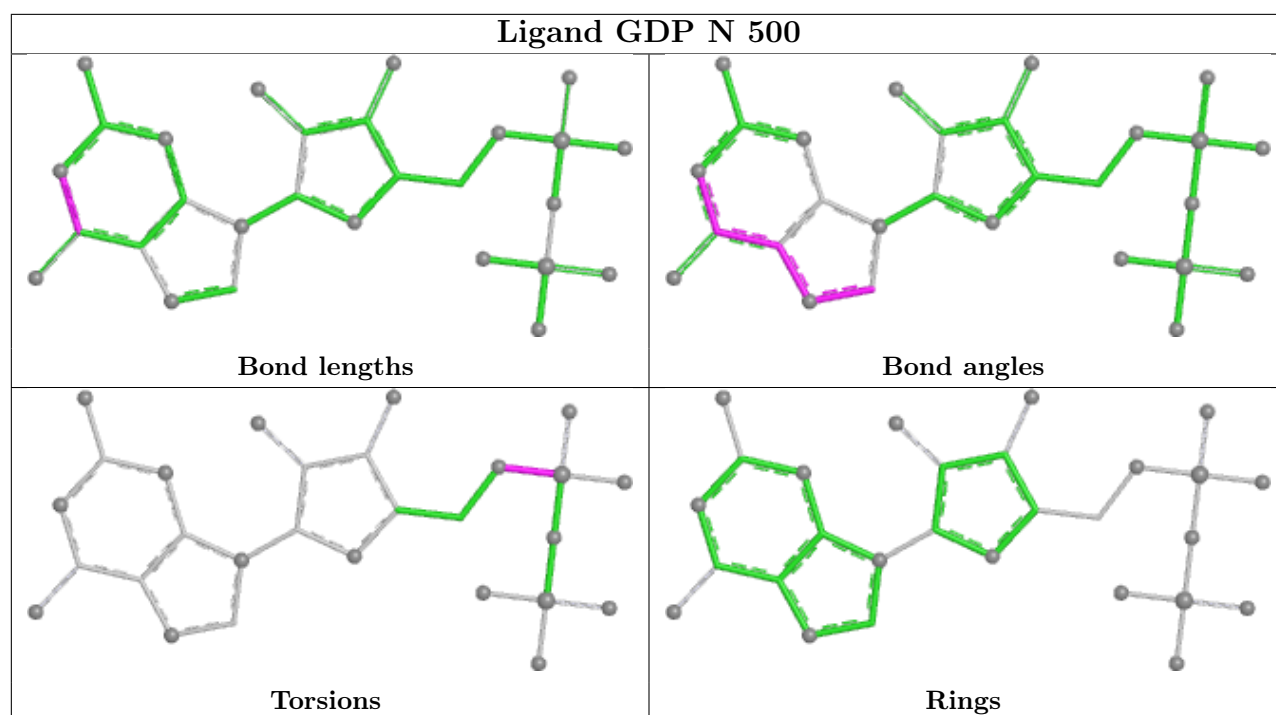
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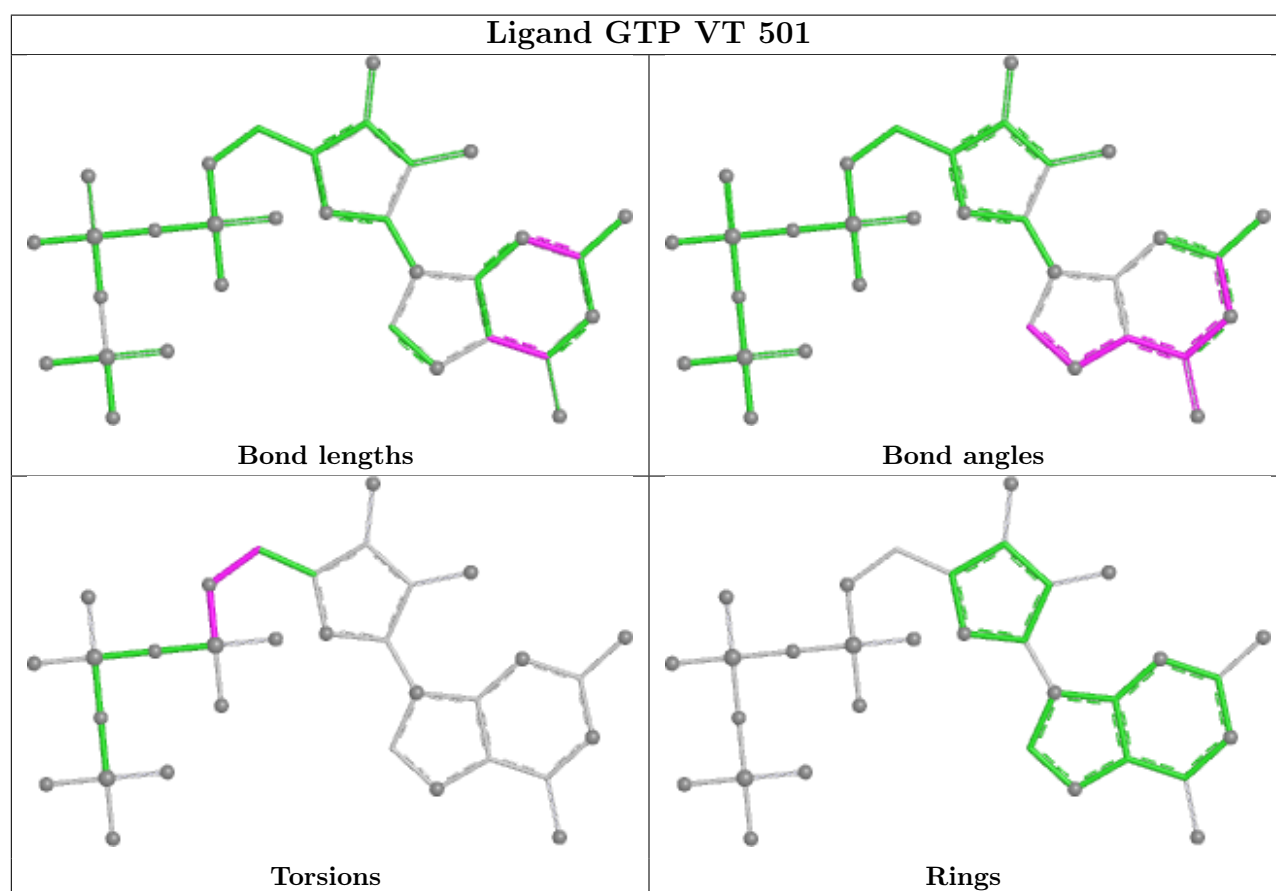
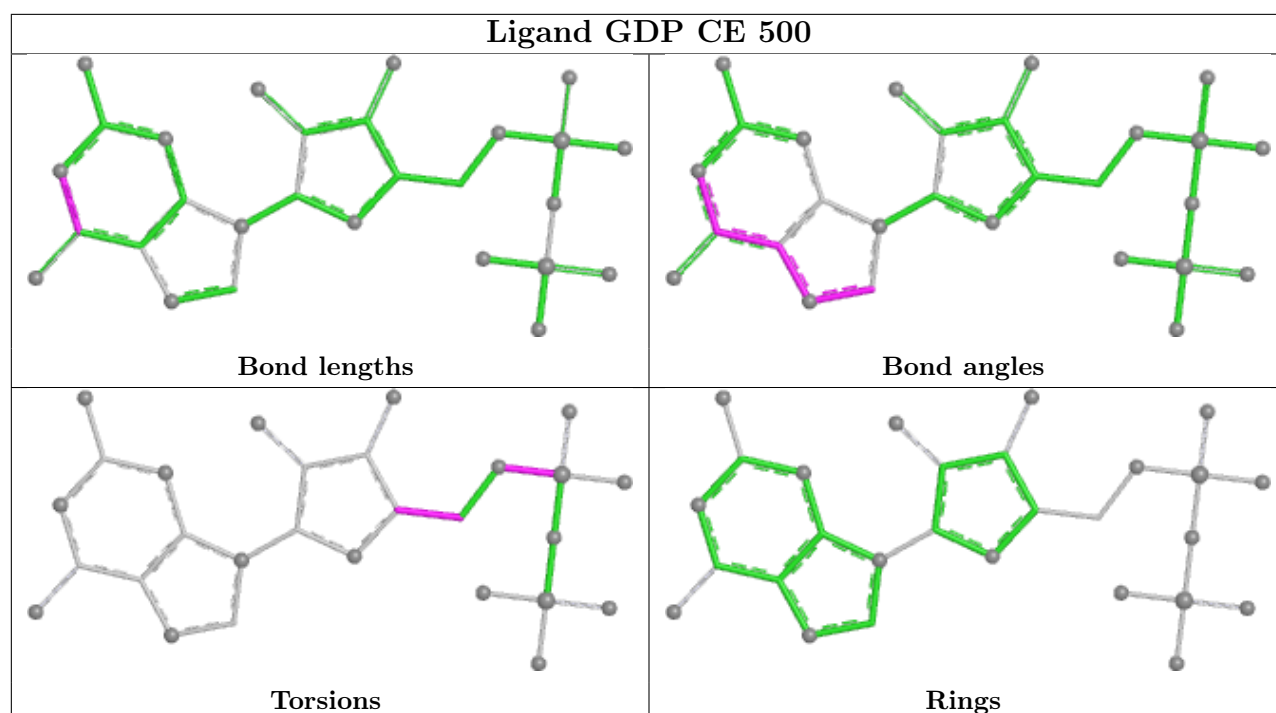




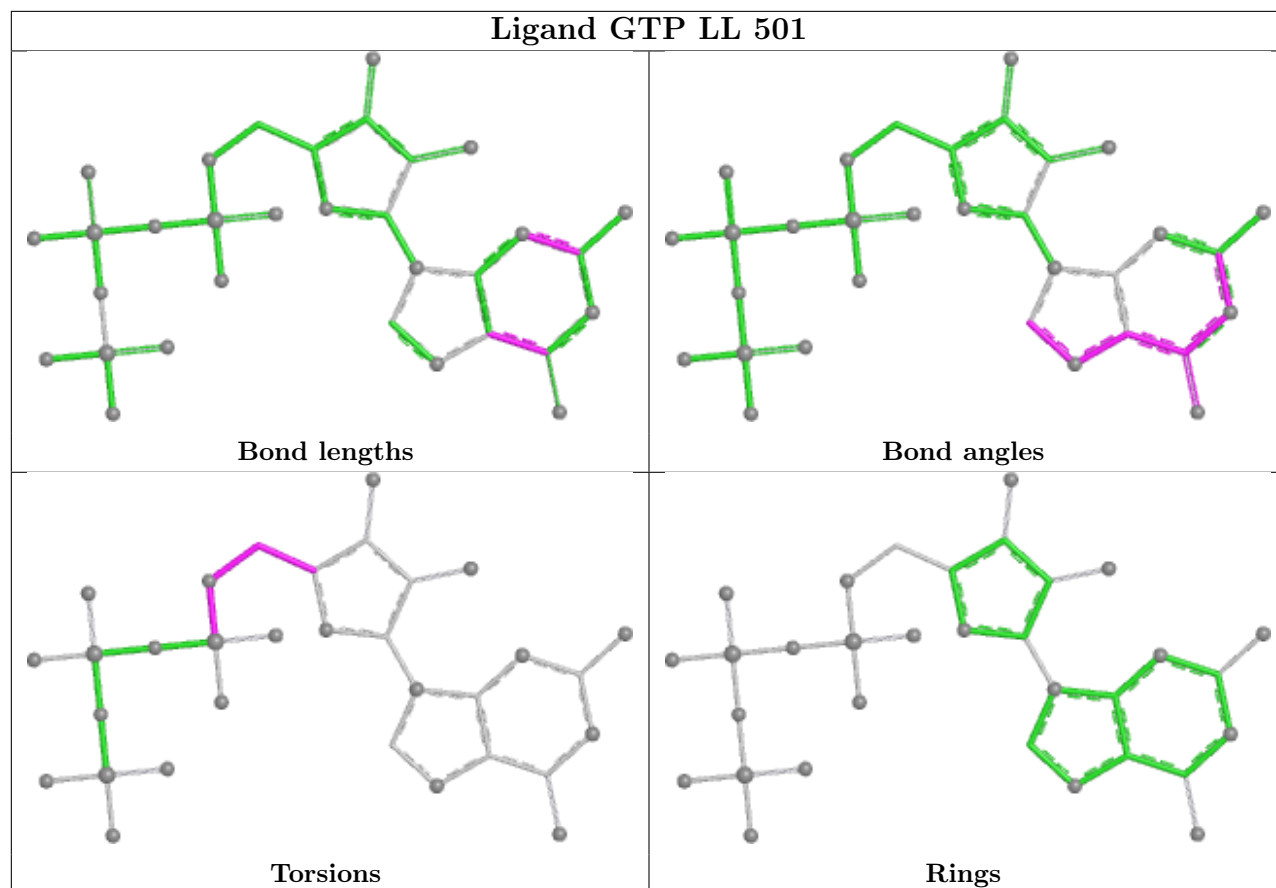




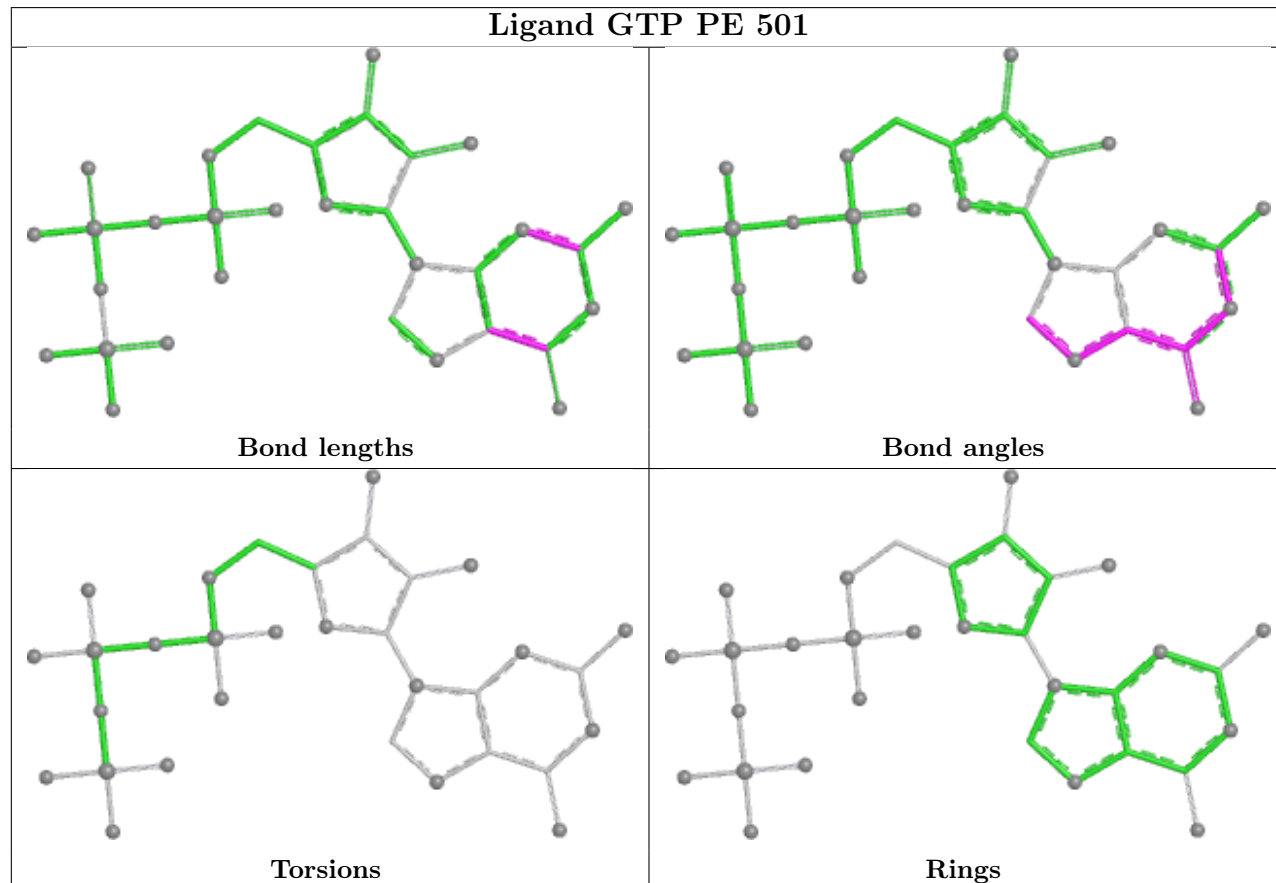


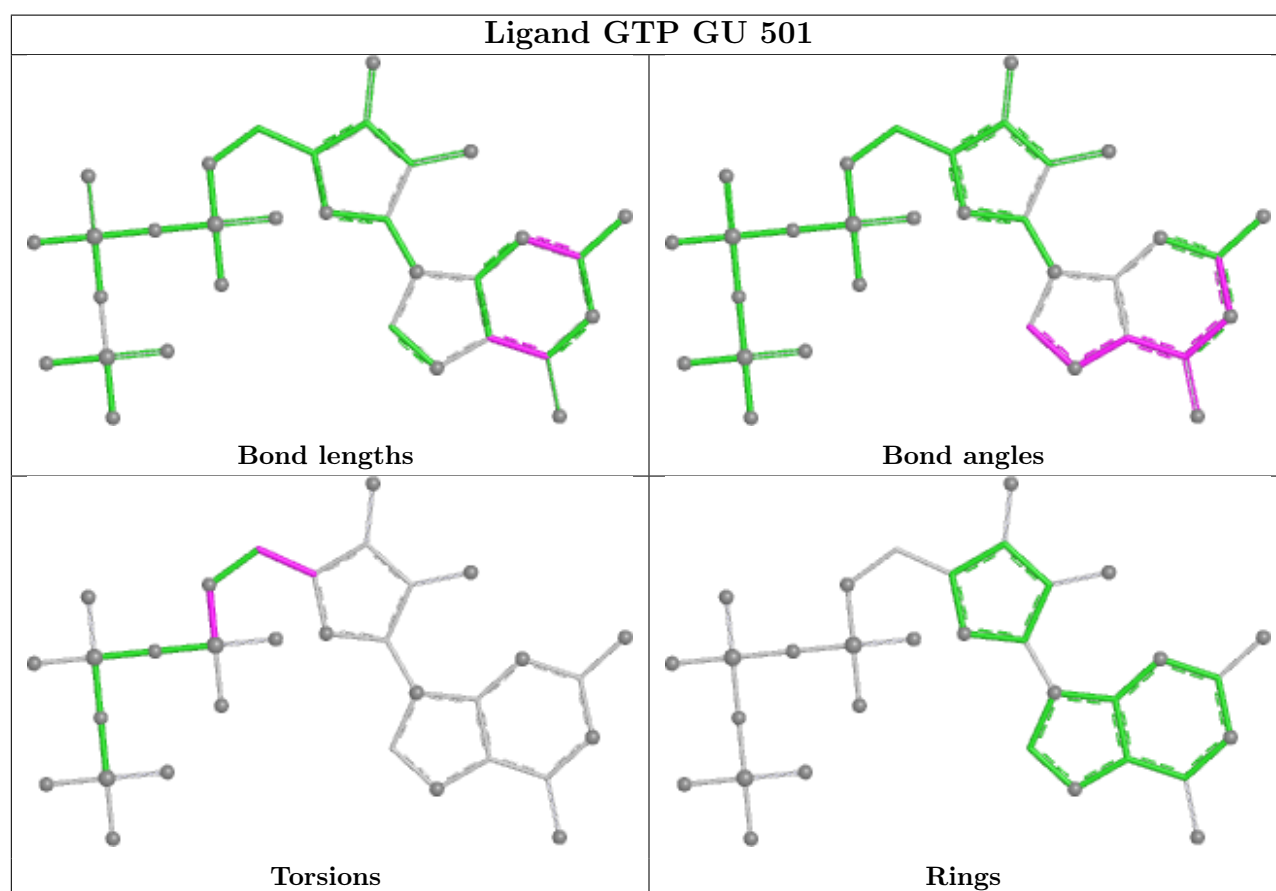
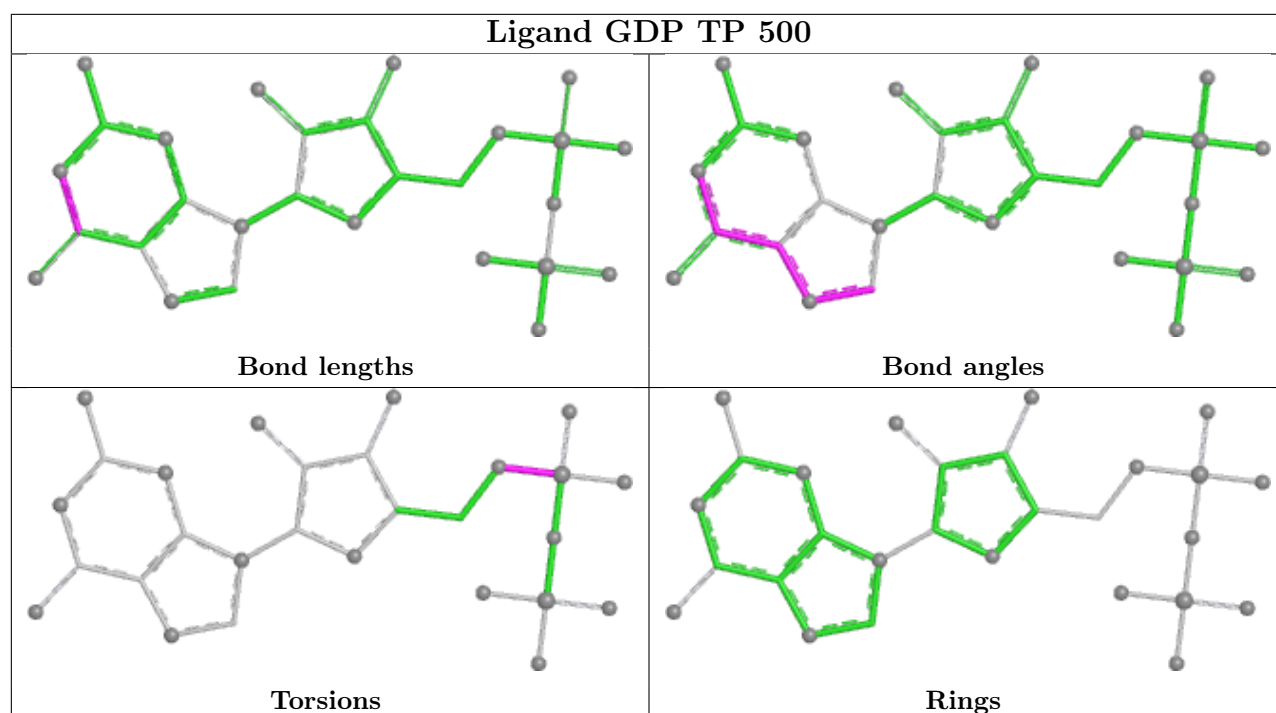


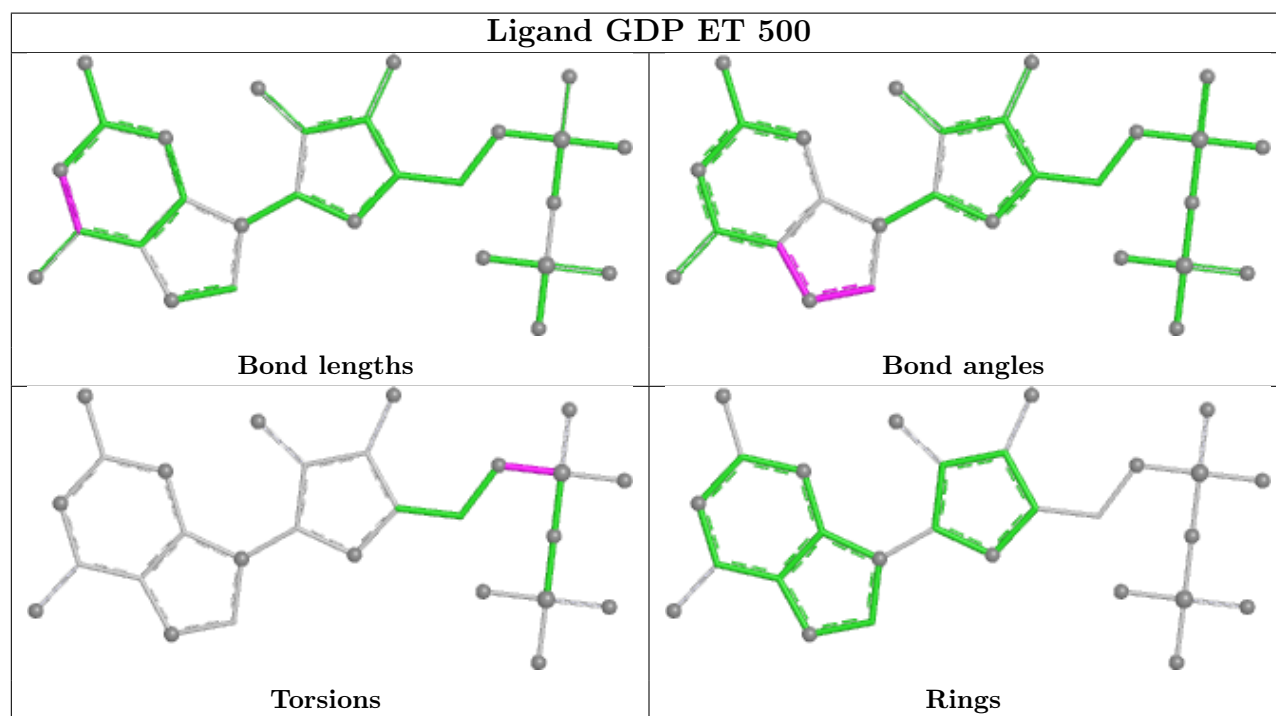
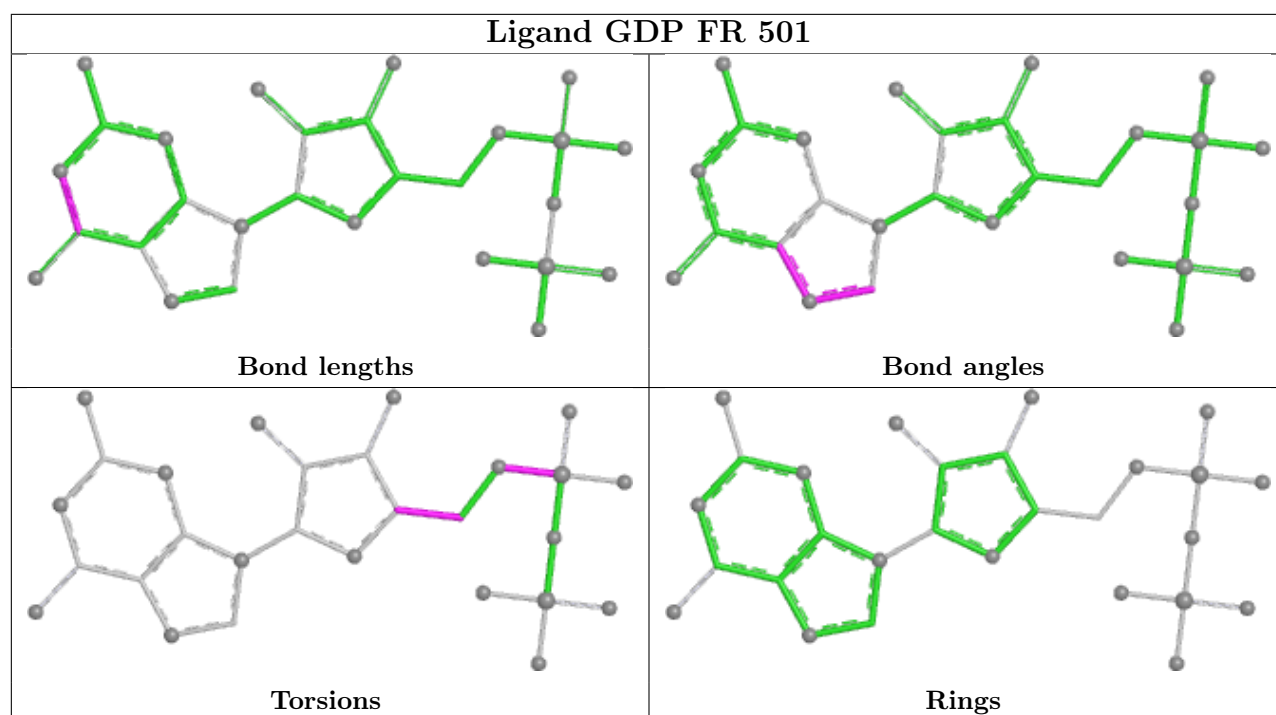
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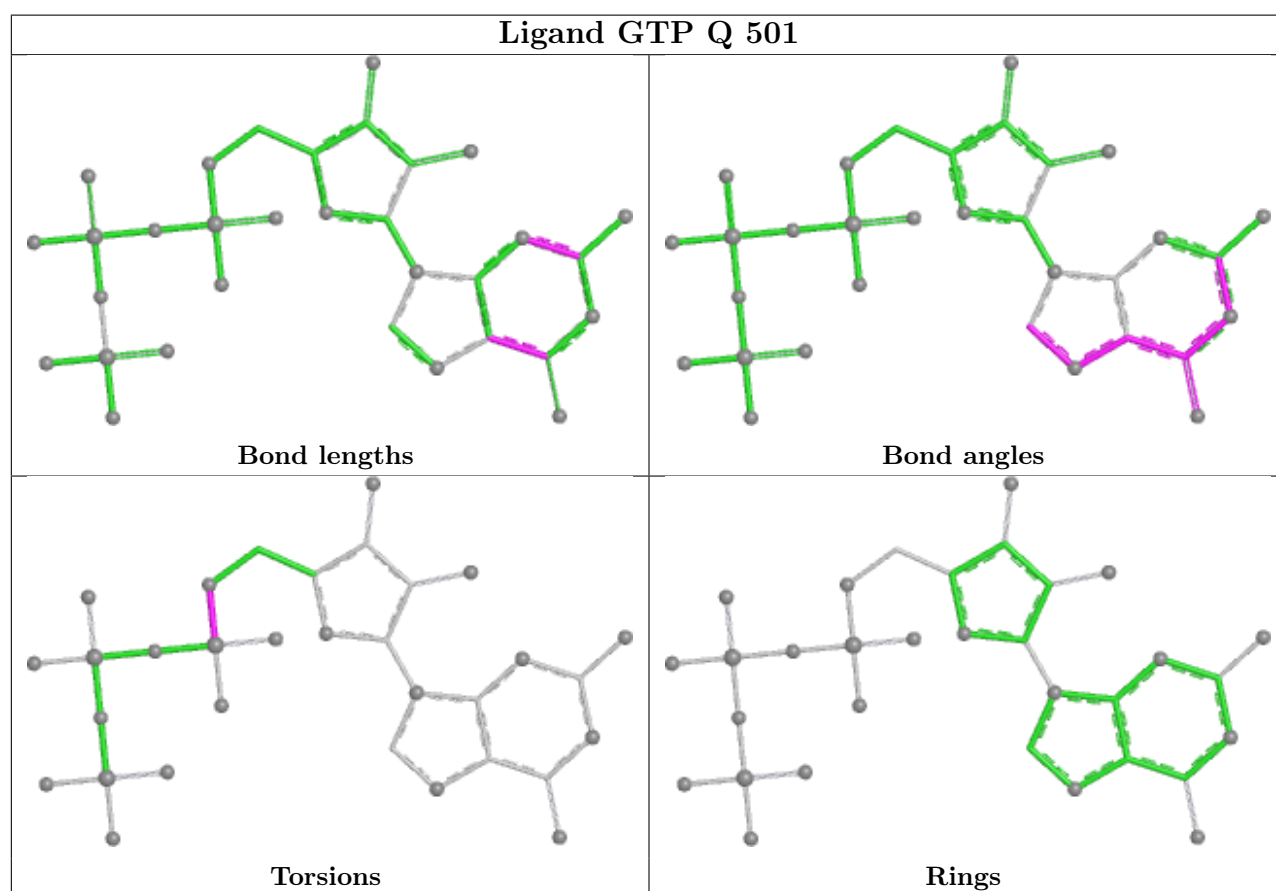
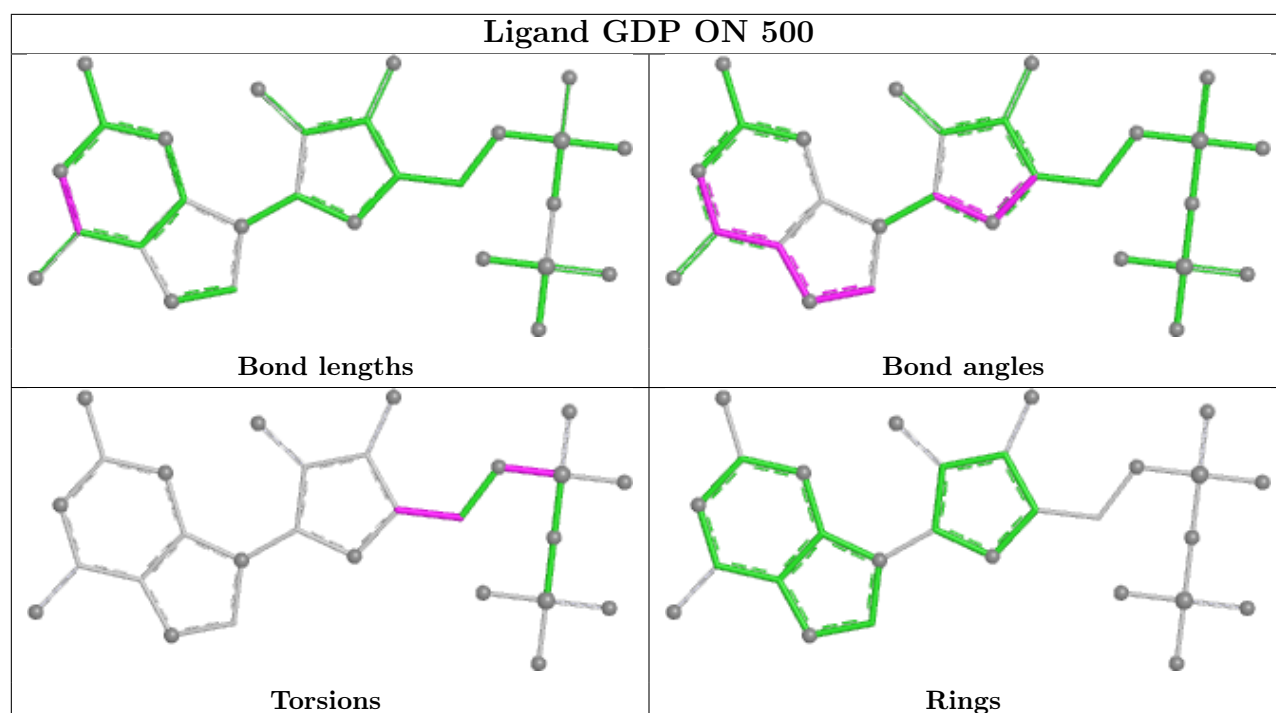


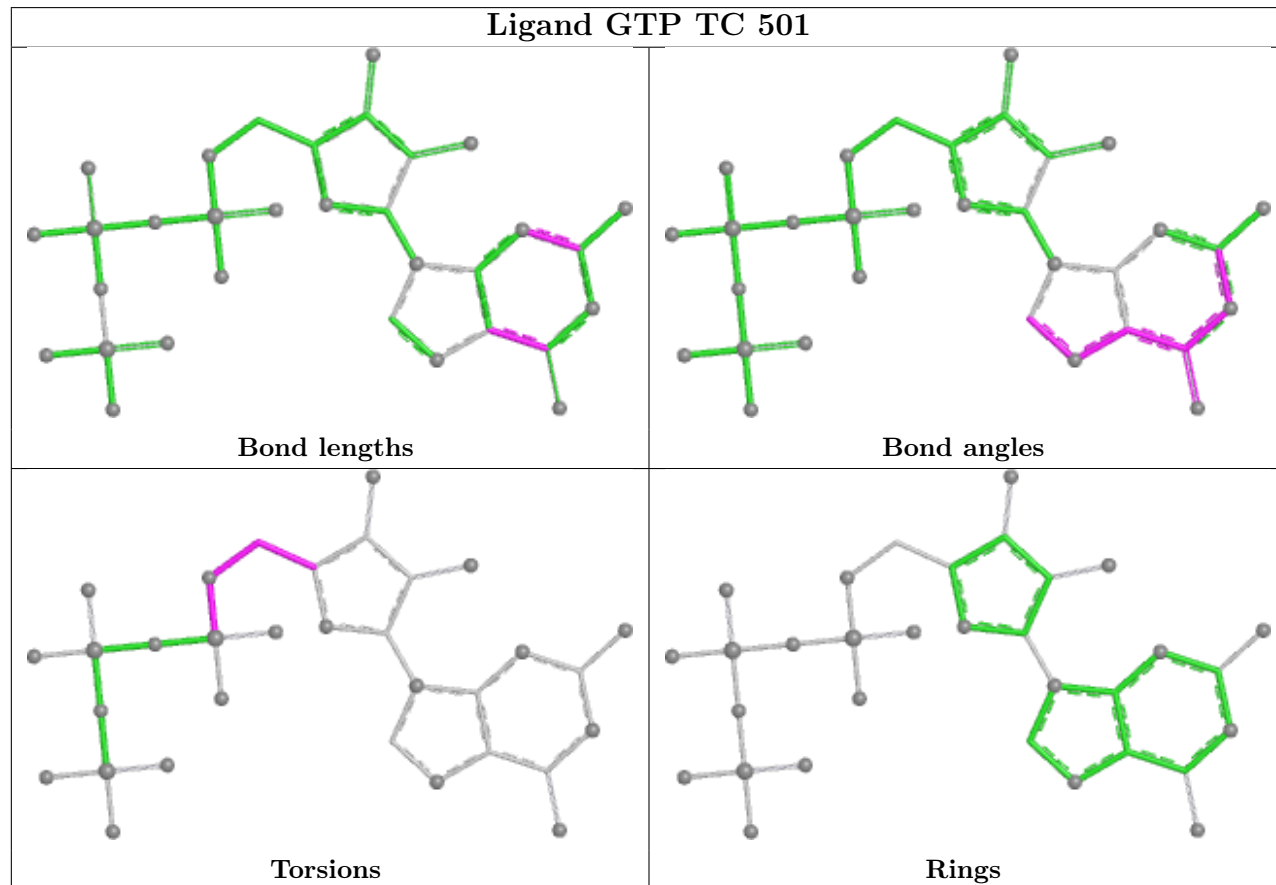
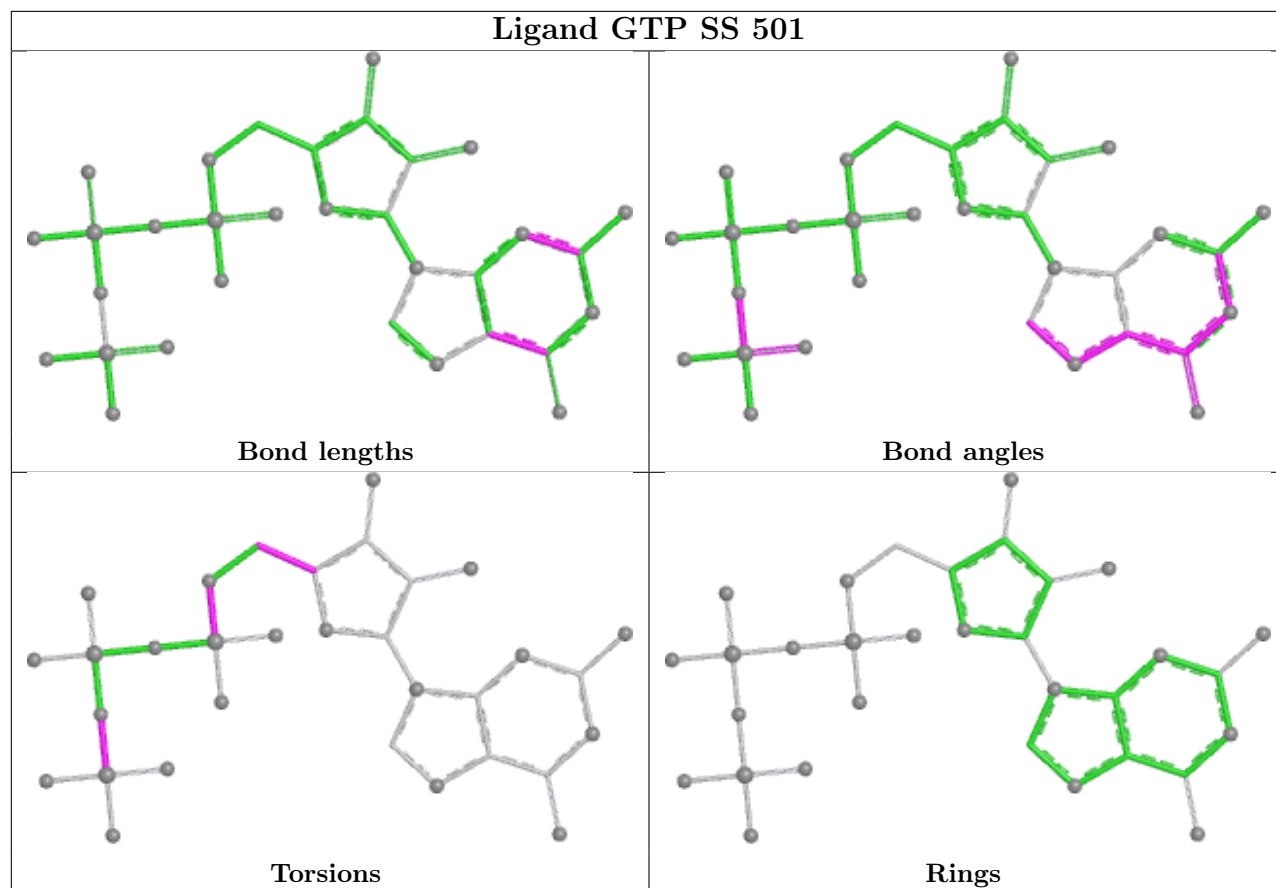
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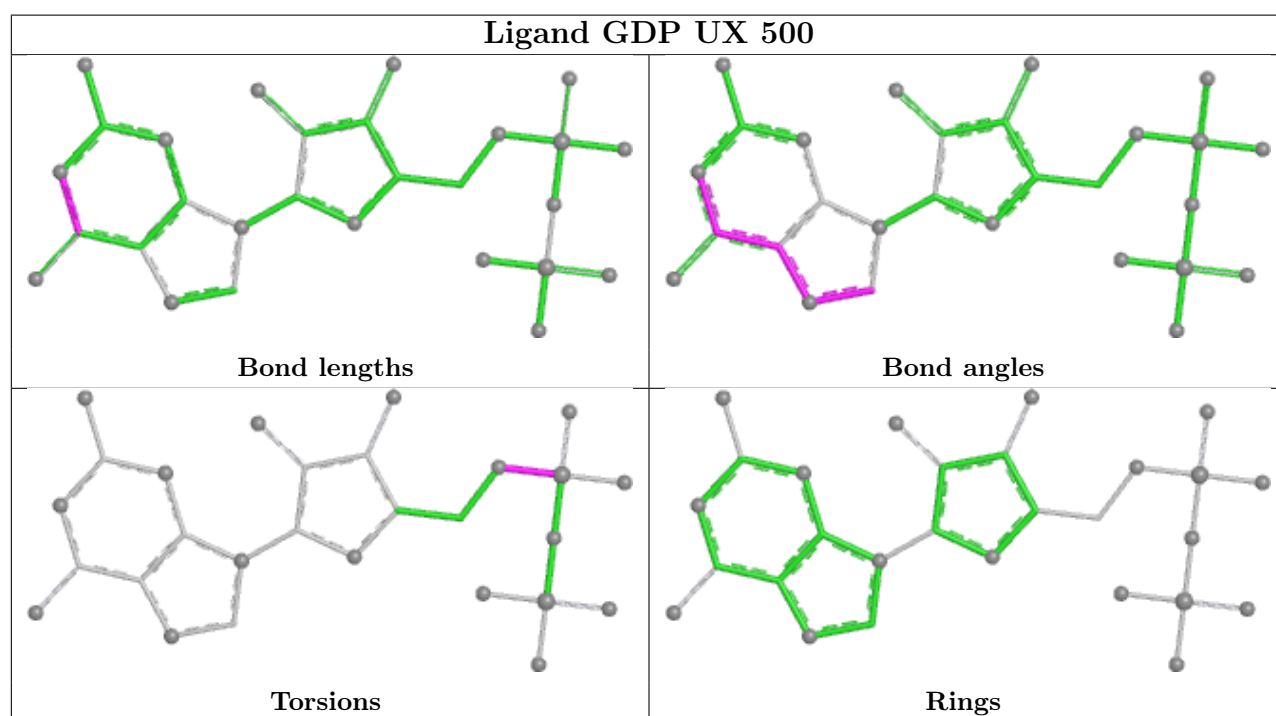
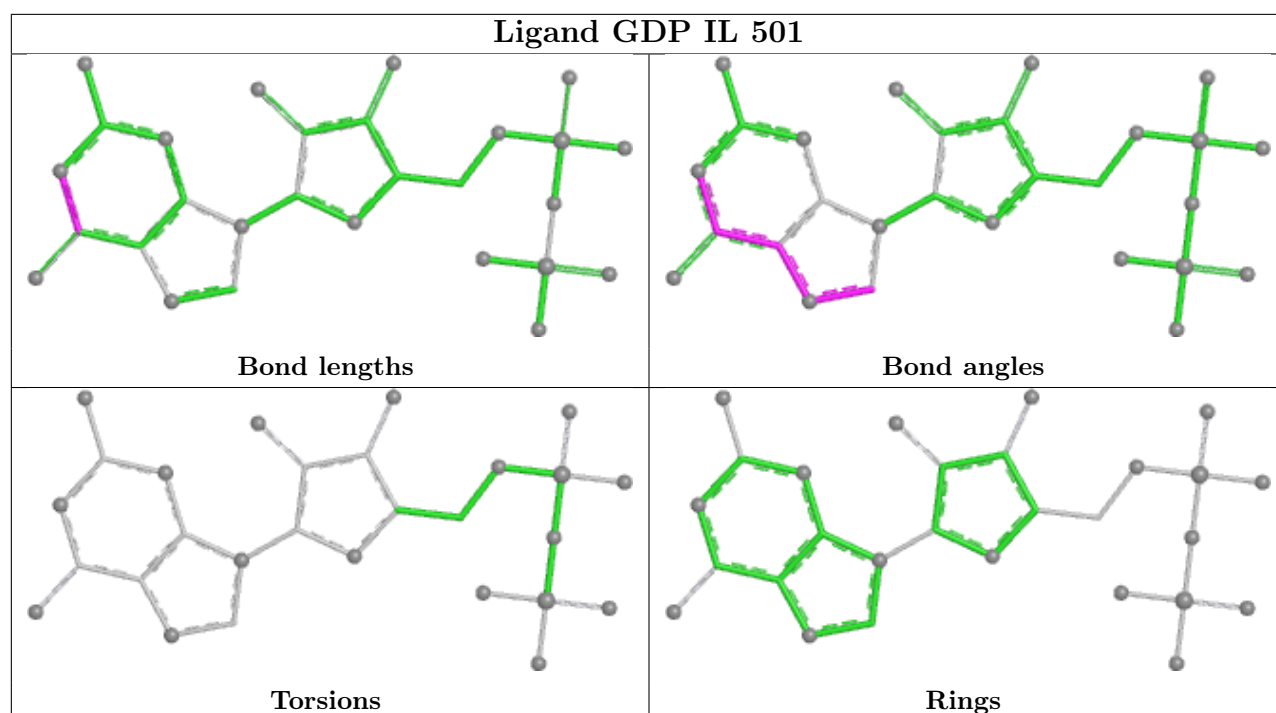


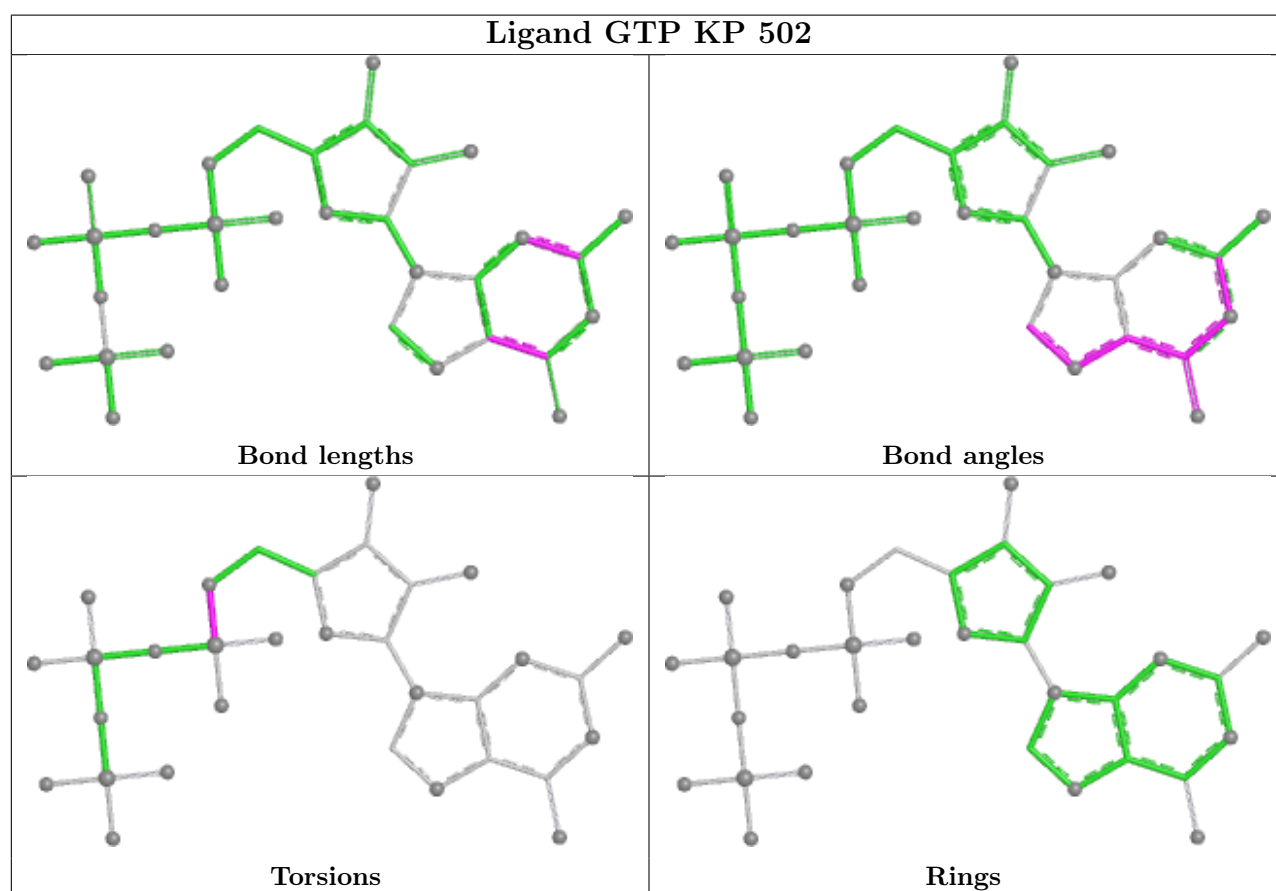
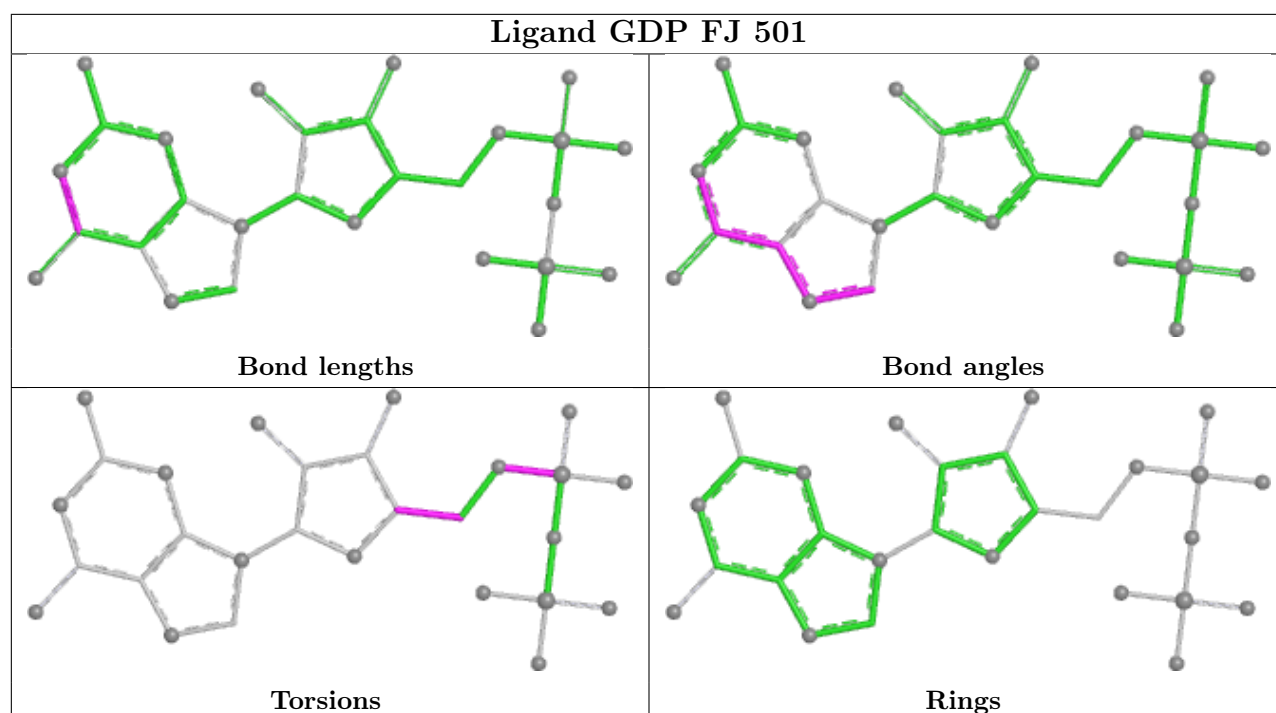


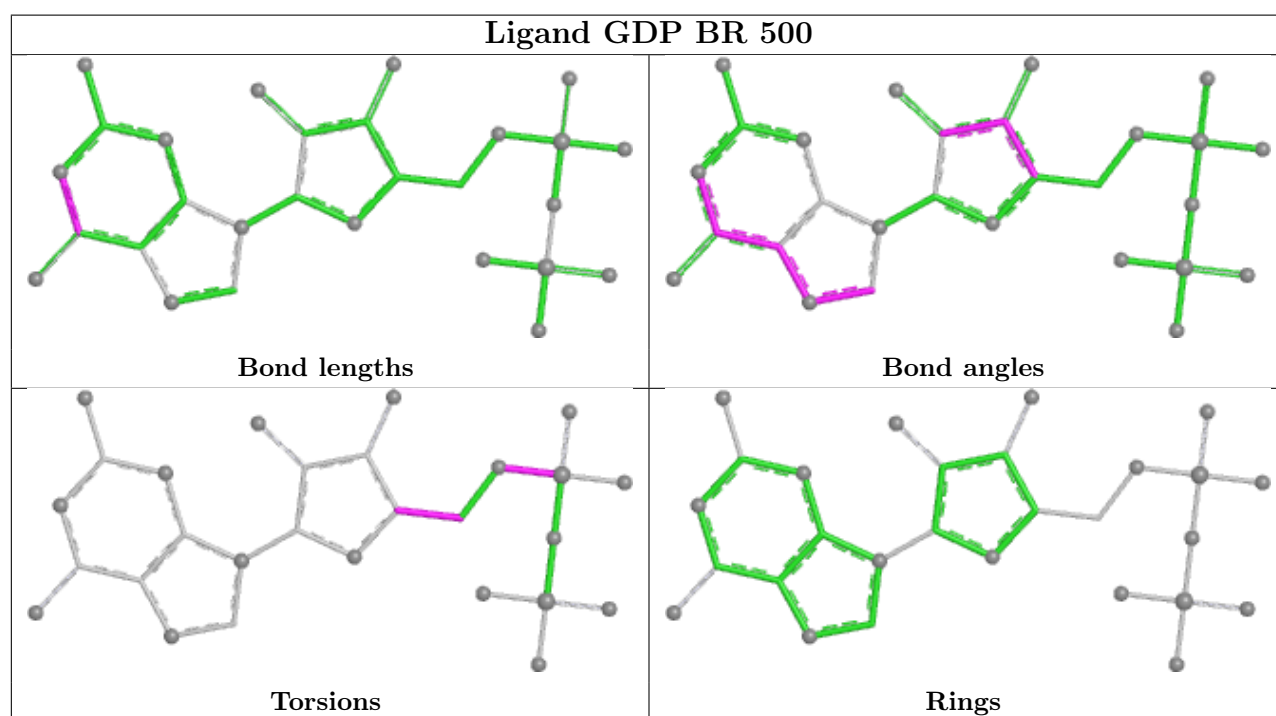
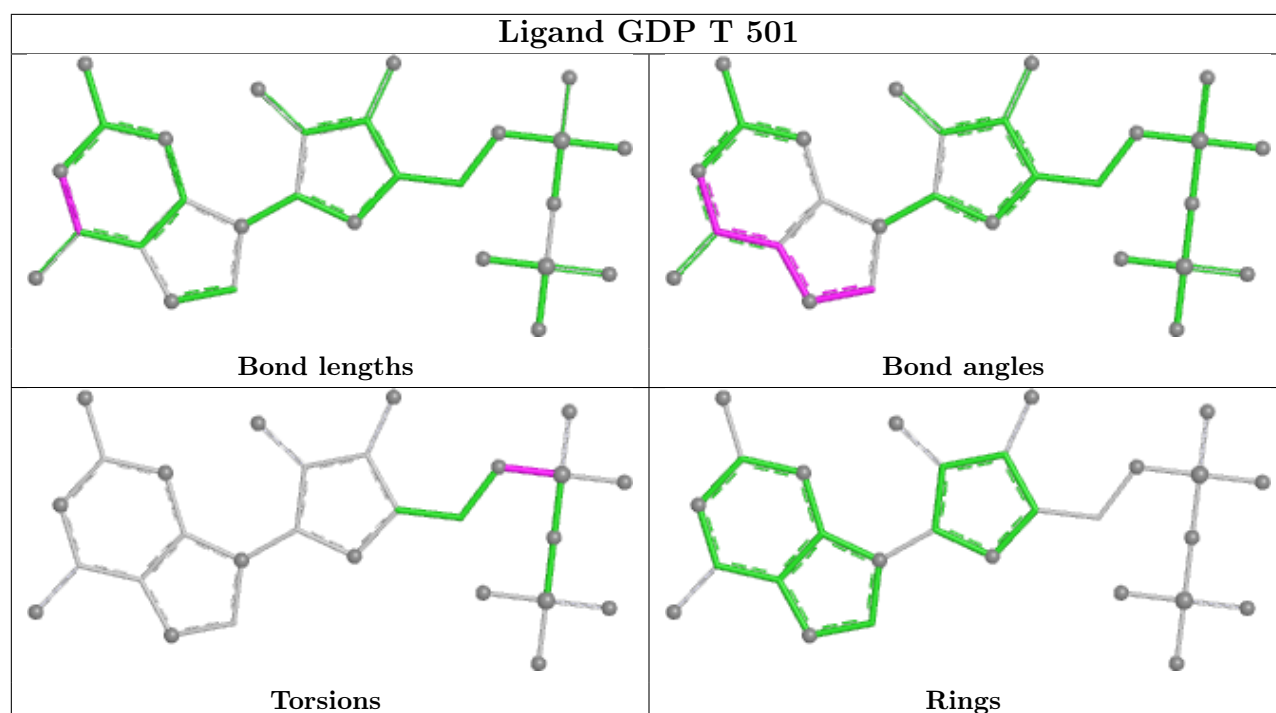




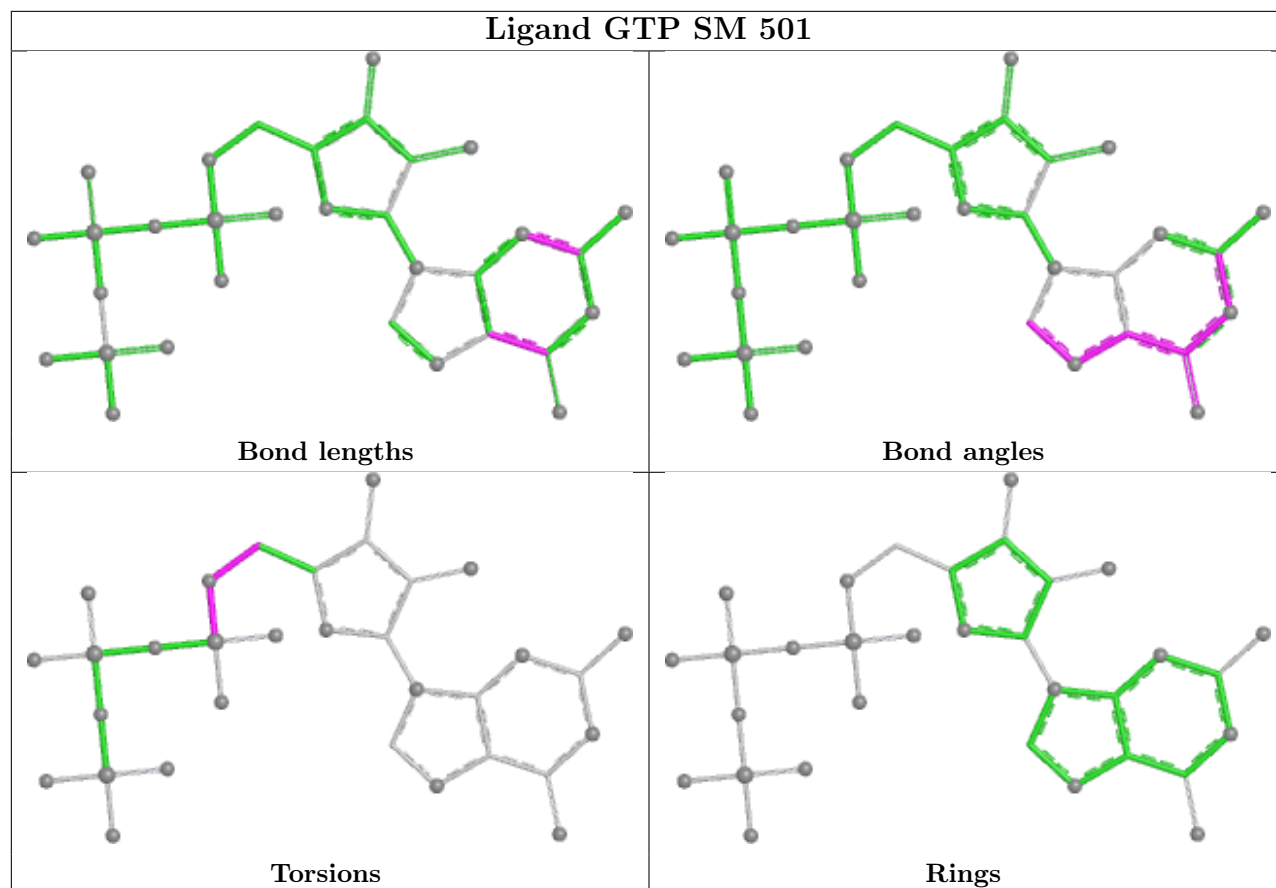




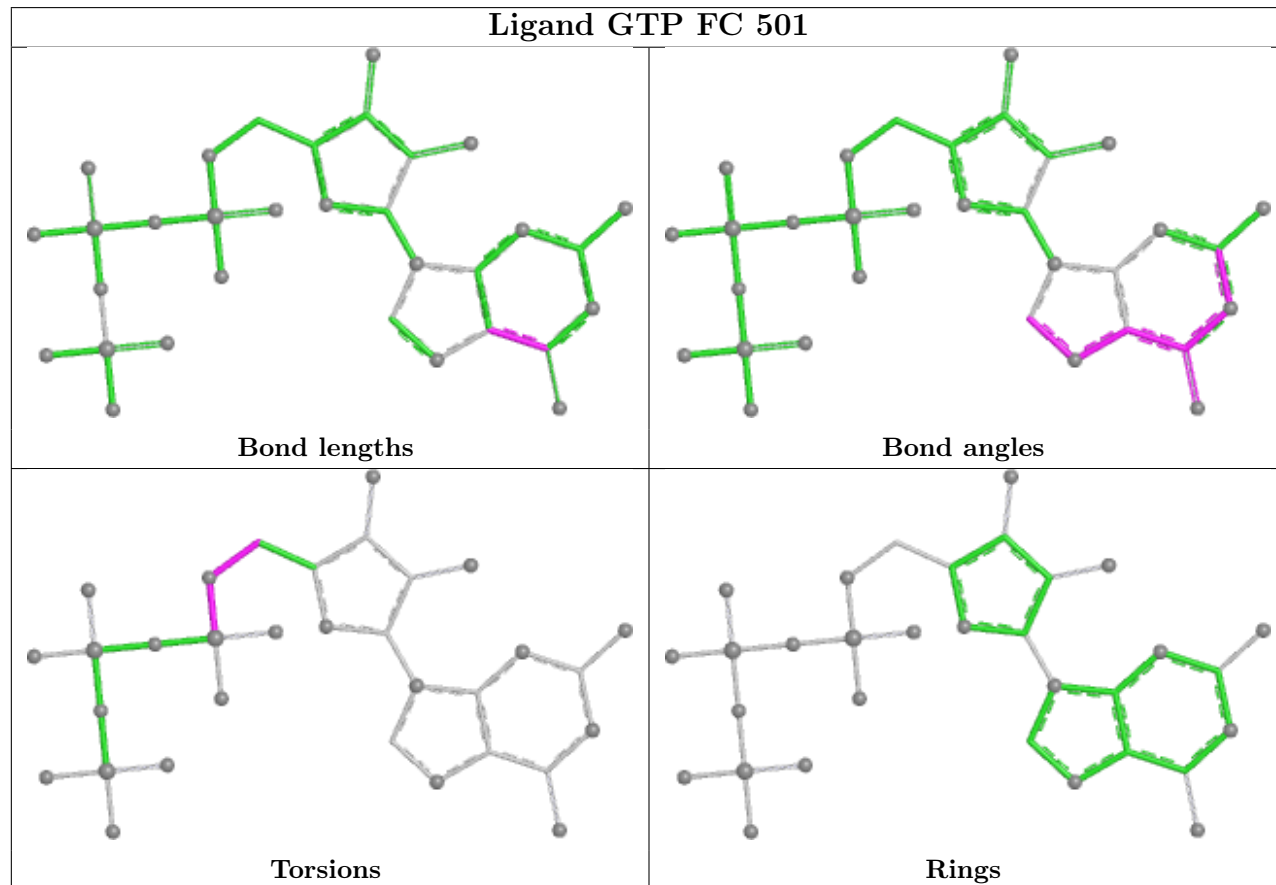


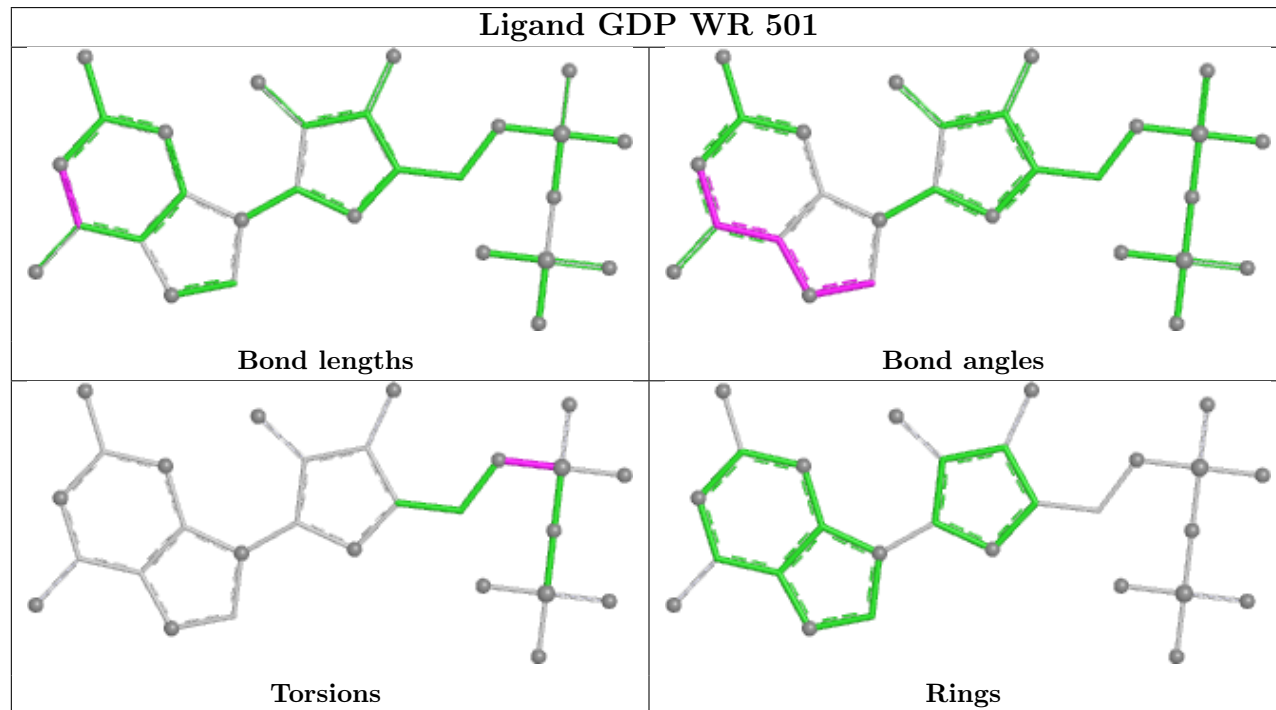
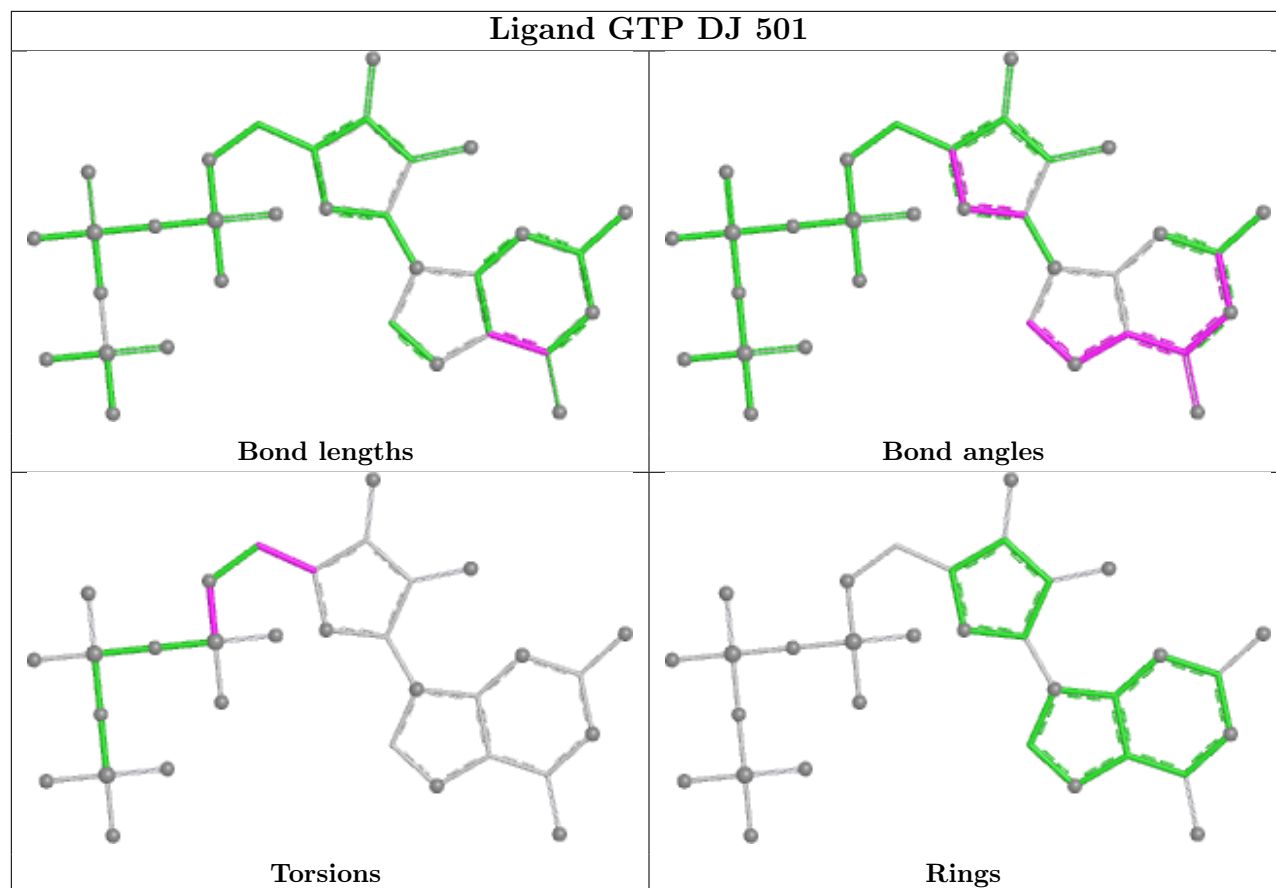


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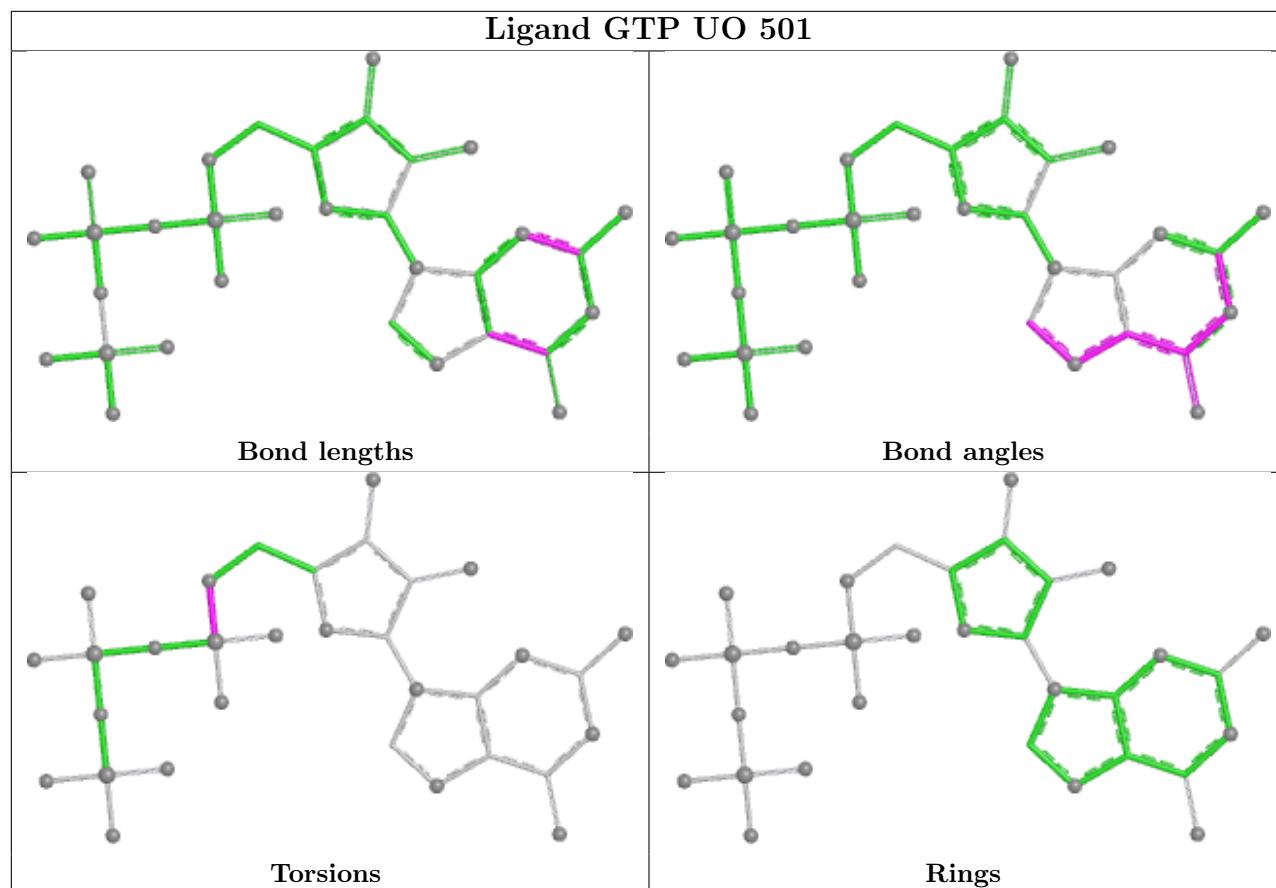


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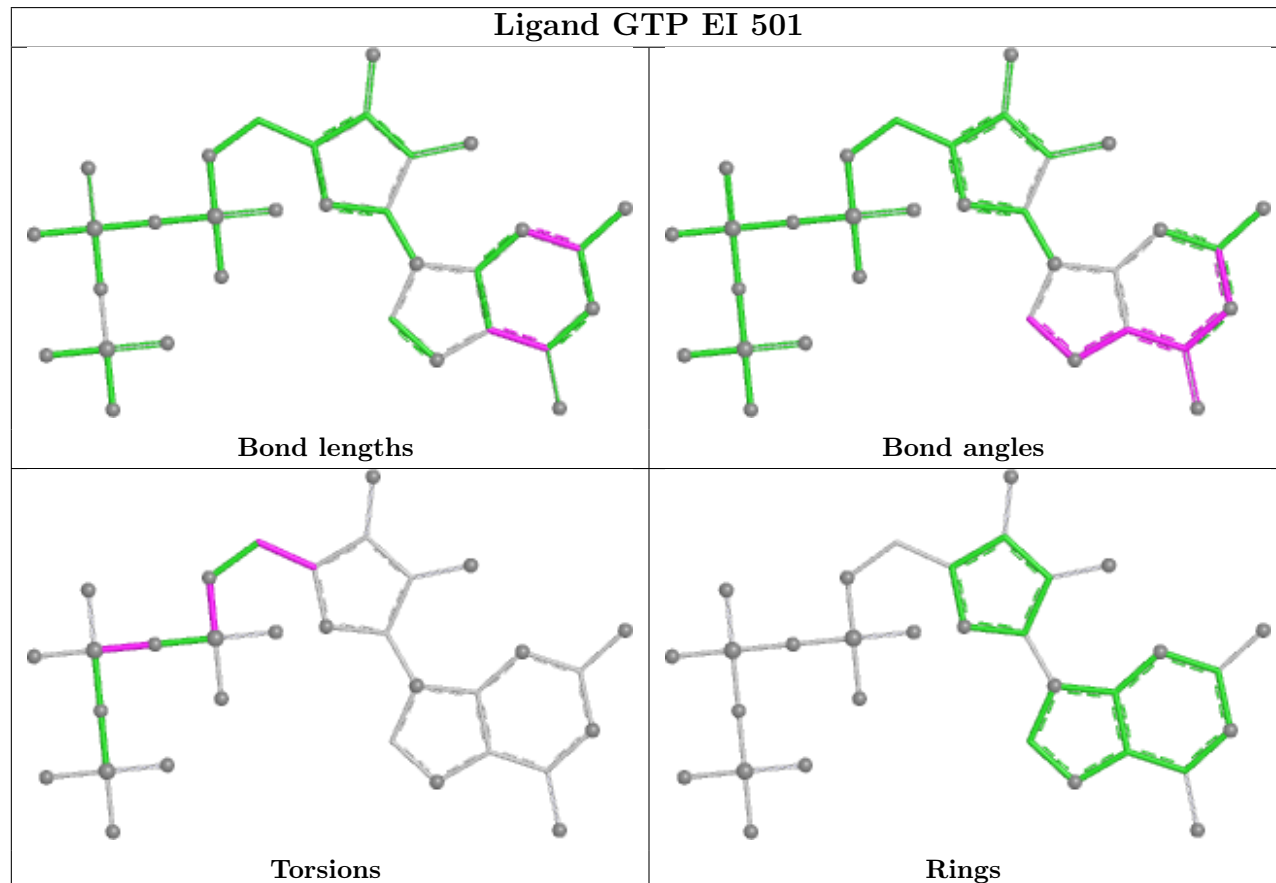


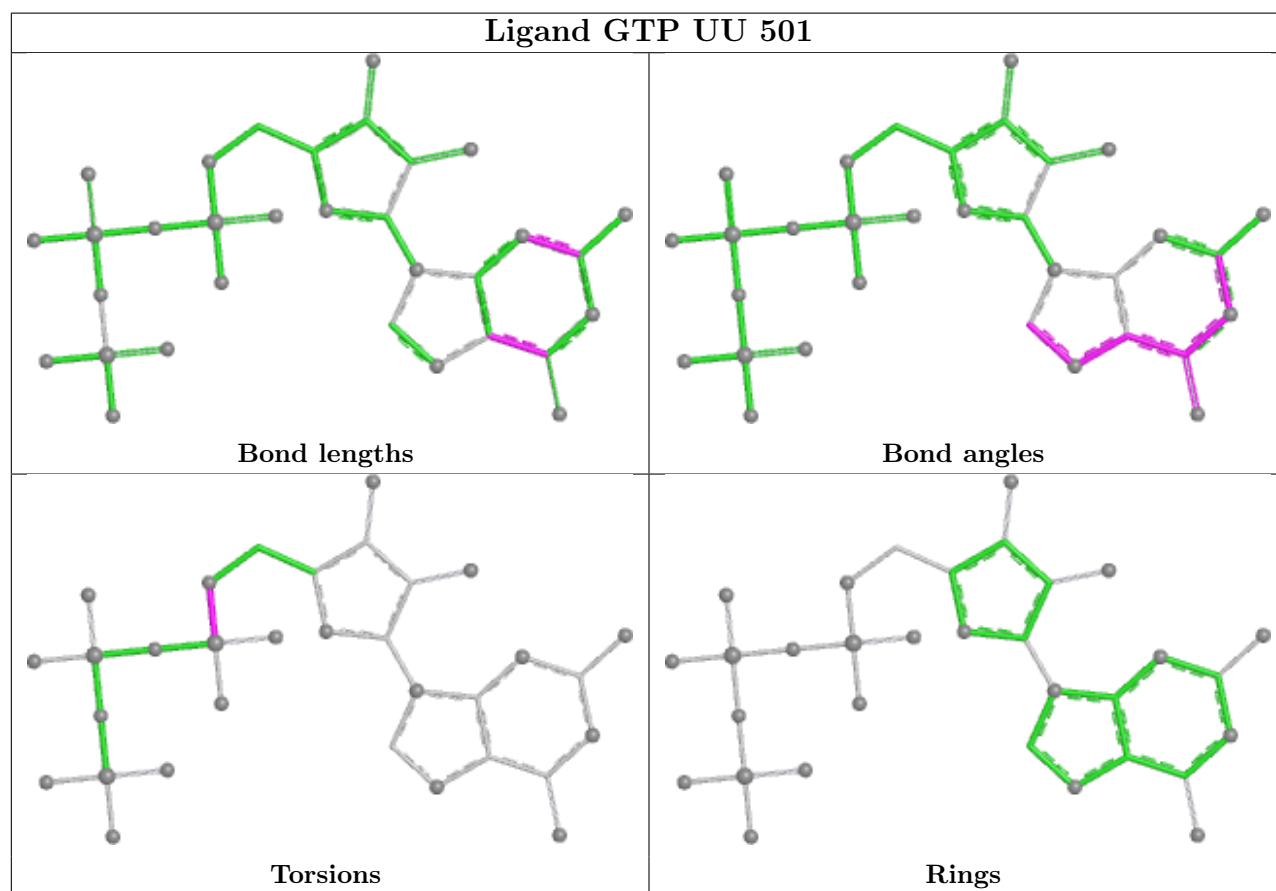
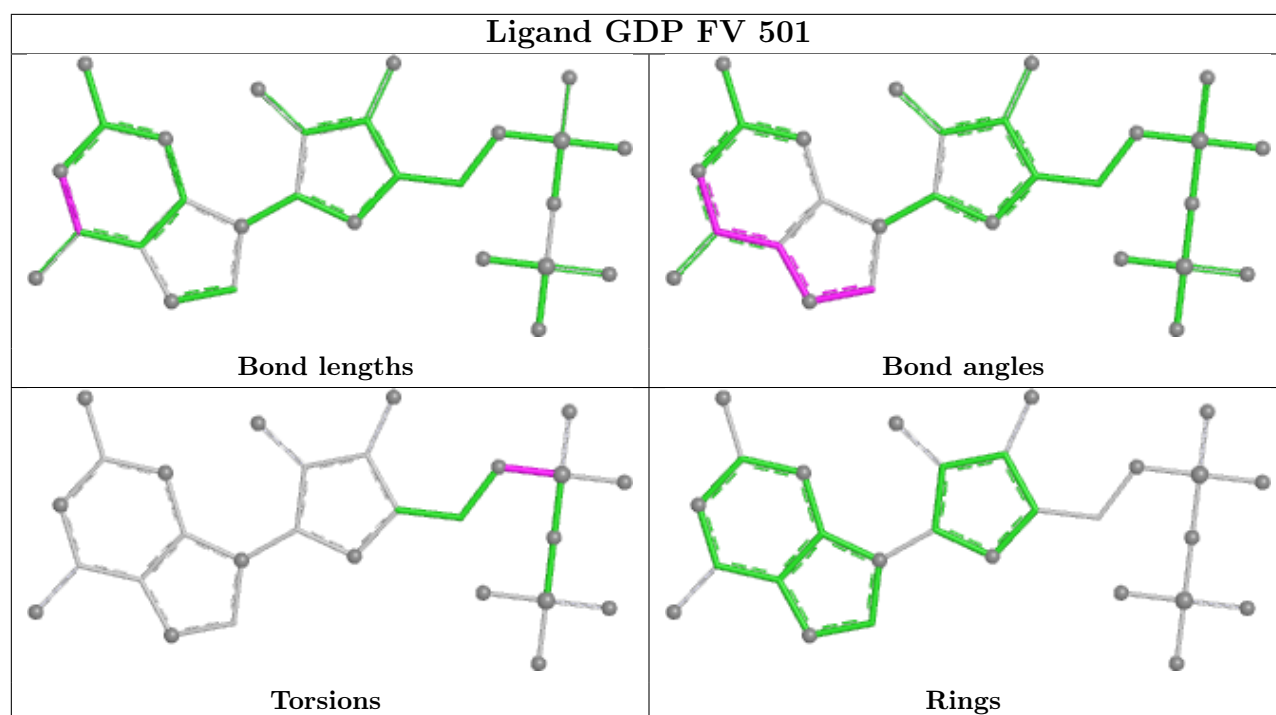


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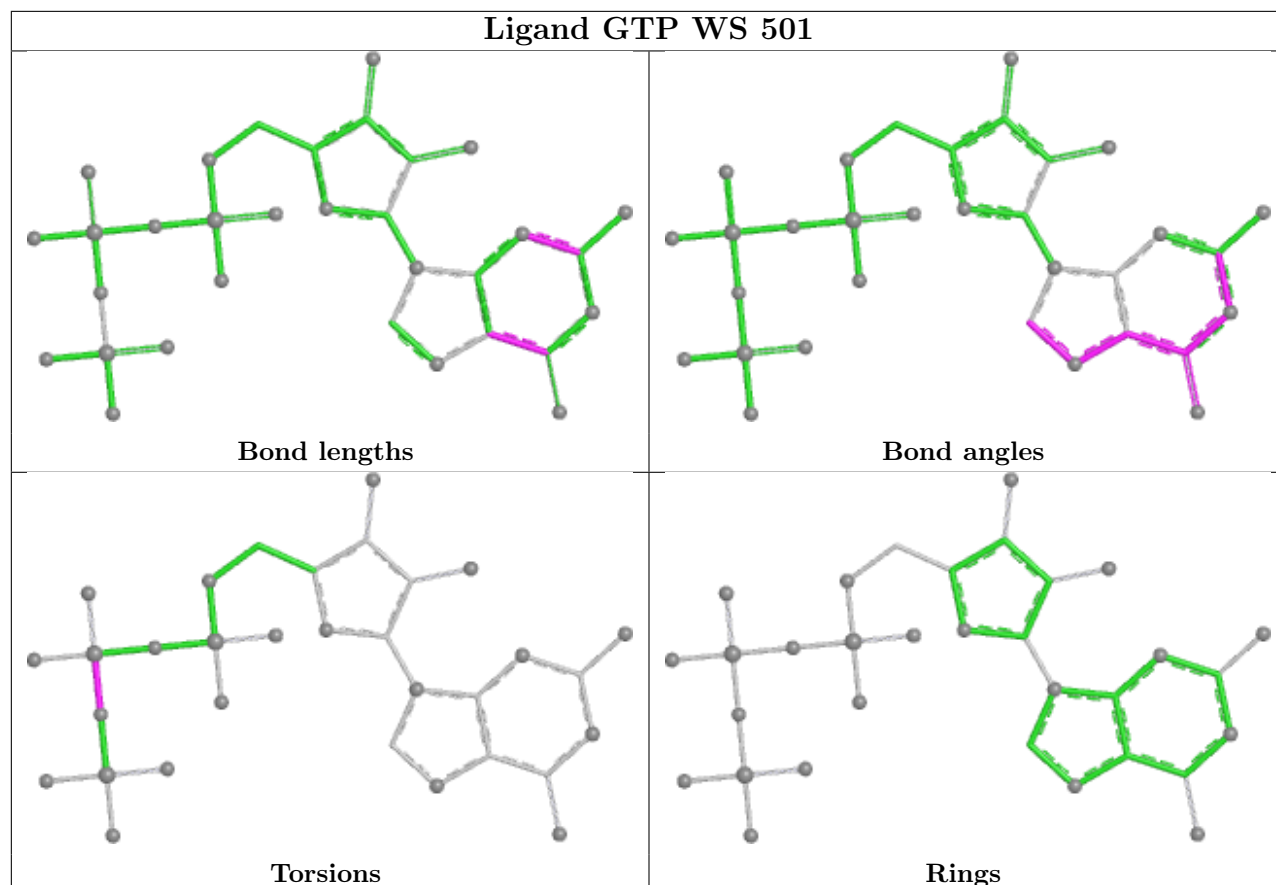


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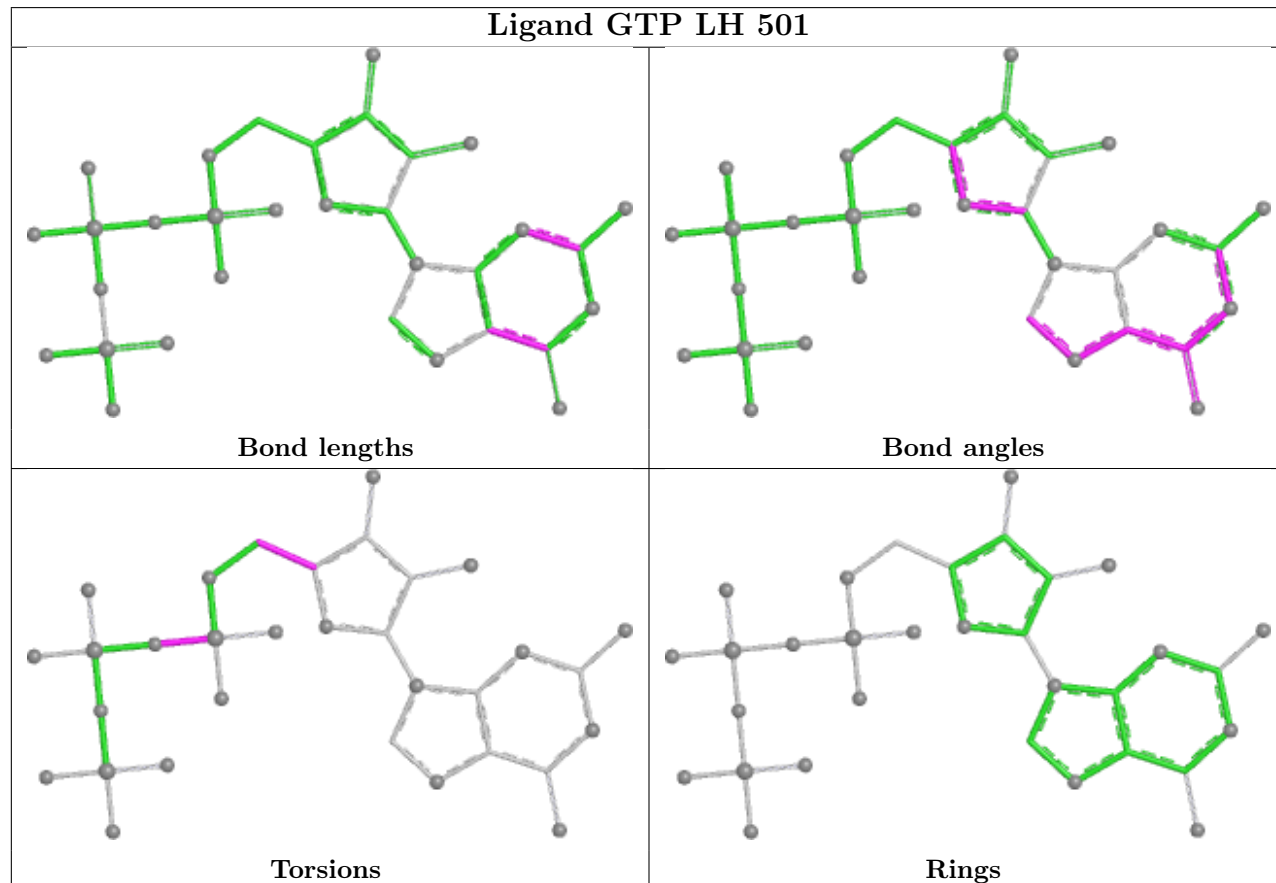


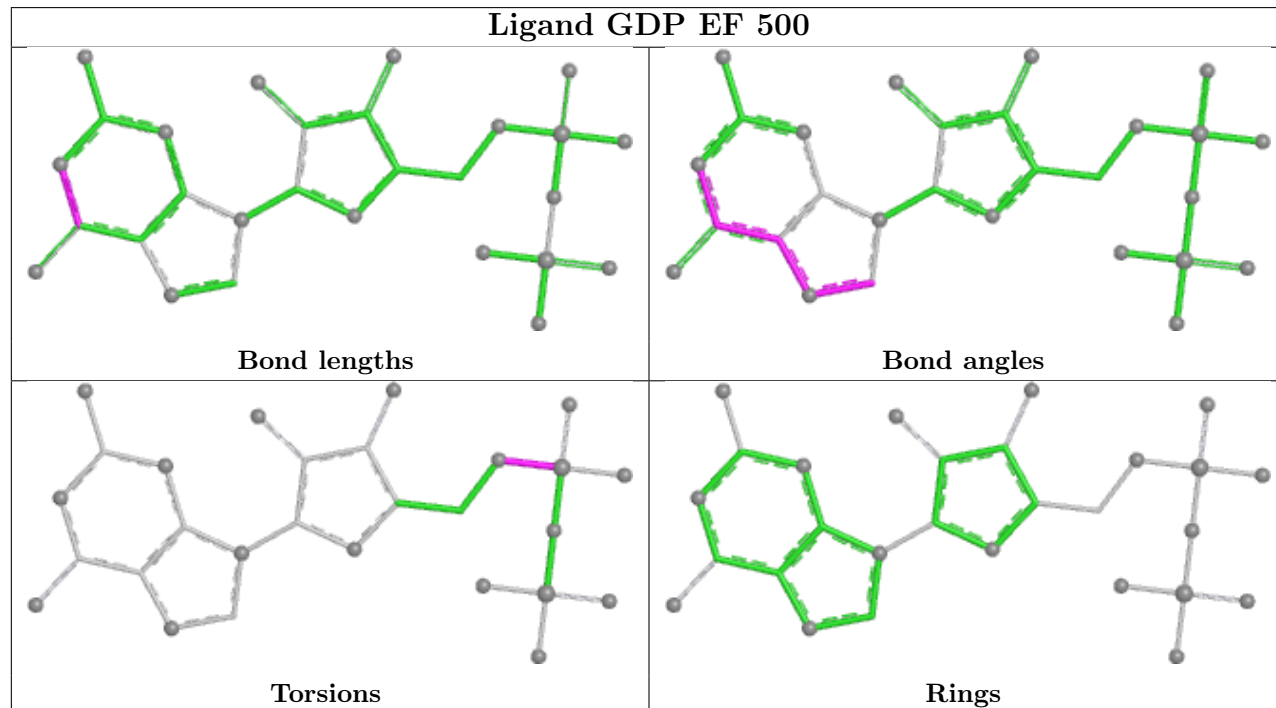
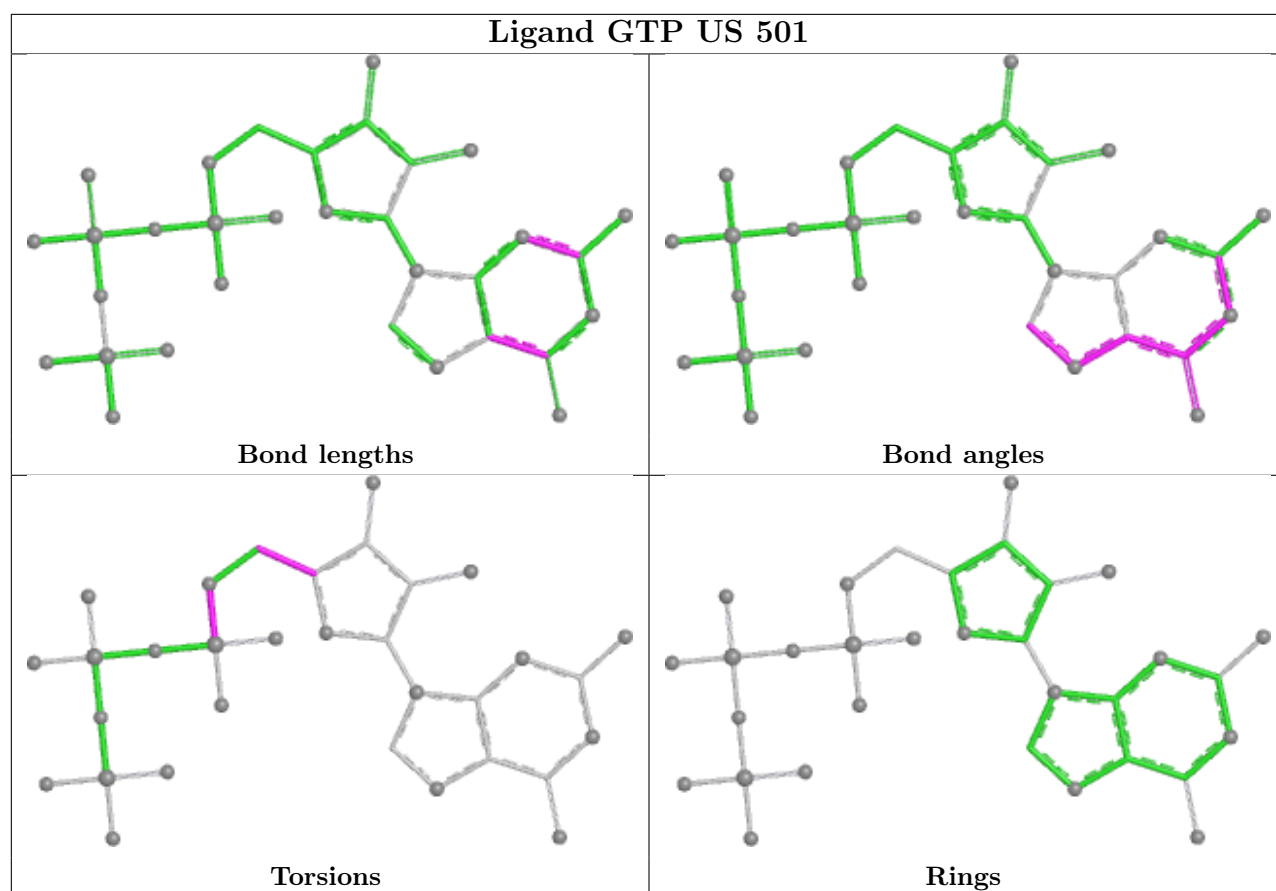


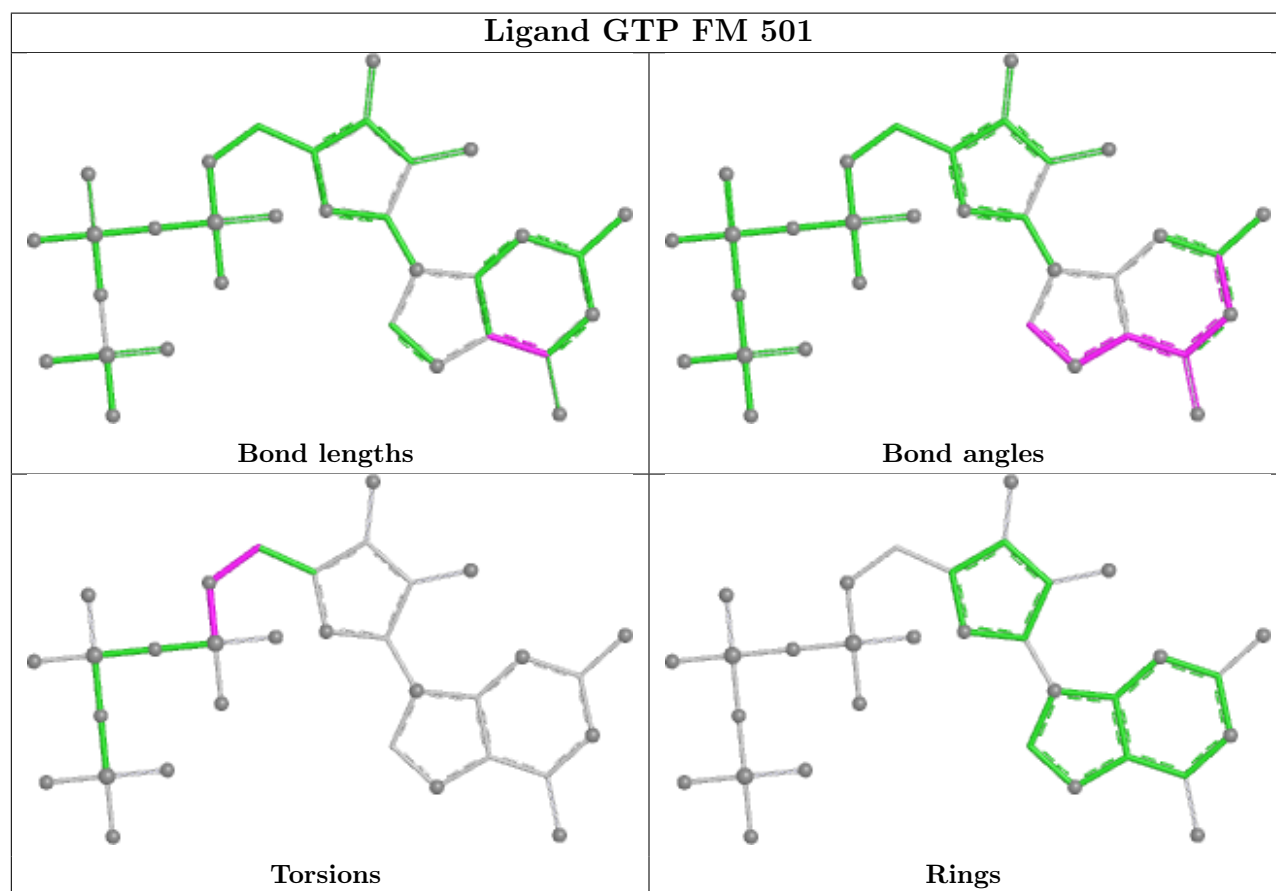
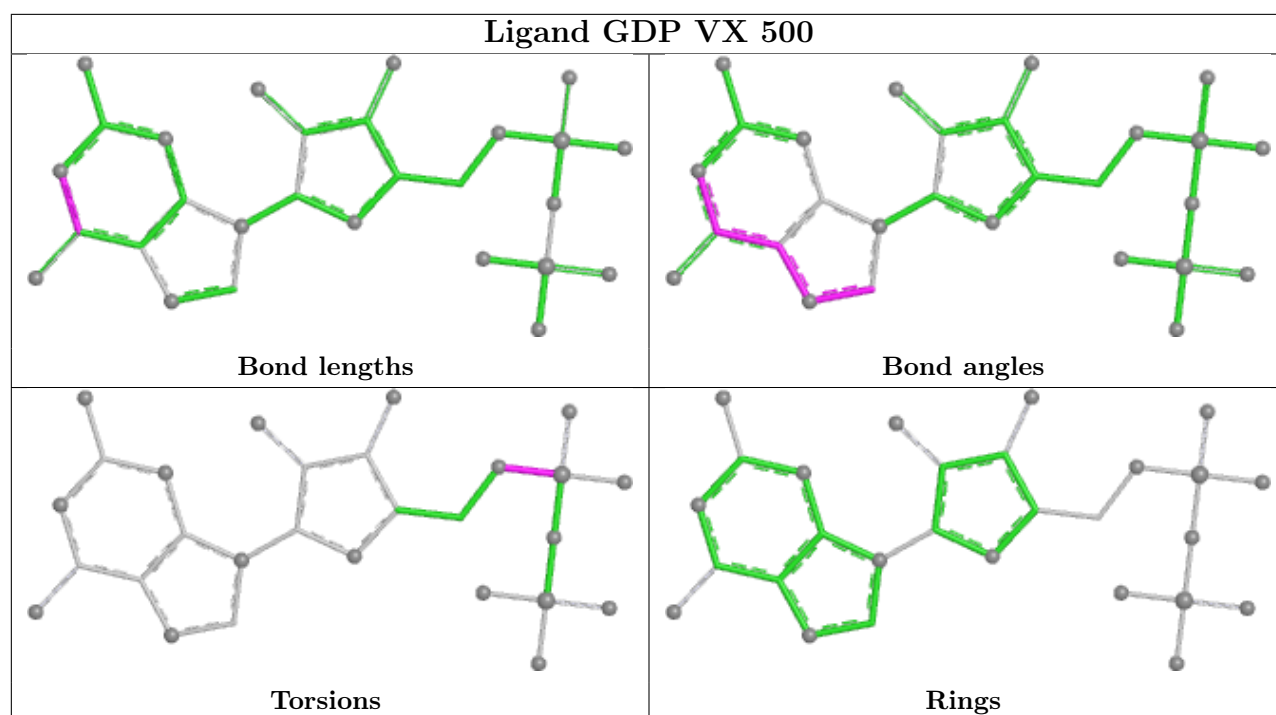
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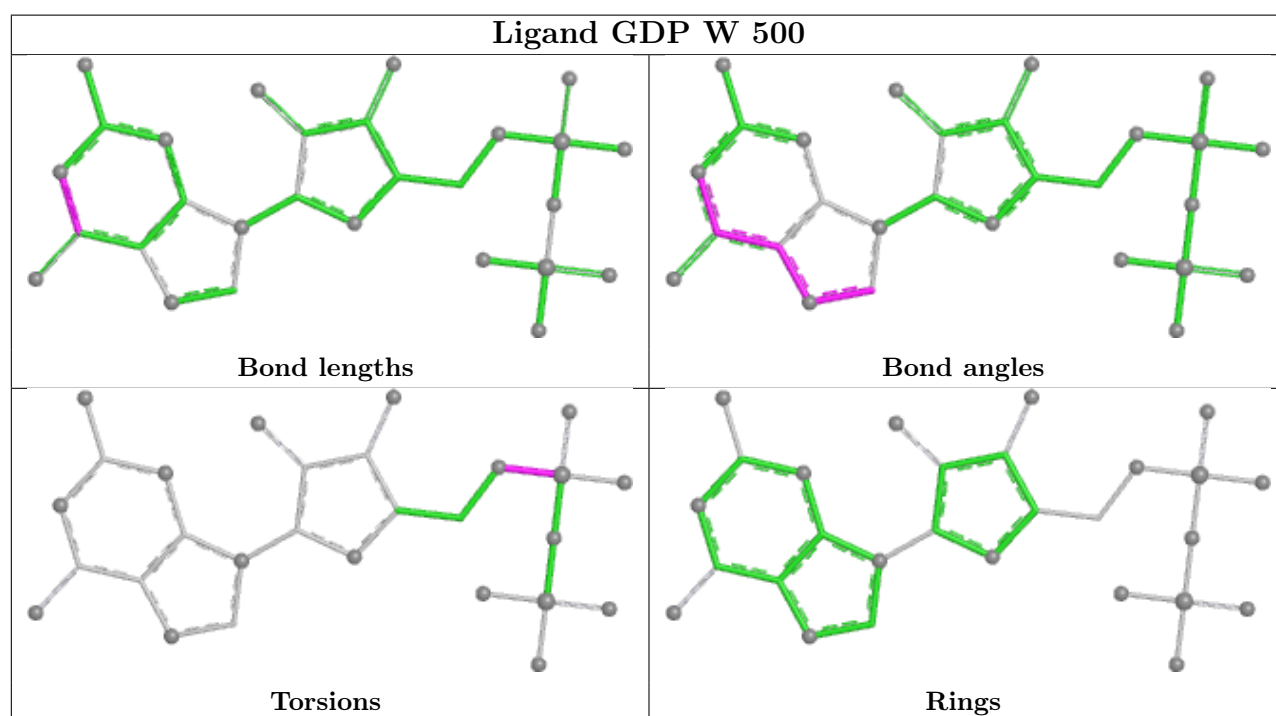
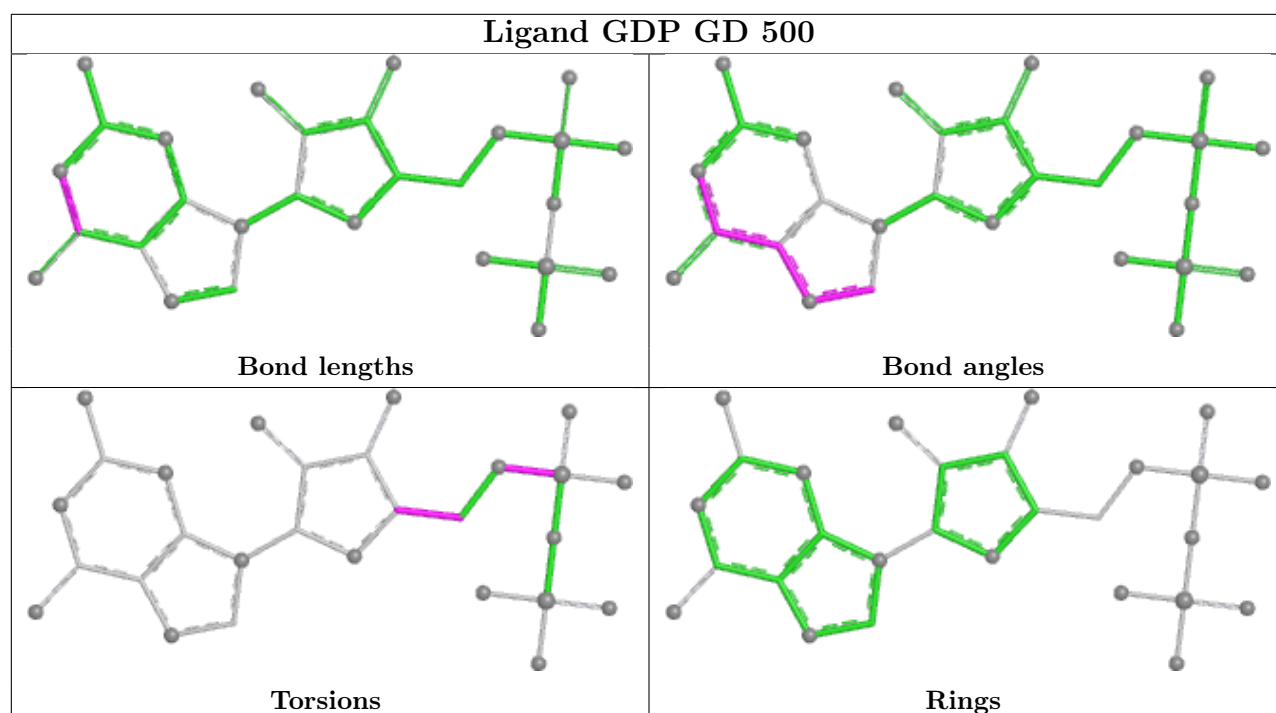


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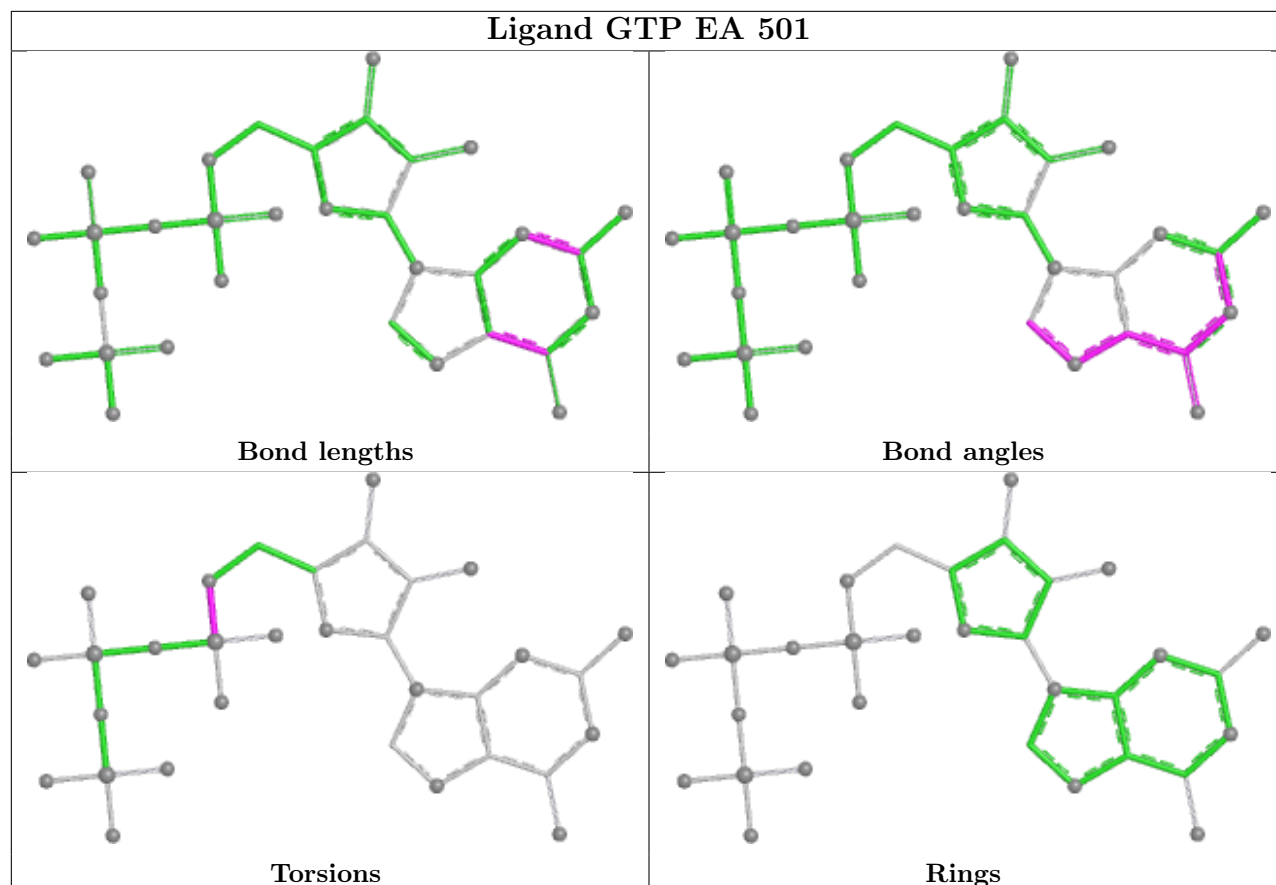




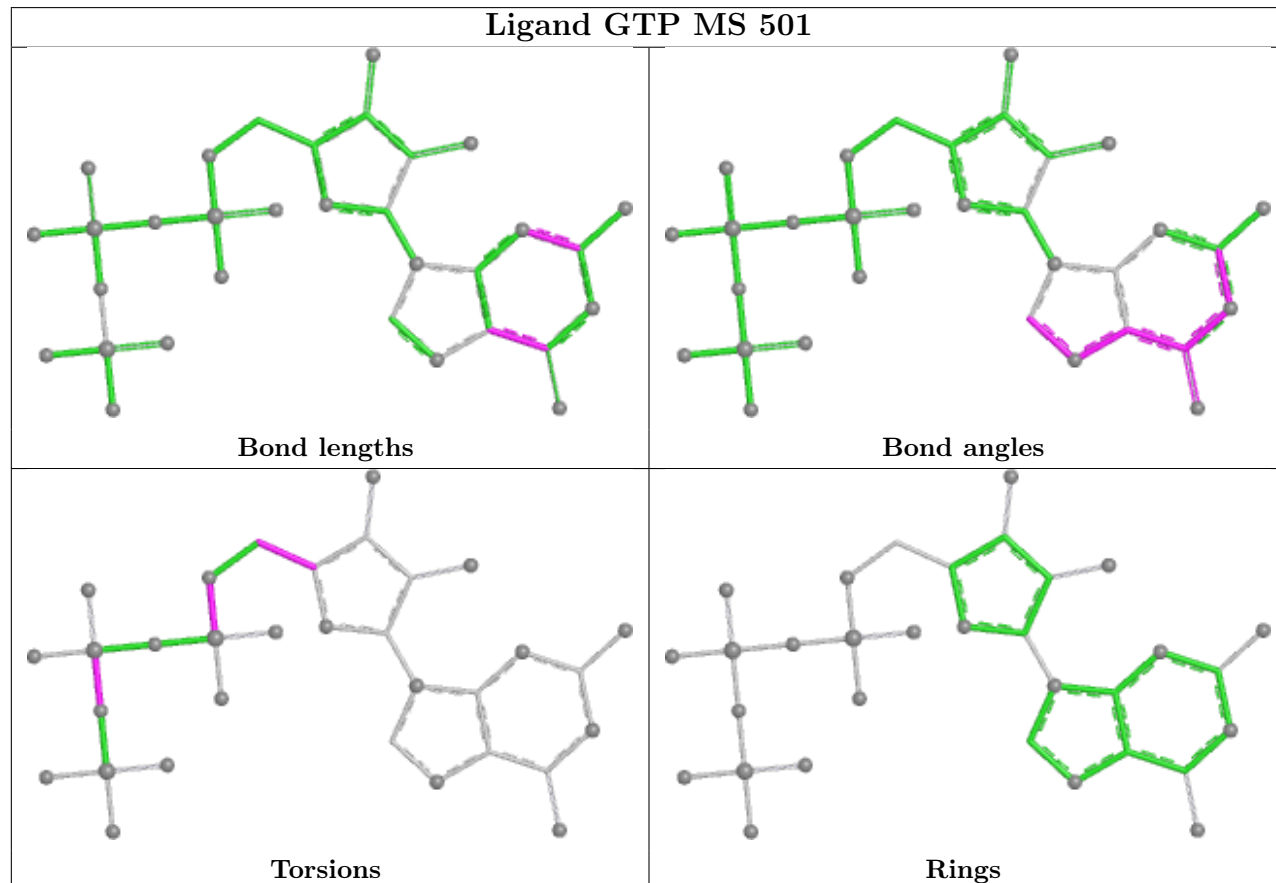




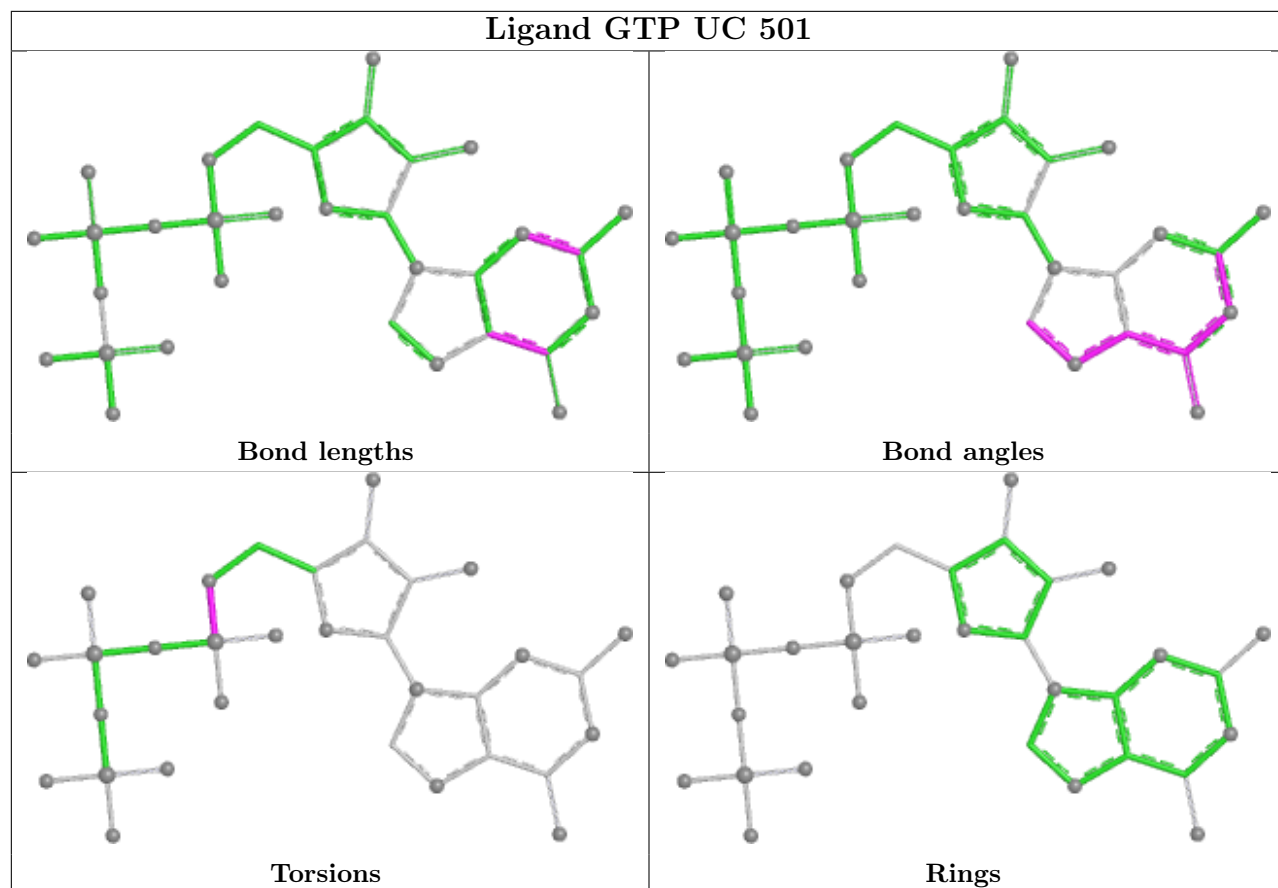
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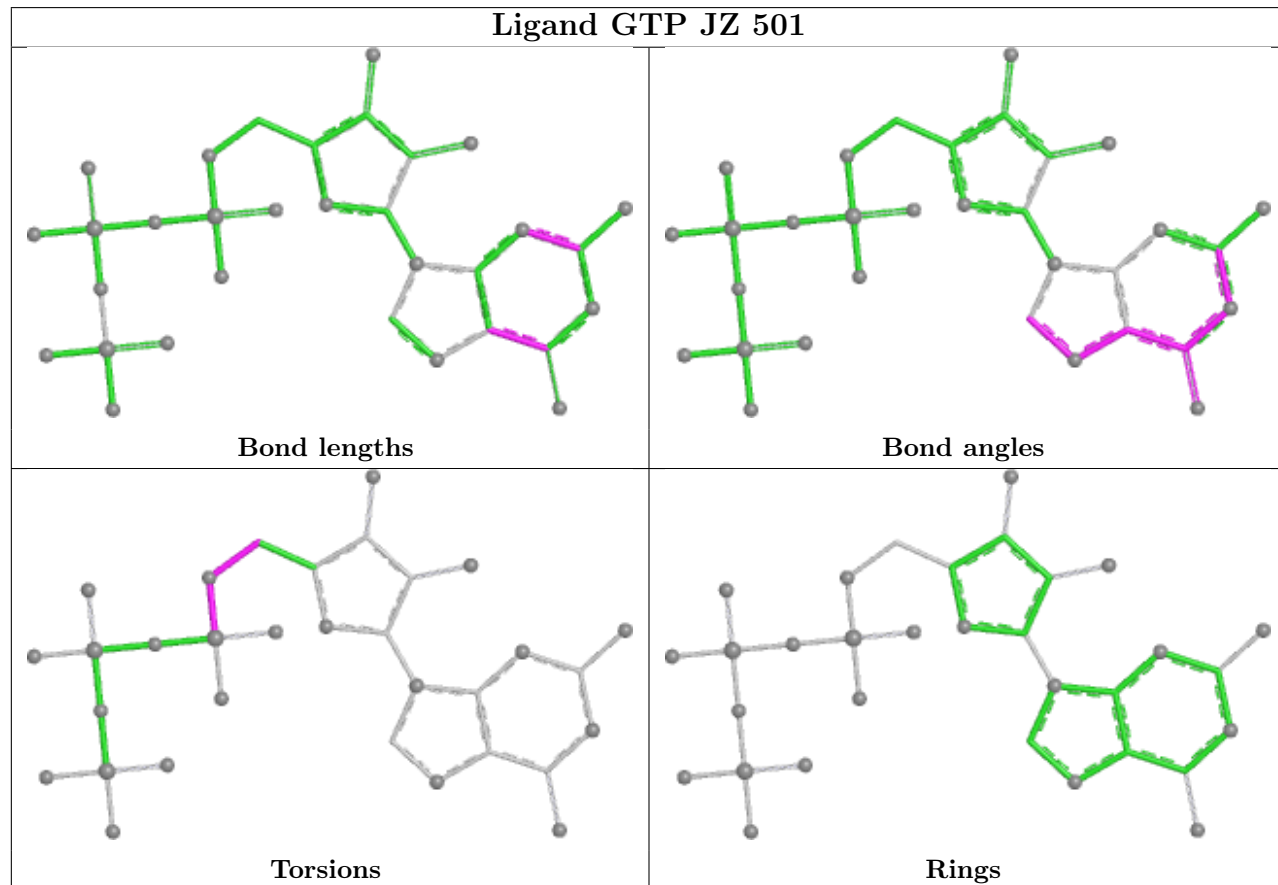
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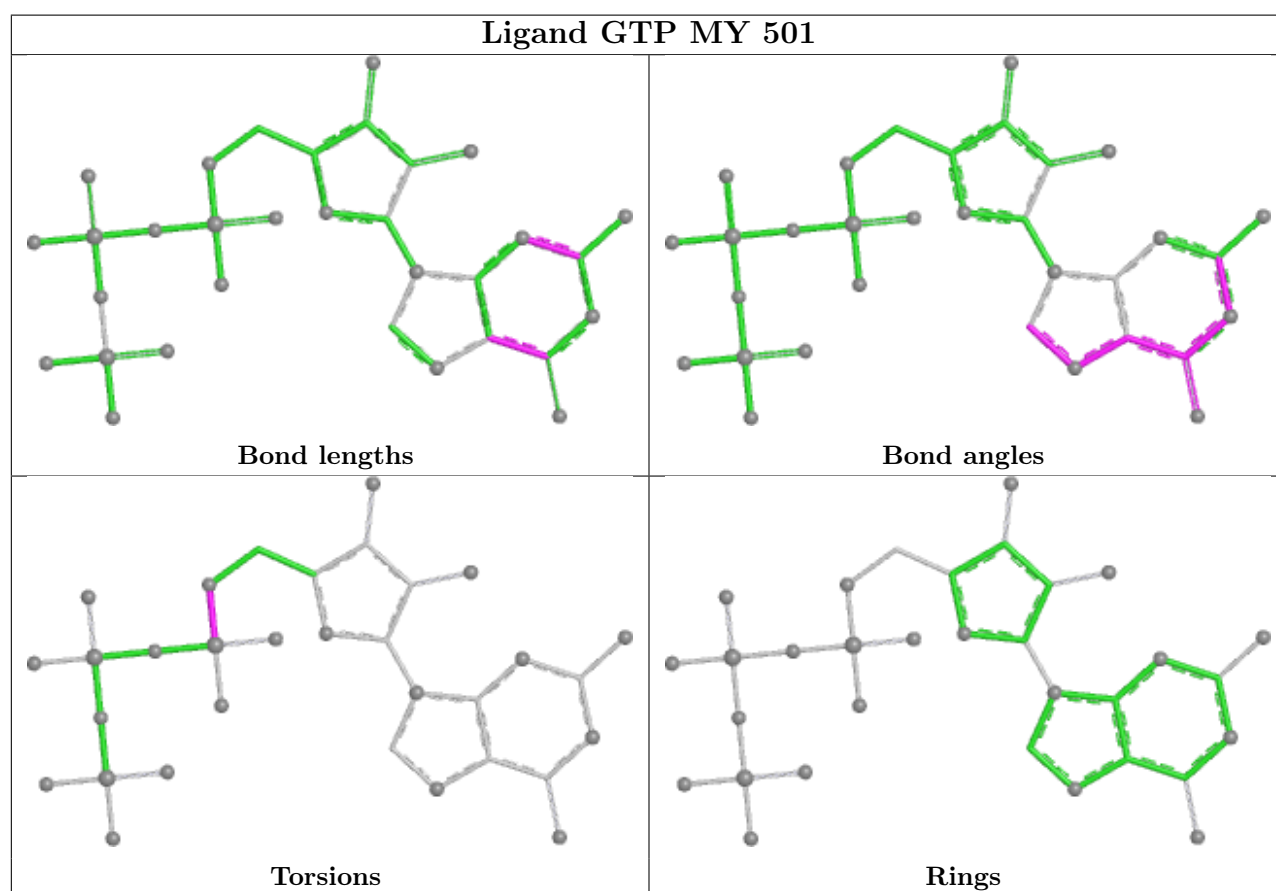
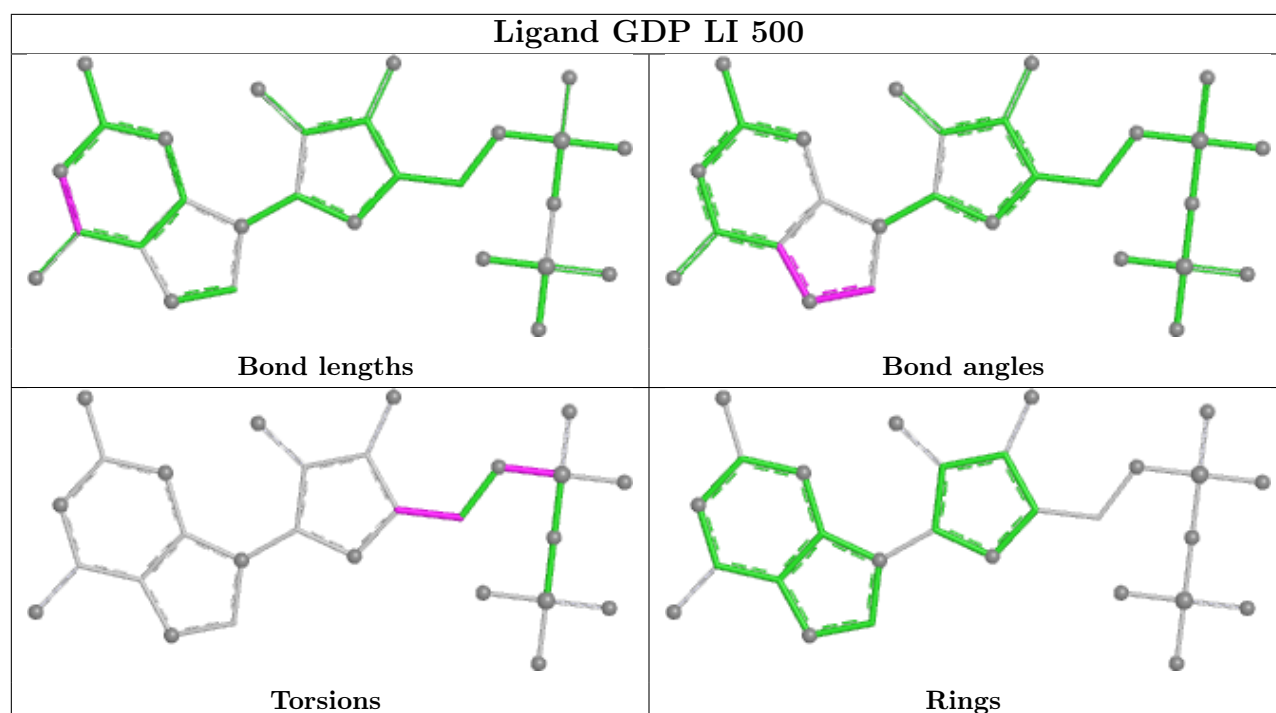


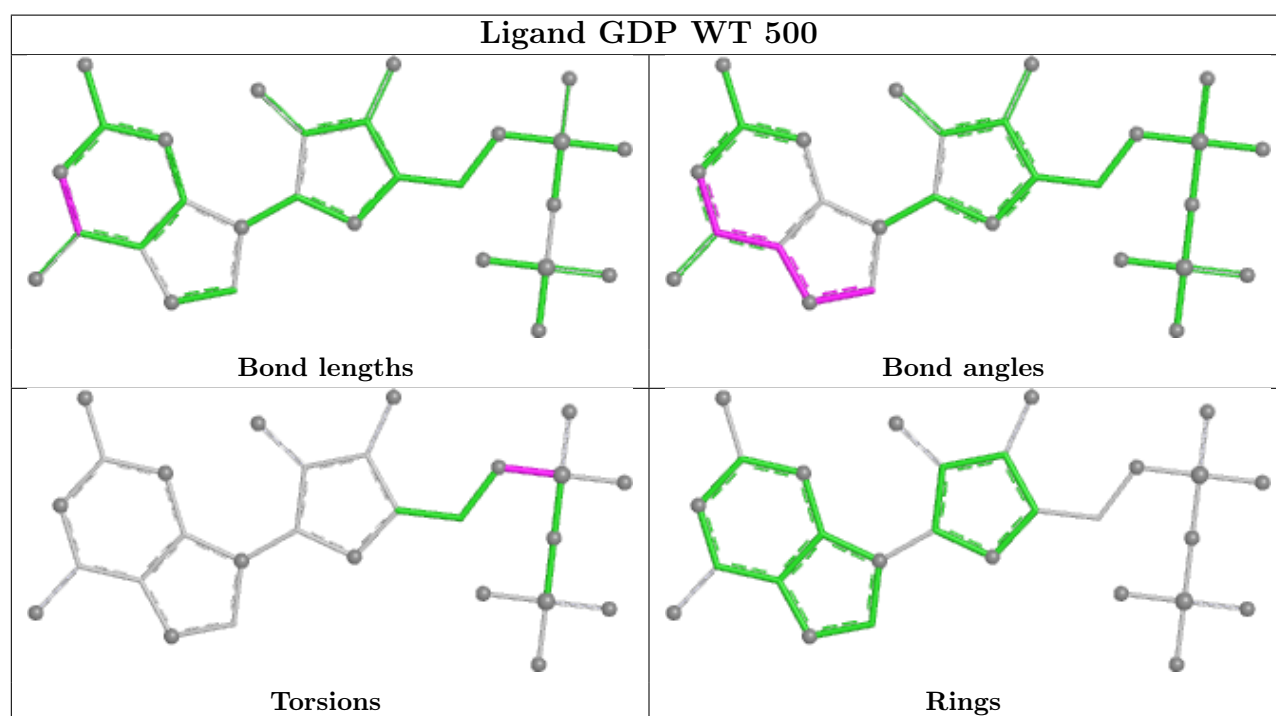
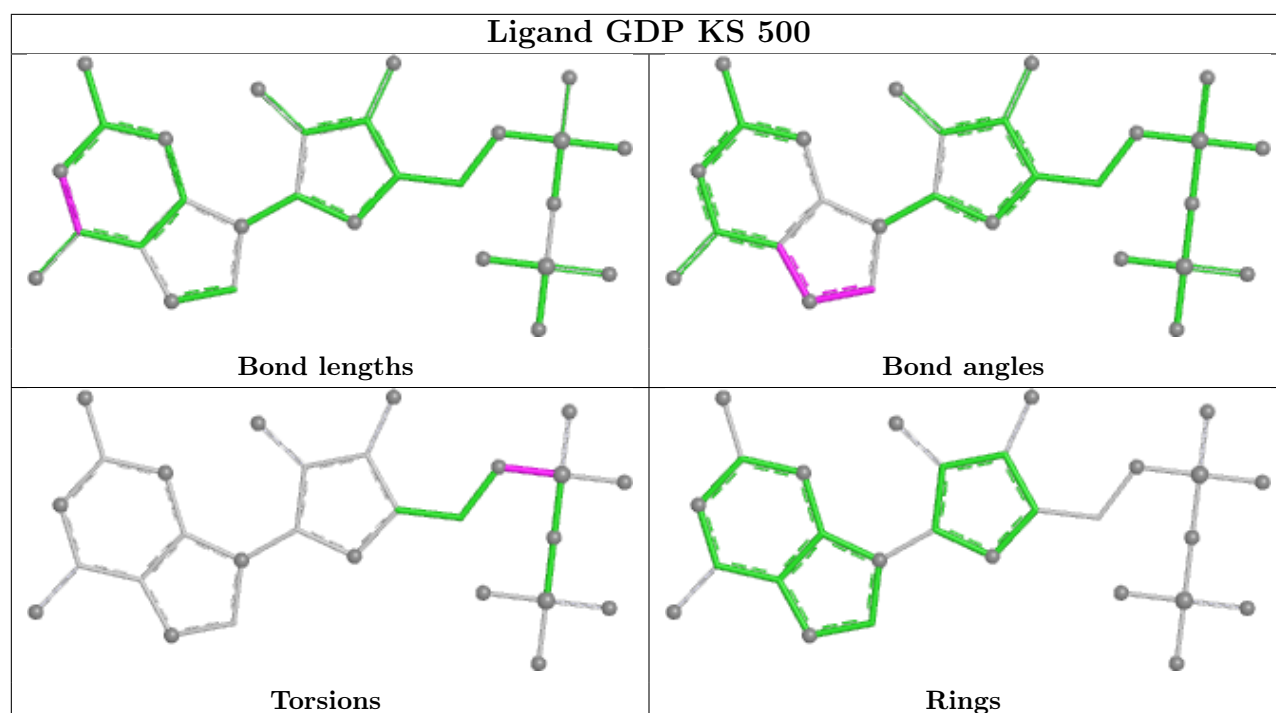
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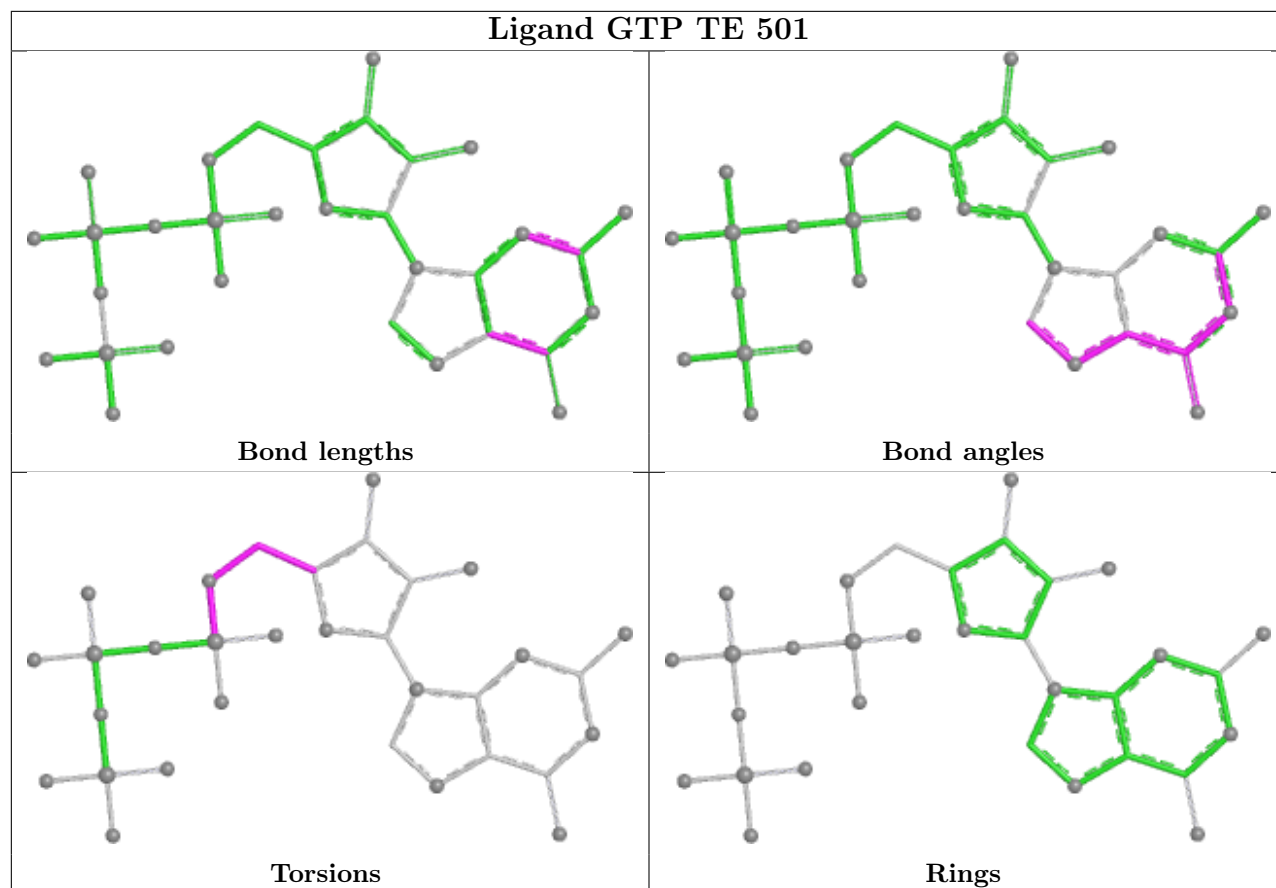
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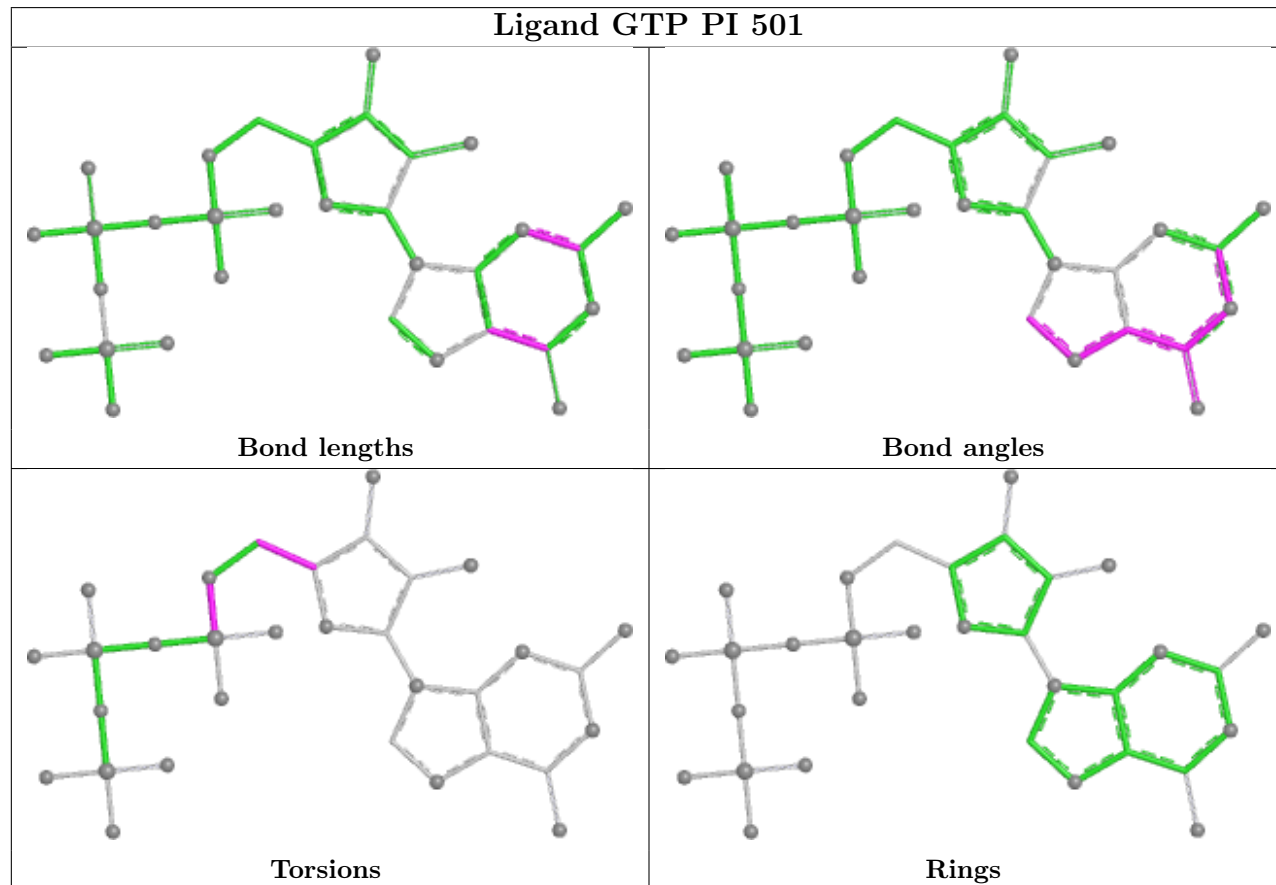




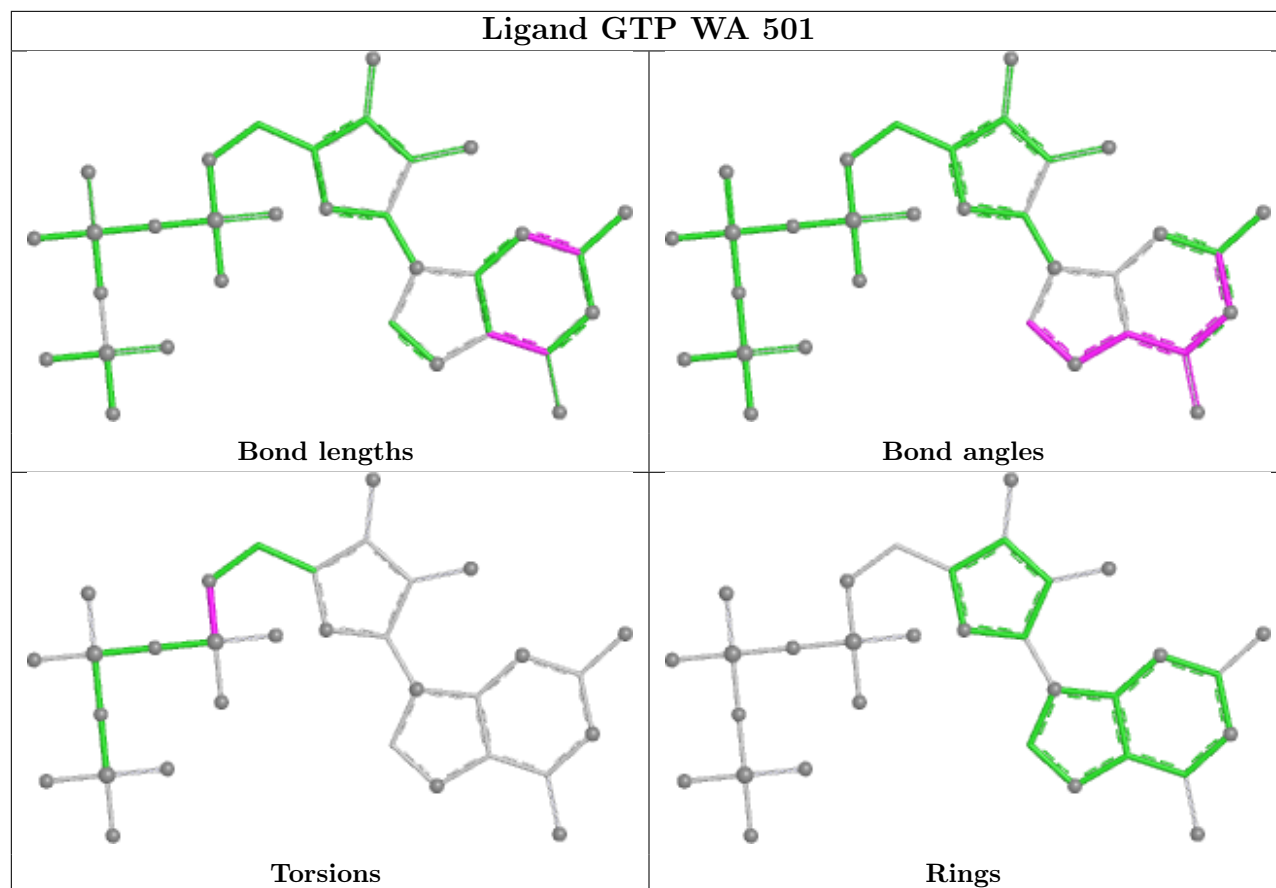
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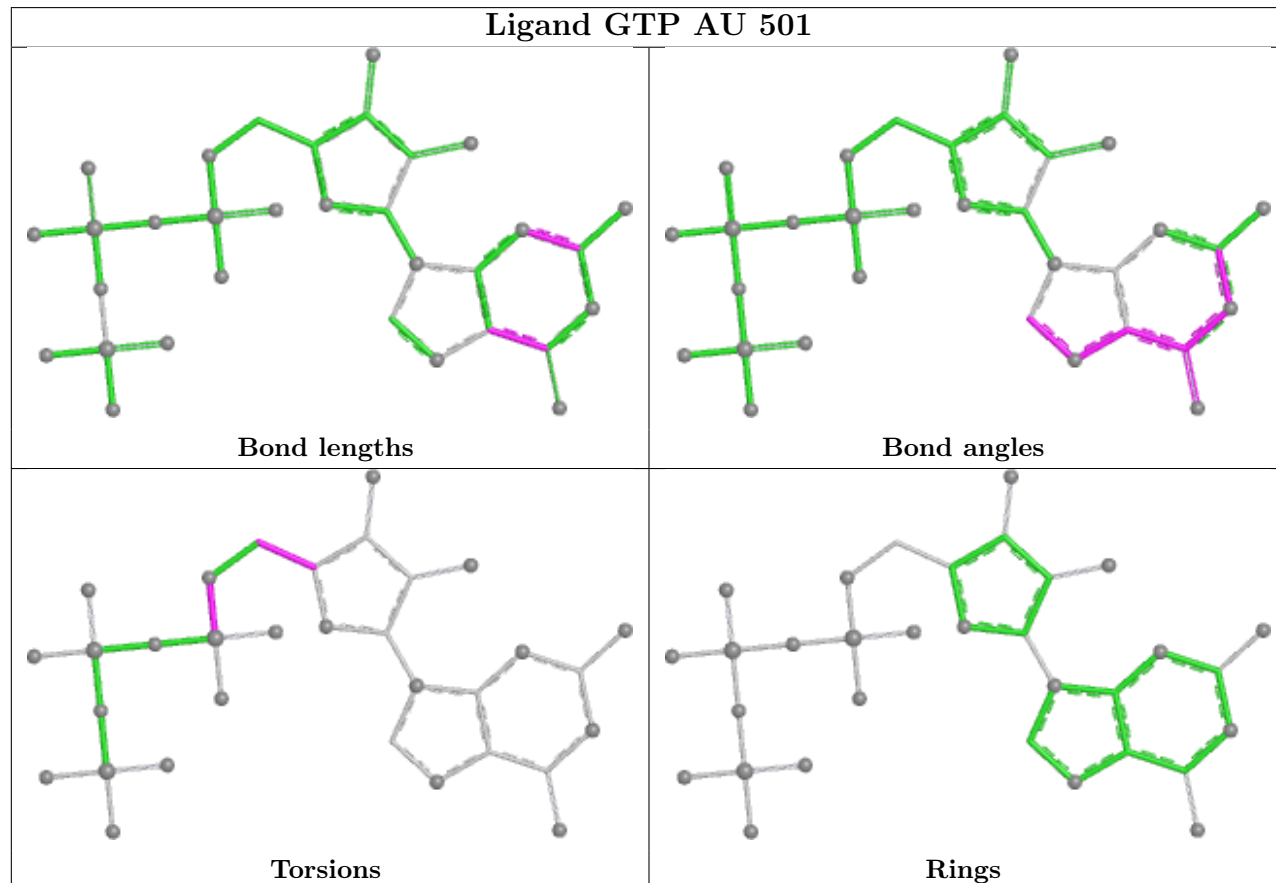
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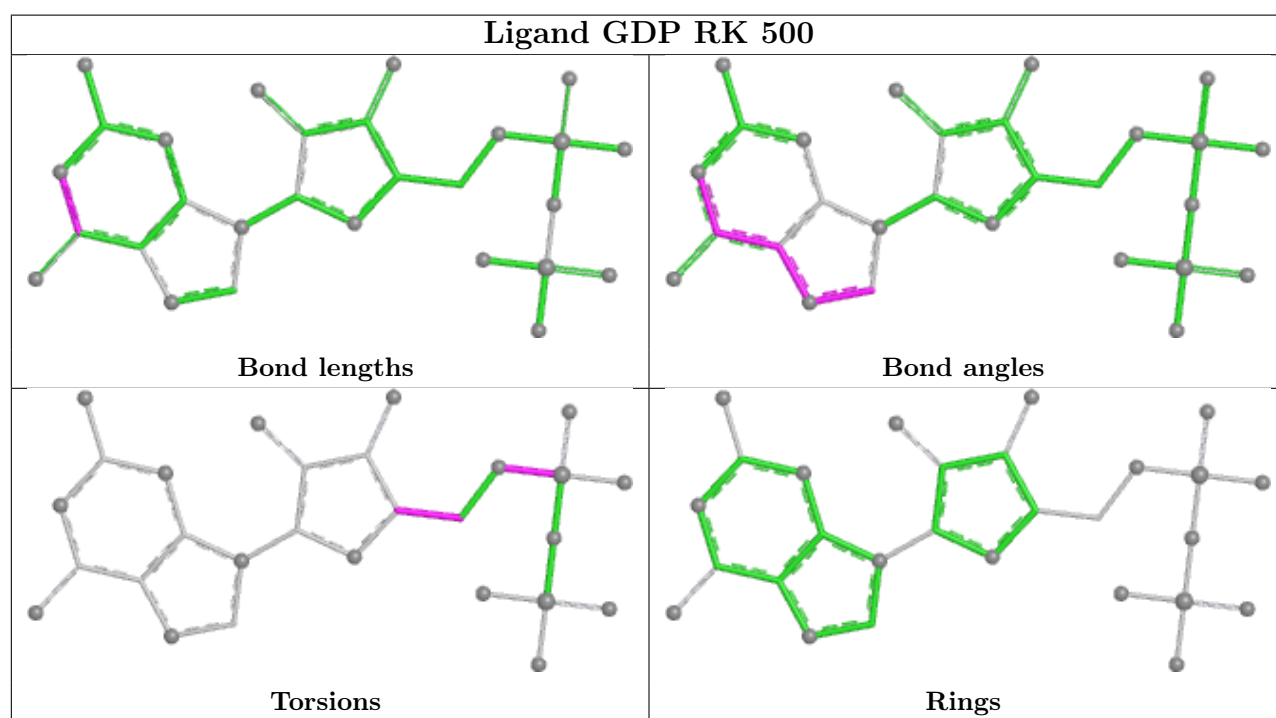
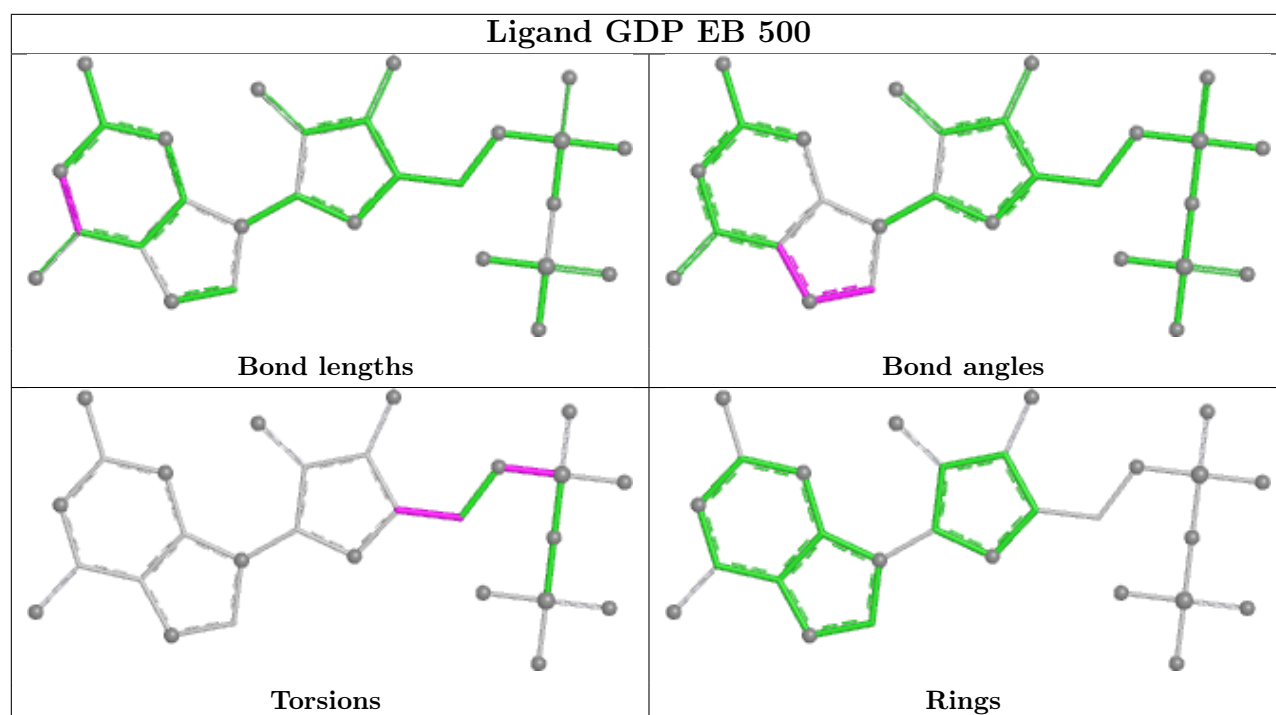


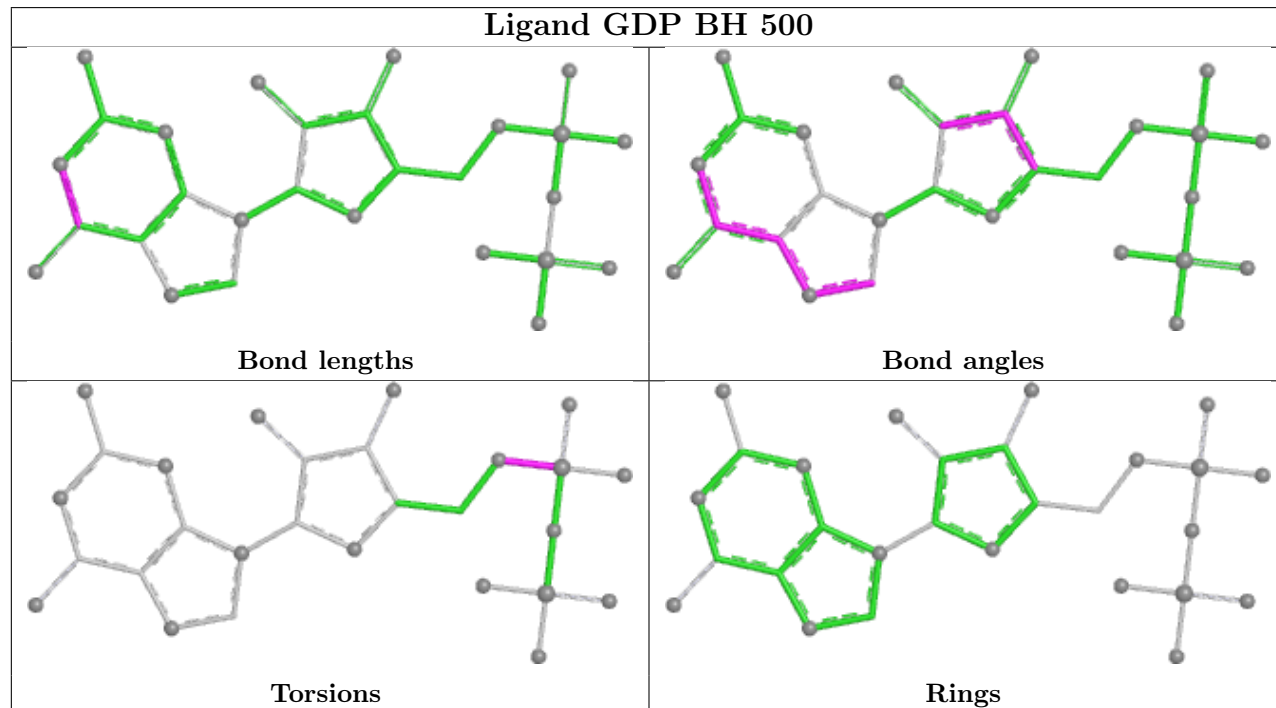
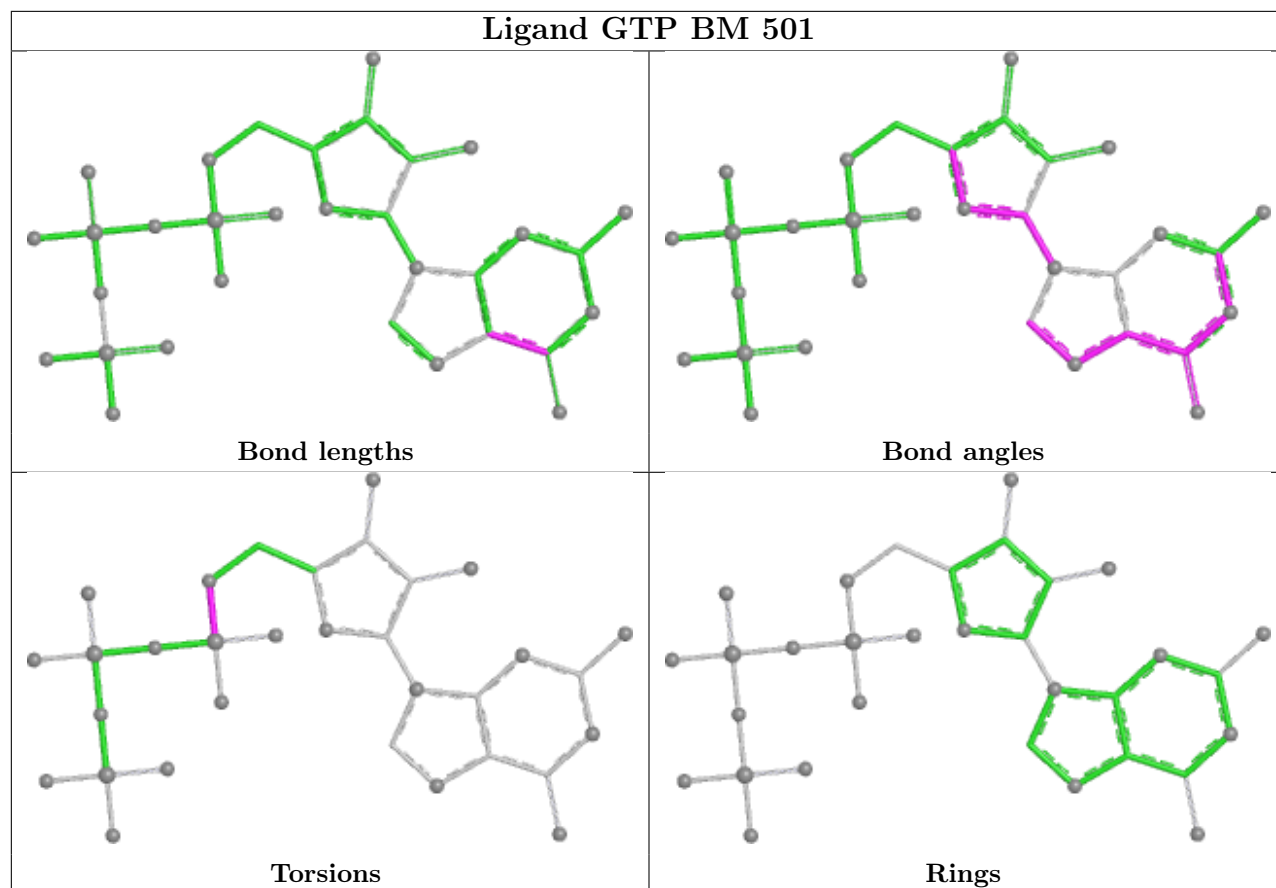
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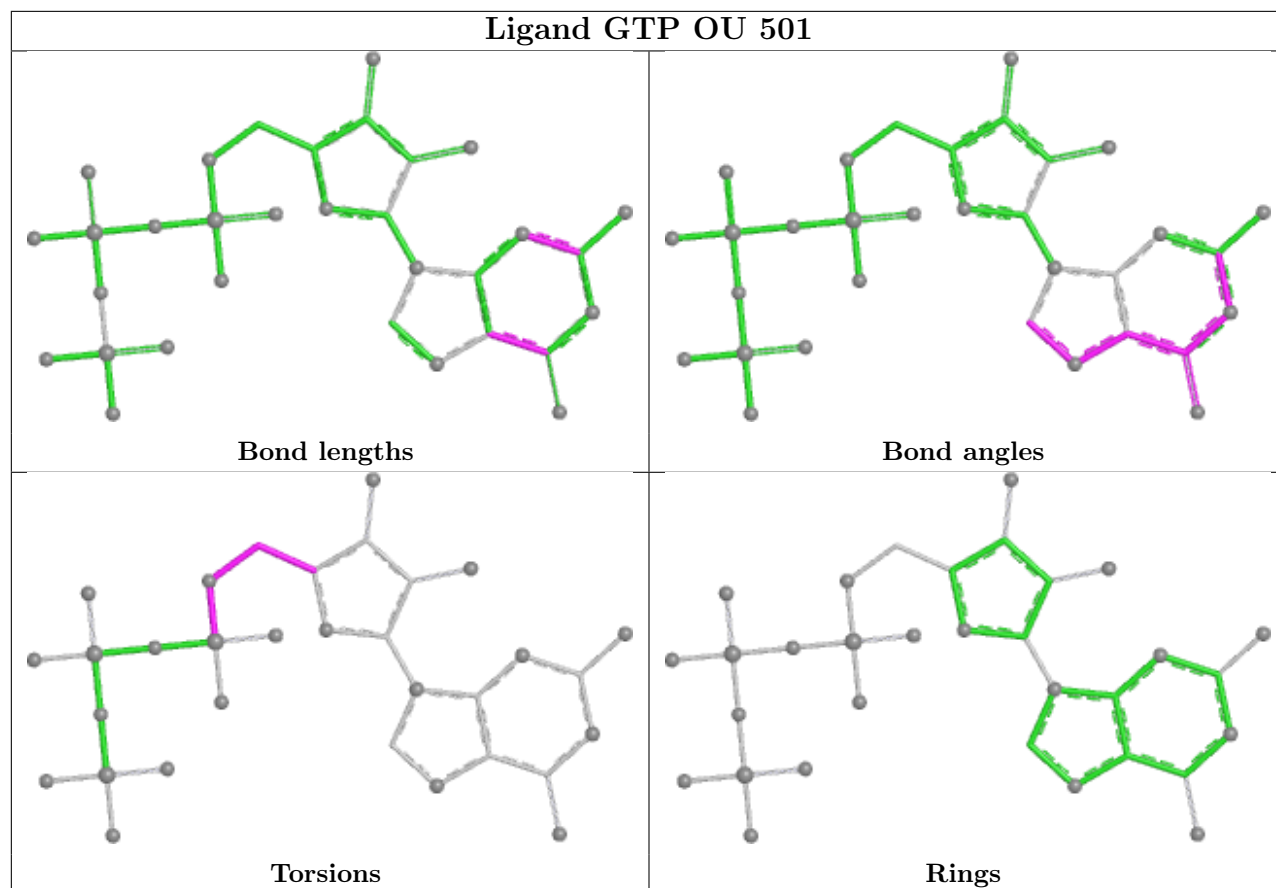
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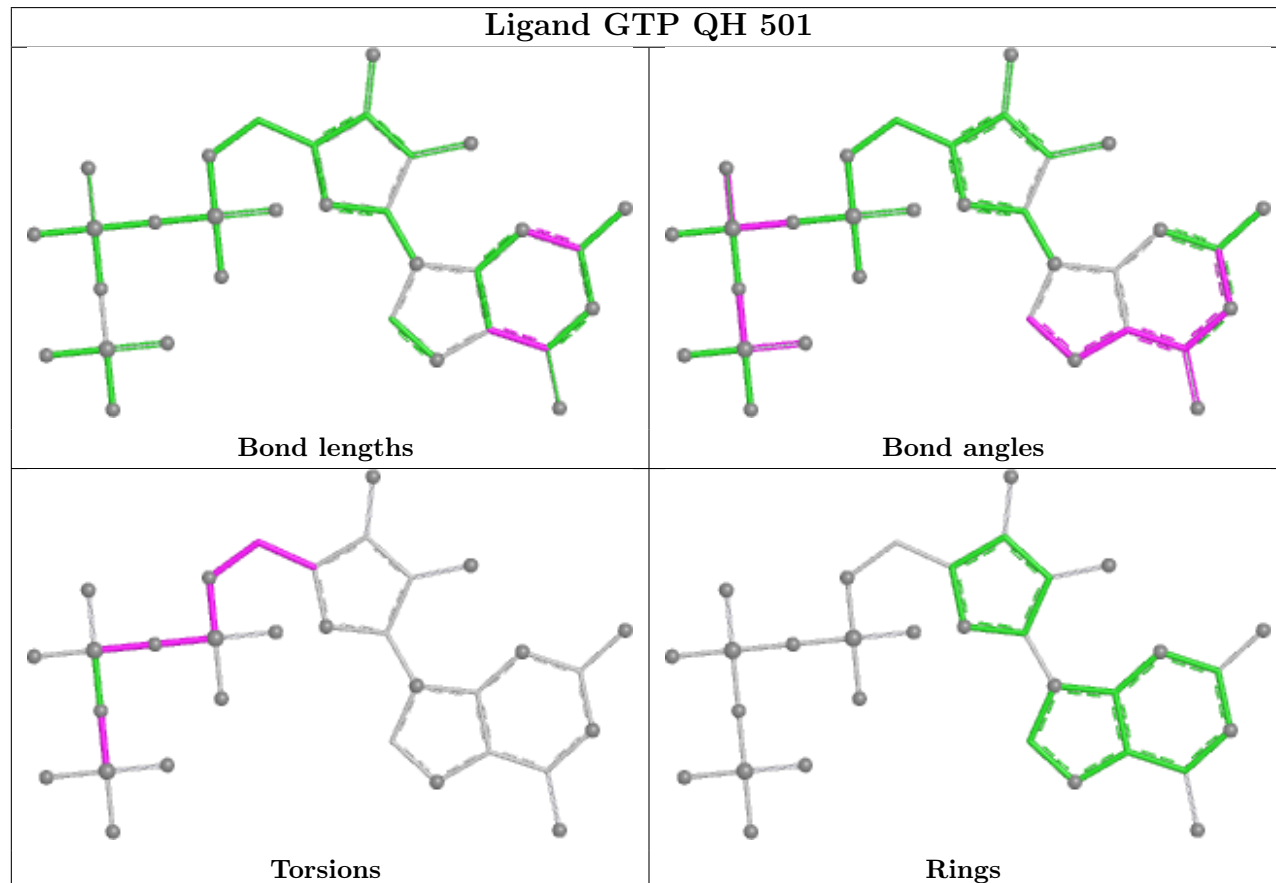


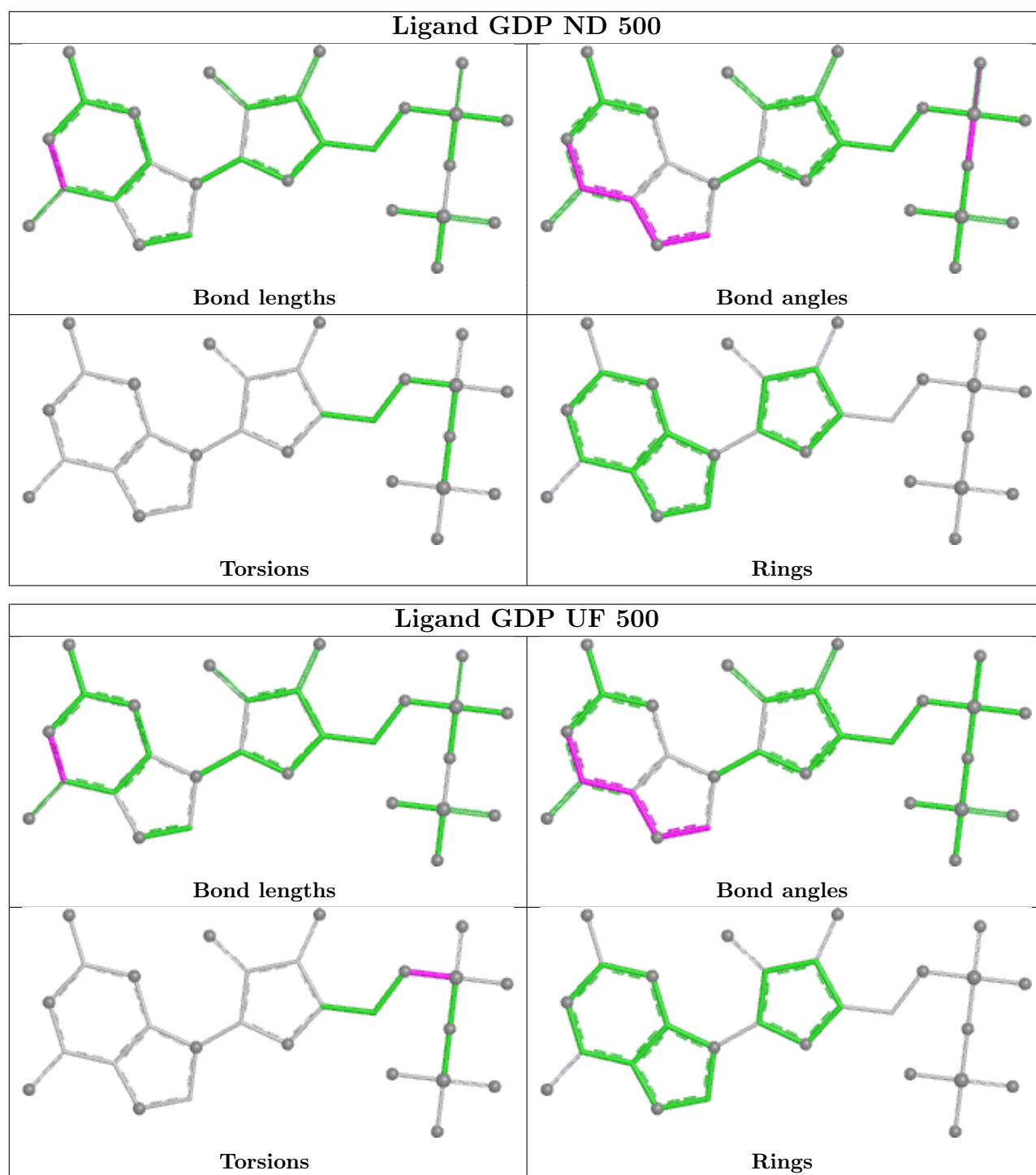


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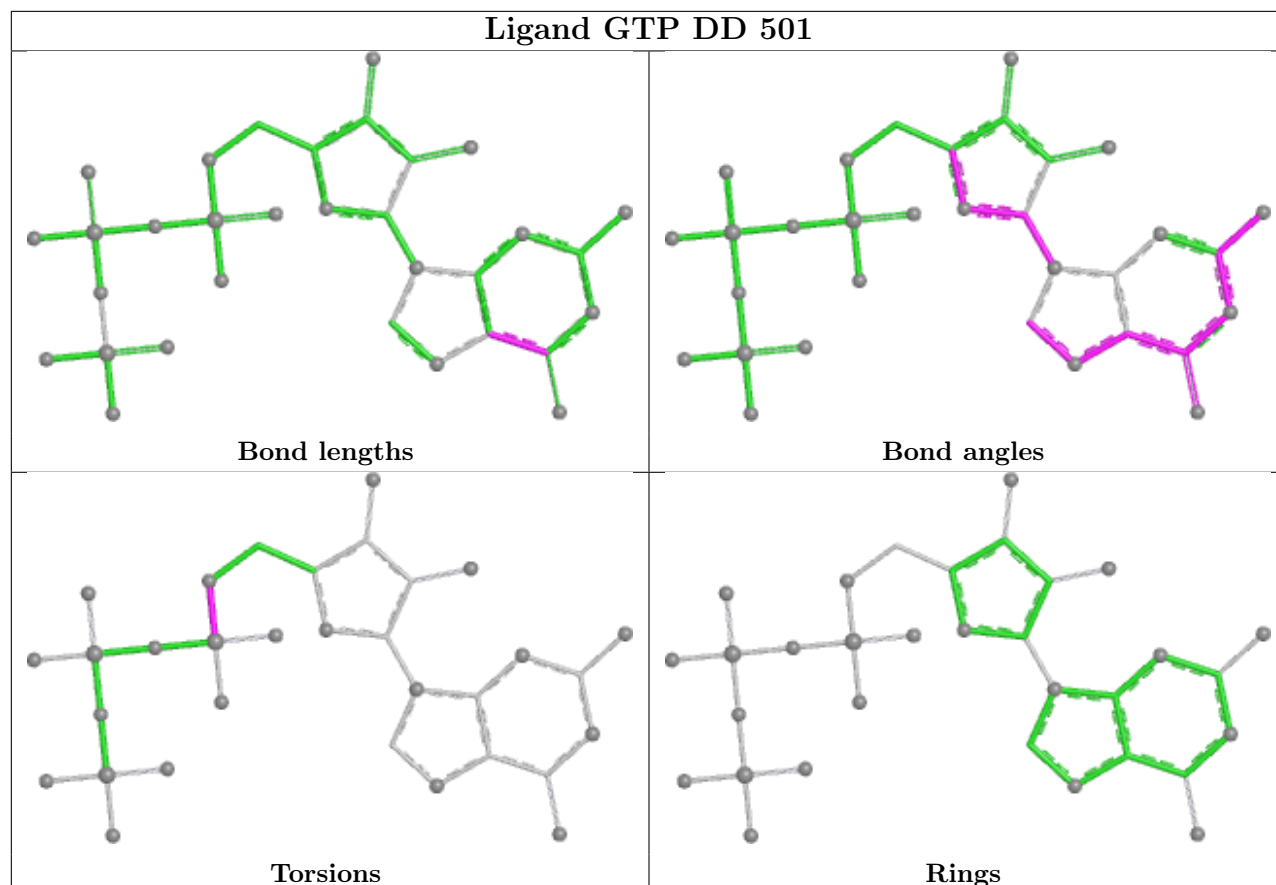


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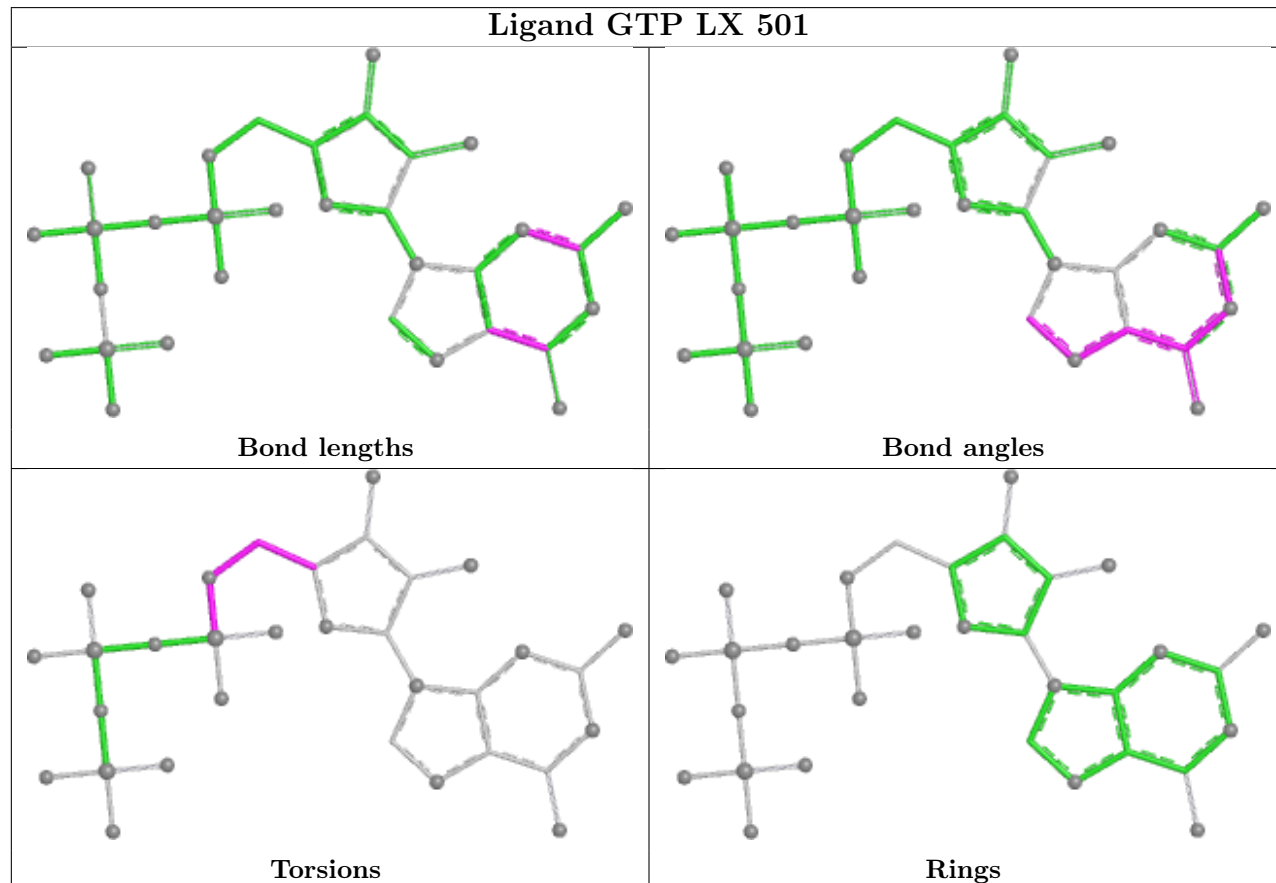


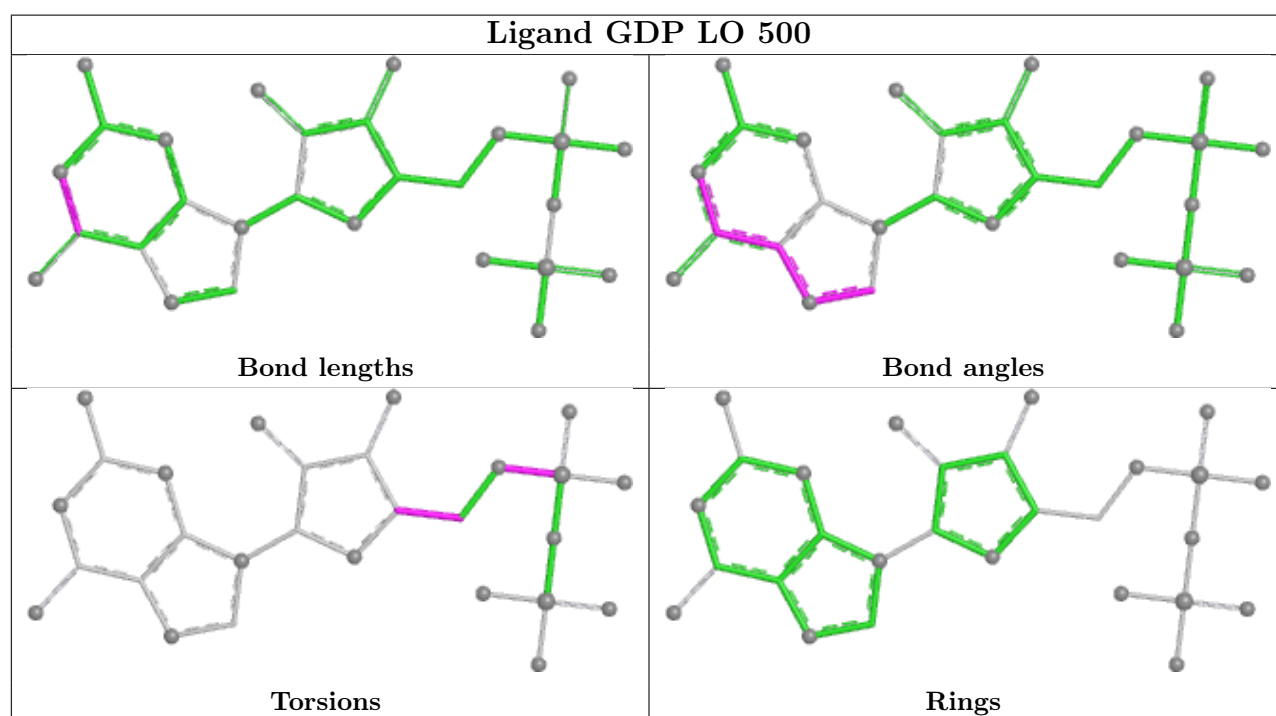
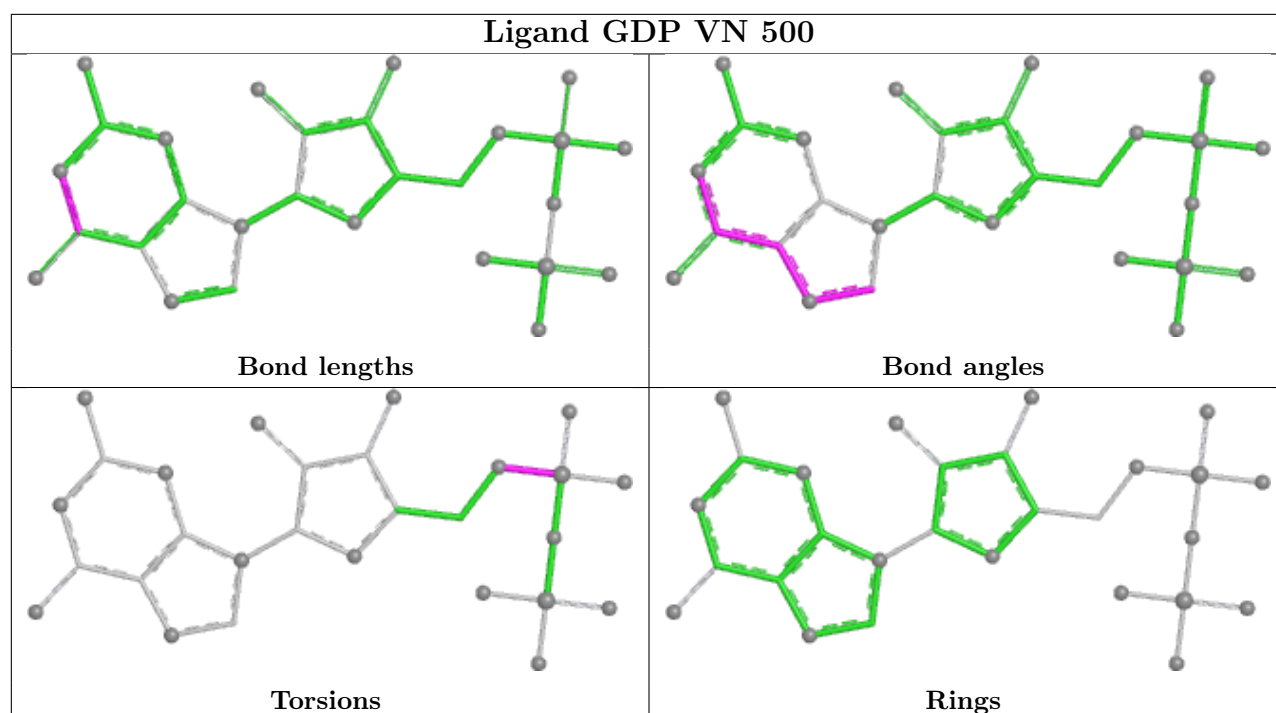


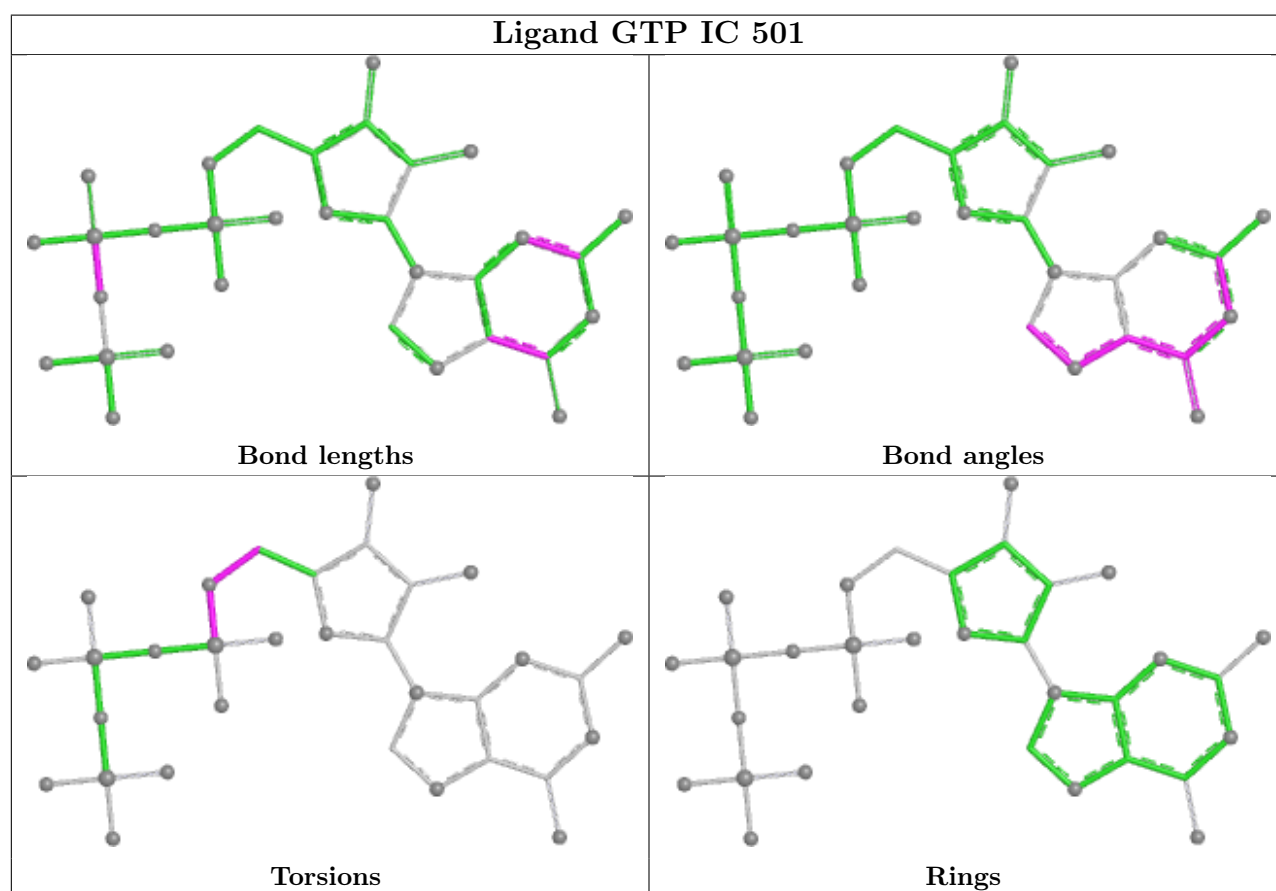
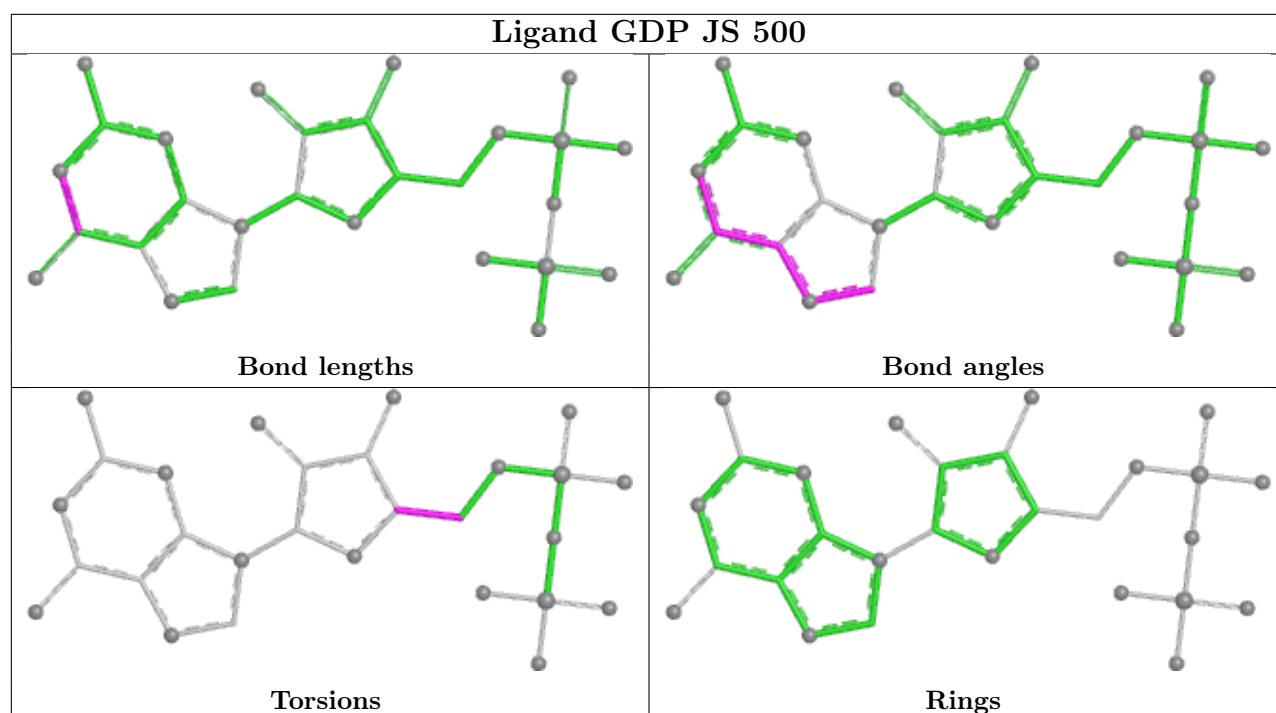
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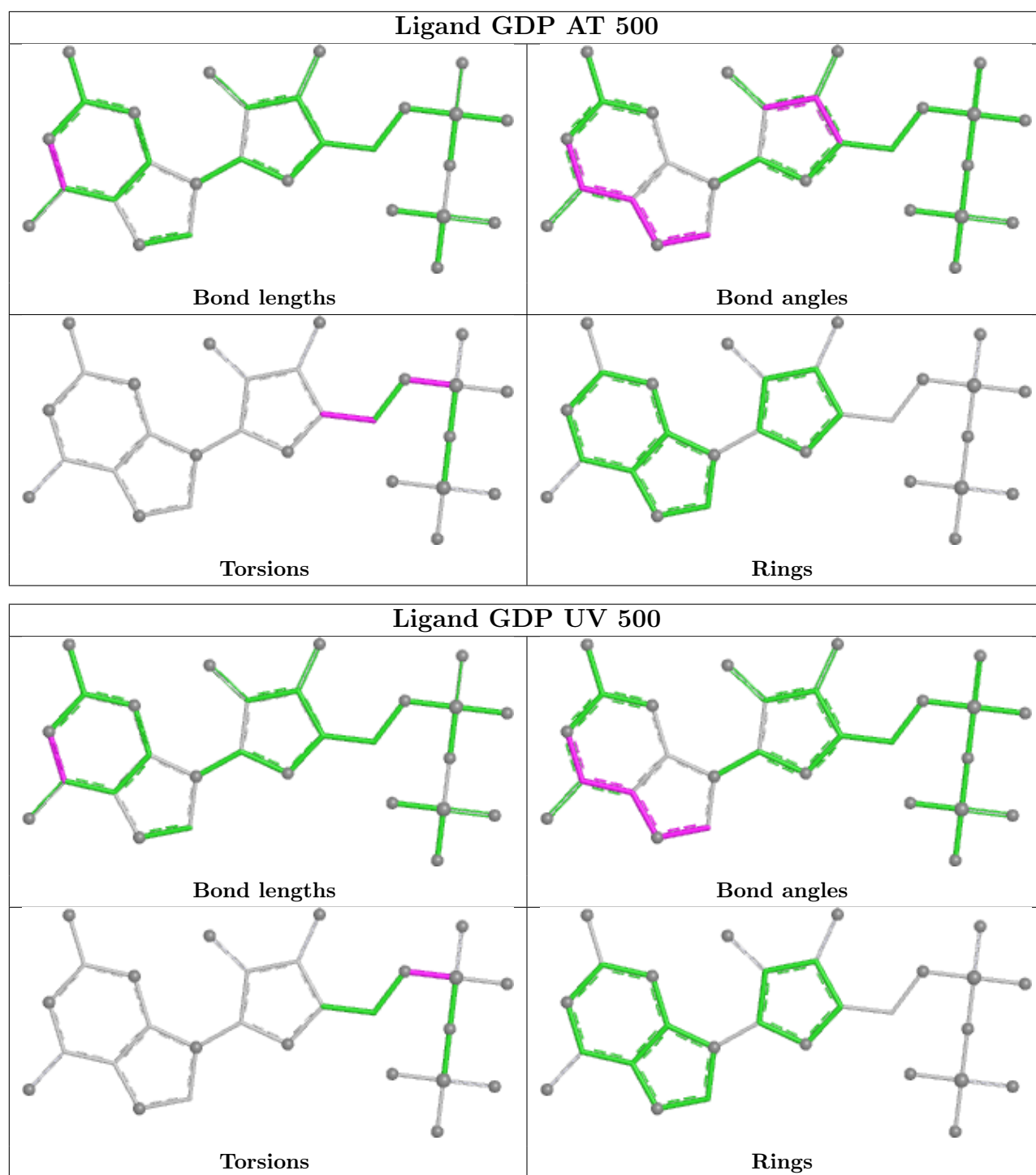


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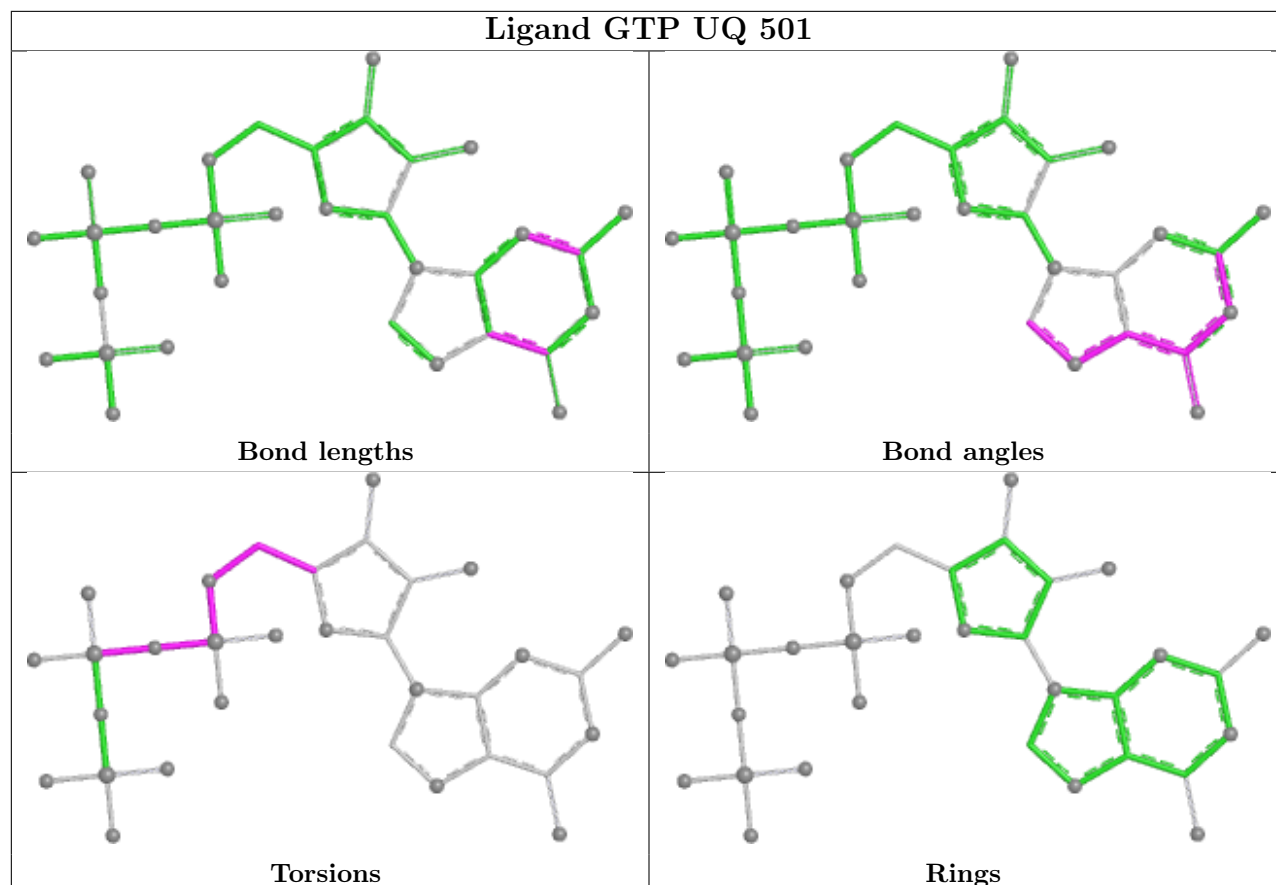




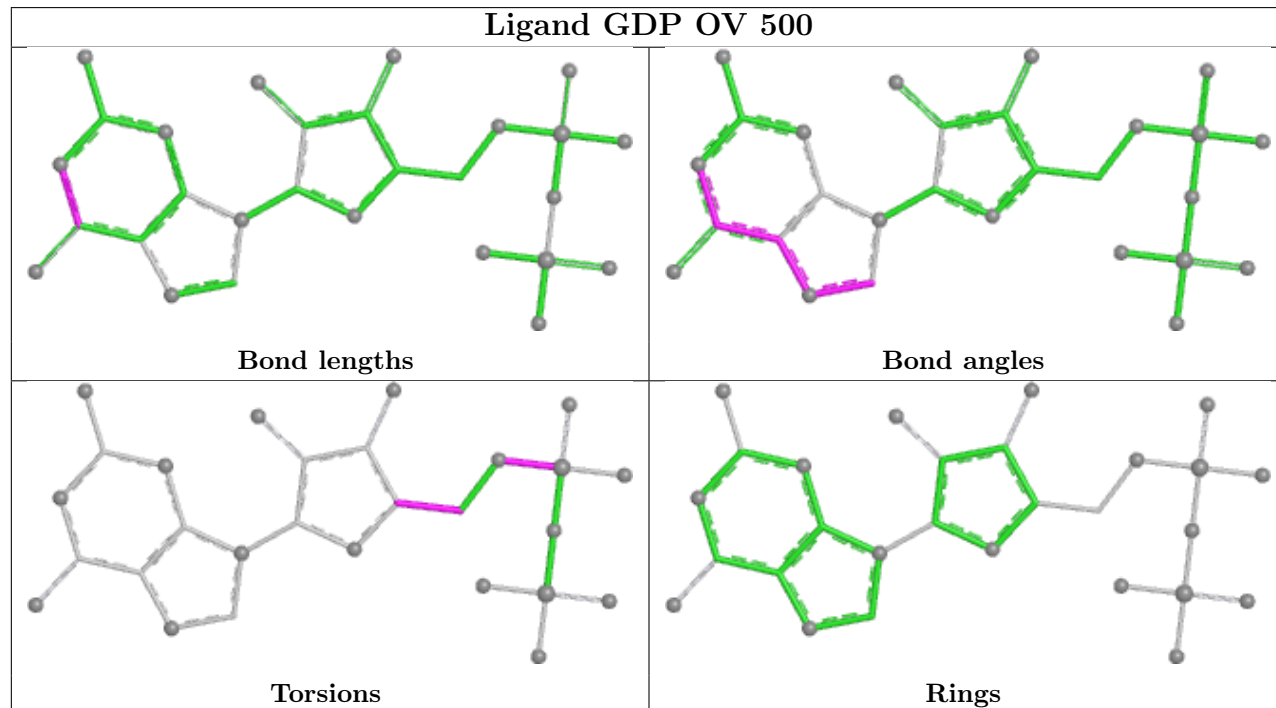


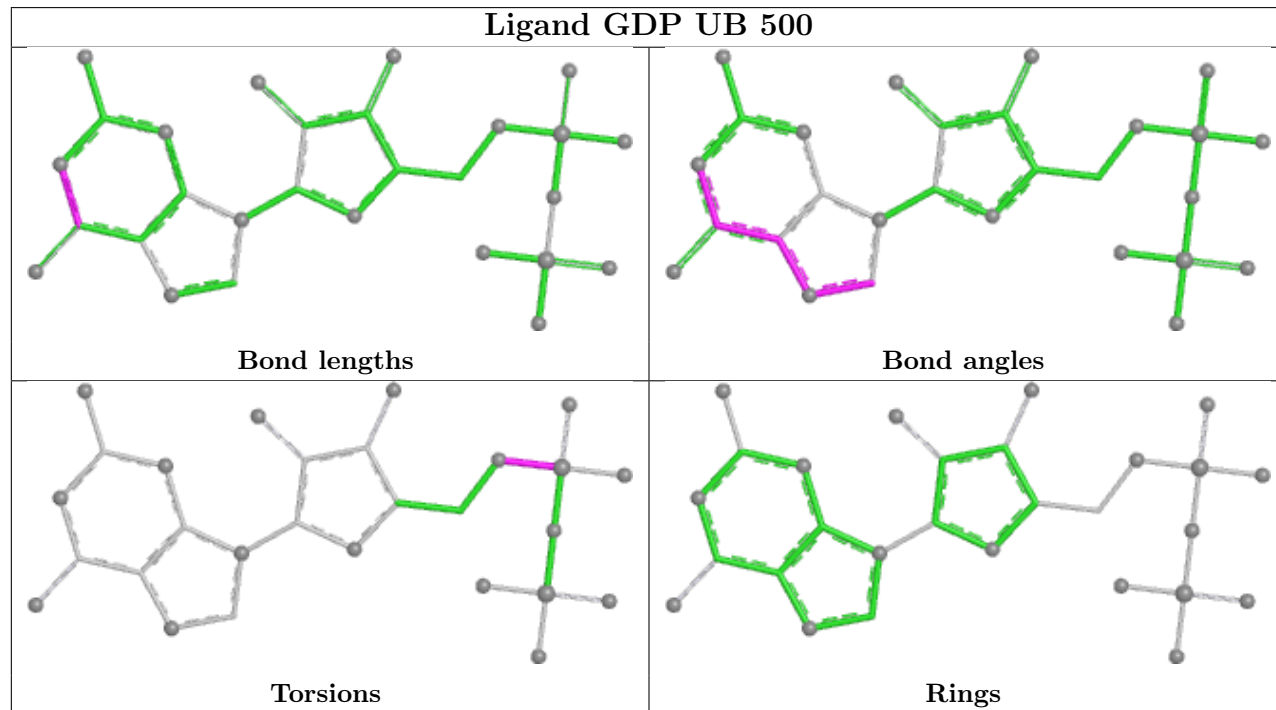
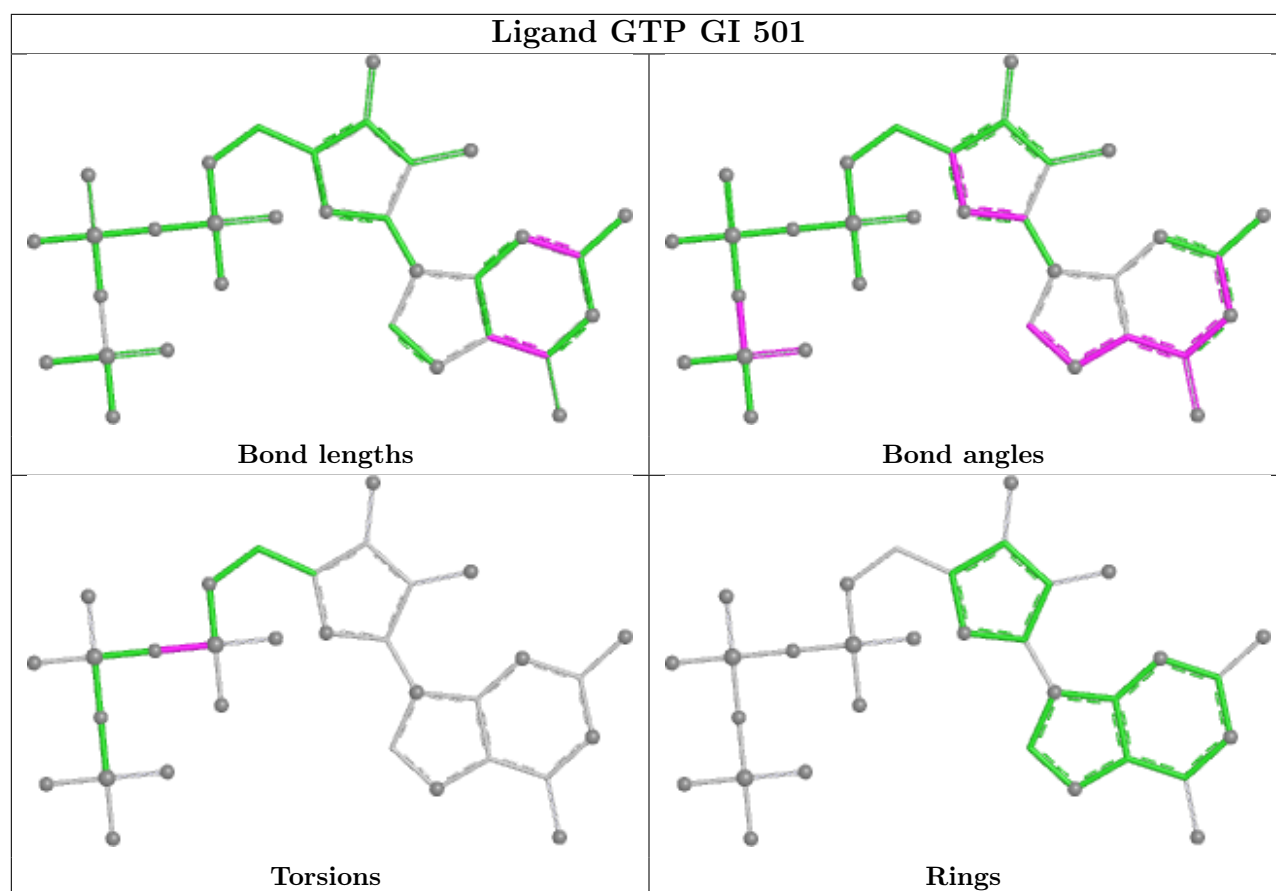


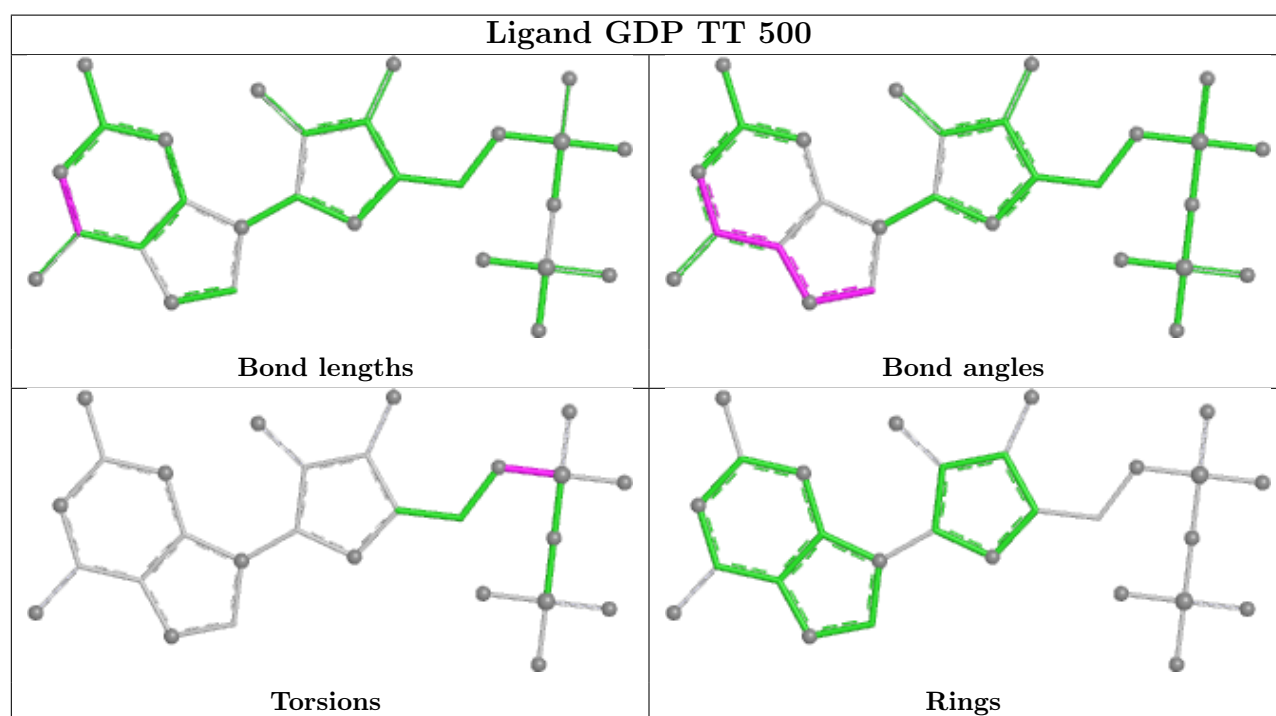
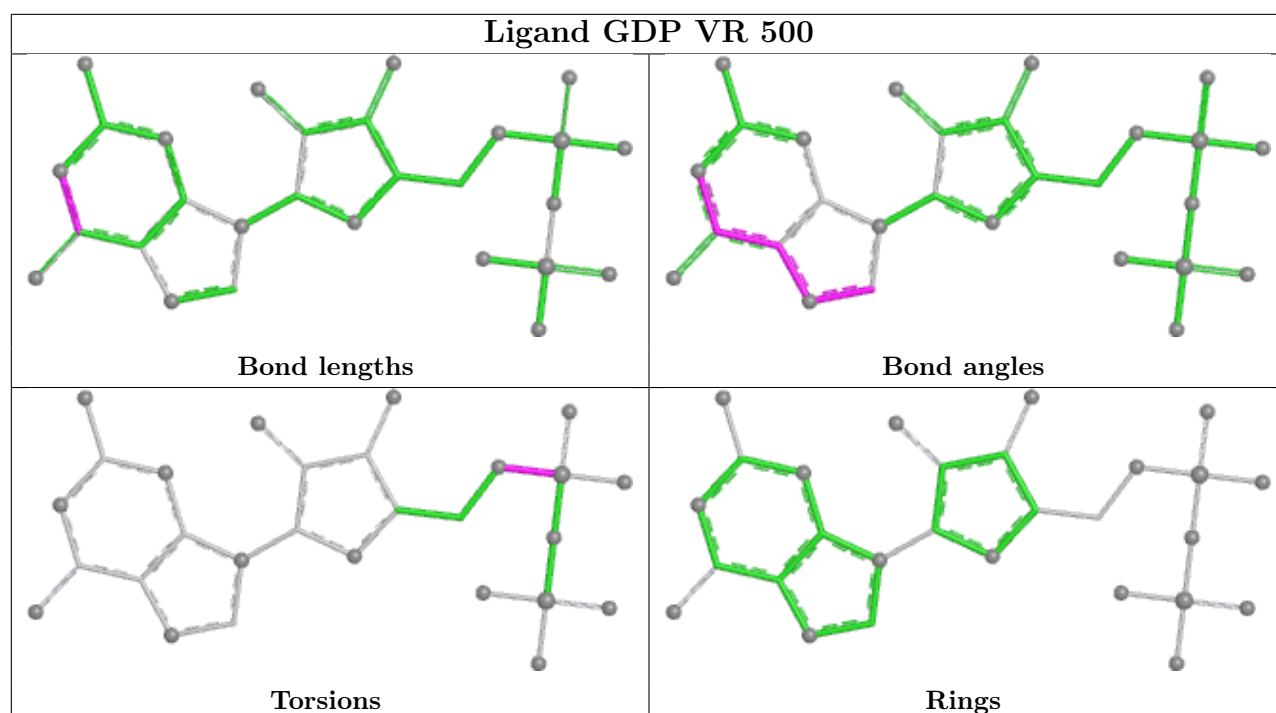
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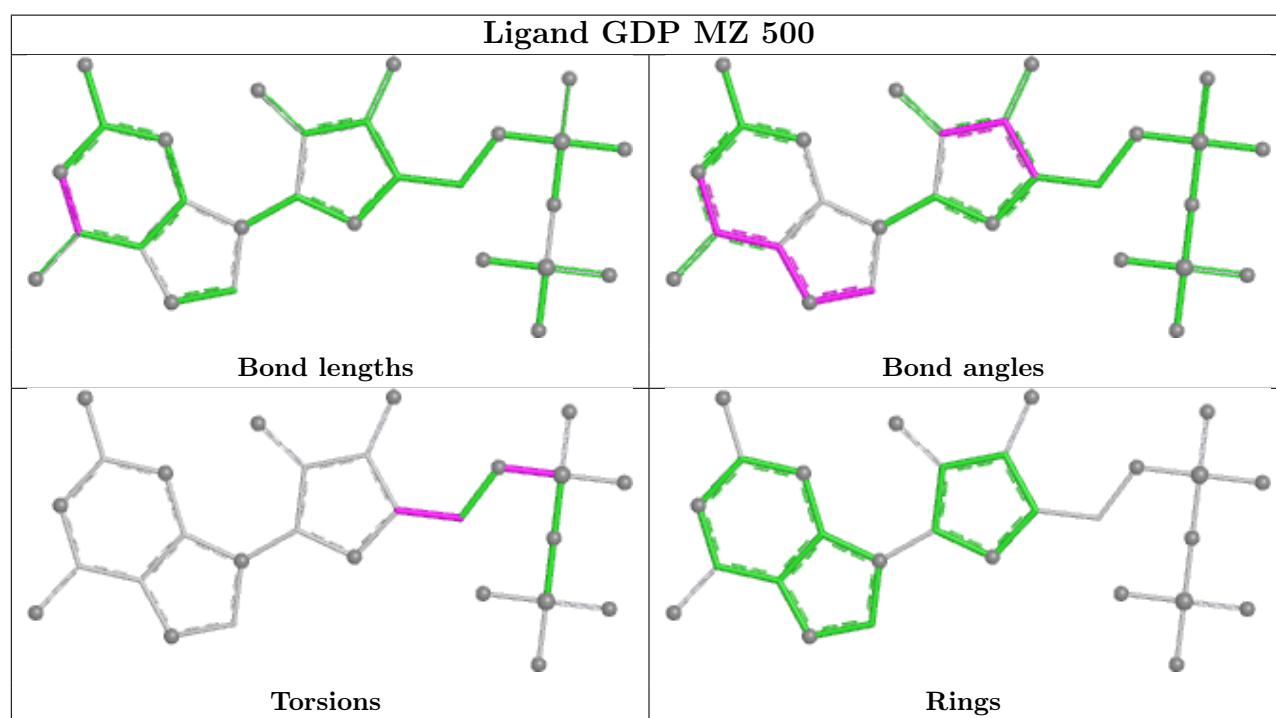
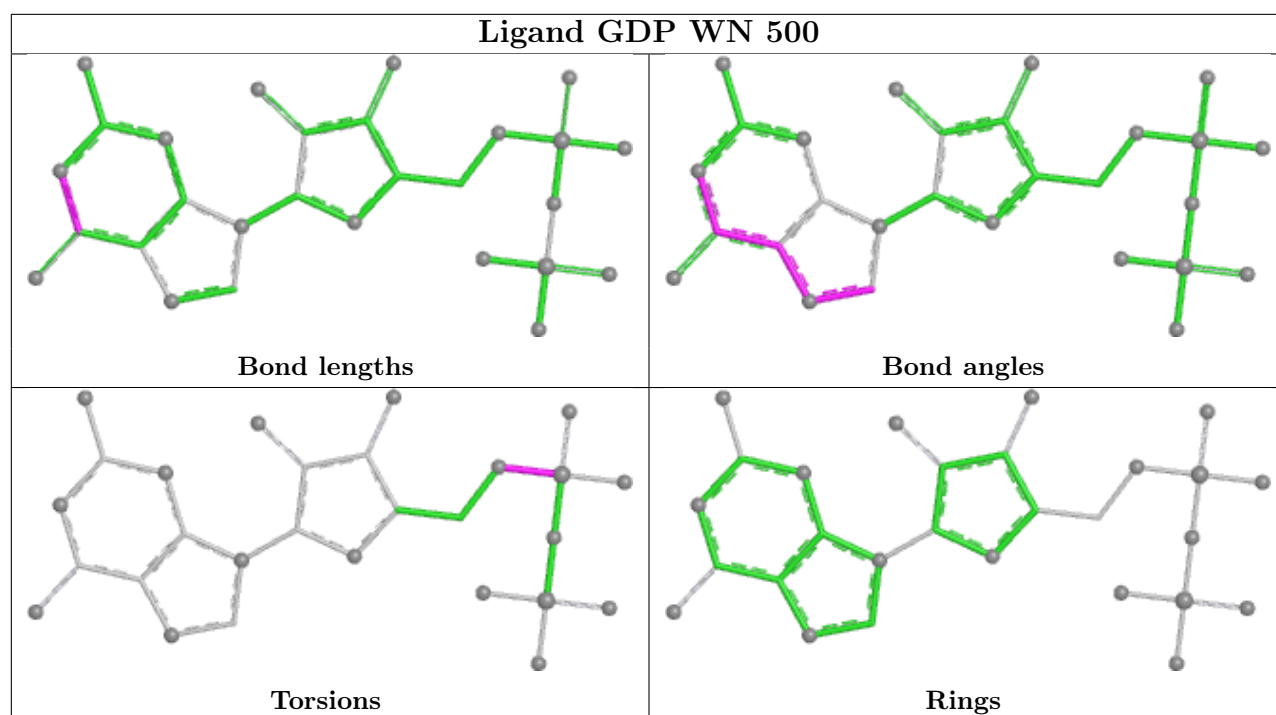


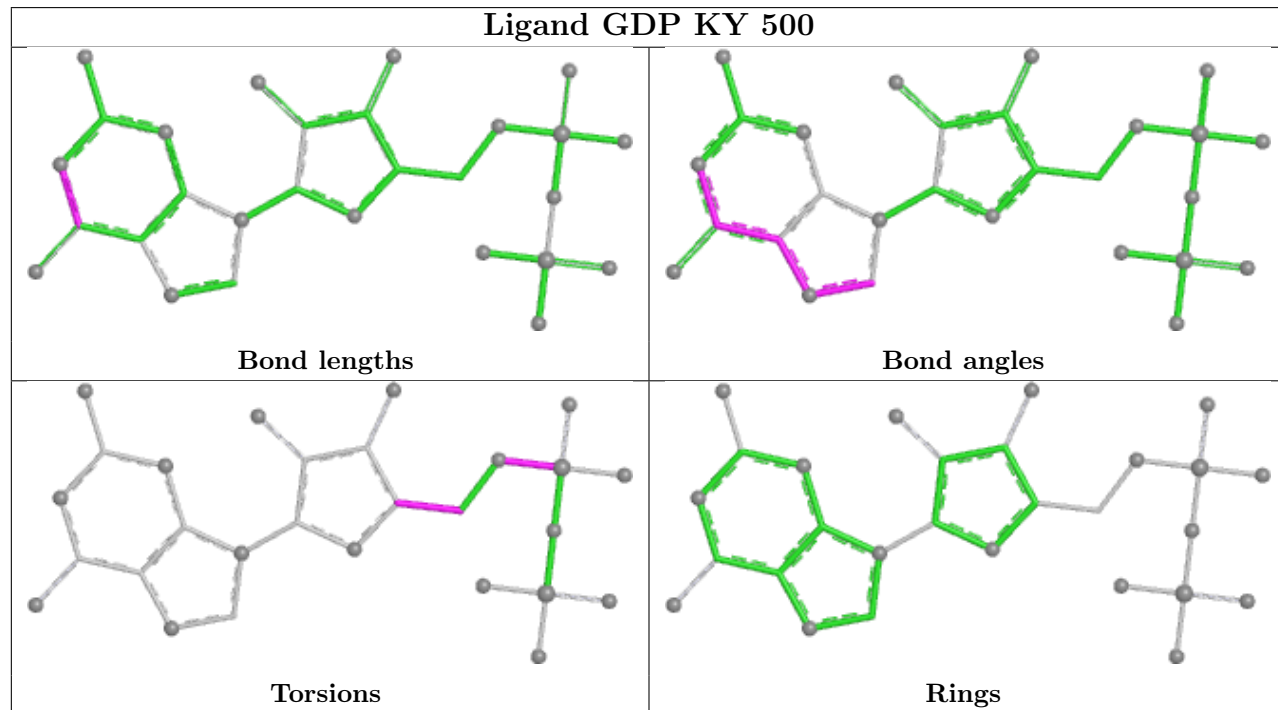
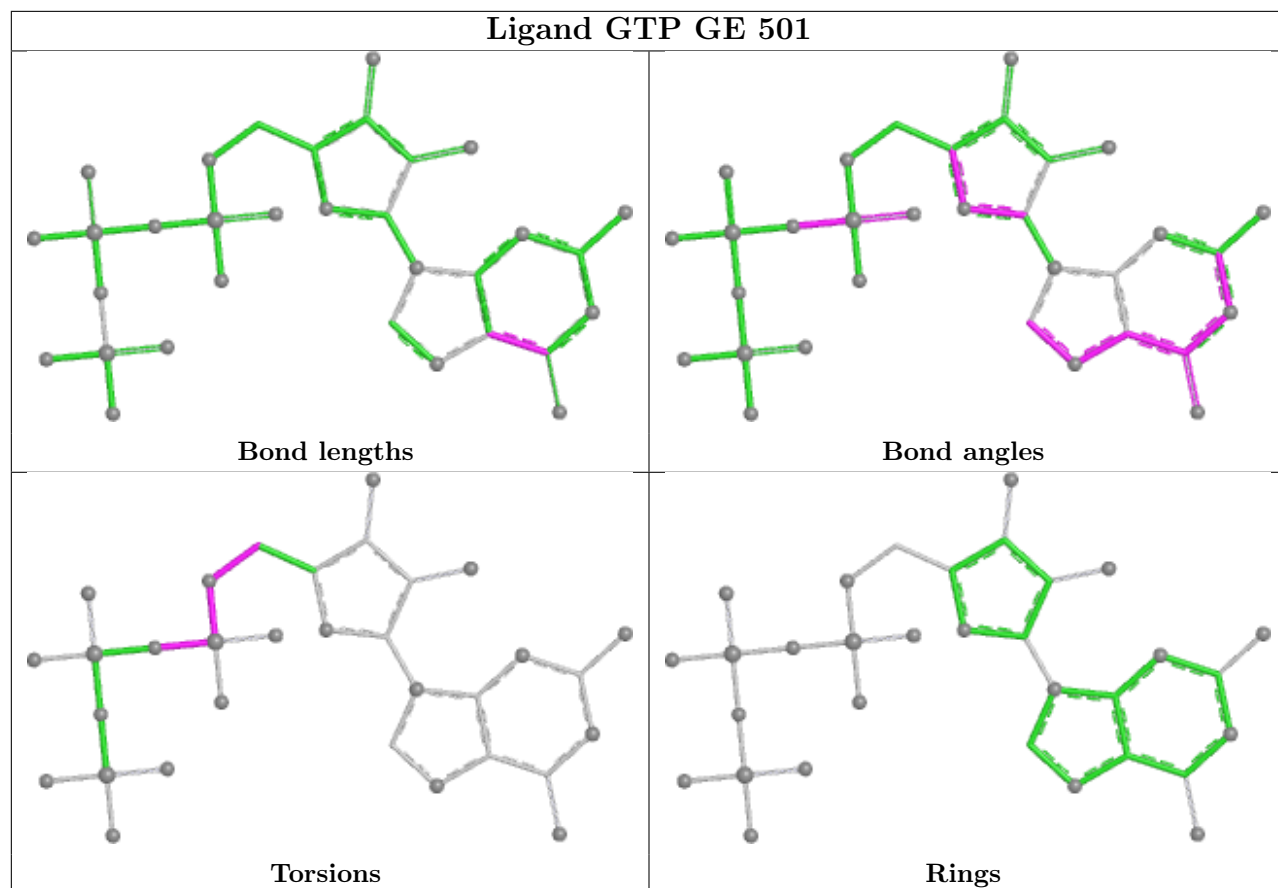
Ligand GDP OV 500

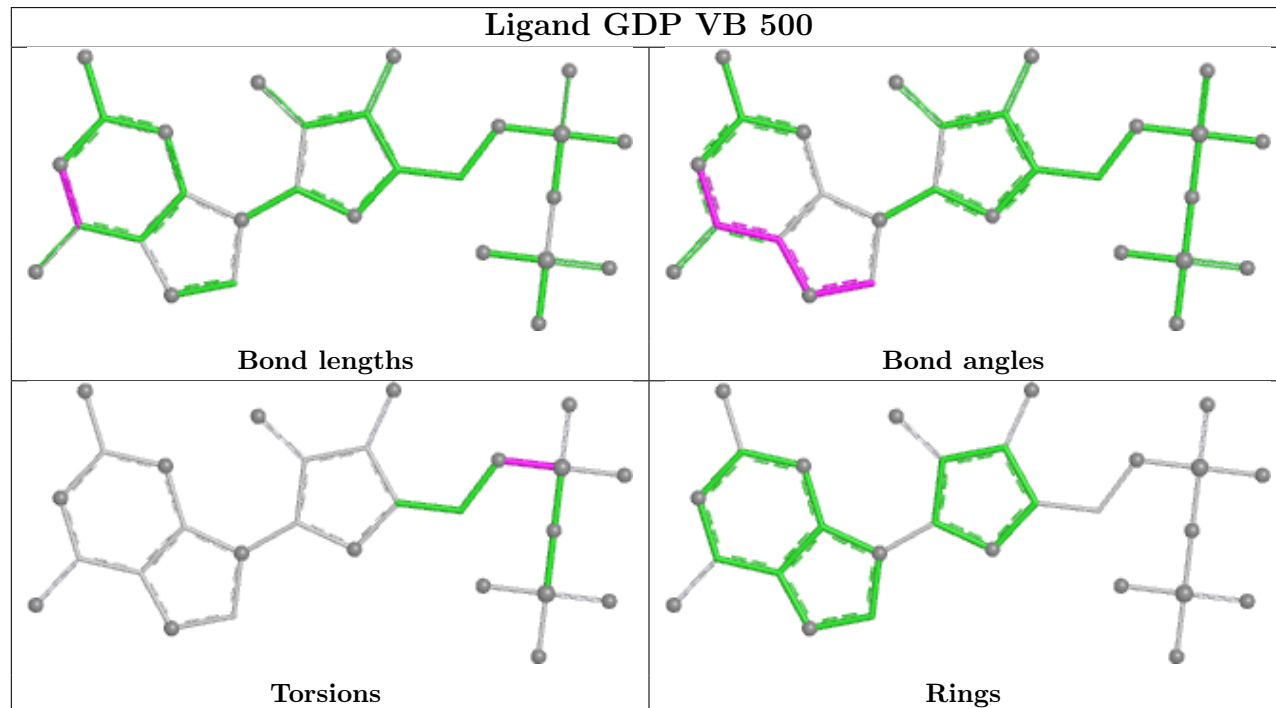
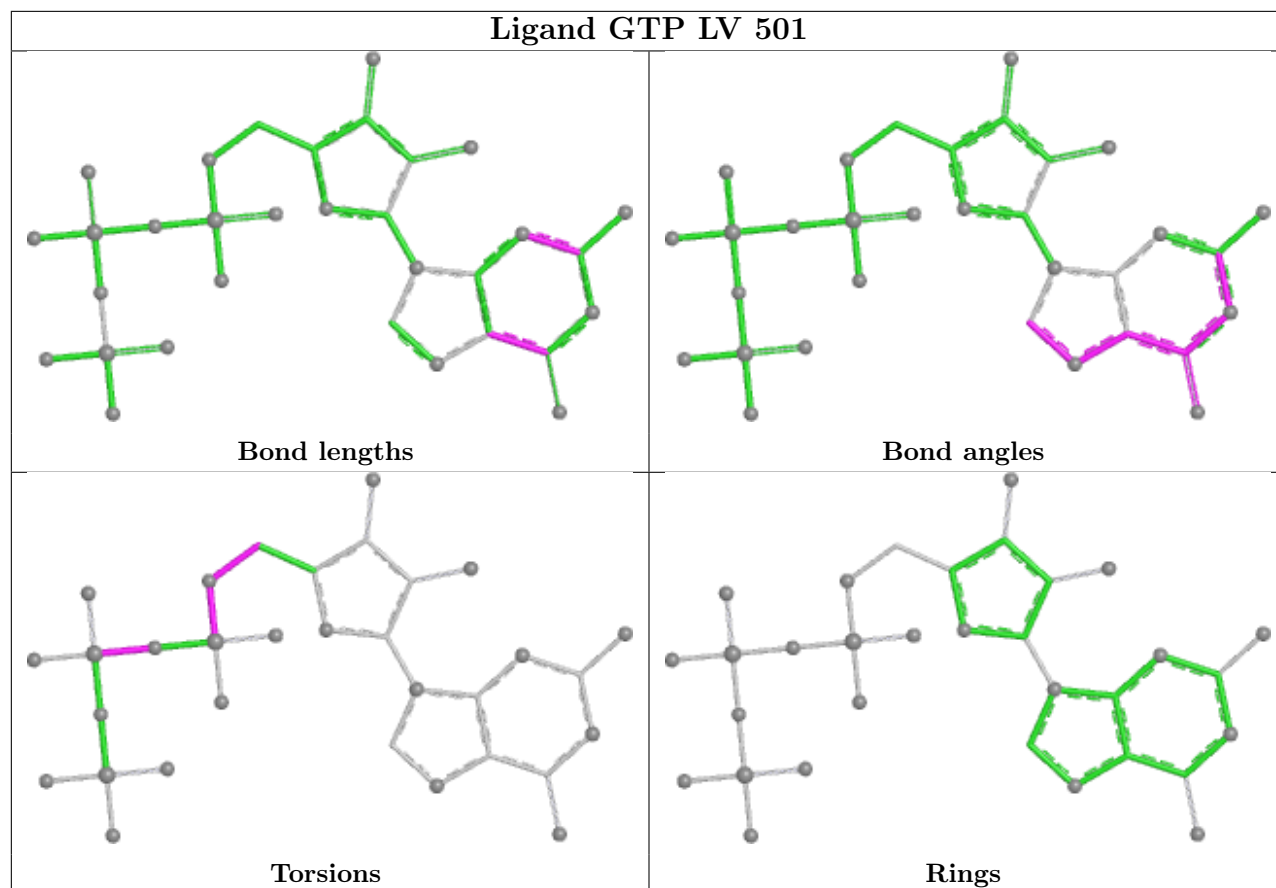




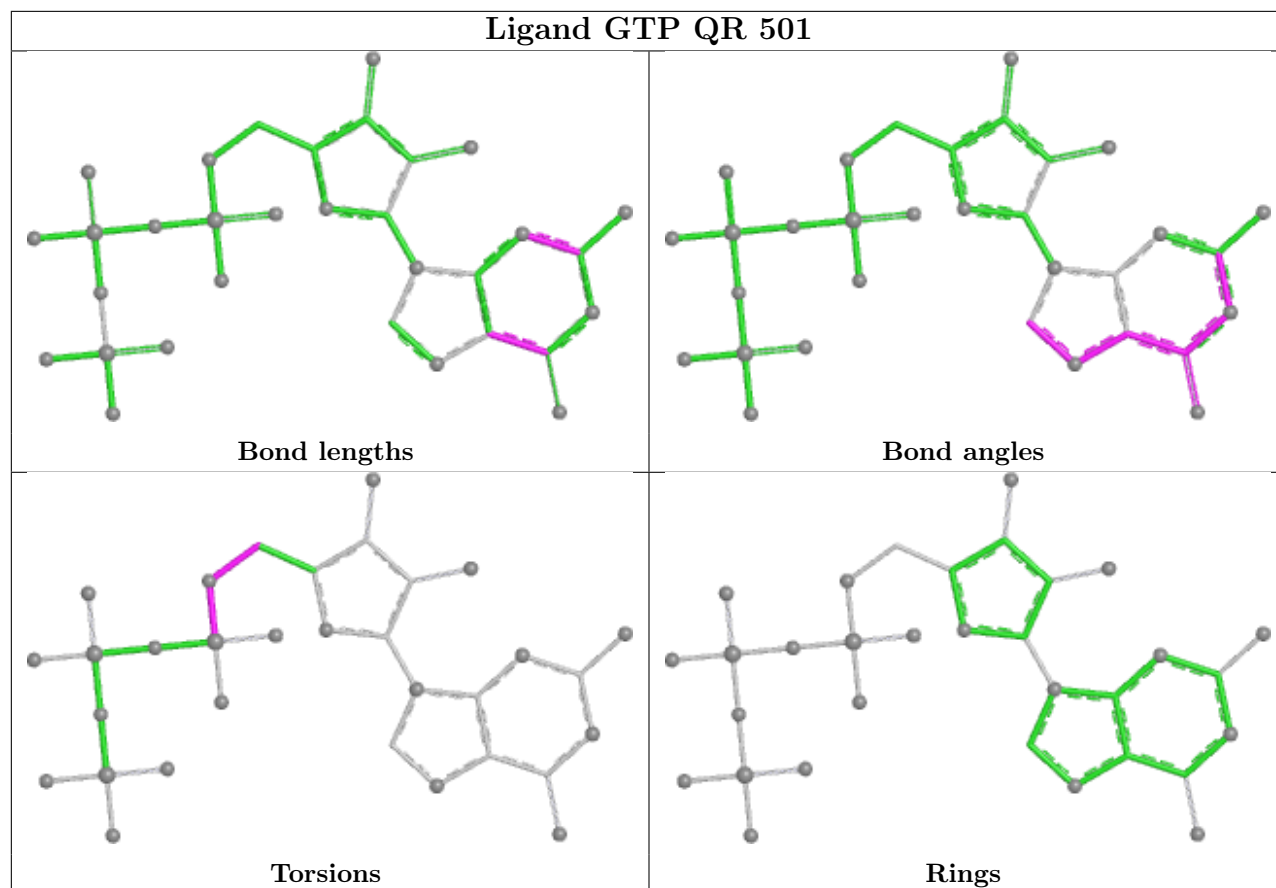




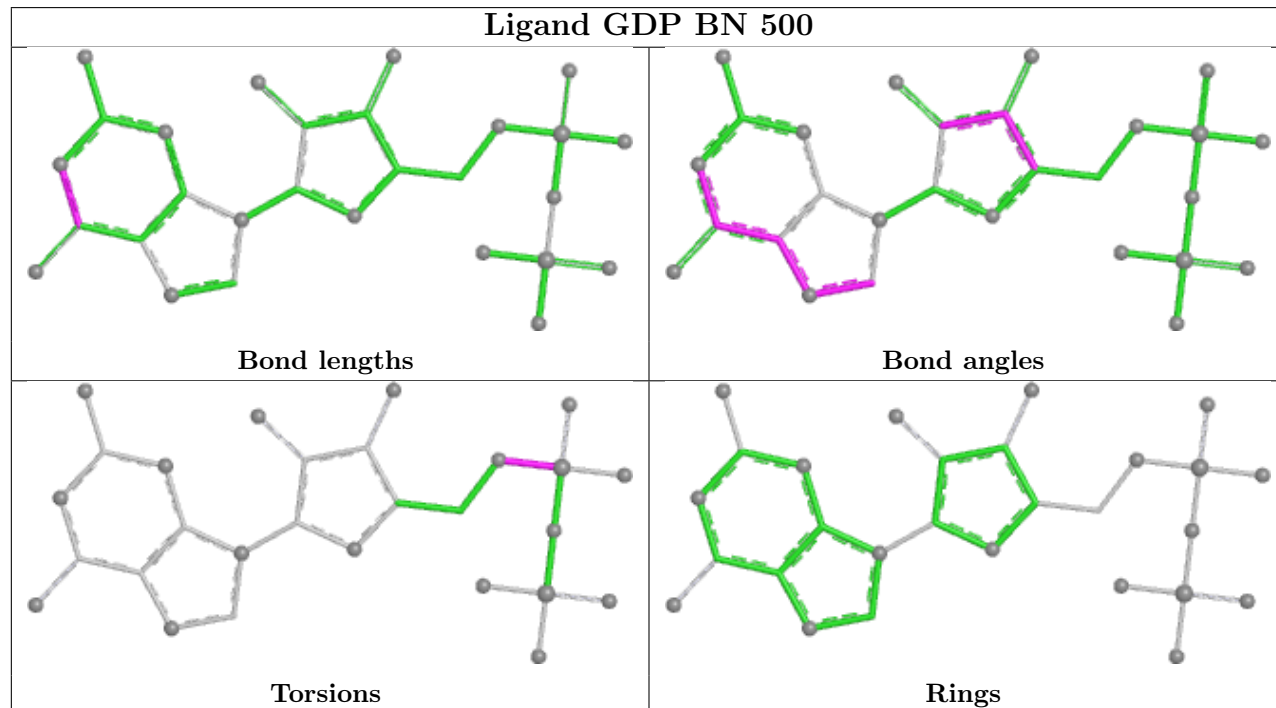


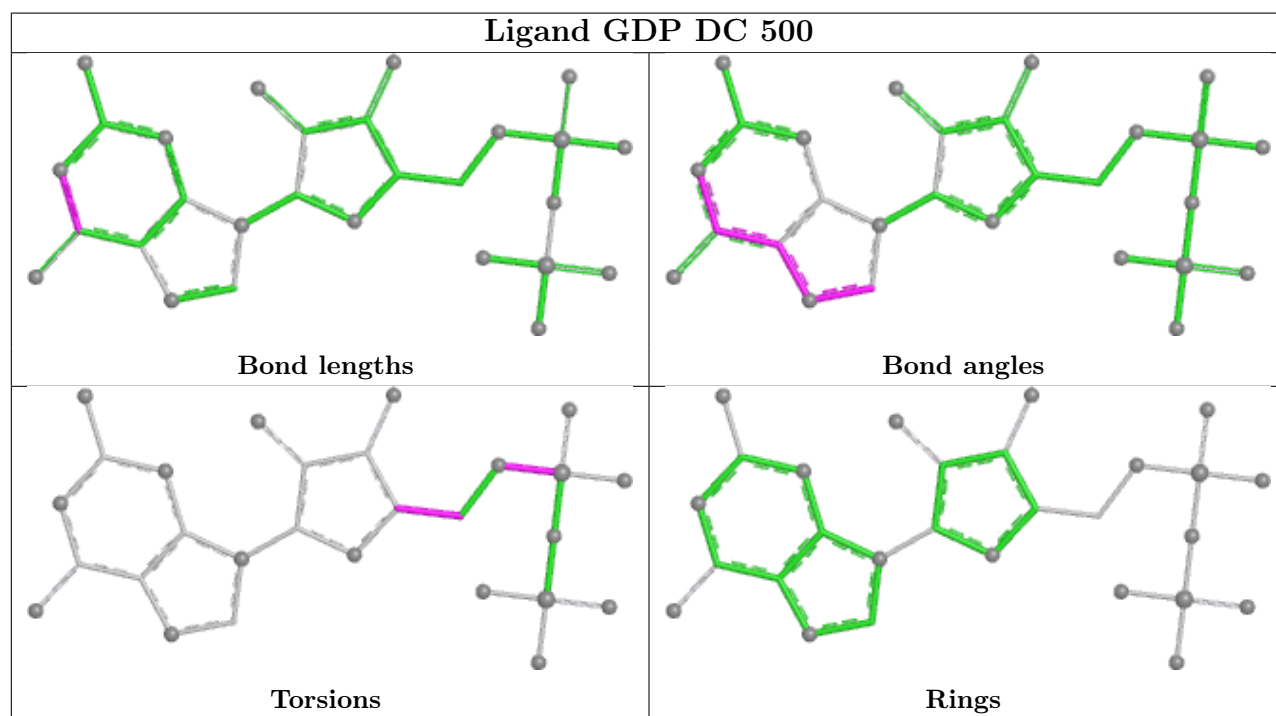
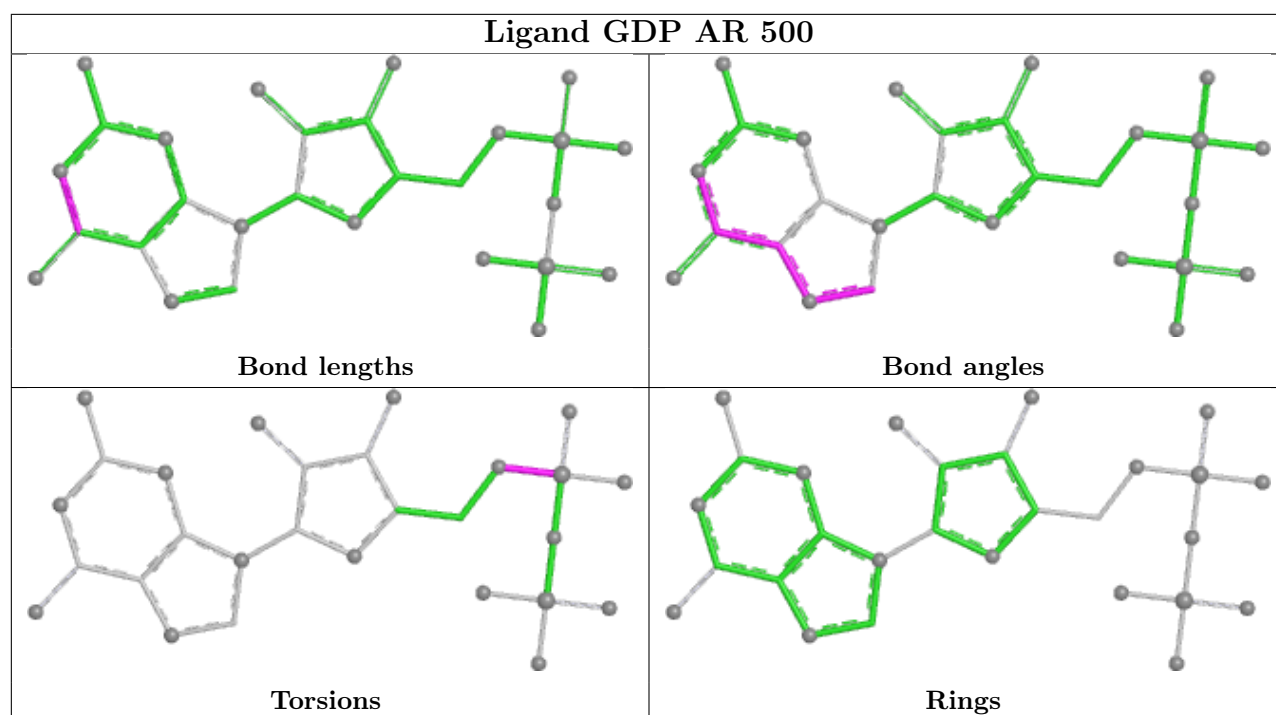


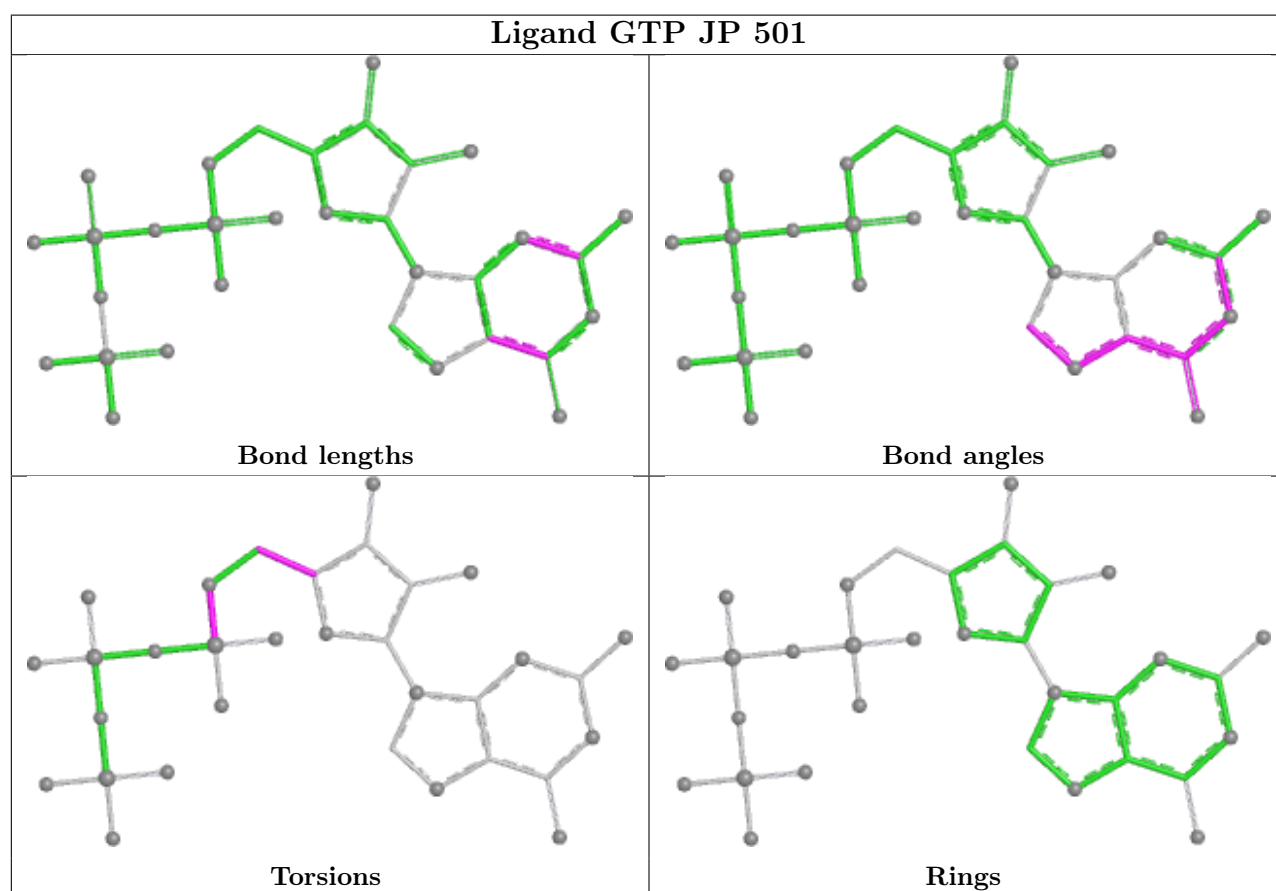
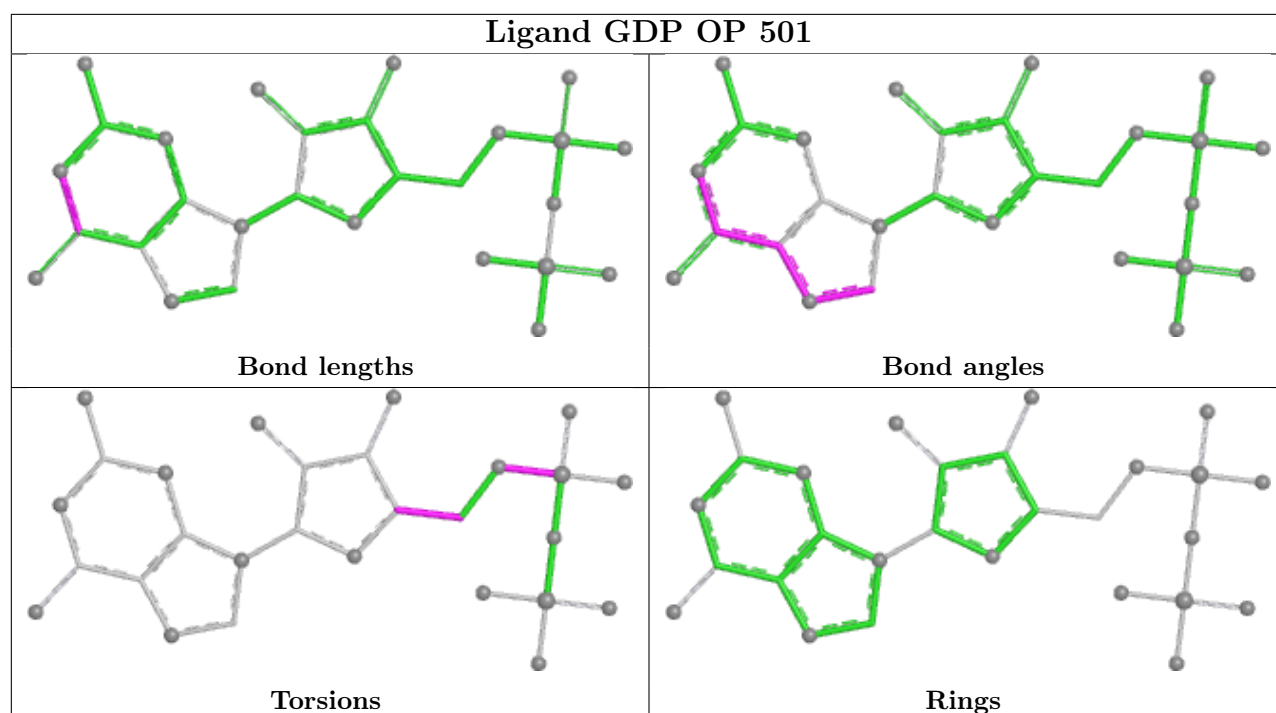
Ligand GTP QR 501



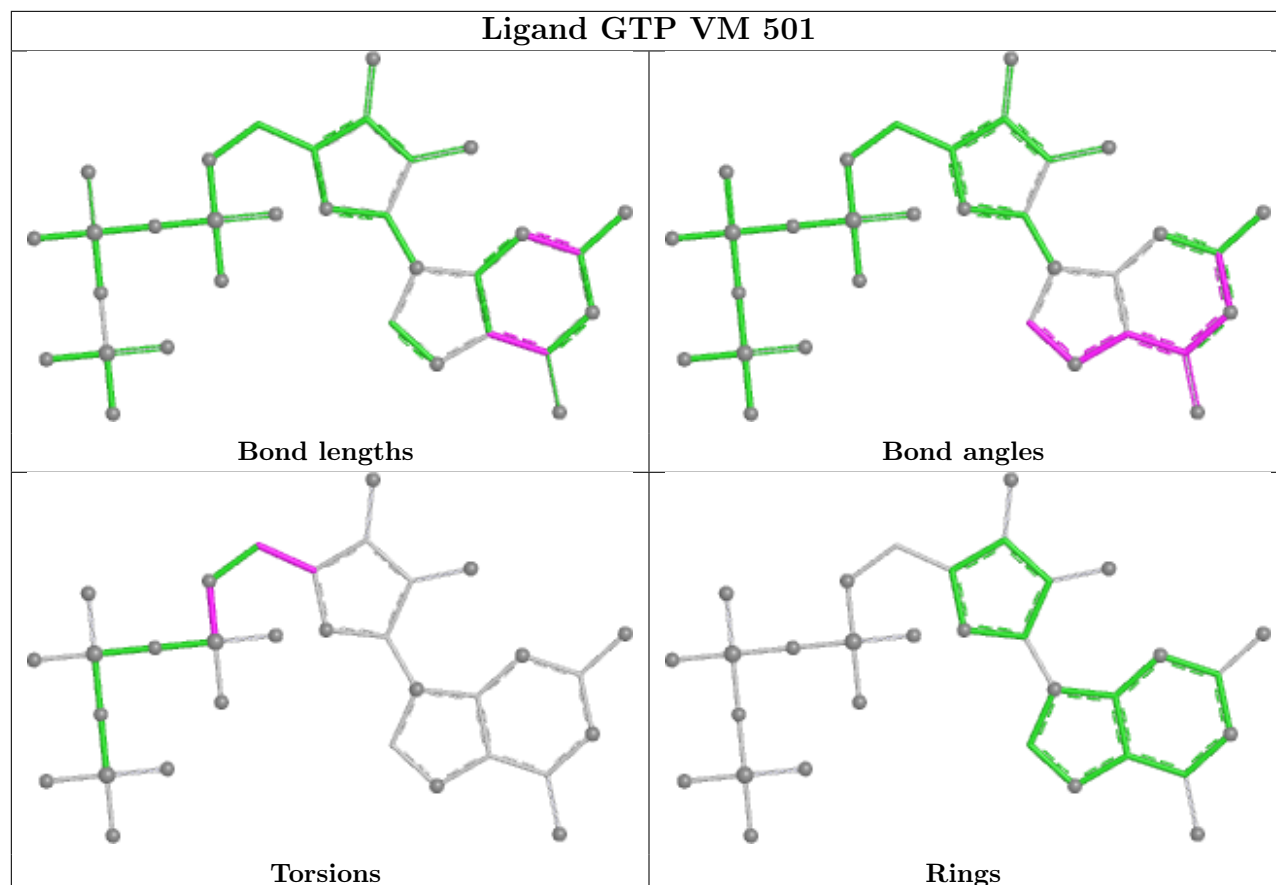
Ligand GDP BN 500



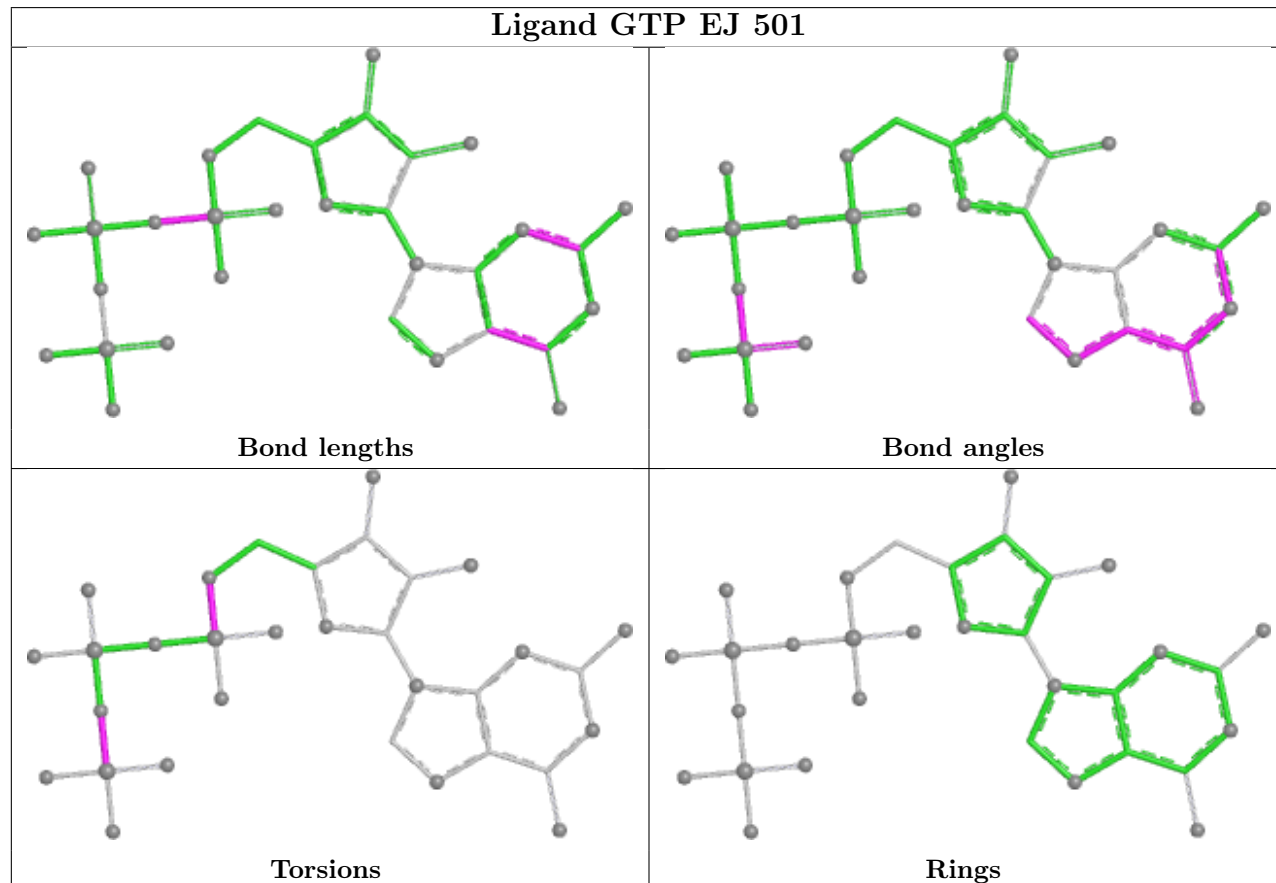


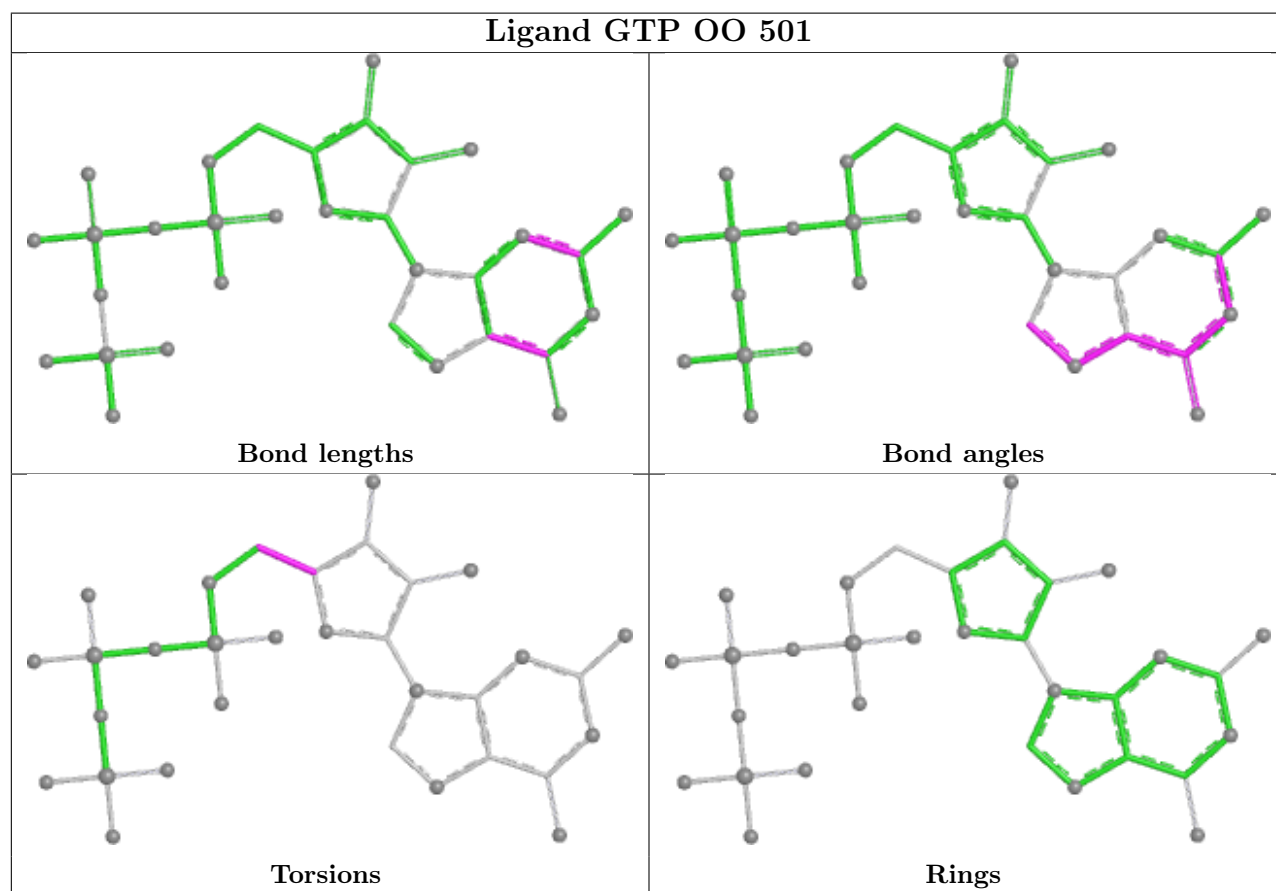
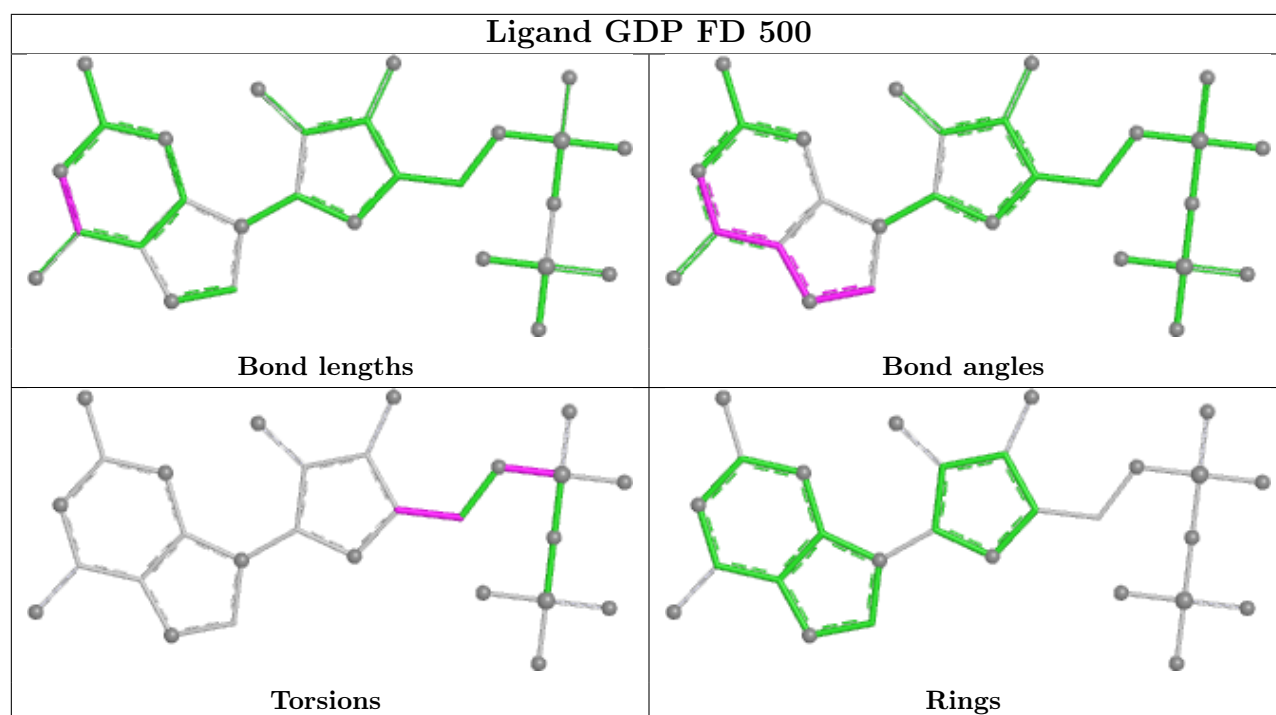


Ligand GTP VM 501

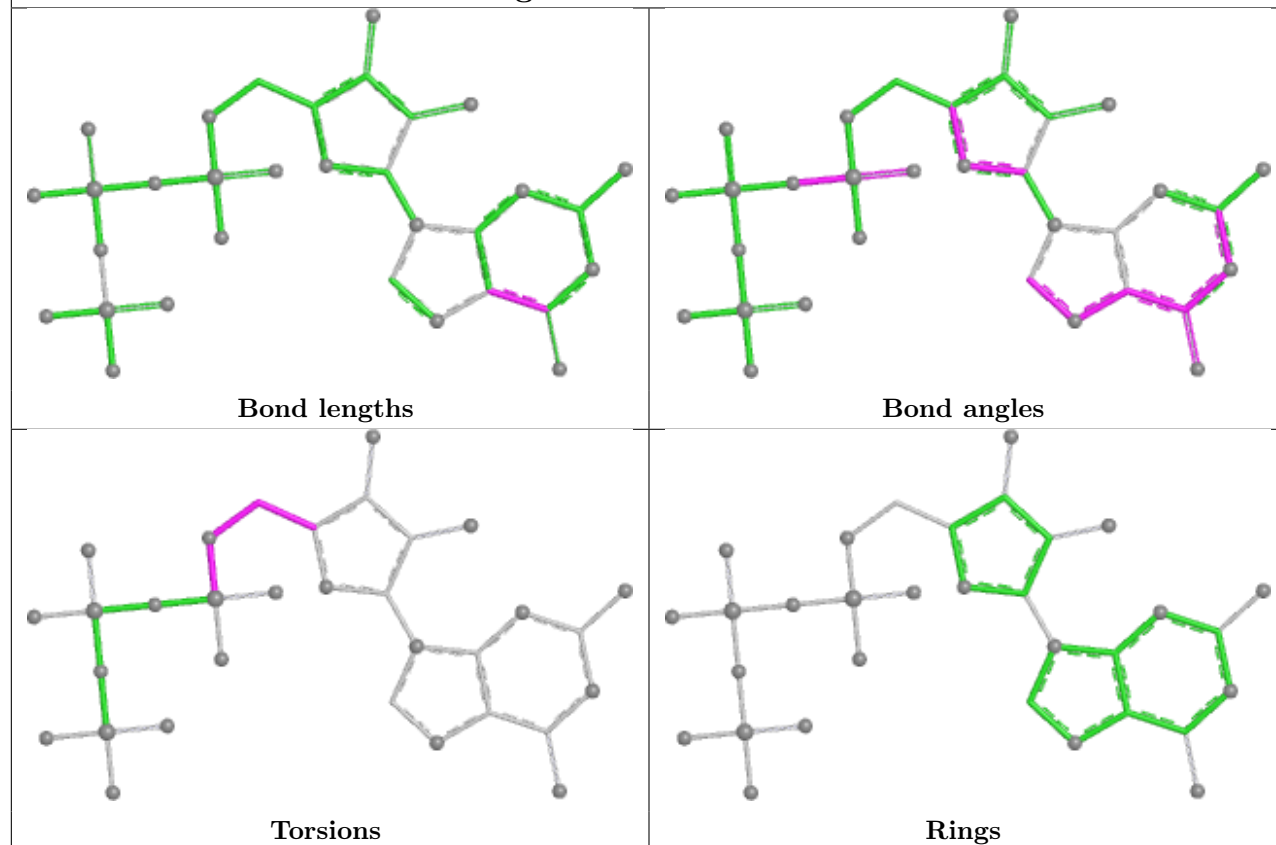


Ligand GTP EJ 501

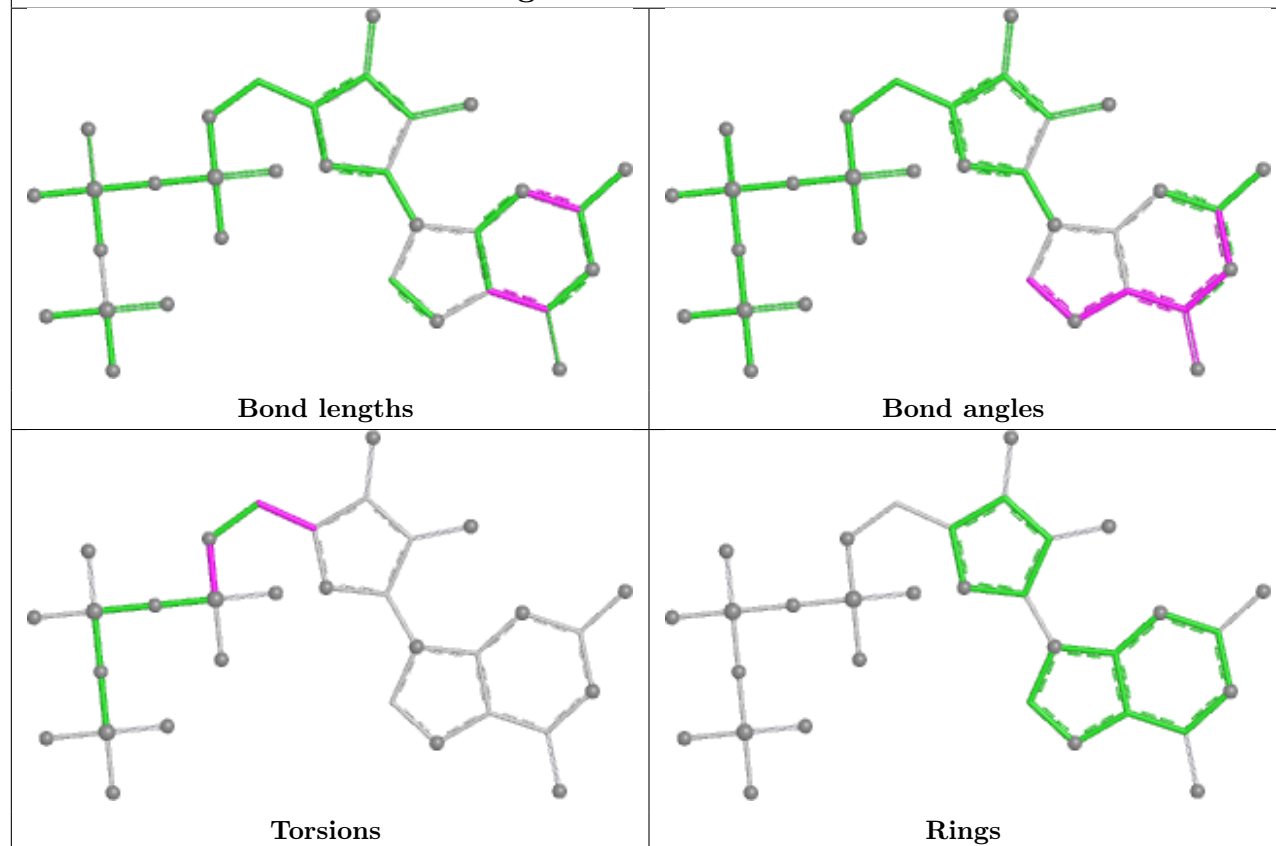




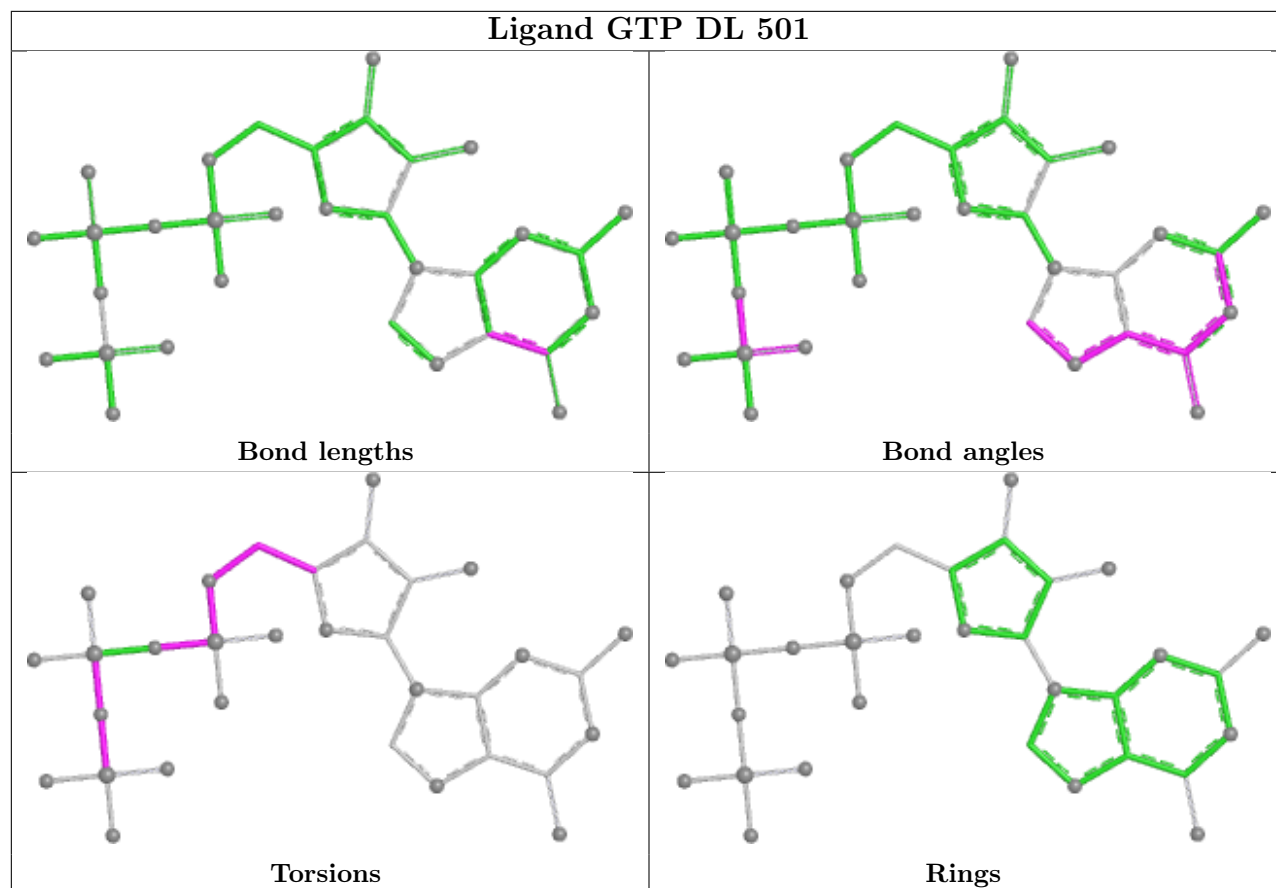
Ligand GTP GG 501



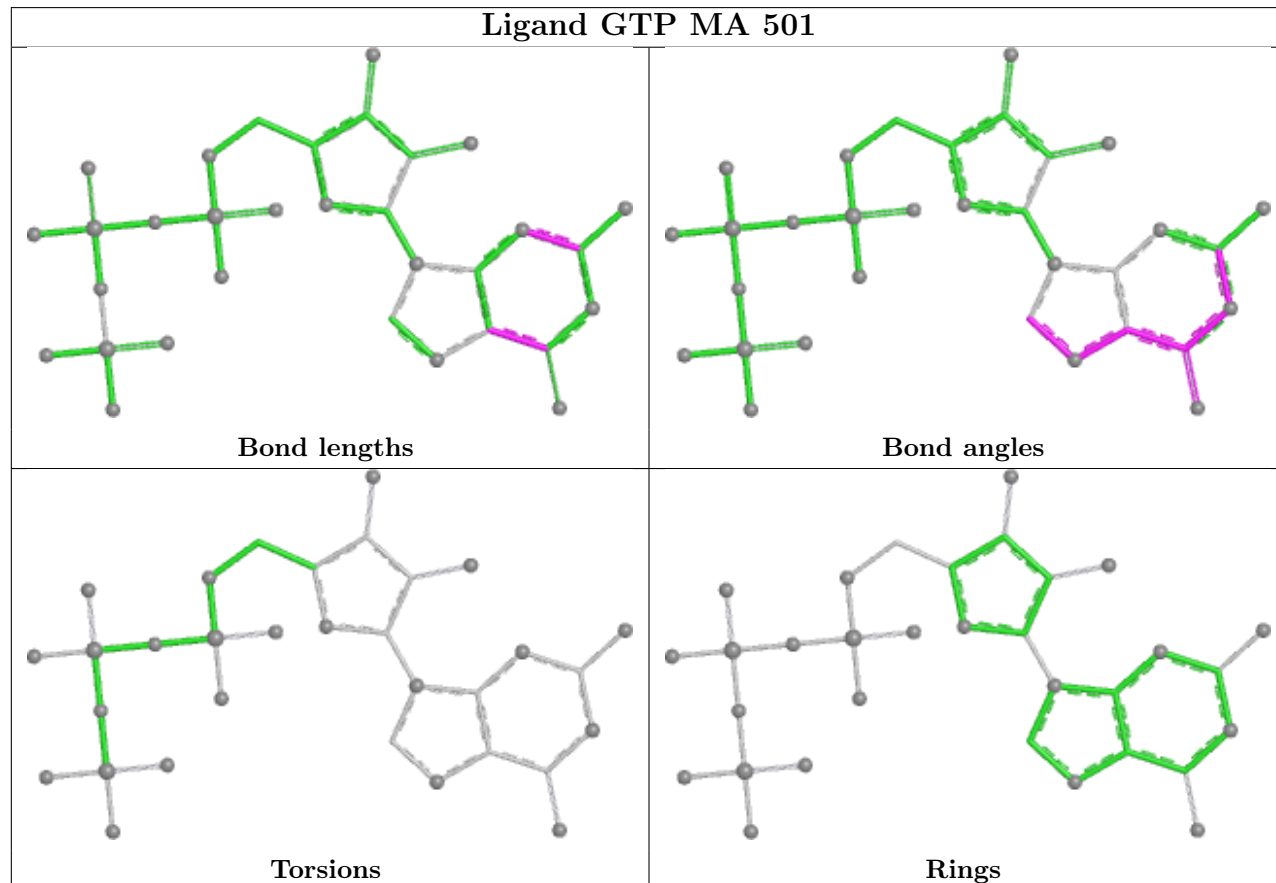
Ligand GTP PU 501

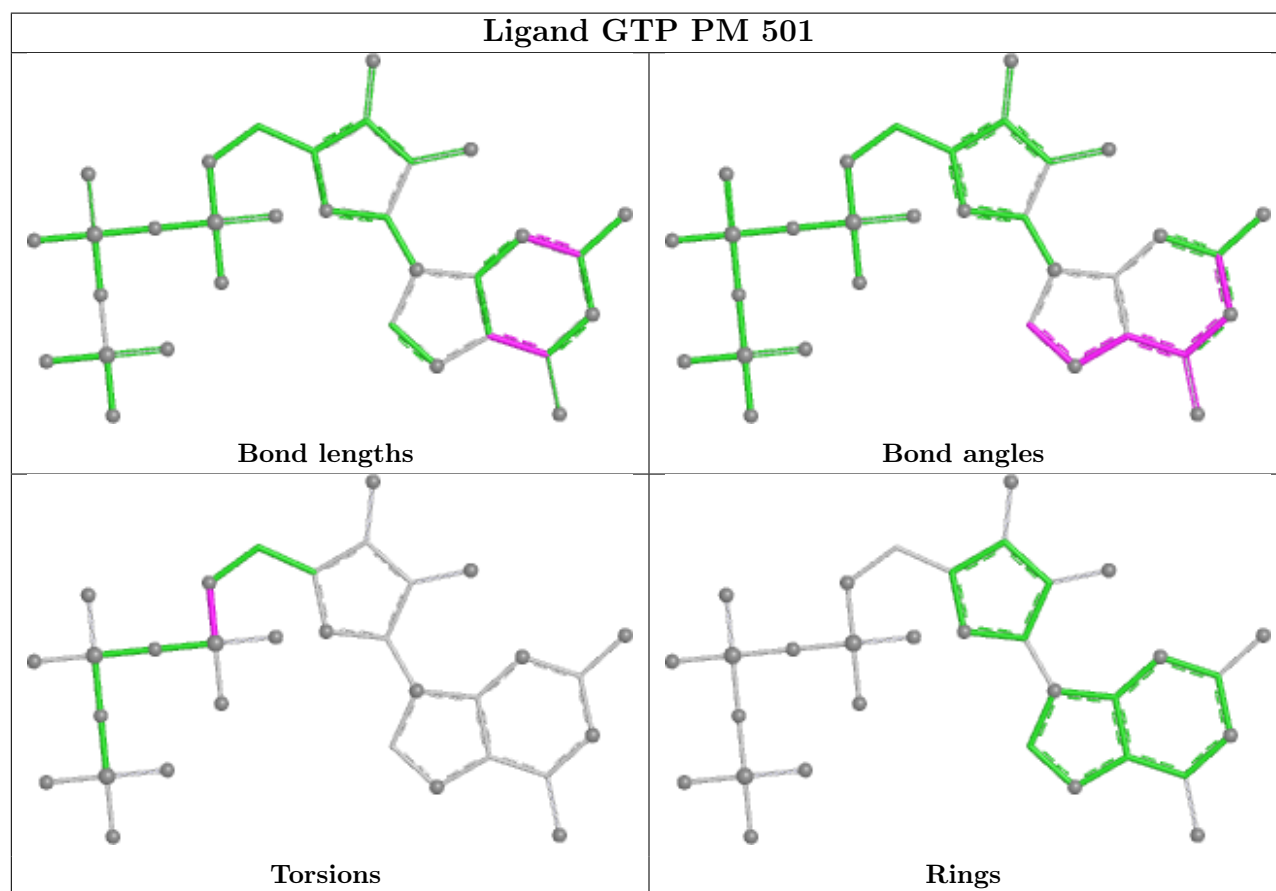
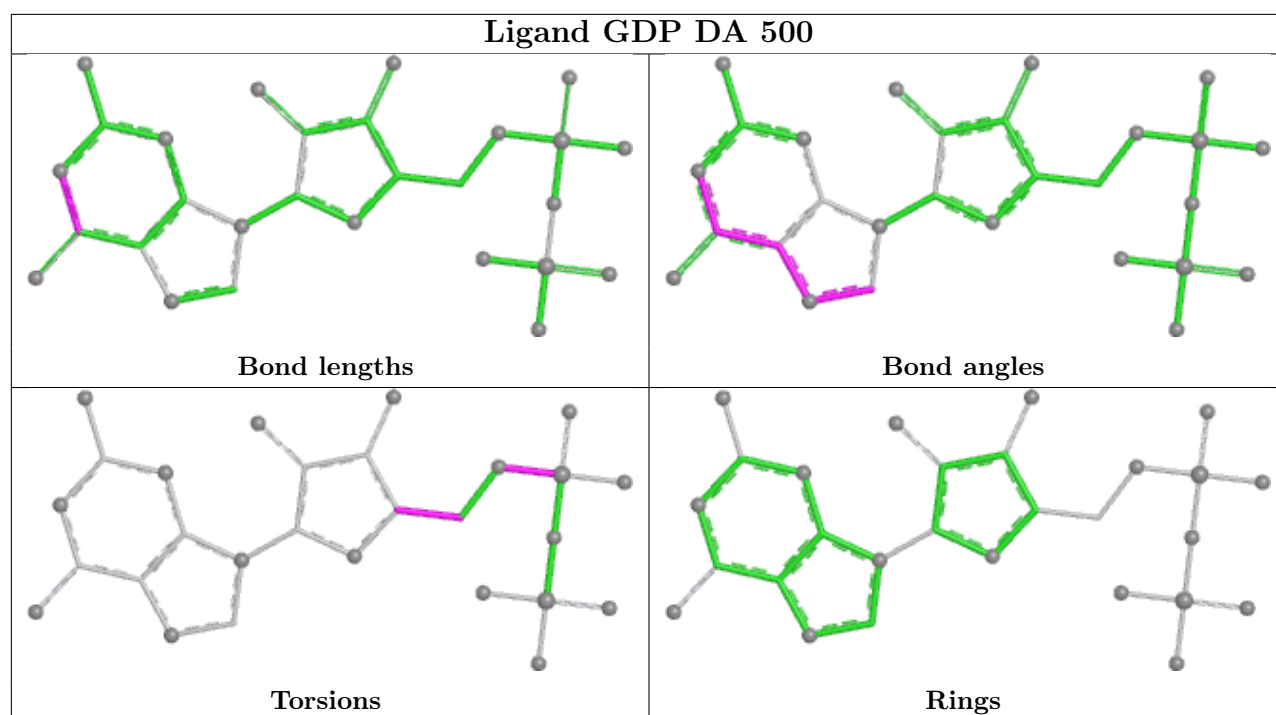


Ligand GTP DL 501

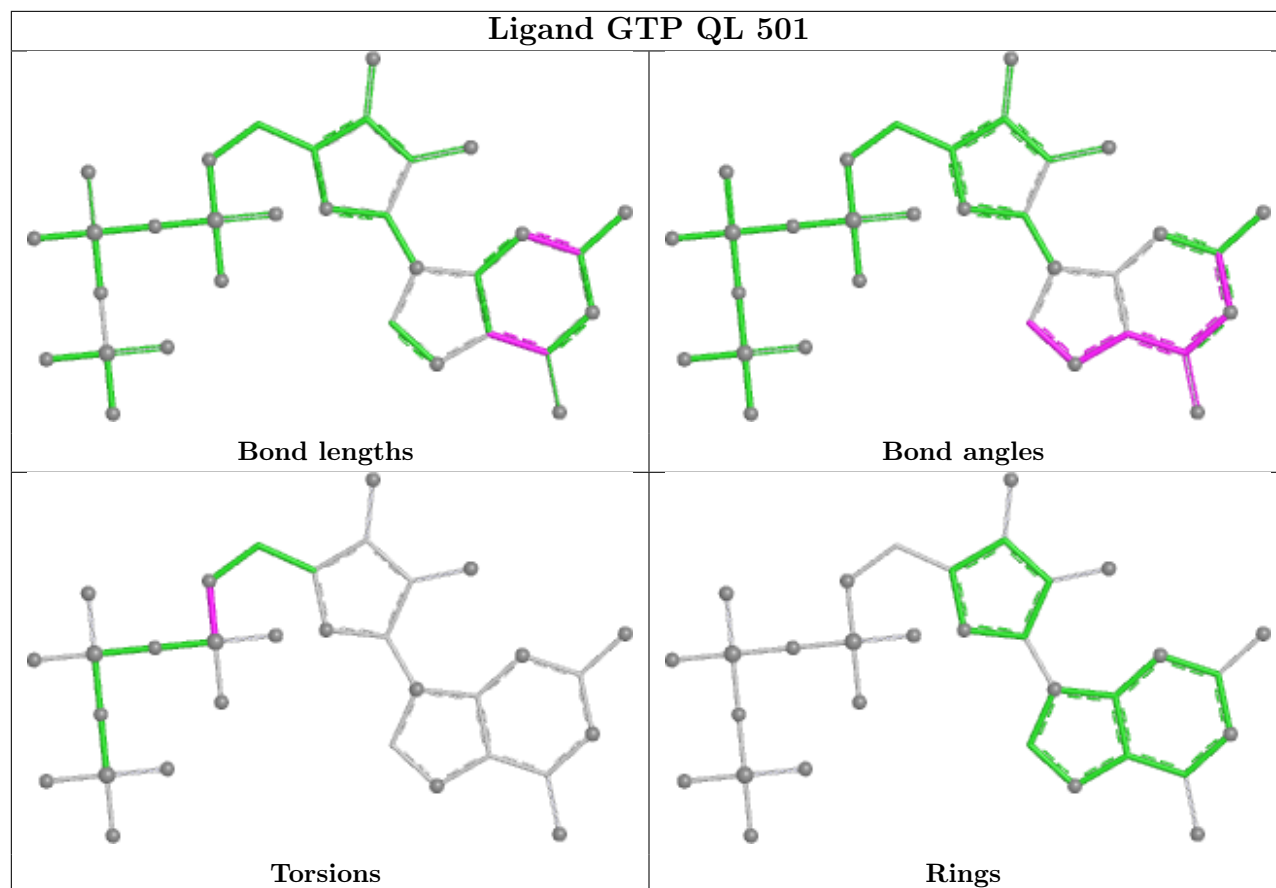


Ligand GTP MA 501

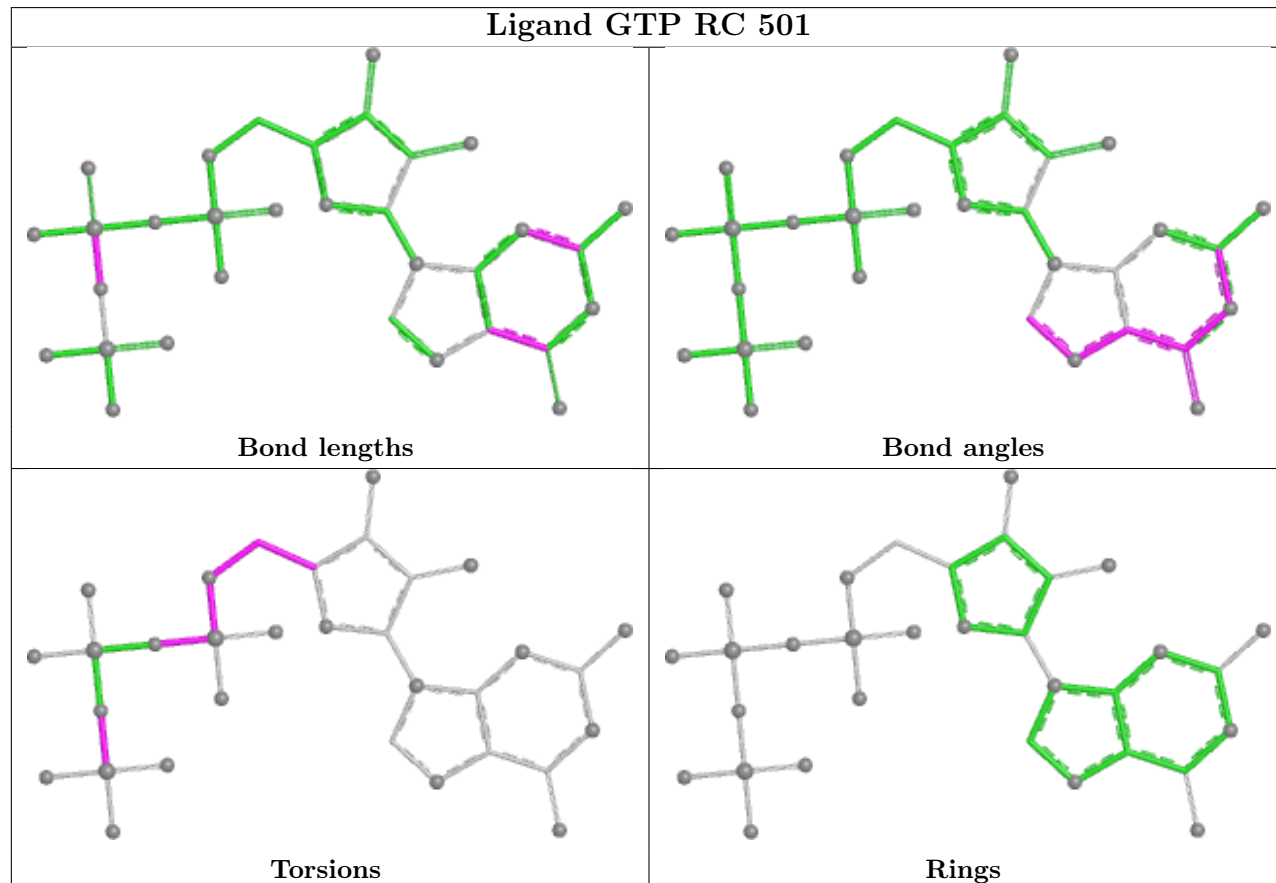


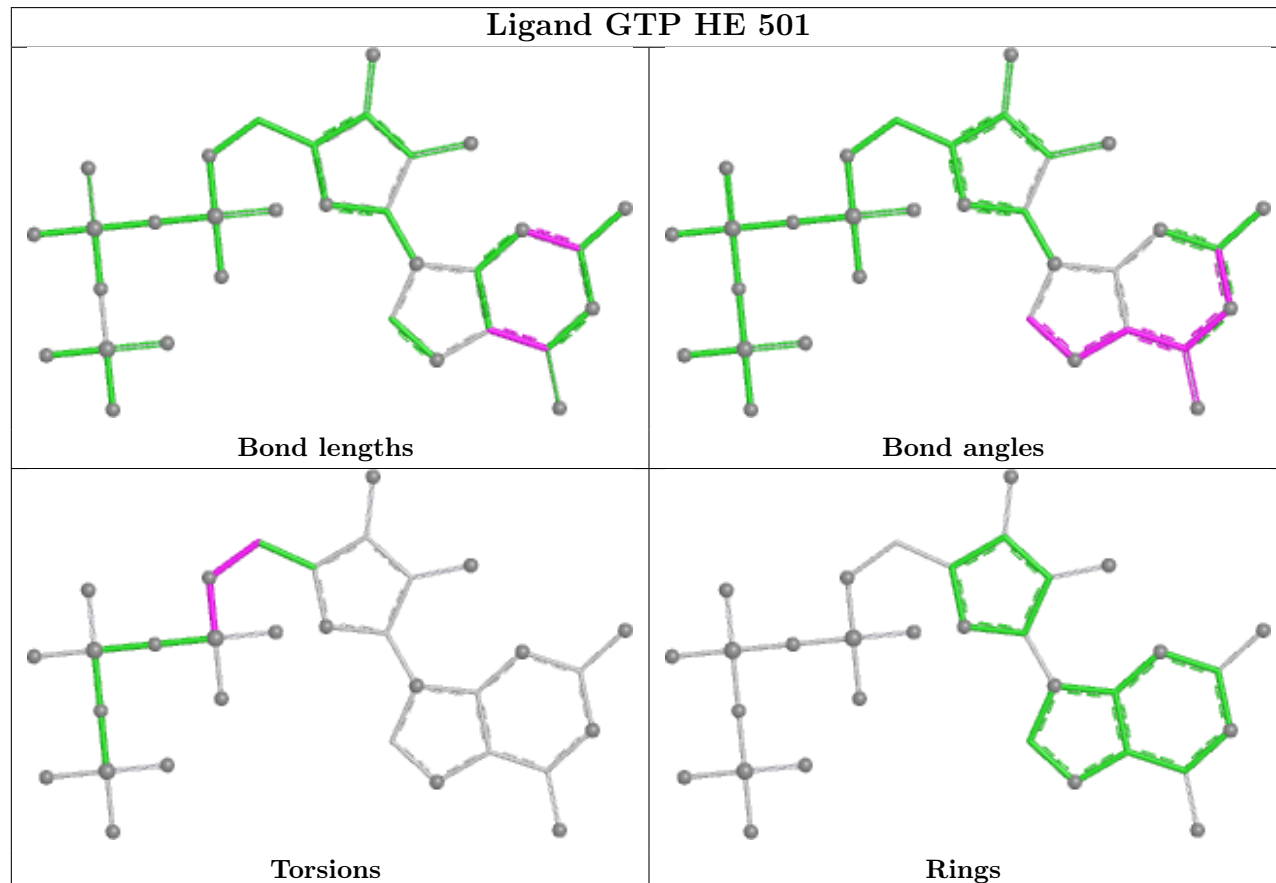
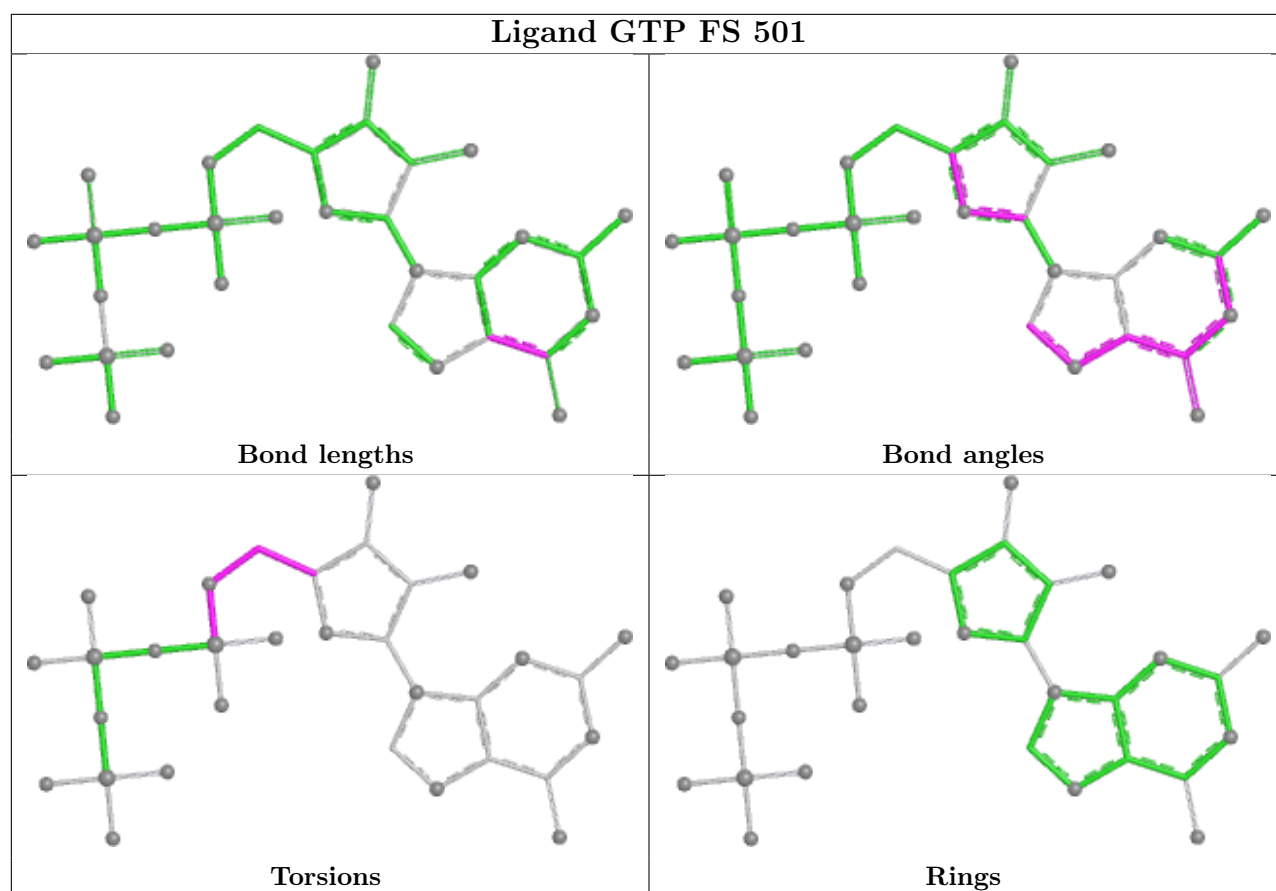


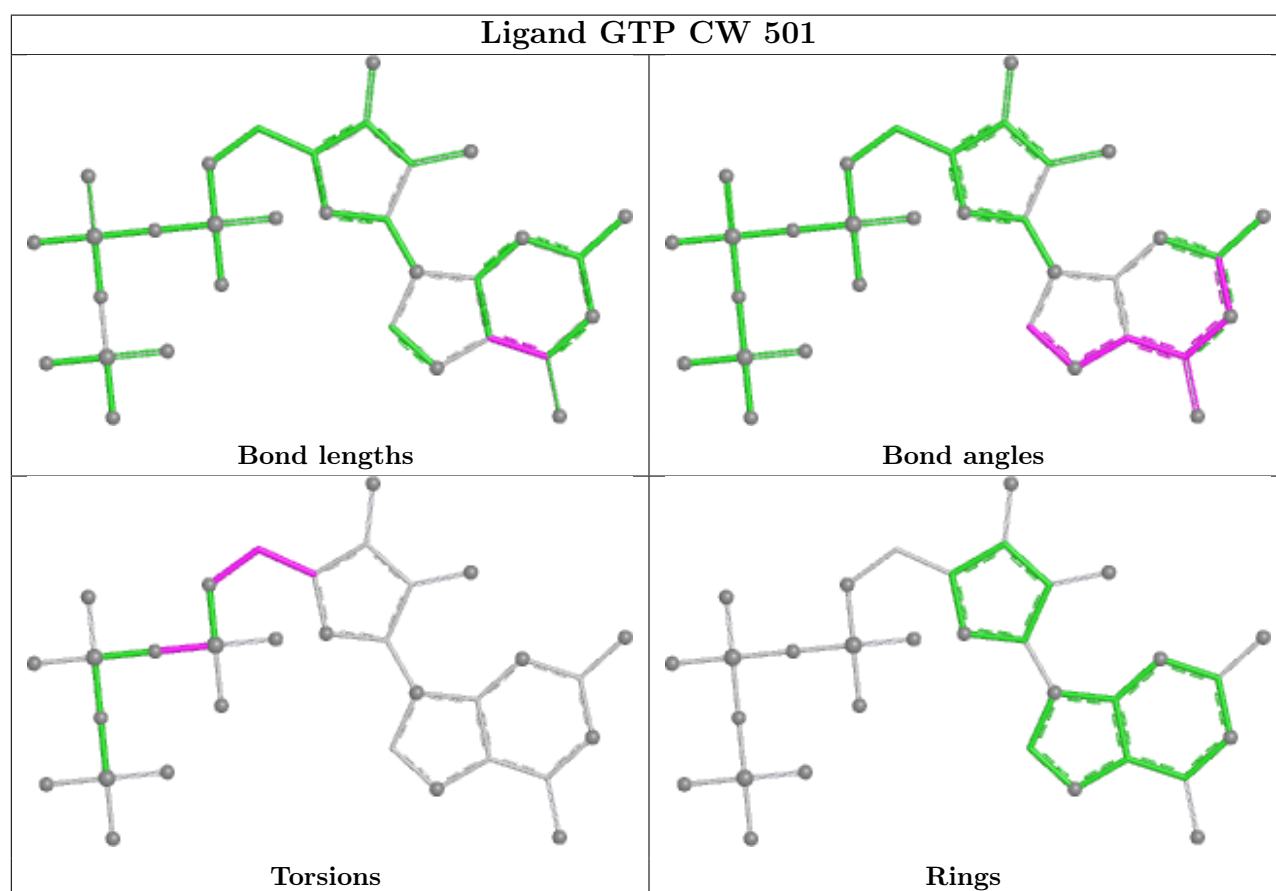
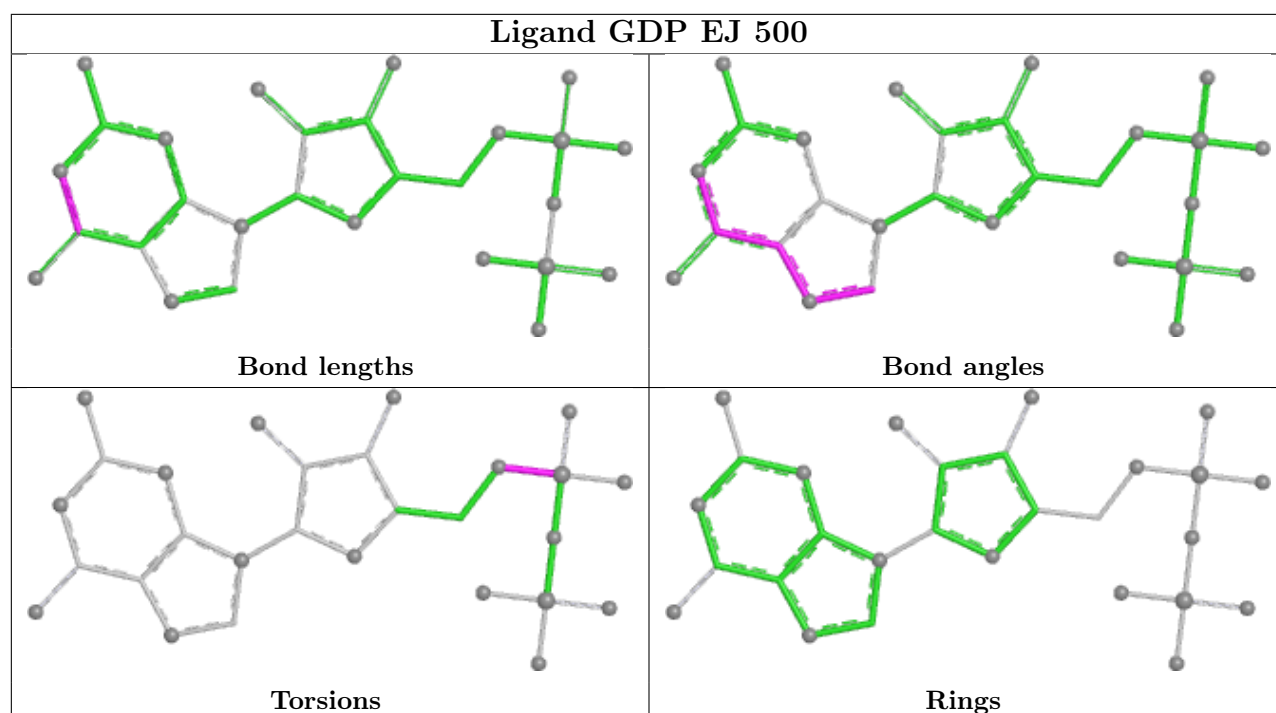
Ligand GTP QL 501

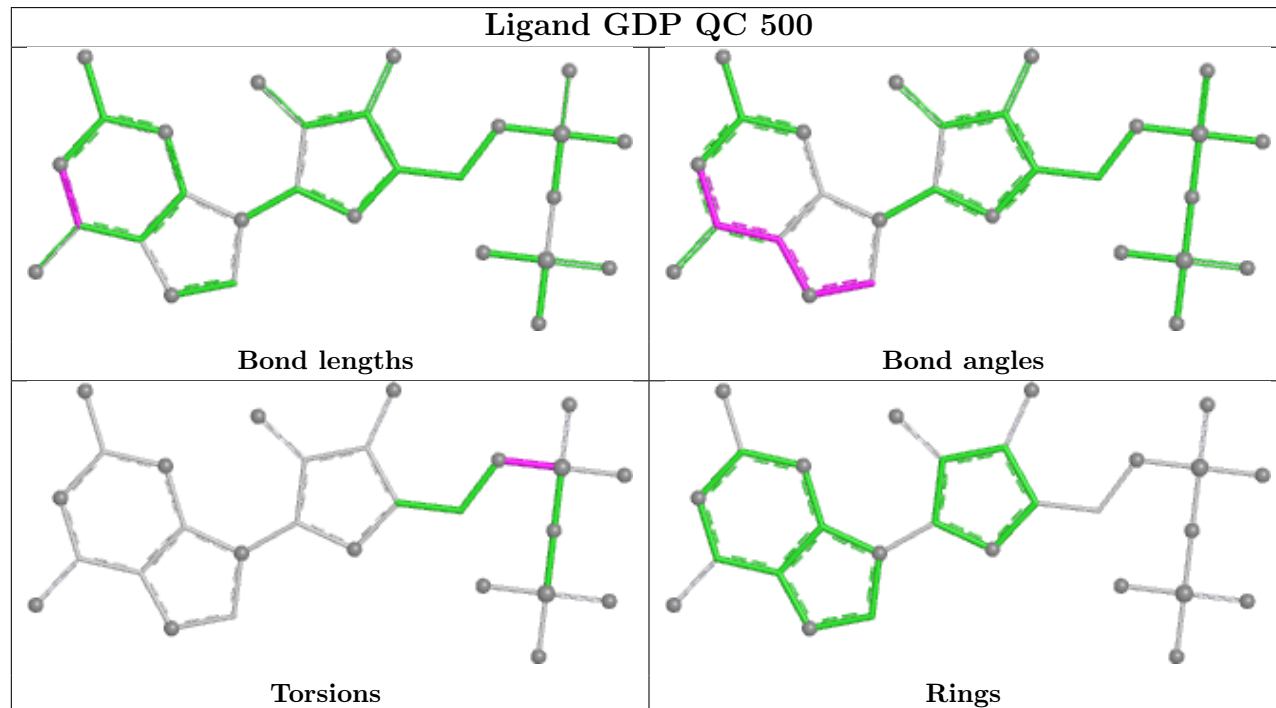
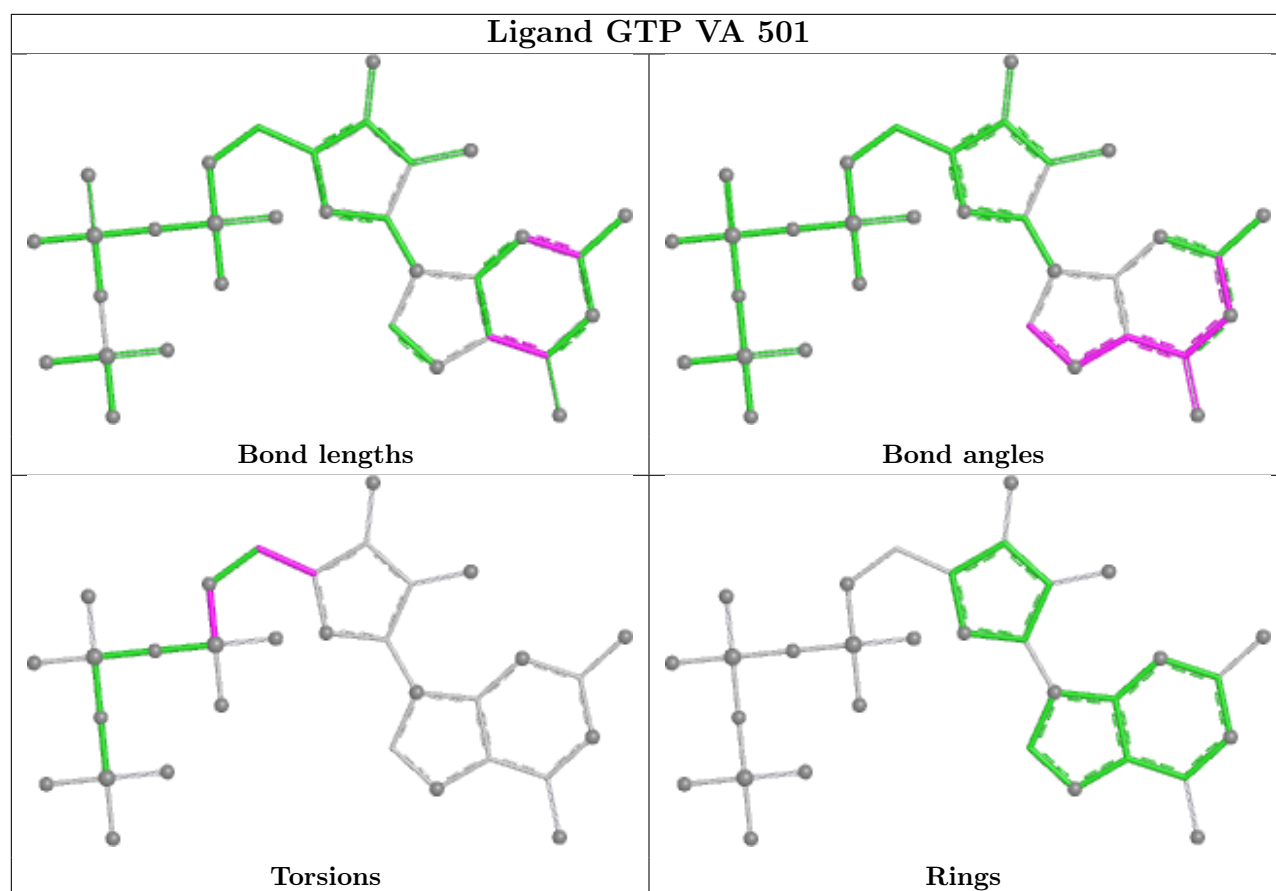


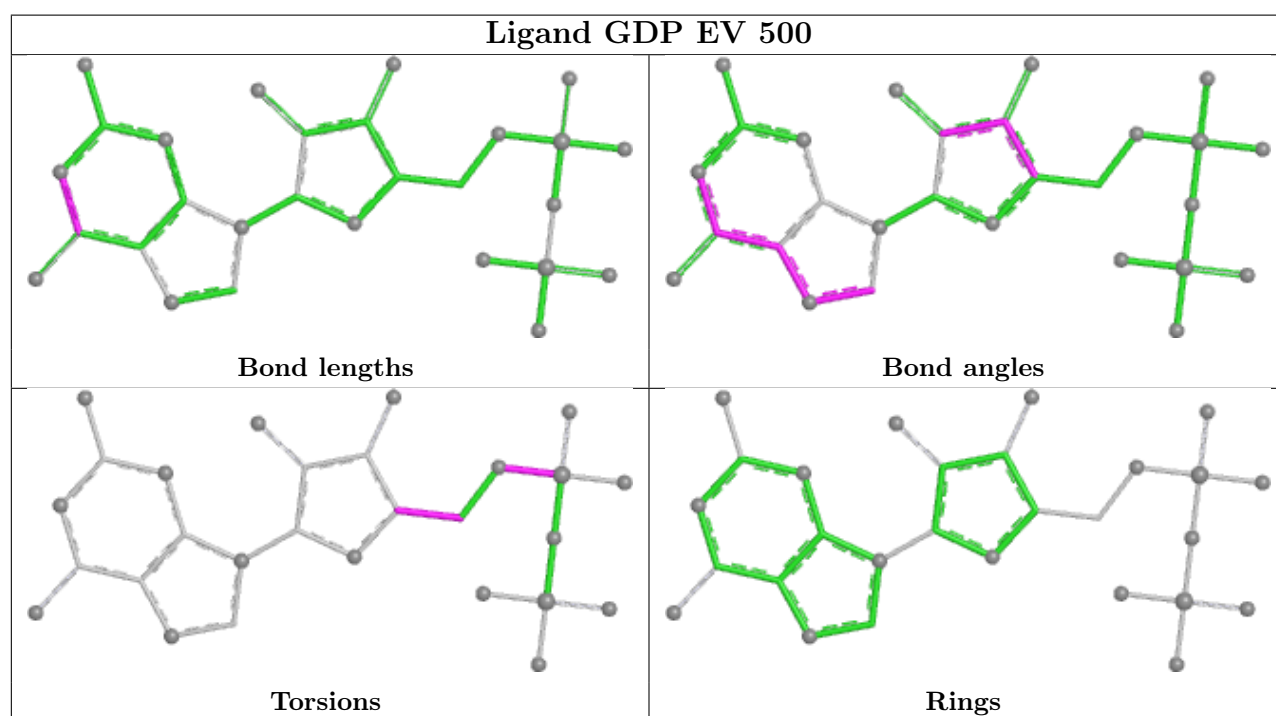
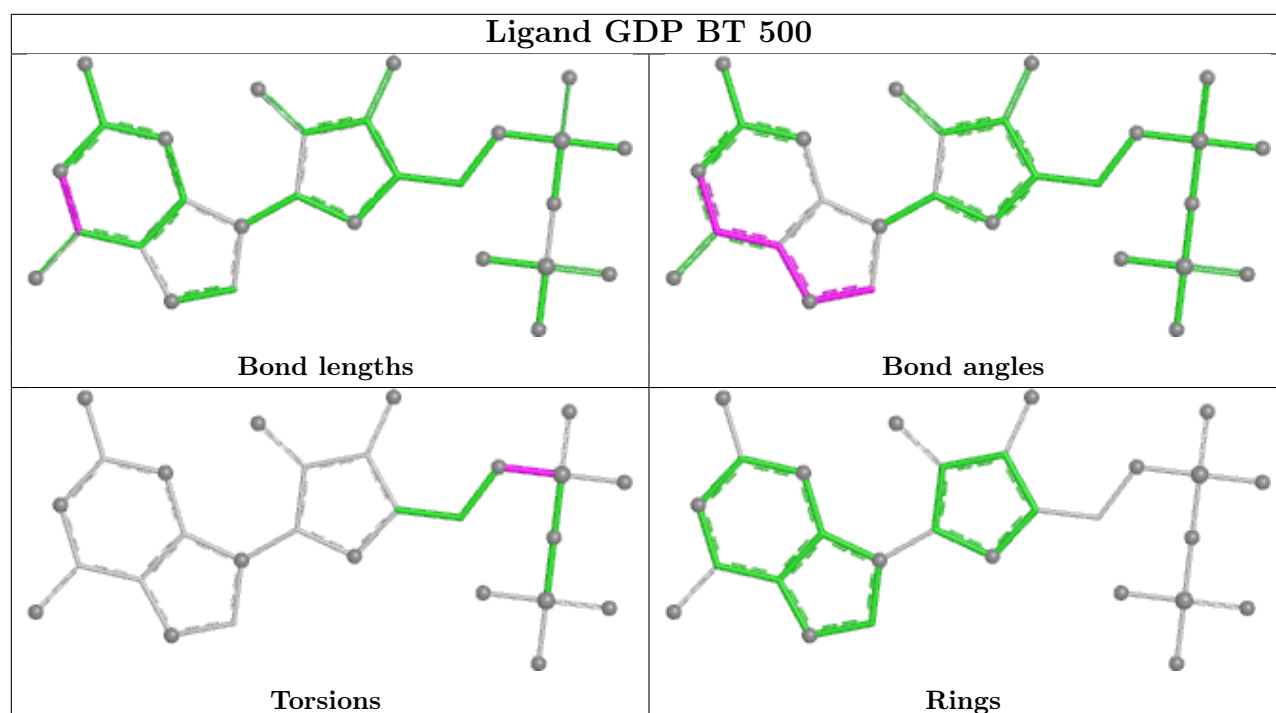
Ligand GTP RC 501



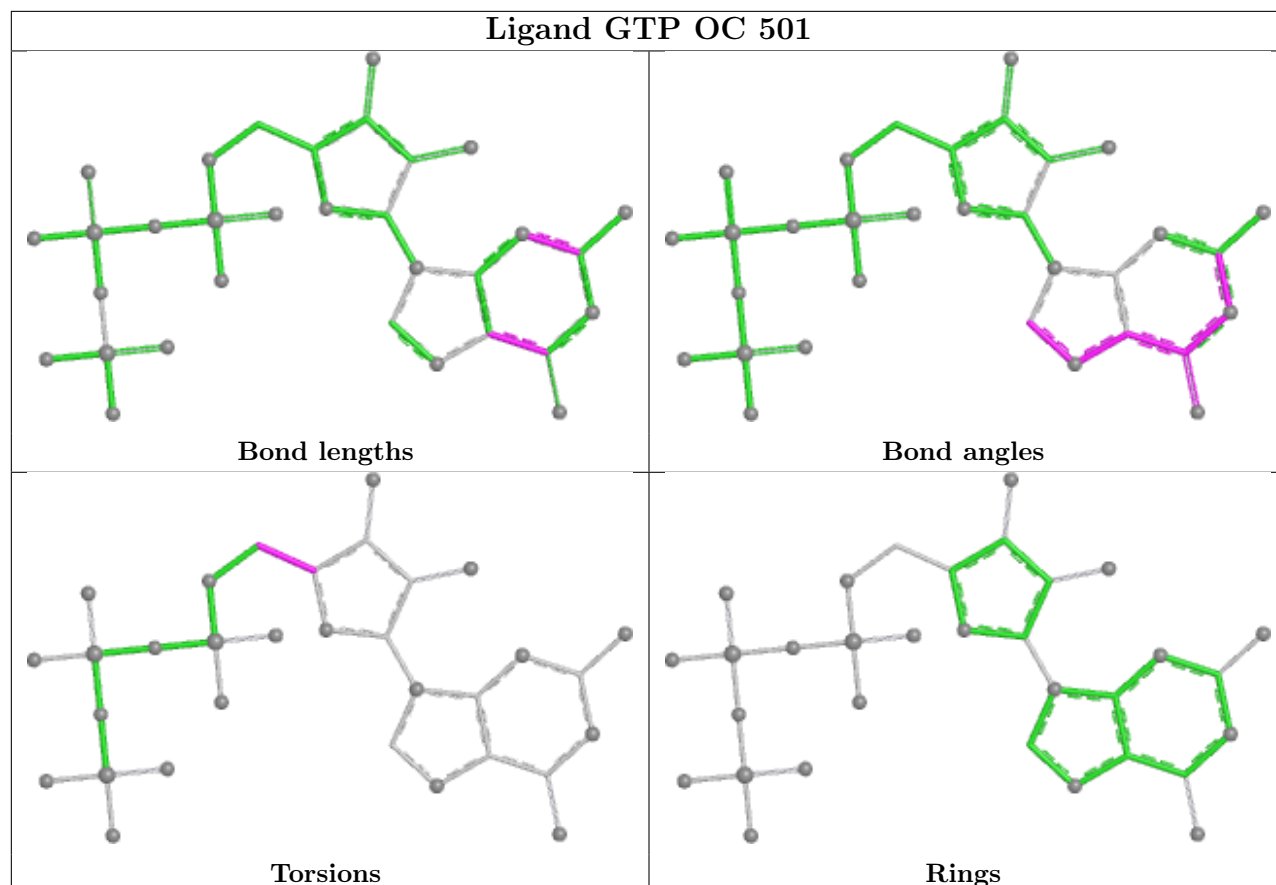




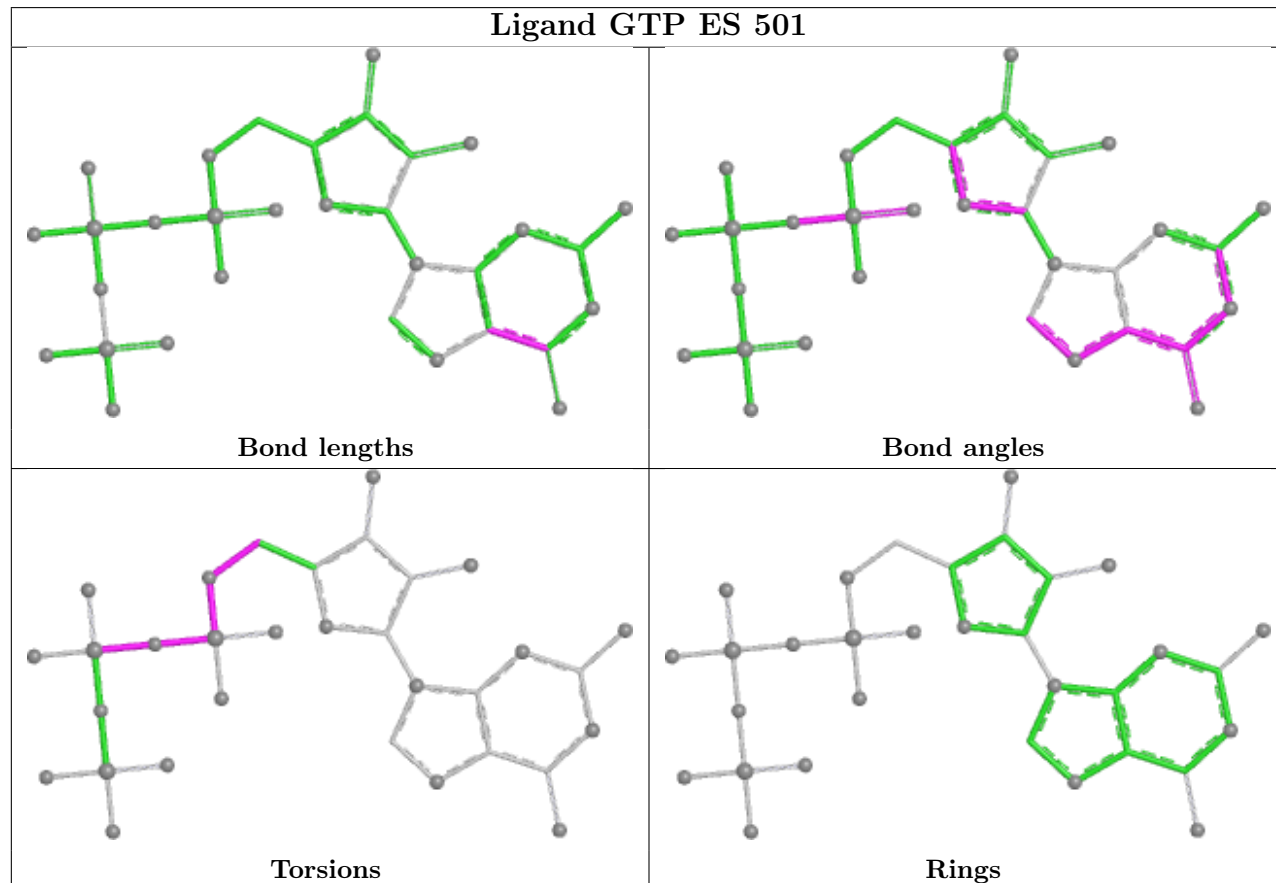




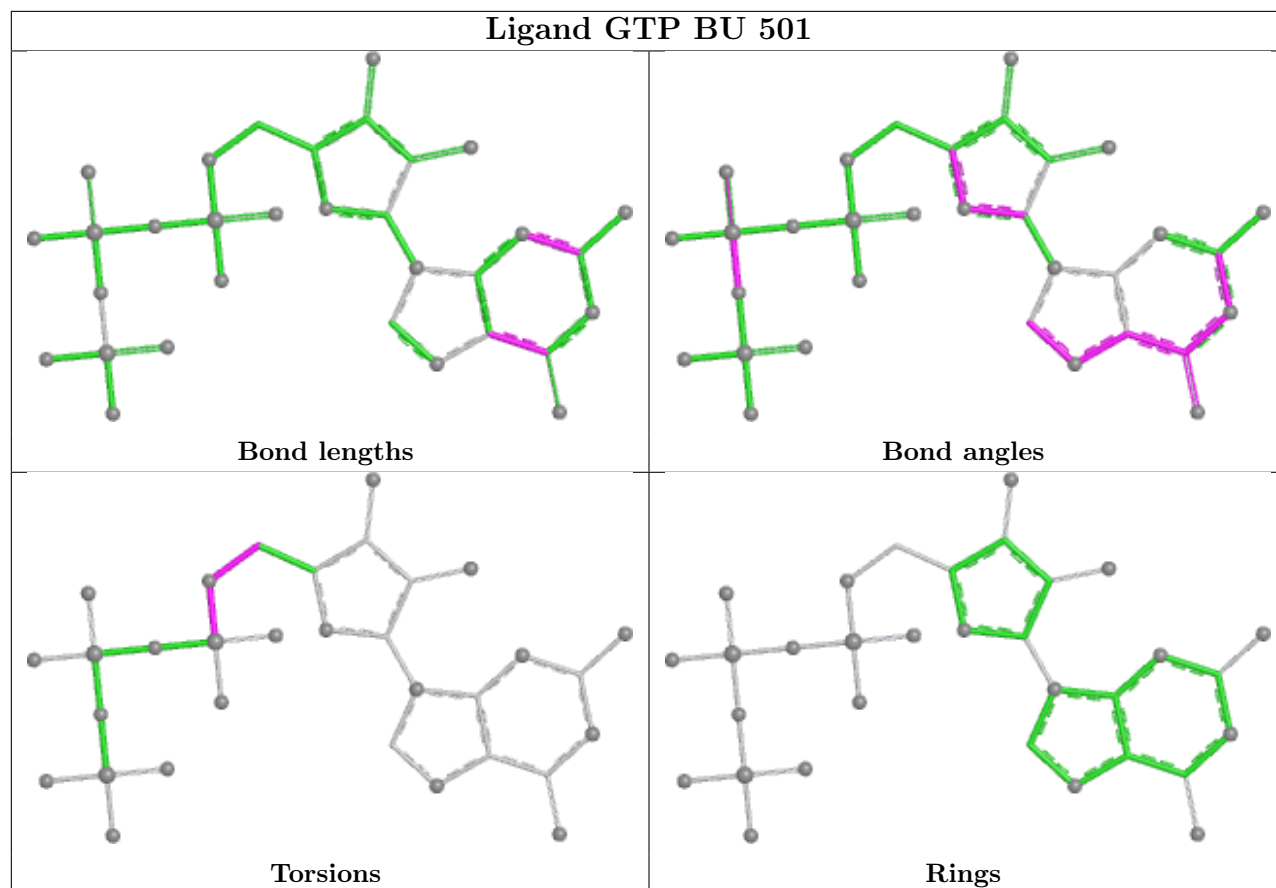
Ligand GTP OC 501



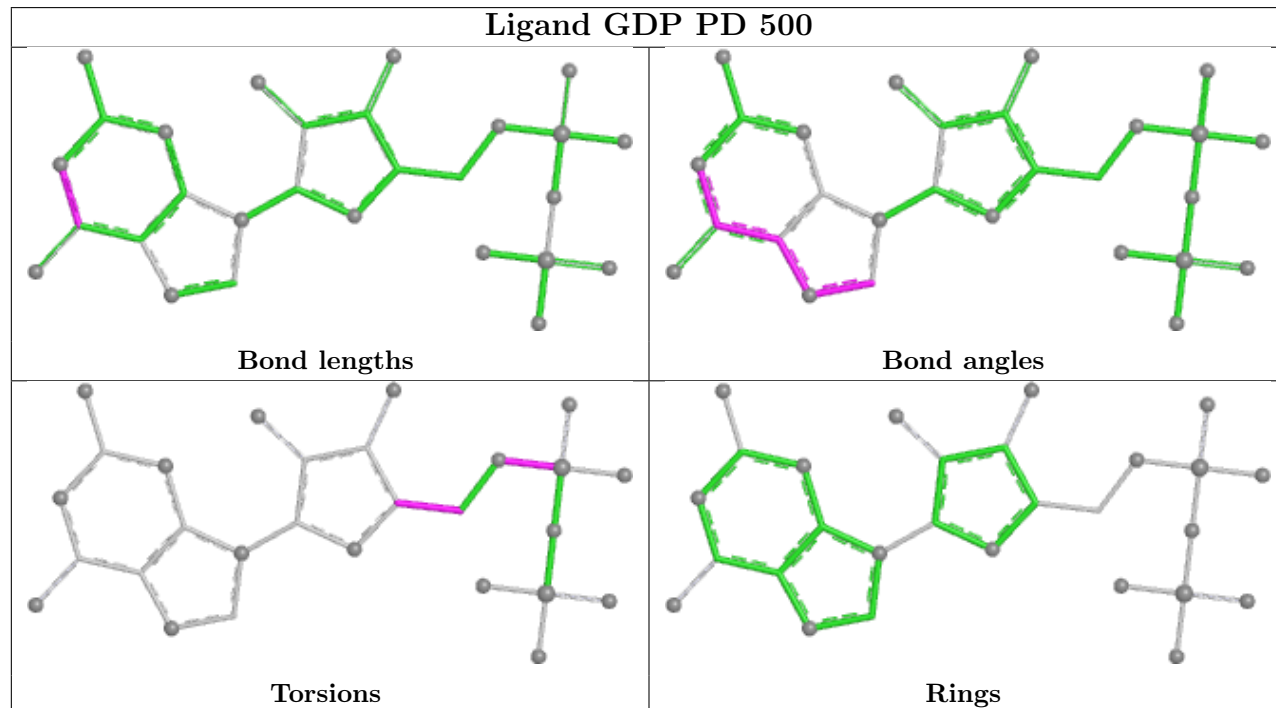
Ligand GTP ES 501

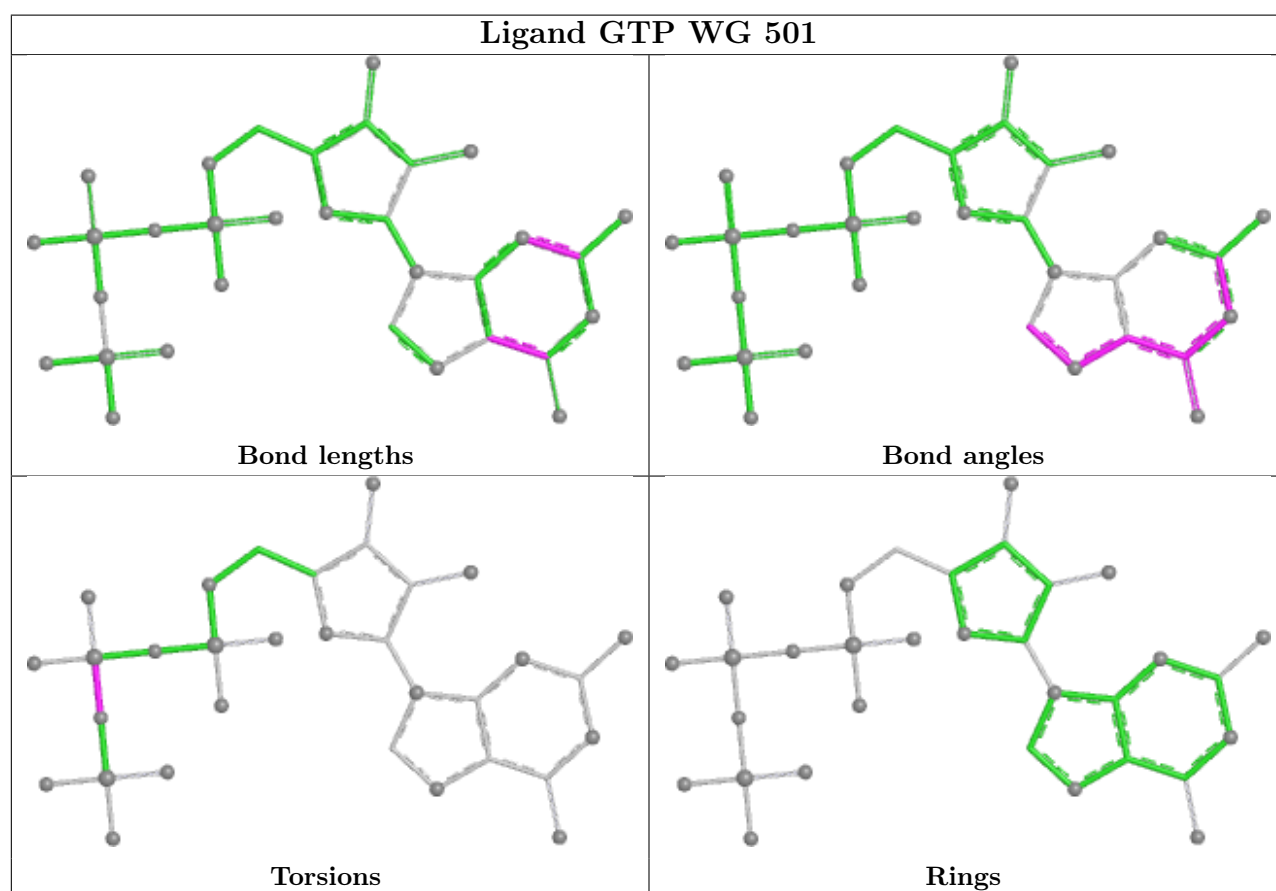
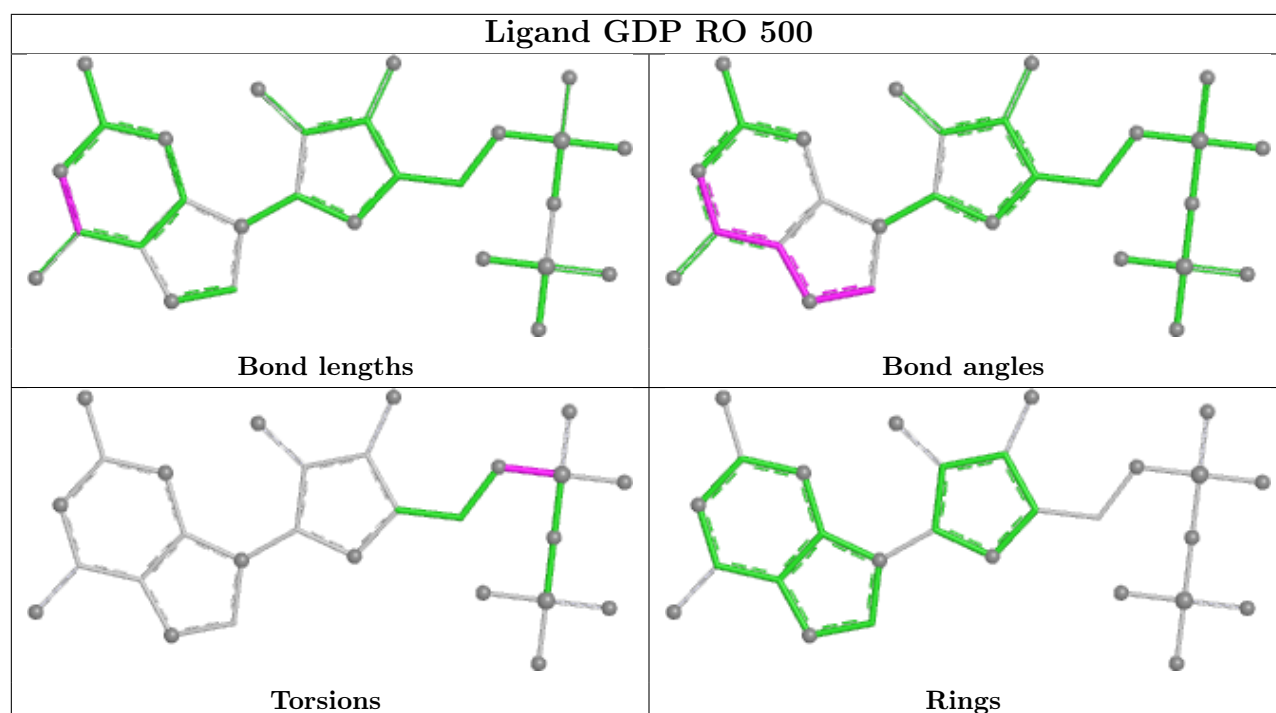


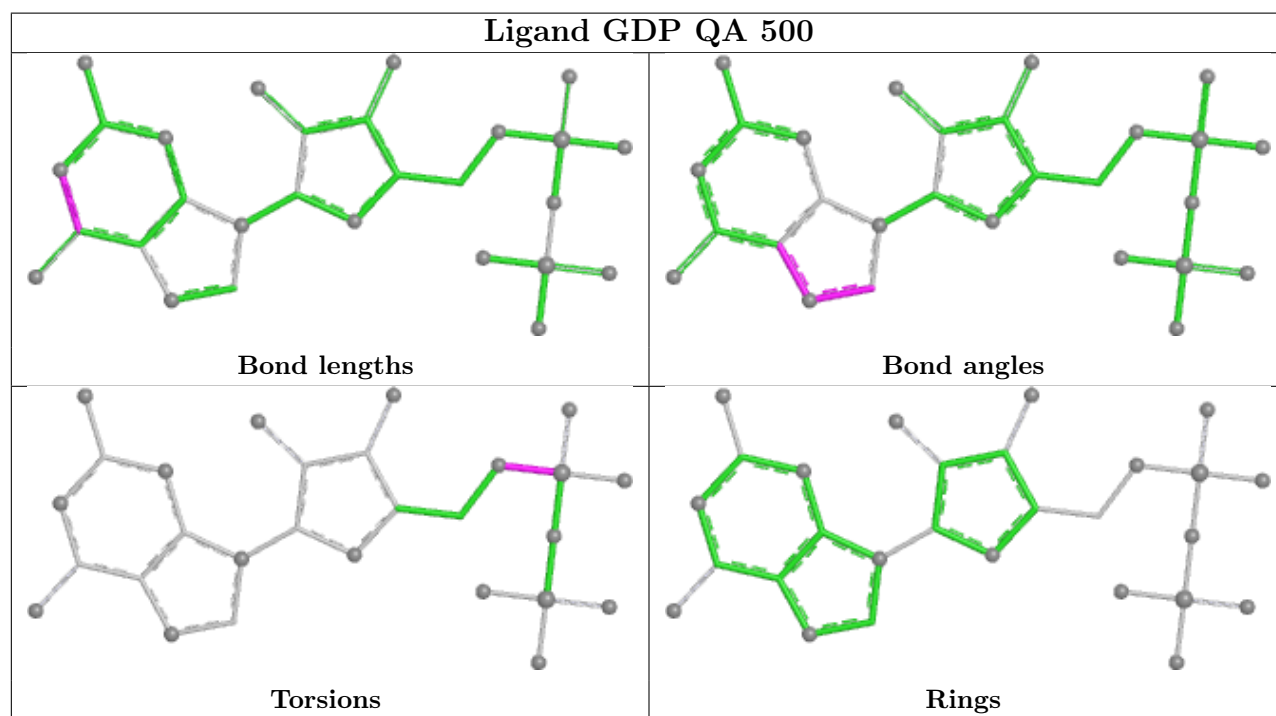
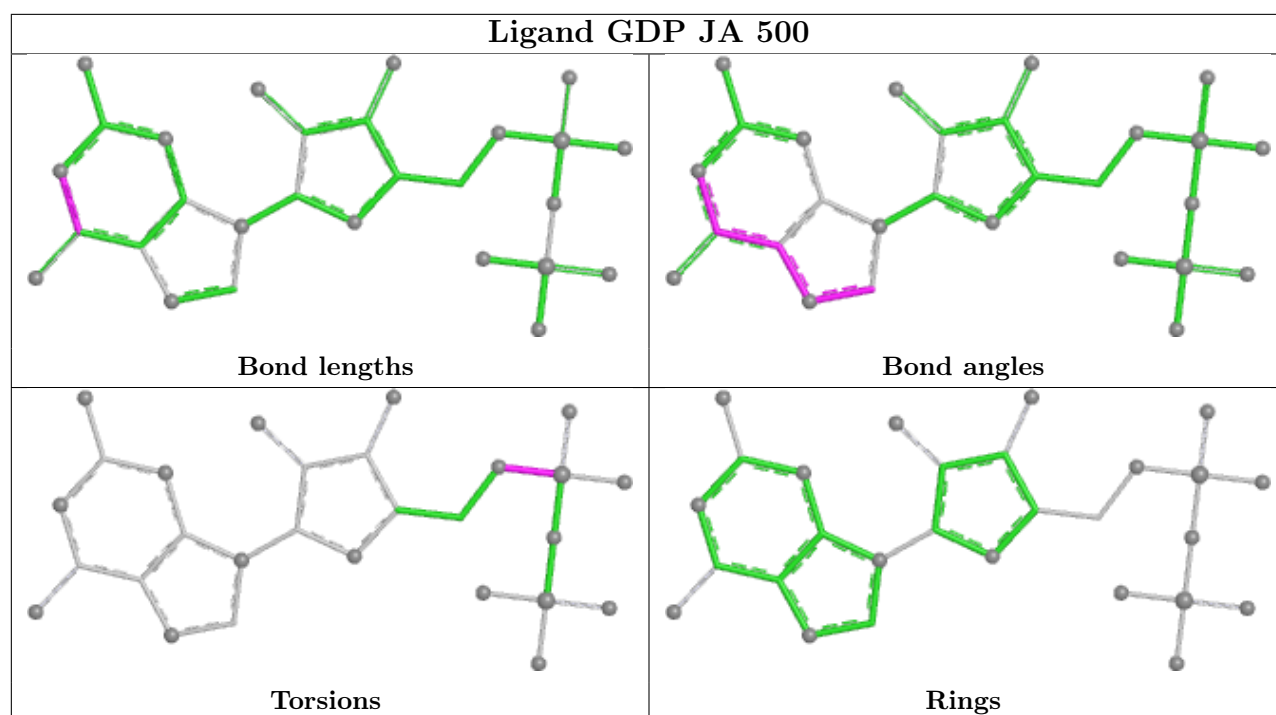
Ligand GTP BU 501

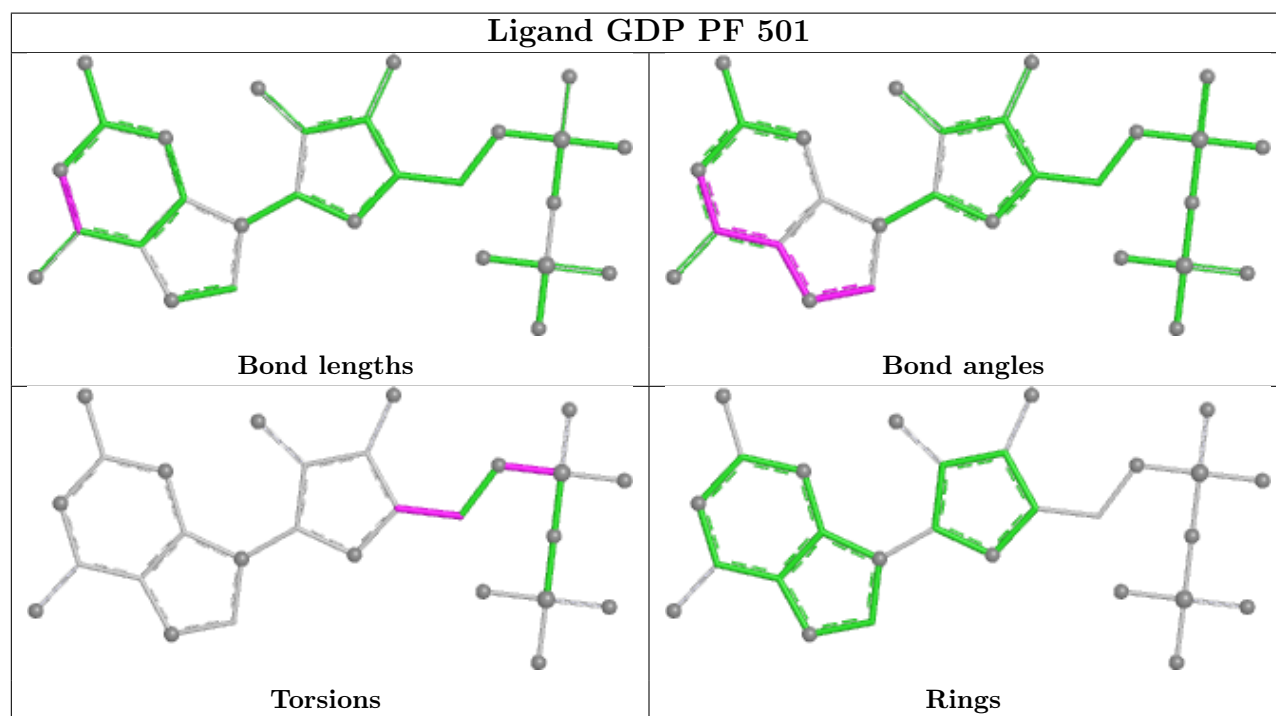
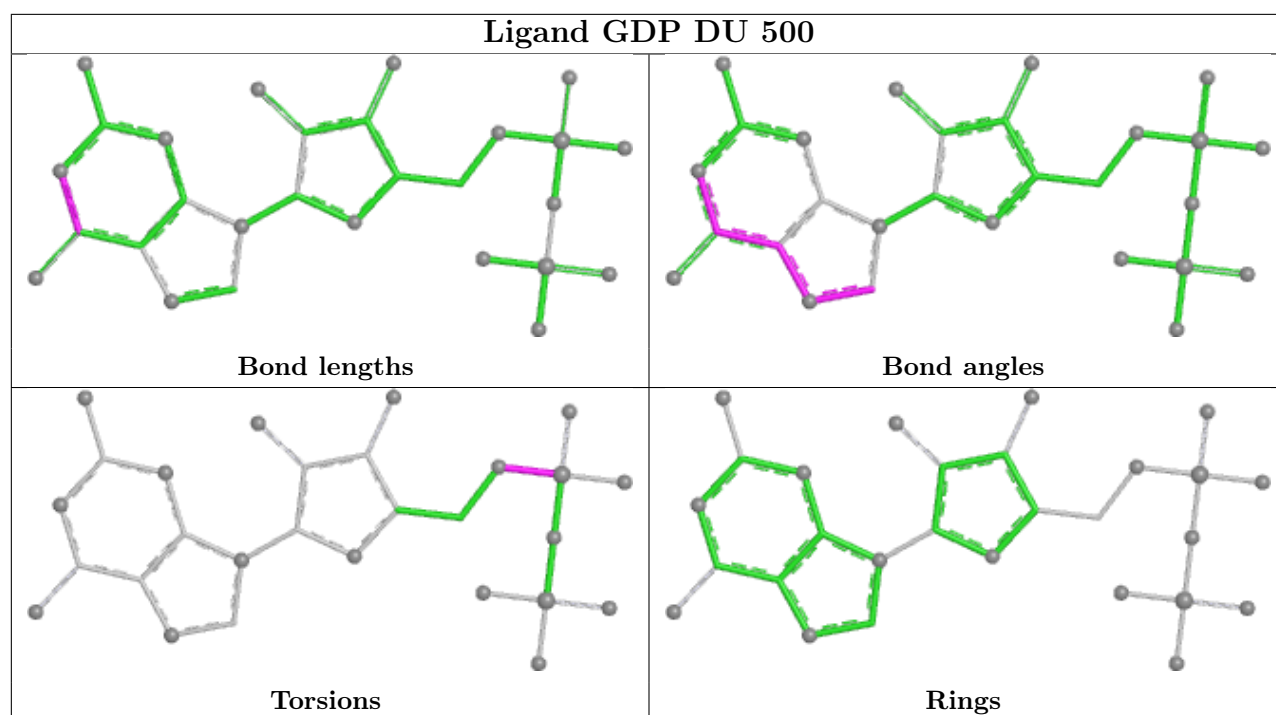


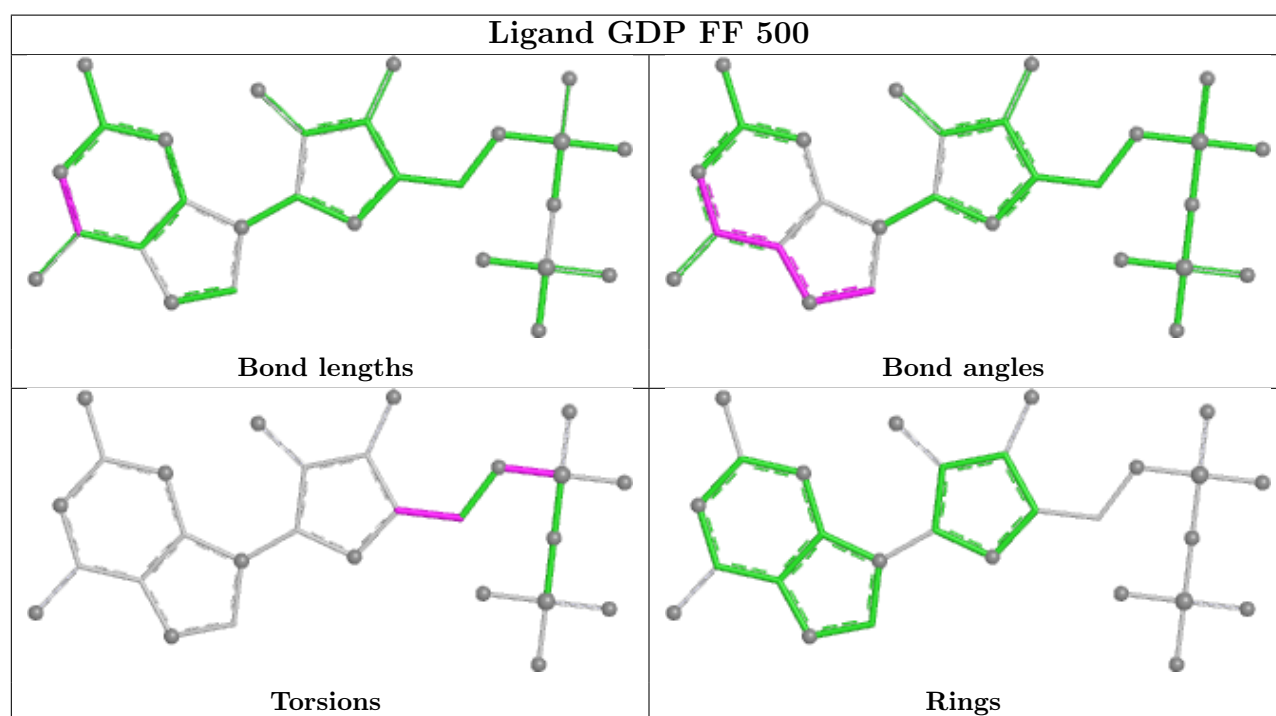
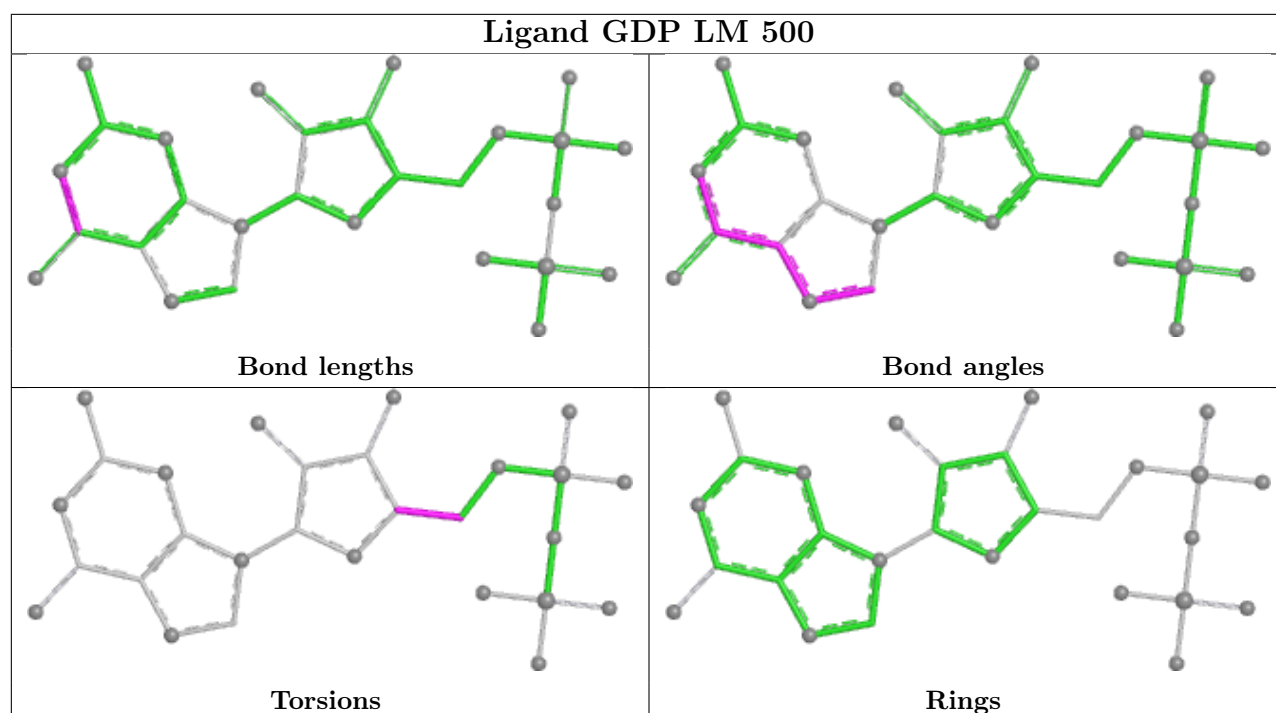
Ligand GDP PD 500



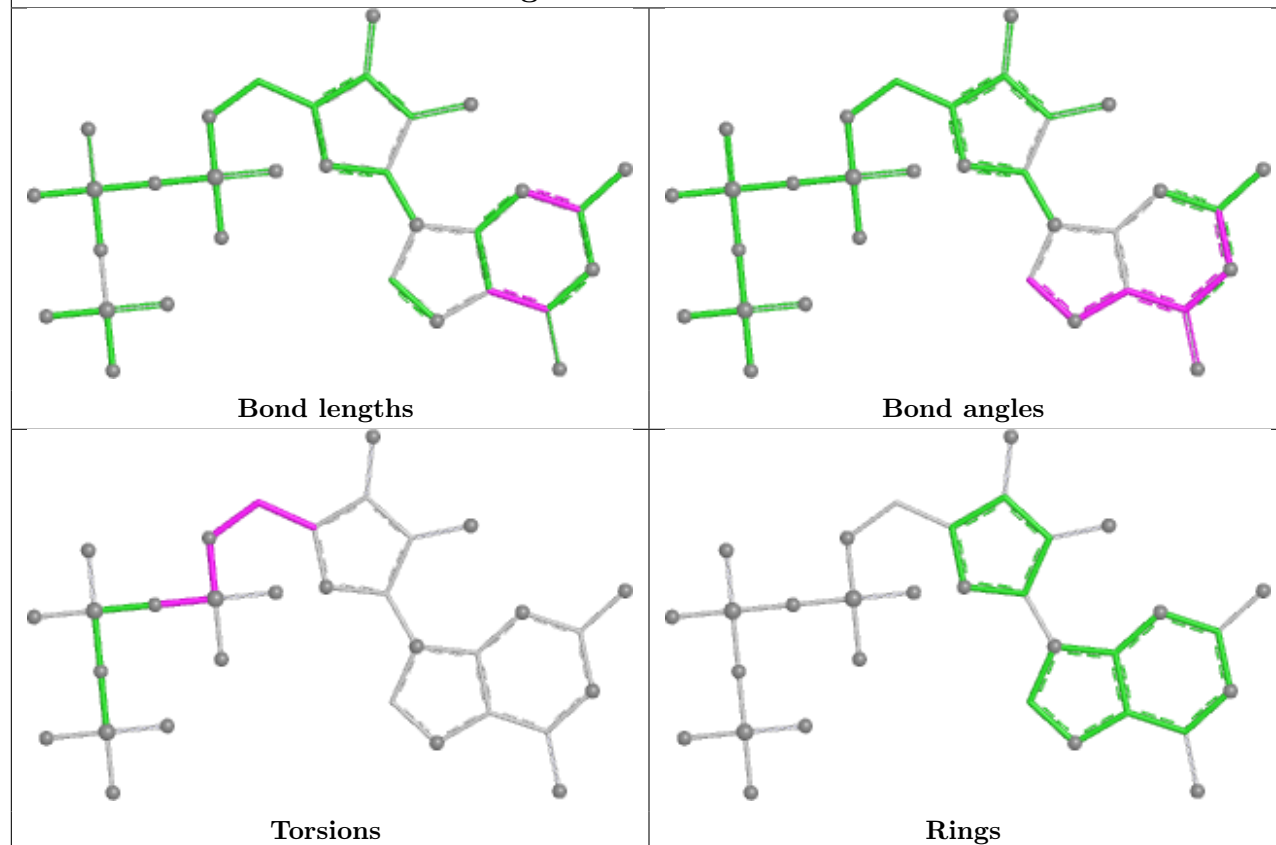




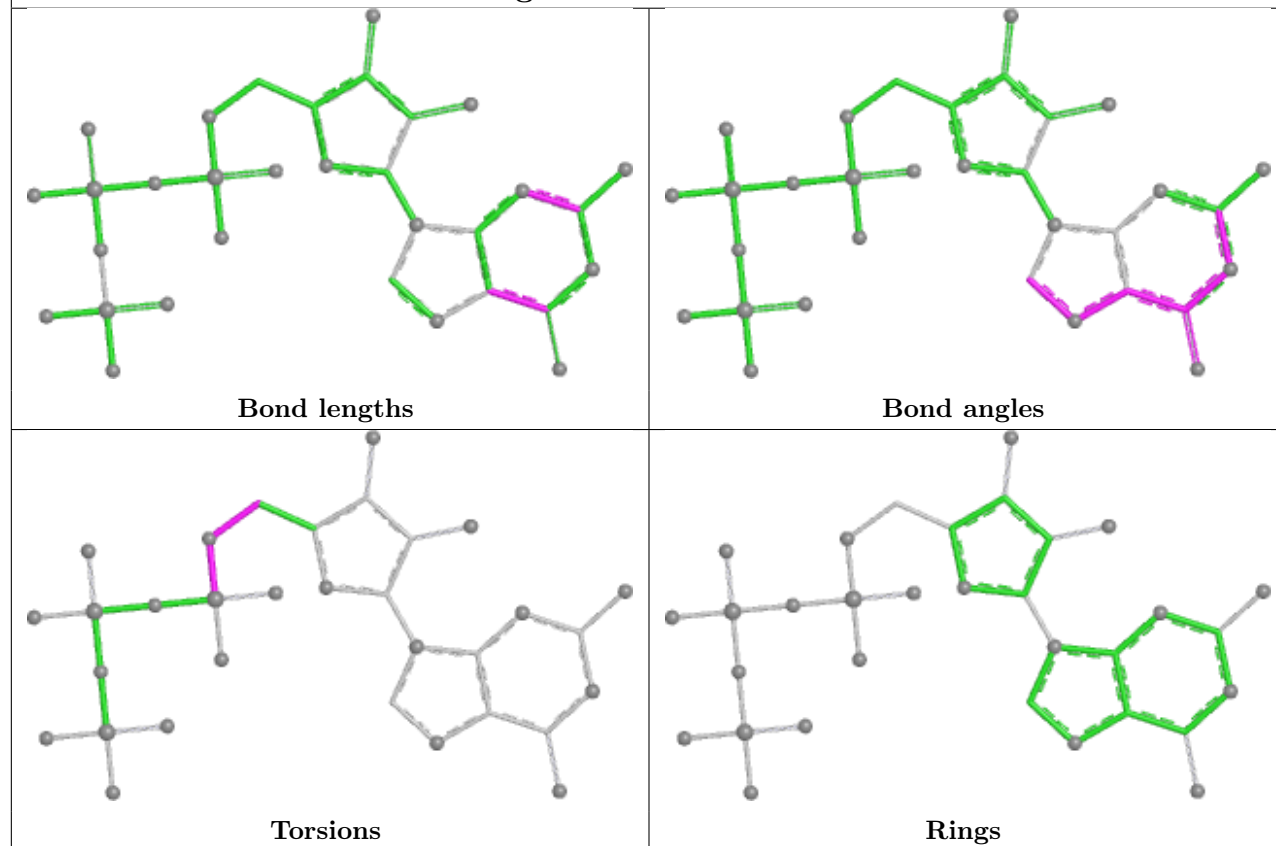




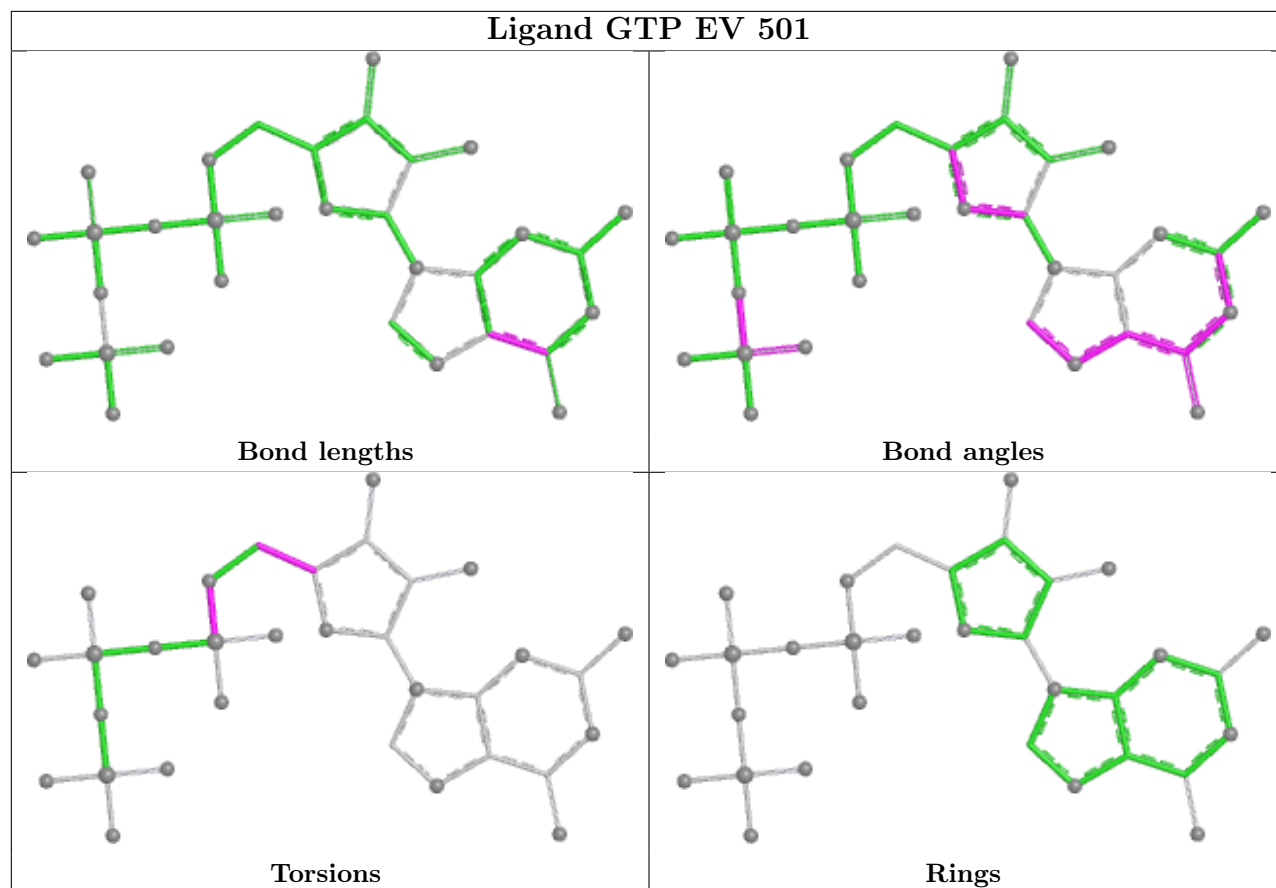
Ligand GTP LP 502



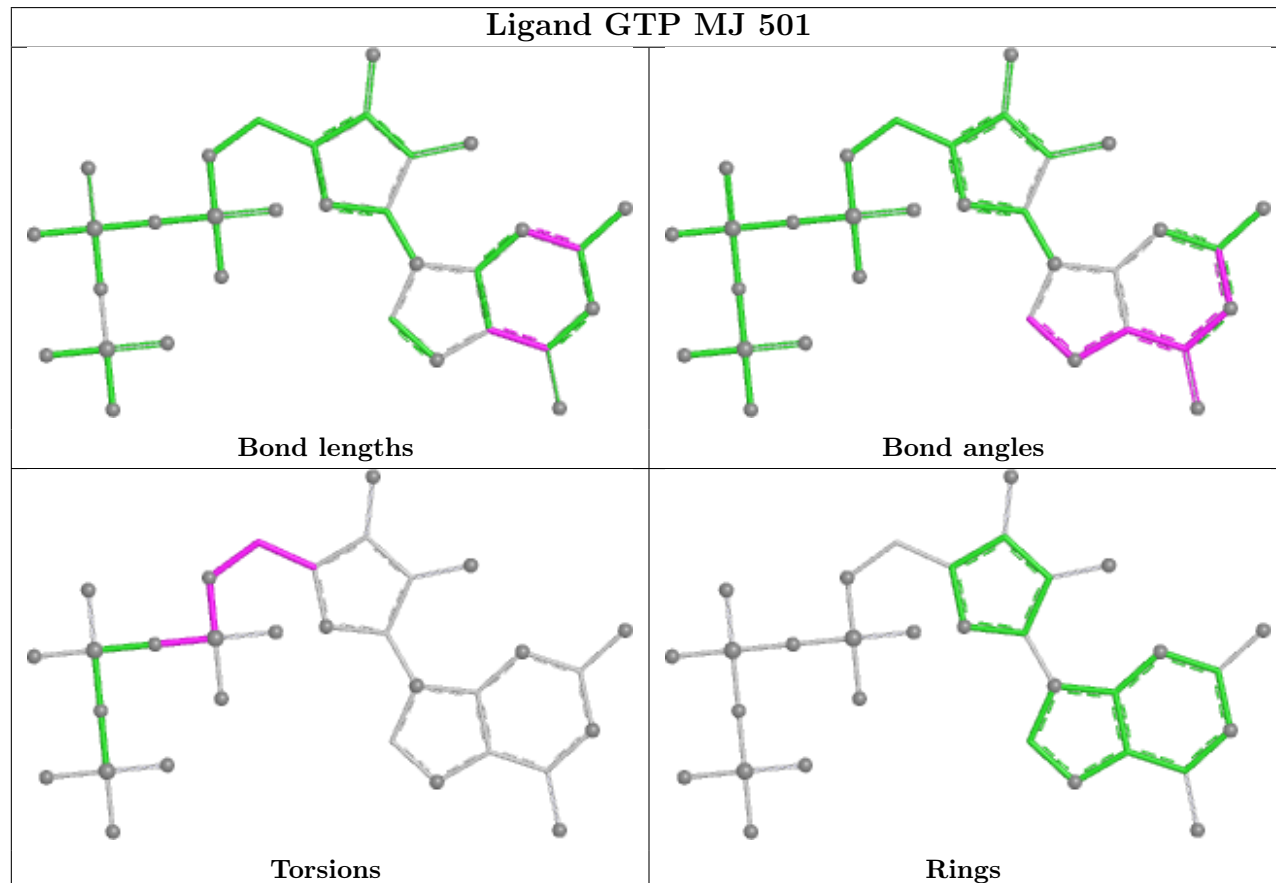
Ligand GTP HK 501

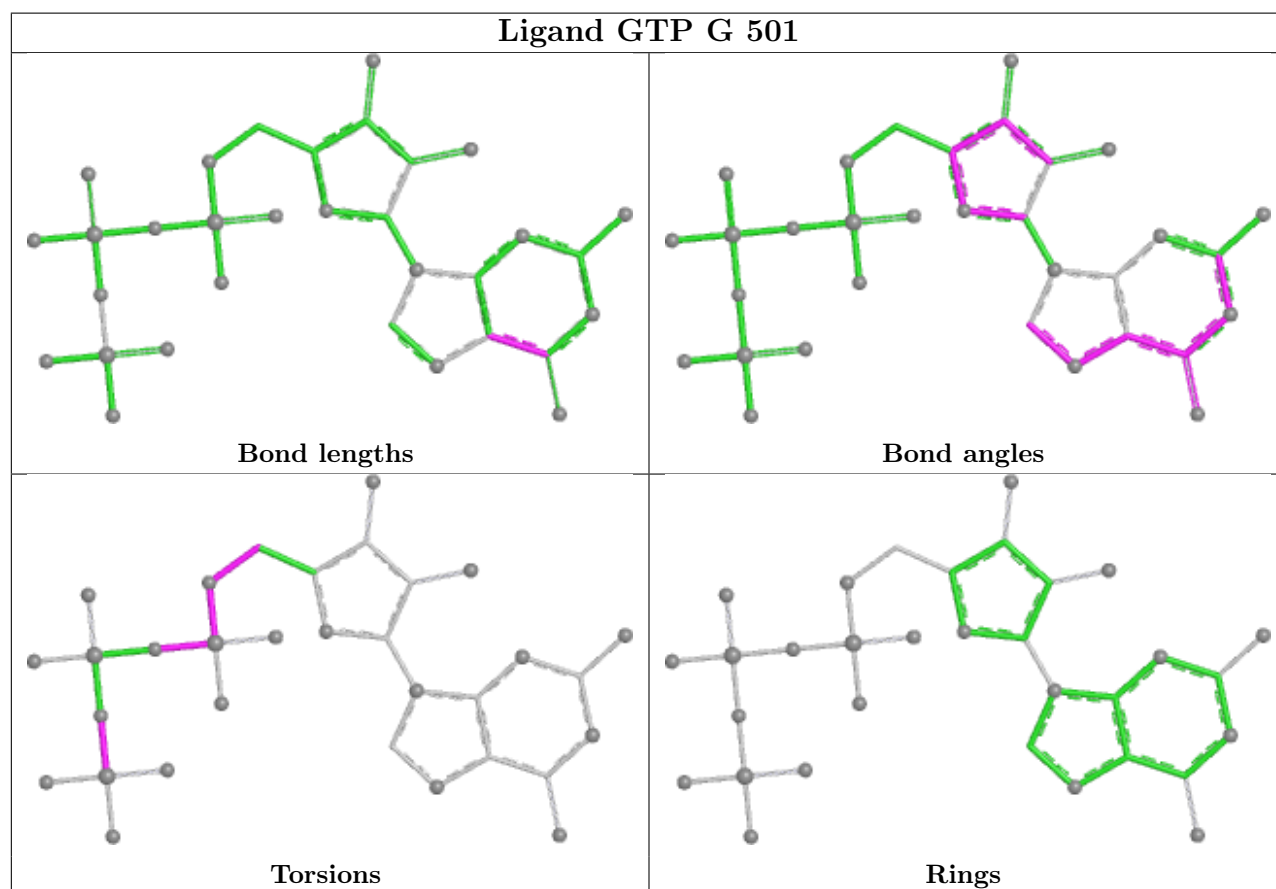
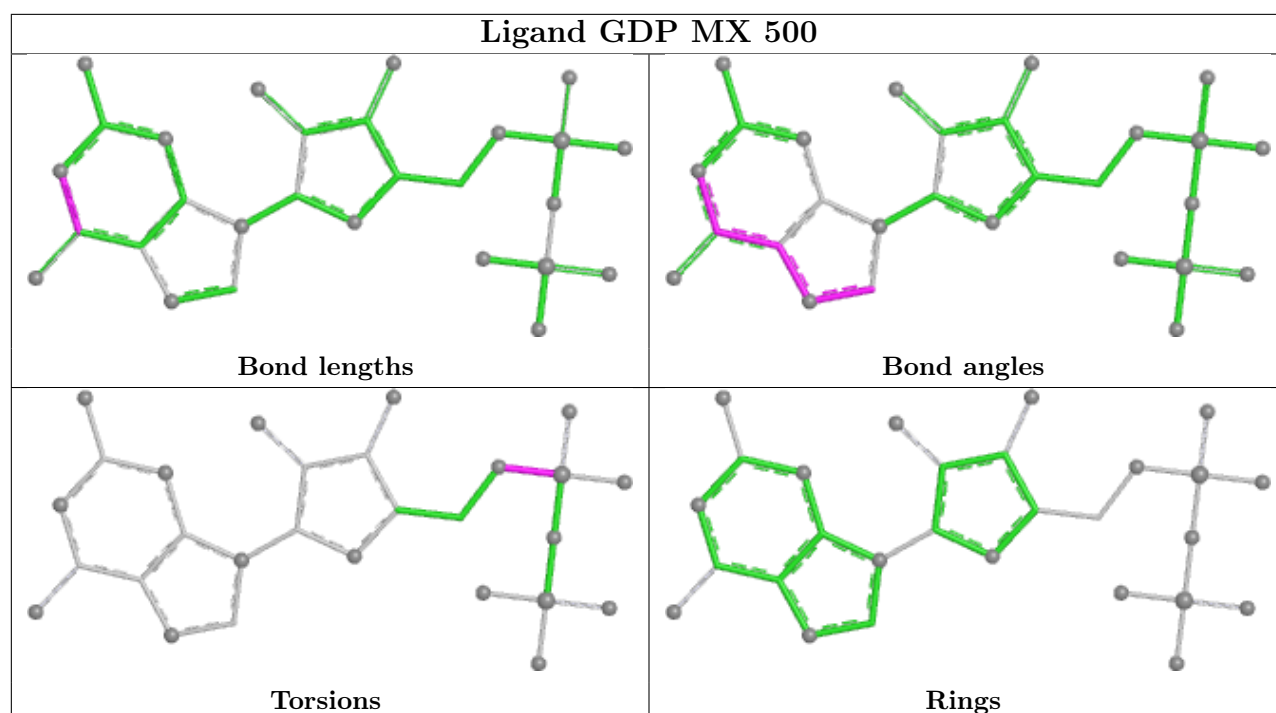


Ligand GTP EV 501

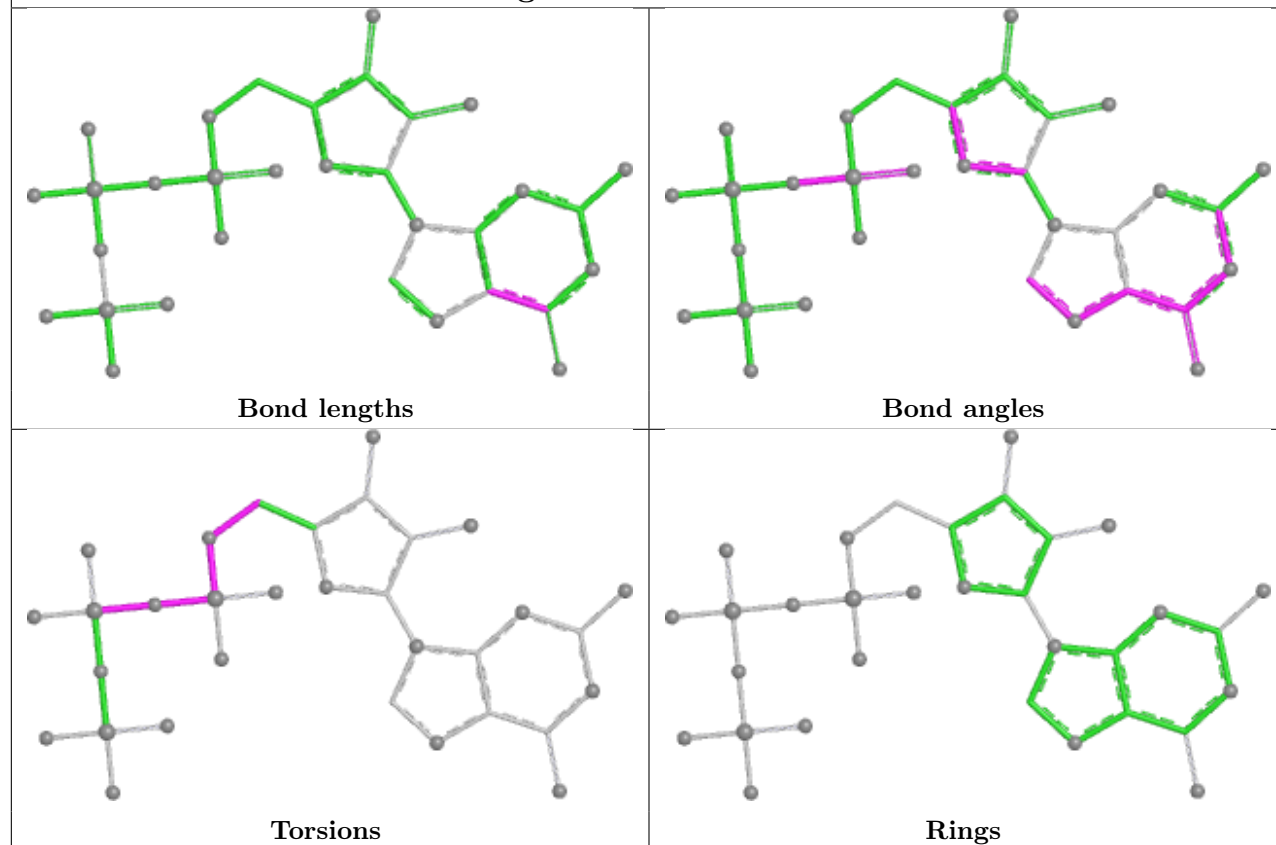


Ligand GTP MJ 501

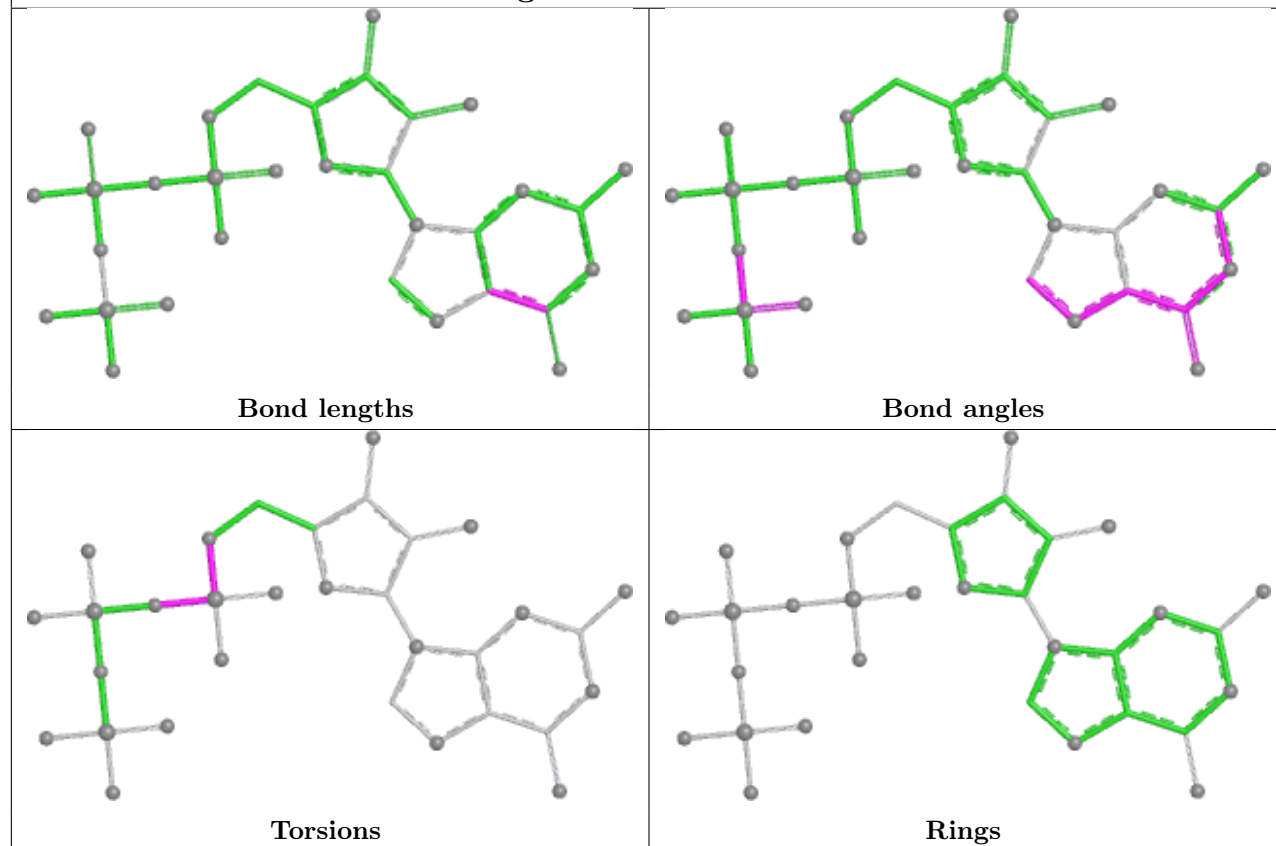


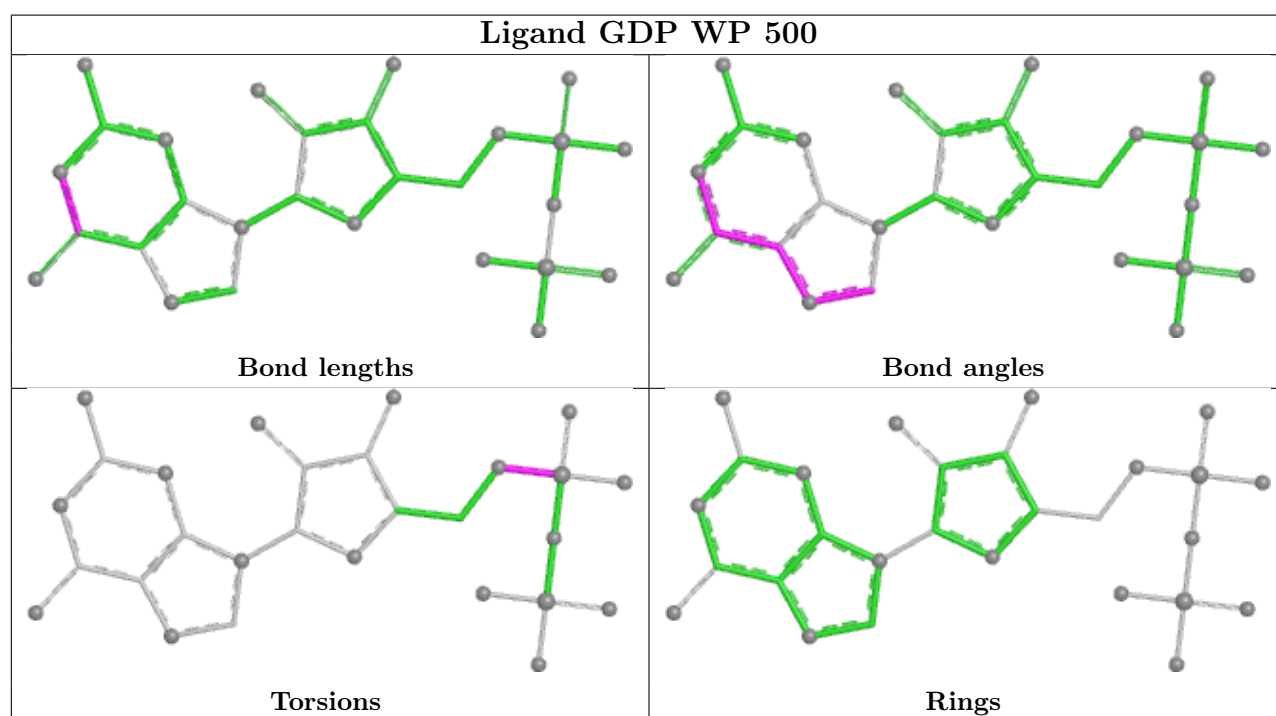
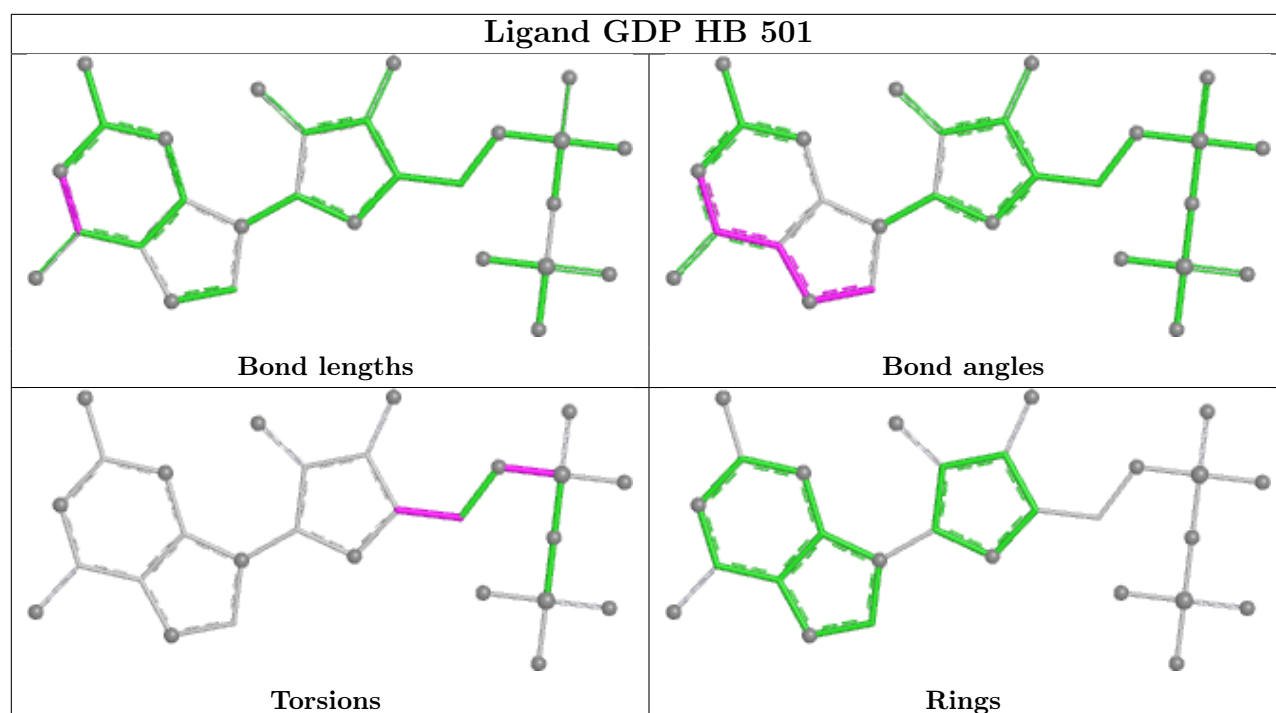


Ligand GTP EG 501

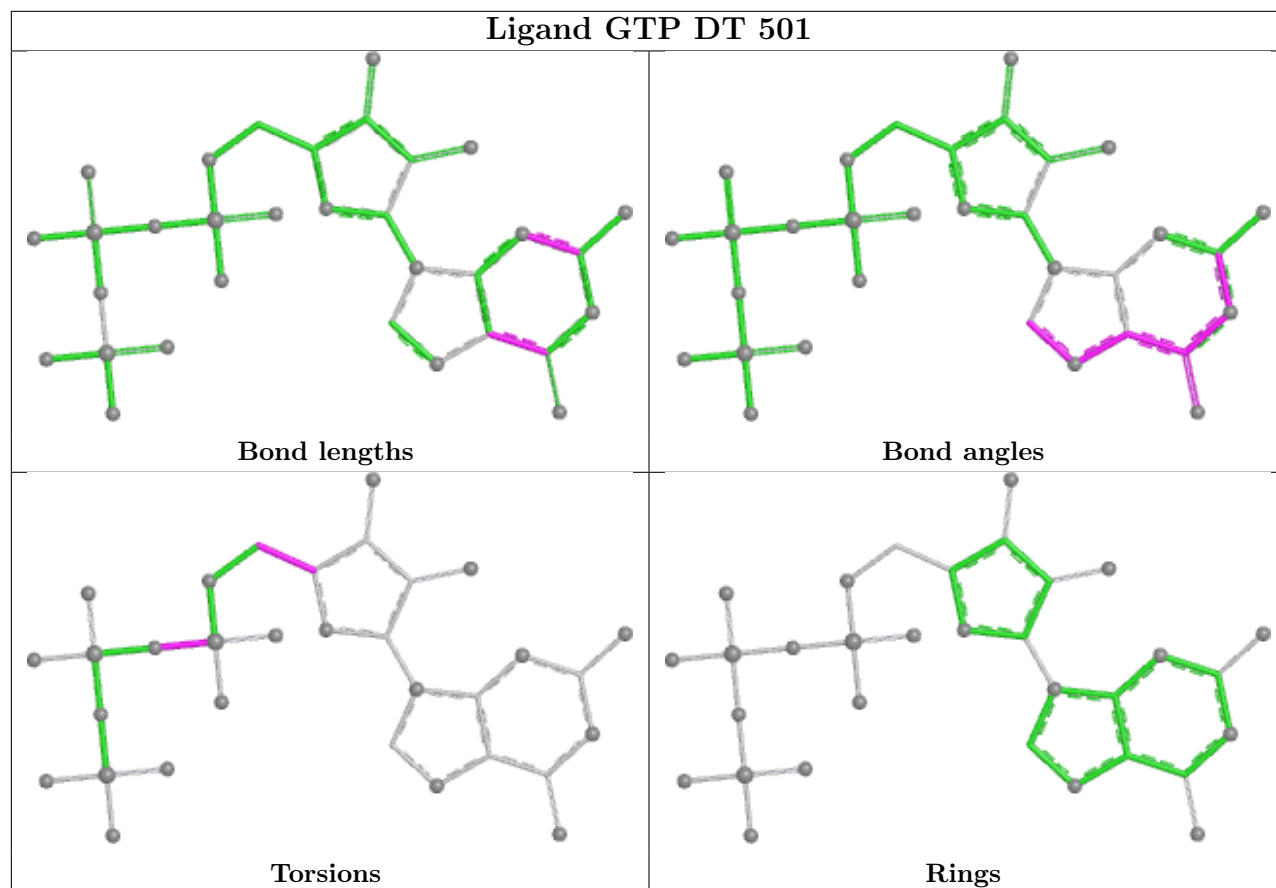


Ligand GTP BO 501

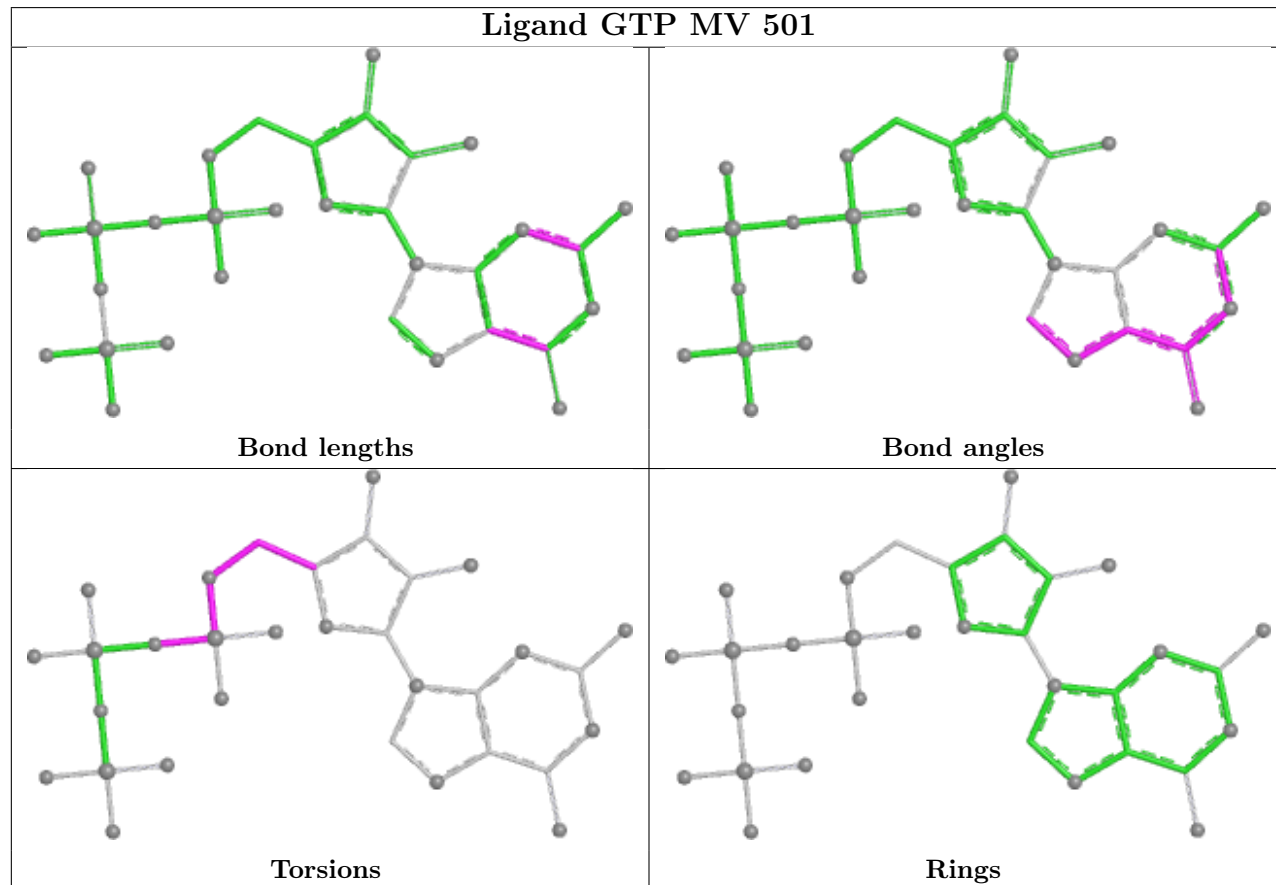




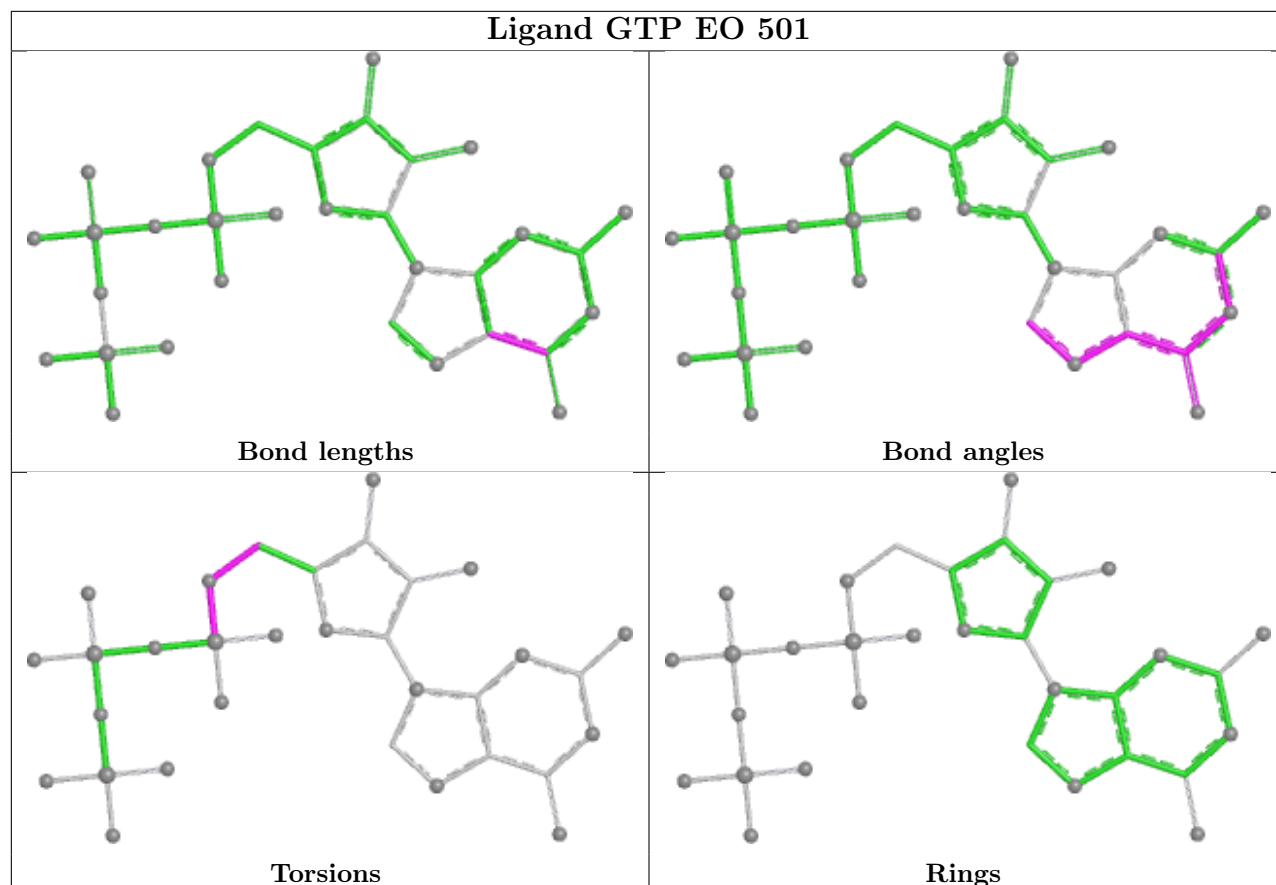
Ligand GTP DT 501



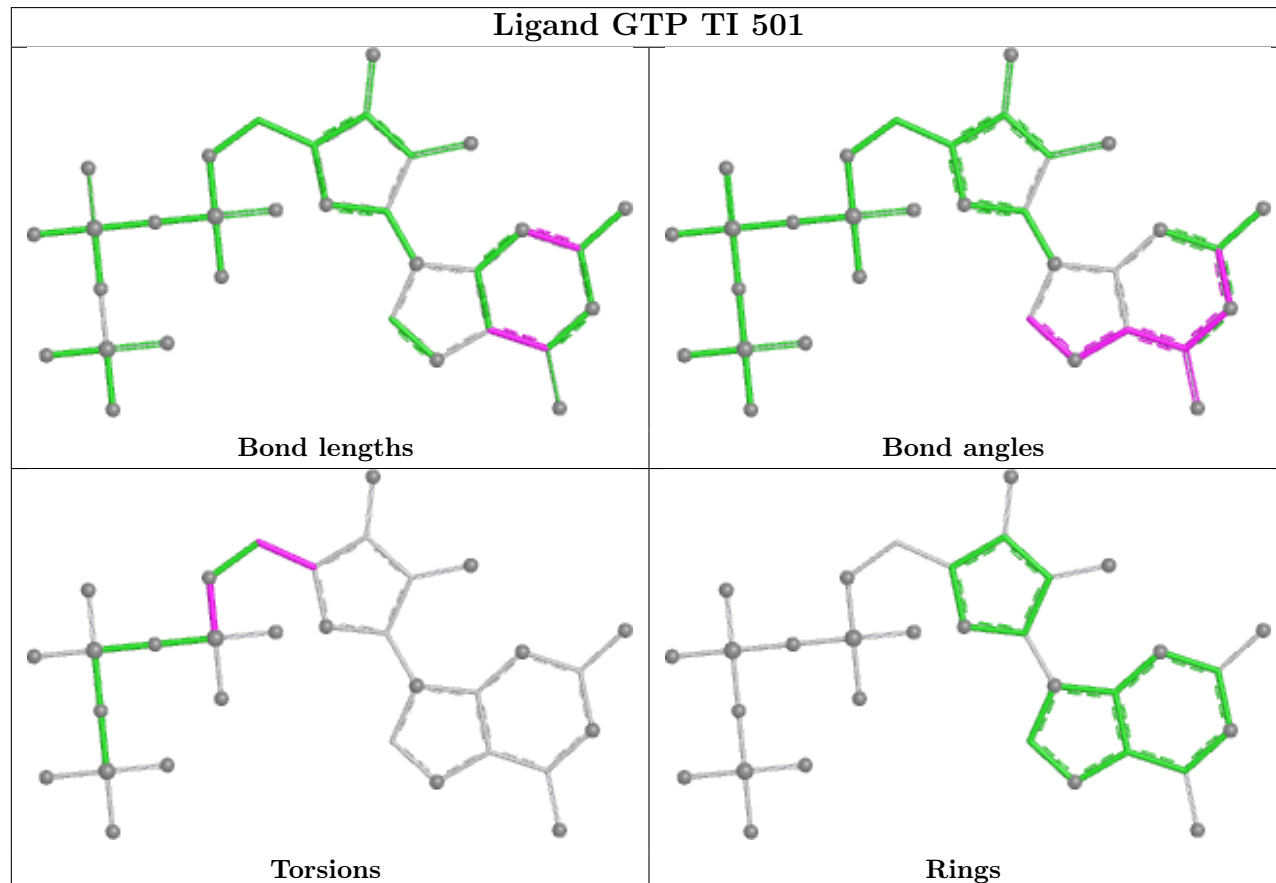
Ligand GTP MV 501



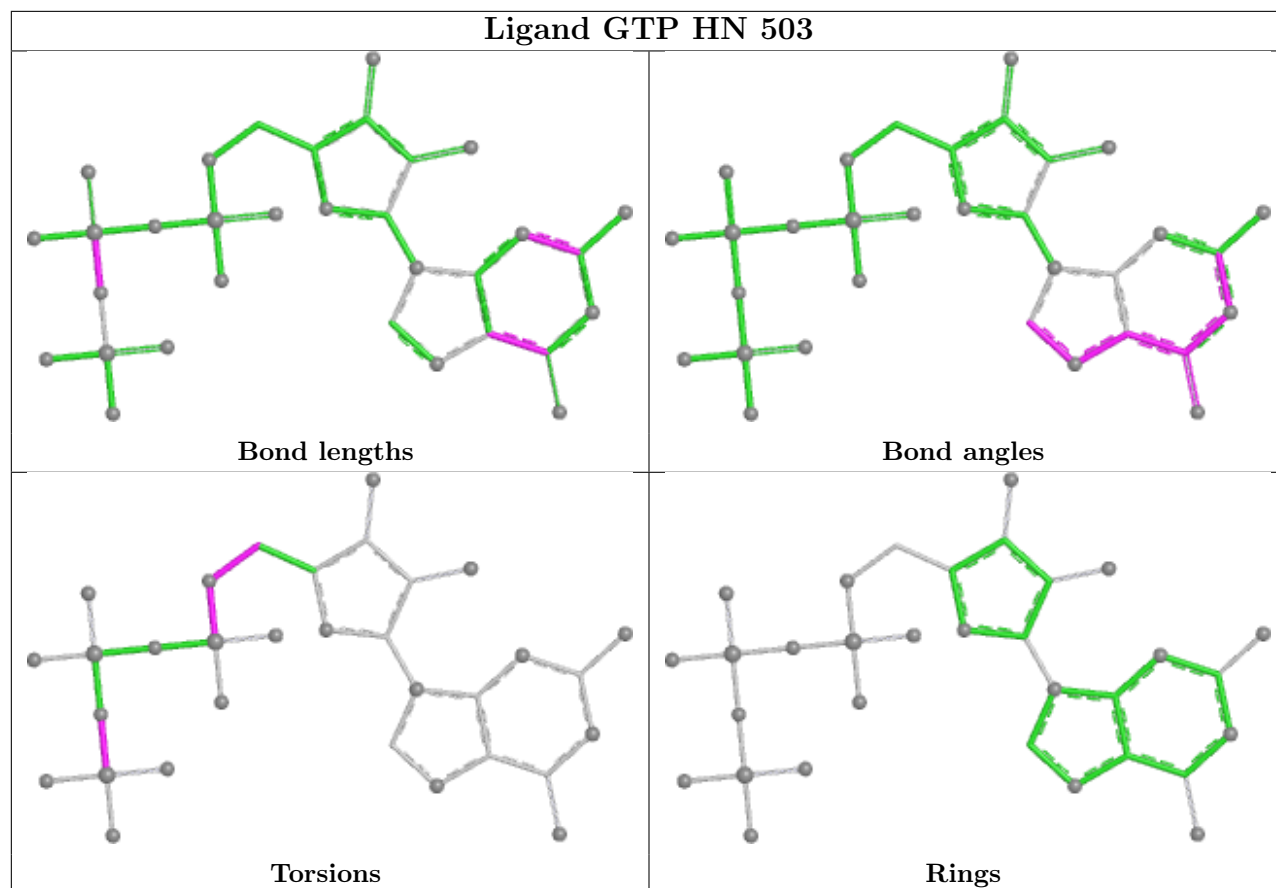
Ligand GTP EO 501



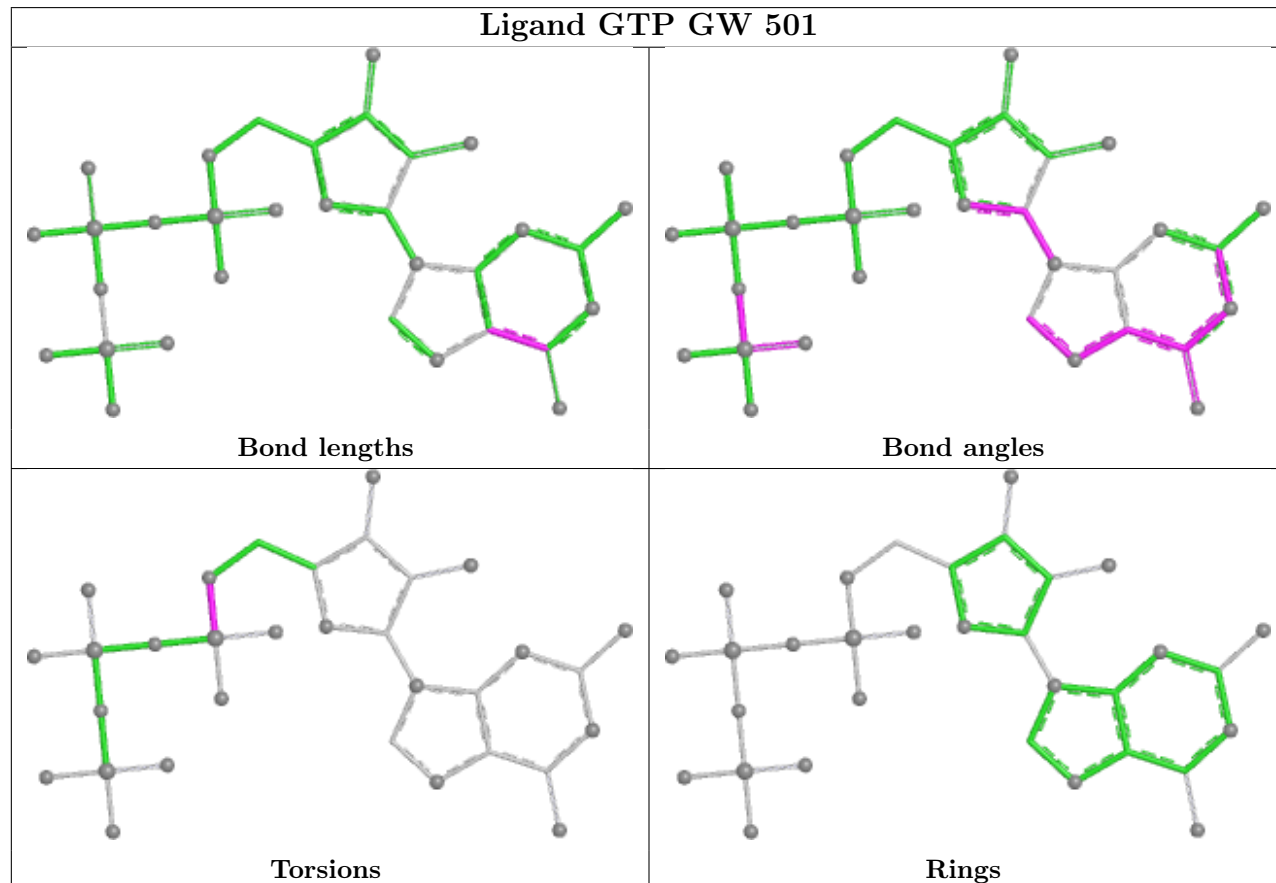
Ligand GTP TI 501

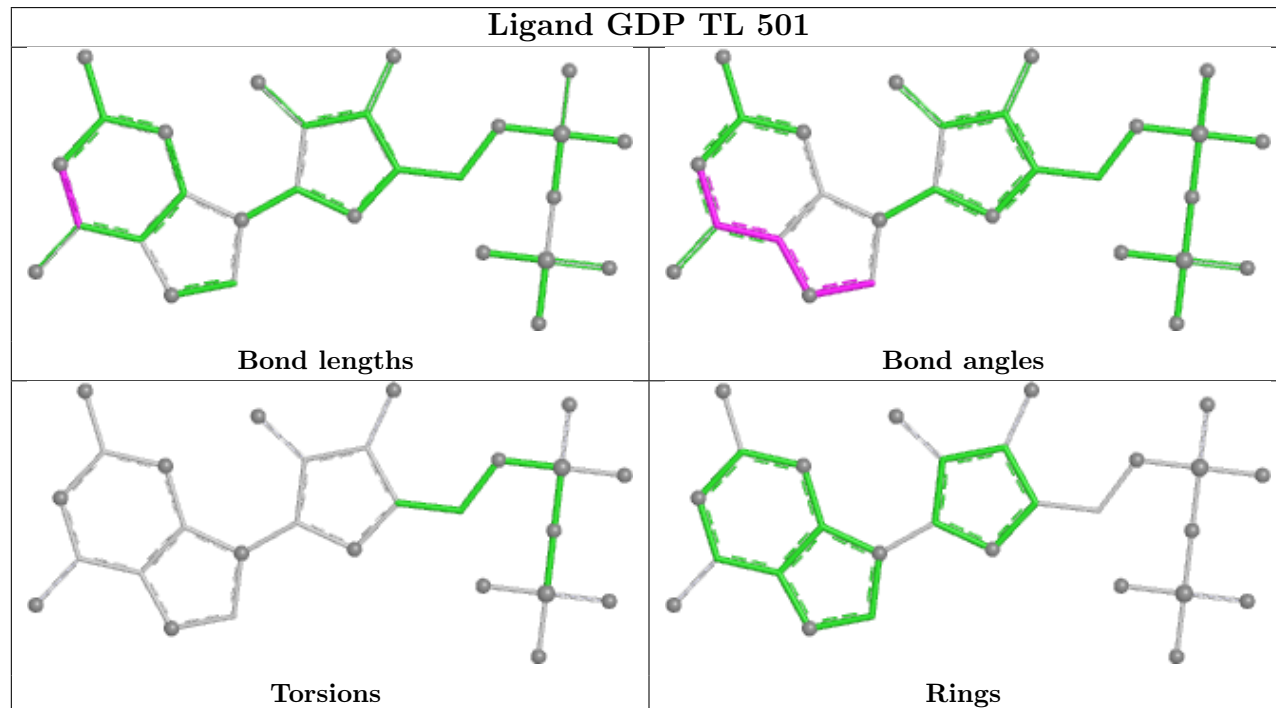
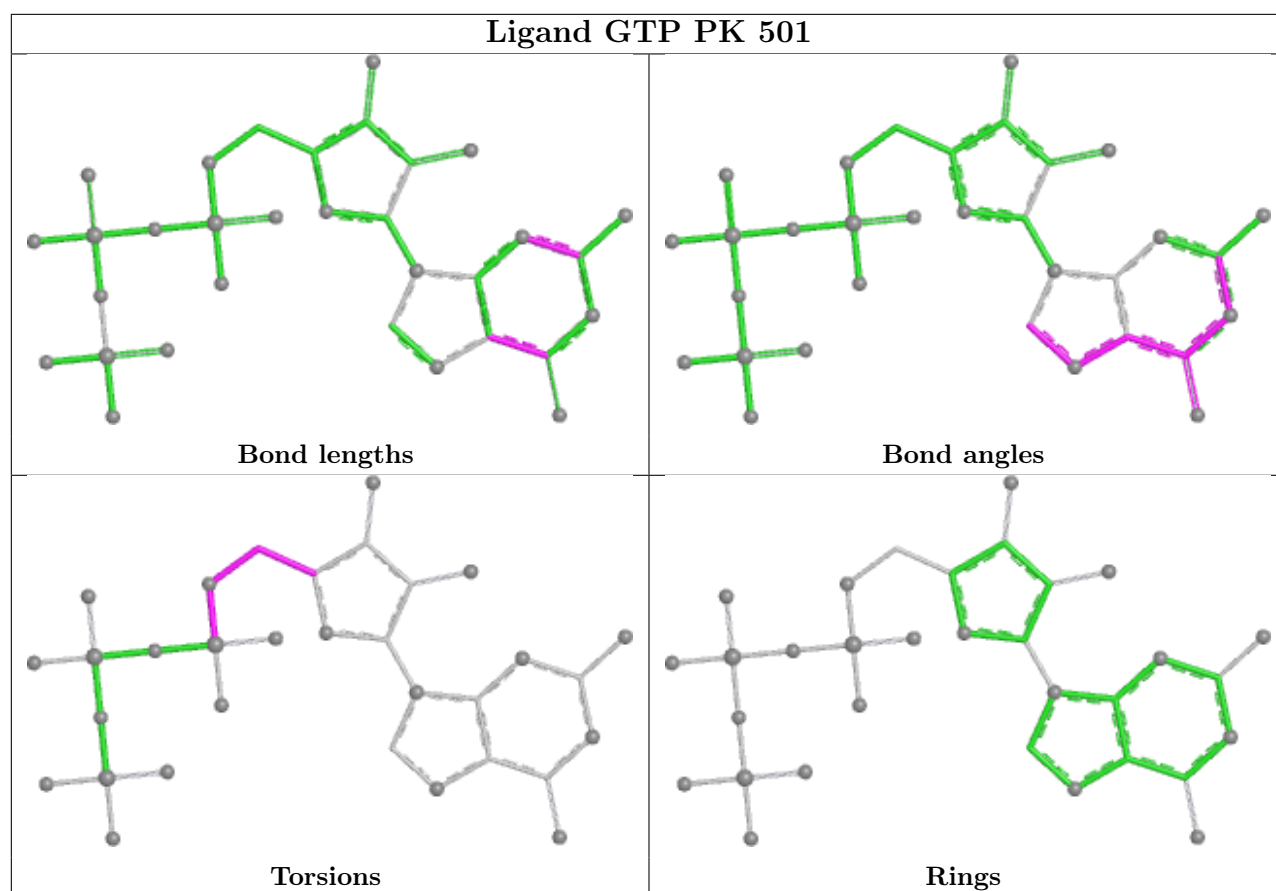


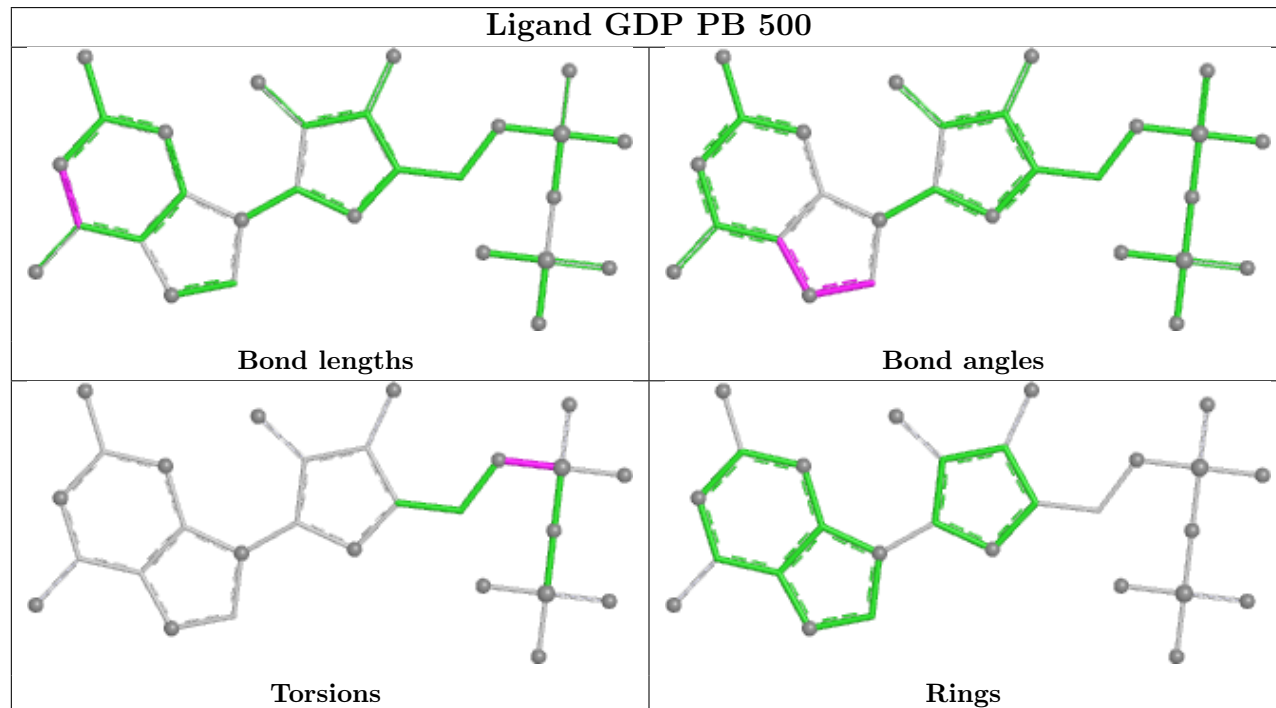
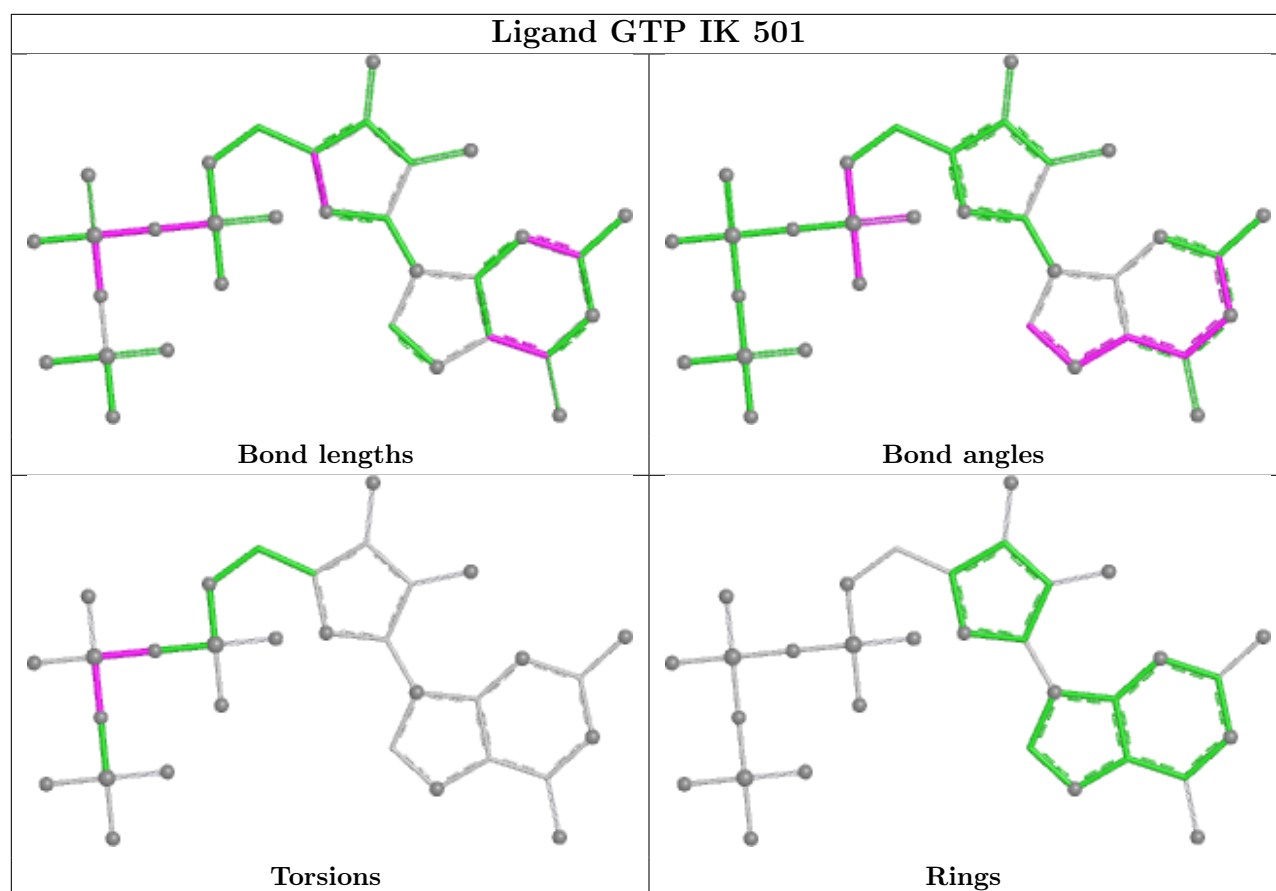
Ligand GTP HN 503

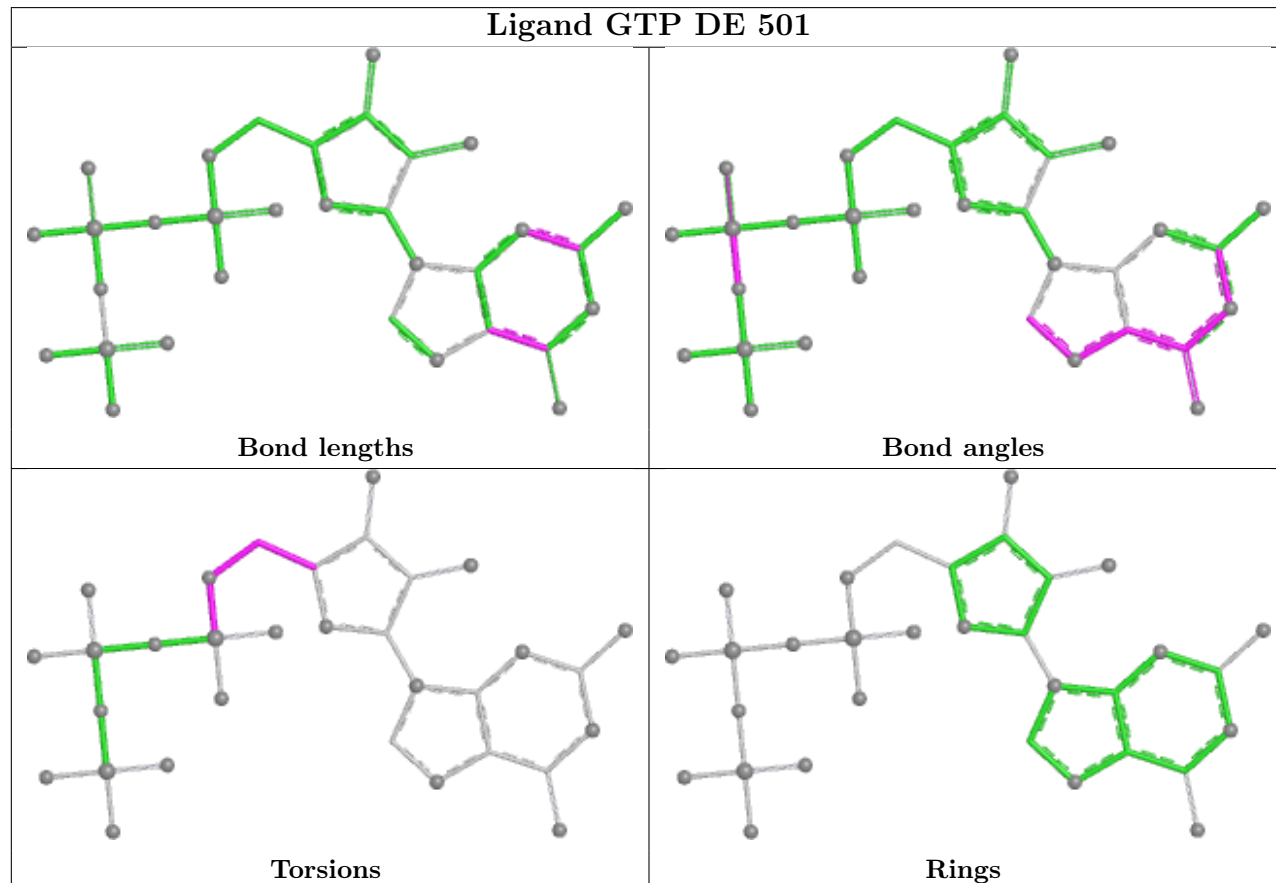
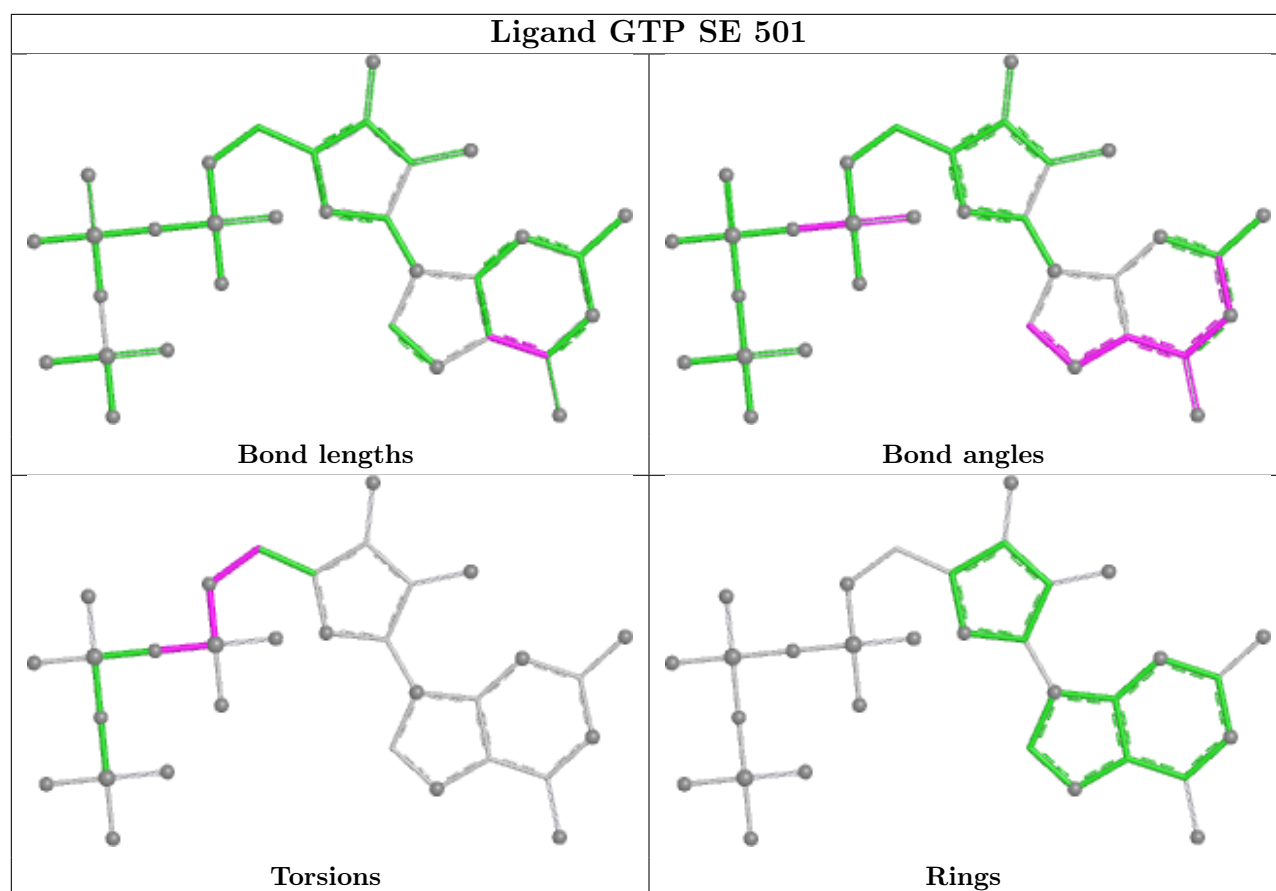


Ligand GTP GW 501









4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
67	5Z	4
67	5Y	4
67	5X	4
67	5a	3
68	5f	2
95	6t	1
68	5c	1
68	5d	1
109	9a	1
68	5e	1
67	5W	1
83	6k	1
16	0i	1
126	9N	1
2	GU	1
2	CB	1

The worst 5 of 28 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	5a	233:ASP	C	234:ASP	N	8.58
1	5Z	233:ASP	C	234:ASP	N	8.37
1	5Y	233:ASP	C	234:ASP	N	7.90
1	5X	233:ASP	C	234:ASP	N	7.70
1	5Z	496:PHE	C	497:LEU	N	7.54

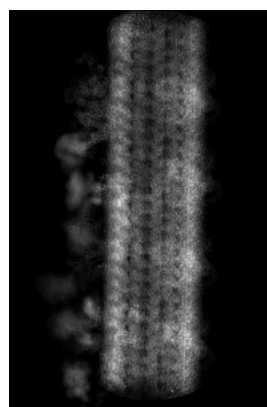
5 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-72629. These allow visual inspection of the internal detail of the map and identification of artifacts.

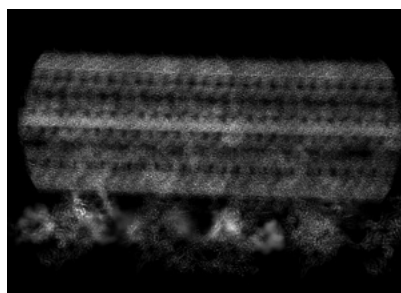
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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: 323



Y Index: 292

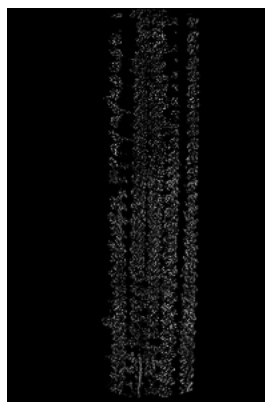


Z Index: 451

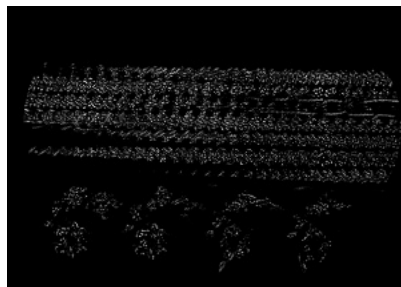
The images above show central slices of the map in three orthogonal directions.

5.3 Largest variance slices [i](#)

5.3.1 Primary map



X Index: 387



Y Index: 409

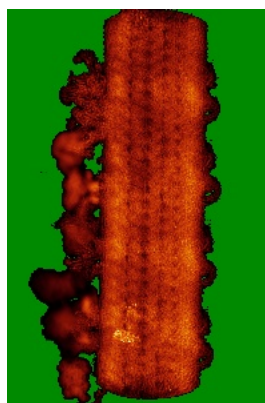


Z Index: 168

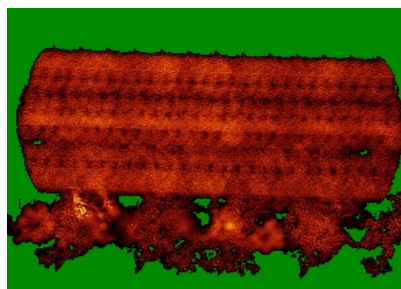
The images above show the largest variance slices of the map in three orthogonal directions.

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

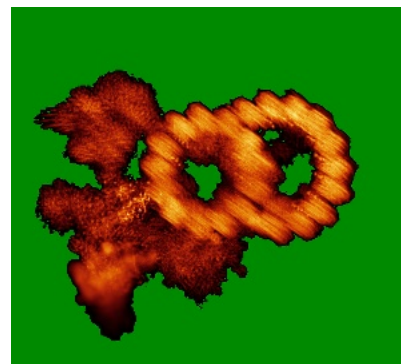
5.4.1 Primary map



X



Y

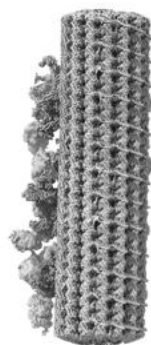


Z

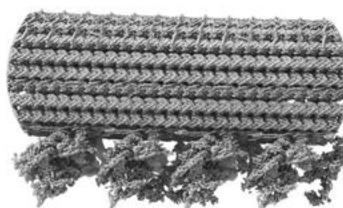
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

5.5 Orthogonal surface views [i](#)

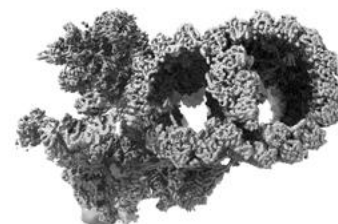
5.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.00285. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

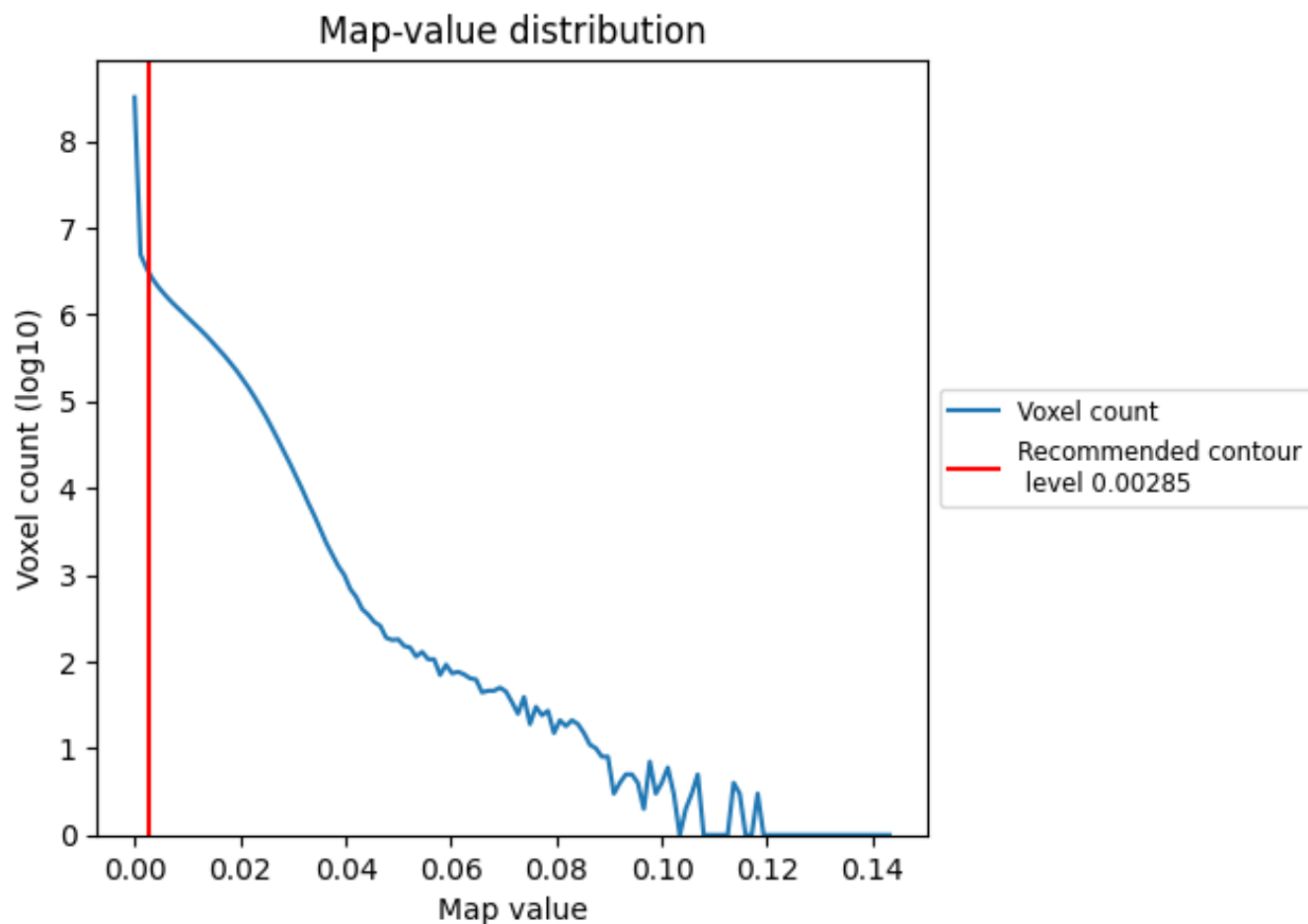
5.6 Mask visualisation [i](#)

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

6 Map analysis [i](#)

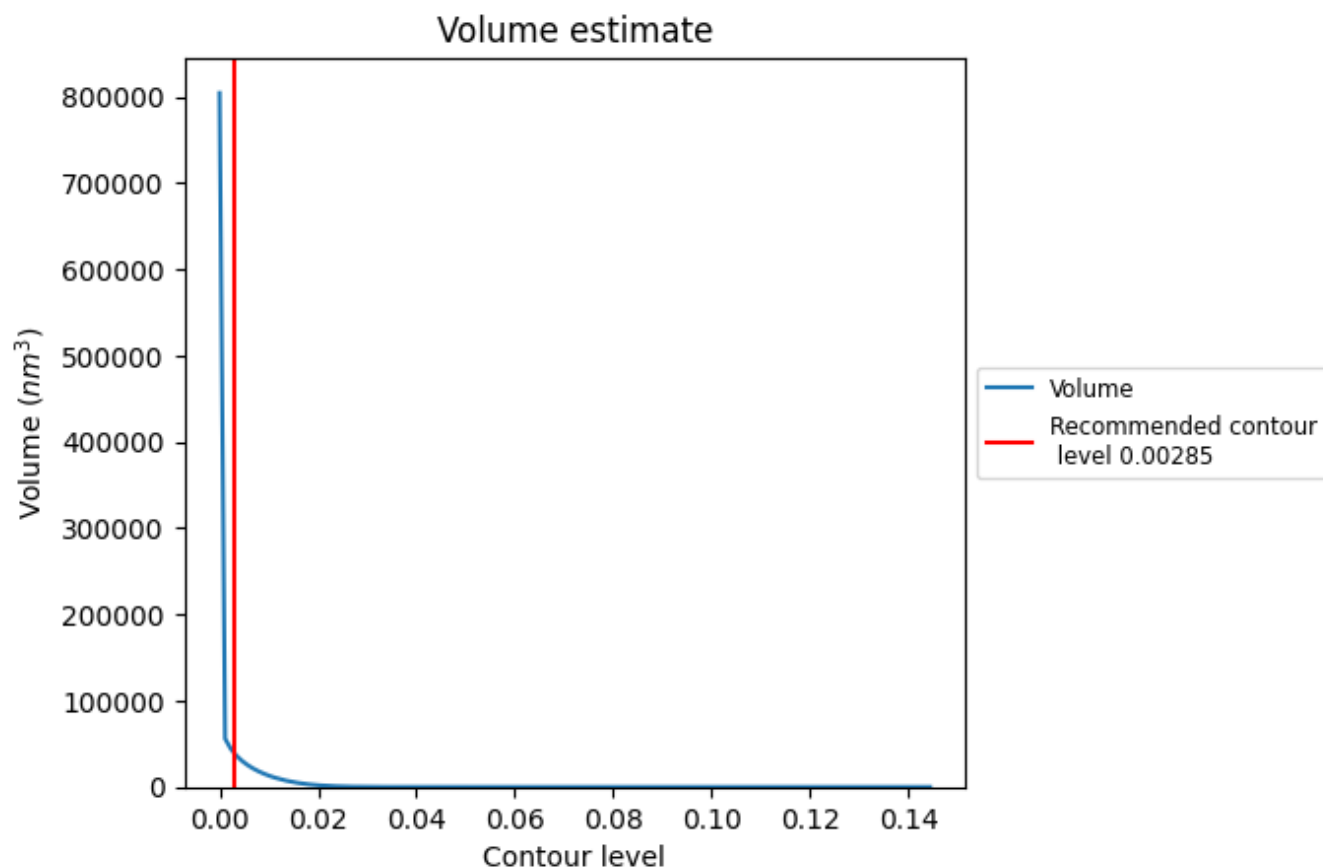
This section contains the results of statistical analysis of the map.

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 40261 nm³; this corresponds to an approximate mass of 36369 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.

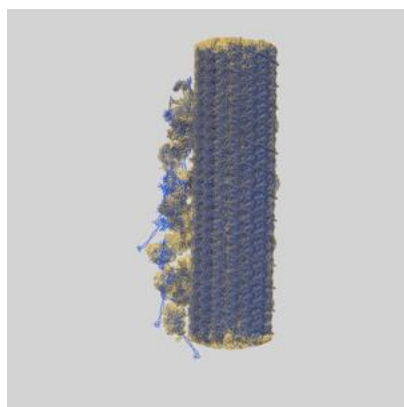
7 Fourier-Shell correlation ⓘ

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

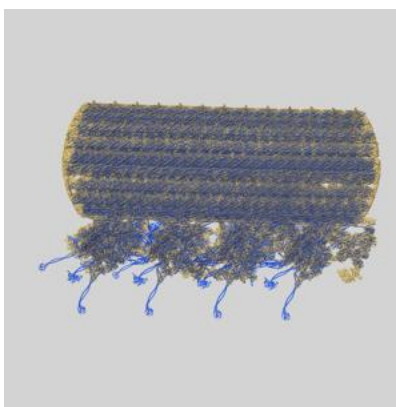
8 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-72629 and PDB model 9Y6S. Per-residue inclusion information can be found in section ?? on page ??.

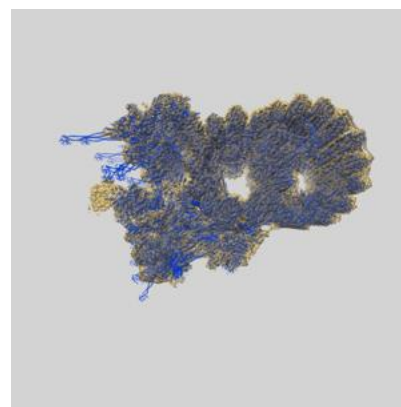
8.1 Map-model overlay [i](#)



X



Y



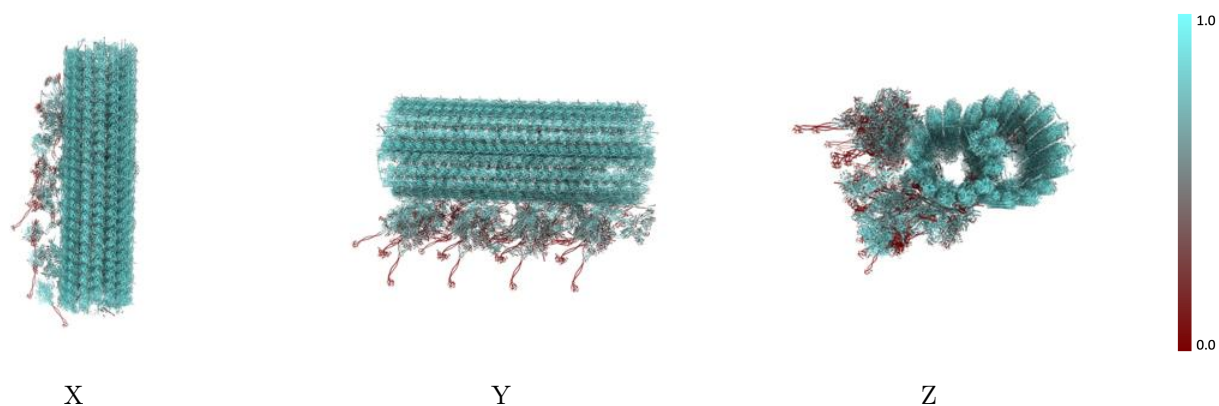
Z

The images above show the 3D surface view of the map at the recommended contour level 0.00285 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](#)

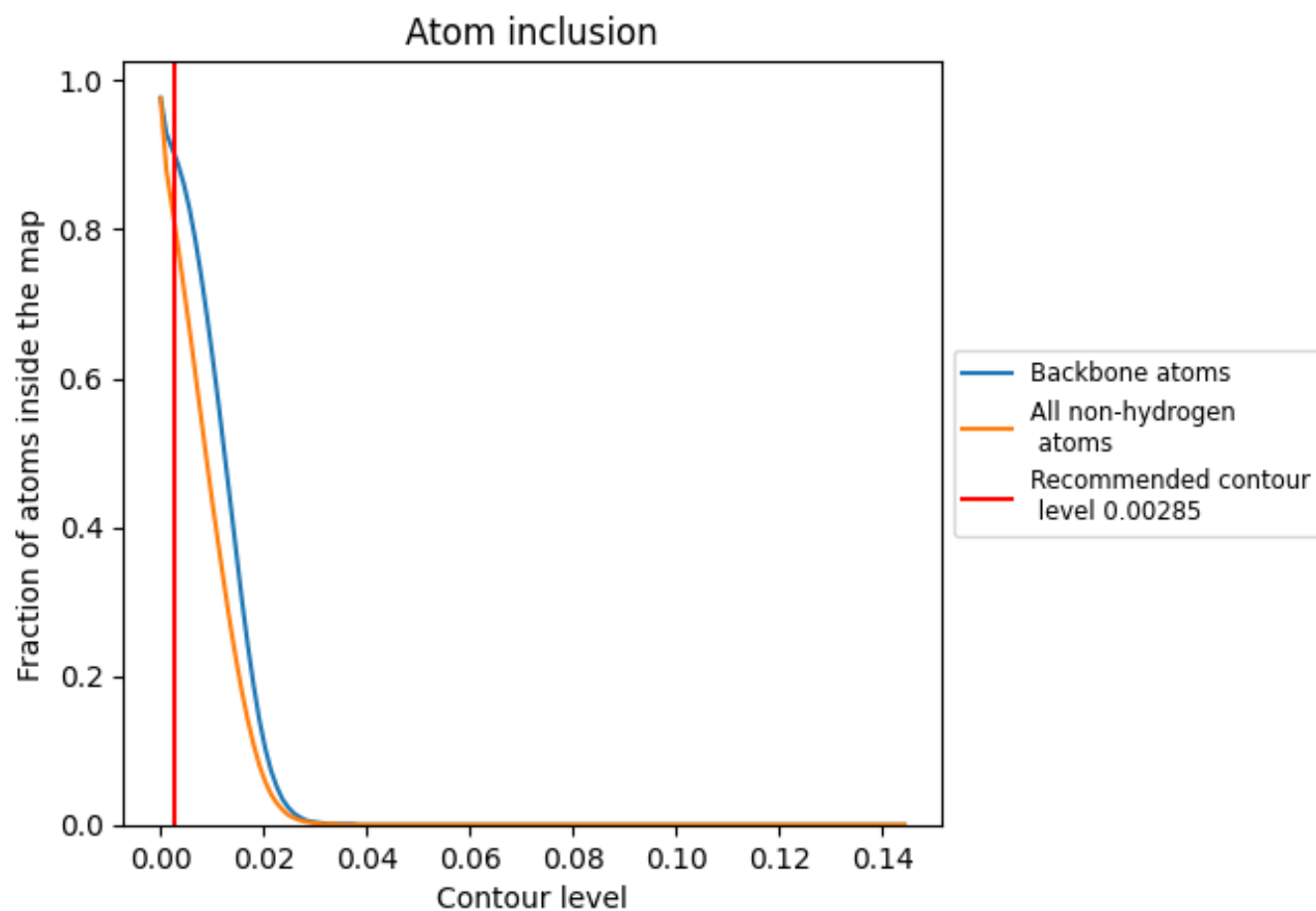
This section was not generated.

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 (0.00285).




































8.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 80% 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 (0.00285) and Q-score for the entire model and for each chain.

Chain	Atom inclusion
All	 0.8020
0	 0.8710
0A	 0.9280
0B	 0.9090
0C	 0.8280
0D	 0.8730
0E	 0.8890
0F	 0.7480
0G	 0.7360
0H	 0.7460
0I	 0.7140
0J	 0.7540
0K	 0.7890
0L	 0.8610
0M	 0.8560
0N	 0.8860
0O	 0.9080
0P	 0.8970
0Q	 0.8960
0R	 0.7770
0S	 0.8190
0T	 0.7940
0U	 0.8870
0V	 0.9180
0W	 0.8700
0X	 0.9050
0Y	 0.8440
0Z	 0.8100
0a	 0.8690
0b	 0.8520
0c	 0.7580
0d	 0.8470
0e	 0.8060
0f	 0.8930
0g	 0.9320













































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Chain	Atom inclusion
0h	 0.8840
0i	 0.7980
0j	 0.7980
0k	 0.8610
0l	 0.8050
0m	 0.7520
0n	 0.7350
0o	 0.7580
0p	 0.8020
0q	 0.8490
0r	 0.8500
0s	 0.8960
0t	 0.8970
0u	 0.9410
0v	 0.6740
0w	 0.7990
0x	 0.7890
0y	 0.8490
0z	 0.6000
1A	 0.8530
1B	 0.8730
1C	 0.8300
1D	 0.8340
1E	 0.8800
1F	 0.9190
1G	 0.8820
1H	 0.5880
1I	 0.7740
1J	 0.7890
1K	 0.8520
1L	 0.8430
1M	 0.8230
1N	 0.6460
1O	 0.7990
1P	 0.8700
1Q	 0.8410
1R	 0.8880
1S	 0.8270
1T	 0.8770
1U	 0.7780
1V	 0.8330
1W	 0.9060











































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Chain	Atom inclusion
1X	 0.7500
1Y	 0.7980
1Z	 0.8080
1a	 0.7200
1b	 0.8290
1c	 0.8550
1d	 0.7590
1e	 0.8150
1f	 0.8840
1g	 0.6760
1h	 0.7680
1i	 0.8120
1j	 0.8250
1k	 0.8570
1l	 0.9030
1m	 0.9060
1n	 0.8800
1o	 0.8700
1p	 0.9110
1q	 0.6560
1r	 0.5910
1s	 0.6180
1t	 0.7320
1u	 0.6510
1v	 0.6350
1w	 0.6050
1x	 0.7170
1y	 0.6960
1z	 0.7830
2A	 0.6200
2B	 0.8750
2C	 0.8640
2D	 0.9050
2E	 0.8910
2F	 0.8850
2G	 0.8770
2H	 0.8910
2I	 0.9300
2J	 0.9150
2K	 0.9000
2L	 0.7900
2M	 0.8370











































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Chain	Atom inclusion
2N	 0.8730
2O	 0.9020
2P	 0.9300
2Q	 0.8600
2R	 0.8930
2S	 0.8530
2U	 0.8070
2V	 0.8700
2W	 0.7900
2X	 0.7940
2Y	 0.8250
2Z	 0.7850
2a	 0.8370
2b	 0.7880
2c	 0.7890
2d	 0.8000
2e	 0.7780
2f	 0.8050
2g	 0.8050
2h	 0.7300
2i	 0.7910
2j	 0.7470
2k	 0.7120
2l	 0.7720
2m	 0.7660
2n	 0.6990
2o	 0.7160
2p	 0.7740
2q	 0.7710
2r	 0.7690
2s	 0.8520
2t	 0.8480
2u	 0.8870
2v	 0.7960
2w	 0.9280
2x	 0.9290
2y	 0.8440
2z	 0.8900
3A	 0.8570
3B	 0.8390
3C	 0.8910
3D	 0.7870











































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Chain	Atom inclusion
3E	 0.8410
3F	 0.3470
3G	 0.5420
3H	 0.3670
3I	 0.7090
3J	 0.6180
3K	 0.3790
3L	 0.7310
3M	 0.4630
3N	 0.8020
3O	 0.3680
3P	 0.8310
3Q	 0.9270
3R	 0.9230
3S	 0.8490
3T	 0.9150
3U	 0.8940
3V	 0.8900
3W	 0.7840
3X	 0.8440
3Y	 0.8090
3Z	 0.8070
3a	 0.6670
3b	 0.7750
3c	 0.8230
3d	 0.6500
3e	 0.7370
3f	 0.6590
3g	 0.7640
3h	 0.7400
3i	 0.7990
3j	 0.7850
3k	 0.7600
3l	 0.7550
3m	 0.7620
3n	 0.7610
3o	 0.6820
3p	 0.8320
3q	 0.8230
3r	 0.6890
3s	 0.7230
3t	 0.7740











































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Chain	Atom inclusion
3u	 0.8030
3v	 0.6850
3w	 0.8660
3x	 0.8880
3y	 0.8240
4A	 0.8050
4B	 0.8390
4C	 0.8540
4D	 0.8570
4E	 0.8370
4F	 0.8430
4G	 0.8710
4H	 0.8260
4I	 0.8440
4J	 0.9010
4K	 0.8040
4L	 0.8520
4M	 0.5810
4N	 0.8750
4O	 0.8300
4P	 0.8500
4Q	 0.8730
4R	 0.6810
4S	 0.8120
4T	 0.7120
4U	 0.8080
4V	 0.7830
4W	 0.7930
4X	 0.8280
4Y	 0.7670
4a	 0.7750
4b	 0.8810
4c	 0.8870
4d	 0.7020
4e	 0.7210
4f	 0.7230
4g	 0.7970
5A	 0.5230
5B	 0.5630
5C	 0.5510
5D	 0.5700
5E	 0.5890











































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Chain	Atom inclusion
5F	 0.4270
5G	 0.5440
5H	 0.5250
5I	 0.5580
5J	 0.6100
5K	 0.7190
5L	 0.6260
5M	 0.7100
5N	 0.6600
5O	 0.7230
5P	 0.5210
5Q	 0.7080
5R	 0.5340
5S	 0.7330
5T	 0.5840
5U	 0.7450
5V	 0.5950
5W	 0.4720
5X	 0.4880
5Y	 0.4910
5Z	 0.4700
5a	 0.6060
5b	 0.4340
5c	 0.4310
5d	 0.4380
5e	 0.4350
5f	 0.5210
5g	 0.6570
5h	 0.6600
5i	 0.6650
5j	 0.6600
5k	 0.6270
5l	 0.6330
5m	 0.6190
5n	 0.6080
5o	 0.0000
5p	 0.0000
5q	 0.0000
5r	 0.0000
5s	 0.4980
5t	 0.4930
5u	 0.4900











































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Chain	Atom inclusion
5v	 0.4960
5w	 0.6050
5x	 0.6100
5y	 0.6140
5z	 0.6370
6A	 0.6270
6B	 0.6510
6C	 0.6440
6D	 0.6360
6E	 0.6610
6F	 0.6560
6G	 0.6320
6H	 0.6630
6I	 0.6650
6J	 0.6760
6K	 0.6630
6L	 0.6550
6M	 0.4260
6N	 0.4550
6O	 0.4610
6P	 0.4860
6Q	 0.5620
6R	 0.5510
6S	 0.5470
6T	 0.5560
6U	 0.4300
6V	 0.4150
6W	 0.4030
6X	 0.4220
6Y	 0.5330
6Z	 0.5390
6a	 0.5330
6b	 0.5480
6c	 0.2800
6d	 0.2620
6e	 0.2660
6f	 0.2460
6g	 0.2750
6h	 0.3030
6i	 0.3120
6j	 0.3050
6k	 0.8310











































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Chain	Atom inclusion
6l	 0.8400
6m	 0.7950
6n	 0.8130
6o	 0.6570
6p	 0.8240
6q	 0.7770
6r	 0.7900
6s	 0.8500
6t	 0.7800
6u	 0.8220
6v	 0.5720
6w	 0.6370
6x	 0.4840
6y	 0.5280
6z	 0.4250
7A	 0.6980
7B	 0.7760
7C	 0.5120
7D	 0.7270
7E	 0.7140
7F	 0.4850
7G	 0.6320
7I	 0.6280
7K	 0.4390
7L	 0.4820
7M	 0.4450
7N	 0.5730
7O	 0.5840
7Q	 0.6110
7R	 0.5300
7S	 0.6900
7T	 0.7550
7U	 0.7170
7V	 0.7180
7W	 0.5700
7X	 0.5930
8A	 0.7180
8B	 0.6990
8C	 0.6760
8D	 0.7290
8E	 0.6940
8F	 0.6180











































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Chain	Atom inclusion
8G	 0.4230
8H	 0.4100
8I	 0.3610
8J	 0.5690
8K	 0.7030
8L	 0.5310
8M	 0.4110
8N	 0.5500
8O	 0.4790
8P	 0.5760
8R	 0.4920
8a	 0.7420
8b	 0.6420
8c	 0.4310
8d	 0.3030
8e	 0.6240
8f	 0.4750
8g	 0.7130
8h	 0.7020
8i	 0.7210
8j	 0.6250
8k	 0.6490
8l	 0.5940
8m	 0.4230
8n	 0.3260
8o	 0.3730
8p	 0.5520
8q	 0.4590
8r	 0.7810
8s	 0.7180
8t	 0.6510
8u	 0.6100
8v	 0.7670
8w	 0.6310
9A	 0.7140
9B	 0.8190
9C	 0.8170
9D	 0.8400
9E	 0.8230
9F	 0.8800
9G	 0.6730
9H	 0.3220











































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Chain	Atom inclusion
9I	 0.8730
9J	 0.5100
9K	 0.5610
9L	 0.3620
9M	 0.2620
9N	 0.4290
9O	 0.5440
9Q	 0.4430
9R	 0.6250
9S	 0.6060
9T	 0.6190
9U	 0.3950
9V	 0.3870
9W	 0.1320
9X	 0.1210
9Y	 0.4340
9Z	 0.4320
9a	 0.5280
9b	 0.5310
9c	 0.5640
9d	 0.7790
9e	 0.5080
9f	 0.5590
9g	 0.5960
9h	 0.5540
9i	 0.6850
9j	 0.7550
9k	 0.6770
9l	 0.7160
9m	 0.5640
9n	 0.5760
9o	 0.3740
9p	 0.2630
9q	 0.7370
9r	 0.2910
9s	 0.3390
9t	 0.5040
9u	 0.4650
A	 0.9080
AA	 0.9220
AB	 0.9160
AC	 0.8990











































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Chain	Atom inclusion
AD	 0.9230
AE	 0.9100
AF	 0.9150
AG	 0.8850
AH	 0.9090
AI	 0.9200
AJ	 0.9190
AK	 0.9300
AL	 0.9630
AM	 0.9630
AN	 0.9620
AO	 0.9330
AP	 0.9500
AQ	 0.9410
AR	 0.9410
AS	 0.9270
AT	 0.9380
AU	 0.9410
AV	 0.9450
AW	 0.9310
AX	 0.9440
AY	 0.9440
AZ	 0.8870
B	 0.8350
BA	 0.8550
BD	 0.9070
BE	 0.9310
BF	 0.9090
BG	 0.8990
BH	 0.9070
BI	 0.9100
BJ	 0.9200
BK	 0.9210
BL	 0.9520
BM	 0.9560
BN	 0.9570
BO	 0.9440
BP	 0.9470
BQ	 0.9530
BR	 0.9360
BS	 0.9320
BT	 0.9330











































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Chain	Atom inclusion
BU	 0.9340
BV	 0.9450
BW	 0.9310
BX	 0.9470
BY	 0.9220
C	 0.8430
CA	 0.8890
CB	 0.8820
CC	 0.9130
CD	 0.9320
CE	 0.9030
CF	 0.9010
CG	 0.8900
CH	 0.9080
CI	 0.9240
CJ	 0.9130
CK	 0.9460
CL	 0.9440
CM	 0.9500
CN	 0.9290
CO	 0.9470
CP	 0.9530
CQ	 0.9360
CR	 0.9280
CS	 0.9260
CT	 0.9490
CU	 0.9570
CV	 0.9380
CW	 0.9350
CX	 0.9260
CY	 0.8370
D	 0.7630
DA	 0.8960
DB	 0.9140
DC	 0.9210
DD	 0.9340
DE	 0.9040
DF	 0.9070
DG	 0.8980
DH	 0.9160
DI	 0.9320
DJ	 0.9080











































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Chain	Atom inclusion
DK	 0.9260
DL	 0.9530
DM	 0.9590
DN	 0.9520
DO	 0.9470
DP	 0.9560
DQ	 0.9430
DR	 0.9430
DS	 0.9250
DT	 0.9420
DU	 0.9590
DV	 0.9350
DW	 0.9370
DX	 0.9360
DY	 0.8570
E	 0.8390
EA	 0.8790
EB	 0.8880
EC	 0.9200
ED	 0.9130
EE	 0.9020
EF	 0.8990
EG	 0.9020
EH	 0.9260
EI	 0.8990
EJ	 0.8840
EK	 0.9260
EL	 0.9300
EM	 0.9350
EN	 0.9380
EO	 0.9540
EP	 0.9370
EQ	 0.9350
ER	 0.9440
ES	 0.9490
ET	 0.9500
EU	 0.9410
EV	 0.9350
EW	 0.9400
EX	 0.8610
F	 0.8400
FA	 0.8740











































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Chain	Atom inclusion
FB	 0.9060
FC	 0.9330
FD	 0.9210
FE	 0.9160
FF	 0.9160
FG	 0.9240
FH	 0.9310
FI	 0.9200
FJ	 0.9050
FK	 0.9330
FL	 0.9530
FM	 0.9230
FN	 0.9430
FO	 0.9600
FP	 0.9470
FQ	 0.9380
FR	 0.9520
FS	 0.9500
FT	 0.9600
FU	 0.9520
FV	 0.9380
FW	 0.9390
FX	 0.9030
G	 0.7340
GA	 0.8280
GB	 0.8790
GC	 0.9070
GD	 0.9220
GE	 0.8890
GF	 0.8900
GG	 0.8870
GH	 0.9060
GI	 0.9190
GJ	 0.9050
GK	 0.9180
GL	 0.9130
GM	 0.9180
GN	 0.9140
GO	 0.9390
GP	 0.9540
GQ	 0.9250
GR	 0.9210











































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Chain	Atom inclusion
GS	 0.9370
GT	 0.9460
GU	 0.9470
GV	 0.9410
GW	 0.9290
GX	 0.8940
H	 0.7530
HA	 0.8480
HB	 0.8630
HC	 0.8710
HD	 0.8930
HE	 0.8670
HF	 0.8590
HG	 0.8780
HH	 0.8840
HI	 0.9060
HJ	 0.8840
HK	 0.9020
HL	 0.9090
HM	 0.9170
HN	 0.8990
HO	 0.9000
HP	 0.9230
HQ	 0.9020
HR	 0.9040
HS	 0.9100
HT	 0.9190
HU	 0.9290
HV	 0.9220
HW	 0.9250
HX	 0.9010
HY	 0.8780
I	 0.7620
IA	 0.8270
IB	 0.8570
IC	 0.8850
ID	 0.8820
IE	 0.8810
IF	 0.8780
IG	 0.8840
IH	 0.8910
II	 0.8900











































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Chain	Atom inclusion
IJ	 0.8990
IK	 0.9000
IL	 0.8930
IM	 0.9110
IN	 0.9100
IO	 0.9130
IP	 0.9230
IQ	 0.9290
IR	 0.9210
IS	 0.9300
IT	 0.9300
IU	 0.9290
IV	 0.9270
IW	 0.9220
IX	 0.8760
IY	 0.8590
J	 0.7850
JA	 0.8590
JB	 0.8730
JC	 0.8880
JD	 0.9020
JE	 0.9050
JF	 0.8920
JG	 0.8860
JH	 0.8930
JI	 0.9060
JJ	 0.8920
JK	 0.9150
JL	 0.9280
JM	 0.9320
JN	 0.9240
JO	 0.9220
JP	 0.9300
JQ	 0.9380
JR	 0.9340
JS	 0.9260
JT	 0.9230
JU	 0.9290
JV	 0.9300
JW	 0.9320
JX	 0.9090
JY	 0.8830











































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Chain	Atom inclusion
JZ	 0.8610
K	 0.8800
KA	 0.8990
KB	 0.9120
KC	 0.8990
KD	 0.9230
KE	 0.9230
KF	 0.9050
KG	 0.8930
KH	 0.8980
KI	 0.9100
KJ	 0.9250
KK	 0.9310
KL	 0.9460
KM	 0.9400
KN	 0.9480
KO	 0.9470
KP	 0.9470
KQ	 0.9500
KR	 0.9280
KS	 0.9250
KT	 0.9290
KU	 0.9360
KV	 0.9420
KW	 0.9430
KX	 0.9390
KY	 0.9340
KZ	 0.9300
L	 0.8680
LA	 0.9370
LB	 0.9260
LC	 0.9220
LD	 0.9220
LE	 0.9190
LF	 0.9170
LG	 0.9120
LH	 0.9130
LI	 0.9240
LJ	 0.9170
LK	 0.9300
LL	 0.9490
LM	 0.9690











































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Chain	Atom inclusion
LN	 0.9610
LO	 0.9560
LP	 0.9510
LQ	 0.9540
LR	 0.9400
LS	 0.9390
LT	 0.9480
LU	 0.9500
LV	 0.9400
LW	 0.9450
LX	 0.9470
LY	 0.9650
LZ	 0.9470
M	 0.9100
MA	 0.9240
MB	 0.9090
MC	 0.9000
MD	 0.8920
ME	 0.9050
MF	 0.9070
MG	 0.8730
MH	 0.9050
MI	 0.8880
MJ	 0.9170
MK	 0.9300
ML	 0.9430
MM	 0.9530
MN	 0.9400
MO	 0.9300
MP	 0.9270
MQ	 0.9360
MR	 0.9350
MS	 0.9080
MT	 0.9300
MU	 0.9220
MV	 0.9370
MW	 0.9130
MX	 0.9300
MY	 0.9430
MZ	 0.8550
N	 0.7990
NA	 0.8130











































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Chain	Atom inclusion
NB	 0.8590
NC	 0.8650
ND	 0.8840
NE	 0.8670
NF	 0.8550
NG	 0.8360
NH	 0.8900
NI	 0.8840
NJ	 0.9040
NK	 0.8960
NL	 0.8970
NM	 0.8910
NN	 0.9200
NO	 0.8970
NP	 0.9200
NQ	 0.9050
NR	 0.9000
NS	 0.8920
NT	 0.9160
NU	 0.9090
NV	 0.9240
NW	 0.8960
NX	 0.8840
NY	 0.8530
O	 0.8000
OA	 0.8420
OB	 0.8680
OC	 0.8830
OD	 0.9180
OE	 0.9090
OF	 0.8790
OG	 0.8480
OH	 0.9100
OI	 0.9050
OJ	 0.9090
OK	 0.9110
OL	 0.9000
OM	 0.9200
ON	 0.9300
OO	 0.9200
OP	 0.9410
OQ	 0.9380











































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Chain	Atom inclusion
OR	 0.9290
OS	 0.9000
OT	 0.9390
OU	 0.9260
OV	 0.9320
OW	 0.9160
OX	 0.8740
OY	 0.8560
P	 0.7780
PA	 0.8290
PB	 0.8860
PC	 0.8980
PD	 0.9080
PE	 0.9090
PF	 0.9100
PG	 0.9010
PH	 0.9200
PI	 0.9150
PJ	 0.9150
PK	 0.9210
PL	 0.9060
PM	 0.9200
PN	 0.9290
PO	 0.9310
PP	 0.9310
PQ	 0.9380
PR	 0.9350
PS	 0.9180
PT	 0.9400
PU	 0.9350
PV	 0.9300
PW	 0.9360
PX	 0.9140
PY	 0.8900
Q	 0.8100
QA	 0.8830
QB	 0.9010
QC	 0.9260
QD	 0.9290
QE	 0.9280
QF	 0.9140
QG	 0.9320











































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Chain	Atom inclusion
QH	 0.9130
QI	 0.9370
QJ	 0.9350
QK	 0.9110
QL	 0.9350
QM	 0.9320
QN	 0.9300
QO	 0.9420
QP	 0.9510
QQ	 0.9430
QR	 0.9280
QS	 0.9370
QT	 0.9350
QU	 0.9510
QV	 0.9510
QW	 0.9110
QX	 0.9080
R	 0.7950
RA	 0.8710
RB	 0.8940
RC	 0.9140
RD	 0.9400
RE	 0.9330
RF	 0.9190
RG	 0.9100
RH	 0.9310
RI	 0.9400
RJ	 0.9270
RK	 0.8980
RL	 0.9220
RM	 0.9320
RN	 0.9300
RO	 0.9430
RP	 0.9530
RQ	 0.9440
RR	 0.9290
RS	 0.9270
RT	 0.9420
RU	 0.9510
RV	 0.9430
RW	 0.9180
RX	 0.8950











































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Chain	Atom inclusion
S	 0.8700
SA	 0.9110
SB	 0.9090
SC	 0.9290
SD	 0.9120
SE	 0.9020
SF	 0.8930
SG	 0.9110
SH	 0.9100
SI	 0.9210
SJ	 0.8890
SK	 0.9220
SL	 0.9300
SM	 0.9340
SN	 0.9370
SO	 0.9550
SP	 0.9400
SQ	 0.9300
SR	 0.9260
SS	 0.9330
ST	 0.9380
SU	 0.9420
SV	 0.9280
SW	 0.9120
T	 0.8590
TA	 0.9010
TB	 0.9090
TC	 0.9210
TD	 0.9140
TE	 0.9050
TF	 0.9030
TG	 0.8970
TH	 0.9260
TI	 0.9180
TJ	 0.9020
TK	 0.9160
TL	 0.9270
TM	 0.9370
TN	 0.9420
TO	 0.9500
TP	 0.9410
TQ	 0.9340











































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Chain	Atom inclusion
TR	 0.9370
TS	 0.9320
TT	 0.9480
TU	 0.9450
TV	 0.9260
TW	 0.9170
TX	 0.8550
U	 0.8210
UA	 0.8720
UB	 0.8760
UC	 0.8970
UD	 0.9090
UE	 0.8860
UF	 0.8870
UG	 0.8950
UH	 0.8950
UI	 0.8960
UJ	 0.8680
UK	 0.9050
UL	 0.9170
UM	 0.9240
UN	 0.9150
UO	 0.9260
UP	 0.9410
UQ	 0.9200
UR	 0.9190
US	 0.9190
UT	 0.9290
UU	 0.9220
UV	 0.9080
UW	 0.9060
UX	 0.8700
V	 0.8570
VA	 0.8900
VB	 0.8940
VC	 0.9040
VD	 0.9160
VE	 0.8890
VF	 0.8900
VG	 0.8850
VH	 0.8920
VI	 0.9010


























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Chain	Atom inclusion
VJ	 0.8870
VK	 0.9210
VL	 0.9300
VM	 0.9240
VN	 0.9220
VO	 0.9290
VP	 0.9430
VQ	 0.9170
VR	 0.9160
VS	 0.9150
VT	 0.9290
VU	 0.9350
VV	 0.9080
VW	 0.9230
VX	 0.9130
VY	 0.8290
W	 0.8470
WA	 0.8840
WB	 0.8820
WC	 0.8940
WD	 0.9070
WE	 0.8890
WF	 0.8820
WG	 0.8860
WH	 0.8840
WI	 0.9020
WJ	 0.8780
WK	 0.9110
WL	 0.9200
WM	 0.9330
WN	 0.9260
WO	 0.9260
WP	 0.9330
WQ	 0.9120
WR	 0.9070
WS	 0.9080
WT	 0.9160
WU	 0.9300
WV	 0.9130
WW	 0.9110
WX	 0.8970
WY	 0.8710

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Chain	Atom inclusion
X	 0.8970
X1	 0.8710
XA	 0.9080
XB	 0.9380
XC	 0.9150
XD	 0.9270
XE	 0.9450
XF	 0.9490
XG	 0.9320
XH	 0.9410
XI	 0.9220
XJ	 0.9450
XK	 0.9260
XL	 0.9270
XM	 0.8880
XN	 0.9010
XO	 0.9130
XP	 0.8660
XQ	 0.8940
XR	 0.9340
XS	 0.9280
XT	 0.9130
XU	 0.8940
XV	 0.9240
XW	 0.8580