



## wwPDB EM Validation Summary Report ⓘ

Mar 23, 2025 – 01:40 pm GMT

PDB ID : 9FQR  
EMDB ID : EMD-50664  
Title : 96-nm repeat of axonemal doublet microtubules from bovine sperm  
Authors : Leung, M.R.; Sun, C.; Zeng, J.; Anderson, J.R.; Niu, Q.; Huang, W.; Noteborn, W.E.M.; Brown, A.; Zeev-Ben-Mordehai, T.; Zhang, R.  
Deposited on : 2024-06-21  
Resolution : 5.00 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis	:	0.0.1.dev117
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	<b>FAILED</b>
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	<b>FAILED</b>
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.5

# 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 5.00 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 4527463 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 UPF0602 protein C4orf47 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	27	Total	C	N	O	S	0	0
			238	149	44	43	2		
1	W	124	Total	C	N	O	S	0	0
			990	626	176	185	3		
1	Wh	124	Total	C	N	O	S	0	0
			990	626	176	185	3		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
0	199	PRO	THR	variant	UNP Q2T9M0
W	199	PRO	THR	variant	UNP Q2T9M0
Wh	199	PRO	THR	variant	UNP Q2T9M0

- Molecule 2 is a protein called Sperm acrosome associated 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	0A	156	Total	C	N	O	S	0	0
			1252	782	224	236	10		
2	0B	156	Total	C	N	O	S	0	0
			1252	782	224	236	10		
2	0C	156	Total	C	N	O	S	0	0
			1252	782	224	236	10		
2	0D	156	Total	C	N	O	S	0	0
			1252	782	224	236	10		
2	0E	157	Total	C	N	O	S	0	0
			1260	787	225	237	11		
2	0F	157	Total	C	N	O	S	0	0
			1260	787	225	237	11		
2	0G	156	Total	C	N	O	S	0	0
			1252	782	224	236	10		
2	0H	156	Total	C	N	O	S	0	0
			1252	782	224	236	10		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	0Y	156	Total	C	N	O	S	0	0
			1252	782	224	236	10		
2	0Z	156	Total	C	N	O	S	0	0
			1252	782	224	236	10		
2	0a	156	Total	C	N	O	S	0	0
			1252	782	224	236	10		
2	0c	156	Total	C	N	O	S	0	0
			1252	782	224	236	10		
2	0d	156	Total	C	N	O	S	0	0
			1252	782	224	236	10		
2	0e	155	Total	C	N	O	S	0	0
			1244	777	223	235	9		
2	0f	155	Total	C	N	O	S	0	0
			1244	777	223	235	9		
2	0g	156	Total	C	N	O	S	0	0
			1252	782	224	236	10		
2	0h	155	Total	C	N	O	S	0	0
			1244	777	223	235	9		
2	0i	156	Total	C	N	O	S	0	0
			1252	782	224	236	10		
2	0j	156	Total	C	N	O	S	0	0
			1252	782	224	236	10		
2	0k	156	Total	C	N	O	S	0	0
			1252	782	224	236	10		
2	CT	157	Total	C	N	O	S	0	0
			1260	787	225	237	11		
2	CU	155	Total	C	N	O	S	0	0
			1244	777	223	235	9		
2	CV	156	Total	C	N	O	S	0	0
			1252	782	224	236	10		
2	CX	156	Total	C	N	O	S	0	0
			1252	782	224	236	10		
2	CY	156	Total	C	N	O	S	0	0
			1252	782	224	236	10		
2	CZ	156	Total	C	N	O	S	0	0
			1252	782	224	236	10		
2	Ca	156	Total	C	N	O	S	0	0
			1252	782	224	236	10		
2	Cb	156	Total	C	N	O	S	0	0
			1252	782	224	236	10		
2	Cc	156	Total	C	N	O	S	0	0
			1252	782	224	236	10		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	Cd	156	Total	C	N	O	S	0	0
			1252	782	224	236	10		
2	Ce	155	Total	C	N	O	S	0	0
			1244	777	223	235	9		
2	Cf	155	Total	C	N	O	S	0	0
			1244	777	223	235	9		
2	Cg	156	Total	C	N	O	S	0	0
			1252	782	224	236	10		
2	Ch	156	Total	C	N	O	S	0	0
			1252	782	224	236	10		
2	Ci	156	Total	C	N	O	S	0	0
			1252	782	224	236	10		
2	Cj	155	Total	C	N	O	S	0	0
			1244	777	223	235	9		
2	Ck	156	Total	C	N	O	S	0	0
			1252	782	224	236	10		
2	El	156	Total	C	N	O	S	0	0
			1252	782	224	236	10		
2	Em	156	Total	C	N	O	S	0	0
			1252	782	224	236	10		
2	En	156	Total	C	N	O	S	0	0
			1252	782	224	236	10		
2	Eo	156	Total	C	N	O	S	0	0
			1252	782	224	236	10		
2	Ep	156	Total	C	N	O	S	0	0
			1252	782	224	236	10		
2	Et	156	Total	C	N	O	S	0	0
			1252	782	224	236	10		
2	Eu	156	Total	C	N	O	S	0	0
			1252	782	224	236	10		
2	Ev	156	Total	C	N	O	S	0	0
			1252	782	224	236	10		
2	Ew	155	Total	C	N	O	S	0	0
			1244	777	223	235	9		
2	Ex	156	Total	C	N	O	S	0	0
			1252	782	224	236	10		
2	M0	156	Total	C	N	O	S	0	0
			1252	782	224	236	10		
2	M2	157	Total	C	N	O	S	0	0
			1260	787	225	237	11		
2	M3	155	Total	C	N	O	S	0	0
			1244	777	223	235	9		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	M4	156	Total	C	N	O	S	0	0
			1252	782	224	236	10		
2	M6	156	Total	C	N	O	S	0	0
			1252	782	224	236	10		
2	M7	156	Total	C	N	O	S	0	0
			1252	782	224	236	10		
2	M8	156	Total	C	N	O	S	0	0
			1252	782	224	236	10		
2	M9	156	Total	C	N	O	S	0	0
			1252	782	224	236	10		
2	NR	156	Total	C	N	O	S	0	0
			1252	782	224	236	10		
2	NS	156	Total	C	N	O	S	0	0
			1252	782	224	236	10		
2	NT	155	Total	C	N	O	S	0	0
			1244	777	223	235	9		
2	NU	155	Total	C	N	O	S	0	0
			1244	777	223	235	9		
2	NV	156	Total	C	N	O	S	0	0
			1252	782	224	236	10		
2	NW	156	Total	C	N	O	S	0	0
			1252	782	224	236	10		
2	NX	156	Total	C	N	O	S	0	0
			1252	782	224	236	10		
2	NY	155	Total	C	N	O	S	0	0
			1244	777	223	235	9		
2	NZ	156	Total	C	N	O	S	0	0
			1252	782	224	236	10		

- Molecule 3 is a protein called Chromosome 19 C17orf98 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	1	142	Total	C	N	O	S	0	0
			1173	737	232	199	5		
3	N	142	Total	C	N	O	S	0	0
			1173	737	232	199	5		
3	O	137	Total	C	N	O	S	0	0
			1134	715	222	194	3		
3	T0	137	Total	C	N	O	S	0	0
			1134	715	222	194	3		
3	Tw	142	Total	C	N	O	S	0	0
			1173	737	232	199	5		

- Molecule 4 is a protein called Testis specific serine kinase 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	2	258	Total	C	N	O	S	0	0
			2027	1292	370	357	8		
4	4	258	Total	C	N	O	S	0	0
			2027	1292	370	357	8		
4	Ef	258	Total	C	N	O	S	0	0
			2027	1292	370	357	8		
4	XZ	258	Total	C	N	O	S	0	0
			2027	1292	370	357	8		
4	x	258	Total	C	N	O	S	0	0
			2027	1292	370	357	8		

- Molecule 5 is a protein called EF-hand calcium binding domain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	3	178	Total	C	N	O	S	0	0
			1469	941	252	265	11		
5	5	178	Total	C	N	O	S	0	0
			1469	941	252	265	11		
5	Fm	178	Total	C	N	O	S	0	0
			1469	941	252	265	11		
5	Gq	178	Total	C	N	O	S	0	0
			1469	941	252	265	11		
5	Xa	178	Total	C	N	O	S	0	0
			1469	941	252	265	11		
5	Xb	178	Total	C	N	O	S	0	0
			1469	941	252	265	11		
5	y	178	Total	C	N	O	S	0	0
			1469	941	252	265	11		
5	z	178	Total	C	N	O	S	0	0
			1469	941	252	265	11		

- Molecule 6 is a protein called Chromosome 13 C20orf85 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	6	105	Total	C	N	O	S	0	0
			870	564	151	153	2		
6	P	105	Total	C	N	O	S	0	0
			870	564	151	153	2		
6	Ud	105	Total	C	N	O	S	0	0
			870	564	151	153	2		

- Molecule 7 is a protein called Cilia and flagella associated protein 77.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	8	140	Total	C	N	O	S	0	0
			1162	731	225	200	6		
7	R	140	Total	C	N	O	S	0	0
			1162	731	225	200	6		
7	S	140	Total	C	N	O	S	0	0
			1162	731	225	200	6		
7	T	140	Total	C	N	O	S	0	0
			1165	734	226	199	6		
7	U4	140	Total	C	N	O	S	0	0
			1162	731	225	200	6		
7	VX	140	Total	C	N	O	S	0	0
			1162	731	225	200	6		
7	Vl	140	Total	C	N	O	S	0	0
			1165	734	226	199	6		
7	Vy	97	Total	C	N	O	S	0	0
			818	518	155	141	4		

- Molecule 8 is a protein called Outer dense fiber of sperm tails 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	9	219	Total	C	N	O		0	0
			1078	640	219	219			
8	A1	239	Total	C	N	O	S	0	0
			1828	1173	321	324	10		
8	A2	124	Total	C	N	O	S	0	0
			930	590	162	171	7		
8	A3	244	Total	C	N	O		0	0
			1200	712	244	244			
8	A4	64	Total	C	N	O		0	0
			316	188	64	64			
8	A6	38	Total	C	N	O	S	0	0
			282	180	48	51	3		
8	A8	169	Total	C	N	O	S	0	0
			1281	815	222	237	7		
8	AT	234	Total	C	N	O	S	0	0
			1793	1155	315	314	9		
8	AY	248	Total	C	N	O	S	0	0
			1900	1218	335	337	10		
8	Ai	249	Total	C	N	O	S	0	0
			1907	1223	336	338	10		
8	Au	71	Total	C	N	O	S	0	0
			540	344	93	99	4		
8	Av	121	Total	C	N	O	S	0	0
			905	576	155	167	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
8	Aw	228	Total	C	N	O	S	0	0
			1744	1120	307	308	9		
8	BO	109	Total	C	N	O		0	0
			536	318	109	109			
8	BU	134	Total	C	N	O		0	0
			659	391	134	134			
8	BX	101	Total	C	N	O	S	0	0
			775	493	133	145	4		
8	Bd	38	Total	C	N	O	S	0	0
			282	180	48	51	3		
8	Bf	79	Total	C	N	O	S	0	0
			619	403	113	100	3		
8	Bm	129	Total	C	N	O	S	0	0
			1009	652	182	172	3		
8	Bo	96	Total	C	N	O	S	0	0
			728	465	124	136	3		
8	Ju	239	Total	C	N	O	S	0	0
			1828	1173	321	324	10		
8	Jv	49	Total	C	N	O	S	0	0
			385	252	72	60	1		
8	Jw	244	Total	C	N	O		0	0
			1200	712	244	244			
8	Jx	155	Total	C	N	O		0	0
			762	452	155	155			
8	Jy	226	Total	C	N	O	S	0	0
			1726	1110	305	303	8		
8	Jz	112	Total	C	N	O	S	0	0
			879	573	156	147	3		
8	K3	129	Total	C	N	O	S	0	0
			1009	652	182	172	3		
8	K5	183	Total	C	N	O	S	0	0
			1412	909	250	248	5		

- Molecule 9 is a protein called ATP6V1F neighbor.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	A	39	Total	C	N	O	S	0	0
			338	216	64	56	2		
9	B	91	Total	C	N	O	S	0	0
			751	486	129	132	4		
9	C	91	Total	C	N	O	S	0	0
			751	486	129	132	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
9	Js	39	Total	C	N	O	S	0	0
			338	216	64	56	2		
9	K6	91	Total	C	N	O	S	0	0
			751	486	129	132	4		
9	M	39	Total	C	N	O	S	0	0
			338	216	64	56	2		
9	Ma	91	Total	C	N	O	S	0	0
			751	486	129	132	4		
9	U	91	Total	C	N	O	S	0	0
			751	486	129	132	4		

- Molecule 10 is a protein called Tektin-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	A0	427	Total	C	N	O	S	0	0
			3478	2146	640	677	15		
10	Cq	421	Total	C	N	O	S	0	0
			3427	2114	632	667	14		
10	Cr	415	Total	C	N	O	S	0	0
			3386	2087	626	659	14		
10	Cs	183	Total	C	N	O	S	0	0
			1496	915	282	293	6		
10	Ct	337	Total	C	N	O	S	0	0
			2727	1689	496	529	13		
10	Cu	376	Total	C	N	O	S	0	0
			3055	1887	556	598	14		
10	Cv	422	Total	C	N	O	S	0	0
			3436	2120	634	668	14		
10	Cw	422	Total	C	N	O	S	0	0
			3436	2120	634	668	14		
10	Cy	44	Total	C	N	O	S	0	0
			365	224	71	68	2		
10	E6	403	Total	C	N	O	S	0	0
			3279	2018	605	642	14		
10	E7	101	Total	C	N	O	S	0	0
			834	517	155	160	2		
10	E8	91	Total	C	N	O	S	0	0
			756	460	145	149	2		
10	E9	376	Total	C	N	O	S	0	0
			3055	1887	556	598	14		
10	FA	298	Total	C	N	O	S	0	0
			2418	1491	446	471	10		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	Nd	421	Total	C	N	O	S	0	0
			3427	2114	632	667	14		
10	Ne	415	Total	C	N	O	S	0	0
			3386	2087	626	659	14		
10	Nf	376	Total	C	N	O	S	0	0
			3055	1887	556	598	14		
10	Ng	422	Total	C	N	O	S	0	0
			3436	2120	634	668	14		
10	Nh	422	Total	C	N	O	S	0	0
			3436	2120	634	668	14		

- Molecule 11 is a protein called Tektin-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	A5	407	Total	C	N	O	S	0	0
			3314	2044	605	649	16		
11	A7	415	Total	C	N	O	S	0	0
			3378	2080	617	664	17		
11	By	423	Total	C	N	O	S	0	0
			3449	2133	626	674	16		
11	C2	407	Total	C	N	O	S	0	0
			3314	2044	605	649	16		
11	C3	407	Total	C	N	O	S	0	0
			3314	2044	605	649	16		
11	C4	342	Total	C	N	O	S	0	0
			2779	1715	505	545	14		
11	C5	164	Total	C	N	O	S	0	0
			1328	823	240	258	7		
11	C7	425	Total	C	N	O	S	0	0
			3454	2128	630	678	18		
11	C8	424	Total	C	N	O	S	0	0
			3446	2124	629	675	18		
11	C9	381	Total	C	N	O	S	0	0
			3089	1897	568	609	15		
11	D6	243	Total	C	N	O	S	0	0
			1986	1221	365	391	9		
11	D7	193	Total	C	N	O	S	0	0
			1564	954	290	316	4		
11	DO	88	Total	C	N	O	S	0	0
			731	441	140	148	2		
11	Dy	294	Total	C	N	O	S	0	0
			2387	1482	429	462	14		

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Mol	Chain	Residues	Atoms					AltConf	Trace
11	EB	327	Total	C	N	O	S	0	0
			2647	1639	477	516	15		
11	F0	184	Total	C	N	O	S	0	0
			1498	928	271	289	10		
11	F2	418	Total	C	N	O	S	0	0
			3411	2107	621	667	16		
11	F3	417	Total	C	N	O	S	0	0
			3400	2102	616	666	16		
11	F4	387	Total	C	N	O	S	0	0
			3141	1931	577	618	15		
11	F6	127	Total	C	N	O	S	0	0
			1047	643	194	208	2		
11	GA	417	Total	C	N	O	S	0	0
			3400	2102	616	666	16		
11	Mb	105	Total	C	N	O	S	0	0
			851	527	155	166	3		
11	Md	407	Total	C	N	O	S	0	0
			3314	2044	605	649	16		
11	Me	407	Total	C	N	O	S	0	0
			3314	2044	605	649	16		
11	Mf	41	Total	C	N	O	S	0	0
			352	218	65	68	1		
11	Mg	425	Total	C	N	O	S	0	0
			3454	2128	630	678	18		
11	Mh	424	Total	C	N	O	S	0	0
			3446	2124	629	675	18		
11	Px	418	Total	C	N	O	S	0	0
			3411	2107	621	667	16		
11	Py	417	Total	C	N	O	S	0	0
			3400	2102	616	666	16		

- Molecule 12 is a protein called Tektin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	A9	399	Total	C	N	O	S	0	0
			3286	2047	598	632	9		
12	Cm	396	Total	C	N	O	S	0	0
			3264	2032	594	629	9		
12	Cn	399	Total	C	N	O	S	0	0
			3286	2047	598	632	9		
12	Co	243	Total	C	N	O	S	0	0
			2027	1263	365	395	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
12	Cp	208	Total	C	N	O	S	0	0
			1690	1058	306	319	7		
12	E4	390	Total	C	N	O	S	0	0
			3209	2001	580	620	8		
12	E5	156	Total	C	N	O	S	0	0
			1259	784	233	237	5		
12	Ez	84	Total	C	N	O	S	0	0
			697	426	134	136	1		
12	Nb	396	Total	C	N	O	S	0	0
			3264	2032	594	629	9		
12	Nc	399	Total	C	N	O	S	0	0
			3286	2047	598	632	9		

- Molecule 13 is a protein called Tubulin alpha-3 chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	AA	438	Total	C	N	O	S	0	0
			3413	2161	581	650	21		
13	AC	440	Total	C	N	O	S	0	0
			3428	2171	583	652	22		
13	AE	440	Total	C	N	O	S	0	0
			3428	2171	583	652	22		
13	AG	440	Total	C	N	O	S	0	0
			3428	2171	583	652	22		
13	AI	440	Total	C	N	O	S	0	0
			3428	2171	583	652	22		
13	AK	440	Total	C	N	O	S	0	0
			3428	2171	583	652	22		
13	AN	440	Total	C	N	O	S	0	0
			3428	2171	583	652	22		
13	AR	440	Total	C	N	O	S	0	0
			3428	2171	583	652	22		
13	BA	429	Total	C	N	O	S	0	0
			3355	2128	571	635	21		
13	BC	438	Total	C	N	O	S	0	0
			3415	2163	581	649	22		
13	BE	430	Total	C	N	O	S	0	0
			3363	2133	572	636	22		
13	BG	439	Total	C	N	O	S	0	0
			3421	2166	582	651	22		
13	BI	429	Total	C	N	O	S	0	0
			3357	2130	571	634	22		

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Mol	Chain	Residues	Atoms					AltConf	Trace
13	BK	437	Total	C	N	O	S	0	0
			3407	2159	580	646	22		
13	Bt	438	Total	C	N	O	S	0	0
			3415	2163	581	649	22		
13	Bw	430	Total	C	N	O	S	0	0
			3363	2133	572	636	22		
13	CA	437	Total	C	N	O	S	0	0
			3407	2158	580	648	21		
13	CC	438	Total	C	N	O	S	0	0
			3415	2163	581	649	22		
13	CE	438	Total	C	N	O	S	0	0
			3415	2163	581	649	22		
13	CG	436	Total	C	N	O	S	0	0
			3400	2154	579	645	22		
13	CI	438	Total	C	N	O	S	0	0
			3415	2163	581	649	22		
13	CK	438	Total	C	N	O	S	0	0
			3415	2163	581	649	22		
13	DA	380	Total	C	N	O	S	0	0
			2965	1881	509	556	19		
13	DC	428	Total	C	N	O	S	0	0
			3349	2126	570	631	22		
13	DE	428	Total	C	N	O	S	0	0
			3349	2126	570	631	22		
13	DG	431	Total	C	N	O	S	0	0
			3370	2138	573	637	22		
13	DI	428	Total	C	N	O	S	0	0
			3348	2124	570	632	22		
13	DK	427	Total	C	N	O	S	0	0
			3342	2121	569	630	22		
13	DM	427	Total	C	N	O	S	0	0
			3342	2121	569	630	22		
13	EC	434	Total	C	N	O	S	0	0
			3392	2150	577	643	22		
13	EE	439	Total	C	N	O	S	0	0
			3421	2166	582	651	22		
13	EG	437	Total	C	N	O	S	0	0
			3407	2159	580	646	22		
13	EI	436	Total	C	N	O	S	0	0
			3400	2154	579	645	22		
13	EK	437	Total	C	N	O	S	0	0
			3413	2162	580	649	22		

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Mol	Chain	Residues	Atoms					AltConf	Trace
13	EM	428	Total	C	N	O	S	0	0
			3349	2126	570	631	22		
13	EW	438	Total	C	N	O	S	0	0
			3415	2163	581	649	22		
13	Eb	438	Total	C	N	O	S	0	0
			3415	2163	581	649	22		
13	FC	429	Total	C	N	O	S	0	0
			3357	2130	571	634	22		
13	FE	424	Total	C	N	O	S	0	0
			3323	2110	566	625	22		
13	FG	430	Total	C	N	O	S	0	0
			3363	2133	572	636	22		
13	FI	425	Total	C	N	O	S	0	0
			3325	2109	567	627	22		
13	FK	428	Total	C	N	O	S	0	0
			3350	2125	570	633	22		
13	FM	429	Total	C	N	O	S	0	0
			3356	2128	571	635	22		
13	FU	428	Total	C	N	O	S	0	0
			3349	2126	570	631	22		
13	FW	428	Total	C	N	O	S	0	0
			3349	2126	570	631	22		
13	Fr	434	Total	C	N	O	S	0	0
			3392	2150	577	643	22		
13	Ft	439	Total	C	N	O	S	0	0
			3421	2166	582	651	22		
13	Fv	437	Total	C	N	O	S	0	0
			3407	2159	580	646	22		
13	GB	429	Total	C	N	O	S	0	0
			3357	2130	571	634	22		
13	GC	439	Total	C	N	O	S	0	0
			3421	2166	582	651	22		
13	GE	431	Total	C	N	O	S	0	0
			3370	2138	573	637	22		
13	GG	433	Total	C	N	O	S	0	0
			3384	2145	575	642	22		
13	GI	436	Total	C	N	O	S	0	0
			3398	2154	578	644	22		
13	GK	430	Total	C	N	O	S	0	0
			3364	2132	572	638	22		
13	GM	439	Total	C	N	O	S	0	0
			3421	2166	582	651	22		

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Mol	Chain	Residues	Atoms					AltConf	Trace
13	GP	424	Total	C	N	O	S	0	0
			3323	2110	566	625	22		
13	GR	430	Total	C	N	O	S	0	0
			3363	2133	572	636	22		
13	GT	439	Total	C	N	O	S	0	0
			3421	2166	582	651	22		
13	GV	431	Total	C	N	O	S	0	0
			3370	2138	573	637	22		
13	GX	433	Total	C	N	O	S	0	0
			3384	2145	575	642	22		
13	HE	429	Total	C	N	O	S	0	0
			3357	2130	571	634	22		
13	HG	431	Total	C	N	O	S	0	0
			3370	2138	573	637	22		
13	HI	430	Total	C	N	O	S	0	0
			3362	2134	572	634	22		
13	HK	431	Total	C	N	O	S	0	0
			3370	2138	573	637	22		
13	HM	434	Total	C	N	O	S	0	0
			3393	2150	577	644	22		
13	HO	387	Total	C	N	O	S	0	0
			3035	1925	518	571	21		
13	HP	429	Total	C	N	O	S	0	0
			3357	2130	571	634	22		
13	HR	431	Total	C	N	O	S	0	0
			3370	2138	573	637	22		
13	IC	433	Total	C	N	O	S	0	0
			3384	2145	575	642	22		
13	IE	430	Total	C	N	O	S	0	0
			3363	2133	572	636	22		
13	IG	439	Total	C	N	O	S	0	0
			3421	2166	582	651	22		
13	II	431	Total	C	N	O	S	0	0
			3371	2137	573	639	22		
13	IK	436	Total	C	N	O	S	0	0
			3400	2154	579	645	22		
13	IM	437	Total	C	N	O	S	0	0
			3407	2159	580	646	22		
13	IN	433	Total	C	N	O	S	0	0
			3384	2145	575	642	22		
13	IP	430	Total	C	N	O	S	0	0
			3363	2133	572	636	22		

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Mol	Chain	Residues	Atoms					AltConf	Trace
13	IR	439	Total	C	N	O	S	0	0
			3421	2166	582	651	22		
13	J1	438	Total	C	N	O	S	0	0
			3413	2161	581	650	21		
13	J3	440	Total	C	N	O	S	0	0
			3428	2171	583	652	22		
13	J5	440	Total	C	N	O	S	0	0
			3428	2171	583	652	22		
13	J7	440	Total	C	N	O	S	0	0
			3428	2171	583	652	22		
13	J9	440	Total	C	N	O	S	0	0
			3428	2171	583	652	22		
13	JC	433	Total	C	N	O	S	0	0
			3382	2144	575	641	22		
13	JE	430	Total	C	N	O	S	0	0
			3363	2133	572	636	22		
13	JG	428	Total	C	N	O	S	0	0
			3349	2126	570	631	22		
13	JI	429	Total	C	N	O	S	0	0
			3357	2130	571	634	22		
13	JK	438	Total	C	N	O	S	0	0
			3415	2163	581	649	22		
13	JM	430	Total	C	N	O	S	0	0
			3363	2133	572	636	22		
13	JO	433	Total	C	N	O	S	0	0
			3382	2144	575	641	22		
13	JQ	430	Total	C	N	O	S	0	0
			3363	2133	572	636	22		
13	JS	428	Total	C	N	O	S	0	0
			3349	2126	570	631	22		
13	KA	440	Total	C	N	O	S	0	0
			3428	2171	583	652	22		
13	KC	434	Total	C	N	O	S	0	0
			3389	2146	576	645	22		
13	KE	431	Total	C	N	O	S	0	0
			3371	2137	573	639	22		
13	KG	430	Total	C	N	O	S	0	0
			3361	2132	572	635	22		
13	KI	428	Total	C	N	O	S	0	0
			3349	2126	570	631	22		
13	KK	431	Total	C	N	O	S	0	0
			3371	2137	573	639	22		

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Mol	Chain	Residues	Atoms					AltConf	Trace
13	KM	434	Total	C	N	O	S	0	0
			3383	2143	576	642	22		
13	KO	434	Total	C	N	O	S	0	0
			3389	2146	576	645	22		
13	KQ	431	Total	C	N	O	S	0	0
			3371	2137	573	639	22		
13	KS	430	Total	C	N	O	S	0	0
			3361	2132	572	635	22		
13	KV	439	Total	C	N	O	S	0	0
			3421	2166	582	651	22		
13	LC	440	Total	C	N	O	S	0	0
			3428	2171	583	652	22		
13	LE	445	Total	C	N	O	S	0	0
			3465	2192	588	663	22		
13	LG	440	Total	C	N	O	S	0	0
			3428	2171	583	652	22		
13	LI	445	Total	C	N	O	S	0	0
			3465	2192	588	663	22		
13	LK	440	Total	C	N	O	S	0	0
			3428	2171	583	652	22		
13	LM	436	Total	C	N	O	S	0	0
			3404	2157	578	647	22		
13	LN	440	Total	C	N	O	S	0	0
			3428	2171	583	652	22		
13	LP	445	Total	C	N	O	S	0	0
			3465	2192	588	663	22		
13	LR	440	Total	C	N	O	S	0	0
			3428	2171	583	652	22		
13	LY	429	Total	C	N	O	S	0	0
			3355	2128	571	635	21		
13	La	438	Total	C	N	O	S	0	0
			3415	2163	581	649	22		
13	Lc	430	Total	C	N	O	S	0	0
			3363	2133	572	636	22		
13	Le	439	Total	C	N	O	S	0	0
			3421	2166	582	651	22		
13	Lg	429	Total	C	N	O	S	0	0
			3357	2130	571	634	22		
13	Li	437	Total	C	N	O	S	0	0
			3407	2159	580	646	22		
13	Lk	430	Total	C	N	O	S	0	0
			3363	2133	572	636	22		

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Mol	Chain	Residues	Atoms					AltConf	Trace
13	MC	439	Total	C	N	O	S	0	0
			3421	2166	582	651	22		
13	ME	429	Total	C	N	O	S	0	0
			3357	2130	571	634	22		
13	MG	432	Total	C	N	O	S	0	0
			3377	2140	574	641	22		
13	MI	431	Total	C	N	O	S	0	0
			3369	2136	573	638	22		
13	MK	440	Total	C	N	O	S	0	0
			3428	2171	583	652	22		
13	MM	437	Total	C	N	O	S	0	0
			3407	2158	580	648	21		
13	MN	439	Total	C	N	O	S	0	0
			3421	2166	582	651	22		
13	MP	429	Total	C	N	O	S	0	0
			3357	2130	571	634	22		
13	MR	432	Total	C	N	O	S	0	0
			3377	2140	574	641	22		
13	Mi	437	Total	C	N	O	S	0	0
			3407	2158	580	648	21		
13	Mk	438	Total	C	N	O	S	0	0
			3415	2163	581	649	22		
13	Mm	438	Total	C	N	O	S	0	0
			3415	2163	581	649	22		
13	Mo	436	Total	C	N	O	S	0	0
			3400	2154	579	645	22		
13	Mq	438	Total	C	N	O	S	0	0
			3415	2163	581	649	22		
13	Ms	438	Total	C	N	O	S	0	0
			3415	2163	581	649	22		
13	Mu	438	Total	C	N	O	S	0	0
			3415	2163	581	649	22		
13	N1	427	Total	C	N	O	S	0	0
			3342	2121	569	630	22		
13	N3	427	Total	C	N	O	S	0	0
			3342	2121	569	630	22		
13	NA	426	Total	C	N	O	S	0	0
			3333	2117	568	627	21		
13	NC	427	Total	C	N	O	S	0	0
			3343	2123	569	629	22		
13	NE	430	Total	C	N	O	S	0	0
			3363	2133	572	636	22		

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Mol	Chain	Residues	Atoms					AltConf	Trace
13	NG	430	Total 3363	C 2133	N 572	O 636	S 22	0	0
13	NI	429	Total 3357	C 2130	N 571	O 634	S 22	0	0
13	NK	429	Total 3357	C 2130	N 571	O 634	S 22	0	0
13	NM	426	Total 3333	C 2117	N 568	O 627	S 21	0	0
13	NO	427	Total 3343	C 2123	N 569	O 629	S 22	0	0
13	NQ	430	Total 3363	C 2133	N 572	O 636	S 22	0	0
13	Ns	428	Total 3349	C 2126	N 570	O 631	S 22	0	0
13	Nu	428	Total 3349	C 2126	N 570	O 631	S 22	0	0
13	Nw	431	Total 3370	C 2138	N 573	O 637	S 22	0	0
13	Ny	428	Total 3348	C 2124	N 570	O 632	S 22	0	0
13	O1	434	Total 3392	C 2150	N 577	O 643	S 22	0	0
13	O3	439	Total 3421	C 2166	N 582	O 651	S 22	0	0
13	O5	437	Total 3407	C 2159	N 580	O 646	S 22	0	0
13	O7	436	Total 3400	C 2154	N 579	O 645	S 22	0	0
13	O9	437	Total 3413	C 2162	N 580	O 649	S 22	0	0
13	OA	428	Total 3349	C 2125	N 570	O 633	S 21	0	0
13	OC	429	Total 3357	C 2130	N 571	O 634	S 22	0	0
13	OE	432	Total 3378	C 2142	N 574	O 640	S 22	0	0
13	OG	432	Total 3375	C 2139	N 574	O 640	S 22	0	0
13	OI	432	Total 3378	C 2142	N 574	O 640	S 22	0	0
13	OK	430	Total 3365	C 2134	N 572	O 637	S 22	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
13	OM	428	Total	C	N	O	S	0	0
			3349	2125	570	633	21		
13	OO	429	Total	C	N	O	S	0	0
			3357	2130	571	634	22		
13	OQ	432	Total	C	N	O	S	0	0
			3378	2142	574	640	22		
13	P0	430	Total	C	N	O	S	0	0
			3363	2133	572	636	22		
13	P6	429	Total	C	N	O	S	0	0
			3357	2130	571	634	22		
13	P8	424	Total	C	N	O	S	0	0
			3323	2110	566	625	22		
13	PA	430	Total	C	N	O	S	0	0
			3363	2132	572	638	21		
13	PC	434	Total	C	N	O	S	0	0
			3385	2144	576	643	22		
13	PE	431	Total	C	N	O	S	0	0
			3371	2137	573	639	22		
13	PG	433	Total	C	N	O	S	0	0
			3384	2145	575	642	22		
13	PI	427	Total	C	N	O	S	0	0
			3341	2121	569	630	21		
13	PK	429	Total	C	N	O	S	0	0
			3355	2129	571	633	22		
13	PM	431	Total	C	N	O	S	0	0
			3369	2136	573	638	22		
13	PO	434	Total	C	N	O	S	0	0
			3385	2144	576	643	22		
13	PQ	431	Total	C	N	O	S	0	0
			3371	2137	573	639	22		
13	PT	428	Total	C	N	O	S	0	0
			3349	2126	570	631	22		
13	Q0	436	Total	C	N	O	S	0	0
			3398	2154	578	644	22		
13	Q4	439	Total	C	N	O	S	0	0
			3421	2166	582	651	22		
13	Q6	431	Total	C	N	O	S	0	0
			3370	2138	573	637	22		
13	Q8	433	Total	C	N	O	S	0	0
			3384	2145	575	642	22		
13	QA	428	Total	C	N	O	S	0	0
			3347	2124	570	632	21		

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Mol	Chain	Residues	Atoms					AltConf	Trace
13	QC	428	Total	C	N	O	S	0	0
			3349	2126	570	631	22		
13	QE	430	Total	C	N	O	S	0	0
			3363	2133	572	636	22		
13	QG	431	Total	C	N	O	S	0	0
			3371	2137	573	639	22		
13	QI	428	Total	C	N	O	S	0	0
			3349	2126	570	631	22		
13	QK	430	Total	C	N	O	S	0	0
			3363	2133	572	636	22		
13	QM	428	Total	C	N	O	S	0	0
			3347	2124	570	632	21		
13	QO	428	Total	C	N	O	S	0	0
			3349	2126	570	631	22		
13	QQ	430	Total	C	N	O	S	0	0
			3363	2133	572	636	22		
13	QT	425	Total	C	N	O	S	0	0
			3325	2109	567	627	22		
13	QV	428	Total	C	N	O	S	0	0
			3350	2125	570	633	22		
13	QX	429	Total	C	N	O	S	0	0
			3356	2128	571	635	22		
13	R0	431	Total	C	N	O	S	0	0
			3370	2138	573	637	22		
13	R2	429	Total	C	N	O	S	0	0
			3357	2130	571	634	22		
13	R4	429	Total	C	N	O	S	0	0
			3357	2130	571	634	22		
13	R6	431	Total	C	N	O	S	0	0
			3370	2138	573	637	22		
13	R8	430	Total	C	N	O	S	0	0
			3362	2134	572	634	22		
13	RA	429	Total	C	N	O	S	0	0
			3355	2128	571	635	21		
13	RC	432	Total	C	N	O	S	0	0
			3378	2142	574	640	22		
13	RE	429	Total	C	N	O	S	0	0
			3357	2130	571	634	22		
13	RG	432	Total	C	N	O	S	0	0
			3376	2141	574	639	22		
13	RI	432	Total	C	N	O	S	0	0
			3376	2141	574	639	22		

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Mol	Chain	Residues	Atoms					AltConf	Trace
13	RK	433	Total	C	N	O	S	0	0
			3384	2145	575	642	22		
13	RM	428	Total	C	N	O	S	0	0
			3348	2124	570	632	22		
13	RO	432	Total	C	N	O	S	0	0
			3378	2142	574	640	22		
13	RQ	429	Total	C	N	O	S	0	0
			3357	2130	571	634	22		
13	RT	430	Total	C	N	O	S	0	0
			3364	2132	572	638	22		
13	RV	439	Total	C	N	O	S	0	0
			3421	2166	582	651	22		
13	S0	434	Total	C	N	O	S	0	0
			3383	2143	576	642	22		
13	S2	431	Total	C	N	O	S	0	0
			3371	2137	573	639	22		
13	S4	430	Total	C	N	O	S	0	0
			3361	2132	572	635	22		
13	S6	428	Total	C	N	O	S	0	0
			3349	2126	570	631	22		
13	S8	431	Total	C	N	O	S	0	0
			3371	2137	573	639	22		
13	SA	428	Total	C	N	O	S	0	0
			3349	2125	570	633	21		
13	SC	430	Total	C	N	O	S	0	0
			3363	2133	572	636	22		
13	SE	431	Total	C	N	O	S	0	0
			3372	2138	573	639	22		
13	SG	431	Total	C	N	O	S	0	0
			3370	2138	573	637	22		
13	SI	426	Total	C	N	O	S	0	0
			3341	2121	567	631	22		
13	SK	432	Total	C	N	O	S	0	0
			3378	2142	574	640	22		
13	SN	430	Total	C	N	O	S	0	0
			3363	2133	572	636	22		
13	SP	431	Total	C	N	O	S	0	0
			3372	2138	573	639	22		
13	ST	434	Total	C	N	O	S	0	0
			3393	2150	577	644	22		
13	SV	387	Total	C	N	O	S	0	0
			3035	1925	518	571	21		

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Mol	Chain	Residues	Atoms					AltConf	Trace
13	SY	433	Total	C	N	O	S	0	0
			3384	2145	575	642	22		
13	Sa	430	Total	C	N	O	S	0	0
			3363	2133	572	636	22		
13	Sc	439	Total	C	N	O	S	0	0
			3421	2166	582	651	22		
13	Se	431	Total	C	N	O	S	0	0
			3371	2137	573	639	22		
13	Sg	436	Total	C	N	O	S	0	0
			3400	2154	579	645	22		
13	Si	437	Total	C	N	O	S	0	0
			3407	2159	580	646	22		
13	Sm	433	Total	C	N	O	S	0	0
			3382	2144	575	641	22		
13	So	430	Total	C	N	O	S	0	0
			3363	2133	572	636	22		
13	Sq	428	Total	C	N	O	S	0	0
			3349	2126	570	631	22		
13	Ss	429	Total	C	N	O	S	0	0
			3357	2130	571	634	22		
13	Su	438	Total	C	N	O	S	0	0
			3415	2163	581	649	22		
13	Sw	430	Total	C	N	O	S	0	0
			3363	2133	572	636	22		
13	Sz	434	Total	C	N	O	S	0	0
			3389	2146	576	645	22		
13	T1	427	Total	C	N	O	S	0	0
			3343	2123	569	629	22		
13	T3	430	Total	C	N	O	S	0	0
			3363	2133	572	636	22		
13	T5	430	Total	C	N	O	S	0	0
			3363	2133	572	636	22		
13	T7	429	Total	C	N	O	S	0	0
			3357	2130	571	634	22		
13	T9	429	Total	C	N	O	S	0	0
			3357	2130	571	634	22		
13	TC	429	Total	C	N	O	S	0	0
			3357	2130	571	634	22		
13	TE	432	Total	C	N	O	S	0	0
			3378	2142	574	640	22		
13	TG	429	Total	C	N	O	S	0	0
			3355	2129	571	633	22		

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Mol	Chain	Residues	Atoms					AltConf	Trace
13	TI	430	Total	C	N	O	S	0	0
			3363	2133	572	636	22		
13	TK	431	Total	C	N	O	S	0	0
			3371	2137	573	639	22		
13	TM	430	Total	C	N	O	S	0	0
			3363	2133	572	636	22		
13	TO	429	Total	C	N	O	S	0	0
			3357	2130	571	634	22		
13	TQ	432	Total	C	N	O	S	0	0
			3378	2142	574	640	22		
13	TW	440	Total	C	N	O	S	0	0
			3428	2171	583	652	22		
13	TY	445	Total	C	N	O	S	0	0
			3465	2192	588	663	22		
13	Ta	440	Total	C	N	O	S	0	0
			3428	2171	583	652	22		
13	Tc	445	Total	C	N	O	S	0	0
			3465	2192	588	663	22		
13	Te	440	Total	C	N	O	S	0	0
			3428	2171	583	652	22		
13	Tg	436	Total	C	N	O	S	0	0
			3404	2157	578	647	22		
13	Tk	439	Total	C	N	O	S	0	0
			3421	2166	582	651	22		
13	Tm	429	Total	C	N	O	S	0	0
			3357	2130	571	634	22		
13	To	432	Total	C	N	O	S	0	0
			3377	2140	574	641	22		
13	Tq	431	Total	C	N	O	S	0	0
			3369	2136	573	638	22		
13	Ts	440	Total	C	N	O	S	0	0
			3428	2171	583	652	22		
13	Tu	437	Total	C	N	O	S	0	0
			3407	2158	580	648	21		
13	Ty	426	Total	C	N	O	S	0	0
			3333	2117	568	627	21		
13	U2	430	Total	C	N	O	S	0	0
			3363	2133	572	636	22		
13	U5	429	Total	C	N	O	S	0	0
			3355	2128	571	635	21		
13	U7	432	Total	C	N	O	S	0	0
			3378	2142	574	640	22		

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Mol	Chain	Residues	Atoms					AltConf	Trace
13	U9	429	Total	C	N	O	S	0	0
			3357	2130	571	634	22		
13	UA	428	Total	C	N	O	S	0	0
			3349	2125	570	633	21		
13	UC	431	Total	C	N	O	S	0	0
			3371	2137	573	639	22		
13	UE	431	Total	C	N	O	S	0	0
			3371	2137	573	639	22		
13	UG	432	Total	C	N	O	S	0	0
			3375	2139	574	640	22		
13	UI	431	Total	C	N	O	S	0	0
			3371	2137	573	639	22		
13	UK	430	Total	C	N	O	S	0	0
			3363	2133	572	636	22		
13	UM	429	Total	C	N	O	S	0	0
			3357	2130	571	634	22		
13	UN	431	Total	C	N	O	S	0	0
			3371	2137	573	639	22		
13	UP	431	Total	C	N	O	S	0	0
			3371	2137	573	639	22		
13	UR	432	Total	C	N	O	S	0	0
			3375	2139	574	640	22		
13	UT	429	Total	C	N	O	S	0	0
			3357	2130	571	634	22		
13	UV	432	Total	C	N	O	S	0	0
			3378	2142	574	640	22		
13	UX	432	Total	C	N	O	S	0	0
			3375	2139	574	640	22		
13	UZ	432	Total	C	N	O	S	0	0
			3378	2142	574	640	22		
13	Ub	430	Total	C	N	O	S	0	0
			3365	2134	572	637	22		
13	Ue	430	Total	C	N	O	S	0	0
			3363	2132	572	638	21		
13	Ug	434	Total	C	N	O	S	0	0
			3385	2144	576	643	22		
13	Ui	431	Total	C	N	O	S	0	0
			3371	2137	573	639	22		
13	Uk	433	Total	C	N	O	S	0	0
			3384	2145	575	642	22		
13	Um	427	Total	C	N	O	S	0	0
			3341	2121	569	630	21		

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Mol	Chain	Residues	Atoms					AltConf	Trace
13	Uo	429	Total 3355	C 2129	N 571	O 633	S 22	0	0
13	Ur	428	Total 3347	C 2124	N 570	O 632	S 21	0	0
13	Ut	428	Total 3349	C 2126	N 570	O 631	S 22	0	0
13	Uv	430	Total 3363	C 2133	N 572	O 636	S 22	0	0
13	Ux	431	Total 3371	C 2137	N 573	O 639	S 22	0	0
13	Uz	428	Total 3349	C 2126	N 570	O 631	S 22	0	0
13	V1	431	Total 3371	C 2137	N 573	O 639	S 22	0	0
13	V3	431	Total 3371	C 2137	N 573	O 639	S 22	0	0
13	V5	432	Total 3375	C 2139	N 574	O 640	S 22	0	0
13	V7	431	Total 3371	C 2137	N 573	O 639	S 22	0	0
13	V9	430	Total 3363	C 2133	N 572	O 636	S 22	0	0
13	VA	432	Total 3376	C 2141	N 574	O 639	S 22	0	0
13	VC	436	Total 3400	C 2154	N 579	O 645	S 22	0	0
13	VE	430	Total 3365	C 2134	N 573	O 636	S 22	0	0
13	VG	439	Total 3421	C 2166	N 582	O 651	S 22	0	0
13	VI	428	Total 3350	C 2125	N 570	O 633	S 22	0	0
13	VK	437	Total 3407	C 2159	N 580	O 646	S 22	0	0
13	VM	432	Total 3377	C 2140	N 574	O 641	S 22	0	0
13	VN	436	Total 3400	C 2154	N 579	O 645	S 22	0	0
13	VP	430	Total 3365	C 2134	N 573	O 636	S 22	0	0
13	VR	439	Total 3421	C 2166	N 582	O 651	S 22	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
13	VT	432	Total	C	N	O	S	0	0
			3376	2141	574	639	22		
13	VV	433	Total	C	N	O	S	0	0
			3384	2145	575	642	22		
13	VY	428	Total	C	N	O	S	0	0
			3349	2125	570	633	21		
13	Va	430	Total	C	N	O	S	0	0
			3363	2133	572	636	22		
13	Vc	431	Total	C	N	O	S	0	0
			3372	2138	573	639	22		
13	Ve	431	Total	C	N	O	S	0	0
			3370	2138	573	637	22		
13	Vg	426	Total	C	N	O	S	0	0
			3341	2121	567	631	22		
13	Vi	432	Total	C	N	O	S	0	0
			3378	2142	574	640	22		
13	Vk	430	Total	C	N	O	S	0	0
			3363	2133	572	636	22		
13	Vn	429	Total	C	N	O	S	0	0
			3357	2130	571	634	22		
13	Vp	432	Total	C	N	O	S	0	0
			3378	2142	574	640	22		
13	Vr	429	Total	C	N	O	S	0	0
			3355	2129	571	633	22		
13	Vt	430	Total	C	N	O	S	0	0
			3363	2133	572	636	22		
13	Vv	431	Total	C	N	O	S	0	0
			3371	2137	573	639	22		
13	Vx	430	Total	C	N	O	S	0	0
			3363	2133	572	636	22		
13	WA	429	Total	C	N	O	S	0	0
			3357	2130	571	634	22		
13	WC	437	Total	C	N	O	S	0	0
			3407	2159	580	646	22		
13	WE	430	Total	C	N	O	S	0	0
			3361	2132	572	635	22		
13	WG	436	Total	C	N	O	S	0	0
			3400	2154	579	645	22		
13	WI	429	Total	C	N	O	S	0	0
			3357	2130	571	634	22		
13	WK	437	Total	C	N	O	S	0	0
			3407	2159	580	646	22		

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Mol	Chain	Residues	Atoms					AltConf	Trace
13	WM	430	Total	C	N	O	S	0	0
			3363	2133	572	636	22		
13	WN	437	Total	C	N	O	S	0	0
			3407	2159	580	646	22		
13	WP	430	Total	C	N	O	S	0	0
			3361	2132	572	635	22		
13	WR	436	Total	C	N	O	S	0	0
			3400	2154	579	645	22		
13	WV	436	Total	C	N	O	S	0	0
			3400	2154	579	645	22		
13	WX	430	Total	C	N	O	S	0	0
			3365	2134	573	636	22		
13	WZ	439	Total	C	N	O	S	0	0
			3421	2166	582	651	22		
13	Wb	428	Total	C	N	O	S	0	0
			3350	2125	570	633	22		
13	Wd	437	Total	C	N	O	S	0	0
			3407	2159	580	646	22		
13	Wf	432	Total	C	N	O	S	0	0
			3377	2140	574	641	22		
13	Wj	437	Total	C	N	O	S	0	0
			3407	2159	580	646	22		
13	Wl	430	Total	C	N	O	S	0	0
			3361	2132	572	635	22		
13	Wn	436	Total	C	N	O	S	0	0
			3400	2154	579	645	22		
13	Wp	429	Total	C	N	O	S	0	0
			3357	2130	571	634	22		
13	Wr	437	Total	C	N	O	S	0	0
			3407	2159	580	646	22		
13	Wt	430	Total	C	N	O	S	0	0
			3363	2133	572	636	22		

- Molecule 14 is a protein called Tubulin beta-4B chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	AB	436	Total	C	N	O	S	0	0
			3424	2150	584	664	26		
14	AD	436	Total	C	N	O	S	0	0
			3424	2150	584	664	26		
14	AF	436	Total	C	N	O	S	0	0
			3424	2150	584	664	26		

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Mol	Chain	Residues	Atoms					AltConf	Trace
14	AH	436	Total	C	N	O	S	0	0
			3424	2150	584	664	26		
14	AJ	436	Total	C	N	O	S	0	0
			3424	2150	584	664	26		
14	AL	431	Total	C	N	O	S	0	0
			3383	2124	579	655	25		
14	AM	436	Total	C	N	O	S	0	0
			3424	2150	584	664	26		
14	AO	436	Total	C	N	O	S	0	0
			3424	2150	584	664	26		
14	AX	436	Total	C	N	O	S	0	0
			3424	2150	584	664	26		
14	BB	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
14	BD	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
14	BF	428	Total	C	N	O	S	0	0
			3361	2112	576	647	26		
14	BH	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
14	BJ	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
14	BL	425	Total	C	N	O	S	0	0
			3340	2100	573	642	25		
14	Bp	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
14	Bv	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
14	Bx	428	Total	C	N	O	S	0	0
			3361	2112	576	647	26		
14	CB	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
14	CD	425	Total	C	N	O	S	0	0
			3339	2100	572	641	26		
14	CF	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
14	CH	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
14	CJ	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
14	CL	425	Total	C	N	O	S	0	0
			3340	2100	573	642	25		

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Mol	Chain	Residues	Atoms					AltConf	Trace
14	DB	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
14	DD	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
14	DF	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
14	DH	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
14	DJ	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
14	DL	425	Total	C	N	O	S	0	0
			3340	2100	573	642	25		
14	DN	387	Total	C	N	O	S	0	0
			3035	1911	519	582	23		
14	ED	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
14	EF	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
14	EH	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
14	EJ	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
14	EL	425	Total	C	N	O	S	0	0
			3340	2100	573	642	25		
14	EN	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
14	ER	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
14	Ea	425	Total	C	N	O	S	0	0
			3339	2100	572	641	26		
14	Ec	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
14	FB	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
14	FD	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
14	FF	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
14	FH	428	Total	C	N	O	S	0	0
			3361	2112	576	647	26		
14	FJ	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		

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Mol	Chain	Residues	Atoms					AltConf	Trace
14	FL	425	Total 3340	C 2100	N 573	O 642	S 25	0	0
14	FN	428	Total 3361	C 2112	N 576	O 647	S 26	0	0
14	FV	426	Total 3348	C 2105	N 574	O 643	S 26	0	0
14	FX	426	Total 3348	C 2105	N 574	O 643	S 26	0	0
14	Fs	426	Total 3348	C 2105	N 574	O 643	S 26	0	0
14	Fu	426	Total 3348	C 2105	N 574	O 643	S 26	0	0
14	GD	427	Total 3356	C 2109	N 575	O 646	S 26	0	0
14	GF	428	Total 3361	C 2112	N 576	O 647	S 26	0	0
14	GH	428	Total 3361	C 2112	N 576	O 647	S 26	0	0
14	GJ	428	Total 3361	C 2112	N 576	O 647	S 26	0	0
14	GL	425	Total 3340	C 2100	N 573	O 642	S 25	0	0
14	GN	427	Total 3356	C 2109	N 575	O 646	S 26	0	0
14	GO	427	Total 3356	C 2109	N 575	O 646	S 26	0	0
14	GQ	426	Total 3348	C 2105	N 574	O 643	S 26	0	0
14	GU	427	Total 3356	C 2109	N 575	O 646	S 26	0	0
14	GW	428	Total 3361	C 2112	N 576	O 647	S 26	0	0
14	HB	426	Total 3348	C 2105	N 574	O 643	S 26	0	0
14	HD	427	Total 3356	C 2109	N 575	O 646	S 26	0	0
14	HF	426	Total 3348	C 2105	N 574	O 643	S 26	0	0
14	HH	427	Total 3356	C 2109	N 575	O 646	S 26	0	0
14	HJ	428	Total 3361	C 2112	N 576	O 647	S 26	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
14	HL	425	Total	C	N	O	S	0	0
			3340	2100	573	642	25		
14	HN	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
14	HQ	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
14	IB	368	Total	C	N	O	S	0	0
			2892	1817	499	553	23		
14	ID	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
14	IF	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
14	IH	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
14	IJ	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
14	IL	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
14	IO	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
14	IQ	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
14	J0	436	Total	C	N	O	S	0	0
			3424	2150	584	664	26		
14	J2	436	Total	C	N	O	S	0	0
			3424	2150	584	664	26		
14	J4	436	Total	C	N	O	S	0	0
			3424	2150	584	664	26		
14	J6	436	Total	C	N	O	S	0	0
			3424	2150	584	664	26		
14	J8	436	Total	C	N	O	S	0	0
			3424	2150	584	664	26		
14	JB	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
14	JD	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
14	JF	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
14	JH	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
14	JJ	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		

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Mol	Chain	Residues	Atoms					AltConf	Trace
14	JL	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
14	JN	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
14	JP	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
14	JR	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
14	KB	403	Total	C	N	O	S	0	0
			3165	1989	539	613	24		
14	KD	429	Total	C	N	O	S	0	0
			3368	2116	577	649	26		
14	KF	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
14	KH	429	Total	C	N	O	S	0	0
			3368	2116	577	649	26		
14	KJ	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
14	KL	429	Total	C	N	O	S	0	0
			3368	2116	577	649	26		
14	KN	428	Total	C	N	O	S	0	0
			3361	2112	576	647	26		
14	KP	429	Total	C	N	O	S	0	0
			3368	2116	577	649	26		
14	KR	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
14	KU	431	Total	C	N	O	S	0	0
			3383	2124	579	655	25		
14	LB	437	Total	C	N	O	S	0	0
			3433	2155	585	667	26		
14	LD	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
14	LF	436	Total	C	N	O	S	0	0
			3424	2150	584	664	26		
14	LH	428	Total	C	N	O	S	0	0
			3361	2112	576	647	26		
14	LJ	437	Total	C	N	O	S	0	0
			3433	2155	585	667	26		
14	LL	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
14	LO	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		

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Mol	Chain	Residues	Atoms					AltConf	Trace
14	LQ	436	Total	C	N	O	S	0	0
			3424	2150	584	664	26		
14	LZ	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
14	Lb	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
14	Ld	428	Total	C	N	O	S	0	0
			3361	2112	576	647	26		
14	Lf	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
14	Lh	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
14	Lj	425	Total	C	N	O	S	0	0
			3340	2100	573	642	25		
14	MB	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
14	MD	429	Total	C	N	O	S	0	0
			3368	2116	577	649	26		
14	MF	429	Total	C	N	O	S	0	0
			3368	2116	577	649	26		
14	MH	429	Total	C	N	O	S	0	0
			3368	2116	577	649	26		
14	MJ	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
14	ML	429	Total	C	N	O	S	0	0
			3368	2116	577	649	26		
14	MO	429	Total	C	N	O	S	0	0
			3368	2116	577	649	26		
14	MQ	429	Total	C	N	O	S	0	0
			3368	2116	577	649	26		
14	Mj	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
14	Ml	425	Total	C	N	O	S	0	0
			3339	2100	572	641	26		
14	Mn	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
14	Mp	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
14	Mr	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
14	Mt	425	Total	C	N	O	S	0	0
			3340	2100	573	642	25		

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Mol	Chain	Residues	Atoms					AltConf	Trace
14	N0	425	Total	C	N	O	S	0	0
			3339	2100	572	641	26		
14	N2	425	Total	C	N	O	S	0	0
			3340	2100	573	642	25		
14	NB	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
14	ND	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
14	NF	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
14	NH	428	Total	C	N	O	S	0	0
			3361	2112	576	647	26		
14	NJ	428	Total	C	N	O	S	0	0
			3361	2112	576	647	26		
14	NL	425	Total	C	N	O	S	0	0
			3339	2100	572	641	26		
14	NN	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
14	NP	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
14	Nr	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
14	Nt	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
14	Nv	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
14	Nx	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
14	Nz	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
14	O0	391	Total	C	N	O	S	0	0
			3078	1937	526	592	23		
14	O2	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
14	O4	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
14	O6	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
14	O8	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
14	OB	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		

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Mol	Chain	Residues	Atoms					AltConf	Trace
14	OD	424	Total	C	N	O	S	0	0
			3327	2091	571	639	26		
14	OF	425	Total	C	N	O	S	0	0
			3339	2100	572	641	26		
14	OH	428	Total	C	N	O	S	0	0
			3361	2112	576	647	26		
14	OJ	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
14	OL	424	Total	C	N	O	S	0	0
			3327	2091	571	639	26		
14	ON	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
14	OP	424	Total	C	N	O	S	0	0
			3327	2091	571	639	26		
14	Oz	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
14	P5	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
14	P7	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
14	P9	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
14	PB	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
14	PD	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
14	PF	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
14	PH	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
14	PJ	428	Total	C	N	O	S	0	0
			3361	2112	576	647	26		
14	PL	425	Total	C	N	O	S	0	0
			3340	2100	573	642	25		
14	PN	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
14	PP	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
14	PR	418	Total	C	N	O	S	0	0
			3283	2066	564	629	24		
14	PS	425	Total	C	N	O	S	0	0
			3340	2100	573	642	25		

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Mol	Chain	Residues	Atoms					AltConf	Trace
14	PU	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
14	Q3	428	Total	C	N	O	S	0	0
			3361	2112	576	647	26		
14	Q5	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
14	Q7	428	Total	C	N	O	S	0	0
			3361	2112	576	647	26		
14	Q9	428	Total	C	N	O	S	0	0
			3361	2112	576	647	26		
14	QB	428	Total	C	N	O	S	0	0
			3361	2112	576	647	26		
14	QD	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
14	QF	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
14	QH	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
14	QJ	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
14	QL	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
14	QN	428	Total	C	N	O	S	0	0
			3361	2112	576	647	26		
14	QP	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
14	QR	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
14	QS	428	Total	C	N	O	S	0	0
			3361	2112	576	647	26		
14	QU	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
14	QW	425	Total	C	N	O	S	0	0
			3340	2100	573	642	25		
14	R1	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
14	R3	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
14	R5	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
14	R7	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		

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Mol	Chain	Residues	Atoms					AltConf	Trace
14	R9	428	Total 3361	C 2112	N 576	O 647	S 26	0	0
14	RB	428	Total 3361	C 2112	N 576	O 647	S 26	0	0
14	RD	427	Total 3356	C 2109	N 575	O 646	S 26	0	0
14	RF	427	Total 3356	C 2109	N 575	O 646	S 26	0	0
14	RH	428	Total 3361	C 2112	N 576	O 647	S 26	0	0
14	RJ	428	Total 3361	C 2112	N 576	O 647	S 26	0	0
14	RL	426	Total 3348	C 2105	N 574	O 643	S 26	0	0
14	RN	428	Total 3361	C 2112	N 576	O 647	S 26	0	0
14	RP	427	Total 3356	C 2109	N 575	O 646	S 26	0	0
14	RR	427	Total 3356	C 2109	N 575	O 646	S 26	0	0
14	RS	428	Total 3361	C 2112	N 576	O 647	S 26	0	0
14	RU	425	Total 3340	C 2100	N 573	O 642	S 25	0	0
14	RW	427	Total 3356	C 2109	N 575	O 646	S 26	0	0
14	S1	429	Total 3368	C 2116	N 577	O 649	S 26	0	0
14	S3	427	Total 3356	C 2109	N 575	O 646	S 26	0	0
14	S5	429	Total 3368	C 2116	N 577	O 649	S 26	0	0
14	S7	426	Total 3348	C 2105	N 574	O 643	S 26	0	0
14	S9	429	Total 3368	C 2116	N 577	O 649	S 26	0	0
14	SB	428	Total 3361	C 2112	N 576	O 647	S 26	0	0
14	SD	427	Total 3356	C 2109	N 575	O 646	S 26	0	0
14	SF	428	Total 3361	C 2112	N 576	O 647	S 26	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
14	SH	428	Total 3361	C 2112	N 576	O 647	S 26	0	0
14	SJ	428	Total 3361	C 2112	N 576	O 647	S 26	0	0
14	SL	426	Total 3348	C 2105	N 574	O 643	S 26	0	0
14	SM	428	Total 3361	C 2112	N 576	O 647	S 26	0	0
14	SO	427	Total 3356	C 2109	N 575	O 646	S 26	0	0
14	SQ	428	Total 3361	C 2112	N 576	O 647	S 26	0	0
14	SS	425	Total 3340	C 2100	N 573	O 642	S 25	0	0
14	SU	427	Total 3356	C 2109	N 575	O 646	S 26	0	0
14	SX	368	Total 2892	C 1817	N 499	O 553	S 23	0	0
14	SZ	427	Total 3356	C 2109	N 575	O 646	S 26	0	0
14	Sb	427	Total 3356	C 2109	N 575	O 646	S 26	0	0
14	Sd	426	Total 3348	C 2105	N 574	O 643	S 26	0	0
14	Sf	427	Total 3356	C 2109	N 575	O 646	S 26	0	0
14	Sh	426	Total 3348	C 2105	N 574	O 643	S 26	0	0
14	Sj	426	Total 3348	C 2105	N 574	O 643	S 26	0	0
14	Sl	426	Total 3348	C 2105	N 574	O 643	S 26	0	0
14	Sn	427	Total 3356	C 2109	N 575	O 646	S 26	0	0
14	Sp	426	Total 3348	C 2105	N 574	O 643	S 26	0	0
14	Sr	426	Total 3348	C 2105	N 574	O 643	S 26	0	0
14	St	426	Total 3348	C 2105	N 574	O 643	S 26	0	0
14	Sv	426	Total 3348	C 2105	N 574	O 643	S 26	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
14	T2	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
14	T4	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
14	T6	428	Total	C	N	O	S	0	0
			3361	2112	576	647	26		
14	T8	428	Total	C	N	O	S	0	0
			3361	2112	576	647	26		
14	TA	428	Total	C	N	O	S	0	0
			3361	2112	576	647	26		
14	TB	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
14	TD	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
14	TF	428	Total	C	N	O	S	0	0
			3361	2112	576	647	26		
14	TH	428	Total	C	N	O	S	0	0
			3361	2112	576	647	26		
14	TJ	428	Total	C	N	O	S	0	0
			3361	2112	576	647	26		
14	TL	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
14	TN	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
14	TP	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
14	TR	428	Total	C	N	O	S	0	0
			3361	2112	576	647	26		
14	TV	437	Total	C	N	O	S	0	0
			3433	2155	585	667	26		
14	TX	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
14	TZ	436	Total	C	N	O	S	0	0
			3424	2150	584	664	26		
14	Tb	428	Total	C	N	O	S	0	0
			3361	2112	576	647	26		
14	Td	437	Total	C	N	O	S	0	0
			3433	2155	585	667	26		
14	Tf	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
14	Th	437	Total	C	N	O	S	0	0
			3433	2155	585	667	26		

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Mol	Chain	Residues	Atoms					AltConf	Trace
14	Tj	426	Total 3348	C 2105	N 574	O 643	S 26	0	0
14	Tl	429	Total 3368	C 2116	N 577	O 649	S 26	0	0
14	Tn	429	Total 3368	C 2116	N 577	O 649	S 26	0	0
14	Tp	429	Total 3368	C 2116	N 577	O 649	S 26	0	0
14	Tr	426	Total 3348	C 2105	N 574	O 643	S 26	0	0
14	Tt	429	Total 3368	C 2116	N 577	O 649	S 26	0	0
14	Tv	429	Total 3368	C 2116	N 577	O 649	S 26	0	0
14	Tx	425	Total 3339	C 2100	N 572	O 641	S 26	0	0
14	Tz	426	Total 3348	C 2105	N 574	O 643	S 26	0	0
14	U0	427	Total 3356	C 2109	N 575	O 646	S 26	0	0
14	U1	426	Total 3348	C 2105	N 574	O 643	S 26	0	0
14	U3	426	Total 3348	C 2105	N 574	O 643	S 26	0	0
14	U6	428	Total 3361	C 2112	N 576	O 647	S 26	0	0
14	U8	427	Total 3356	C 2109	N 575	O 646	S 26	0	0
14	UB	426	Total 3348	C 2105	N 574	O 643	S 26	0	0
14	UD	427	Total 3356	C 2109	N 575	O 646	S 26	0	0
14	UF	427	Total 3356	C 2109	N 575	O 646	S 26	0	0
14	UH	427	Total 3356	C 2109	N 575	O 646	S 26	0	0
14	UJ	427	Total 3356	C 2109	N 575	O 646	S 26	0	0
14	UL	426	Total 3348	C 2105	N 574	O 643	S 26	0	0
14	UO	427	Total 3356	C 2109	N 575	O 646	S 26	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
14	UQ	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
14	US	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
14	UU	424	Total	C	N	O	S	0	0
			3327	2091	571	639	26		
14	UW	425	Total	C	N	O	S	0	0
			3339	2100	572	641	26		
14	UY	428	Total	C	N	O	S	0	0
			3361	2112	576	647	26		
14	Ua	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
14	Uc	424	Total	C	N	O	S	0	0
			3327	2091	571	639	26		
14	Uf	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
14	Uh	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
14	Uj	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
14	Ul	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
14	Un	428	Total	C	N	O	S	0	0
			3361	2112	576	647	26		
14	Up	425	Total	C	N	O	S	0	0
			3340	2100	573	642	25		
14	Us	428	Total	C	N	O	S	0	0
			3361	2112	576	647	26		
14	Uu	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
14	Uw	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
14	Uy	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
14	V0	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
14	V2	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
14	V4	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
14	V6	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		

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Mol	Chain	Residues	Atoms					AltConf	Trace
14	V8	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
14	VB	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
14	VD	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
14	VF	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
14	VH	428	Total	C	N	O	S	0	0
			3361	2112	576	647	26		
14	VJ	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
14	VL	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
14	VO	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
14	VQ	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
14	VS	428	Total	C	N	O	S	0	0
			3361	2112	576	647	26		
14	VU	428	Total	C	N	O	S	0	0
			3361	2112	576	647	26		
14	VW	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
14	VZ	428	Total	C	N	O	S	0	0
			3361	2112	576	647	26		
14	Vb	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
14	Vd	428	Total	C	N	O	S	0	0
			3361	2112	576	647	26		
14	Vf	428	Total	C	N	O	S	0	0
			3361	2112	576	647	26		
14	Vh	428	Total	C	N	O	S	0	0
			3361	2112	576	647	26		
14	Vj	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
14	Vm	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
14	Vo	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
14	Vq	428	Total	C	N	O	S	0	0
			3361	2112	576	647	26		

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Mol	Chain	Residues	Atoms					AltConf	Trace
14	Vs	428	Total 3361	C 2112	N 576	O 647	S 26	0	0
14	Vu	428	Total 3361	C 2112	N 576	O 647	S 26	0	0
14	Vw	426	Total 3348	C 2105	N 574	O 643	S 26	0	0
14	Vz	426	Total 3348	C 2105	N 574	O 643	S 26	0	0
14	WB	426	Total 3348	C 2105	N 574	O 643	S 26	0	0
14	WD	426	Total 3348	C 2105	N 574	O 643	S 26	0	0
14	WF	426	Total 3348	C 2105	N 574	O 643	S 26	0	0
14	WH	426	Total 3348	C 2105	N 574	O 643	S 26	0	0
14	WJ	426	Total 3348	C 2105	N 574	O 643	S 26	0	0
14	WL	426	Total 3348	C 2105	N 574	O 643	S 26	0	0
14	WO	426	Total 3348	C 2105	N 574	O 643	S 26	0	0
14	WQ	426	Total 3348	C 2105	N 574	O 643	S 26	0	0
14	WS	427	Total 3356	C 2109	N 575	O 646	S 26	0	0
14	WU	426	Total 3348	C 2105	N 574	O 643	S 26	0	0
14	WW	426	Total 3348	C 2105	N 574	O 643	S 26	0	0
14	WY	426	Total 3348	C 2105	N 574	O 643	S 26	0	0
14	Wa	428	Total 3361	C 2112	N 576	O 647	S 26	0	0
14	Wc	426	Total 3348	C 2105	N 574	O 643	S 26	0	0
14	We	426	Total 3348	C 2105	N 574	O 643	S 26	0	0
14	Wg	426	Total 3348	C 2105	N 574	O 643	S 26	0	0
14	Wi	426	Total 3348	C 2105	N 574	O 643	S 26	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
14	Wk	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
14	Wm	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
14	Wo	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
14	Wq	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
14	Ws	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
14	Wu	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		

- Molecule 15 is a protein called Protein Flattop.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	AP	117	Total	C	N	O	S	0	0
			920	586	168	164	2		
15	AQ	117	Total	C	N	O	S	0	0
			920	586	168	164	2		
15	AS	117	Total	C	N	O	S	0	0
			920	586	168	164	2		
15	AZ	117	Total	C	N	O	S	0	0
			920	586	168	164	2		
15	Ae	117	Total	C	N	O	S	0	0
			920	586	168	164	2		
15	KY	117	Total	C	N	O	S	0	0
			920	586	168	164	2		
15	KZ	117	Total	C	N	O	S	0	0
			920	586	168	164	2		
15	Kb	117	Total	C	N	O	S	0	0
			920	586	168	164	2		

- Molecule 16 is a protein called Cilia- and flagella-associated protein 53.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	AU	217	Total	C	N	O	S	0	0
			1855	1127	350	364	14		
16	Af	200	Total	C	N	O	S	0	0
			1679	1032	323	318	6		
16	Ag	465	Total	C	N	O	S	0	0
			3952	2415	749	766	22		

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Mol	Chain	Residues	Atoms					AltConf	Trace
16	Kc	297	Total	C	N	O	S	0	0
			2521	1541	478	489	13		

- Molecule 17 is a protein called Nucleoside diphosphate kinase 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	AV	366	Total	C	N	O	S	0	0
			2901	1853	491	536	21		
17	AW	372	Total	C	N	O	S	0	0
			2947	1880	499	546	22		
17	Ah	366	Total	C	N	O	S	0	0
			2901	1853	491	536	21		
17	Kd	366	Total	C	N	O	S	0	0
			2901	1853	491	536	21		
17	Ke	372	Total	C	N	O	S	0	0
			2947	1880	499	546	22		

- Molecule 18 is a protein called EF-hand domain-containing family member C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Aa	585	Total	C	N	O	S	0	0
			4829	3100	812	892	25		
18	Ab	598	Total	C	N	O	S	0	0
			4935	3171	827	912	25		
18	Ac	600	Total	C	N	O	S	0	0
			4948	3179	831	913	25		
18	Ad	512	Total	C	N	O	S	0	0
			4235	2727	705	782	21		
18	Aj	600	Total	C	N	O	S	0	0
			4948	3179	831	913	25		
18	Kj	598	Total	C	N	O	S	0	0
			4935	3171	827	912	25		
18	Kk	600	Total	C	N	O	S	0	0
			4948	3179	831	913	25		
18	Kl	512	Total	C	N	O	S	0	0
			4235	2727	705	782	21		

- Molecule 19 is a protein called EF-hand domain-containing protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Ak	448	Total	C	N	O	S	0	0
			3692	2385	621	672	14		

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Mol	Chain	Residues	Atoms					AltConf	Trace
19	I	447	Total	C	N	O	S	0	0
			3689	2376	623	676	14		
19	SW	447	Total	C	N	O	S	0	0
			3689	2376	623	676	14		
19	Wv	448	Total	C	N	O	S	0	0
			3692	2385	621	672	14		
19	Ww	454	Total	C	N	O	S	0	0
			3743	2416	631	682	14		
19	X	448	Total	C	N	O	S	0	0
			3692	2385	621	672	14		
19	Y	454	Total	C	N	O	S	0	0
			3743	2416	631	682	14		

- Molecule 20 is a protein called Family with sequence similarity 166 member A.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Al	43	Total	C	N	O	S	0	0
			338	217	58	62	1		
20	Am	43	Total	C	N	O	S	0	0
			338	217	58	62	1		
20	An	43	Total	C	N	O	S	0	0
			338	217	58	62	1		
20	Ao	43	Total	C	N	O	S	0	0
			338	217	58	62	1		
20	B7	86	Total	C	N	O	S	0	0
			686	443	117	122	4		
20	BY	106	Total	C	N	O	S	0	0
			866	553	155	152	6		
20	BZ	106	Total	C	N	O	S	0	0
			866	553	155	152	6		
20	Ba	191	Total	C	N	O	S	0	0
			1587	1026	281	271	9		
20	Bb	191	Total	C	N	O	S	0	0
			1587	1026	281	271	9		
20	Bc	190	Total	C	N	O	S	0	0
			1575	1017	280	269	9		
20	Be	106	Total	C	N	O	S	0	0
			866	553	155	152	6		
20	CN	84	Total	C	N	O	S	0	0
			670	431	115	120	4		
20	CO	87	Total	C	N	O	S	0	0
			697	449	121	123	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
20	Do	106	Total	C	N	O	S	0	0
			866	553	155	152	6		
20	Dp	191	Total	C	N	O	S	0	0
			1587	1026	281	271	9		
20	Dq	191	Total	C	N	O	S	0	0
			1587	1026	281	271	9		
20	Eg	84	Total	C	N	O	S	0	0
			670	431	115	120	4		
20	Eh	87	Total	C	N	O	S	0	0
			697	449	121	123	4		
20	Kt	43	Total	C	N	O	S	0	0
			338	217	58	62	1		
20	Ku	43	Total	C	N	O	S	0	0
			338	217	58	62	1		
20	Kv	43	Total	C	N	O	S	0	0
			338	217	58	62	1		
20	L3	106	Total	C	N	O	S	0	0
			866	553	155	152	6		
20	L4	106	Total	C	N	O	S	0	0
			866	553	155	152	6		
20	LV	86	Total	C	N	O	S	0	0
			686	443	117	122	4		
20	Lv	106	Total	C	N	O	S	0	0
			866	553	155	152	6		
20	Lw	106	Total	C	N	O	S	0	0
			866	553	155	152	6		
20	Lx	191	Total	C	N	O	S	0	0
			1587	1026	281	271	9		
20	Ly	191	Total	C	N	O	S	0	0
			1587	1026	281	271	9		
20	Lz	190	Total	C	N	O	S	0	0
			1575	1017	280	269	9		
20	Mv	84	Total	C	N	O	S	0	0
			670	431	115	120	4		
20	Mw	87	Total	C	N	O	S	0	0
			697	449	121	123	4		

- Molecule 21 is a protein called Protein FAM166C.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Ap	130	Total	C	N	O	S	0	0
			1101	710	202	187	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
21	Aq	88	Total	C	N	O	S	0	0
			766	493	146	126	1		
21	Ar	152	Total	C	N	O	S	0	0
			1257	809	228	218	2		
21	Az	152	Total	C	N	O	S	0	0
			1257	809	228	218	2		
21	Kx	130	Total	C	N	O	S	0	0
			1101	710	202	187	2		
21	Ky	88	Total	C	N	O	S	0	0
			766	493	146	126	1		
21	Kz	152	Total	C	N	O	S	0	0
			1257	809	228	218	2		

- Molecule 22 is a protein called Ciliary microtubule associated protein 1B.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	As	219	Total	C	N	O	S	0	0
			1686	1085	317	277	7		
22	At	100	Total	C	N	O	S	0	0
			772	495	138	135	4		
22	Bn	107	Total	C	N	O	S	0	0
			804	517	154	130	3		
22	K4	119	Total	C	N	O	S	0	0
			914	590	179	142	3		

- Molecule 23 is a protein called RIB43A-like with coiled-coils protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Ax	364	Total	C	N	O	S	0	0
			3026	1840	595	576	15		
23	BV	371	Total	C	N	O	S	0	0
			3087	1881	602	589	15		
23	Bk	174	Total	C	N	O	S	0	0
			1444	876	285	276	7		
23	DT	189	Total	C	N	O	S	0	0
			1570	955	306	302	7		
23	Ds	141	Total	C	N	O	S	0	0
			1189	725	227	230	7		
23	L9	247	Total	C	N	O	S	0	0
			2029	1233	393	393	10		
23	Lr	36	Total	C	N	O	S	0	0
			307	192	64	50	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
23	Ls	371	Total	C	N	O	S	0	0
			3087	1881	602	589	15		

- Molecule 24 is a protein called Meiosis-specific nuclear structural protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Ay	470	Total	C	N	O	S	0	0
			4020	2484	742	774	20		
24	Bs	355	Total	C	N	O	S	0	0
			3042	1886	556	583	17		
24	Dt	115	Total	C	N	O	S	0	0
			978	598	186	191	3		
24	Du	160	Total	C	N	O	S	0	0
			1364	856	242	259	7		
24	MV	165	Total	C	N	O	S	0	0
			1380	842	259	272	7		

- Molecule 25 is a protein called Spermatid-specific manchette-related protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	B0	45	Total	C	N	O		0	0
			367	240	59	68			
25	B1	37	Total	C	N	O		0	0
			300	198	46	56			
25	B2	41	Total	C	N	O	S	0	0
			307	190	56	55	6		
25	B3	26	Total	C	N	O	S	0	0
			200	124	35	37	4		
25	B4	39	Total	C	N	O	S	0	0
			305	188	57	54	6		
25	B8	41	Total	C	N	O	S	0	0
			307	190	56	55	6		
25	B9	38	Total	C	N	O		0	0
			307	202	47	58			
25	CM	45	Total	C	N	O		0	0
			367	240	59	68			
25	CQ	45	Total	C	N	O		0	0
			367	240	59	68			
25	CR	39	Total	C	N	O		0	0
			316	208	49	59			
25	CS	38	Total	C	N	O		0	0
			307	202	47	58			

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Mol	Chain	Residues	Atoms					AltConf	Trace
25	Ei	45	Total	C	N	O		0	0
			367	240	59	68			
25	Ej	39	Total	C	N	O		0	0
			316	208	49	59			
25	K0	26	Total	C	N	O	S	0	0
			200	124	35	37	4		
25	K7	45	Total	C	N	O		0	0
			367	240	59	68			
25	K8	37	Total	C	N	O		0	0
			300	198	46	56			
25	K9	41	Total	C	N	O	S	0	0
			307	190	56	55	6		
25	LA	39	Total	C	N	O	S	0	0
			305	188	57	54	6		
25	LW	41	Total	C	N	O	S	0	0
			320	196	62	56	6		
25	LX	38	Total	C	N	O		0	0
			307	202	47	58			
25	M1	38	Total	C	N	O		0	0
			307	202	47	58			
25	My	45	Total	C	N	O		0	0
			367	240	59	68			
25	Mz	39	Total	C	N	O		0	0
			316	208	49	59			

- Molecule 26 is a protein called Enkurin.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	B5	244	Total	C	N	O	S	0	0
			2008	1283	348	369	8		
26	B6	248	Total	C	N	O	S	0	0
			2040	1306	352	374	8		
26	Bz	244	Total	C	N	O	S	0	0
			2008	1283	348	369	8		
26	Dw	244	Total	C	N	O	S	0	0
			2008	1283	348	369	8		
26	LT	244	Total	C	N	O	S	0	0
			2008	1283	348	369	8		
26	LU	248	Total	C	N	O	S	0	0
			2040	1306	352	374	8		
26	MY	160	Total	C	N	O	S	0	0
			1316	833	228	250	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
26	MZ	244	Total	C	N	O	S	0	0
			2008	1283	348	369	8		

- Molecule 27 is a protein called Ciliary microtubule associated protein 1C.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	BM	57	Total	C	N	O	S	0	0
			454	297	77	75	5		
27	BN	78	Total	C	N	O	S	0	0
			606	382	119	101	4		
27	Jt	130	Total	C	N	O	S	0	0
			1017	656	177	175	9		
27	p	176	Total	C	N	O	S	0	0
			1376	885	247	233	11		

- Molecule 28 is a protein called Coiled-coil domain-containing protein 105.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	BP	418	Total	C	N	O	S	1	0
			3394	2101	651	616	26		
28	BQ	367	Total	C	N	O	S	1	0
			2989	1843	580	545	21		
28	BR	427	Total	C	N	O	S	1	0
			3465	2147	665	627	26		
28	C0	367	Total	C	N	O	S	1	0
			2989	1843	580	545	21		
28	C6	314	Total	C	N	O	S	1	0
			2540	1568	485	468	19		
28	Ll	61	Total	C	N	O	S	0	0
			487	310	89	83	5		
28	Lm	418	Total	C	N	O	S	1	0
			3394	2101	651	616	26		
28	Ln	367	Total	C	N	O	S	1	0
			2989	1843	580	545	21		
28	Lo	427	Total	C	N	O	S	1	0
			3465	2147	665	627	26		

- Molecule 29 is a protein called Protein phosphatase 1 regulatory subunit 32.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	BS	110	Total	C	N	O	S	0	0
			879	552	160	166	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
29	BT	240	Total	C	N	O	S	0	0
			1886	1193	327	362	4		
29	Lp	151	Total	C	N	O	S	0	0
			1192	756	212	223	1		
29	Lq	240	Total	C	N	O	S	0	0
			1886	1193	327	362	4		

- Molecule 30 is a protein called Cilia- and flagella-associated protein 107.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	BW	189	Total	C	N	O	S	0	0
			1586	1022	284	279	1		
30	Di	189	Total	C	N	O	S	0	0
			1586	1022	284	279	1		
30	Lt	189	Total	C	N	O	S	0	0
			1586	1022	284	279	1		

- Molecule 31 is a protein called Piercer of microtubule wall 1 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Bg	115	Total	C	N	O	S	0	0
			950	602	168	175	5		
31	L5	62	Total	C	N	O	S	0	0
			508	324	87	93	4		
31	L6	115	Total	C	N	O	S	0	0
			950	602	168	175	5		

- Molecule 32 is a protein called Piercer of microtubule wall 2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Bh	96	Total	C	N	O	S	0	0
			775	496	130	142	7		
32	Dr	76	Total	C	N	O	S	0	0
			609	392	99	111	7		
32	L7	96	Total	C	N	O	S	0	0
			775	496	130	142	7		

- Molecule 33 is a protein called Tektin-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Bi	387	Total	C	N	O	S	0	0
			3169	1945	592	603	29		

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Mol	Chain	Residues	Atoms					AltConf	Trace
33	Bj	354	Total	C	N	O	S	0	0
			2896	1777	538	555	26		
33	C1	330	Total	C	N	O	S	0	0
			2710	1677	498	513	22		
33	CP	397	Total	C	N	O	S	0	0
			3243	1994	602	616	31		
33	Cz	297	Total	C	N	O	S	0	0
			2435	1509	445	461	20		
33	D1	358	Total	C	N	O	S	0	0
			2933	1802	545	560	26		
33	D2	387	Total	C	N	O	S	0	0
			3169	1945	592	603	29		
33	D3	386	Total	C	N	O	S	0	0
			3160	1939	590	602	29		
33	D4	385	Total	C	N	O	S	0	0
			3152	1936	587	601	28		
33	D5	362	Total	C	N	O	S	0	0
			2961	1818	552	564	27		
33	D8	387	Total	C	N	O	S	0	0
			3169	1945	592	603	29		
33	D9	160	Total	C	N	O	S	0	0
			1305	789	247	258	11		
33	DP	204	Total	C	N	O	S	0	0
			1668	1010	317	327	14		
33	DQ	150	Total	C	N	O	S	0	0
			1228	767	221	228	12		
33	DR	261	Total	C	N	O	S	0	0
			2151	1327	399	407	18		
33	DS	257	Total	C	N	O	S	0	0
			2118	1308	392	401	17		
33	DU	300	Total	C	N	O	S	0	0
			2497	1547	463	466	21		
33	DV	301	Total	C	N	O	S	0	0
			2502	1550	464	467	21		
33	DW	301	Total	C	N	O	S	0	0
			2502	1550	464	467	21		
33	DX	229	Total	C	N	O	S	0	0
			1897	1171	354	357	15		
33	Dx	330	Total	C	N	O	S	0	0
			2710	1677	498	513	22		
33	EA	399	Total	C	N	O	S	0	0
			3259	2006	604	618	31		

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Mol	Chain	Residues	Atoms					AltConf	Trace
33	EO	398	Total	C	N	O	S	0	0
			3251	2000	603	617	31		
33	EP	360	Total	C	N	O	S	0	0
			2940	1805	544	563	28		
33	EQ	178	Total	C	N	O	S	0	0
			1458	909	265	270	14		
33	FO	111	Total	C	N	O	S	0	0
			908	565	165	171	7		
33	FQ	212	Total	C	N	O	S	0	0
			1736	1055	327	338	16		
33	FR	362	Total	C	N	O	S	0	0
			2961	1818	552	564	27		
33	FS	381	Total	C	N	O	S	0	0
			3118	1914	582	594	28		
33	FT	30	Total	C	N	O	S	0	0
			243	147	48	45	3		
33	Fa	204	Total	C	N	O	S	0	0
			1668	1010	317	327	14		
33	Fc	257	Total	C	N	O	S	0	0
			2118	1308	392	401	17		
33	Fd	295	Total	C	N	O	S	0	0
			2447	1515	457	454	21		
33	Fe	301	Total	C	N	O	S	0	0
			2502	1550	464	467	21		
33	Ff	229	Total	C	N	O	S	0	0
			1897	1171	354	357	15		
33	Fq	109	Total	C	N	O	S	0	0
			877	539	159	170	9		
33	Fx	398	Total	C	N	O	S	0	0
			3251	2000	603	617	31		
33	Mc	330	Total	C	N	O	S	0	0
			2710	1677	498	513	22		
33	N4	261	Total	C	N	O	S	0	0
			2151	1327	399	407	18		
33	N5	257	Total	C	N	O	S	0	0
			2118	1308	392	401	17		
33	N6	300	Total	C	N	O	S	0	0
			2497	1547	463	466	21		
33	N7	301	Total	C	N	O	S	0	0
			2502	1550	464	467	21		
33	N8	301	Total	C	N	O	S	0	0
			2502	1550	464	467	21		

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Mol	Chain	Residues	Atoms					AltConf	Trace
33	N9	229	Total	C	N	O	S	0	0
			1897	1171	354	357	15		
33	Ni	297	Total	C	N	O	S	0	0
			2435	1509	445	461	20		
33	Nk	387	Total	C	N	O	S	0	0
			3169	1945	592	603	29		
33	Nl	386	Total	C	N	O	S	0	0
			3160	1939	590	602	29		
33	Nm	385	Total	C	N	O	S	0	0
			3152	1936	587	601	28		
33	Nn	362	Total	C	N	O	S	0	0
			2961	1818	552	564	27		
33	Np	73	Total	C	N	O	S	0	0
			603	374	111	113	5		
33	Nq	387	Total	C	N	O	S	0	0
			3169	1945	592	603	29		
33	Oy	399	Total	C	N	O	S	0	0
			3259	2006	604	618	31		
33	PV	398	Total	C	N	O	S	0	0
			3251	2000	603	617	31		

There are 53 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Bi	245	ASP	GLU	variant	UNP Q2YDI7
Bj	245	ASP	GLU	variant	UNP Q2YDI7
C1	245	ASP	GLU	variant	UNP Q2YDI7
CP	245	ASP	GLU	variant	UNP Q2YDI7
Cz	245	ASP	GLU	variant	UNP Q2YDI7
D1	245	ASP	GLU	variant	UNP Q2YDI7
D2	245	ASP	GLU	variant	UNP Q2YDI7
D3	245	ASP	GLU	variant	UNP Q2YDI7
D4	245	ASP	GLU	variant	UNP Q2YDI7
D5	245	ASP	GLU	variant	UNP Q2YDI7
D8	245	ASP	GLU	variant	UNP Q2YDI7
D9	245	ASP	GLU	variant	UNP Q2YDI7
DP	245	ASP	GLU	variant	UNP Q2YDI7
DQ	245	ASP	GLU	variant	UNP Q2YDI7
DR	245	ASP	GLU	variant	UNP Q2YDI7
DS	245	ASP	GLU	variant	UNP Q2YDI7
DU	245	ASP	GLU	variant	UNP Q2YDI7
DV	245	ASP	GLU	variant	UNP Q2YDI7
DW	245	ASP	GLU	variant	UNP Q2YDI7

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Chain	Residue	Modelled	Actual	Comment	Reference
DX	245	ASP	GLU	variant	UNP Q2YDI7
Dx	245	ASP	GLU	variant	UNP Q2YDI7
EA	245	ASP	GLU	variant	UNP Q2YDI7
EO	245	ASP	GLU	variant	UNP Q2YDI7
EP	245	ASP	GLU	variant	UNP Q2YDI7
EQ	245	ASP	GLU	variant	UNP Q2YDI7
FO	245	ASP	GLU	variant	UNP Q2YDI7
FQ	245	ASP	GLU	variant	UNP Q2YDI7
FR	245	ASP	GLU	variant	UNP Q2YDI7
FS	245	ASP	GLU	variant	UNP Q2YDI7
FT	245	ASP	GLU	variant	UNP Q2YDI7
Fa	245	ASP	GLU	variant	UNP Q2YDI7
Fc	245	ASP	GLU	variant	UNP Q2YDI7
Fd	245	ASP	GLU	variant	UNP Q2YDI7
Fe	245	ASP	GLU	variant	UNP Q2YDI7
Ff	245	ASP	GLU	variant	UNP Q2YDI7
Fq	245	ASP	GLU	variant	UNP Q2YDI7
Fx	245	ASP	GLU	variant	UNP Q2YDI7
Mc	245	ASP	GLU	variant	UNP Q2YDI7
N4	245	ASP	GLU	variant	UNP Q2YDI7
N5	245	ASP	GLU	variant	UNP Q2YDI7
N6	245	ASP	GLU	variant	UNP Q2YDI7
N7	245	ASP	GLU	variant	UNP Q2YDI7
N8	245	ASP	GLU	variant	UNP Q2YDI7
N9	245	ASP	GLU	variant	UNP Q2YDI7
Ni	245	ASP	GLU	variant	UNP Q2YDI7
Nk	245	ASP	GLU	variant	UNP Q2YDI7
Nl	245	ASP	GLU	variant	UNP Q2YDI7
Nm	245	ASP	GLU	variant	UNP Q2YDI7
Nn	245	ASP	GLU	variant	UNP Q2YDI7
Np	245	ASP	GLU	variant	UNP Q2YDI7
Nq	245	ASP	GLU	variant	UNP Q2YDI7
Oy	245	ASP	GLU	variant	UNP Q2YDI7
PV	245	ASP	GLU	variant	UNP Q2YDI7

- Molecule 34 is a protein called Tektin-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Bl	425	Total	C	N	O	S	0	0
			3483	2143	653	672	15		
34	Br	443	Total	C	N	O	S	0	0
			3615	2228	673	698	16		

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Mol	Chain	Residues	Atoms					AltConf	Trace
34	ES	425	Total	C	N	O	S	0	0
			3483	2143	653	672	15		
34	ET	278	Total	C	N	O	S	0	0
			2273	1404	416	445	8		
34	EU	163	Total	C	N	O	S	0	0
			1338	823	261	247	7		
34	EV	425	Total	C	N	O	S	0	0
			3483	2143	653	672	15		
34	EX	436	Total	C	N	O	S	0	0
			3560	2192	665	687	16		
34	EY	311	Total	C	N	O	S	0	0
			2552	1578	476	486	12		
34	EZ	443	Total	C	N	O	S	0	0
			3615	2228	673	698	16		
34	F1	59	Total	C	N	O	S	0	0
			468	293	88	86	1		
34	F5	364	Total	C	N	O	S	0	0
			2988	1839	559	575	15		
34	F7	311	Total	C	N	O	S	0	0
			2552	1578	476	486	12		
34	F8	71	Total	C	N	O	S	0	0
			564	354	101	107	2		
34	Fy	368	Total	C	N	O	S	0	0
			3010	1851	560	585	14		
34	Fz	263	Total	C	N	O	S	0	0
			2153	1326	393	426	8		
34	PX	425	Total	C	N	O	S	0	0
			3483	2143	653	672	15		
34	PY	425	Total	C	N	O	S	0	0
			3483	2143	653	672	15		
34	PZ	436	Total	C	N	O	S	0	0
			3560	2192	665	687	16		
34	Pa	443	Total	C	N	O	S	0	0
			3615	2228	673	698	16		

- Molecule 35 is a protein called Stabilizer of axonemal microtubules 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Bq	100	Total	C	N	O		0	0
			782	505	139	138			
35	Bu	147	Total	C	N	O	S	0	0
			1177	755	219	202	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
35	Dv	124	Total	C	N	O	S	0	0
			998	641	188	168	1		
35	MU	100	Total	C	N	O		0	0
			782	505	139	138			
35	MX	147	Total	C	N	O	S	0	0
			1177	755	219	202	1		

- Molecule 36 is a protein called Sperm-associated antigen 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	CW	163	Total	C	N	O	S	0	0
			1319	827	236	249	7		
36	Ek	89	Total	C	N	O	S	0	0
			725	450	133	136	6		
36	M5	163	Total	C	N	O	S	0	0
			1319	827	236	249	7		

- Molecule 37 is a protein called Sperm microtubule inner protein 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	Cl	127	Total	C	N	O	S	0	0
			977	615	168	190	4		
37	Ey	127	Total	C	N	O	S	0	0
			977	615	168	190	4		
37	Na	127	Total	C	N	O	S	0	0
			977	615	168	190	4		

- Molecule 38 is a protein called Cilia- and flagella-associated protein 95.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Cx	40	Total	C	N	O	S	0	0
			330	205	63	61	1		
38	V	183	Total	C	N	O	S	0	0
			1487	932	258	288	9		
38	WT	183	Total	C	N	O	S	0	0
			1487	932	258	288	9		

- Molecule 39 is a protein called Dynein axonemal heavy chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	D	62	Total	C	N	O	S	0	0
			537	344	94	98	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
39	Nj	62	Total	C	N	O	S	0	0
			537	344	94	98	1		

- Molecule 40 is a protein called Dynein axonemal heavy chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	D0	3128	Total	C	N	O	S	0	0
			25215	16097	4275	4707	136		
40	G2	3720	Total	C	N	O	S	0	0
			30098	19263	5134	5541	160		

- Molecule 41 is a protein called TEPP protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	DY	38	Total	C	N	O	S	0	0
			308	187	53	63	5		
41	DZ	51	Total	C	N	O	S	0	0
			416	250	82	79	5		
41	Da	134	Total	C	N	O	S	0	0
			1095	704	194	193	4		
41	Ee	45	Total	C	N	O	S	0	0
			386	248	71	66	1		
41	F9	45	Total	C	N	O	S	0	0
			386	248	71	66	1		
41	Fg	38	Total	C	N	O	S	0	0
			308	187	53	63	5		
41	Fh	134	Total	C	N	O	S	0	0
			1095	704	194	193	4		
41	OR	38	Total	C	N	O	S	0	0
			308	187	53	63	5		
41	OS	51	Total	C	N	O	S	0	0
			416	250	82	79	5		
41	OT	134	Total	C	N	O	S	0	0
			1095	704	194	193	4		
41	Pc	45	Total	C	N	O	S	0	0
			386	248	71	66	1		

- Molecule 42 is a protein called Ciliary Microtubule Inner Protein 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	Db	52	Total	C	N	O	S	0	0
			450	290	81	78	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
42	Dc	51	Total	C	N	O	S	0	0
			442	284	80	77	1		
42	Dd	47	Total	C	N	O	S	0	0
			406	262	72	71	1		
42	Fi	52	Total	C	N	O	S	0	0
			450	290	81	78	1		
42	OU	52	Total	C	N	O	S	0	0
			450	290	81	78	1		
42	OV	51	Total	C	N	O	S	0	0
			442	284	80	77	1		
42	OW	47	Total	C	N	O	S	0	0
			406	262	72	71	1		

- Molecule 43 is a protein called Testis expressed 33.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	De	66	Total	C	N	O	S	0	0
			545	343	97	101	4		
43	OX	66	Total	C	N	O	S	0	0
			545	343	97	101	4		

- Molecule 44 is a protein called Testis-expressed sequence 37 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	Df	133	Total	C	N	O	S	0	0
			1060	685	176	196	3		
44	Dg	123	Total	C	N	O	S	0	0
			981	629	167	181	4		
44	Dh	109	Total	C	N	O	S	0	0
			873	561	143	166	3		
44	Fk	109	Total	C	N	O	S	0	0
			873	561	143	166	3		
44	OY	133	Total	C	N	O	S	0	0
			1060	685	176	196	3		
44	OZ	123	Total	C	N	O	S	0	0
			981	629	167	181	4		
44	Oa	109	Total	C	N	O	S	0	0
			873	561	143	166	3		

- Molecule 45 is a protein called Testis-expressed protein 43.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	Dj	99	Total	C	N	O	S	0	0
			806	513	154	133	6		
45	Dk	99	Total	C	N	O	S	0	0
			806	513	154	133	6		
45	Dl	99	Total	C	N	O	S	0	0
			806	513	154	133	6		
45	Fl	99	Total	C	N	O	S	0	0
			806	513	154	133	6		
45	Ob	78	Total	C	N	O	S	0	0
			632	405	120	102	5		
45	Oc	99	Total	C	N	O	S	0	0
			806	513	154	133	6		
45	Od	99	Total	C	N	O	S	0	0
			806	513	154	133	6		
45	Oe	99	Total	C	N	O	S	0	0
			806	513	154	133	6		

- Molecule 46 is a protein called Testis expressed 49.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	Dm	87	Total	C	N	O	S	0	0
			725	458	136	127	4		
46	Of	87	Total	C	N	O	S	0	0
			725	458	136	127	4		

- Molecule 47 is a protein called Theg spermatid protein like.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	Dn	56	Total	C	N	O	S	0	0
			468	289	97	81	1		
47	Fn	56	Total	C	N	O	S	0	0
			468	289	97	81	1		
47	Og	56	Total	C	N	O	S	0	0
			468	289	97	81	1		

- Molecule 48 is a protein called Coiled-coil domain containing 40.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	Dz	356	Total	C	N	O	S	0	0
			2911	1795	527	569	20		
48	Iv	381	Total	C	N	O	S	0	0
			3107	1916	567	604	20		

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Mol	Chain	Residues	Atoms					AltConf	Trace
48	Pi	73	Total	C	N	O	S	0	0
			600	372	119	106	3		

- Molecule 49 is a protein called EF-hand domain-containing family member B.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	E	148	Total	C	N	O	S	0	0
			1181	742	206	230	3		
49	F	455	Total	C	N	O	S	0	0
			3679	2344	655	667	13		
49	On	148	Total	C	N	O	S	0	0
			1181	742	206	230	3		
49	Pu	409	Total	C	N	O	S	0	0
			3332	2129	597	594	12		
49	n	114	Total	C	N	O	S	0	0
			919	596	164	154	5		

- Molecule 50 is a protein called Tektin bundle interacting protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	E1	197	Total	C	N	O	S	1	0
			1648	1052	300	292	4		
50	E2	197	Total	C	N	O	S	1	0
			1648	1052	300	292	4		
50	E3	197	Total	C	N	O	S	0	0
			1641	1047	299	291	4		
50	Fo	197	Total	C	N	O	S	1	0
			1648	1052	300	292	4		
50	Op	197	Total	C	N	O	S	1	0
			1648	1052	300	292	4		
50	Oq	197	Total	C	N	O	S	1	0
			1648	1052	300	292	4		
50	Or	197	Total	C	N	O	S	0	0
			1641	1047	299	291	4		
50	Os	145	Total	C	N	O	S	1	0
			1221	782	222	214	3		

- Molecule 51 is a protein called Outer dynein arm-docking complex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	Ed	425	Total	C	N	O	S	0	0
			3545	2210	654	671	10		

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Mol	Chain	Residues	Atoms					AltConf	Trace
51	Iy	425	Total	C	N	O	S	0	0
			3545	2210	654	671	10		
51	Ja	425	Total	C	N	O	S	0	0
			3545	2210	654	671	10		
51	RX	379	Total	C	N	O	S	0	0
			3152	1965	581	596	10		
51	Rl	195	Total	C	N	O	S	0	0
			1613	1008	295	303	7		

- Molecule 52 is a protein called Calcium/calmodulin dependent protein kinase IV.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	Er	294	Total	C	N	O	S	0	0
			2354	1520	400	424	10		
52	G9	294	Total	C	N	O	S	0	0
			2354	1520	400	424	10		

- Molecule 53 is a protein called Radial spoke head 6 homolog A.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	FP	391	Total	C	N	O	S	0	0
			3175	2041	538	582	14		
53	H4	396	Total	C	N	O	S	0	0
			3204	2067	538	586	13		
53	H5	403	Total	C	N	O	S	0	0
			3267	2099	551	603	14		
53	H6	396	Total	C	N	O	S	0	0
			3204	2067	538	586	13		
53	Hh	403	Total	C	N	O	S	0	0
			3267	2099	551	603	14		
53	QZ	387	Total	C	N	O	S	0	0
			3137	2024	528	572	13		
53	Qa	391	Total	C	N	O	S	0	0
			3175	2041	538	582	14		
53	Qb	387	Total	C	N	O	S	0	0
			3137	2024	528	572	13		

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
FP	50	ILE	-	insertion	UNP E1BJG2
FP	51	LEU	ARG	conflict	UNP E1BJG2

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Chain	Residue	Modelled	Actual	Comment	Reference
H4	50	ILE	-	insertion	UNP E1BJG2
H4	51	LEU	ARG	conflict	UNP E1BJG2
H5	50	ILE	-	insertion	UNP E1BJG2
H5	51	LEU	ARG	conflict	UNP E1BJG2
H6	50	ILE	-	insertion	UNP E1BJG2
H6	51	LEU	ARG	conflict	UNP E1BJG2
Hh	50	ILE	-	insertion	UNP E1BJG2
Hh	51	LEU	ARG	conflict	UNP E1BJG2
QZ	50	ILE	-	insertion	UNP E1BJG2
QZ	51	LEU	ARG	conflict	UNP E1BJG2
Qa	50	ILE	-	insertion	UNP E1BJG2
Qa	51	LEU	ARG	conflict	UNP E1BJG2
Qb	50	ILE	-	insertion	UNP E1BJG2
Qb	51	LEU	ARG	conflict	UNP E1BJG2

- Molecule 54 is a protein called Dynein light chain 1, cytoplasmic.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	FZ	85	Total	C	N	O	S	0	0
			695	447	115	129	4		
54	Fb	85	Total	C	N	O	S	0	0
			695	447	115	129	4		
54	GY	89	Total	C	N	O	S	0	0
			728	465	122	135	6		
54	GZ	89	Total	C	N	O	S	0	0
			728	465	122	135	6		
54	Ga	89	Total	C	N	O	S	0	0
			728	465	122	135	6		
54	Gp	89	Total	C	N	O	S	0	0
			728	465	122	135	6		
54	Hp	89	Total	C	N	O	S	0	0
			728	465	122	135	6		
54	Hq	89	Total	C	N	O	S	0	0
			728	465	122	135	6		
54	Hr	89	Total	C	N	O	S	0	0
			728	465	122	135	6		
54	Hs	89	Total	C	N	O	S	0	0
			728	465	122	135	6		
54	Ht	89	Total	C	N	O	S	0	0
			728	465	122	135	6		
54	Hu	89	Total	C	N	O	S	0	0
			728	465	122	135	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
54	I0	89	Total 728	C 465	N 122	O 135	S 6	0	0
54	I7	36	Total 302	C 203	N 50	O 48	S 1	0	0
54	I8	89	Total 728	C 465	N 122	O 135	S 6	0	0
54	I9	89	Total 728	C 465	N 122	O 135	S 6	0	0
54	IA	83	Total 681	C 439	N 112	O 126	S 4	0	0
54	IU	83	Total 681	C 439	N 112	O 126	S 4	0	0
54	IV	83	Total 681	C 439	N 112	O 126	S 4	0	0
54	IW	83	Total 681	C 439	N 112	O 126	S 4	0	0
54	If	85	Total 695	C 447	N 115	O 129	S 4	0	0
54	Ig	85	Total 695	C 447	N 115	O 129	S 4	0	0
54	Ih	85	Total 695	C 447	N 115	O 129	S 4	0	0
54	Ii	85	Total 695	C 447	N 115	O 129	S 4	0	0
54	JA	89	Total 728	C 465	N 122	O 135	S 6	0	0
54	JU	89	Total 728	C 465	N 122	O 135	S 6	0	0
54	Ji	89	Total 728	C 465	N 122	O 135	S 6	0	0
54	Jj	89	Total 728	C 465	N 122	O 135	S 6	0	0
54	Jk	89	Total 728	C 465	N 122	O 135	S 6	0	0
54	Jl	89	Total 728	C 465	N 122	O 135	S 6	0	0
54	Jm	89	Total 728	C 465	N 122	O 135	S 6	0	0
54	Jn	89	Total 728	C 465	N 122	O 135	S 6	0	0
54	KX	89	Total 728	C 465	N 122	O 135	S 6	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
54	Ka	89	Total	C	N	O	S	0	0
			728	465	122	135	6		
54	Kf	89	Total	C	N	O	S	0	0
			728	465	122	135	6		
54	Kg	89	Total	C	N	O	S	0	0
			728	465	122	135	6		
54	Kh	89	Total	C	N	O	S	0	0
			728	465	122	135	6		
54	Ki	89	Total	C	N	O	S	0	0
			728	465	122	135	6		
54	L0	85	Total	C	N	O	S	0	0
			695	447	115	129	4		
54	L8	85	Total	C	N	O	S	0	0
			695	447	115	129	4		
54	Qf	85	Total	C	N	O	S	0	0
			695	447	115	129	4		
54	Qg	85	Total	C	N	O	S	0	0
			695	447	115	129	4		
54	Qh	85	Total	C	N	O	S	0	0
			695	447	115	129	4		
54	Qi	85	Total	C	N	O	S	0	0
			695	447	115	129	4		
54	Qj	85	Total	C	N	O	S	0	0
			695	447	115	129	4		
54	Qk	85	Total	C	N	O	S	0	0
			695	447	115	129	4		
54	Ql	85	Total	C	N	O	S	0	0
			695	447	115	129	4		
54	Qm	85	Total	C	N	O	S	0	0
			695	447	115	129	4		
54	Re	89	Total	C	N	O	S	0	0
			728	465	122	135	6		
54	Rf	89	Total	C	N	O	S	0	0
			728	465	122	135	6		
54	Rg	89	Total	C	N	O	S	0	0
			728	465	122	135	6		
54	Rr	89	Total	C	N	O	S	0	0
			728	465	122	135	6		
54	Rs	89	Total	C	N	O	S	0	0
			728	465	122	135	6		
54	Rt	89	Total	C	N	O	S	0	0
			728	465	122	135	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
54	Ru	89	Total	C	N	O	S	0	0
			728	465	122	135	6		
54	Rv	89	Total	C	N	O	S	0	0
			728	465	122	135	6		

- Molecule 55 is a protein called Radial spoke head 14 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	Fj	319	Total	C	N	O	S	0	0
			2458	1554	428	463	13		
55	Ib	325	Total	C	N	O	S	0	0
			2505	1584	438	470	13		

- Molecule 56 is a protein called Tetratricopeptide repeat protein 29.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	Fp	422	Total	C	N	O	S	0	0
			3431	2175	586	654	16		

- Molecule 57 is a protein called Dynein regulatory complex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	Fw	416	Total	C	N	O	S	0	0
			3478	2165	636	660	17		
57	Qw	411	Total	C	N	O	S	0	0
			3373	2099	615	642	17		

- Molecule 58 is a protein called Sperm associated microtubule inner protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	G	282	Total	C	N	O	S	0	0
			2317	1475	409	427	6		
58	Q1	282	Total	C	N	O	S	0	0
			2317	1475	409	427	6		

- Molecule 59 is a protein called Cytochrome b5 domain-containing protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	G0	222	Total	C	N	O	S	0	0
			1849	1184	317	344	4		
59	Pm	222	Total	C	N	O	S	0	0
			1849	1184	317	344	4		

- Molecule 60 is a protein called Axonemal dynein light intermediate polypeptide 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	G1	207	Total	C	N	O	S	0	0
			1696	1051	309	328	8		
60	G4	216	Total	C	N	O	S	0	0
			1780	1098	331	343	8		
60	G5	187	Total	C	N	O	S	0	0
			1538	954	279	297	8		
60	Gr	156	Total	C	N	O	S	0	0
			1292	789	245	250	8		
60	Mx	198	Total	C	N	O	S	0	0
			1630	1009	298	315	8		
60	Pe	214	Total	C	N	O	S	0	0
			1752	1087	318	338	9		
60	Pf	156	Total	C	N	O	S	0	0
			1292	789	245	250	8		
60	Pg	165	Total	C	N	O	S	0	0
			1360	833	257	262	8		
60	Qr	210	Total	C	N	O	S	0	0
			1719	1064	313	334	8		
60	Qs	197	Total	C	N	O	S	0	0
			1628	1005	298	317	8		

- Molecule 61 is a protein called Outer dynein arm-docking complex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	G3	599	Total	C	N	O	S	0	0
			4601	2871	834	864	32		
61	Iz	599	Total	C	N	O	S	0	0
			4601	2871	834	864	32		
61	Jb	599	Total	C	N	O	S	0	0
			4601	2871	834	864	32		
61	RY	599	Total	C	N	O	S	0	0
			4601	2871	834	864	32		
61	Rm	599	Total	C	N	O	S	0	0
			4601	2871	834	864	32		

- Molecule 62 is a protein called Actin, cytoplasmic 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	G6	375	Total	C	N	O	S	0	0
			2929	1854	491	561	23		
62	Gz	375	Total	C	N	O	S	0	0
			2929	1854	491	561	23		

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Mol	Chain	Residues	Atoms					AltConf	Trace
62	Oi	375	Total	C	N	O	S	0	0
			2929	1854	491	561	23		
62	Pj	375	Total	C	N	O	S	0	0
			2929	1854	491	561	23		
62	Pl	374	Total	C	N	O	S	0	0
			2917	1845	490	559	23		
62	Qp	375	Total	C	N	O	S	0	0
			2929	1854	491	561	23		

- Molecule 63 is a protein called Outer dynein arm-docking complex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	G7	224	Total	C	N	O	S	0	0
			1806	1147	307	342	10		
63	I1	224	Total	C	N	O	S	0	0
			1806	1147	307	342	10		
63	Jc	224	Total	C	N	O	S	0	0
			1806	1147	307	342	10		
63	RZ	224	Total	C	N	O	S	0	0
			1806	1147	307	342	10		
63	Rn	224	Total	C	N	O	S	0	0
			1806	1147	307	342	10		

- Molecule 64 is a protein called Adenylate kinase 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	G8	475	Total	C	N	O	S	0	0
			3831	2454	661	696	20		
64	Oh	475	Total	C	N	O	S	0	0
			3831	2454	661	696	20		

- Molecule 65 is a protein called Cilia- and flagella-associated protein 45.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	Gb	185	Total	C	N	O	S	0	0
			1559	959	297	294	9		
65	Gc	144	Total	C	N	O	S	0	0
			1234	751	253	228	2		
65	Gd	182	Total	C	N	O	S	0	0
			1567	949	305	302	11		
65	W1	162	Total	C	N	O	S	0	0
			1380	835	284	259	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
65	Wy	185	Total	C	N	O	S	0	0
			1559	959	297	294	9		
65	Wz	297	Total	C	N	O	S	0	0
			2525	1544	478	487	16		
65	b	275	Total	C	N	O	S	0	0
			2356	1427	467	453	9		
65	c	297	Total	C	N	O	S	0	0
			2525	1544	478	487	16		
65	d	162	Total	C	N	O	S	0	0
			1380	835	284	259	2		
65	o	464	Total	C	N	O	S	0	0
			3948	2406	769	754	19		

- Molecule 66 is a protein called Dynein light chain Tctex-type 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	Ge	113	Total	C	N	O	S	0	0
			872	548	142	175	7		
66	JX	113	Total	C	N	O	S	0	0
			872	548	142	175	7		
66	Jq	113	Total	C	N	O	S	0	0
			872	548	142	175	7		
66	P3	113	Total	C	N	O	S	0	0
			872	548	142	175	7		
66	Ry	113	Total	C	N	O	S	0	0
			872	548	142	175	7		

- Molecule 67 is a protein called Cilia- and flagella-associated protein 52.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	Gf	610	Total	C	N	O	S	0	0
			4722	2990	823	877	32		
67	Gg	289	Total	C	N	O	S	0	0
			2195	1398	376	403	18		
67	W2	610	Total	C	N	O	S	0	0
			4722	2990	823	877	32		
67	W3	609	Total	C	N	O	S	0	0
			4713	2985	822	874	32		
67	W4	609	Total	C	N	O	S	0	0
			4713	2985	822	874	32		
67	e	610	Total	C	N	O	S	0	0
			4722	2990	823	877	32		

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Mol	Chain	Residues	Atoms					AltConf	Trace
67	f	609	Total	C	N	O	S	0	0
			4713	2985	822	874	32		
67	g	609	Total	C	N	O	S	0	0
			4713	2985	822	874	32		

- Molecule 68 is a protein called Cilia- and flagella-associated protein 161.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	Gh	255	Total	C	N	O	S	0	0
			2055	1302	369	373	11		
68	W6	255	Total	C	N	O	S	0	0
			2055	1302	369	373	11		
68	W7	268	Total	C	N	O	S	0	0
			2158	1367	386	394	11		
68	i	255	Total	C	N	O	S	0	0
			2055	1302	369	373	11		
68	j	268	Total	C	N	O	S	0	0
			2158	1367	386	394	11		

- Molecule 69 is a protein called Dual specificity phosphatase 21.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	Gi	137	Total	C	N	O	S	0	0
			1098	706	185	199	8		
69	W0	159	Total	C	N	O	S	0	0
			1263	807	211	234	11		
69	W8	157	Total	C	N	O	S	0	0
			1245	797	207	230	11		
69	W9	137	Total	C	N	O	S	0	0
			1098	706	185	199	8		
69	XA	114	Total	C	N	O	S	0	0
			908	587	147	167	7		
69	k	157	Total	C	N	O	S	0	0
			1245	797	207	230	11		
69	l	137	Total	C	N	O	S	0	0
			1098	706	185	199	8		
69	m	159	Total	C	N	O	S	0	0
			1263	807	211	234	11		

- Molecule 70 is a protein called Cilia- and flagella- associated protein 210.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	Gj	179	Total	C	N	O	S	0	0
			1537	951	288	292	6		
70	H	59	Total	C	N	O	S	0	0
			483	306	80	96	1		
70	XB	397	Total	C	N	O	S	0	0
			3401	2106	640	644	11		
70	a	455	Total	C	N	O	S	0	0
			3879	2409	719	739	12		

- Molecule 71 is a protein called CFAP97 domain containing 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	Gk	96	Total	C	N	O	S	0	0
			829	510	169	148	2		
71	Wx	117	Total	C	N	O	S	0	0
			1014	632	205	175	2		
71	XC	21	Total	C	N	O		0	0
			185	122	36	27			
71	XD	96	Total	C	N	O	S	0	0
			829	510	169	148	2		
71	Z	117	Total	C	N	O	S	0	0
			1014	632	205	175	2		
71	q	96	Total	C	N	O	S	0	0
			829	510	169	148	2		

- Molecule 72 is a protein called Cilia- and flagella-associated protein 276.

Mol	Chain	Residues	Atoms				AltConf	Trace
72	Gm	78	Total	C	N	O	0	0
			624	391	115	118		
72	XE	77	Total	C	N	O	0	0
			615	386	113	116		
72	XF	78	Total	C	N	O	0	0
			624	391	115	118		
72	XV	78	Total	C	N	O	0	0
			624	391	115	118		
72	r	77	Total	C	N	O	0	0
			615	386	113	116		
72	s	78	Total	C	N	O	0	0
			624	391	115	118		
72	t	78	Total	C	N	O	0	0
			624	391	115	118		

- Molecule 73 is a protein called Dynein axonemal intermediate chain 1.



Mol	Chain	Residues	Atoms					AltConf	Trace
73	Gn	416	Total	C	N	O	S	0	0
			3342	2137	563	624	18		
73	I5	416	Total	C	N	O	S	0	0
			3342	2137	563	624	18		
73	JT	416	Total	C	N	O	S	0	0
			3342	2137	563	624	18		
73	Jg	416	Total	C	N	O	S	0	0
			3342	2137	563	624	18		
73	Rc	416	Total	C	N	O	S	0	0
			3342	2137	563	624	18		

- Molecule 74 is a protein called EF-hand calcium-binding domain-containing protein 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	Go	128	Total	C	N	O	S	0	0
			1081	697	188	192	4		
74	XW	128	Total	C	N	O	S	0	0
			1081	697	188	192	4		
74	XY	128	Total	C	N	O	S	0	0
			1081	697	188	192	4		
74	u	128	Total	C	N	O	S	0	0
			1081	697	188	192	4		
74	w	128	Total	C	N	O	S	0	0
			1081	697	188	192	4		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Go	290	ALA	GLU	variant	UNP Q2T9P0
Go	303	SER	THR	variant	UNP Q2T9P0
XW	290	ALA	GLU	variant	UNP Q2T9P0
XW	303	SER	THR	variant	UNP Q2T9P0
XY	290	ALA	GLU	variant	UNP Q2T9P0
XY	303	SER	THR	variant	UNP Q2T9P0
u	290	ALA	GLU	variant	UNP Q2T9P0
u	303	SER	THR	variant	UNP Q2T9P0
w	290	ALA	GLU	variant	UNP Q2T9P0
w	303	SER	THR	variant	UNP Q2T9P0

- Molecule 75 is a protein called T-complex protein 1 subunit epsilon.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	Gs	514	Total	C	N	O	S	0	0
			3952	2472	692	758	30		
75	Is	514	Total	C	N	O	S	0	0
			3952	2472	692	758	30		

- Molecule 76 is a protein called T-complex protein 1 subunit zeta.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	Gt	520	Total	C	N	O	S	0	0
			3984	2507	694	762	21		
76	Gu	520	Total	C	N	O	S	0	0
			3984	2507	694	762	21		

- Molecule 77 is a protein called T-complex protein 1 subunit eta.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	Gv	517	Total	C	N	O	S	0	0
			3973	2510	683	755	25		
77	Gw	517	Total	C	N	O	S	0	0
			3973	2510	683	755	25		

- Molecule 78 is a protein called T-complex protein 1 subunit theta.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	Gx	515	Total	C	N	O	S	0	0
			3929	2474	668	760	27		
78	Gy	515	Total	C	N	O	S	0	0
			3929	2474	668	760	27		

- Molecule 79 is a protein called Testis expressed 47.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	H0	189	Total	C	N	O	S	0	0
			1534	1001	248	274	11		
79	Pz	189	Total	C	N	O	S	0	0
			1534	1001	248	274	11		

- Molecule 80 is a protein called Dynein light chain roadblock-type 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	H1	96	Total	C	N	O	S	0	0
			758	475	133	145	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
80	H2	96	Total	C	N	O	S	0	0
			758	475	133	145	5		
80	JV	96	Total	C	N	O	S	0	0
			758	475	133	145	5		
80	JW	96	Total	C	N	O	S	0	0
			758	475	133	145	5		
80	Jo	96	Total	C	N	O	S	0	0
			758	475	133	145	5		
80	Jp	96	Total	C	N	O	S	0	0
			758	475	133	145	5		
80	P1	96	Total	C	N	O	S	0	0
			758	475	133	145	5		
80	P2	96	Total	C	N	O	S	0	0
			758	475	133	145	5		
80	Rh	96	Total	C	N	O	S	0	0
			758	475	133	145	5		
80	Ri	96	Total	C	N	O	S	0	0
			758	475	133	145	5		
80	Rw	96	Total	C	N	O	S	0	0
			758	475	133	145	5		
80	Rx	96	Total	C	N	O	S	0	0
			758	475	133	145	5		

- Molecule 81 is a protein called Leucine-rich repeat-containing protein 51.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	H3	176	Total	C	N	O	S	0	0
			1423	902	251	266	4		

- Molecule 82 is a protein called Radial spoke head protein 9 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	H7	263	Total	C	N	O	S	0	0
			2096	1346	351	390	9		
82	Hi	251	Total	C	N	O	S	0	0
			2000	1282	335	374	9		
82	Hj	262	Total	C	N	O	S	0	0
			2088	1340	350	389	9		
82	Hk	258	Total	C	N	O	S	0	0
			2058	1321	346	382	9		
82	Lu	251	Total	C	N	O	S	0	0
			2000	1282	335	374	9		

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Mol	Chain	Residues	Atoms					AltConf	Trace
82	Qc	263	Total	C	N	O	S	0	0
			2096	1346	351	390	9		
82	Qd	262	Total	C	N	O	S	0	0
			2088	1340	350	389	9		
82	Qe	258	Total	C	N	O	S	0	0
			2058	1321	346	382	9		

- Molecule 83 is a protein called Cilia- and flagella-associated protein 43.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	H8	1508	Total	C	N	O	S	0	0
			12248	7779	2099	2306	64		
83	Pb	1508	Total	C	N	O	S	0	0
			12248	7779	2099	2306	64		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H8	?	-	VAL	deletion	UNP E1BMD1
H8	?	-	THR	deletion	UNP E1BMD1
H8	?	-	GLU	deletion	UNP E1BMD1
Pb	?	-	VAL	deletion	UNP E1BMD1
Pb	?	-	THR	deletion	UNP E1BMD1
Pb	?	-	GLU	deletion	UNP E1BMD1

- Molecule 84 is a protein called Cilia and flagella associated protein 44.

Mol	Chain	Residues	Atoms					AltConf	Trace
84	H9	1531	Total	C	N	O	S	0	0
			12481	7935	2110	2375	61		
84	Pw	1531	Total	C	N	O	S	0	0
			12481	7935	2110	2375	61		

- Molecule 85 is a protein called DnaJ (Hsp40) related, subfamily B, member 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
85	HA	291	Total	C	N	O	S	0	0
			2359	1519	404	430	6		
85	HC	288	Total	C	N	O	S	0	0
			2333	1499	401	427	6		
85	Pn	291	Total	C	N	O	S	0	0
			2359	1519	404	430	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
85	Po	288	Total	C	N	O	S	0	0
			2333	1499	401	427	6		

- Molecule 86 is a protein called Calaxin.

Mol	Chain	Residues	Atoms					AltConf	Trace
86	HT	166	Total	C	N	O	S	0	0
			1371	879	225	254	13		
86	I2	166	Total	C	N	O	S	0	0
			1371	879	225	254	13		
86	Jd	166	Total	C	N	O	S	0	0
			1371	879	225	254	13		
86	Ra	166	Total	C	N	O	S	0	0
			1371	879	225	254	13		
86	Ro	166	Total	C	N	O	S	0	0
			1371	879	225	254	13		

- Molecule 87 is a protein called DPY30 domain-containing protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
87	HU	84	Total	C	N	O	S	0	0
			708	448	120	132	8		
87	HV	98	Total	C	N	O	S	0	0
			836	527	141	161	7		
87	Pp	84	Total	C	N	O	S	0	0
			708	448	120	132	8		
87	Pq	98	Total	C	N	O	S	0	0
			836	527	141	161	7		

- Molecule 88 is a protein called EF-hand calcium binding domain 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
88	HW	128	Total	C	N	O	S	0	0
			1048	667	182	194	5		
88	Pr	128	Total	C	N	O	S	0	0
			1048	667	182	194	5		

- Molecule 89 is a protein called NME/NM23 family member 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
89	HX	207	Total	C	N	O	S	0	0
			1659	1077	276	297	9		

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Mol	Chain	Residues	Atoms					AltConf	Trace
89	HY	202	Total	C	N	O	S	0	0
			1618	1051	269	290	8		
89	Ps	207	Total	C	N	O	S	0	0
			1659	1077	276	297	9		
89	Pt	202	Total	C	N	O	S	0	0
			1618	1051	269	290	8		

- Molecule 90 is a protein called Probable inactive peptidyl-prolyl cis-trans isomerase-like 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
90	HZ	291	Total	C	N	O	S	0	0
			2333	1504	389	433	7		
90	Ot	291	Total	C	N	O	S	0	0
			2333	1504	389	433	7		

- Molecule 91 is a protein called Regulator of G protein signaling 22.

Mol	Chain	Residues	Atoms					AltConf	Trace
91	Ha	540	Total	C	N	O	S	0	0
			4534	2959	756	797	22		
91	Ou	644	Total	C	N	O	S	0	0
			5437	3542	911	958	26		

- Molecule 92 is a protein called Probable inactive peptidyl-prolyl cis-trans isomerase-like 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
92	Hb	181	Total	C	N	O	S	0	0
			1484	940	267	276	1		
92	Hc	181	Total	C	N	O	S	0	0
			1484	940	267	276	1		
92	Hd	181	Total	C	N	O	S	0	0
			1484	940	267	276	1		
92	He	181	Total	C	N	O	S	0	0
			1484	940	267	276	1		
92	Oo	181	Total	C	N	O	S	0	0
			1484	940	267	276	1		
92	Ov	181	Total	C	N	O	S	0	0
			1484	940	267	276	1		
92	Ow	181	Total	C	N	O	S	0	0
			1484	940	267	276	1		
92	Ox	181	Total	C	N	O	S	0	0
			1484	940	267	276	1		

- Molecule 93 is a protein called Radial spoke head protein 3 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
93	Hf	164	Total	C	N	O	S	0	0
			1372	861	241	264	6		
93	Hg	158	Total	C	N	O	S	0	0
			1321	826	235	254	6		
93	P4	214	Total	C	N	O	S	0	0
			1766	1113	299	346	8		
93	QY	212	Total	C	N	O	S	0	0
			1750	1103	296	343	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
94	Hl	4122	Total	C	N	O	S	0	0
			33465	21426	5667	6190	182		

- Molecule 95 is a protein called Dynein axonemal intermediate chain 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
95	Hn	590	Total	C	N	O	S	0	0
			4819	3084	795	916	24		

- Molecule 96 is a protein called Cilia and flagella associated protein 73.

Mol	Chain	Residues	Atoms					AltConf	Trace
96	Ho	260	Total	C	N	O	S	0	0
			2153	1330	421	394	8		

- Molecule 97 is a protein called Coiled-coil domain containing 37.

Mol	Chain	Residues	Atoms					AltConf	Trace
97	Hv	249	Total	C	N	O	S	0	0
			2052	1285	334	422	11		

- Molecule 98 is a protein called WD repeat domain 63.

Mol	Chain	Residues	Atoms					AltConf	Trace
98	Hw	595	Total	C	N	O	S	0	0
			4783	3064	796	896	27		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Hw	217	PRO	SER	conflict	UNP A0A4W2D1C0

- Molecule 99 is a protein called Cilia and flagella associated protein 100.

Mol	Chain	Residues	Atoms					AltConf	Trace
99	Hx	504	Total	C	N	O	S	0	0
			4016	2550	673	772	21		

- Molecule 100 is a protein called Dynein axonemal intermediate chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
100	Hy	731	Total	C	N	O	S	0	0
			5809	3686	967	1119	37		
100	Hx	731	Total	C	N	O	S	0	0
			5809	3686	967	1119	37		
100	Kn	183	Total	C	N	O	S	0	0
			1573	983	291	293	6		
100	Ko	196	Total	C	N	O	S	0	0
			1677	1052	307	312	6		

- Molecule 101 is a protein called Cilia and flagella associated protein 57.

Mol	Chain	Residues	Atoms					AltConf	Trace
101	I3	1203	Total	C	N	O	S	0	0
			9764	6248	1647	1819	50		
101	X0	1353	Total	C	N	O	S	0	0
			10983	7018	1848	2061	56		
101	X2	1353	Total	C	N	O	S	0	0
			10983	7018	1848	2061	56		
101	X4	1353	Total	C	N	O	S	0	0
			10983	7018	1848	2061	56		
101	X8	1353	Total	C	N	O	S	0	0
			10983	7018	1848	2061	56		
101	Yc	2775	Total	C	N	O	S	0	0
			22387	14359	3762	4139	127		
101	Ye	2775	Total	C	N	O	S	0	0
			22387	14359	3762	4139	127		
101	Yg	2775	Total	C	N	O	S	0	0
			22387	14359	3762	4139	127		
101	Yi	2775	Total	C	N	O	S	0	0
			22387	14359	3762	4139	127		

- Molecule 102 is a protein called Dynein axonemal heavy chain 17.



Mol	Chain	Residues	Atoms					AltConf	Trace
102	I4	888	Total	C	N	O	S	0	0
			7201	4625	1187	1347	42		
102	X3	1003	Total	C	N	O	S	0	0
			8128	5210	1336	1534	48		
102	X5	1003	Total	C	N	O	S	0	0
			8128	5210	1336	1534	48		
102	X9	1003	Total	C	N	O	S	0	0
			8128	5210	1336	1534	48		
102	YA	1003	Total	C	N	O	S	0	0
			8128	5210	1336	1534	48		
102	Yd	2772	Total	C	N	O	S	0	0
			22214	14286	3705	4108	115		
102	Yf	2772	Total	C	N	O	S	0	0
			22214	14286	3705	4108	115		
102	Yh	2772	Total	C	N	O	S	0	0
			22214	14286	3705	4108	115		
102	Yj	2772	Total	C	N	O	S	0	0
			22214	14286	3705	4108	115		

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I4	400	LYS	-	insertion	UNP E1BLB4
X3	400	LYS	-	insertion	UNP E1BLB4
X5	400	LYS	-	insertion	UNP E1BLB4
X9	400	LYS	-	insertion	UNP E1BLB4
YA	400	LYS	-	insertion	UNP E1BLB4
Yd	400	LYS	-	insertion	UNP E1BLB4
Yf	400	LYS	-	insertion	UNP E1BLB4
Yh	400	LYS	-	insertion	UNP E1BLB4
Yj	400	LYS	-	insertion	UNP E1BLB4

- Molecule 103 is a protein called Dynein intermediate chain 2, axonemal isoform X2.

Mol	Chain	Residues	Atoms					AltConf	Trace
103	I6	448	Total	C	N	O	S	0	0
			3605	2285	615	681	24		
103	Jh	448	Total	C	N	O	S	0	0
			3605	2285	615	681	24		
103	KW	448	Total	C	N	O	S	0	0
			3605	2285	615	681	24		
103	Rd	448	Total	C	N	O	S	0	0
			3605	2285	615	681	24		

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Mol	Chain	Residues	Atoms					AltConf	Trace
103	Rq	448	Total	C	N	O	S	0	0
			3605	2285	615	681	24		

- Molecule 104 is a protein called Ropporin-1-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
104	IX	197	Total	C	N	O	S	0	0
			1549	994	256	289	10		
104	IY	138	Total	C	N	O	S	0	0
			1084	694	177	205	8		
104	MT	208	Total	C	N	O	S	0	0
			1631	1045	270	305	11		

- Molecule 105 is a protein called T-complex protein 1 subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
105	IZ	514	Total	C	N	O	S	0	0
			3900	2442	684	753	21		
105	Ia	523	Total	C	N	O	S	0	0
			3966	2482	695	767	22		

- Molecule 106 is a protein called Sperm surface protein Sp17.

Mol	Chain	Residues	Atoms				AltConf	Trace
106	Ic	39	Total	C	N	O	0	0
			317	202	54	61		
106	Id	39	Total	C	N	O	0	0
			317	202	54	61		
106	Ie	39	Total	C	N	O	0	0
			317	202	54	61		
106	MW	39	Total	C	N	O	0	0
			317	202	54	61		
106	Qn	39	Total	C	N	O	0	0
			317	202	54	61		
106	Qo	39	Total	C	N	O	0	0
			317	202	54	61		

- Molecule 107 is a protein called IQ motif and ubiquitin domain containing.

Mol	Chain	Residues	Atoms					AltConf	Trace
107	Ij	520	Total	C	N	O	S	0	0
			4374	2795	773	786	20		

- Molecule 108 is a protein called Calmodulin 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
108	Ik	142	Total	C	N	O	S	0	0
			1121	687	180	245	9		

- Molecule 109 is a protein called LRP2-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
109	Il	309	Total	C	N	O	S	0	0
			2485	1582	427	461	15		

- Molecule 110 is a protein called T-complex protein 1 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
110	Im	516	Total	C	N	O	S	0	0
			3882	2430	683	750	19		
110	In	516	Total	C	N	O	S	0	0
			3882	2430	683	750	19		

- Molecule 111 is a protein called T-complex protein 1 subunit gamma.

Mol	Chain	Residues	Atoms					AltConf	Trace
111	Io	510	Total	C	N	O	S	0	0
			3966	2470	702	766	28		
111	Ip	510	Total	C	N	O	S	0	0
			3966	2470	702	766	28		

- Molecule 112 is a protein called T-complex protein 1 subunit delta.

Mol	Chain	Residues	Atoms					AltConf	Trace
112	Iq	516	Total	C	N	O	S	0	0
			3900	2440	676	761	23		
112	Ir	516	Total	C	N	O	S	0	0
			3900	2440	676	761	23		

- Molecule 113 is a protein called Cilia and flagella associated protein 58.

Mol	Chain	Residues	Atoms					AltConf	Trace
113	It	141	Total	C	N	O	S	0	0
			1195	755	213	224	3		
113	Iu	130	Total	C	N	O	S	0	0
			1098	692	193	210	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
113	Kp	471	Total	C	N	O	S	0	0
			3967	2475	723	758	11		
113	Kq	457	Total	C	N	O	S	0	0
			3842	2395	697	739	11		

- Molecule 114 is a protein called Coiled-coil domain-containing protein 39.

Mol	Chain	Residues	Atoms					AltConf	Trace
114	Iw	382	Total	C	N	O	S	0	0
			3165	1940	577	635	13		
114	Kw	360	Total	C	N	O	S	0	0
			2976	1856	521	587	12		
114	Ph	75	Total	C	N	O	S	0	0
			624	382	108	131	3		

- Molecule 115 is a protein called Coiled-coil domain-containing protein 63.

Mol	Chain	Residues	Atoms					AltConf	Trace
115	Ix	415	Total	C	N	O	S	0	0
			3488	2192	613	668	15		
115	JZ	415	Total	C	N	O	S	0	0
			3488	2192	613	668	15		
115	Q2	382	Total	C	N	O	S	0	0
			3205	2020	560	611	14		
115	Rk	210	Total	C	N	O	S	0	0
			1764	1114	296	347	7		
115	XX	415	Total	C	N	O	S	0	0
			3488	2192	613	668	15		

- Molecule 116 is a protein called Sperm-associated microtubule inner protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
116	J	116	Total	C	N	O	S	0	0
			951	599	178	165	9		
116	K	116	Total	C	N	O	S	0	0
			951	599	178	165	9		
116	L	108	Total	C	N	O	S	0	0
			891	562	167	155	7		
116	Sk	116	Total	C	N	O	S	0	0
			951	599	178	165	9		
116	Sx	116	Total	C	N	O	S	0	0
			951	599	178	165	9		

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Mol	Chain	Residues	Atoms					AltConf	Trace
116	TT	108	Total	C	N	O	S	0	0
			891	562	167	155	7		
116	Ti	89	Total	C	N	O	S	0	0
			728	459	135	127	7		
116	v	116	Total	C	N	O	S	0	0
			951	599	178	165	9		

- Molecule 117 is a protein called Dynein light chain Tctex-type protein 2B.

Mol	Chain	Residues	Atoms					AltConf	Trace
117	JY	90	Total	C	N	O	S	0	0
			727	464	121	133	9		
117	Jr	104	Total	C	N	O	S	0	0
			837	533	137	157	10		
117	Pv	104	Total	C	N	O	S	0	0
			837	533	137	157	10		
117	Rj	104	Total	C	N	O	S	0	0
			837	533	137	157	10		
117	Rz	104	Total	C	N	O	S	0	0
			837	533	137	157	10		

- Molecule 118 is a protein called Cilia- and flagella-associated protein 144.

Mol	Chain	Residues	Atoms					AltConf	Trace
118	K1	116	Total	C	N	O	S	0	0
			992	627	186	177	2		
118	Sy	116	Total	C	N	O	S	0	0
			992	627	186	177	2		

- Molecule 119 is a protein called Dynein axonemal heavy chain 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
119	K2	3083	Total	C	N	O	S	0	0
			24830	15886	4187	4622	135		

There are 31 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K2	?	-	ALA	deletion	UNP F1MSP8
K2	?	-	LYS	deletion	UNP F1MSP8
K2	?	-	ASN	deletion	UNP F1MSP8
K2	?	-	LEU	deletion	UNP F1MSP8

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Chain	Residue	Modelled	Actual	Comment	Reference
K2	165	GLU	GLN	conflict	UNP F1MSP8
K2	168	CYS	MET	conflict	UNP F1MSP8
K2	169	THR	TYR	conflict	UNP F1MSP8
K2	170	GLN	SER	conflict	UNP F1MSP8
K2	172	LEU	HIS	conflict	UNP F1MSP8
K2	173	GLY	ARG	conflict	UNP F1MSP8
K2	174	ASP	-	insertion	UNP F1MSP8
K2	175	LEU	-	insertion	UNP F1MSP8
K2	176	GLY	-	insertion	UNP F1MSP8
K2	177	ALA	PRO	conflict	UNP F1MSP8
K2	180	TYR	SER	conflict	UNP F1MSP8
K2	182	ARG	GLU	conflict	UNP F1MSP8
K2	183	GLY	GLU	conflict	UNP F1MSP8
K2	184	THR	GLU	conflict	UNP F1MSP8
K2	185	PHE	GLU	conflict	UNP F1MSP8
K2	186	LEU	MET	conflict	UNP F1MSP8
K2	?	-	ASP	deletion	UNP F1MSP8
K2	?	-	LEU	deletion	UNP F1MSP8
K2	?	-	GLU	deletion	UNP F1MSP8
K2	?	-	SER	deletion	UNP F1MSP8
K2	?	-	ILE	deletion	UNP F1MSP8
K2	?	-	GLU	deletion	UNP F1MSP8
K2	?	-	ASN	deletion	UNP F1MSP8
K2	187	VAL	LEU	conflict	UNP F1MSP8
K2	189	MET	VAL	conflict	UNP F1MSP8
K2	190	PHE	-	insertion	UNP F1MSP8
K2	191	GLN	LYS	conflict	UNP F1MSP8

- Molecule 120 is a protein called Tubulin alpha-3 chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
120	Km	376	Total	C	N	O	S	0	0
			2936	1863	490	566	17		

- Molecule 121 is a protein called Cilia and flagella associated protein 299.

Mol	Chain	Residues	Atoms					AltConf	Trace
121	Kr	209	Total	C	N	O	S	0	0
			1707	1083	293	330	1		

- Molecule 122 is a protein called CCDC96 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
122	Ks	142	Total	C	N	O	S	0	0
			1156	719	215	216	6		

- Molecule 123 is a protein called Chromosome 20 C5orf49 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
123	L1	134	Total	C	N	O	S	0	0
			1090	685	208	195	2		
123	L2	134	Total	C	N	O	S	0	0
			1090	685	208	195	2		
123	TU	134	Total	C	N	O	S	0	0
			1090	685	208	195	2		

- Molecule 124 is a protein called Leucine rich repeat containing 34.

Mol	Chain	Residues	Atoms					AltConf	Trace
124	MA	375	Total	C	N	O	S	0	0
			2935	1845	504	564	22		

- Molecule 125 is a protein called MORN repeat-containing protein 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
125	MS	226	Total	C	N	O	S	0	0
			1849	1177	328	337	7		

- Molecule 126 is a protein called WD repeat domain 64.

Mol	Chain	Residues	Atoms					AltConf	Trace
126	No	812	Total	C	N	O	S	0	0
			6544	4197	1114	1198	35		

- Molecule 127 is a protein called Dynein regulatory complex protein 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
127	Oj	320	Total	C	N	O	S	0	0
			2627	1631	469	518	9		

- Molecule 128 is a protein called IQ motif containing with AAA domain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
128	Ok	677	Total	C	N	O	S	0	0
			5505	3526	943	1008	28		

- Molecule 129 is a protein called Ankyrin repeat and EF-hand domain containing 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
129	Ol	649	Total	C	N	O	S	0	0
			5105	3218	901	953	33		

- Molecule 130 is a protein called Cilia- and flagella-associated protein 263.

Mol	Chain	Residues	Atoms					AltConf	Trace
130	Om	143	Total	C	N	O	S	0	0
			1197	761	214	215	7		

- Molecule 131 is a protein called Dynein axonemal heavy chain 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
131	PW	2678	Total	C	N	O	S	0	0
			21531	13851	3596	3960	124		
131	Xv	3582	Total	C	N	O	S	0	0
			28933	18580	4828	5360	165		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
PW	2621	PRO	ALA	conflict	UNP A0A3Q1M7D1
PW	2622	ALA	THR	conflict	UNP A0A3Q1M7D1
Xv	2621	PRO	ALA	conflict	UNP A0A3Q1M7D1
Xv	2622	ALA	THR	conflict	UNP A0A3Q1M7D1

- Molecule 132 is a protein called Centrin-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
132	Pk	147	Total	C	N	O	S	0	0
			1186	740	192	247	7		

- Molecule 133 is a protein called Cilia- and flagella-associated protein 68.

Mol	Chain	Residues	Atoms					AltConf	Trace
133	Q	107	Total	C	N	O	S	0	0
			919	584	160	170	5		
133	Uq	107	Total	C	N	O	S	0	0
			919	584	160	170	5		

- Molecule 134 is a protein called Zinc finger MYND-type containing 12.



Mol	Chain	Residues	Atoms					AltConf	Trace
134	Qq	366	Total	C	N	O	S	0	0
			2935	1869	506	543	17		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Qq	287	LEU	ILE	conflict	UNP A0A4W2F7K6

- Molecule 135 is a protein called Dynein regulatory complex protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
135	Qt	521	Total	C	N	O	S	0	0
			4389	2780	760	833	16		

- Molecule 136 is a protein called Dynein regulatory complex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
136	Qu	440	Total	C	N	O	S	0	0
			3684	2315	646	710	13		

- Molecule 137 is a protein called Dynein regulatory complex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
137	Qv	516	Total	C	N	O	S	0	0
			4219	2657	710	830	22		

- Molecule 138 is a protein called T-complex-associated-testis-expressed 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
138	Qx	402	Total	C	N	O	S	0	0
			3170	1997	576	581	16		

- Molecule 139 is a protein called Dynein regulatory complex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
139	Qy	590	Total	C	N	O	S	0	0
			4884	3103	836	908	37		

- Molecule 140 is a protein called Dynein regulatory complex protein 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
140	Qz	238	Total	C	N	O	S	0	0
			1991	1245	346	392	8		

- Molecule 141 is a protein called Cilia- and flagella-associated protein 141.

Mol	Chain	Residues	Atoms					AltConf	Trace
141	W5	91	Total	C	N	O	S	0	0
			785	495	151	133	6		
141	h	91	Total	C	N	O	S	0	0
			785	495	151	133	6		

- Molecule 142 is a protein called Dynein axonemal heavy chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
142	X1	3787	Total	C	N	O	S	0	0
			30514	19533	5116	5690	175		

- Molecule 143 is a protein called Cilia- and flagella-associated protein 20.

Mol	Chain	Residues	Atoms					AltConf	Trace
143	XG	182	Total	C	N	O	S	0	0
			1512	969	266	270	7		
143	XH	182	Total	C	N	O	S	0	0
			1512	969	266	270	7		
143	XI	182	Total	C	N	O	S	0	0
			1512	969	266	270	7		
143	XJ	182	Total	C	N	O	S	0	0
			1512	969	266	270	7		
143	XK	182	Total	C	N	O	S	0	0
			1512	969	266	270	7		
143	XL	181	Total	C	N	O	S	0	0
			1503	963	264	269	7		
143	XM	180	Total	C	N	O	S	0	0
			1494	958	262	267	7		
143	XN	182	Total	C	N	O	S	0	0
			1512	969	266	270	7		
143	XO	182	Total	C	N	O	S	0	0
			1512	969	266	270	7		
143	XP	181	Total	C	N	O	S	0	0
			1503	963	264	269	7		
143	XQ	182	Total	C	N	O	S	0	0
			1512	969	266	270	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
143	XR	182	Total	C	N	O	S	0	0
			1512	969	266	270	7		
143	XS	182	Total	C	N	O	S	0	0
			1512	969	266	270	7		
143	XT	181	Total	C	N	O	S	0	0
			1503	963	264	269	7		
143	XU	180	Total	C	N	O	S	0	0
			1494	958	262	267	7		

- Molecule 144 is a protein called Adenylate kinase 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
144	Xc	665	Total	C	N	O	S	0	0
			5389	3429	911	1026	23		
144	Xd	653	Total	C	N	O	S	0	0
			5286	3371	894	998	23		

- Molecule 145 is a protein called Cilia- and flagella-associated protein 97 domain containing 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
145	Xe	122	Total	C	N	O	S	0	0
			1044	685	179	176	4		

- Molecule 146 is a protein called Cilia- and flagella-associated protein 276.

Mol	Chain	Residues	Atoms					AltConf	Trace
146	Xf	1415	Total	C	N	O	S	0	0
			11545	7440	1917	2133	55		

- Molecule 147 is a protein called Cilia- and flagella-associated protein 20.

Mol	Chain	Residues	Atoms					AltConf	Trace
147	Xg	1135	Total	C	N	O	S	0	0
			9167	5898	1549	1670	50		

- Molecule 148 is a protein called Ciliogenesis-associated TTC17-interacting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
148	Xh	332	Total	C	N	O	S	0	0
			2669	1713	445	496	15		

- Molecule 149 is a protein called Cilia- and flagella-associated protein 91.

Mol	Chain	Residues	Atoms					AltConf	Trace
149	Xi	644	Total	C	N	O	S	0	0
			5346	3351	978	996	21		

- Molecule 150 is a protein called Adenylate kinase 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
150	Xj	911	Total	C	N	O	S	0	0
			7253	4652	1206	1357	38		

- Molecule 151 is a protein called cAMP-dependent protein kinase type I-alpha regulatory subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
151	Xk	261	Total	C	N	O	S	0	0
			2067	1309	353	397	8		

- Molecule 152 is a protein called A-kinase anchoring protein 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
152	Xl	1096	Total	C	N	O	S	0	0
			8922	5701	1530	1647	44		

- Molecule 153 is a protein called Leucine-rich repeat-containing protein 23.

Mol	Chain	Residues	Atoms					AltConf	Trace
153	Xm	276	Total	C	N	O	S	0	0
			2220	1391	397	424	8		
153	Xn	276	Total	C	N	O	S	0	0
			2220	1391	397	424	8		

- Molecule 154 is a protein called Leucine rich repeats and death domain containing 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
154	Xo	719	Total	C	N	O	S	0	0
			5792	3723	971	1072	26		

- Molecule 155 is a protein called Malate dehydrogenase, cytoplasmic.

Mol	Chain	Residues	Atoms					AltConf	Trace
155	Xp	334	Total	C	N	O	S	0	0
			2557	1628	428	487	14		

- Molecule 156 is a protein called Putative malate dehydrogenase 1B.

Mol	Chain	Residues	Atoms					AltConf	Trace
156	Xq	448	Total	C	N	O	S	0	0
			3536	2271	606	641	18		

- Molecule 157 is a protein called Cilia and flagella associated protein 251.

Mol	Chain	Residues	Atoms					AltConf	Trace
157	Xr	580	Total	C	N	O	S	0	0
			4560	2909	772	852	27		

- Molecule 158 is a protein called Serine/threonine/tyrosine interacting like 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
158	Xs	300	Total	C	N	O	S	0	0
			2417	1561	408	431	17		

- Molecule 159 is a protein called cAMP-dependent protein kinase catalytic subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
159	Xt	294	Total	C	N	O	S	0	0
			2432	1585	414	424	9		

- Molecule 160 is a protein called MORN repeat-containing protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
160	Xu	128	Total	C	N	O	S	0	0
			1042	660	174	201	7		

- Molecule 161 is a protein called Dynein axonemal heavy chain 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
161	Xw	3528	Total	C	N	O	S	0	0
			28562	18304	4789	5303	166		
161	Xy	3397	Total	C	N	O	S	0	0
			27446	17571	4607	5110	158		

- Molecule 162 is a protein called putative malate dehydrogenase 1B.

Mol	Chain	Residues	Atoms					AltConf	Trace
162	Xx	3523	Total	C	N	O	S	0	0
			28503	18349	4712	5276	166		

- Molecule 163 is a protein called Dynein axonemal heavy chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
163	Xz	3595	Total	C	N	O	S	0	0
			29070	18634	4881	5400	155		

- Molecule 164 is a protein called Parkin coregulated gene protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
164	YG	210	Total	C	N	O	S	0	0
			1706	1108	288	301	9		
164	YH	218	Total	C	N	O	S	0	0
			1759	1138	297	315	9		
164	YI	218	Total	C	N	O	S	0	0
			1759	1138	297	315	9		
164	YJ	218	Total	C	N	O	S	0	0
			1759	1138	297	315	9		
164	YK	218	Total	C	N	O	S	0	0
			1759	1138	297	315	9		
164	YL	218	Total	C	N	O	S	0	0
			1759	1138	297	315	9		
164	YM	218	Total	C	N	O	S	0	0
			1759	1138	297	315	9		
164	YN	218	Total	C	N	O	S	0	0
			1759	1138	297	315	9		
164	YO	218	Total	C	N	O	S	0	0
			1759	1138	297	315	9		
164	YP	218	Total	C	N	O	S	0	0
			1759	1138	297	315	9		
164	YQ	218	Total	C	N	O	S	0	0
			1759	1138	297	315	9		
164	YR	218	Total	C	N	O	S	0	0
			1759	1138	297	315	9		
164	YS	218	Total	C	N	O	S	0	0
			1759	1138	297	315	9		
164	YT	218	Total	C	N	O	S	0	0
			1759	1138	297	315	9		

- Molecule 165 is a protein called Dynein axonemal heavy chain 6.

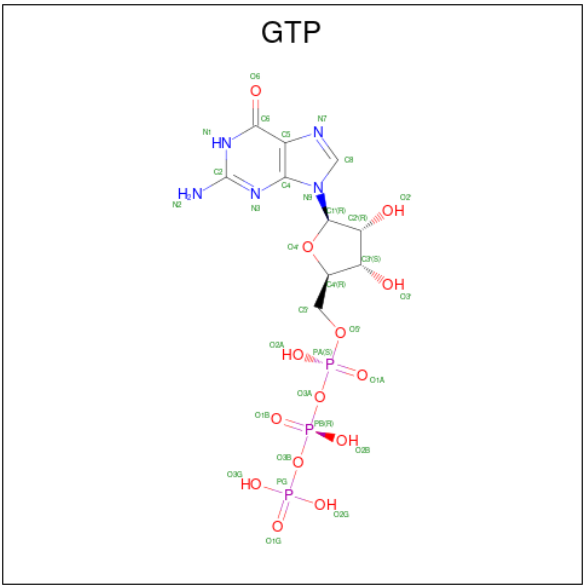
Mol	Chain	Residues	Atoms					AltConf	Trace
165	ke	97	Total	C	N	O	S	0	0
			796	516	138	141	1		
165	kf	97	Total	C	N	O	S	0	0
			796	516	138	141	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
165	kg	97	796	516	138	141	1	0	0

- Molecule 166 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>14</sub>P<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
166	AA	1	Total 32	10	5	14	3	0
166	AC	1	Total 32	10	5	14	3	0
166	AE	1	Total 32	10	5	14	3	0
166	AG	1	Total 32	10	5	14	3	0
166	AI	1	Total 32	10	5	14	3	0
166	AK	1	Total 32	10	5	14	3	0
166	AN	1	Total 32	10	5	14	3	0
166	AR	1	Total 32	10	5	14	3	0
166	BA	1	Total 32	10	5	14	3	0
166	BC	1	Total 32	10	5	14	3	0

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Mol	Chain	Residues	Atoms					AltConf
166	BE	1	Total 32	C 10	N 5	O 14	P 3	0
166	BG	1	Total 32	C 10	N 5	O 14	P 3	0
166	BI	1	Total 32	C 10	N 5	O 14	P 3	0
166	BK	1	Total 32	C 10	N 5	O 14	P 3	0
166	Bt	1	Total 32	C 10	N 5	O 14	P 3	0
166	Bw	1	Total 32	C 10	N 5	O 14	P 3	0
166	CA	1	Total 32	C 10	N 5	O 14	P 3	0
166	CC	1	Total 32	C 10	N 5	O 14	P 3	0
166	CE	1	Total 32	C 10	N 5	O 14	P 3	0
166	CG	1	Total 32	C 10	N 5	O 14	P 3	0
166	CI	1	Total 32	C 10	N 5	O 14	P 3	0
166	CK	1	Total 32	C 10	N 5	O 14	P 3	0
166	DA	1	Total 32	C 10	N 5	O 14	P 3	0
166	DC	1	Total 32	C 10	N 5	O 14	P 3	0
166	DE	1	Total 32	C 10	N 5	O 14	P 3	0
166	DG	1	Total 32	C 10	N 5	O 14	P 3	0
166	DI	1	Total 32	C 10	N 5	O 14	P 3	0
166	DK	1	Total 32	C 10	N 5	O 14	P 3	0
166	DM	1	Total 32	C 10	N 5	O 14	P 3	0
166	EC	1	Total 32	C 10	N 5	O 14	P 3	0
166	EE	1	Total 32	C 10	N 5	O 14	P 3	0

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Mol	Chain	Residues	Atoms					AltConf
166	EG	1	Total 32	C 10	N 5	O 14	P 3	0
166	EI	1	Total 32	C 10	N 5	O 14	P 3	0
166	EK	1	Total 32	C 10	N 5	O 14	P 3	0
166	EM	1	Total 32	C 10	N 5	O 14	P 3	0
166	EW	1	Total 32	C 10	N 5	O 14	P 3	0
166	Eb	1	Total 32	C 10	N 5	O 14	P 3	0
166	FC	1	Total 32	C 10	N 5	O 14	P 3	0
166	FE	1	Total 32	C 10	N 5	O 14	P 3	0
166	FG	1	Total 32	C 10	N 5	O 14	P 3	0
166	FI	1	Total 32	C 10	N 5	O 14	P 3	0
166	FK	1	Total 32	C 10	N 5	O 14	P 3	0
166	FM	1	Total 32	C 10	N 5	O 14	P 3	0
166	FU	1	Total 32	C 10	N 5	O 14	P 3	0
166	FW	1	Total 32	C 10	N 5	O 14	P 3	0
166	FX	1	Total 32	C 10	N 5	O 14	P 3	0
166	Fr	1	Total 32	C 10	N 5	O 14	P 3	0
166	Ft	1	Total 32	C 10	N 5	O 14	P 3	0
166	Fv	1	Total 32	C 10	N 5	O 14	P 3	0
166	GB	1	Total 32	C 10	N 5	O 14	P 3	0
166	GC	1	Total 32	C 10	N 5	O 14	P 3	0
166	GE	1	Total 32	C 10	N 5	O 14	P 3	0

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Mol	Chain	Residues	Atoms					AltConf
166	GG	1	Total 32	C 10	N 5	O 14	P 3	0
166	GI	1	Total 32	C 10	N 5	O 14	P 3	0
166	GK	1	Total 32	C 10	N 5	O 14	P 3	0
166	GM	1	Total 32	C 10	N 5	O 14	P 3	0
166	GP	1	Total 32	C 10	N 5	O 14	P 3	0
166	GR	1	Total 32	C 10	N 5	O 14	P 3	0
166	GT	1	Total 32	C 10	N 5	O 14	P 3	0
166	GV	1	Total 32	C 10	N 5	O 14	P 3	0
166	GX	1	Total 32	C 10	N 5	O 14	P 3	0
166	HE	1	Total 32	C 10	N 5	O 14	P 3	0
166	HG	1	Total 32	C 10	N 5	O 14	P 3	0
166	HI	1	Total 32	C 10	N 5	O 14	P 3	0
166	HK	1	Total 32	C 10	N 5	O 14	P 3	0
166	HM	1	Total 32	C 10	N 5	O 14	P 3	0
166	HP	1	Total 32	C 10	N 5	O 14	P 3	0
166	HR	1	Total 32	C 10	N 5	O 14	P 3	0
166	IC	1	Total 32	C 10	N 5	O 14	P 3	0
166	IE	1	Total 32	C 10	N 5	O 14	P 3	0
166	IG	1	Total 32	C 10	N 5	O 14	P 3	0
166	II	1	Total 32	C 10	N 5	O 14	P 3	0
166	IK	1	Total 32	C 10	N 5	O 14	P 3	0

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Mol	Chain	Residues	Atoms					AltConf
166	IM	1	Total 32	C 10	N 5	O 14	P 3	0
166	IN	1	Total 32	C 10	N 5	O 14	P 3	0
166	IP	1	Total 32	C 10	N 5	O 14	P 3	0
166	IR	1	Total 32	C 10	N 5	O 14	P 3	0
166	J1	1	Total 32	C 10	N 5	O 14	P 3	0
166	J3	1	Total 32	C 10	N 5	O 14	P 3	0
166	J5	1	Total 32	C 10	N 5	O 14	P 3	0
166	J7	1	Total 32	C 10	N 5	O 14	P 3	0
166	J9	1	Total 32	C 10	N 5	O 14	P 3	0
166	JC	1	Total 32	C 10	N 5	O 14	P 3	0
166	JE	1	Total 32	C 10	N 5	O 14	P 3	0
166	JG	1	Total 32	C 10	N 5	O 14	P 3	0
166	JI	1	Total 32	C 10	N 5	O 14	P 3	0
166	JK	1	Total 32	C 10	N 5	O 14	P 3	0
166	JM	1	Total 32	C 10	N 5	O 14	P 3	0
166	JO	1	Total 32	C 10	N 5	O 14	P 3	0
166	JQ	1	Total 32	C 10	N 5	O 14	P 3	0
166	JS	1	Total 32	C 10	N 5	O 14	P 3	0
166	KA	1	Total 32	C 10	N 5	O 14	P 3	0
166	KC	1	Total 32	C 10	N 5	O 14	P 3	0
166	KE	1	Total 32	C 10	N 5	O 14	P 3	0

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Mol	Chain	Residues	Atoms					AltConf
166	KG	1	Total 32	C 10	N 5	O 14	P 3	0
166	KI	1	Total 32	C 10	N 5	O 14	P 3	0
166	KK	1	Total 32	C 10	N 5	O 14	P 3	0
166	KM	1	Total 32	C 10	N 5	O 14	P 3	0
166	KO	1	Total 32	C 10	N 5	O 14	P 3	0
166	KQ	1	Total 32	C 10	N 5	O 14	P 3	0
166	KS	1	Total 32	C 10	N 5	O 14	P 3	0
166	KV	1	Total 32	C 10	N 5	O 14	P 3	0
166	LC	1	Total 32	C 10	N 5	O 14	P 3	0
166	LE	1	Total 32	C 10	N 5	O 14	P 3	0
166	LG	1	Total 32	C 10	N 5	O 14	P 3	0
166	LI	1	Total 32	C 10	N 5	O 14	P 3	0
166	LK	1	Total 32	C 10	N 5	O 14	P 3	0
166	LM	1	Total 32	C 10	N 5	O 14	P 3	0
166	LN	1	Total 32	C 10	N 5	O 14	P 3	0
166	LP	1	Total 32	C 10	N 5	O 14	P 3	0
166	LR	1	Total 32	C 10	N 5	O 14	P 3	0
166	LY	1	Total 32	C 10	N 5	O 14	P 3	0
166	La	1	Total 32	C 10	N 5	O 14	P 3	0
166	Lc	1	Total 32	C 10	N 5	O 14	P 3	0
166	Le	1	Total 32	C 10	N 5	O 14	P 3	0

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Mol	Chain	Residues	Atoms					AltConf
166	Lg	1	Total 32	C 10	N 5	O 14	P 3	0
166	Li	1	Total 32	C 10	N 5	O 14	P 3	0
166	Lk	1	Total 32	C 10	N 5	O 14	P 3	0
166	MC	1	Total 32	C 10	N 5	O 14	P 3	0
166	ME	1	Total 32	C 10	N 5	O 14	P 3	0
166	MG	1	Total 32	C 10	N 5	O 14	P 3	0
166	MI	1	Total 32	C 10	N 5	O 14	P 3	0
166	MK	1	Total 32	C 10	N 5	O 14	P 3	0
166	MM	1	Total 32	C 10	N 5	O 14	P 3	0
166	MN	1	Total 32	C 10	N 5	O 14	P 3	0
166	MP	1	Total 32	C 10	N 5	O 14	P 3	0
166	MR	1	Total 32	C 10	N 5	O 14	P 3	0
166	Mi	1	Total 32	C 10	N 5	O 14	P 3	0
166	Mk	1	Total 32	C 10	N 5	O 14	P 3	0
166	Mm	1	Total 32	C 10	N 5	O 14	P 3	0
166	Mo	1	Total 32	C 10	N 5	O 14	P 3	0
166	Mq	1	Total 32	C 10	N 5	O 14	P 3	0
166	Ms	1	Total 32	C 10	N 5	O 14	P 3	0
166	Mu	1	Total 32	C 10	N 5	O 14	P 3	0
166	N1	1	Total 32	C 10	N 5	O 14	P 3	0
166	N3	1	Total 32	C 10	N 5	O 14	P 3	0

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Mol	Chain	Residues	Atoms					AltConf
166	NA	1	Total 32	C 10	N 5	O 14	P 3	0
166	NC	1	Total 32	C 10	N 5	O 14	P 3	0
166	NE	1	Total 32	C 10	N 5	O 14	P 3	0
166	NG	1	Total 32	C 10	N 5	O 14	P 3	0
166	NI	1	Total 32	C 10	N 5	O 14	P 3	0
166	NK	1	Total 32	C 10	N 5	O 14	P 3	0
166	NM	1	Total 32	C 10	N 5	O 14	P 3	0
166	NO	1	Total 32	C 10	N 5	O 14	P 3	0
166	NQ	1	Total 32	C 10	N 5	O 14	P 3	0
166	Ns	1	Total 32	C 10	N 5	O 14	P 3	0
166	Nu	1	Total 32	C 10	N 5	O 14	P 3	0
166	Nw	1	Total 32	C 10	N 5	O 14	P 3	0
166	Ny	1	Total 32	C 10	N 5	O 14	P 3	0
166	O1	1	Total 32	C 10	N 5	O 14	P 3	0
166	O3	1	Total 32	C 10	N 5	O 14	P 3	0
166	O5	1	Total 32	C 10	N 5	O 14	P 3	0
166	O7	1	Total 32	C 10	N 5	O 14	P 3	0
166	O9	1	Total 32	C 10	N 5	O 14	P 3	0
166	OC	1	Total 32	C 10	N 5	O 14	P 3	0
166	OE	1	Total 32	C 10	N 5	O 14	P 3	0
166	OG	1	Total 32	C 10	N 5	O 14	P 3	0

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Mol	Chain	Residues	Atoms					AltConf
166	OI	1	Total 32	C 10	N 5	O 14	P 3	0
166	OK	1	Total 32	C 10	N 5	O 14	P 3	0
166	OO	1	Total 32	C 10	N 5	O 14	P 3	0
166	OQ	1	Total 32	C 10	N 5	O 14	P 3	0
166	P0	1	Total 32	C 10	N 5	O 14	P 3	0
166	P6	1	Total 32	C 10	N 5	O 14	P 3	0
166	P8	1	Total 32	C 10	N 5	O 14	P 3	0
166	PA	1	Total 32	C 10	N 5	O 14	P 3	0
166	PC	1	Total 32	C 10	N 5	O 14	P 3	0
166	PE	1	Total 32	C 10	N 5	O 14	P 3	0
166	PG	1	Total 32	C 10	N 5	O 14	P 3	0
166	PI	1	Total 32	C 10	N 5	O 14	P 3	0
166	PK	1	Total 32	C 10	N 5	O 14	P 3	0
166	PM	1	Total 32	C 10	N 5	O 14	P 3	0
166	PO	1	Total 32	C 10	N 5	O 14	P 3	0
166	PQ	1	Total 32	C 10	N 5	O 14	P 3	0
166	PT	1	Total 32	C 10	N 5	O 14	P 3	0
166	Q0	1	Total 32	C 10	N 5	O 14	P 3	0
166	Q4	1	Total 32	C 10	N 5	O 14	P 3	0
166	Q6	1	Total 32	C 10	N 5	O 14	P 3	0
166	Q8	1	Total 32	C 10	N 5	O 14	P 3	0

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Mol	Chain	Residues	Atoms					AltConf
166	QA	1	Total 32	C 10	N 5	O 14	P 3	0
166	QC	1	Total 32	C 10	N 5	O 14	P 3	0
166	QE	1	Total 32	C 10	N 5	O 14	P 3	0
166	QG	1	Total 32	C 10	N 5	O 14	P 3	0
166	QI	1	Total 32	C 10	N 5	O 14	P 3	0
166	QK	1	Total 32	C 10	N 5	O 14	P 3	0
166	QM	1	Total 32	C 10	N 5	O 14	P 3	0
166	QO	1	Total 32	C 10	N 5	O 14	P 3	0
166	QQ	1	Total 32	C 10	N 5	O 14	P 3	0
166	QT	1	Total 32	C 10	N 5	O 14	P 3	0
166	QV	1	Total 32	C 10	N 5	O 14	P 3	0
166	QX	1	Total 32	C 10	N 5	O 14	P 3	0
166	R0	1	Total 32	C 10	N 5	O 14	P 3	0
166	R2	1	Total 32	C 10	N 5	O 14	P 3	0
166	R4	1	Total 32	C 10	N 5	O 14	P 3	0
166	R6	1	Total 32	C 10	N 5	O 14	P 3	0
166	R8	1	Total 32	C 10	N 5	O 14	P 3	0
166	RA	1	Total 32	C 10	N 5	O 14	P 3	0
166	RC	1	Total 32	C 10	N 5	O 14	P 3	0
166	RE	1	Total 32	C 10	N 5	O 14	P 3	0
166	RG	1	Total 32	C 10	N 5	O 14	P 3	0

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Mol	Chain	Residues	Atoms					AltConf
166	RI	1	Total 32	C 10	N 5	O 14	P 3	0
166	RK	1	Total 32	C 10	N 5	O 14	P 3	0
166	RM	1	Total 32	C 10	N 5	O 14	P 3	0
166	RO	1	Total 32	C 10	N 5	O 14	P 3	0
166	RQ	1	Total 32	C 10	N 5	O 14	P 3	0
166	RT	1	Total 32	C 10	N 5	O 14	P 3	0
166	RV	1	Total 32	C 10	N 5	O 14	P 3	0
166	S0	1	Total 32	C 10	N 5	O 14	P 3	0
166	S2	1	Total 32	C 10	N 5	O 14	P 3	0
166	S4	1	Total 32	C 10	N 5	O 14	P 3	0
166	S6	1	Total 32	C 10	N 5	O 14	P 3	0
166	S8	1	Total 32	C 10	N 5	O 14	P 3	0
166	SA	1	Total 32	C 10	N 5	O 14	P 3	0
166	SC	1	Total 32	C 10	N 5	O 14	P 3	0
166	SE	1	Total 32	C 10	N 5	O 14	P 3	0
166	SG	1	Total 32	C 10	N 5	O 14	P 3	0
166	SI	1	Total 32	C 10	N 5	O 14	P 3	0
166	SK	1	Total 32	C 10	N 5	O 14	P 3	0
166	SN	1	Total 32	C 10	N 5	O 14	P 3	0
166	SP	1	Total 32	C 10	N 5	O 14	P 3	0
166	ST	1	Total 32	C 10	N 5	O 14	P 3	0

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Mol	Chain	Residues	Atoms					AltConf
166	SV	1	Total 32	C 10	N 5	O 14	P 3	0
166	SY	1	Total 32	C 10	N 5	O 14	P 3	0
166	Sa	1	Total 32	C 10	N 5	O 14	P 3	0
166	Sc	1	Total 32	C 10	N 5	O 14	P 3	0
166	Se	1	Total 32	C 10	N 5	O 14	P 3	0
166	Sg	1	Total 32	C 10	N 5	O 14	P 3	0
166	Si	1	Total 32	C 10	N 5	O 14	P 3	0
166	Sm	1	Total 32	C 10	N 5	O 14	P 3	0
166	So	1	Total 32	C 10	N 5	O 14	P 3	0
166	Sq	1	Total 32	C 10	N 5	O 14	P 3	0
166	Ss	1	Total 32	C 10	N 5	O 14	P 3	0
166	Su	1	Total 32	C 10	N 5	O 14	P 3	0
166	Sw	1	Total 32	C 10	N 5	O 14	P 3	0
166	Sz	1	Total 32	C 10	N 5	O 14	P 3	0
166	T1	1	Total 32	C 10	N 5	O 14	P 3	0
166	T3	1	Total 32	C 10	N 5	O 14	P 3	0
166	T5	1	Total 32	C 10	N 5	O 14	P 3	0
166	T7	1	Total 32	C 10	N 5	O 14	P 3	0
166	T9	1	Total 32	C 10	N 5	O 14	P 3	0
166	TC	1	Total 32	C 10	N 5	O 14	P 3	0
166	TE	1	Total 32	C 10	N 5	O 14	P 3	0

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Mol	Chain	Residues	Atoms					AltConf
166	TG	1	Total 32	C 10	N 5	O 14	P 3	0
166	TI	1	Total 32	C 10	N 5	O 14	P 3	0
166	TK	1	Total 32	C 10	N 5	O 14	P 3	0
166	TM	1	Total 32	C 10	N 5	O 14	P 3	0
166	TO	1	Total 32	C 10	N 5	O 14	P 3	0
166	TQ	1	Total 32	C 10	N 5	O 14	P 3	0
166	TW	1	Total 32	C 10	N 5	O 14	P 3	0
166	TY	1	Total 32	C 10	N 5	O 14	P 3	0
166	Ta	1	Total 32	C 10	N 5	O 14	P 3	0
166	Tc	1	Total 32	C 10	N 5	O 14	P 3	0
166	Te	1	Total 32	C 10	N 5	O 14	P 3	0
166	Tg	1	Total 32	C 10	N 5	O 14	P 3	0
166	Tk	1	Total 32	C 10	N 5	O 14	P 3	0
166	Tm	1	Total 32	C 10	N 5	O 14	P 3	0
166	To	1	Total 32	C 10	N 5	O 14	P 3	0
166	Tq	1	Total 32	C 10	N 5	O 14	P 3	0
166	Ts	1	Total 32	C 10	N 5	O 14	P 3	0
166	Tu	1	Total 32	C 10	N 5	O 14	P 3	0
166	Ty	1	Total 32	C 10	N 5	O 14	P 3	0
166	U2	1	Total 32	C 10	N 5	O 14	P 3	0
166	U5	1	Total 32	C 10	N 5	O 14	P 3	0

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Mol	Chain	Residues	Atoms					AltConf
166	U7	1	Total 32	C 10	N 5	O 14	P 3	0
166	U9	1	Total 32	C 10	N 5	O 14	P 3	0
166	UA	1	Total 32	C 10	N 5	O 14	P 3	0
166	UC	1	Total 32	C 10	N 5	O 14	P 3	0
166	UE	1	Total 32	C 10	N 5	O 14	P 3	0
166	UG	1	Total 32	C 10	N 5	O 14	P 3	0
166	UI	1	Total 32	C 10	N 5	O 14	P 3	0
166	UK	1	Total 32	C 10	N 5	O 14	P 3	0
166	UM	1	Total 32	C 10	N 5	O 14	P 3	0
166	UN	1	Total 32	C 10	N 5	O 14	P 3	0
166	UP	1	Total 32	C 10	N 5	O 14	P 3	0
166	UR	1	Total 32	C 10	N 5	O 14	P 3	0
166	UT	1	Total 32	C 10	N 5	O 14	P 3	0
166	UV	1	Total 32	C 10	N 5	O 14	P 3	0
166	UX	1	Total 32	C 10	N 5	O 14	P 3	0
166	UZ	1	Total 32	C 10	N 5	O 14	P 3	0
166	Ub	1	Total 32	C 10	N 5	O 14	P 3	0
166	Ue	1	Total 32	C 10	N 5	O 14	P 3	0
166	Ug	1	Total 32	C 10	N 5	O 14	P 3	0
166	Ui	1	Total 32	C 10	N 5	O 14	P 3	0
166	Uk	1	Total 32	C 10	N 5	O 14	P 3	0

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Mol	Chain	Residues	Atoms					AltConf
166	Um	1	Total 32	C 10	N 5	O 14	P 3	0
166	Uo	1	Total 32	C 10	N 5	O 14	P 3	0
166	Ur	1	Total 32	C 10	N 5	O 14	P 3	0
166	Ut	1	Total 32	C 10	N 5	O 14	P 3	0
166	Uv	1	Total 32	C 10	N 5	O 14	P 3	0
166	Ux	1	Total 32	C 10	N 5	O 14	P 3	0
166	Uz	1	Total 32	C 10	N 5	O 14	P 3	0
166	V1	1	Total 32	C 10	N 5	O 14	P 3	0
166	V3	1	Total 32	C 10	N 5	O 14	P 3	0
166	V5	1	Total 32	C 10	N 5	O 14	P 3	0
166	V7	1	Total 32	C 10	N 5	O 14	P 3	0
166	V9	1	Total 32	C 10	N 5	O 14	P 3	0
166	VA	1	Total 32	C 10	N 5	O 14	P 3	0
166	VC	1	Total 32	C 10	N 5	O 14	P 3	0
166	VE	1	Total 32	C 10	N 5	O 14	P 3	0
166	VG	1	Total 32	C 10	N 5	O 14	P 3	0
166	VI	1	Total 32	C 10	N 5	O 14	P 3	0
166	VK	1	Total 32	C 10	N 5	O 14	P 3	0
166	VM	1	Total 32	C 10	N 5	O 14	P 3	0
166	VN	1	Total 32	C 10	N 5	O 14	P 3	0
166	VP	1	Total 32	C 10	N 5	O 14	P 3	0

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Mol	Chain	Residues	Atoms					AltConf
166	VR	1	Total 32	C 10	N 5	O 14	P 3	0
166	VT	1	Total 32	C 10	N 5	O 14	P 3	0
166	VV	1	Total 32	C 10	N 5	O 14	P 3	0
166	VY	1	Total 32	C 10	N 5	O 14	P 3	0
166	Va	1	Total 32	C 10	N 5	O 14	P 3	0
166	Vc	1	Total 32	C 10	N 5	O 14	P 3	0
166	Ve	1	Total 32	C 10	N 5	O 14	P 3	0
166	Vg	1	Total 32	C 10	N 5	O 14	P 3	0
166	Vi	1	Total 32	C 10	N 5	O 14	P 3	0
166	Vk	1	Total 32	C 10	N 5	O 14	P 3	0
166	Vn	1	Total 32	C 10	N 5	O 14	P 3	0
166	Vp	1	Total 32	C 10	N 5	O 14	P 3	0
166	Vr	1	Total 32	C 10	N 5	O 14	P 3	0
166	Vt	1	Total 32	C 10	N 5	O 14	P 3	0
166	Vv	1	Total 32	C 10	N 5	O 14	P 3	0
166	Vx	1	Total 32	C 10	N 5	O 14	P 3	0
166	WA	1	Total 32	C 10	N 5	O 14	P 3	0
166	WC	1	Total 32	C 10	N 5	O 14	P 3	0
166	WE	1	Total 32	C 10	N 5	O 14	P 3	0
166	WG	1	Total 32	C 10	N 5	O 14	P 3	0
166	WI	1	Total 32	C 10	N 5	O 14	P 3	0

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Mol	Chain	Residues	Atoms					AltConf
166	WK	1	Total	C	N	O	P	0
			32	10	5	14	3	
166	WM	1	Total	C	N	O	P	0
			32	10	5	14	3	
166	WN	1	Total	C	N	O	P	0
			32	10	5	14	3	
166	WP	1	Total	C	N	O	P	0
			32	10	5	14	3	
166	WR	1	Total	C	N	O	P	0
			32	10	5	14	3	
166	WV	1	Total	C	N	O	P	0
			32	10	5	14	3	
166	WX	1	Total	C	N	O	P	0
			32	10	5	14	3	
166	WZ	1	Total	C	N	O	P	0
			32	10	5	14	3	
166	Wb	1	Total	C	N	O	P	0
			32	10	5	14	3	
166	Wd	1	Total	C	N	O	P	0
			32	10	5	14	3	
166	Wf	1	Total	C	N	O	P	0
			32	10	5	14	3	
166	Wj	1	Total	C	N	O	P	0
			32	10	5	14	3	
166	Wl	1	Total	C	N	O	P	0
			32	10	5	14	3	
166	Wn	1	Total	C	N	O	P	0
			32	10	5	14	3	
166	Wp	1	Total	C	N	O	P	0
			32	10	5	14	3	
166	Wr	1	Total	C	N	O	P	0
			32	10	5	14	3	
166	Wt	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 167 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
167	AA	1	Total	Mg	0
			1	1	
167	AC	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
167	AE	1	Total 1	Mg 1	0
167	AG	1	Total 1	Mg 1	0
167	AI	1	Total 1	Mg 1	0
167	AK	1	Total 1	Mg 1	0
167	AN	1	Total 1	Mg 1	0
167	AR	1	Total 1	Mg 1	0
167	BA	1	Total 1	Mg 1	0
167	BC	1	Total 1	Mg 1	0
167	BE	1	Total 1	Mg 1	0
167	BG	1	Total 1	Mg 1	0
167	BI	1	Total 1	Mg 1	0
167	BK	1	Total 1	Mg 1	0
167	Bt	1	Total 1	Mg 1	0
167	Bw	1	Total 1	Mg 1	0
167	CA	1	Total 1	Mg 1	0
167	CC	1	Total 1	Mg 1	0
167	CE	1	Total 1	Mg 1	0
167	CG	1	Total 1	Mg 1	0
167	CI	1	Total 1	Mg 1	0
167	CK	1	Total 1	Mg 1	0
167	DA	1	Total 1	Mg 1	0

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Mol	Chain	Residues	Atoms		AltConf
167	DC	1	Total 1	Mg 1	0
167	DE	1	Total 1	Mg 1	0
167	DG	1	Total 1	Mg 1	0
167	DI	1	Total 1	Mg 1	0
167	DK	1	Total 1	Mg 1	0
167	DM	1	Total 1	Mg 1	0
167	EC	1	Total 1	Mg 1	0
167	EE	1	Total 1	Mg 1	0
167	EG	1	Total 1	Mg 1	0
167	EI	1	Total 1	Mg 1	0
167	EJ	1	Total 1	Mg 1	0
167	EM	1	Total 1	Mg 1	0
167	EW	1	Total 1	Mg 1	0
167	Eb	1	Total 1	Mg 1	0
167	FC	1	Total 1	Mg 1	0
167	FE	1	Total 1	Mg 1	0
167	FG	1	Total 1	Mg 1	0
167	FI	1	Total 1	Mg 1	0
167	FK	1	Total 1	Mg 1	0
167	FM	1	Total 1	Mg 1	0
167	FU	1	Total 1	Mg 1	0

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Mol	Chain	Residues	Atoms		AltConf
167	FW	1	Total 1	Mg 1	0
167	Fr	1	Total 1	Mg 1	0
167	Ft	1	Total 1	Mg 1	0
167	Fv	1	Total 1	Mg 1	0
167	GB	1	Total 1	Mg 1	0
167	GC	1	Total 1	Mg 1	0
167	GE	1	Total 1	Mg 1	0
167	GG	1	Total 1	Mg 1	0
167	GI	1	Total 1	Mg 1	0
167	GK	1	Total 1	Mg 1	0
167	GM	1	Total 1	Mg 1	0
167	GP	1	Total 1	Mg 1	0
167	GR	1	Total 1	Mg 1	0
167	GT	1	Total 1	Mg 1	0
167	GV	1	Total 1	Mg 1	0
167	GX	1	Total 1	Mg 1	0
167	HE	1	Total 1	Mg 1	0
167	HG	1	Total 1	Mg 1	0
167	HI	1	Total 1	Mg 1	0
167	HK	1	Total 1	Mg 1	0
167	HM	1	Total 1	Mg 1	0

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Mol	Chain	Residues	Atoms		AltConf
167	HO	1	Total 1	Mg 1	0
167	HP	1	Total 1	Mg 1	0
167	HR	1	Total 1	Mg 1	0
167	IB	1	Total 1	Mg 1	0
167	IC	1	Total 1	Mg 1	0
167	IE	1	Total 1	Mg 1	0
167	IG	1	Total 1	Mg 1	0
167	II	1	Total 1	Mg 1	0
167	IK	1	Total 1	Mg 1	0
167	IM	1	Total 1	Mg 1	0
167	IP	1	Total 1	Mg 1	0
167	IR	1	Total 1	Mg 1	0
167	J1	1	Total 1	Mg 1	0
167	J3	1	Total 1	Mg 1	0
167	J5	1	Total 1	Mg 1	0
167	J7	1	Total 1	Mg 1	0
167	J9	1	Total 1	Mg 1	0
167	JC	1	Total 1	Mg 1	0
167	JE	1	Total 1	Mg 1	0
167	JG	1	Total 1	Mg 1	0
167	JI	1	Total 1	Mg 1	0

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Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
167	JK	1	1	1	0
167	JM	1	1	1	0
167	JO	1	1	1	0
167	JQ	1	1	1	0
167	JS	1	1	1	0
167	KA	1	1	1	0
167	KC	1	1	1	0
167	KE	1	1	1	0
167	KG	1	1	1	0
167	KI	1	1	1	0
167	KK	1	1	1	0
167	KM	1	1	1	0
167	KO	2	2	2	0
167	KQ	1	1	1	0
167	KS	1	1	1	0
167	KV	1	1	1	0
167	LC	1	1	1	0
167	LE	1	1	1	0
167	LG	1	1	1	0
167	LH	1	1	1	0
167	LK	1	1	1	0

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Mol	Chain	Residues	Atoms		AltConf
167	LM	1	Total 1	Mg 1	0
167	LN	1	Total 1	Mg 1	0
167	LP	1	Total 1	Mg 1	0
167	LR	1	Total 1	Mg 1	0
167	LY	1	Total 1	Mg 1	0
167	La	1	Total 1	Mg 1	0
167	Lc	1	Total 1	Mg 1	0
167	Le	1	Total 1	Mg 1	0
167	Lg	1	Total 1	Mg 1	0
167	Li	1	Total 1	Mg 1	0
167	Lk	1	Total 1	Mg 1	0
167	MC	1	Total 1	Mg 1	0
167	ME	1	Total 1	Mg 1	0
167	MG	1	Total 1	Mg 1	0
167	MI	1	Total 1	Mg 1	0
167	MK	1	Total 1	Mg 1	0
167	MM	1	Total 1	Mg 1	0
167	MN	1	Total 1	Mg 1	0
167	MP	1	Total 1	Mg 1	0
167	MR	1	Total 1	Mg 1	0
167	Mi	1	Total 1	Mg 1	0

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Mol	Chain	Residues	Atoms		AltConf
167	Mk	1	Total 1	Mg 1	0
167	Mm	1	Total 1	Mg 1	0
167	Mo	1	Total 1	Mg 1	0
167	Mq	1	Total 1	Mg 1	0
167	Ms	1	Total 1	Mg 1	0
167	Mu	1	Total 1	Mg 1	0
167	N1	1	Total 1	Mg 1	0
167	N3	1	Total 1	Mg 1	0
167	NA	1	Total 1	Mg 1	0
167	NC	1	Total 1	Mg 1	0
167	NE	1	Total 1	Mg 1	0
167	NG	1	Total 1	Mg 1	0
167	NI	1	Total 1	Mg 1	0
167	NK	1	Total 1	Mg 1	0
167	NM	1	Total 1	Mg 1	0
167	NO	1	Total 1	Mg 1	0
167	NQ	1	Total 1	Mg 1	0
167	Ns	1	Total 1	Mg 1	0
167	Nu	1	Total 1	Mg 1	0
167	Nw	1	Total 1	Mg 1	0
167	Ny	1	Total 1	Mg 1	0

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Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
167	O1	1	1	1	0
167	O3	1	1	1	0
167	O5	1	1	1	0
167	O7	1	1	1	0
167	O9	1	1	1	0
167	OA	1	1	1	0
167	OC	1	1	1	0
167	OE	1	1	1	0
167	OG	1	1	1	0
167	OI	1	1	1	0
167	OK	1	1	1	0
167	OM	1	1	1	0
167	OO	1	1	1	0
167	OQ	1	1	1	0
167	P0	1	1	1	0
167	P6	1	1	1	0
167	P8	1	1	1	0
167	PA	1	1	1	0
167	PC	1	1	1	0
167	PE	1	1	1	0
167	PG	1	1	1	0

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Mol	Chain	Residues	Atoms		AltConf
167	PI	1	Total 1	Mg 1	0
167	PK	1	Total 1	Mg 1	0
167	PM	1	Total 1	Mg 1	0
167	PO	1	Total 1	Mg 1	0
167	PQ	1	Total 1	Mg 1	0
167	PT	1	Total 1	Mg 1	0
167	Q0	1	Total 1	Mg 1	0
167	Q4	1	Total 1	Mg 1	0
167	Q6	1	Total 1	Mg 1	0
167	Q8	1	Total 1	Mg 1	0
167	QA	1	Total 1	Mg 1	0
167	QC	1	Total 1	Mg 1	0
167	QE	1	Total 1	Mg 1	0
167	QG	1	Total 1	Mg 1	0
167	QI	1	Total 1	Mg 1	0
167	QK	1	Total 1	Mg 1	0
167	QM	1	Total 1	Mg 1	0
167	QO	1	Total 1	Mg 1	0
167	QQ	1	Total 1	Mg 1	0
167	QT	1	Total 1	Mg 1	0
167	QV	1	Total 1	Mg 1	0

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Mol	Chain	Residues	Atoms		AltConf
167	QX	1	Total 1	Mg 1	0
167	R0	1	Total 1	Mg 1	0
167	R2	1	Total 1	Mg 1	0
167	R4	1	Total 1	Mg 1	0
167	R6	1	Total 1	Mg 1	0
167	R8	1	Total 1	Mg 1	0
167	RA	1	Total 1	Mg 1	0
167	RC	1	Total 1	Mg 1	0
167	RE	1	Total 1	Mg 1	0
167	RG	1	Total 1	Mg 1	0
167	RI	1	Total 1	Mg 1	0
167	RK	1	Total 1	Mg 1	0
167	RM	1	Total 1	Mg 1	0
167	RO	1	Total 1	Mg 1	0
167	RQ	1	Total 1	Mg 1	0
167	RT	1	Total 1	Mg 1	0
167	RV	1	Total 1	Mg 1	0
167	S0	1	Total 1	Mg 1	0
167	S2	1	Total 1	Mg 1	0
167	S4	1	Total 1	Mg 1	0
167	S6	1	Total 1	Mg 1	0

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Mol	Chain	Residues	Atoms		AltConf
167	S8	1	Total 1	Mg 1	0
167	SA	1	Total 1	Mg 1	0
167	SC	1	Total 1	Mg 1	0
167	SE	1	Total 1	Mg 1	0
167	SG	1	Total 1	Mg 1	0
167	SI	1	Total 1	Mg 1	0
167	SK	1	Total 1	Mg 1	0
167	SN	1	Total 1	Mg 1	0
167	SP	1	Total 1	Mg 1	0
167	ST	1	Total 1	Mg 1	0
167	SV	1	Total 1	Mg 1	0
167	SY	1	Total 1	Mg 1	0
167	Sa	1	Total 1	Mg 1	0
167	Sc	1	Total 1	Mg 1	0
167	Se	1	Total 1	Mg 1	0
167	Sg	1	Total 1	Mg 1	0
167	Si	1	Total 1	Mg 1	0
167	Sm	1	Total 1	Mg 1	0
167	So	1	Total 1	Mg 1	0
167	Sq	1	Total 1	Mg 1	0
167	Ss	1	Total 1	Mg 1	0

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Mol	Chain	Residues	Atoms		AltConf
167	Su	1	Total 1	Mg 1	0
167	Sw	1	Total 1	Mg 1	0
167	Sz	1	Total 1	Mg 1	0
167	T1	1	Total 1	Mg 1	0
167	T3	1	Total 1	Mg 1	0
167	T5	1	Total 1	Mg 1	0
167	T7	1	Total 1	Mg 1	0
167	T9	1	Total 1	Mg 1	0
167	TC	1	Total 1	Mg 1	0
167	TD	1	Total 1	Mg 1	0
167	TG	1	Total 1	Mg 1	0
167	TI	1	Total 1	Mg 1	0
167	TK	1	Total 1	Mg 1	0
167	TL	1	Total 1	Mg 1	0
167	TO	1	Total 1	Mg 1	0
167	TQ	1	Total 1	Mg 1	0
167	TW	1	Total 1	Mg 1	0
167	TY	1	Total 1	Mg 1	0
167	Ta	1	Total 1	Mg 1	0
167	Tc	1	Total 1	Mg 1	0
167	Te	1	Total 1	Mg 1	0

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Mol	Chain	Residues	Atoms		AltConf
167	Tf	1	Total 1	Mg 1	0
167	Tk	1	Total 1	Mg 1	0
167	Tm	1	Total 1	Mg 1	0
167	To	1	Total 1	Mg 1	0
167	Tq	1	Total 1	Mg 1	0
167	Ts	1	Total 1	Mg 1	0
167	Tu	1	Total 1	Mg 1	0
167	Ty	1	Total 1	Mg 1	0
167	U2	1	Total 1	Mg 1	0
167	U5	1	Total 1	Mg 1	0
167	U7	1	Total 1	Mg 1	0
167	U9	1	Total 1	Mg 1	0
167	UA	1	Total 1	Mg 1	0
167	UC	1	Total 1	Mg 1	0
167	UE	1	Total 1	Mg 1	0
167	UG	1	Total 1	Mg 1	0
167	UI	1	Total 1	Mg 1	0
167	UK	1	Total 1	Mg 1	0
167	UM	1	Total 1	Mg 1	0
167	UN	1	Total 1	Mg 1	0
167	UP	1	Total 1	Mg 1	0

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Mol	Chain	Residues	Atoms		AltConf
167	UQ	1	Total 1	Mg 1	0
167	UT	1	Total 1	Mg 1	0
167	UV	1	Total 1	Mg 1	0
167	UX	1	Total 1	Mg 1	0
167	UZ	1	Total 1	Mg 1	0
167	Ub	1	Total 1	Mg 1	0
167	Ue	1	Total 1	Mg 1	0
167	Ug	1	Total 1	Mg 1	0
167	Ui	1	Total 1	Mg 1	0
167	Uk	1	Total 1	Mg 1	0
167	Um	1	Total 1	Mg 1	0
167	Uo	1	Total 1	Mg 1	0
167	Ur	1	Total 1	Mg 1	0
167	Ut	1	Total 1	Mg 1	0
167	Uv	1	Total 1	Mg 1	0
167	Ux	1	Total 1	Mg 1	0
167	Uz	1	Total 1	Mg 1	0
167	V1	1	Total 1	Mg 1	0
167	V3	1	Total 1	Mg 1	0
167	V5	1	Total 1	Mg 1	0
167	V7	1	Total 1	Mg 1	0

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Mol	Chain	Residues	Atoms		AltConf
167	V9	1	Total 1	Mg 1	0
167	VA	1	Total 1	Mg 1	0
167	VC	1	Total 1	Mg 1	0
167	VE	1	Total 1	Mg 1	0
167	VG	1	Total 1	Mg 1	0
167	VI	1	Total 1	Mg 1	0
167	VK	1	Total 1	Mg 1	0
167	VM	1	Total 1	Mg 1	0
167	VN	1	Total 1	Mg 1	0
167	VP	1	Total 1	Mg 1	0
167	VR	1	Total 1	Mg 1	0
167	VT	1	Total 1	Mg 1	0
167	VV	1	Total 1	Mg 1	0
167	VY	1	Total 1	Mg 1	0
167	Va	1	Total 1	Mg 1	0
167	Vc	1	Total 1	Mg 1	0
167	Ve	1	Total 1	Mg 1	0
167	Vg	1	Total 1	Mg 1	0
167	Vi	1	Total 1	Mg 1	0
167	Vk	1	Total 1	Mg 1	0
167	Vm	1	Total 1	Mg 1	0

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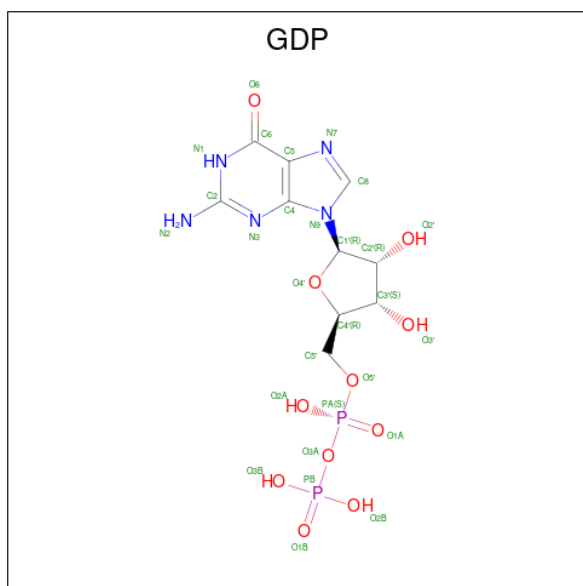
Mol	Chain	Residues	Atoms		AltConf
167	Vo	1	Total 1	Mg 1	0
167	Vq	1	Total 1	Mg 1	0
167	Vs	1	Total 1	Mg 1	0
167	Vu	1	Total 1	Mg 1	0
167	Vw	1	Total 1	Mg 1	0
167	WA	1	Total 1	Mg 1	0
167	WC	1	Total 1	Mg 1	0
167	WE	1	Total 1	Mg 1	0
167	WG	1	Total 1	Mg 1	0
167	WI	1	Total 1	Mg 1	0
167	WK	1	Total 1	Mg 1	0
167	WM	1	Total 1	Mg 1	0
167	WN	1	Total 1	Mg 1	0
167	WP	1	Total 1	Mg 1	0
167	WR	1	Total 1	Mg 1	0
167	WV	1	Total 1	Mg 1	0
167	WX	1	Total 1	Mg 1	0
167	WZ	1	Total 1	Mg 1	0
167	Wb	1	Total 1	Mg 1	0
167	Wd	1	Total 1	Mg 1	0
167	Wf	1	Total 1	Mg 1	0

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Mol	Chain	Residues	Atoms		AltConf
167	Wj	1	Total	Mg	0
			1	1	
167	Wl	1	Total	Mg	0
			1	1	
167	Wn	1	Total	Mg	0
			1	1	
167	Wp	1	Total	Mg	0
			1	1	
167	Wr	1	Total	Mg	0
			1	1	
167	Wt	1	Total	Mg	0
			1	1	

- Molecule 168 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula:  $C_{10}H_{15}N_5O_{11}P_2$ ).



Mol	Chain	Residues	Atoms					AltConf
168	AB	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	AD	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	AF	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	AH	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	AJ	1	Total	C	N	O	P	0
			28	10	5	11	2	

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Mol	Chain	Residues	Atoms					AltConf
168	AL	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	AM	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	AO	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	AX	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	BB	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	BD	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	BF	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	BH	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	BJ	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	BL	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	Bp	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	Bv	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	Bx	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	CB	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	CD	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	CF	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	CH	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	CJ	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	CL	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	DB	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	DD	1	Total	C	N	O	P	0
			28	10	5	11	2	

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Mol	Chain	Residues	Atoms					AltConf
168	DF	1	Total 28	C 10	N 5	O 11	P 2	0
168	DH	1	Total 28	C 10	N 5	O 11	P 2	0
168	DJ	1	Total 28	C 10	N 5	O 11	P 2	0
168	DL	1	Total 28	C 10	N 5	O 11	P 2	0
168	DN	1	Total 28	C 10	N 5	O 11	P 2	0
168	ED	1	Total 28	C 10	N 5	O 11	P 2	0
168	EF	1	Total 28	C 10	N 5	O 11	P 2	0
168	EH	1	Total 28	C 10	N 5	O 11	P 2	0
168	EJ	1	Total 28	C 10	N 5	O 11	P 2	0
168	EL	1	Total 28	C 10	N 5	O 11	P 2	0
168	EN	1	Total 28	C 10	N 5	O 11	P 2	0
168	ER	1	Total 28	C 10	N 5	O 11	P 2	0
168	Ea	1	Total 28	C 10	N 5	O 11	P 2	0
168	Ec	1	Total 28	C 10	N 5	O 11	P 2	0
168	FB	1	Total 28	C 10	N 5	O 11	P 2	0
168	FD	1	Total 28	C 10	N 5	O 11	P 2	0
168	FF	1	Total 28	C 10	N 5	O 11	P 2	0
168	FH	1	Total 28	C 10	N 5	O 11	P 2	0
168	FJ	1	Total 28	C 10	N 5	O 11	P 2	0
168	FL	1	Total 28	C 10	N 5	O 11	P 2	0
168	FN	1	Total 28	C 10	N 5	O 11	P 2	0

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Mol	Chain	Residues	Atoms					AltConf
168	FV	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	FX	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	Fs	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	Fu	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	GD	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	GF	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	GH	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	GJ	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	GL	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	GN	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	GO	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	GQ	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	GU	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	GW	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	HB	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	HD	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	HF	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	HH	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	HJ	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	HL	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	HN	1	Total	C	N	O	P	0
			28	10	5	11	2	

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Mol	Chain	Residues	Atoms					AltConf
168	HQ	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	IB	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	ID	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	IF	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	IH	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	IJ	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	IL	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	IO	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	IQ	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	J0	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	J2	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	J4	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	J6	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	J8	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	JB	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	JD	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	JF	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	JH	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	JJ	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	JL	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	JN	1	Total	C	N	O	P	0
			28	10	5	11	2	

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Mol	Chain	Residues	Atoms					AltConf
168	JP	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	JR	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	KB	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	KD	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	KF	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	KH	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	KJ	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	KL	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	KN	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	KP	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	KR	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	KU	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	LB	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	LD	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	LF	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	LH	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	LJ	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	LL	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	LO	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	LQ	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	LZ	1	Total	C	N	O	P	0
			28	10	5	11	2	

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Mol	Chain	Residues	Atoms					AltConf
168	Lb	1	Total 28	C 10	N 5	O 11	P 2	0
168	Ld	1	Total 28	C 10	N 5	O 11	P 2	0
168	Lf	1	Total 28	C 10	N 5	O 11	P 2	0
168	Lh	1	Total 28	C 10	N 5	O 11	P 2	0
168	Lj	1	Total 28	C 10	N 5	O 11	P 2	0
168	MB	1	Total 28	C 10	N 5	O 11	P 2	0
168	MD	1	Total 28	C 10	N 5	O 11	P 2	0
168	MF	1	Total 28	C 10	N 5	O 11	P 2	0
168	MH	1	Total 28	C 10	N 5	O 11	P 2	0
168	MJ	1	Total 28	C 10	N 5	O 11	P 2	0
168	ML	1	Total 28	C 10	N 5	O 11	P 2	0
168	MO	1	Total 28	C 10	N 5	O 11	P 2	0
168	MQ	1	Total 28	C 10	N 5	O 11	P 2	0
168	Mj	1	Total 28	C 10	N 5	O 11	P 2	0
168	Ml	1	Total 28	C 10	N 5	O 11	P 2	0
168	Mn	1	Total 28	C 10	N 5	O 11	P 2	0
168	Mp	1	Total 28	C 10	N 5	O 11	P 2	0
168	Mr	1	Total 28	C 10	N 5	O 11	P 2	0
168	Mt	1	Total 28	C 10	N 5	O 11	P 2	0
168	N0	1	Total 28	C 10	N 5	O 11	P 2	0
168	N2	1	Total 28	C 10	N 5	O 11	P 2	0

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Mol	Chain	Residues	Atoms					AltConf
168	NB	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	ND	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	NF	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	NH	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	NJ	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	NL	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	NN	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	NP	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	Nr	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	Nt	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	Nv	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	Nx	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	Nz	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	O0	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	O2	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	O4	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	O6	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	O8	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	OB	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	OD	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	OF	1	Total	C	N	O	P	0
			28	10	5	11	2	

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Mol	Chain	Residues	Atoms					AltConf
168	OH	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	OJ	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	OL	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	ON	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	OP	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	Oz	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	P5	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	P7	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	P9	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	PB	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	PD	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	PF	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	PH	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	PJ	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	PL	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	PN	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	PP	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	PR	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	PS	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	PU	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	Q3	1	Total	C	N	O	P	0
			28	10	5	11	2	

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Mol	Chain	Residues	Atoms					AltConf
168	Q5	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	Q7	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	Q9	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	QB	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	QD	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	QF	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	QH	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	QJ	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	QL	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	QN	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	QP	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	QR	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	QS	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	QU	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	QW	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	R1	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	R3	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	R5	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	R7	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	R9	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	RB	1	Total	C	N	O	P	0
			28	10	5	11	2	

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Mol	Chain	Residues	Atoms					AltConf
168	RD	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	RF	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	RH	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	RJ	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	RL	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	RN	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	RP	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	RR	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	RS	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	RU	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	RW	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	S1	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	S3	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	S5	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	S7	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	S9	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	SB	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	SD	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	SF	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	SH	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	SJ	1	Total	C	N	O	P	0
			28	10	5	11	2	

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Mol	Chain	Residues	Atoms					AltConf
168	SL	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	SM	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	SO	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	SQ	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	SS	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	SU	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	SX	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	SZ	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	Sb	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	Sd	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	Sf	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	Sh	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	Sj	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	Sl	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	Sn	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	Sp	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	Sr	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	St	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	Sv	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	T2	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	T4	1	Total	C	N	O	P	0
			28	10	5	11	2	

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Mol	Chain	Residues	Atoms					AltConf
168	T6	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	T8	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	TA	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	TB	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	TD	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	TF	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	TH	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	TJ	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	TL	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	TN	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	TP	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	TR	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	TV	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	TX	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	TZ	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	Tb	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	Td	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	Tf	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	Th	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	Tj	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	Tl	1	Total	C	N	O	P	0
			28	10	5	11	2	

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Mol	Chain	Residues	Atoms					AltConf
168	Tn	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	Tp	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	Tr	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	Tt	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	Tv	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	Tx	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	Tz	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	U0	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	U1	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	U3	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	U6	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	U8	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	UB	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	UD	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	UF	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	UH	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	UJ	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	UL	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	UO	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	UQ	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	US	1	Total	C	N	O	P	0
			28	10	5	11	2	

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Mol	Chain	Residues	Atoms					AltConf
168	UU	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	UW	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	UY	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	Ua	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	Uc	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	Uf	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	Uh	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	Uj	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	Ul	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	Un	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	Up	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	Us	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	Uu	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	Uw	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	Uy	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	V0	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	V2	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	V4	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	V6	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	V8	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	VB	1	Total	C	N	O	P	0
			28	10	5	11	2	

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Mol	Chain	Residues	Atoms					AltConf
168	VD	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	VF	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	VH	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	VJ	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	VL	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	VO	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	VQ	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	VS	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	VU	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	VW	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	VZ	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	Vb	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	Vd	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	Vf	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	Vh	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	Vj	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	Vm	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	Vo	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	Vq	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	Vs	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	Vu	1	Total	C	N	O	P	0
			28	10	5	11	2	

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Mol	Chain	Residues	Atoms					AltConf
168	Vw	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	Vz	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	WB	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	WD	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	WF	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	WH	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	WJ	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	WL	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	WO	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	WQ	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	WS	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	WU	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	WW	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	WY	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	Wa	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	Wc	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	We	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	Wg	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	Wi	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	Wk	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	Wm	1	Total	C	N	O	P	0
			28	10	5	11	2	

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Mol	Chain	Residues	Atoms					AltConf
168	Wo	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	Wq	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	Ws	1	Total	C	N	O	P	0
			28	10	5	11	2	
168	Wu	1	Total	C	N	O	P	0
			28	10	5	11	2	

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	203560	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor

## 4 Model quality [i](#)

### 4.1 Standard geometry [i](#)

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

### 4.2 Too-close contacts [i](#)

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

### 4.3 Torsion angles [i](#)

#### 4.3.1 Protein backbone [i](#)

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

#### 4.3.2 Protein sidechains [i](#)

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

#### 4.3.3 RNA [i](#)

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

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

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

### 4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 4.6 Ligand geometry [i](#)

Of 1032 ligands modelled in this entry, 345 are monoatomic - leaving 687 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
168	GDP	Sb	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.32	4 (13%)
168	GDP	Wi	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.32	4 (13%)
166	GTP	EC	501	-	26,34,34	1.14	2 (7%)	32,54,54	1.61	7 (21%)
168	GDP	S1	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.35	4 (13%)
168	GDP	JJ	501	-	24,30,30	0.97	1 (4%)	30,47,47	1.34	5 (16%)
168	GDP	Lh	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.25	4 (13%)
168	GDP	Sl	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.41	4 (13%)
166	GTP	Bt	501	-	26,34,34	1.14	2 (7%)	32,54,54	1.73	7 (21%)
166	GTP	SC	501	167	26,34,34	1.15	2 (7%)	32,54,54	1.69	7 (21%)
166	GTP	Wt	501	167	26,34,34	1.16	2 (7%)	32,54,54	1.66	7 (21%)
166	GTP	OO	501	167	26,34,34	1.13	2 (7%)	32,54,54	1.66	7 (21%)
168	GDP	CB	501	-	24,30,30	0.99	1 (4%)	30,47,47	1.35	5 (16%)
168	GDP	Mn	501	-	24,30,30	0.96	1 (4%)	30,47,47	1.37	5 (16%)
168	GDP	Tj	501	-	24,30,30	0.89	1 (4%)	30,47,47	1.34	5 (16%)
168	GDP	LF	501	-	24,30,30	0.88	0	30,47,47	1.35	4 (13%)
168	GDP	SH	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.21	5 (16%)
168	GDP	PR	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.22	4 (13%)
166	GTP	LG	502	167	26,34,34	1.14	2 (7%)	32,54,54	1.59	7 (21%)
168	GDP	WU	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.31	4 (13%)
168	GDP	T4	501	-	24,30,30	0.90	1 (4%)	30,47,47	1.34	4 (13%)
168	GDP	PL	501	-	24,30,30	0.91	1 (4%)	30,47,47	1.44	6 (20%)
168	GDP	Ua	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.33	4 (13%)
166	GTP	JI	501	167	26,34,34	1.15	2 (7%)	32,54,54	1.72	7 (21%)
166	GTP	ME	501	167	26,34,34	1.15	2 (7%)	32,54,54	1.63	7 (21%)
166	GTP	Uo	501	167	26,34,34	1.16	2 (7%)	32,54,54	1.57	7 (21%)
168	GDP	GJ	501	-	24,30,30	0.97	1 (4%)	30,47,47	1.26	5 (16%)
168	GDP	OH	501	-	24,30,30	0.96	1 (4%)	30,47,47	1.18	3 (10%)
166	GTP	WV	501	167	26,34,34	1.14	2 (7%)	32,54,54	1.70	7 (21%)
168	GDP	RR	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.34	4 (13%)
166	GTP	J1	501	167	26,34,34	1.17	1 (3%)	32,54,54	1.73	8 (25%)
166	GTP	RG	501	167	26,34,34	1.14	2 (7%)	32,54,54	1.52	7 (21%)
166	GTP	V7	501	167	26,34,34	1.15	2 (7%)	32,54,54	1.75	7 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
166	GTP	RM	501	-	26,34,34	1.16	2 (7%)	32,54,54	1.66	7 (21%)
166	GTP	Uv	501	167	26,34,34	1.17	2 (7%)	32,54,54	1.71	7 (21%)
168	GDP	Wu	501	-	24,30,30	0.96	1 (4%)	30,47,47	1.29	4 (13%)
166	GTP	SA	501	167	26,34,34	1.16	2 (7%)	32,54,54	1.71	7 (21%)
168	GDP	IO	501	-	24,30,30	0.99	1 (4%)	30,47,47	1.36	4 (13%)
166	GTP	Ui	501	-	26,34,34	1.15	2 (7%)	32,54,54	1.53	8 (25%)
166	GTP	Vn	501	167	26,34,34	1.15	2 (7%)	32,54,54	1.57	7 (21%)
168	GDP	CH	501	-	24,30,30	0.96	1 (4%)	30,47,47	1.24	4 (13%)
168	GDP	HF	501	-	24,30,30	1.01	2 (8%)	30,47,47	1.44	6 (20%)
168	GDP	ER	501	-	24,30,30	0.92	1 (4%)	30,47,47	1.17	4 (13%)
168	GDP	JD	501	-	24,30,30	0.97	1 (4%)	30,47,47	1.40	4 (13%)
168	GDP	Td	501	-	24,30,30	0.91	1 (4%)	30,47,47	1.39	5 (16%)
166	GTP	UX	501	-	26,34,34	1.15	2 (7%)	32,54,54	1.71	8 (25%)
166	GTP	NQ	501	167	26,34,34	1.15	2 (7%)	32,54,54	1.68	7 (21%)
168	GDP	Lj	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.29	4 (13%)
168	GDP	AF	501	-	24,30,30	0.96	1 (4%)	30,47,47	1.27	4 (13%)
168	GDP	RH	501	-	24,30,30	0.92	1 (4%)	30,47,47	1.29	5 (16%)
166	GTP	Vi	502	167	26,34,34	1.16	2 (7%)	32,54,54	1.66	7 (21%)
168	GDP	P9	501	-	24,30,30	0.92	1 (4%)	30,47,47	1.30	4 (13%)
168	GDP	GQ	501	-	24,30,30	0.98	1 (4%)	30,47,47	1.36	5 (16%)
168	GDP	GW	501	-	24,30,30	0.92	1 (4%)	30,47,47	1.32	4 (13%)
166	GTP	GP	501	167	26,34,34	1.15	2 (7%)	32,54,54	1.69	7 (21%)
168	GDP	J4	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.35	4 (13%)
166	GTP	BA	501	167	26,34,34	1.14	2 (7%)	32,54,54	1.71	7 (21%)
166	GTP	Sw	502	167	26,34,34	1.16	2 (7%)	32,54,54	1.59	7 (21%)
168	GDP	BH	501	-	24,30,30	0.97	1 (4%)	30,47,47	1.20	5 (16%)
168	GDP	NB	501	-	24,30,30	0.90	1 (4%)	30,47,47	1.37	4 (13%)
168	GDP	HL	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.33	4 (13%)
168	GDP	CD	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.29	4 (13%)
168	GDP	OL	501	-	24,30,30	0.89	0	30,47,47	1.56	8 (26%)
168	GDP	QH	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.32	4 (13%)
168	GDP	TB	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.35	4 (13%)
168	GDP	UW	501	-	24,30,30	1.00	1 (4%)	30,47,47	1.79	10 (33%)
168	GDP	Vd	501	-	24,30,30	0.93	1 (4%)	30,47,47	1.32	4 (13%)
166	GTP	KA	501	-	26,34,34	1.17	2 (7%)	32,54,54	1.58	7 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
168	GDP	LB	501	-	24,30,30	0.96	0	30,47,47	1.30	4 (13%)
166	GTP	O7	501	167	26,34,34	1.13	2 (7%)	32,54,54	1.63	7 (21%)
166	GTP	GG	501	167	26,34,34	1.13	2 (7%)	32,54,54	1.56	7 (21%)
168	GDP	OD	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.31	5 (16%)
166	GTP	S8	501	167	26,34,34	1.16	2 (7%)	32,54,54	1.59	7 (21%)
166	GTP	HI	501	167	26,34,34	1.14	2 (7%)	32,54,54	1.67	7 (21%)
168	GDP	T8	501	-	24,30,30	0.92	1 (4%)	30,47,47	1.38	4 (13%)
166	GTP	V3	501	167	26,34,34	1.14	2 (7%)	32,54,54	1.64	6 (18%)
166	GTP	V5	501	167	26,34,34	1.14	2 (7%)	32,54,54	1.69	7 (21%)
166	GTP	HG	502	167	26,34,34	1.15	2 (7%)	32,54,54	1.68	7 (21%)
166	GTP	LP	501	167	26,34,34	1.16	2 (7%)	32,54,54	1.92	8 (25%)
166	GTP	PG	501	167	26,34,34	1.20	2 (7%)	32,54,54	1.62	8 (25%)
168	GDP	KR	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.28	5 (16%)
168	GDP	N0	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.26	3 (10%)
168	GDP	Vz	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.31	4 (13%)
166	GTP	V9	501	167	26,34,34	1.14	2 (7%)	32,54,54	1.72	7 (21%)
166	GTP	Se	501	167	26,34,34	1.17	2 (7%)	32,54,54	1.65	7 (21%)
168	GDP	BJ	501	-	24,30,30	0.93	1 (4%)	30,47,47	1.31	4 (13%)
166	GTP	Wp	501	167	26,34,34	1.16	2 (7%)	32,54,54	1.62	7 (21%)
166	GTP	UP	502	167	26,34,34	1.12	2 (7%)	32,54,54	1.64	6 (18%)
166	GTP	KM	501	167	26,34,34	1.14	2 (7%)	32,54,54	1.52	7 (21%)
166	GTP	IN	501	167	26,34,34	1.18	2 (7%)	32,54,54	1.69	7 (21%)
166	GTP	JQ	501	167	26,34,34	1.15	2 (7%)	32,54,54	1.62	7 (21%)
166	GTP	VT	501	167	26,34,34	1.14	1 (3%)	32,54,54	1.73	8 (25%)
168	GDP	IB	501	-	24,30,30	1.02	1 (4%)	30,47,47	1.32	4 (13%)
166	GTP	RC	501	-	26,34,34	1.17	2 (7%)	32,54,54	1.64	7 (21%)
168	GDP	Sd	501	-	24,30,30	0.96	1 (4%)	30,47,47	1.35	4 (13%)
166	GTP	T7	502	167	26,34,34	1.16	2 (7%)	32,54,54	1.70	7 (21%)
168	GDP	S7	501	-	24,30,30	0.98	1 (4%)	30,47,47	1.36	5 (16%)
166	GTP	UC	501	167	26,34,34	1.12	2 (7%)	32,54,54	1.65	6 (18%)
168	GDP	U0	501	-	24,30,30	0.93	1 (4%)	30,47,47	1.36	4 (13%)
168	GDP	AJ	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.34	4 (13%)
168	GDP	WW	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.31	4 (13%)
166	GTP	Tg	501	167	26,34,34	1.16	2 (7%)	32,54,54	1.62	7 (21%)
166	GTP	AG	501	167	26,34,34	1.14	1 (3%)	32,54,54	1.67	9 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
168	GDP	Wm	501	-	24,30,30	0.96	1 (4%)	30,47,47	1.36	5 (16%)
166	GTP	Mi	501	-	26,34,34	1.16	2 (7%)	32,54,54	1.70	8 (25%)
168	GDP	AO	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.33	4 (13%)
166	GTP	NC	501	-	26,34,34	1.16	2 (7%)	32,54,54	1.51	7 (21%)
168	GDP	NL	501	-	24,30,30	0.96	1 (4%)	30,47,47	1.29	4 (13%)
168	GDP	KF	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.28	5 (16%)
168	GDP	U8	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.34	4 (13%)
168	GDP	MI	501	-	24,30,30	0.98	1 (4%)	30,47,47	1.28	4 (13%)
168	GDP	RP	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.34	5 (16%)
168	GDP	Nz	501	-	24,30,30	0.96	1 (4%)	30,47,47	1.29	4 (13%)
168	GDP	Lb	501	-	24,30,30	0.98	1 (4%)	30,47,47	1.26	4 (13%)
166	GTP	OC	501	167	26,34,34	1.13	2 (7%)	32,54,54	1.66	6 (18%)
166	GTP	Ts	501	167	26,34,34	1.16	2 (7%)	32,54,54	1.63	7 (21%)
168	GDP	TN	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.31	4 (13%)
166	GTP	OK	501	167	26,34,34	1.12	2 (7%)	32,54,54	1.43	5 (15%)
166	GTP	Vp	501	167	26,34,34	1.14	2 (7%)	32,54,54	1.57	7 (21%)
168	GDP	Wo	501	-	24,30,30	0.98	1 (4%)	30,47,47	1.34	4 (13%)
168	GDP	DB	501	-	24,30,30	0.93	1 (4%)	30,47,47	1.50	5 (16%)
168	GDP	RW	501	-	24,30,30	0.92	1 (4%)	30,47,47	1.29	3 (10%)
168	GDP	FH	501	-	24,30,30	0.93	1 (4%)	30,47,47	1.33	4 (13%)
166	GTP	Vc	501	167	26,34,34	1.17	2 (7%)	32,54,54	1.73	7 (21%)
166	GTP	Va	501	167	26,34,34	1.16	2 (7%)	32,54,54	1.73	7 (21%)
168	GDP	LQ	501	-	24,30,30	0.85	0	30,47,47	1.61	6 (20%)
166	GTP	VV	501	-	26,34,34	1.16	2 (7%)	32,54,54	1.58	7 (21%)
166	GTP	Um	502	167	26,34,34	1.17	2 (7%)	32,54,54	1.74	7 (21%)
168	GDP	Sf	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.34	4 (13%)
166	GTP	J7	501	167	26,34,34	1.16	2 (7%)	32,54,54	1.71	9 (28%)
168	GDP	Nt	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.34	4 (13%)
168	GDP	PF	501	-	24,30,30	0.96	1 (4%)	30,47,47	1.31	5 (16%)
166	GTP	Mm	501	-	26,34,34	1.14	2 (7%)	32,54,54	1.62	6 (18%)
168	GDP	SZ	501	-	24,30,30	0.96	1 (4%)	30,47,47	1.31	5 (16%)
168	GDP	Uh	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.32	4 (13%)
166	GTP	J3	501	-	26,34,34	1.12	2 (7%)	32,54,54	1.60	7 (21%)
166	GTP	JO	501	167	26,34,34	1.14	1 (3%)	32,54,54	1.76	9 (28%)
166	GTP	KV	501	167	26,34,34	1.14	2 (7%)	32,54,54	1.65	7 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
168	GDP	Ld	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.20	4 (13%)
168	GDP	ED	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.40	4 (13%)
168	GDP	Vq	501	-	24,30,30	0.93	1 (4%)	30,47,47	1.33	4 (13%)
168	GDP	ID	501	-	24,30,30	0.99	1 (4%)	30,47,47	1.32	5 (16%)
166	GTP	EG	501	167	26,34,34	1.13	2 (7%)	32,54,54	1.67	7 (21%)
168	GDP	CJ	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.34	4 (13%)
168	GDP	QR	501	-	24,30,30	0.96	1 (4%)	30,47,47	1.43	4 (13%)
168	GDP	MJ	501	-	24,30,30	0.90	1 (4%)	30,47,47	1.33	5 (16%)
166	GTP	Wd	501	167	26,34,34	1.16	2 (7%)	32,54,54	1.60	7 (21%)
166	GTP	MI	501	167	26,34,34	1.16	1 (3%)	32,54,54	1.76	9 (28%)
168	GDP	DH	501	-	24,30,30	0.96	1 (4%)	30,47,47	1.43	4 (13%)
168	GDP	OF	501	-	24,30,30	1.16	3 (12%)	30,47,47	1.45	6 (20%)
166	GTP	SN	501	167	26,34,34	1.16	2 (7%)	32,54,54	1.67	7 (21%)
166	GTP	AN	501	-	26,34,34	1.14	1 (3%)	32,54,54	1.66	10 (31%)
168	GDP	QN	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.33	5 (16%)
166	GTP	Uz	501	-	26,34,34	1.16	2 (7%)	32,54,54	1.71	7 (21%)
168	GDP	DJ	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.27	5 (16%)
166	GTP	CK	501	-	26,34,34	1.15	2 (7%)	32,54,54	1.49	8 (25%)
168	GDP	RJ	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.32	5 (16%)
166	GTP	PC	501	-	26,34,34	1.16	2 (7%)	32,54,54	1.66	7 (21%)
166	GTP	Eb	501	-	26,34,34	1.14	2 (7%)	32,54,54	1.65	6 (18%)
168	GDP	KU	501	-	24,30,30	0.99	1 (4%)	30,47,47	1.29	5 (16%)
168	GDP	Ul	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.38	4 (13%)
168	GDP	Tx	501	-	24,30,30	0.89	0	30,47,47	1.37	4 (13%)
168	GDP	NF	501	-	24,30,30	0.88	0	30,47,47	1.73	6 (20%)
168	GDP	Sr	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.40	4 (13%)
166	GTP	AK	501	-	26,34,34	1.15	1 (3%)	32,54,54	1.65	10 (31%)
166	GTP	NA	502	167	26,34,34	1.17	2 (7%)	32,54,54	1.70	8 (25%)
166	GTP	RV	501	167	26,34,34	1.15	2 (7%)	32,54,54	1.70	7 (21%)
168	GDP	Vu	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.34	4 (13%)
166	GTP	Ub	501	167	26,34,34	1.14	2 (7%)	32,54,54	1.55	7 (21%)
168	GDP	FB	501	-	24,30,30	0.93	1 (4%)	30,47,47	1.32	4 (13%)
168	GDP	WL	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.30	4 (13%)
166	GTP	RI	501	167	26,34,34	1.14	2 (7%)	32,54,54	1.70	7 (21%)
166	GTP	S4	501	167	26,34,34	1.17	2 (7%)	32,54,54	1.66	9 (28%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
168	GDP	SU	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.37	4 (13%)
166	GTP	Sg	501	167	26,34,34	1.16	2 (7%)	32,54,54	1.70	7 (21%)
168	GDP	EN	501	-	24,30,30	0.98	1 (4%)	30,47,47	1.45	5 (16%)
166	GTP	EI	501	167	26,34,34	1.14	2 (7%)	32,54,54	1.57	7 (21%)
166	GTP	FW	501	167	26,34,34	1.16	2 (7%)	32,54,54	1.65	7 (21%)
166	GTP	GK	501	-	26,34,34	1.14	2 (7%)	32,54,54	1.75	8 (25%)
166	GTP	SE	501	167	26,34,34	1.14	2 (7%)	32,54,54	1.74	7 (21%)
166	GTP	JM	502	167	26,34,34	1.15	2 (7%)	32,54,54	1.56	7 (21%)
168	GDP	S3	501	-	24,30,30	0.93	1 (4%)	30,47,47	1.27	5 (16%)
166	GTP	GC	501	167	26,34,34	1.14	2 (7%)	32,54,54	1.66	7 (21%)
166	GTP	U7	501	-	26,34,34	1.16	2 (7%)	32,54,54	1.65	7 (21%)
168	GDP	Sp	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.36	4 (13%)
166	GTP	SK	501	167	26,34,34	1.15	2 (7%)	32,54,54	1.57	8 (25%)
168	GDP	Vs	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.33	4 (13%)
168	GDP	Vh	501	-	24,30,30	0.93	1 (4%)	30,47,47	1.43	4 (13%)
166	GTP	CG	501	167	26,34,34	1.15	2 (7%)	32,54,54	1.73	7 (21%)
168	GDP	TZ	501	-	24,30,30	0.90	1 (4%)	30,47,47	1.38	5 (16%)
168	GDP	Q3	501	-	24,30,30	0.92	1 (4%)	30,47,47	1.27	4 (13%)
166	GTP	TO	501	167	26,34,34	1.29	3 (11%)	32,54,54	1.73	8 (25%)
168	GDP	DF	501	-	24,30,30	0.99	1 (4%)	30,47,47	1.38	4 (13%)
166	GTP	IE	501	-	26,34,34	1.16	2 (7%)	32,54,54	1.59	8 (25%)
166	GTP	WI	502	167	26,34,34	1.15	2 (7%)	32,54,54	1.53	7 (21%)
168	GDP	WD	501	-	24,30,30	0.97	1 (4%)	30,47,47	1.31	5 (16%)
168	GDP	Wg	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.32	4 (13%)
166	GTP	Nw	501	-	26,34,34	1.14	2 (7%)	32,54,54	1.58	8 (25%)
168	GDP	Vm	501	-	24,30,30	0.96	1 (4%)	30,47,47	1.39	5 (16%)
168	GDP	WF	501	-	24,30,30	0.99	1 (4%)	30,47,47	1.34	5 (16%)
168	GDP	Nv	501	-	24,30,30	0.97	1 (4%)	30,47,47	1.42	4 (13%)
168	GDP	UH	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.19	4 (13%)
166	GTP	LC	501	167	26,34,34	1.15	2 (7%)	32,54,54	1.68	7 (21%)
168	GDP	V8	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.34	4 (13%)
166	GTP	N3	501	167	26,34,34	1.16	2 (7%)	32,54,54	1.71	7 (21%)
166	GTP	R2	501	167	26,34,34	1.15	2 (7%)	32,54,54	1.76	7 (21%)
166	GTP	KO	502	167	26,34,34	1.14	2 (7%)	32,54,54	1.73	7 (21%)
166	GTP	SP	501	167	26,34,34	1.17	2 (7%)	32,54,54	1.72	7 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
166	GTP	Ur	501	167	26,34,34	1.21	2 (7%)	32,54,54	1.68	8 (25%)
168	GDP	DL	501	-	24,30,30	0.97	1 (4%)	30,47,47	1.34	5 (16%)
168	GDP	Uc	501	-	24,30,30	0.96	1 (4%)	30,47,47	1.29	4 (13%)
168	GDP	V0	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.29	4 (13%)
166	GTP	HE	501	167	26,34,34	1.13	2 (7%)	32,54,54	1.67	6 (18%)
166	GTP	UR	501	167	26,34,34	1.11	2 (7%)	32,54,54	1.76	6 (18%)
166	GTP	Le	501	167	26,34,34	1.14	2 (7%)	32,54,54	1.66	7 (21%)
166	GTP	JC	501	167	26,34,34	1.25	1 (3%)	32,54,54	1.81	8 (25%)
168	GDP	O8	501	-	24,30,30	0.97	1 (4%)	30,47,47	1.22	3 (10%)
166	GTP	TC	501	167	26,34,34	1.19	2 (7%)	32,54,54	1.58	7 (21%)
166	GTP	LN	501	167	26,34,34	1.16	2 (7%)	32,54,54	1.66	7 (21%)
166	GTP	JG	501	167	26,34,34	1.14	2 (7%)	32,54,54	1.55	7 (21%)
166	GTP	FX	502	-	26,34,34	1.16	2 (7%)	32,54,54	1.56	7 (21%)
166	GTP	AC	501	-	26,34,34	1.38	2 (7%)	32,54,54	1.96	6 (18%)
166	GTP	PM	501	167	26,34,34	1.17	2 (7%)	32,54,54	1.76	7 (21%)
166	GTP	Q6	501	167	26,34,34	1.15	2 (7%)	32,54,54	1.65	7 (21%)
166	GTP	NO	501	-	26,34,34	1.17	2 (7%)	32,54,54	1.51	7 (21%)
168	GDP	J6	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.30	4 (13%)
168	GDP	MQ	501	-	24,30,30	0.90	0	30,47,47	1.42	5 (16%)
168	GDP	UQ	501	-	24,30,30	0.97	1 (4%)	30,47,47	1.34	5 (16%)
166	GTP	QG	501	-	26,34,34	1.19	2 (7%)	32,54,54	1.60	7 (21%)
168	GDP	Vj	501	-	24,30,30	0.96	1 (4%)	30,47,47	1.33	4 (13%)
168	GDP	KB	501	-	24,30,30	0.93	1 (4%)	30,47,47	1.34	4 (13%)
166	GTP	Wl	501	167	26,34,34	1.17	2 (7%)	32,54,54	1.61	7 (21%)
166	GTP	Vg	501	167	26,34,34	1.17	2 (7%)	32,54,54	1.71	7 (21%)
166	GTP	R0	501	167	26,34,34	1.16	2 (7%)	32,54,54	1.67	7 (21%)
168	GDP	JN	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.33	4 (13%)
166	GTP	R6	502	167	26,34,34	1.15	2 (7%)	32,54,54	1.70	7 (21%)
168	GDP	NP	501	-	24,30,30	0.90	0	30,47,47	1.53	6 (20%)
168	GDP	PN	501	-	24,30,30	0.92	1 (4%)	30,47,47	1.27	3 (10%)
168	GDP	RL	501	-	24,30,30	0.89	0	30,47,47	1.38	5 (16%)
168	GDP	QS	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.36	4 (13%)
168	GDP	UO	501	-	24,30,30	0.96	1 (4%)	30,47,47	1.29	5 (16%)
168	GDP	UU	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.32	4 (13%)
166	GTP	VP	501	-	26,34,34	1.13	2 (7%)	32,54,54	1.62	8 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
168	GDP	NJ	501	-	24,30,30	0.91	1 (4%)	30,47,47	1.32	4 (13%)
166	GTP	J5	501	-	26,34,34	1.14	2 (7%)	32,54,54	1.58	7 (21%)
168	GDP	Tr	501	-	24,30,30	0.91	1 (4%)	30,47,47	1.35	3 (10%)
166	GTP	TK	501	167	26,34,34	1.18	2 (7%)	32,54,54	1.54	7 (21%)
166	GTP	O9	502	167	26,34,34	1.17	2 (7%)	32,54,54	1.62	7 (21%)
166	GTP	DC	501	-	26,34,34	1.15	2 (7%)	32,54,54	1.56	7 (21%)
168	GDP	UF	501	-	24,30,30	1.02	1 (4%)	30,47,47	1.48	3 (10%)
166	GTP	UK	501	167	26,34,34	1.13	2 (7%)	32,54,54	1.70	6 (18%)
166	GTP	Sm	501	167	26,34,34	1.15	2 (7%)	32,54,54	1.71	7 (21%)
166	GTP	Mk	501	-	26,34,34	1.16	2 (7%)	32,54,54	1.56	7 (21%)
166	GTP	QX	501	167	26,34,34	1.14	2 (7%)	32,54,54	1.64	7 (21%)
166	GTP	T9	501	167	26,34,34	1.16	2 (7%)	32,54,54	1.61	7 (21%)
166	GTP	Uk	501	167	26,34,34	1.19	1 (3%)	32,54,54	1.63	8 (25%)
168	GDP	RN	501	-	24,30,30	0.92	1 (4%)	30,47,47	1.38	6 (20%)
166	GTP	Vt	501	167	26,34,34	1.16	2 (7%)	32,54,54	1.59	7 (21%)
168	GDP	DN	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.43	4 (13%)
166	GTP	RT	501	-	26,34,34	1.13	2 (7%)	32,54,54	1.65	8 (25%)
166	GTP	WZ	501	167	26,34,34	1.14	2 (7%)	32,54,54	1.65	6 (18%)
168	GDP	TD	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.30	5 (16%)
166	GTP	GR	501	167	26,34,34	1.11	1 (3%)	32,54,54	1.69	6 (18%)
168	GDP	SS	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.34	4 (13%)
168	GDP	AD	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.30	4 (13%)
166	GTP	CC	501	-	26,34,34	1.17	2 (7%)	32,54,54	1.62	7 (21%)
168	GDP	U1	501	-	24,30,30	0.97	1 (4%)	30,47,47	1.34	4 (13%)
166	GTP	VM	501	-	26,34,34	1.13	1 (3%)	32,54,54	1.64	9 (28%)
168	GDP	SO	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.34	4 (13%)
168	GDP	Tb	501	-	24,30,30	0.89	1 (4%)	30,47,47	1.35	3 (10%)
166	GTP	VY	501	167	26,34,34	1.16	2 (7%)	32,54,54	1.75	7 (21%)
168	GDP	UL	501	-	24,30,30	0.97	1 (4%)	30,47,47	1.21	5 (16%)
166	GTP	Mo	501	167	26,34,34	1.16	2 (7%)	32,54,54	1.66	7 (21%)
166	GTP	Ny	501	167	26,34,34	1.15	2 (7%)	32,54,54	1.67	7 (21%)
168	GDP	J2	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.32	4 (13%)
168	GDP	RB	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.36	6 (20%)
168	GDP	Oz	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.37	4 (13%)
166	GTP	Fr	501	-	26,34,34	1.15	2 (7%)	32,54,54	1.64	7 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
166	GTP	CA	501	-	26,34,34	1.14	1 (3%)	32,54,54	2.42	9 (28%)
166	GTP	OQ	501	167	26,34,34	1.14	2 (7%)	32,54,54	1.60	7 (21%)
166	GTP	VG	501	167	26,34,34	1.14	2 (7%)	32,54,54	1.65	7 (21%)
168	GDP	Th	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.39	4 (13%)
166	GTP	KS	501	167	26,34,34	1.15	2 (7%)	32,54,54	1.55	7 (21%)
168	GDP	Sh	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.34	4 (13%)
166	GTP	EM	501	-	26,34,34	1.20	2 (7%)	32,54,54	1.65	7 (21%)
168	GDP	ON	501	-	24,30,30	0.96	1 (4%)	30,47,47	1.28	4 (13%)
168	GDP	LL	501	-	24,30,30	0.88	0	30,47,47	1.33	6 (20%)
166	GTP	Wf	501	-	26,34,34	1.15	1 (3%)	32,54,54	1.51	8 (25%)
168	GDP	O6	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.34	4 (13%)
168	GDP	HJ	501	-	24,30,30	1.03	1 (4%)	30,47,47	1.31	5 (16%)
166	GTP	DK	501	167	26,34,34	1.17	2 (7%)	32,54,54	1.51	7 (21%)
168	GDP	Tz	501	-	24,30,30	0.92	1 (4%)	30,47,47	1.34	4 (13%)
168	GDP	T2	501	-	24,30,30	0.92	1 (4%)	30,47,47	1.35	4 (13%)
166	GTP	PI	502	167	26,34,34	1.15	2 (7%)	32,54,54	1.70	7 (21%)
166	GTP	VC	501	167	26,34,34	1.14	2 (7%)	32,54,54	1.68	5 (15%)
168	GDP	GU	501	-	24,30,30	0.91	1 (4%)	30,47,47	1.28	4 (13%)
166	GTP	Vr	501	167	26,34,34	1.15	2 (7%)	32,54,54	1.62	7 (21%)
168	GDP	Sj	502	-	24,30,30	0.94	1 (4%)	30,47,47	1.34	4 (13%)
166	GTP	EE	501	-	26,34,34	1.16	2 (7%)	32,54,54	1.50	6 (18%)
166	GTP	DA	501	167	26,34,34	1.17	2 (7%)	32,54,54	1.61	7 (21%)
168	GDP	TH	501	-	24,30,30	0.93	1 (4%)	30,47,47	1.25	4 (13%)
166	GTP	GX	501	167	26,34,34	1.13	1 (3%)	32,54,54	1.56	6 (18%)
168	GDP	S5	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.35	4 (13%)
166	GTP	II	502	167	26,34,34	1.13	2 (7%)	32,54,54	1.59	7 (21%)
168	GDP	SJ	501	-	24,30,30	0.93	1 (4%)	30,47,47	1.34	4 (13%)
168	GDP	OP	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.34	4 (13%)
168	GDP	Uf	501	-	24,30,30	0.90	1 (4%)	30,47,47	1.40	5 (16%)
168	GDP	Bv	501	-	24,30,30	0.98	1 (4%)	30,47,47	1.34	4 (13%)
168	GDP	O0	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.30	4 (13%)
168	GDP	TV	501	-	24,30,30	0.90	0	30,47,47	1.38	4 (13%)
166	GTP	La	501	-	26,34,34	1.14	2 (7%)	32,54,54	1.68	7 (21%)
168	GDP	VZ	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.40	4 (13%)
166	GTP	PE	501	-	26,34,34	1.16	2 (7%)	32,54,54	1.59	7 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
166	GTP	P8	501	167	26,34,34	1.17	2 (7%)	32,54,54	1.72	7 (21%)
166	GTP	AA	501	167	26,34,34	1.41	2 (7%)	32,54,54	1.93	7 (21%)
166	GTP	Tq	501	167	26,34,34	1.18	2 (7%)	32,54,54	1.68	7 (21%)
168	GDP	FN	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.34	4 (13%)
168	GDP	FV	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.35	4 (13%)
166	GTP	HK	501	167	26,34,34	1.17	1 (3%)	32,54,54	1.60	7 (21%)
168	GDP	UD	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.27	4 (13%)
166	GTP	Q4	501	167	26,34,34	1.17	2 (7%)	32,54,54	1.67	7 (21%)
166	GTP	PT	502	-	26,34,34	1.17	2 (7%)	32,54,54	1.70	7 (21%)
166	GTP	VA	501	167	26,34,34	1.16	2 (7%)	32,54,54	1.57	7 (21%)
166	GTP	VN	501	167	26,34,34	1.15	2 (7%)	32,54,54	1.73	7 (21%)
166	GTP	UZ	501	-	26,34,34	1.14	2 (7%)	32,54,54	1.68	7 (21%)
168	GDP	V4	501	-	24,30,30	0.97	1 (4%)	30,47,47	1.27	5 (16%)
166	GTP	Ta	501	167	26,34,34	1.17	2 (7%)	32,54,54	1.61	7 (21%)
168	GDP	RF	501	-	24,30,30	0.92	1 (4%)	30,47,47	1.30	5 (16%)
168	GDP	Ec	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.35	4 (13%)
168	GDP	JR	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.38	4 (13%)
168	GDP	JB	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.30	4 (13%)
166	GTP	Ss	501	167	26,34,34	1.17	2 (7%)	32,54,54	1.72	7 (21%)
166	GTP	Ut	501	167	26,34,34	1.16	2 (7%)	32,54,54	1.69	7 (21%)
166	GTP	NG	501	-	26,34,34	1.13	2 (7%)	32,54,54	1.53	7 (21%)
166	GTP	Sa	501	167	26,34,34	1.15	2 (7%)	32,54,54	1.54	7 (21%)
168	GDP	UB	501	-	24,30,30	0.99	1 (4%)	30,47,47	1.20	3 (10%)
168	GDP	WY	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.28	4 (13%)
166	GTP	RQ	501	-	26,34,34	1.12	2 (7%)	32,54,54	1.67	7 (21%)
168	GDP	LJ	501	-	24,30,30	0.90	1 (4%)	30,47,47	1.33	5 (16%)
168	GDP	MF	501	-	24,30,30	0.85	0	30,47,47	1.35	6 (20%)
166	GTP	MR	501	167	26,34,34	1.12	2 (7%)	32,54,54	1.92	8 (25%)
166	GTP	N1	501	167	26,34,34	1.13	2 (7%)	32,54,54	1.57	7 (21%)
168	GDP	Ea	501	-	24,30,30	0.96	1 (4%)	30,47,47	1.15	3 (10%)
166	GTP	PQ	501	-	26,34,34	1.16	2 (7%)	32,54,54	1.53	8 (25%)
168	GDP	ND	501	-	24,30,30	0.91	1 (4%)	30,47,47	1.26	4 (13%)
168	GDP	AL	501	-	24,30,30	0.96	1 (4%)	30,47,47	1.35	5 (16%)
168	GDP	AH	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.41	6 (20%)
168	GDP	UY	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.35	4 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
168	GDP	FX	501	-	24,30,30	1.03	2 (8%)	30,47,47	1.50	5 (16%)
168	GDP	CF	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.22	3 (10%)
166	GTP	RE	501	-	26,34,34	1.14	2 (7%)	32,54,54	1.68	7 (21%)
166	GTP	VK	501	167	26,34,34	1.13	1 (3%)	32,54,54	1.45	7 (21%)
168	GDP	GL	501	-	24,30,30	0.93	1 (4%)	30,47,47	1.31	4 (13%)
168	GDP	ML	501	-	24,30,30	0.88	0	30,47,47	1.37	4 (13%)
168	GDP	DD	501	-	24,30,30	0.91	1 (4%)	30,47,47	1.33	5 (16%)
168	GDP	P5	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.31	4 (13%)
168	GDP	TF	501	-	24,30,30	0.92	1 (4%)	30,47,47	1.31	5 (16%)
168	GDP	Tv	501	-	24,30,30	0.93	1 (4%)	30,47,47	1.38	4 (13%)
168	GDP	TA	501	-	24,30,30	0.98	1 (4%)	30,47,47	1.32	4 (13%)
168	GDP	TJ	501	-	24,30,30	0.90	0	30,47,47	1.38	6 (20%)
166	GTP	MG	501	167	26,34,34	1.09	2 (7%)	32,54,54	1.64	6 (18%)
166	GTP	IG	501	167	26,34,34	1.13	2 (7%)	32,54,54	1.54	7 (21%)
168	GDP	HH	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.31	4 (13%)
166	GTP	SY	501	167	26,34,34	1.16	2 (7%)	32,54,54	1.68	7 (21%)
166	GTP	UA	501	-	26,34,34	1.15	2 (7%)	32,54,54	1.59	6 (18%)
168	GDP	QW	501	-	24,30,30	0.92	1 (4%)	30,47,47	1.37	4 (13%)
168	GDP	Uj	501	-	24,30,30	1.32	3 (12%)	30,47,47	1.28	3 (10%)
168	GDP	Uy	501	-	24,30,30	0.97	1 (4%)	30,47,47	1.38	4 (13%)
168	GDP	V2	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.29	4 (13%)
166	GTP	DI	501	167	26,34,34	1.16	2 (7%)	32,54,54	1.56	7 (21%)
166	GTP	HR	502	167	26,34,34	1.13	2 (7%)	32,54,54	1.68	6 (18%)
168	GDP	We	501	-	24,30,30	0.96	1 (4%)	30,47,47	1.29	4 (13%)
166	GTP	S6	501	167	26,34,34	1.18	2 (7%)	32,54,54	1.64	7 (21%)
166	GTP	DE	501	167	26,34,34	1.18	2 (7%)	32,54,54	1.69	8 (25%)
166	GTP	PA	501	167	26,34,34	1.20	2 (7%)	32,54,54	1.73	7 (21%)
166	GTP	LE	501	167	26,34,34	1.15	2 (7%)	32,54,54	1.68	7 (21%)
168	GDP	PD	501	-	24,30,30	0.97	1 (4%)	30,47,47	1.27	5 (16%)
168	GDP	Th	501	-	24,30,30	0.87	0	30,47,47	1.44	6 (20%)
166	GTP	Ns	501	-	26,34,34	1.15	2 (7%)	32,54,54	1.63	7 (21%)
166	GTP	J9	501	-	26,34,34	1.14	2 (7%)	32,54,54	1.67	7 (21%)
168	GDP	Bp	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.28	4 (13%)
168	GDP	Tt	501	-	24,30,30	0.89	1 (4%)	30,47,47	1.34	3 (10%)
168	GDP	JP	501	-	24,30,30	0.96	1 (4%)	30,47,47	1.34	4 (13%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
166	GTP	EW	501	-	26,34,34	1.14	2 (7%)	32,54,54	1.63	8 (25%)
168	GDP	TX	501	-	24,30,30	0.99	1 (4%)	30,47,47	1.43	6 (20%)
166	GTP	IP	501	167	26,34,34	1.14	2 (7%)	32,54,54	1.54	7 (21%)
168	GDP	JF	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.33	4 (13%)
166	GTP	PO	502	-	26,34,34	1.15	2 (7%)	32,54,54	1.62	7 (21%)
166	GTP	Q8	501	167	26,34,34	1.14	1 (3%)	32,54,54	1.58	7 (21%)
168	GDP	BF	501	-	24,30,30	0.97	1 (4%)	30,47,47	1.12	3 (10%)
166	GTP	Sz	501	167	26,34,34	1.16	2 (7%)	32,54,54	1.66	7 (21%)
166	GTP	BG	501	167	26,34,34	1.13	2 (7%)	32,54,54	1.65	7 (21%)
168	GDP	JL	501	-	24,30,30	0.93	1 (4%)	30,47,47	1.41	4 (13%)
166	GTP	BC	501	-	26,34,34	1.13	2 (7%)	32,54,54	1.68	7 (21%)
166	GTP	Bw	501	-	26,34,34	1.12	2 (7%)	32,54,54	1.65	6 (18%)
166	GTP	GT	501	-	26,34,34	1.14	2 (7%)	32,54,54	1.74	7 (21%)
166	GTP	T5	501	-	26,34,34	1.14	2 (7%)	32,54,54	1.57	7 (21%)
166	GTP	SV	501	-	26,34,34	1.16	1 (3%)	32,54,54	1.57	7 (21%)
168	GDP	WO	501	-	24,30,30	0.97	1 (4%)	30,47,47	1.42	7 (23%)
166	GTP	GI	501	167	26,34,34	1.13	2 (7%)	32,54,54	1.64	8 (25%)
168	GDP	NH	501	-	24,30,30	0.93	0	30,47,47	1.42	5 (16%)
166	GTP	Te	501	167	26,34,34	1.16	2 (7%)	32,54,54	1.59	7 (21%)
168	GDP	KH	501	-	24,30,30	0.92	1 (4%)	30,47,47	1.34	6 (20%)
166	GTP	BE	501	167	26,34,34	1.12	2 (7%)	32,54,54	1.66	6 (18%)
166	GTP	WG	501	-	26,34,34	1.19	2 (7%)	32,54,54	1.61	7 (21%)
166	GTP	U5	501	167	26,34,34	1.16	2 (7%)	32,54,54	1.59	7 (21%)
166	GTP	QV	501	167	26,34,34	1.17	2 (7%)	32,54,54	1.72	7 (21%)
168	GDP	Fu	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.28	3 (10%)
166	GTP	O1	501	167	26,34,34	1.16	2 (7%)	32,54,54	1.71	7 (21%)
168	GDP	JH	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.35	4 (13%)
168	GDP	LO	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.23	3 (10%)
166	GTP	FI	501	167	26,34,34	1.12	2 (7%)	32,54,54	1.55	7 (21%)
168	GDP	MD	501	-	24,30,30	0.91	1 (4%)	30,47,47	1.33	5 (16%)
166	GTP	MN	501	167	26,34,34	1.14	2 (7%)	32,54,54	1.64	7 (21%)
168	GDP	IQ	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.33	3 (10%)
168	GDP	SM	501	-	24,30,30	0.91	1 (4%)	30,47,47	1.33	4 (13%)
166	GTP	FK	501	167	26,34,34	1.16	2 (7%)	32,54,54	1.74	7 (21%)
168	GDP	Ws	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.30	4 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
166	GTP	TY	501	167	26,34,34	1.16	2 (7%)	32,54,54	1.67	7 (21%)
168	GDP	EH	501	-	24,30,30	0.99	1 (4%)	30,47,47	1.32	5 (16%)
166	GTP	Ty	502	167	26,34,34	1.17	2 (7%)	32,54,54	1.69	7 (21%)
168	GDP	WS	501	-	24,30,30	0.92	1 (4%)	30,47,47	1.28	4 (13%)
168	GDP	RS	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.28	4 (13%)
168	GDP	Uw	501	-	24,30,30	0.97	1 (4%)	30,47,47	1.44	4 (13%)
166	GTP	Su	501	-	26,34,34	1.15	2 (7%)	32,54,54	1.70	7 (21%)
168	GDP	SQ	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.28	6 (20%)
168	GDP	S9	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.28	4 (13%)
166	GTP	FG	501	167	26,34,34	1.17	2 (7%)	32,54,54	1.72	7 (21%)
166	GTP	VE	501	167	26,34,34	1.15	2 (7%)	32,54,54	1.62	8 (25%)
166	GTP	TE	501	167	26,34,34	1.18	2 (7%)	32,54,54	1.57	7 (21%)
168	GDP	QJ	501	-	24,30,30	0.96	1 (4%)	30,47,47	1.34	5 (16%)
168	GDP	Tp	501	-	24,30,30	0.91	1 (4%)	30,47,47	1.40	4 (13%)
168	GDP	Mj	501	-	24,30,30	0.96	1 (4%)	30,47,47	1.35	4 (13%)
168	GDP	LZ	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.28	4 (13%)
168	GDP	QU	501	-	24,30,30	0.93	1 (4%)	30,47,47	1.32	4 (13%)
168	GDP	QP	501	-	24,30,30	0.97	1 (4%)	30,47,47	1.32	5 (16%)
168	GDP	J8	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.31	4 (13%)
168	GDP	EF	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.25	4 (13%)
166	GTP	HM	501	-	26,34,34	1.13	2 (7%)	32,54,54	1.60	7 (21%)
166	GTP	UT	501	167	26,34,34	1.13	2 (7%)	32,54,54	1.66	7 (21%)
166	GTP	SG	501	-	26,34,34	1.21	2 (7%)	32,54,54	1.59	7 (21%)
166	GTP	LM	502	167	26,34,34	1.16	2 (7%)	32,54,54	1.64	7 (21%)
166	GTP	RO	501	-	26,34,34	1.17	2 (7%)	32,54,54	1.69	8 (25%)
168	GDP	PP	501	-	24,30,30	2.03	5 (20%)	30,47,47	4.98	10 (33%)
168	GDP	KL	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.21	3 (10%)
168	GDP	Vo	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.34	4 (13%)
166	GTP	KE	501	167	26,34,34	1.14	2 (7%)	32,54,54	1.53	7 (21%)
168	GDP	BD	501	-	24,30,30	0.97	1 (4%)	30,47,47	1.33	4 (13%)
166	GTP	BK	501	167	26,34,34	1.13	2 (7%)	32,54,54	1.63	7 (21%)
166	GTP	MK	501	167	26,34,34	1.16	2 (7%)	32,54,54	1.56	7 (21%)
166	GTP	WA	501	167	26,34,34	76.82	5 (19%)	32,54,54	10.86	8 (25%)
168	GDP	T6	501	-	24,30,30	0.91	0	30,47,47	1.38	4 (13%)
168	GDP	QD	501	-	24,30,30	1.02	2 (8%)	30,47,47	1.63	5 (16%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
166	GTP	WE	501	167	26,34,34	1.13	2 (7%)	32,54,54	1.62	6 (18%)
166	GTP	TG	501	167	26,34,34	1.25	1 (3%)	32,54,54	1.51	7 (21%)
166	GTP	WP	501	167	26,34,34	1.14	2 (7%)	32,54,54	1.62	7 (21%)
168	GDP	MH	501	-	24,30,30	0.90	1 (4%)	30,47,47	1.37	5 (16%)
166	GTP	R8	501	167	26,34,34	1.15	2 (7%)	32,54,54	1.68	7 (21%)
168	GDP	O2	501	-	24,30,30	0.96	1 (4%)	30,47,47	1.39	4 (13%)
168	GDP	EJ	501	-	24,30,30	0.96	1 (4%)	30,47,47	1.24	4 (13%)
166	GTP	TM	501	167	26,34,34	1.11	2 (7%)	32,54,54	1.78	7 (21%)
166	GTP	OG	501	-	26,34,34	1.12	2 (7%)	32,54,54	1.62	8 (25%)
166	GTP	Wb	502	167	26,34,34	1.15	2 (7%)	32,54,54	1.77	6 (18%)
166	GTP	AE	501	-	26,34,34	1.26	2 (7%)	32,54,54	2.01	7 (21%)
166	GTP	LY	501	167	26,34,34	1.16	2 (7%)	32,54,54	1.65	6 (18%)
166	GTP	U2	501	167	26,34,34	1.19	2 (7%)	32,54,54	1.56	7 (21%)
166	GTP	U9	501	-	26,34,34	1.16	2 (7%)	32,54,54	1.72	7 (21%)
168	GDP	UJ	501	-	24,30,30	0.93	1 (4%)	30,47,47	1.32	4 (13%)
168	GDP	VH	501	-	24,30,30	0.96	1 (4%)	30,47,47	1.26	4 (13%)
168	GDP	OJ	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.31	4 (13%)
166	GTP	OE	501	167	26,34,34	1.13	2 (7%)	32,54,54	1.73	7 (21%)
166	GTP	Vv	501	167	26,34,34	1.20	2 (7%)	32,54,54	1.68	7 (21%)
168	GDP	GD	501	-	24,30,30	0.93	1 (4%)	30,47,47	1.28	4 (13%)
168	GDP	Sv	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.34	4 (13%)
166	GTP	Q0	501	167	26,34,34	1.17	2 (7%)	32,54,54	1.45	5 (15%)
168	GDP	GH	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.30	4 (13%)
168	GDP	LH	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.34	3 (10%)
166	GTP	Vk	501	167	26,34,34	1.25	2 (7%)	32,54,54	1.79	7 (21%)
166	GTP	Sc	501	167	26,34,34	1.15	2 (7%)	32,54,54	1.59	7 (21%)
168	GDP	AB	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.31	4 (13%)
168	GDP	HB	501	-	24,30,30	0.97	1 (4%)	30,47,47	1.35	5 (16%)
168	GDP	V6	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.31	4 (13%)
168	GDP	VF	501	-	24,30,30	85.55	5 (20%)	30,47,47	11.56	8 (26%)
166	GTP	Mq	501	-	26,34,34	1.14	2 (7%)	32,54,54	1.59	8 (25%)
166	GTP	CE	501	-	26,34,34	1.16	2 (7%)	32,54,54	1.66	8 (25%)
168	GDP	KN	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.26	6 (20%)
166	GTP	So	502	167	26,34,34	1.17	2 (7%)	32,54,54	1.64	7 (21%)
168	GDP	MB	501	-	24,30,30	0.87	0	30,47,47	1.34	5 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
166	GTP	WR	501	-	26,34,34	1.18	2 (7%)	32,54,54	1.63	7 (21%)
168	GDP	Tf	501	-	24,30,30	0.91	1 (4%)	30,47,47	1.25	3 (10%)
166	GTP	Ms	501	-	26,34,34	1.17	2 (7%)	32,54,54	1.61	7 (21%)
166	GTP	P6	501	-	26,34,34	1.15	2 (7%)	32,54,54	1.69	7 (21%)
168	GDP	VL	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.29	5 (16%)
166	GTP	NM	502	167	26,34,34	1.19	2 (7%)	32,54,54	1.71	7 (21%)
168	GDP	OB	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.35	5 (16%)
166	GTP	JS	501	167	26,34,34	1.13	2 (7%)	32,54,54	1.53	7 (21%)
166	GTP	TQ	501	167	26,34,34	1.19	1 (3%)	32,54,54	1.58	6 (18%)
166	GTP	Ug	501	-	26,34,34	1.16	2 (7%)	32,54,54	1.65	7 (21%)
166	GTP	Ve	501	-	26,34,34	1.20	2 (7%)	32,54,54	1.58	7 (21%)
168	GDP	HQ	501	-	24,30,30	0.96	1 (4%)	30,47,47	1.38	3 (10%)
168	GDP	VJ	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.31	5 (16%)
166	GTP	T1	501	-	26,34,34	1.13	2 (7%)	32,54,54	1.65	7 (21%)
166	GTP	Vx	501	167	26,34,34	1.15	2 (7%)	32,54,54	1.59	6 (18%)
166	GTP	QT	501	167	26,34,34	1.15	2 (7%)	32,54,54	1.63	7 (21%)
168	GDP	SL	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.28	5 (16%)
168	GDP	R1	501	-	24,30,30	0.97	1 (4%)	30,47,47	1.34	4 (13%)
166	GTP	UE	501	167	26,34,34	1.14	2 (7%)	32,54,54	1.62	7 (21%)
166	GTP	P0	501	167	26,34,34	1.14	2 (7%)	32,54,54	1.68	7 (21%)
168	GDP	PB	501	-	24,30,30	0.99	1 (4%)	30,47,47	1.54	5 (16%)
168	GDP	Vb	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.36	4 (13%)
168	GDP	Us	501	-	24,30,30	0.97	1 (4%)	30,47,47	1.34	4 (13%)
166	GTP	MP	501	167	26,34,34	1.15	2 (7%)	32,54,54	1.64	7 (21%)
166	GTP	Sq	501	167	26,34,34	1.17	2 (7%)	32,54,54	1.57	7 (21%)
166	GTP	DM	501	167	26,34,34	1.16	2 (7%)	32,54,54	1.68	7 (21%)
166	GTP	WC	501	167	26,34,34	1.15	2 (7%)	32,54,54	1.66	7 (21%)
168	GDP	VB	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.29	4 (13%)
166	GTP	WX	501	-	26,34,34	1.15	1 (3%)	32,54,54	1.68	7 (21%)
166	GTP	UM	502	167	26,34,34	1.14	1 (3%)	32,54,54	1.78	7 (21%)
168	GDP	SX	501	-	24,30,30	1.00	1 (4%)	30,47,47	1.32	4 (13%)
166	GTP	WK	501	167	26,34,34	1.14	2 (7%)	32,54,54	1.60	6 (18%)
166	GTP	KC	501	167	26,34,34	1.17	2 (7%)	32,54,54	1.73	7 (21%)
168	GDP	Q9	501	-	24,30,30	0.93	1 (4%)	30,47,47	1.30	4 (13%)
166	GTP	BI	501	-	26,34,34	1.14	1 (3%)	32,54,54	1.67	6 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
168	GDP	LD	501	-	24,30,30	0.92	1 (4%)	30,47,47	1.27	3 (10%)
168	GDP	TP	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.33	5 (16%)
166	GTP	S0	501	167	26,34,34	1.16	2 (7%)	32,54,54	1.61	7 (21%)
168	GDP	HN	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.30	4 (13%)
168	GDP	WQ	501	-	24,30,30	0.96	1 (4%)	30,47,47	1.29	4 (13%)
166	GTP	QQ	502	167	26,34,34	1.20	2 (7%)	32,54,54	1.71	8 (25%)
168	GDP	HD	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.29	4 (13%)
168	GDP	Mr	501	-	24,30,30	0.99	1 (4%)	30,47,47	1.38	3 (10%)
166	GTP	R4	501	167	26,34,34	1.15	2 (7%)	32,54,54	1.64	7 (21%)
168	GDP	VQ	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.29	4 (13%)
168	GDP	Bx	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.13	3 (10%)
166	GTP	GM	501	167	26,34,34	1.15	1 (3%)	32,54,54	1.75	6 (18%)
166	GTP	RA	501	167	26,34,34	1.15	2 (7%)	32,54,54	1.61	7 (21%)
166	GTP	Tm	501	167	26,34,34	1.17	2 (7%)	32,54,54	1.65	7 (21%)
168	GDP	TR	501	-	24,30,30	0.93	1 (4%)	30,47,47	1.31	5 (16%)
166	GTP	GV	501	167	26,34,34	1.14	2 (7%)	32,54,54	1.62	7 (21%)
168	GDP	J0	501	-	24,30,30	0.96	1 (4%)	30,47,47	1.33	4 (13%)
168	GDP	GN	501	-	24,30,30	0.92	1 (4%)	30,47,47	1.28	3 (10%)
168	GDP	BB	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.23	4 (13%)
166	GTP	FE	501	167	26,34,34	1.13	2 (7%)	32,54,54	1.68	7 (21%)
168	GDP	N2	501	-	24,30,30	0.93	1 (4%)	30,47,47	1.28	4 (13%)
168	GDP	VD	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.18	3 (10%)
168	GDP	VW	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.32	4 (13%)
168	GDP	Nr	501	-	24,30,30	0.92	1 (4%)	30,47,47	1.37	5 (16%)
168	GDP	Mt	501	-	24,30,30	0.93	1 (4%)	30,47,47	1.32	4 (13%)
166	GTP	Wr	501	167	26,34,34	1.15	2 (7%)	32,54,54	1.67	7 (21%)
168	GDP	U6	501	-	24,30,30	0.92	1 (4%)	30,47,47	1.39	6 (20%)
168	GDP	Mp	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.27	5 (16%)
166	GTP	RK	501	-	26,34,34	1.16	2 (7%)	32,54,54	1.56	6 (18%)
168	GDP	Q5	501	-	24,30,30	0.93	1 (4%)	30,47,47	1.33	4 (13%)
168	GDP	NN	501	-	24,30,30	0.92	1 (4%)	30,47,47	1.30	3 (10%)
166	GTP	FM	501	167	26,34,34	1.13	2 (7%)	32,54,54	1.68	8 (25%)
166	GTP	UI	501	167	26,34,34	1.13	1 (3%)	32,54,54	1.68	6 (18%)
166	GTP	LK	501	167	26,34,34	1.15	2 (7%)	32,54,54	1.58	7 (21%)
166	GTP	Li	501	167	26,34,34	1.14	2 (7%)	32,54,54	1.72	7 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
168	GDP	Lf	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.28	4 (13%)
166	GTP	Nu	501	167	26,34,34	1.16	2 (7%)	32,54,54	1.70	7 (21%)
166	GTP	ST	501	-	26,34,34	1.14	2 (7%)	32,54,54	1.70	8 (25%)
168	GDP	BL	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.21	5 (16%)
166	GTP	LI	501	167	26,34,34	1.13	2 (7%)	32,54,54	1.59	7 (21%)
168	GDP	RU	501	-	24,30,30	0.93	1 (4%)	30,47,47	1.32	4 (13%)
168	GDP	IL	501	-	24,30,30	0.97	1 (4%)	30,47,47	1.29	4 (13%)
166	GTP	S2	501	167	26,34,34	1.15	2 (7%)	32,54,54	1.60	7 (21%)
168	GDP	WJ	501	-	24,30,30	0.99	1 (4%)	30,47,47	1.30	5 (16%)
168	GDP	Wc	501	-	24,30,30	0.97	1 (4%)	30,47,47	1.27	4 (13%)
166	GTP	Si	501	167	26,34,34	1.15	2 (7%)	32,54,54	1.68	7 (21%)
168	GDP	Wk	501	-	24,30,30	0.96	1 (4%)	30,47,47	1.30	4 (13%)
168	GDP	GO	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.40	4 (13%)
166	GTP	JK	501	-	26,34,34	1.15	2 (7%)	32,54,54	1.66	7 (21%)
166	GTP	AR	501	-	26,34,34	1.14	1 (3%)	32,54,54	1.59	10 (31%)
166	GTP	VR	501	167	26,34,34	1.14	2 (7%)	32,54,54	1.64	7 (21%)
166	GTP	TI	502	167	26,34,34	1.17	2 (7%)	32,54,54	1.59	7 (21%)
168	GDP	VO	501	-	24,30,30	0.93	1 (4%)	30,47,47	1.25	4 (13%)
168	GDP	P7	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.31	5 (16%)
166	GTP	DG	501	-	26,34,34	1.17	2 (7%)	32,54,54	1.70	8 (25%)
168	GDP	Un	501	-	24,30,30	0.89	0	30,47,47	1.50	5 (16%)
166	GTP	Wn	501	-	26,34,34	1.16	2 (7%)	32,54,54	1.60	7 (21%)
168	GDP	FF	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.35	5 (16%)
166	GTP	CI	501	-	26,34,34	1.14	2 (7%)	32,54,54	1.50	8 (25%)
166	GTP	WM	501	167	26,34,34	1.14	2 (7%)	32,54,54	1.58	7 (21%)
168	GDP	Vw	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.33	4 (13%)
168	GDP	IJ	501	-	24,30,30	0.96	1 (4%)	30,47,47	1.27	4 (13%)
168	GDP	KP	501	-	24,30,30	0.93	1 (4%)	30,47,47	1.31	4 (13%)
166	GTP	Lg	501	167	26,34,34	1.14	2 (7%)	32,54,54	1.68	7 (21%)
166	GTP	QK	501	167	26,34,34	1.19	2 (7%)	32,54,54	1.58	7 (21%)
166	GTP	UN	501	167	26,34,34	1.14	1 (3%)	32,54,54	1.64	6 (18%)
166	GTP	UV	501	167	26,34,34	1.15	2 (7%)	32,54,54	1.66	7 (21%)
168	GDP	FL	501	-	24,30,30	0.93	1 (4%)	30,47,47	1.35	4 (13%)
166	GTP	HP	501	167	26,34,34	1.14	2 (7%)	32,54,54	1.65	7 (21%)
168	GDP	PU	501	-	24,30,30	0.97	1 (4%)	30,47,47	1.35	4 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
168	GDP	TL	501	-	24,30,30	0.84	1 (4%)	30,47,47	1.43	5 (16%)
166	GTP	NK	501	167	26,34,34	1.15	2 (7%)	32,54,54	1.55	7 (21%)
168	GDP	SB	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.41	6 (20%)
166	GTP	Tu	501	167	26,34,34	1.19	2 (7%)	32,54,54	1.64	7 (21%)
168	GDP	VS	501	-	24,30,30	0.92	1 (4%)	30,47,47	1.34	5 (16%)
166	GTP	Ft	501	-	26,34,34	1.16	2 (7%)	32,54,54	1.49	7 (21%)
166	GTP	O5	501	167	26,34,34	1.15	2 (7%)	32,54,54	1.65	7 (21%)
168	GDP	SF	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.35	5 (16%)
168	GDP	Wa	501	-	24,30,30	0.96	1 (4%)	30,47,47	1.30	4 (13%)
168	GDP	KJ	501	-	24,30,30	0.93	1 (4%)	30,47,47	1.31	4 (13%)
168	GDP	R3	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.34	4 (13%)
168	GDP	MO	501	-	24,30,30	0.89	1 (4%)	30,47,47	1.37	5 (16%)
166	GTP	JE	501	167	26,34,34	1.17	2 (7%)	32,54,54	1.60	7 (21%)
168	GDP	R7	501	-	24,30,30	0.96	1 (4%)	30,47,47	1.31	4 (13%)
166	GTP	V1	501	167	26,34,34	1.14	2 (7%)	32,54,54	1.68	7 (21%)
166	GTP	QE	501	167	26,34,34	1.18	2 (7%)	32,54,54	1.67	7 (21%)
166	GTP	GB	501	-	26,34,34	1.16	2 (7%)	32,54,54	1.76	7 (21%)
168	GDP	PJ	501	-	24,30,30	0.89	1 (4%)	30,47,47	1.31	5 (16%)
168	GDP	QF	501	-	24,30,30	0.98	1 (4%)	30,47,47	1.42	4 (13%)
168	GDP	St	501	-	24,30,30	0.96	1 (4%)	30,47,47	1.37	4 (13%)
168	GDP	Uu	501	-	24,30,30	0.98	1 (4%)	30,47,47	1.33	5 (16%)
166	GTP	Mu	501	-	26,34,34	1.16	2 (7%)	32,54,54	1.61	8 (25%)
168	GDP	WH	501	-	24,30,30	0.96	1 (4%)	30,47,47	1.31	4 (13%)
166	GTP	KQ	501	167	26,34,34	1.14	2 (7%)	32,54,54	1.59	7 (21%)
166	GTP	Lk	501	167	26,34,34	1.17	2 (7%)	32,54,54	1.65	6 (18%)
168	GDP	PS	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.33	4 (13%)
166	GTP	Ux	501	-	26,34,34	1.18	2 (7%)	32,54,54	1.60	7 (21%)
166	GTP	QA	501	-	26,34,34	1.14	2 (7%)	32,54,54	1.52	7 (21%)
168	GDP	WB	501	-	24,30,30	0.97	1 (4%)	30,47,47	1.32	5 (16%)
166	GTP	GE	501	167	26,34,34	1.20	2 (7%)	32,54,54	1.79	7 (21%)
166	GTP	KG	501	167	26,34,34	1.17	2 (7%)	32,54,54	1.60	8 (25%)
166	GTP	Fv	501	167	26,34,34	1.16	2 (7%)	32,54,54	1.61	7 (21%)
166	GTP	TW	501	167	26,34,34	1.15	2 (7%)	32,54,54	1.71	7 (21%)
166	GTP	AI	501	-	26,34,34	1.15	2 (7%)	32,54,54	1.61	9 (28%)
168	GDP	Nx	501	-	24,30,30	0.93	1 (4%)	30,47,47	1.40	5 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
166	GTP	SI	501	167	26,34,34	1.22	2 (7%)	32,54,54	1.74	7 (21%)
168	GDP	CL	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.37	4 (13%)
166	GTP	QC	501	167	26,34,34	1.15	2 (7%)	32,54,54	1.67	7 (21%)
168	GDP	O4	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.30	4 (13%)
166	GTP	KI	501	167	26,34,34	1.15	2 (7%)	32,54,54	1.60	7 (21%)
168	GDP	QL	501	-	24,30,30	0.99	1 (4%)	30,47,47	1.33	4 (13%)
168	GDP	SD	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.34	4 (13%)
168	GDP	Q7	501	-	24,30,30	0.93	1 (4%)	30,47,47	1.34	4 (13%)
166	GTP	Wj	501	167	26,34,34	1.15	2 (7%)	32,54,54	1.68	7 (21%)
166	GTP	LR	501	167	26,34,34	1.14	2 (7%)	32,54,54	1.61	7 (21%)
168	GDP	QB	501	-	24,30,30	0.97	1 (4%)	30,47,47	1.34	5 (16%)
168	GDP	Tl	501	-	24,30,30	0.90	1 (4%)	30,47,47	1.40	4 (13%)
168	GDP	RD	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.28	5 (16%)
168	GDP	KD	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.31	4 (13%)
168	GDP	AX	501	-	24,30,30	0.96	1 (4%)	30,47,47	1.31	4 (13%)
166	GTP	QM	501	-	26,34,34	1.14	2 (7%)	32,54,54	1.56	7 (21%)
168	GDP	EL	501	-	24,30,30	0.96	1 (4%)	30,47,47	1.39	4 (13%)
166	GTP	To	501	167	26,34,34	1.10	1 (3%)	32,54,54	1.65	6 (18%)
166	GTP	T3	501	167	26,34,34	1.14	2 (7%)	32,54,54	1.66	7 (21%)
166	GTP	IM	501	167	26,34,34	1.14	2 (7%)	32,54,54	1.79	8 (25%)
166	GTP	Tk	501	167	26,34,34	1.16	2 (7%)	32,54,54	1.69	7 (21%)
168	GDP	PH	501	-	24,30,30	1.22	4 (16%)	30,47,47	1.63	6 (20%)
166	GTP	Lc	501	167	26,34,34	1.13	2 (7%)	32,54,54	1.64	7 (21%)
168	GDP	GF	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.24	3 (10%)
166	GTP	OI	501	-	26,34,34	1.14	2 (7%)	32,54,54	1.62	8 (25%)
166	GTP	QI	501	-	26,34,34	1.15	2 (7%)	32,54,54	1.65	7 (21%)
166	GTP	VI	502	167	26,34,34	1.14	2 (7%)	32,54,54	1.69	6 (18%)
166	GTP	UG	501	167	26,34,34	1.13	2 (7%)	32,54,54	1.64	7 (21%)
166	GTP	O3	501	-	26,34,34	1.17	2 (7%)	32,54,54	1.54	7 (21%)
168	GDP	US	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.31	4 (13%)
168	GDP	IF	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.25	3 (10%)
168	GDP	IH	501	-	24,30,30	0.96	1 (4%)	30,47,47	1.32	4 (13%)
166	GTP	WN	501	167	26,34,34	1.15	2 (7%)	32,54,54	1.69	7 (21%)
166	GTP	Tc	502	167	26,34,34	1.17	2 (7%)	32,54,54	1.61	7 (21%)
168	GDP	Up	501	-	24,30,30	0.91	1 (4%)	30,47,47	1.44	6 (20%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
166	GTP	EK	501	167	26,34,34	1.16	2 (7%)	32,54,54	1.64	6 (18%)
166	GTP	IK	501	167	26,34,34	1.15	2 (7%)	32,54,54	1.69	7 (21%)
168	GDP	FJ	501	-	24,30,30	0.97	1 (4%)	30,47,47	1.25	4 (13%)
166	GTP	NE	501	167	26,34,34	1.14	2 (7%)	32,54,54	1.66	7 (21%)
168	GDP	U3	502	-	24,30,30	0.99	1 (4%)	30,47,47	1.28	4 (13%)
168	GDP	Fs	501	-	24,30,30	0.96	1 (4%)	30,47,47	1.29	5 (16%)
166	GTP	QO	501	167	26,34,34	1.30	3 (11%)	32,54,54	1.77	7 (21%)
168	GDP	Wq	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.27	4 (13%)
168	GDP	Vf	501	-	24,30,30	0.92	1 (4%)	30,47,47	1.35	4 (13%)
166	GTP	FU	501	-	26,34,34	1.18	2 (7%)	32,54,54	1.57	7 (21%)
166	GTP	PK	501	167	26,34,34	1.14	2 (7%)	32,54,54	1.48	7 (21%)
166	GTP	KK	502	167	26,34,34	1.14	2 (7%)	32,54,54	1.58	7 (21%)
166	GTP	IC	501	-	26,34,34	1.17	2 (7%)	32,54,54	1.67	7 (21%)
168	GDP	Sn	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.42	4 (13%)
166	GTP	IR	501	167	26,34,34	1.13	2 (7%)	32,54,54	1.61	7 (21%)
168	GDP	AM	501	-	24,30,30	0.98	1 (4%)	30,47,47	1.38	5 (16%)
168	GDP	VU	501	-	24,30,30	0.93	1 (4%)	30,47,47	1.38	4 (13%)
166	GTP	FC	501	-	26,34,34	1.15	2 (7%)	32,54,54	1.65	7 (21%)
166	GTP	MM	501	167	26,34,34	1.16	2 (7%)	32,54,54	1.58	7 (21%)
168	GDP	R9	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.34	4 (13%)
166	GTP	NI	501	167	26,34,34	1.14	2 (7%)	32,54,54	1.70	7 (21%)
168	GDP	R5	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.32	5 (16%)
168	GDP	FD	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.40	4 (13%)
166	GTP	Ue	501	167	26,34,34	1.16	2 (7%)	32,54,54	1.69	7 (21%)
166	GTP	MC	501	167	26,34,34	1.16	2 (7%)	32,54,54	1.63	7 (21%)

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
168	GDP	Sb	501	-	-	4/12/32/32	0/3/3/3
168	GDP	Wi	501	-	-	2/12/32/32	0/3/3/3
166	GTP	EC	501	-	-	8/18/38/38	0/3/3/3
168	GDP	S1	501	-	-	3/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
168	GDP	JJ	501	-	-	4/12/32/32	0/3/3/3
168	GDP	Lh	501	-	-	4/12/32/32	0/3/3/3
168	GDP	Sl	501	-	-	1/12/32/32	0/3/3/3
166	GTP	Bt	501	-	-	7/18/38/38	0/3/3/3
166	GTP	SC	501	167	-	4/18/38/38	0/3/3/3
166	GTP	Wt	501	167	-	3/18/38/38	0/3/3/3
166	GTP	OO	501	167	-	6/18/38/38	0/3/3/3
168	GDP	CB	501	-	-	3/12/32/32	0/3/3/3
168	GDP	Mn	501	-	-	3/12/32/32	0/3/3/3
168	GDP	Tj	501	-	-	4/12/32/32	0/3/3/3
168	GDP	LF	501	-	-	3/12/32/32	0/3/3/3
168	GDP	SH	501	-	-	2/12/32/32	0/3/3/3
168	GDP	PR	501	-	-	1/12/32/32	0/3/3/3
166	GTP	LG	502	167	-	8/18/38/38	0/3/3/3
168	GDP	WU	501	-	-	4/12/32/32	0/3/3/3
168	GDP	T4	501	-	-	2/12/32/32	0/3/3/3
168	GDP	PL	501	-	-	4/12/32/32	0/3/3/3
168	GDP	Ua	501	-	-	6/12/32/32	0/3/3/3
166	GTP	JI	501	167	-	3/18/38/38	0/3/3/3
166	GTP	ME	501	167	-	3/18/38/38	0/3/3/3
166	GTP	Uo	501	167	-	3/18/38/38	0/3/3/3
168	GDP	GJ	501	-	-	4/12/32/32	0/3/3/3
168	GDP	OH	501	-	-	3/12/32/32	0/3/3/3
166	GTP	WV	501	167	-	5/18/38/38	0/3/3/3
168	GDP	RR	501	-	-	2/12/32/32	0/3/3/3
166	GTP	J1	501	167	-	5/18/38/38	0/3/3/3
166	GTP	RG	501	167	-	3/18/38/38	0/3/3/3
166	GTP	V7	501	167	-	7/18/38/38	0/3/3/3
166	GTP	RM	501	-	-	6/18/38/38	0/3/3/3
166	GTP	Uv	501	167	-	4/18/38/38	0/3/3/3
168	GDP	Wu	501	-	-	4/12/32/32	0/3/3/3
166	GTP	SA	501	167	-	5/18/38/38	0/3/3/3
168	GDP	IO	501	-	-	2/12/32/32	0/3/3/3
166	GTP	Ui	501	-	-	8/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
166	GTP	Vn	501	167	-	5/18/38/38	0/3/3/3
168	GDP	CH	501	-	-	4/12/32/32	0/3/3/3
168	GDP	HF	501	-	-	4/12/32/32	0/3/3/3
168	GDP	ER	501	-	-	2/12/32/32	0/3/3/3
168	GDP	JD	501	-	-	5/12/32/32	0/3/3/3
168	GDP	Td	501	-	-	3/12/32/32	0/3/3/3
166	GTP	UX	501	-	-	7/18/38/38	0/3/3/3
166	GTP	NQ	501	167	-	5/18/38/38	0/3/3/3
168	GDP	Lj	501	-	-	4/12/32/32	0/3/3/3
168	GDP	AF	501	-	-	1/12/32/32	0/3/3/3
168	GDP	RH	501	-	-	1/12/32/32	0/3/3/3
166	GTP	Vi	502	167	-	2/18/38/38	0/3/3/3
168	GDP	P9	501	-	-	5/12/32/32	0/3/3/3
168	GDP	GQ	501	-	-	6/12/32/32	0/3/3/3
168	GDP	GW	501	-	-	4/12/32/32	0/3/3/3
166	GTP	GP	501	167	-	5/18/38/38	0/3/3/3
168	GDP	J4	501	-	-	1/12/32/32	0/3/3/3
166	GTP	BA	501	167	-	3/18/38/38	0/3/3/3
166	GTP	Sw	502	167	-	4/18/38/38	0/3/3/3
168	GDP	BH	501	-	-	6/12/32/32	0/3/3/3
168	GDP	NB	501	-	-	2/12/32/32	0/3/3/3
168	GDP	HL	501	-	-	3/12/32/32	0/3/3/3
168	GDP	CD	501	-	-	4/12/32/32	0/3/3/3
168	GDP	OL	501	-	-	4/12/32/32	0/3/3/3
168	GDP	QH	501	-	-	0/12/32/32	0/3/3/3
168	GDP	TB	501	-	-	2/12/32/32	0/3/3/3
168	GDP	UW	501	-	-	5/12/32/32	0/3/3/3
168	GDP	Vd	501	-	-	2/12/32/32	0/3/3/3
166	GTP	KA	501	-	-	5/18/38/38	0/3/3/3
168	GDP	LB	501	-	-	3/12/32/32	0/3/3/3
166	GTP	O7	501	167	-	7/18/38/38	0/3/3/3
166	GTP	GG	501	167	-	7/18/38/38	0/3/3/3
168	GDP	OD	501	-	-	6/12/32/32	0/3/3/3
166	GTP	S8	501	167	-	7/18/38/38	0/3/3/3
166	GTP	HI	501	167	-	6/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
168	GDP	T8	501	-	-	3/12/32/32	0/3/3/3
166	GTP	V3	501	167	-	4/18/38/38	0/3/3/3
166	GTP	V5	501	167	-	4/18/38/38	0/3/3/3
166	GTP	HG	502	167	-	2/18/38/38	0/3/3/3
166	GTP	LP	501	167	-	8/18/38/38	0/3/3/3
166	GTP	PG	501	167	-	4/18/38/38	0/3/3/3
168	GDP	KR	501	-	-	5/12/32/32	0/3/3/3
168	GDP	N0	501	-	-	2/12/32/32	0/3/3/3
168	GDP	Vz	501	-	-	1/12/32/32	0/3/3/3
166	GTP	V9	501	167	-	3/18/38/38	0/3/3/3
166	GTP	Se	501	167	-	6/18/38/38	0/3/3/3
168	GDP	BJ	501	-	-	4/12/32/32	0/3/3/3
166	GTP	Wp	501	167	-	2/18/38/38	0/3/3/3
166	GTP	UP	502	167	-	6/18/38/38	0/3/3/3
166	GTP	KM	501	167	-	5/18/38/38	0/3/3/3
166	GTP	IN	501	167	-	6/18/38/38	0/3/3/3
166	GTP	JQ	501	167	-	2/18/38/38	0/3/3/3
166	GTP	VT	501	167	-	7/18/38/38	0/3/3/3
168	GDP	IB	501	-	-	3/12/32/32	0/3/3/3
166	GTP	RC	501	-	-	3/18/38/38	0/3/3/3
168	GDP	Sd	501	-	-	5/12/32/32	0/3/3/3
166	GTP	T7	502	167	-	3/18/38/38	0/3/3/3
168	GDP	S7	501	-	-	2/12/32/32	0/3/3/3
166	GTP	UC	501	167	-	6/18/38/38	0/3/3/3
168	GDP	U0	501	-	-	2/12/32/32	0/3/3/3
168	GDP	AJ	501	-	-	2/12/32/32	0/3/3/3
168	GDP	WW	501	-	-	3/12/32/32	0/3/3/3
166	GTP	Tg	501	167	-	7/18/38/38	0/3/3/3
166	GTP	AG	501	167	-	4/18/38/38	0/3/3/3
168	GDP	Wm	501	-	-	2/12/32/32	0/3/3/3
166	GTP	Mi	501	-	-	3/18/38/38	0/3/3/3
168	GDP	AO	501	-	-	1/12/32/32	0/3/3/3
166	GTP	NC	501	-	-	8/18/38/38	0/3/3/3
168	GDP	NL	501	-	-	2/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
168	GDP	KF	501	-	-	3/12/32/32	0/3/3/3
168	GDP	U8	501	-	-	1/12/32/32	0/3/3/3
168	GDP	MI	501	-	-	1/12/32/32	0/3/3/3
168	GDP	RP	501	-	-	2/12/32/32	0/3/3/3
168	GDP	Nz	501	-	-	4/12/32/32	0/3/3/3
168	GDP	Lb	501	-	-	0/12/32/32	0/3/3/3
166	GTP	OC	501	167	-	6/18/38/38	0/3/3/3
166	GTP	Ts	501	167	-	5/18/38/38	0/3/3/3
168	GDP	TN	501	-	-	2/12/32/32	0/3/3/3
166	GTP	OK	501	167	-	9/18/38/38	0/3/3/3
166	GTP	Vp	501	167	-	3/18/38/38	0/3/3/3
168	GDP	Wo	501	-	-	2/12/32/32	0/3/3/3
168	GDP	DB	501	-	-	4/12/32/32	0/3/3/3
168	GDP	RW	501	-	-	3/12/32/32	0/3/3/3
168	GDP	FH	501	-	-	3/12/32/32	0/3/3/3
166	GTP	Vc	501	167	-	4/18/38/38	0/3/3/3
166	GTP	Va	501	167	-	6/18/38/38	0/3/3/3
168	GDP	LQ	501	-	-	3/12/32/32	0/3/3/3
166	GTP	VV	501	-	-	3/18/38/38	0/3/3/3
166	GTP	Um	502	167	-	6/18/38/38	0/3/3/3
168	GDP	Sf	501	-	-	2/12/32/32	0/3/3/3
166	GTP	J7	501	167	-	4/18/38/38	0/3/3/3
168	GDP	Nt	501	-	-	0/12/32/32	0/3/3/3
168	GDP	PF	501	-	-	2/12/32/32	0/3/3/3
166	GTP	Mm	501	-	-	1/18/38/38	0/3/3/3
168	GDP	SZ	501	-	-	2/12/32/32	0/3/3/3
168	GDP	Uh	501	-	-	2/12/32/32	0/3/3/3
166	GTP	J3	501	-	-	4/18/38/38	0/3/3/3
166	GTP	JO	501	167	-	2/18/38/38	0/3/3/3
166	GTP	KV	501	167	-	3/18/38/38	0/3/3/3
168	GDP	Ld	501	-	-	3/12/32/32	0/3/3/3
168	GDP	ED	501	-	-	4/12/32/32	0/3/3/3
168	GDP	Vq	501	-	-	2/12/32/32	0/3/3/3
168	GDP	ID	501	-	-	2/12/32/32	0/3/3/3
166	GTP	EG	501	167	-	10/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
168	GDP	CJ	501	-	-	5/12/32/32	0/3/3/3
168	GDP	QR	501	-	-	1/12/32/32	0/3/3/3
168	GDP	MJ	501	-	-	6/12/32/32	0/3/3/3
166	GTP	Wd	501	167	-	5/18/38/38	0/3/3/3
166	GTP	MI	501	167	-	5/18/38/38	0/3/3/3
168	GDP	DH	501	-	-	4/12/32/32	0/3/3/3
168	GDP	OF	501	-	-	3/12/32/32	0/3/3/3
166	GTP	SN	501	167	-	6/18/38/38	0/3/3/3
166	GTP	AN	501	-	-	4/18/38/38	0/3/3/3
168	GDP	QN	501	-	-	4/12/32/32	0/3/3/3
166	GTP	Uz	501	-	-	2/18/38/38	0/3/3/3
168	GDP	DJ	501	-	-	4/12/32/32	0/3/3/3
166	GTP	CK	501	-	-	6/18/38/38	0/3/3/3
168	GDP	RJ	501	-	-	2/12/32/32	0/3/3/3
166	GTP	PC	501	-	-	5/18/38/38	0/3/3/3
166	GTP	Eb	501	-	-	3/18/38/38	0/3/3/3
168	GDP	KU	501	-	-	2/12/32/32	0/3/3/3
168	GDP	Ul	501	-	-	2/12/32/32	0/3/3/3
168	GDP	Tx	501	-	-	3/12/32/32	0/3/3/3
168	GDP	NF	501	-	-	2/12/32/32	0/3/3/3
168	GDP	Sr	501	-	-	3/12/32/32	0/3/3/3
166	GTP	AK	501	-	-	4/18/38/38	0/3/3/3
166	GTP	NA	502	167	-	5/18/38/38	0/3/3/3
166	GTP	RV	501	167	-	4/18/38/38	0/3/3/3
168	GDP	Vu	501	-	-	3/12/32/32	0/3/3/3
166	GTP	Ub	501	167	-	6/18/38/38	0/3/3/3
168	GDP	FB	501	-	-	2/12/32/32	0/3/3/3
168	GDP	WL	501	-	-	5/12/32/32	0/3/3/3
166	GTP	RI	501	167	-	6/18/38/38	0/3/3/3
166	GTP	S4	501	167	-	5/18/38/38	0/3/3/3
168	GDP	SU	501	-	-	3/12/32/32	0/3/3/3
166	GTP	Sg	501	167	-	8/18/38/38	0/3/3/3
168	GDP	EN	501	-	-	2/12/32/32	0/3/3/3
166	GTP	EI	501	167	-	8/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
166	GTP	FW	501	167	-	2/18/38/38	0/3/3/3
166	GTP	GK	501	-	-	7/18/38/38	0/3/3/3
166	GTP	SE	501	167	-	4/18/38/38	0/3/3/3
166	GTP	JM	502	167	-	5/18/38/38	0/3/3/3
168	GDP	S3	501	-	-	6/12/32/32	0/3/3/3
166	GTP	GC	501	167	-	5/18/38/38	0/3/3/3
166	GTP	U7	501	-	-	3/18/38/38	0/3/3/3
168	GDP	Sp	501	-	-	2/12/32/32	0/3/3/3
166	GTP	SK	501	167	-	3/18/38/38	0/3/3/3
168	GDP	Vs	501	-	-	2/12/32/32	0/3/3/3
168	GDP	Vh	501	-	-	2/12/32/32	0/3/3/3
166	GTP	CG	501	167	-	5/18/38/38	0/3/3/3
168	GDP	TZ	501	-	-	3/12/32/32	0/3/3/3
168	GDP	Q3	501	-	-	5/12/32/32	0/3/3/3
166	GTP	TO	501	167	-	5/18/38/38	0/3/3/3
168	GDP	DF	501	-	-	4/12/32/32	0/3/3/3
166	GTP	IE	501	-	-	3/18/38/38	0/3/3/3
166	GTP	WI	502	167	-	2/18/38/38	0/3/3/3
168	GDP	WD	501	-	-	5/12/32/32	0/3/3/3
168	GDP	Wg	501	-	-	3/12/32/32	0/3/3/3
166	GTP	Nw	501	-	-	8/18/38/38	0/3/3/3
168	GDP	Vm	501	-	-	2/12/32/32	0/3/3/3
168	GDP	WF	501	-	-	2/12/32/32	0/3/3/3
168	GDP	Nv	501	-	-	4/12/32/32	0/3/3/3
168	GDP	UH	501	-	-	0/12/32/32	0/3/3/3
166	GTP	LC	501	167	-	1/18/38/38	0/3/3/3
168	GDP	V8	501	-	-	1/12/32/32	0/3/3/3
166	GTP	N3	501	167	-	2/18/38/38	0/3/3/3
166	GTP	R2	501	167	-	5/18/38/38	0/3/3/3
166	GTP	KO	502	167	-	6/18/38/38	0/3/3/3
166	GTP	SP	501	167	-	4/18/38/38	0/3/3/3
166	GTP	Ur	501	167	-	3/18/38/38	0/3/3/3
168	GDP	DL	501	-	-	4/12/32/32	0/3/3/3
168	GDP	Uc	501	-	-	4/12/32/32	0/3/3/3
168	GDP	V0	501	-	-	2/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
166	GTP	HE	501	167	-	6/18/38/38	0/3/3/3
166	GTP	UR	501	167	-	8/18/38/38	0/3/3/3
166	GTP	Le	501	167	-	6/18/38/38	0/3/3/3
166	GTP	JC	501	167	-	2/18/38/38	0/3/3/3
168	GDP	O8	501	-	-	6/12/32/32	0/3/3/3
166	GTP	TC	501	167	-	5/18/38/38	0/3/3/3
166	GTP	LN	501	167	-	1/18/38/38	0/3/3/3
166	GTP	JG	501	167	-	4/18/38/38	0/3/3/3
166	GTP	FX	502	-	-	11/18/38/38	0/3/3/3
166	GTP	AC	501	-	-	5/18/38/38	0/3/3/3
166	GTP	PM	501	167	-	2/18/38/38	0/3/3/3
166	GTP	Q6	501	167	-	4/18/38/38	0/3/3/3
166	GTP	NO	501	-	-	10/18/38/38	0/3/3/3
168	GDP	J6	501	-	-	1/12/32/32	0/3/3/3
168	GDP	MQ	501	-	-	1/12/32/32	0/3/3/3
168	GDP	UQ	501	-	-	2/12/32/32	0/3/3/3
166	GTP	QG	501	-	-	2/18/38/38	0/3/3/3
168	GDP	Vj	501	-	-	4/12/32/32	0/3/3/3
168	GDP	KB	501	-	-	5/12/32/32	0/3/3/3
166	GTP	Wl	501	167	-	6/18/38/38	0/3/3/3
166	GTP	Vg	501	167	-	4/18/38/38	0/3/3/3
166	GTP	R0	501	167	-	7/18/38/38	0/3/3/3
168	GDP	JN	501	-	-	5/12/32/32	0/3/3/3
166	GTP	R6	502	167	-	2/18/38/38	0/3/3/3
168	GDP	NP	501	-	-	3/12/32/32	0/3/3/3
168	GDP	PN	501	-	-	3/12/32/32	0/3/3/3
168	GDP	RL	501	-	-	2/12/32/32	0/3/3/3
168	GDP	QS	501	-	-	3/12/32/32	0/3/3/3
168	GDP	UO	501	-	-	4/12/32/32	0/3/3/3
168	GDP	UU	501	-	-	2/12/32/32	0/3/3/3
166	GTP	VP	501	-	-	7/18/38/38	0/3/3/3
168	GDP	NJ	501	-	-	3/12/32/32	0/3/3/3
166	GTP	J5	501	-	-	8/18/38/38	0/3/3/3
168	GDP	Tr	501	-	-	5/12/32/32	0/3/3/3
166	GTP	TK	501	167	-	3/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
166	GTP	O9	502	167	-	3/18/38/38	0/3/3/3
166	GTP	DC	501	-	-	7/18/38/38	0/3/3/3
168	GDP	UF	501	-	-	1/12/32/32	0/3/3/3
166	GTP	UK	501	167	-	3/18/38/38	0/3/3/3
166	GTP	Sm	501	167	-	2/18/38/38	0/3/3/3
166	GTP	Mk	501	-	-	6/18/38/38	0/3/3/3
166	GTP	QX	501	167	-	5/18/38/38	0/3/3/3
166	GTP	T9	501	167	-	5/18/38/38	0/3/3/3
166	GTP	Uk	501	167	-	3/18/38/38	0/3/3/3
168	GDP	RN	501	-	-	1/12/32/32	0/3/3/3
166	GTP	Vt	501	167	-	5/18/38/38	0/3/3/3
168	GDP	DN	501	-	-	3/12/32/32	0/3/3/3
166	GTP	RT	501	-	-	2/18/38/38	0/3/3/3
166	GTP	WZ	501	167	-	6/18/38/38	0/3/3/3
168	GDP	TD	501	-	-	2/12/32/32	0/3/3/3
166	GTP	GR	501	167	-	3/18/38/38	0/3/3/3
168	GDP	SS	501	-	-	2/12/32/32	0/3/3/3
168	GDP	AD	501	-	-	1/12/32/32	0/3/3/3
166	GTP	CC	501	-	-	4/18/38/38	0/3/3/3
168	GDP	U1	501	-	-	1/12/32/32	0/3/3/3
166	GTP	VM	501	-	-	5/18/38/38	0/3/3/3
168	GDP	SO	501	-	-	2/12/32/32	0/3/3/3
168	GDP	Tb	501	-	-	4/12/32/32	0/3/3/3
166	GTP	VY	501	167	-	4/18/38/38	0/3/3/3
168	GDP	UL	501	-	-	2/12/32/32	0/3/3/3
166	GTP	Mo	501	167	-	6/18/38/38	0/3/3/3
166	GTP	Ny	501	167	-	4/18/38/38	0/3/3/3
168	GDP	J2	501	-	-	1/12/32/32	0/3/3/3
168	GDP	RB	501	-	-	1/12/32/32	0/3/3/3
168	GDP	Oz	501	-	-	4/12/32/32	0/3/3/3
166	GTP	Fr	501	-	-	6/18/38/38	0/3/3/3
166	GTP	CA	501	-	-	7/18/38/38	0/3/3/3
166	GTP	OQ	501	167	-	2/18/38/38	0/3/3/3
166	GTP	VG	501	167	-	5/18/38/38	0/3/3/3
168	GDP	Th	501	-	-	3/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
166	GTP	KS	501	167	-	8/18/38/38	0/3/3/3
168	GDP	Sh	501	-	-	4/12/32/32	0/3/3/3
166	GTP	EM	501	-	-	3/18/38/38	0/3/3/3
168	GDP	ON	501	-	-	4/12/32/32	0/3/3/3
168	GDP	LL	501	-	-	3/12/32/32	0/3/3/3
166	GTP	Wf	501	-	-	4/18/38/38	0/3/3/3
168	GDP	O6	501	-	-	4/12/32/32	0/3/3/3
168	GDP	HJ	501	-	-	5/12/32/32	0/3/3/3
166	GTP	DK	501	167	-	3/18/38/38	0/3/3/3
168	GDP	Tz	501	-	-	2/12/32/32	0/3/3/3
168	GDP	T2	501	-	-	2/12/32/32	0/3/3/3
166	GTP	PI	502	167	-	4/18/38/38	0/3/3/3
166	GTP	VC	501	167	-	3/18/38/38	0/3/3/3
168	GDP	GU	501	-	-	5/12/32/32	0/3/3/3
166	GTP	Vr	501	167	-	5/18/38/38	0/3/3/3
168	GDP	Sj	502	-	-	6/12/32/32	0/3/3/3
166	GTP	EE	501	-	-	7/18/38/38	0/3/3/3
166	GTP	DA	501	167	-	2/18/38/38	0/3/3/3
168	GDP	TH	501	-	-	2/12/32/32	0/3/3/3
166	GTP	GX	501	167	-	7/18/38/38	0/3/3/3
168	GDP	S5	501	-	-	6/12/32/32	0/3/3/3
166	GTP	II	502	167	-	5/18/38/38	0/3/3/3
168	GDP	SJ	501	-	-	2/12/32/32	0/3/3/3
168	GDP	OP	501	-	-	5/12/32/32	0/3/3/3
168	GDP	Uf	501	-	-	2/12/32/32	0/3/3/3
168	GDP	Bv	501	-	-	1/12/32/32	0/3/3/3
168	GDP	O0	501	-	-	2/12/32/32	0/3/3/3
168	GDP	TV	501	-	-	3/12/32/32	0/3/3/3
166	GTP	La	501	-	-	6/18/38/38	0/3/3/3
168	GDP	VZ	501	-	-	2/12/32/32	0/3/3/3
166	GTP	PE	501	-	-	8/18/38/38	0/3/3/3
166	GTP	P8	501	167	-	5/18/38/38	0/3/3/3
166	GTP	AA	501	167	-	6/18/38/38	0/3/3/3
166	GTP	Tq	501	167	-	7/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
168	GDP	FN	501	-	-	2/12/32/32	0/3/3/3
168	GDP	FV	501	-	-	4/12/32/32	0/3/3/3
166	GTP	HK	501	167	-	6/18/38/38	0/3/3/3
168	GDP	UD	501	-	-	3/12/32/32	0/3/3/3
166	GTP	Q4	501	167	-	4/18/38/38	0/3/3/3
166	GTP	PT	502	-	-	3/18/38/38	0/3/3/3
166	GTP	VA	501	167	-	3/18/38/38	0/3/3/3
166	GTP	VN	501	167	-	3/18/38/38	0/3/3/3
166	GTP	UZ	501	-	-	5/18/38/38	0/3/3/3
168	GDP	V4	501	-	-	2/12/32/32	0/3/3/3
166	GTP	Ta	501	167	-	9/18/38/38	0/3/3/3
168	GDP	RF	501	-	-	2/12/32/32	0/3/3/3
168	GDP	Ec	501	-	-	4/12/32/32	0/3/3/3
168	GDP	JR	501	-	-	4/12/32/32	0/3/3/3
168	GDP	JB	501	-	-	4/12/32/32	0/3/3/3
166	GTP	Ss	501	167	-	2/18/38/38	0/3/3/3
166	GTP	Ut	501	167	-	5/18/38/38	0/3/3/3
166	GTP	NG	501	-	-	5/18/38/38	0/3/3/3
166	GTP	Sa	501	167	-	4/18/38/38	0/3/3/3
168	GDP	UB	501	-	-	2/12/32/32	0/3/3/3
168	GDP	WY	501	-	-	4/12/32/32	0/3/3/3
166	GTP	RQ	501	-	-	4/18/38/38	0/3/3/3
168	GDP	LJ	501	-	-	3/12/32/32	0/3/3/3
168	GDP	MF	501	-	-	4/12/32/32	0/3/3/3
166	GTP	MR	501	167	-	3/18/38/38	0/3/3/3
166	GTP	N1	501	167	-	4/18/38/38	0/3/3/3
168	GDP	Ea	501	-	-	5/12/32/32	0/3/3/3
166	GTP	PQ	501	-	-	6/18/38/38	0/3/3/3
168	GDP	ND	501	-	-	2/12/32/32	0/3/3/3
168	GDP	AL	501	-	-	1/12/32/32	0/3/3/3
168	GDP	AH	501	-	-	1/12/32/32	0/3/3/3
168	GDP	UY	501	-	-	4/12/32/32	0/3/3/3
168	GDP	FX	501	-	-	2/12/32/32	0/3/3/3
168	GDP	CF	501	-	-	3/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
166	GTP	RE	501	-	-	4/18/38/38	0/3/3/3
166	GTP	VK	501	167	-	4/18/38/38	0/3/3/3
168	GDP	GL	501	-	-	5/12/32/32	0/3/3/3
168	GDP	ML	501	-	-	8/12/32/32	0/3/3/3
168	GDP	DD	501	-	-	4/12/32/32	0/3/3/3
168	GDP	P5	501	-	-	2/12/32/32	0/3/3/3
168	GDP	TF	501	-	-	3/12/32/32	0/3/3/3
168	GDP	Tv	501	-	-	5/12/32/32	0/3/3/3
168	GDP	TA	501	-	-	6/12/32/32	0/3/3/3
168	GDP	TJ	501	-	-	3/12/32/32	0/3/3/3
166	GTP	MG	501	167	-	5/18/38/38	0/3/3/3
166	GTP	IG	501	167	-	2/18/38/38	0/3/3/3
168	GDP	HH	501	-	-	3/12/32/32	0/3/3/3
166	GTP	SY	501	167	-	5/18/38/38	0/3/3/3
166	GTP	UA	501	-	-	3/18/38/38	0/3/3/3
168	GDP	QW	501	-	-	2/12/32/32	0/3/3/3
168	GDP	Uj	501	-	-	2/12/32/32	0/3/3/3
168	GDP	Uy	501	-	-	1/12/32/32	0/3/3/3
168	GDP	V2	501	-	-	2/12/32/32	0/3/3/3
166	GTP	DI	501	167	-	5/18/38/38	0/3/3/3
166	GTP	HR	502	167	-	2/18/38/38	0/3/3/3
168	GDP	We	501	-	-	5/12/32/32	0/3/3/3
166	GTP	S6	501	167	-	9/18/38/38	0/3/3/3
166	GTP	DE	501	167	-	1/18/38/38	0/3/3/3
166	GTP	PA	501	167	-	4/18/38/38	0/3/3/3
166	GTP	LE	501	167	-	7/18/38/38	0/3/3/3
168	GDP	PD	501	-	-	2/12/32/32	0/3/3/3
168	GDP	Tn	501	-	-	2/12/32/32	0/3/3/3
166	GTP	Ns	501	-	-	8/18/38/38	0/3/3/3
166	GTP	J9	501	-	-	2/18/38/38	0/3/3/3
168	GDP	Bp	501	-	-	5/12/32/32	0/3/3/3
168	GDP	Tt	501	-	-	6/12/32/32	0/3/3/3
168	GDP	JP	501	-	-	5/12/32/32	0/3/3/3
166	GTP	EW	501	-	-	3/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
168	GDP	TX	501	-	-	4/12/32/32	0/3/3/3
166	GTP	IP	501	167	-	2/18/38/38	0/3/3/3
168	GDP	JF	501	-	-	3/12/32/32	0/3/3/3
166	GTP	PO	502	-	-	5/18/38/38	0/3/3/3
166	GTP	Q8	501	167	-	7/18/38/38	0/3/3/3
168	GDP	BF	501	-	-	3/12/32/32	0/3/3/3
166	GTP	Sz	501	167	-	8/18/38/38	0/3/3/3
166	GTP	BG	501	167	-	6/18/38/38	0/3/3/3
168	GDP	JL	501	-	-	3/12/32/32	0/3/3/3
166	GTP	BC	501	-	-	5/18/38/38	0/3/3/3
166	GTP	Bw	501	-	-	3/18/38/38	0/3/3/3
166	GTP	GT	501	-	-	5/18/38/38	0/3/3/3
166	GTP	T5	501	-	-	6/18/38/38	0/3/3/3
166	GTP	SV	501	-	-	5/18/38/38	0/3/3/3
168	GDP	WO	501	-	-	4/12/32/32	0/3/3/3
166	GTP	GI	501	167	-	5/18/38/38	0/3/3/3
168	GDP	NH	501	-	-	3/12/32/32	0/3/3/3
166	GTP	Te	501	167	-	6/18/38/38	0/3/3/3
168	GDP	KH	501	-	-	6/12/32/32	0/3/3/3
166	GTP	BE	501	167	-	3/18/38/38	0/3/3/3
166	GTP	WG	501	-	-	6/18/38/38	0/3/3/3
166	GTP	U5	501	167	-	7/18/38/38	0/3/3/3
166	GTP	QV	501	167	-	4/18/38/38	0/3/3/3
168	GDP	Fu	501	-	-	4/12/32/32	0/3/3/3
166	GTP	O1	501	167	-	8/18/38/38	0/3/3/3
168	GDP	JH	501	-	-	5/12/32/32	0/3/3/3
168	GDP	LO	501	-	-	4/12/32/32	0/3/3/3
166	GTP	FI	501	167	-	5/18/38/38	0/3/3/3
168	GDP	MD	501	-	-	4/12/32/32	0/3/3/3
166	GTP	MN	501	167	-	6/18/38/38	0/3/3/3
168	GDP	IQ	501	-	-	3/12/32/32	0/3/3/3
168	GDP	SM	501	-	-	2/12/32/32	0/3/3/3
166	GTP	FK	501	167	-	3/18/38/38	0/3/3/3
168	GDP	Ws	501	-	-	4/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
166	GTP	TY	501	167	-	6/18/38/38	0/3/3/3
168	GDP	EH	501	-	-	2/12/32/32	0/3/3/3
166	GTP	Ty	502	167	-	5/18/38/38	0/3/3/3
168	GDP	WS	501	-	-	1/12/32/32	0/3/3/3
168	GDP	RS	501	-	-	2/12/32/32	0/3/3/3
168	GDP	Uw	501	-	-	3/12/32/32	0/3/3/3
166	GTP	Su	501	-	-	2/18/38/38	0/3/3/3
168	GDP	SQ	501	-	-	2/12/32/32	0/3/3/3
168	GDP	S9	501	-	-	3/12/32/32	0/3/3/3
166	GTP	FG	501	167	-	3/18/38/38	0/3/3/3
166	GTP	VE	501	167	-	7/18/38/38	0/3/3/3
166	GTP	TE	501	167	-	3/18/38/38	0/3/3/3
168	GDP	QJ	501	-	-	0/12/32/32	0/3/3/3
168	GDP	Tp	501	-	-	5/12/32/32	0/3/3/3
168	GDP	Mj	501	-	-	3/12/32/32	0/3/3/3
168	GDP	LZ	501	-	-	4/12/32/32	0/3/3/3
168	GDP	QU	501	-	-	6/12/32/32	0/3/3/3
168	GDP	QP	501	-	-	2/12/32/32	0/3/3/3
168	GDP	J8	501	-	-	1/12/32/32	0/3/3/3
168	GDP	EF	501	-	-	4/12/32/32	0/3/3/3
166	GTP	HM	501	-	-	5/18/38/38	0/3/3/3
166	GTP	UT	501	167	-	7/18/38/38	0/3/3/3
166	GTP	SG	501	-	-	7/18/38/38	0/3/3/3
166	GTP	LM	502	167	-	7/18/38/38	0/3/3/3
166	GTP	RO	501	-	-	3/18/38/38	0/3/3/3
168	GDP	PP	501	-	-	4/12/32/32	0/3/3/3
168	GDP	KL	501	-	-	3/12/32/32	0/3/3/3
168	GDP	Vo	501	-	-	2/12/32/32	0/3/3/3
166	GTP	KE	501	167	-	5/18/38/38	0/3/3/3
168	GDP	BD	501	-	-	0/12/32/32	0/3/3/3
166	GTP	BK	501	167	-	3/18/38/38	0/3/3/3
166	GTP	MK	501	167	-	5/18/38/38	0/3/3/3
166	GTP	WA	501	167	-	4/18/38/38	2/3/3/3
168	GDP	T6	501	-	-	3/12/32/32	0/3/3/3
168	GDP	QD	501	-	-	0/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
166	GTP	WE	501	167	-	5/18/38/38	0/3/3/3
166	GTP	TG	501	167	-	3/18/38/38	0/3/3/3
166	GTP	WP	501	167	-	4/18/38/38	0/3/3/3
168	GDP	MH	501	-	-	7/12/32/32	0/3/3/3
166	GTP	R8	501	167	-	6/18/38/38	0/3/3/3
168	GDP	O2	501	-	-	6/12/32/32	0/3/3/3
168	GDP	EJ	501	-	-	4/12/32/32	0/3/3/3
166	GTP	TM	501	167	-	4/18/38/38	0/3/3/3
166	GTP	OG	501	-	-	6/18/38/38	0/3/3/3
166	GTP	Wb	502	167	-	3/18/38/38	0/3/3/3
166	GTP	AE	501	-	-	6/18/38/38	0/3/3/3
166	GTP	LY	501	167	-	4/18/38/38	0/3/3/3
166	GTP	U2	501	167	-	3/18/38/38	0/3/3/3
166	GTP	U9	501	-	-	4/18/38/38	0/3/3/3
168	GDP	UJ	501	-	-	0/12/32/32	0/3/3/3
168	GDP	VH	501	-	-	5/12/32/32	0/3/3/3
168	GDP	OJ	501	-	-	5/12/32/32	0/3/3/3
166	GTP	OE	501	167	-	4/18/38/38	0/3/3/3
166	GTP	Vv	501	167	-	4/18/38/38	0/3/3/3
168	GDP	GD	501	-	-	4/12/32/32	0/3/3/3
168	GDP	Sv	501	-	-	2/12/32/32	0/3/3/3
166	GTP	Q0	501	167	-	4/18/38/38	0/3/3/3
168	GDP	GH	501	-	-	5/12/32/32	0/3/3/3
168	GDP	LH	501	-	-	4/12/32/32	0/3/3/3
166	GTP	Vk	501	167	-	4/18/38/38	0/3/3/3
166	GTP	Sc	501	167	-	3/18/38/38	0/3/3/3
168	GDP	AB	501	-	-	1/12/32/32	0/3/3/3
168	GDP	HB	501	-	-	3/12/32/32	0/3/3/3
168	GDP	VF	501	-	1/1/6/6	4/12/32/32	2/3/3/3
168	GDP	V6	501	-	-	1/12/32/32	0/3/3/3
166	GTP	Mq	501	-	-	5/18/38/38	0/3/3/3
166	GTP	CE	501	-	-	3/18/38/38	0/3/3/3
168	GDP	KN	501	-	-	5/12/32/32	0/3/3/3
166	GTP	So	502	167	-	2/18/38/38	0/3/3/3
168	GDP	MB	501	-	-	7/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
166	GTP	WR	501	-	-	4/18/38/38	0/3/3/3
168	GDP	Tf	501	-	-	3/12/32/32	0/3/3/3
166	GTP	Ms	501	-	-	6/18/38/38	0/3/3/3
166	GTP	P6	501	-	-	2/18/38/38	0/3/3/3
168	GDP	VL	501	-	-	5/12/32/32	0/3/3/3
166	GTP	NM	502	167	-	5/18/38/38	0/3/3/3
168	GDP	OB	501	-	-	4/12/32/32	0/3/3/3
166	GTP	JS	501	167	-	4/18/38/38	0/3/3/3
166	GTP	TQ	501	167	-	0/18/38/38	0/3/3/3
166	GTP	Ug	501	-	-	5/18/38/38	0/3/3/3
166	GTP	Ve	501	-	-	5/18/38/38	0/3/3/3
168	GDP	HQ	501	-	-	4/12/32/32	0/3/3/3
168	GDP	VJ	501	-	-	2/12/32/32	0/3/3/3
166	GTP	T1	501	-	-	8/18/38/38	0/3/3/3
166	GTP	Vx	501	167	-	5/18/38/38	0/3/3/3
166	GTP	QT	501	167	-	4/18/38/38	0/3/3/3
168	GDP	SL	501	-	-	1/12/32/32	0/3/3/3
168	GDP	R1	501	-	-	3/12/32/32	0/3/3/3
166	GTP	UE	501	167	-	5/18/38/38	0/3/3/3
166	GTP	P0	501	167	-	1/18/38/38	0/3/3/3
168	GDP	PB	501	-	-	3/12/32/32	0/3/3/3
168	GDP	Vb	501	-	-	2/12/32/32	0/3/3/3
168	GDP	Us	501	-	-	4/12/32/32	0/3/3/3
166	GTP	MP	501	167	-	2/18/38/38	0/3/3/3
166	GTP	Sq	501	167	-	3/18/38/38	0/3/3/3
166	GTP	DM	501	167	-	4/18/38/38	0/3/3/3
166	GTP	WC	501	167	-	4/18/38/38	0/3/3/3
168	GDP	VB	501	-	-	4/12/32/32	0/3/3/3
166	GTP	WX	501	-	-	7/18/38/38	0/3/3/3
166	GTP	UM	502	167	-	5/18/38/38	0/3/3/3
168	GDP	SX	501	-	-	4/12/32/32	0/3/3/3
166	GTP	WK	501	167	-	7/18/38/38	0/3/3/3
166	GTP	KC	501	167	-	5/18/38/38	0/3/3/3
168	GDP	Q9	501	-	-	4/12/32/32	0/3/3/3
166	GTP	BI	501	-	-	7/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
168	GDP	LD	501	-	-	4/12/32/32	0/3/3/3
168	GDP	TP	501	-	-	3/12/32/32	0/3/3/3
166	GTP	S0	501	167	-	4/18/38/38	0/3/3/3
168	GDP	HN	501	-	-	3/12/32/32	0/3/3/3
168	GDP	WQ	501	-	-	2/12/32/32	0/3/3/3
166	GTP	QQ	502	167	-	4/18/38/38	0/3/3/3
168	GDP	HD	501	-	-	3/12/32/32	0/3/3/3
168	GDP	Mr	501	-	-	3/12/32/32	0/3/3/3
166	GTP	R4	501	167	-	6/18/38/38	0/3/3/3
168	GDP	VQ	501	-	-	5/12/32/32	0/3/3/3
168	GDP	Bx	501	-	-	3/12/32/32	0/3/3/3
166	GTP	GM	501	167	-	6/18/38/38	0/3/3/3
166	GTP	RA	501	167	-	8/18/38/38	0/3/3/3
166	GTP	Tm	501	167	-	1/18/38/38	0/3/3/3
168	GDP	TR	501	-	-	4/12/32/32	0/3/3/3
166	GTP	GV	501	167	-	4/18/38/38	0/3/3/3
168	GDP	J0	501	-	-	1/12/32/32	0/3/3/3
168	GDP	GN	501	-	-	2/12/32/32	0/3/3/3
168	GDP	BB	501	-	-	5/12/32/32	0/3/3/3
166	GTP	FE	501	167	-	2/18/38/38	0/3/3/3
168	GDP	N2	501	-	-	3/12/32/32	0/3/3/3
168	GDP	VD	501	-	-	2/12/32/32	0/3/3/3
168	GDP	VW	501	-	-	2/12/32/32	0/3/3/3
168	GDP	Nr	501	-	-	4/12/32/32	0/3/3/3
168	GDP	Mt	501	-	-	1/12/32/32	0/3/3/3
166	GTP	Wr	501	167	-	7/18/38/38	0/3/3/3
168	GDP	U6	501	-	-	1/12/32/32	0/3/3/3
168	GDP	Mp	501	-	-	5/12/32/32	0/3/3/3
166	GTP	RK	501	-	-	2/18/38/38	0/3/3/3
168	GDP	Q5	501	-	-	5/12/32/32	0/3/3/3
168	GDP	NN	501	-	-	2/12/32/32	0/3/3/3
166	GTP	FM	501	167	-	5/18/38/38	0/3/3/3
166	GTP	UI	501	167	-	8/18/38/38	0/3/3/3
166	GTP	LK	501	167	-	6/18/38/38	0/3/3/3
166	GTP	Li	501	167	-	4/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
168	GDP	Lf	501	-	-	3/12/32/32	0/3/3/3
166	GTP	Nu	501	167	-	2/18/38/38	0/3/3/3
166	GTP	ST	501	-	-	4/18/38/38	0/3/3/3
168	GDP	BL	501	-	-	4/12/32/32	0/3/3/3
166	GTP	LI	501	167	-	6/18/38/38	0/3/3/3
168	GDP	RU	501	-	-	4/12/32/32	0/3/3/3
168	GDP	IL	501	-	-	2/12/32/32	0/3/3/3
166	GTP	S2	501	167	-	7/18/38/38	0/3/3/3
168	GDP	WJ	501	-	-	2/12/32/32	0/3/3/3
168	GDP	Wc	501	-	-	2/12/32/32	0/3/3/3
166	GTP	Si	501	167	-	3/18/38/38	0/3/3/3
168	GDP	Wk	501	-	-	2/12/32/32	0/3/3/3
168	GDP	GO	501	-	-	3/12/32/32	0/3/3/3
166	GTP	JK	501	-	-	3/18/38/38	0/3/3/3
166	GTP	AR	501	-	-	5/18/38/38	0/3/3/3
166	GTP	VR	501	167	-	6/18/38/38	0/3/3/3
166	GTP	TI	502	167	-	4/18/38/38	0/3/3/3
168	GDP	VO	501	-	-	2/12/32/32	0/3/3/3
168	GDP	P7	501	-	-	3/12/32/32	0/3/3/3
166	GTP	DG	501	-	-	8/18/38/38	0/3/3/3
168	GDP	Un	501	-	-	3/12/32/32	0/3/3/3
166	GTP	Wn	501	-	-	5/18/38/38	0/3/3/3
168	GDP	FF	501	-	-	5/12/32/32	0/3/3/3
166	GTP	CI	501	-	-	4/18/38/38	0/3/3/3
166	GTP	WM	501	167	-	4/18/38/38	0/3/3/3
168	GDP	Vw	501	-	-	2/12/32/32	0/3/3/3
168	GDP	IJ	501	-	-	3/12/32/32	0/3/3/3
168	GDP	KP	501	-	-	3/12/32/32	0/3/3/3
166	GTP	Lg	501	167	-	7/18/38/38	0/3/3/3
166	GTP	QK	501	167	-	3/18/38/38	0/3/3/3
166	GTP	UN	501	167	-	6/18/38/38	0/3/3/3
166	GTP	UV	501	167	-	3/18/38/38	0/3/3/3
168	GDP	FL	501	-	-	3/12/32/32	0/3/3/3
166	GTP	HP	501	167	-	6/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
168	GDP	PU	501	-	-	5/12/32/32	0/3/3/3
168	GDP	TL	501	-	-	2/12/32/32	0/3/3/3
166	GTP	NK	501	167	-	5/18/38/38	0/3/3/3
168	GDP	SB	501	-	-	3/12/32/32	0/3/3/3
166	GTP	Tu	501	167	-	6/18/38/38	0/3/3/3
168	GDP	VS	501	-	-	1/12/32/32	0/3/3/3
166	GTP	Ft	501	-	-	6/18/38/38	0/3/3/3
166	GTP	O5	501	167	-	9/18/38/38	0/3/3/3
168	GDP	SF	501	-	-	6/12/32/32	0/3/3/3
168	GDP	Wa	501	-	-	5/12/32/32	0/3/3/3
168	GDP	KJ	501	-	-	3/12/32/32	0/3/3/3
168	GDP	R3	501	-	-	3/12/32/32	0/3/3/3
168	GDP	MO	501	-	-	6/12/32/32	0/3/3/3
166	GTP	JE	501	167	-	2/18/38/38	0/3/3/3
168	GDP	R7	501	-	-	3/12/32/32	0/3/3/3
166	GTP	V1	501	167	-	6/18/38/38	0/3/3/3
166	GTP	QE	501	167	-	4/18/38/38	0/3/3/3
166	GTP	GB	501	-	-	2/18/38/38	0/3/3/3
168	GDP	PJ	501	-	-	2/12/32/32	0/3/3/3
168	GDP	QF	501	-	-	1/12/32/32	0/3/3/3
168	GDP	St	501	-	-	2/12/32/32	0/3/3/3
168	GDP	Uu	501	-	-	1/12/32/32	0/3/3/3
166	GTP	Mu	501	-	-	1/18/38/38	0/3/3/3
168	GDP	WH	501	-	-	4/12/32/32	0/3/3/3
166	GTP	KQ	501	167	-	4/18/38/38	0/3/3/3
166	GTP	Lk	501	167	-	8/18/38/38	0/3/3/3
168	GDP	PS	501	-	-	4/12/32/32	0/3/3/3
166	GTP	Ux	501	-	-	3/18/38/38	0/3/3/3
166	GTP	QA	501	-	-	4/18/38/38	0/3/3/3
168	GDP	WB	501	-	-	3/12/32/32	0/3/3/3
166	GTP	GE	501	167	-	4/18/38/38	0/3/3/3
166	GTP	KG	501	167	-	6/18/38/38	0/3/3/3
166	GTP	Fv	501	167	-	8/18/38/38	0/3/3/3
166	GTP	TW	501	167	-	1/18/38/38	0/3/3/3
166	GTP	AI	501	-	-	1/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
168	GDP	Nx	501	-	-	4/12/32/32	0/3/3/3
166	GTP	SI	501	167	-	4/18/38/38	0/3/3/3
168	GDP	CL	501	-	-	6/12/32/32	0/3/3/3
166	GTP	QC	501	167	-	5/18/38/38	0/3/3/3
168	GDP	O4	501	-	-	4/12/32/32	0/3/3/3
166	GTP	KI	501	167	-	10/18/38/38	0/3/3/3
168	GDP	QL	501	-	-	0/12/32/32	0/3/3/3
168	GDP	SD	501	-	-	2/12/32/32	0/3/3/3
168	GDP	Q7	501	-	-	5/12/32/32	0/3/3/3
166	GTP	Wj	501	167	-	2/18/38/38	0/3/3/3
166	GTP	LR	501	167	-	7/18/38/38	0/3/3/3
168	GDP	QB	501	-	-	5/12/32/32	0/3/3/3
168	GDP	Tl	501	-	-	2/12/32/32	0/3/3/3
168	GDP	RD	501	-	-	4/12/32/32	0/3/3/3
168	GDP	KD	501	-	-	3/12/32/32	0/3/3/3
168	GDP	AX	501	-	-	1/12/32/32	0/3/3/3
166	GTP	QM	501	-	-	5/18/38/38	0/3/3/3
168	GDP	EL	501	-	-	4/12/32/32	0/3/3/3
166	GTP	To	501	167	-	3/18/38/38	0/3/3/3
166	GTP	T3	501	167	-	4/18/38/38	0/3/3/3
166	GTP	IM	501	167	-	3/18/38/38	0/3/3/3
166	GTP	Tk	501	167	-	5/18/38/38	0/3/3/3
168	GDP	PH	501	-	-	3/12/32/32	0/3/3/3
166	GTP	Lc	501	167	-	3/18/38/38	0/3/3/3
168	GDP	GF	501	-	-	3/12/32/32	0/3/3/3
166	GTP	OI	501	-	-	3/18/38/38	0/3/3/3
166	GTP	QI	501	-	-	3/18/38/38	0/3/3/3
166	GTP	VI	502	167	-	6/18/38/38	0/3/3/3
166	GTP	UG	501	167	-	5/18/38/38	0/3/3/3
166	GTP	O3	501	-	-	7/18/38/38	0/3/3/3
168	GDP	US	501	-	-	3/12/32/32	0/3/3/3
168	GDP	IF	501	-	-	2/12/32/32	0/3/3/3
168	GDP	IH	501	-	-	4/12/32/32	0/3/3/3
166	GTP	WN	501	167	-	0/18/38/38	0/3/3/3
166	GTP	Tc	502	167	-	7/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
168	GDP	Up	501	-	-	2/12/32/32	0/3/3/3
166	GTP	EK	501	167	-	4/18/38/38	0/3/3/3
166	GTP	IK	501	167	-	7/18/38/38	0/3/3/3
168	GDP	FJ	501	-	-	2/12/32/32	0/3/3/3
166	GTP	NE	501	167	-	2/18/38/38	0/3/3/3
168	GDP	U3	502	-	-	2/12/32/32	0/3/3/3
168	GDP	Fs	501	-	-	3/12/32/32	0/3/3/3
166	GTP	QO	501	167	-	5/18/38/38	0/3/3/3
168	GDP	Wq	501	-	-	1/12/32/32	0/3/3/3
168	GDP	Vf	501	-	-	1/12/32/32	0/3/3/3
166	GTP	FU	501	-	-	8/18/38/38	0/3/3/3
166	GTP	PK	501	167	-	3/18/38/38	0/3/3/3
166	GTP	KK	502	167	-	7/18/38/38	0/3/3/3
166	GTP	IC	501	-	-	5/18/38/38	0/3/3/3
168	GDP	Sn	501	-	-	4/12/32/32	0/3/3/3
166	GTP	IR	501	167	-	2/18/38/38	0/3/3/3
168	GDP	AM	501	-	-	1/12/32/32	0/3/3/3
168	GDP	VU	501	-	-	2/12/32/32	0/3/3/3
166	GTP	FC	501	-	-	3/18/38/38	0/3/3/3
166	GTP	MM	501	167	-	7/18/38/38	0/3/3/3
168	GDP	R9	501	-	-	5/12/32/32	0/3/3/3
166	GTP	NI	501	167	-	4/18/38/38	0/3/3/3
168	GDP	R5	501	-	-	3/12/32/32	0/3/3/3
168	GDP	FD	501	-	-	4/12/32/32	0/3/3/3
166	GTP	Ue	501	167	-	1/18/38/38	0/3/3/3
166	GTP	MC	501	167	-	5/18/38/38	0/3/3/3

The worst 5 of 1005 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
168	VF	501	GDP	C5-C6	327.90	8.13	1.47
166	WA	501	GTP	C5-C6	307.57	7.71	1.47
168	VF	501	GDP	C5-C4	173.31	5.86	1.43
166	WA	501	GTP	C5-C4	166.67	5.69	1.43
168	VF	501	GDP	C5'-C4'	138.35	5.82	1.51

The worst 5 of 3919 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
168	VF	501	GDP	C8-N7-C5	-50.69	6.44	102.99
166	WA	501	GTP	C8-N7-C5	-49.09	9.50	102.99
168	VF	501	GDP	O5'-C5'-C4'	-25.71	20.48	108.99
168	VF	501	GDP	O4'-C4'-C5'	-25.23	26.35	109.37
166	WA	501	GTP	O5'-C5'-C4'	-24.77	23.73	108.99

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
168	VF	501	GDP	C4'

5 of 2657 torsion outliers are listed below:

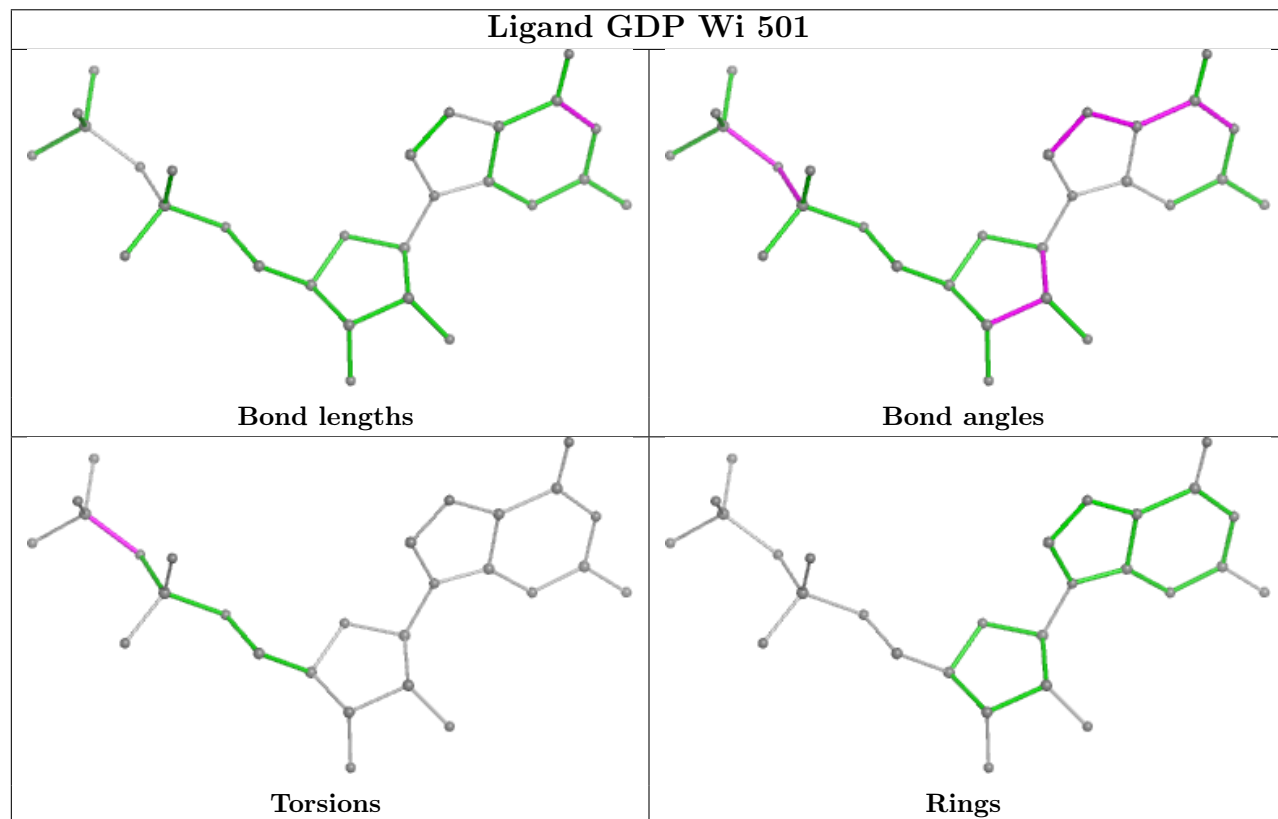
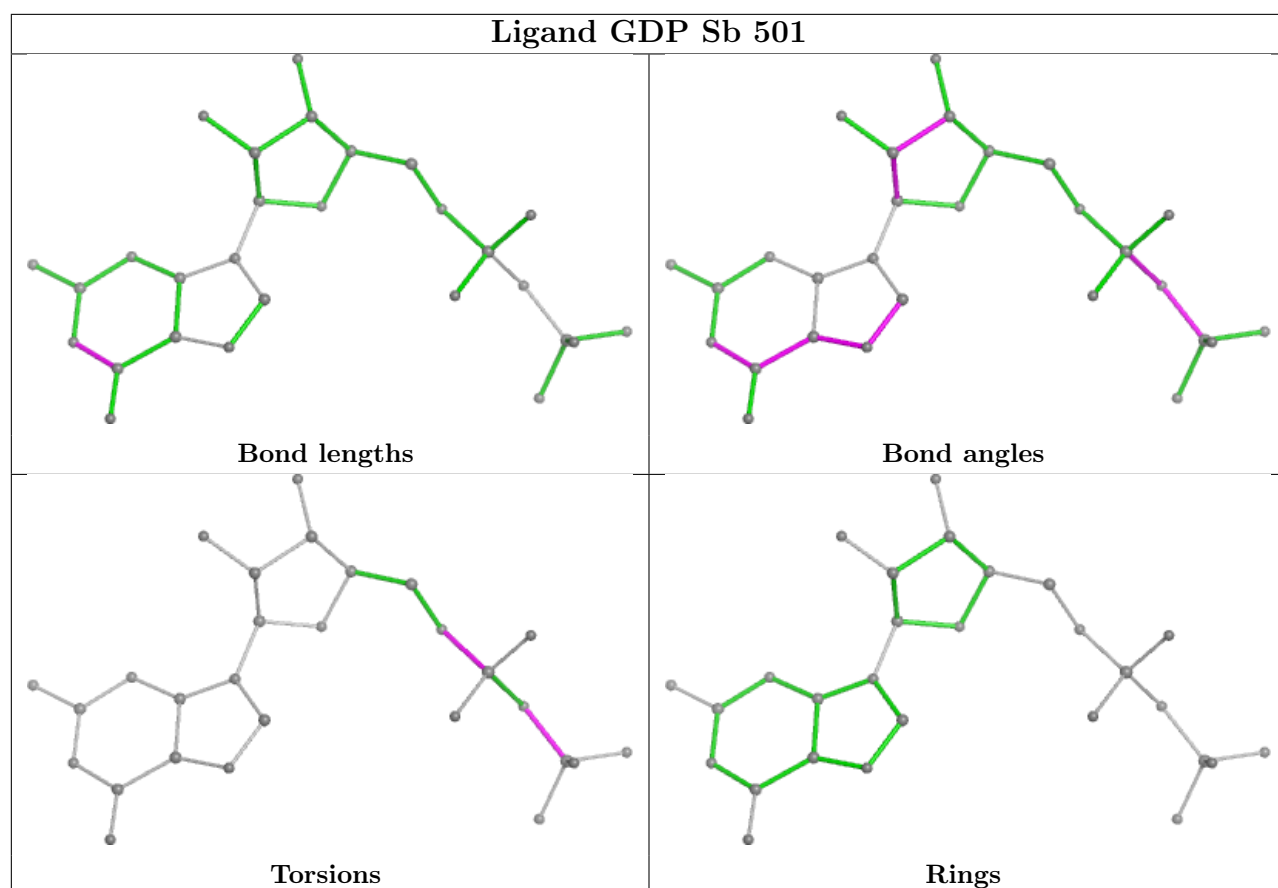
Mol	Chain	Res	Type	Atoms
166	AA	501	GTP	C5'-O5'-PA-O1A
166	AA	501	GTP	C5'-O5'-PA-O2A
166	AC	501	GTP	C5'-O5'-PA-O3A
166	AC	501	GTP	C5'-O5'-PA-O2A
166	AC	501	GTP	C3'-C4'-C5'-O5'

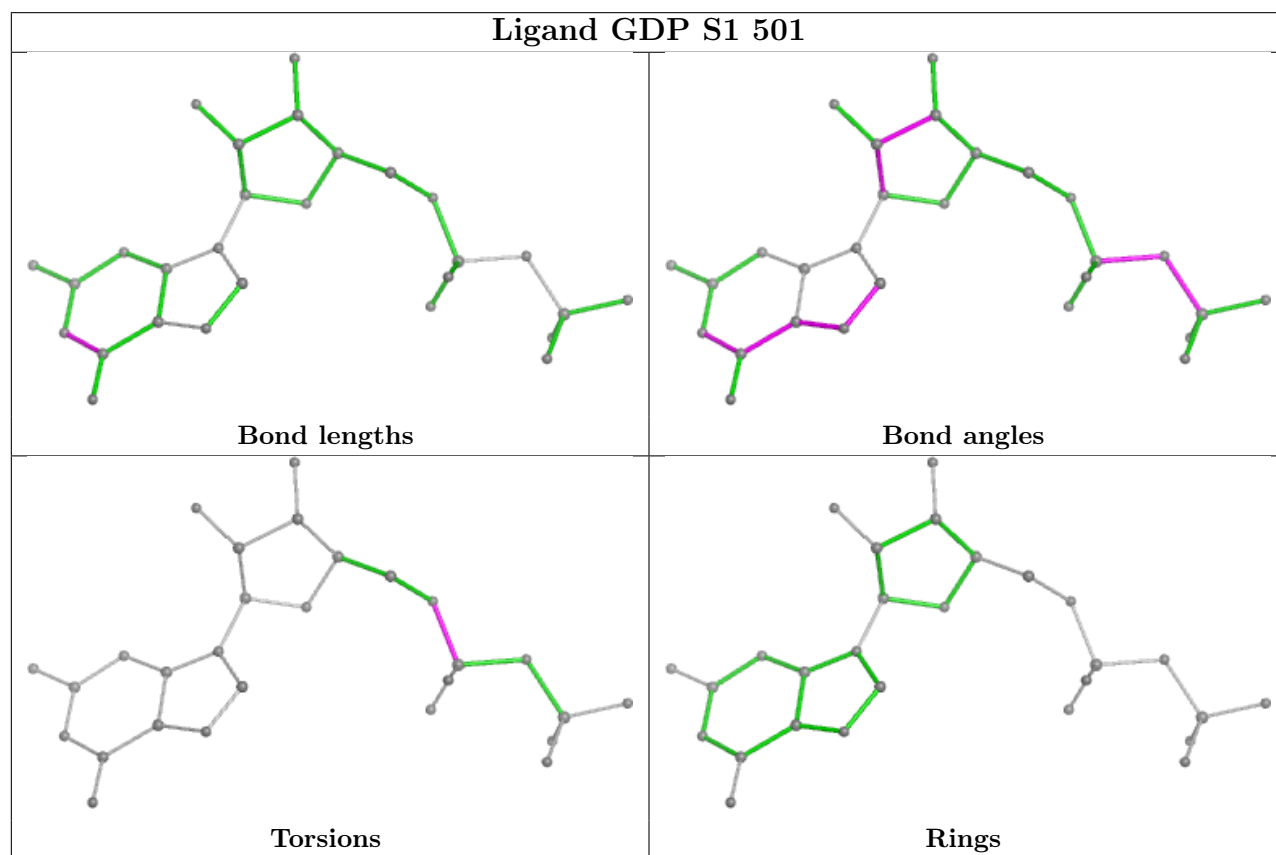
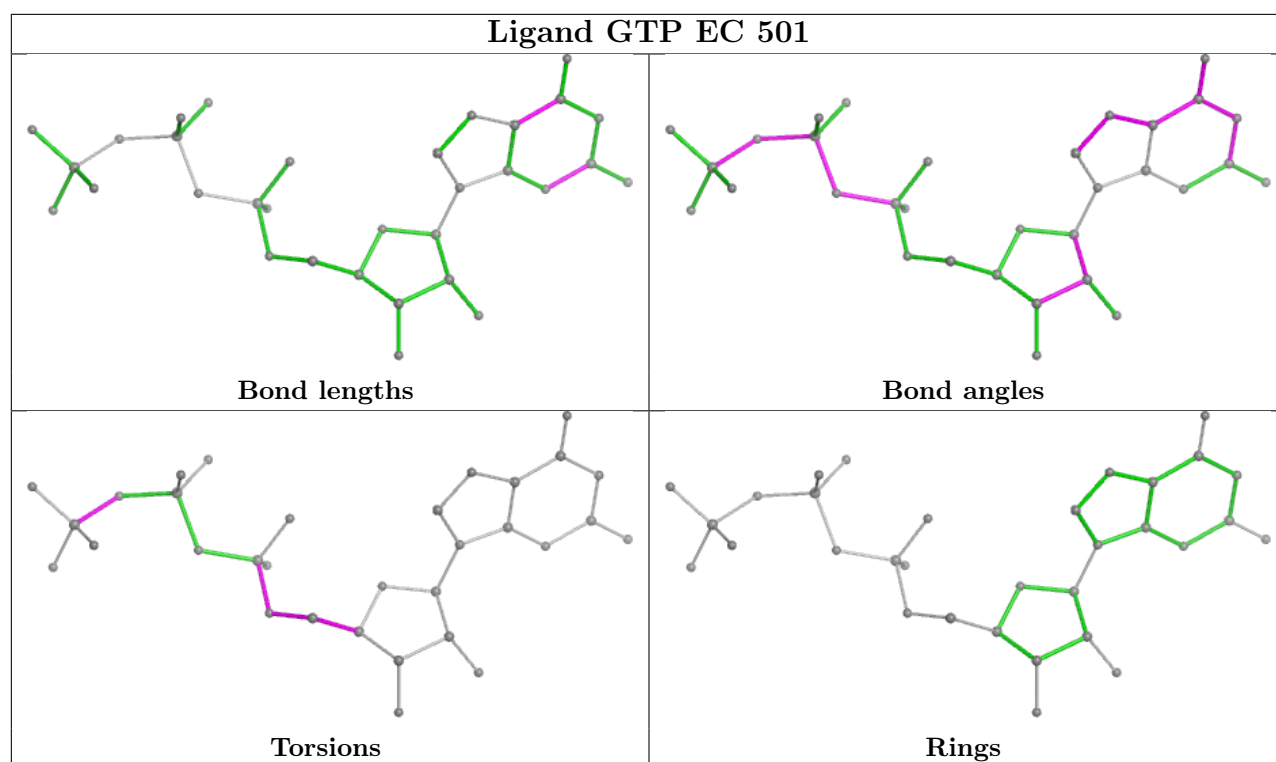
All (4) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
168	VF	501	GDP	C2-C4-C5-C6-N1-N3
166	WA	501	GTP	C2-C4-C5-C6-N1-N3
166	WA	501	GTP	C4-C5-C8-N7-N9
168	VF	501	GDP	C4-C5-C8-N7-N9

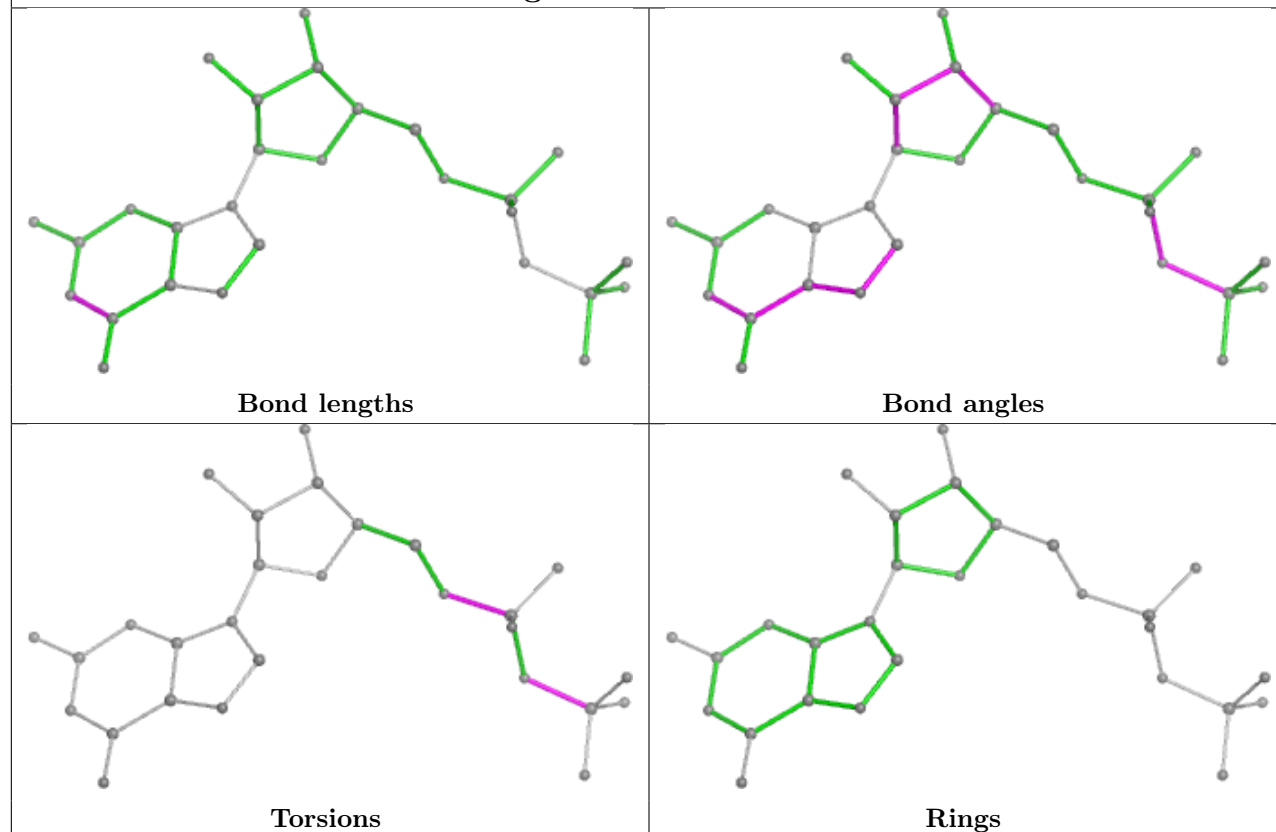
No monomer is involved in short contacts.

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.

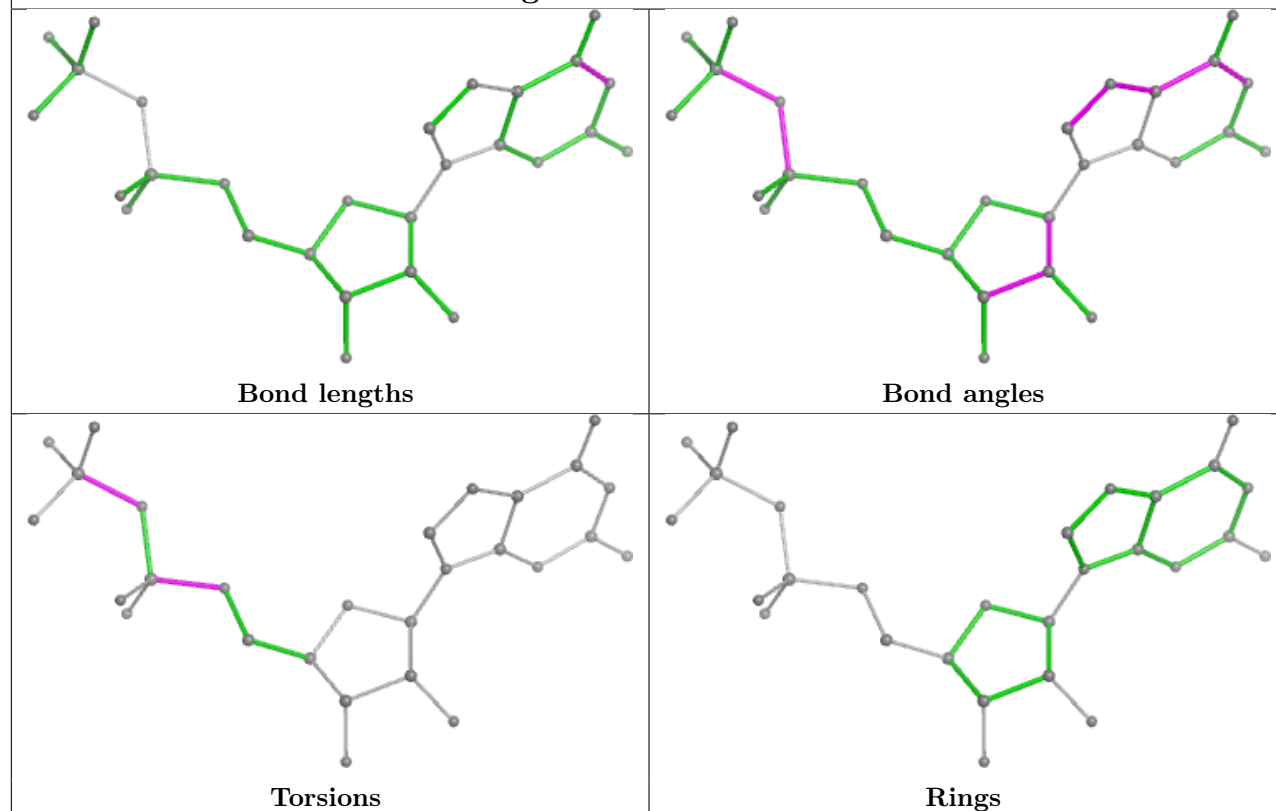


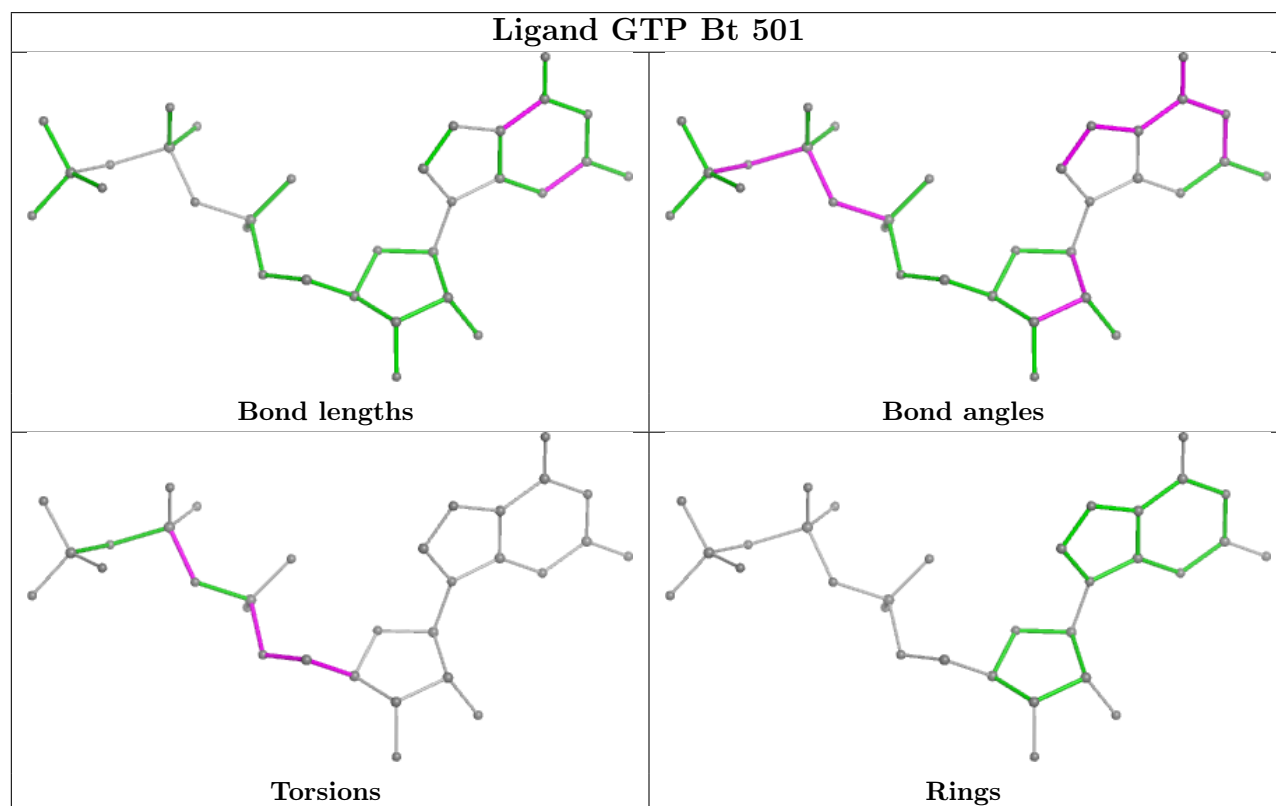
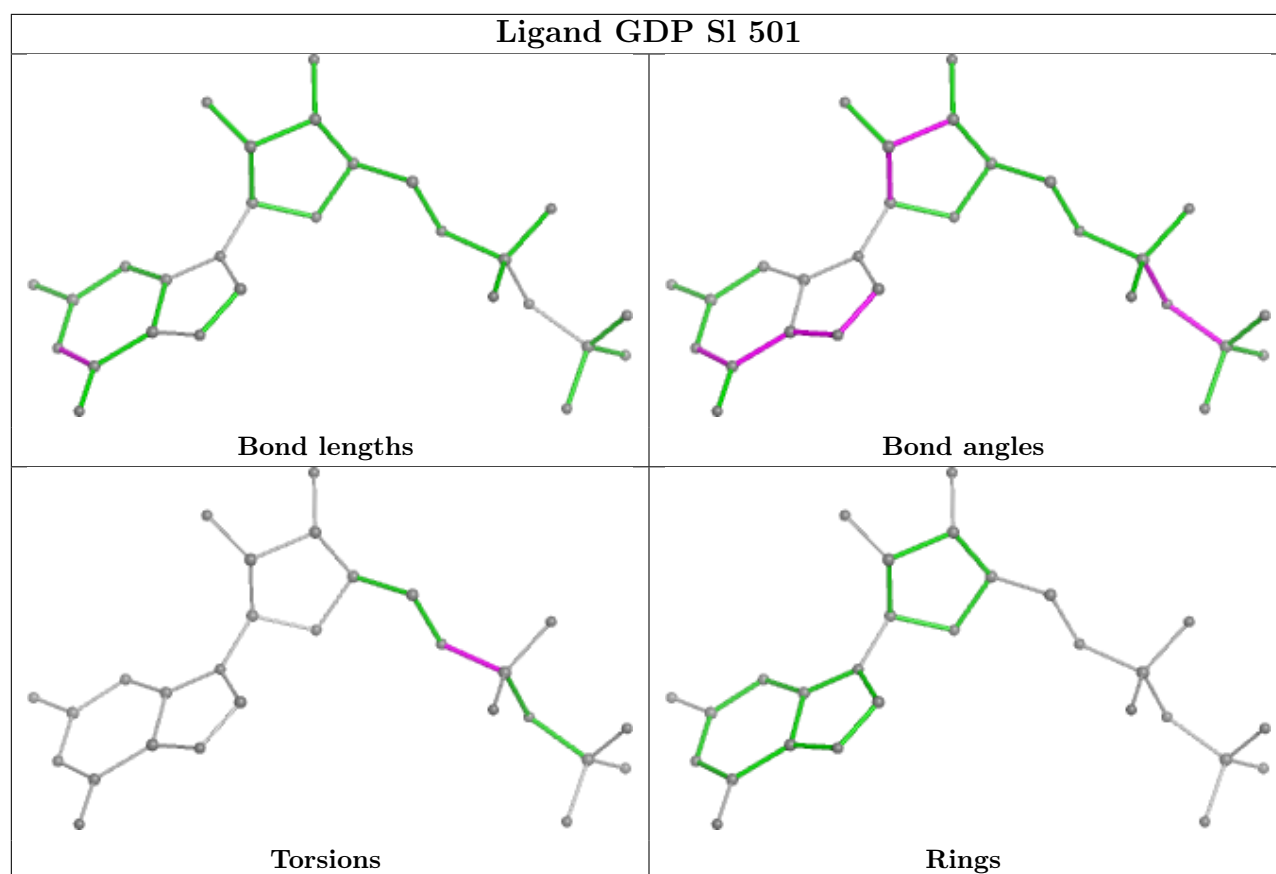


## Ligand GDP JJ 501

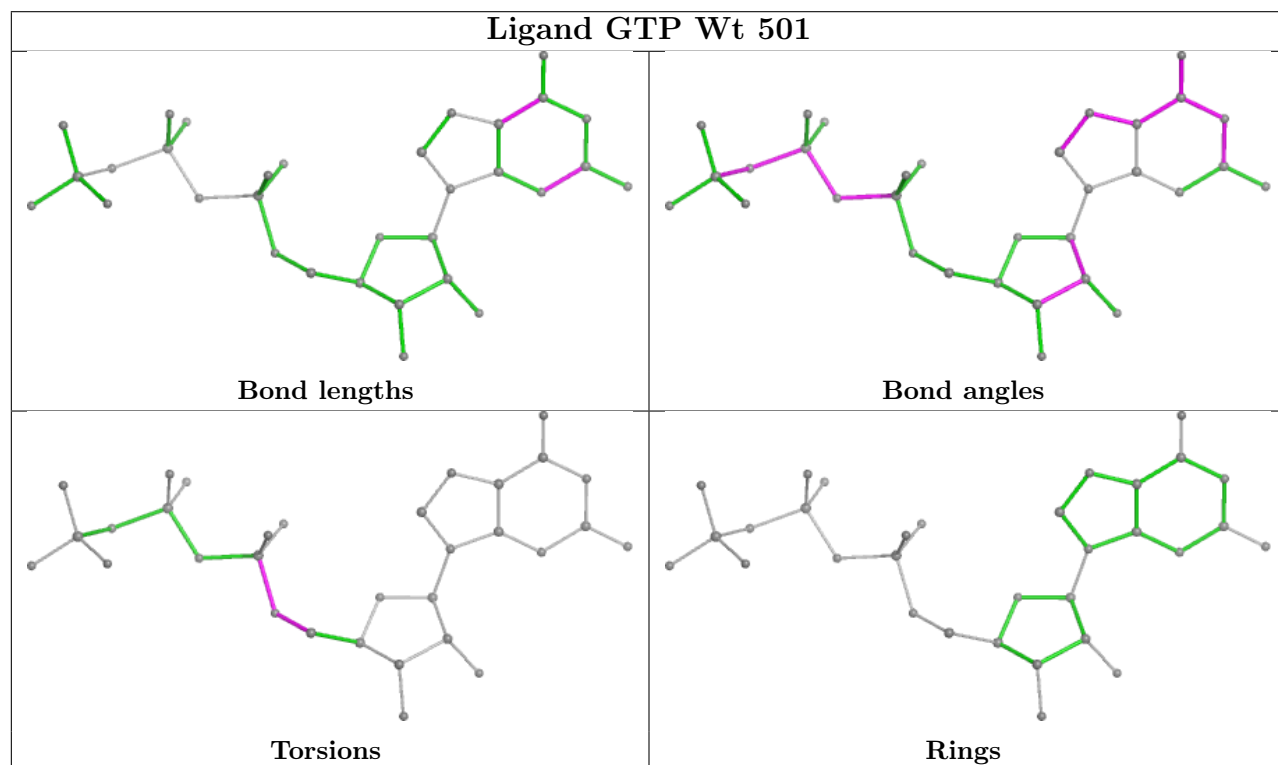
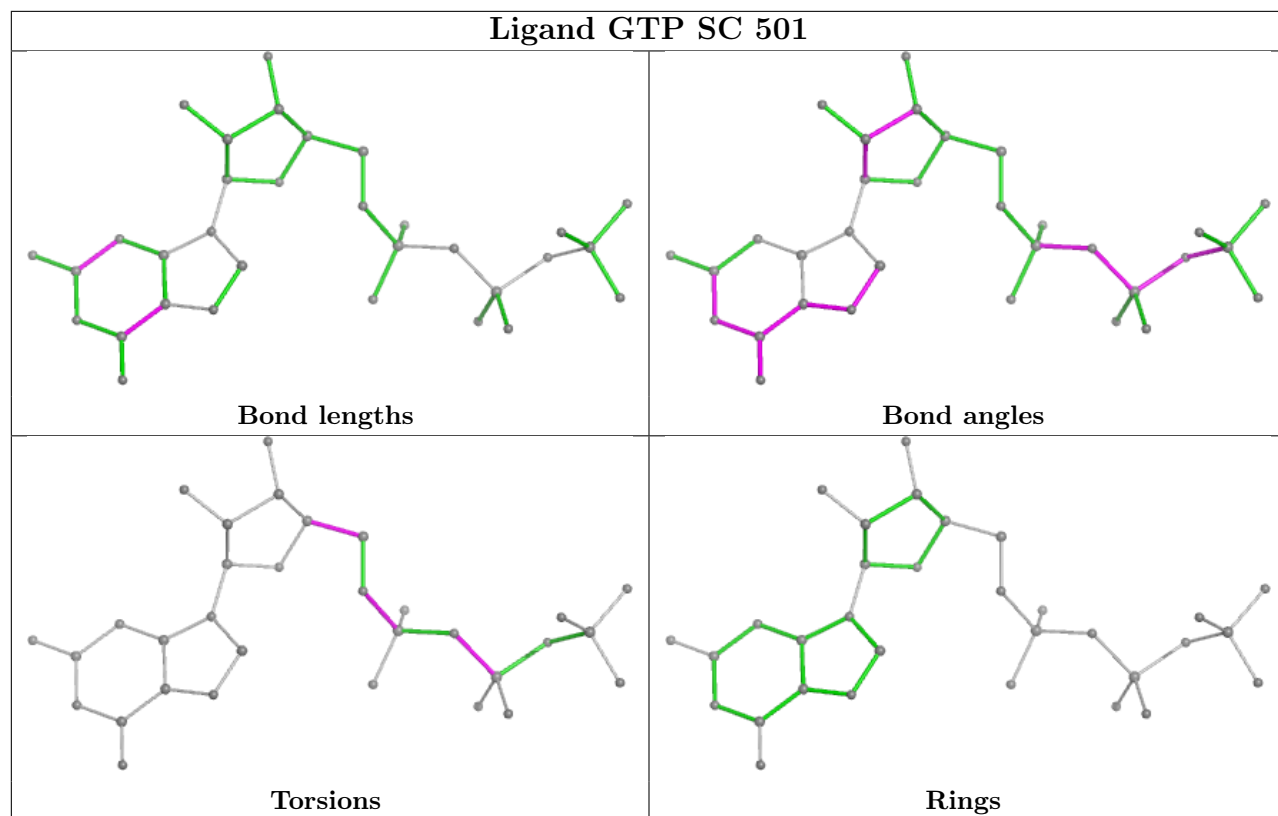


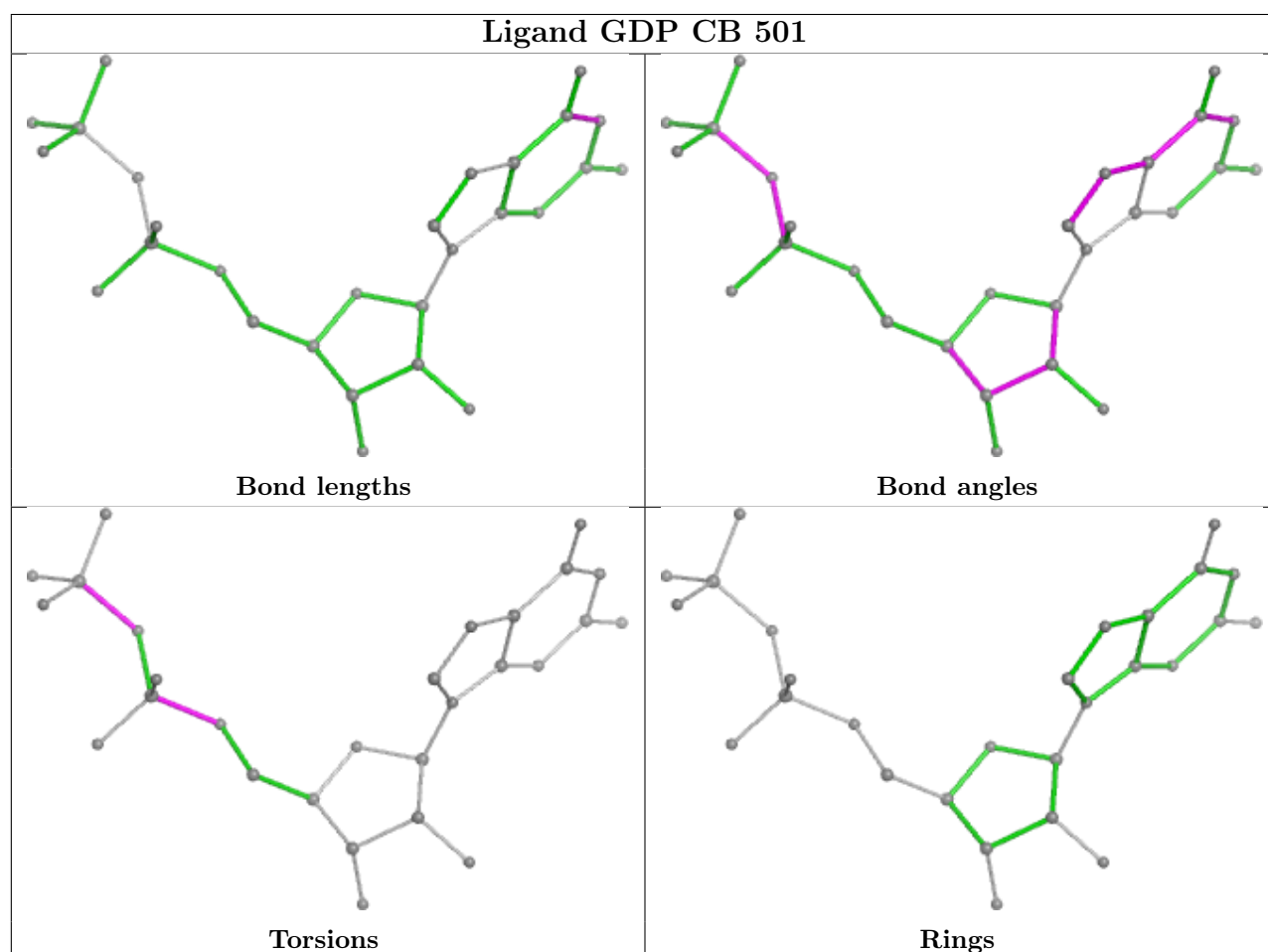
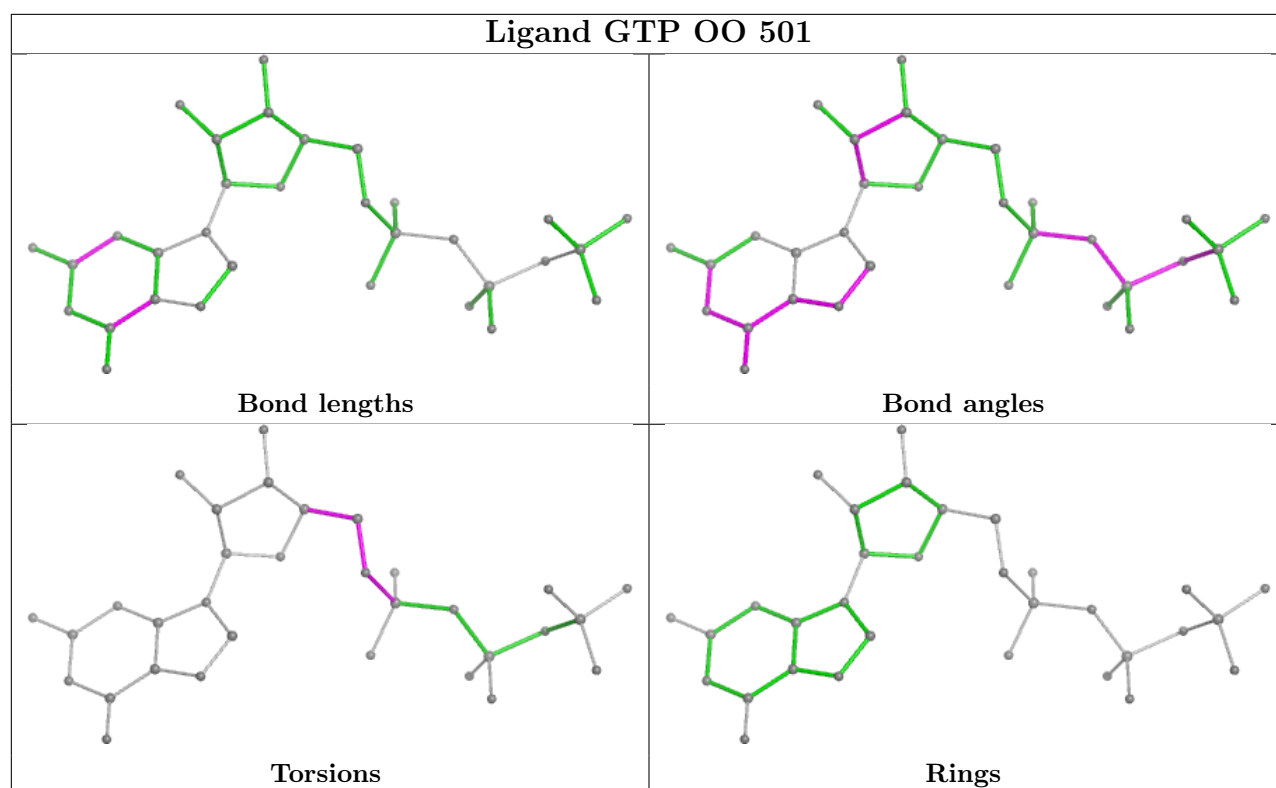
## Ligand GDP Lh 501

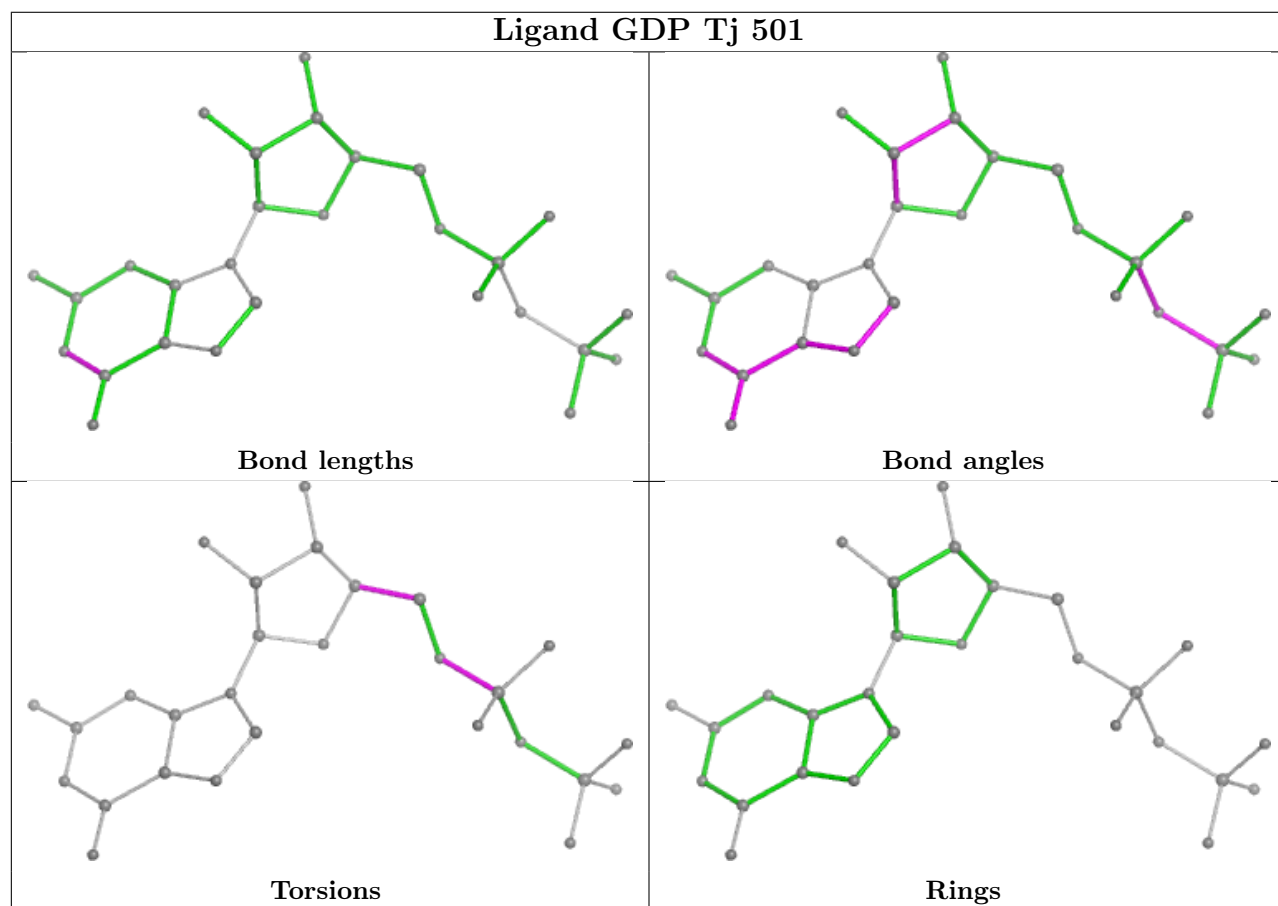
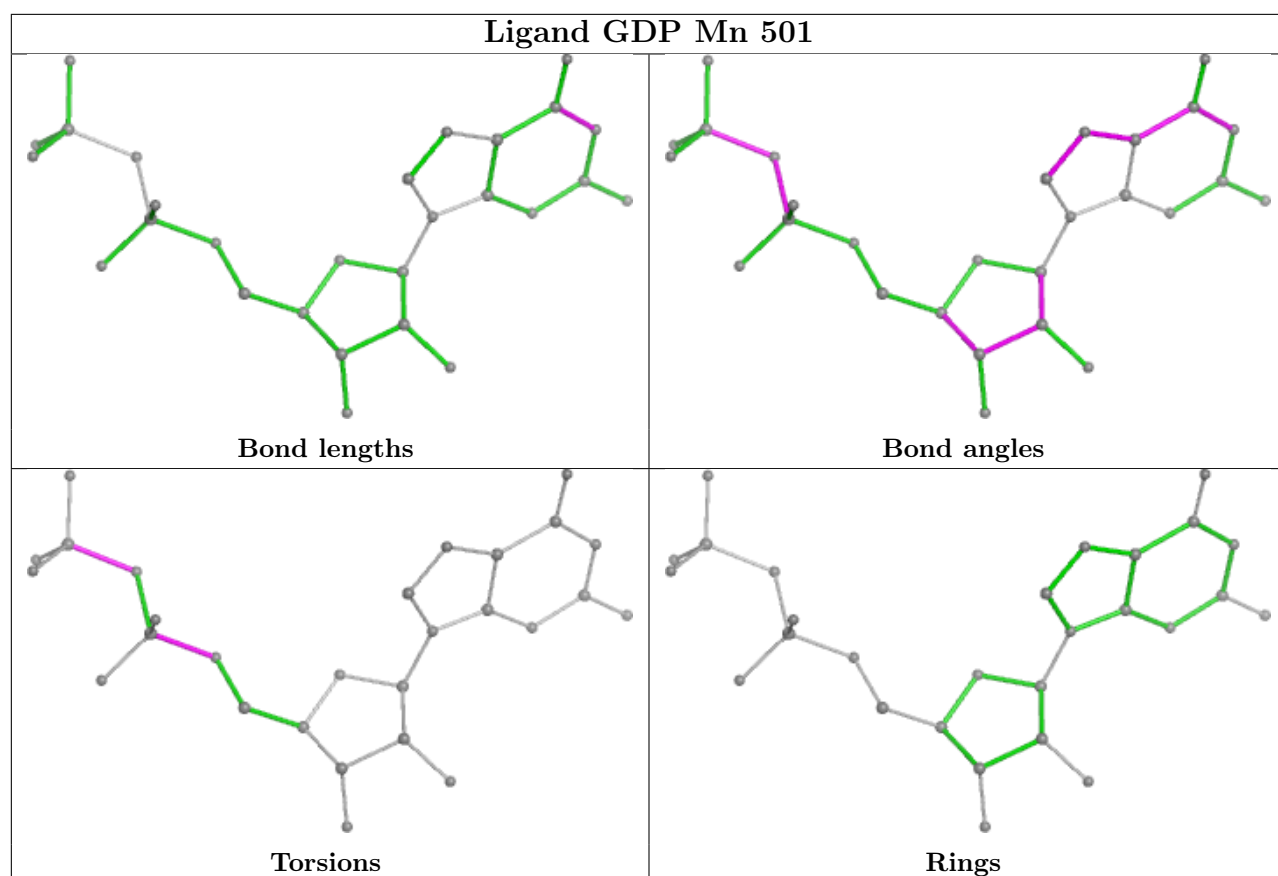


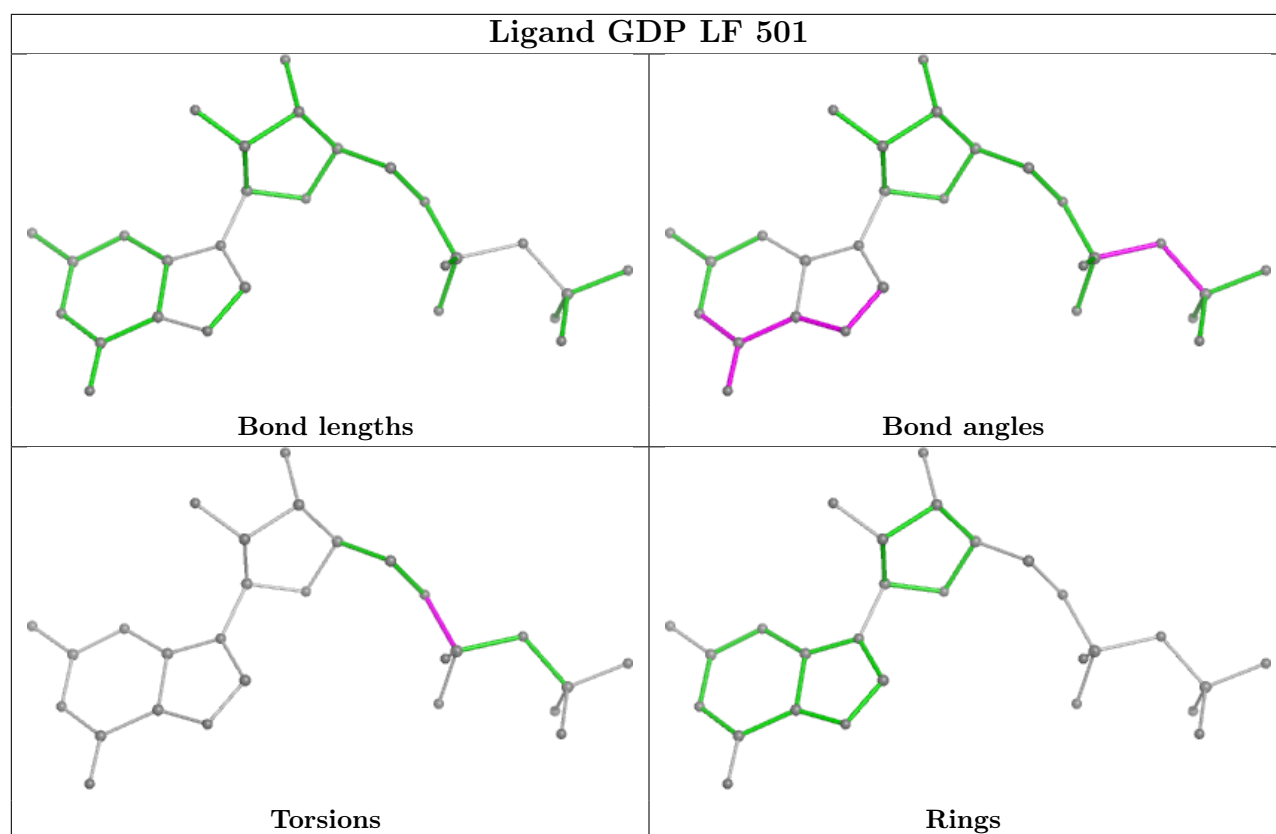




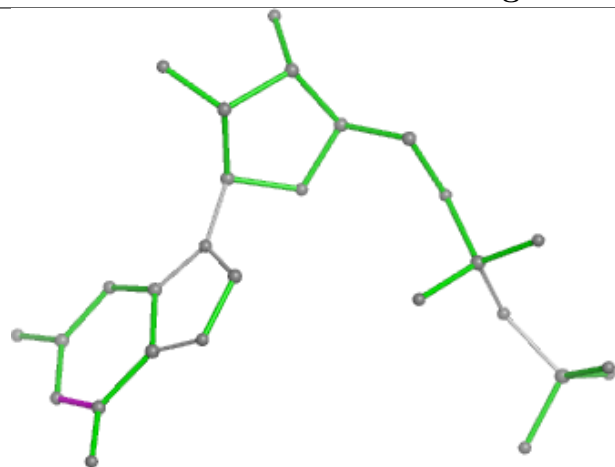




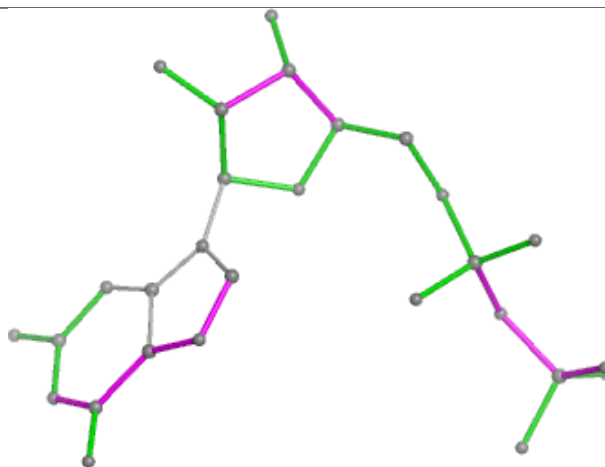




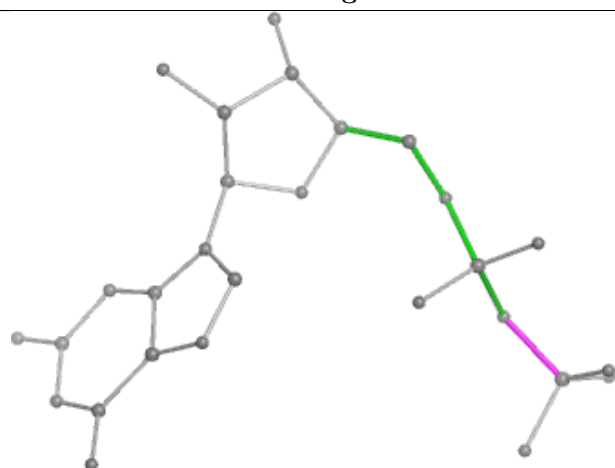
## Ligand GDP SH 501



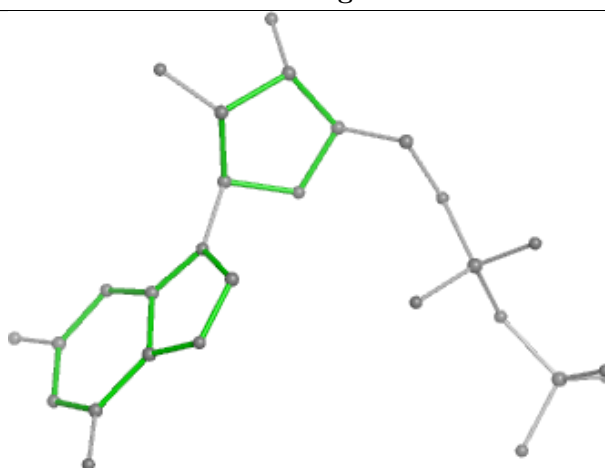
Bond lengths



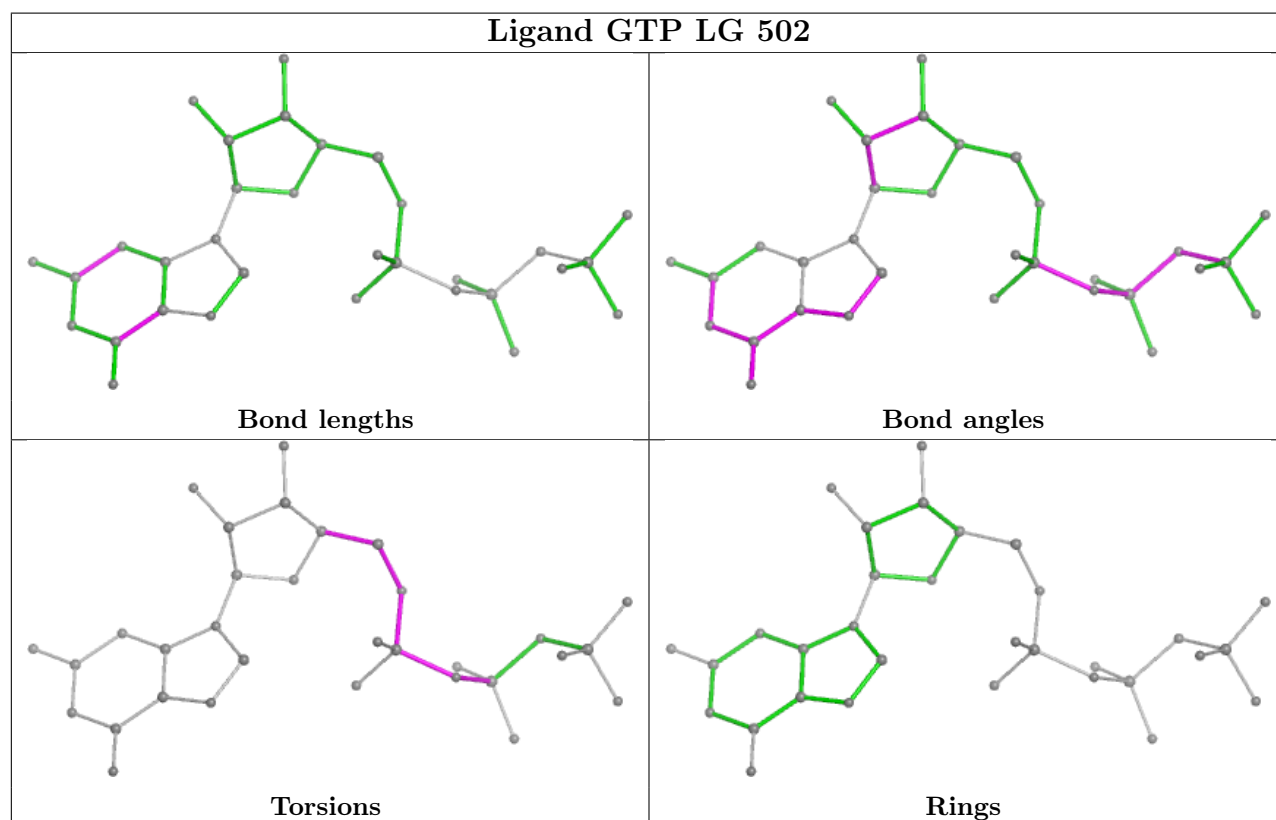
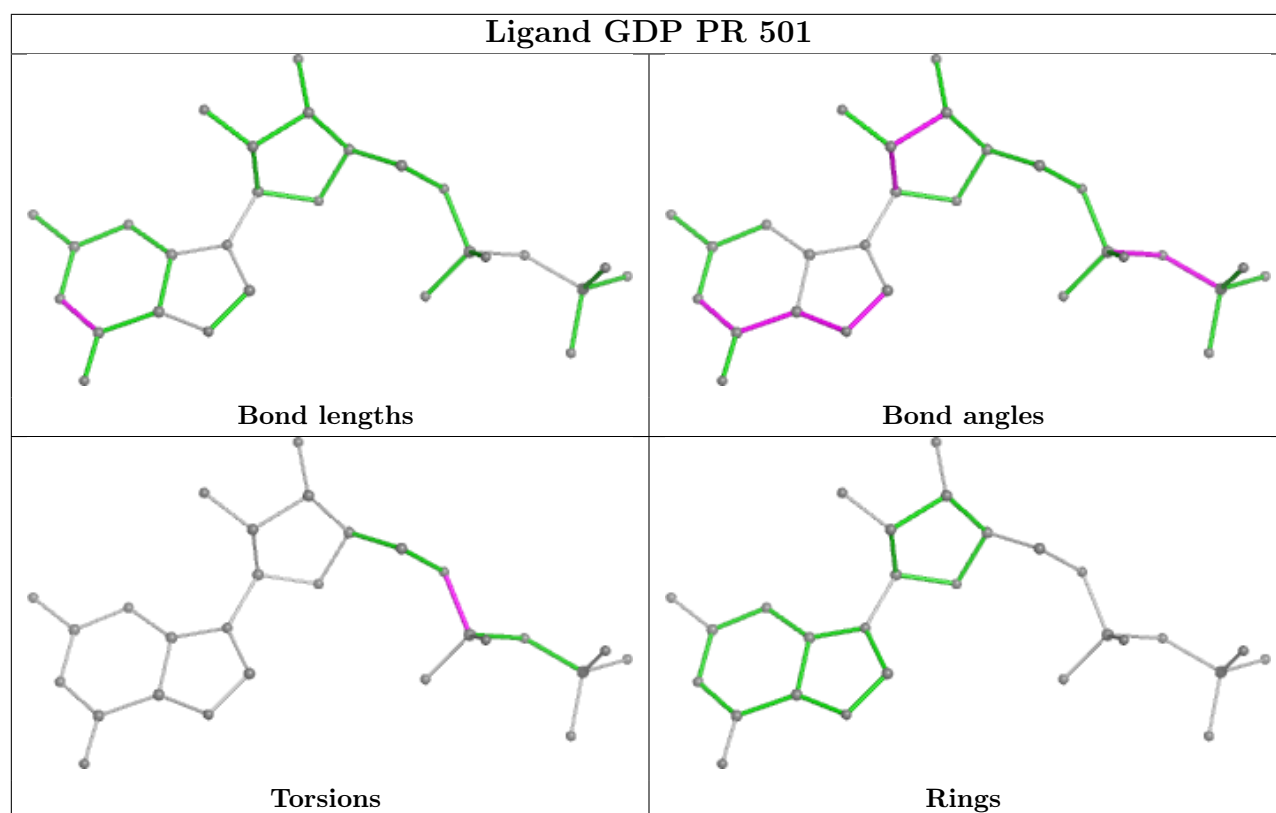
Bond angles



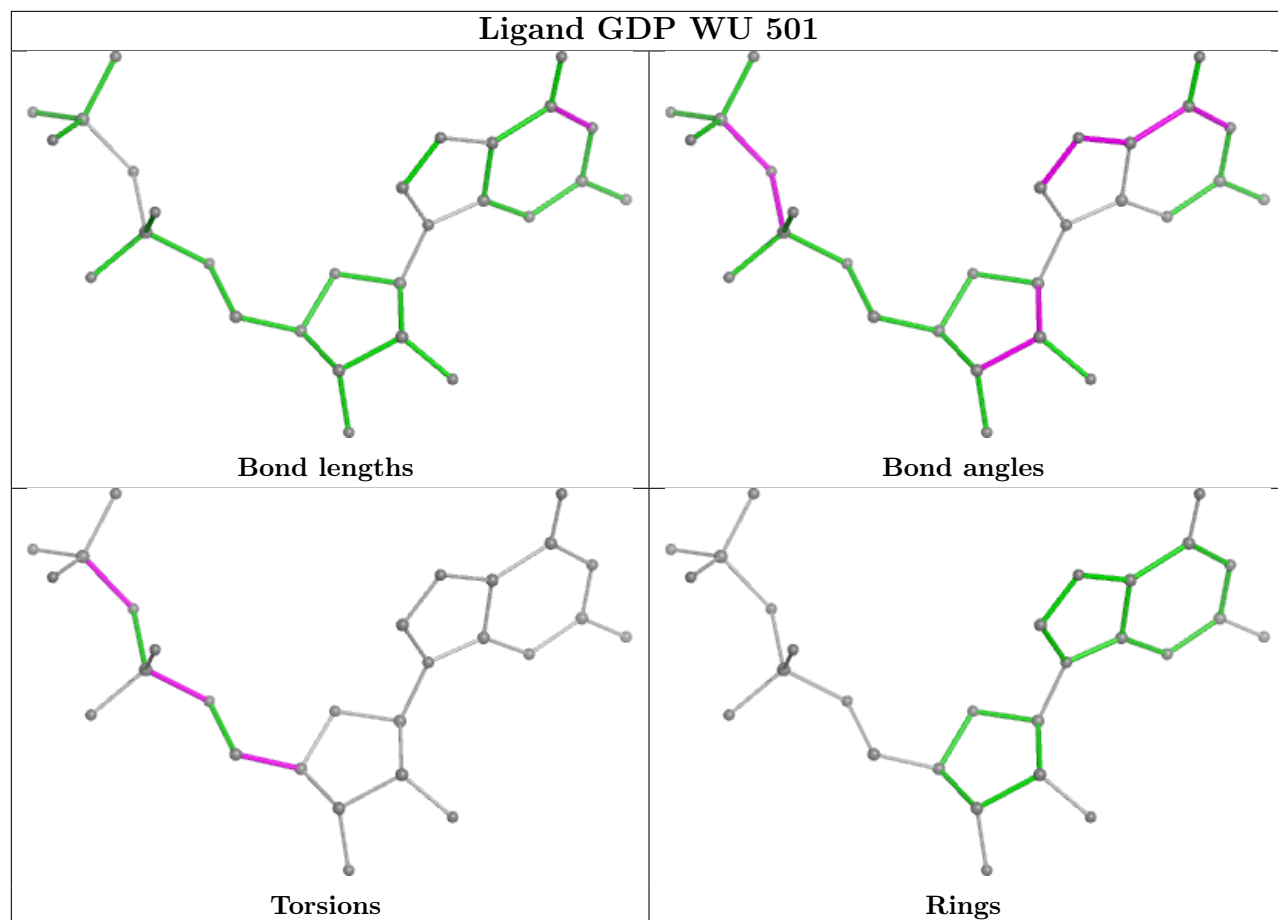
Torsions



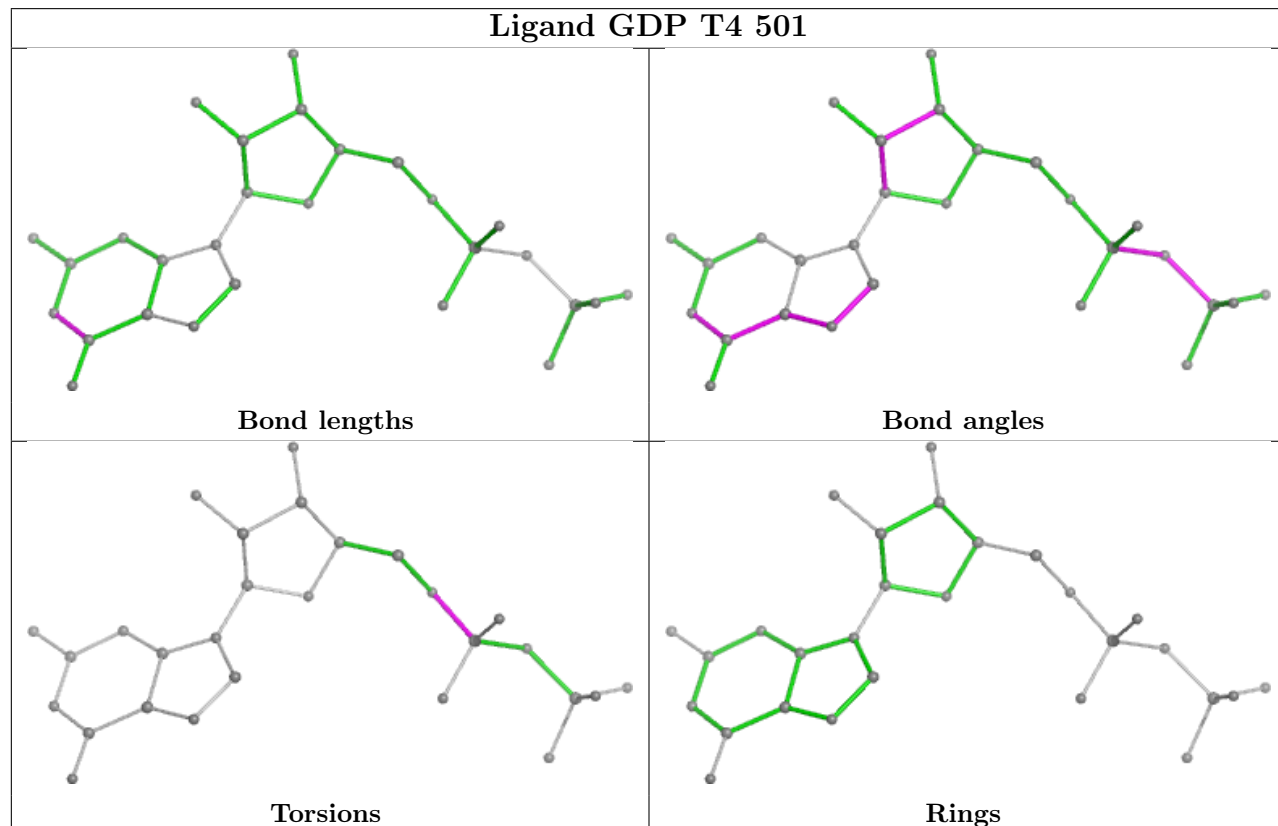
Rings



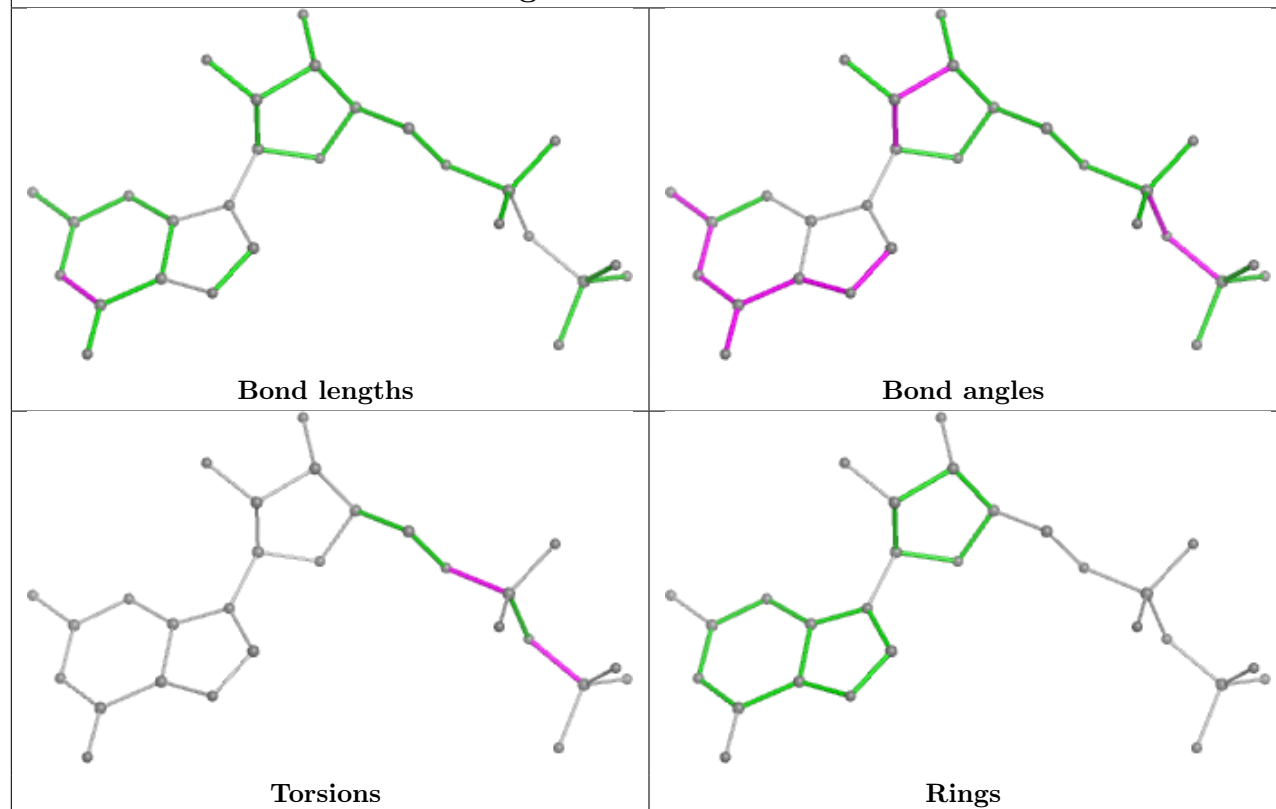
## Ligand GDP WU 501



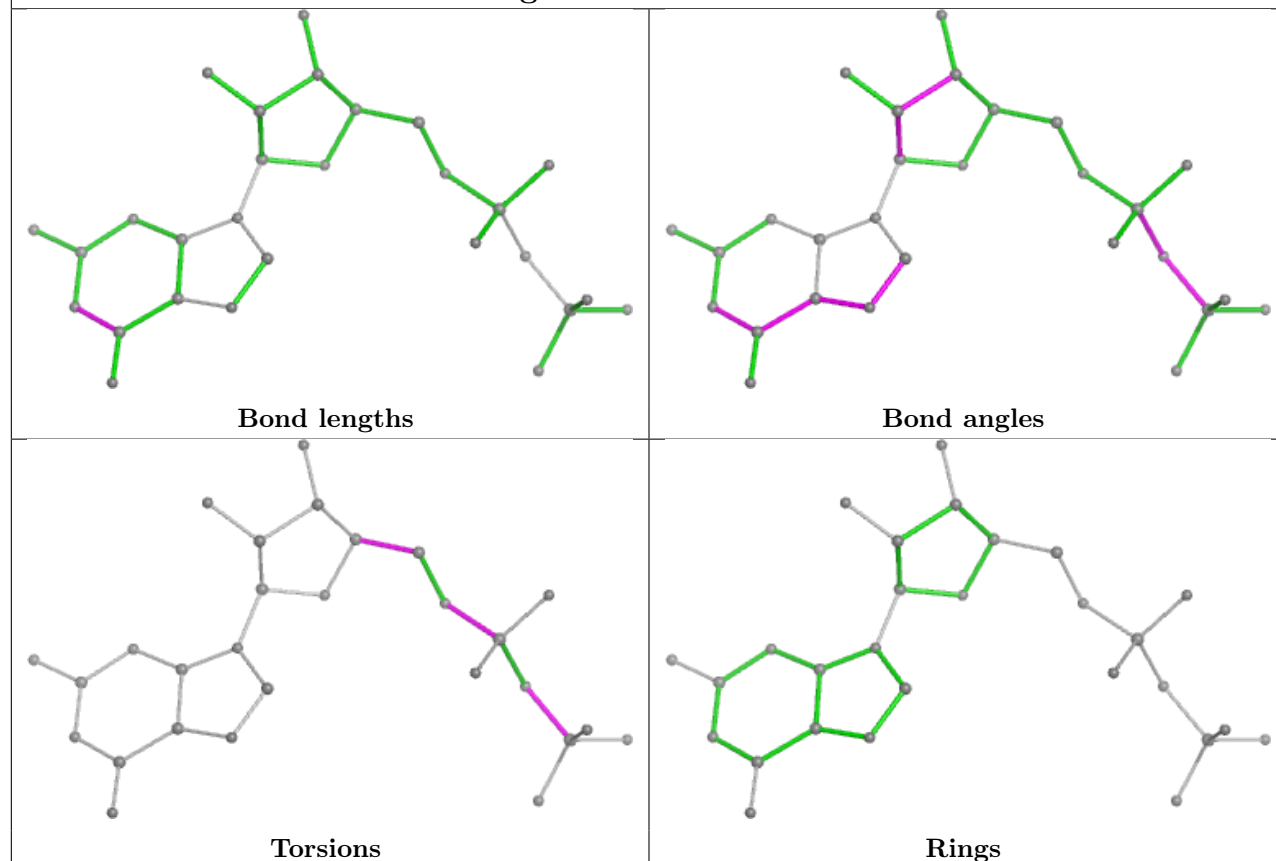
## Ligand GDP T4 501



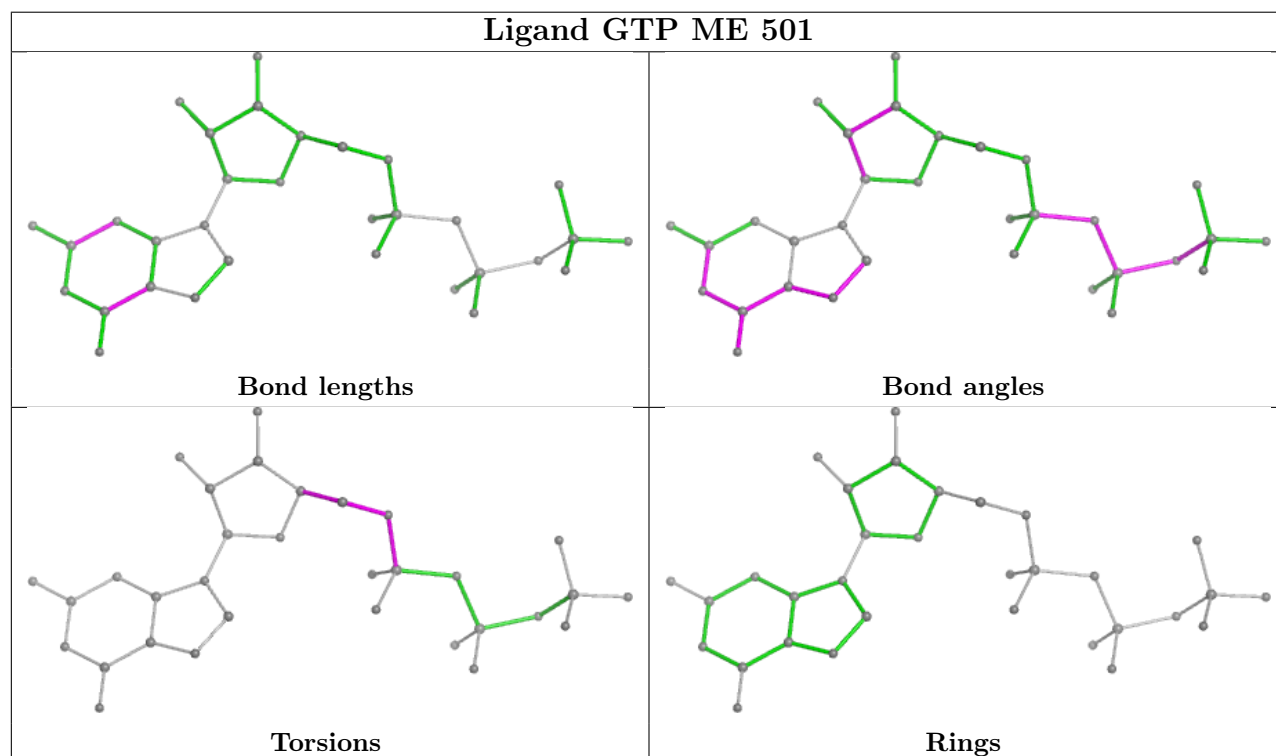
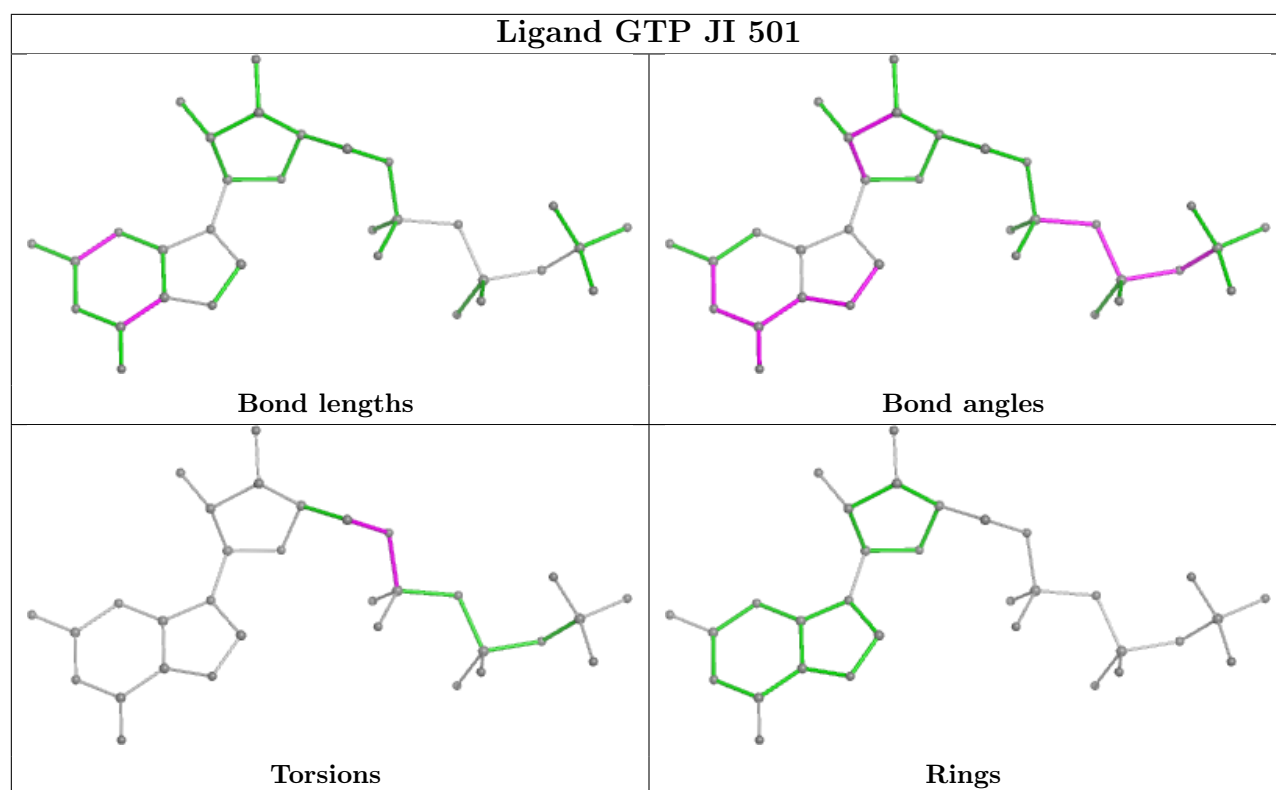
## Ligand GDP PL 501

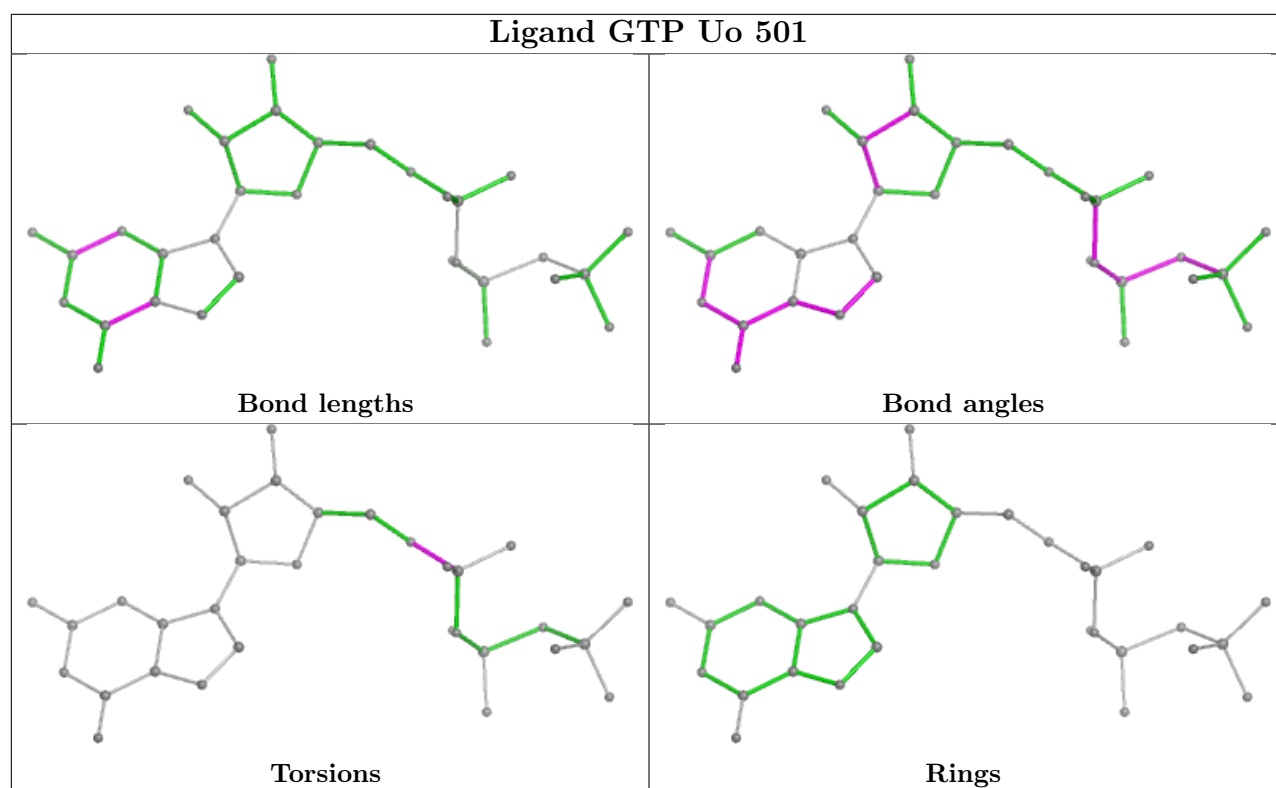


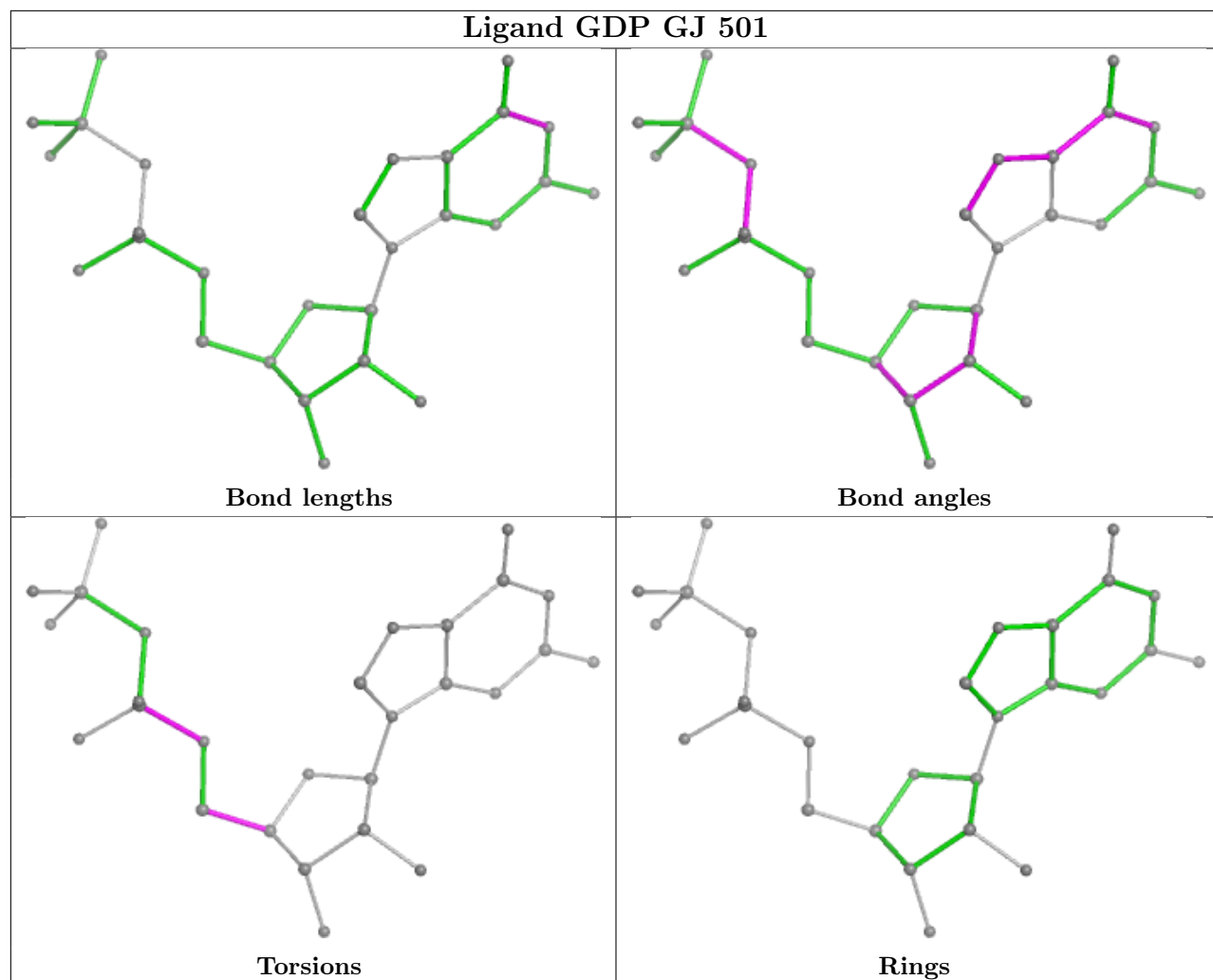
## Ligand GDP Ua 501



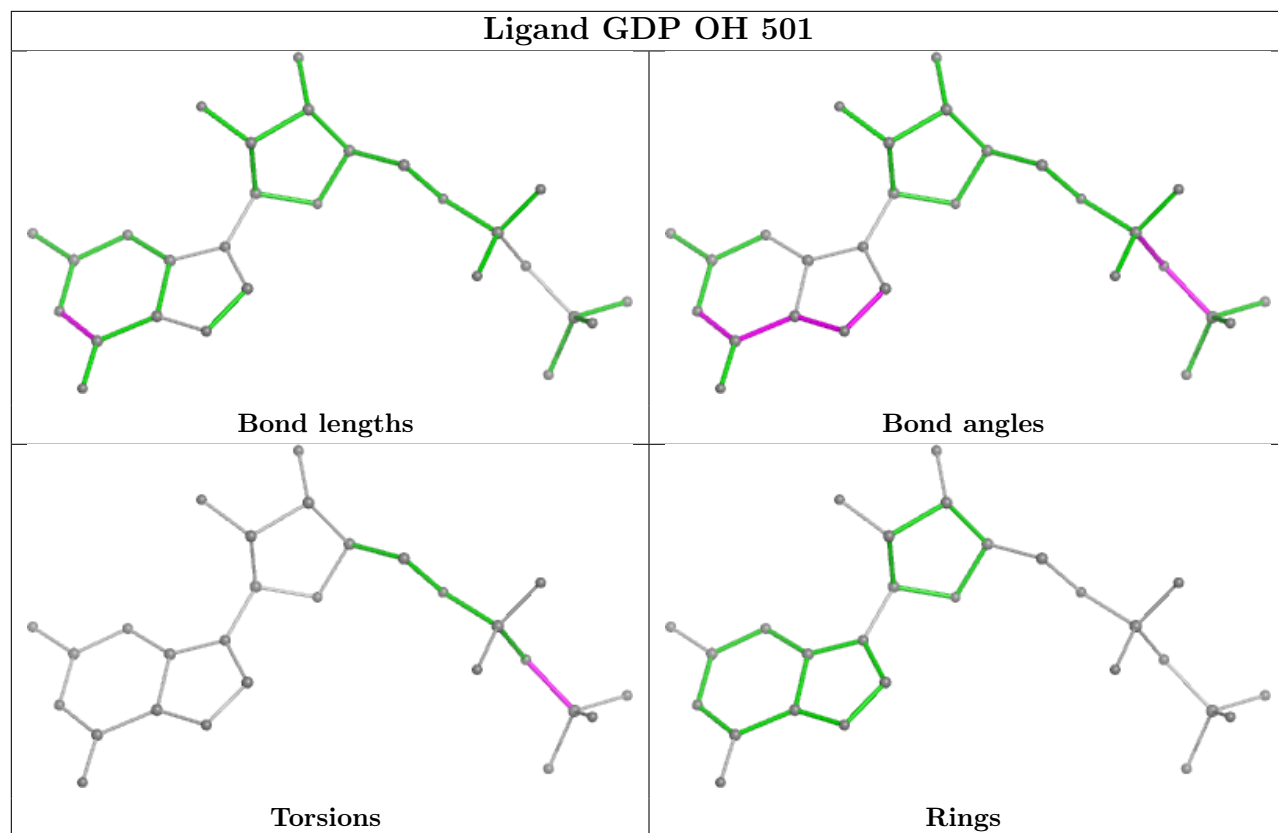




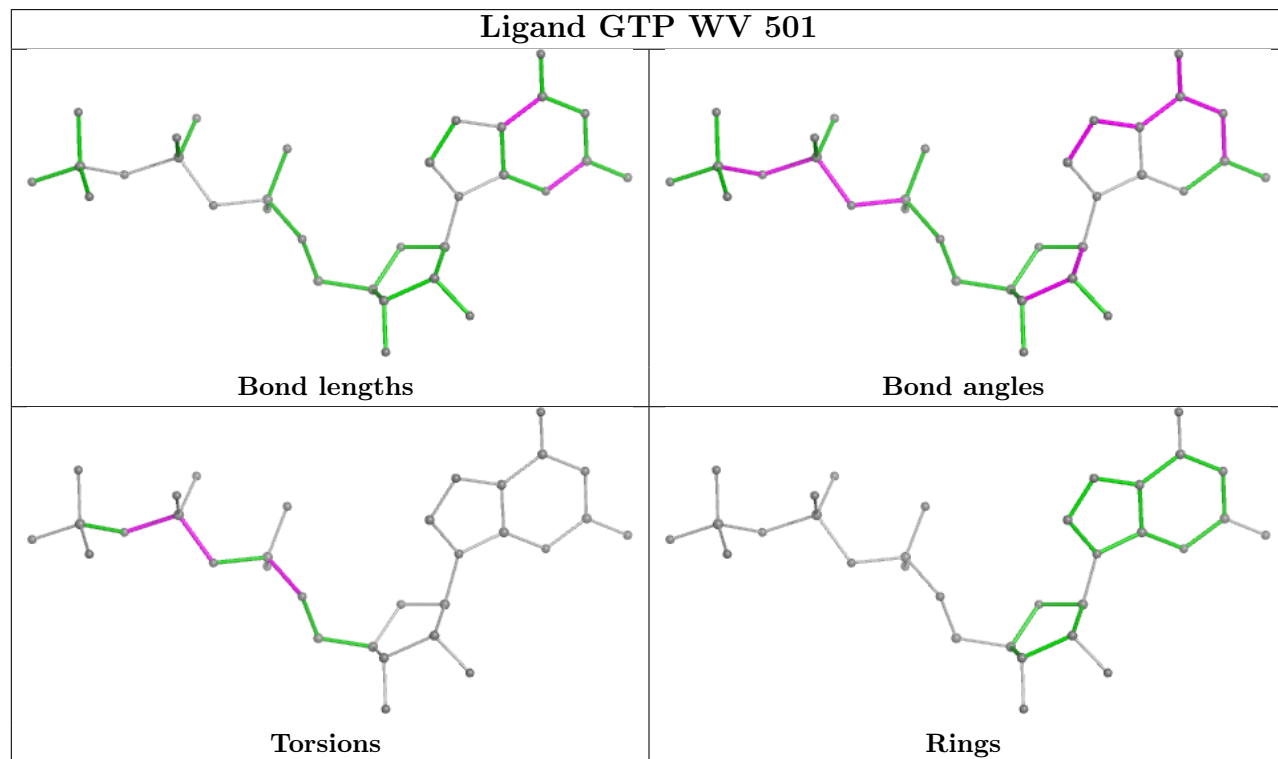




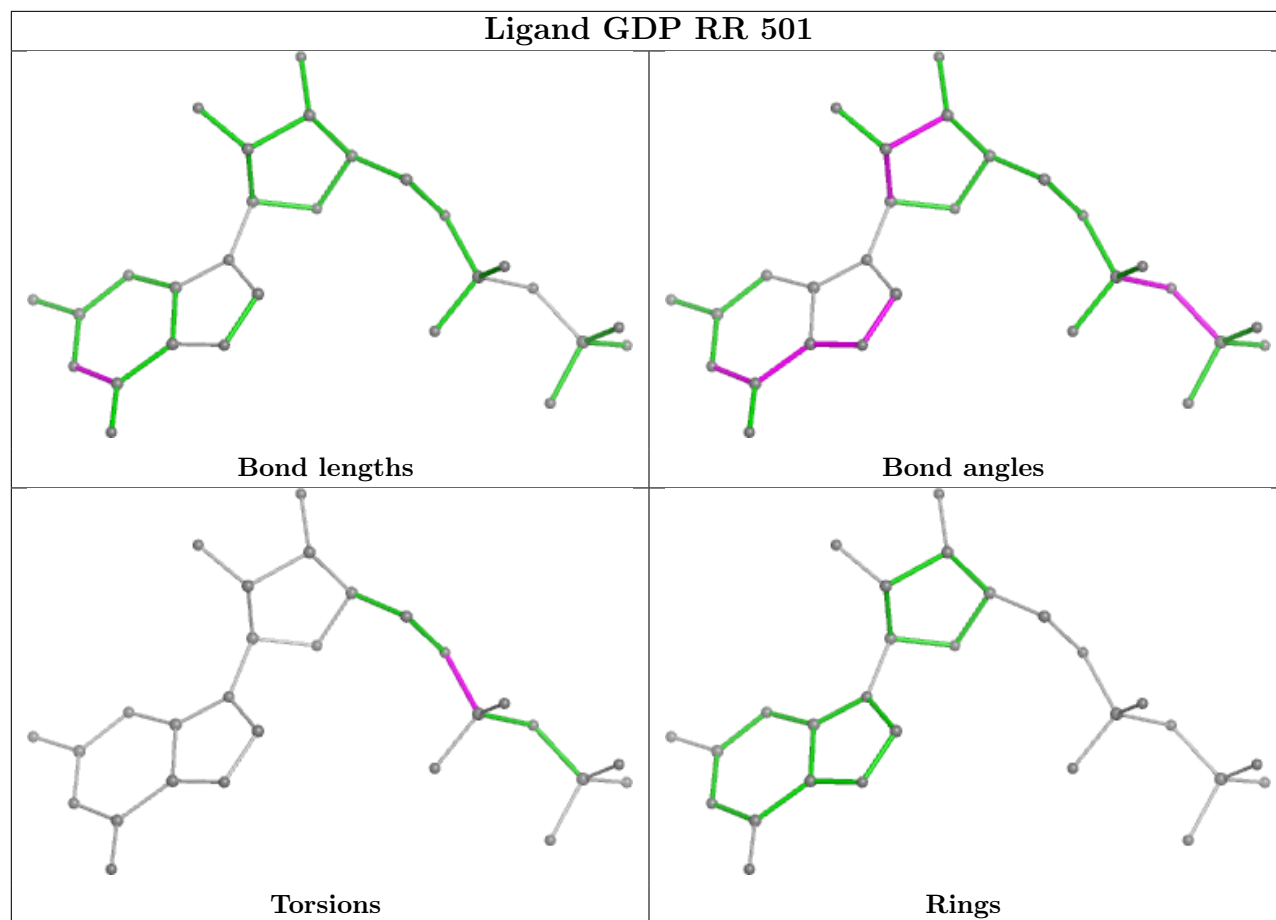
## Ligand GDP OH 501



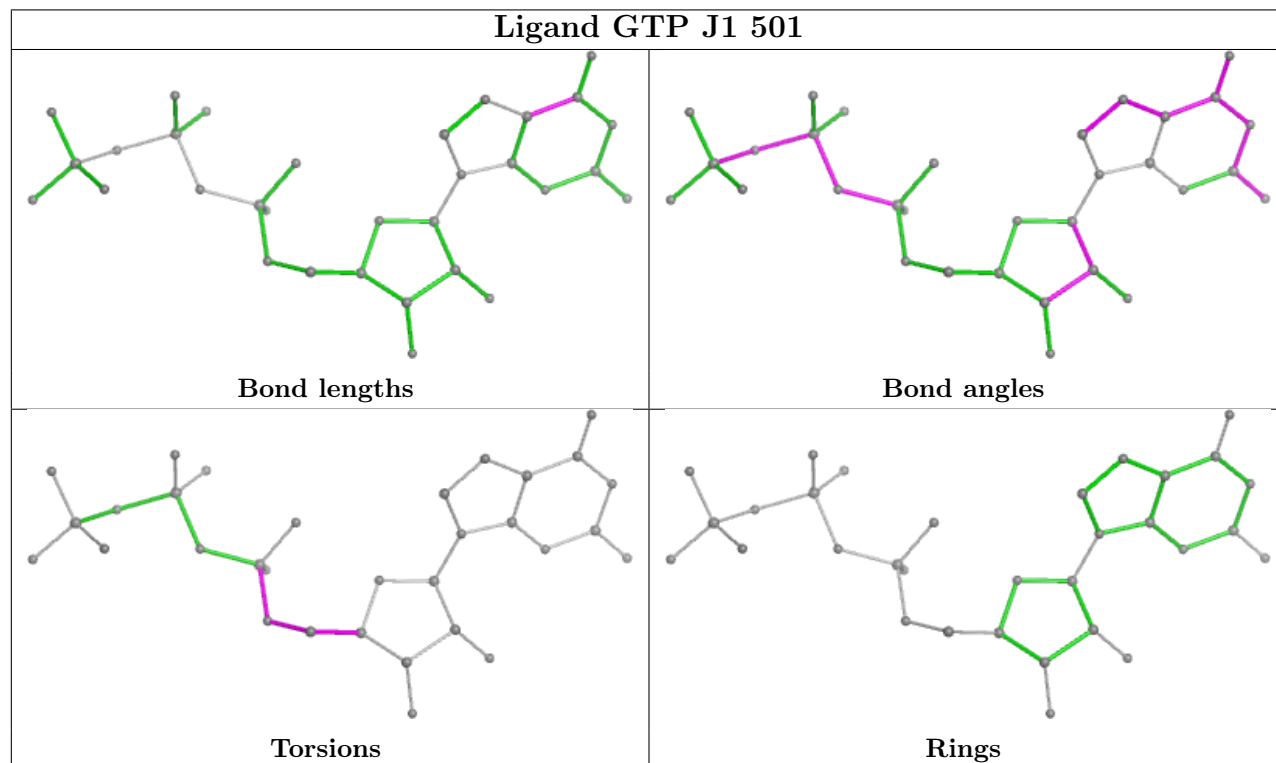
## Ligand GTP WV 501

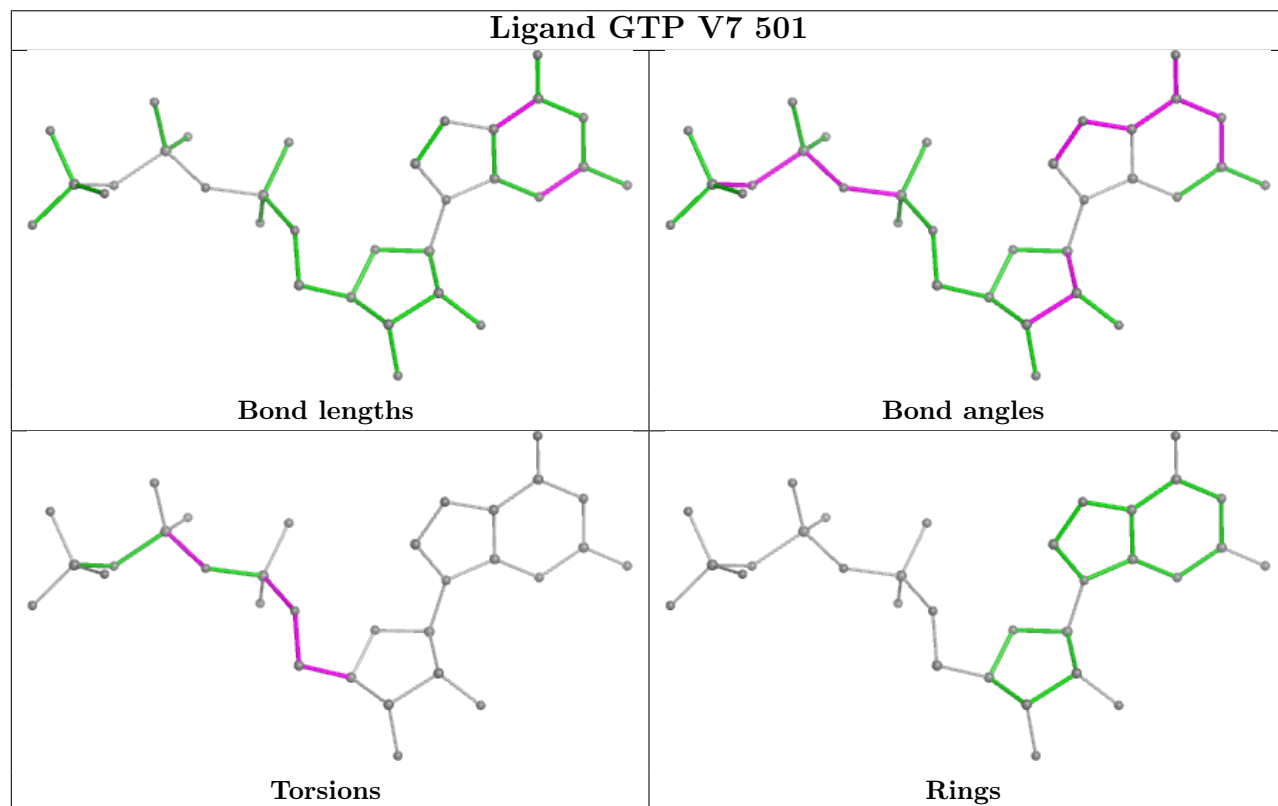
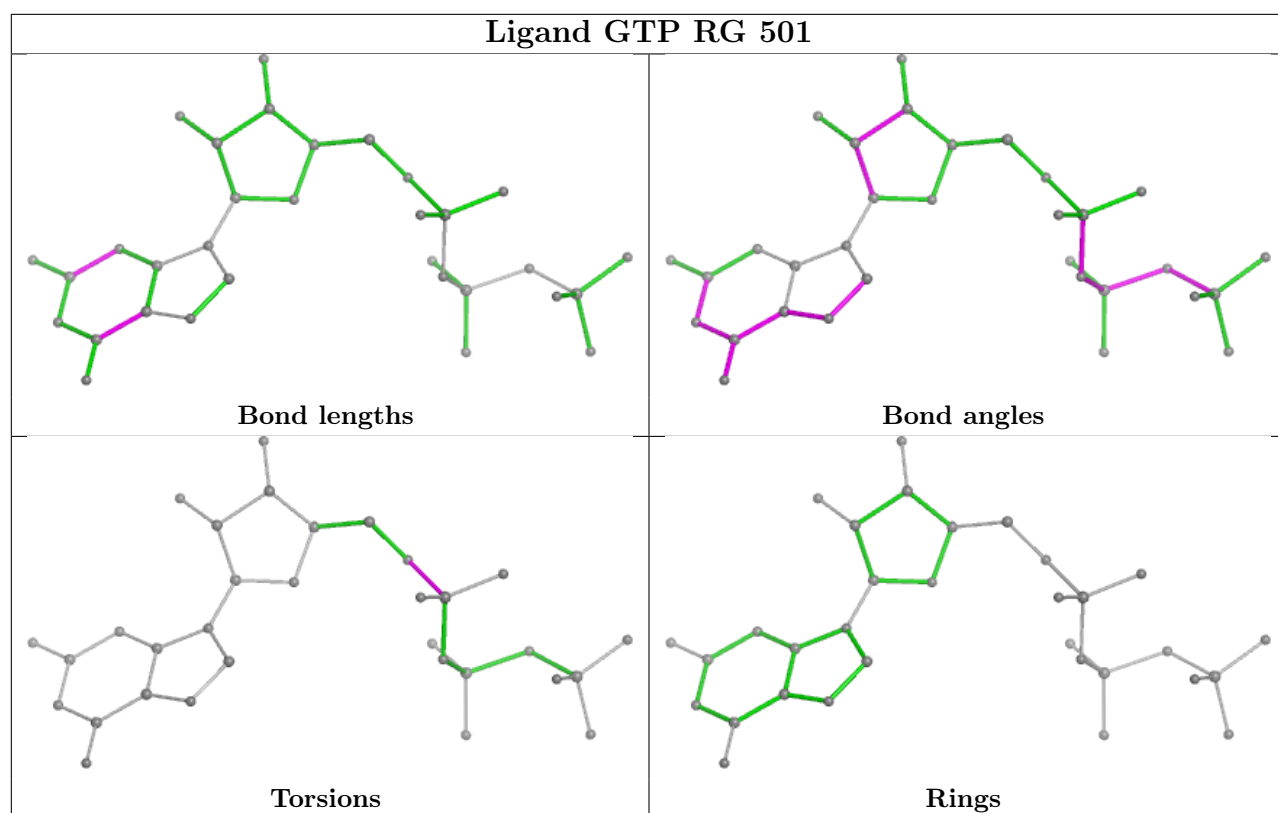


## Ligand GDP RR 501

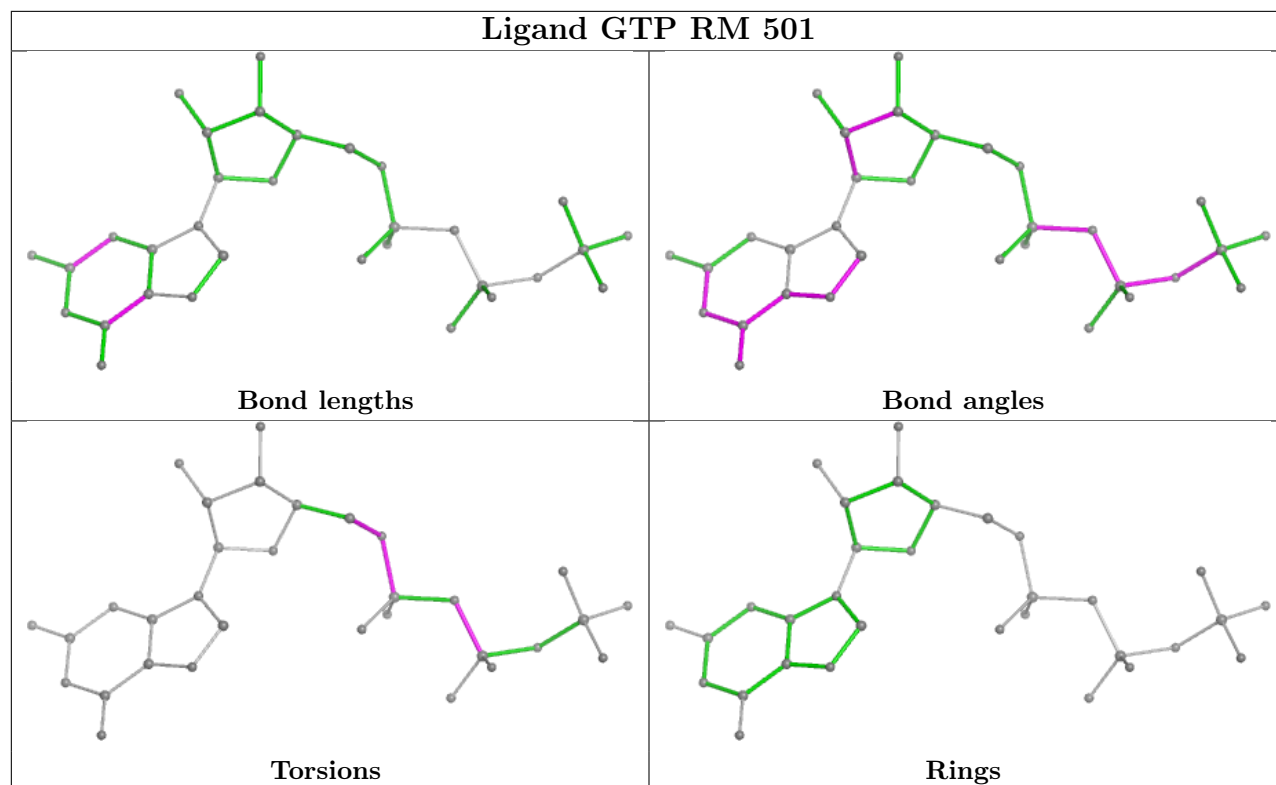


## Ligand GTP J1 501

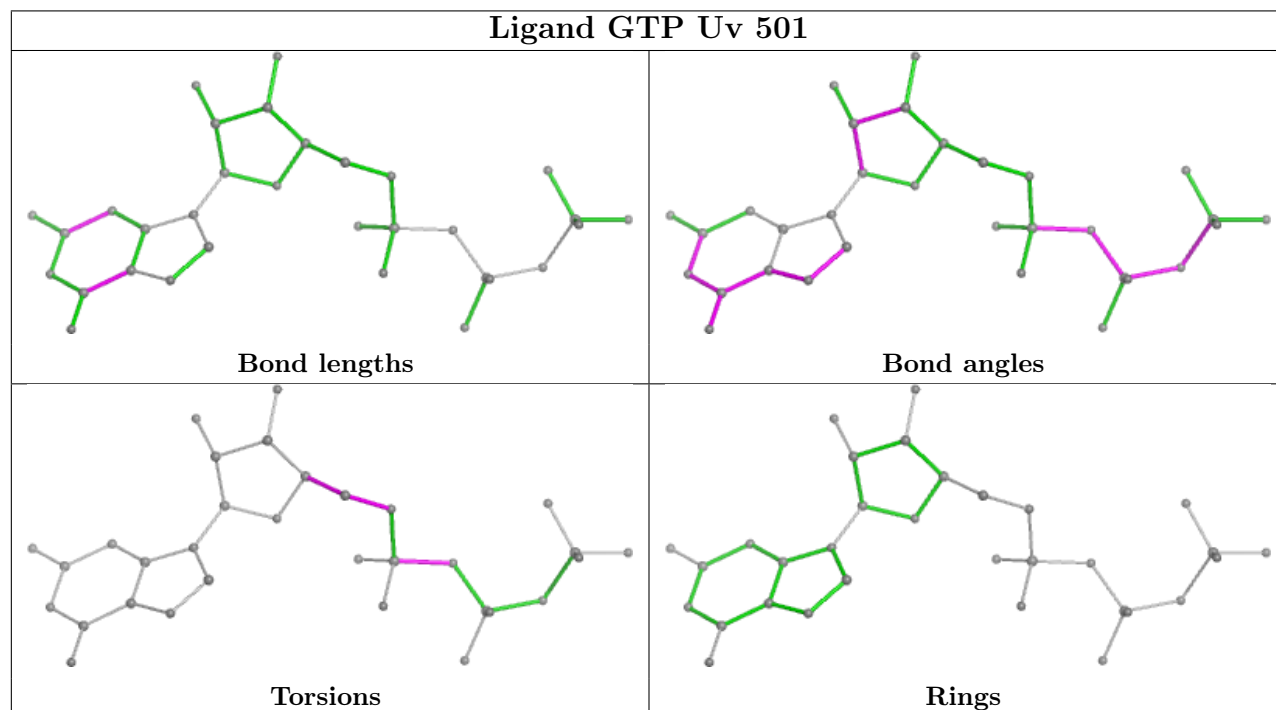




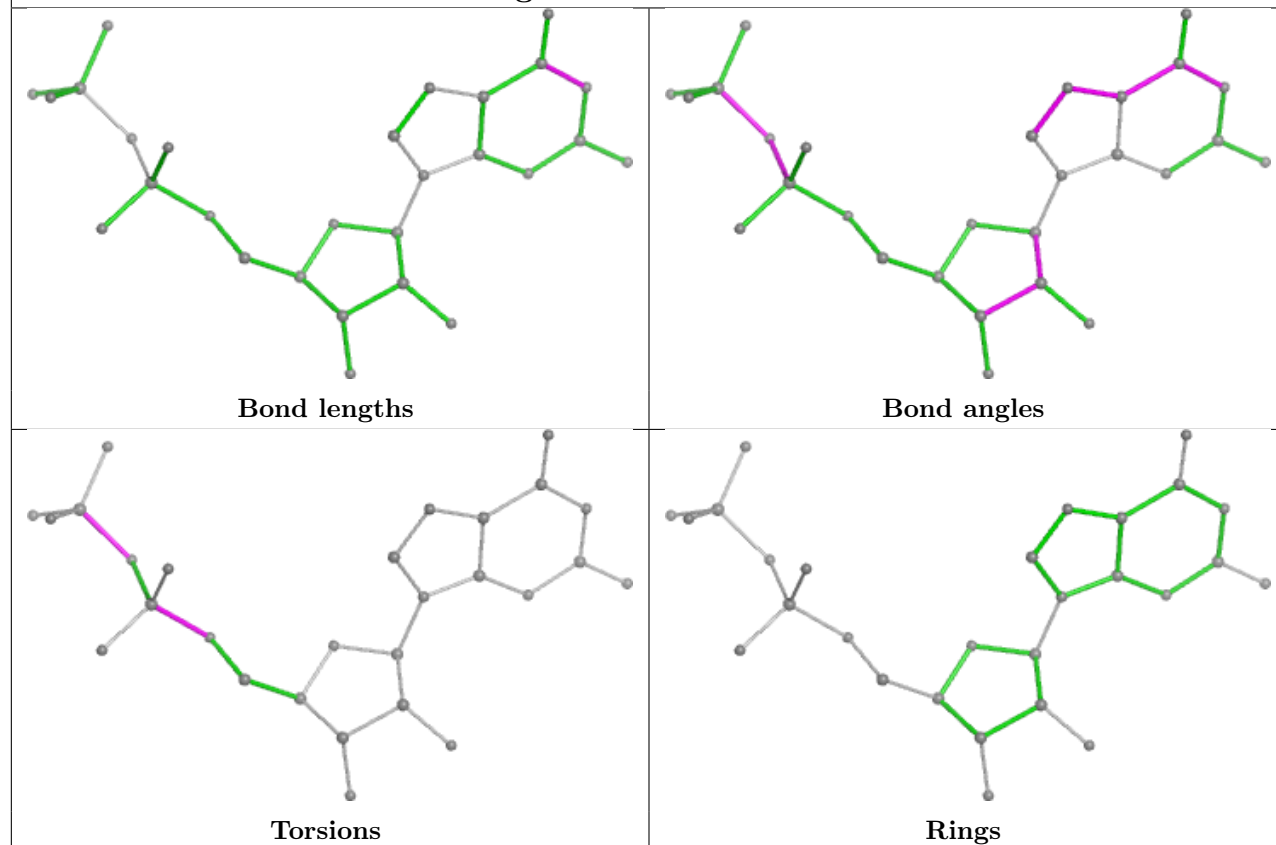
## Ligand GTP RM 501



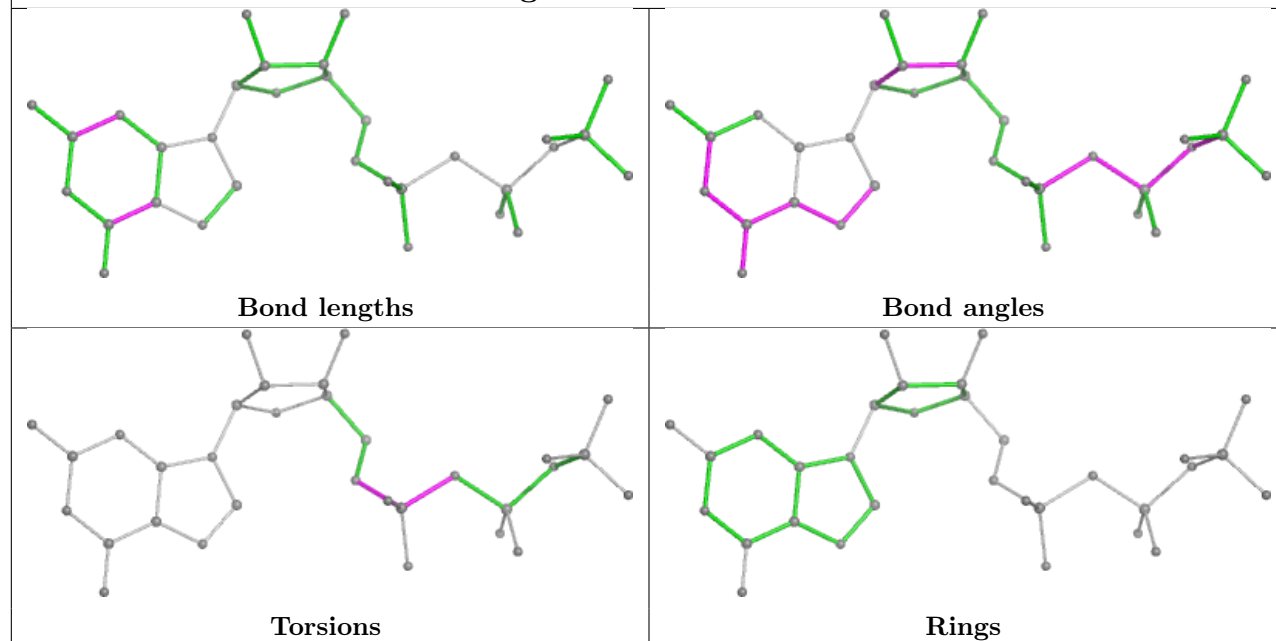
## Ligand GTP Uv 501



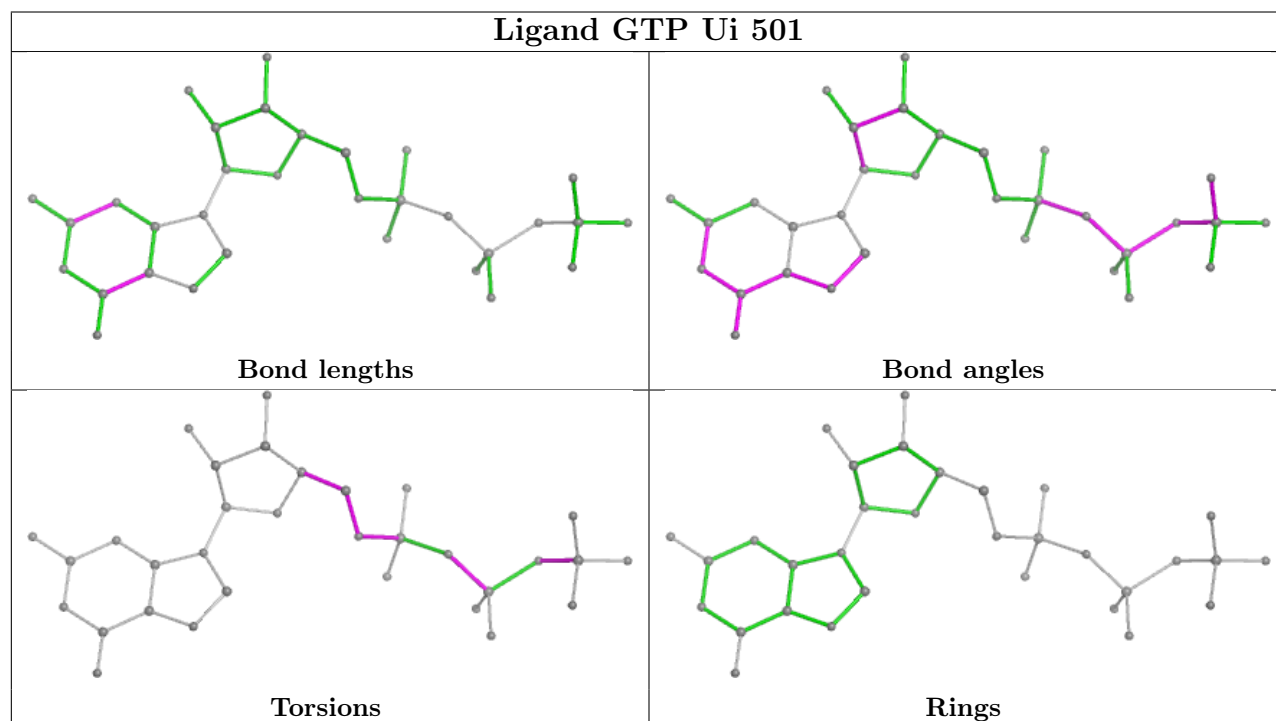
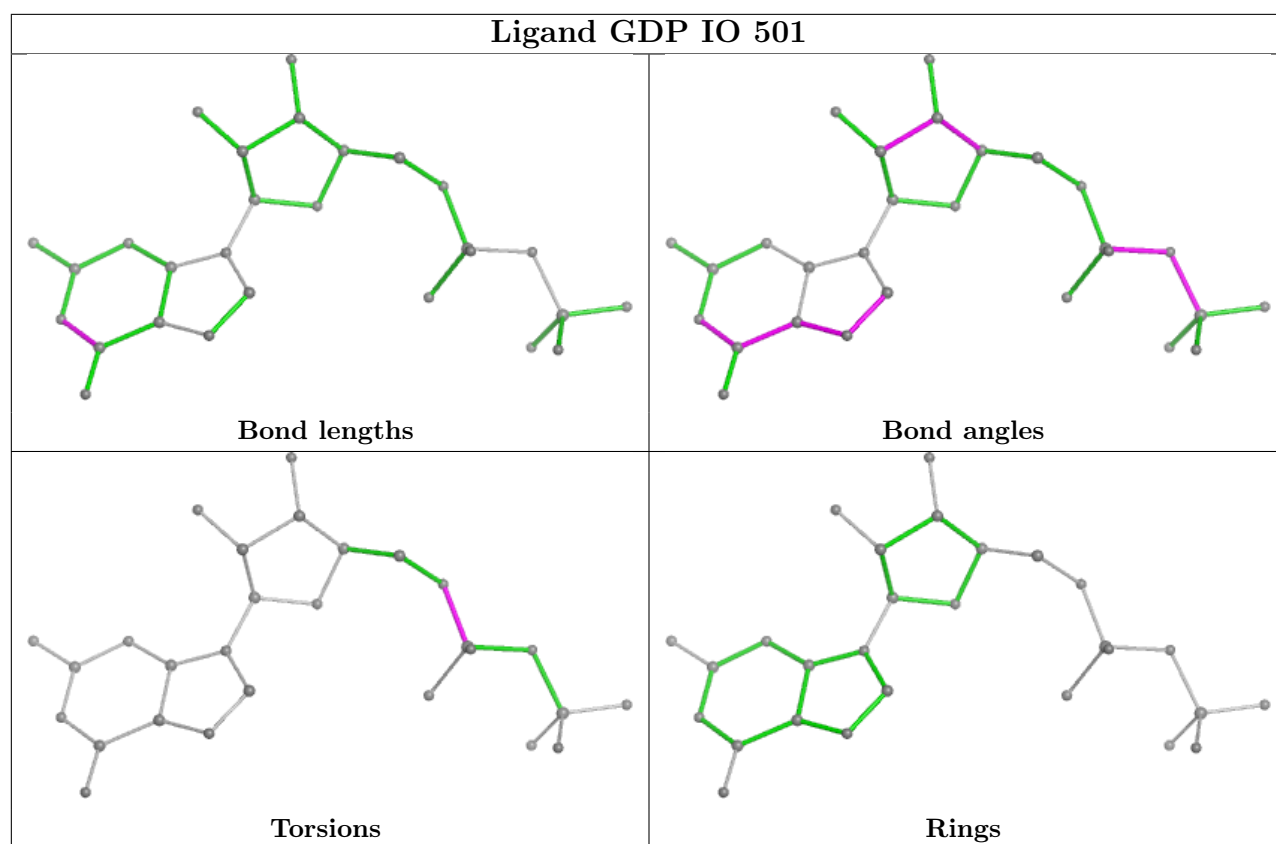
## Ligand GDP Wu 501



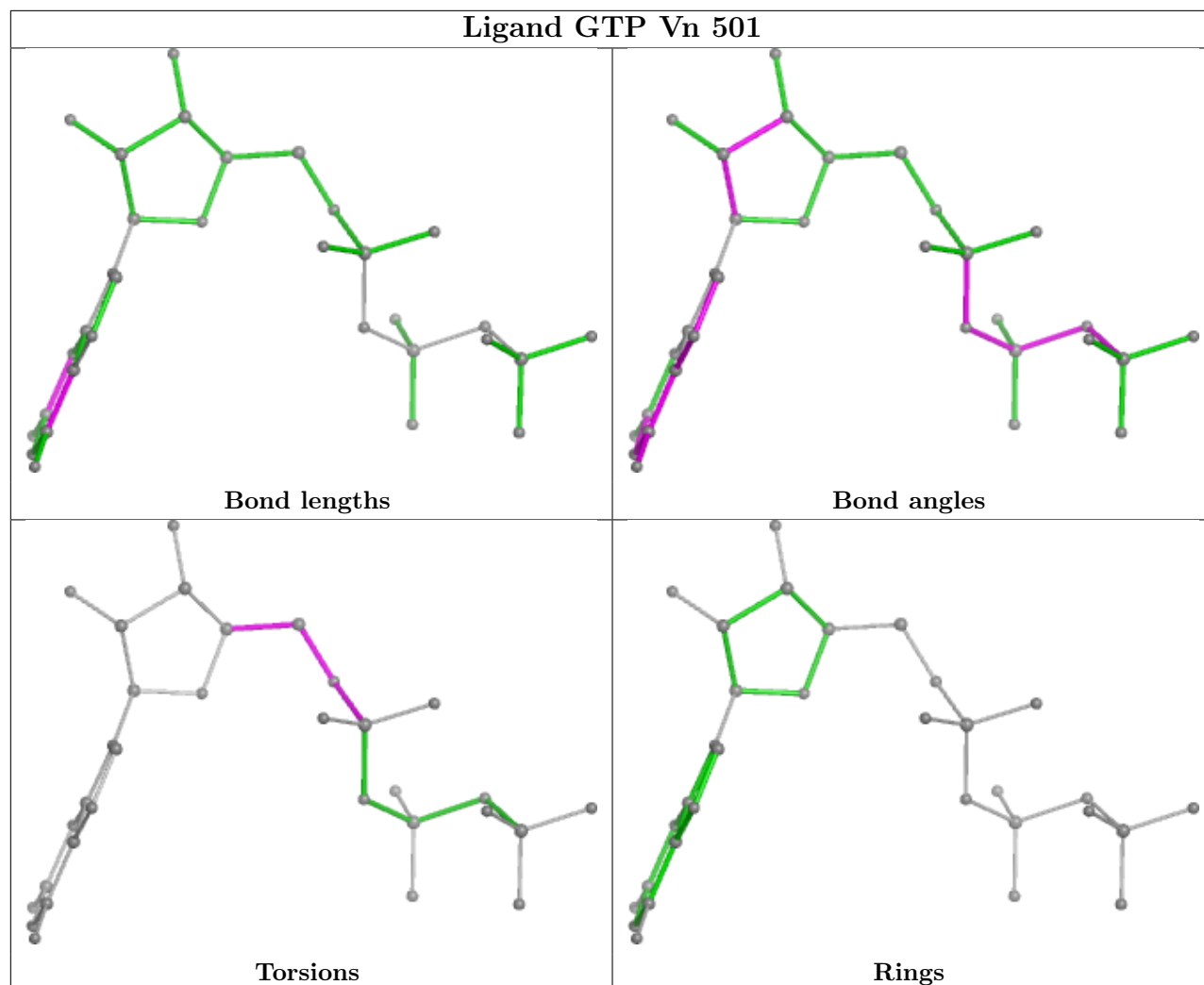
## Ligand GTP SA 501



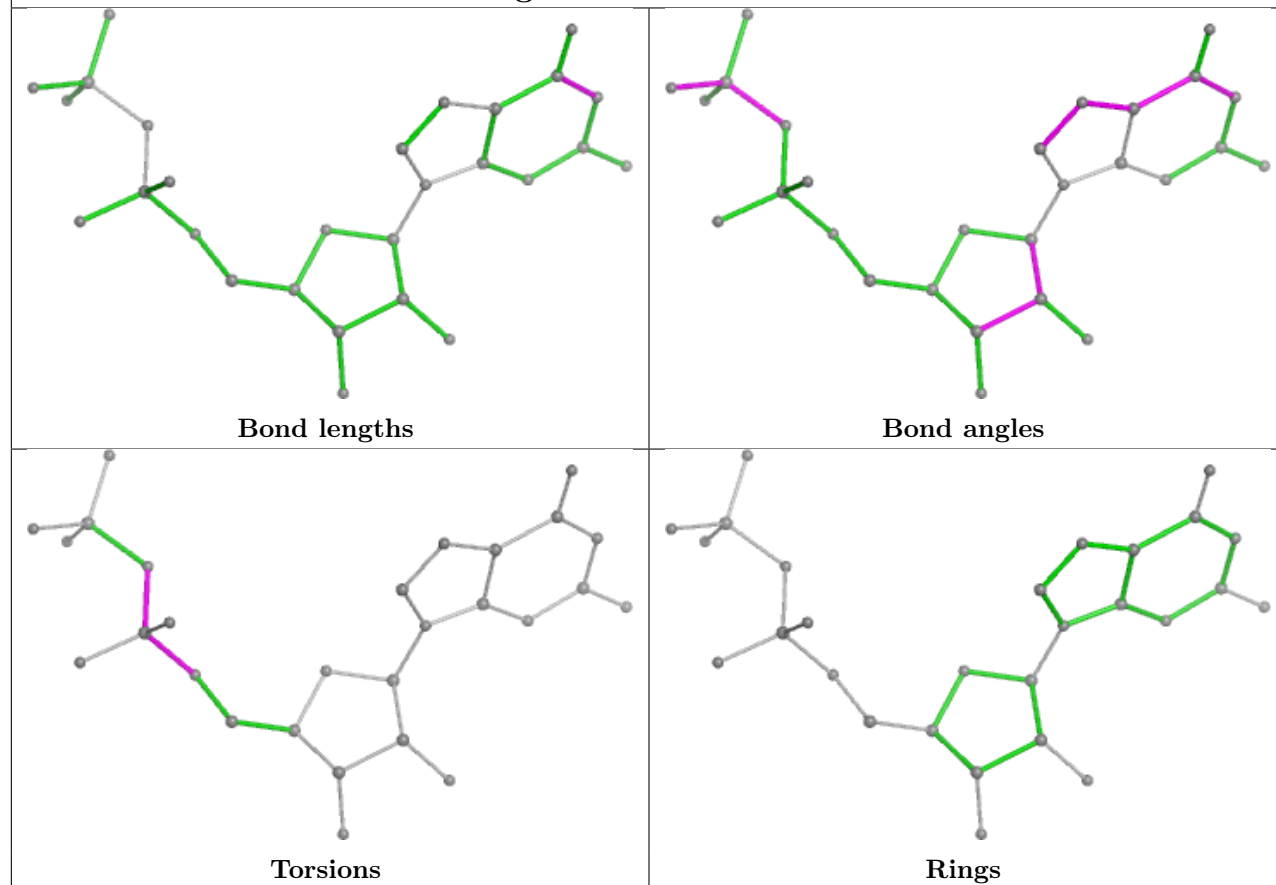




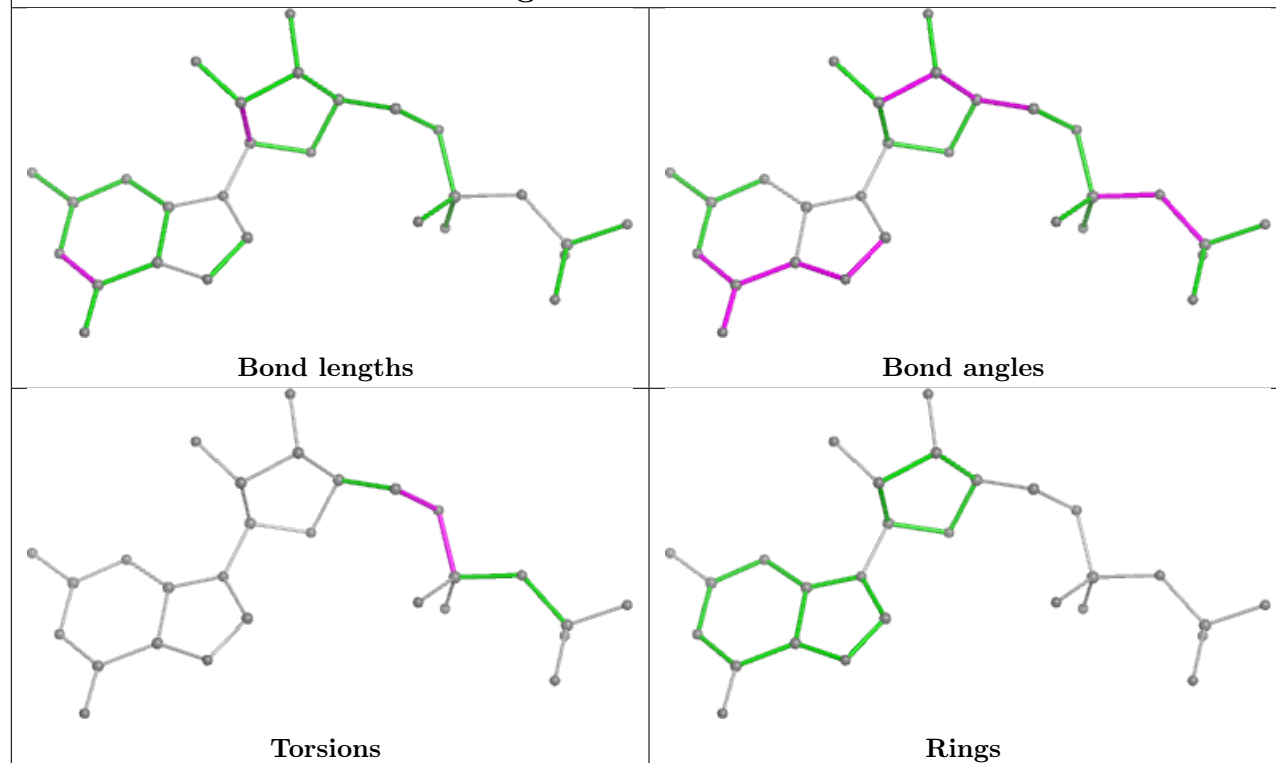
## Ligand GTP Vn 501

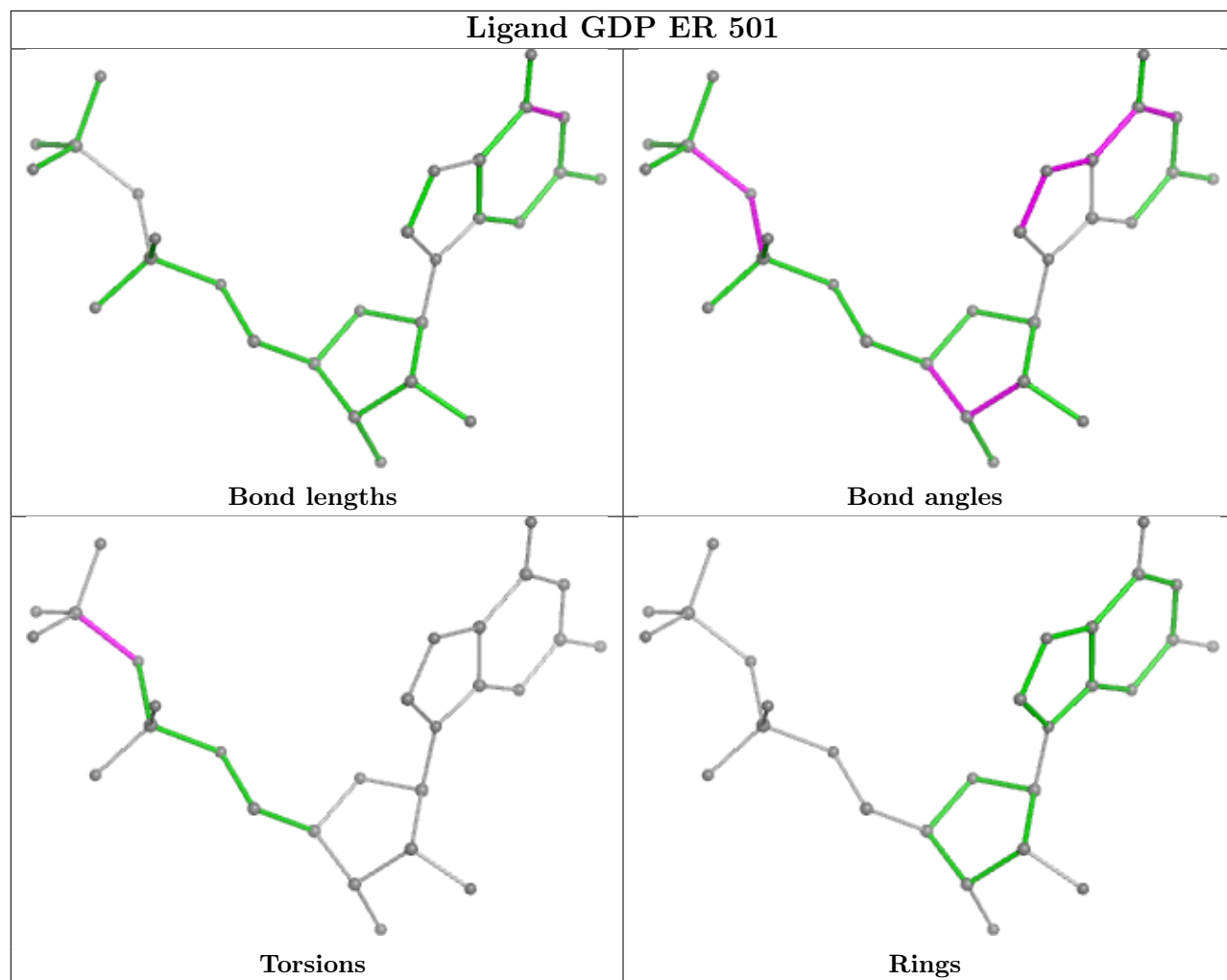


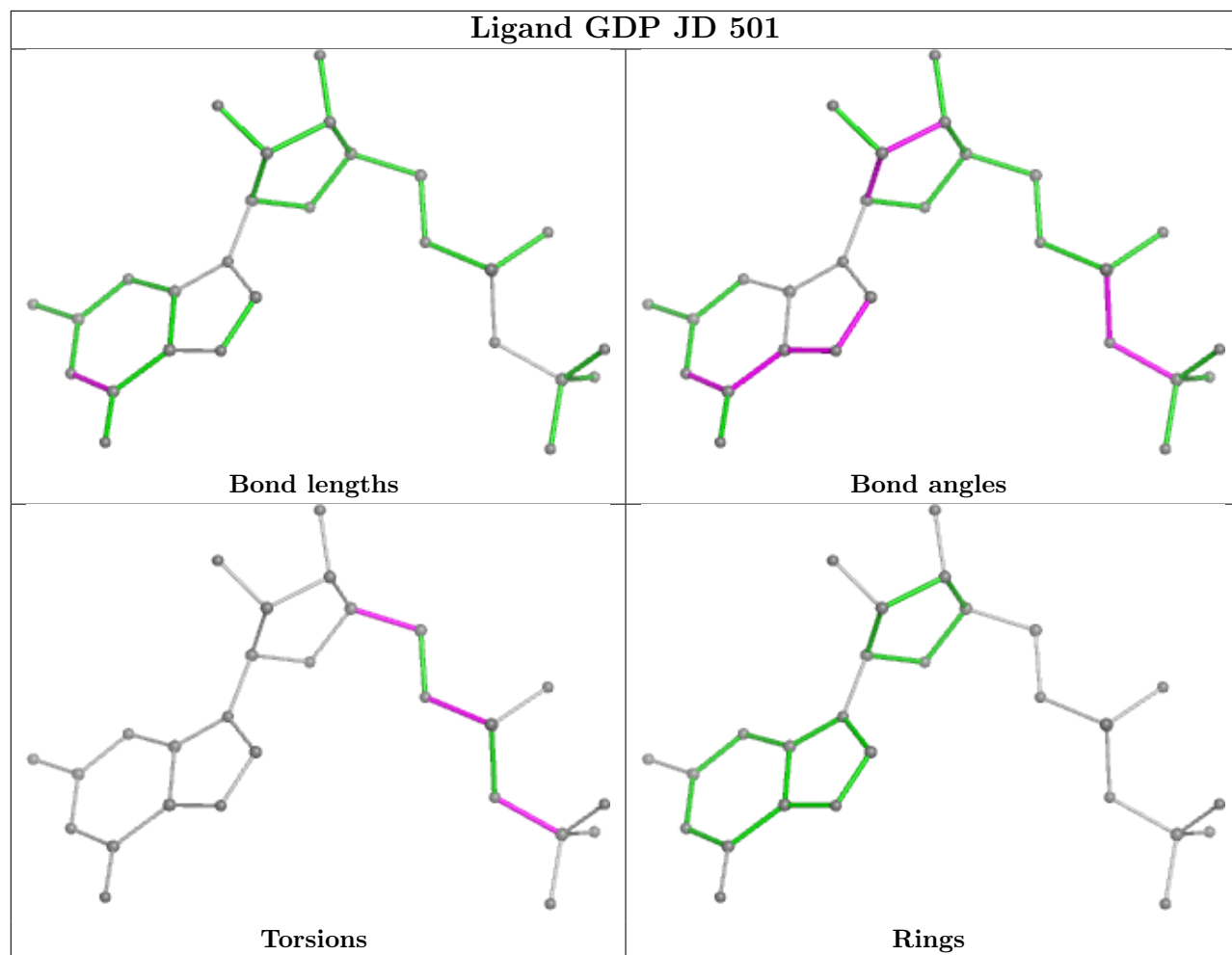
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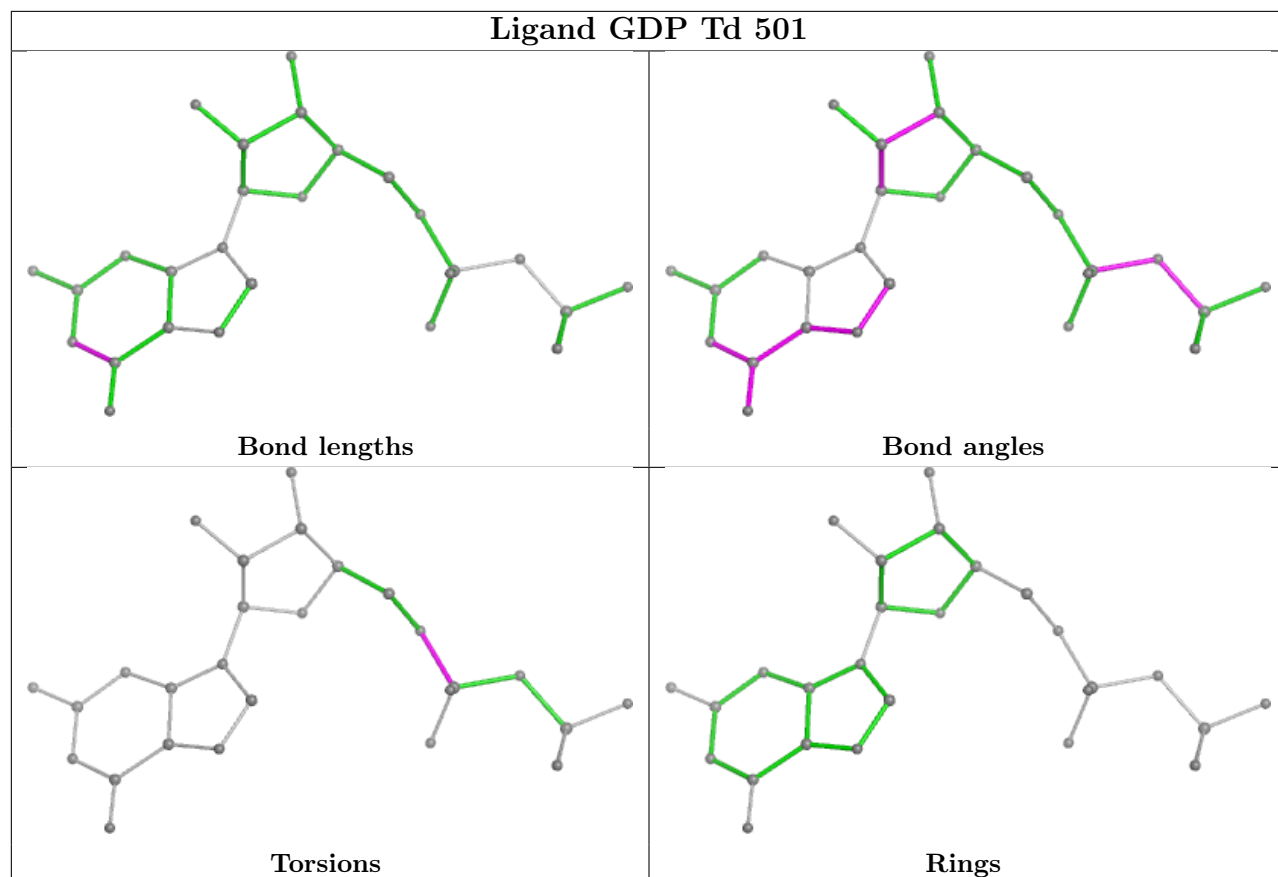
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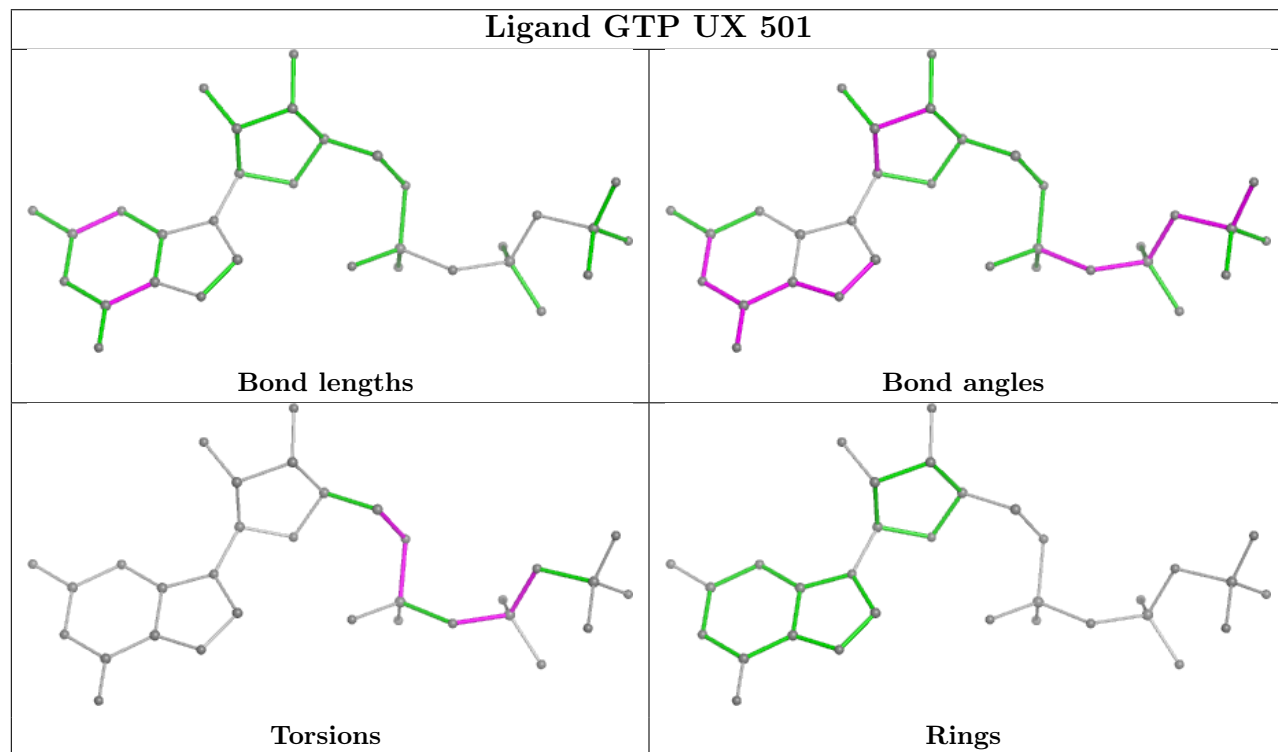


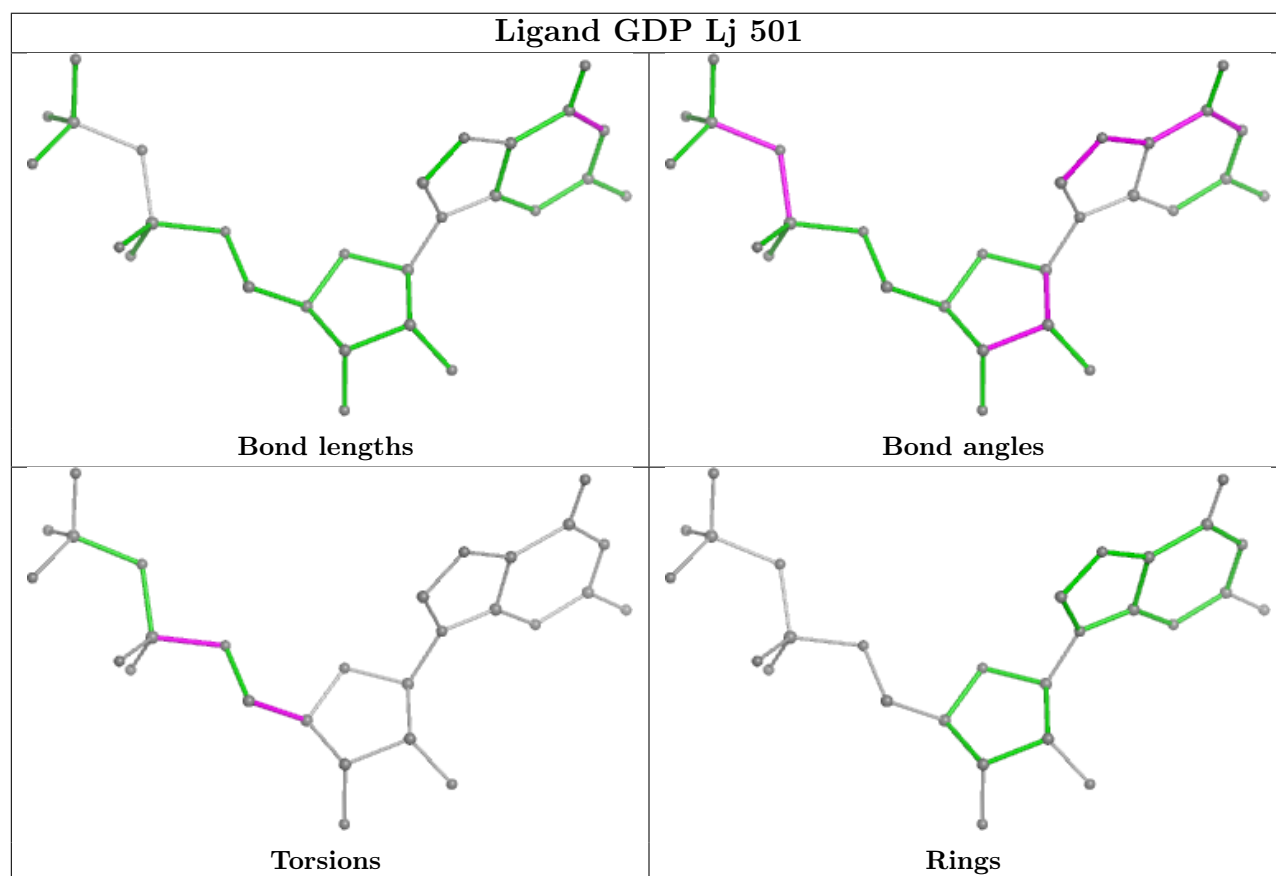
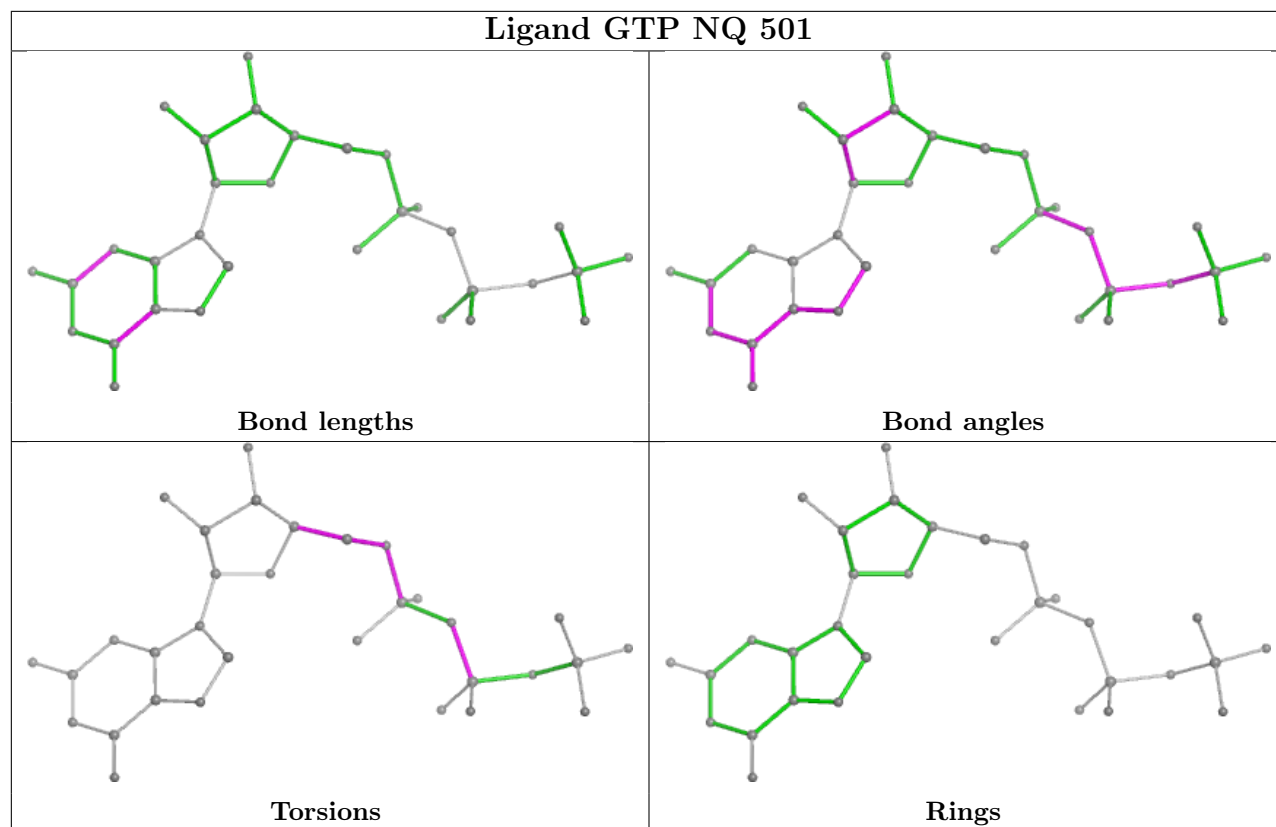


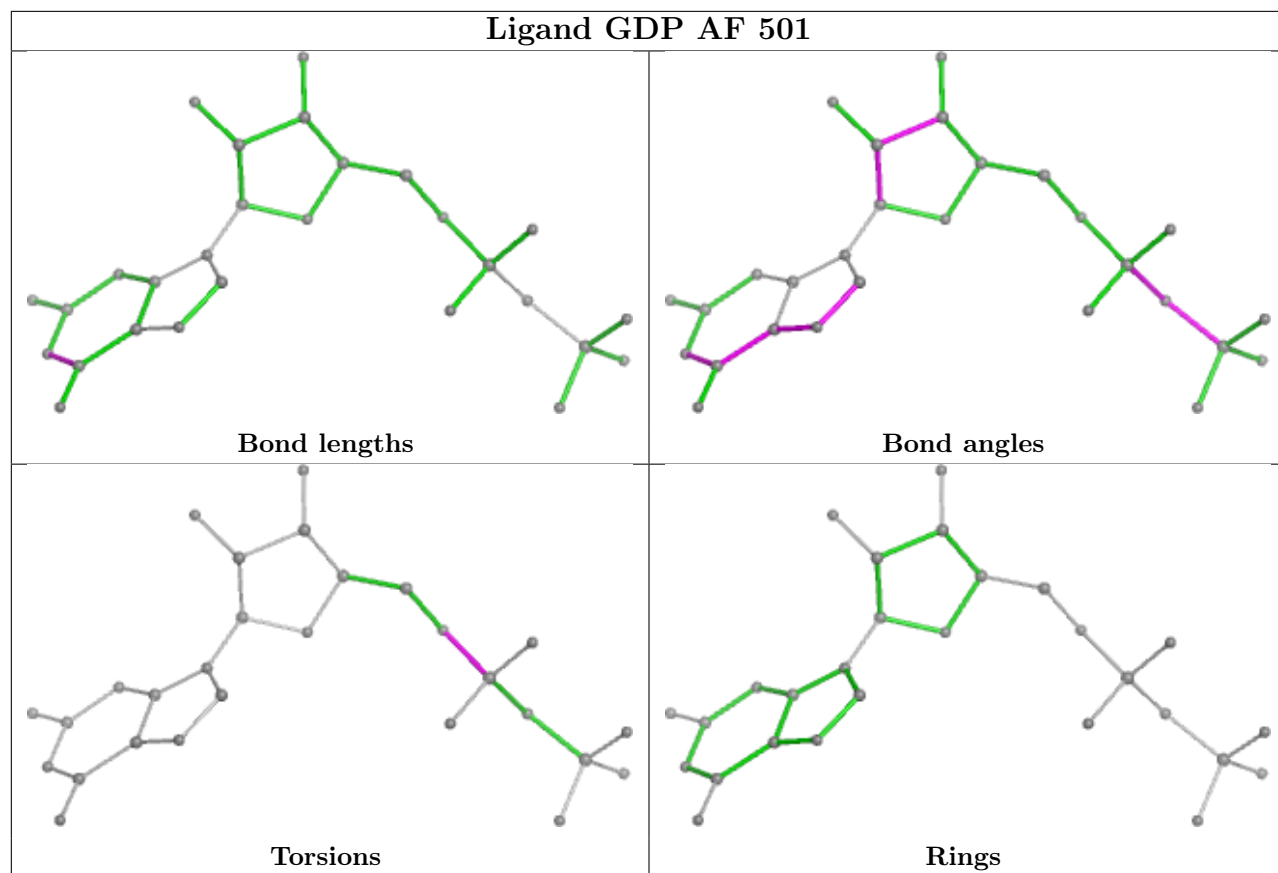
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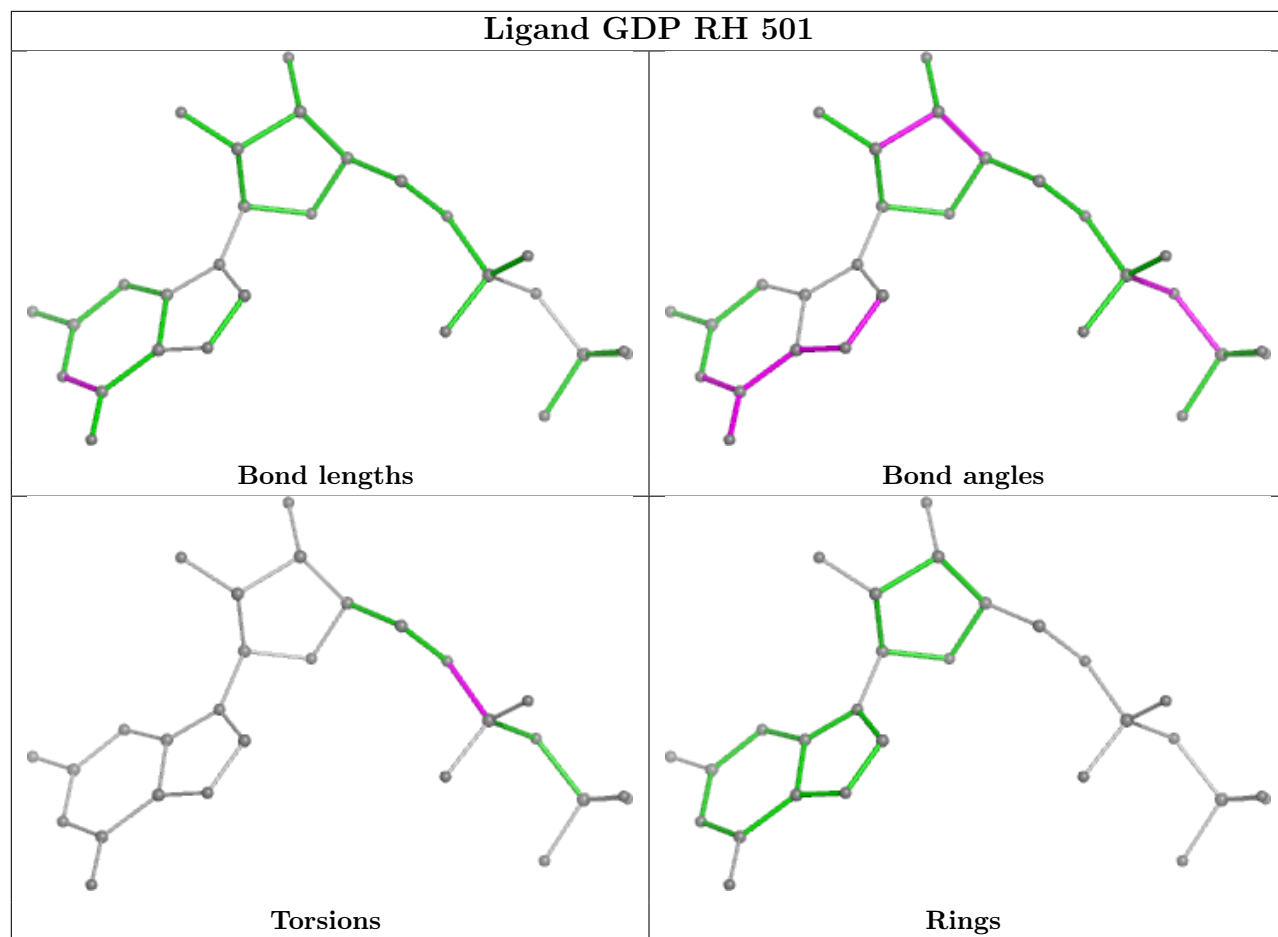
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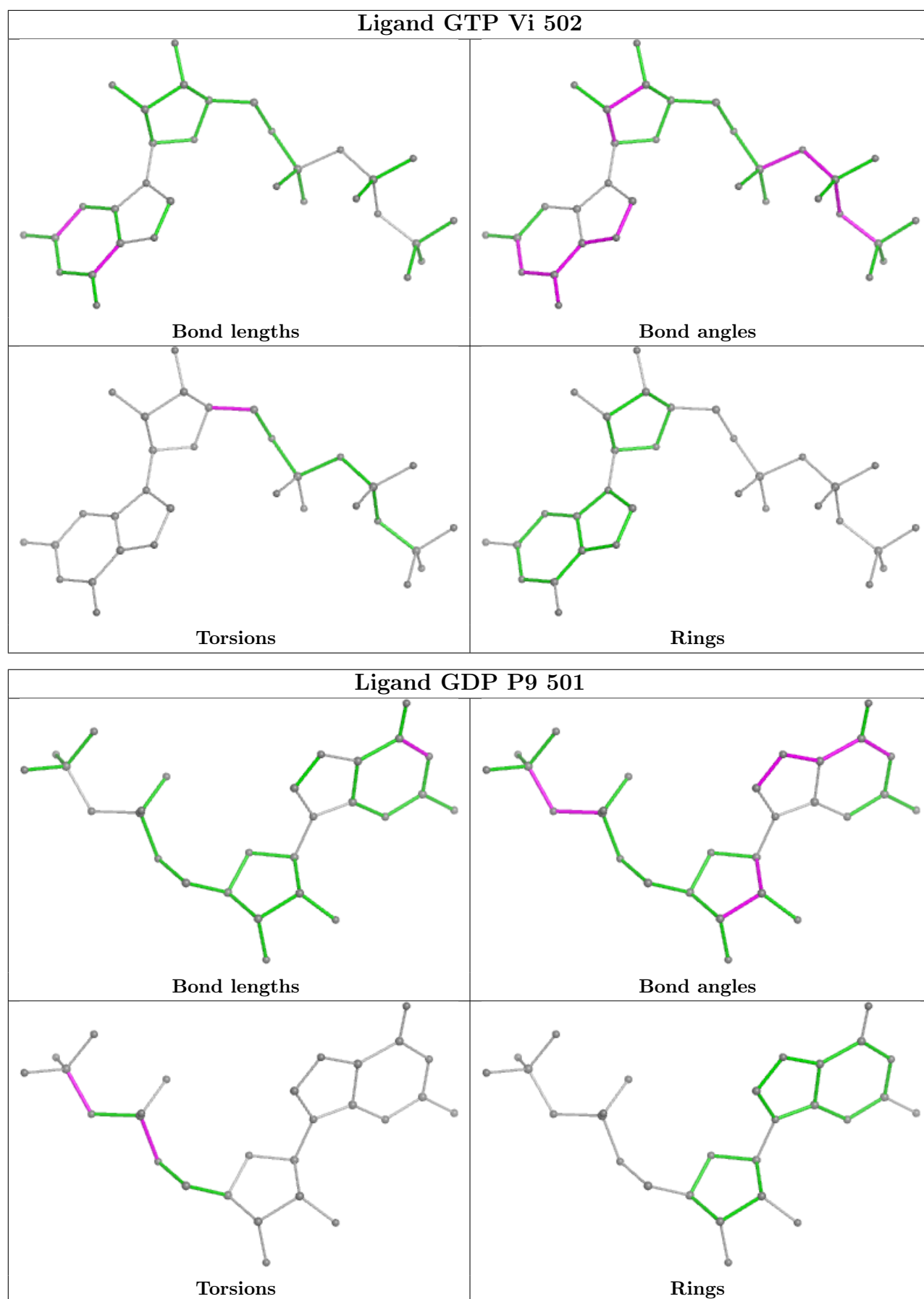


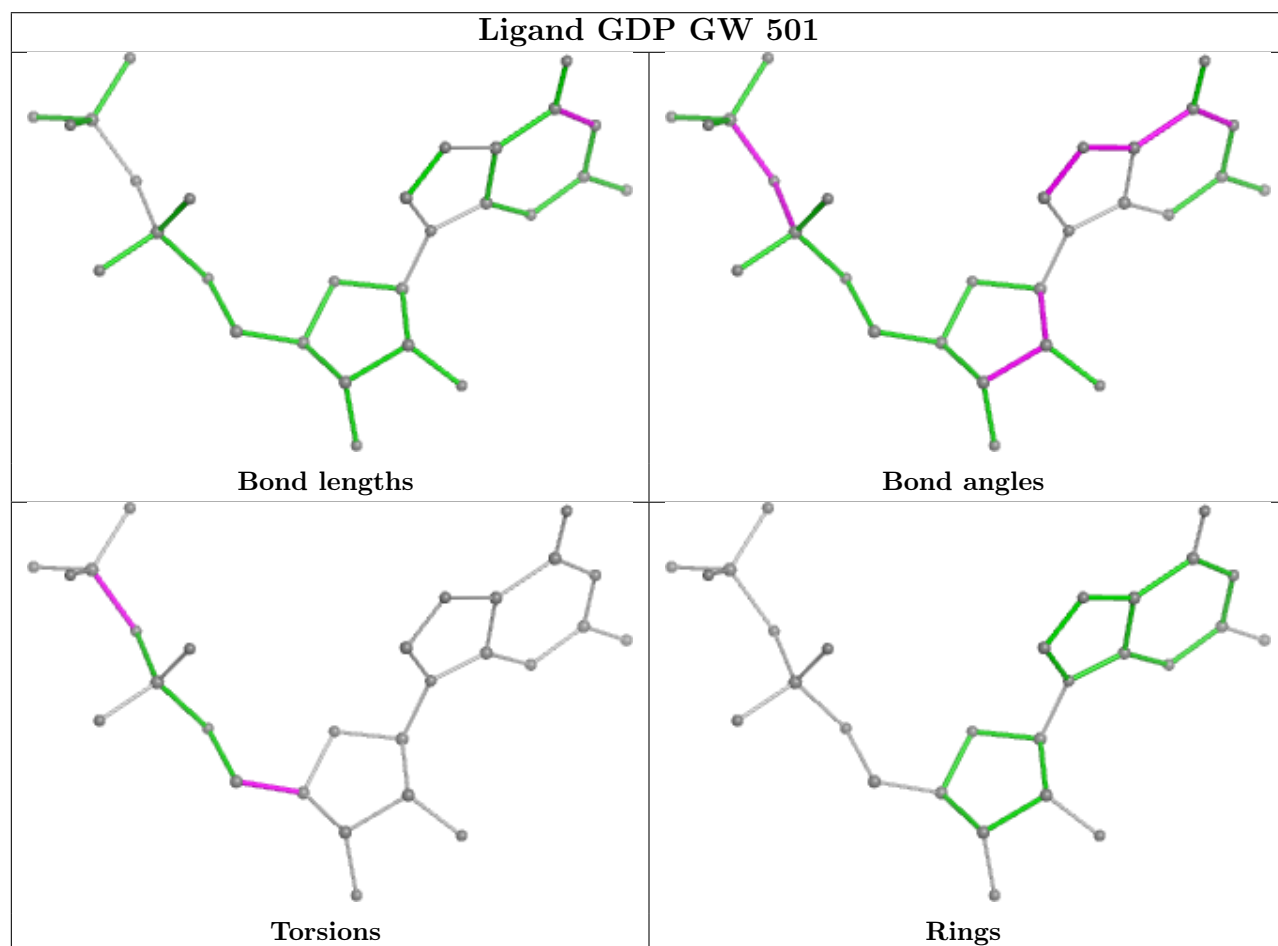
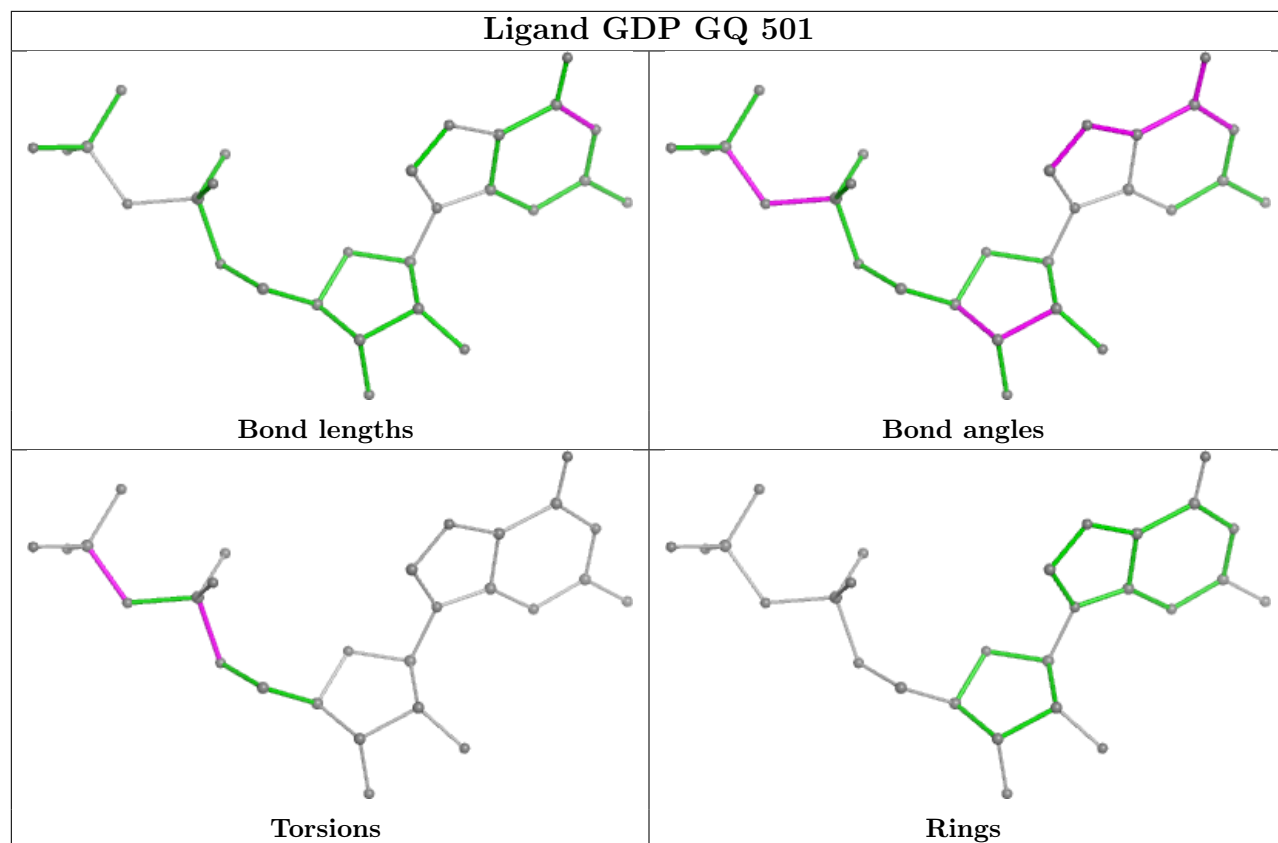


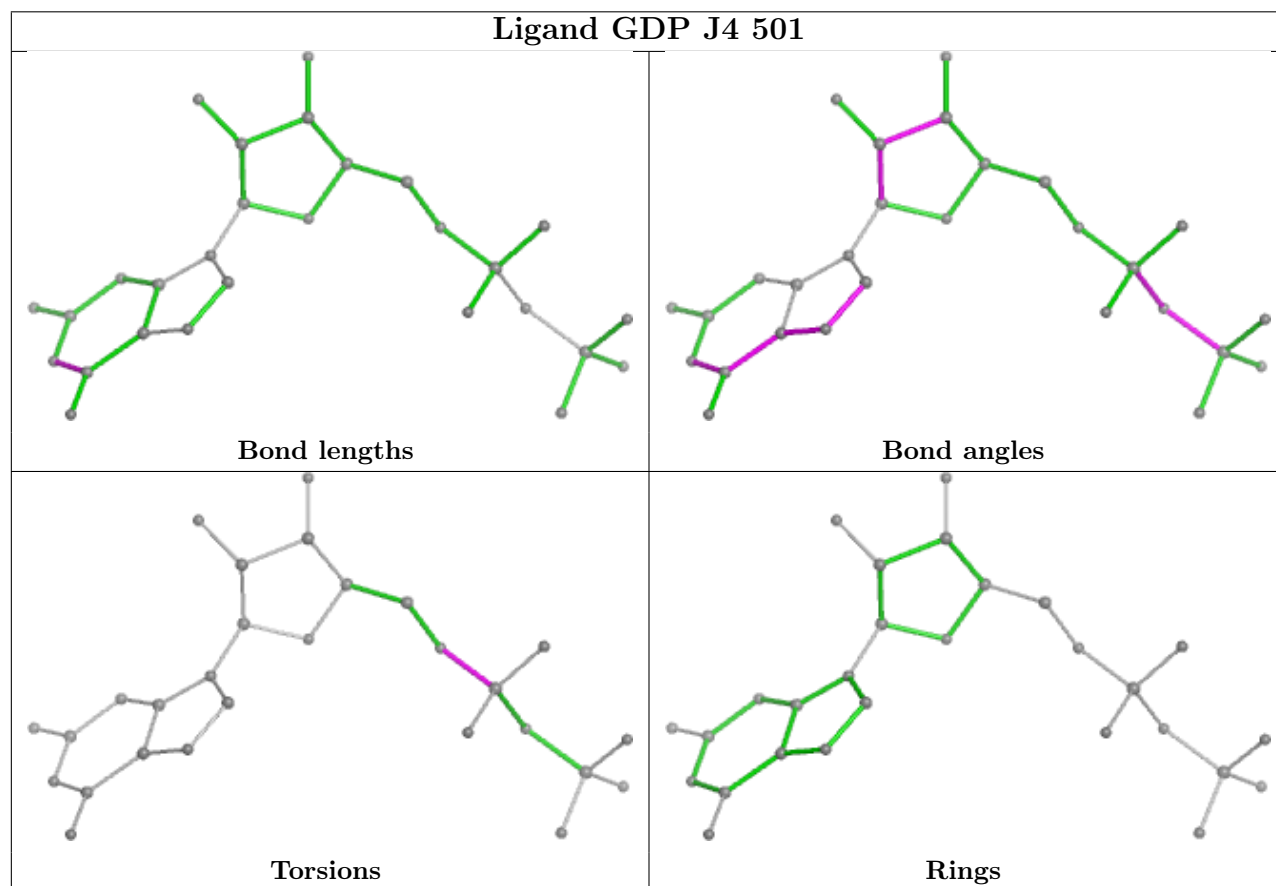
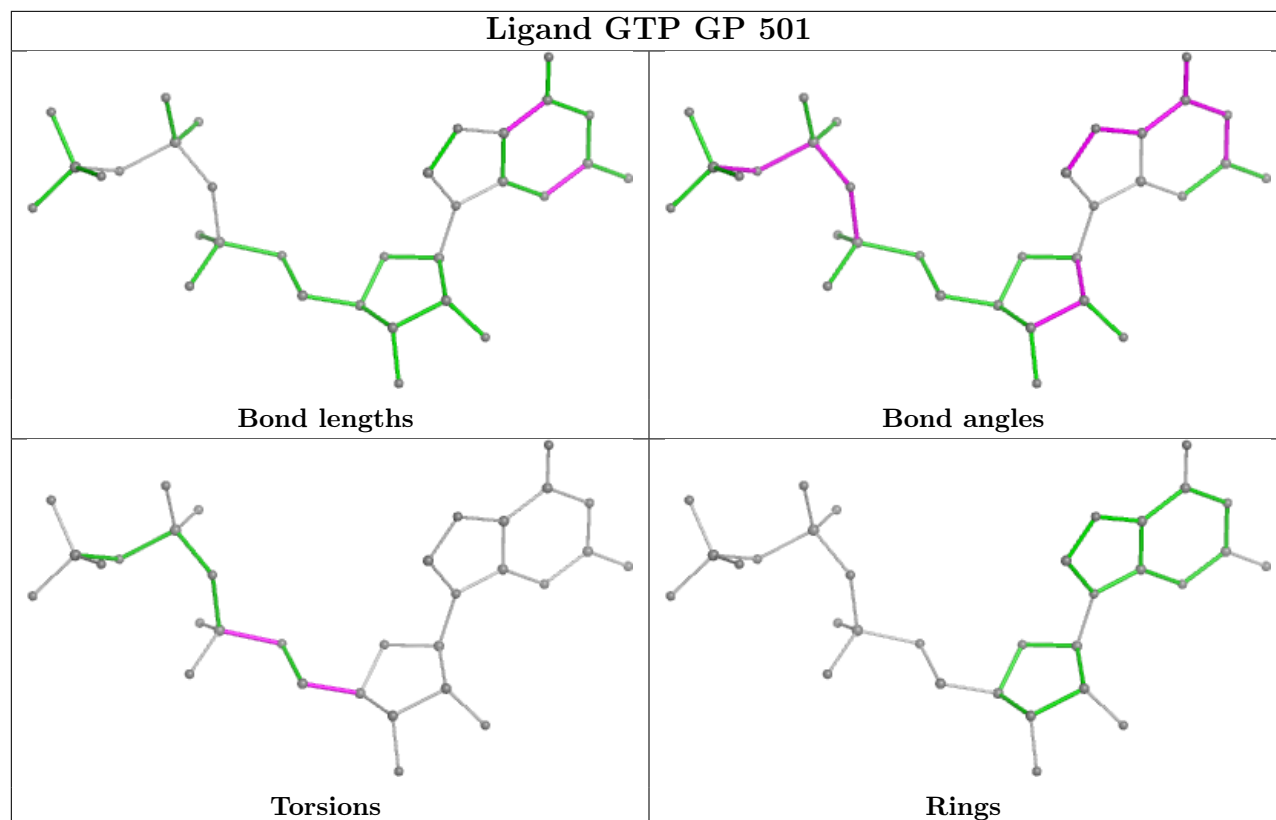


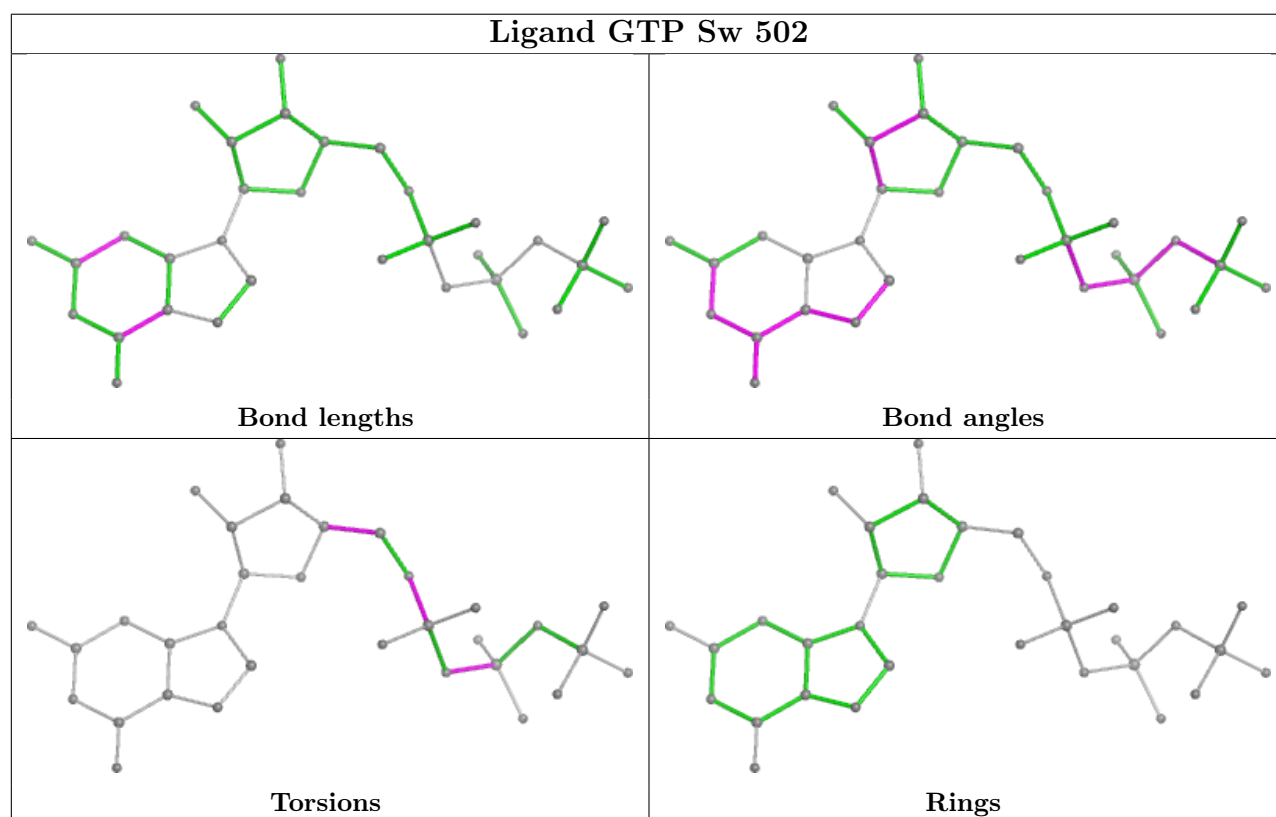
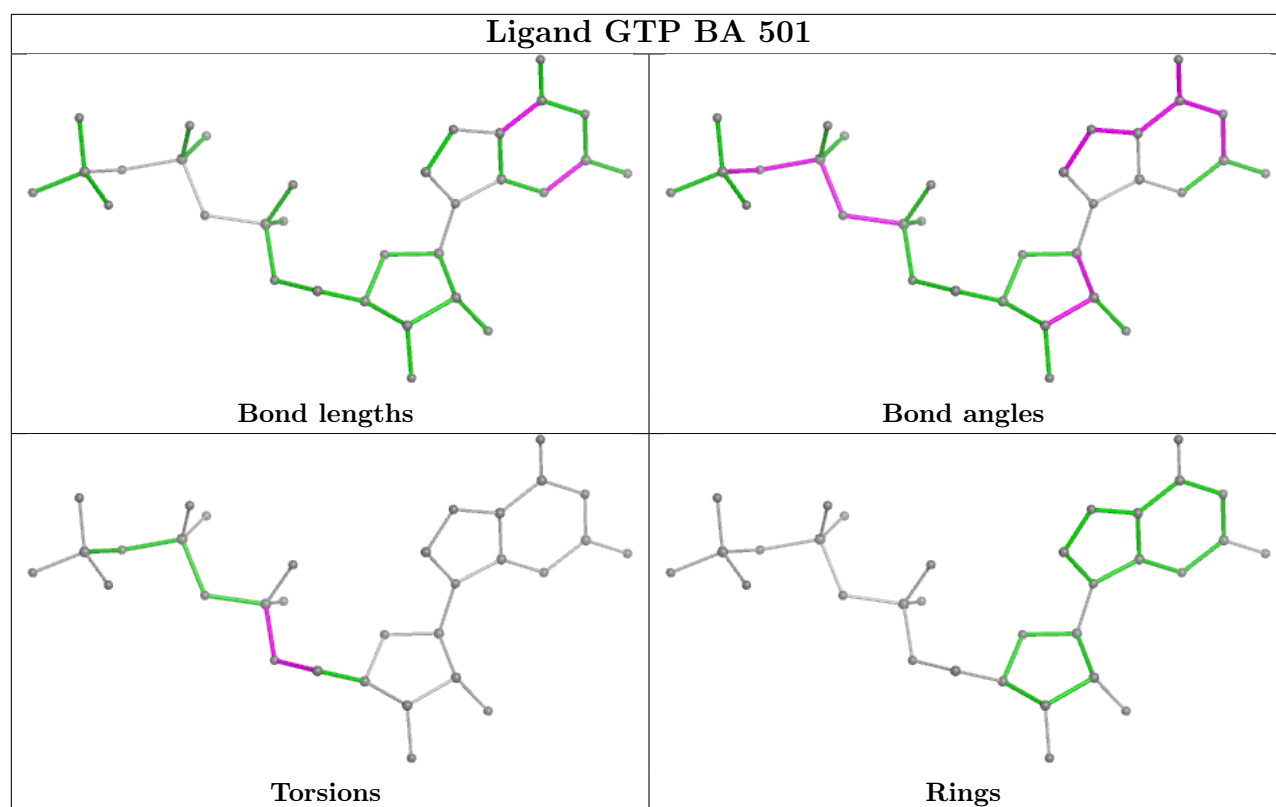




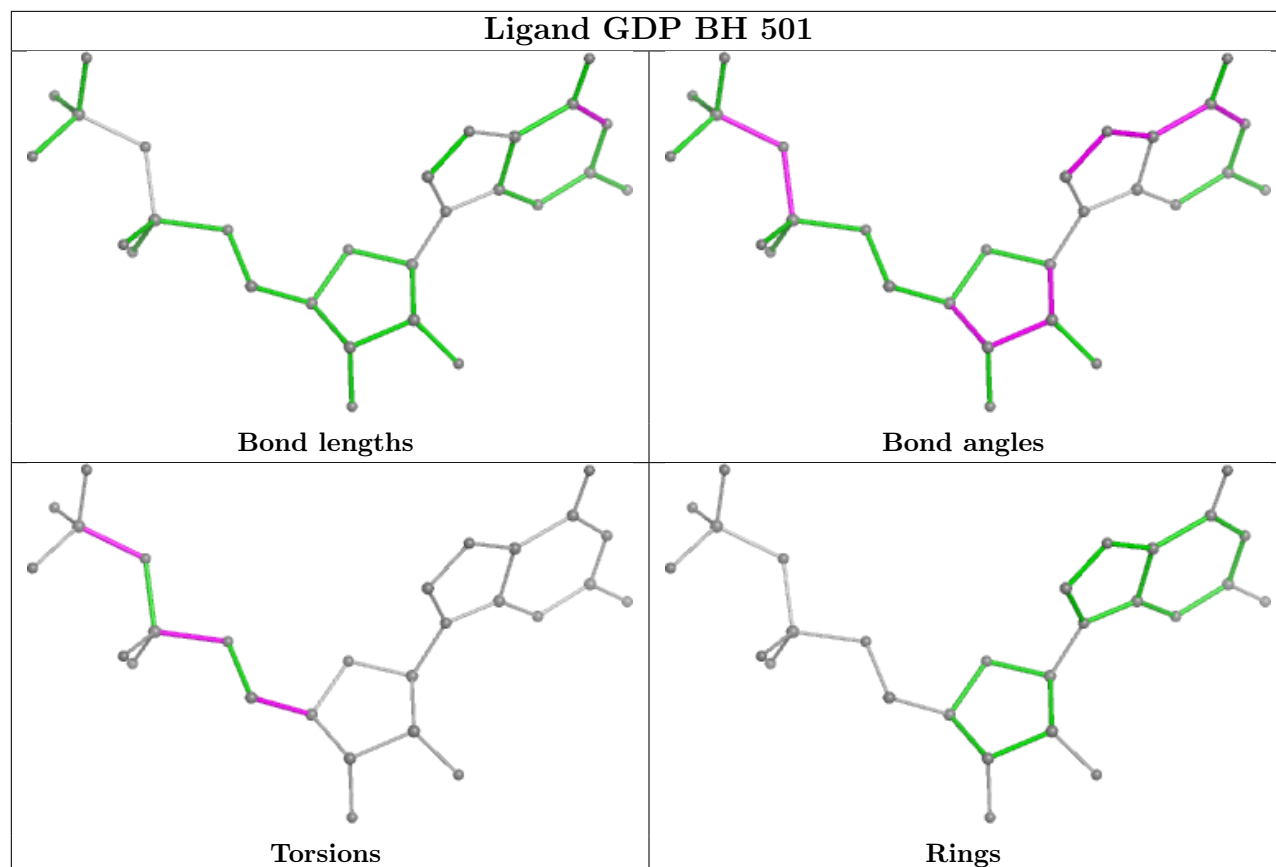




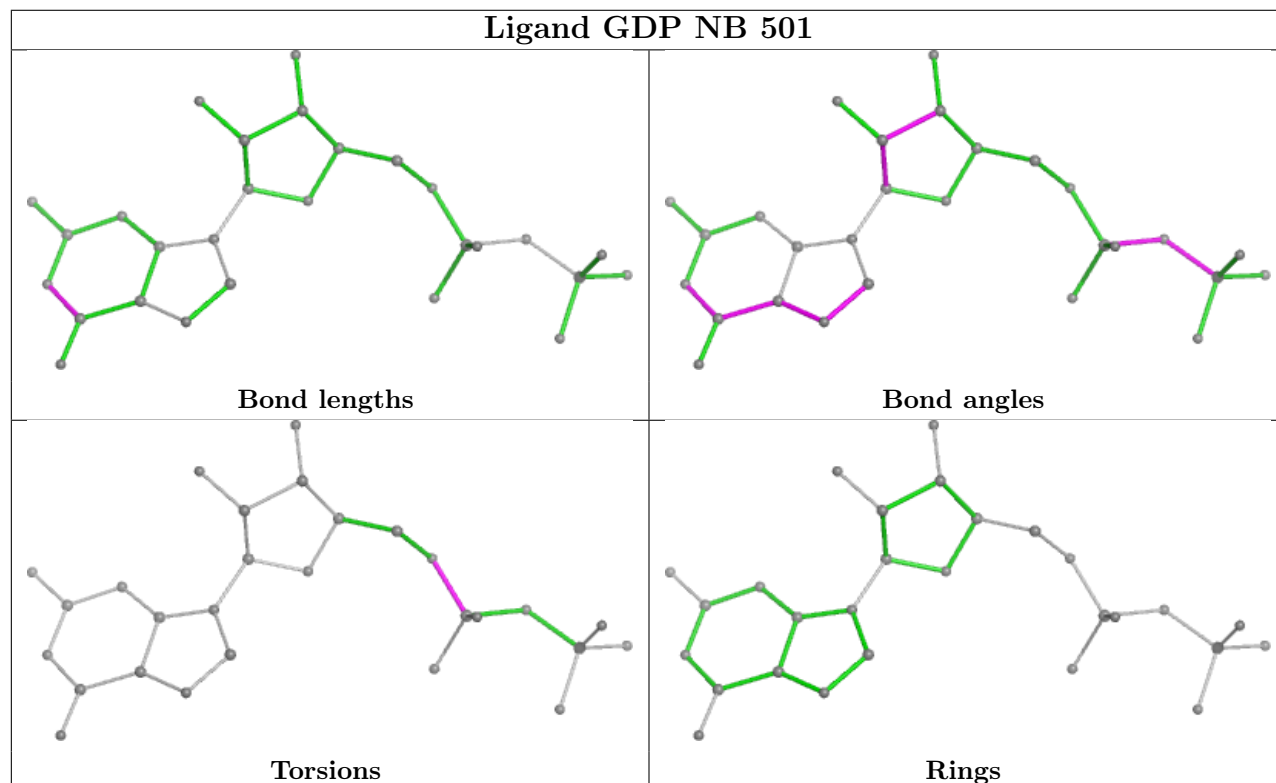




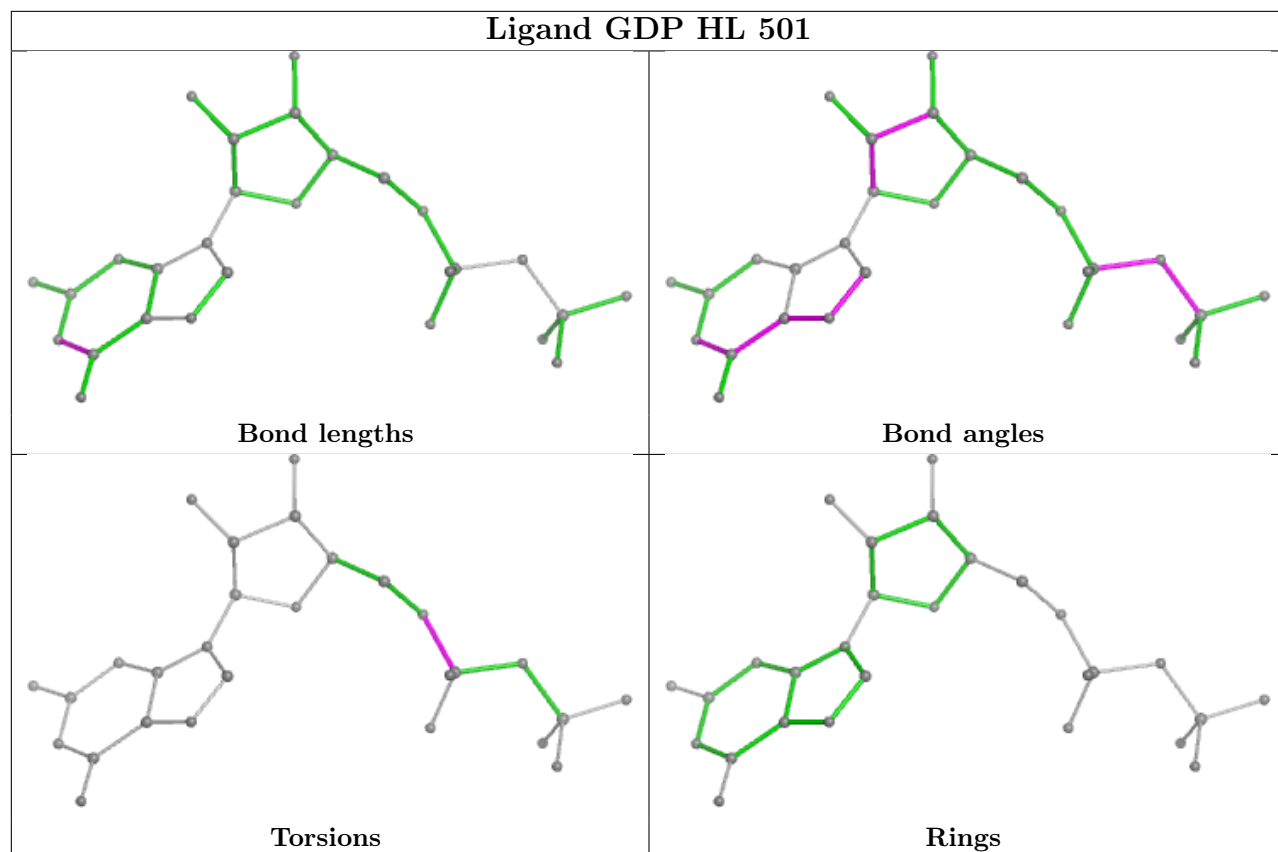
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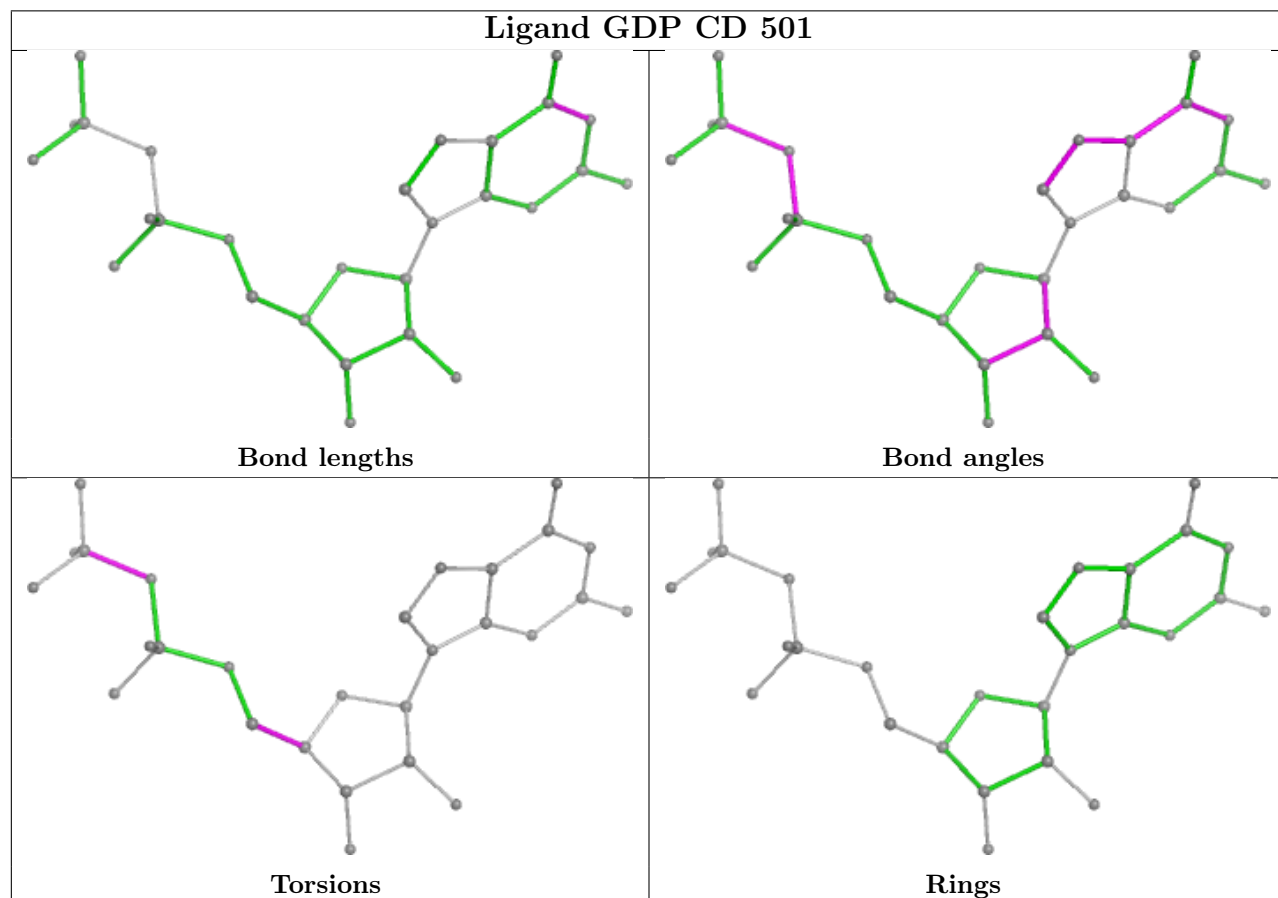
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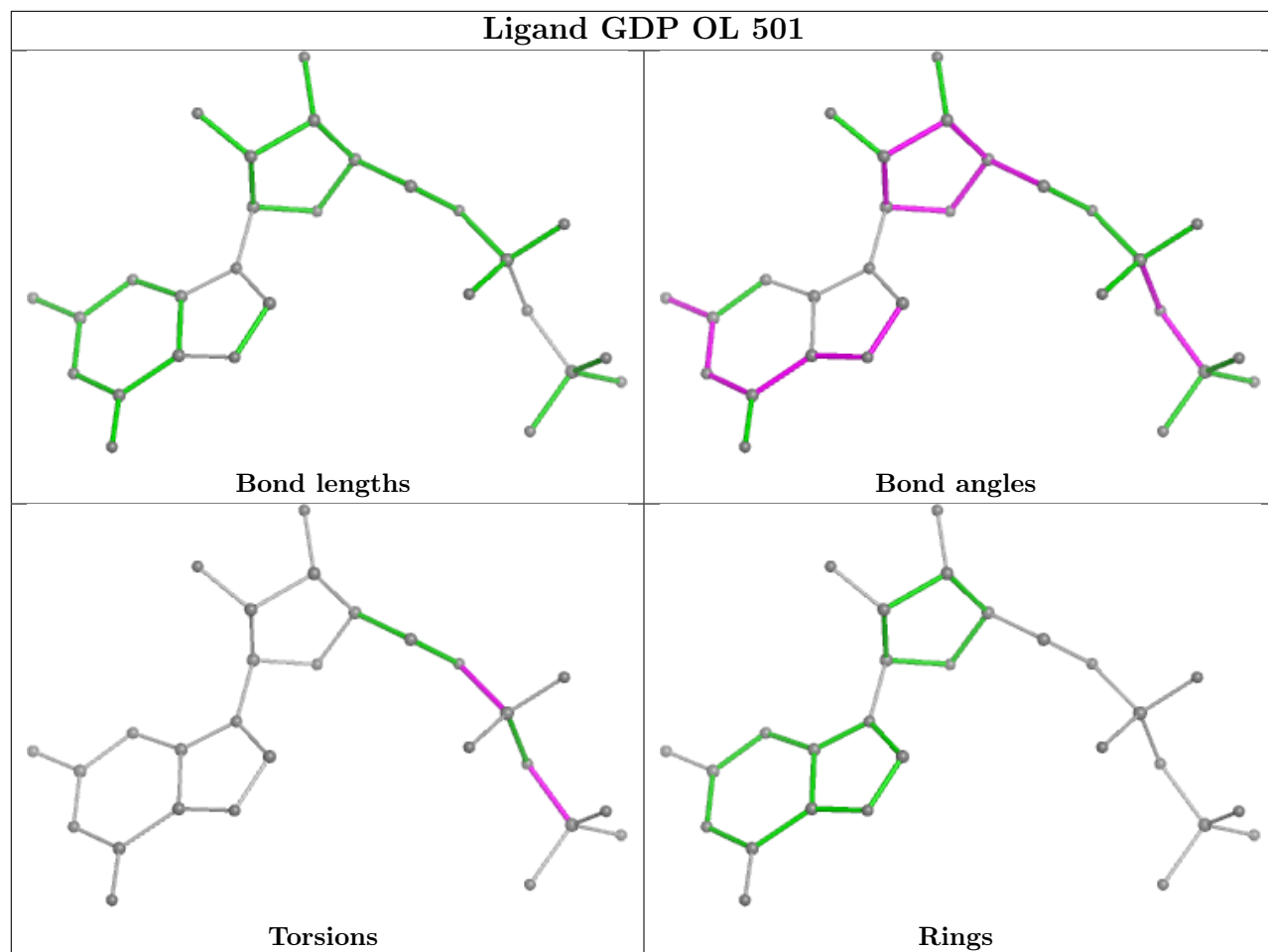
## Ligand GDP HL 501



## Ligand GDP CD 501

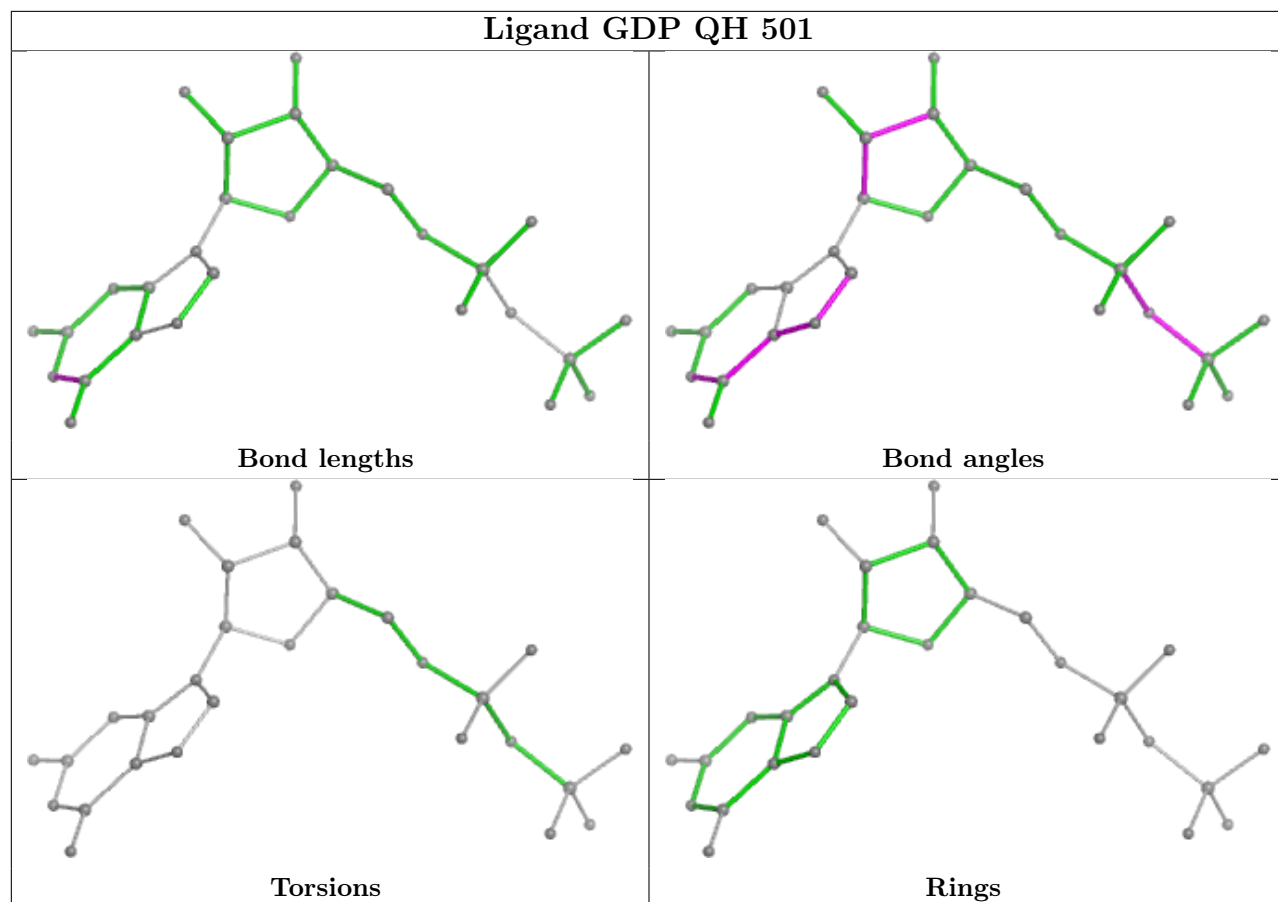


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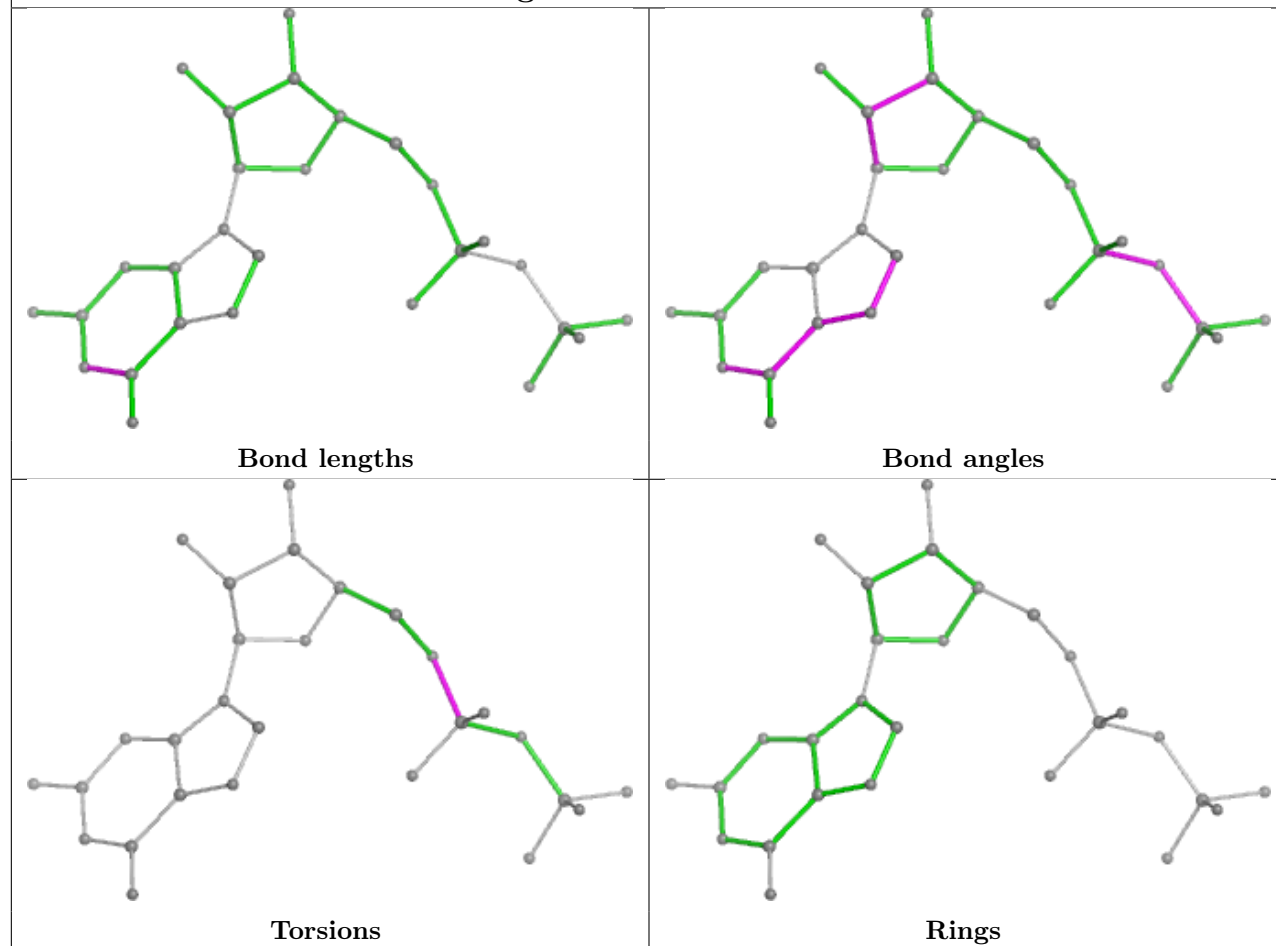




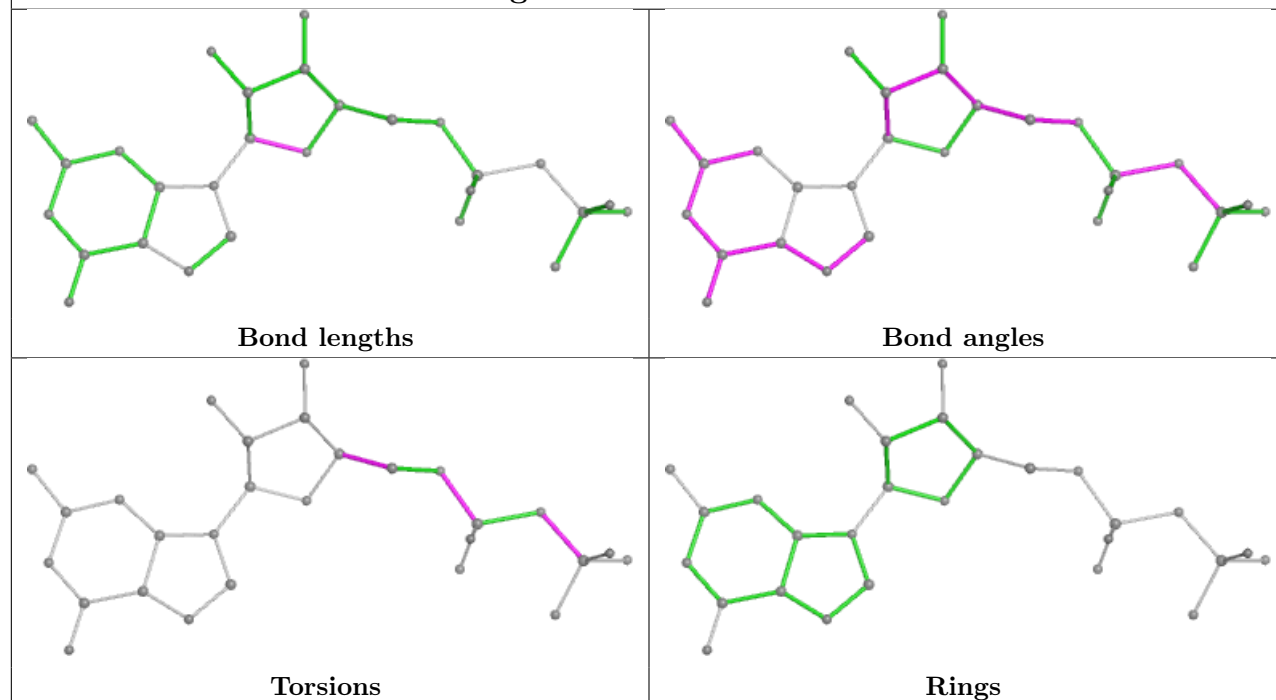
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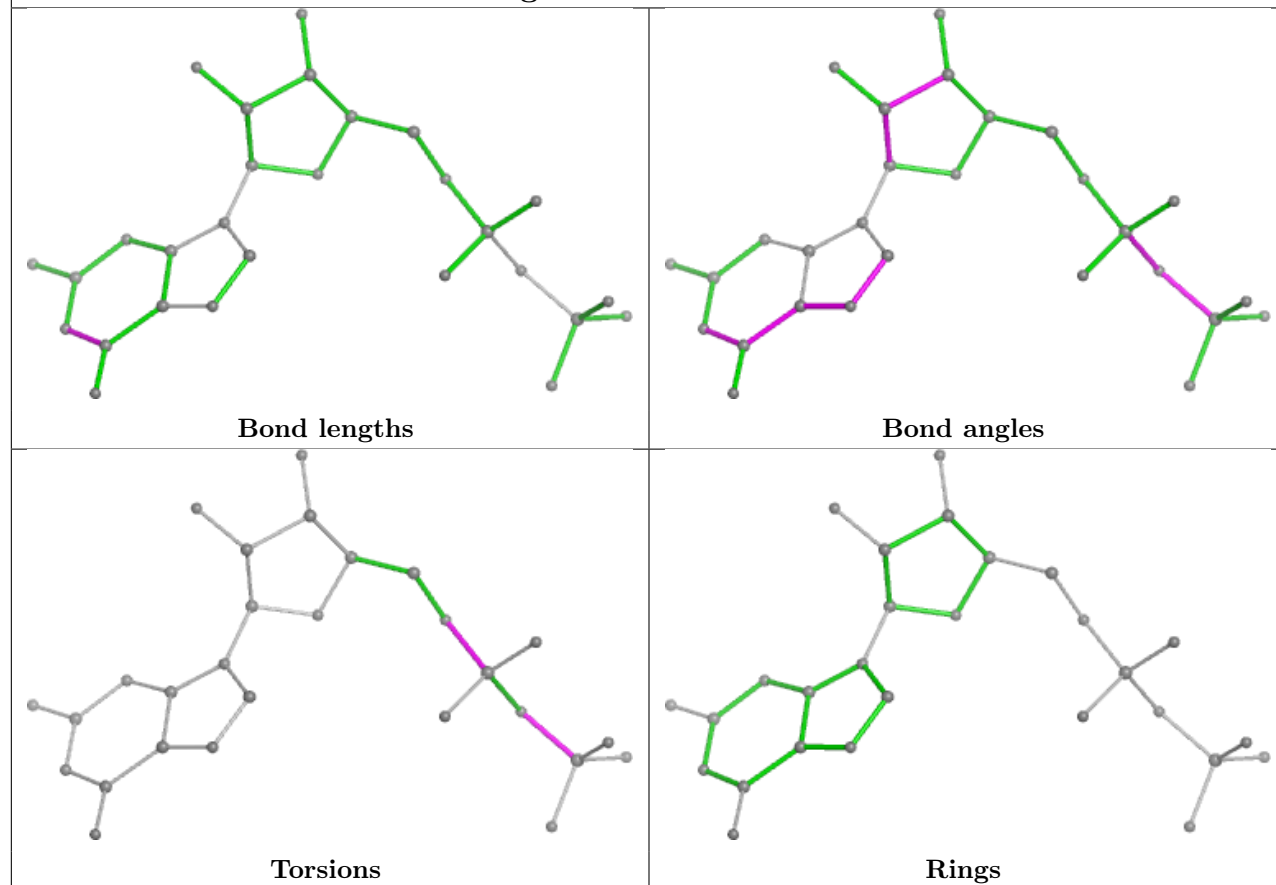
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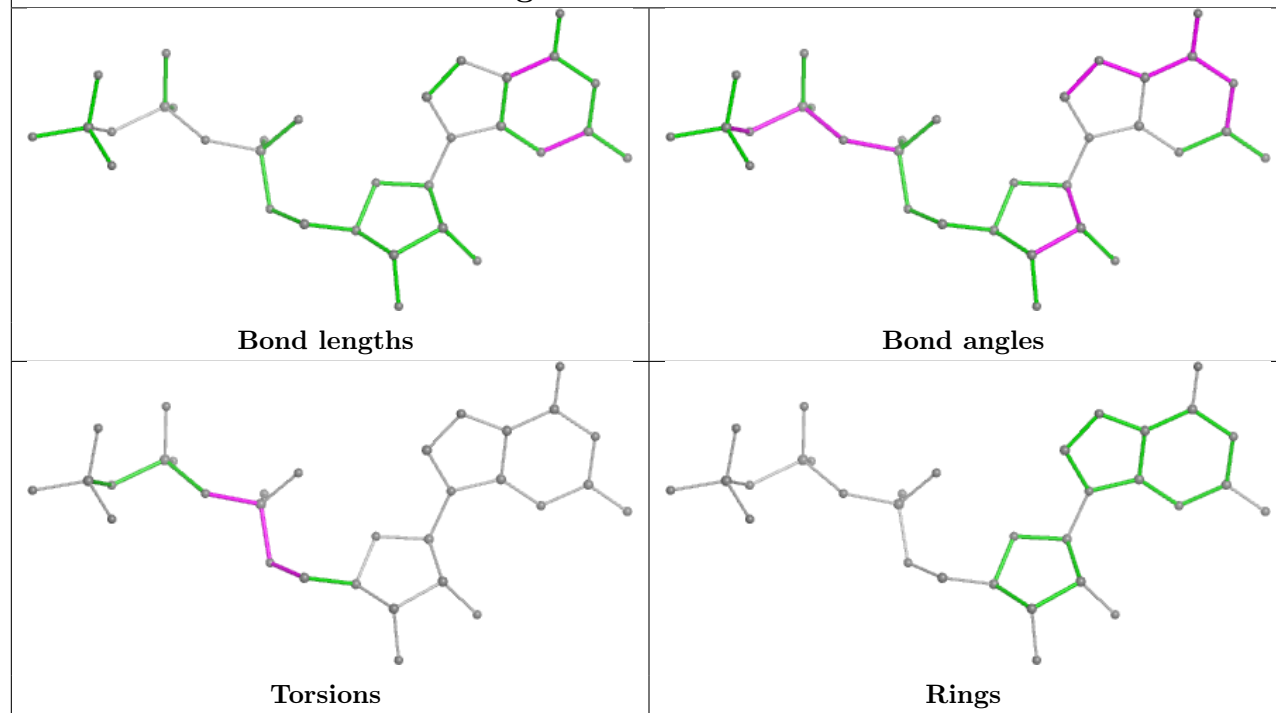
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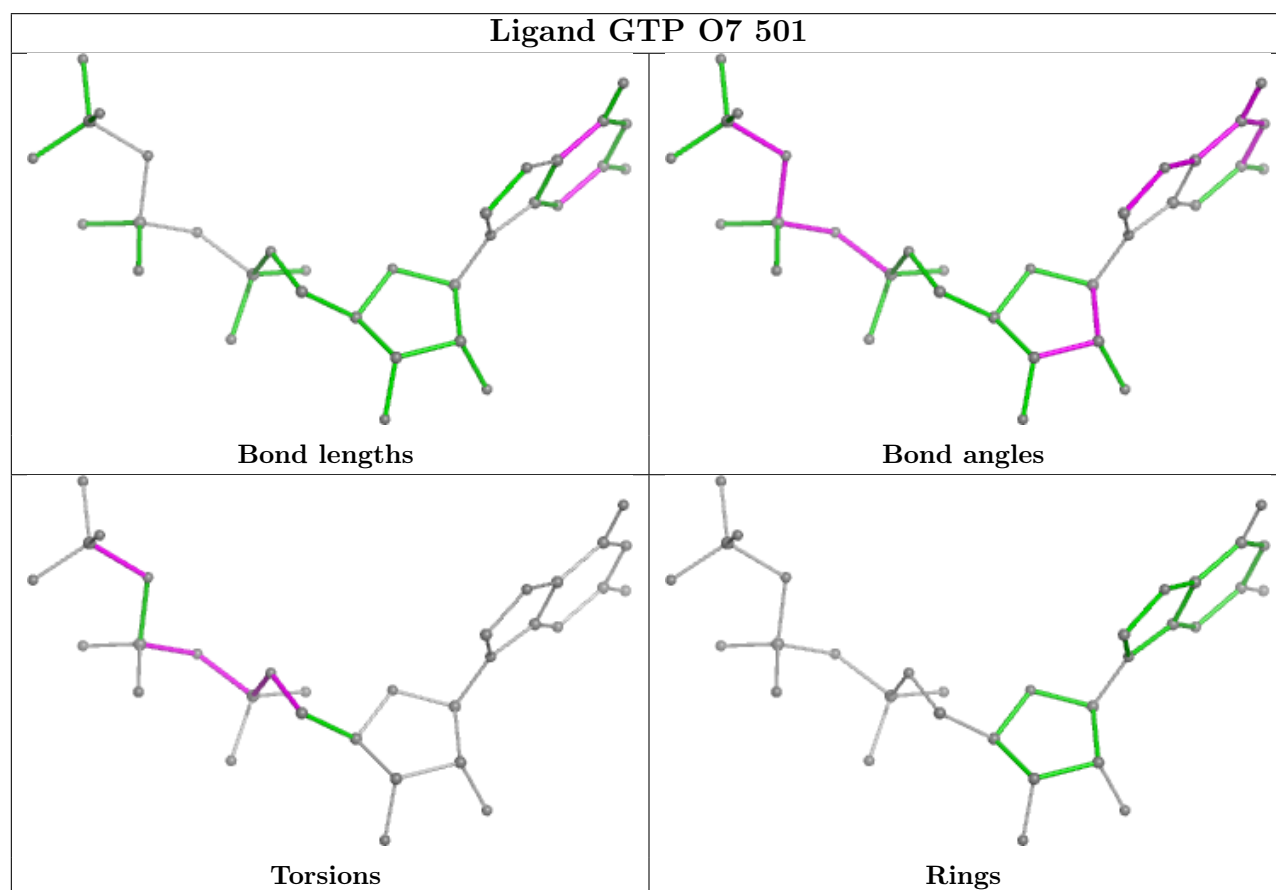
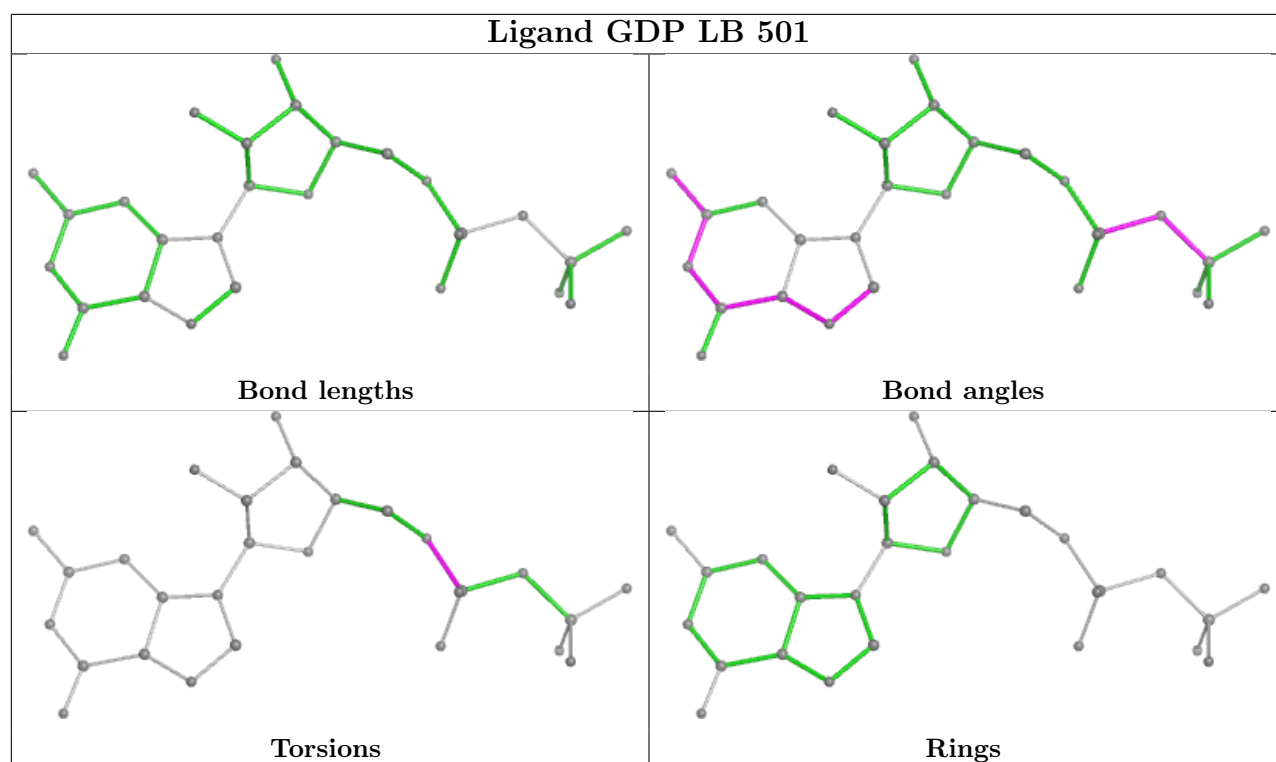


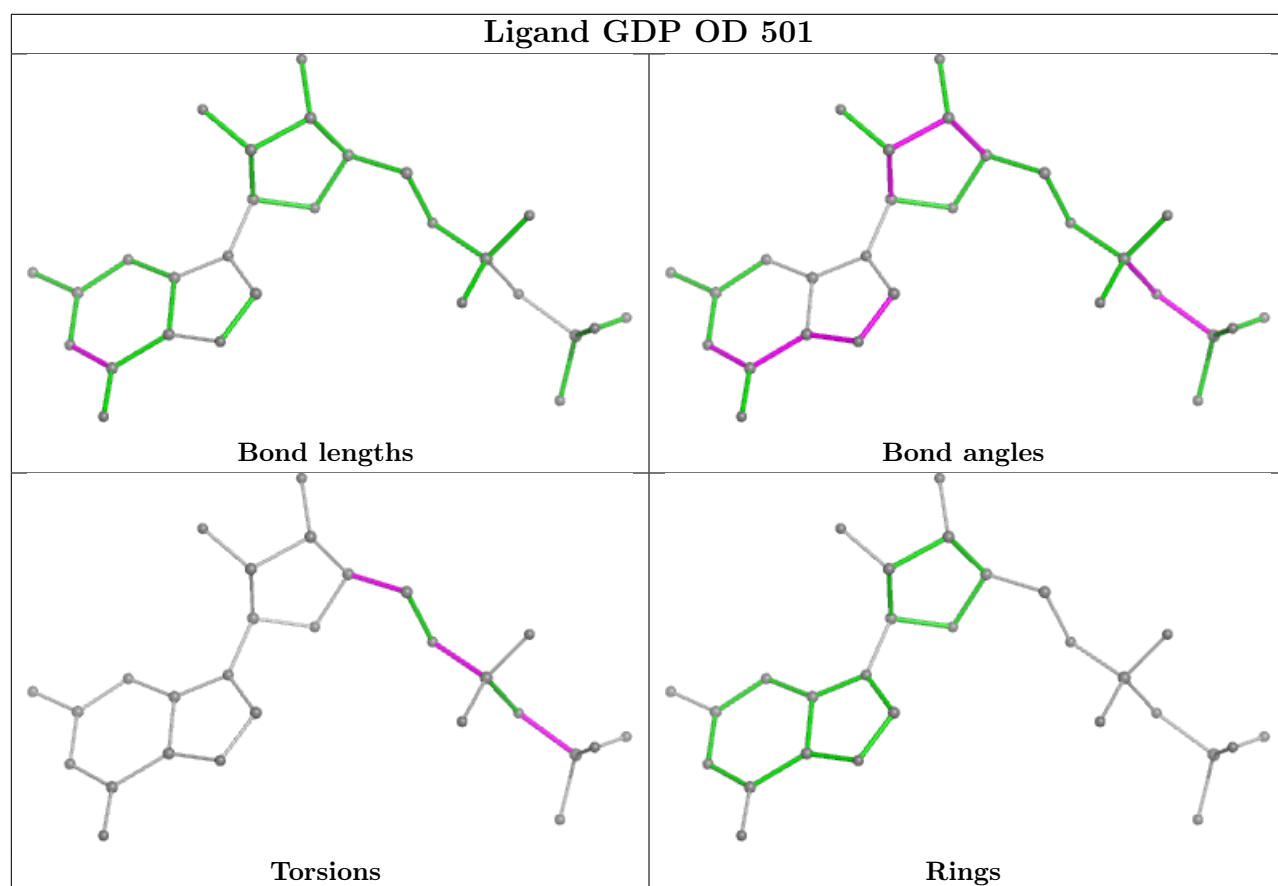
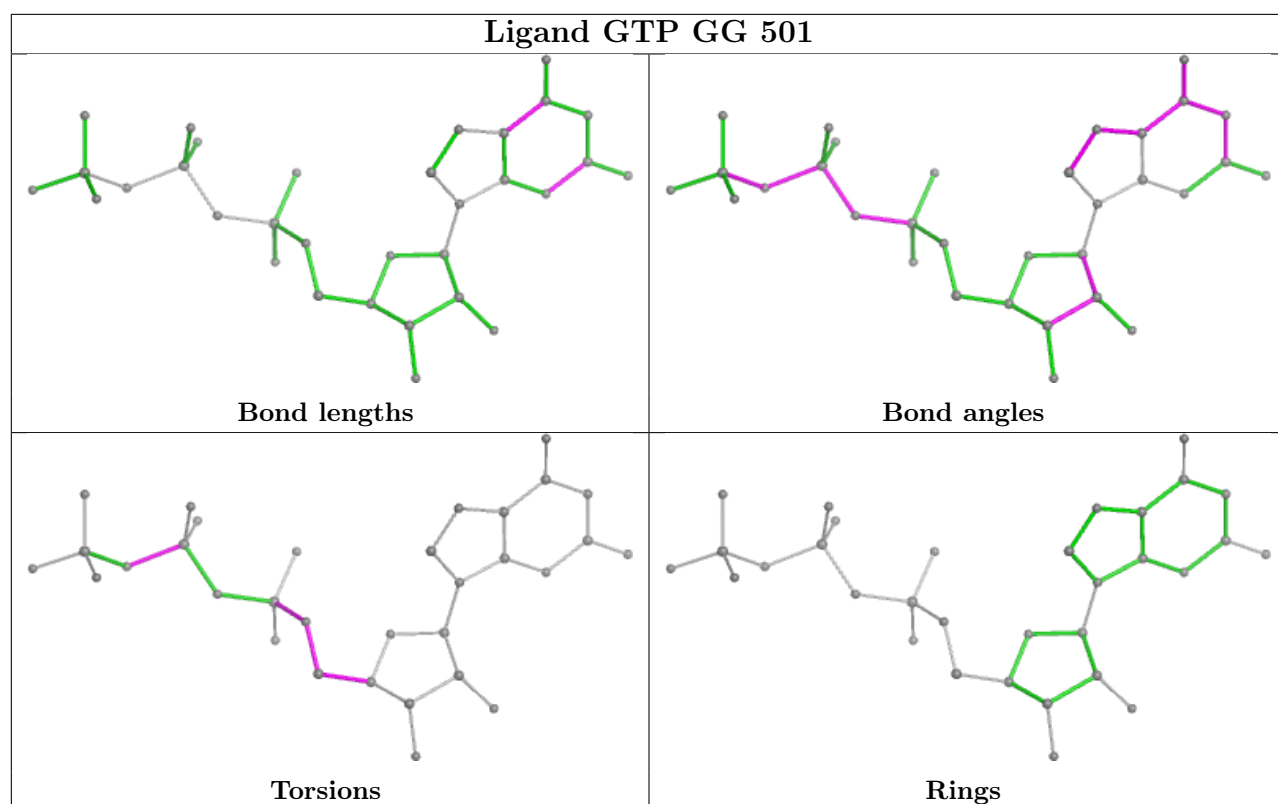
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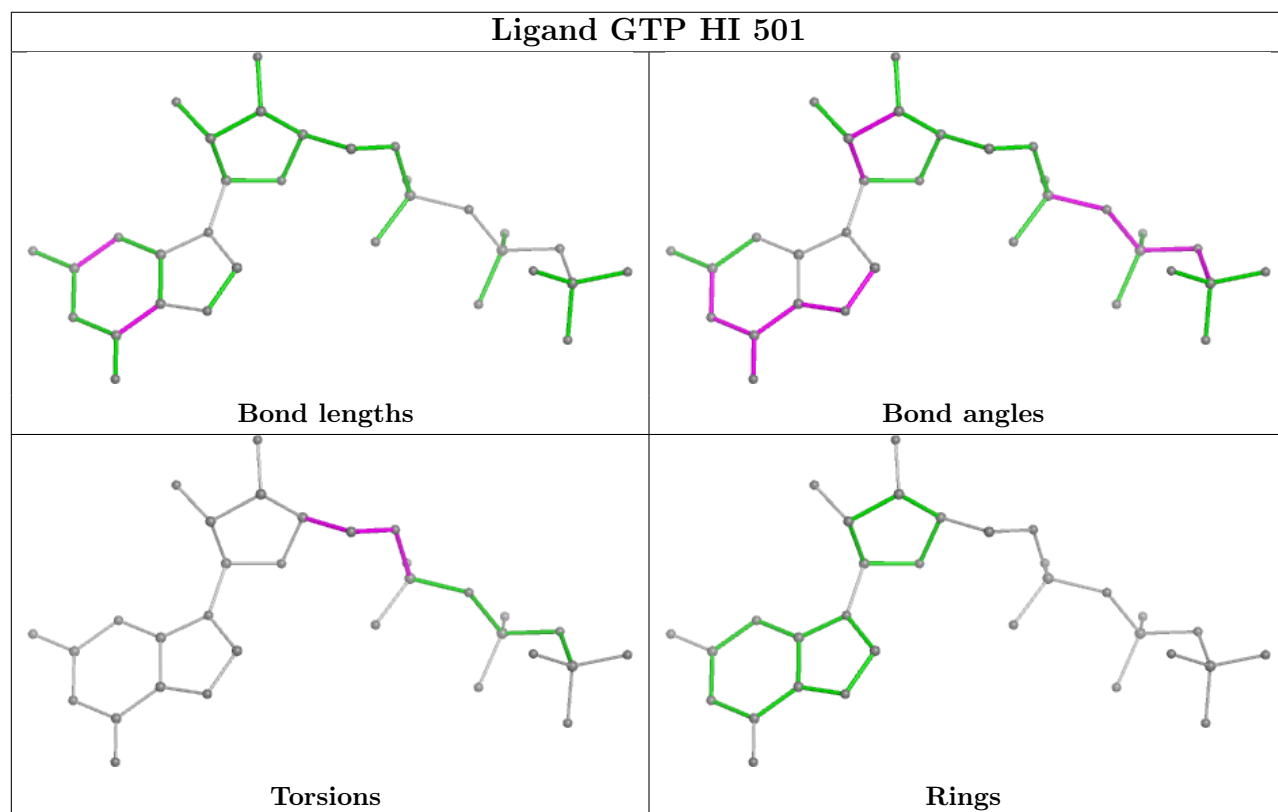
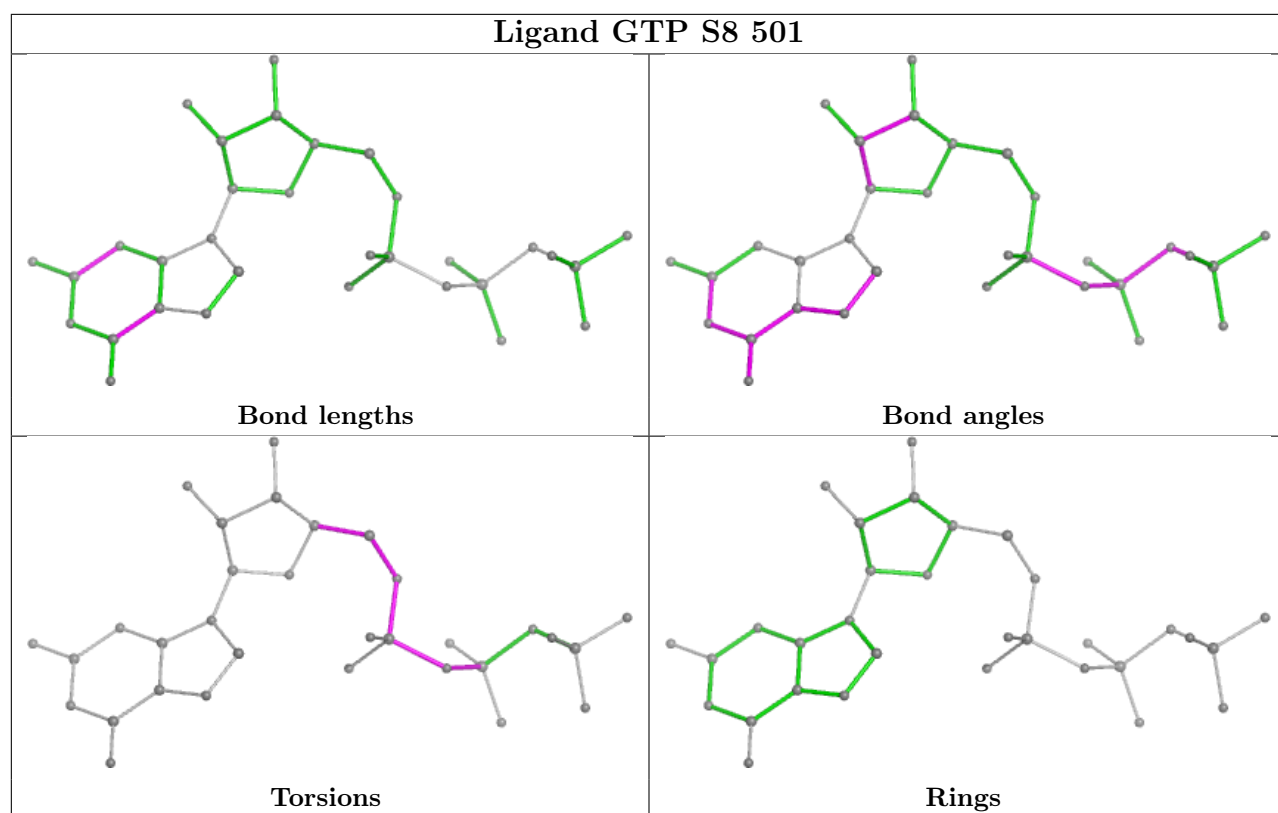


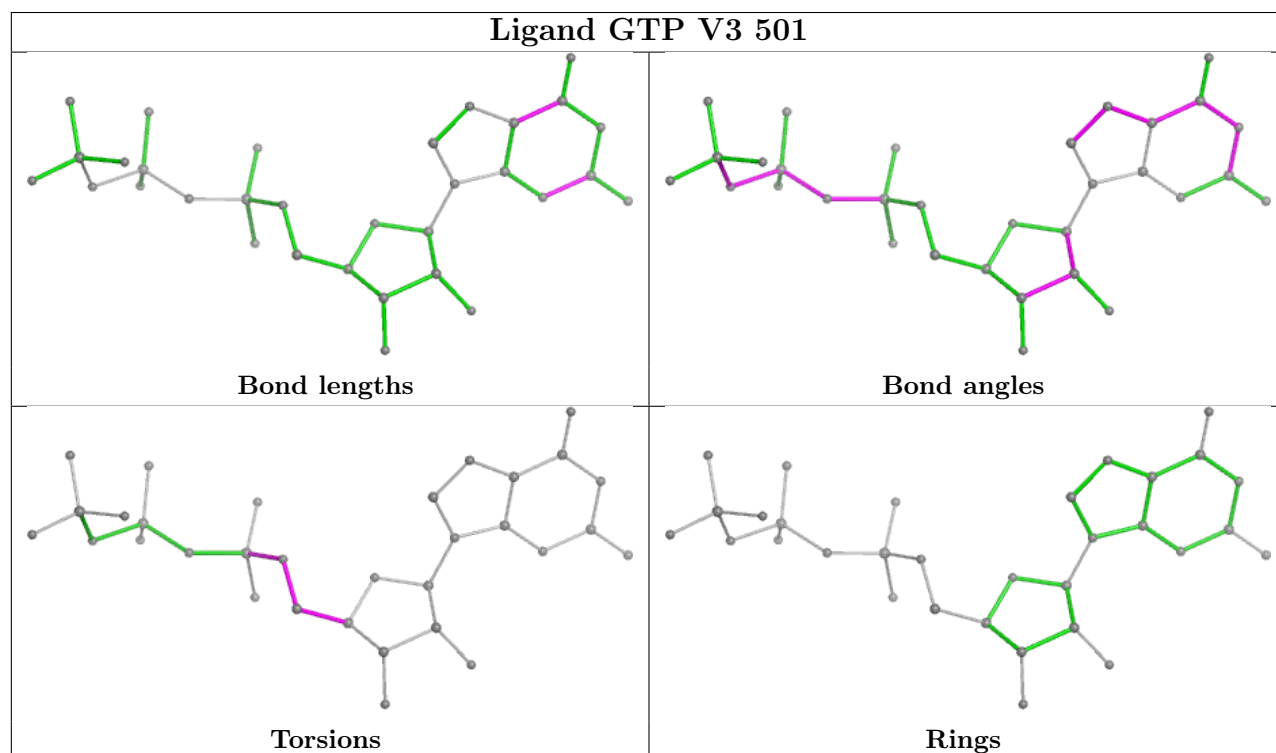
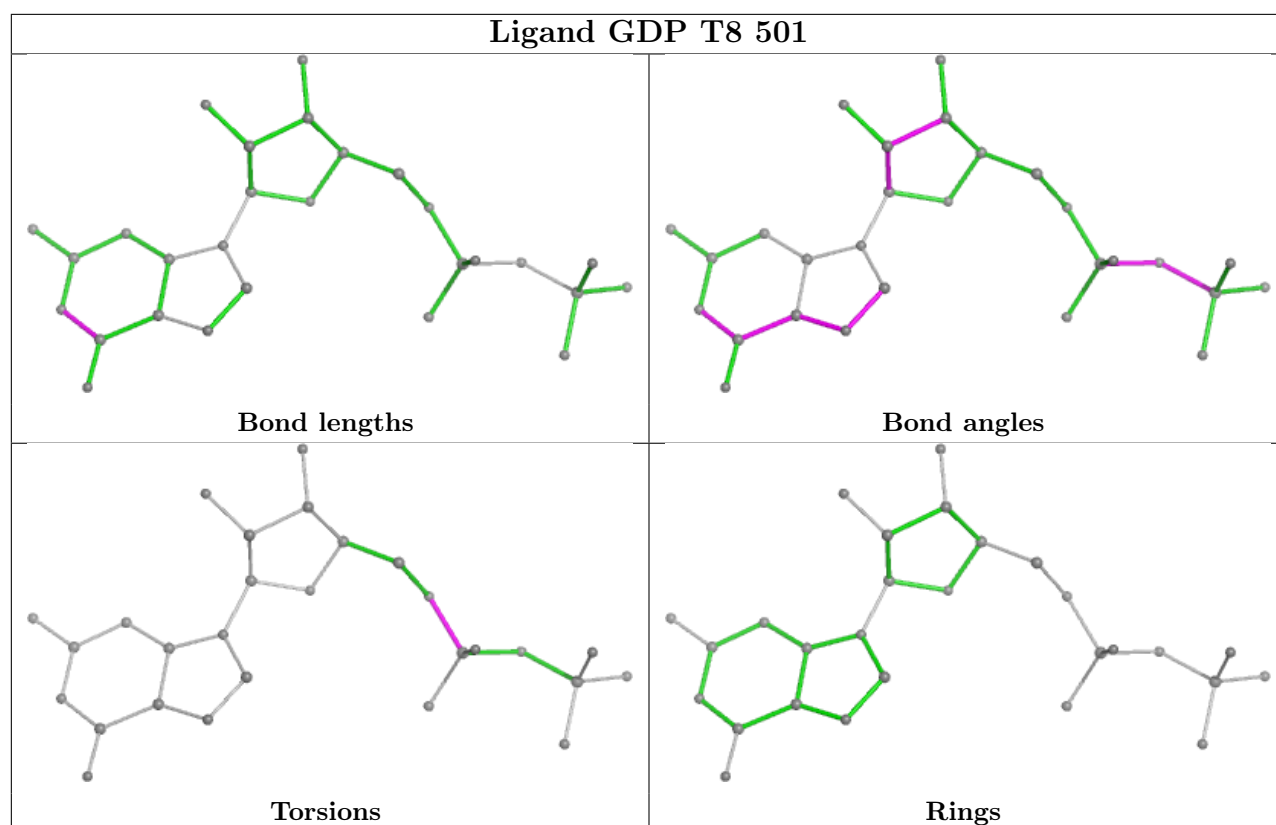
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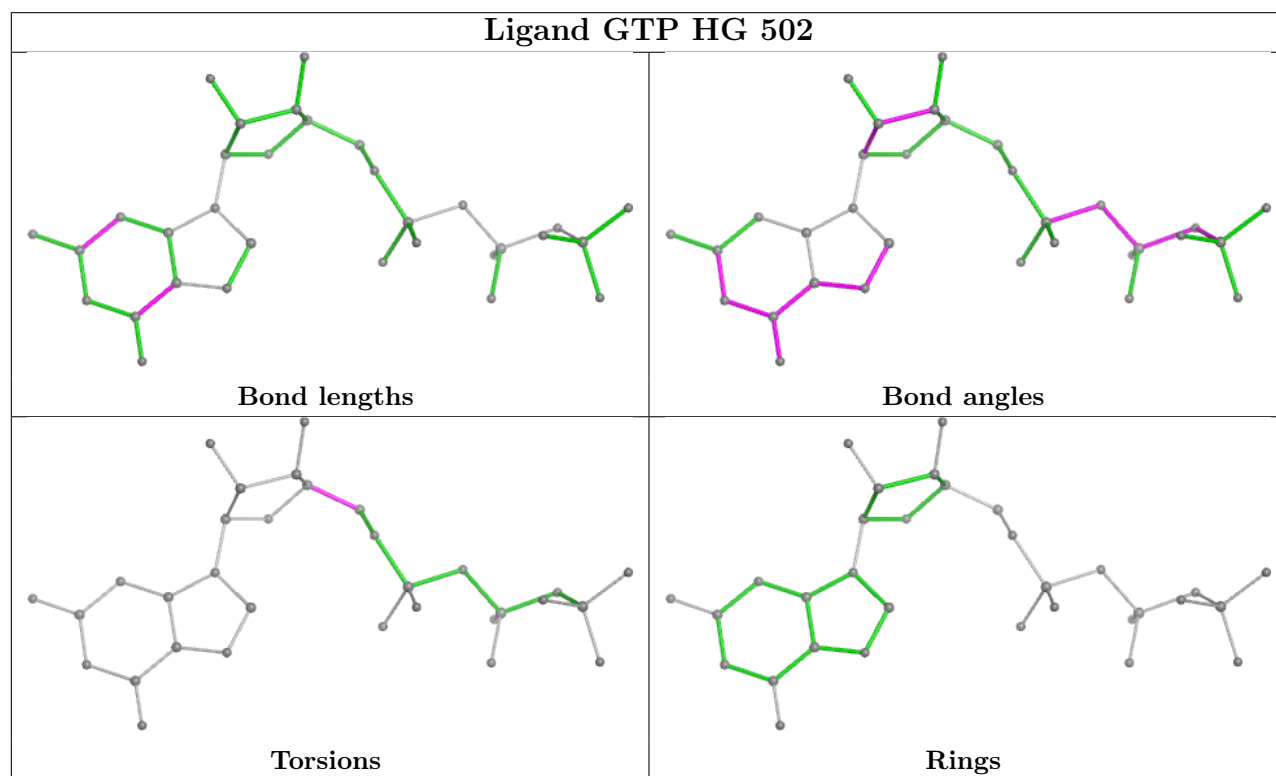
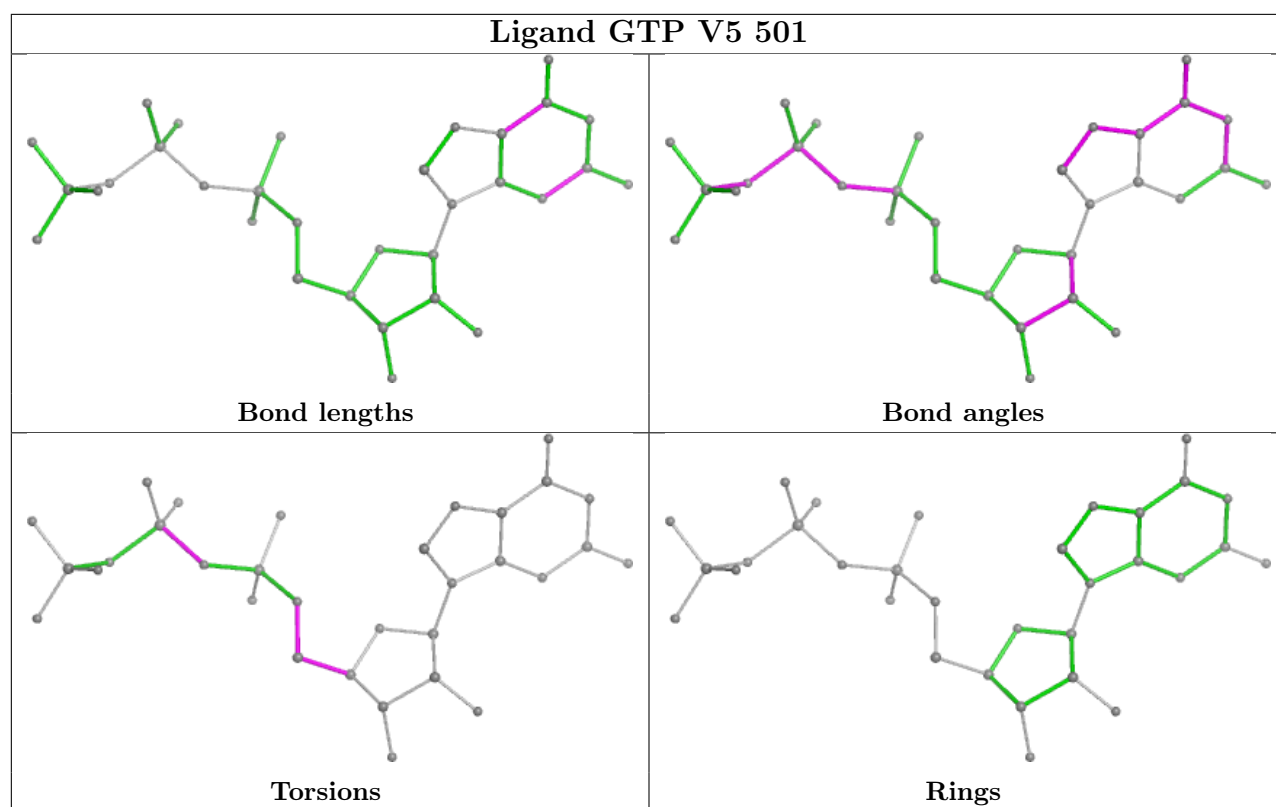






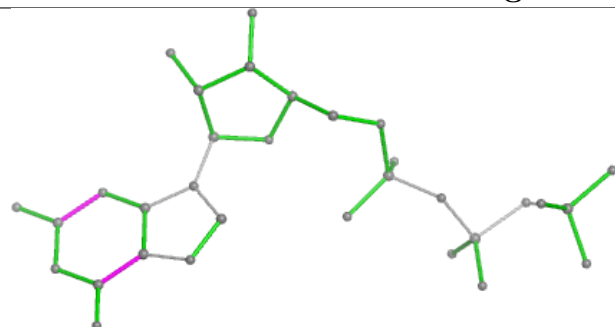




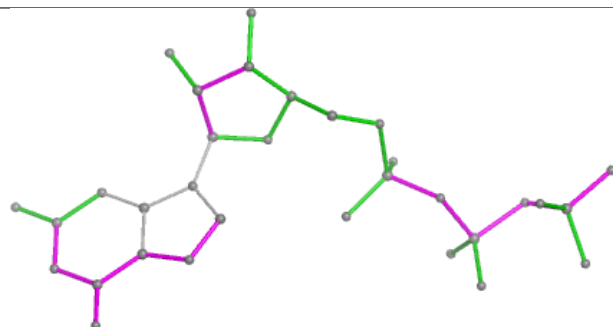




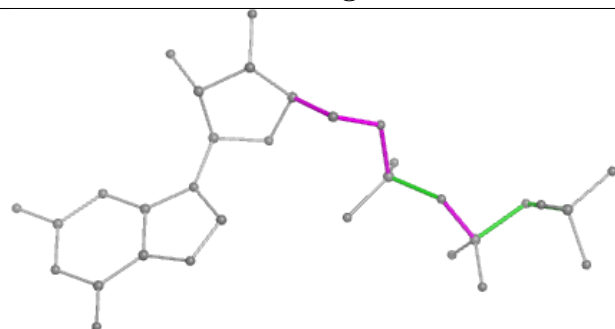
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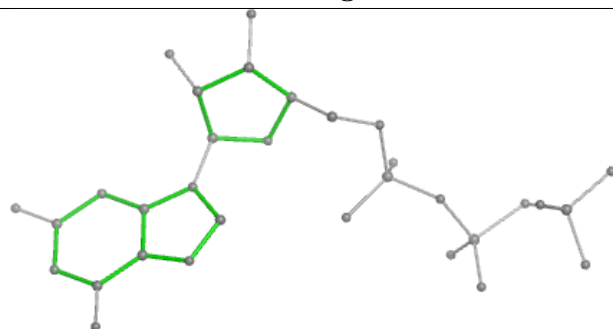
Bond lengths



Bond angles

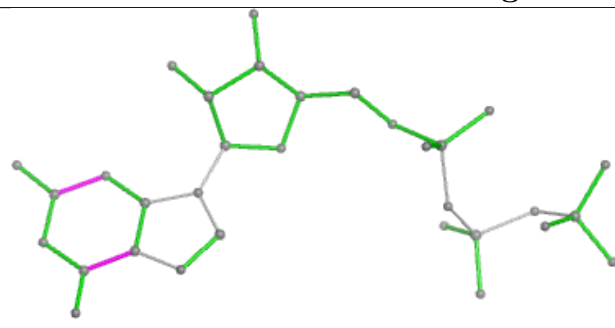


Torsions

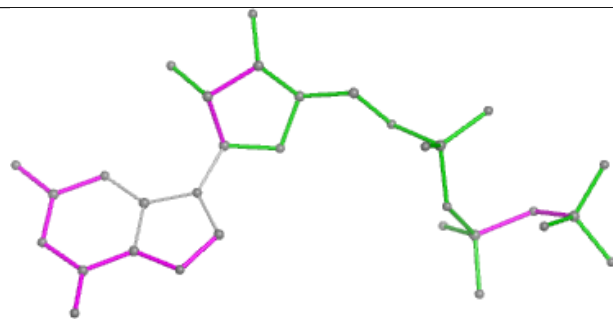


Rings

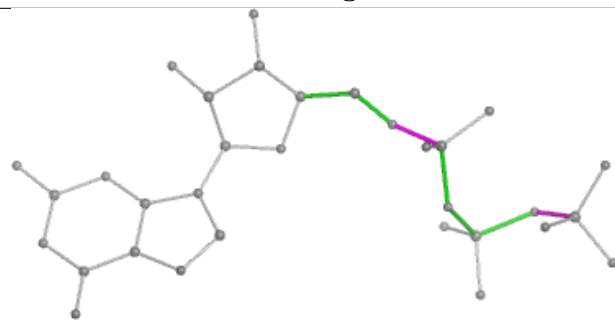
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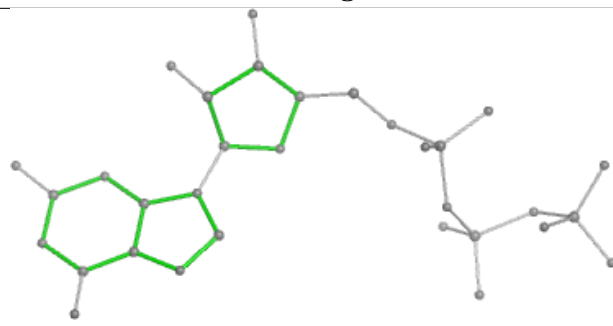
Bond lengths



Bond angles

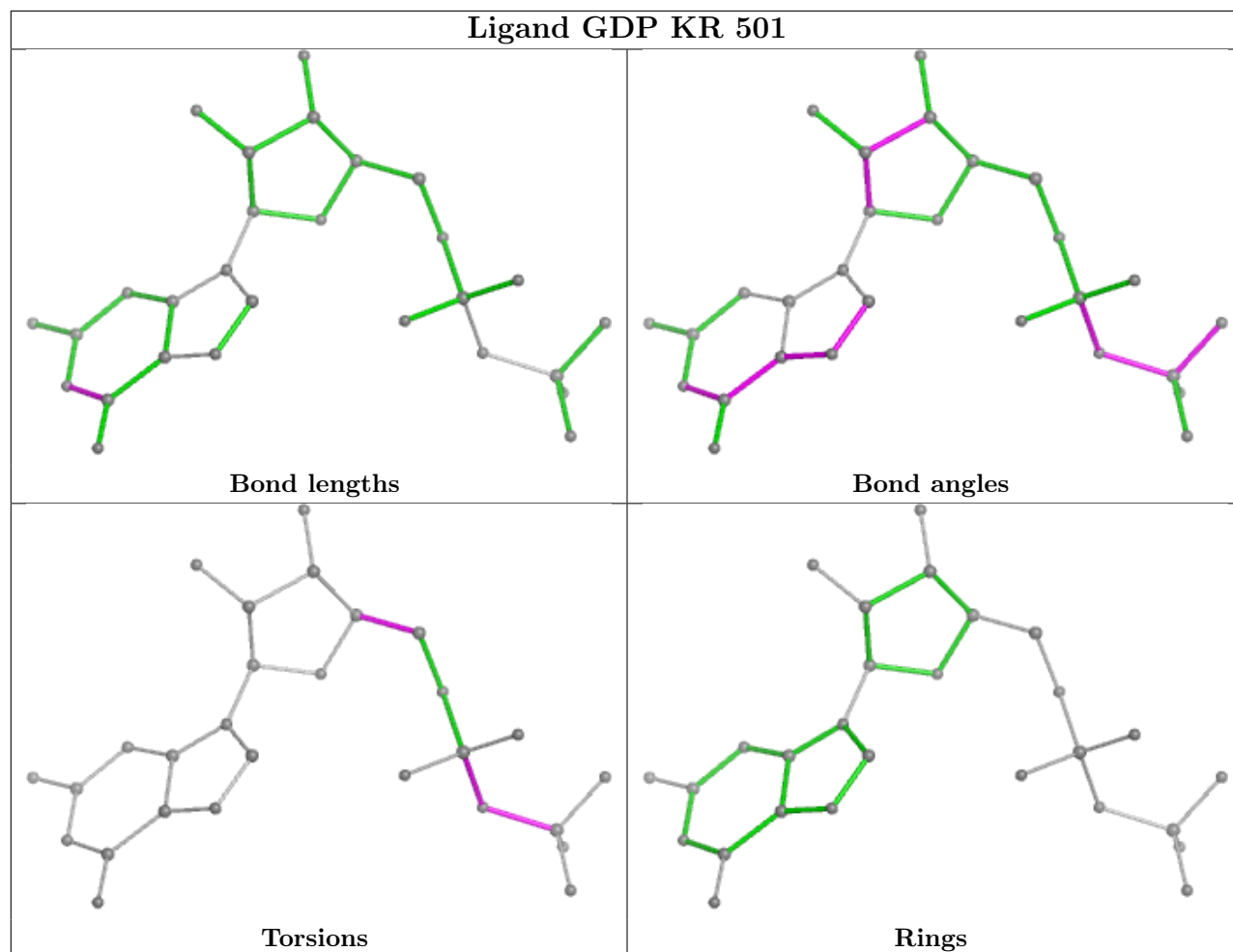


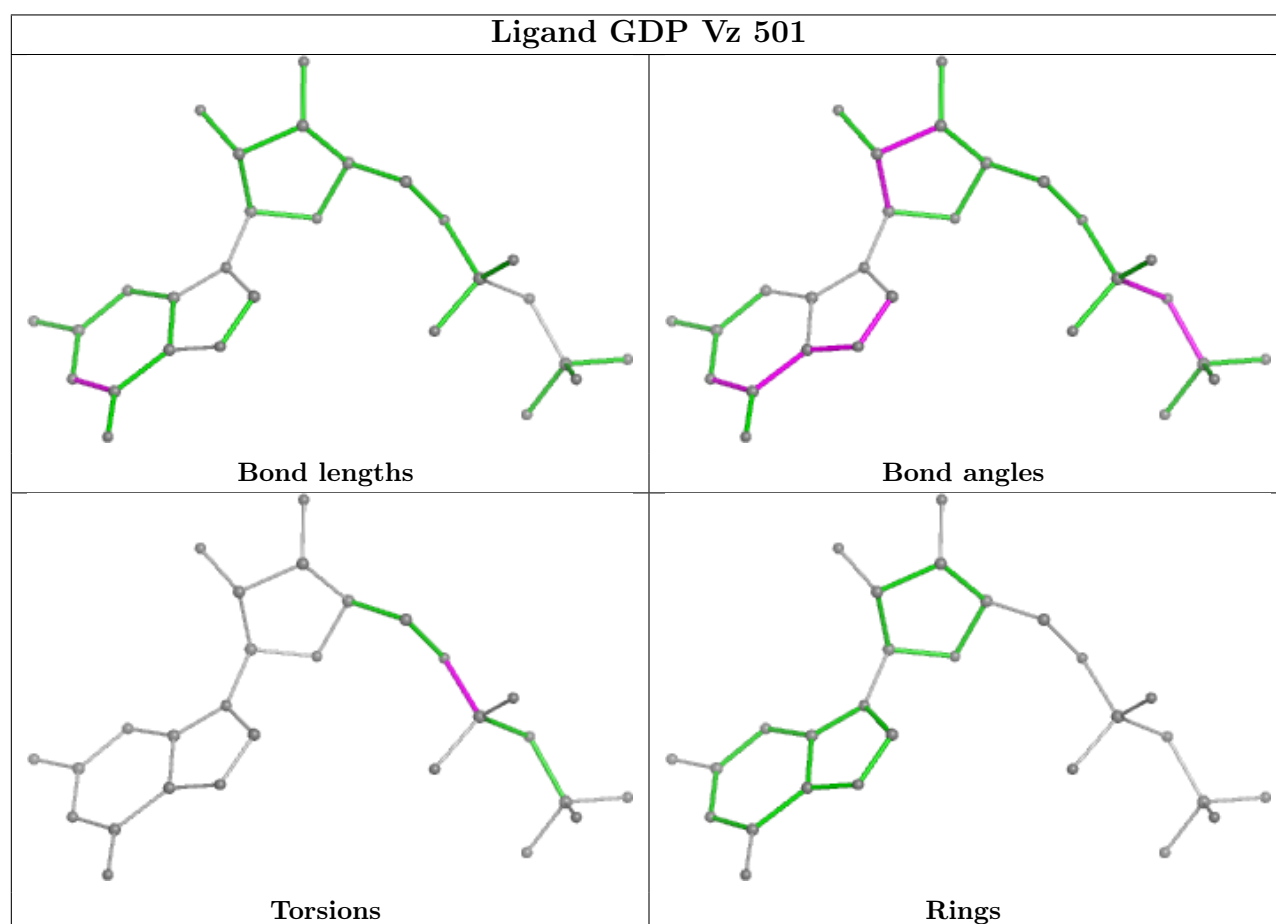
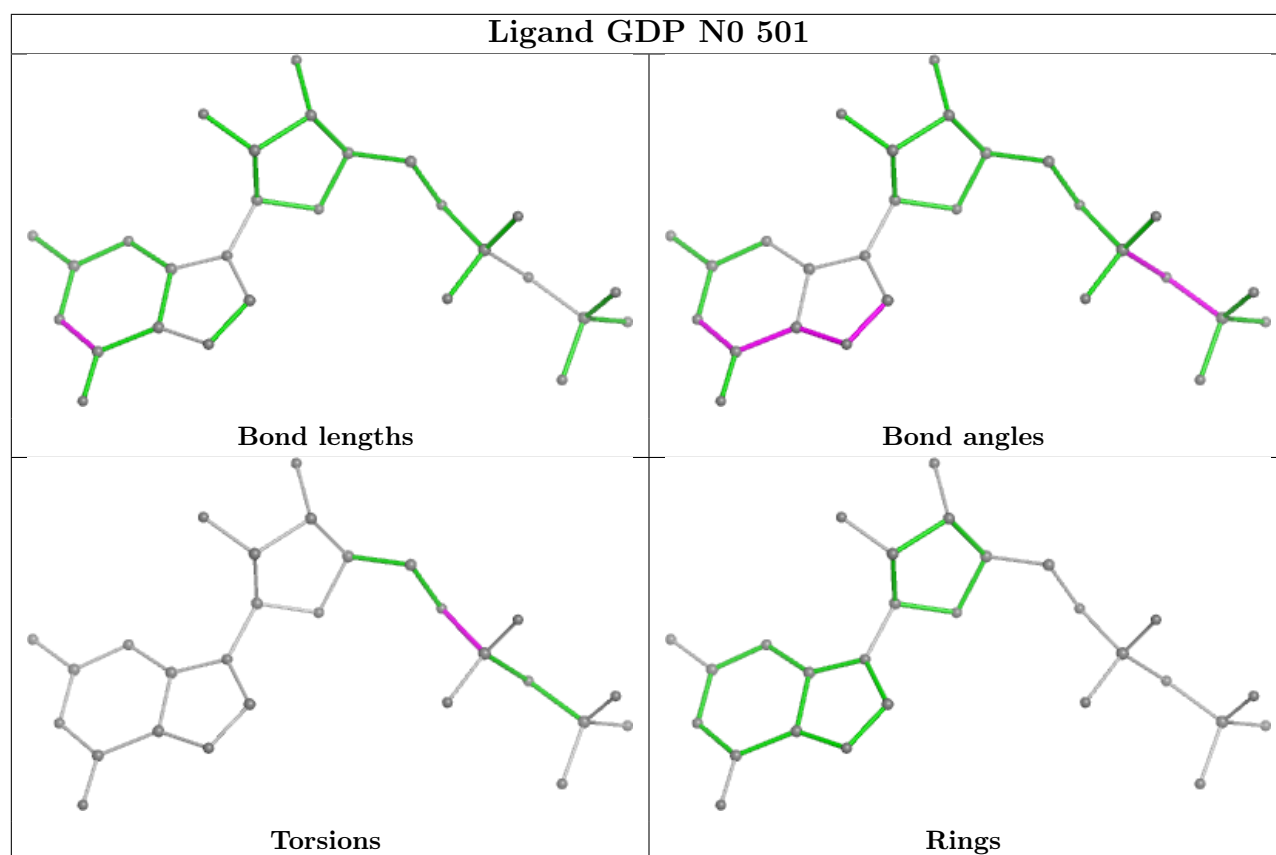
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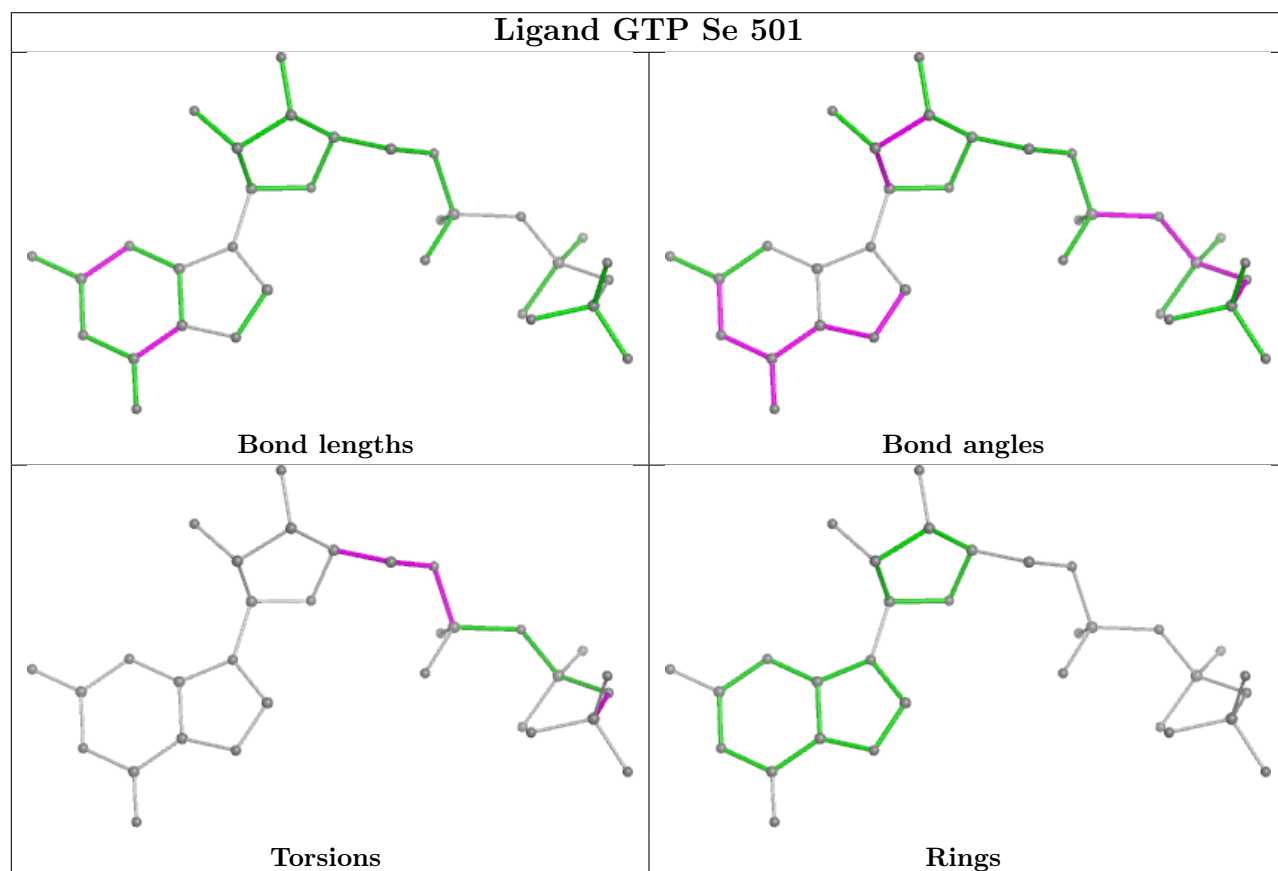
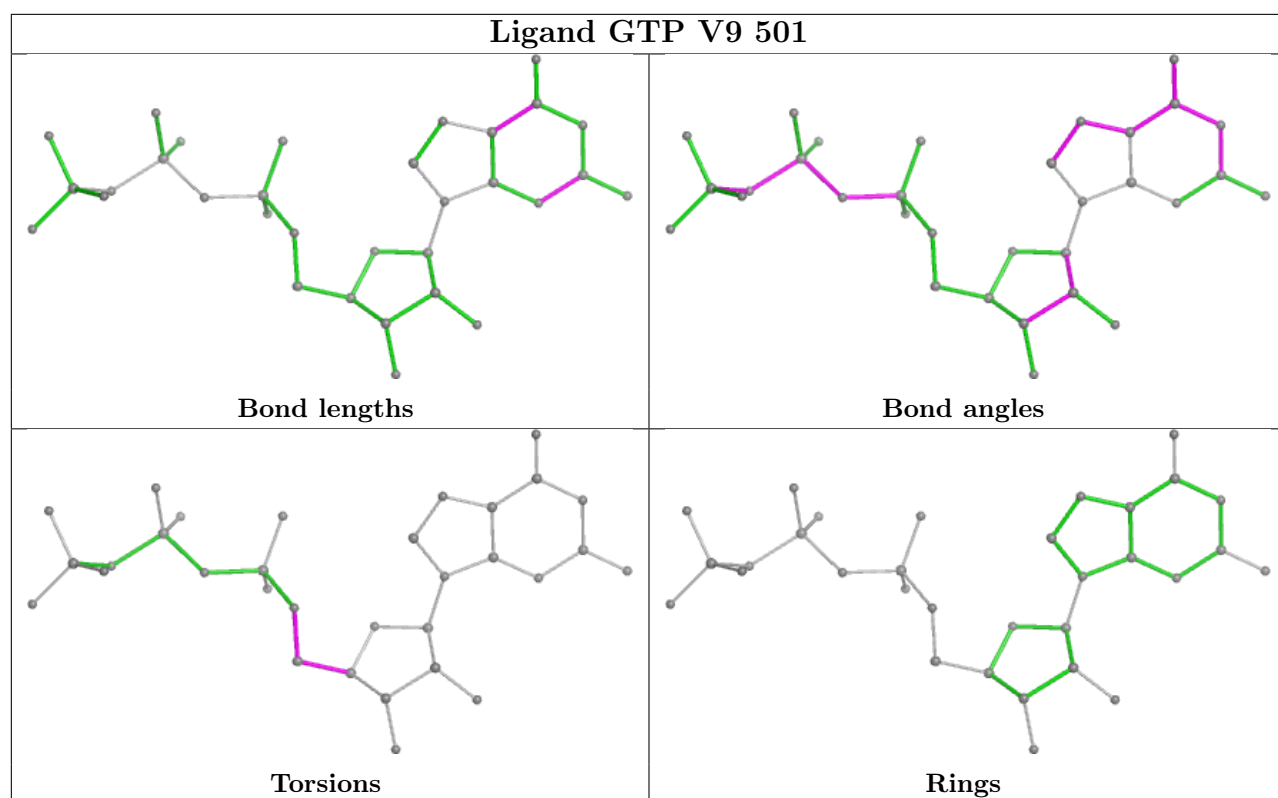


Rings

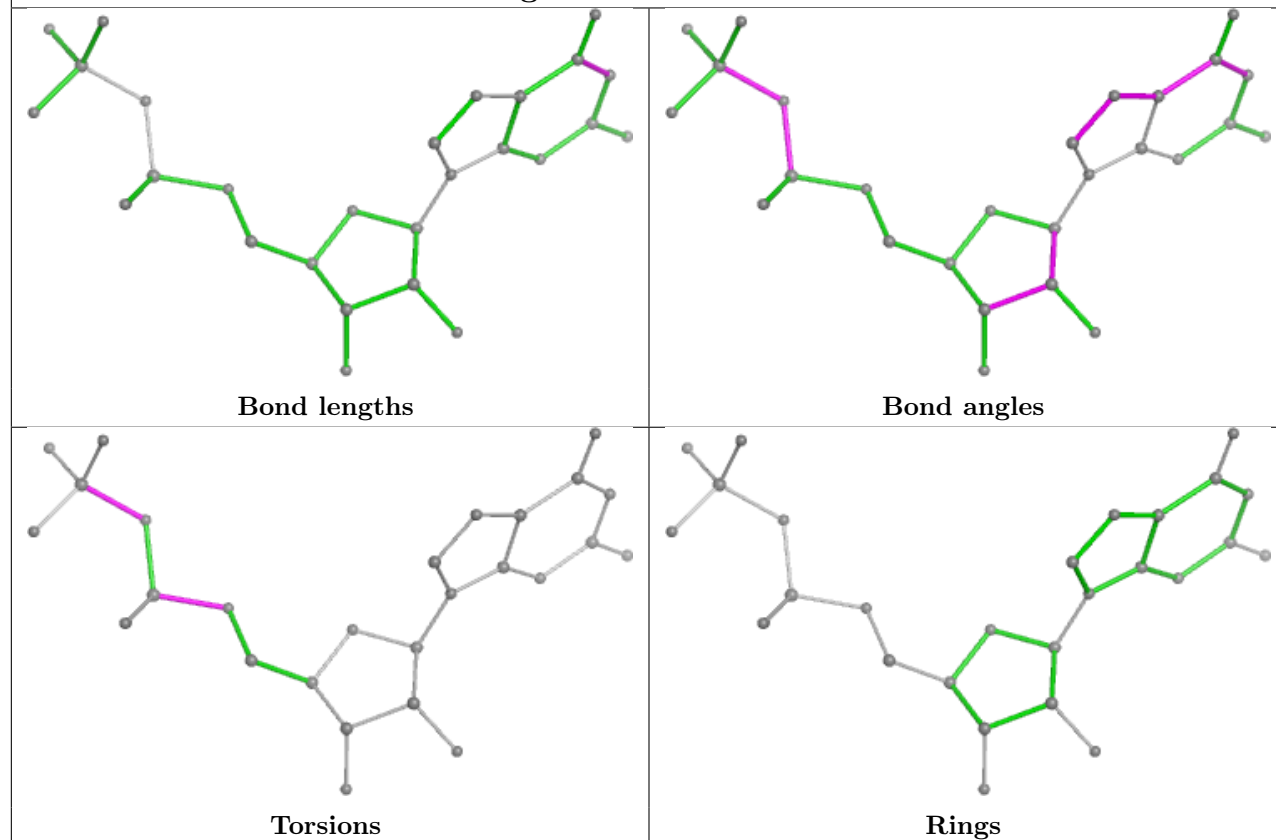
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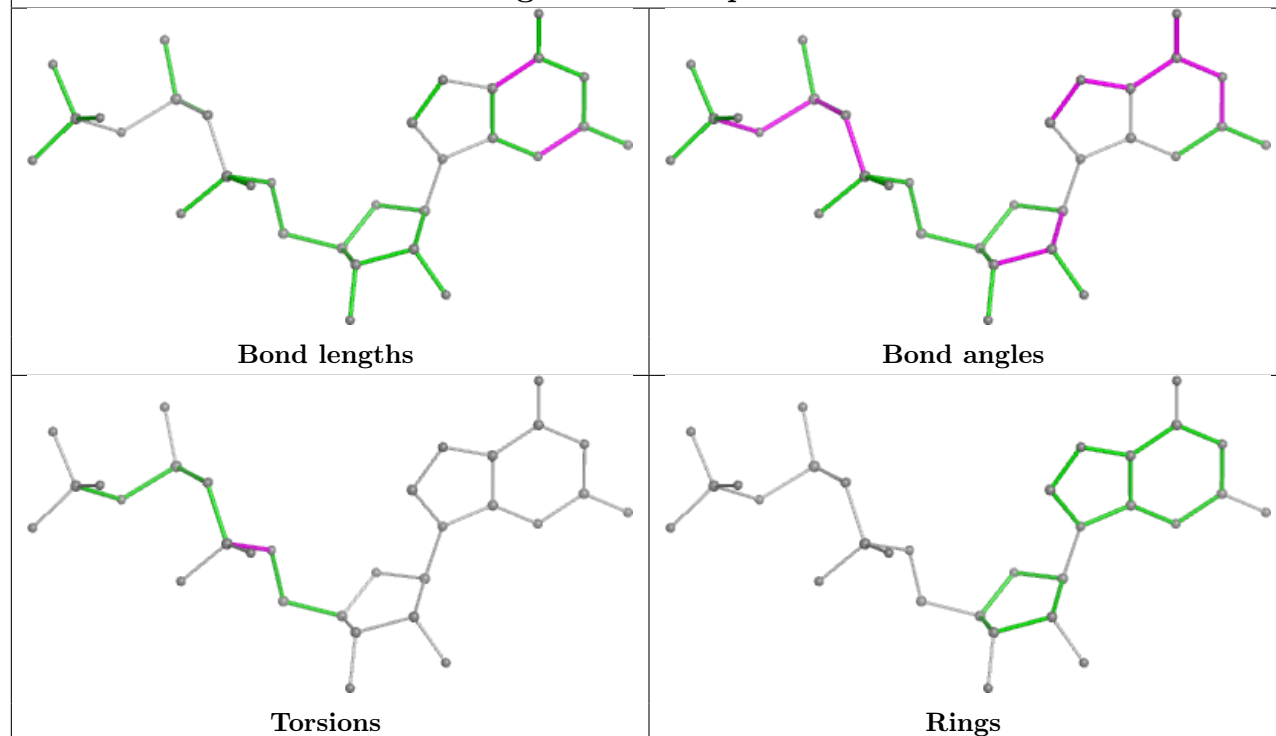




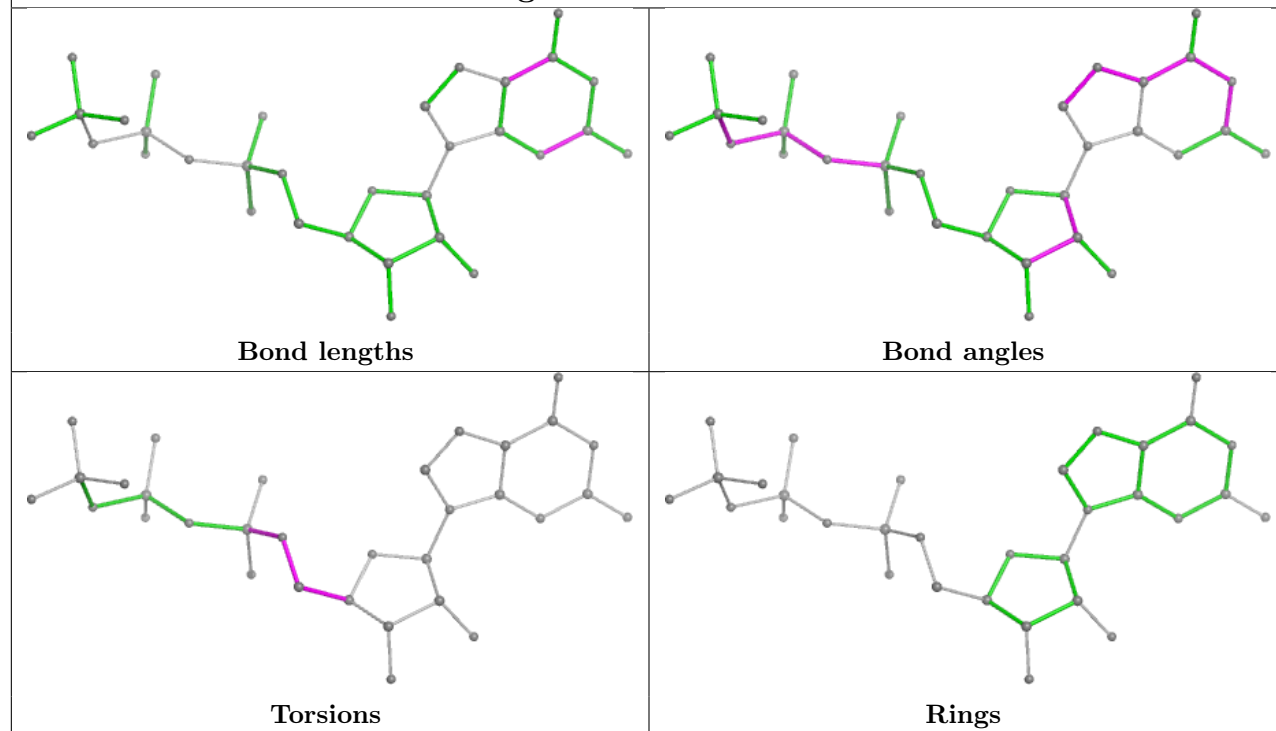
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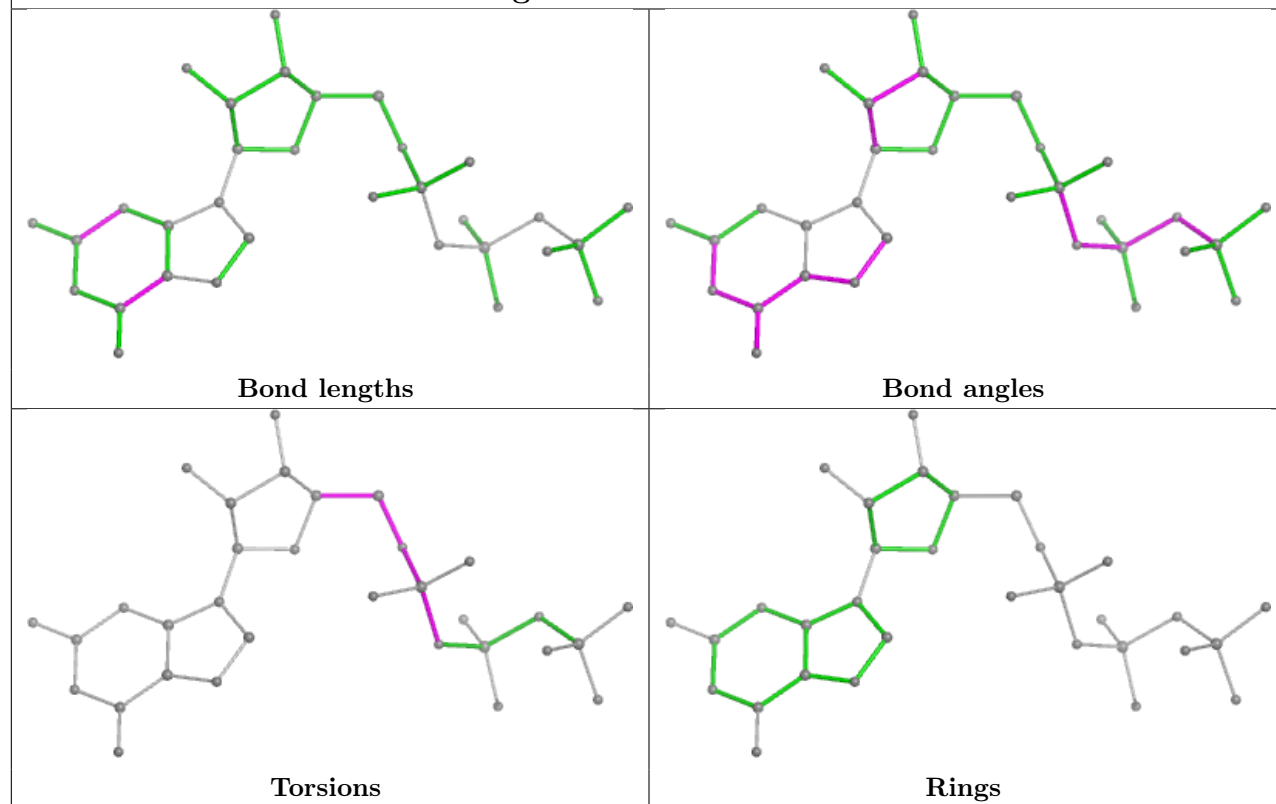
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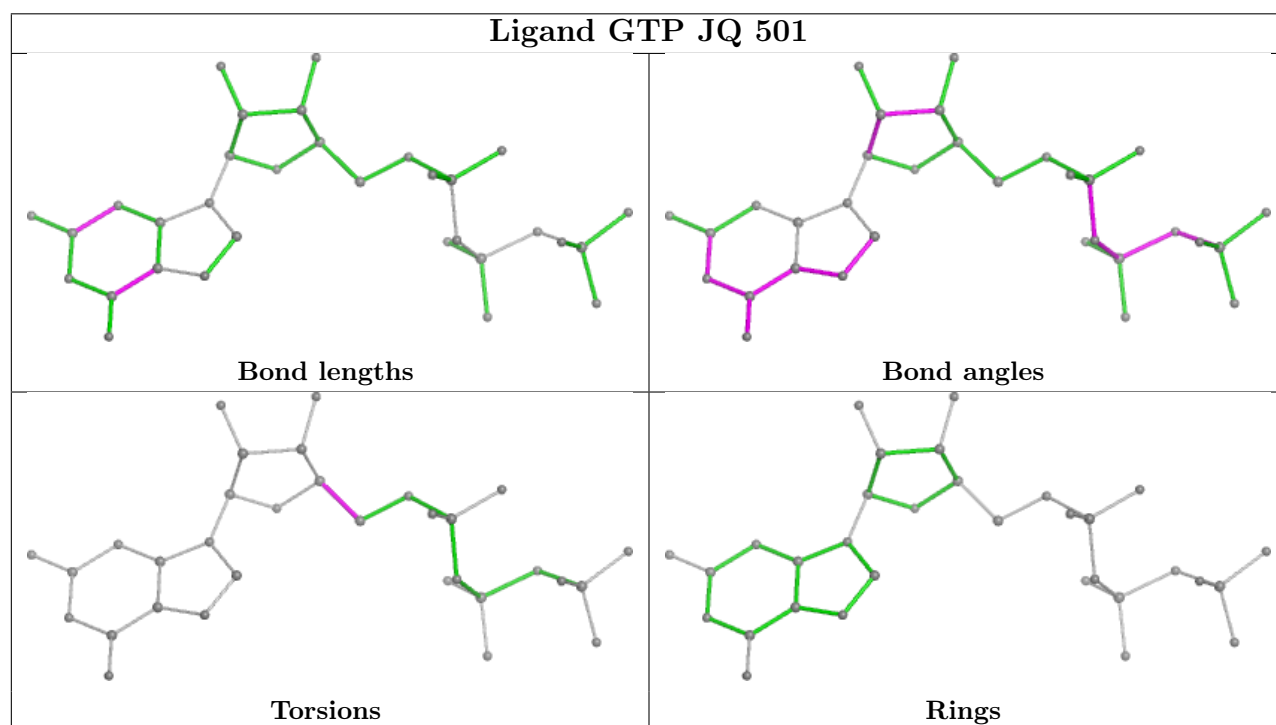
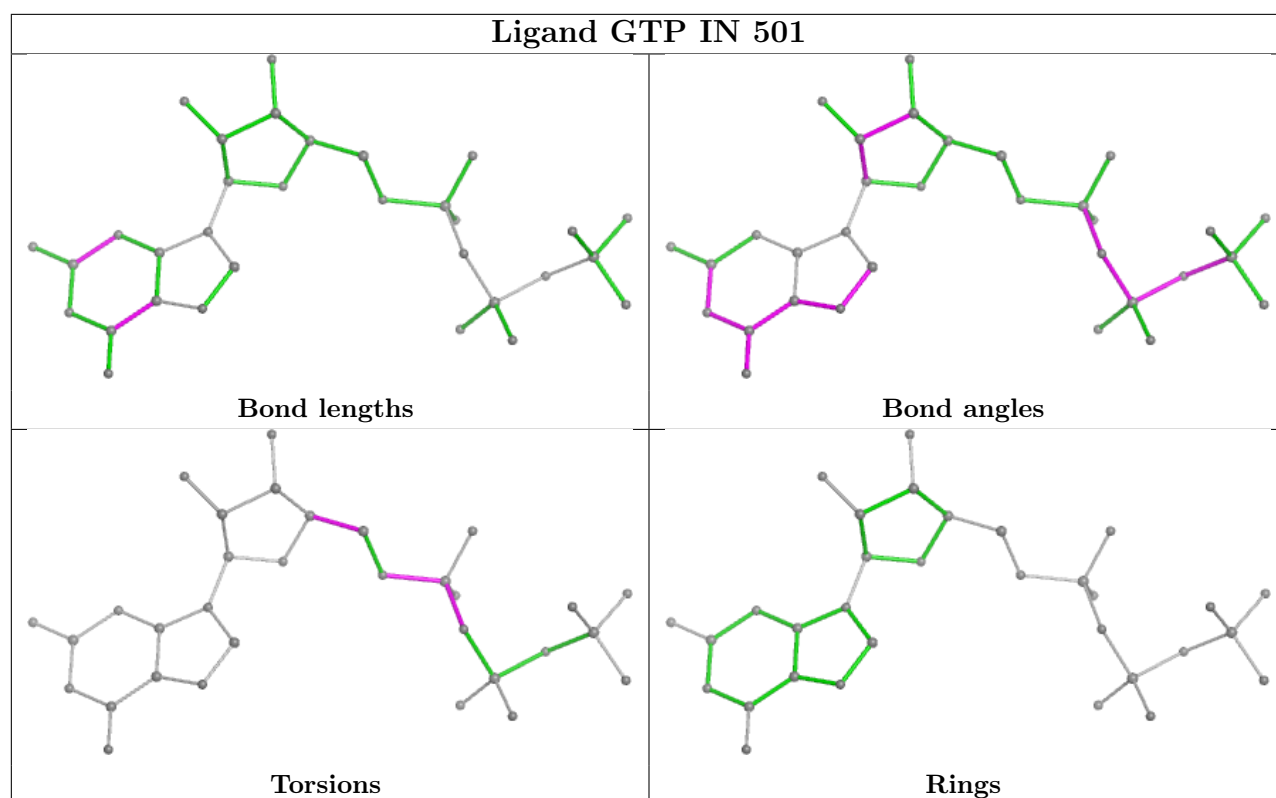


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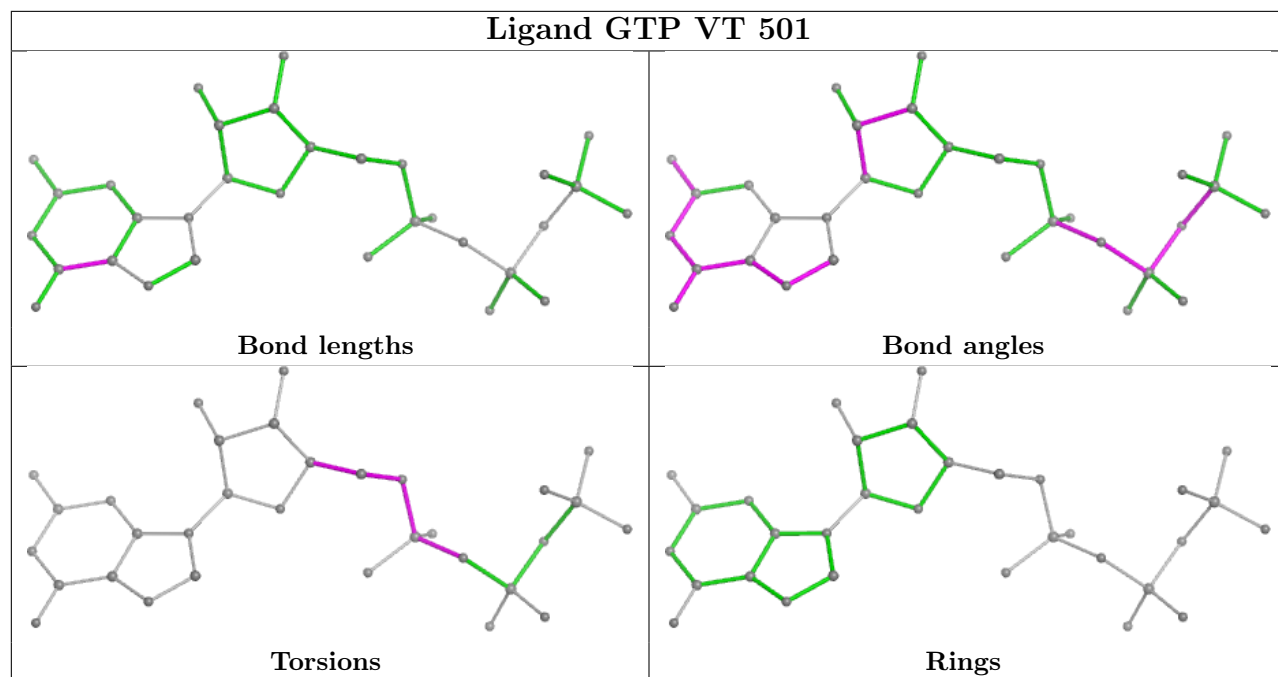


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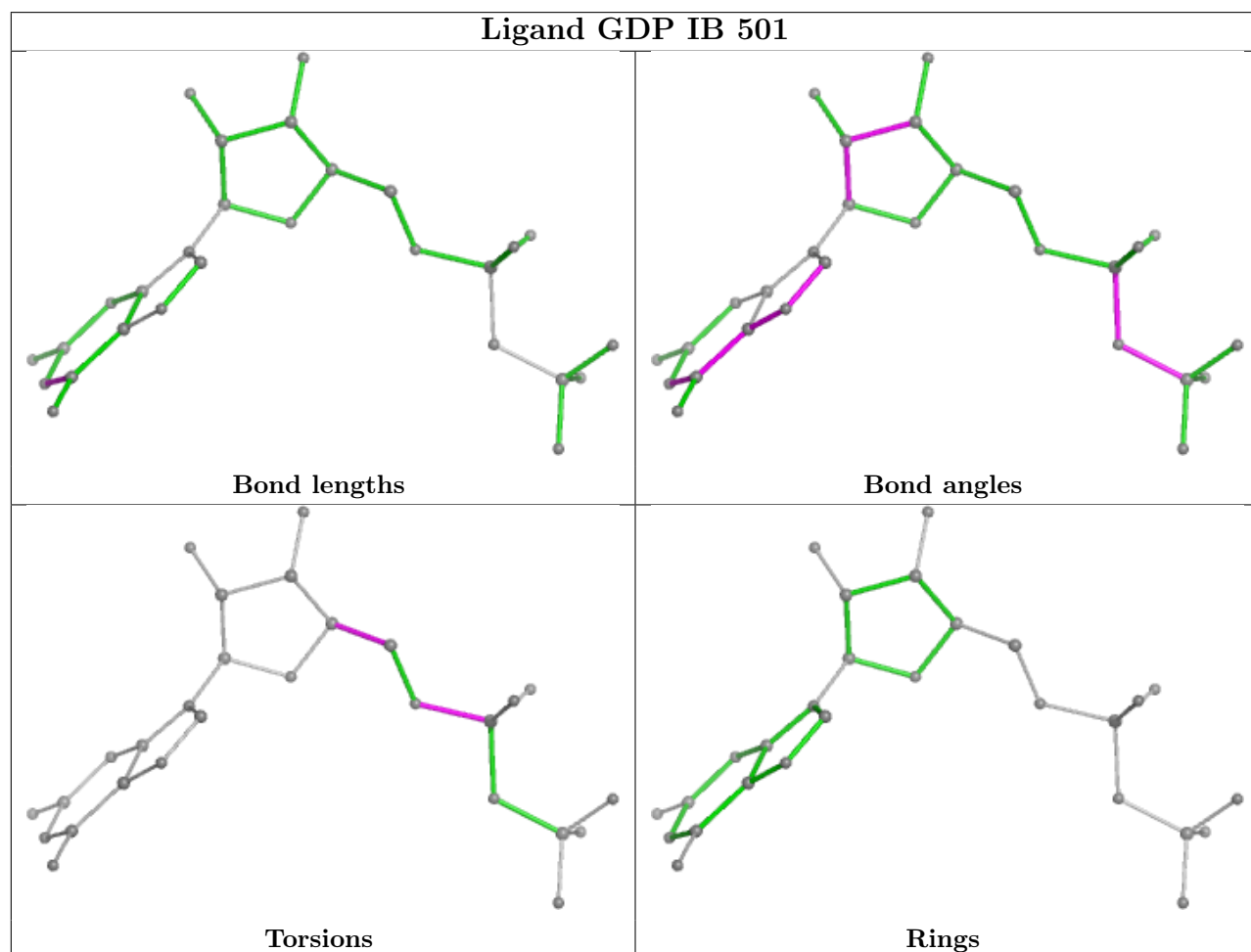




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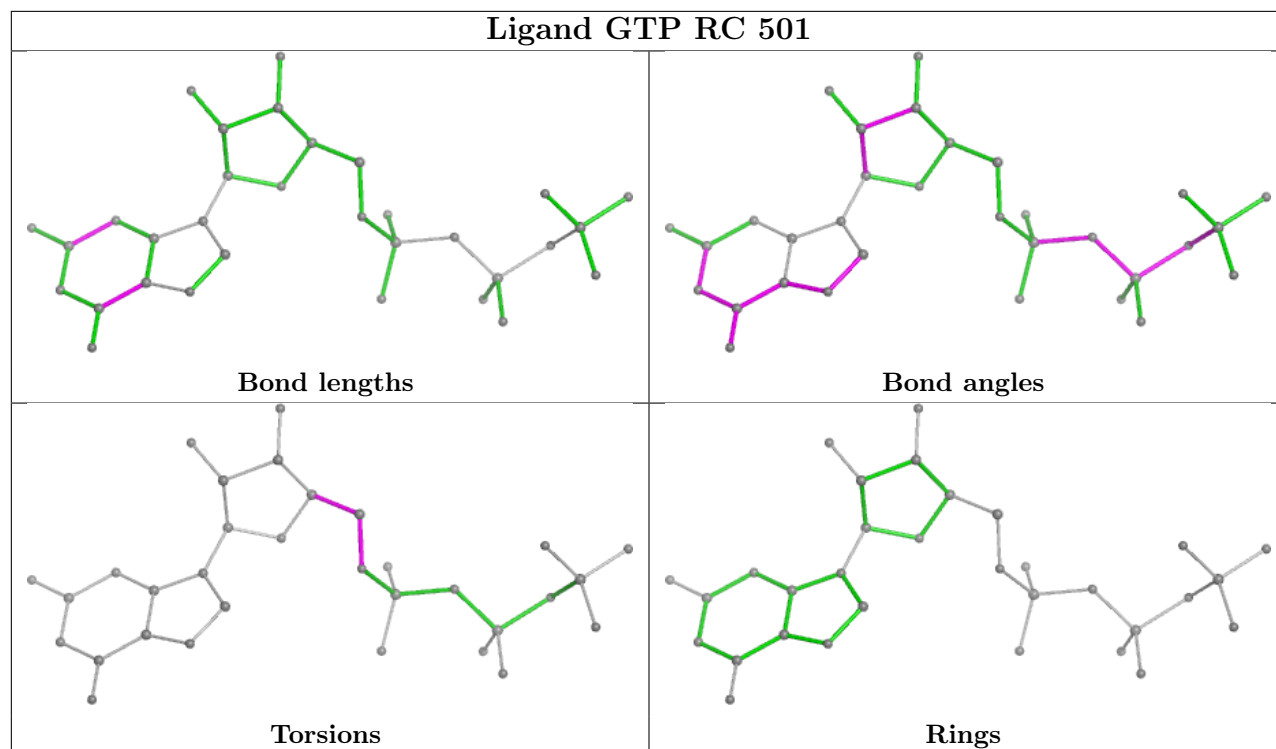


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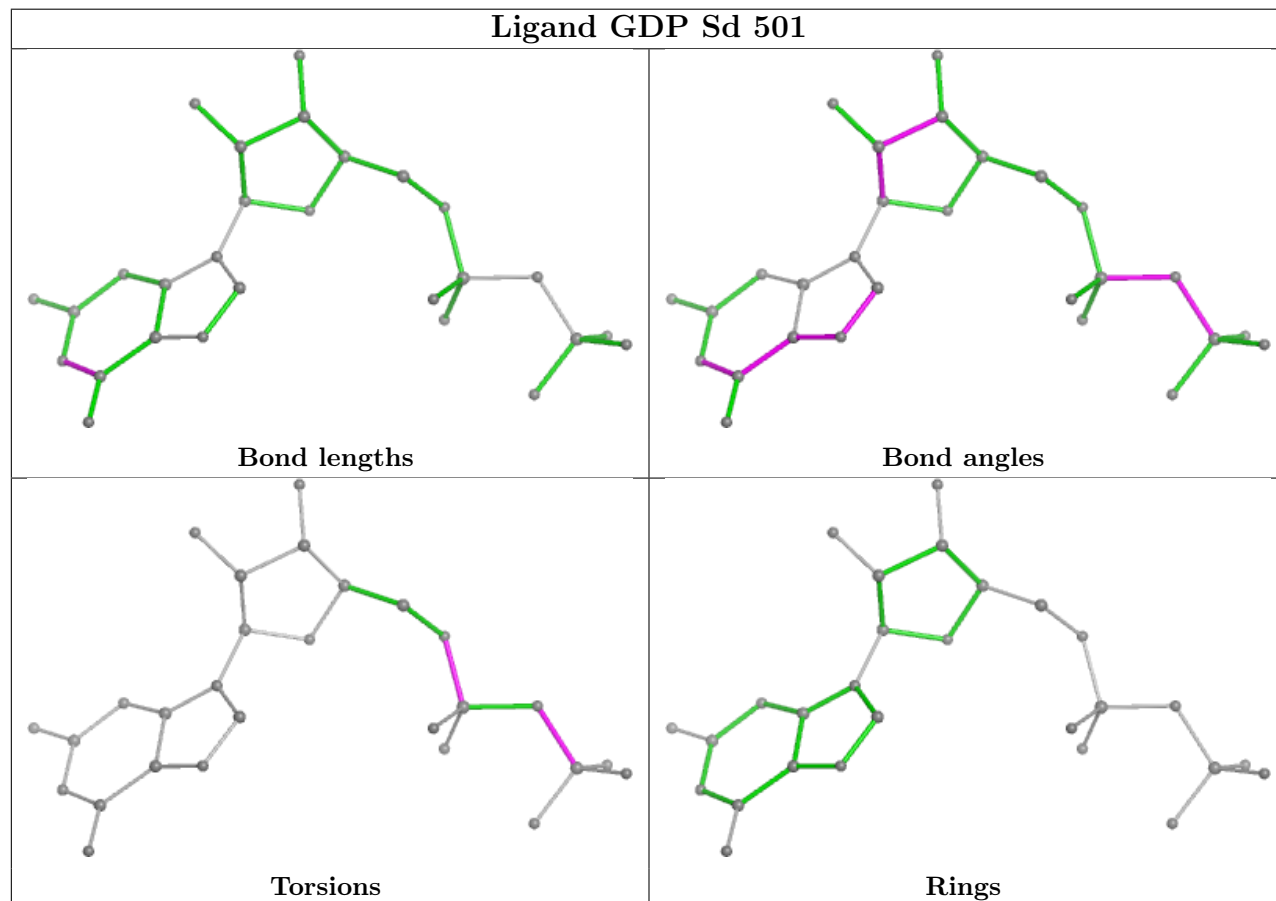


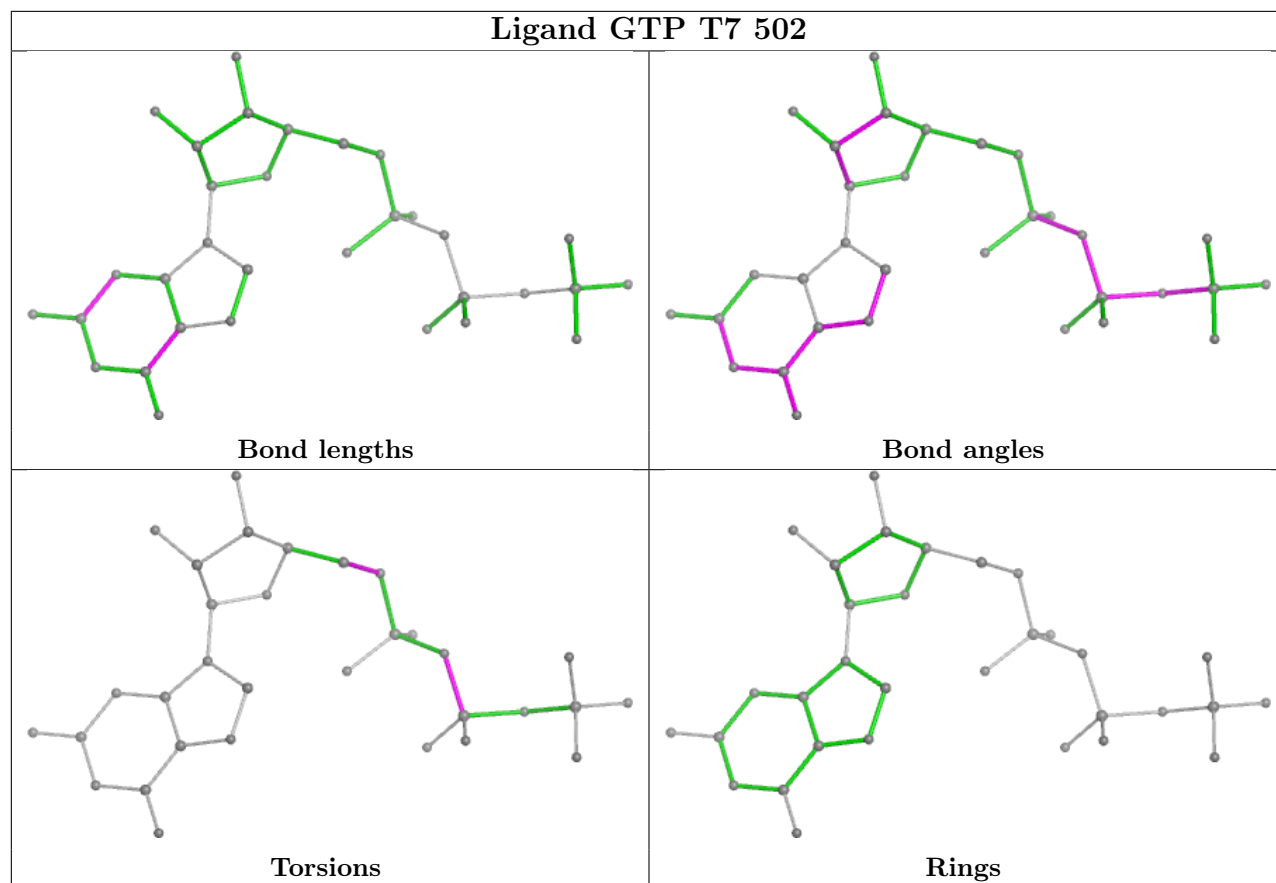


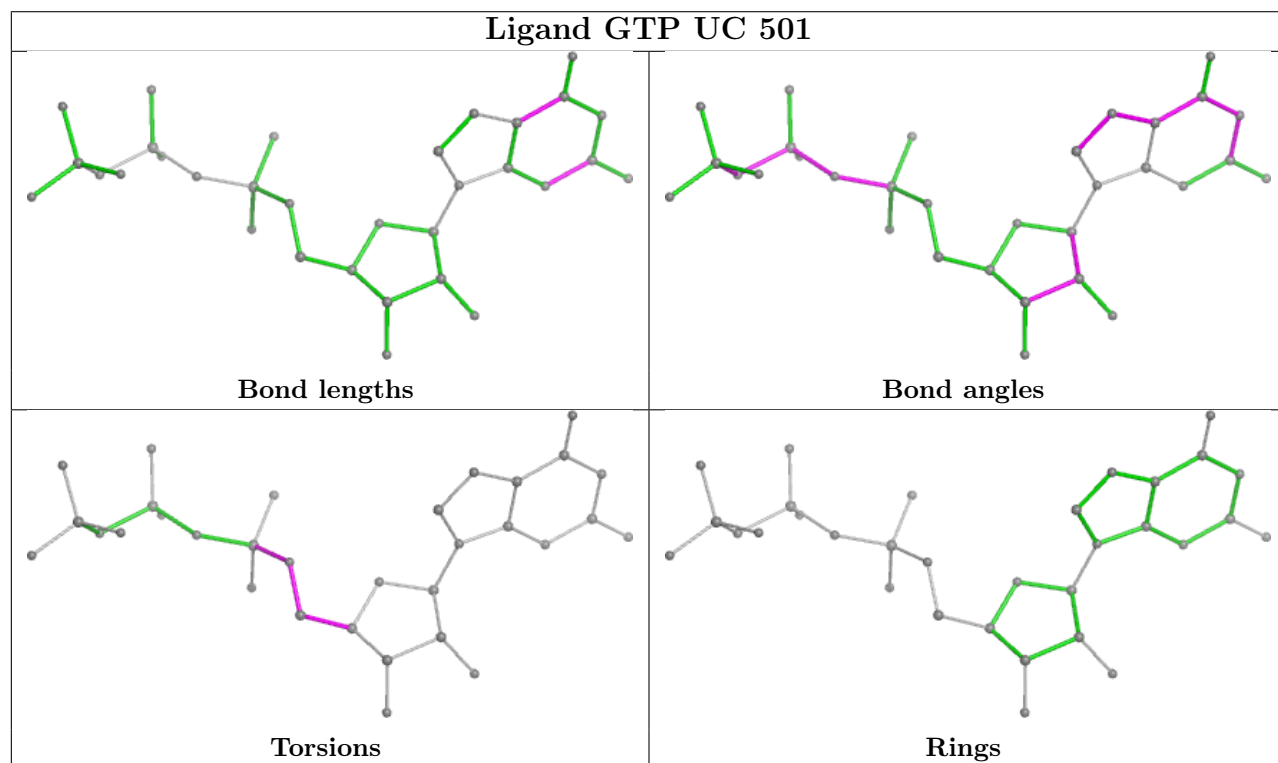
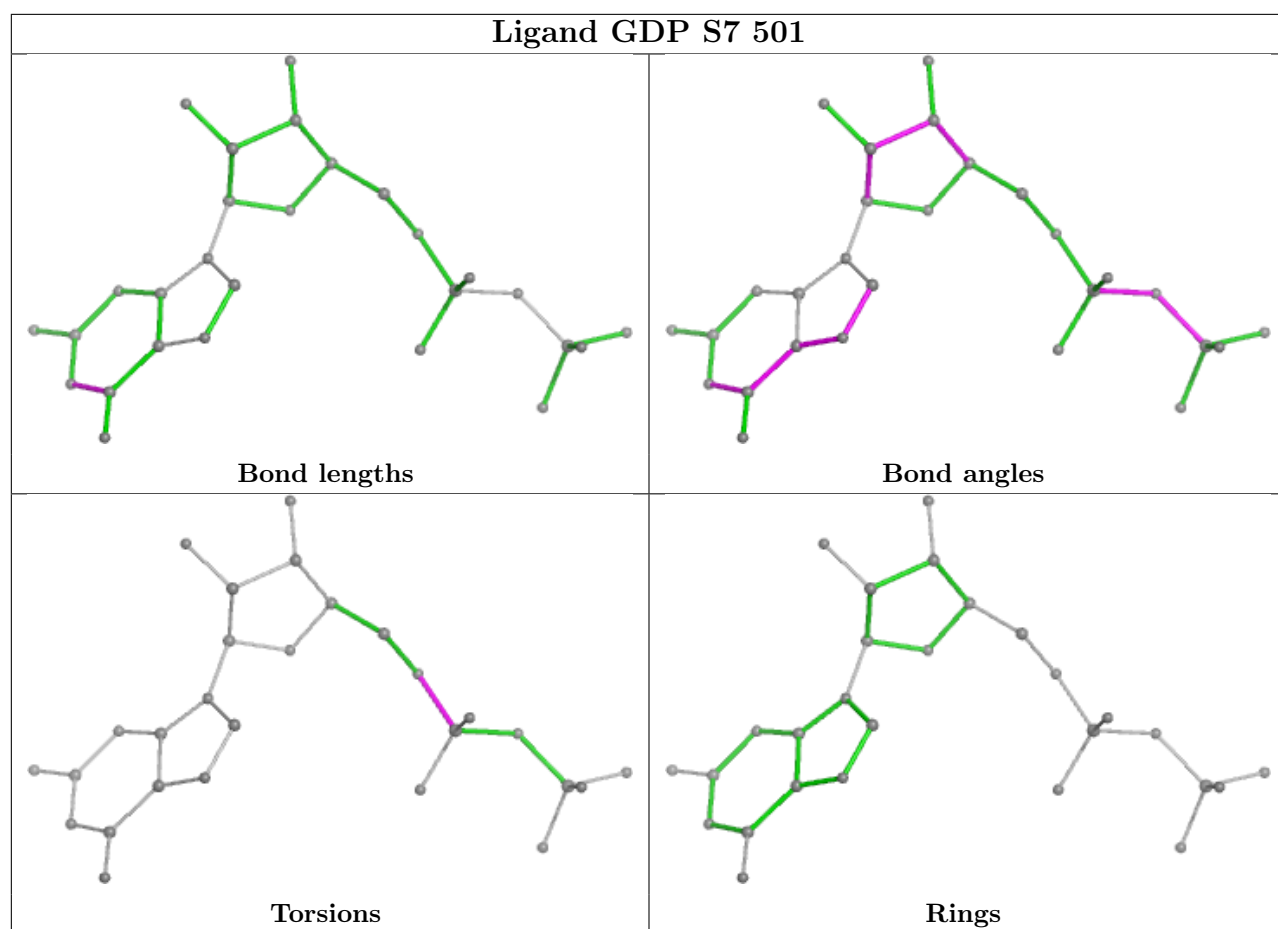
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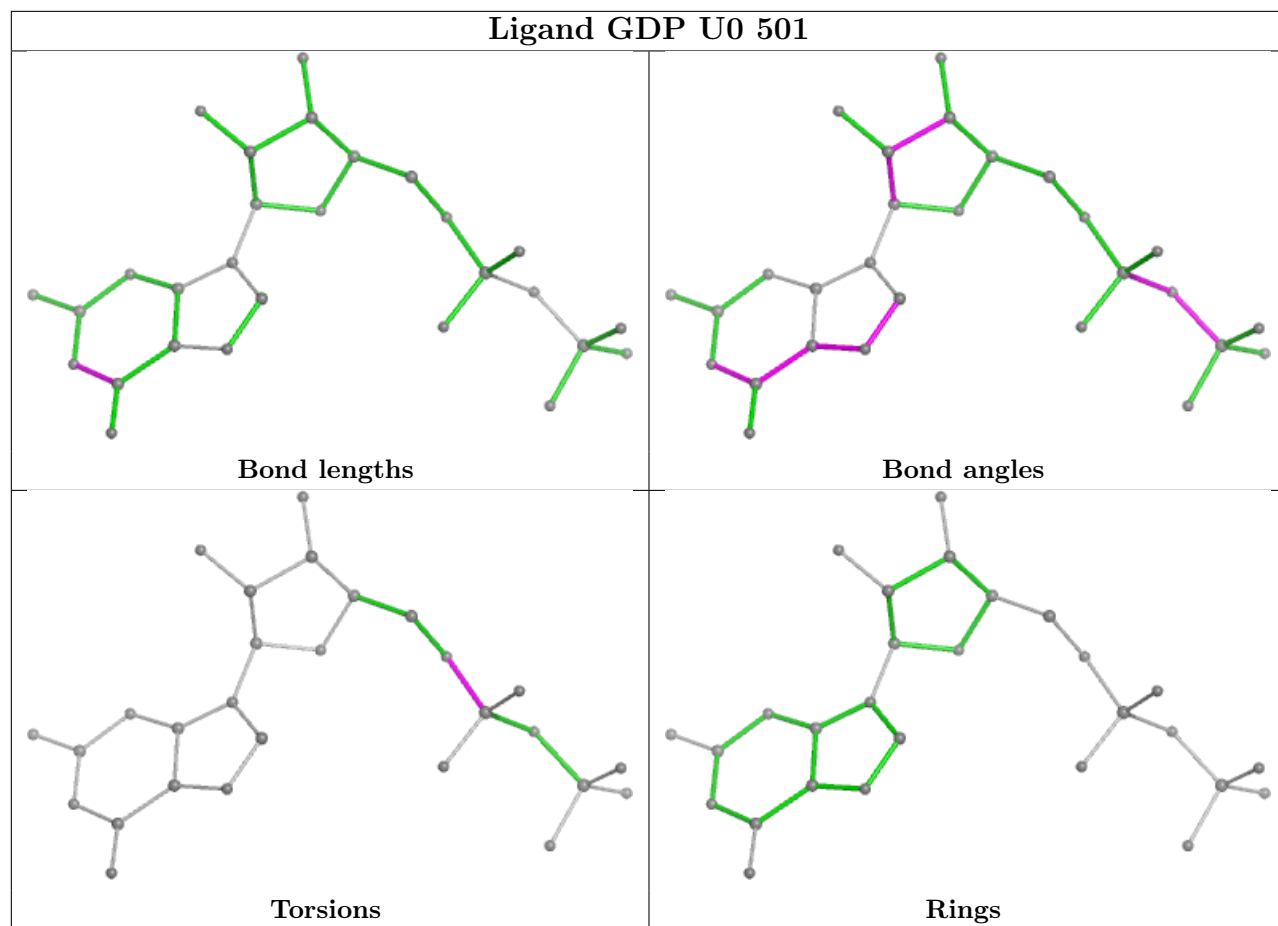


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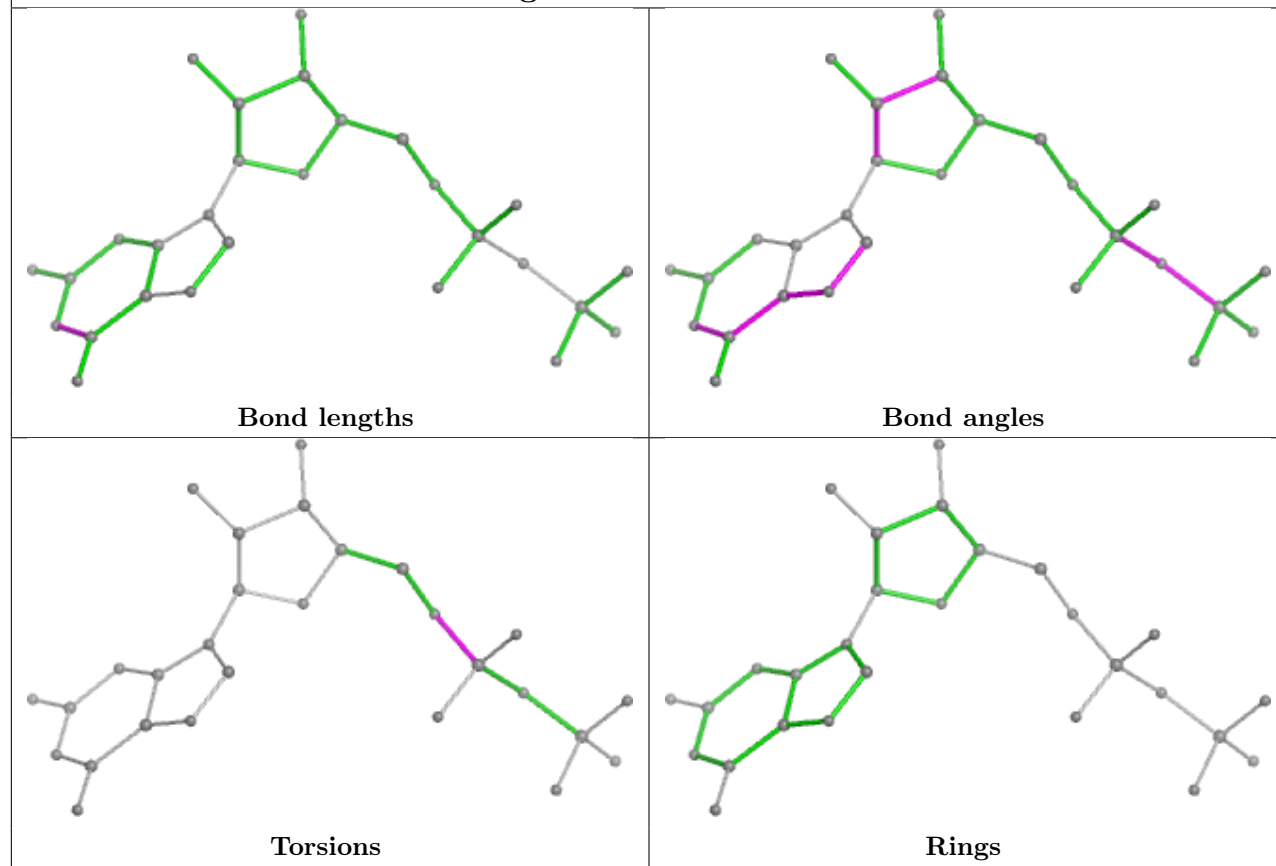




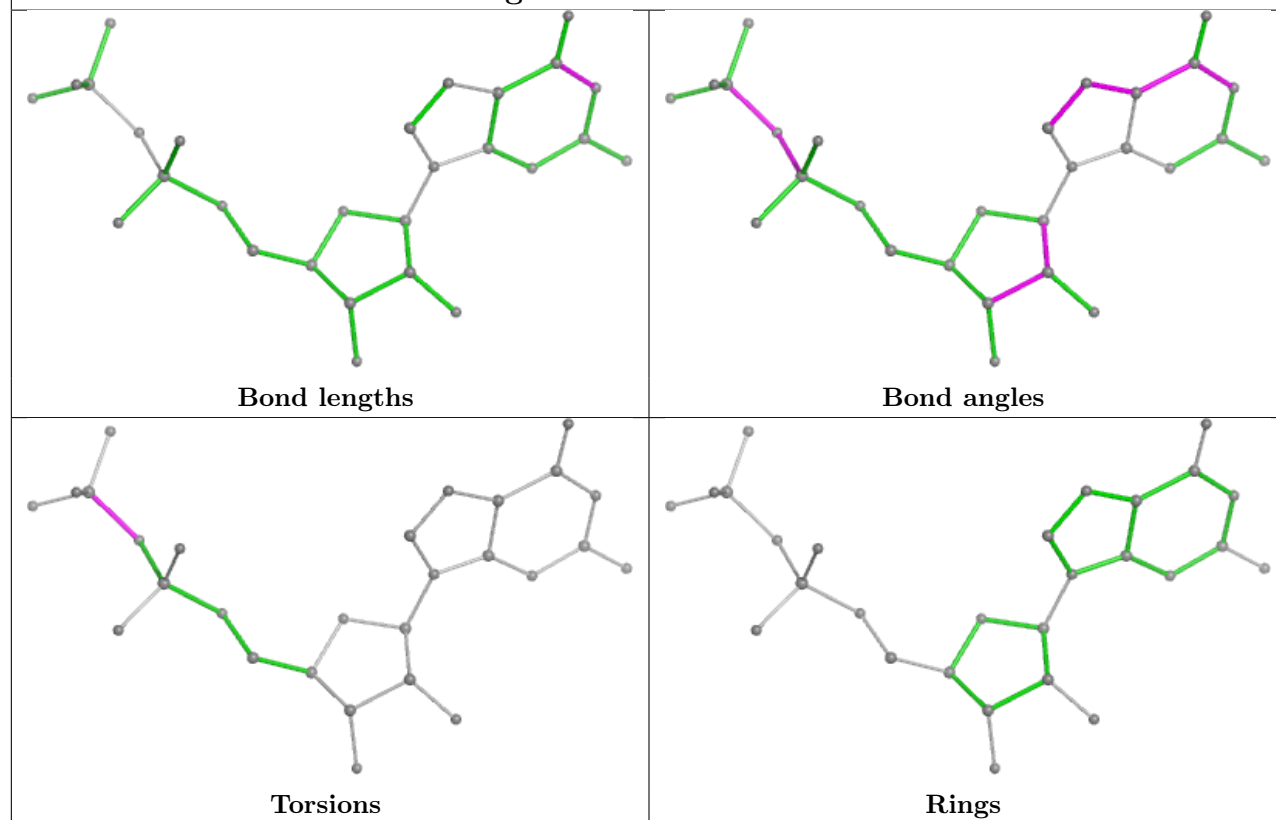


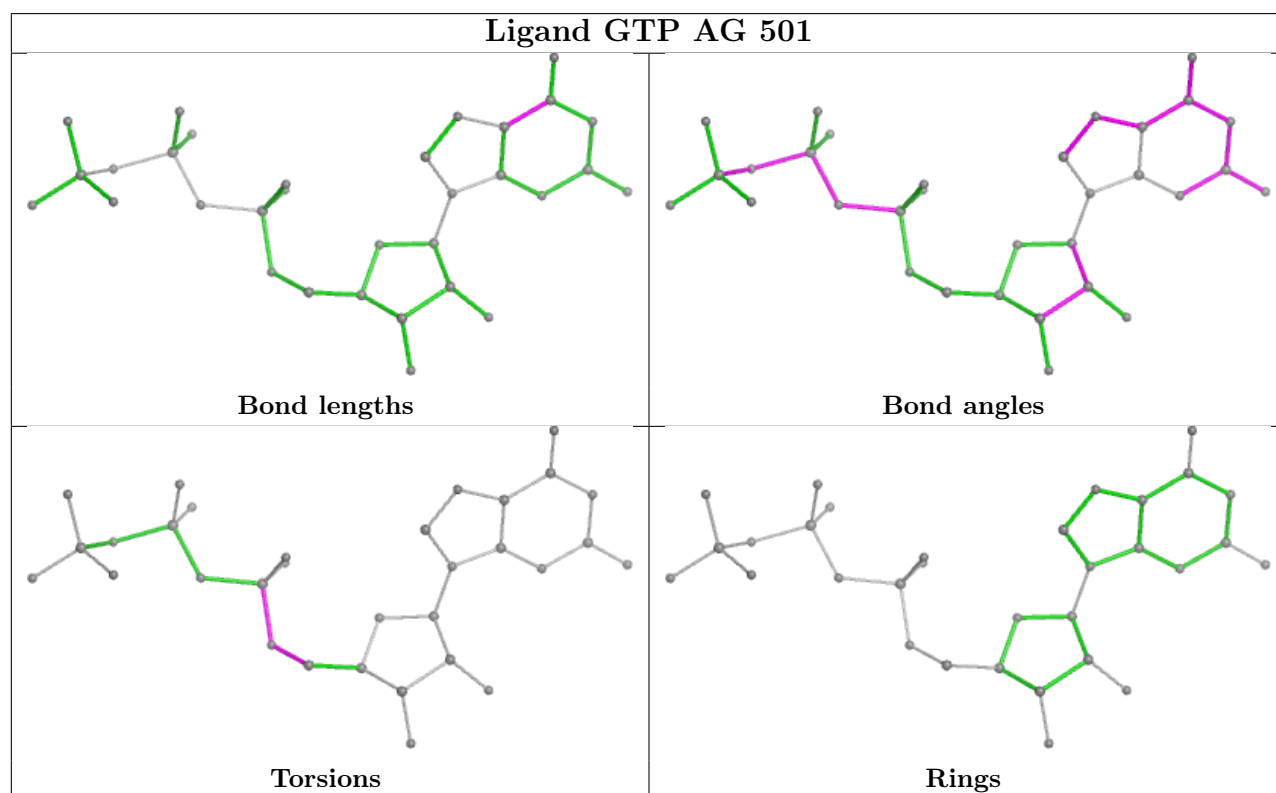
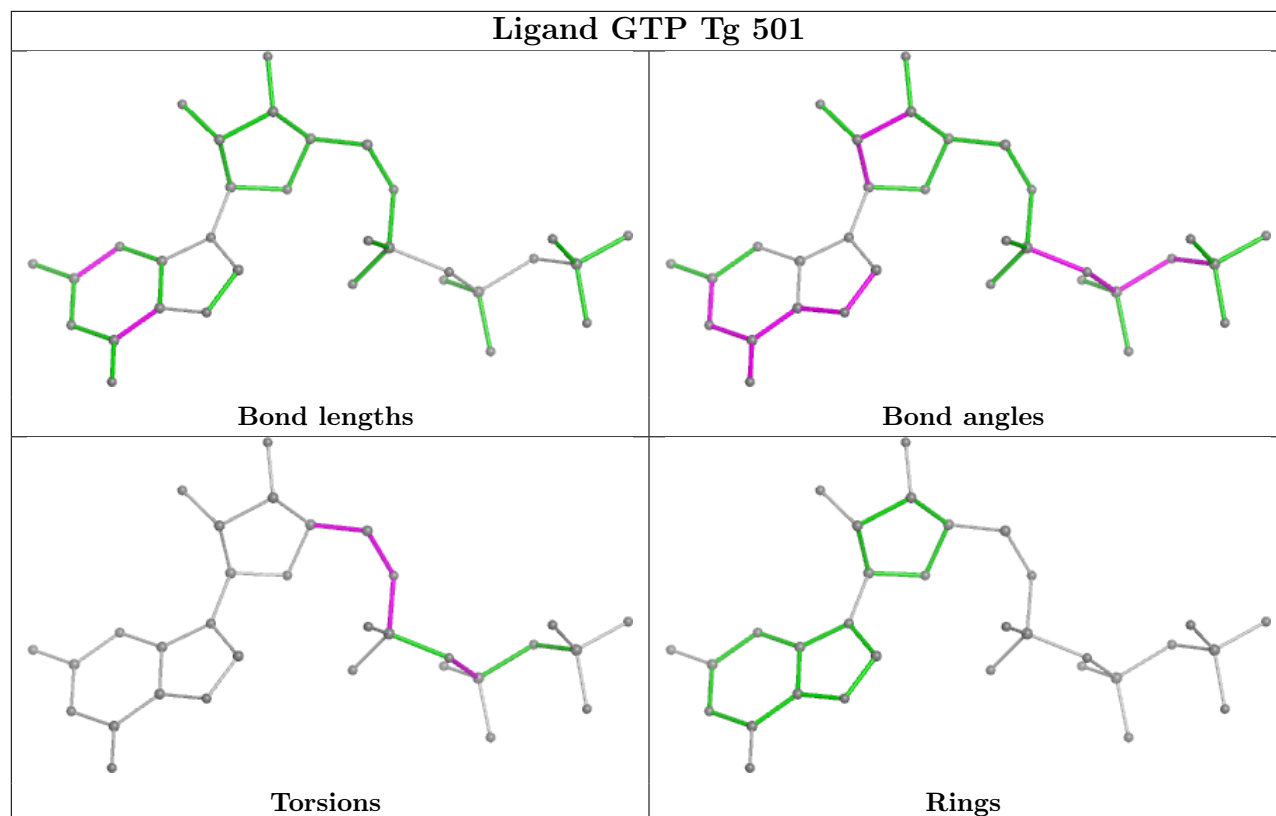


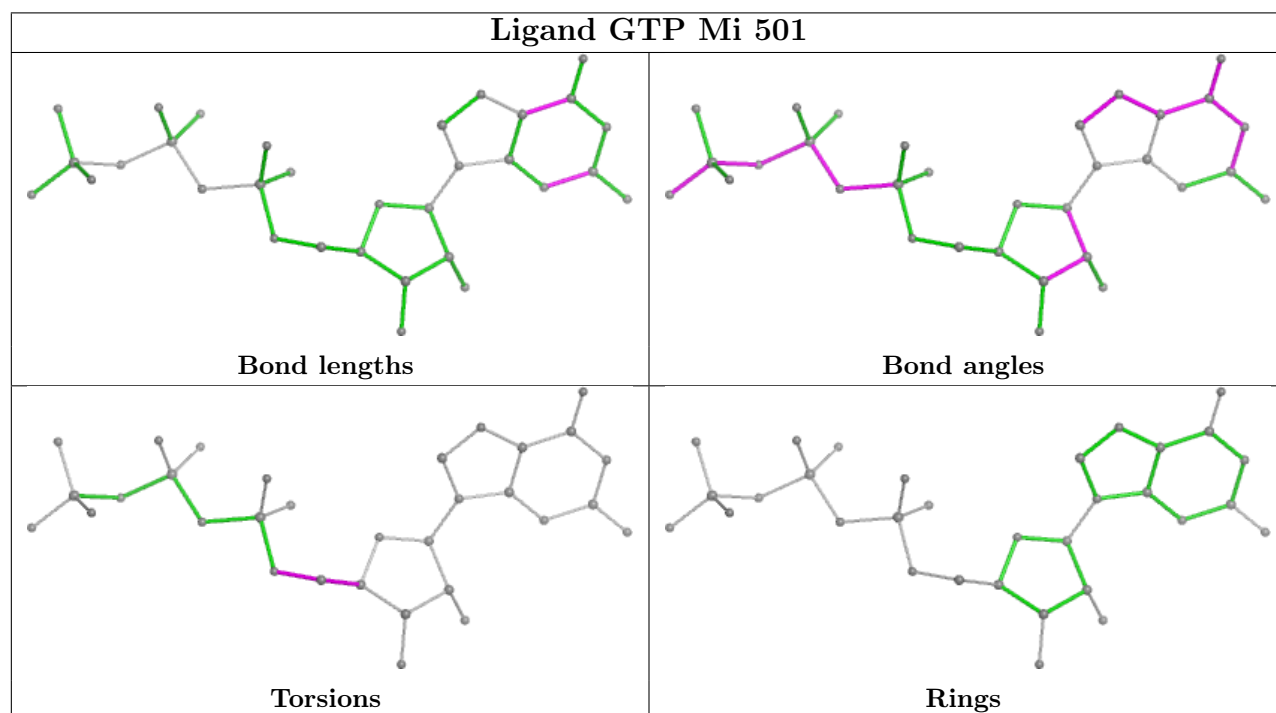
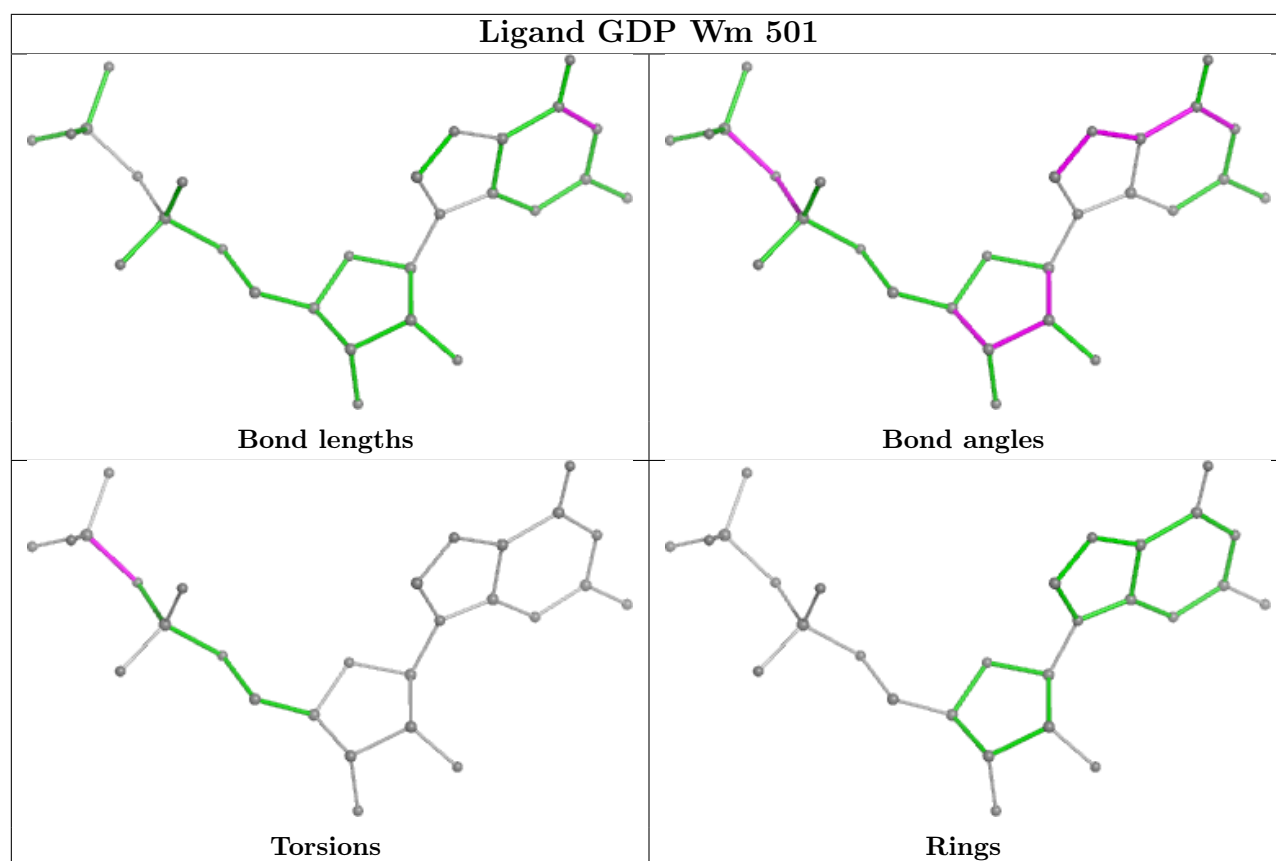
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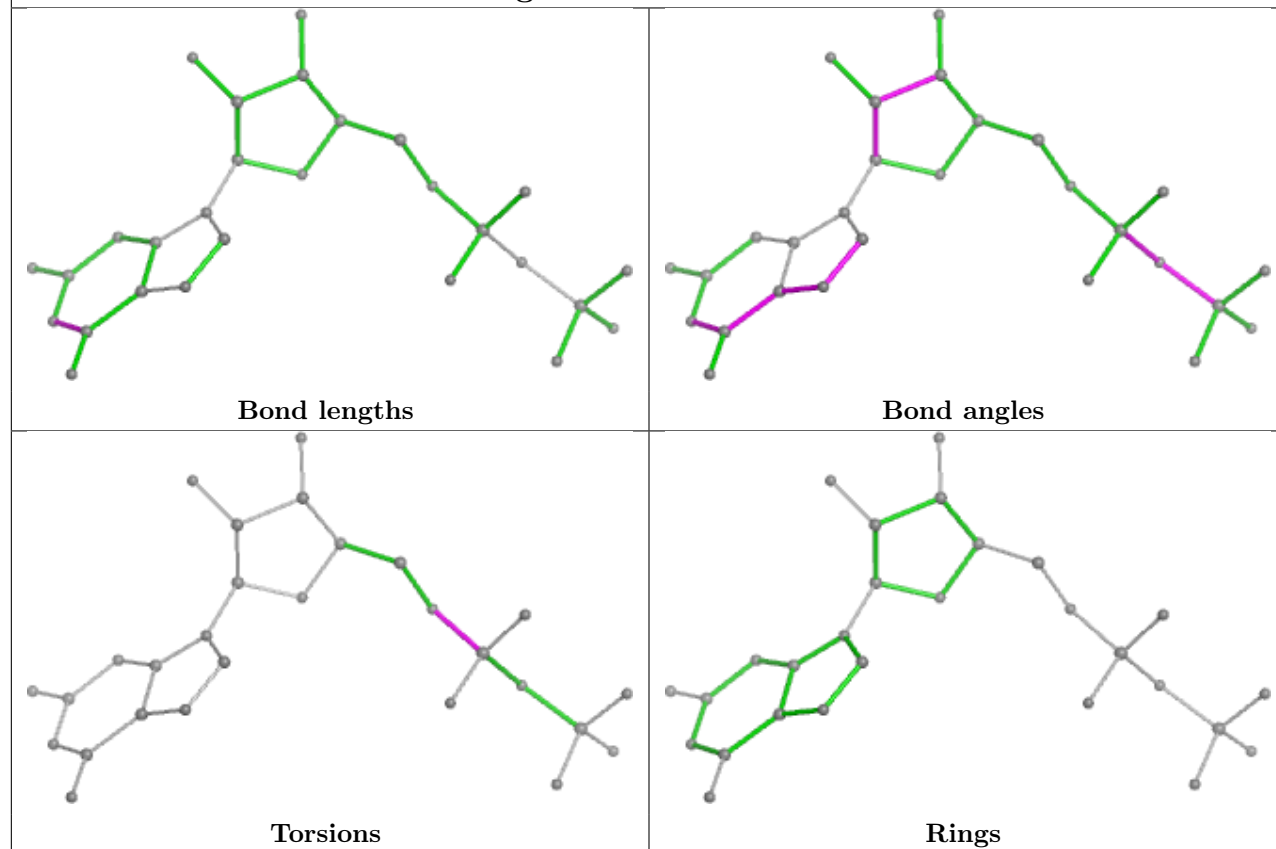
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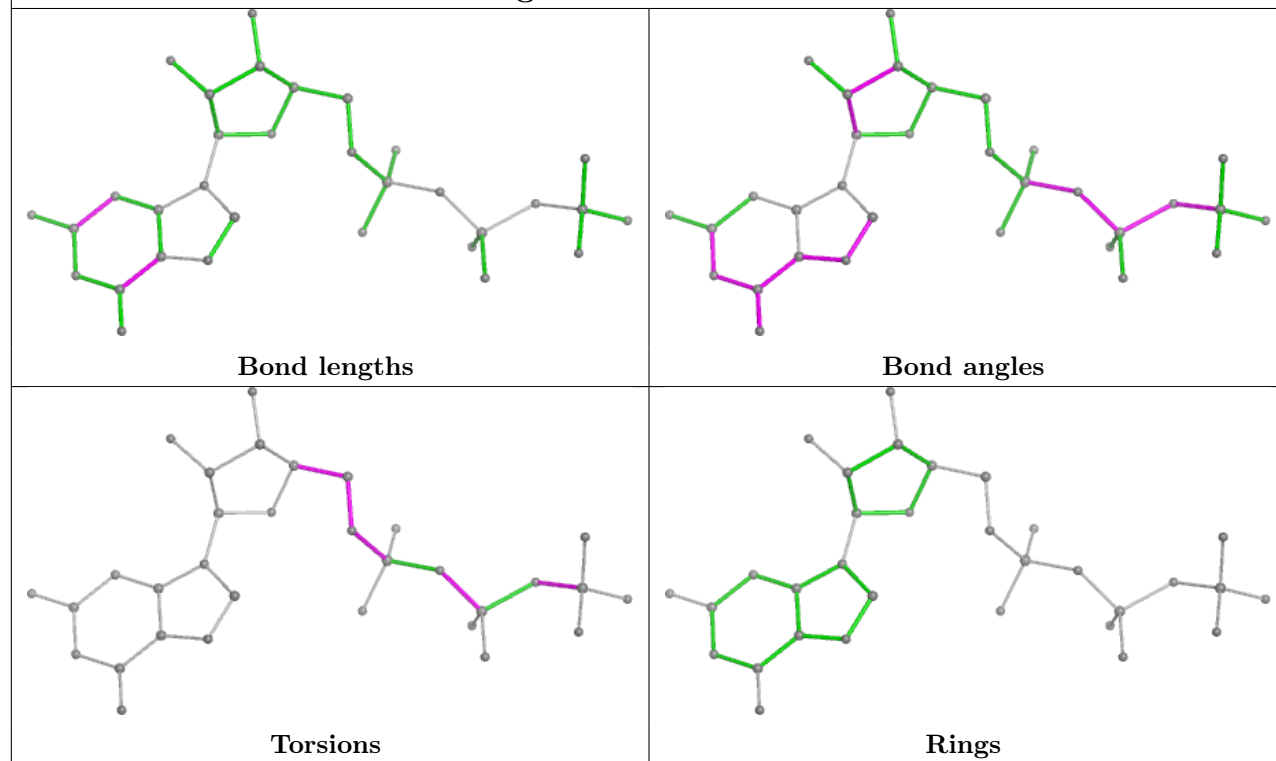




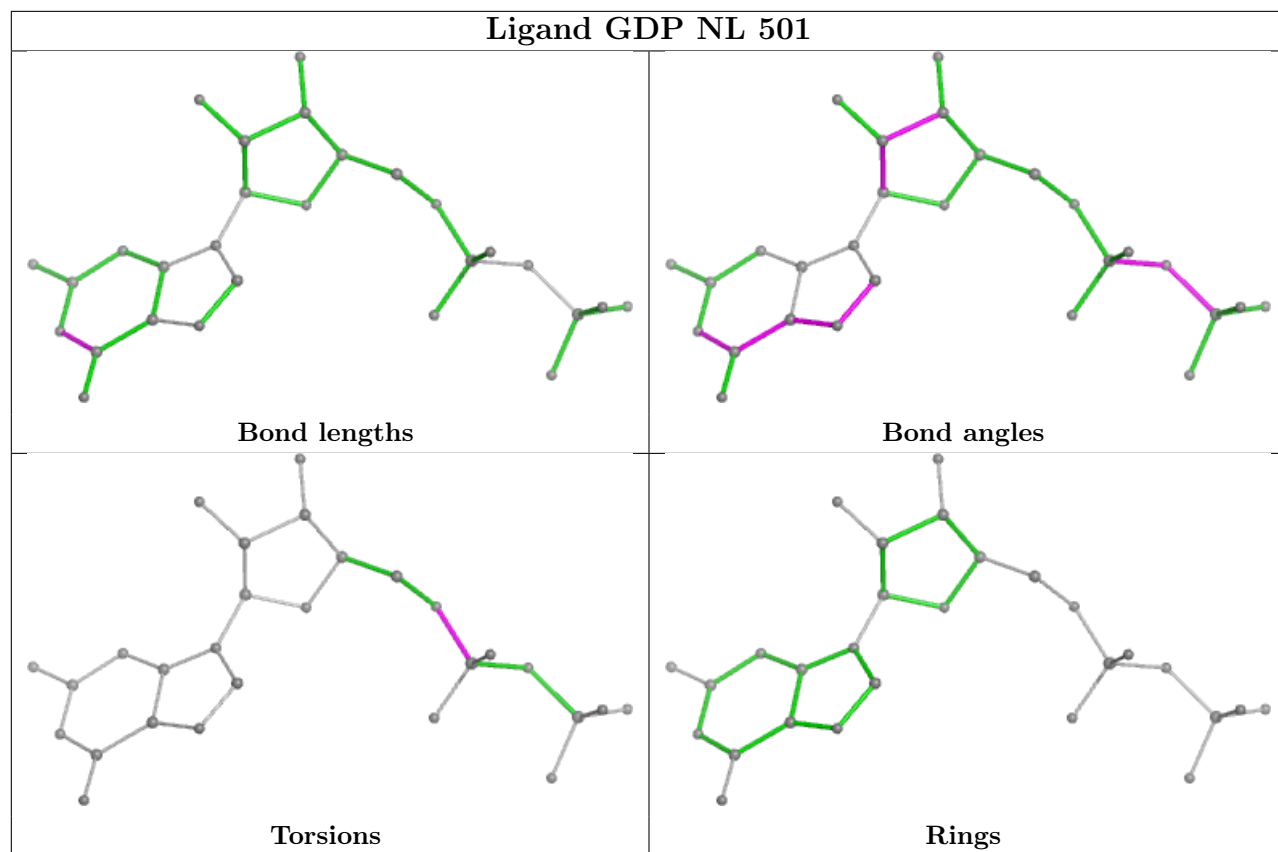
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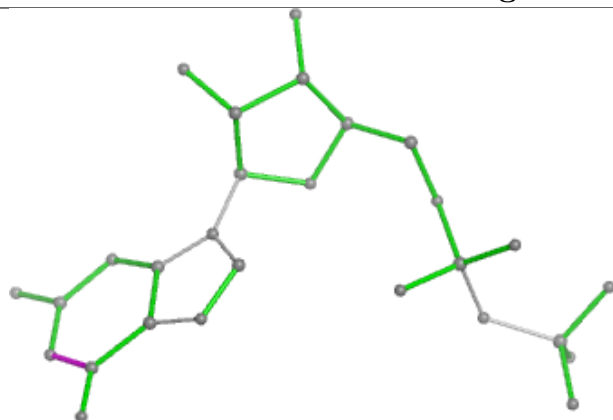
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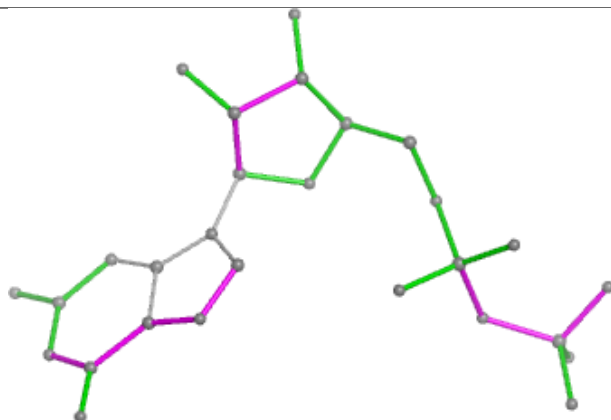




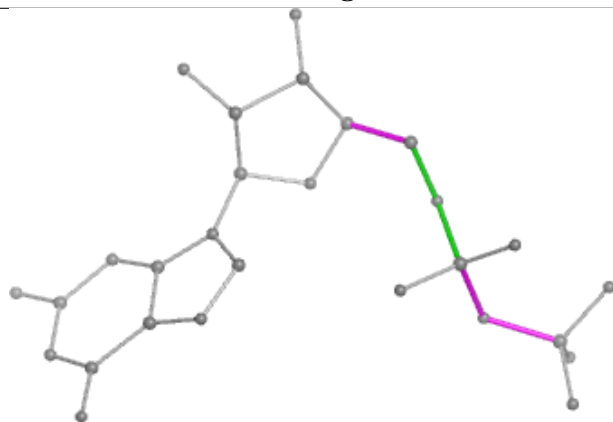
## Ligand GDP KF 501



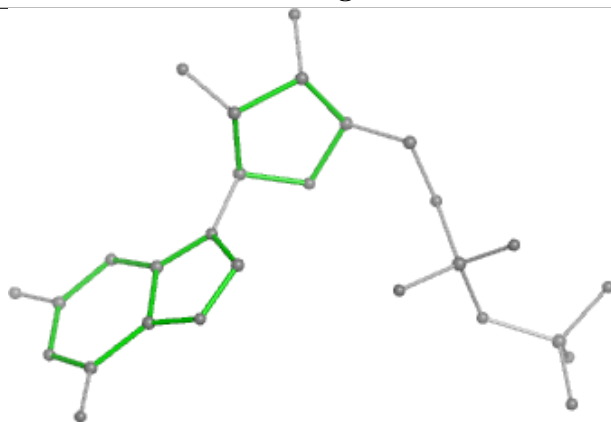
Bond lengths



Bond angles

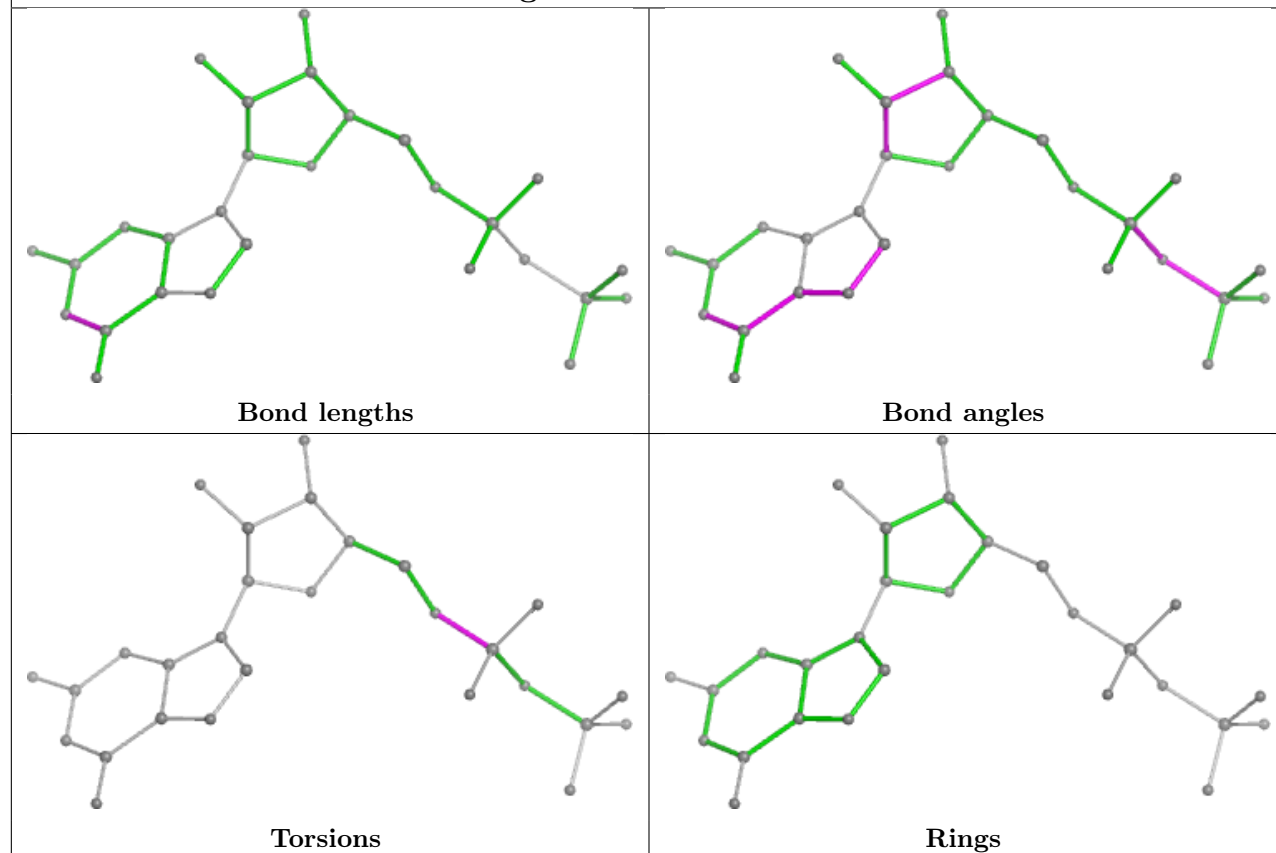


Torsions

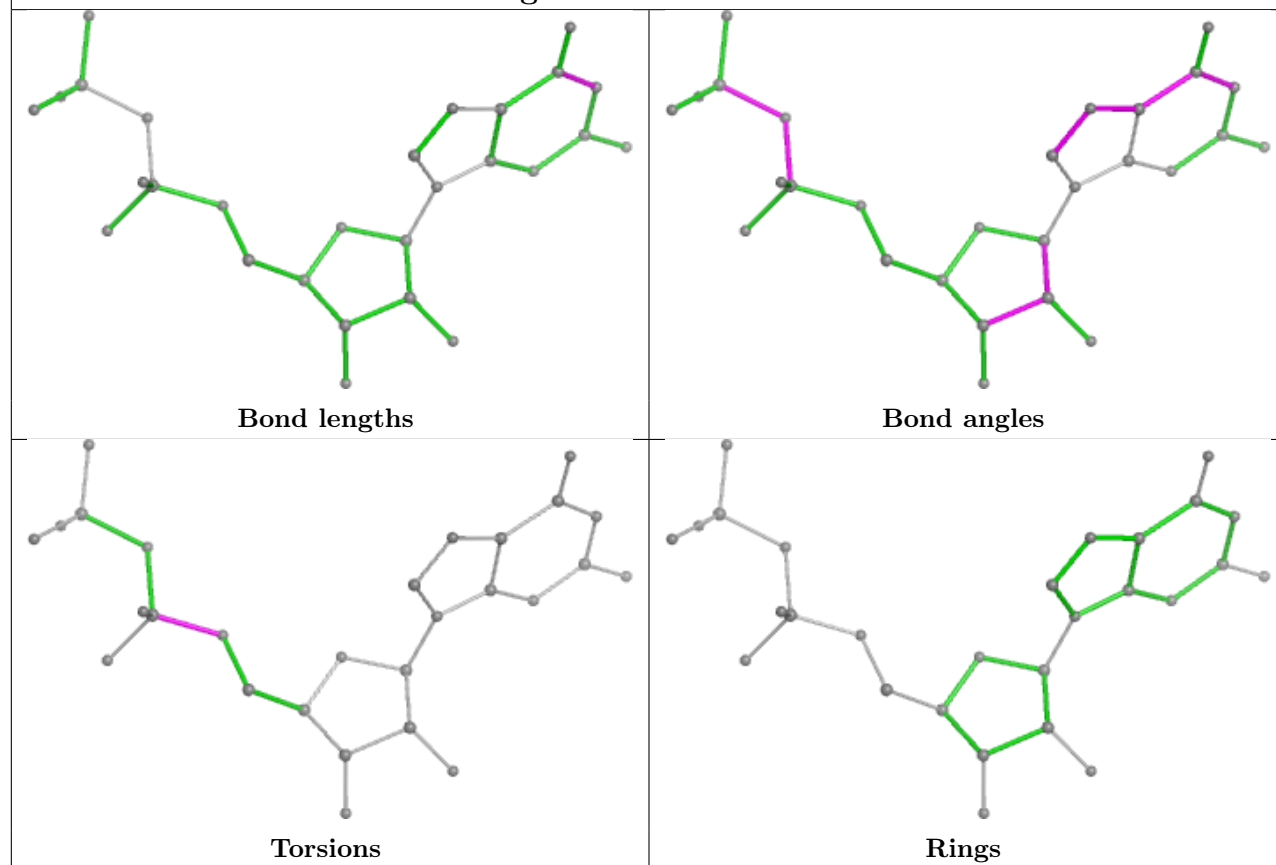


Rings

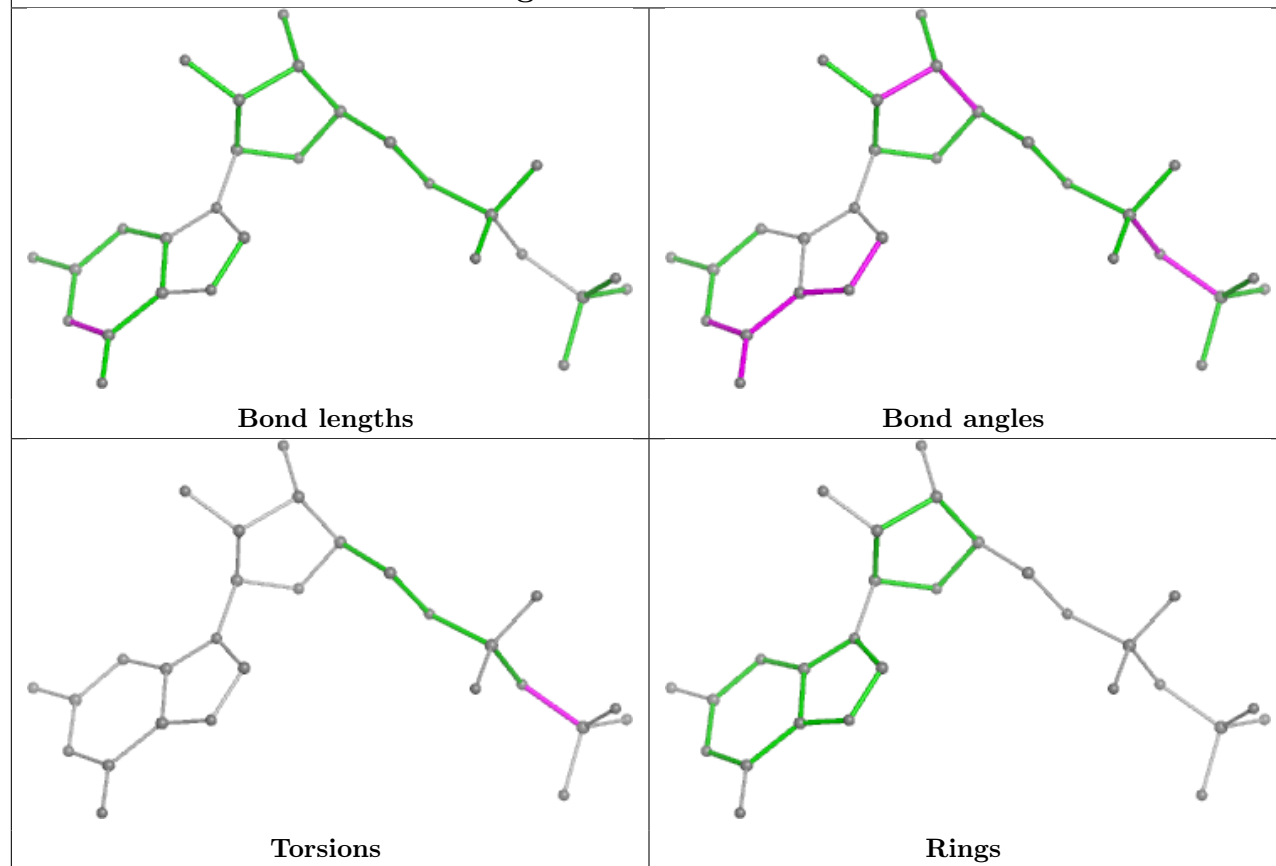
## Ligand GDP U8 501



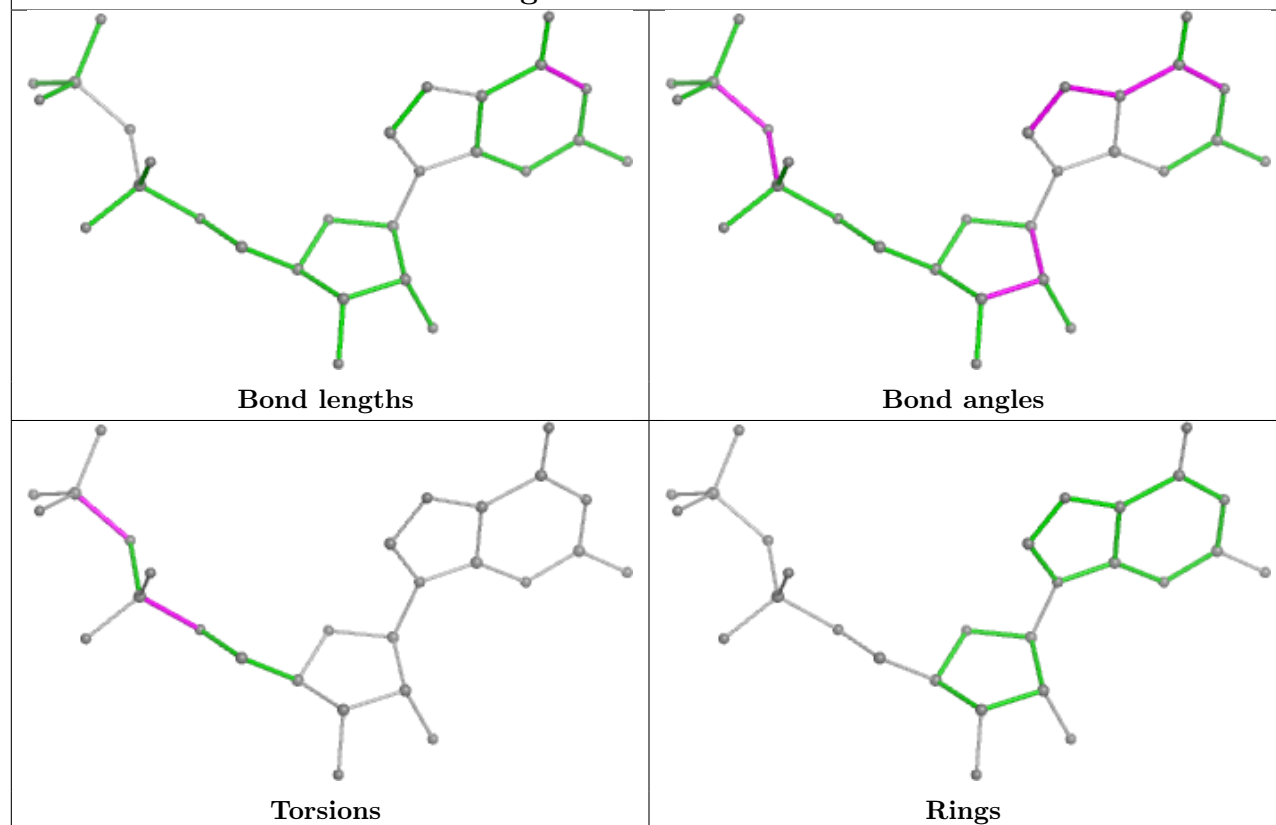
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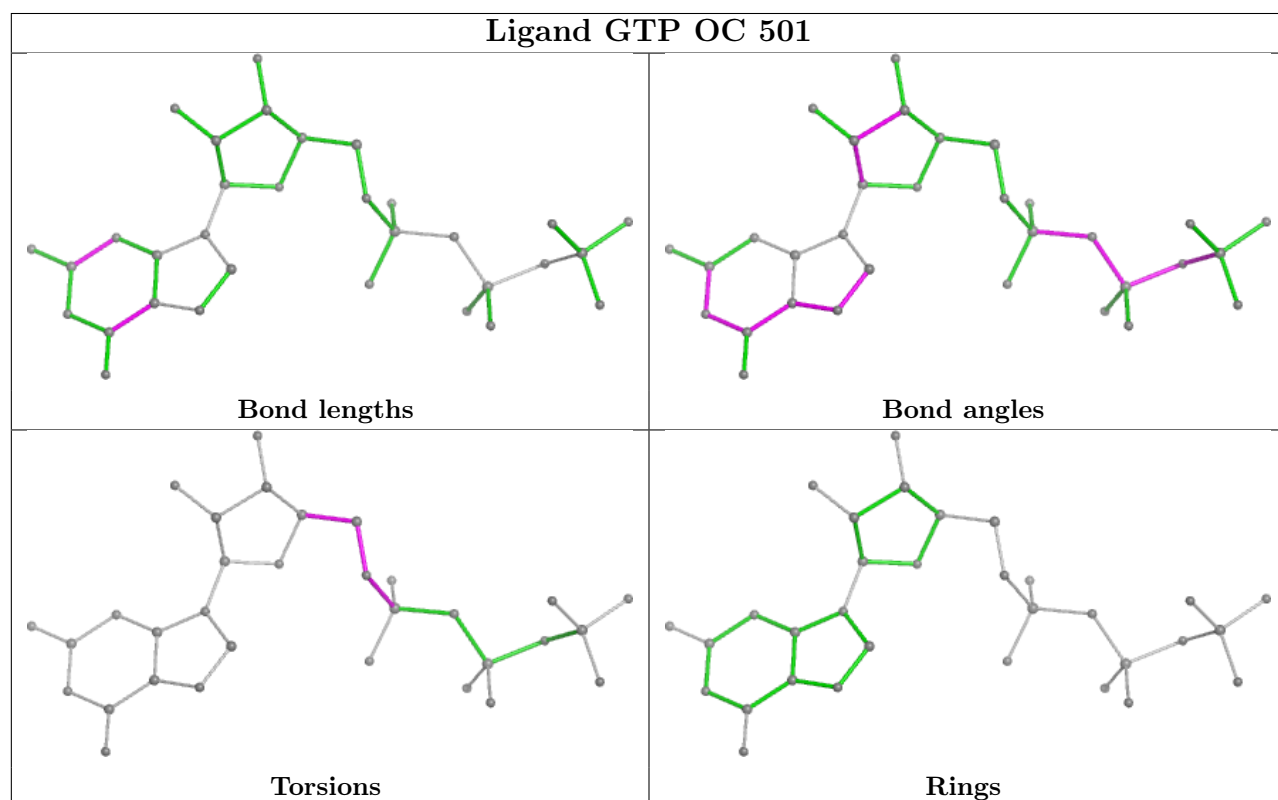
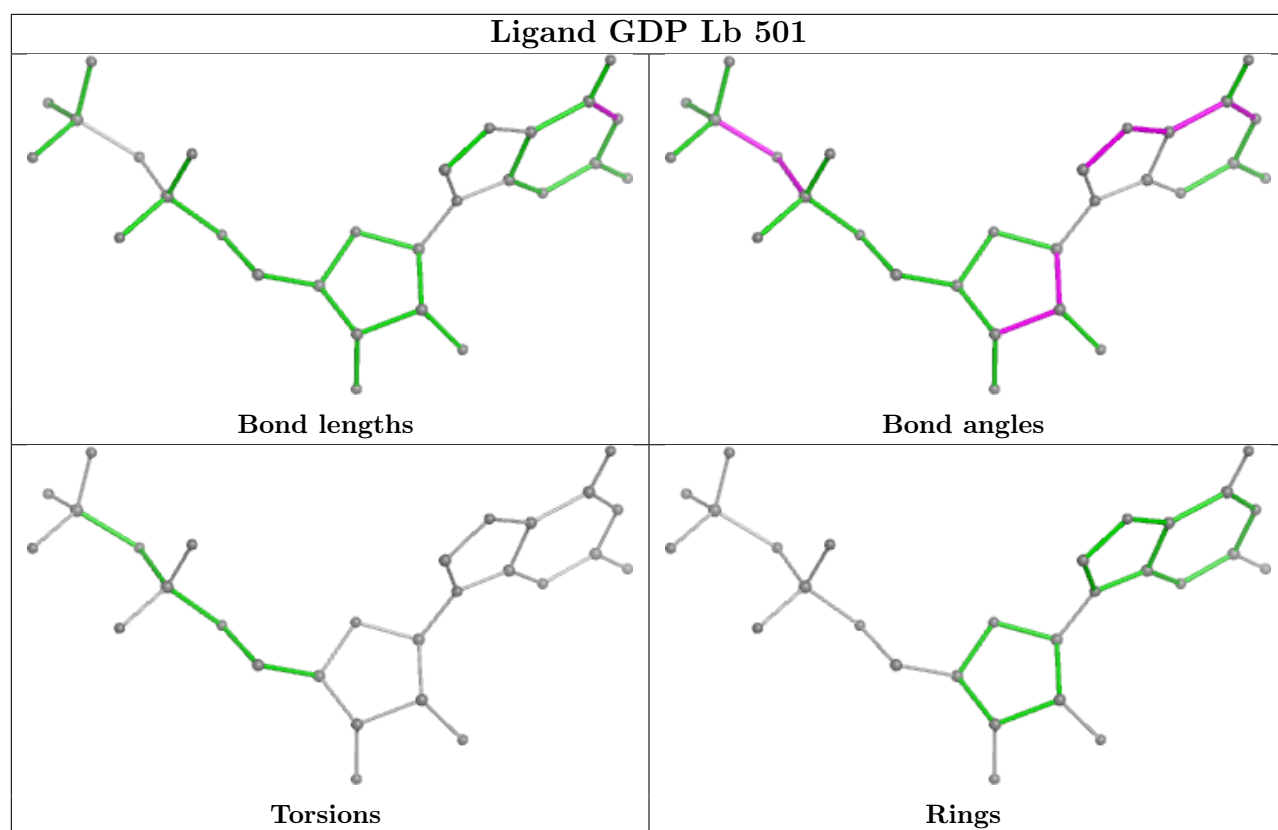


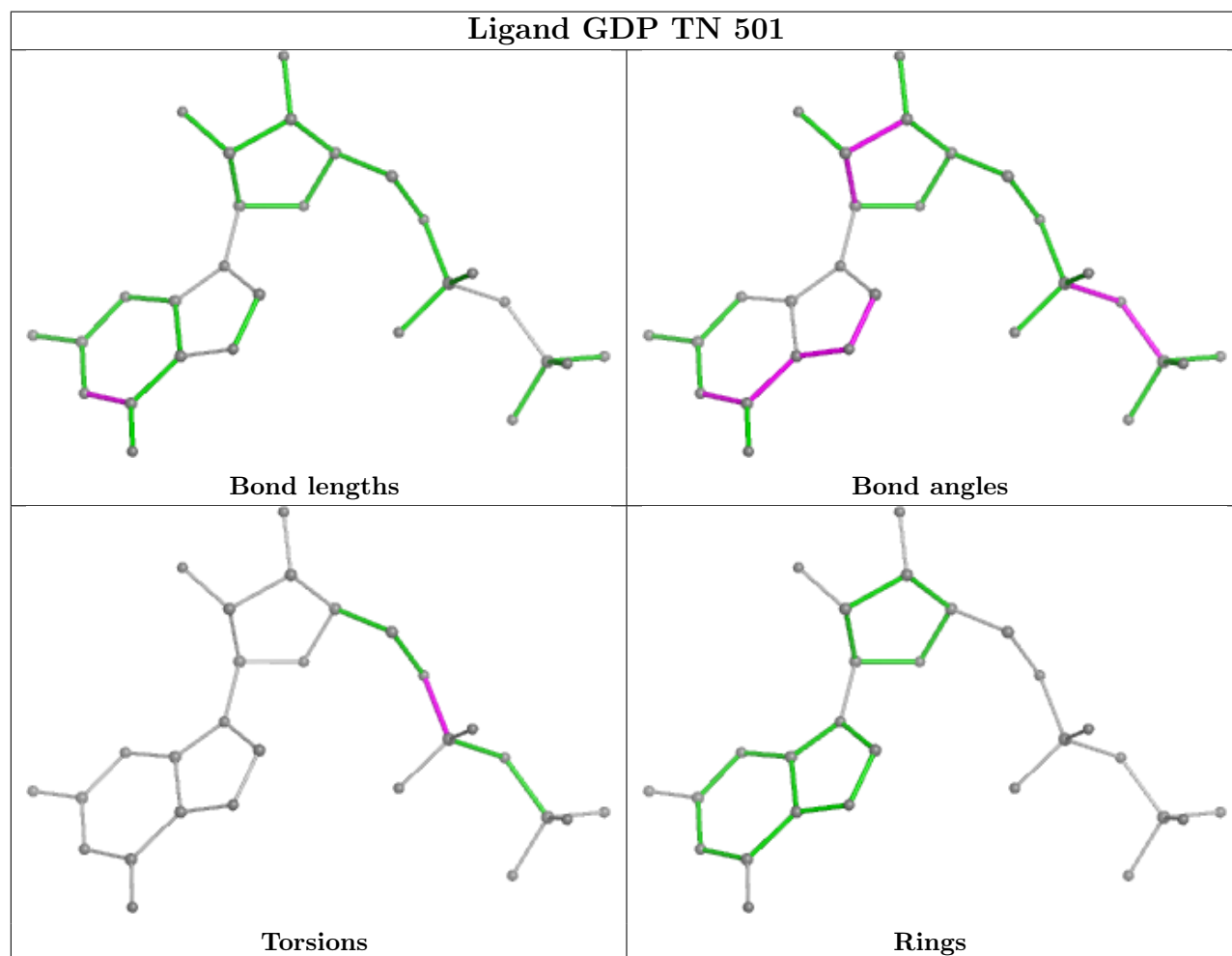
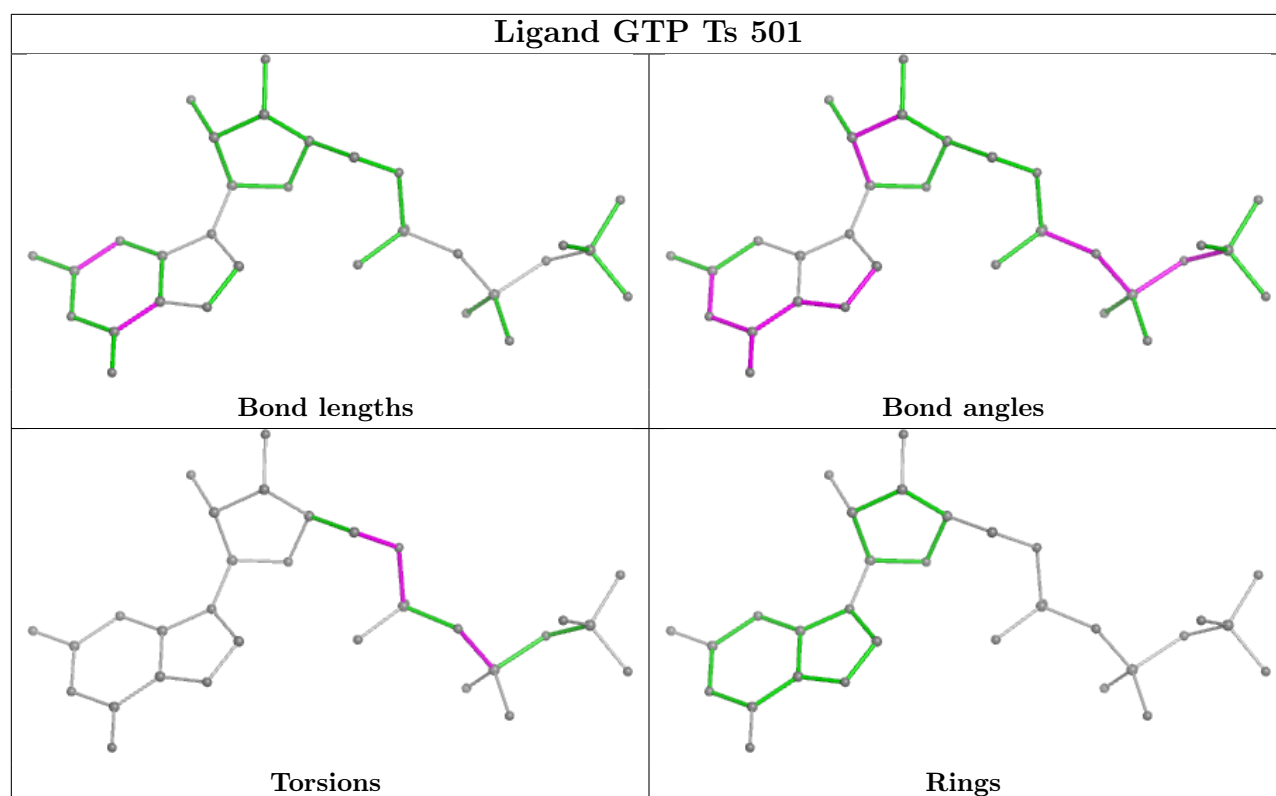
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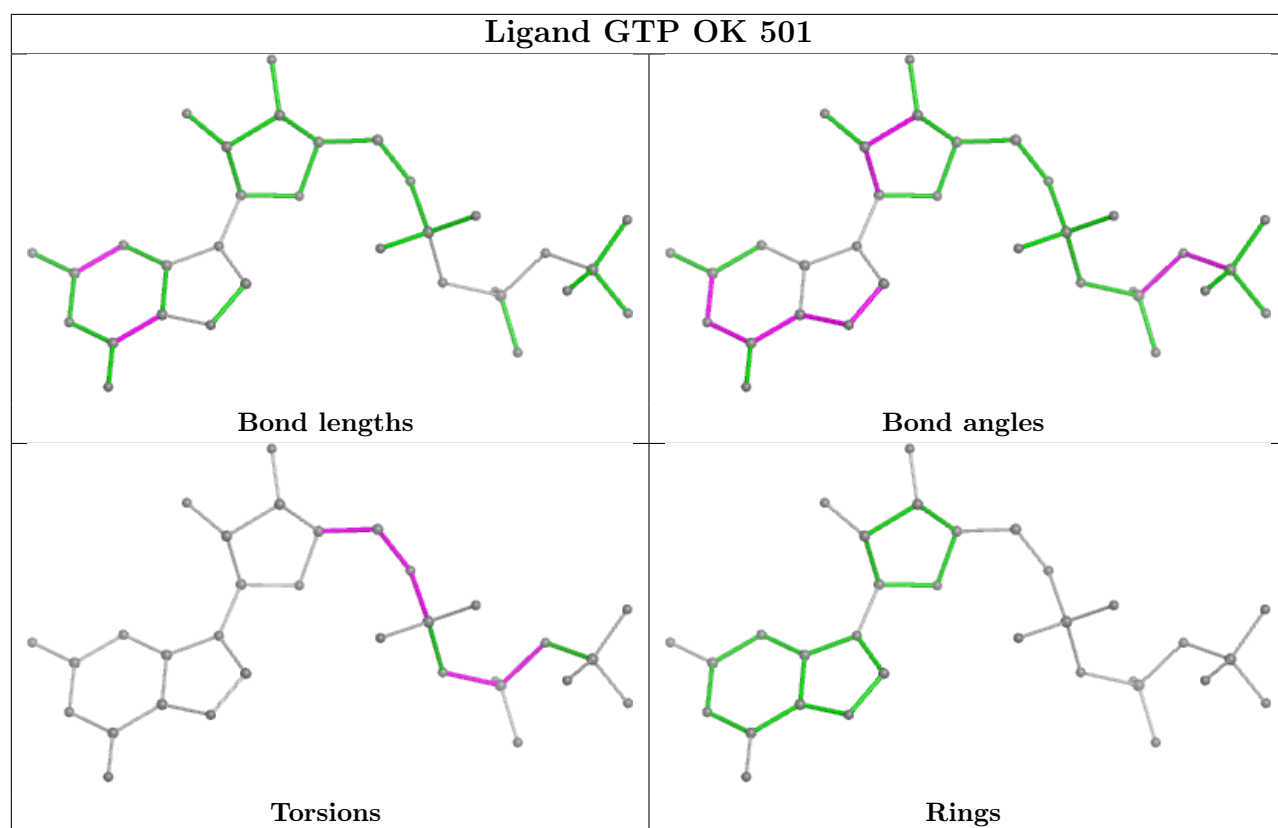


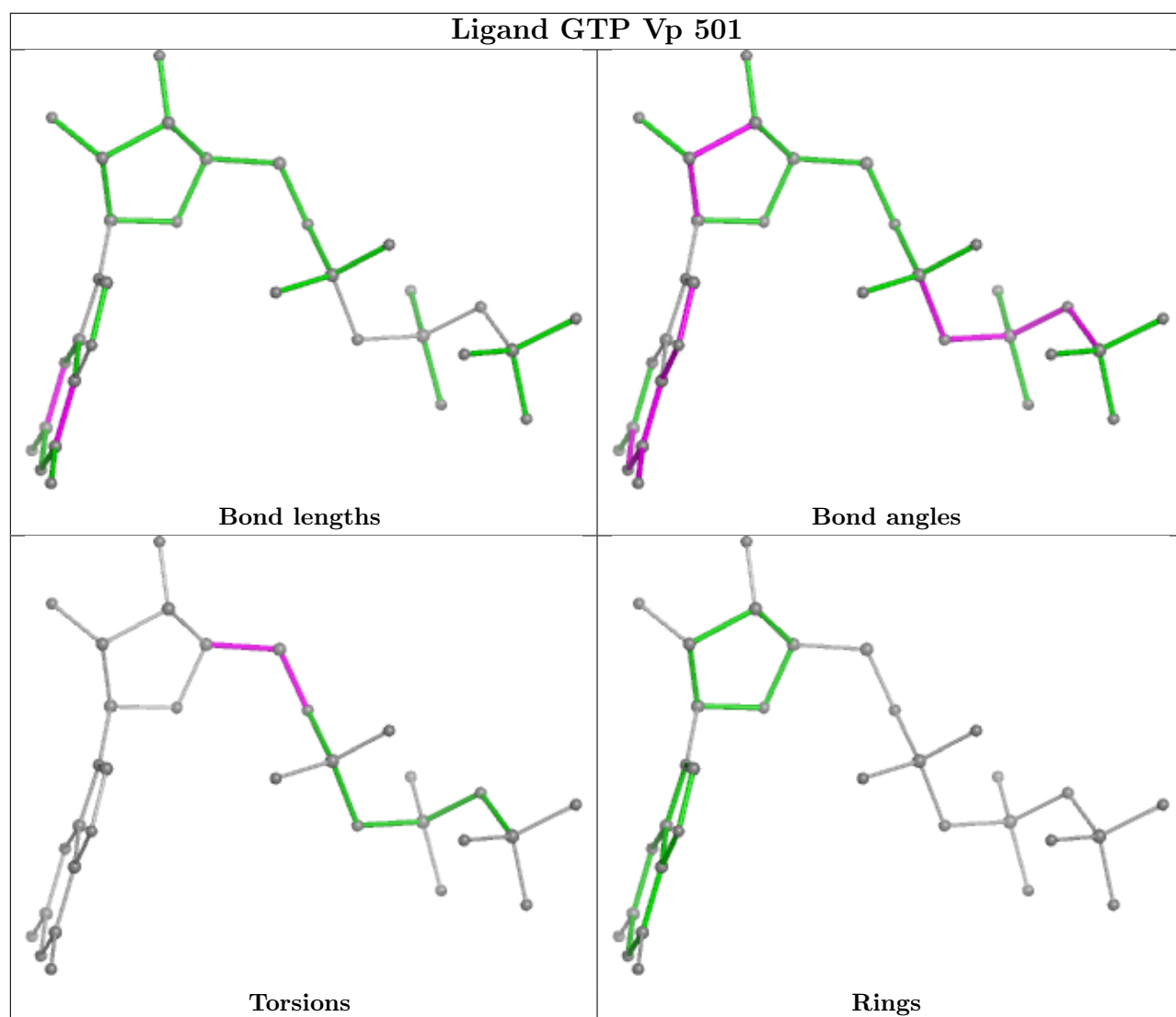
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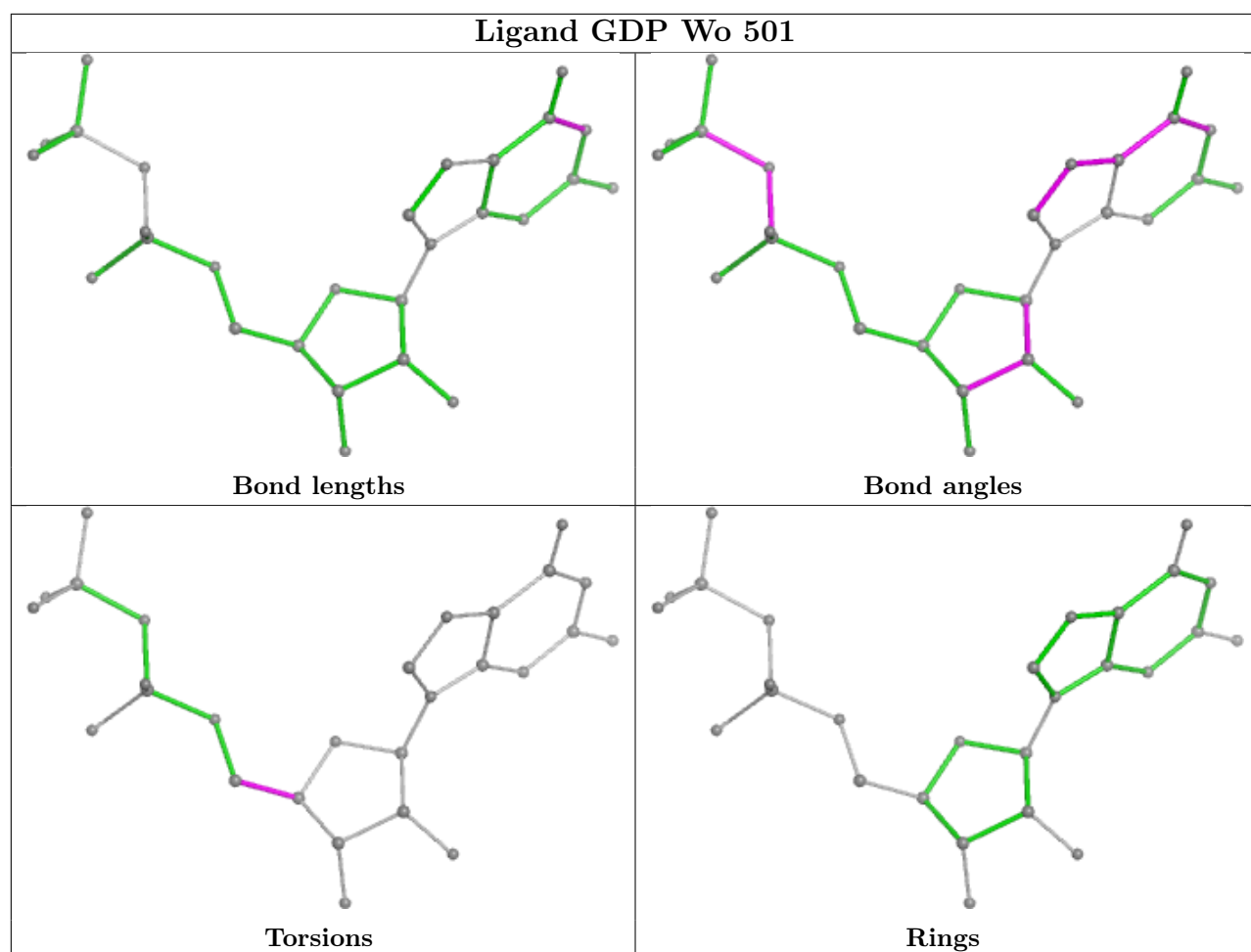


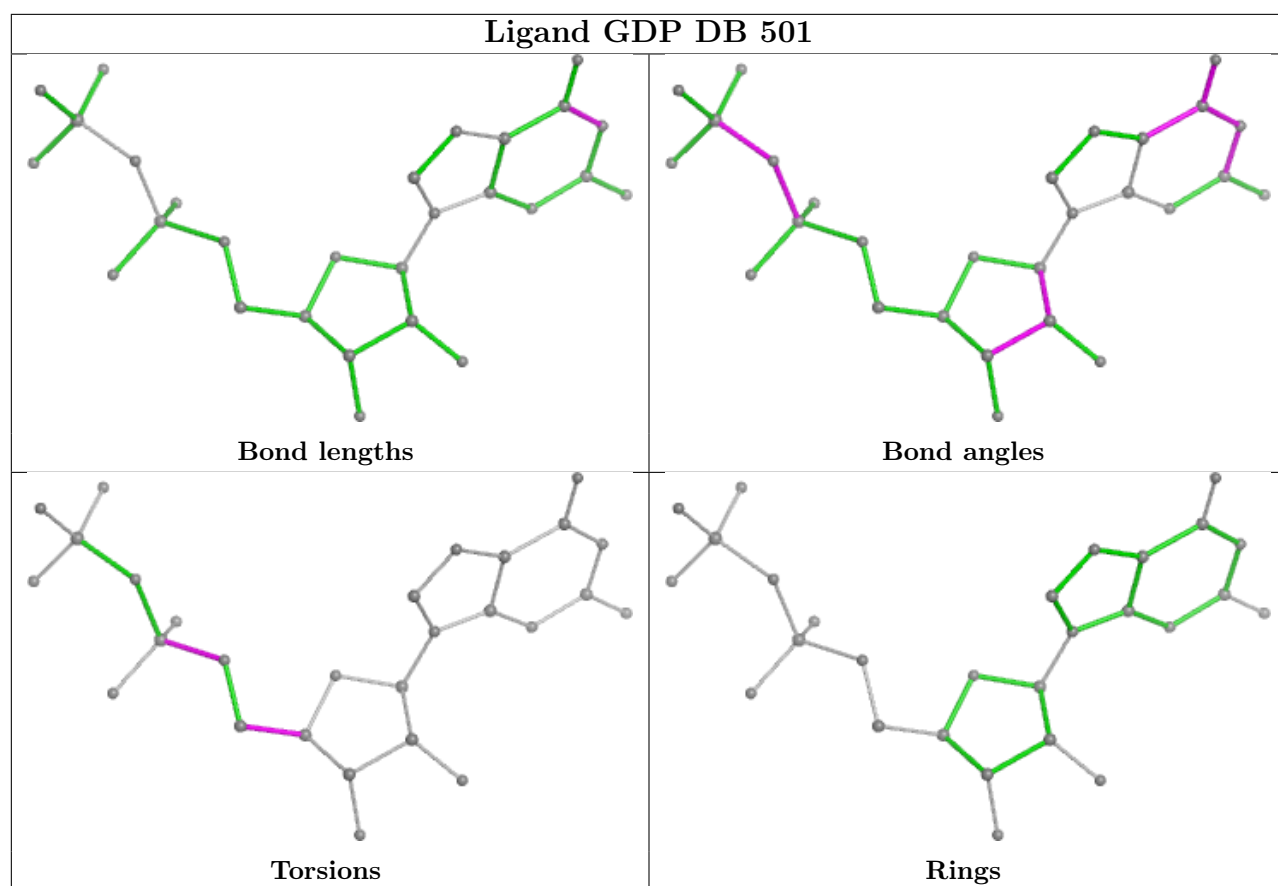


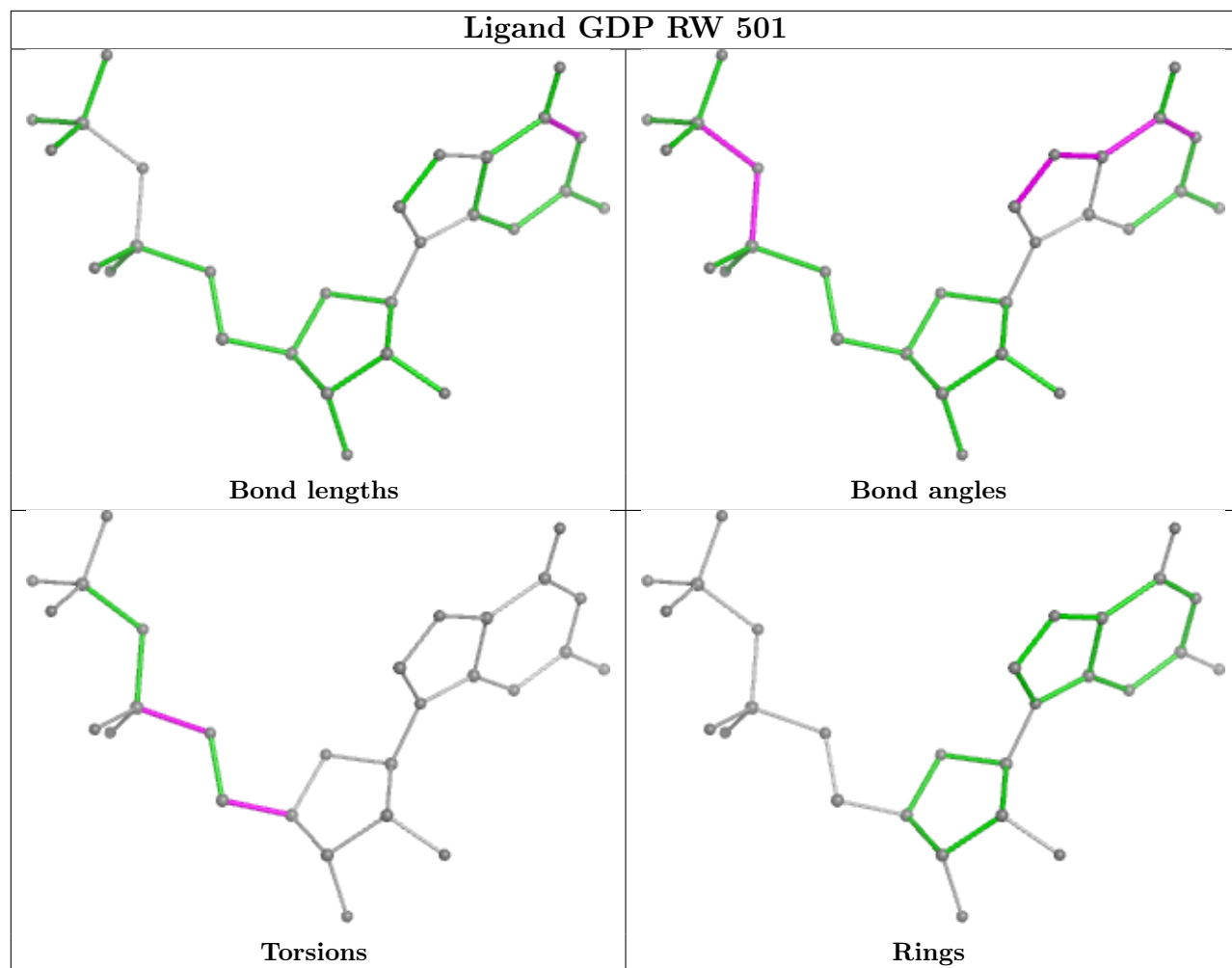


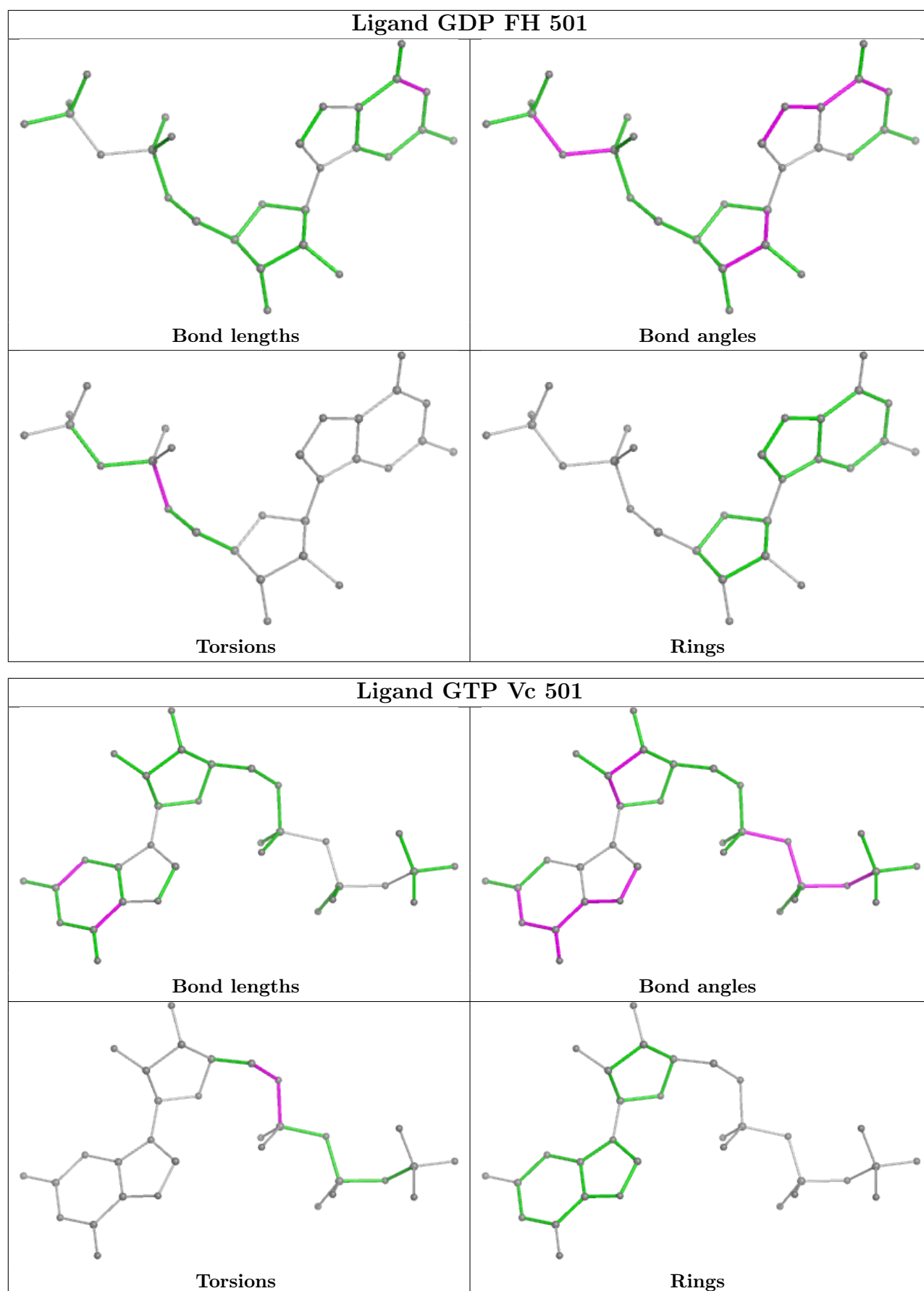


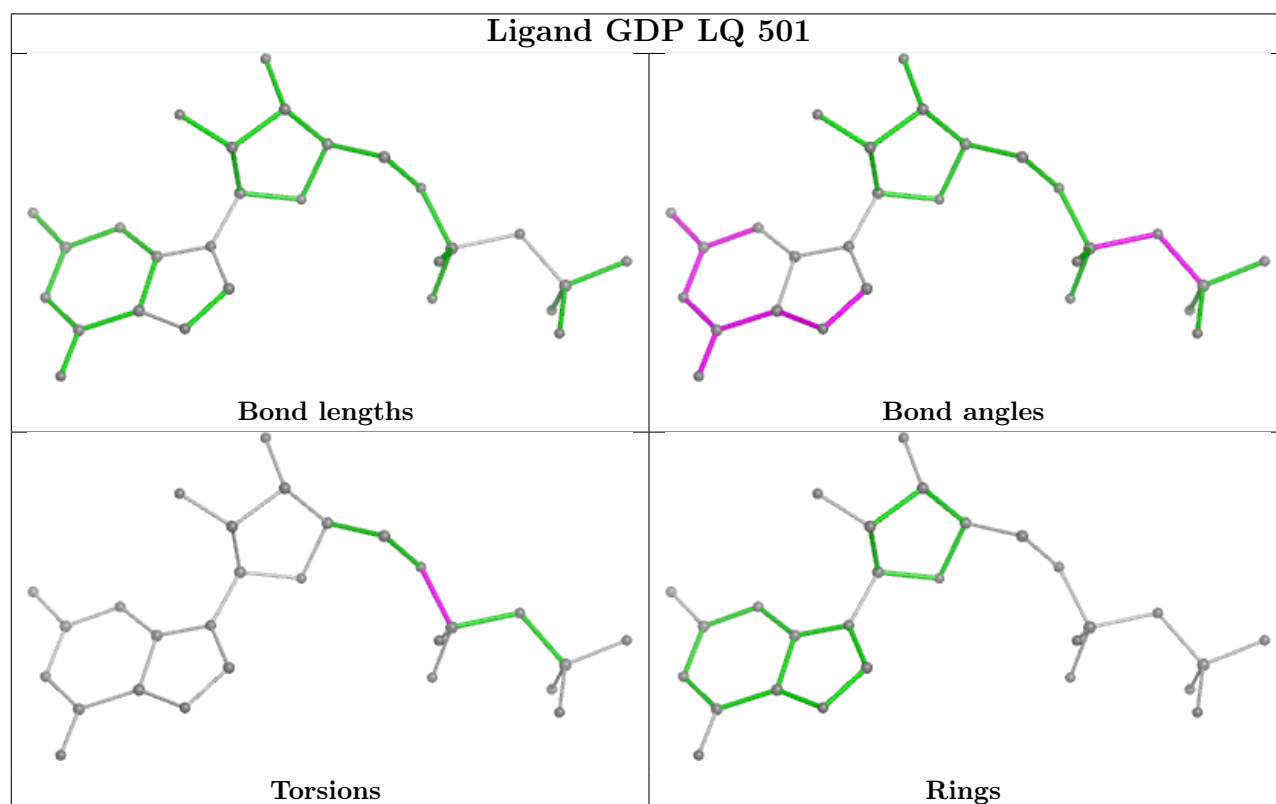
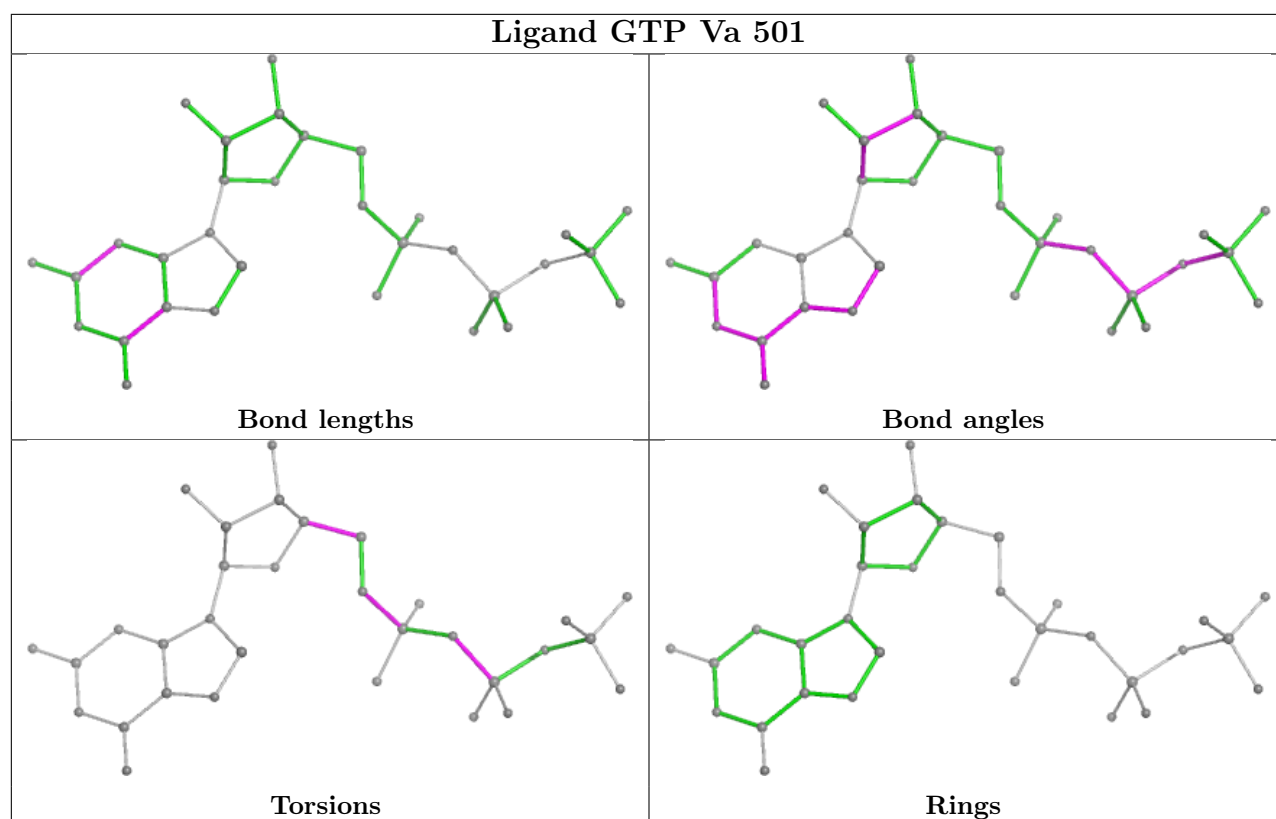


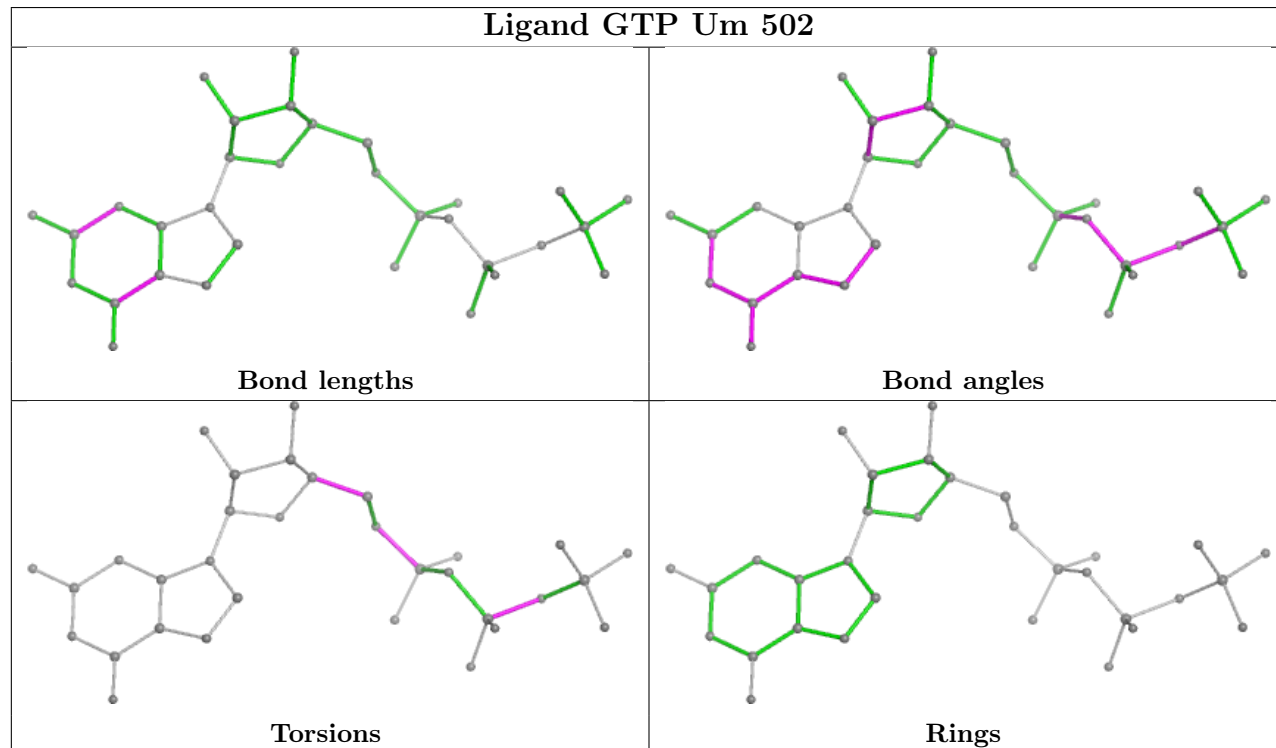
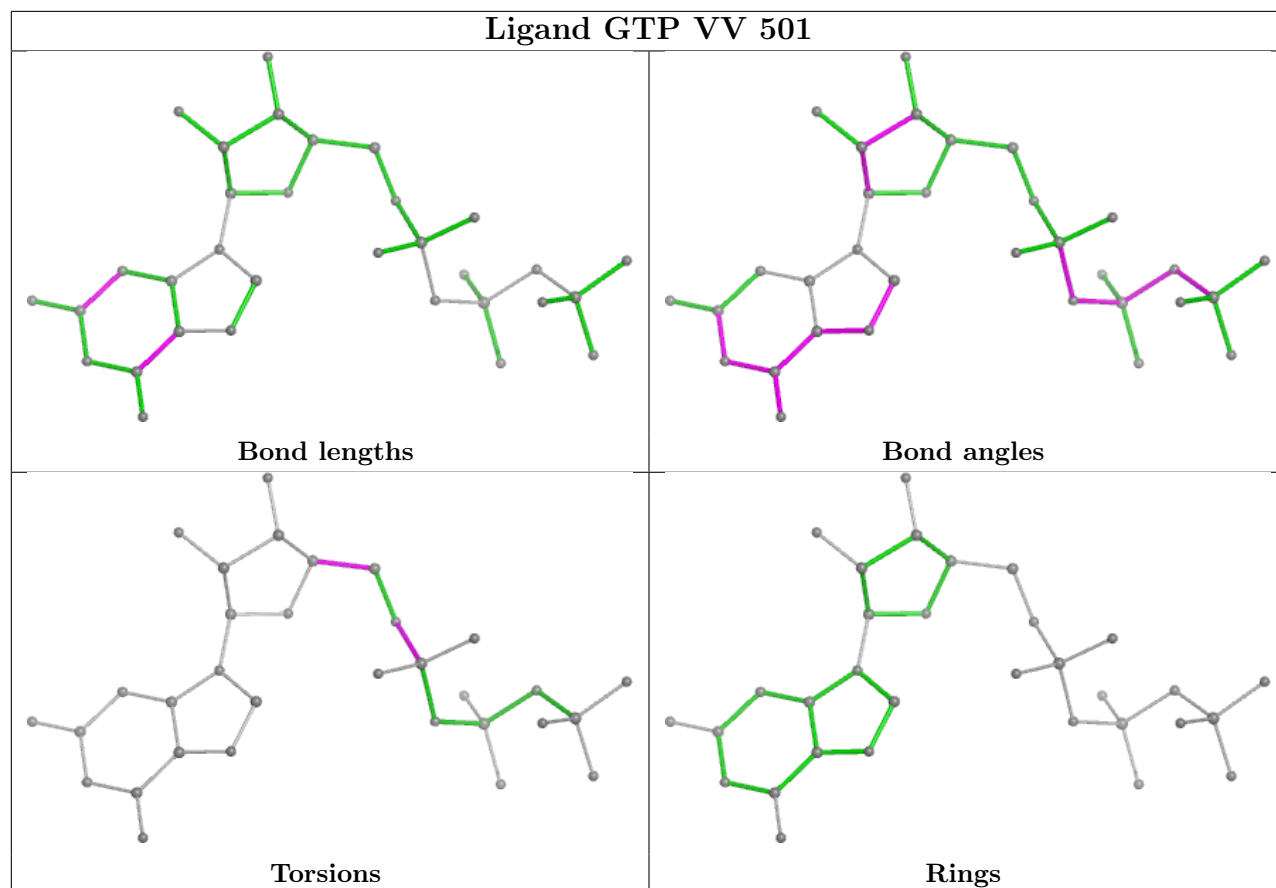


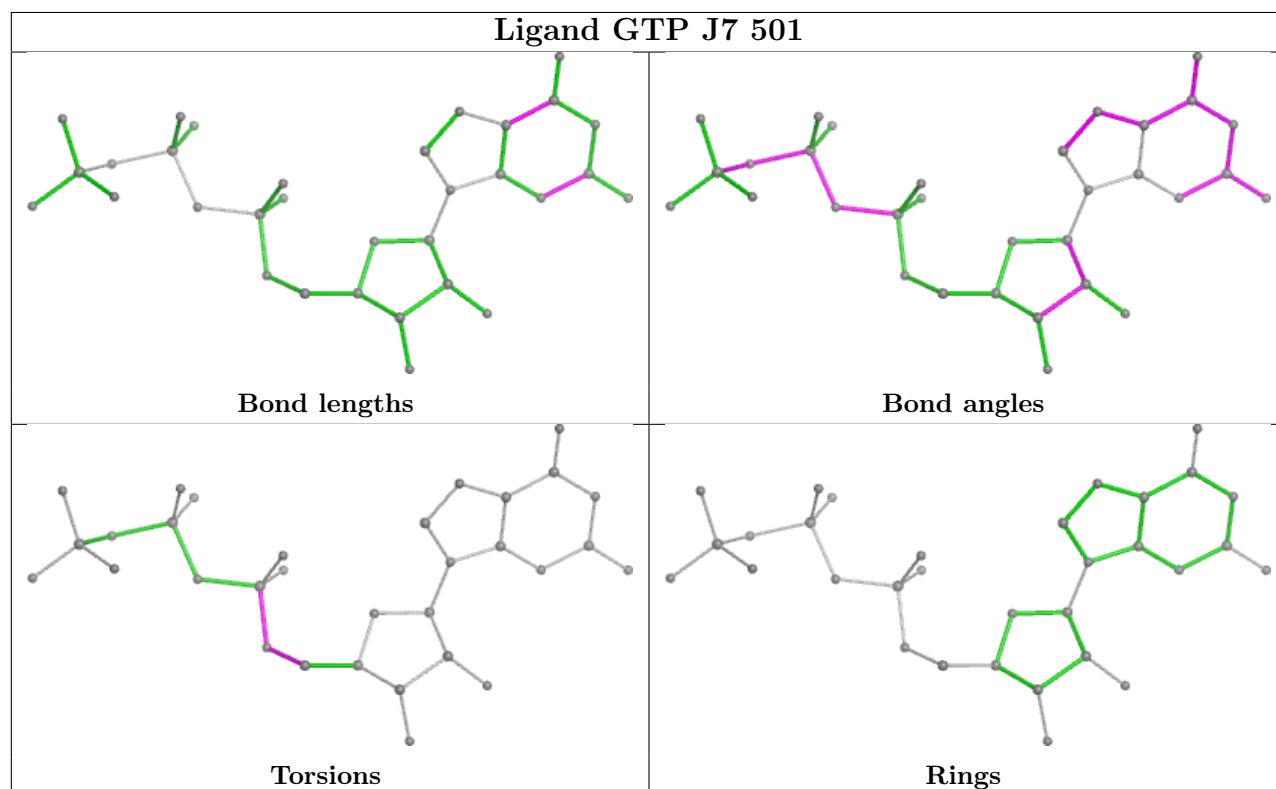
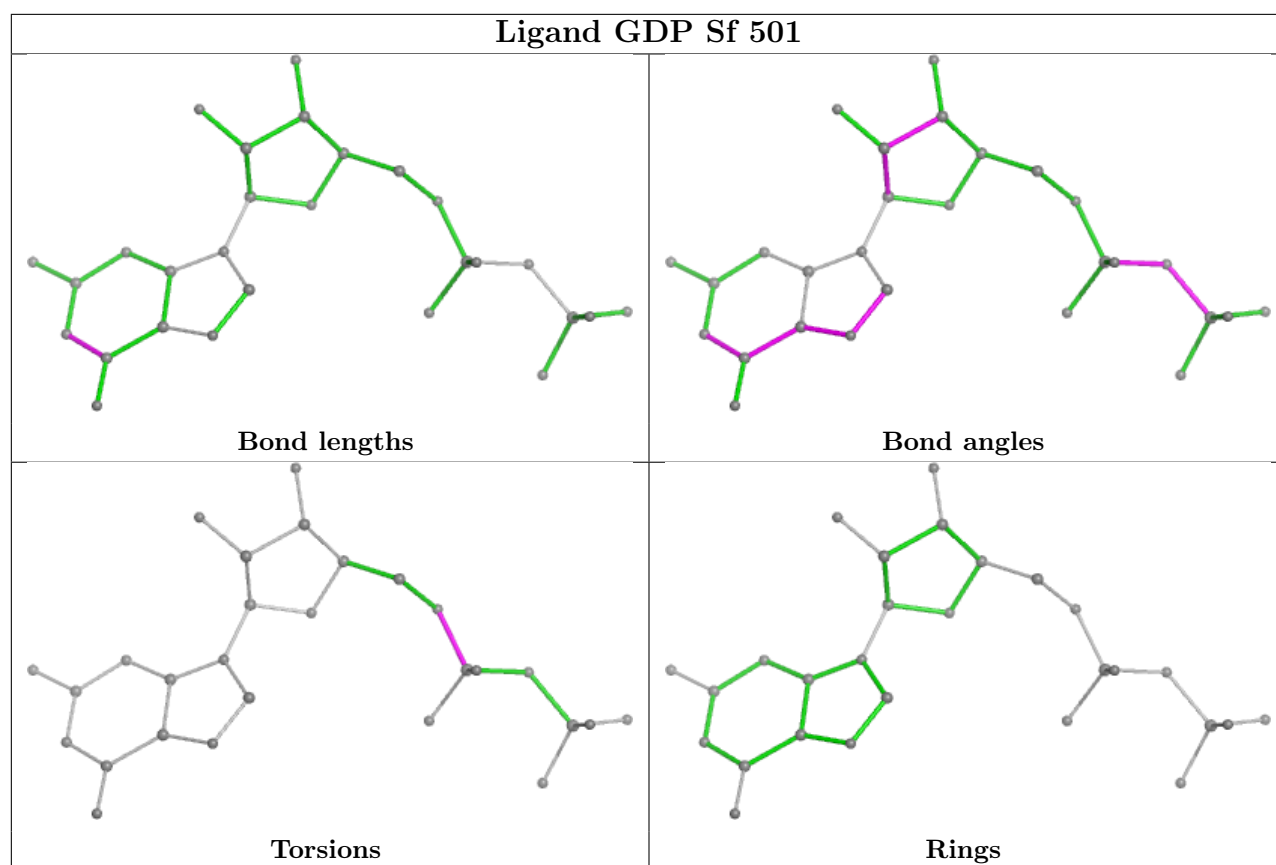


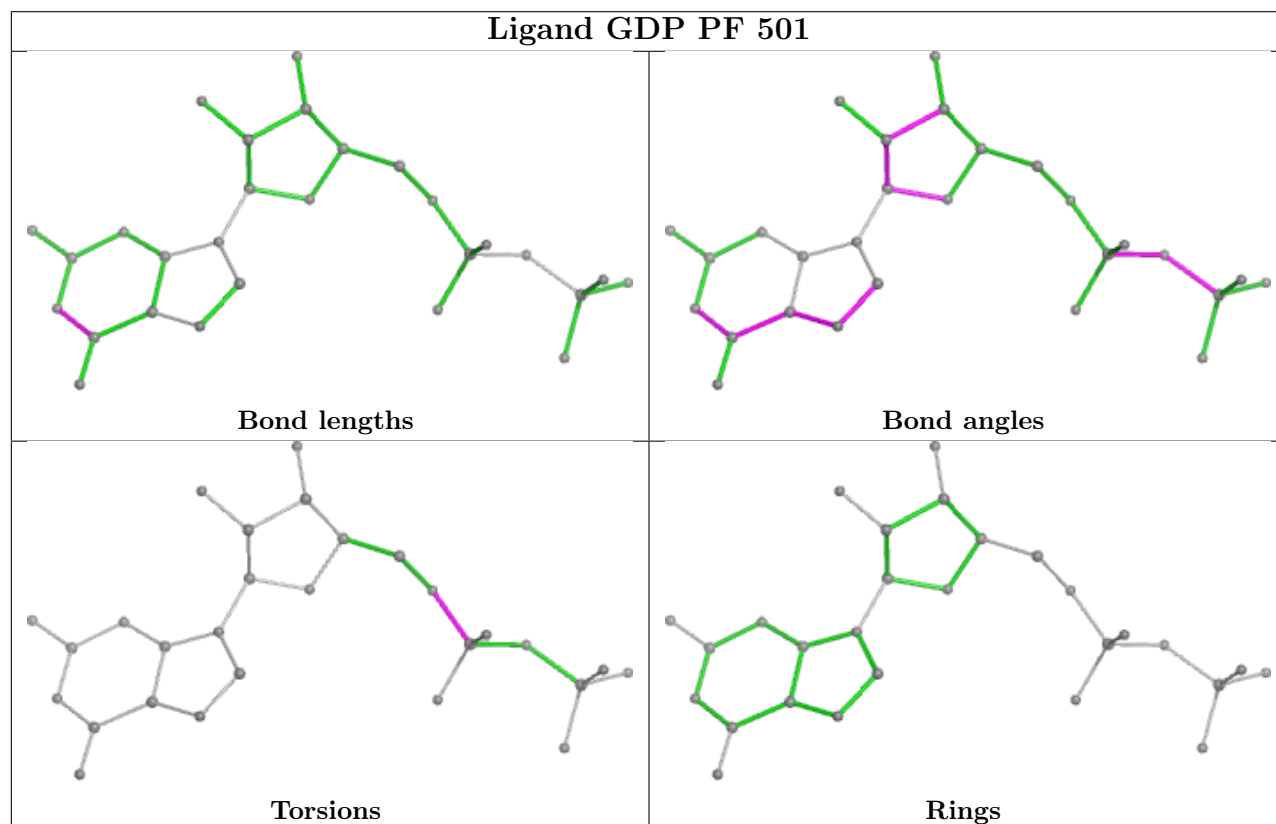
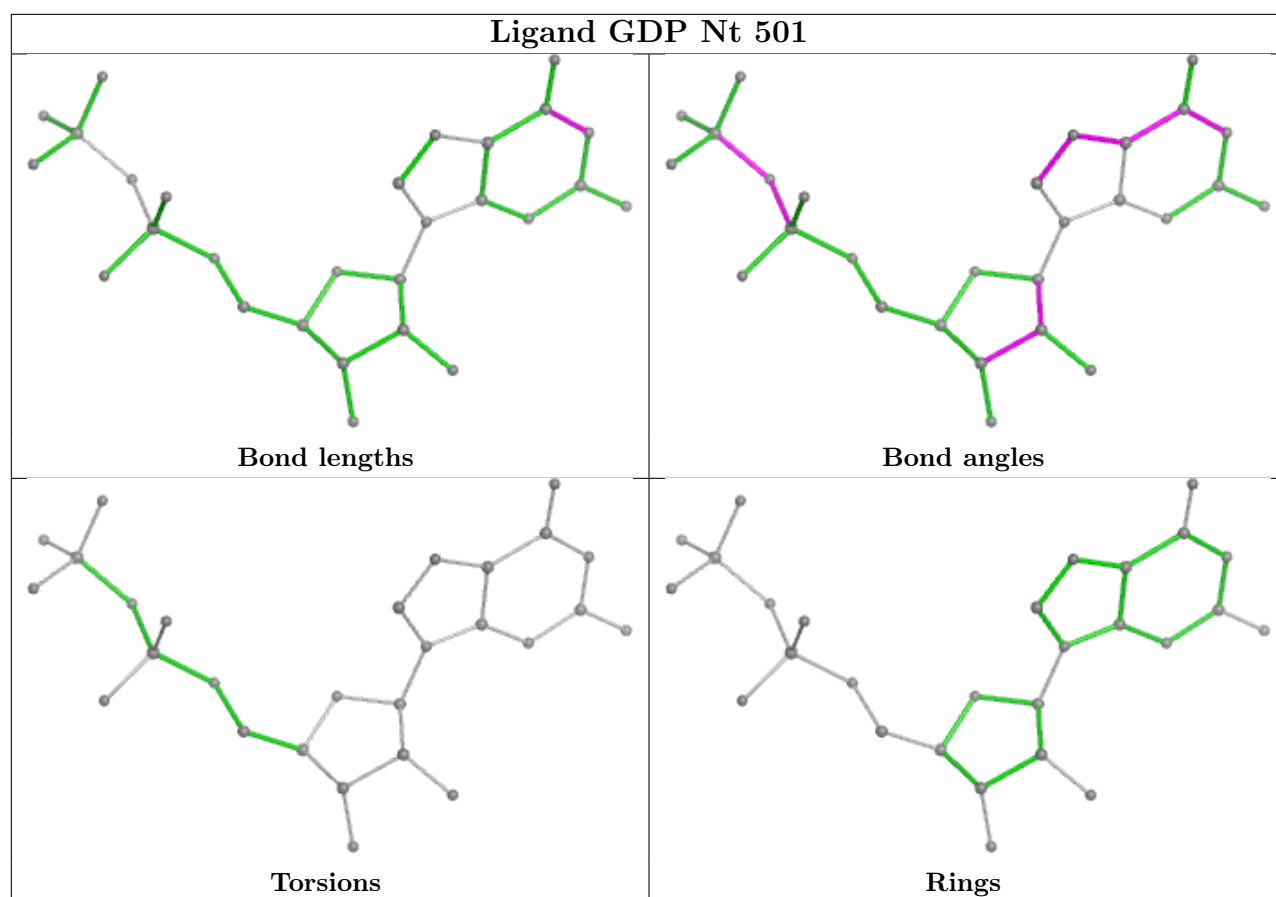




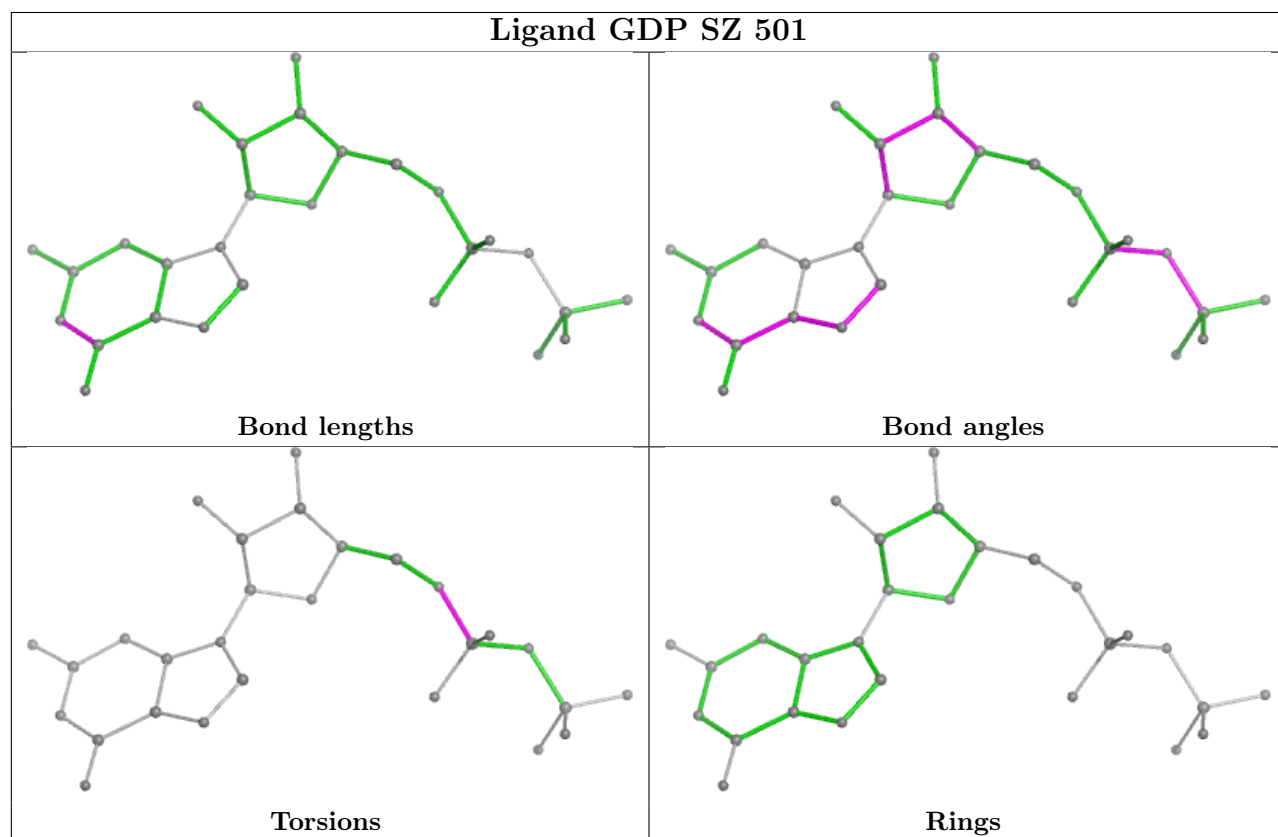
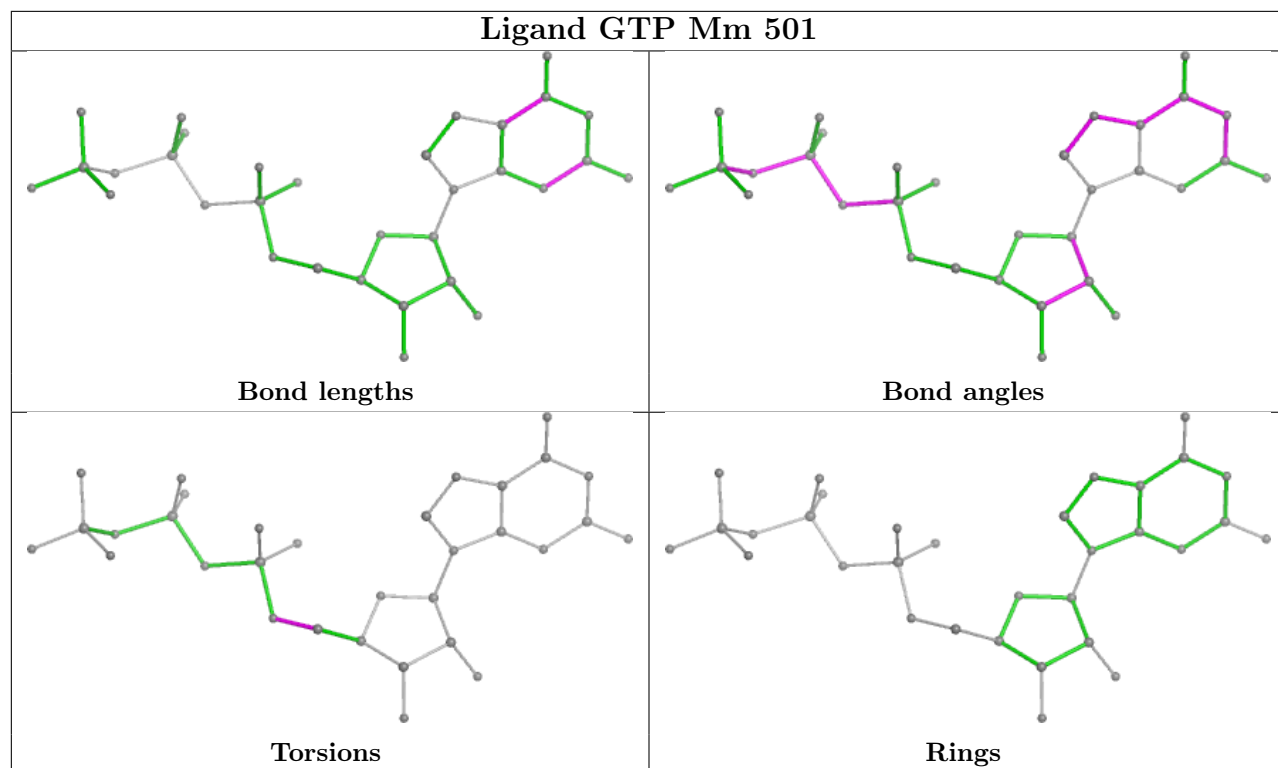


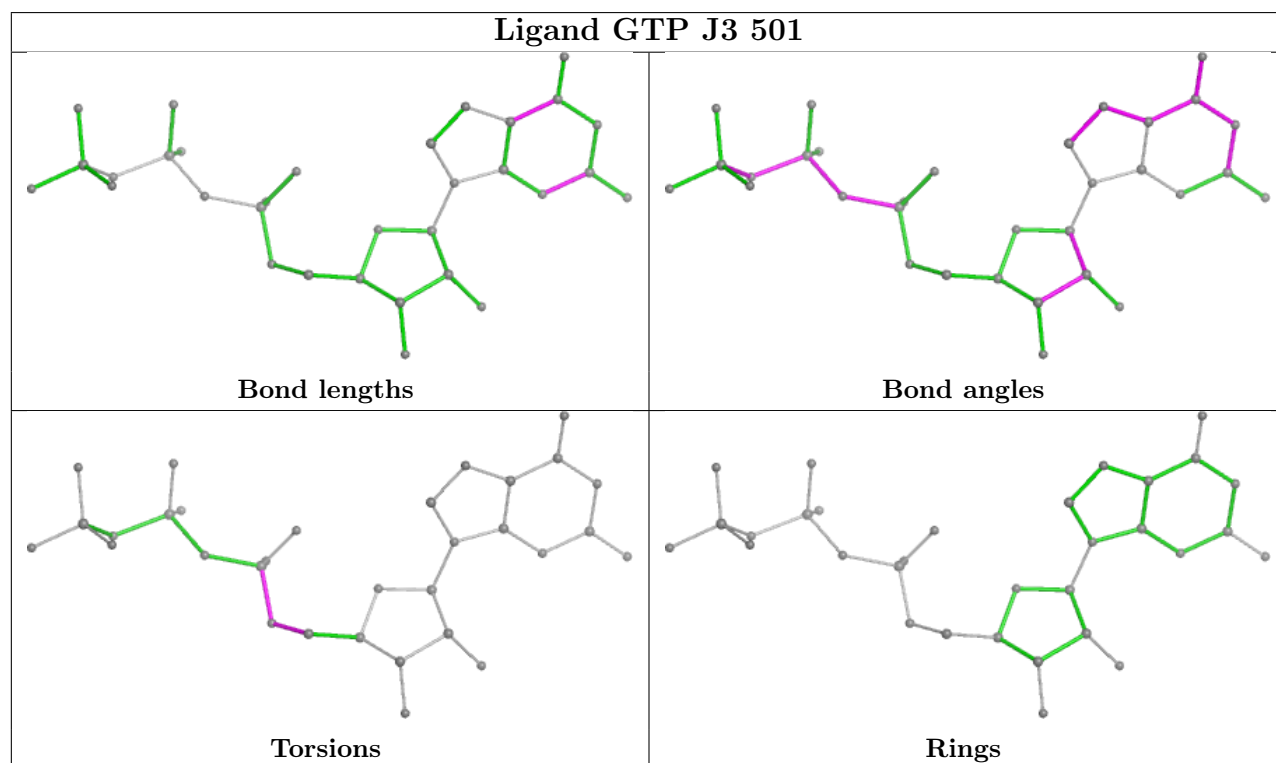
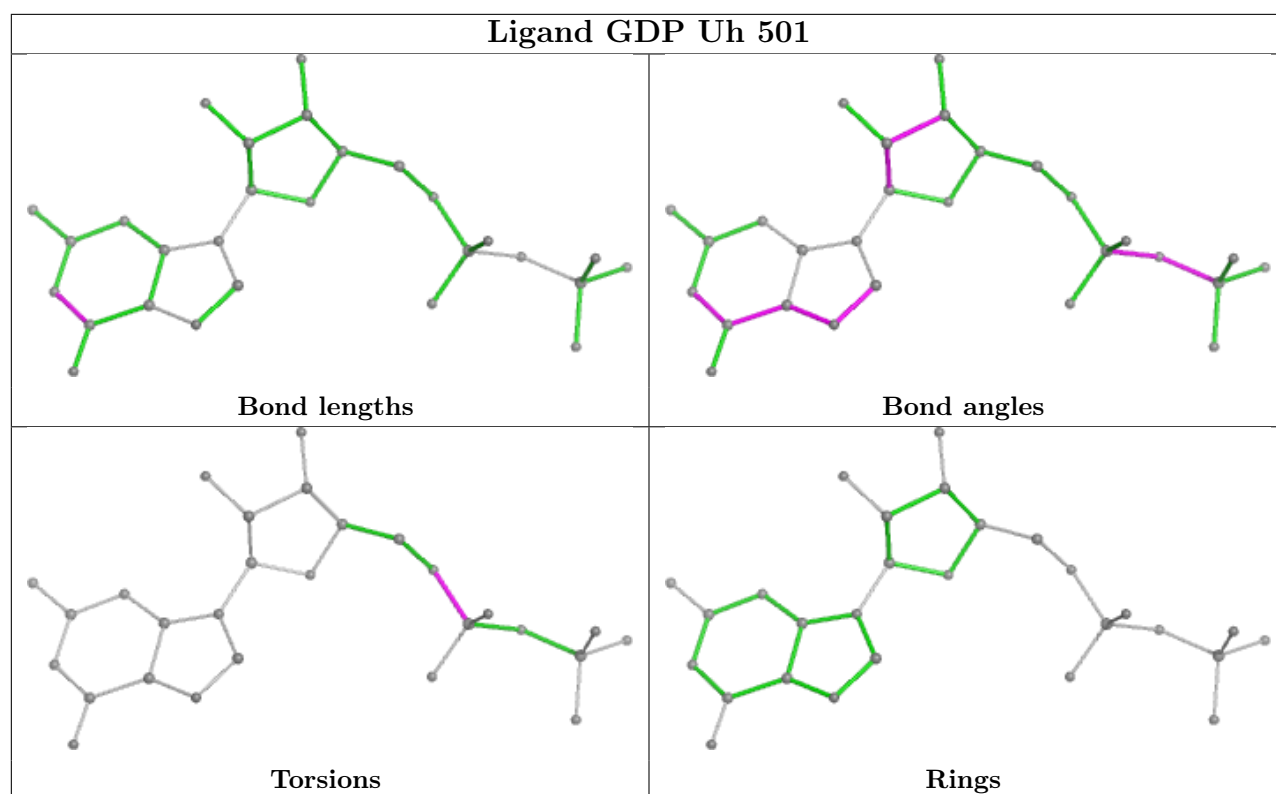




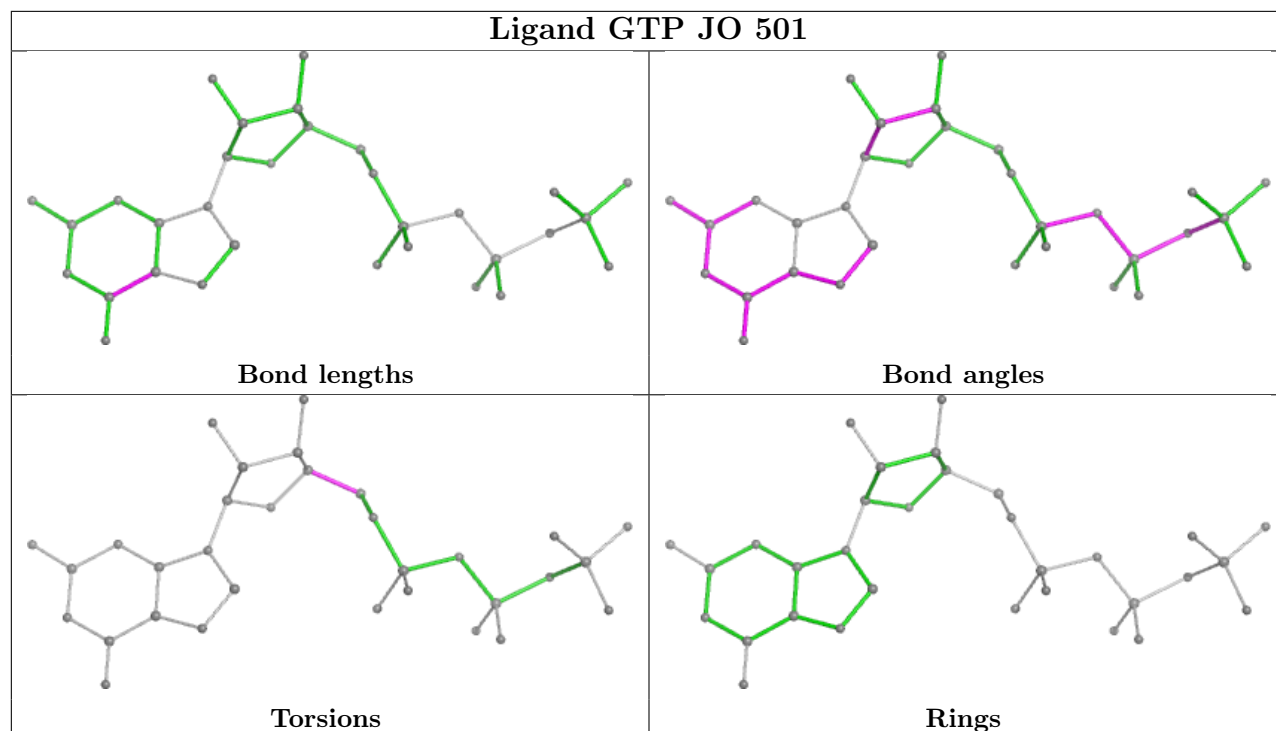




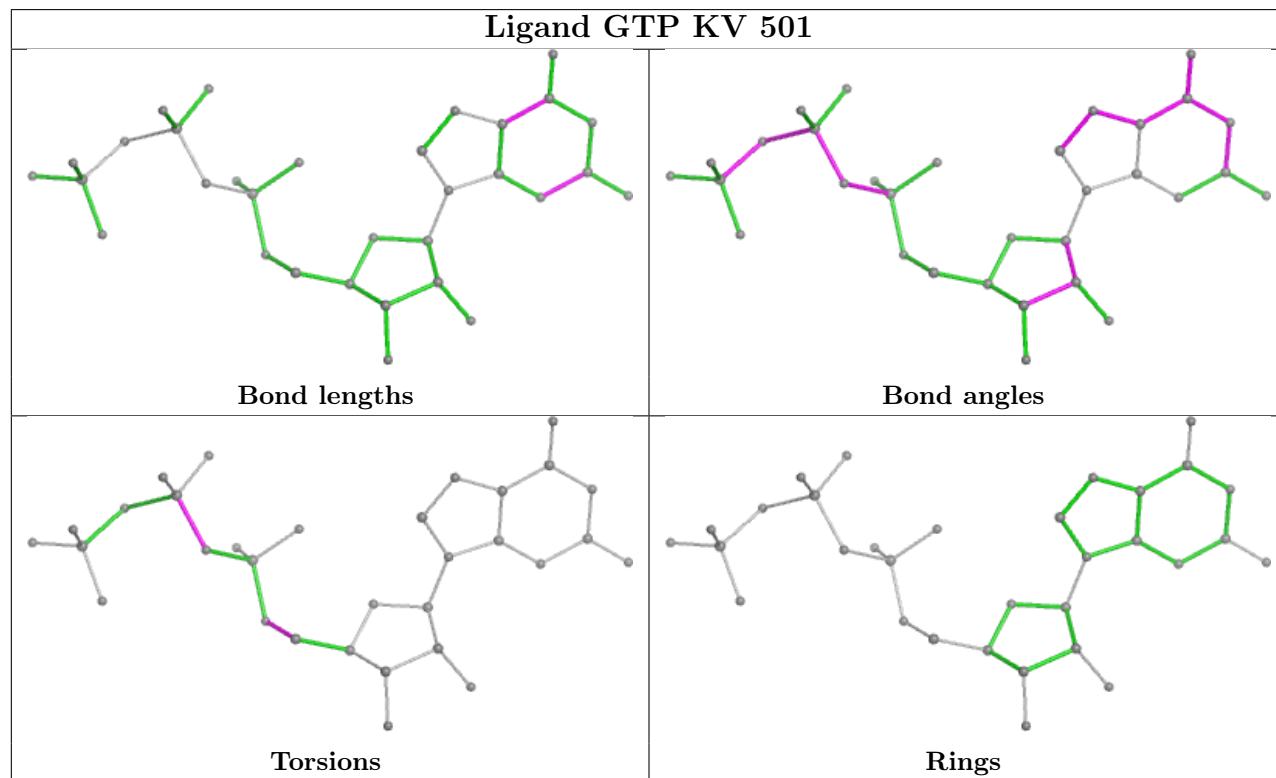


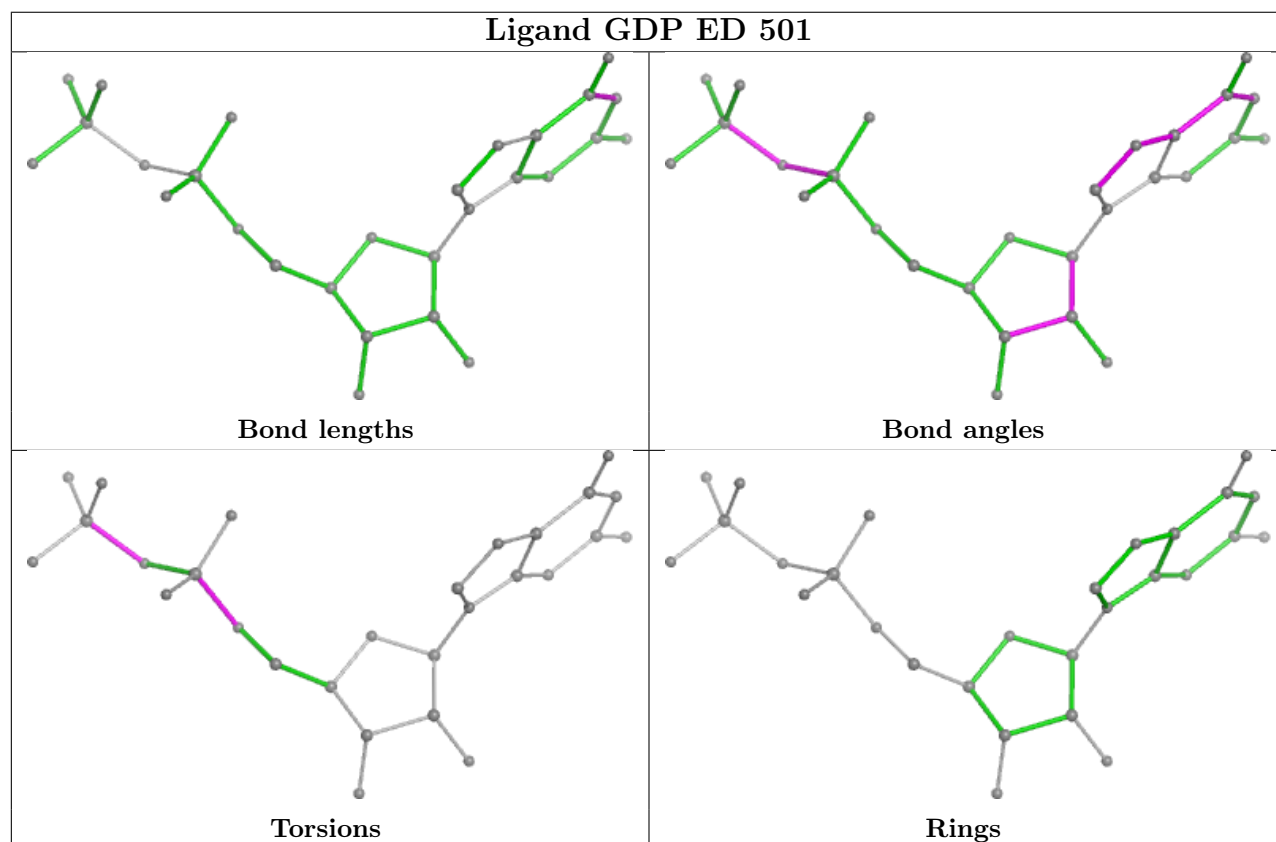
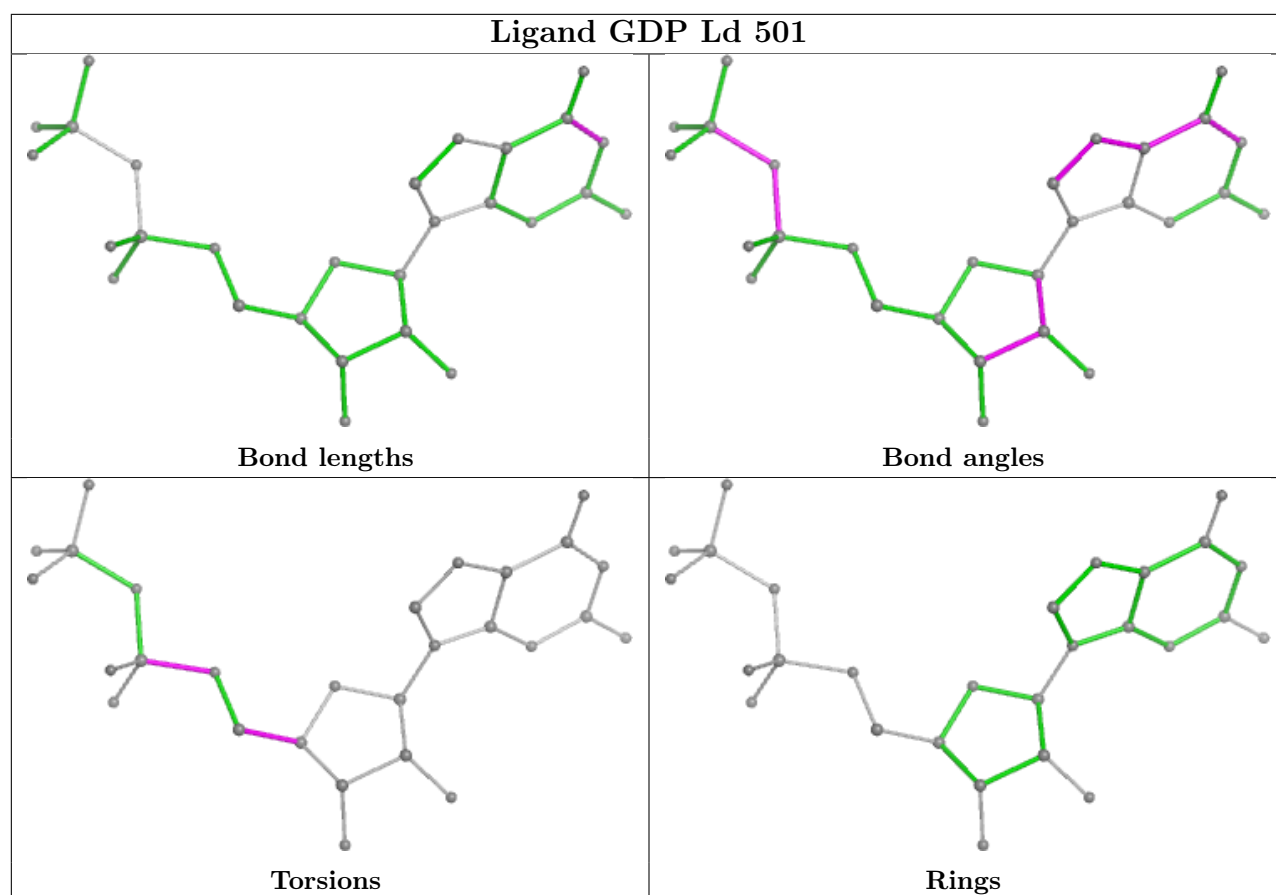


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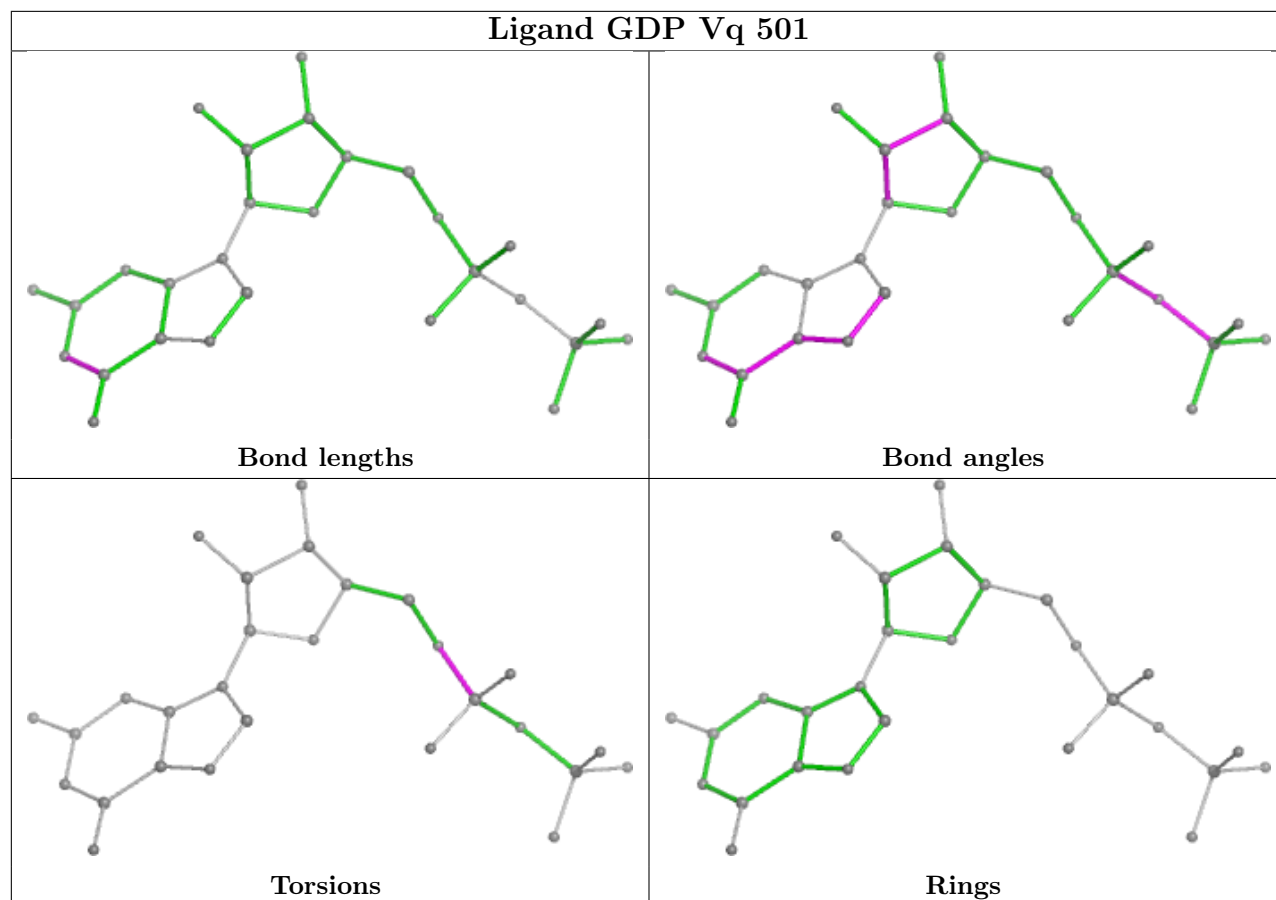


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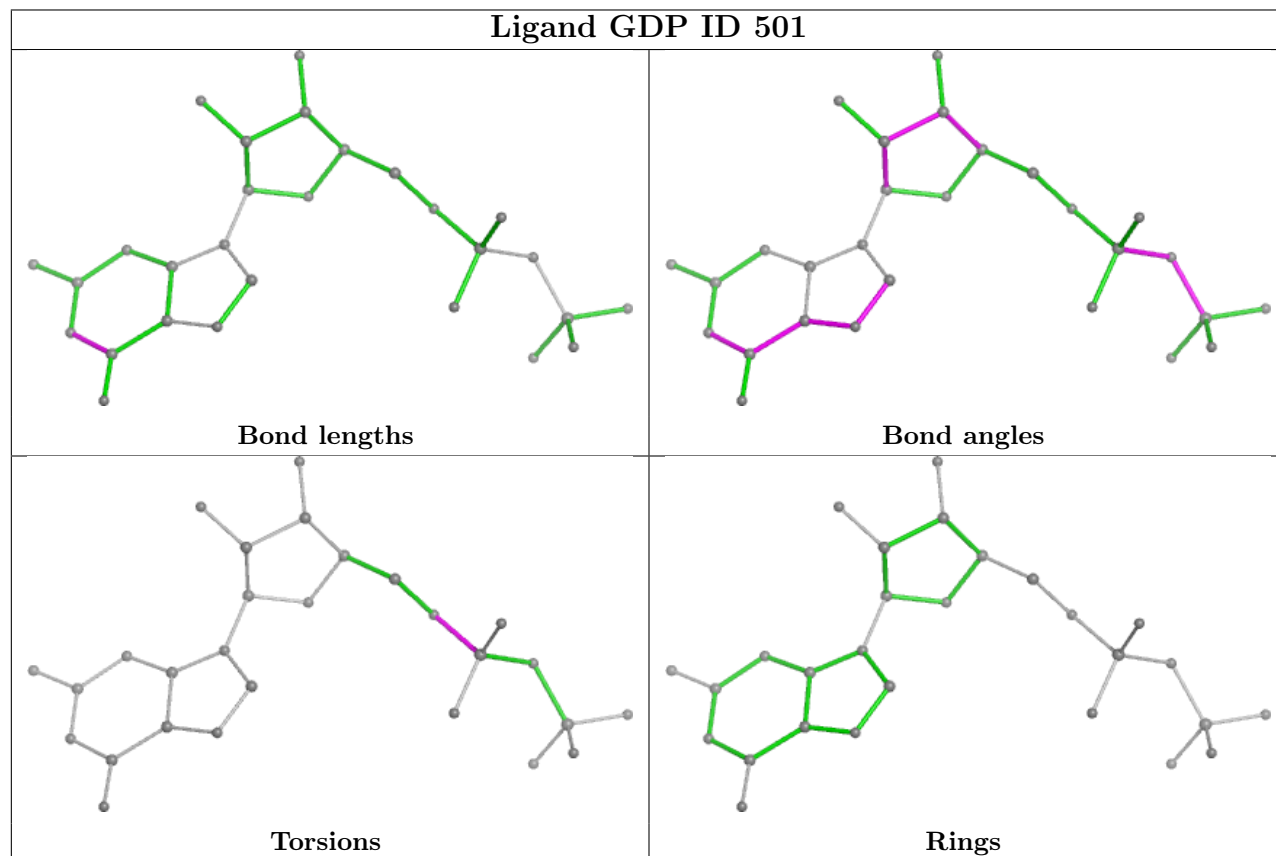


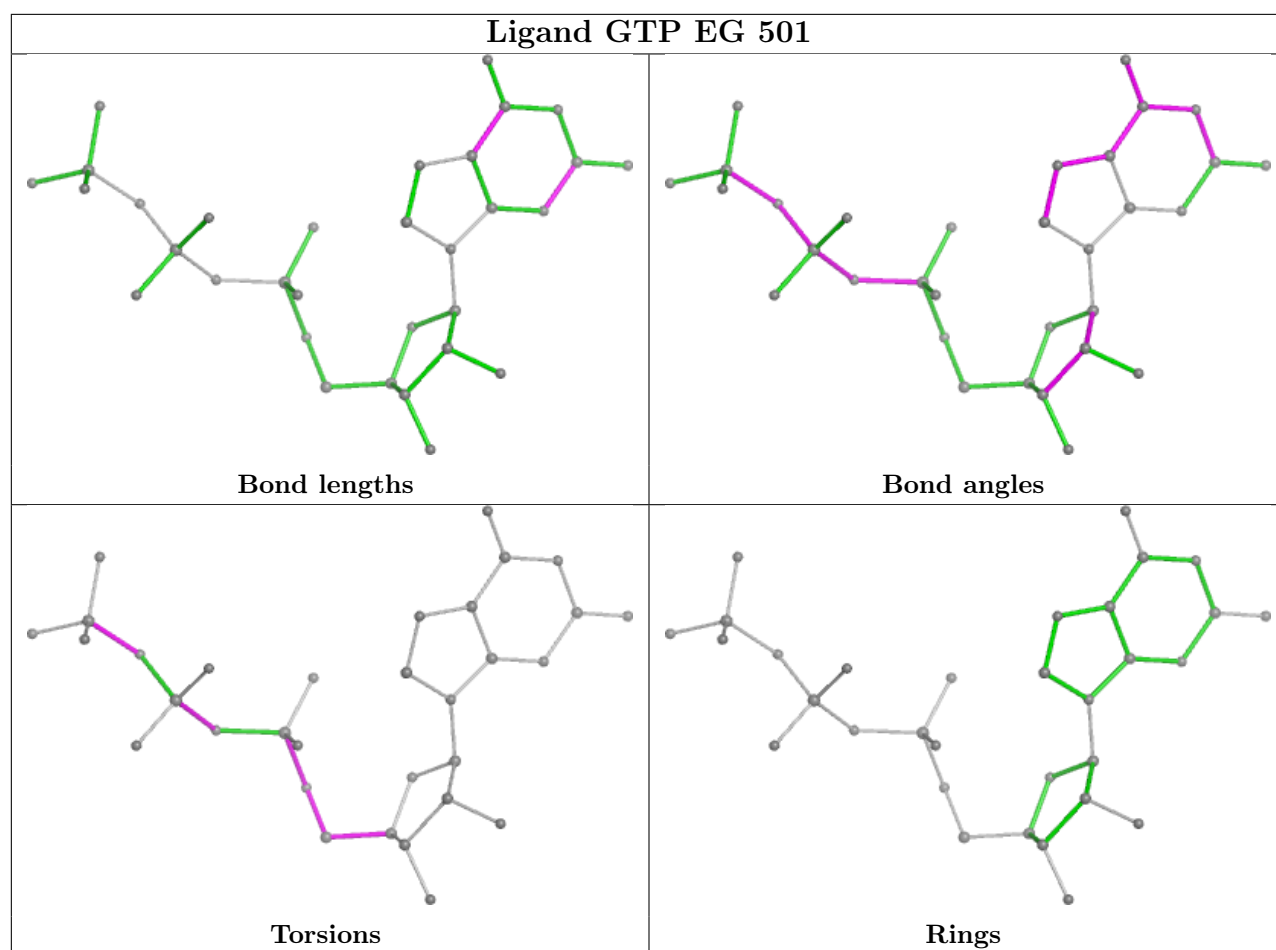


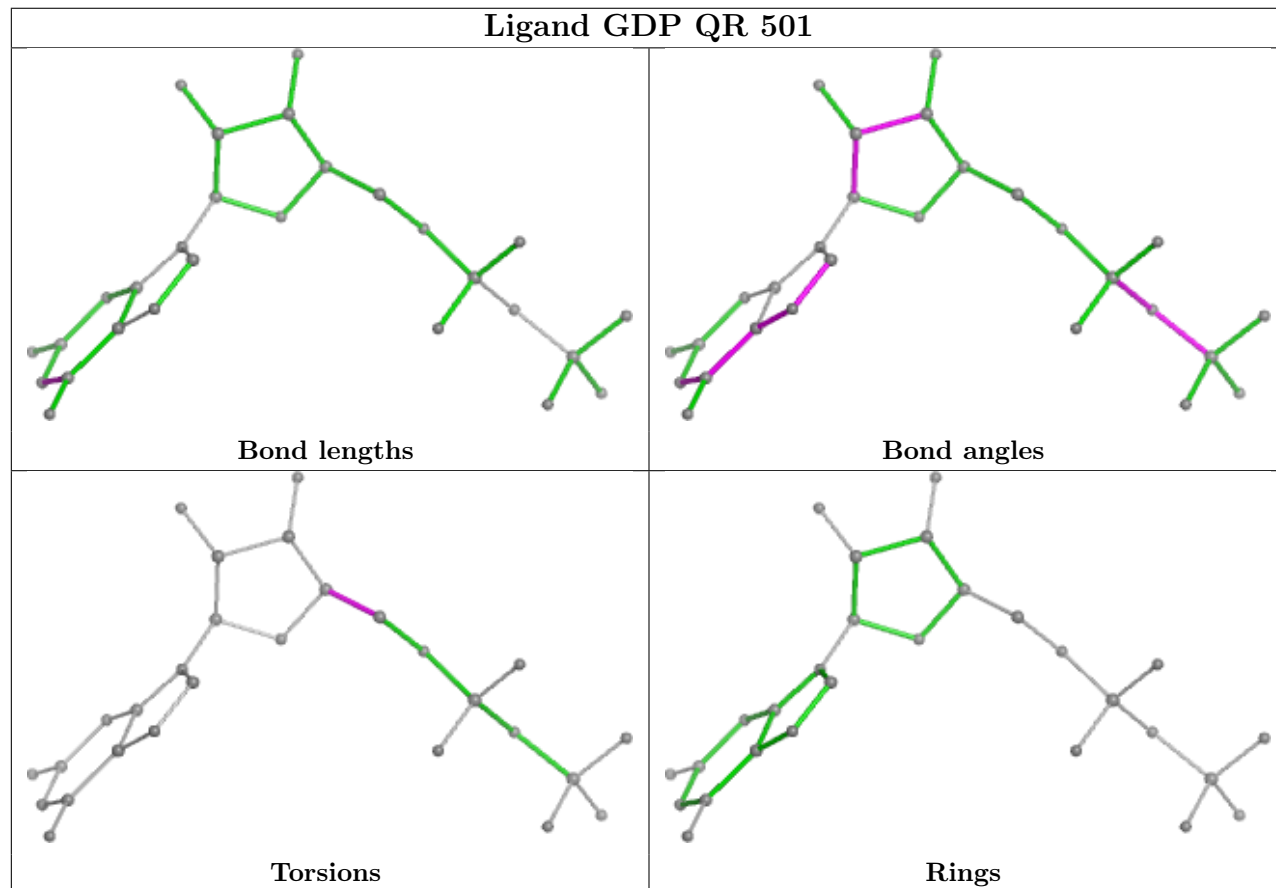
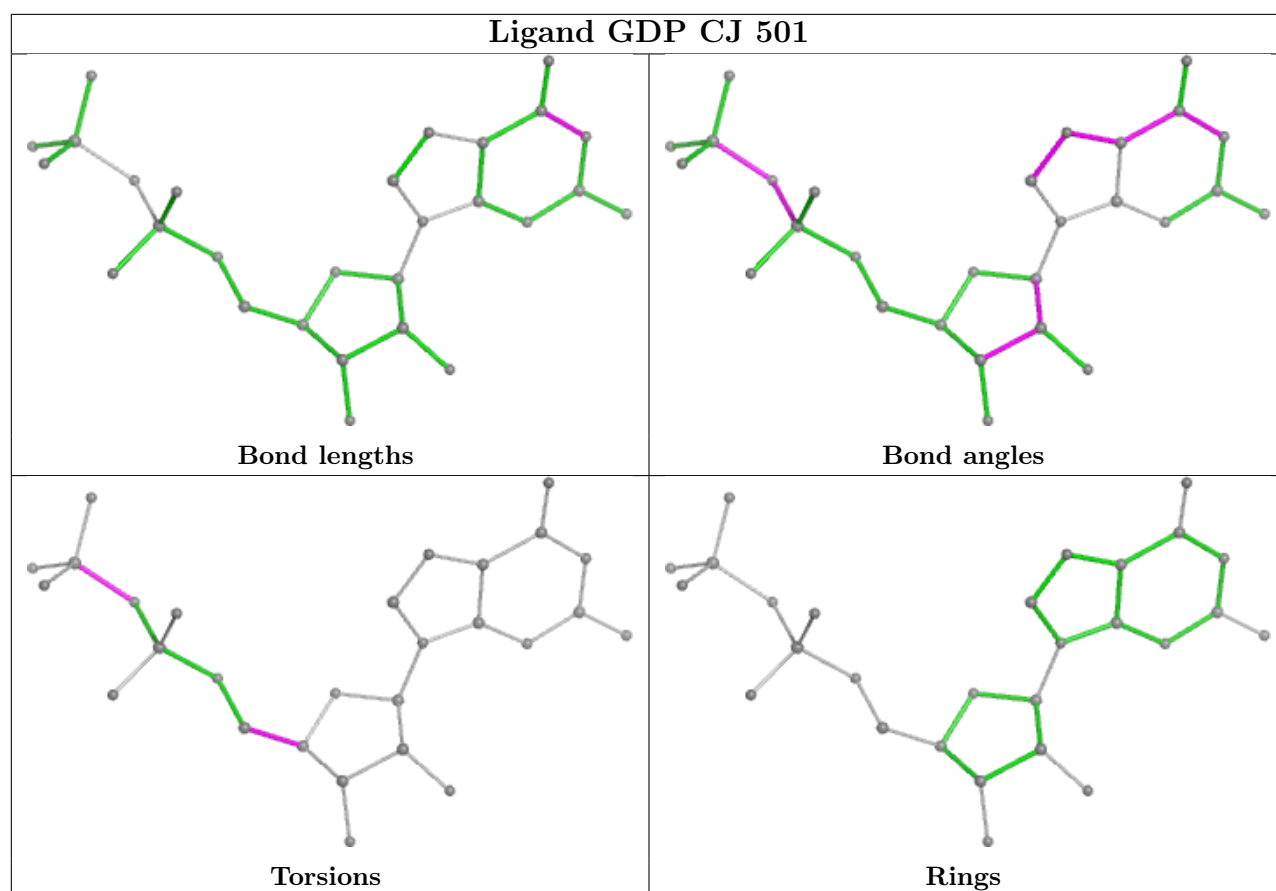
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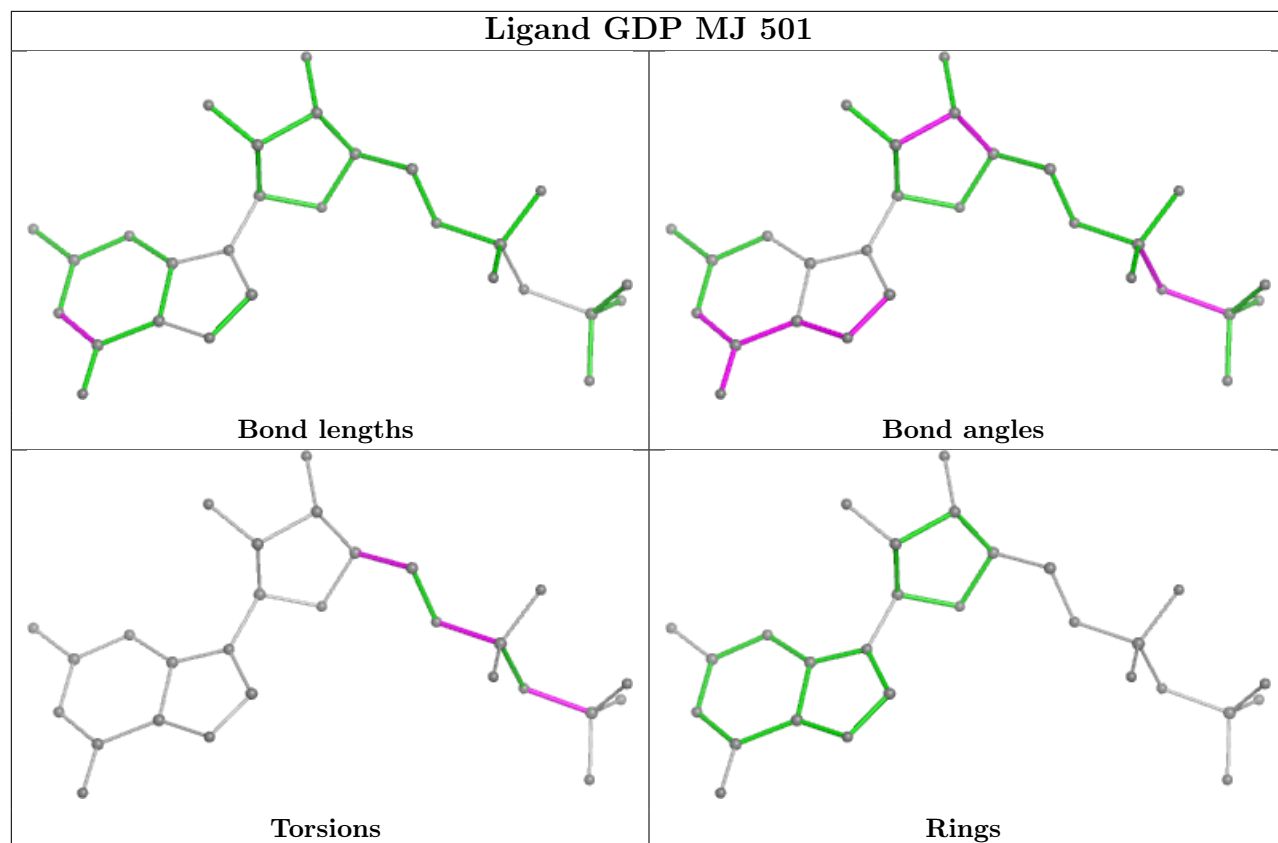
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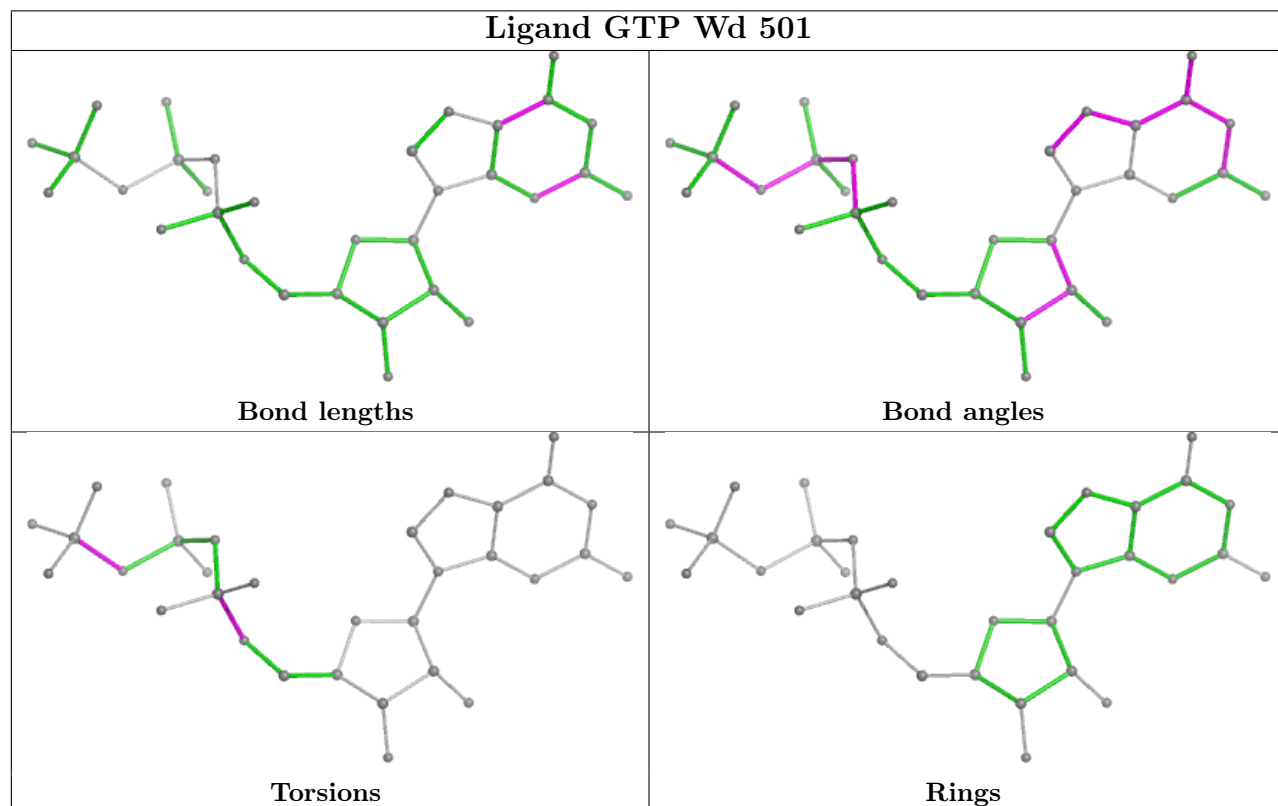




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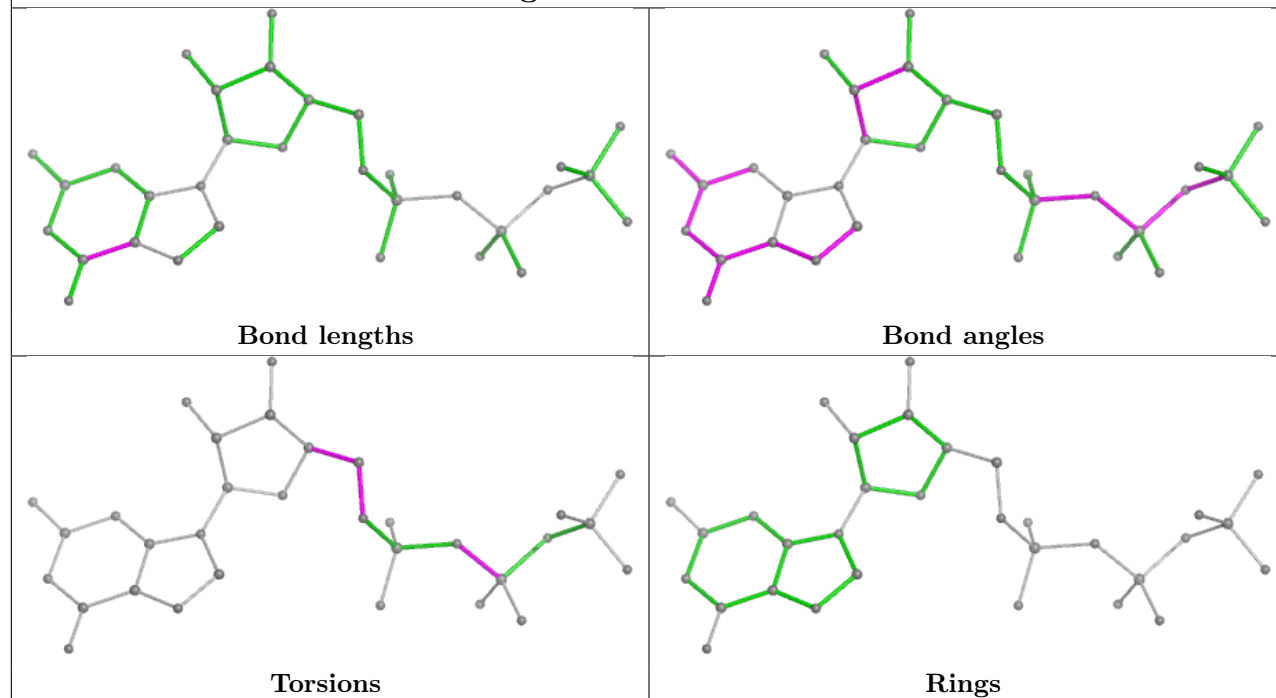


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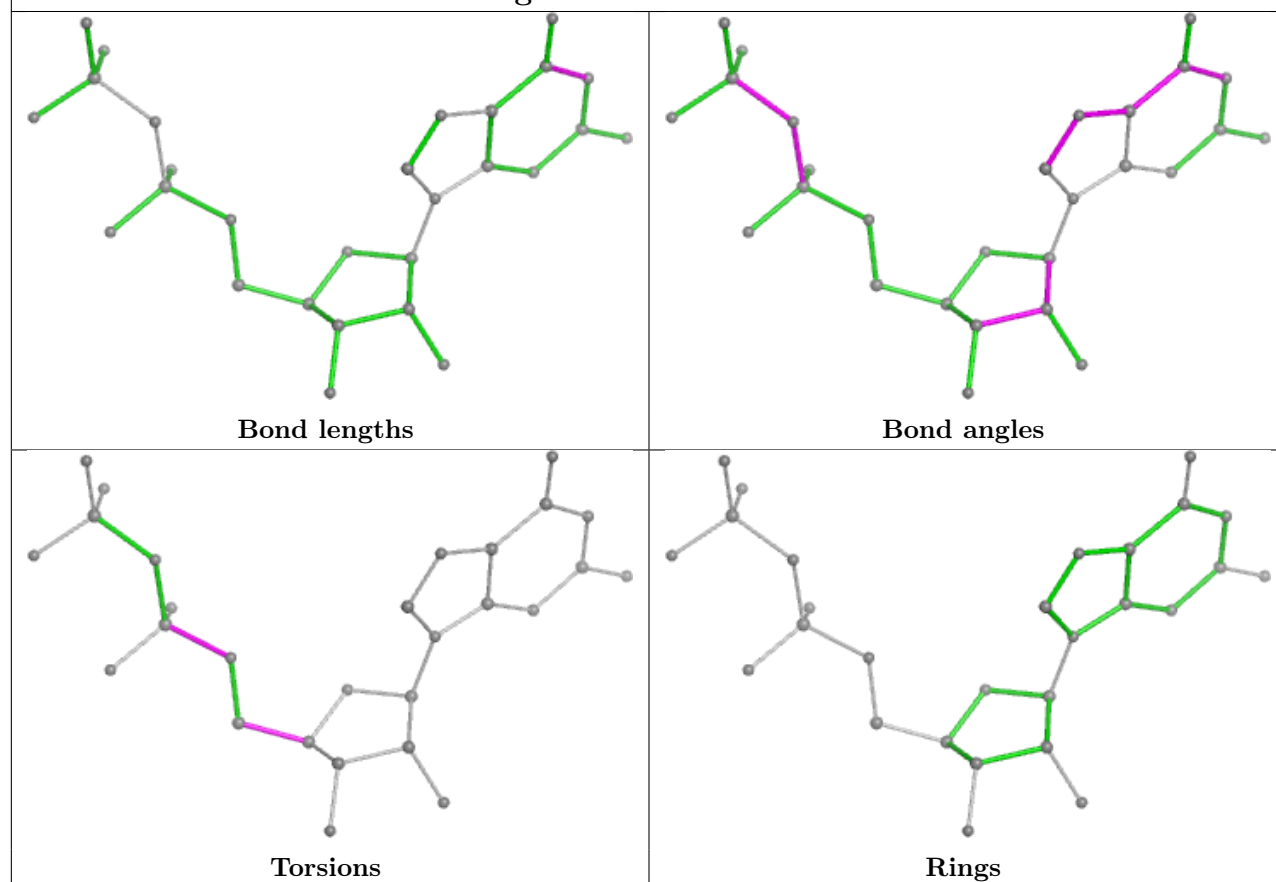




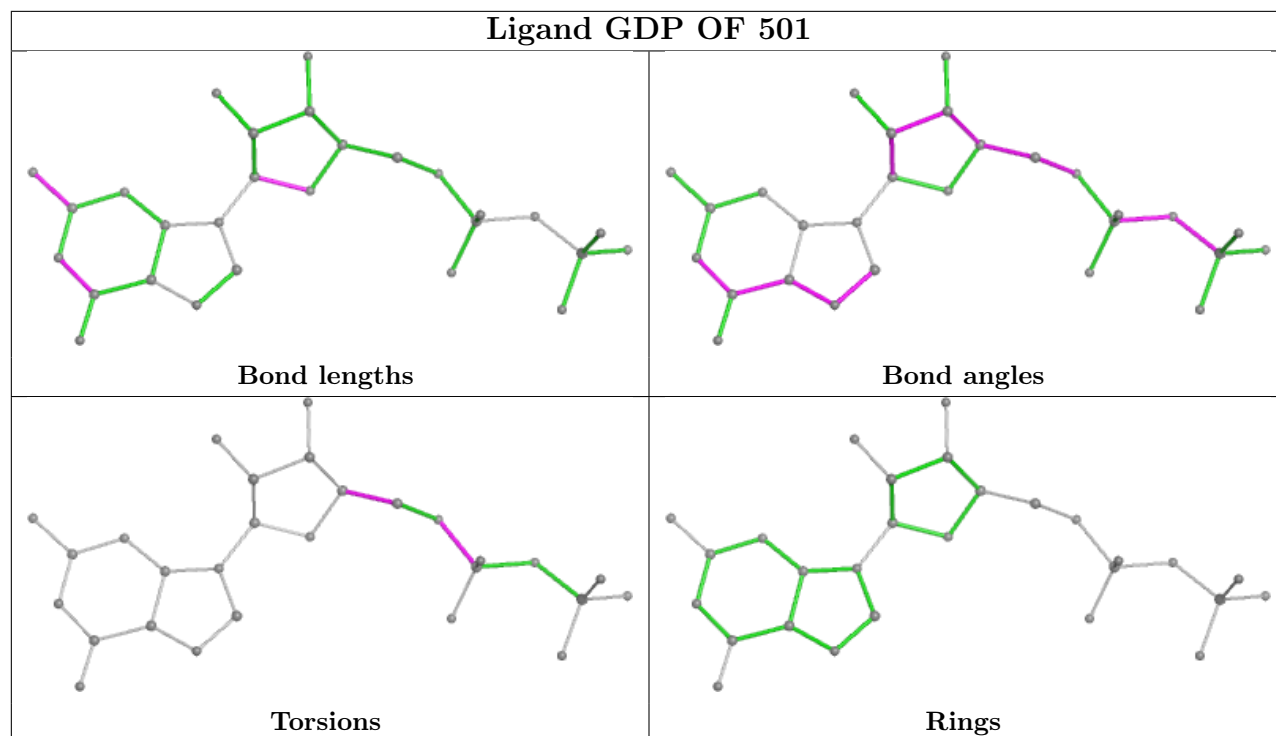
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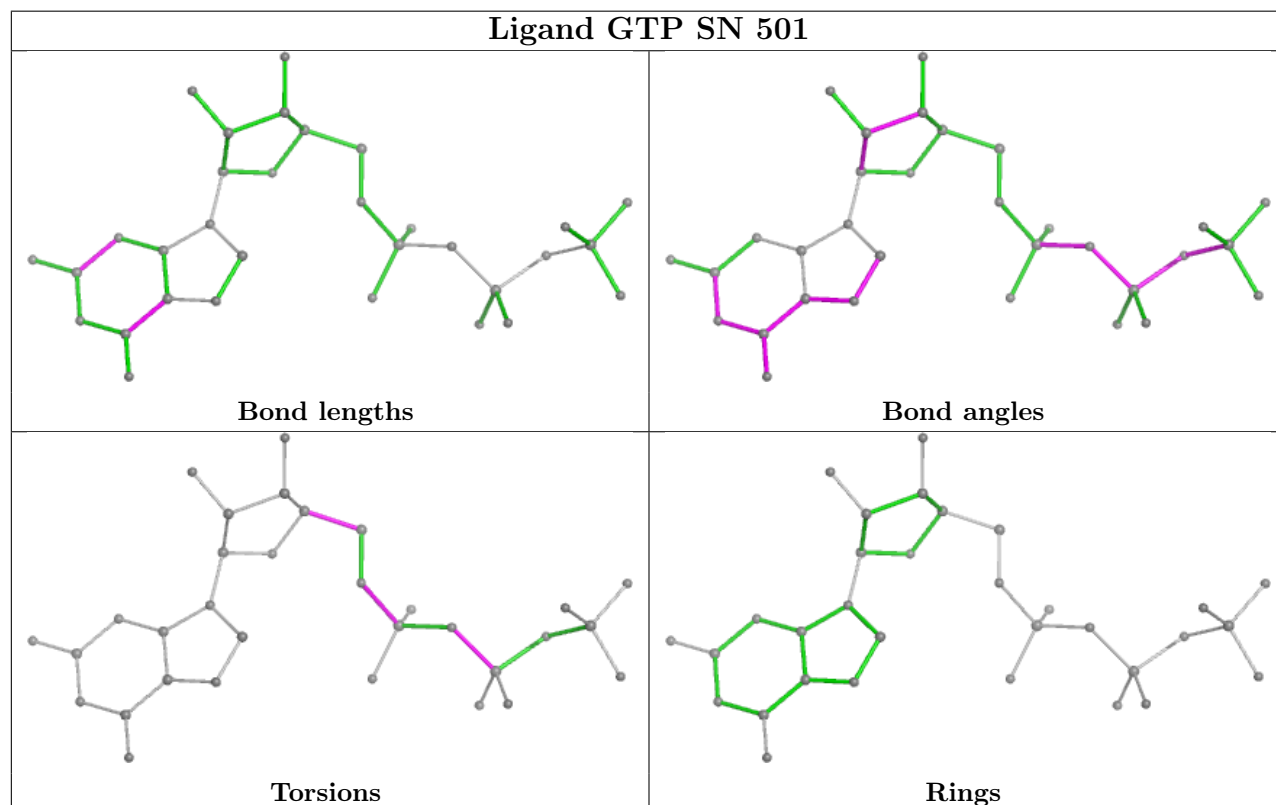
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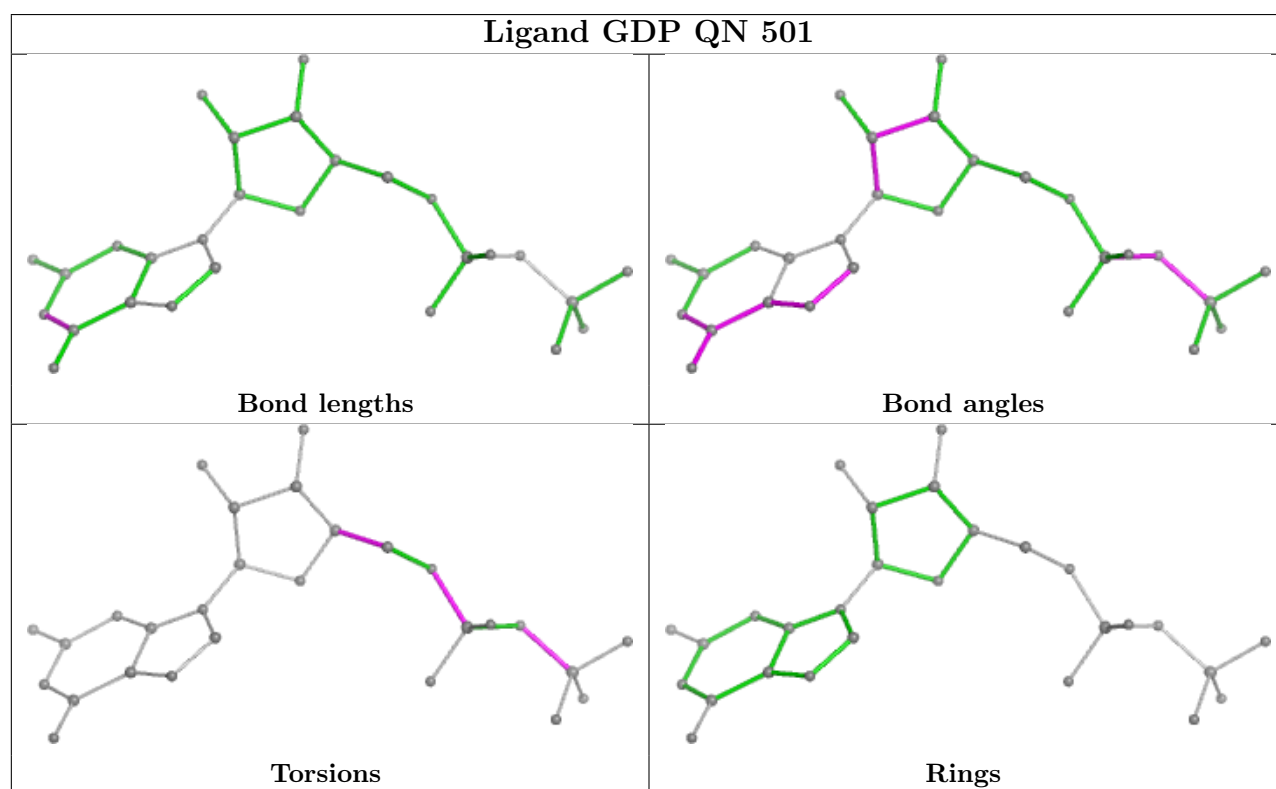
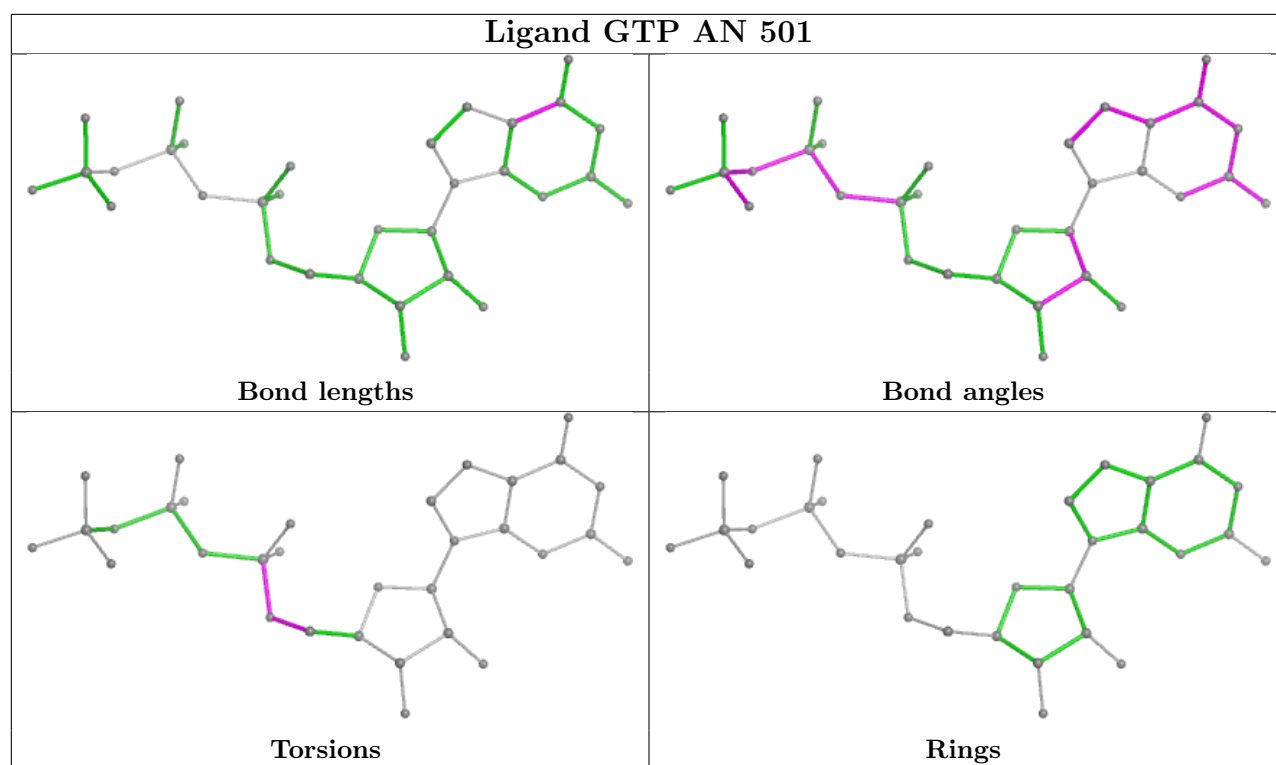


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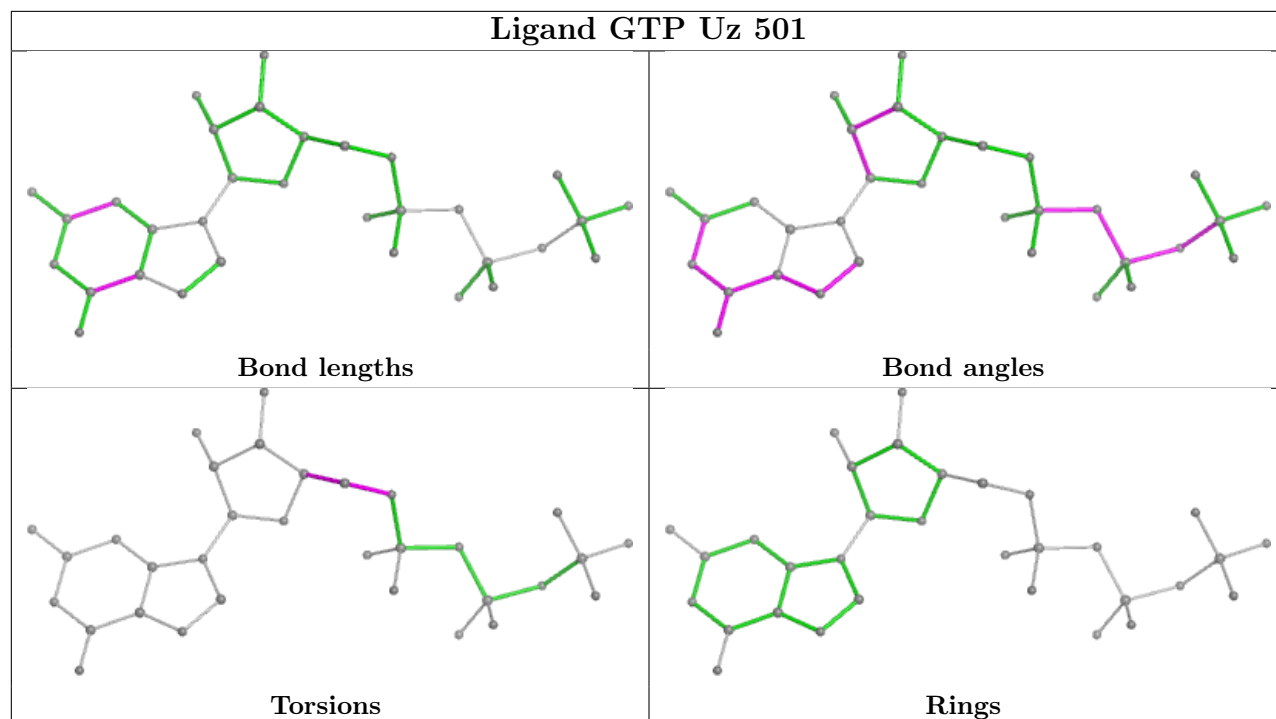


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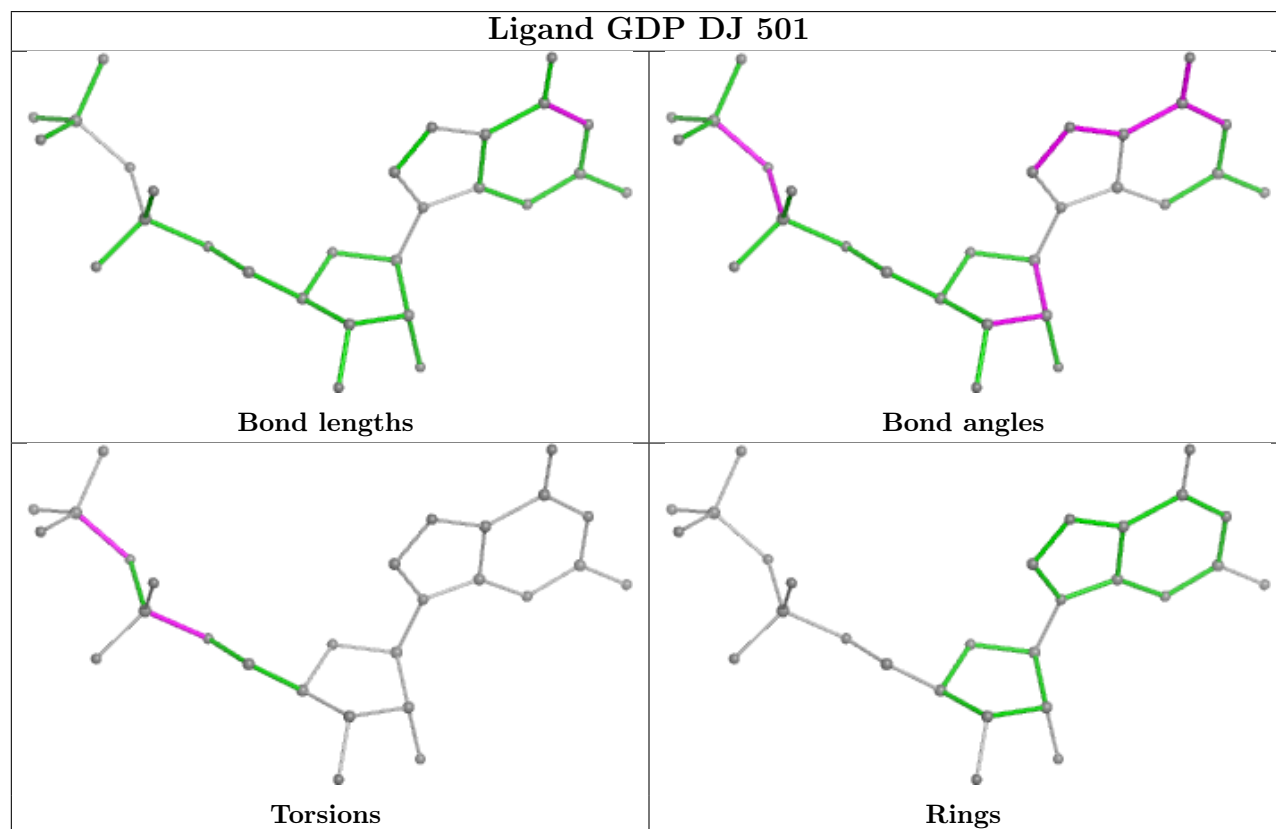


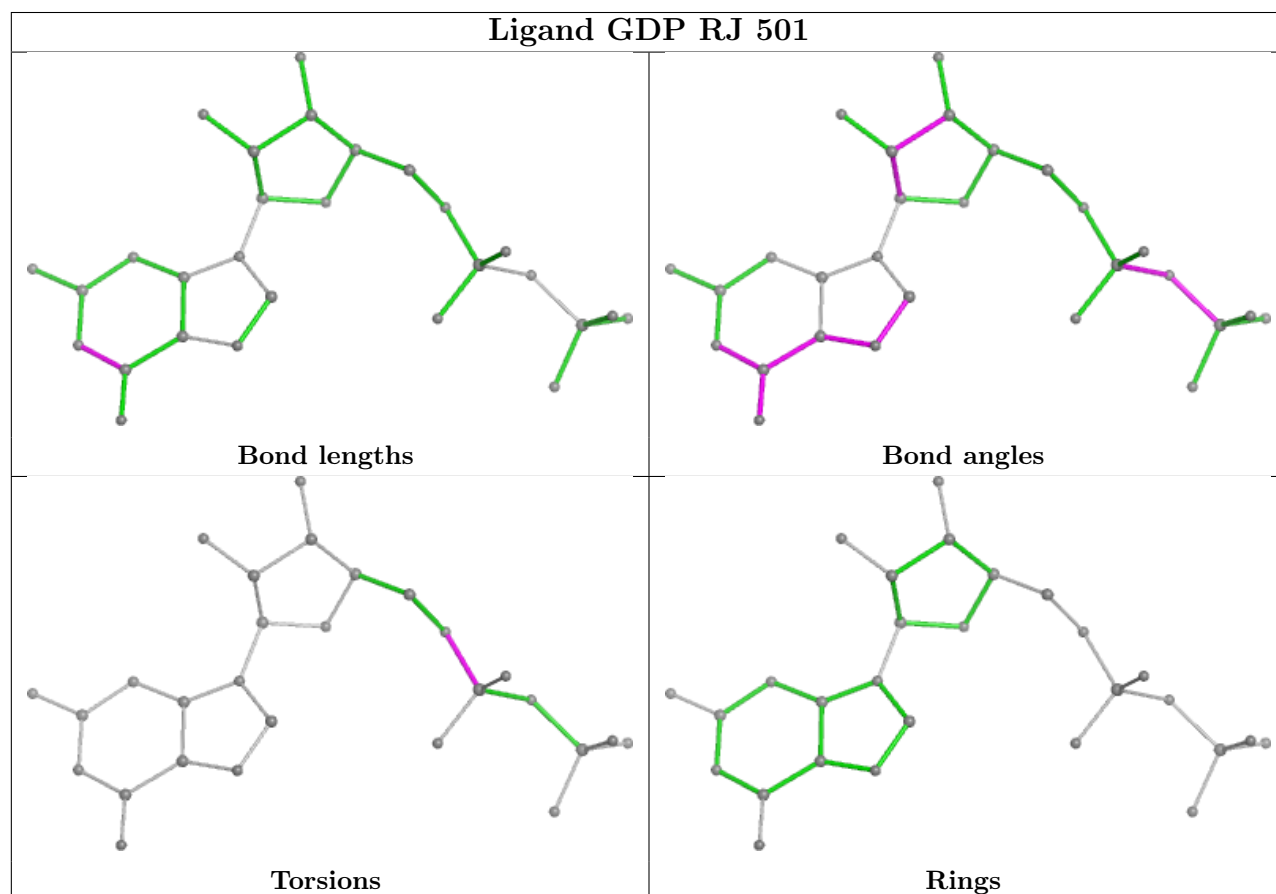
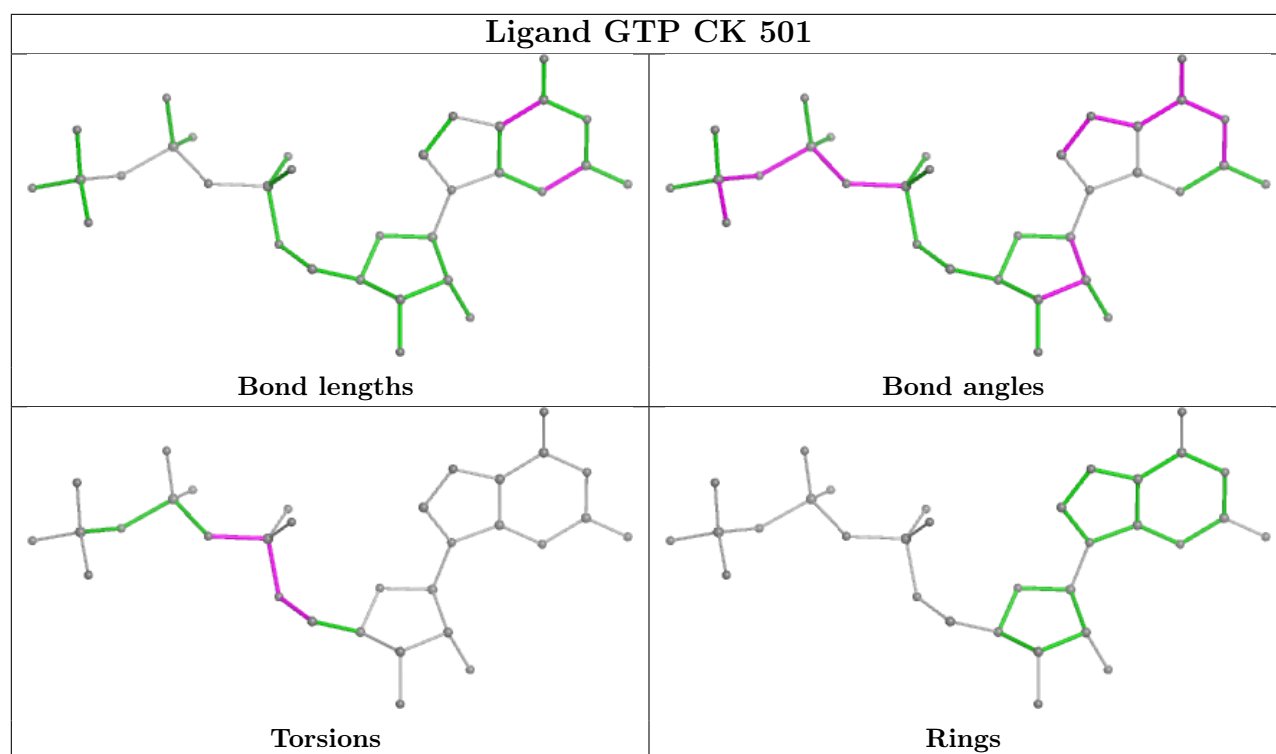


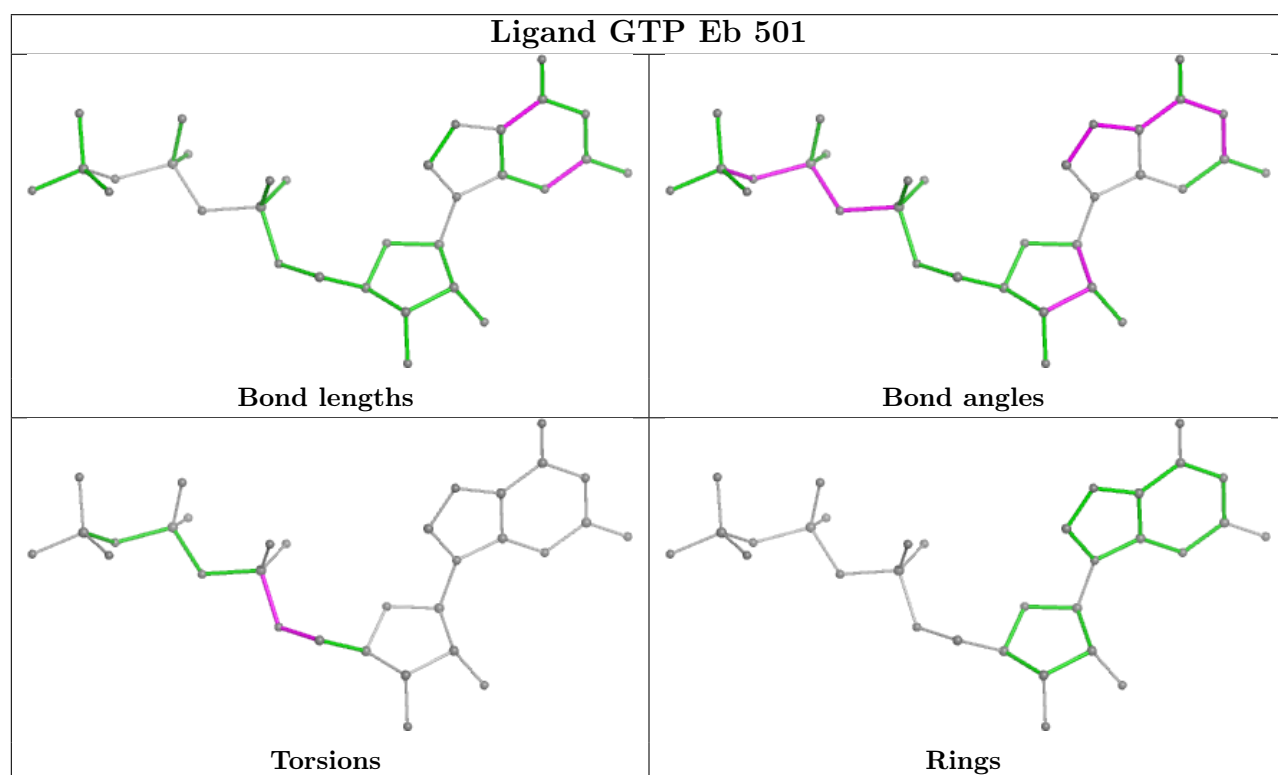
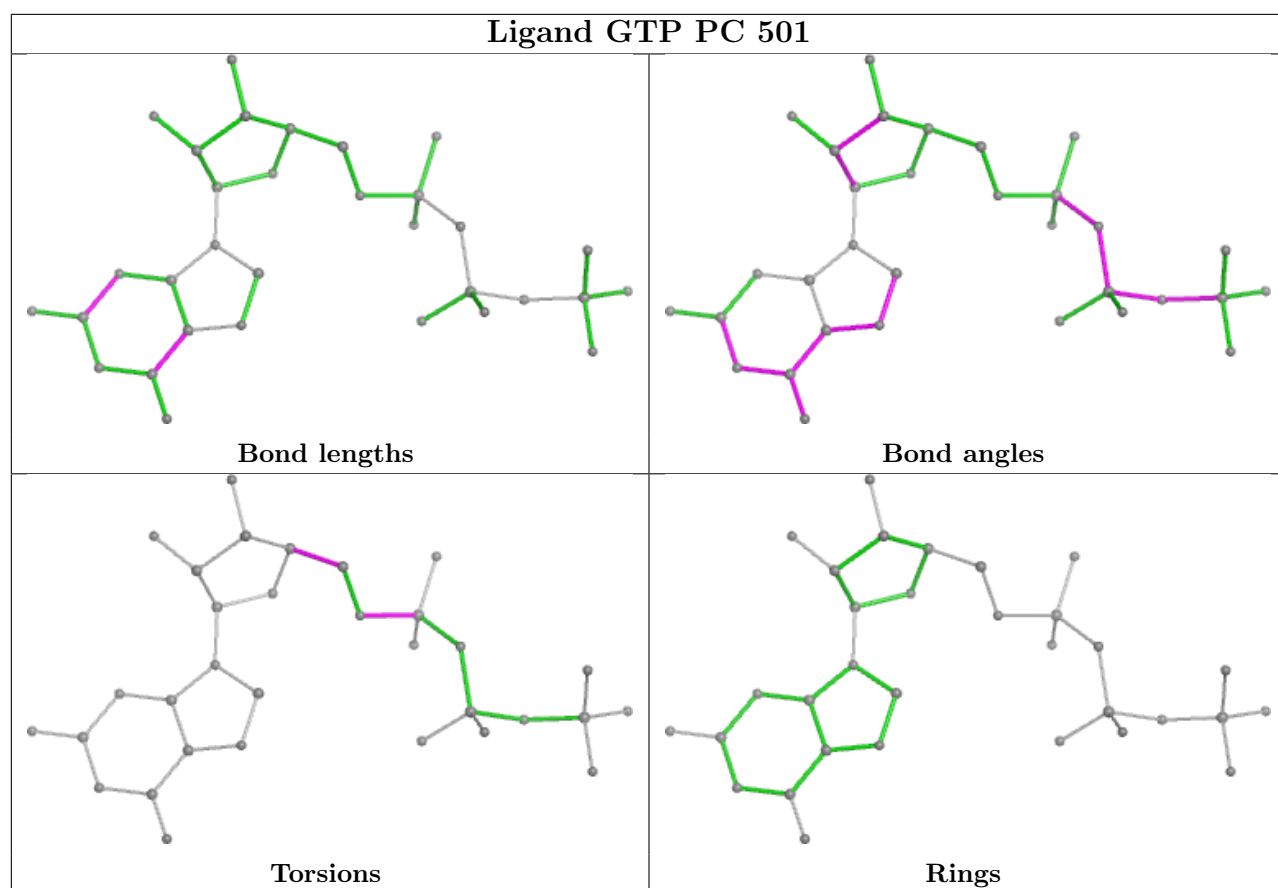
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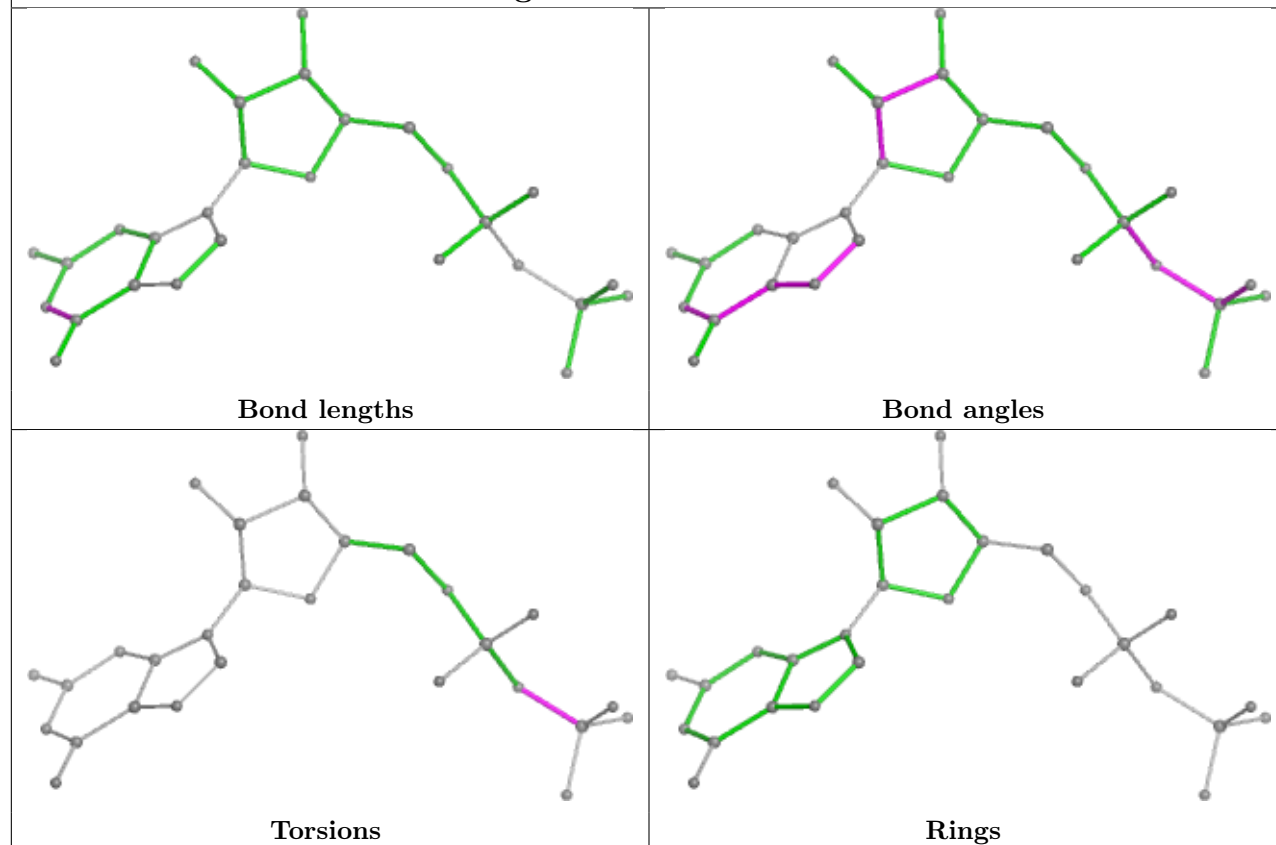
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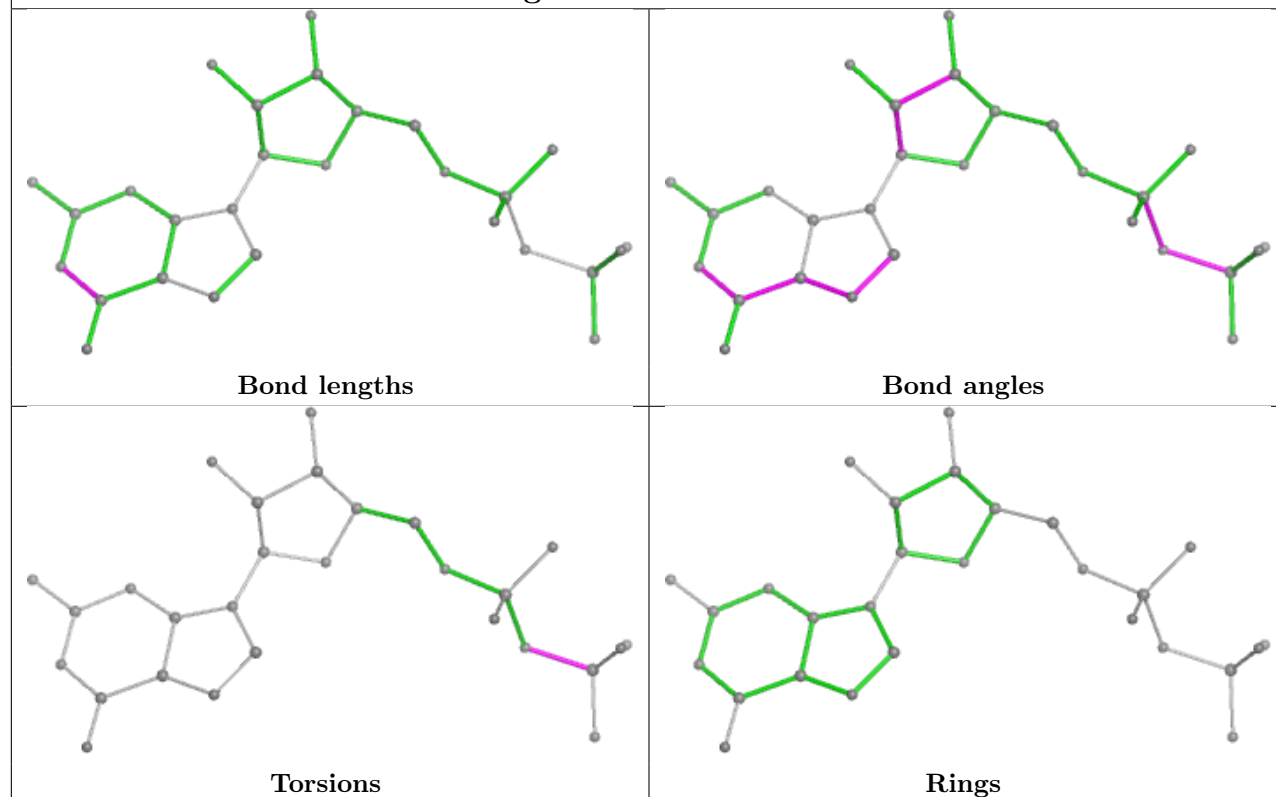


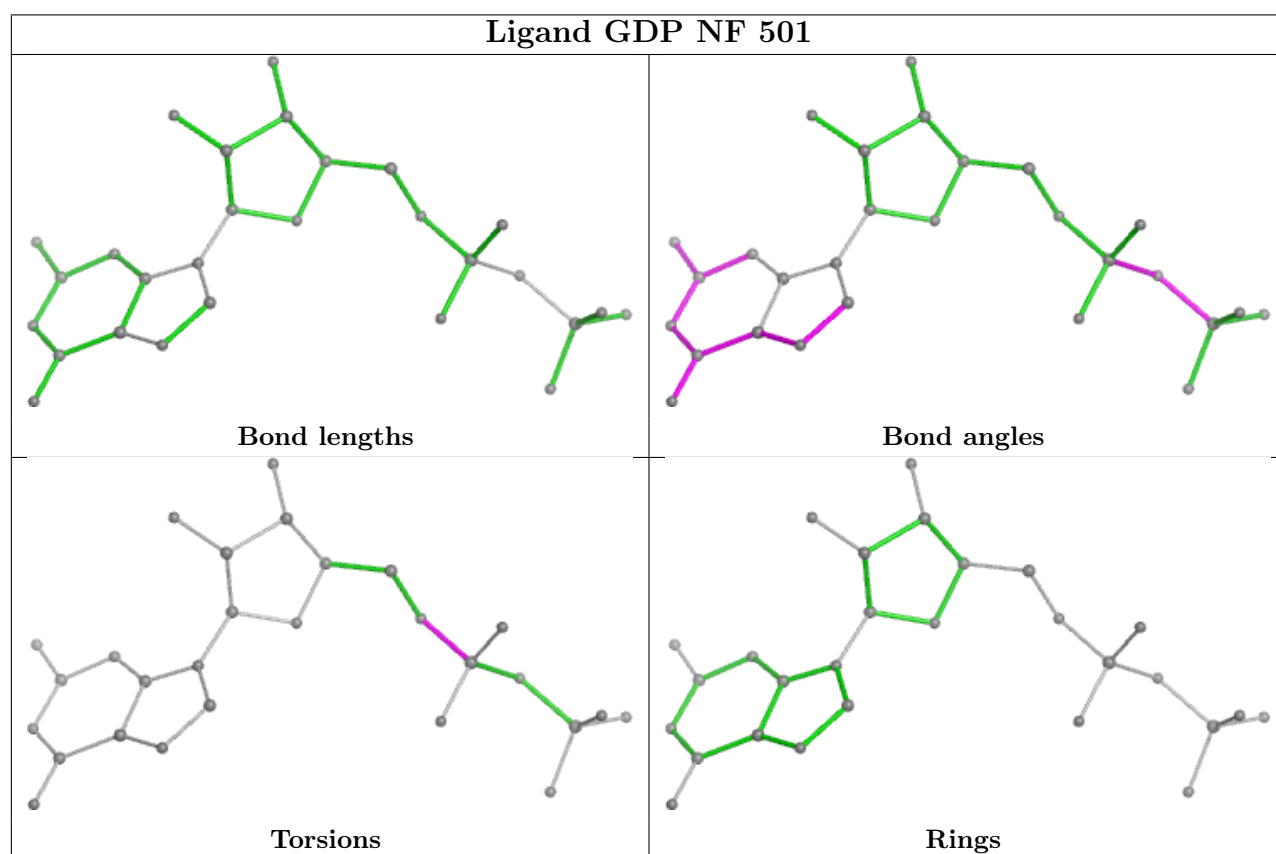
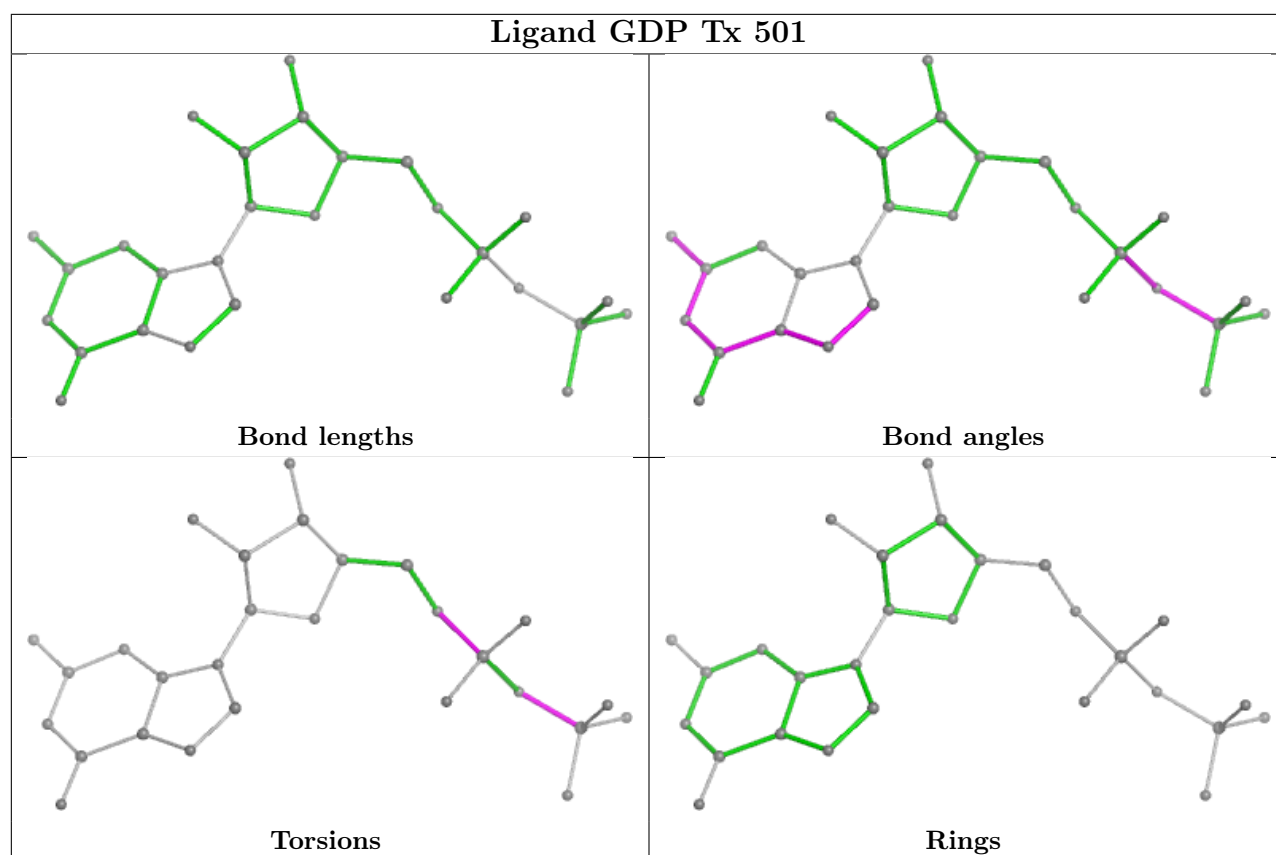


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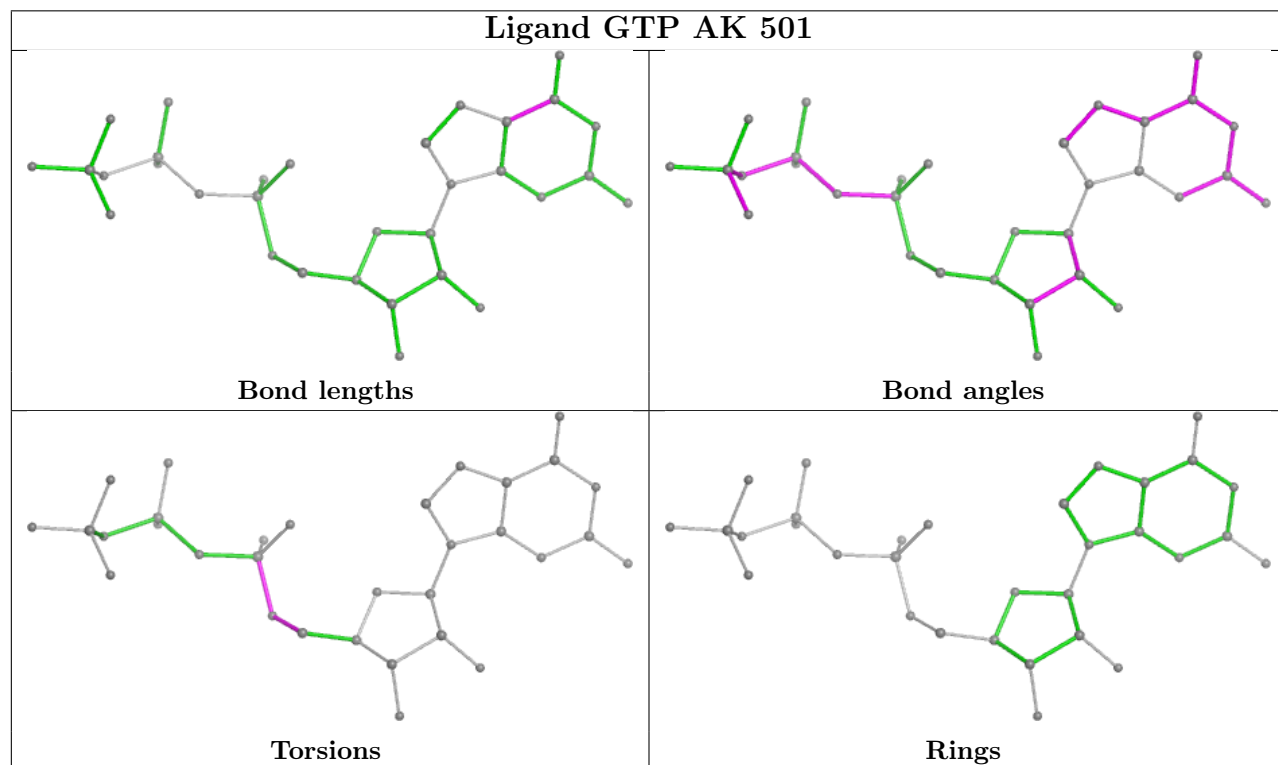
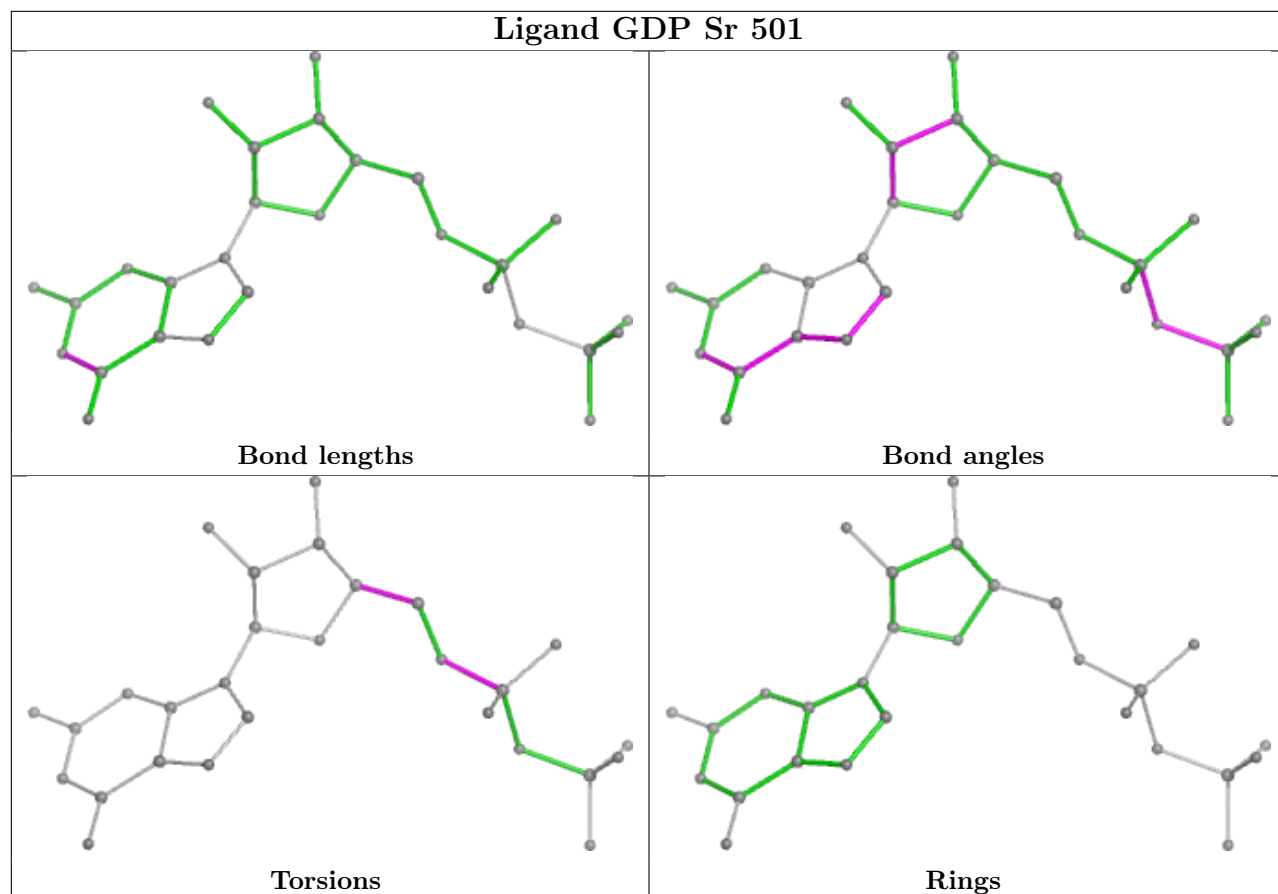


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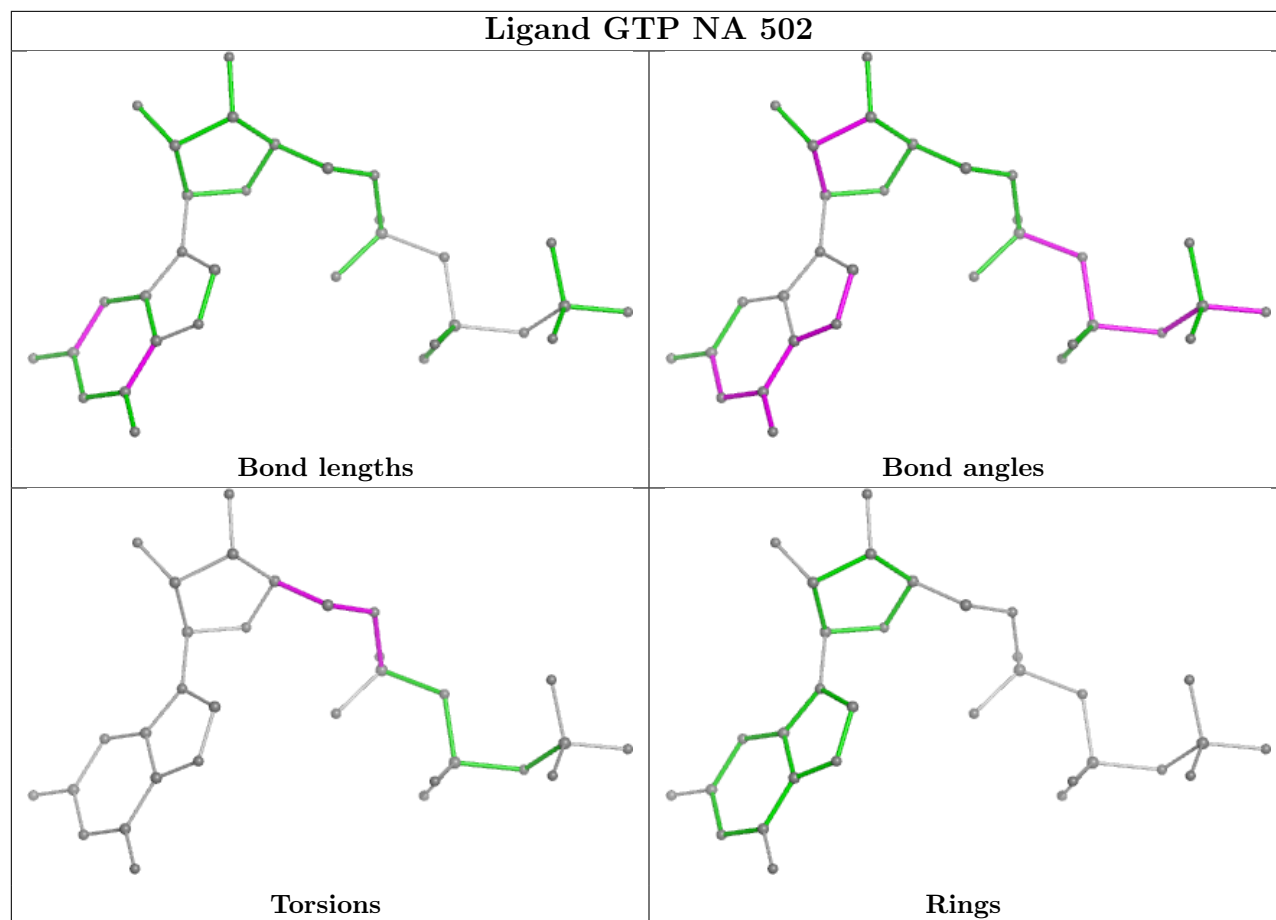




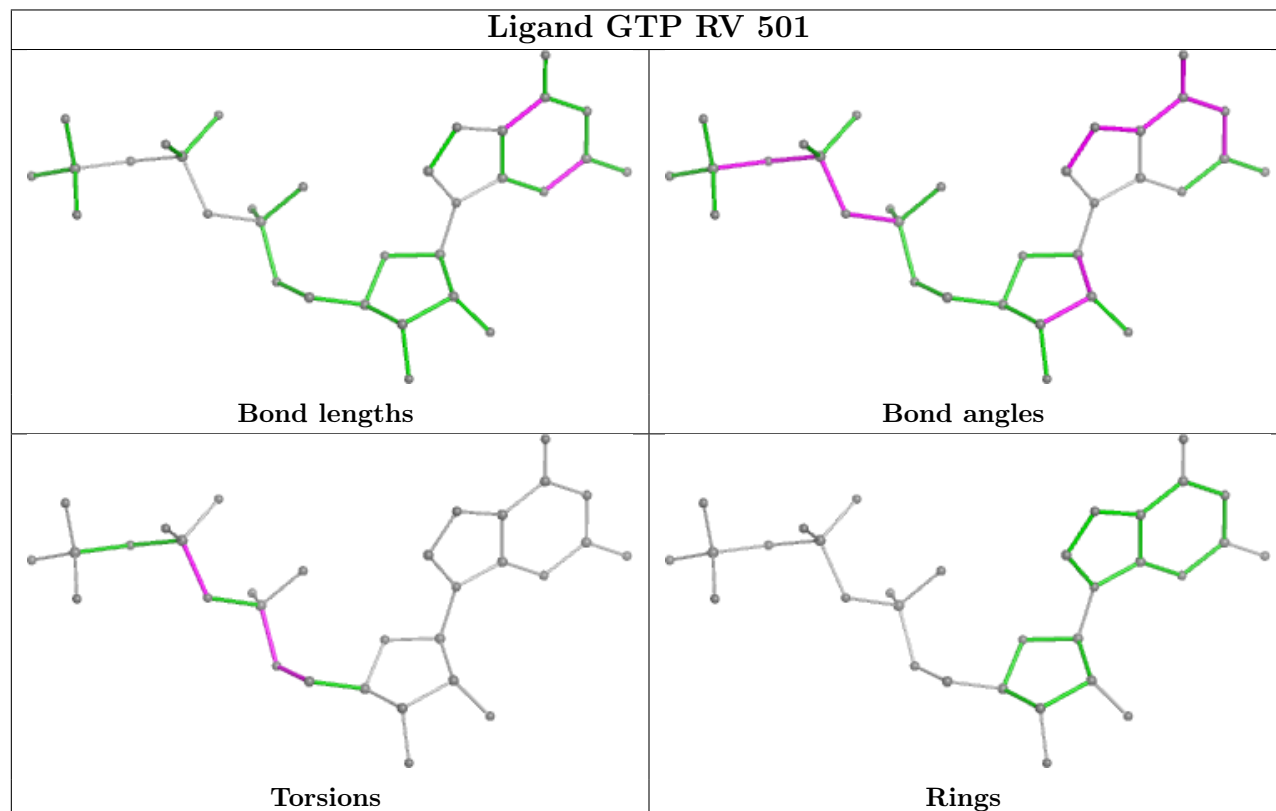




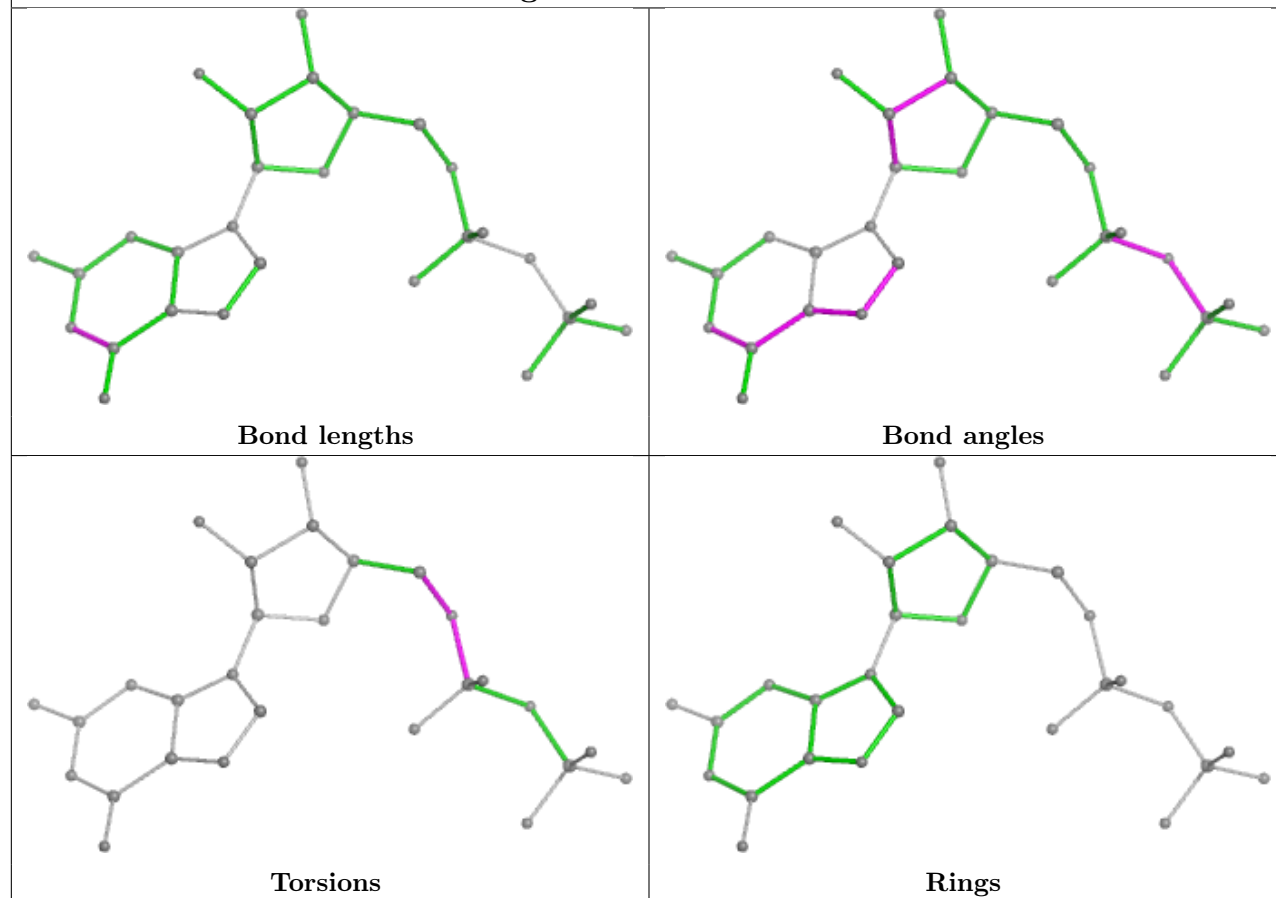
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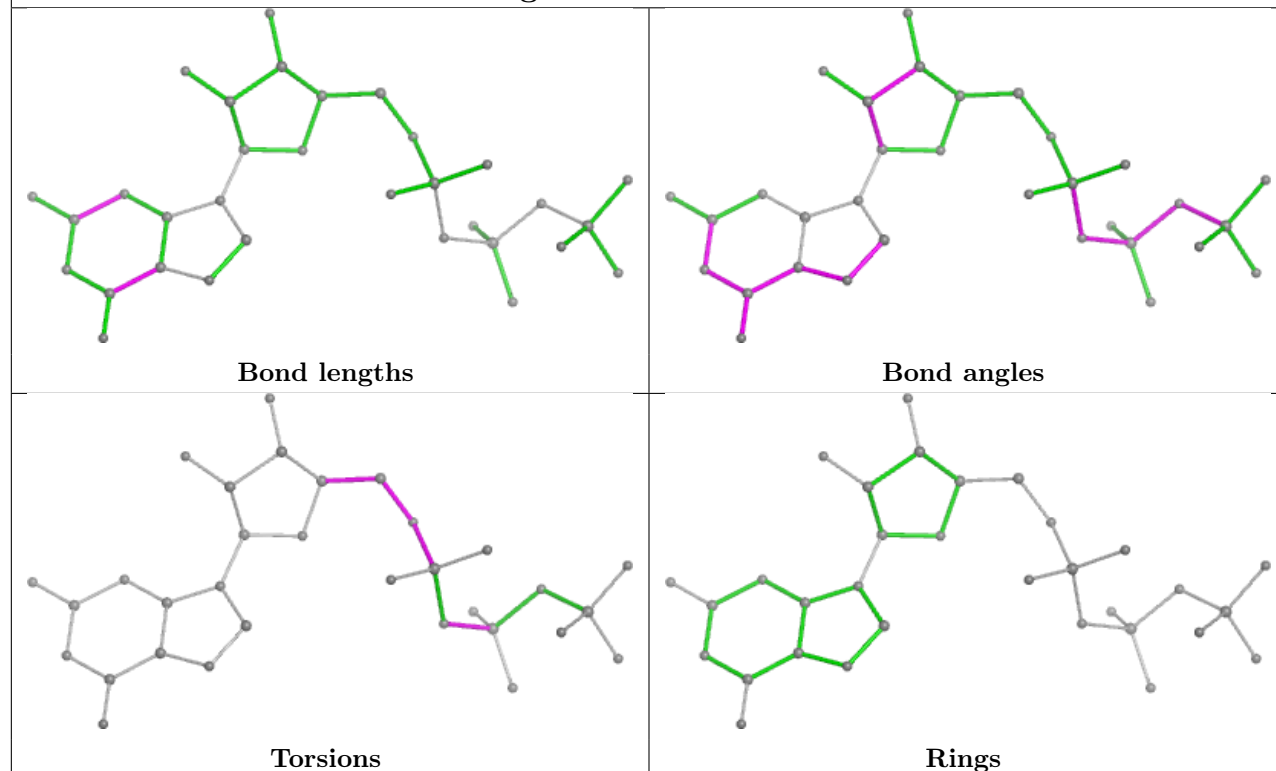
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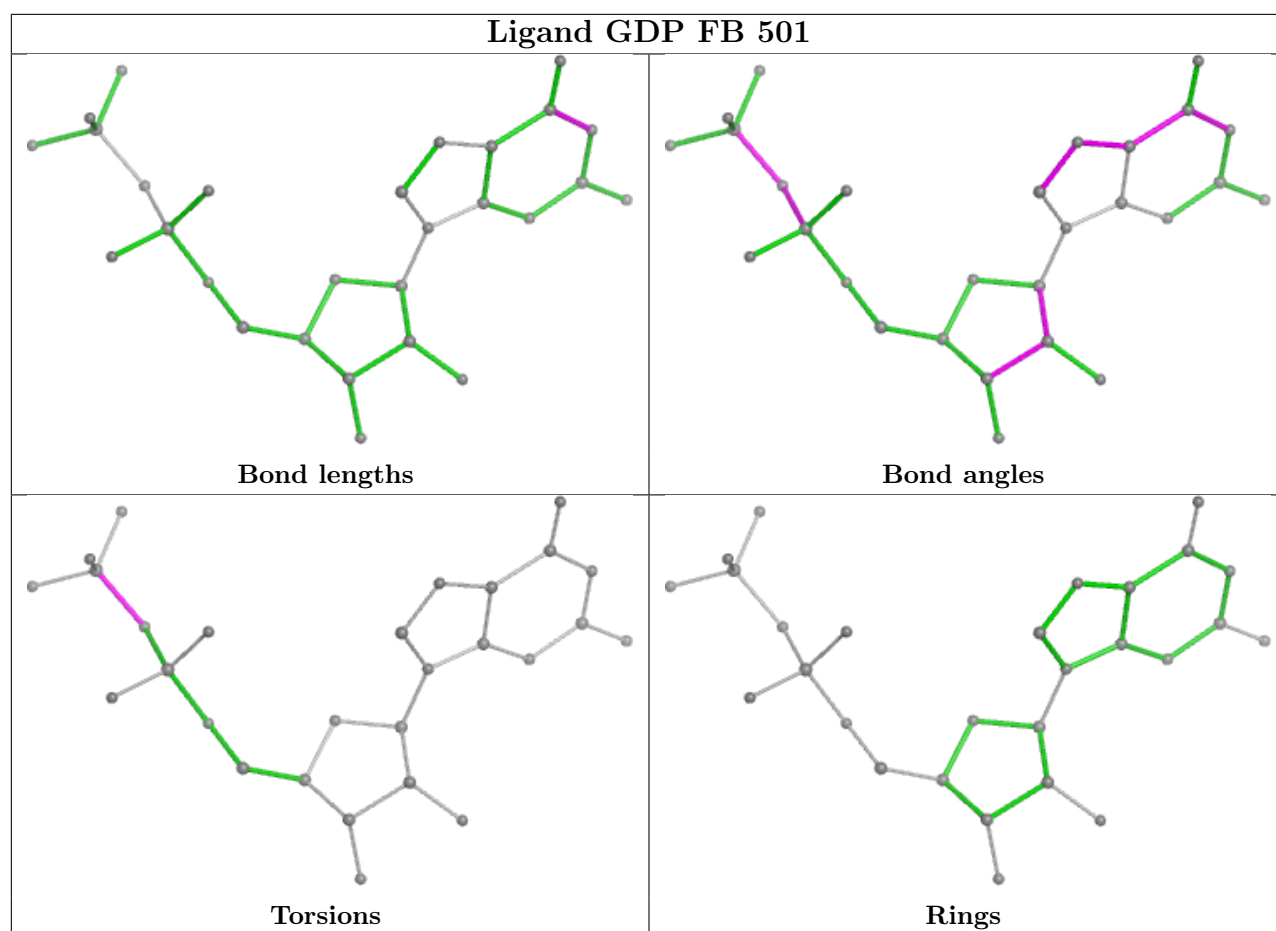


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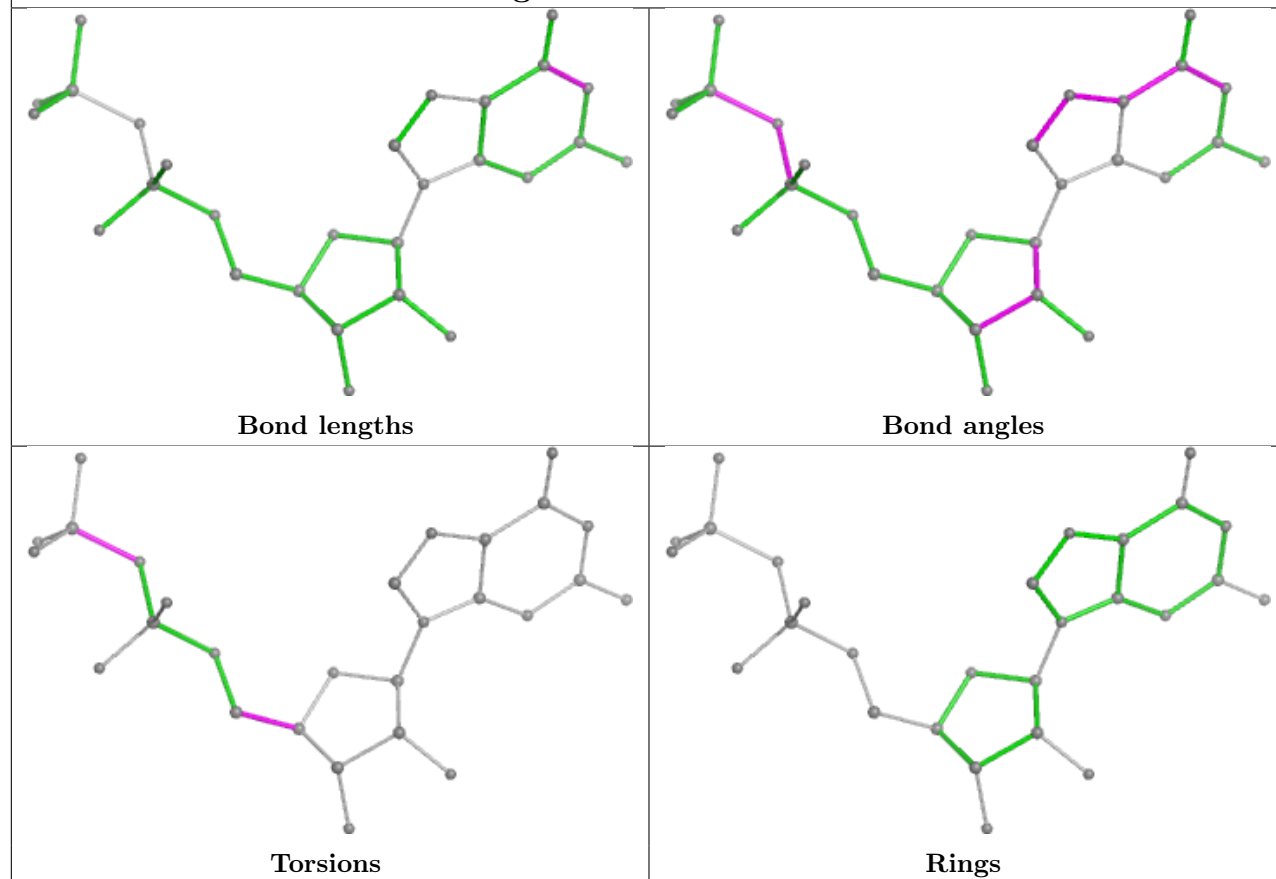


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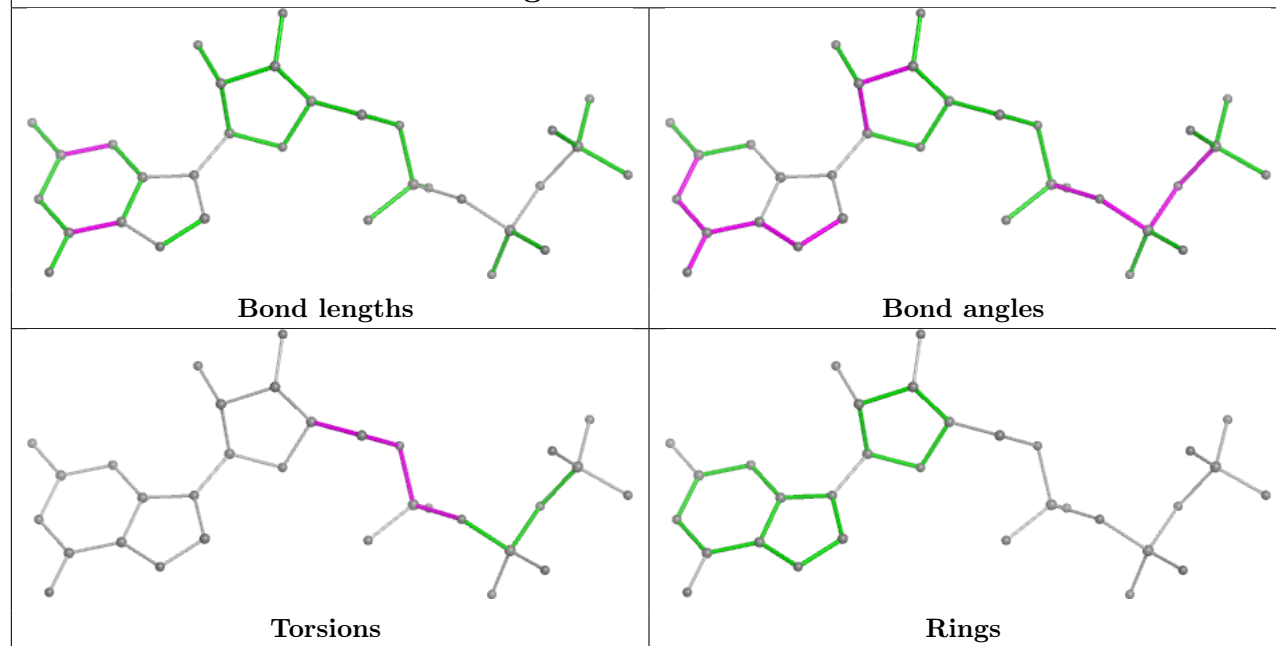


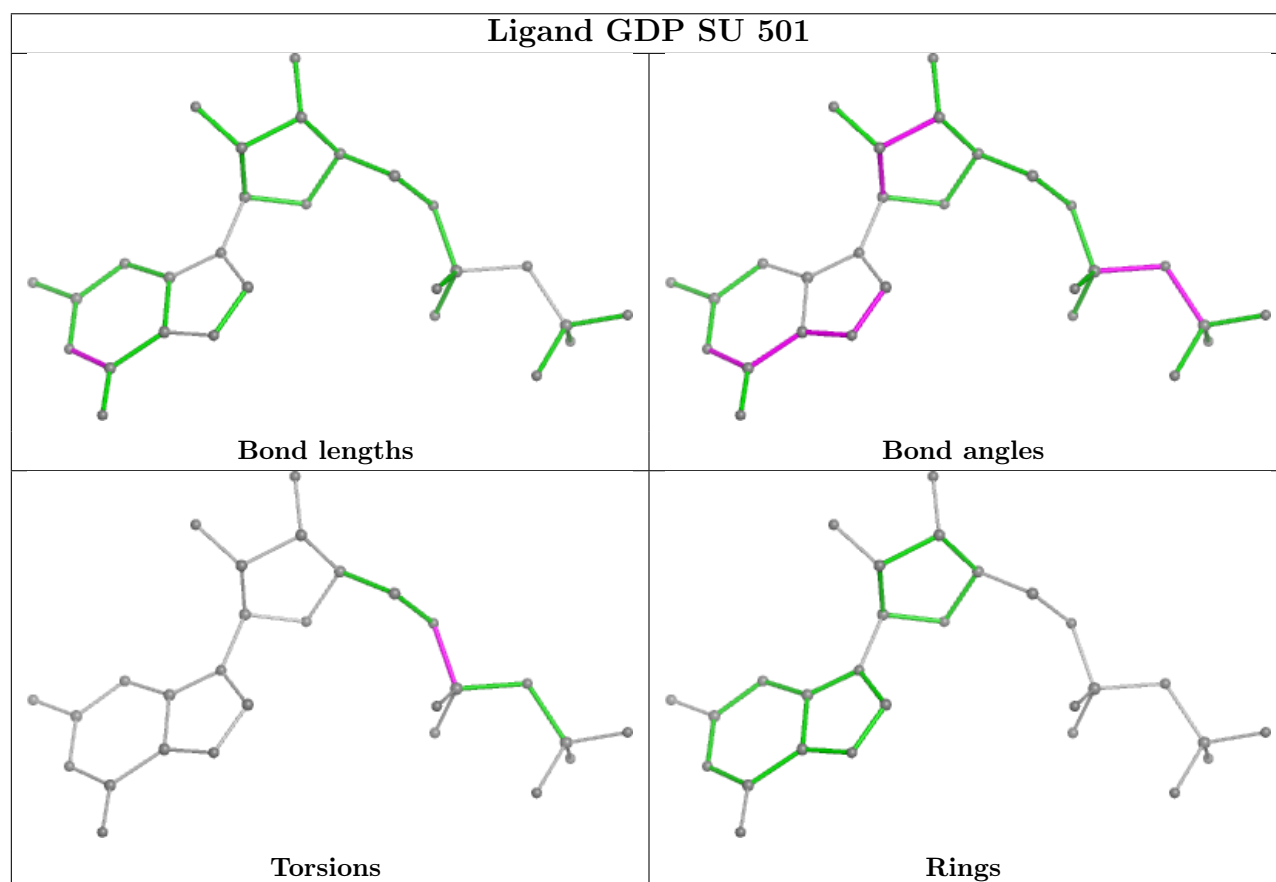
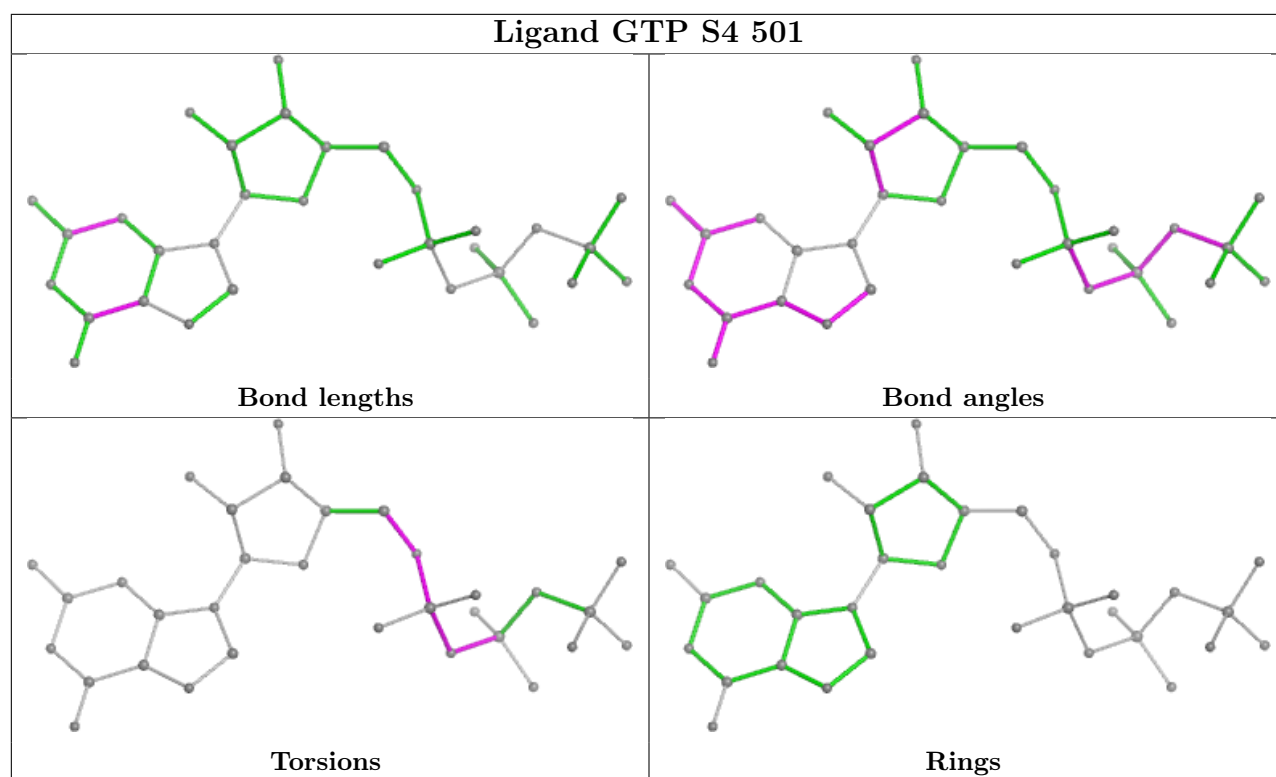


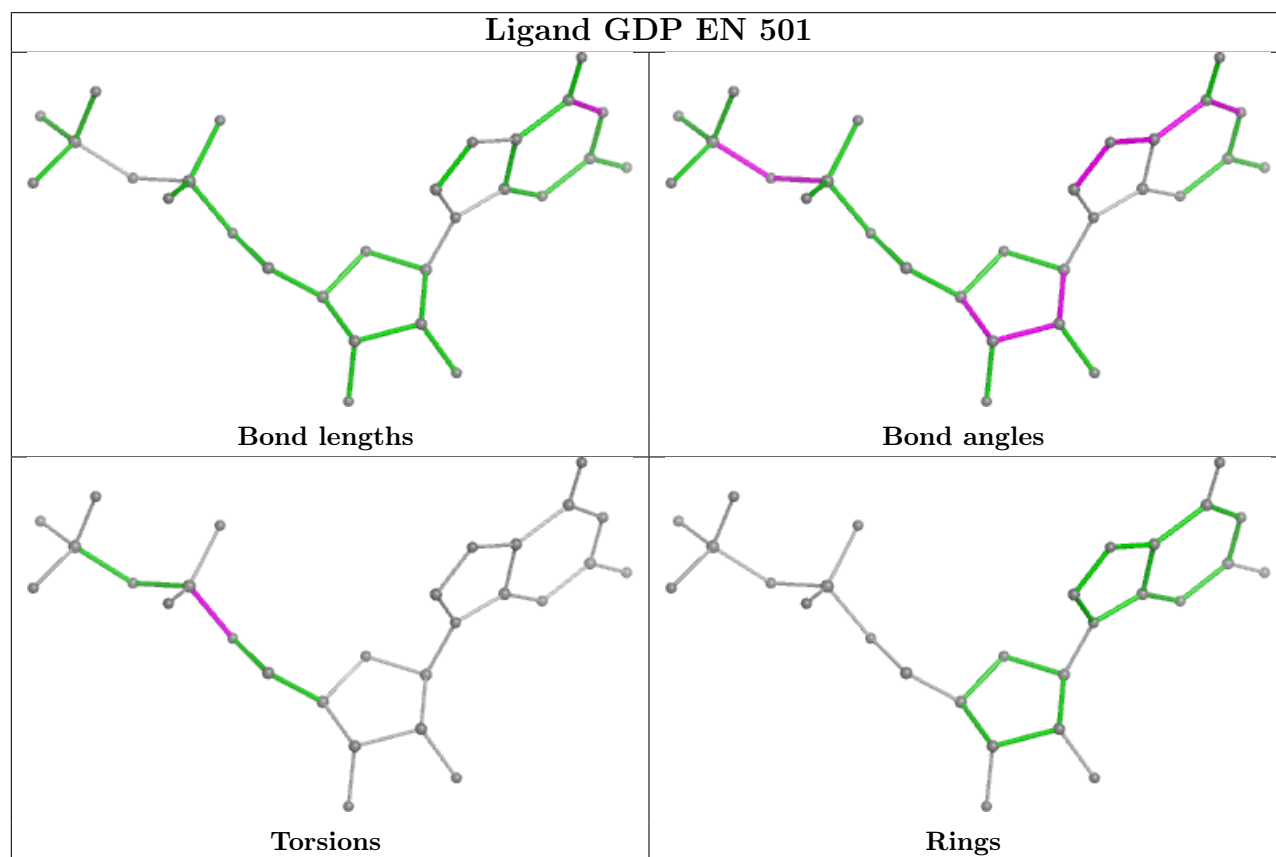
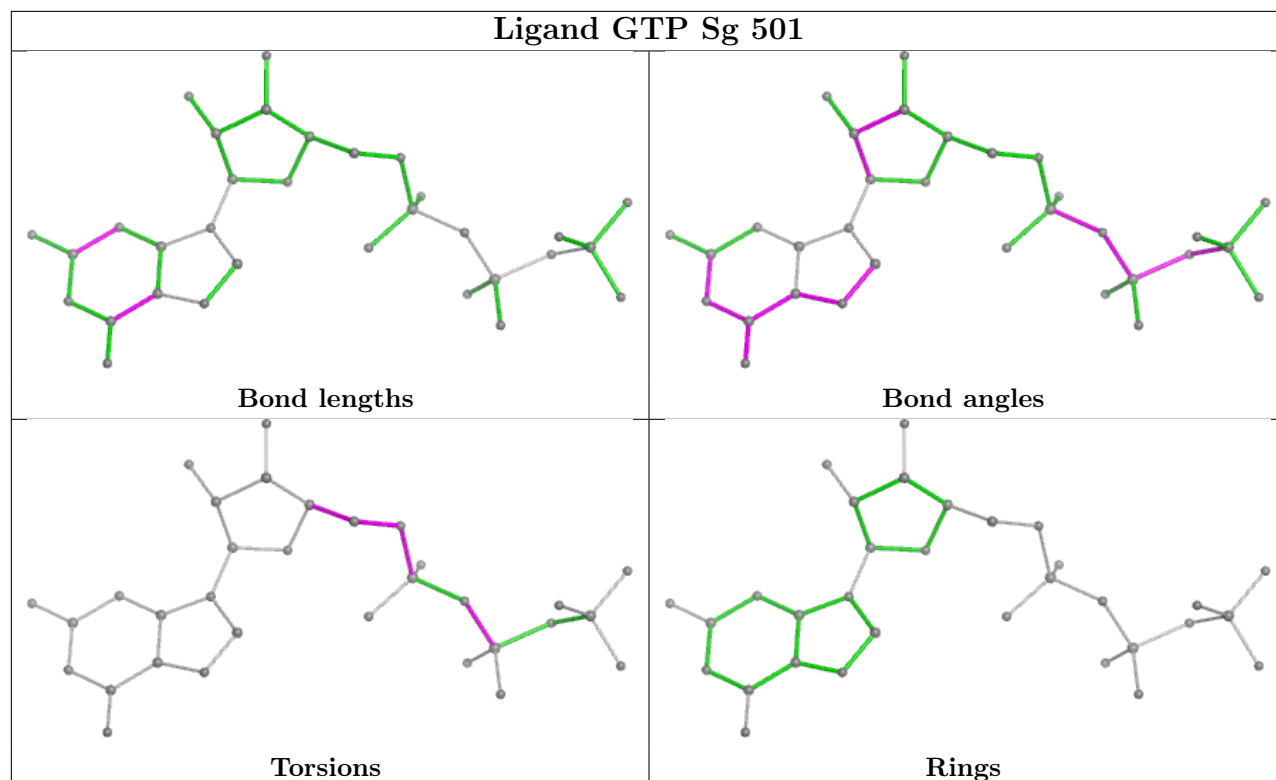
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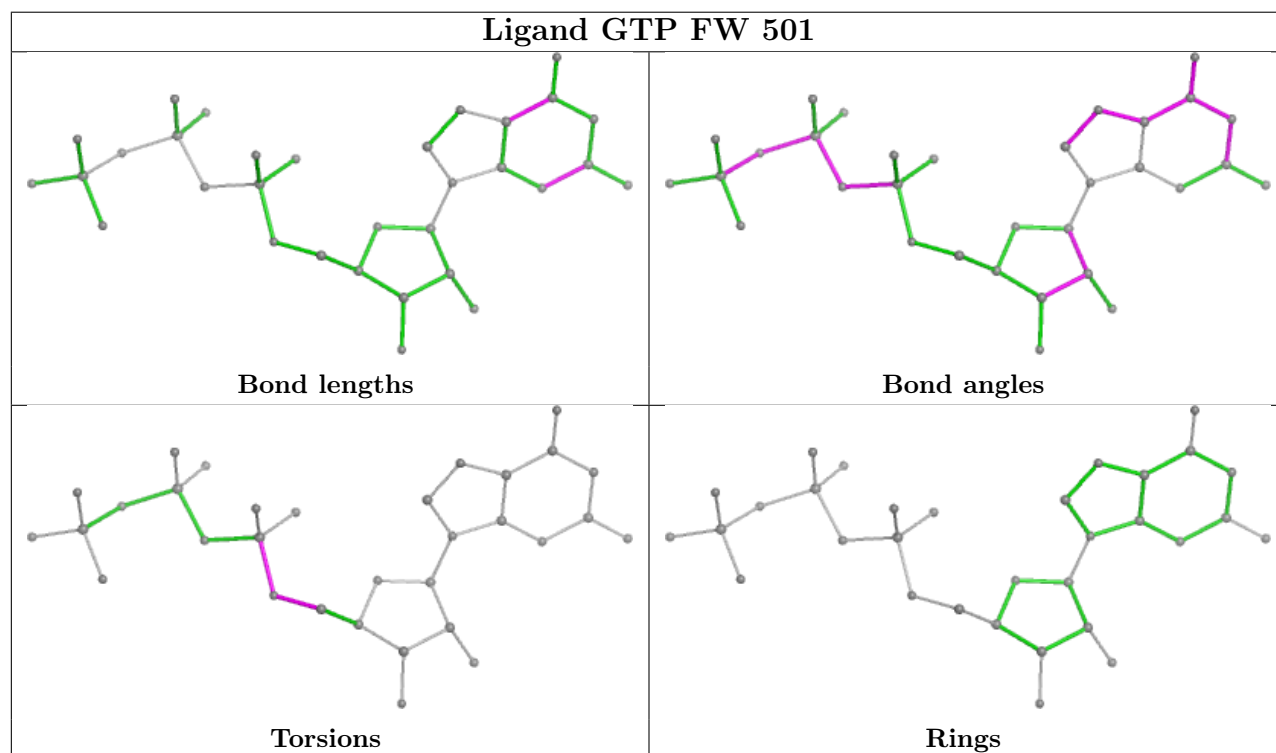
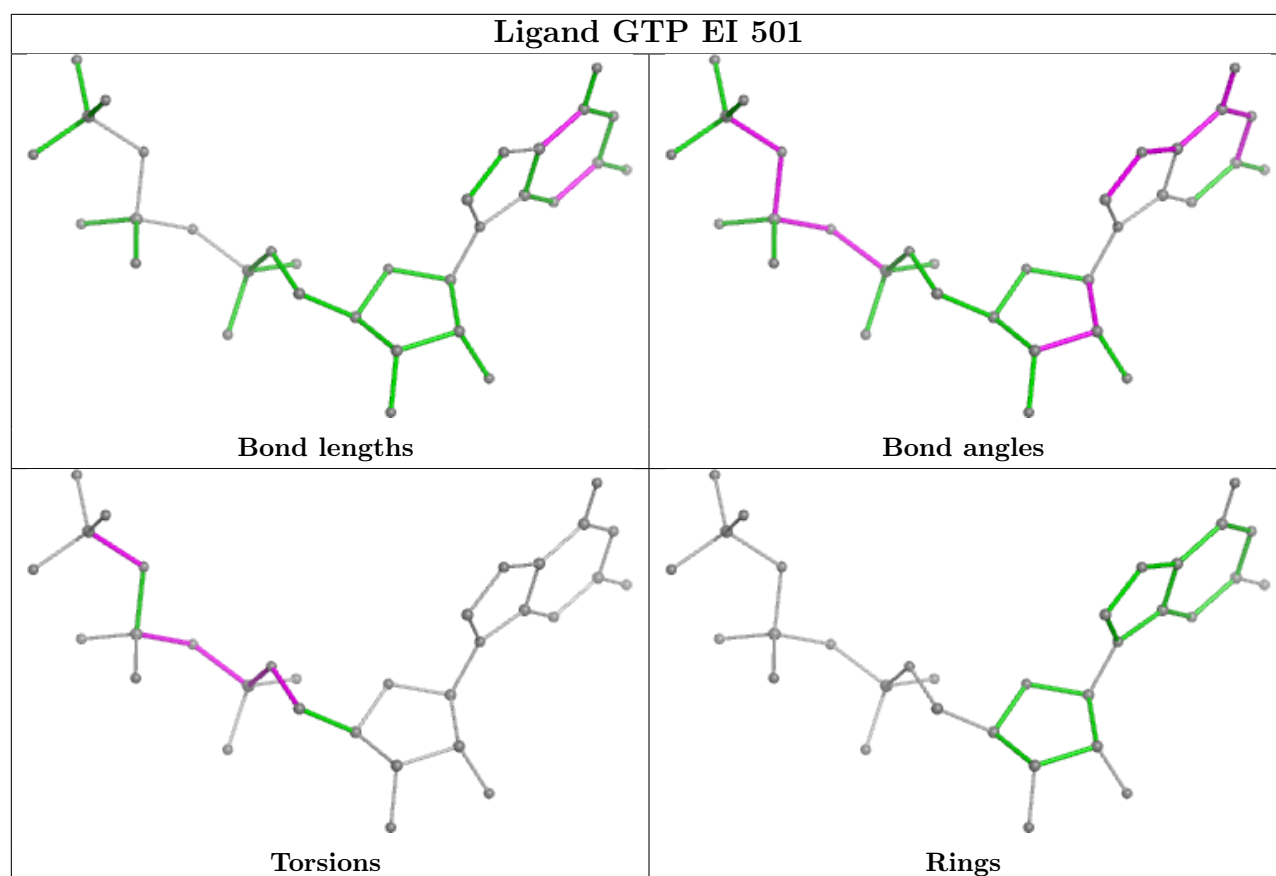


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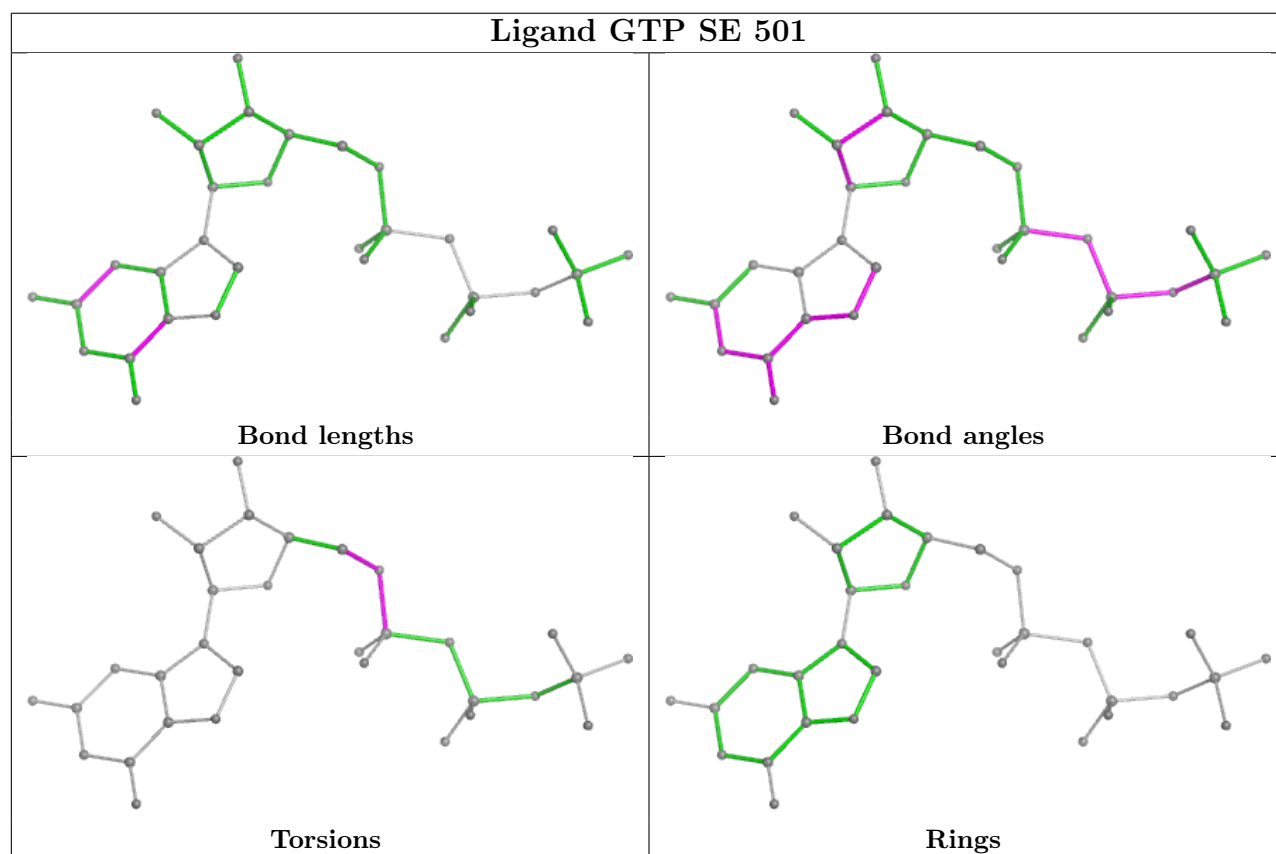
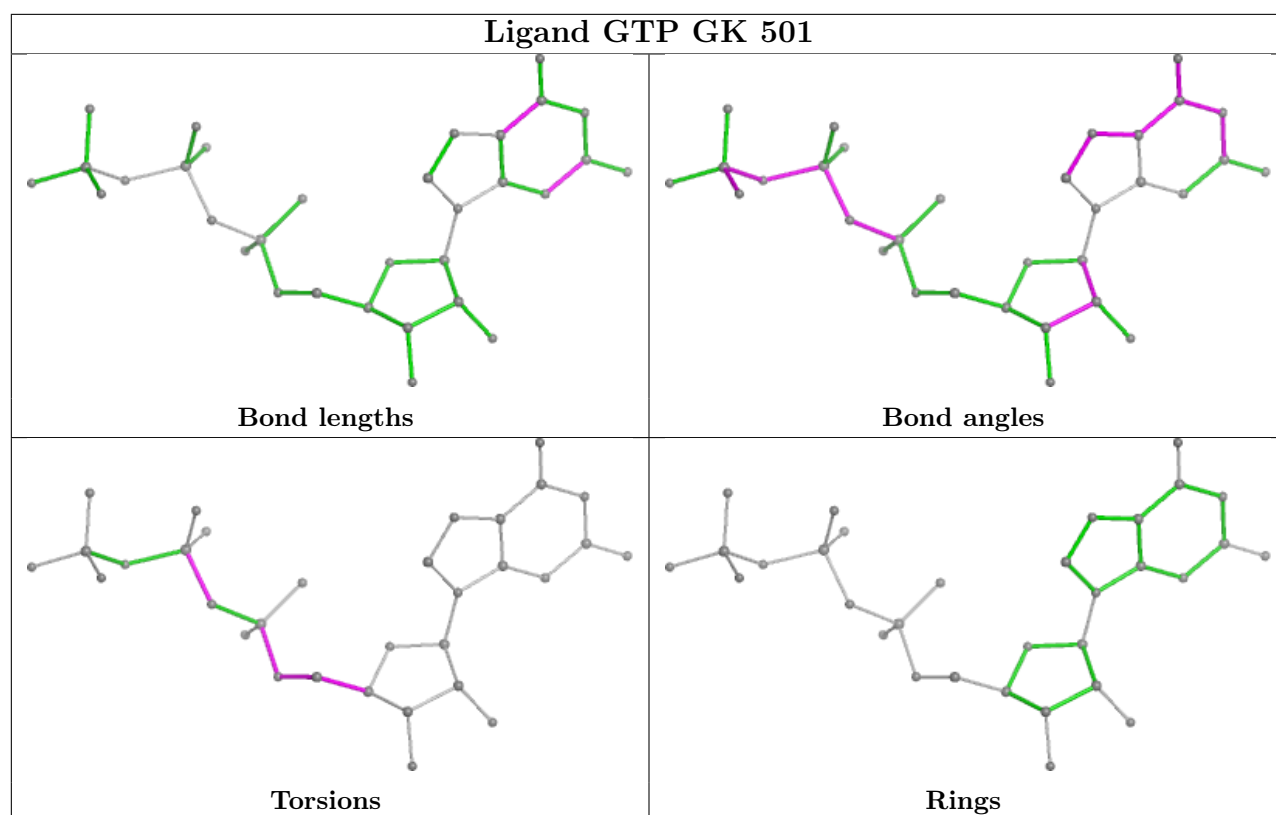


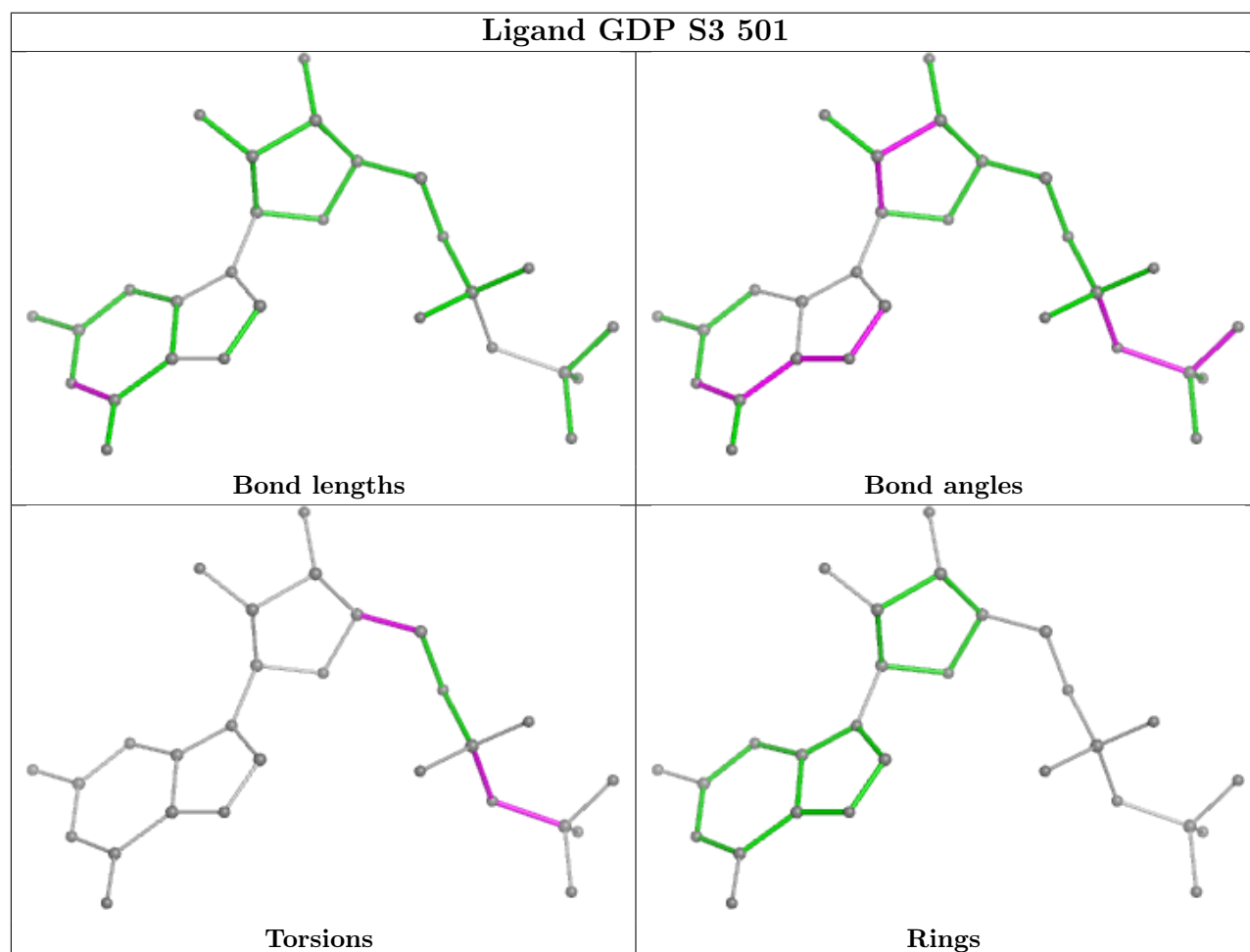
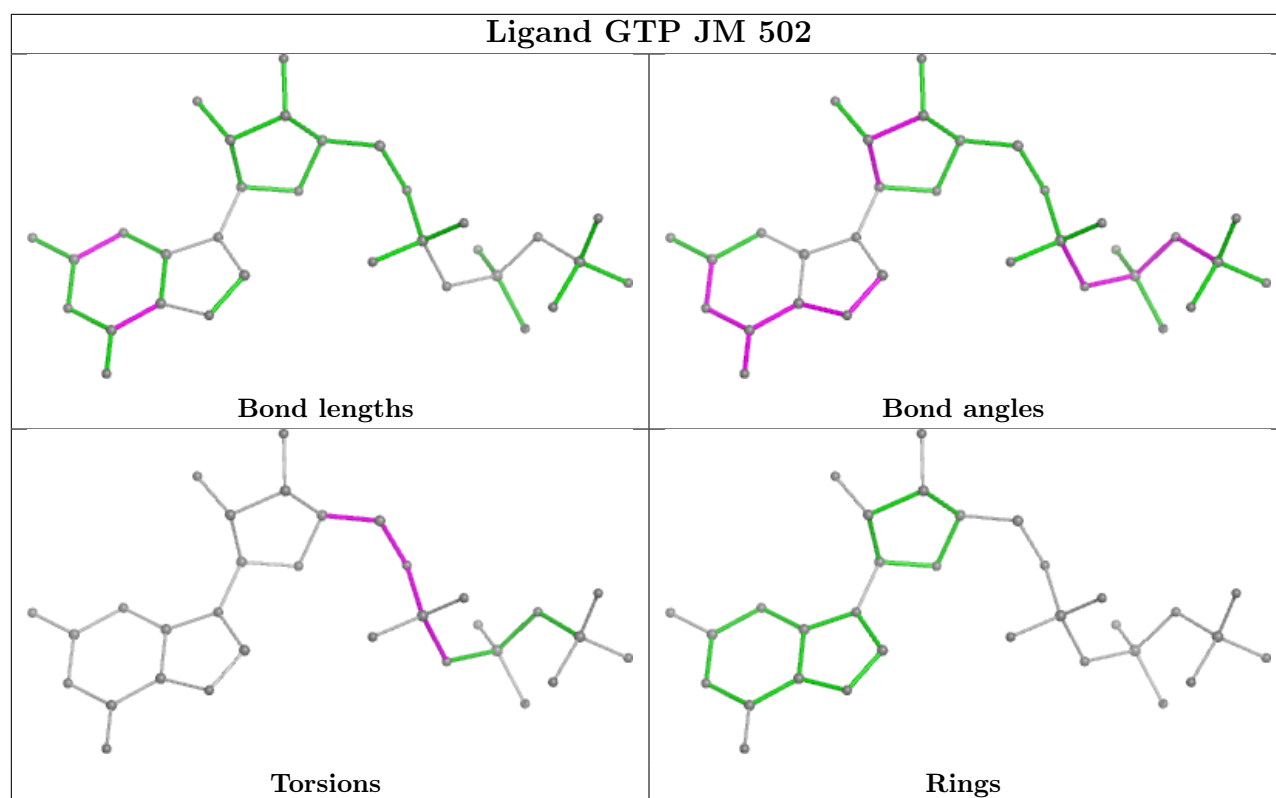




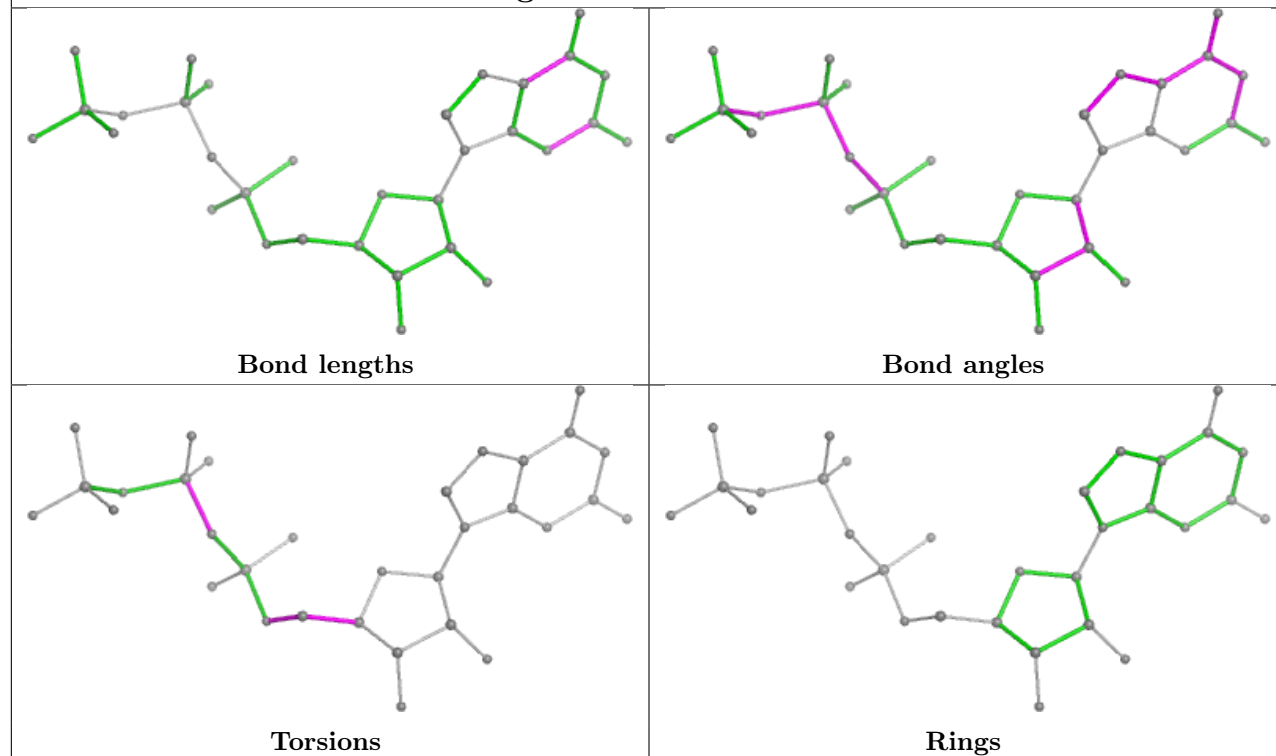




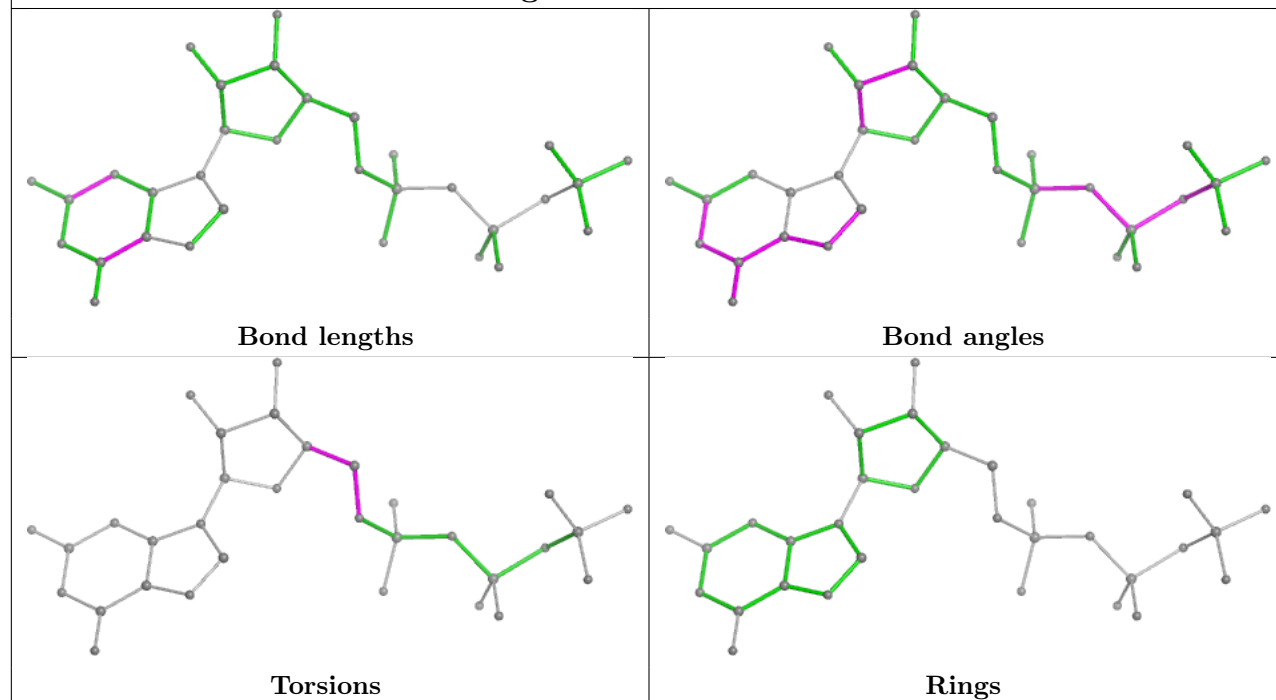




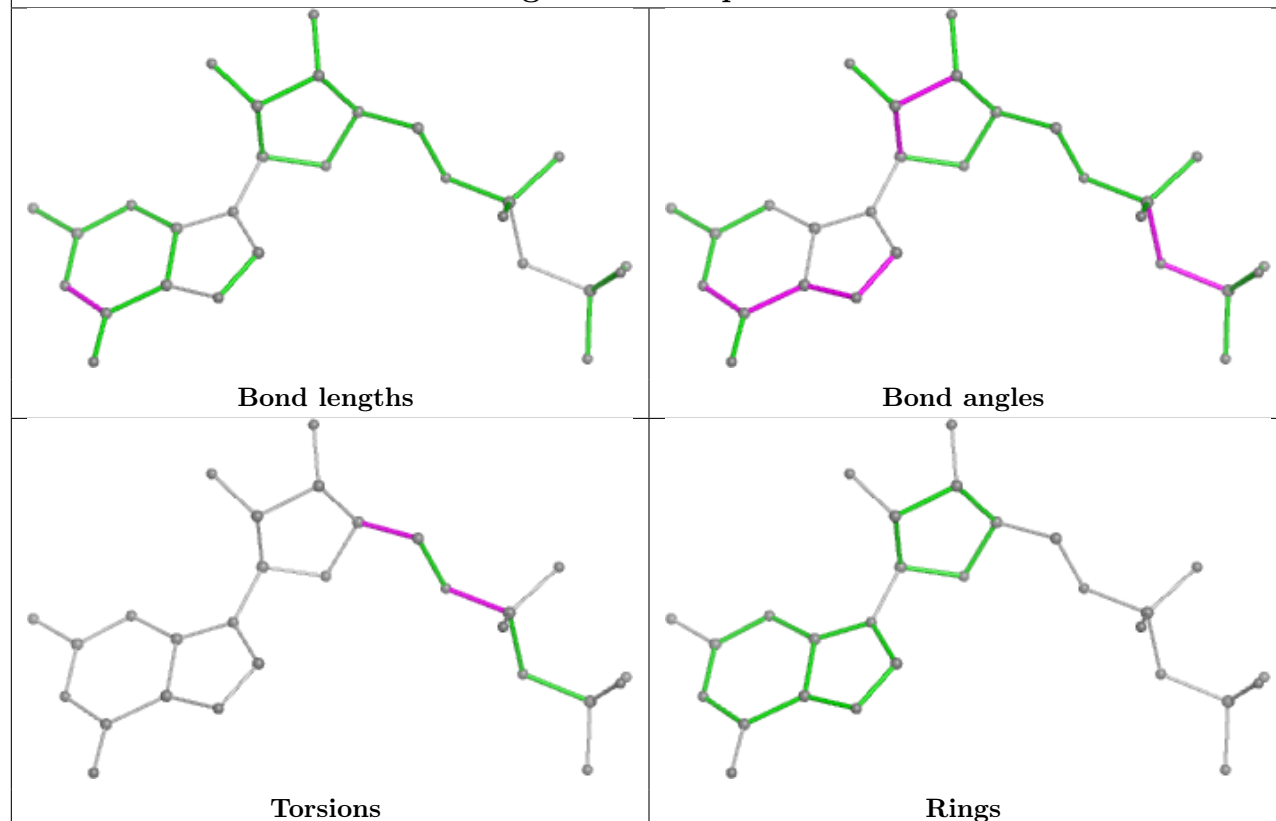
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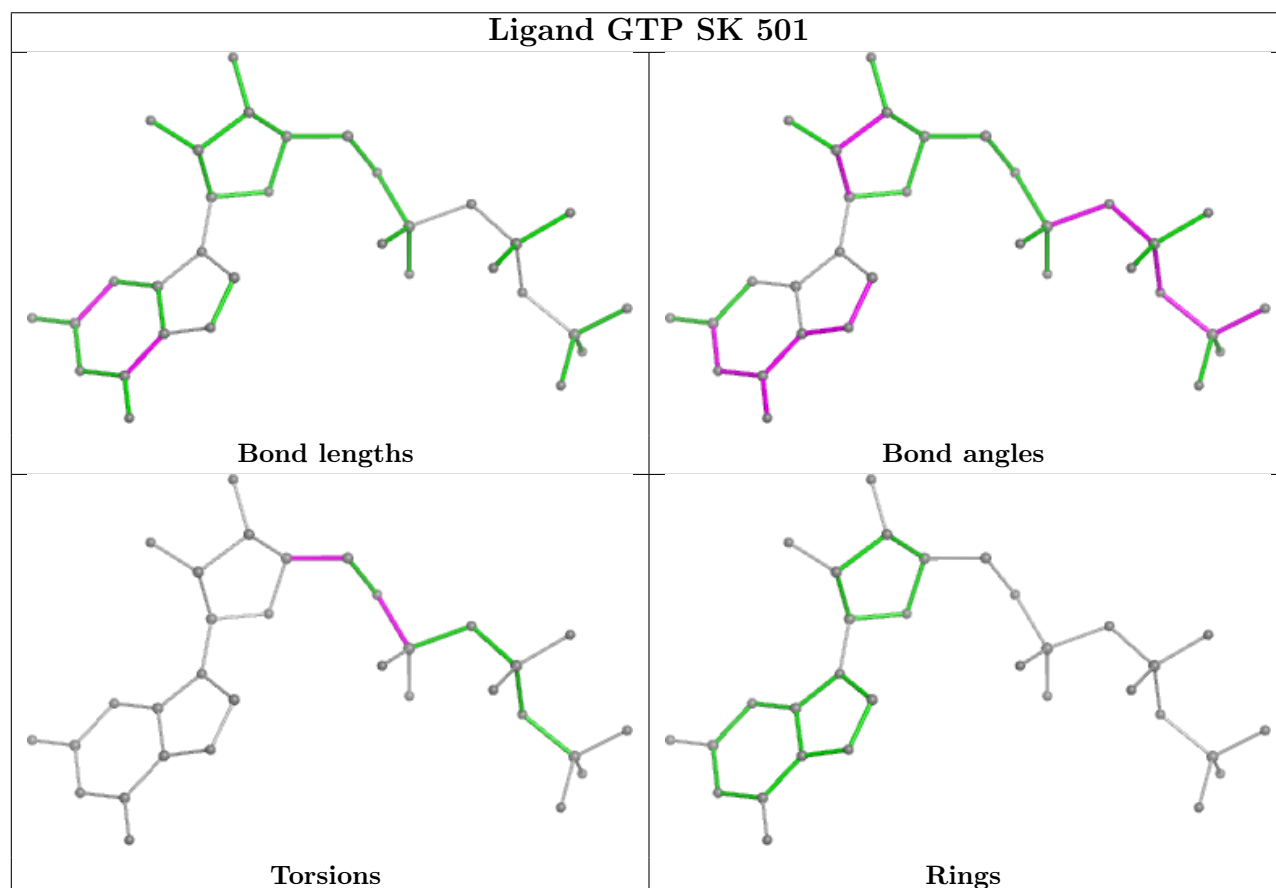
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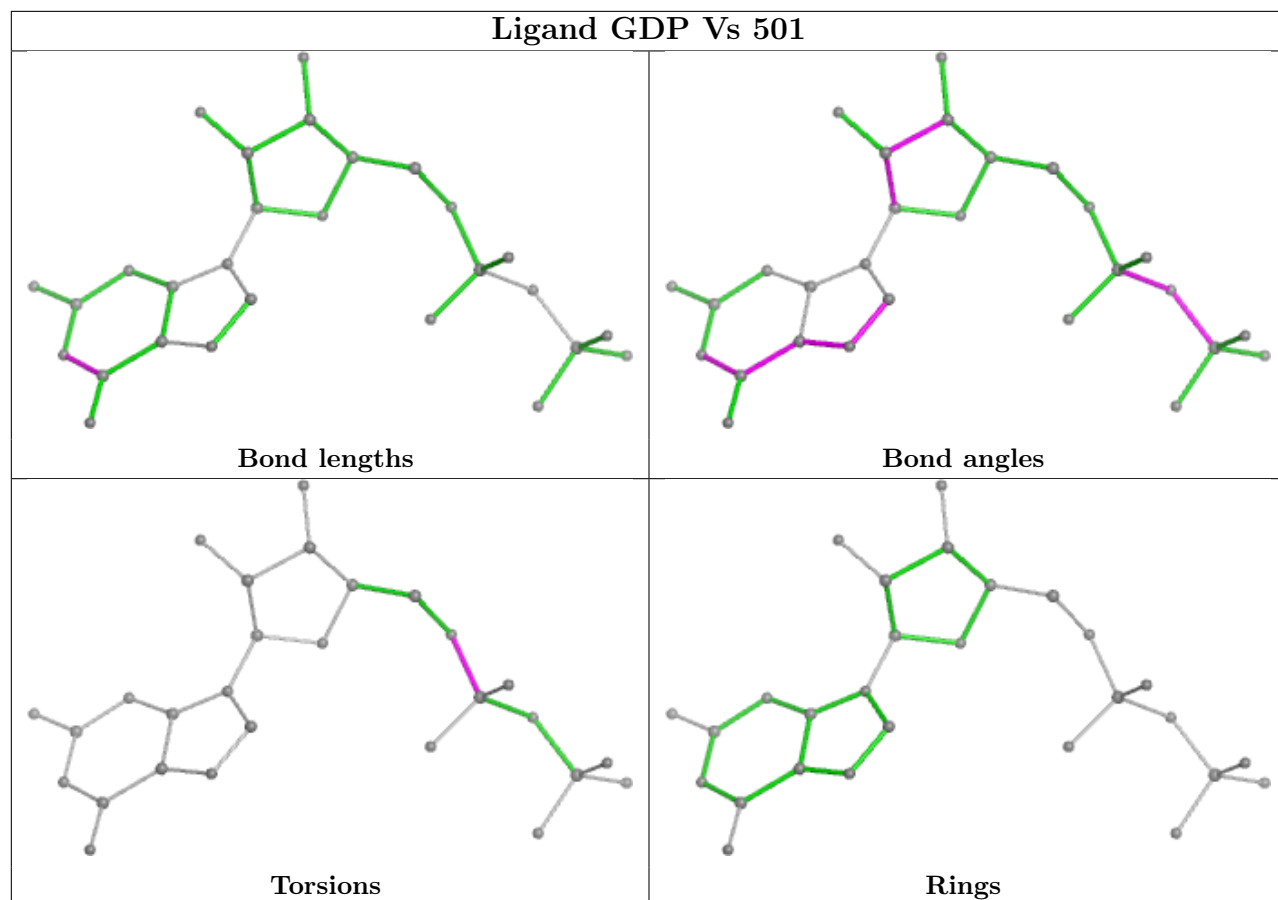


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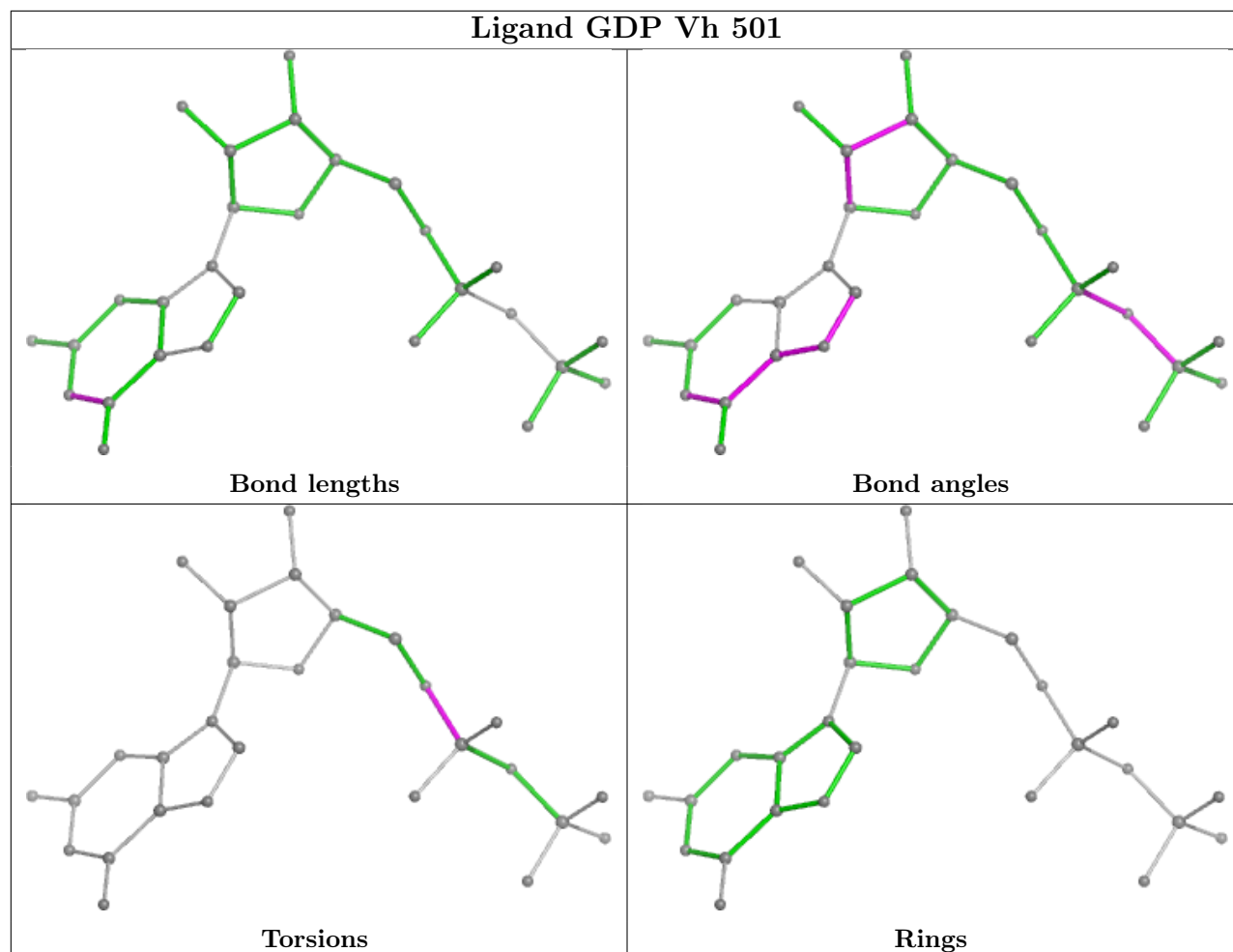


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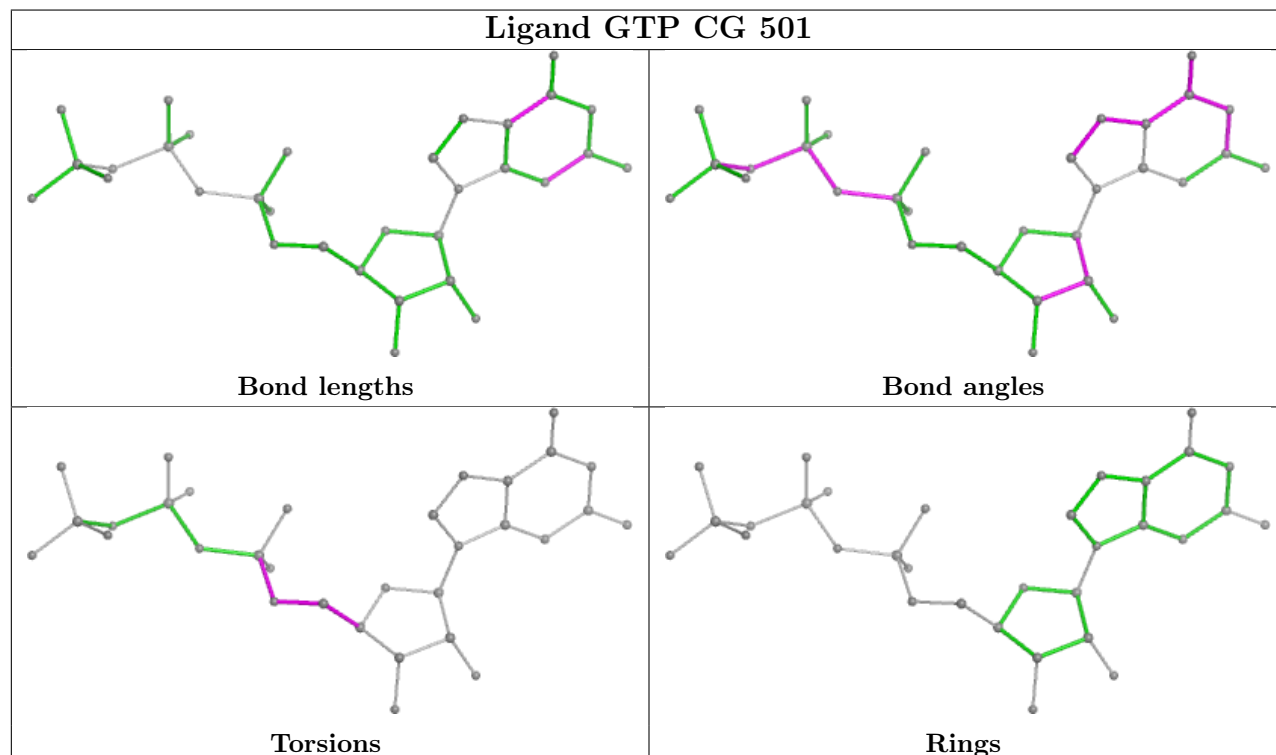




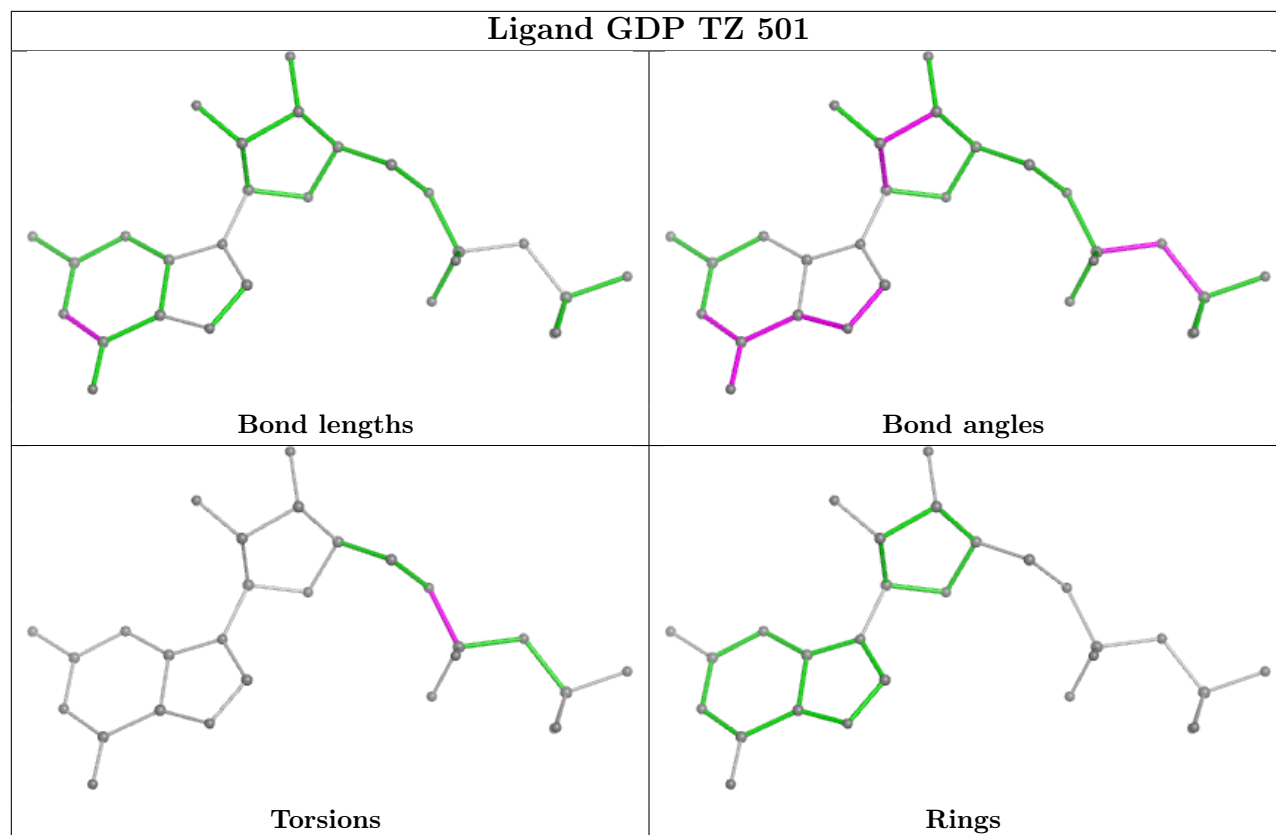
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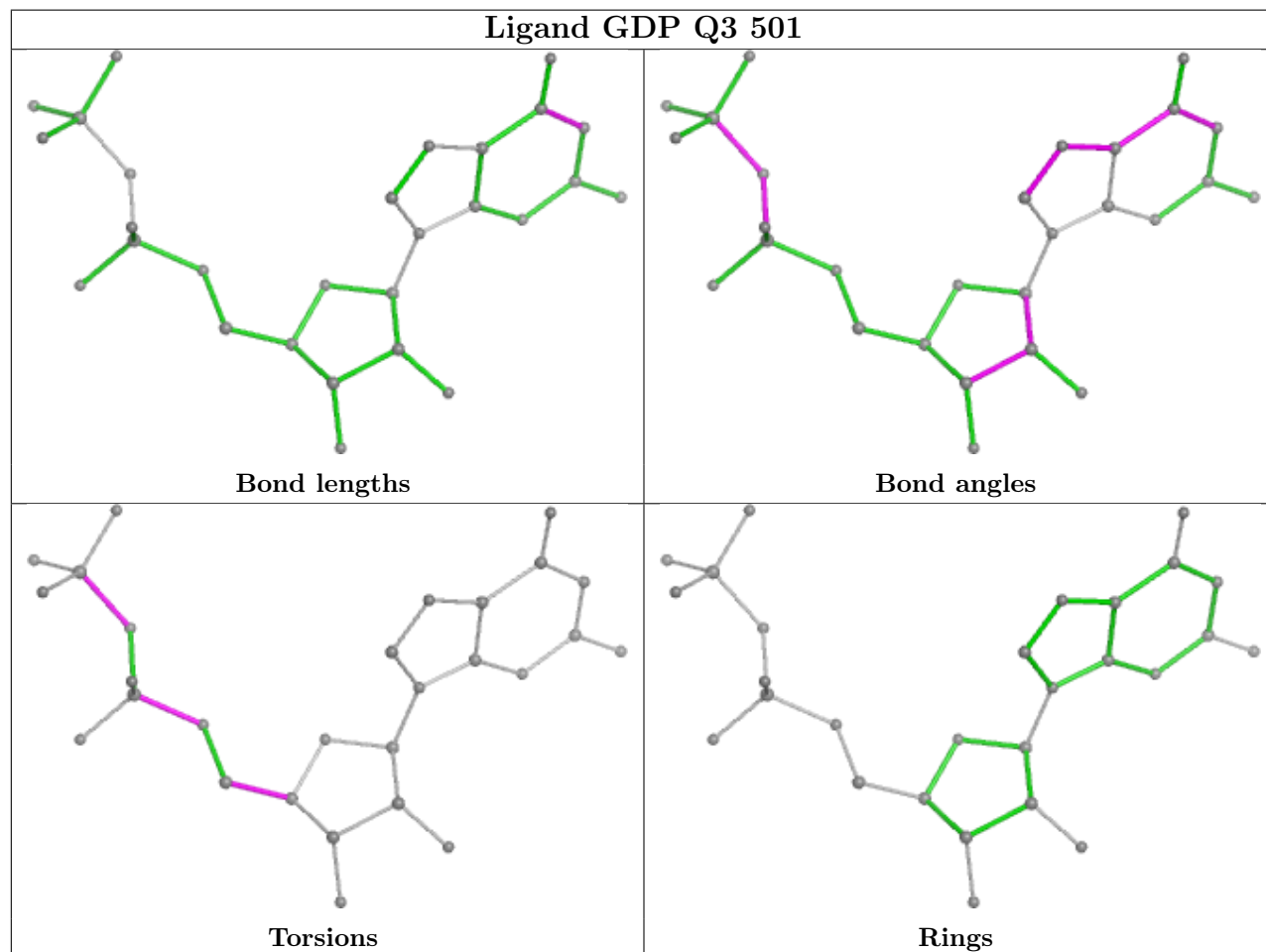
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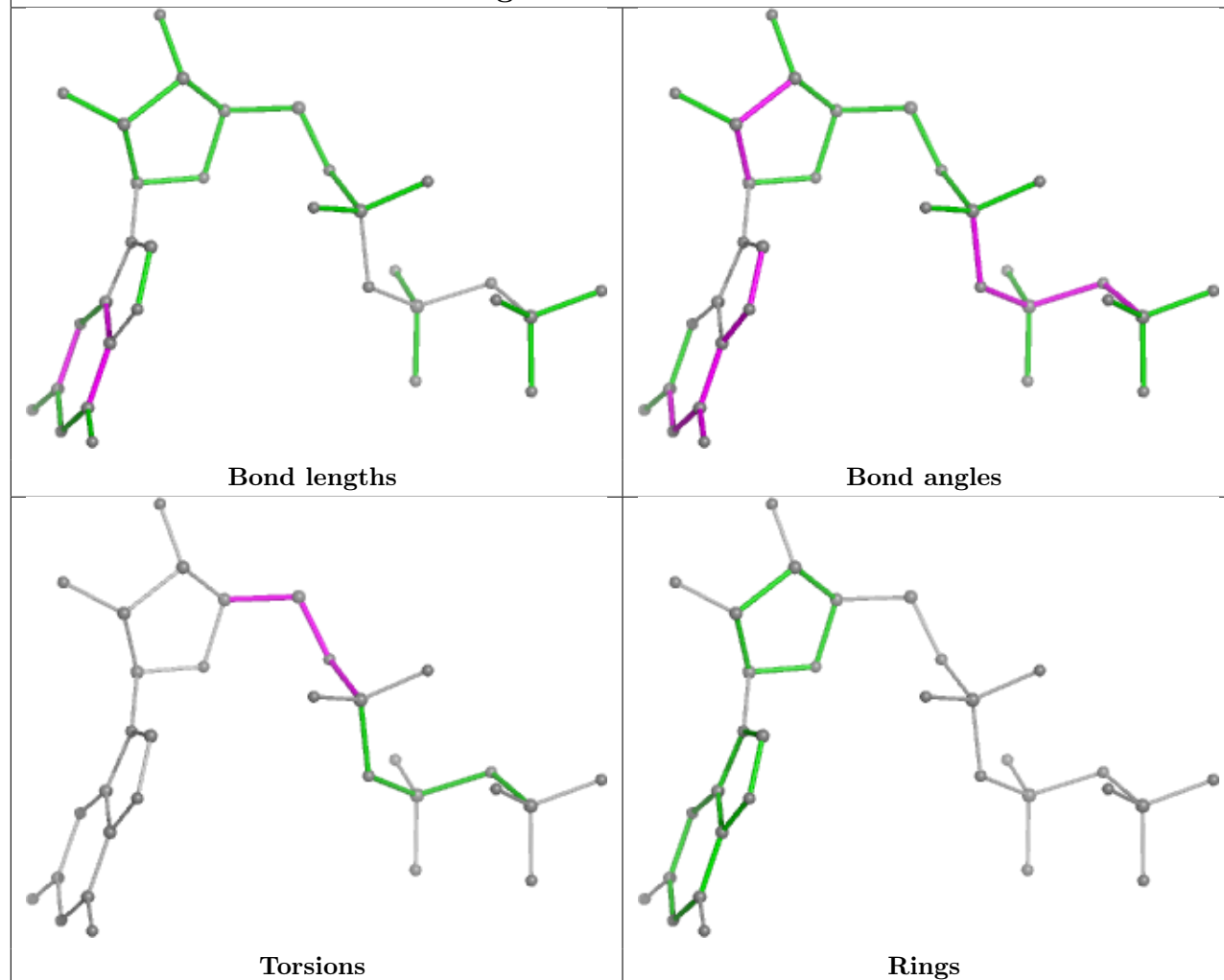
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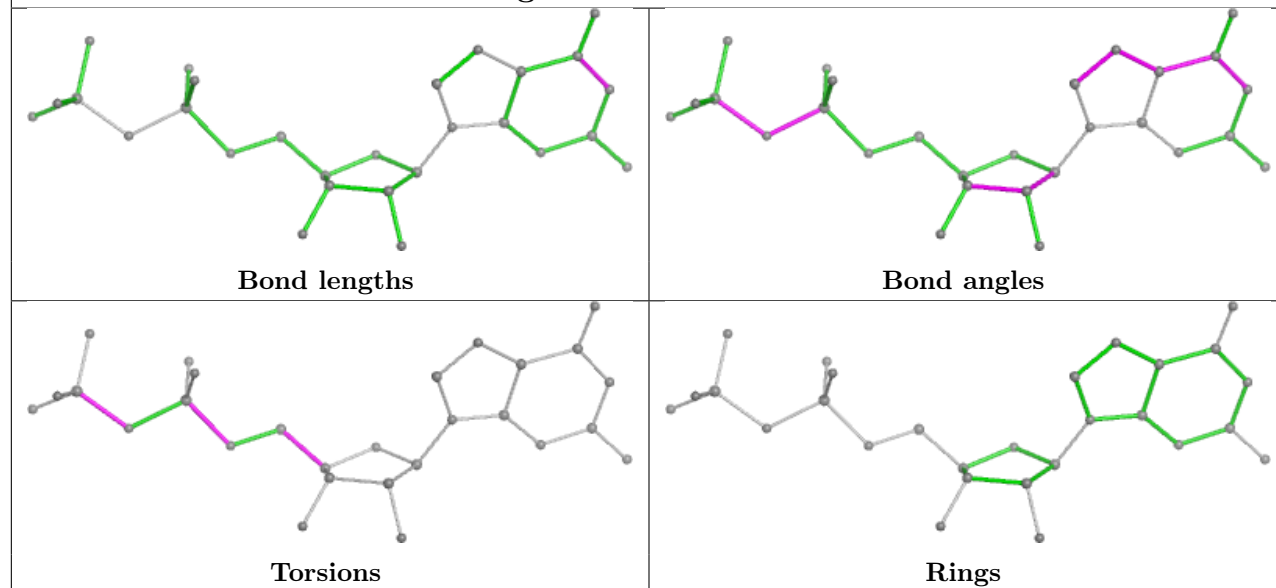
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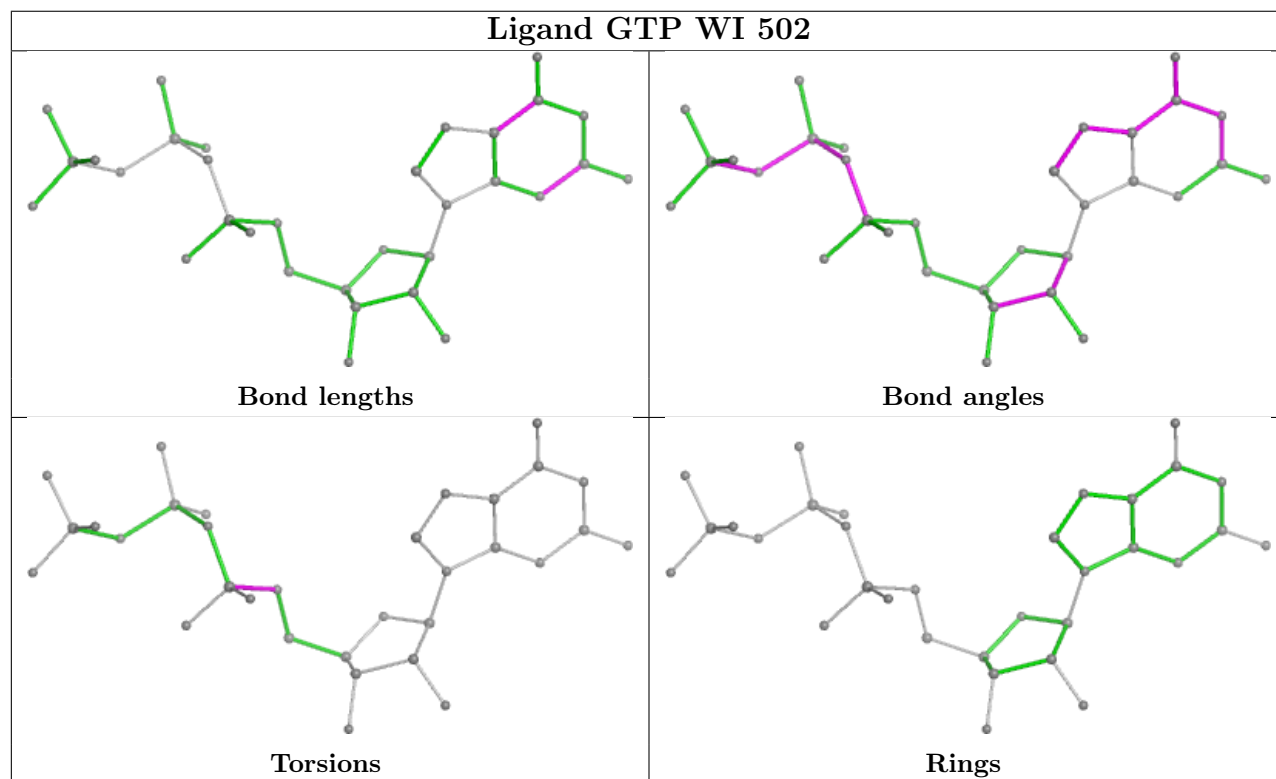
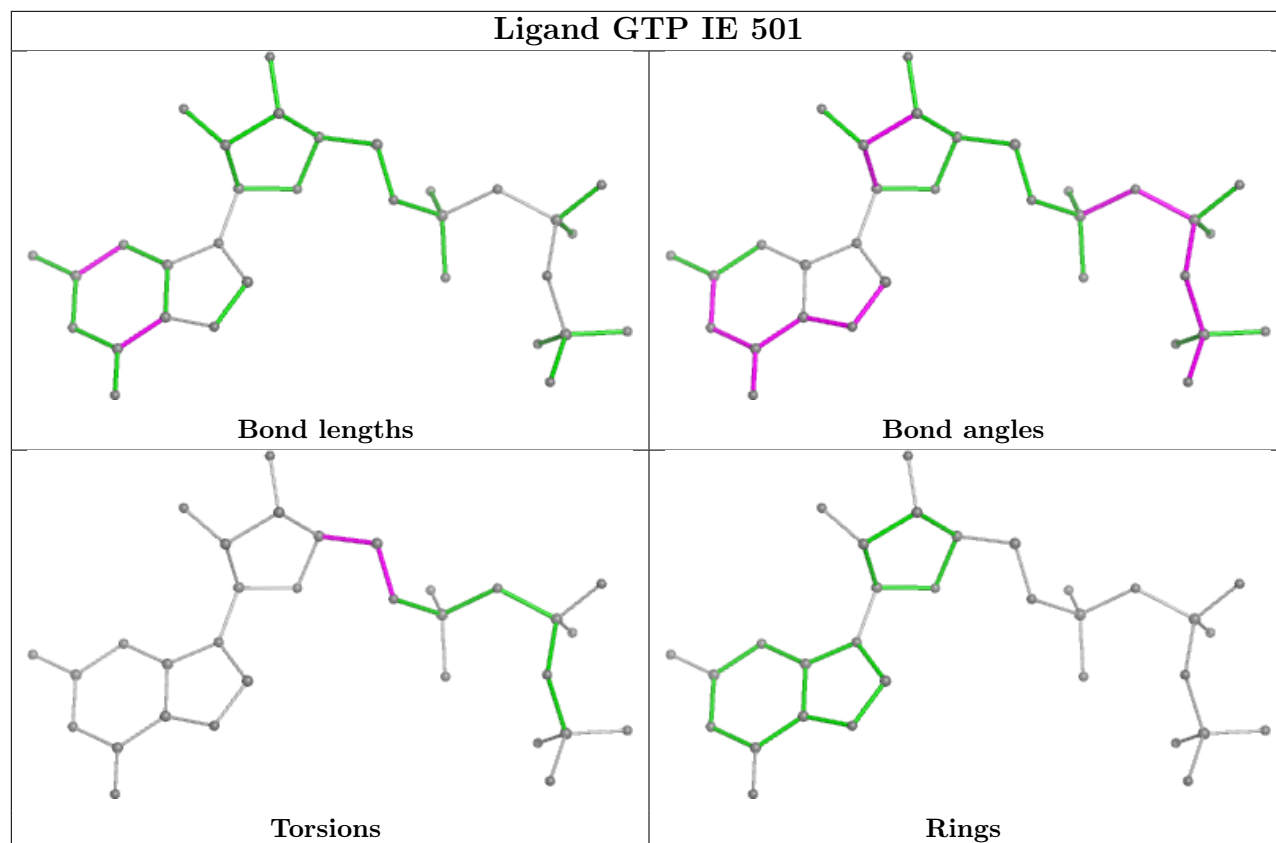
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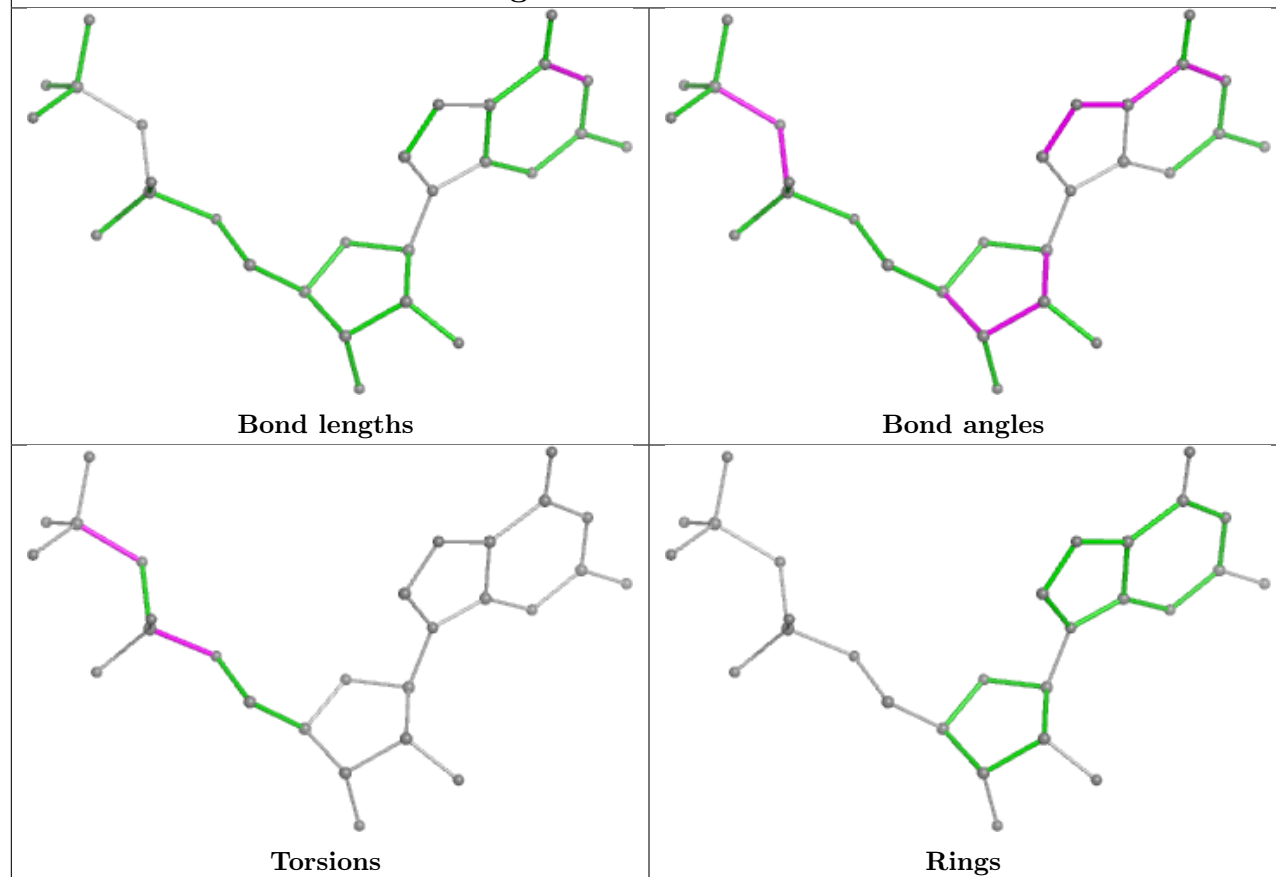
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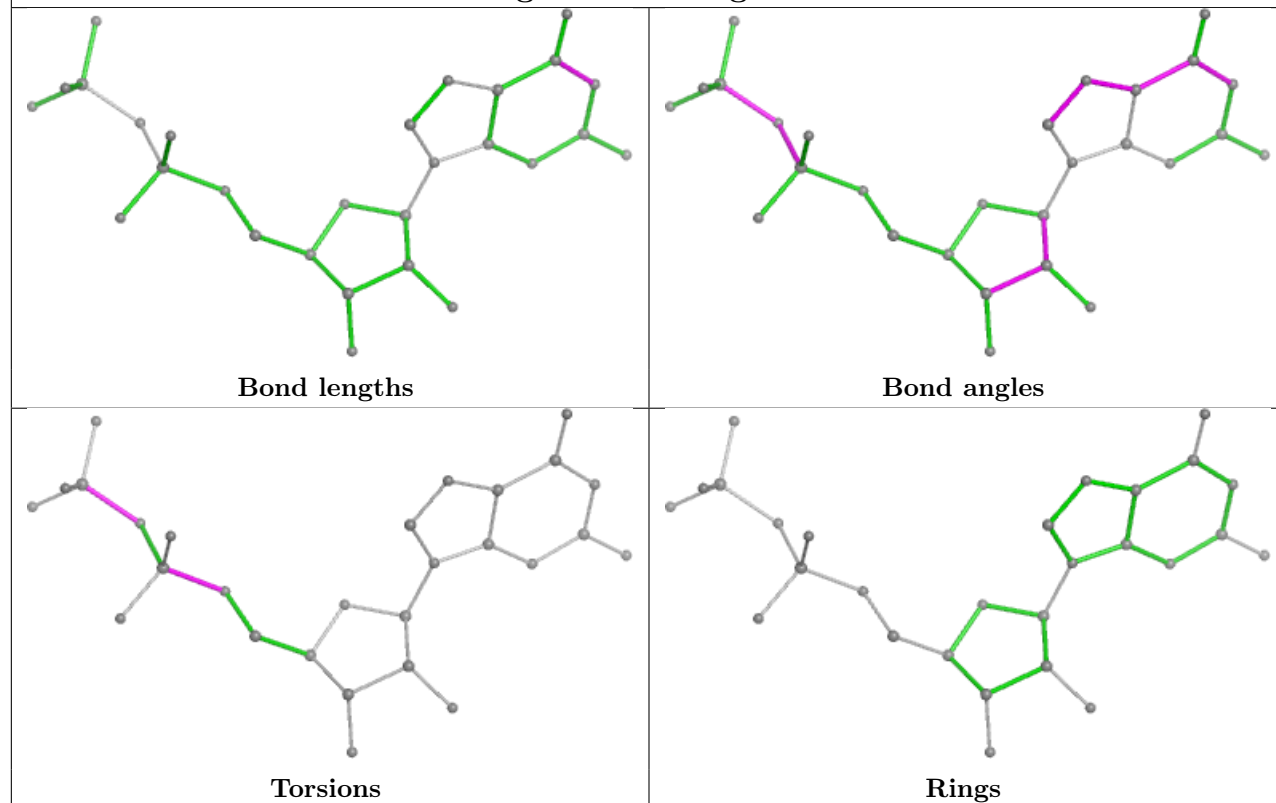


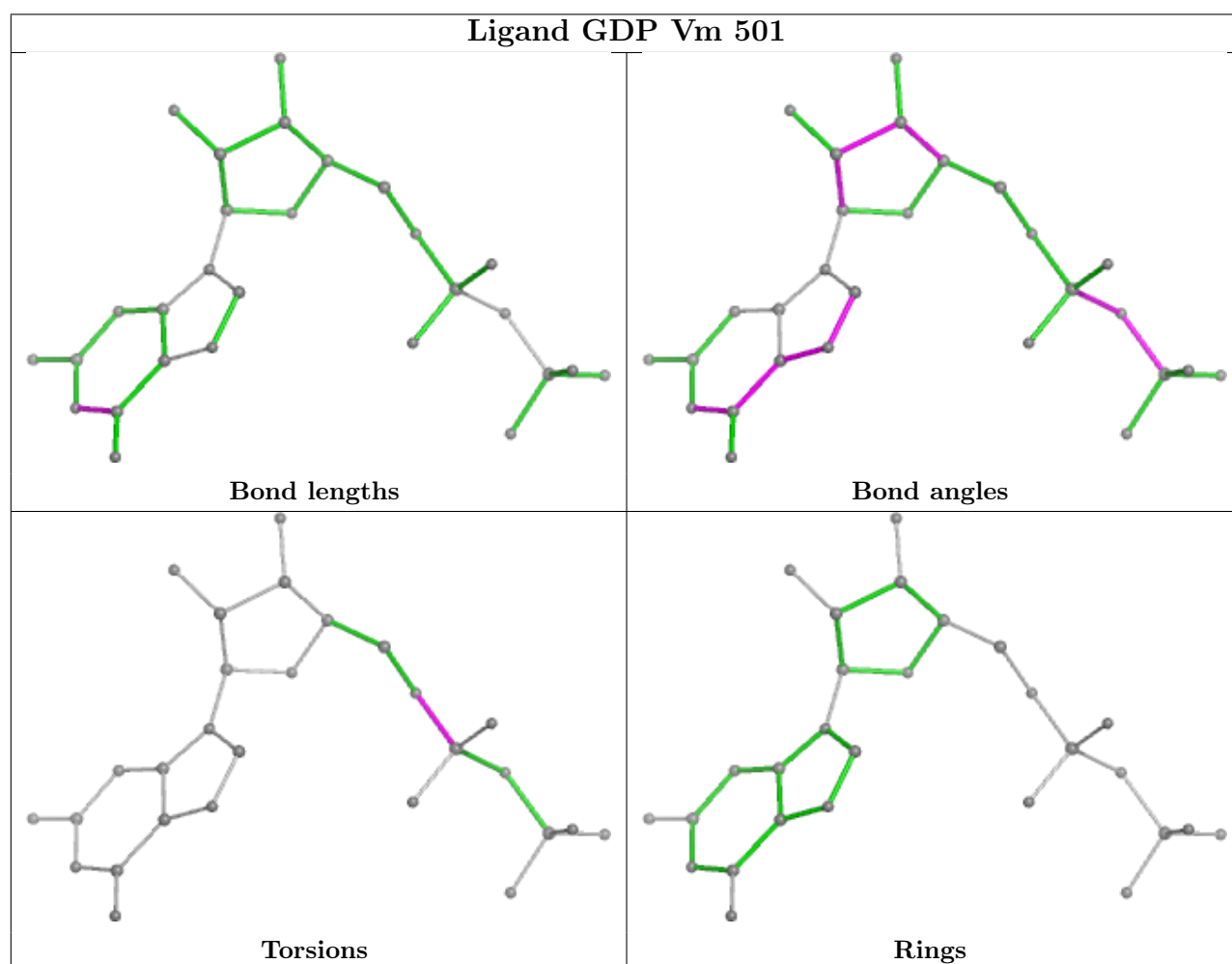
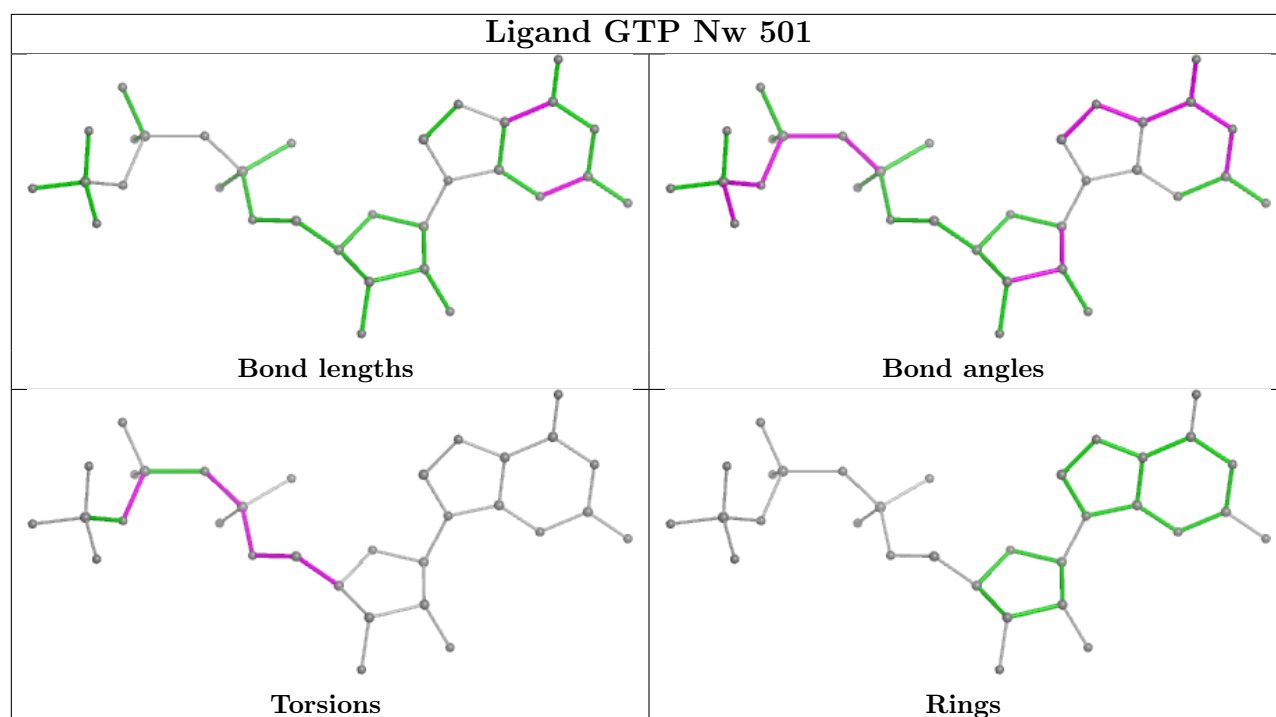


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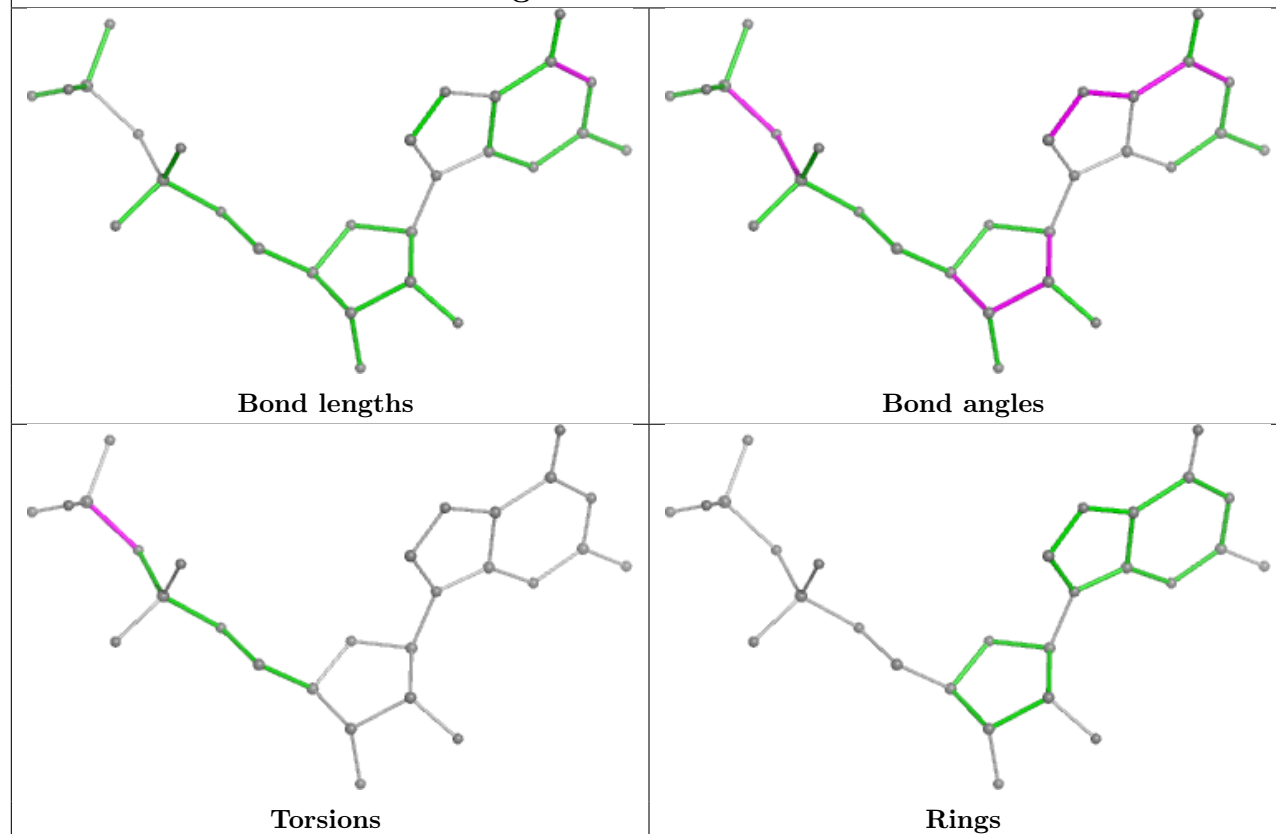


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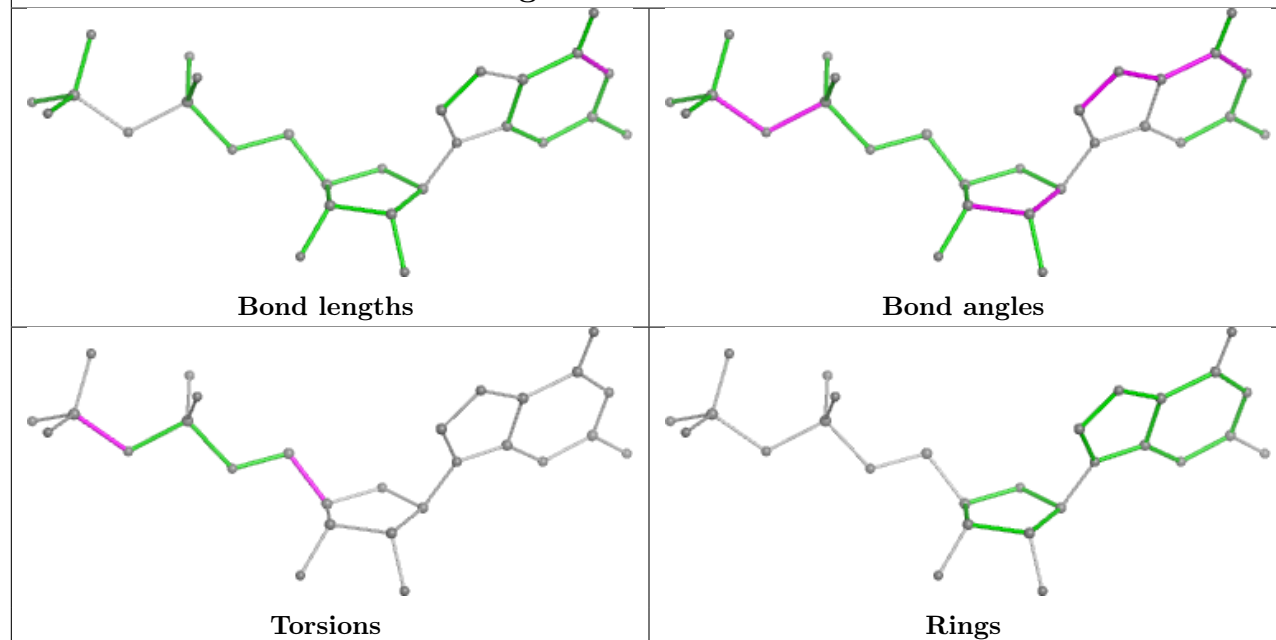




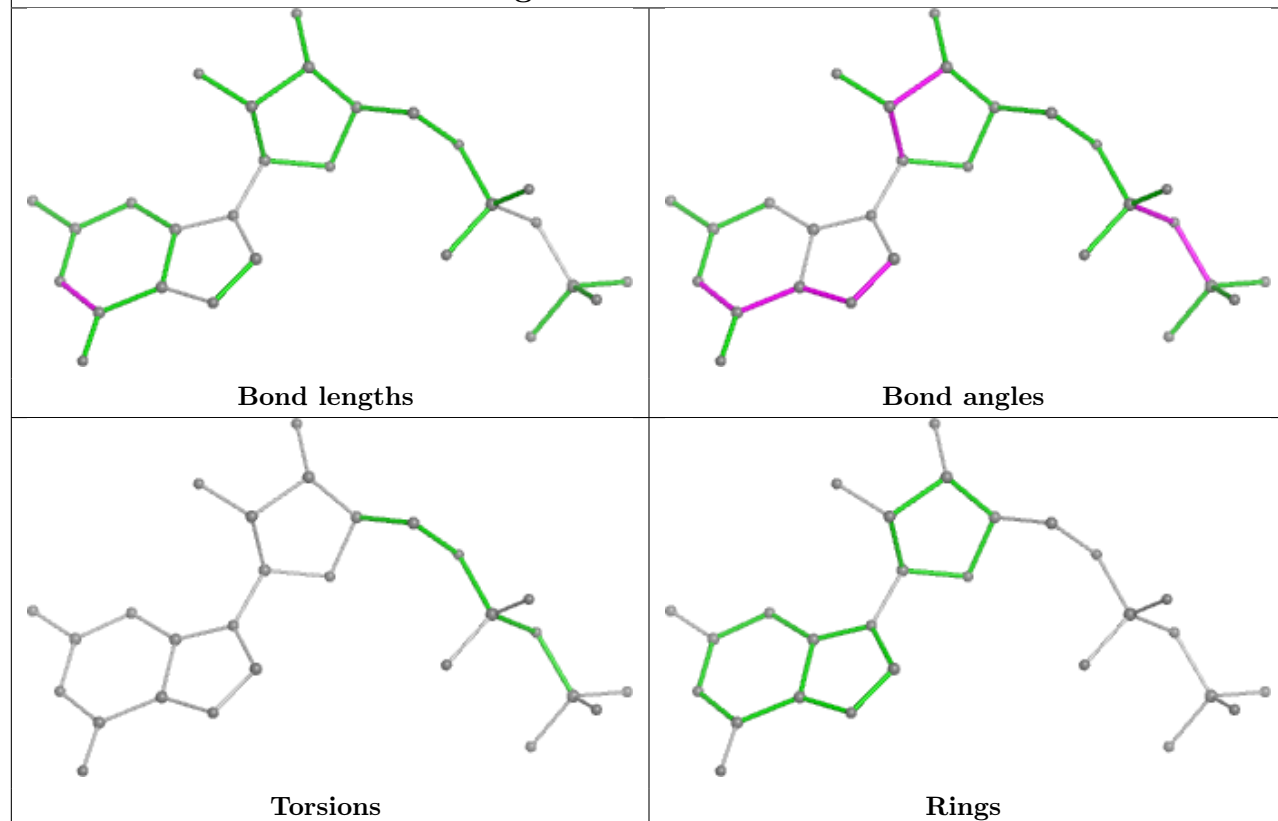
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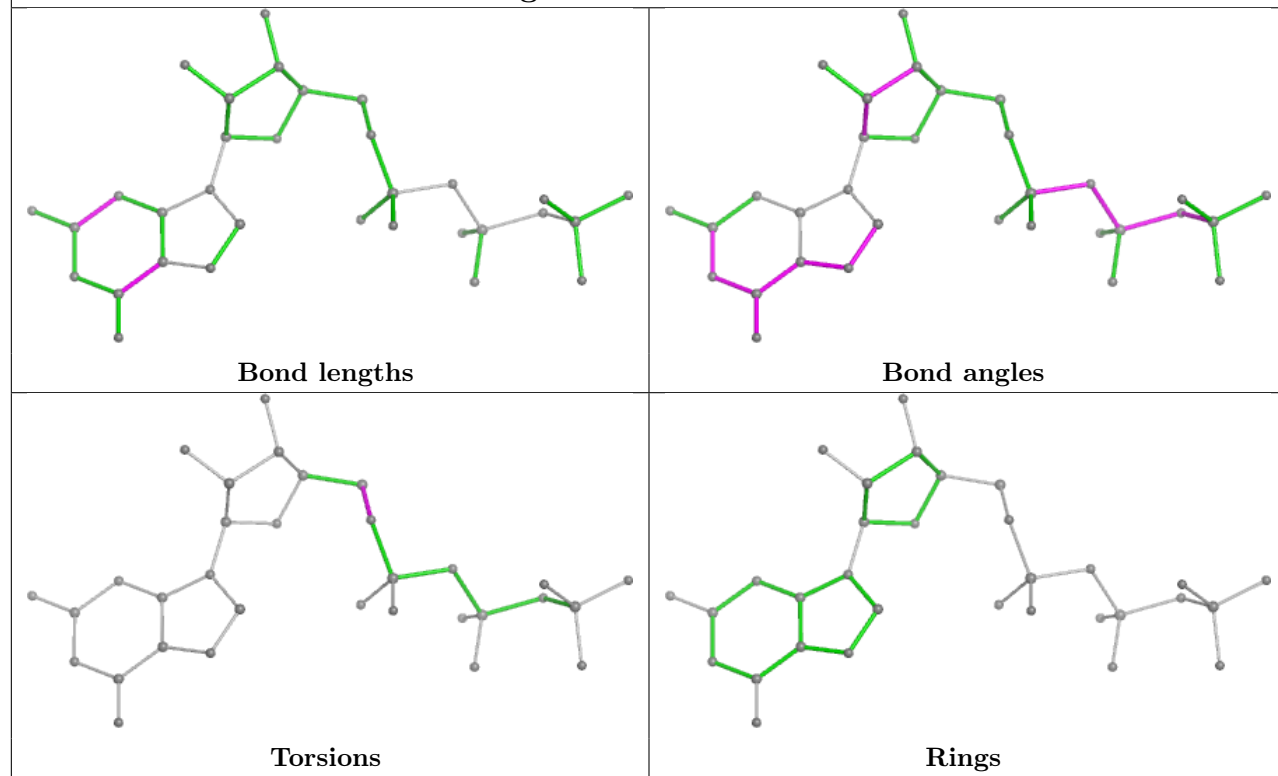
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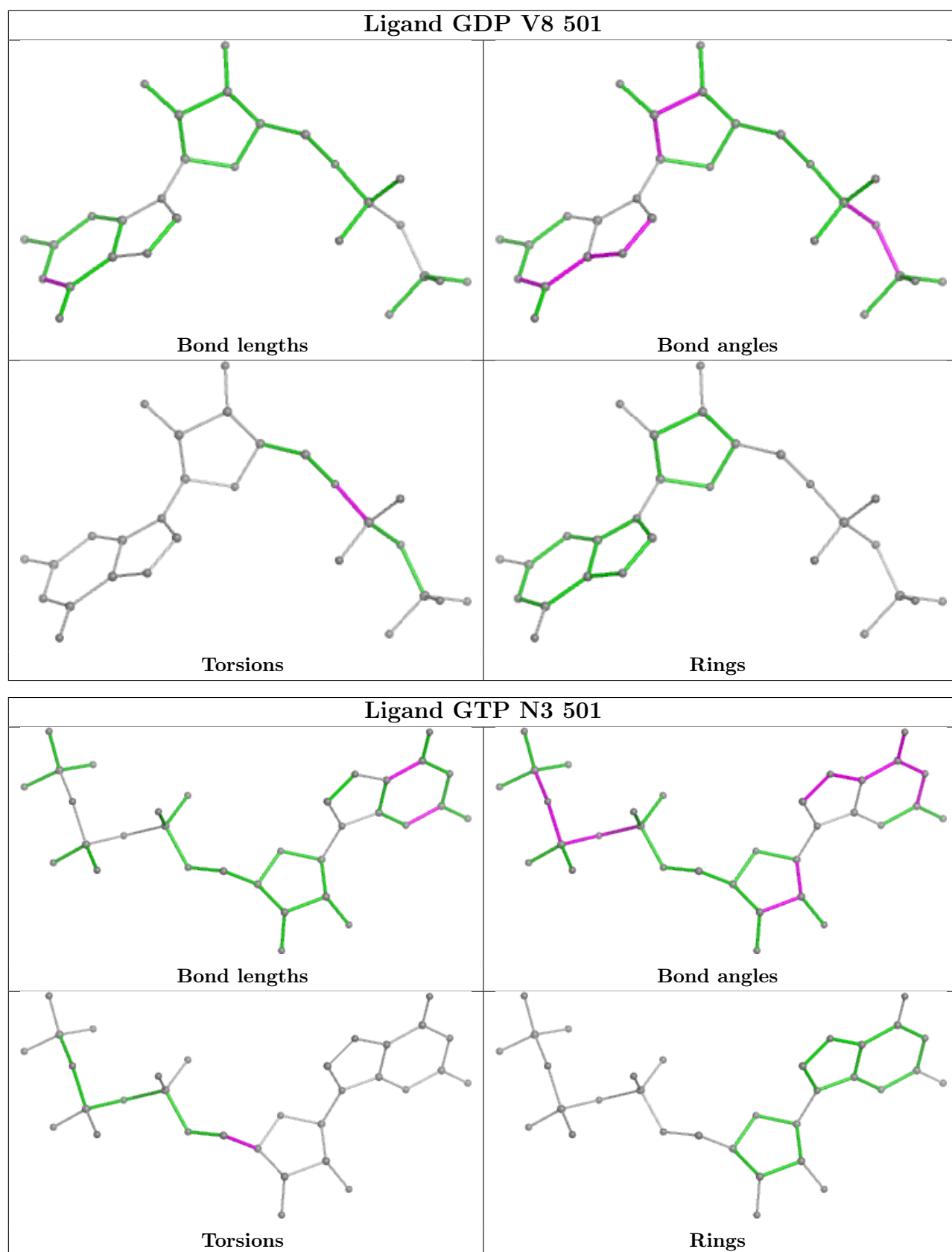


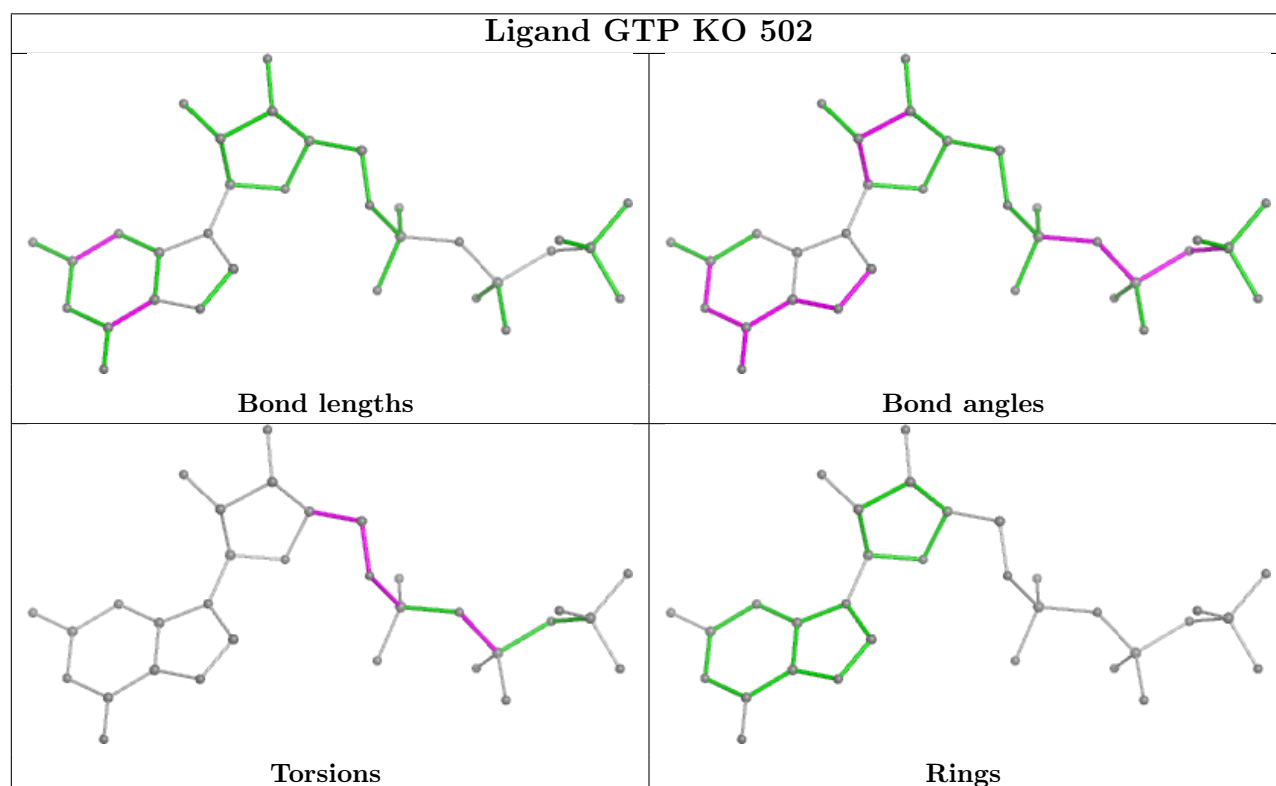
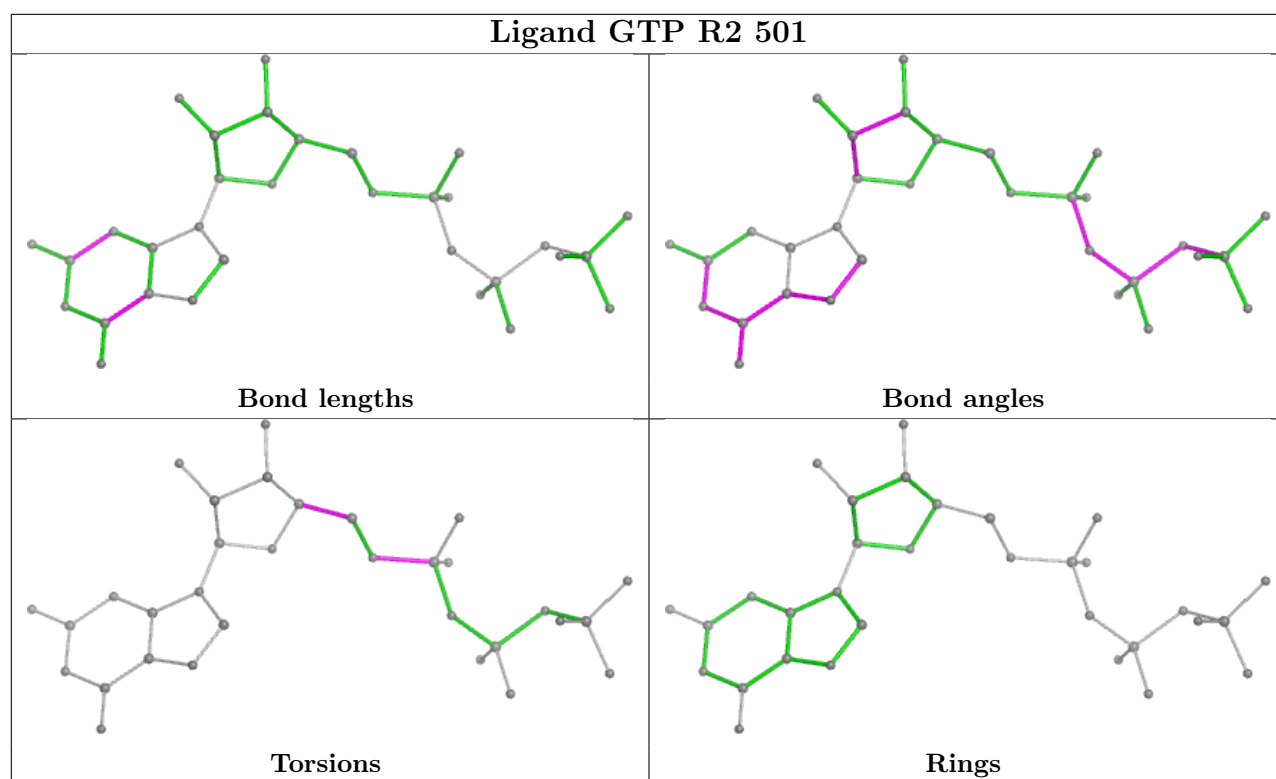
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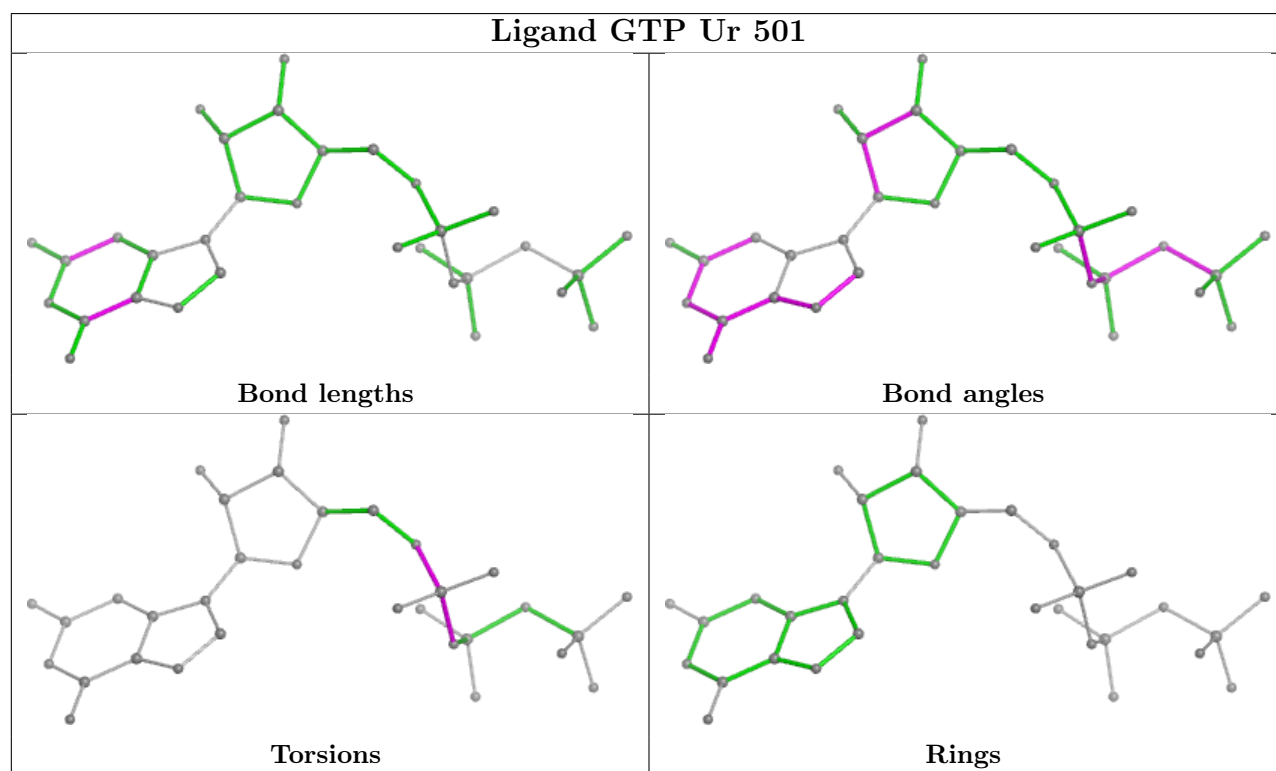
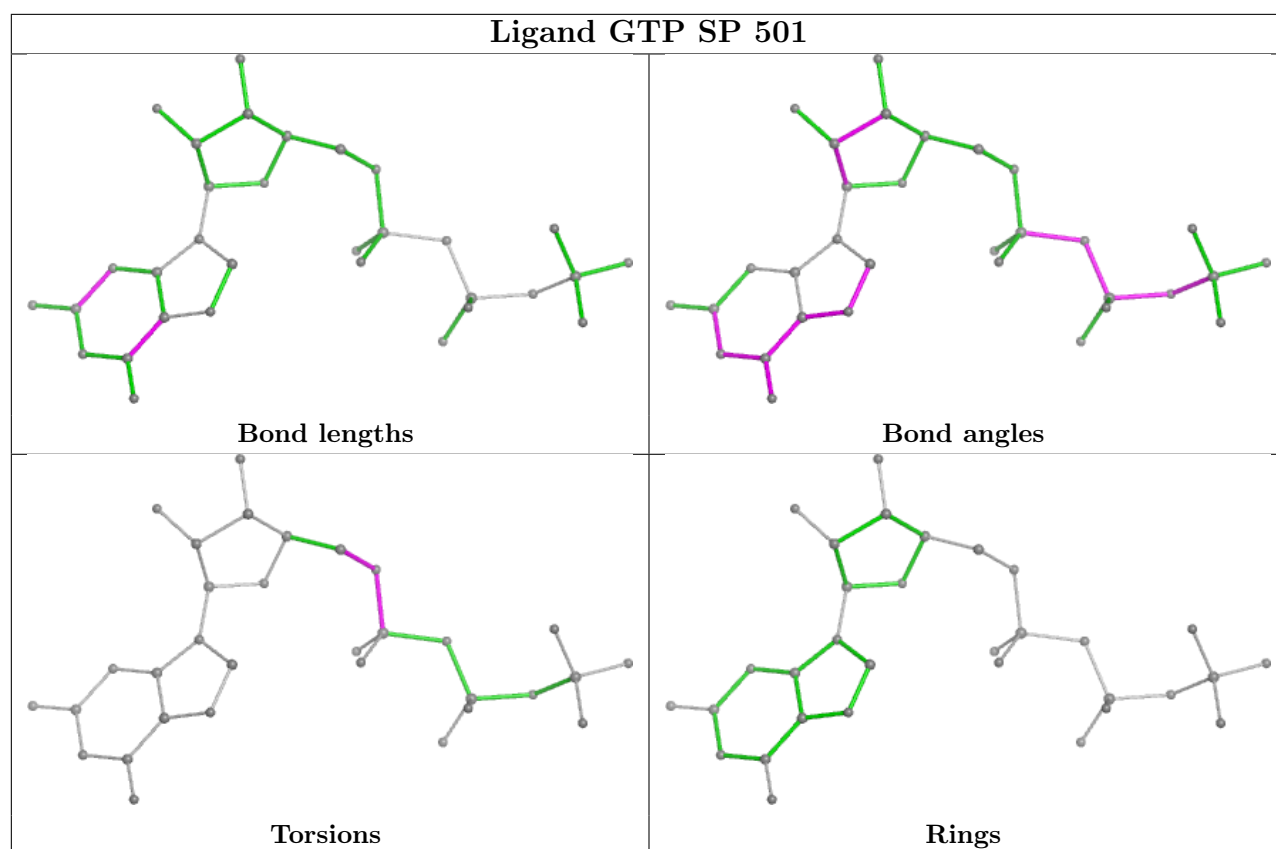


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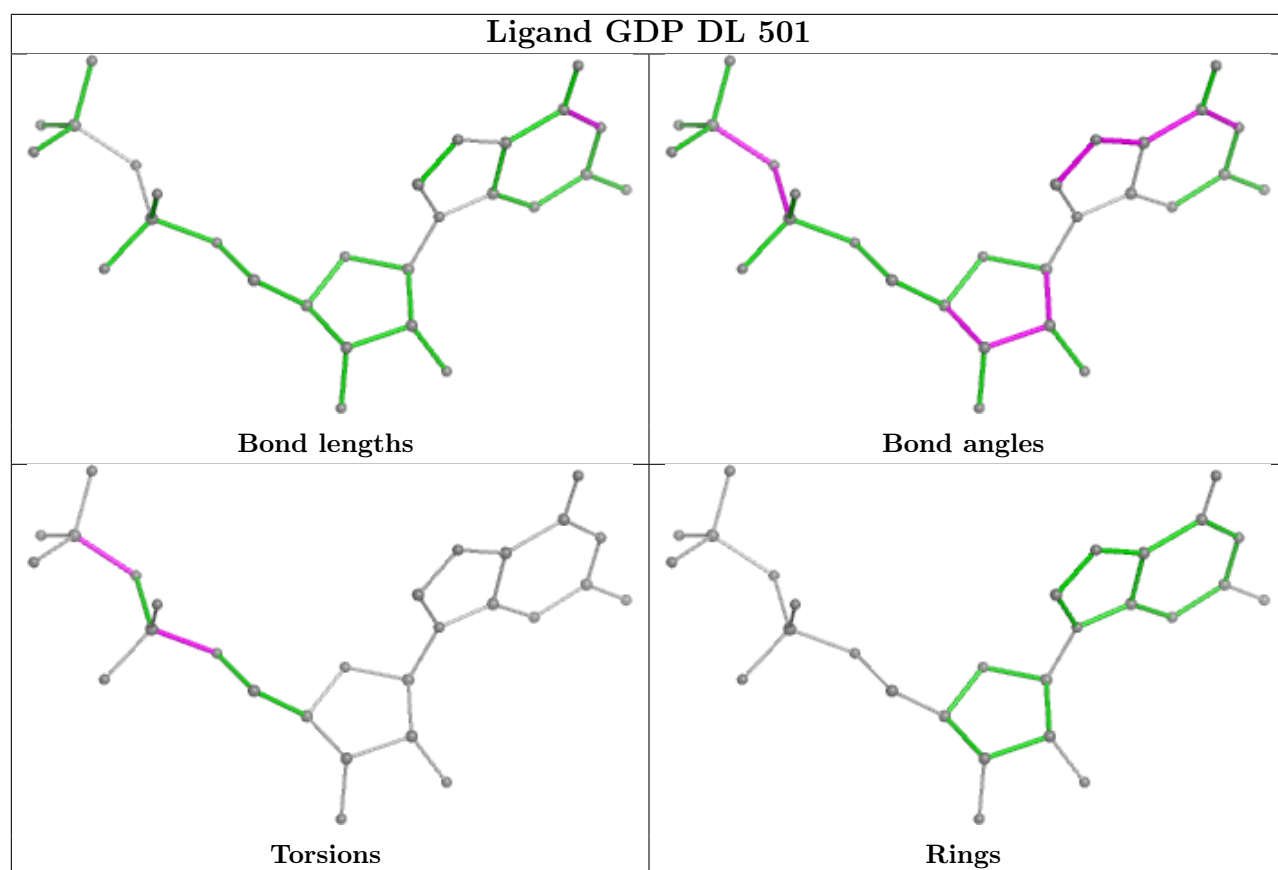


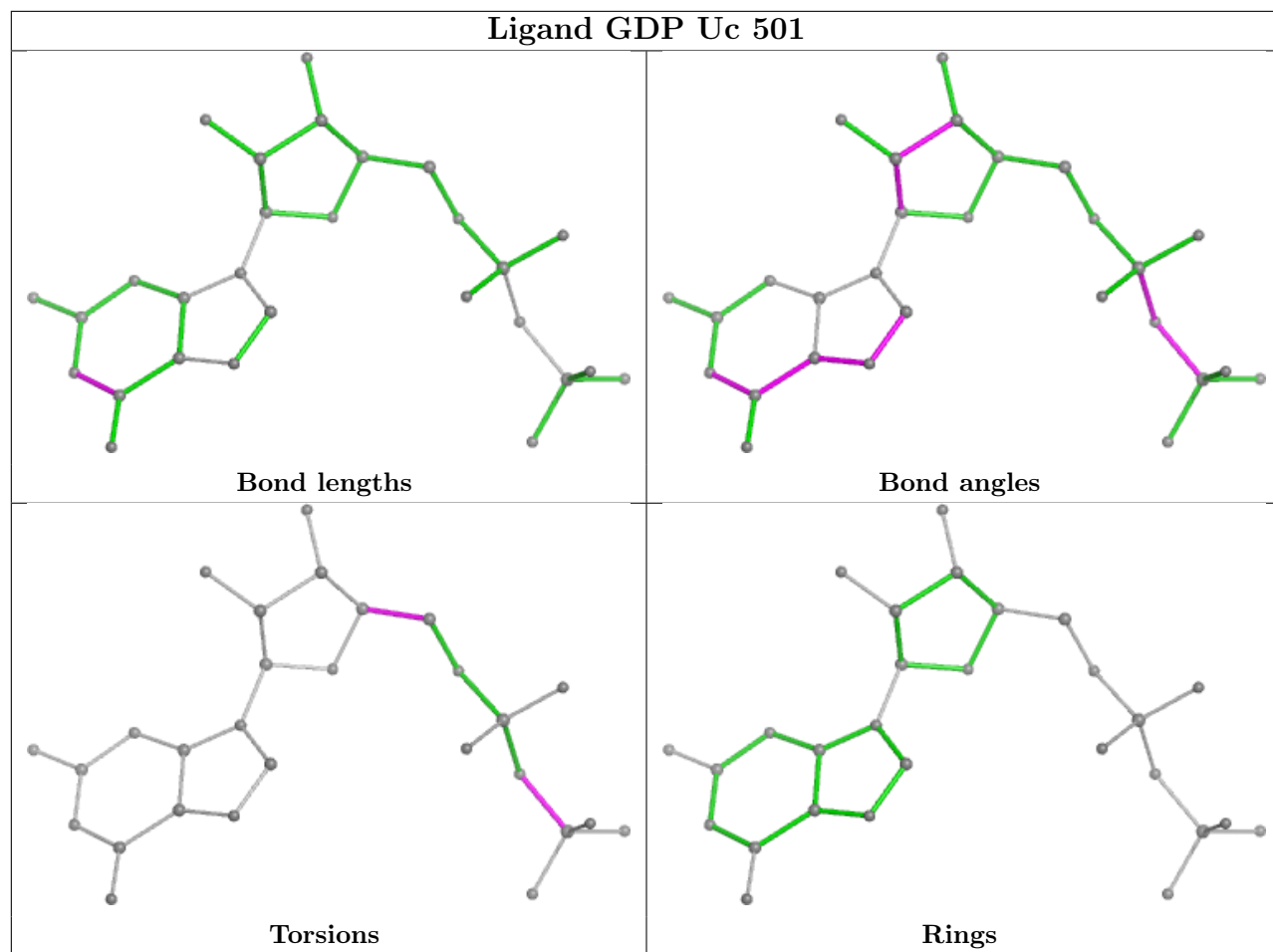




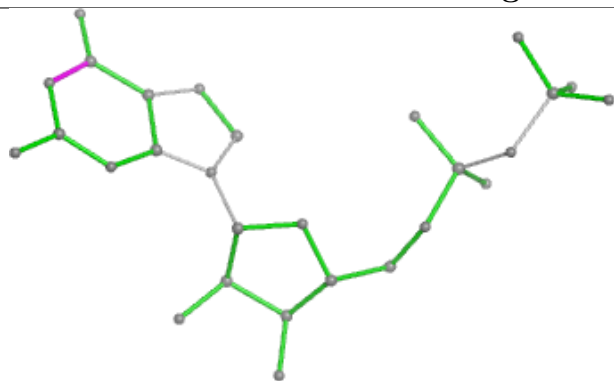




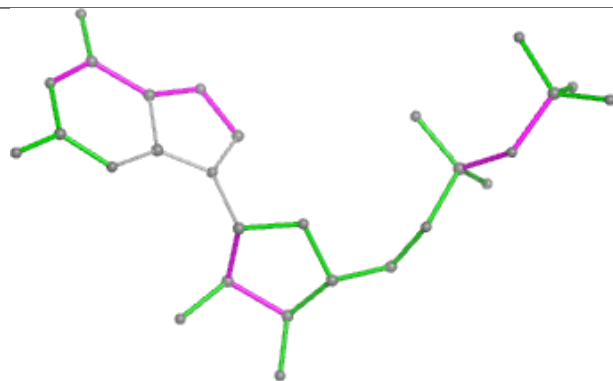




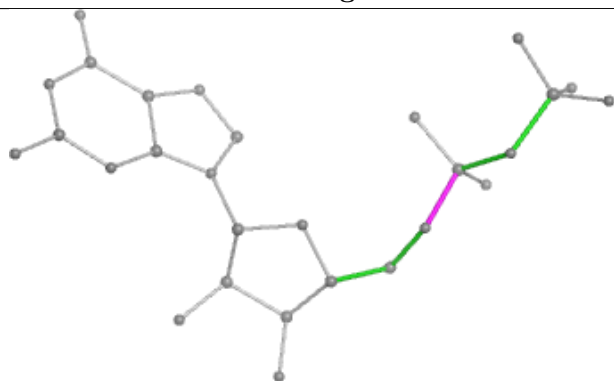
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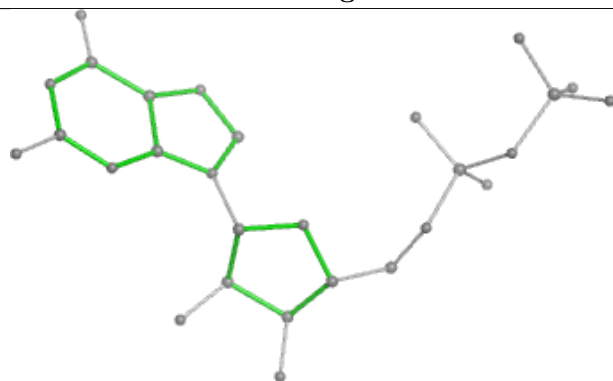
Bond lengths



Bond angles

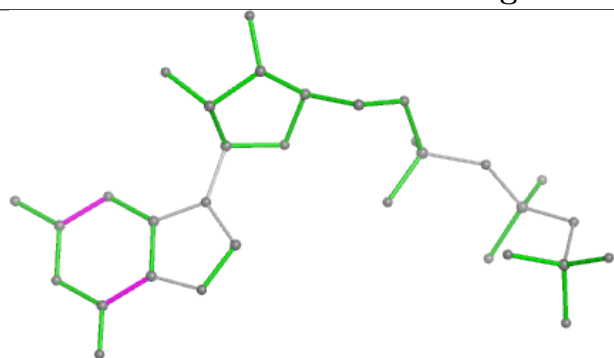


Torsions

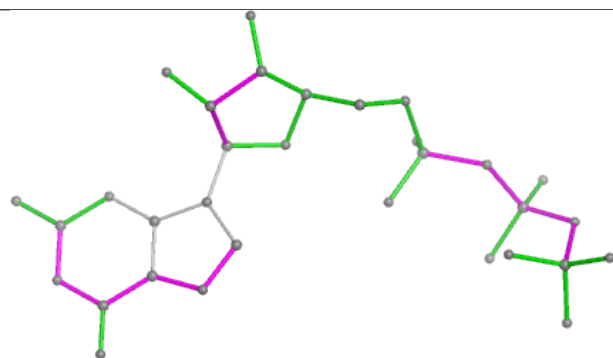


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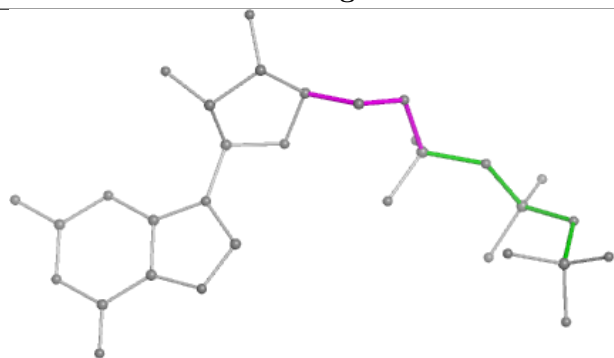
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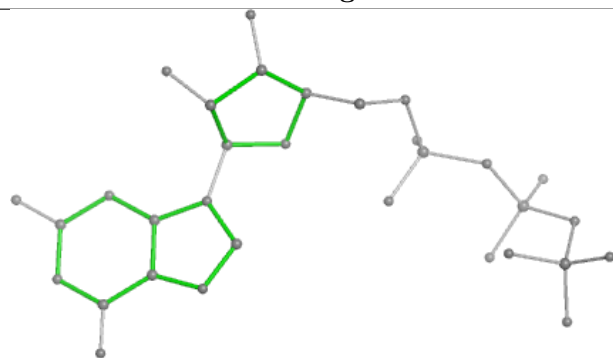
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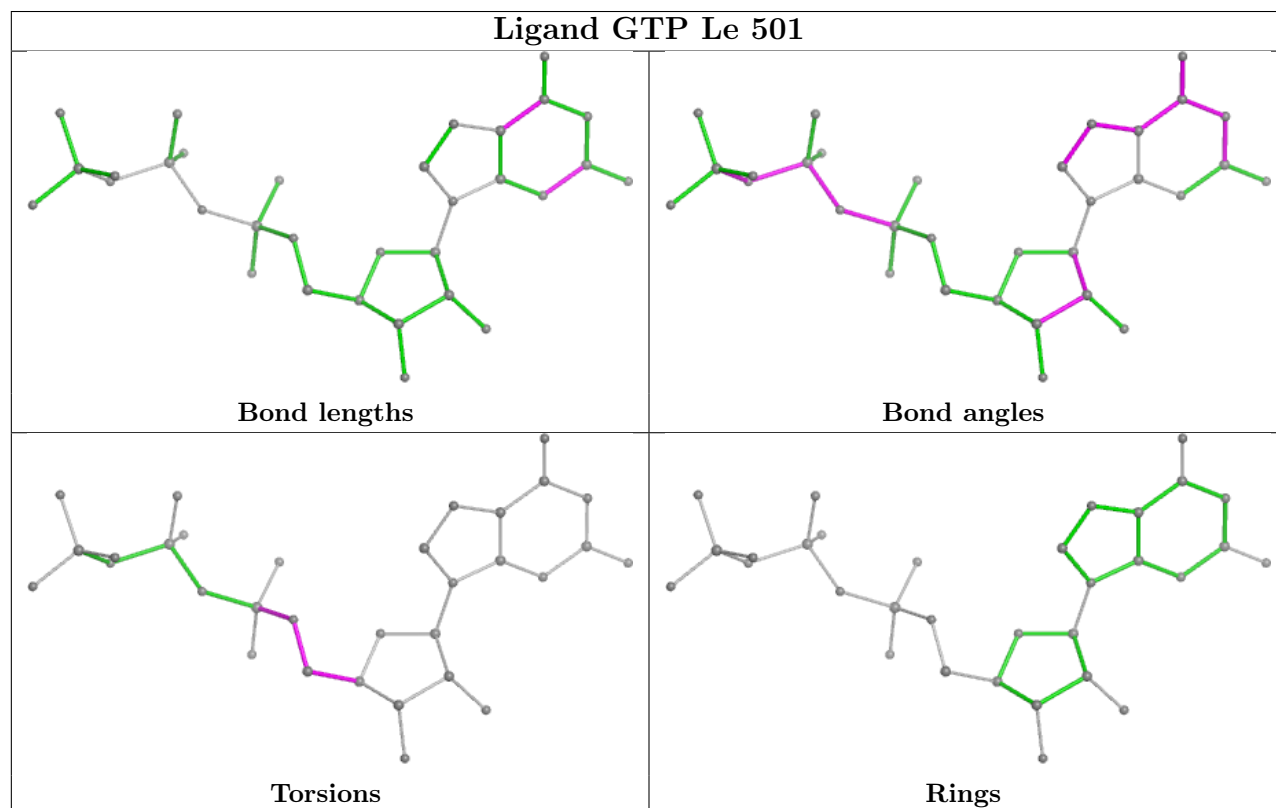
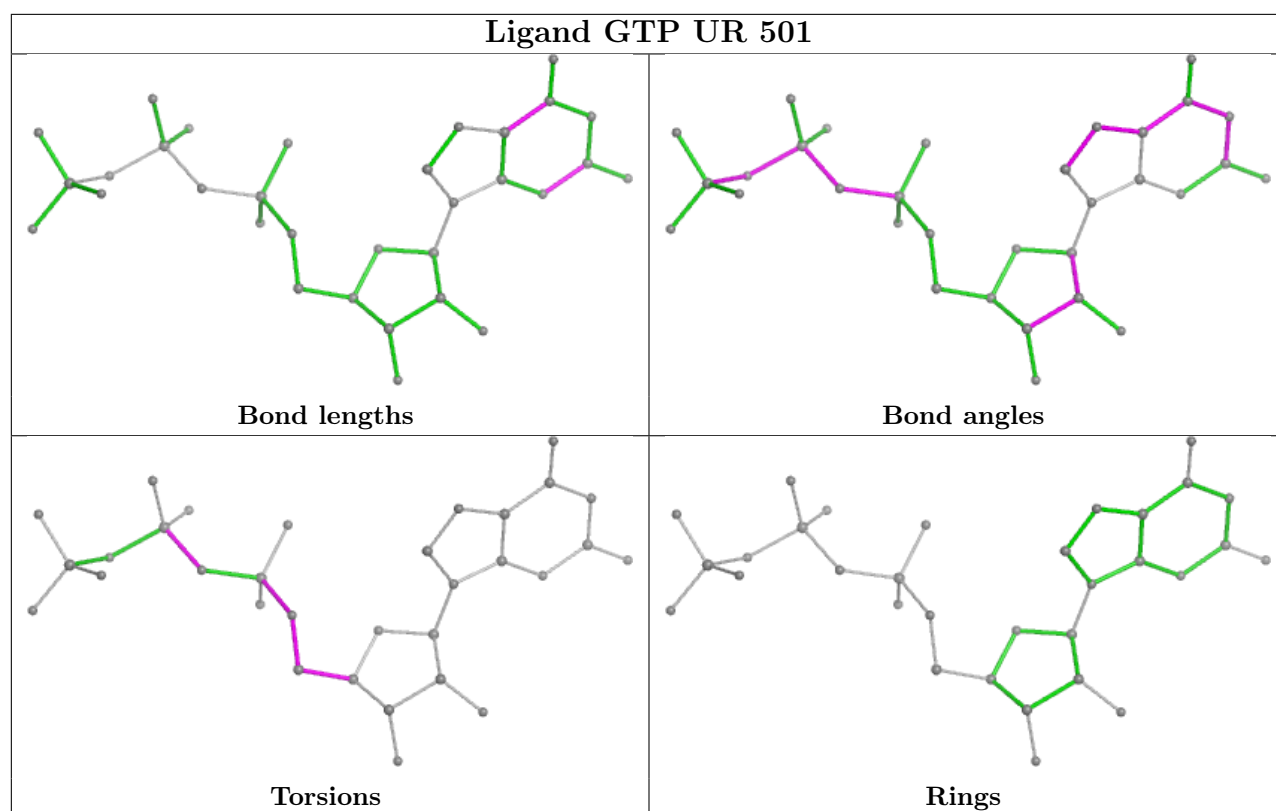
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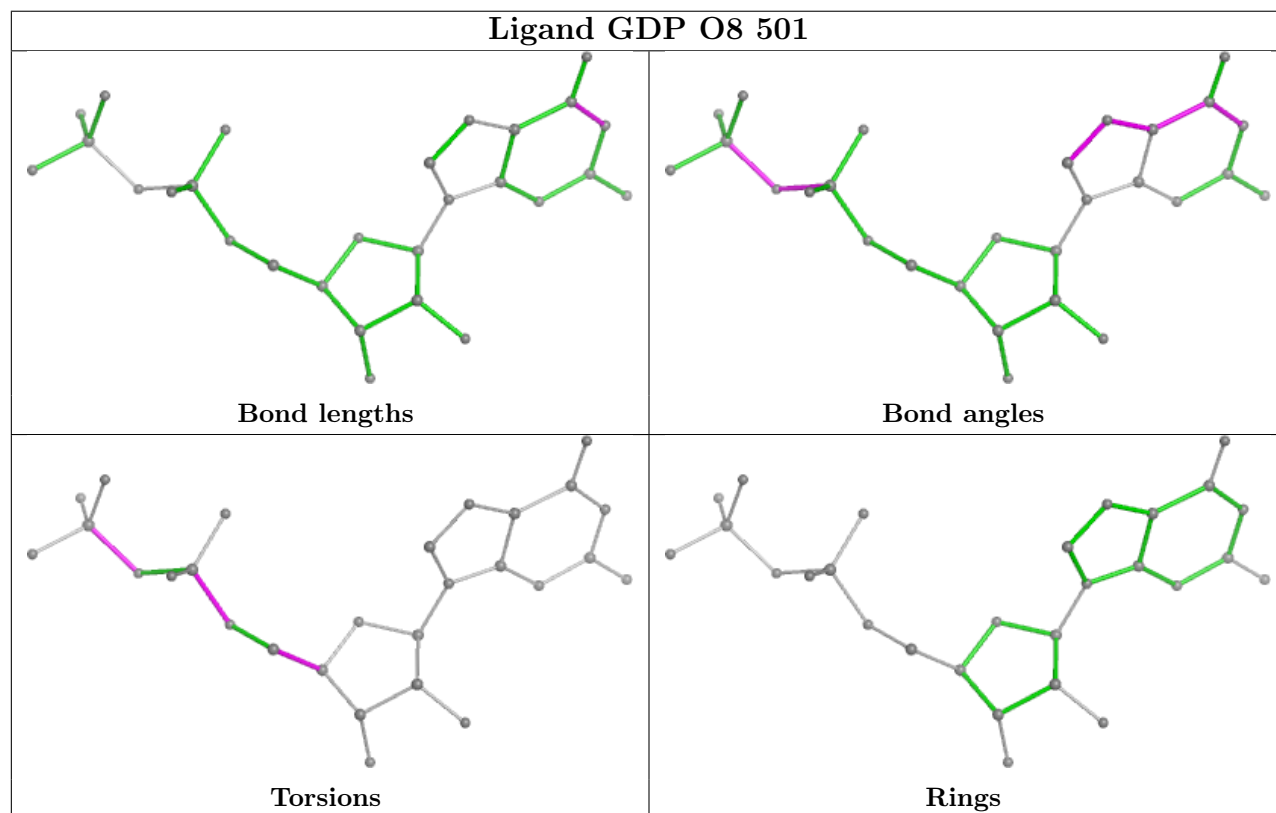
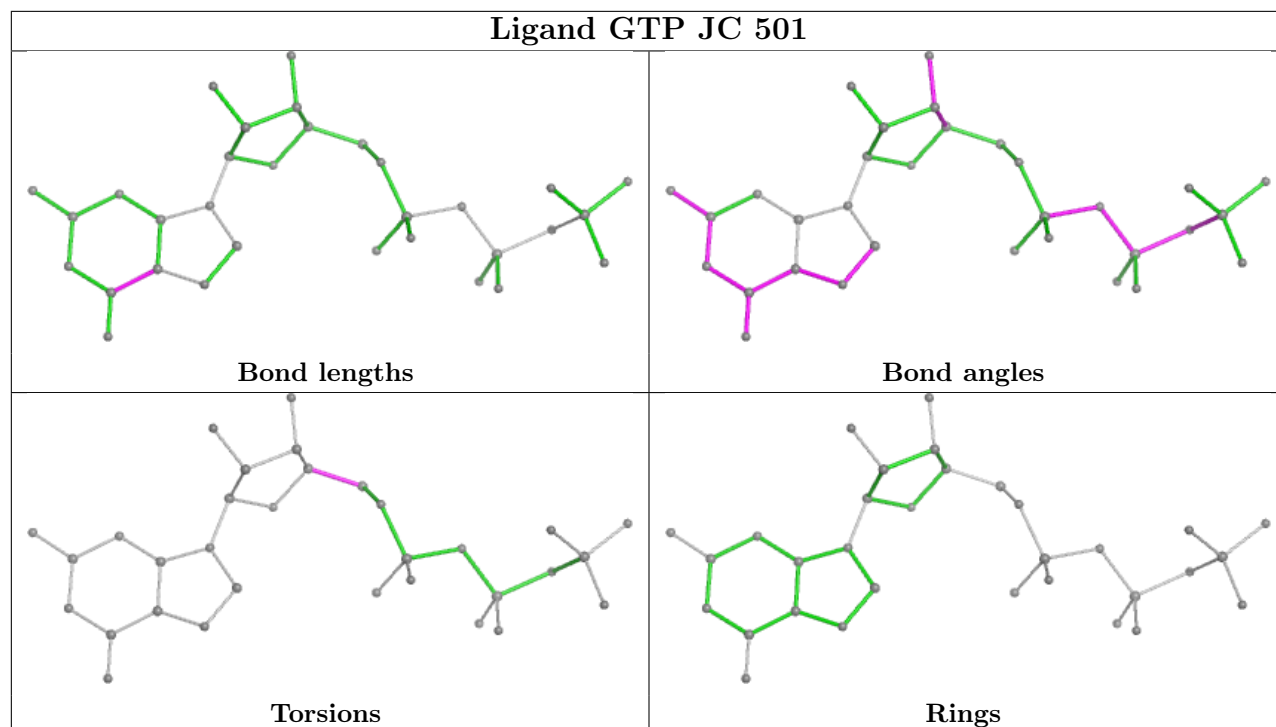


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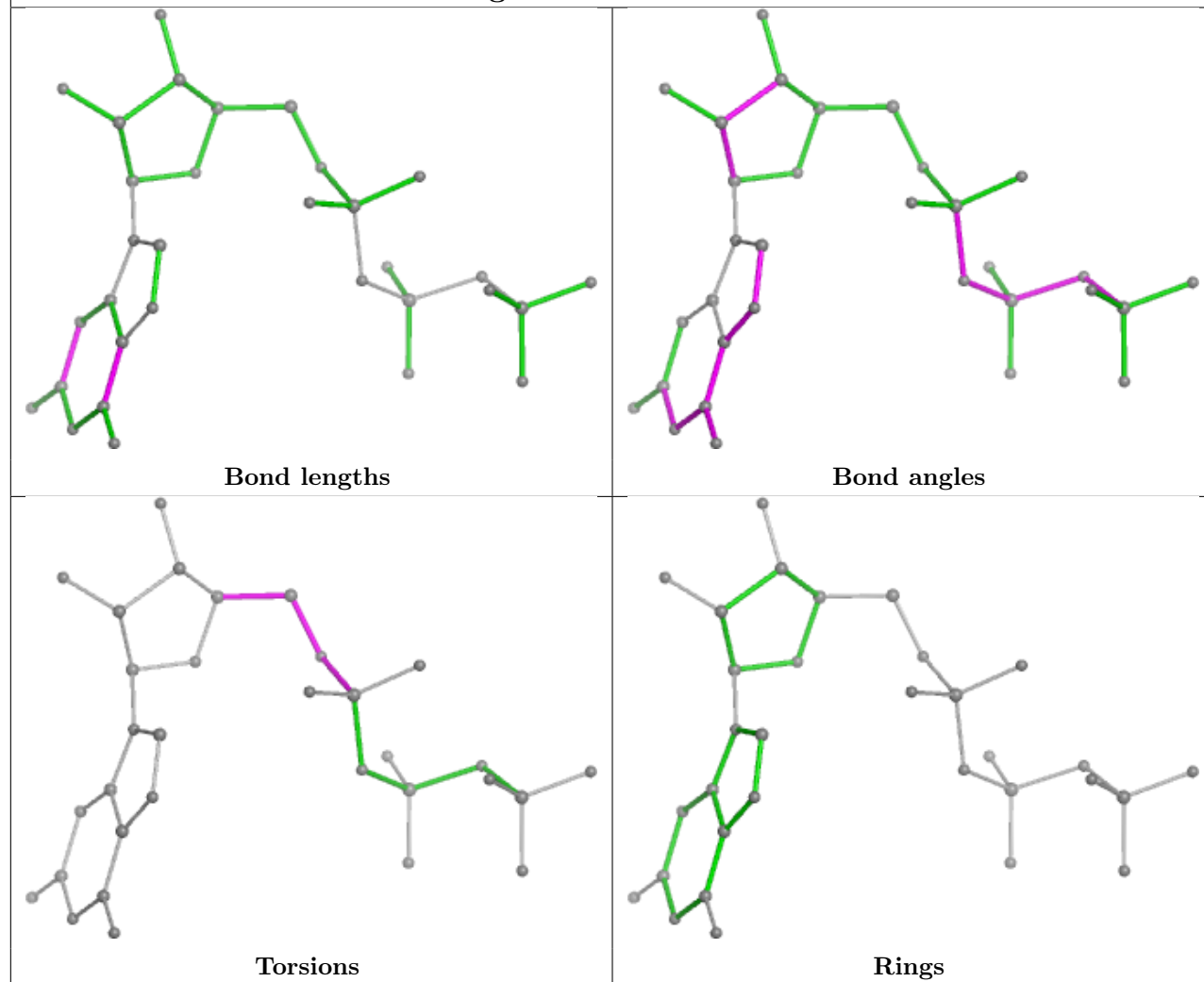


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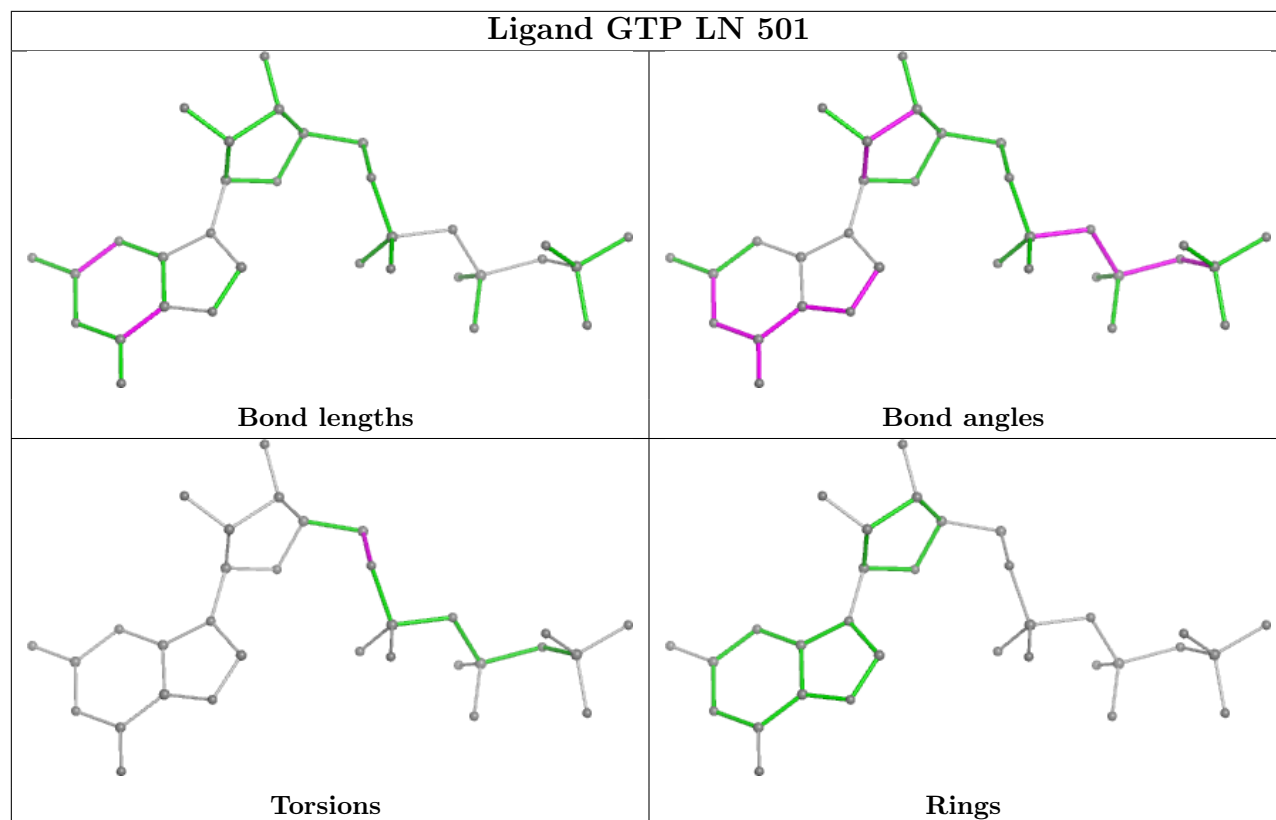




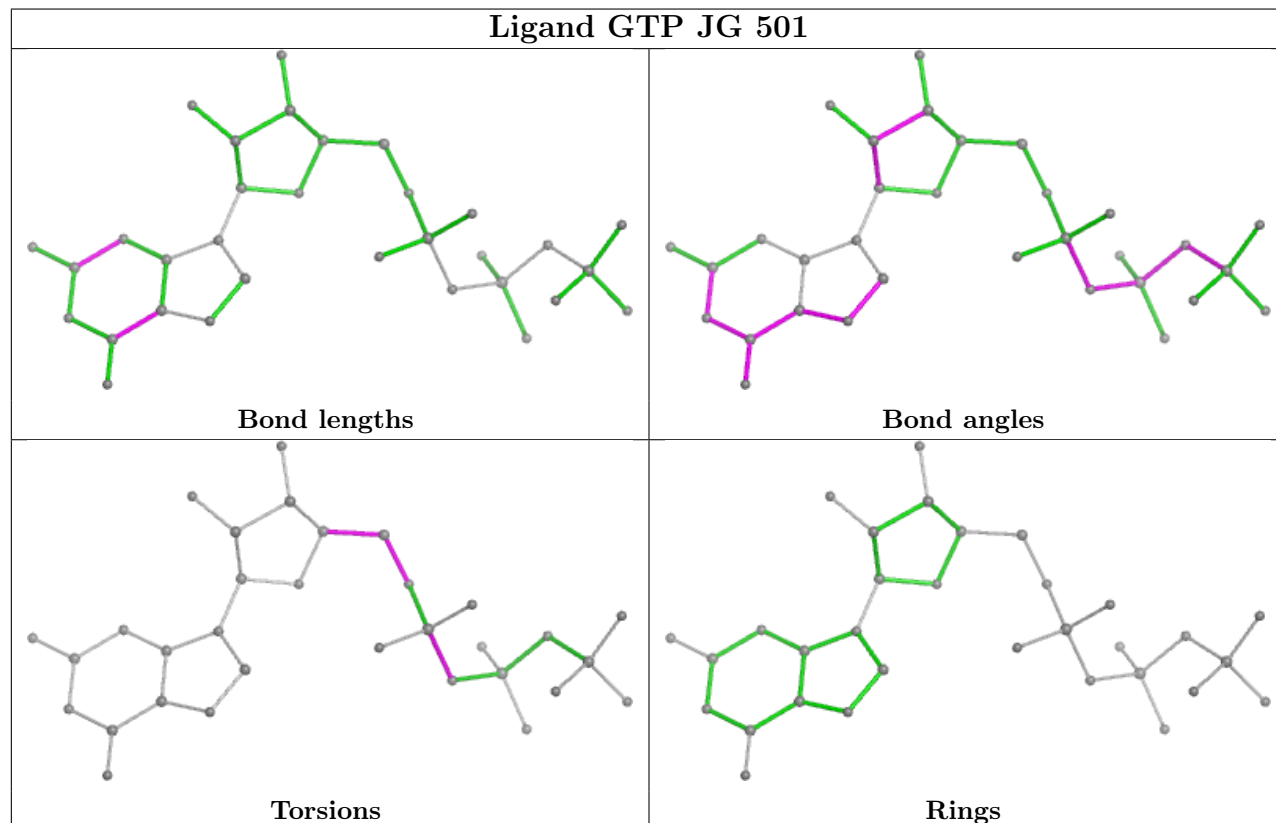
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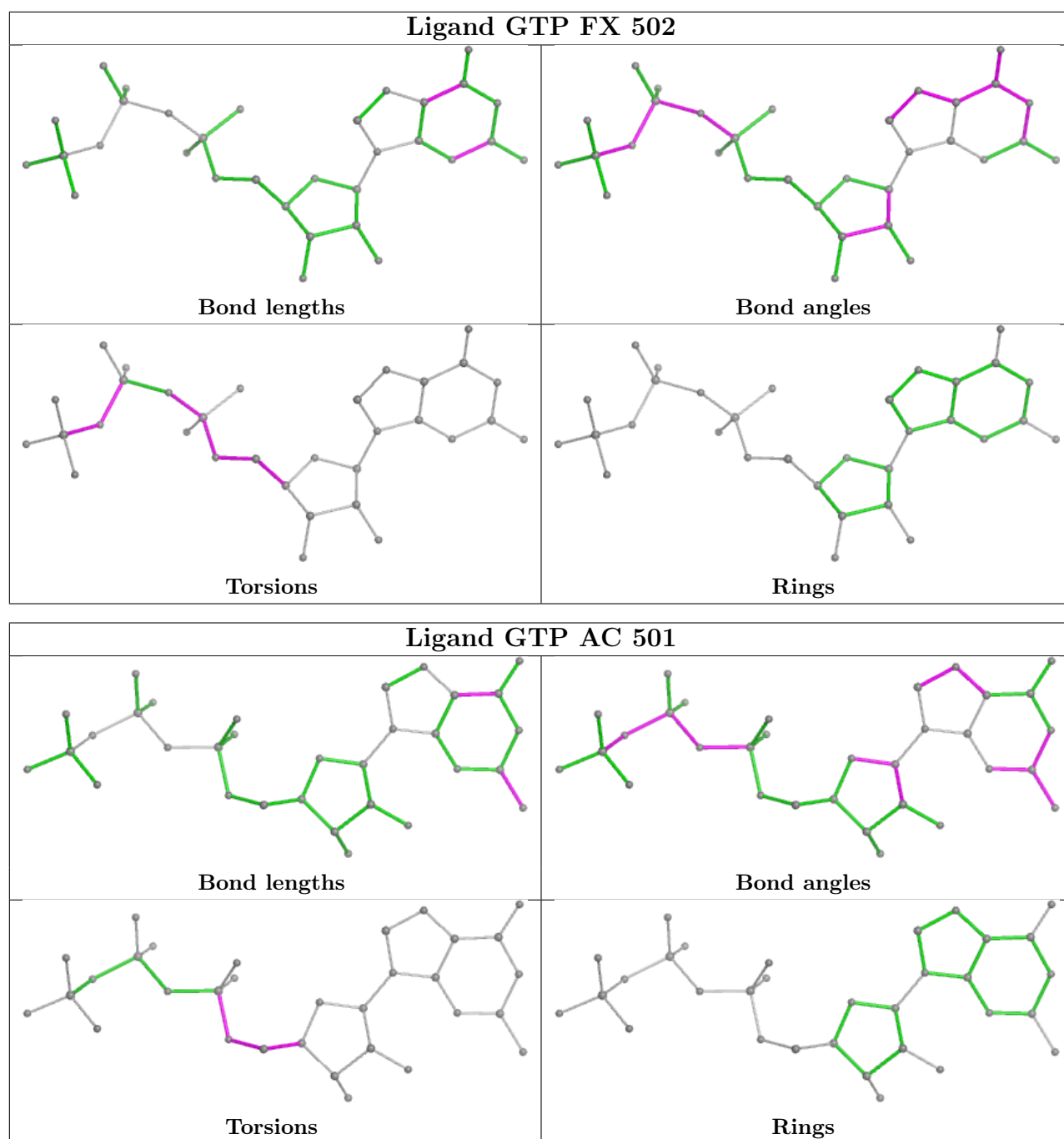


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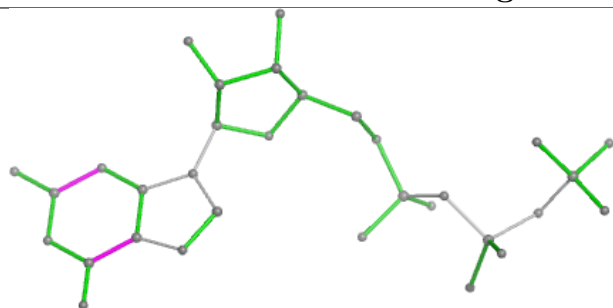
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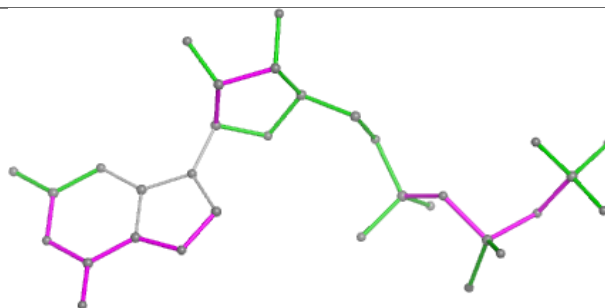




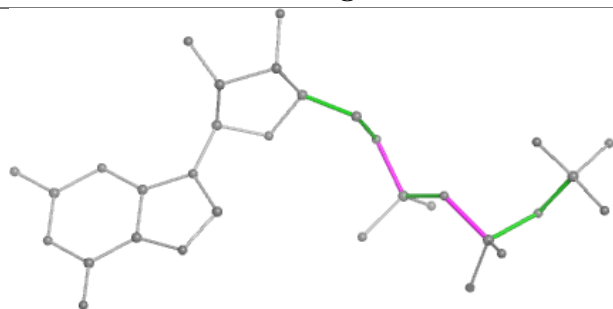
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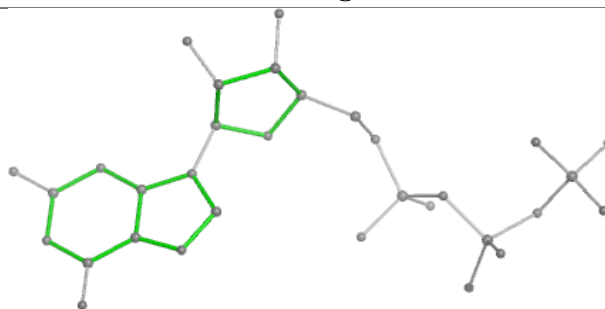
Bond lengths



Bond angles

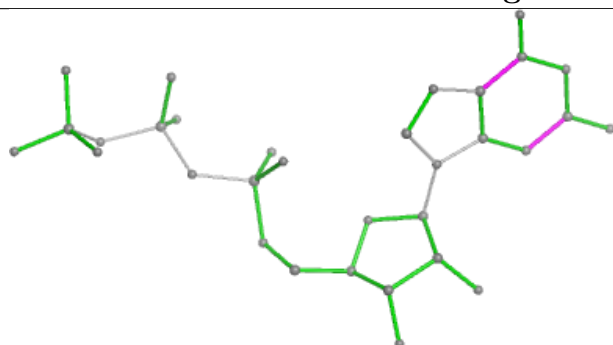


Torsions

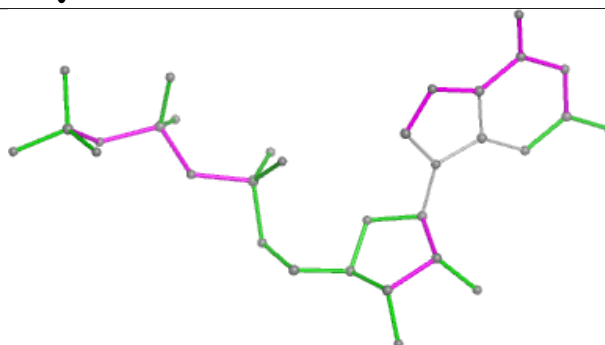


Rings

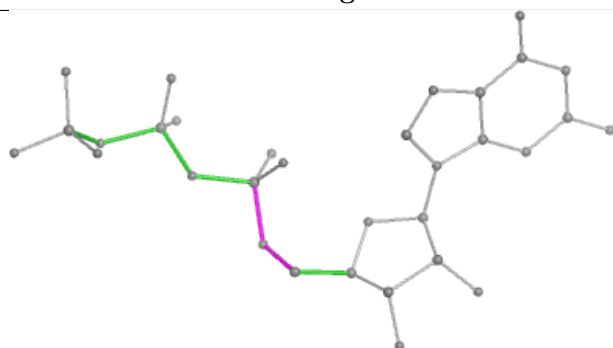
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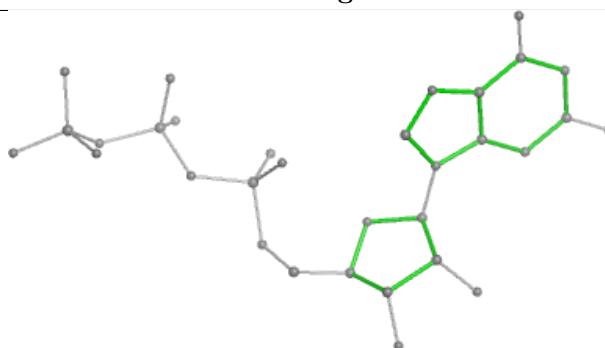
Bond lengths



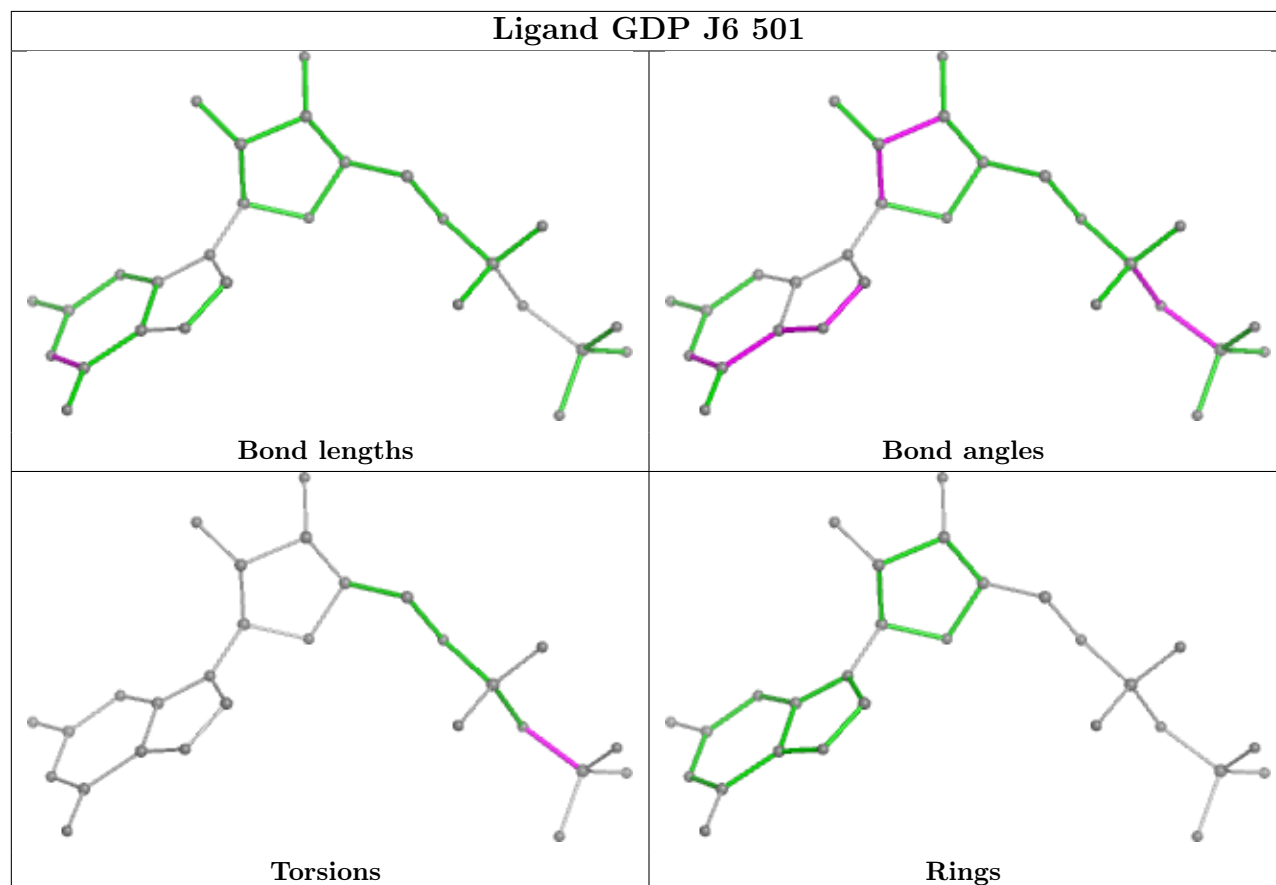
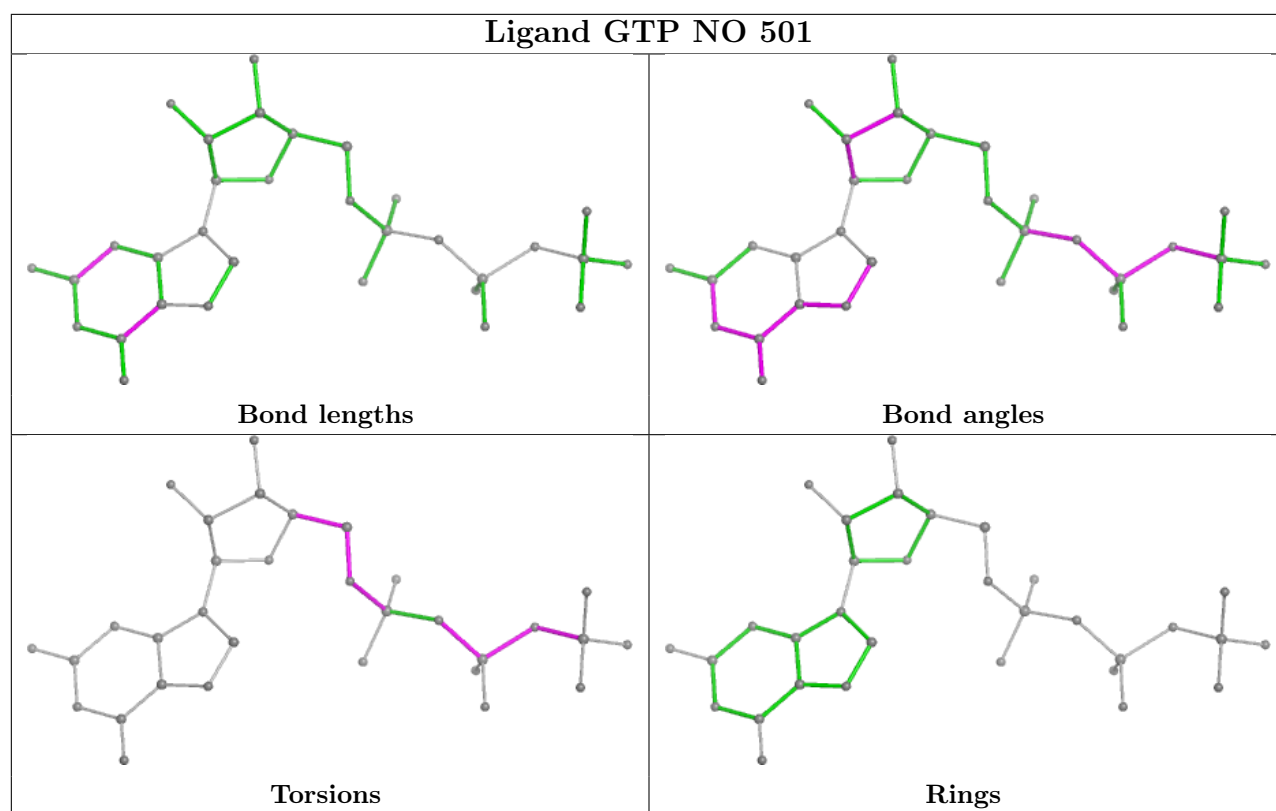
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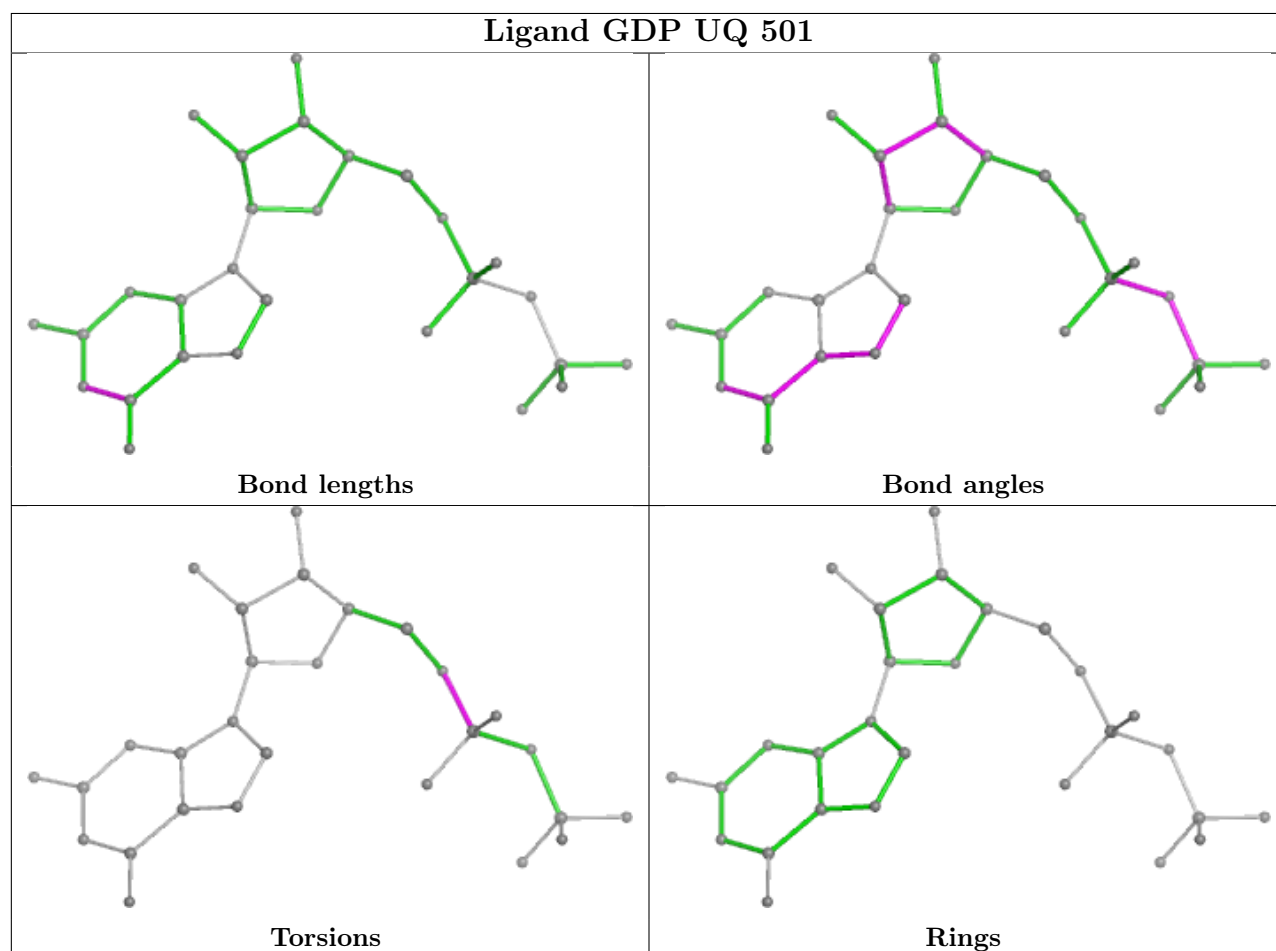
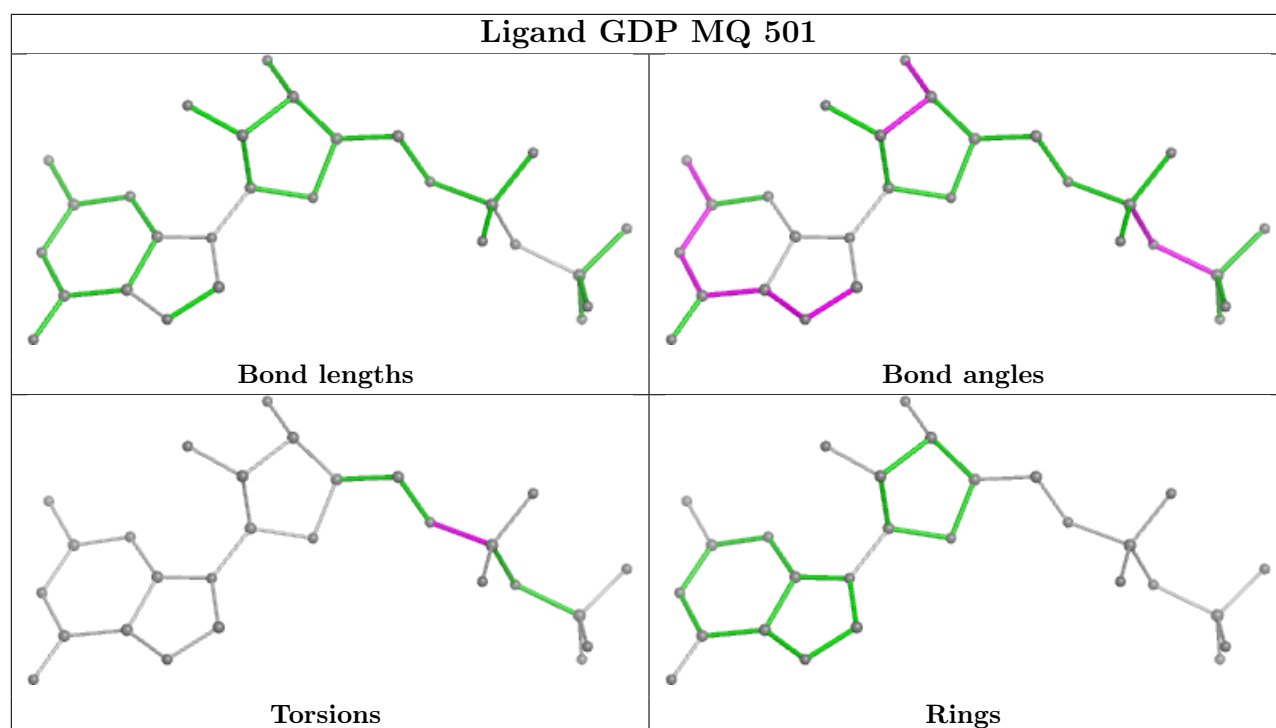


Torsions

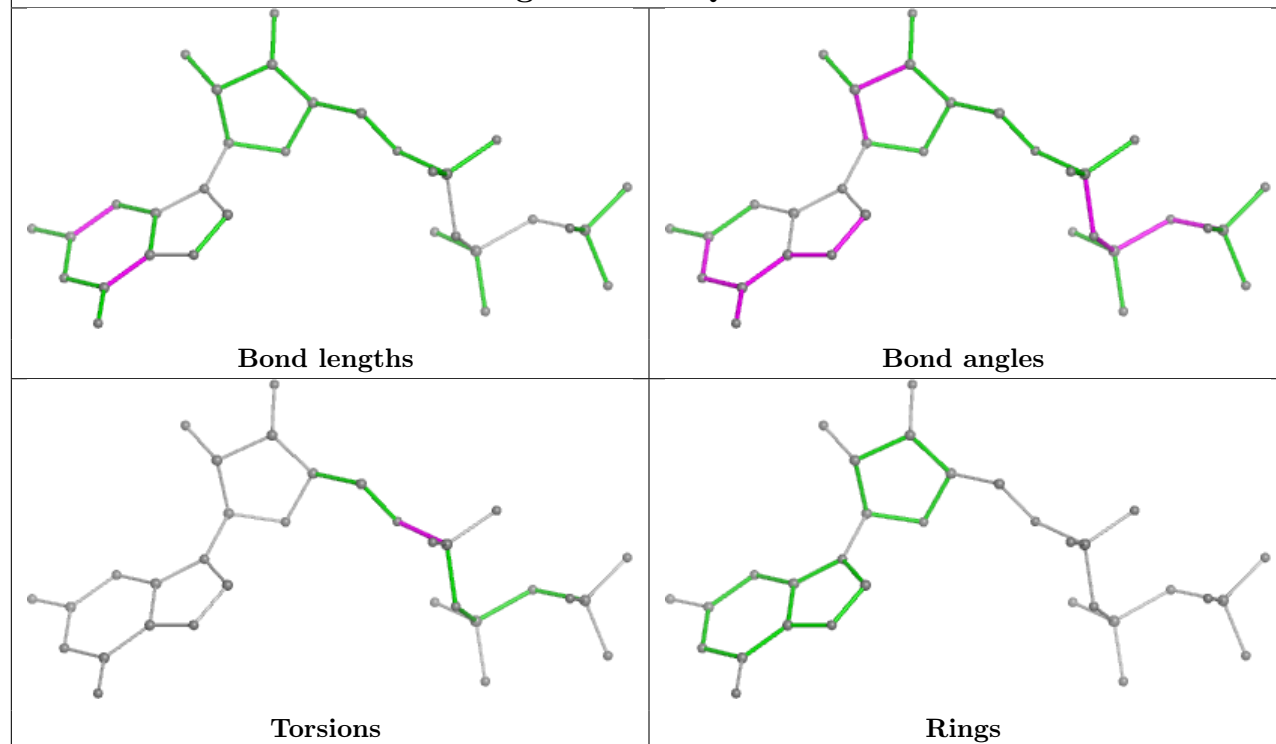


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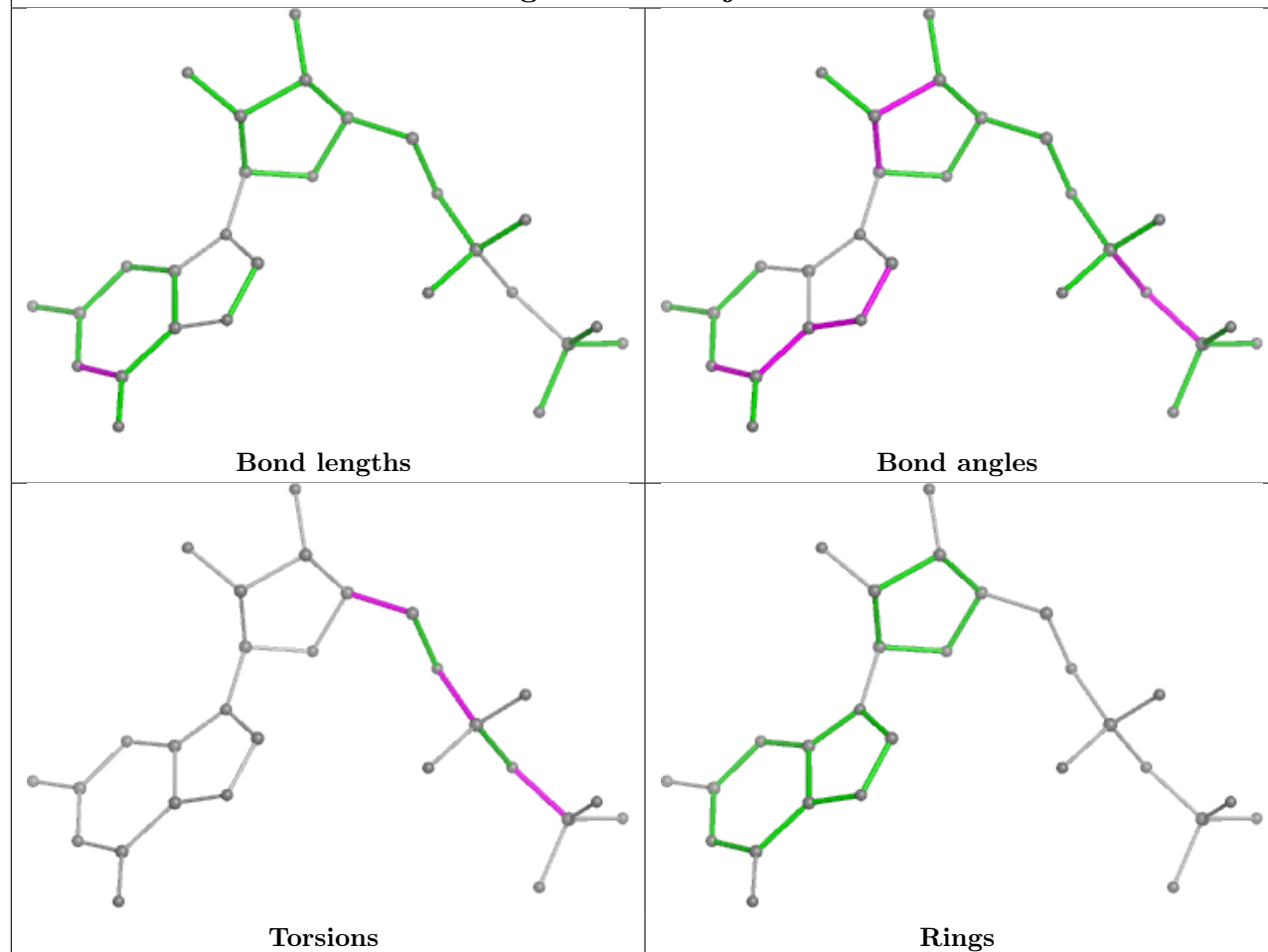


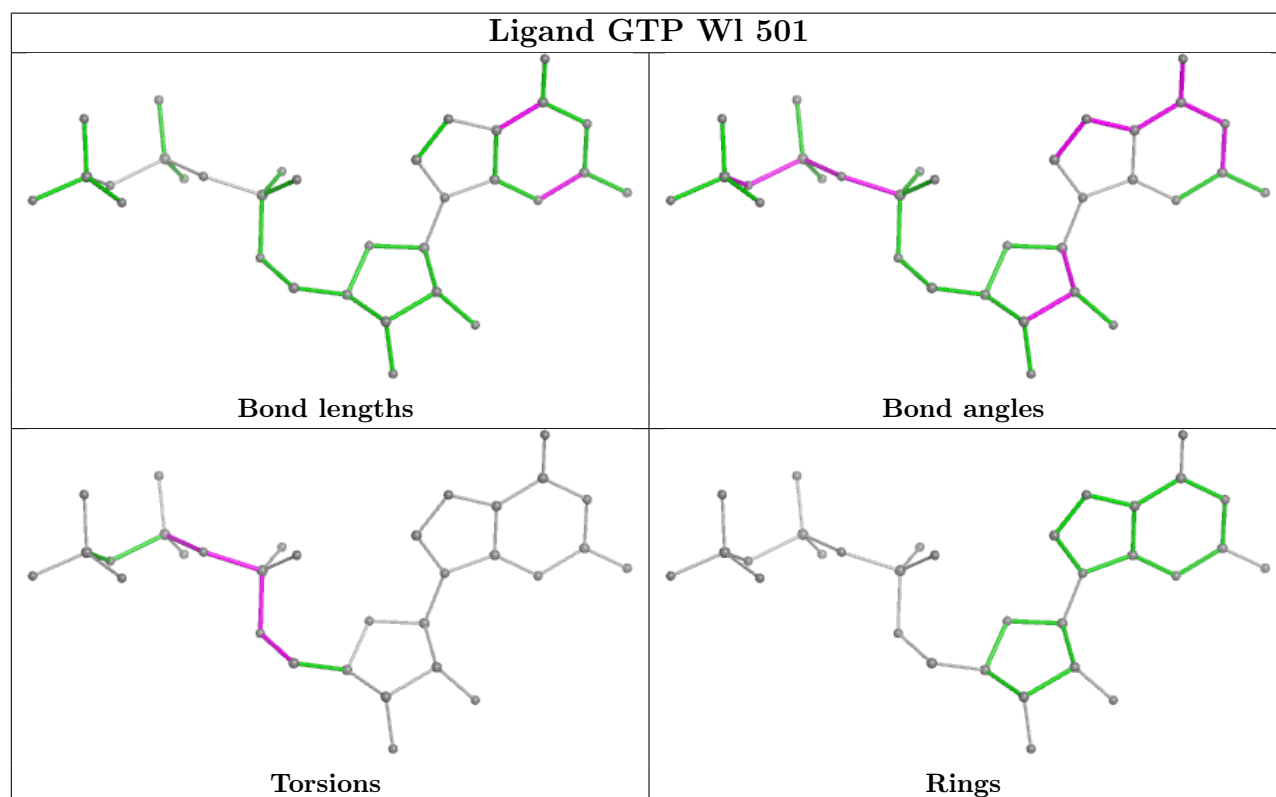
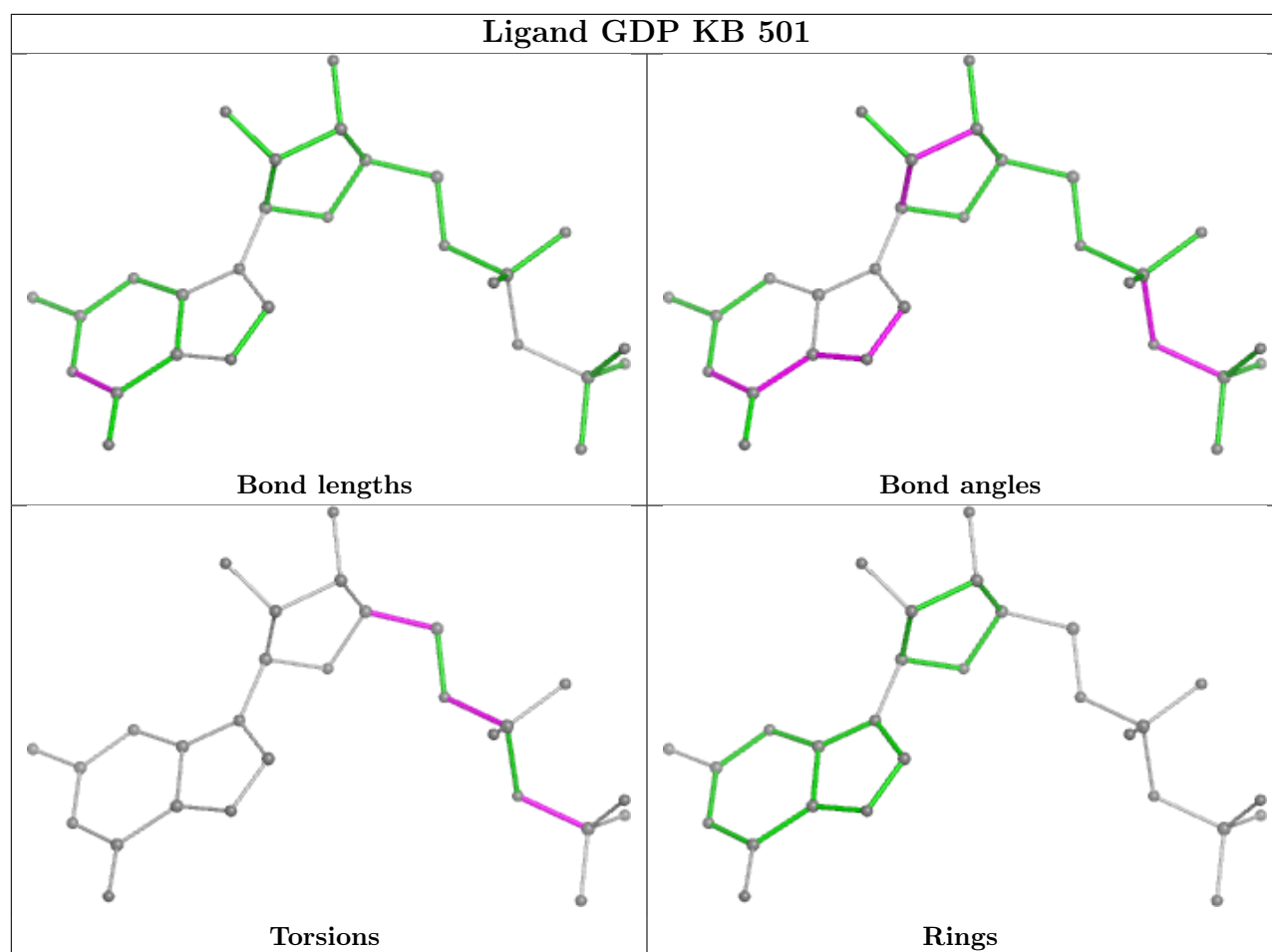


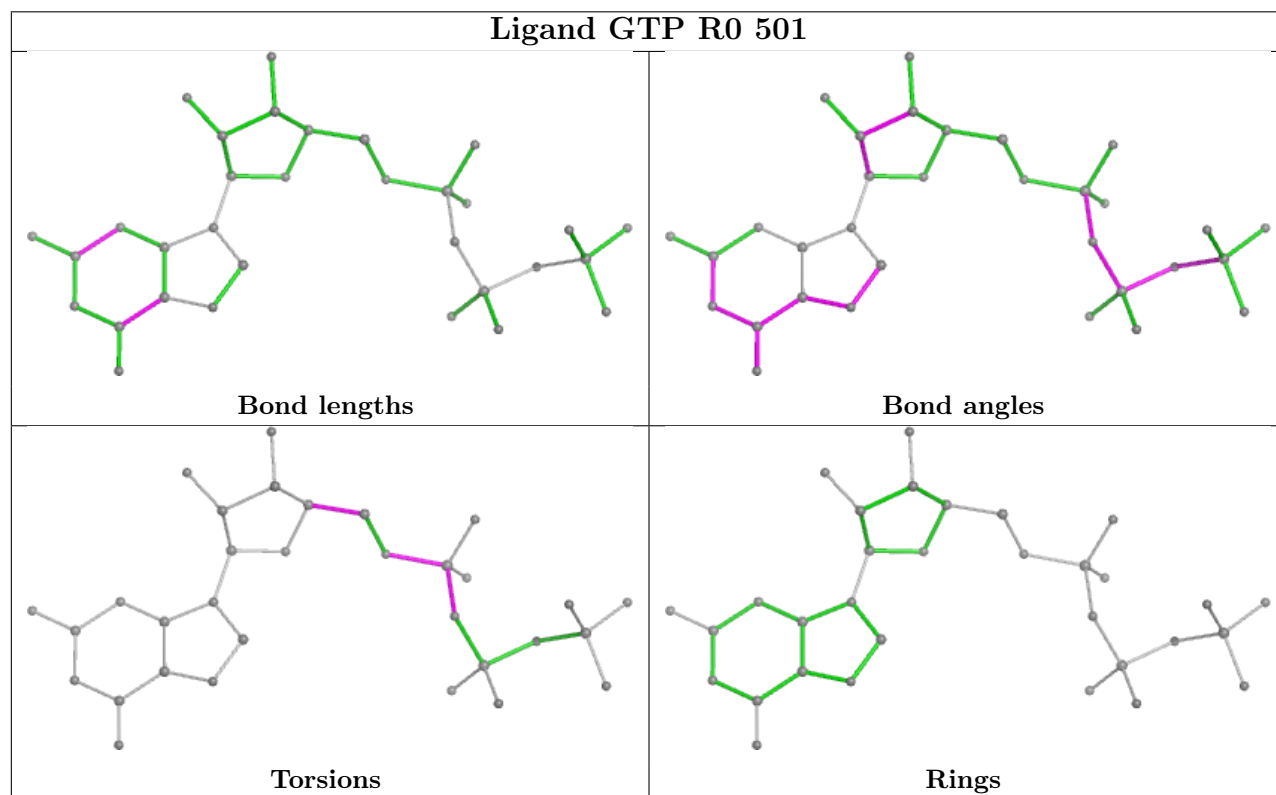
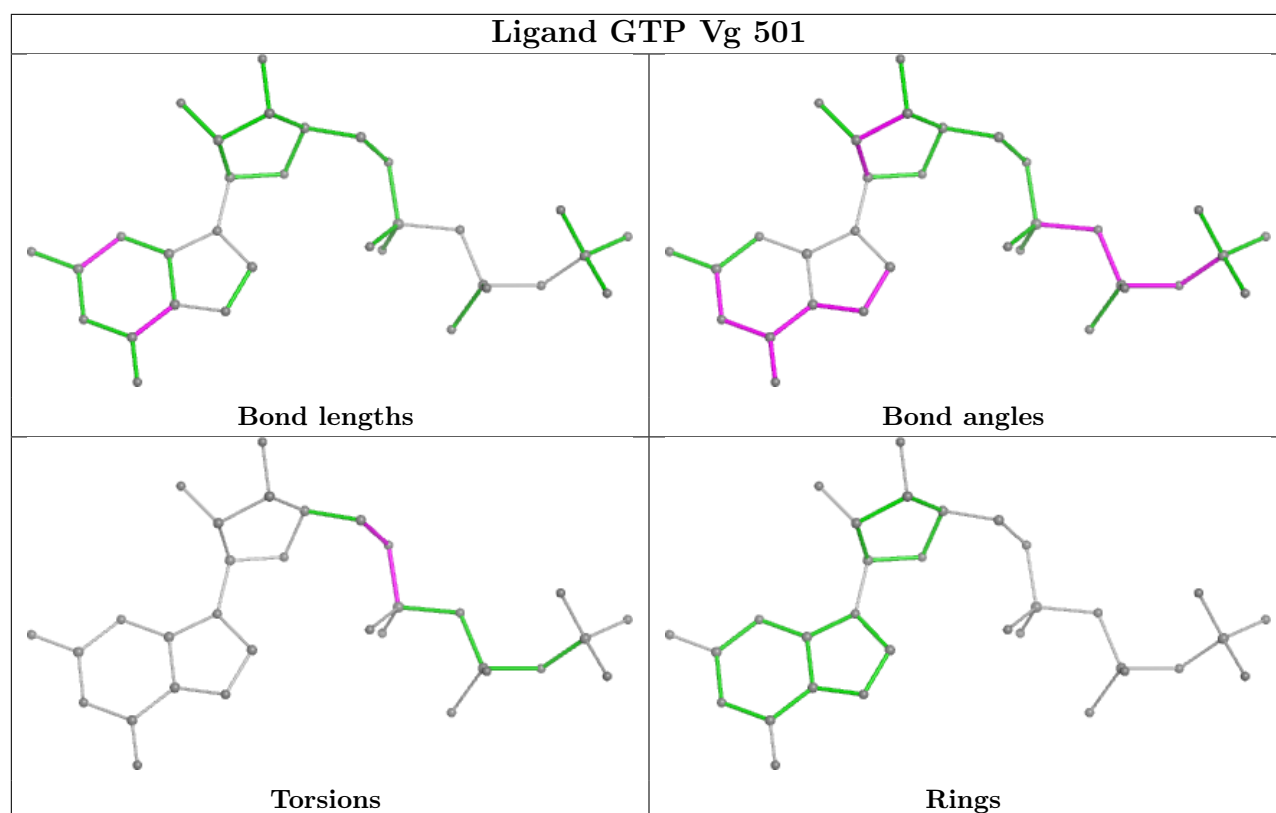
## Ligand GTP QG 501



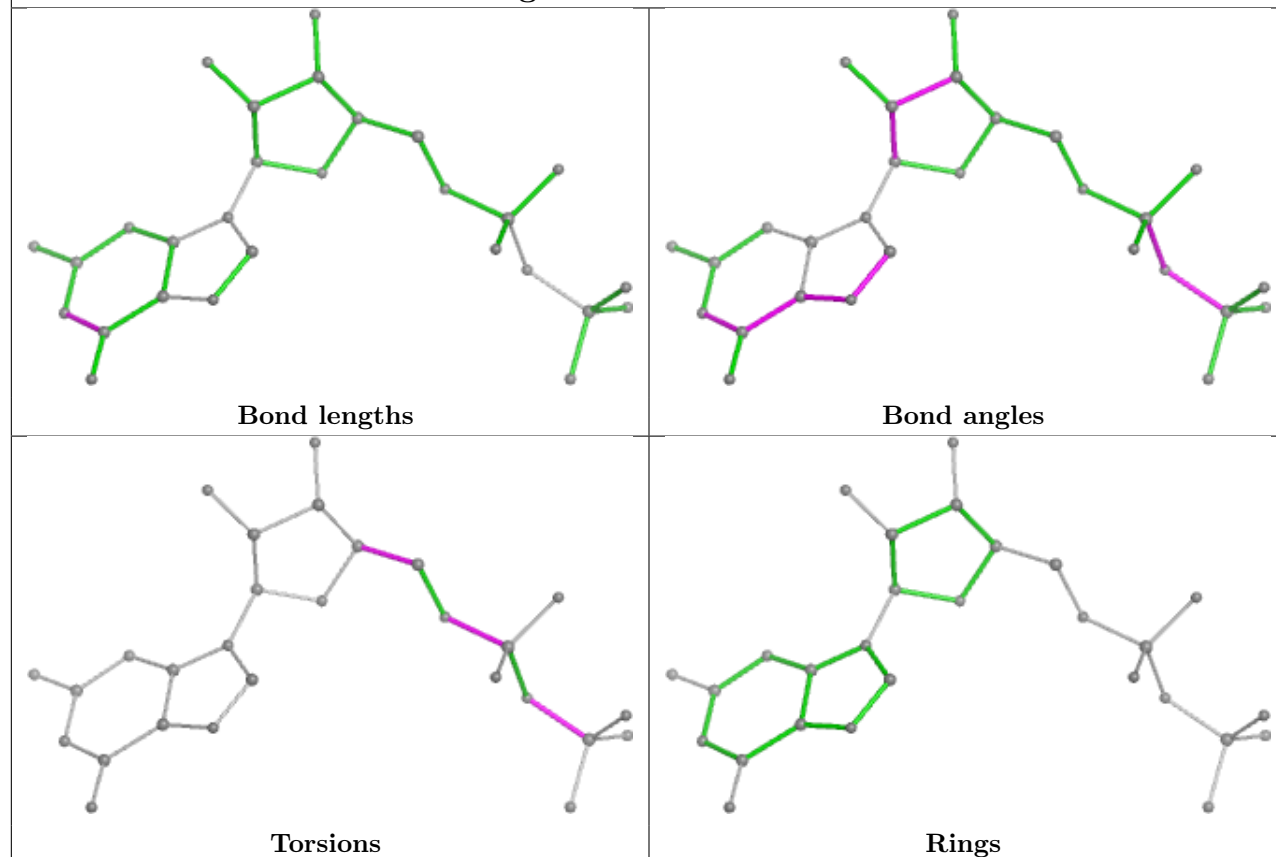
## Ligand GDP Vj 501



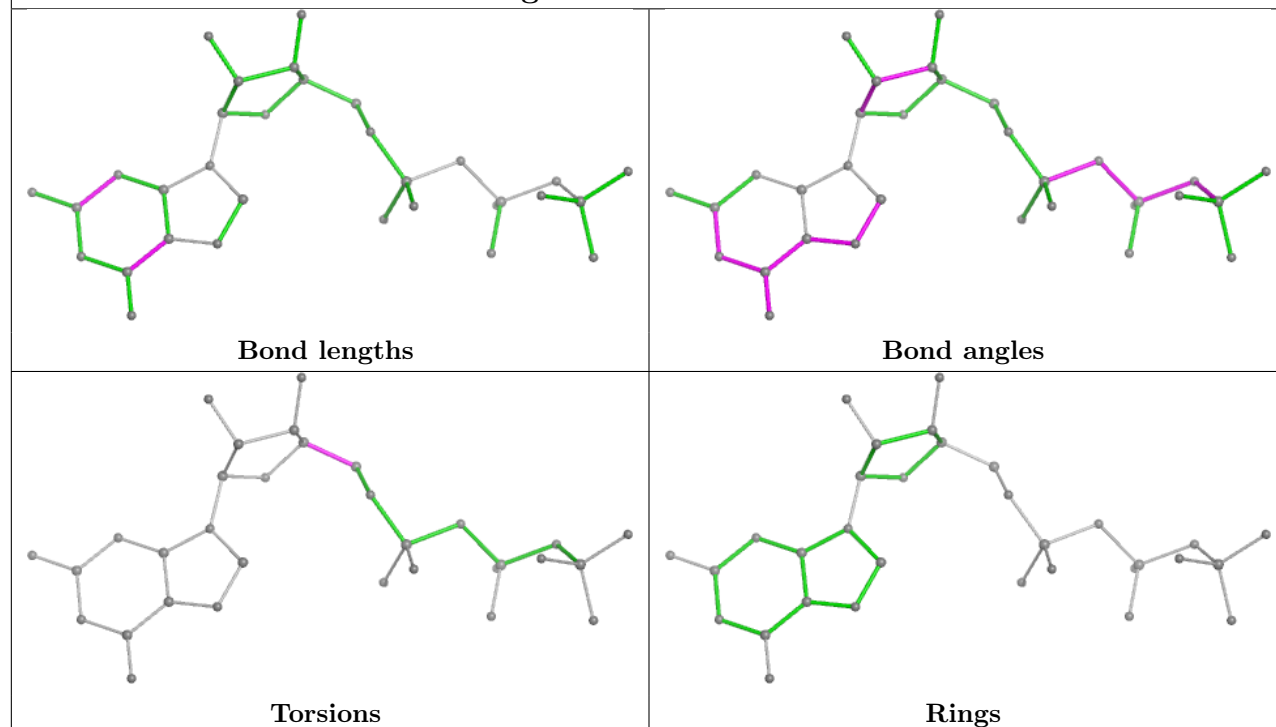


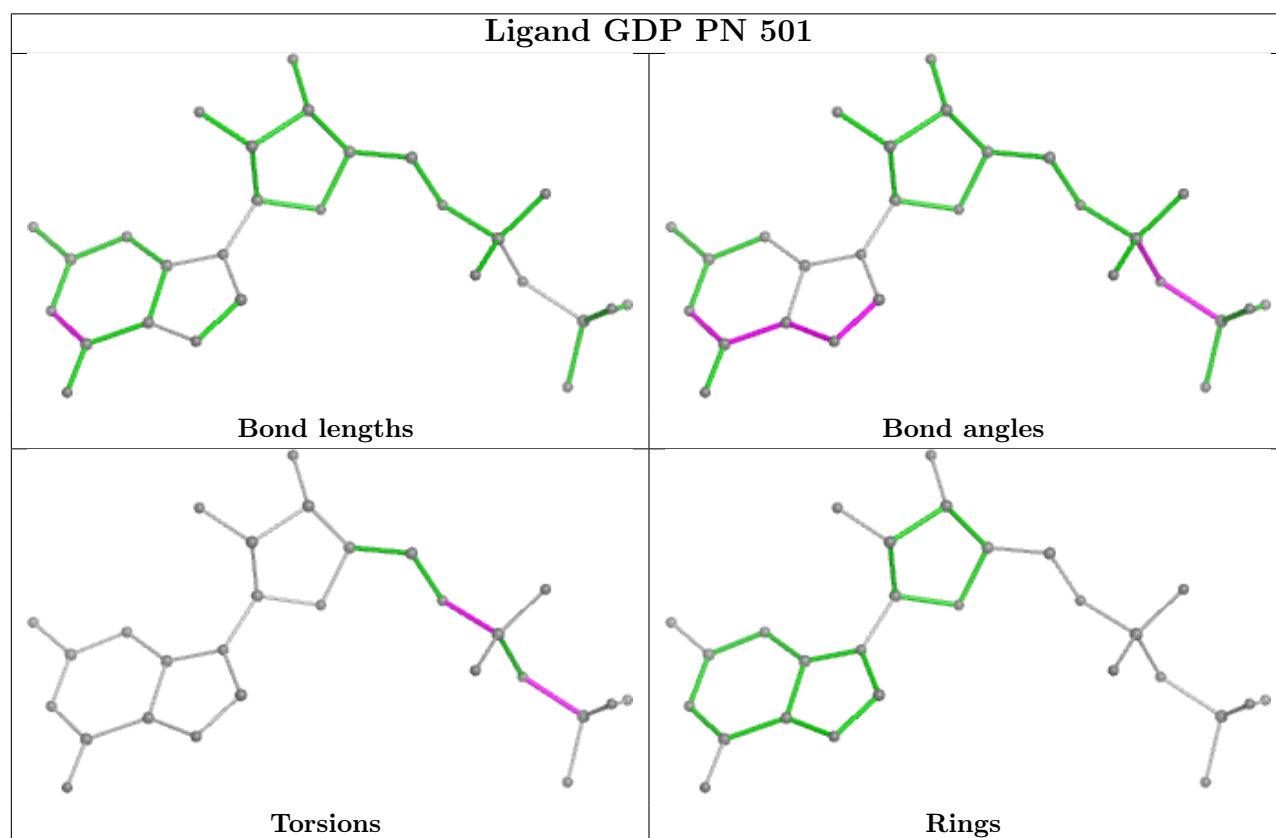
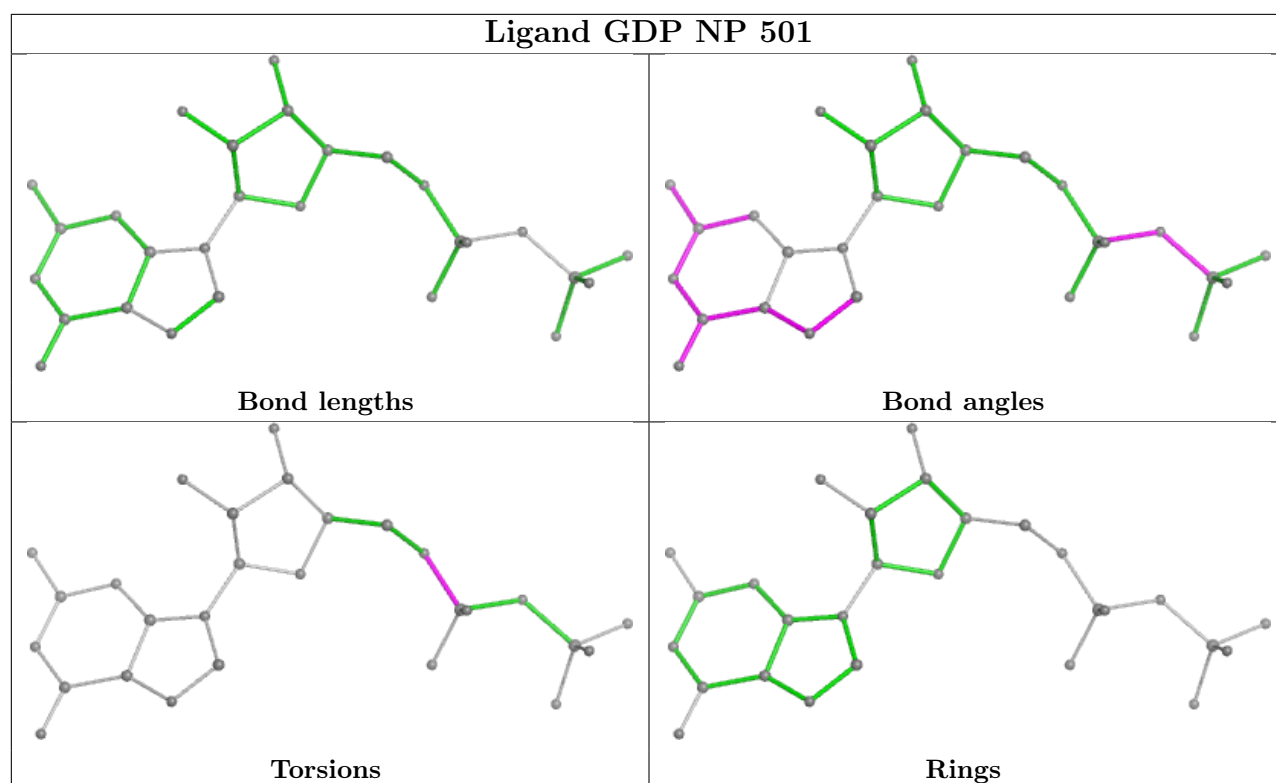


## Ligand GDP JN 501



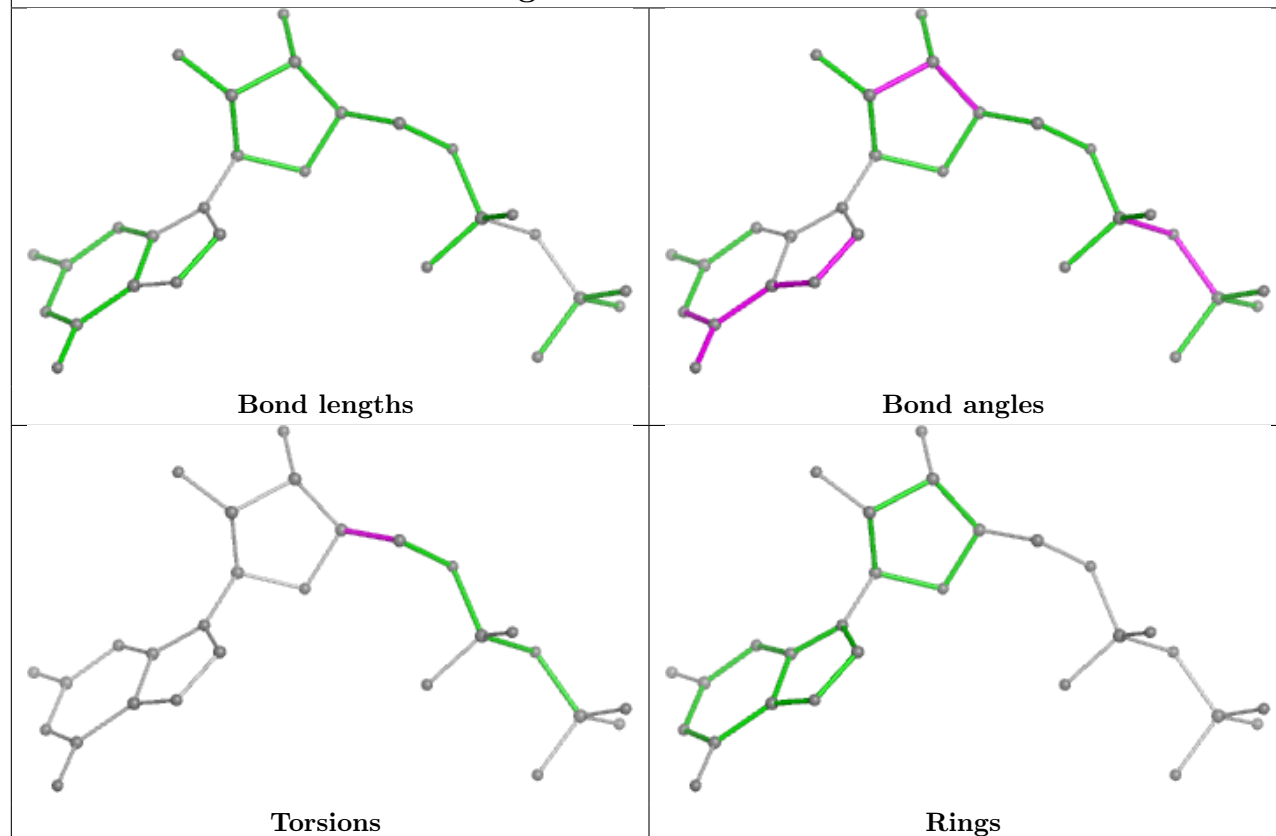
## Ligand GTP R6 502



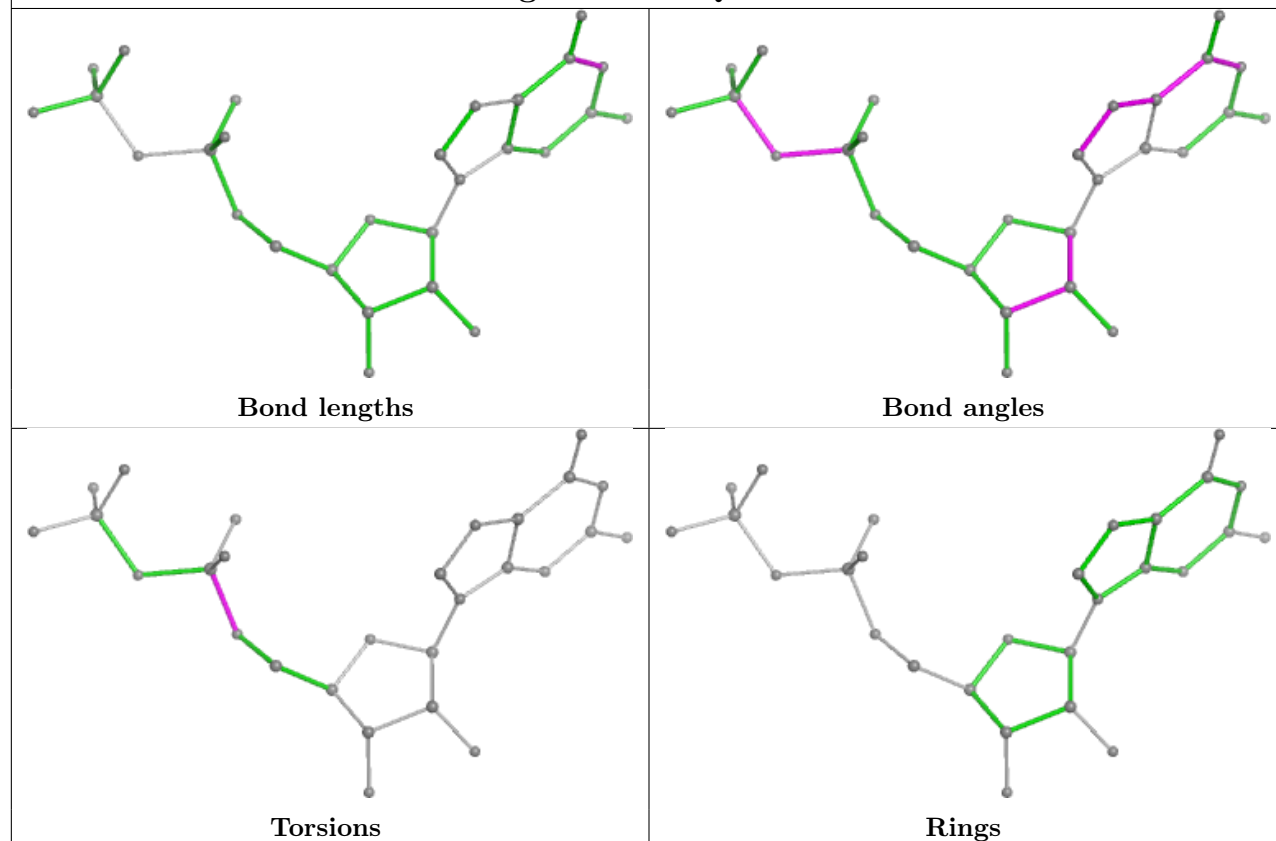


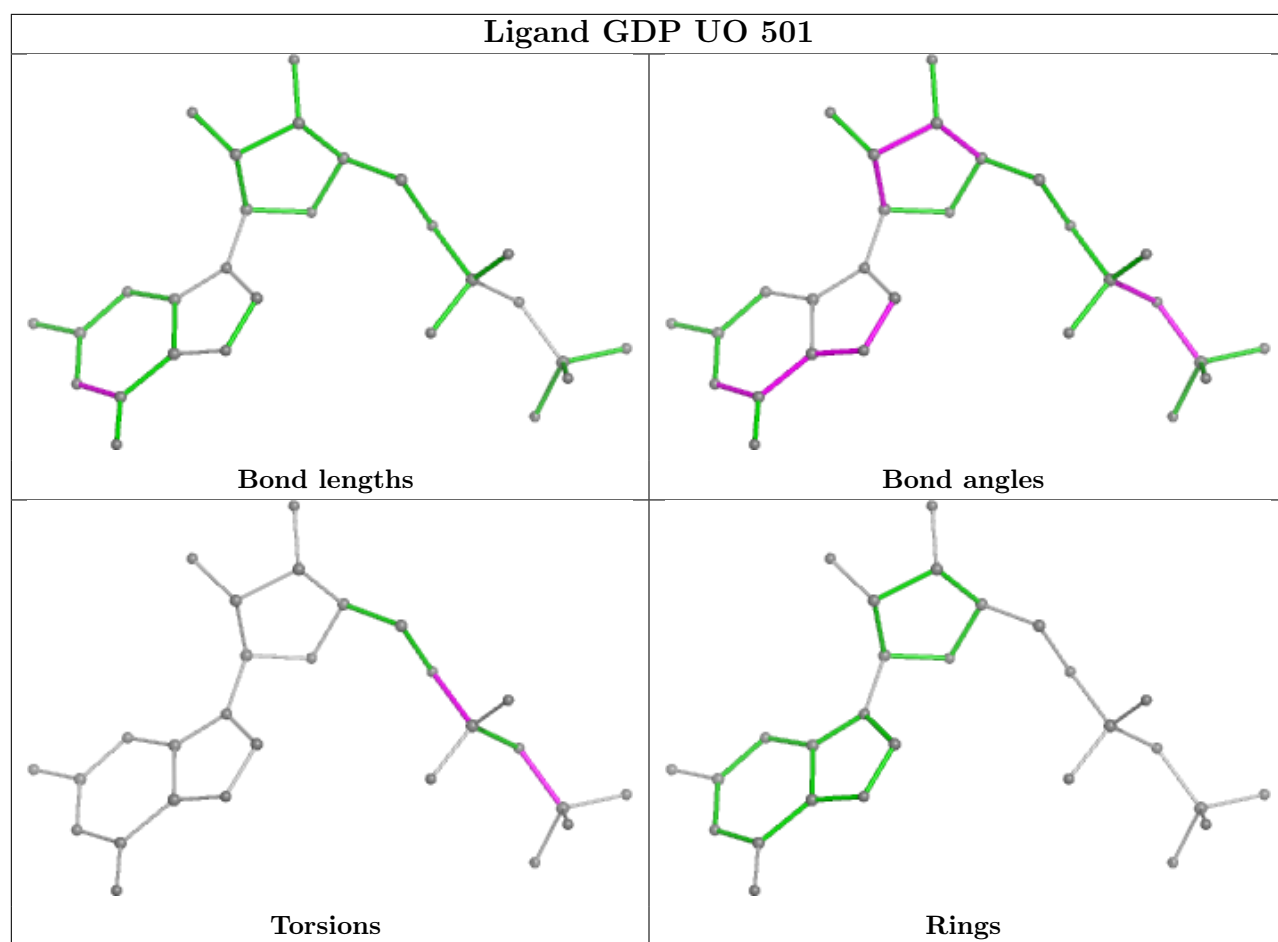


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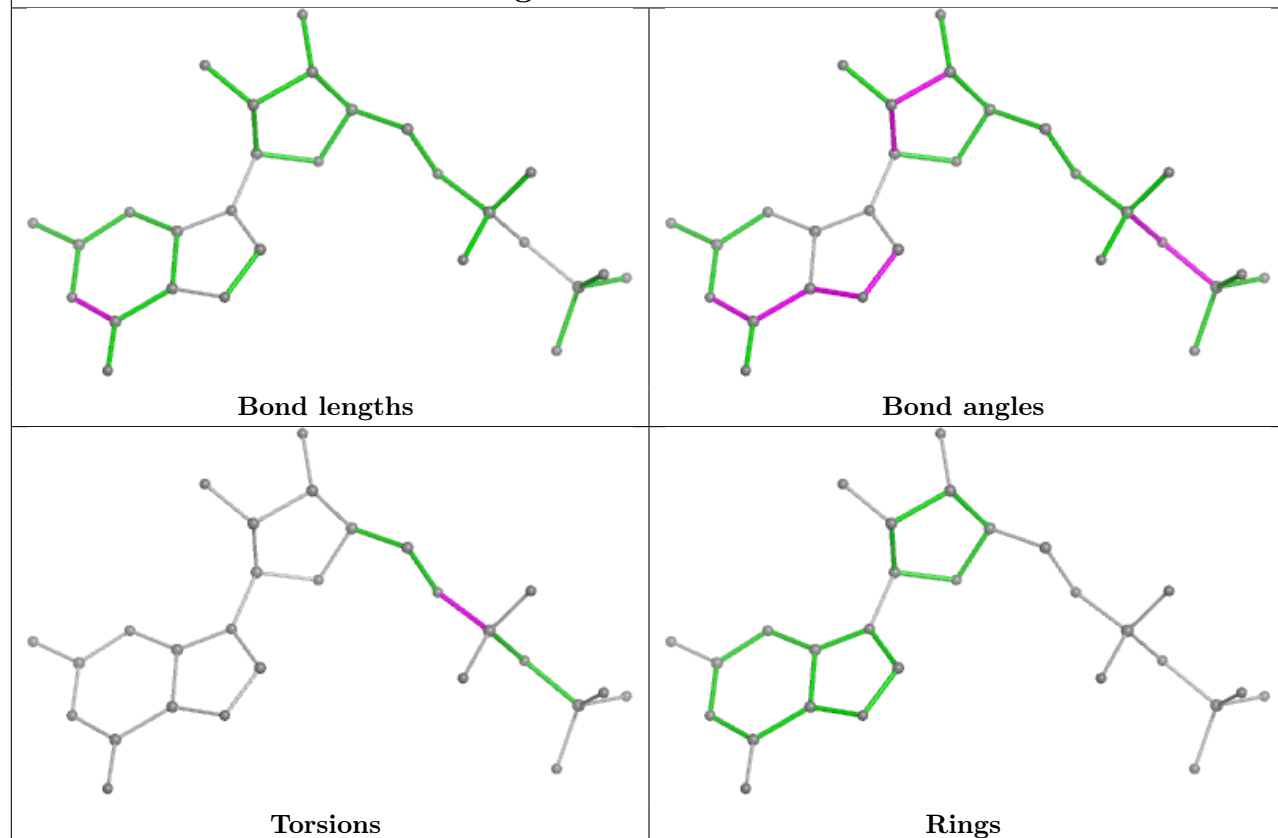


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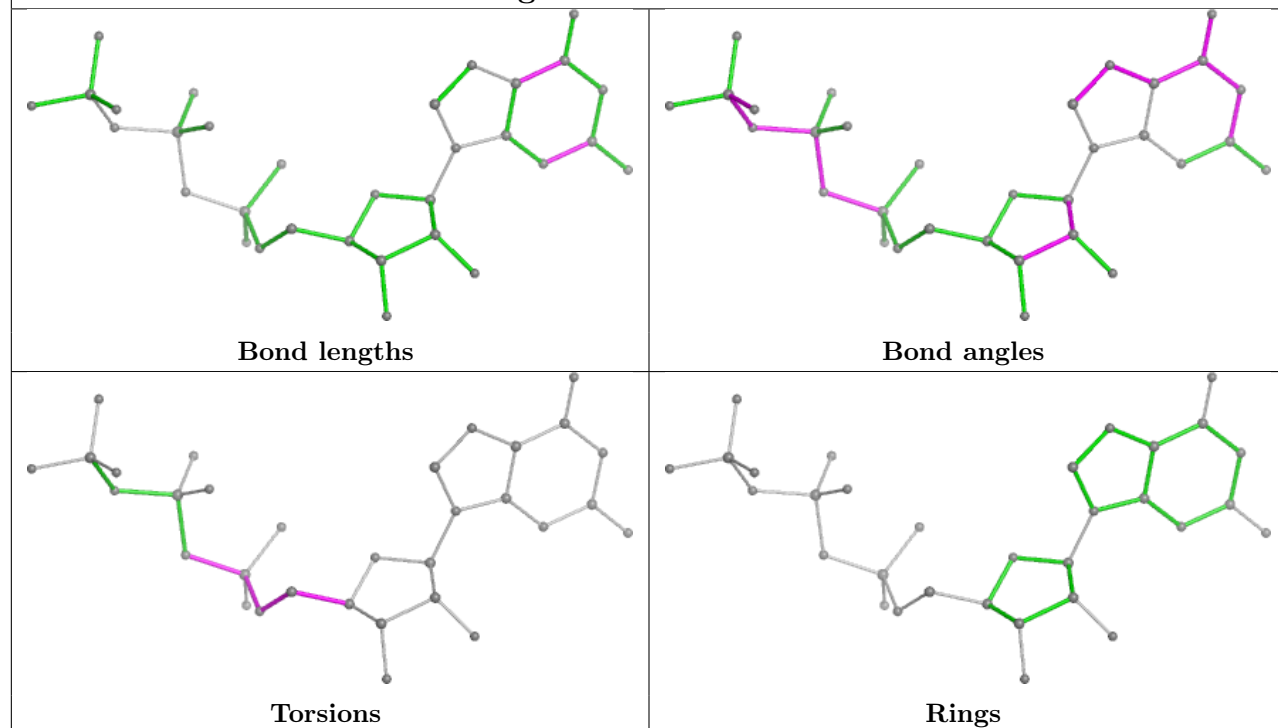




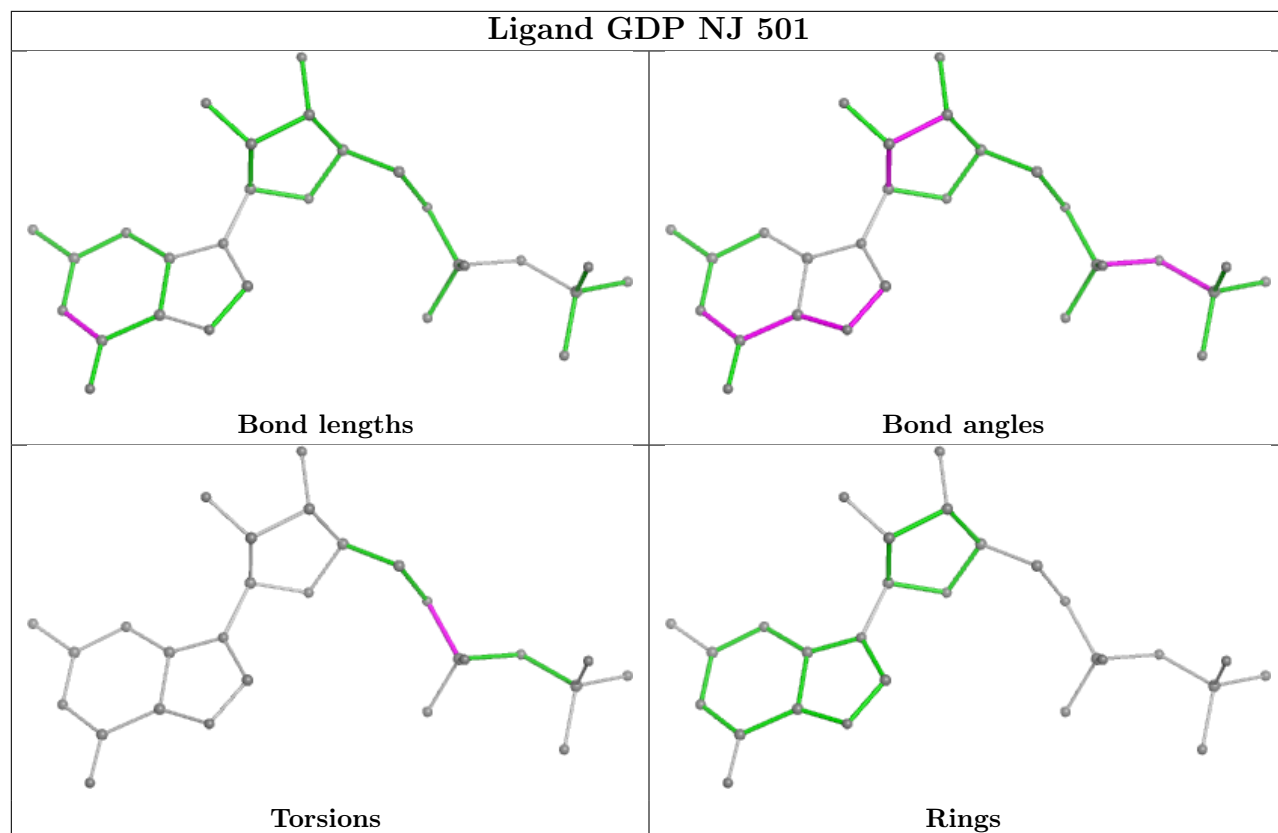
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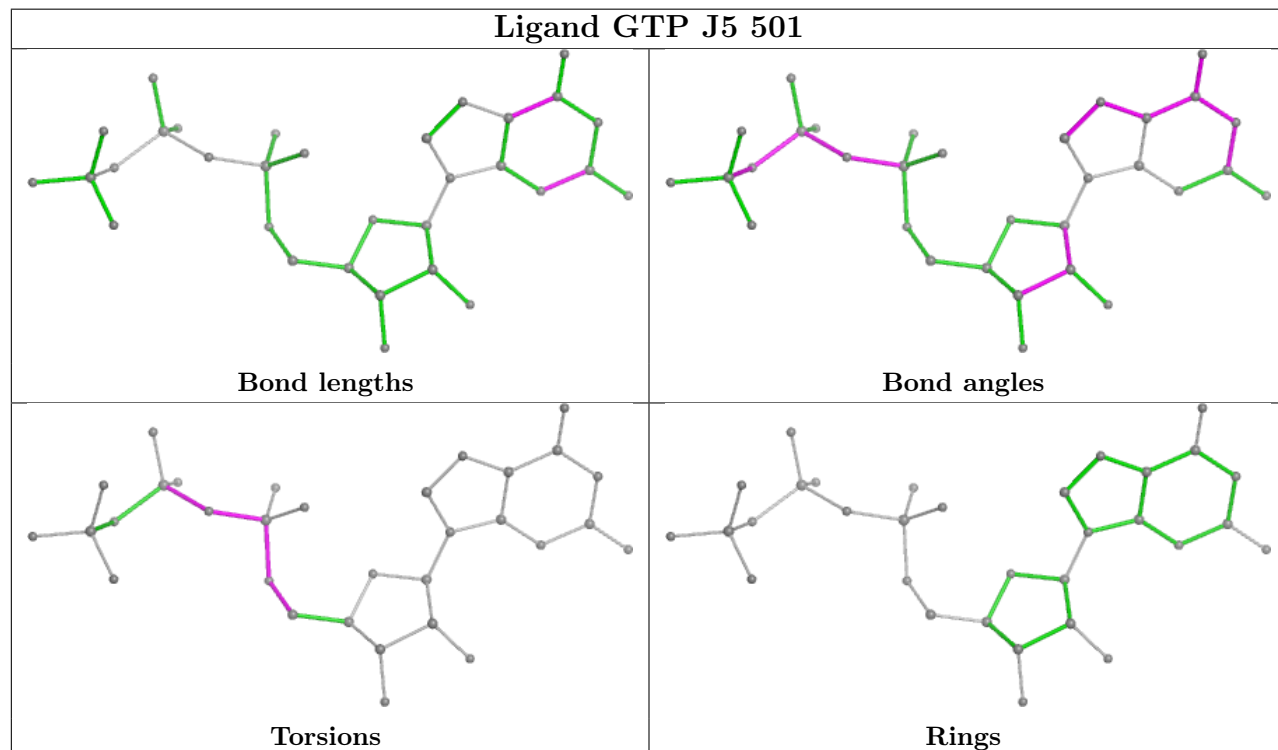
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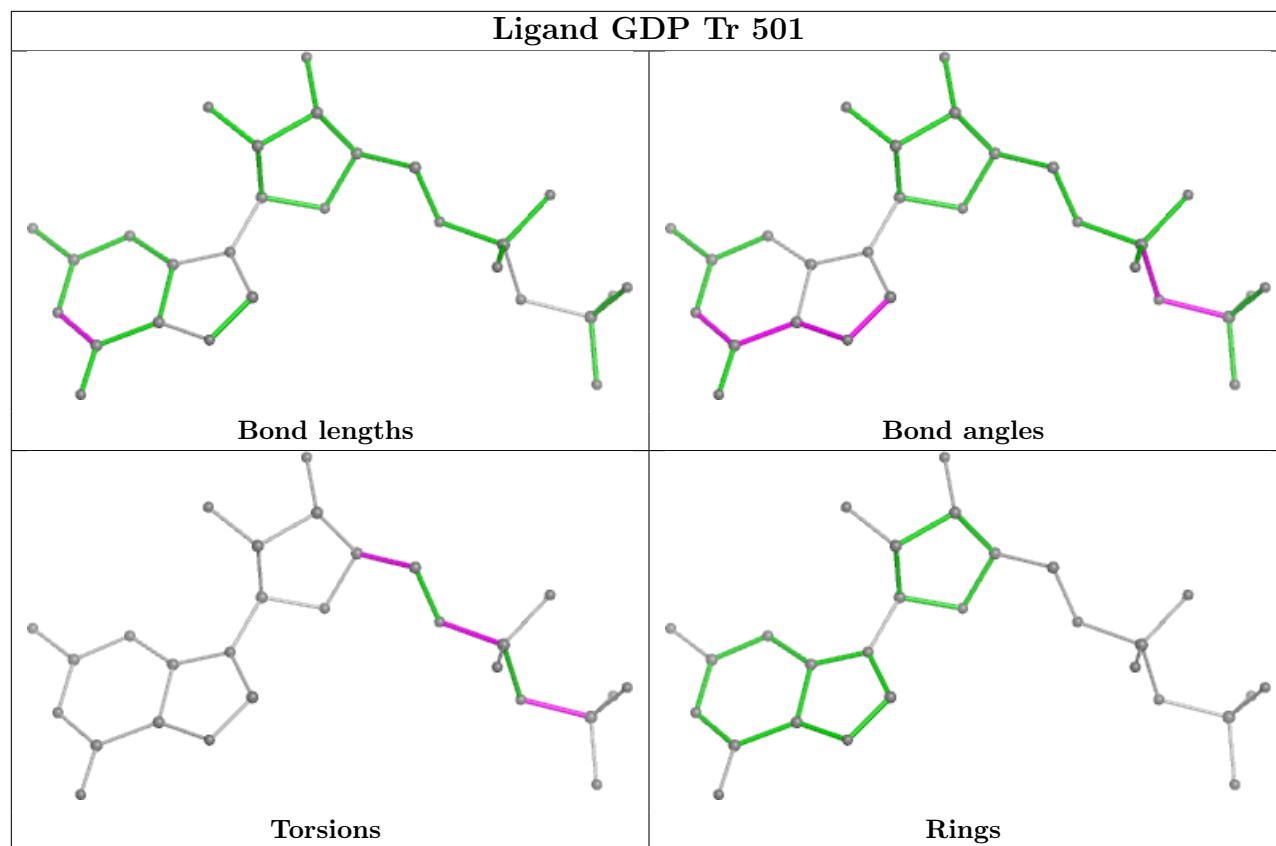


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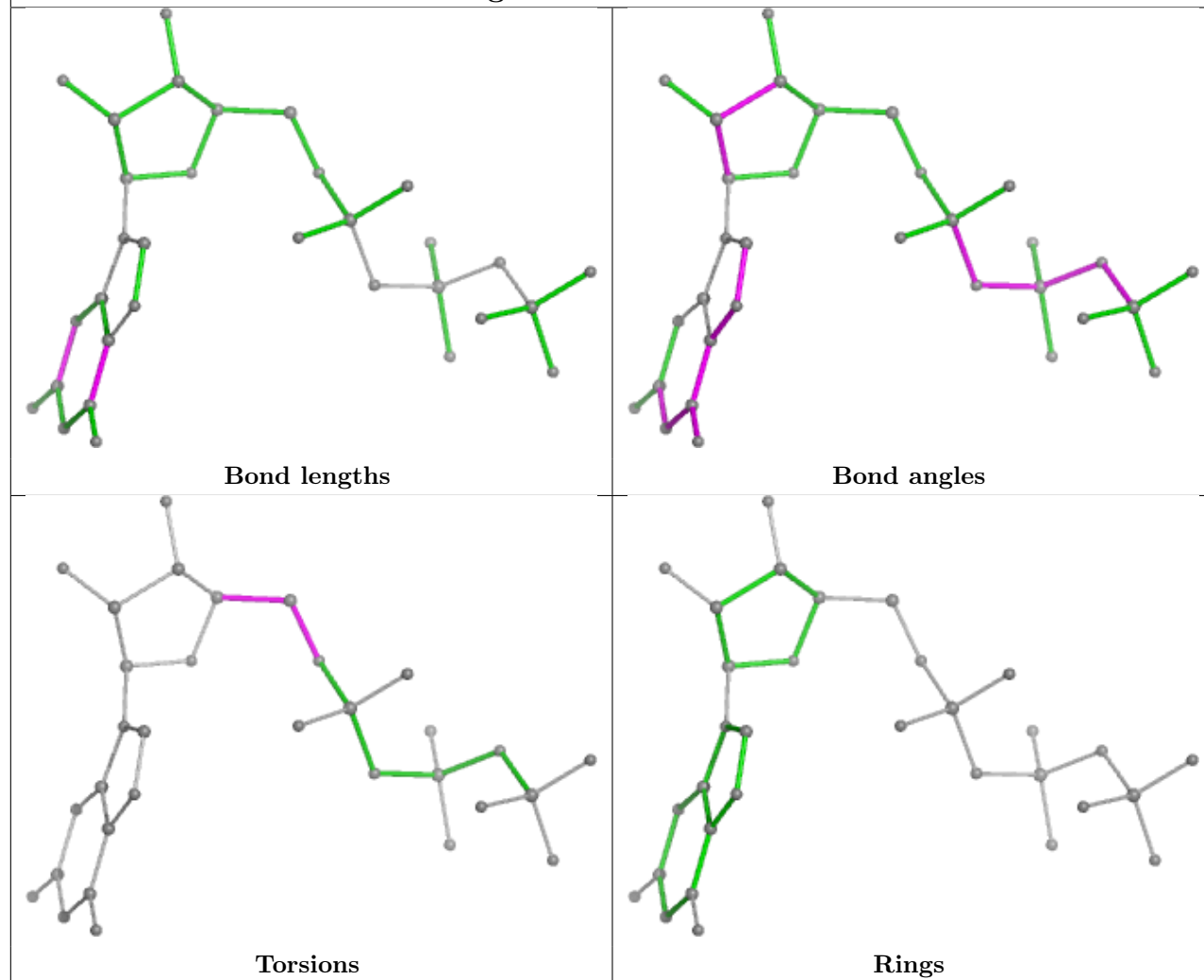


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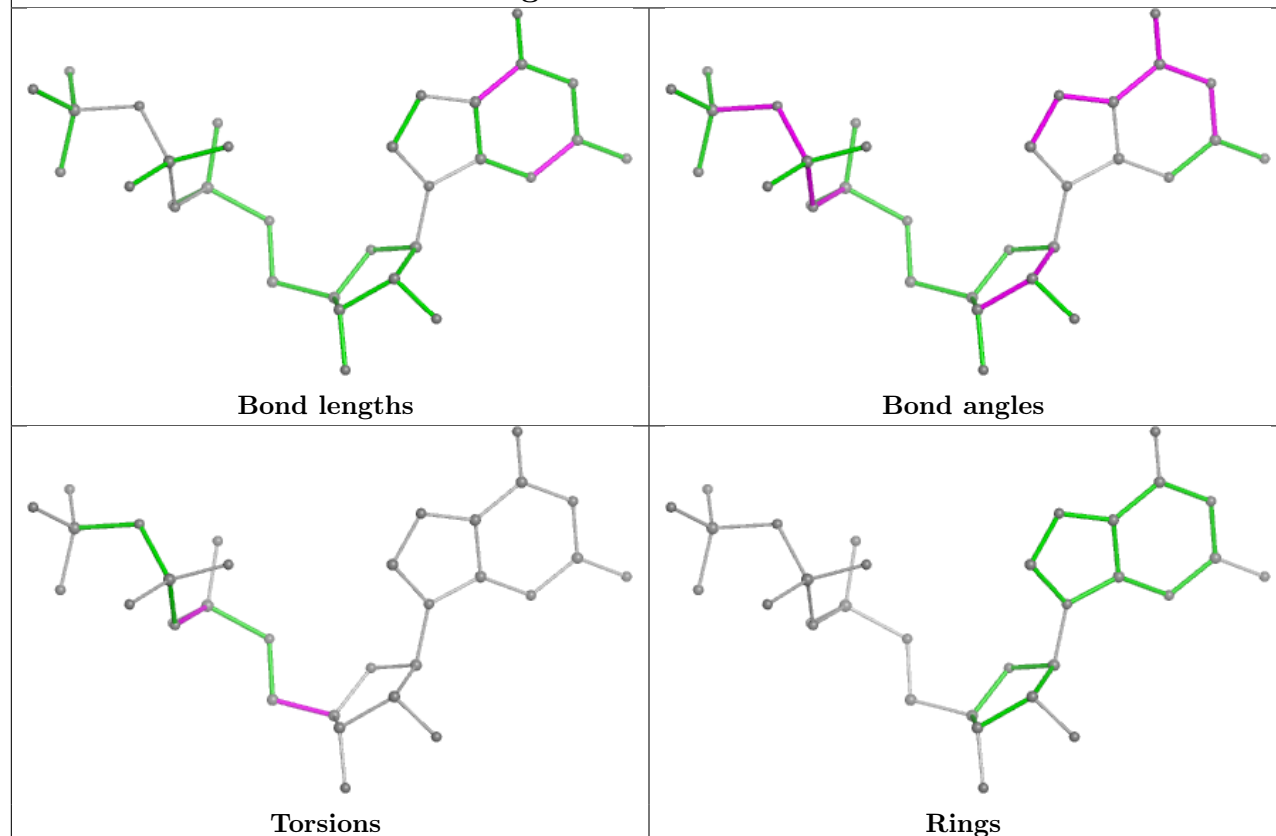




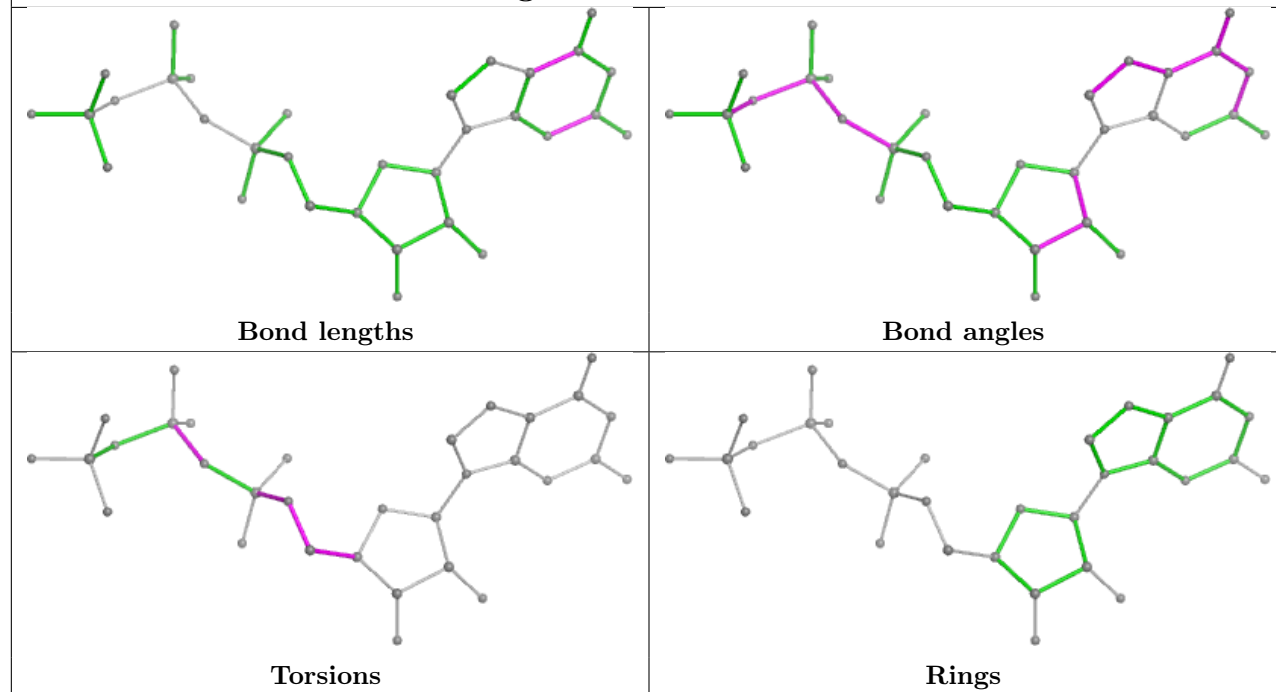
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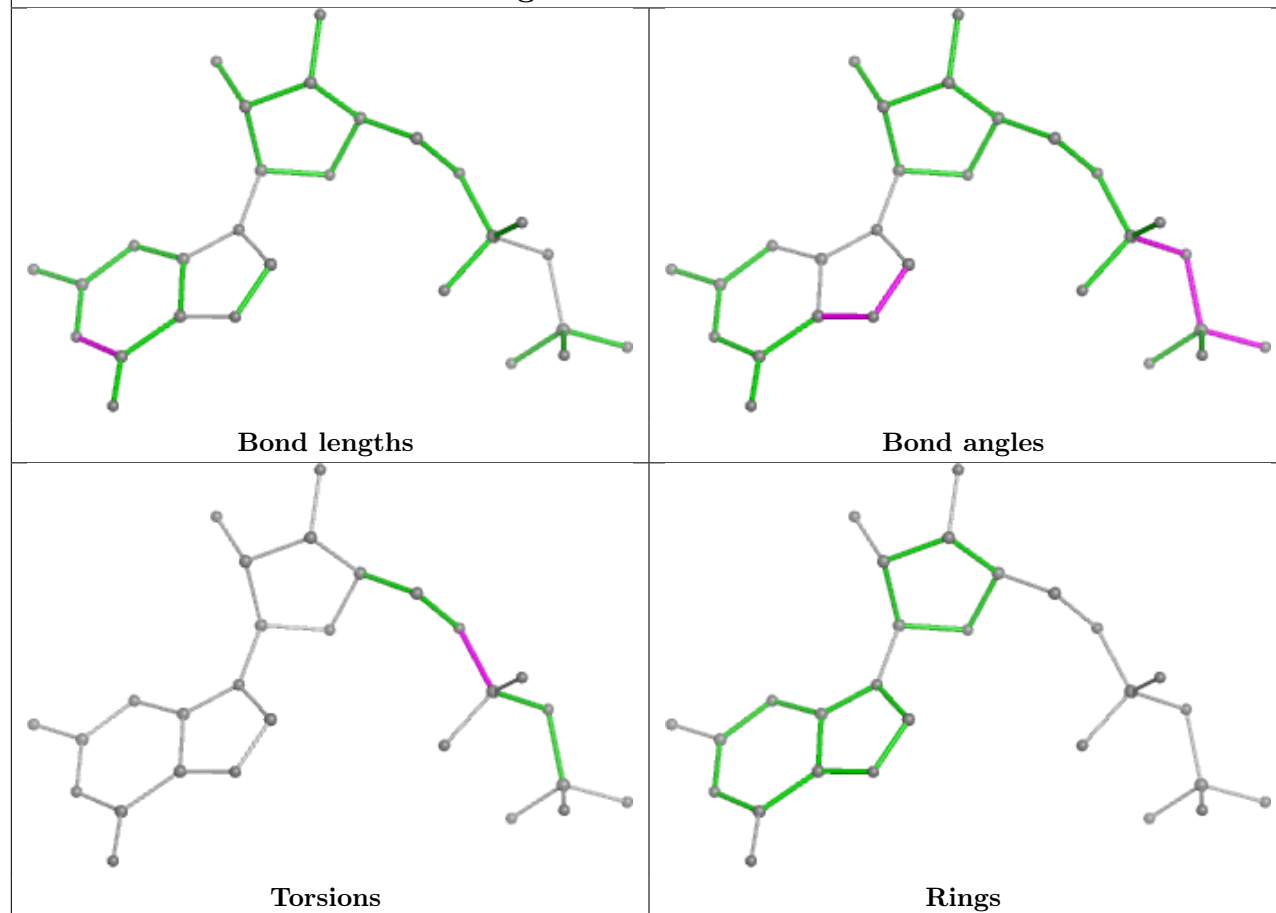
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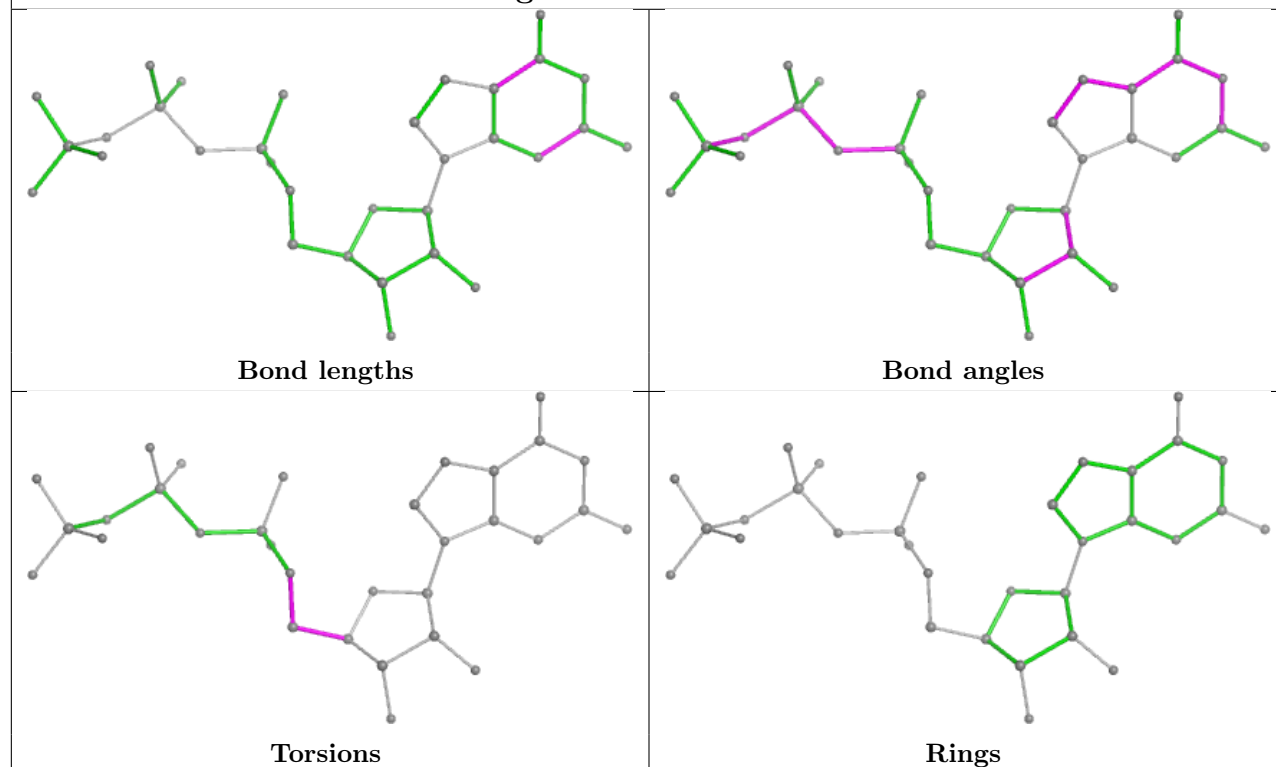
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## Ligand GDP UF 501

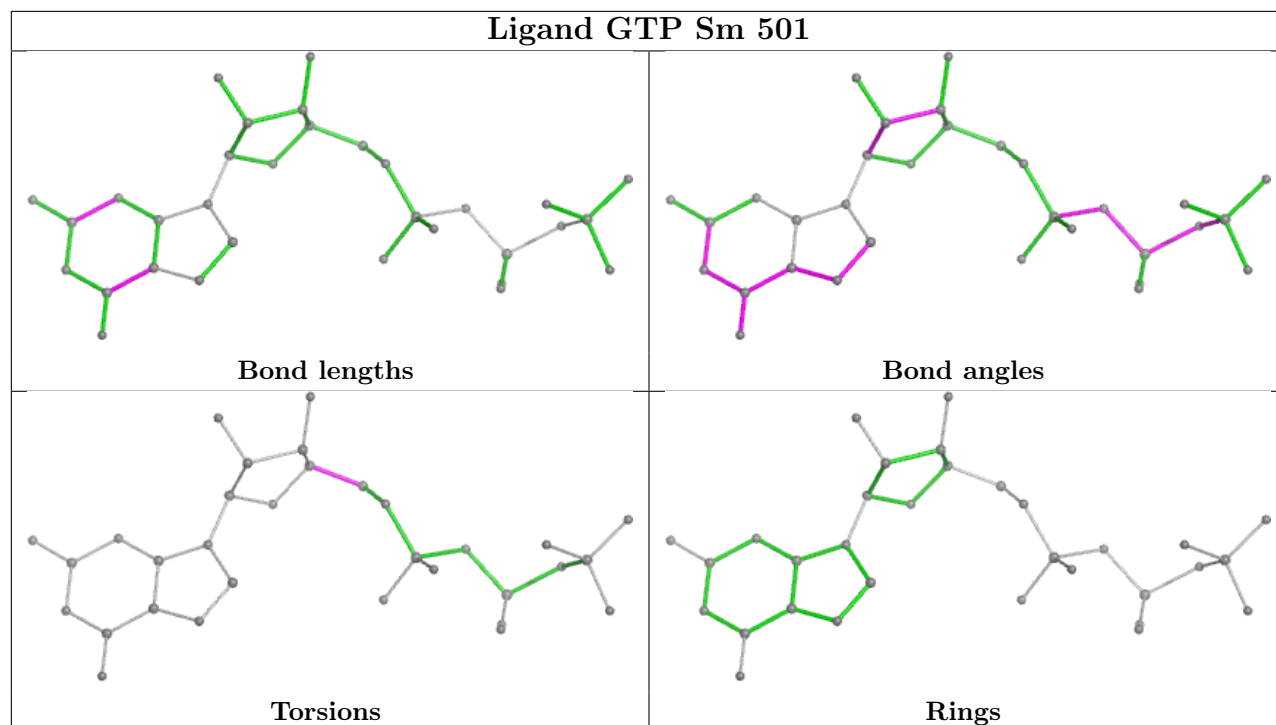


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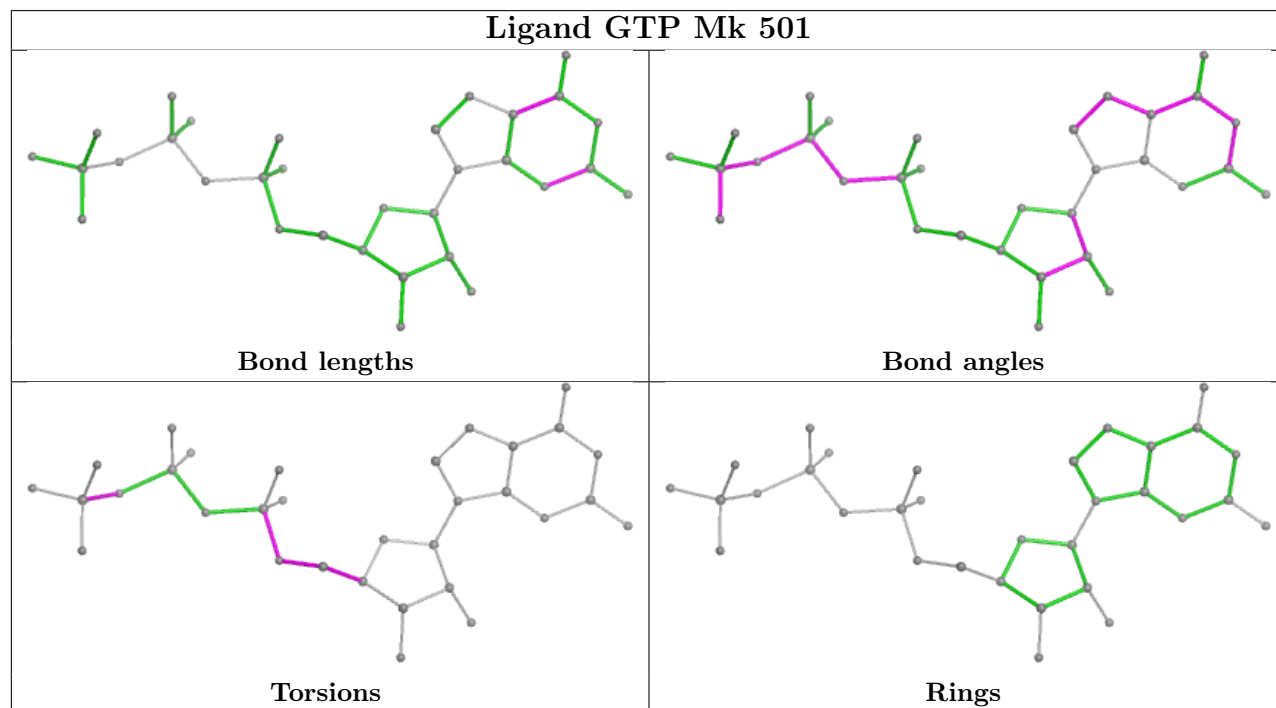


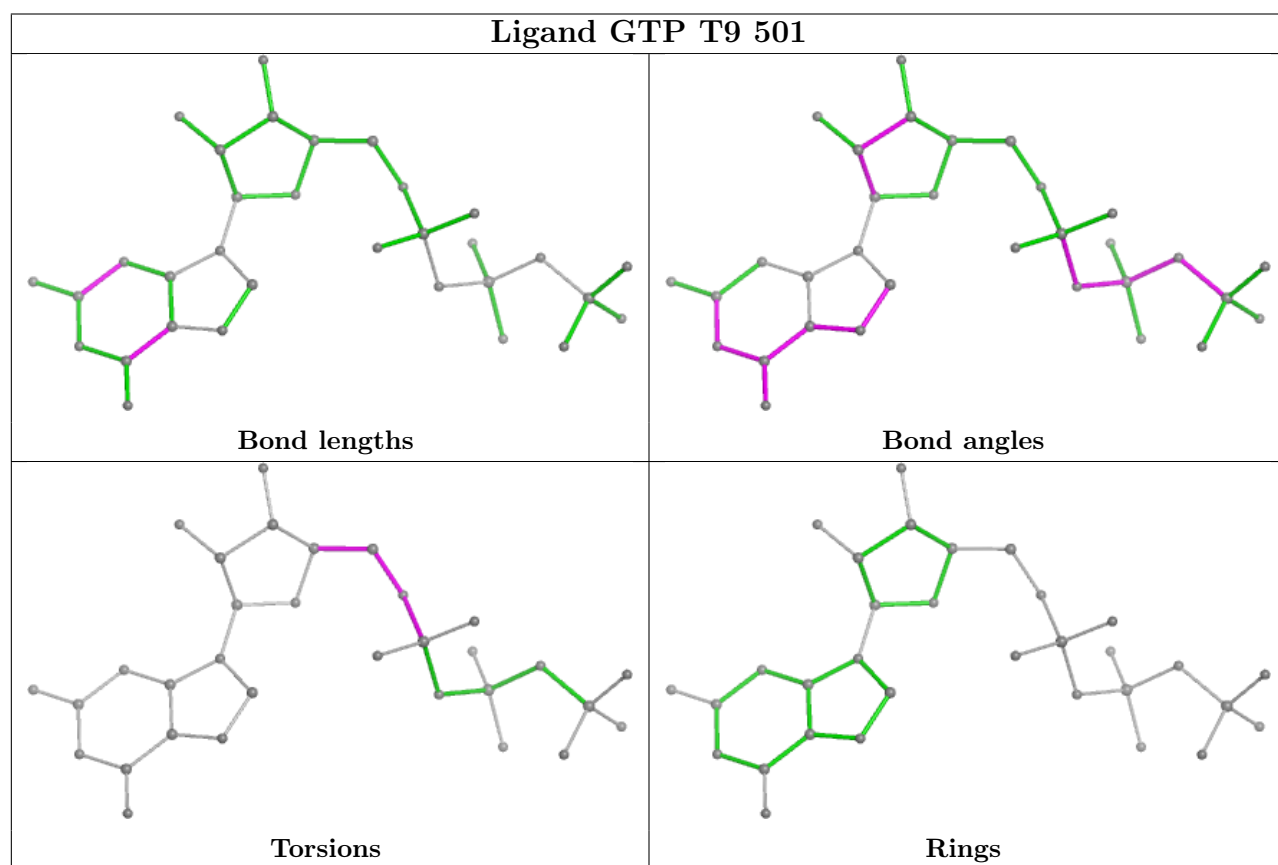
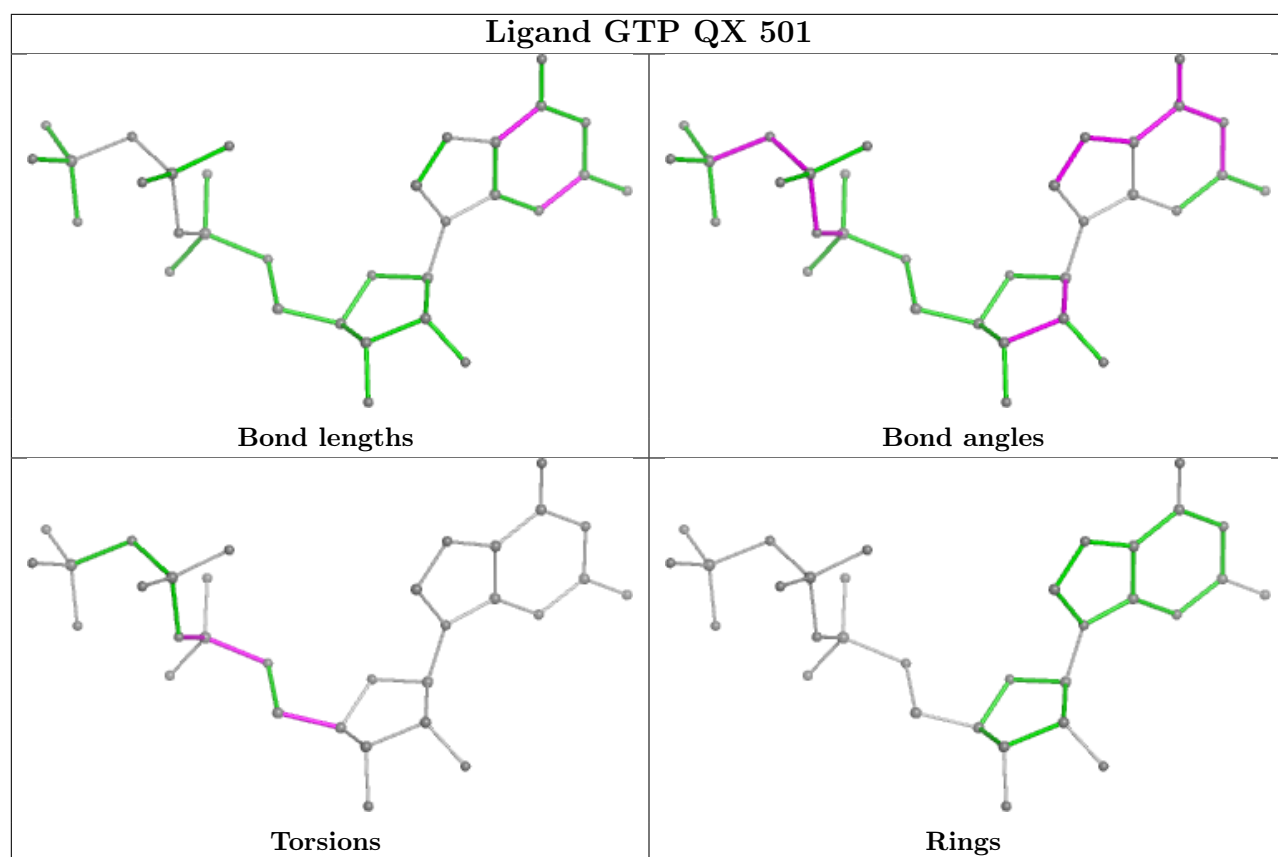


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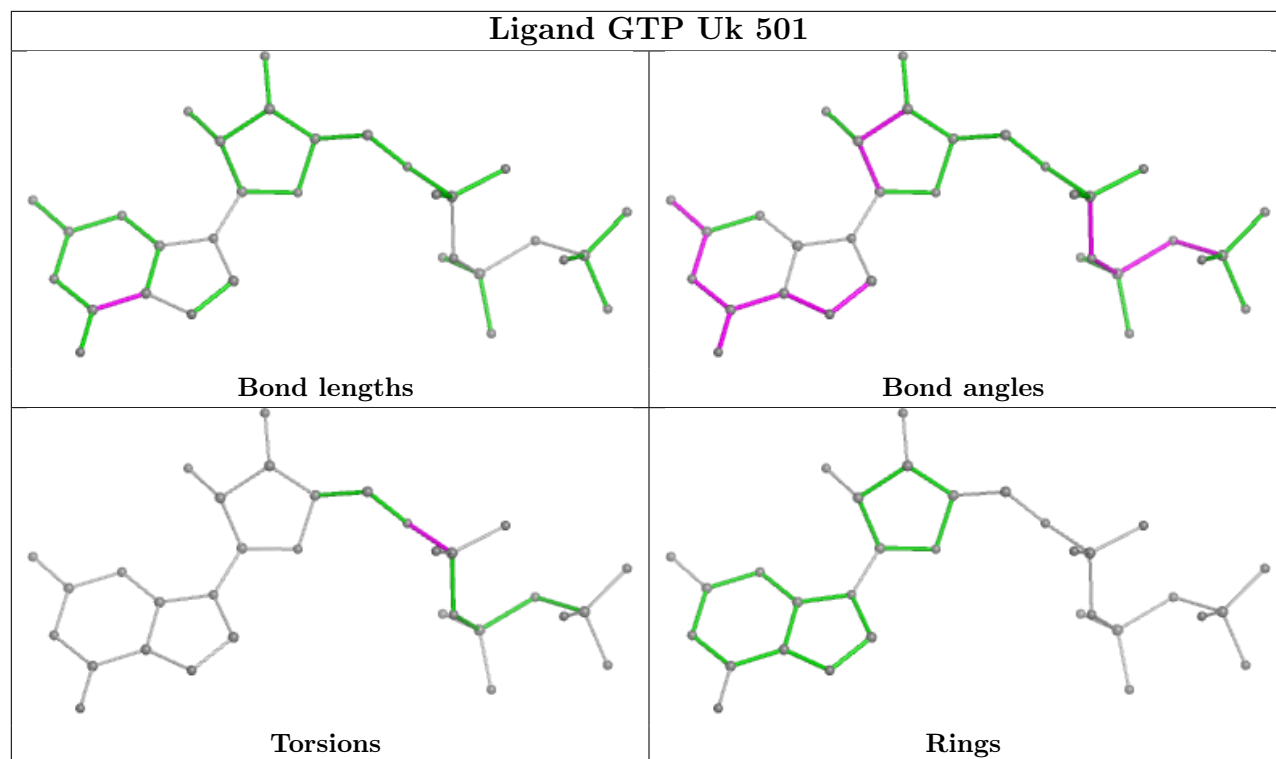


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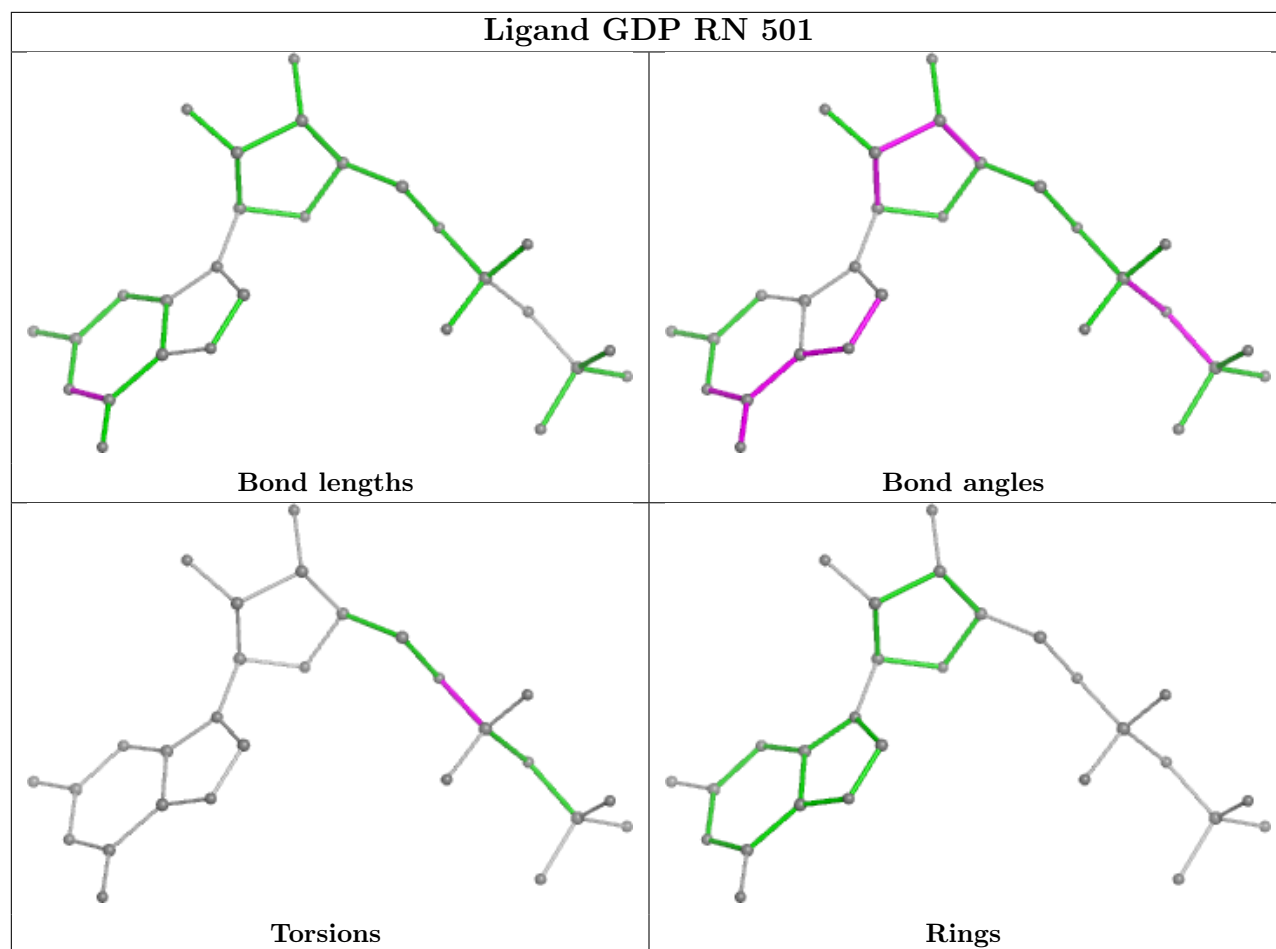


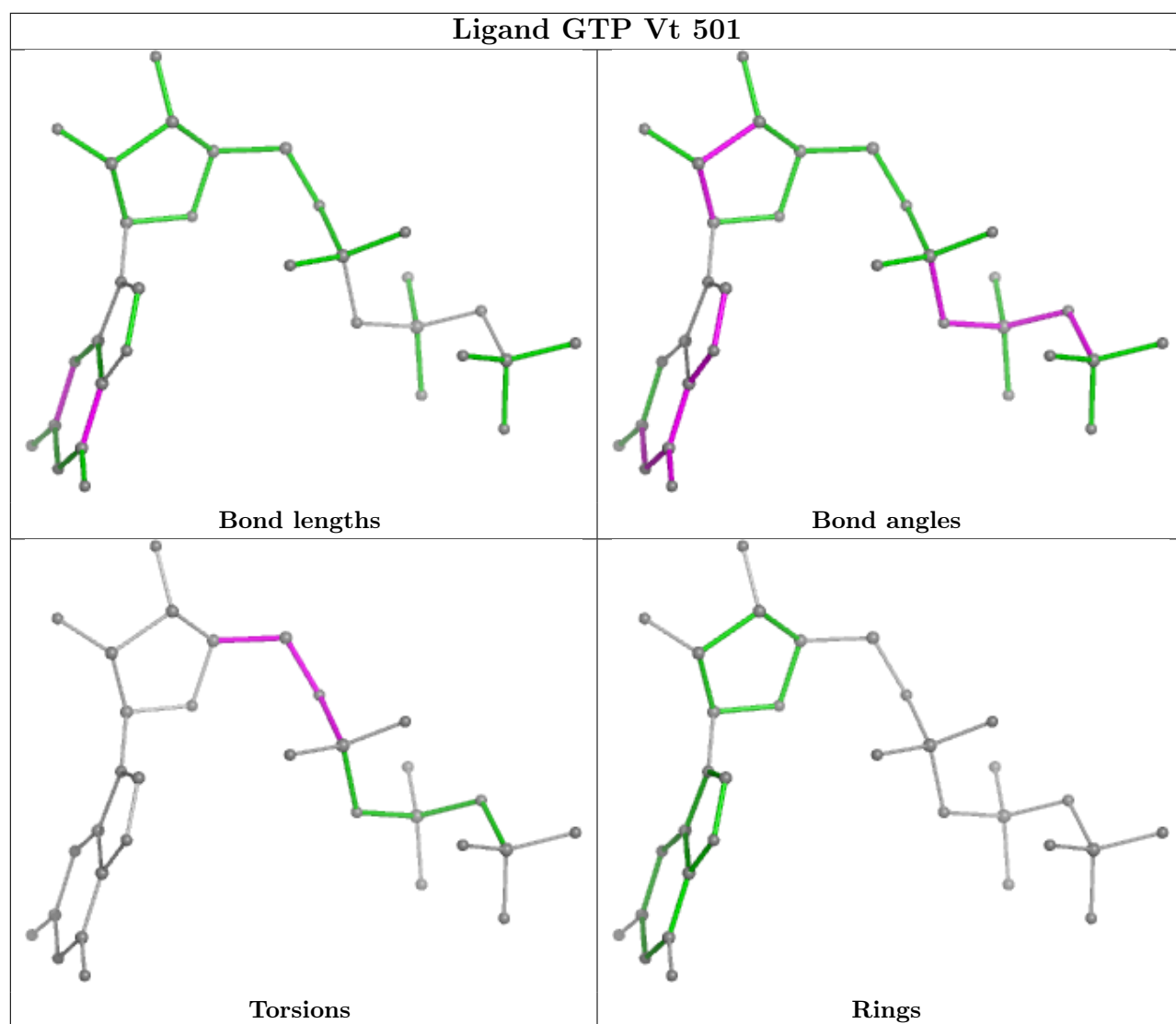


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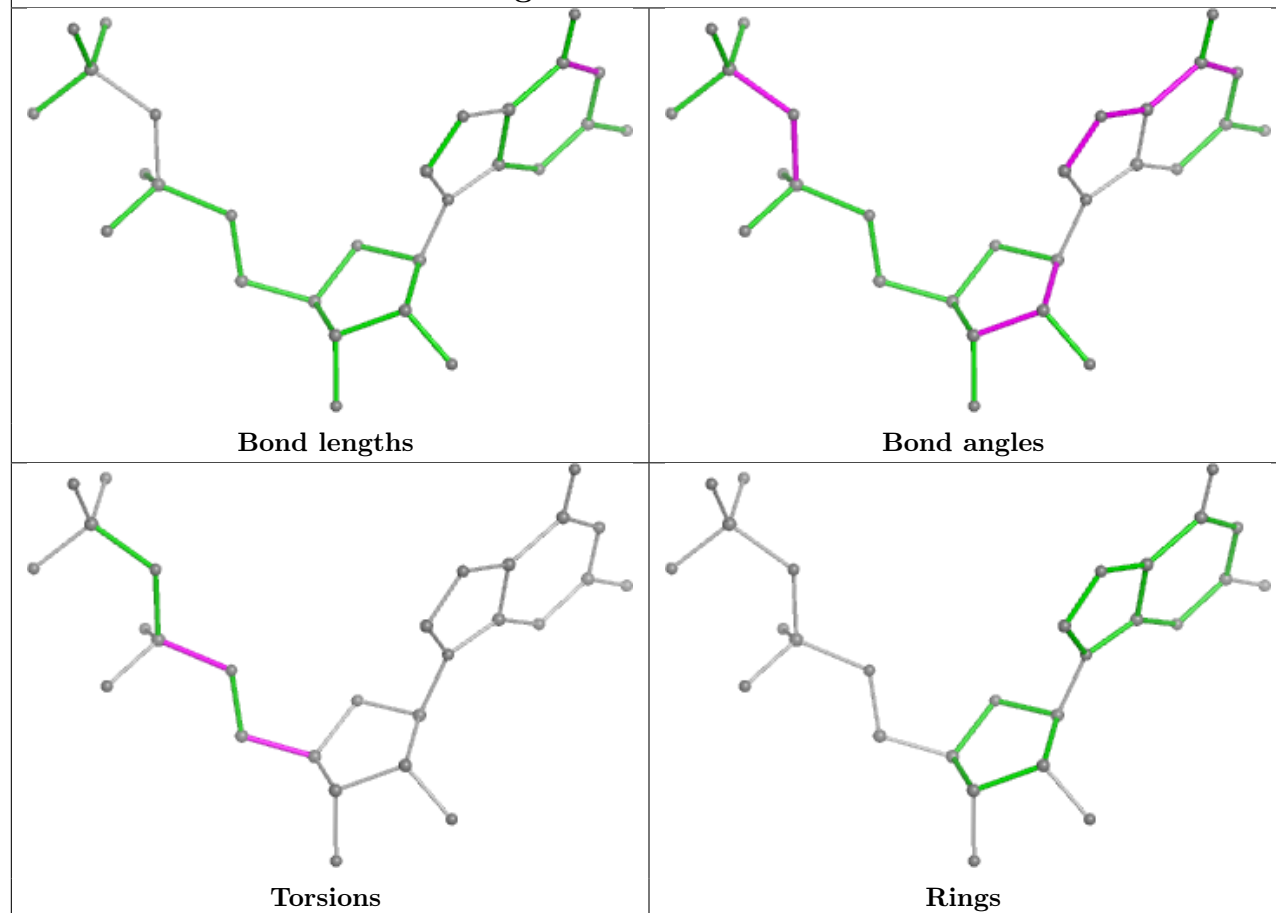


## Ligand GDP RN 501

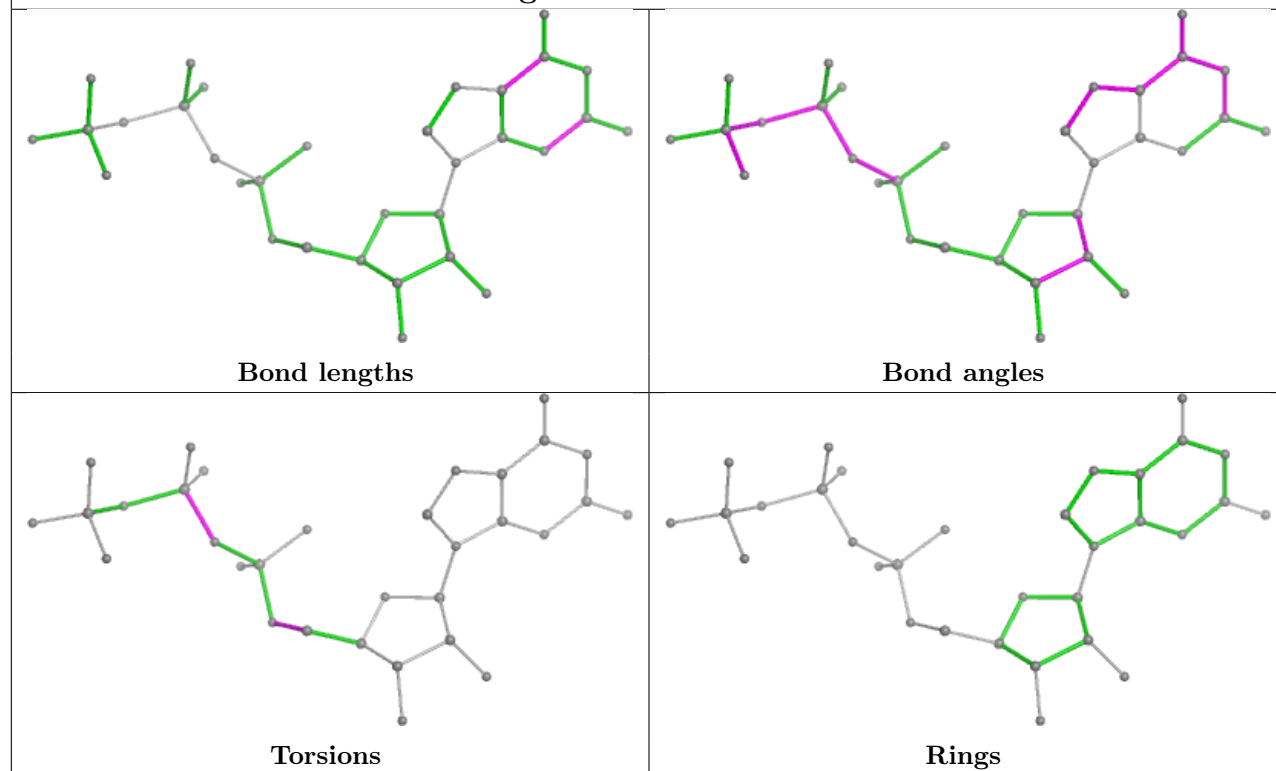


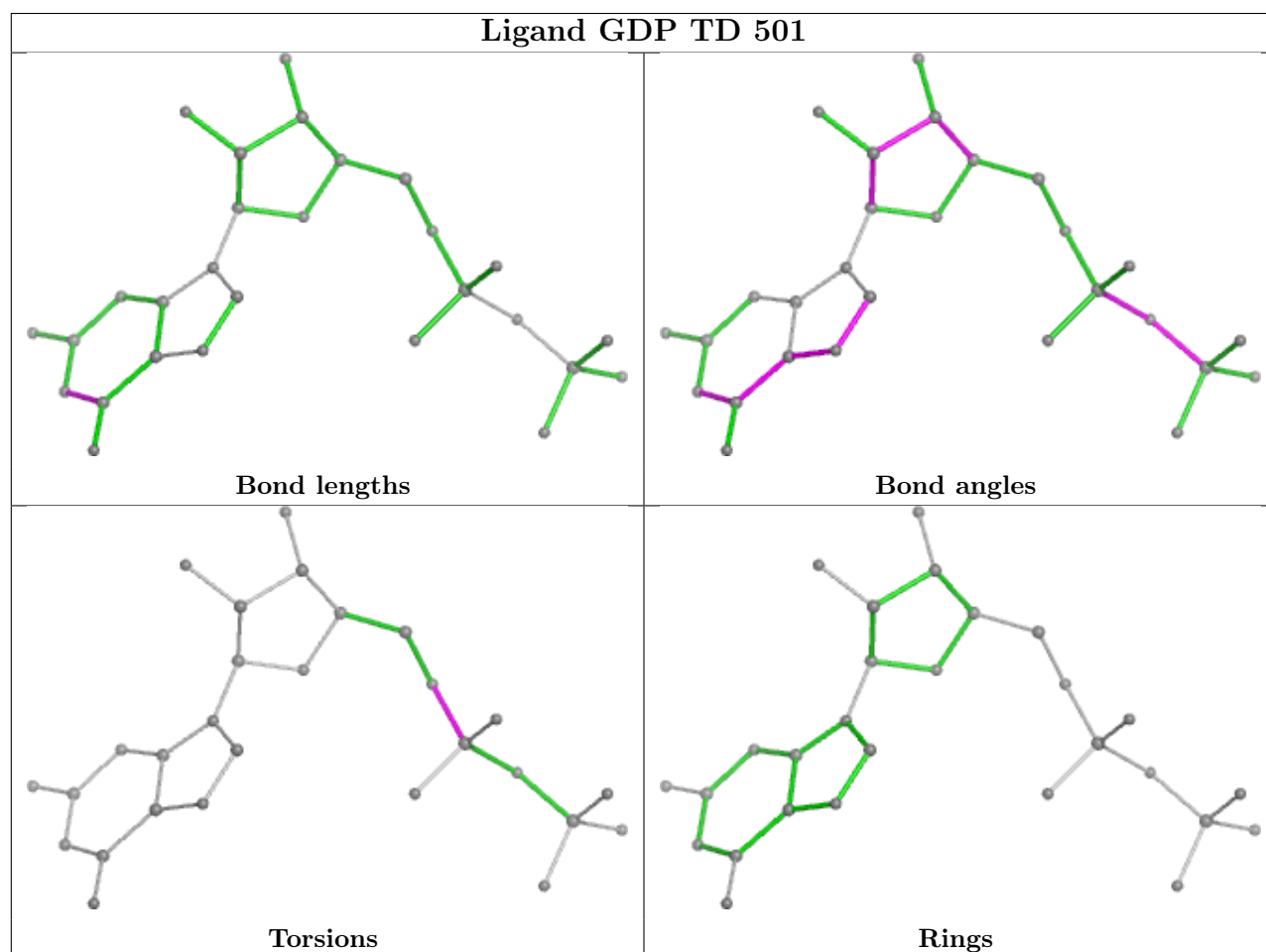
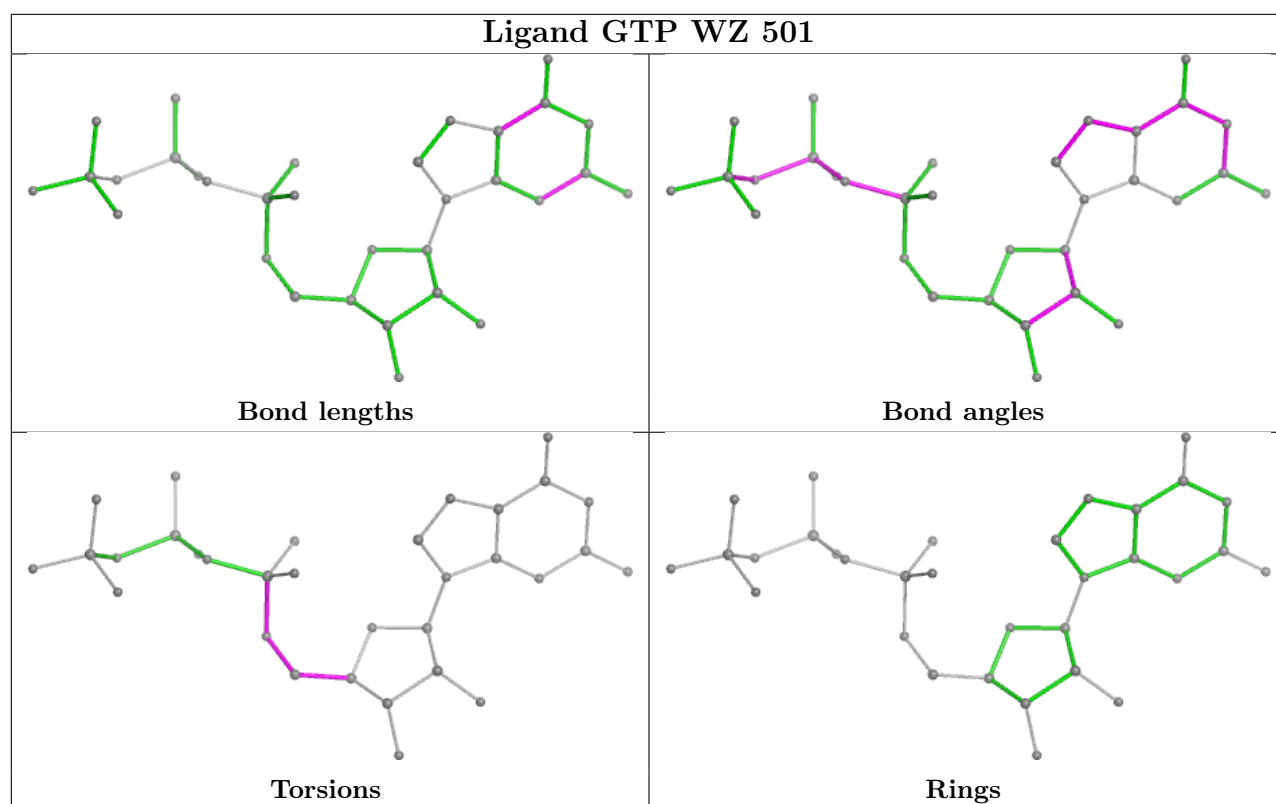


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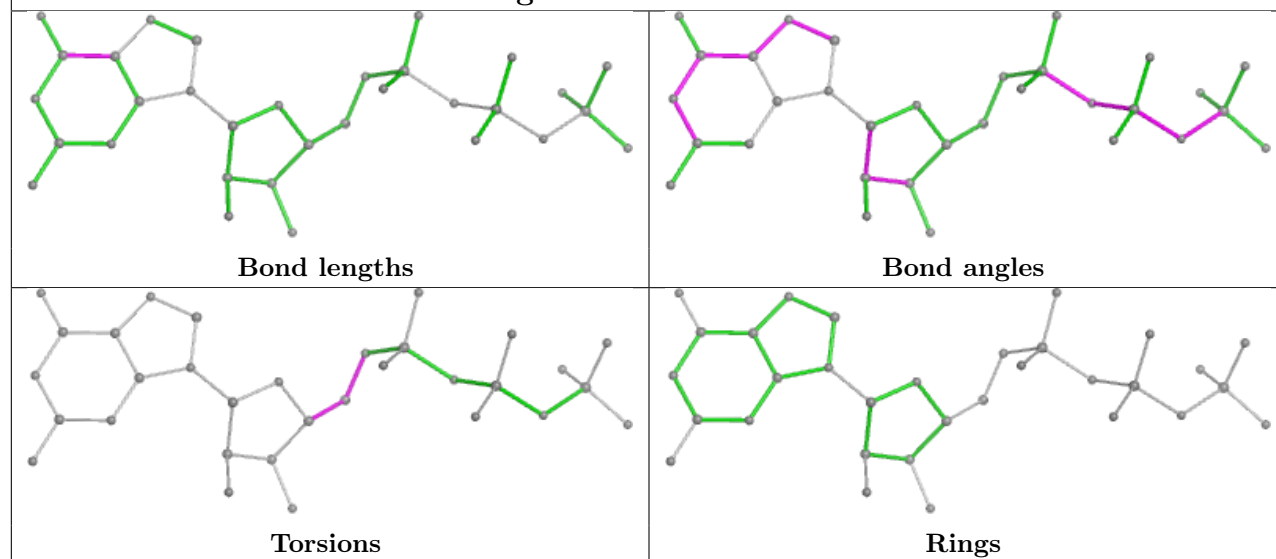


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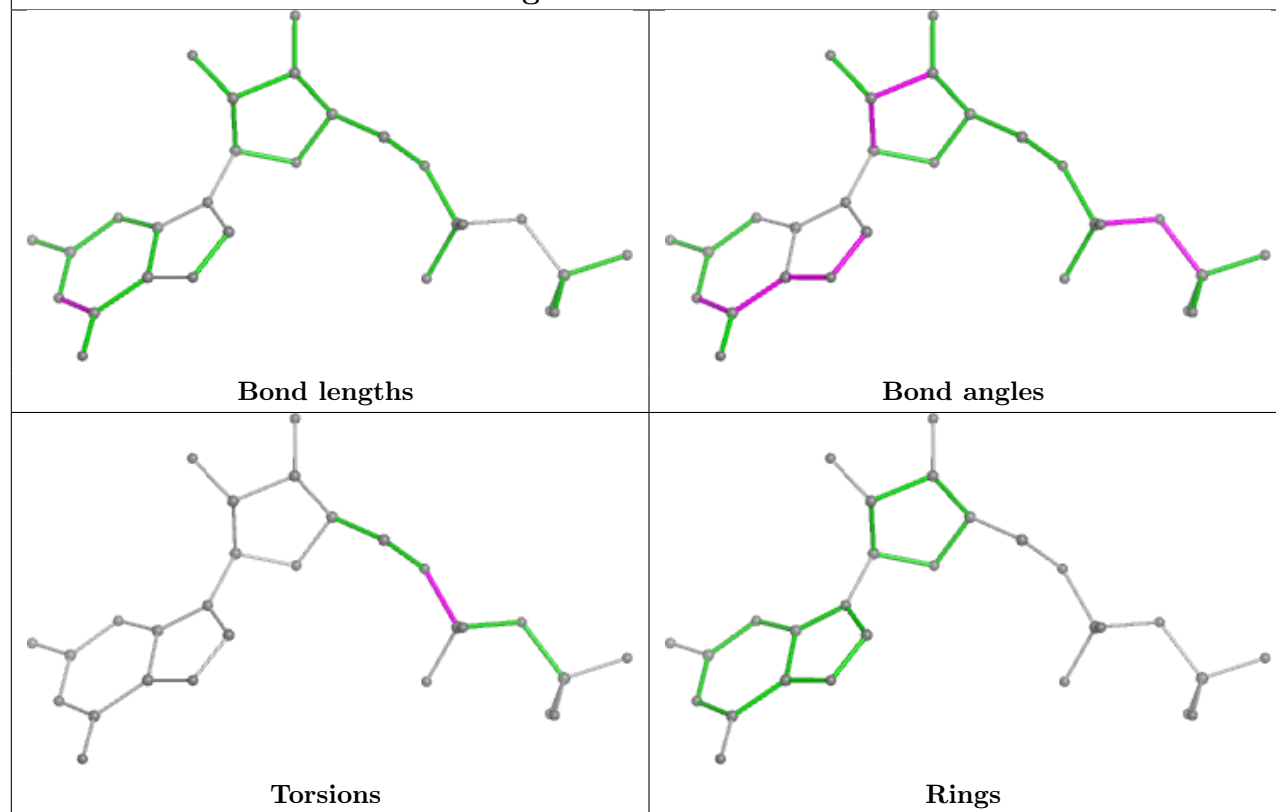




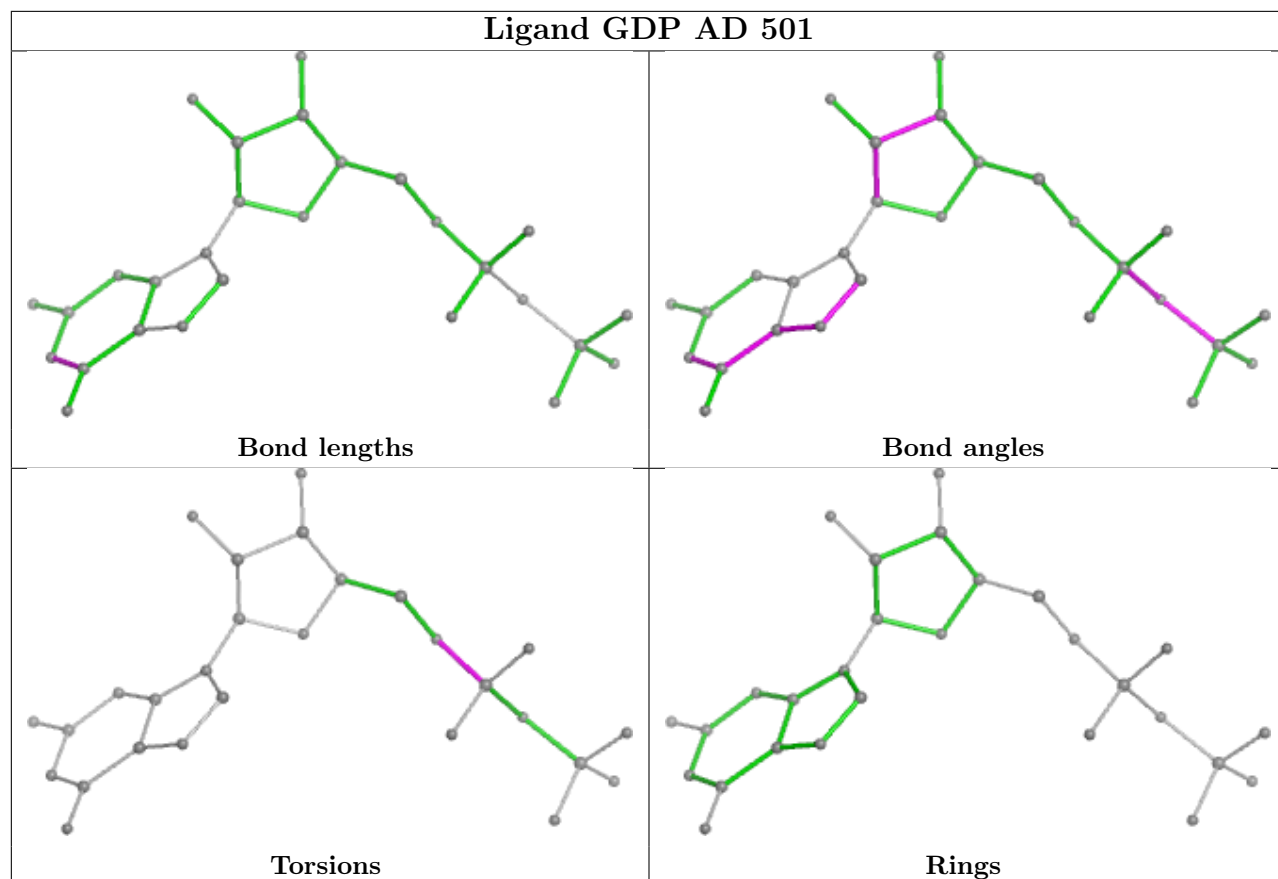
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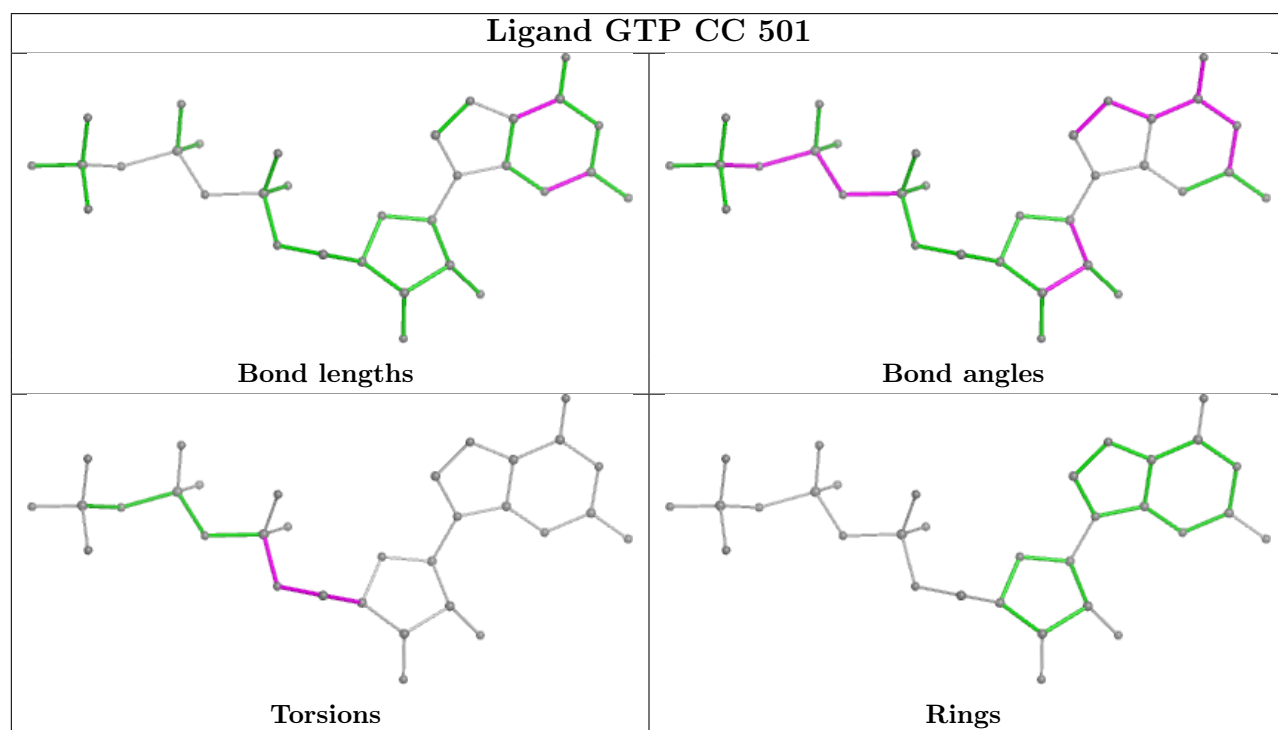
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## Ligand GDP AD 501

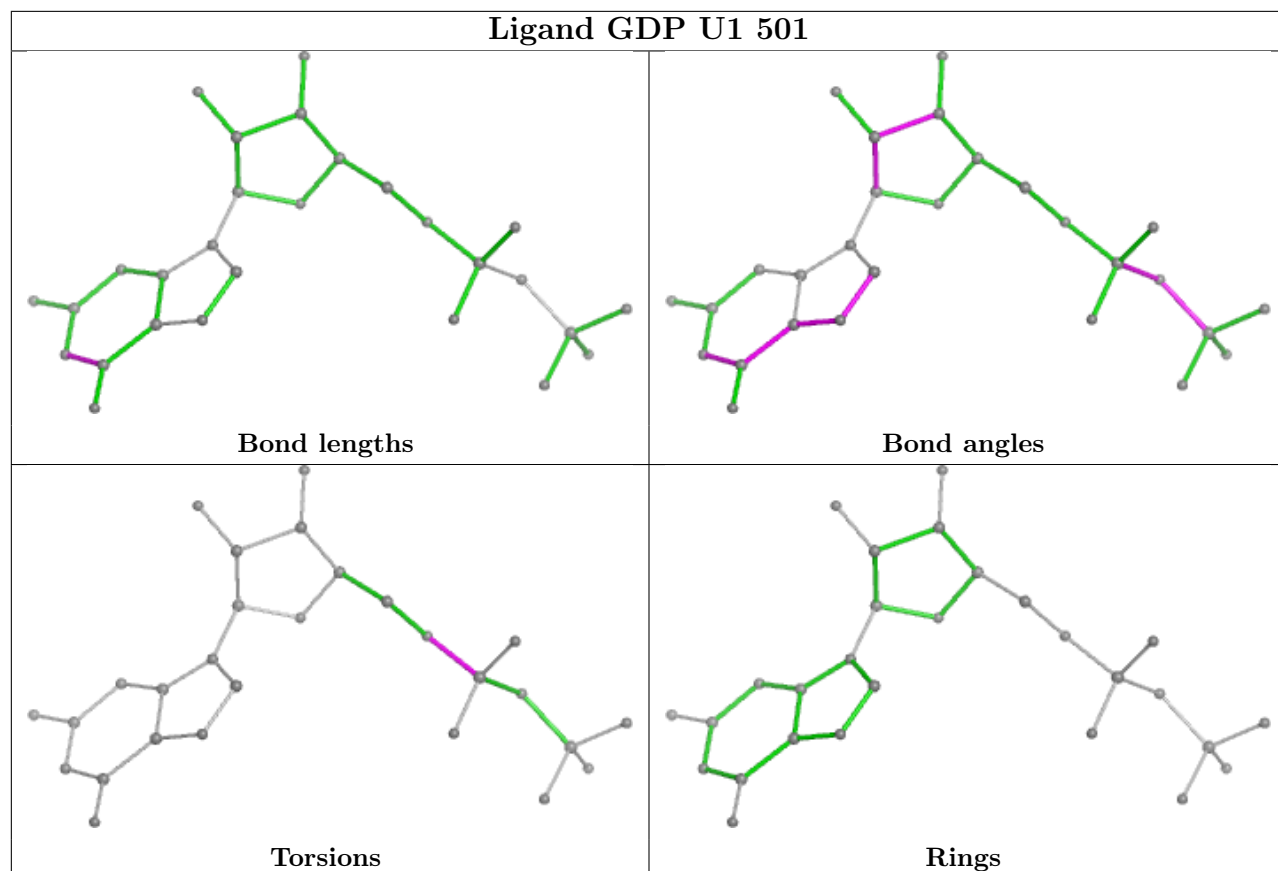


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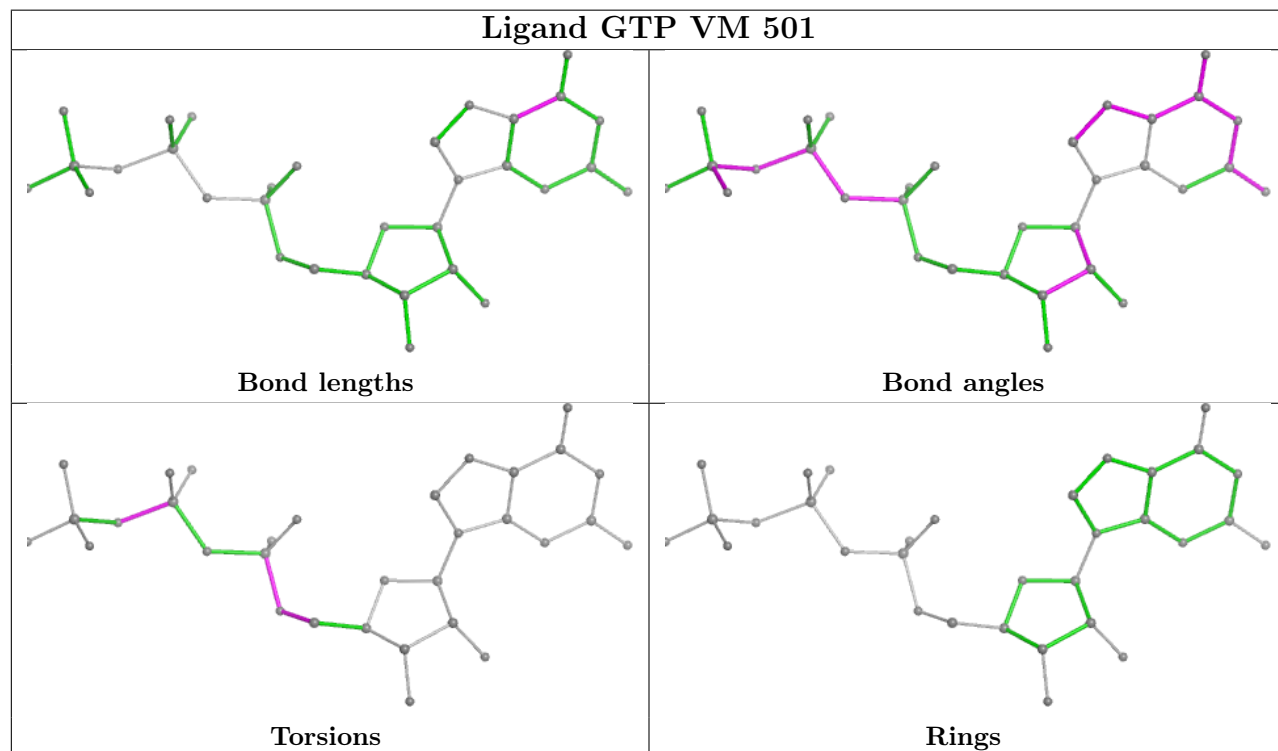


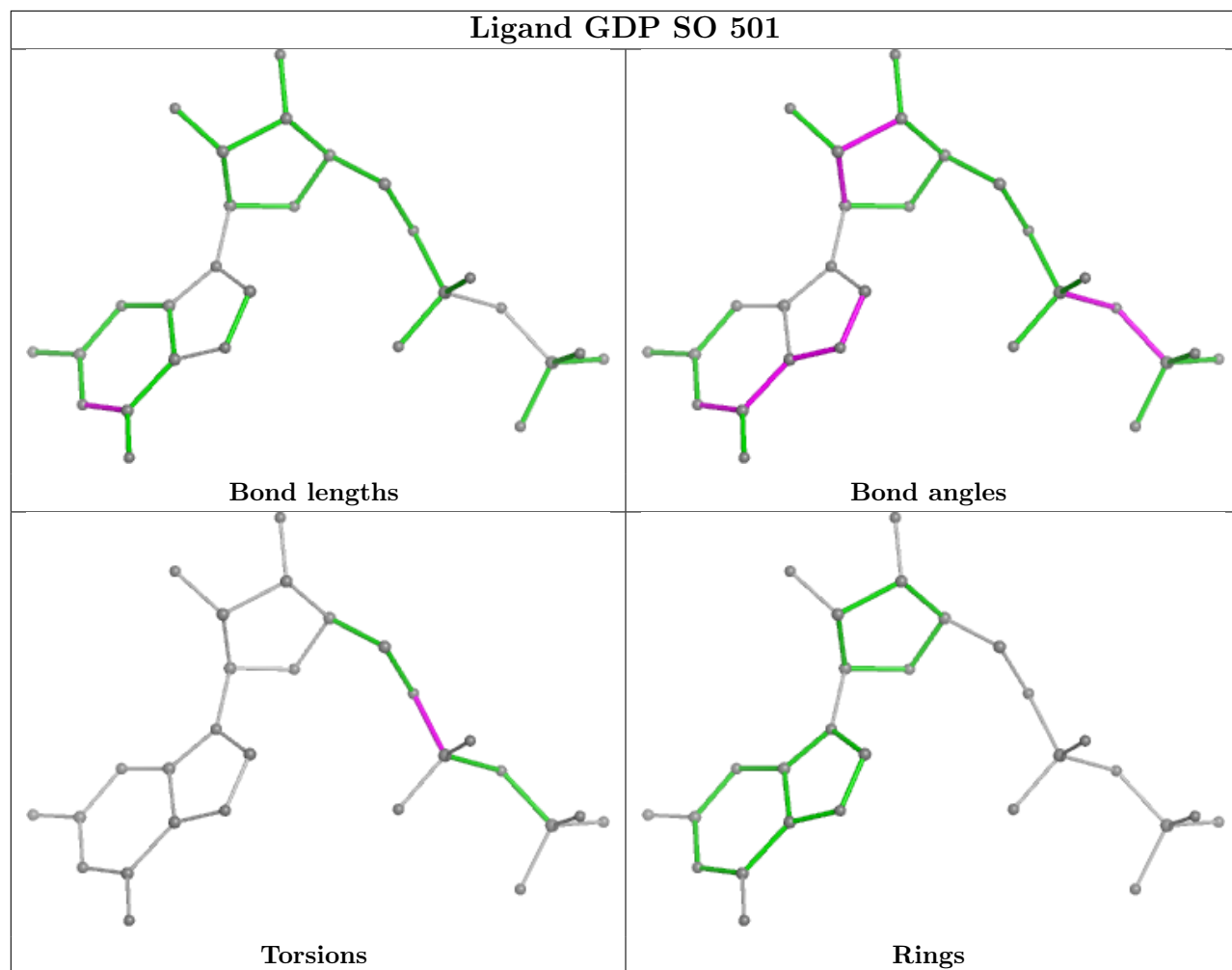


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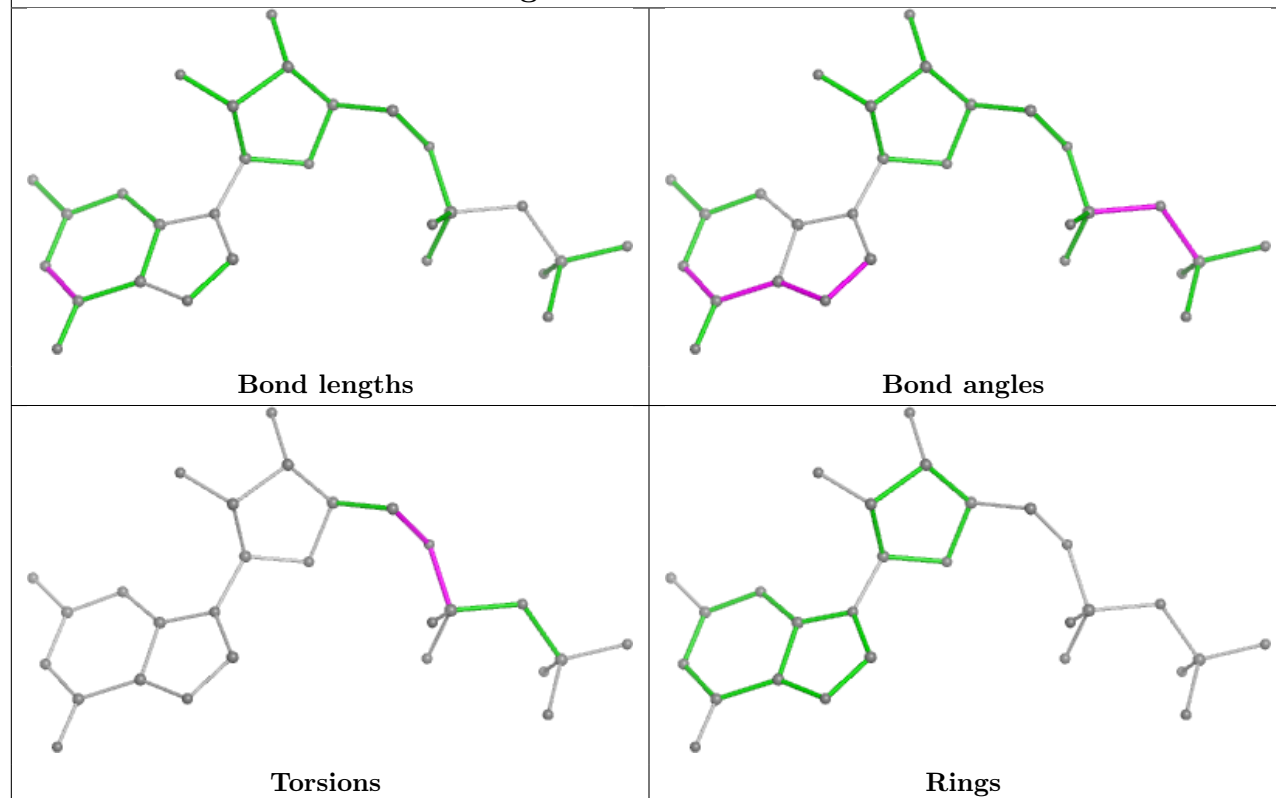


## Ligand GTP VM 501

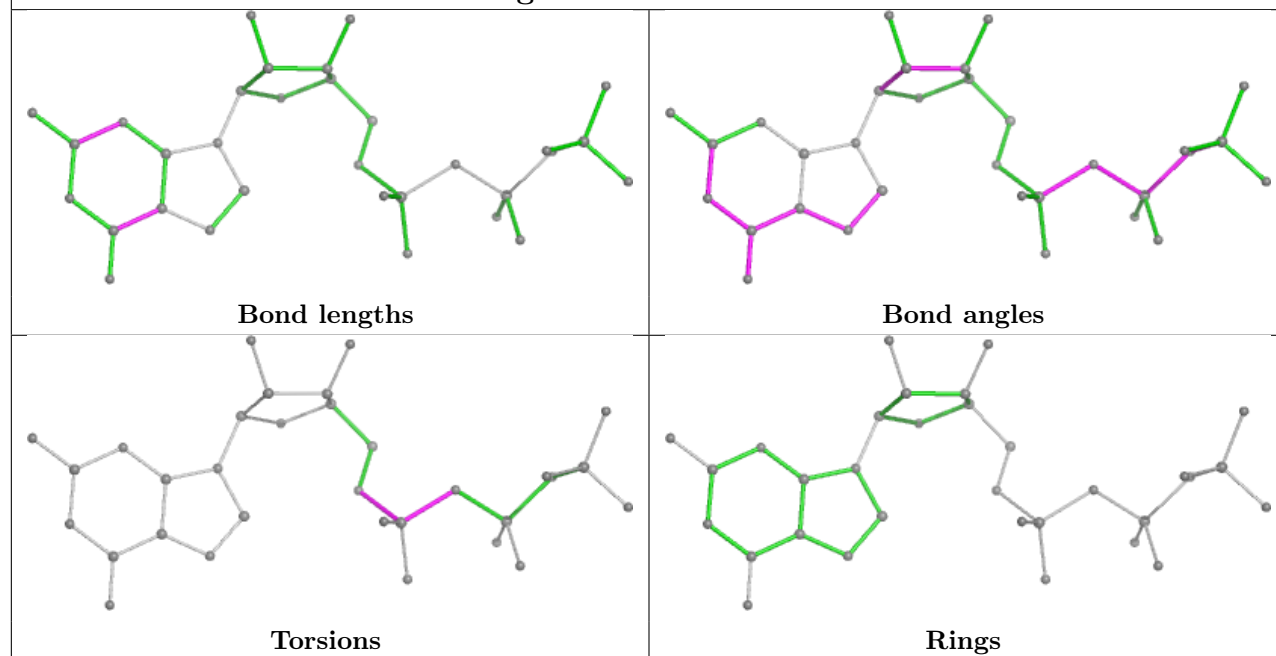




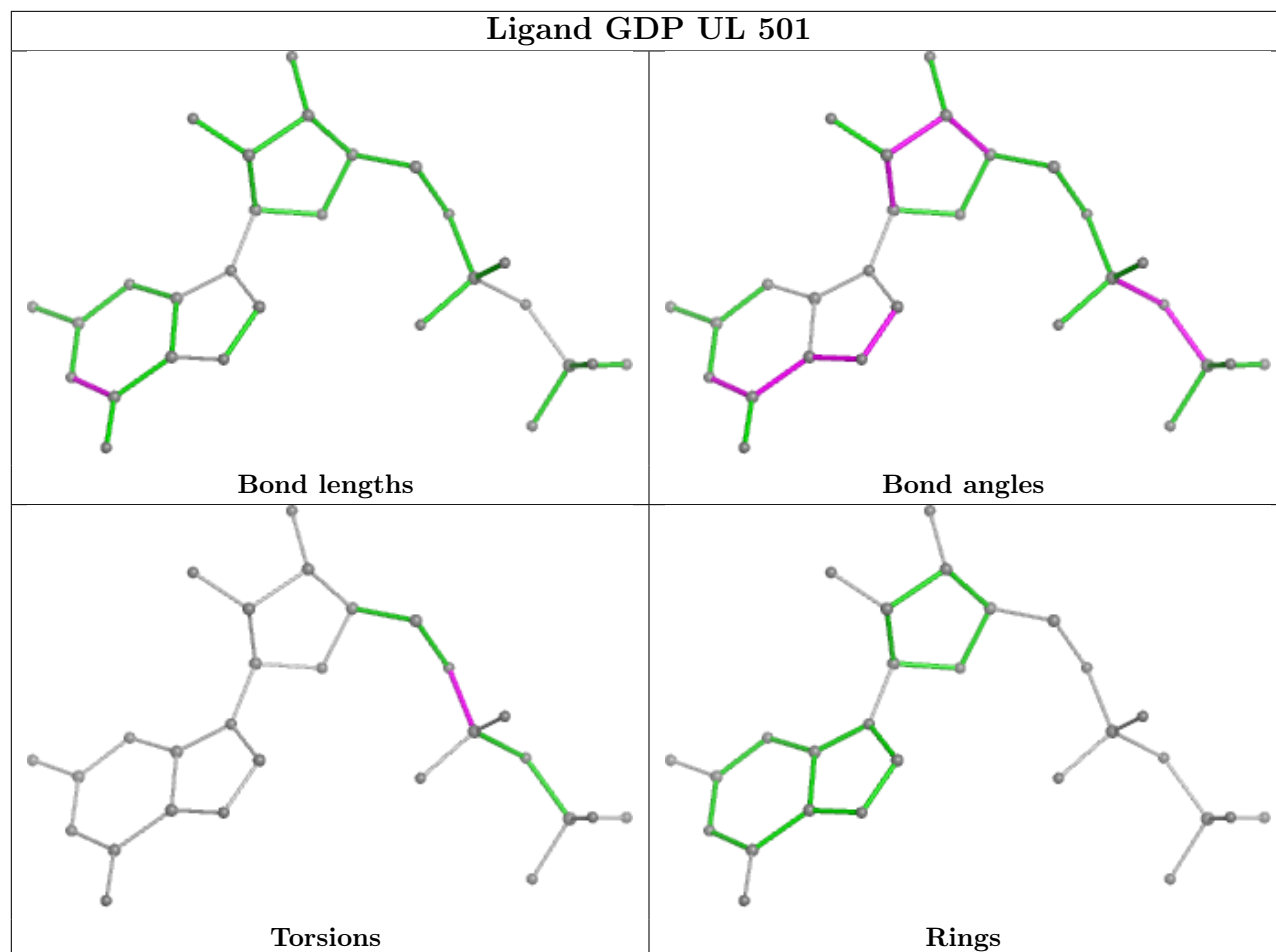
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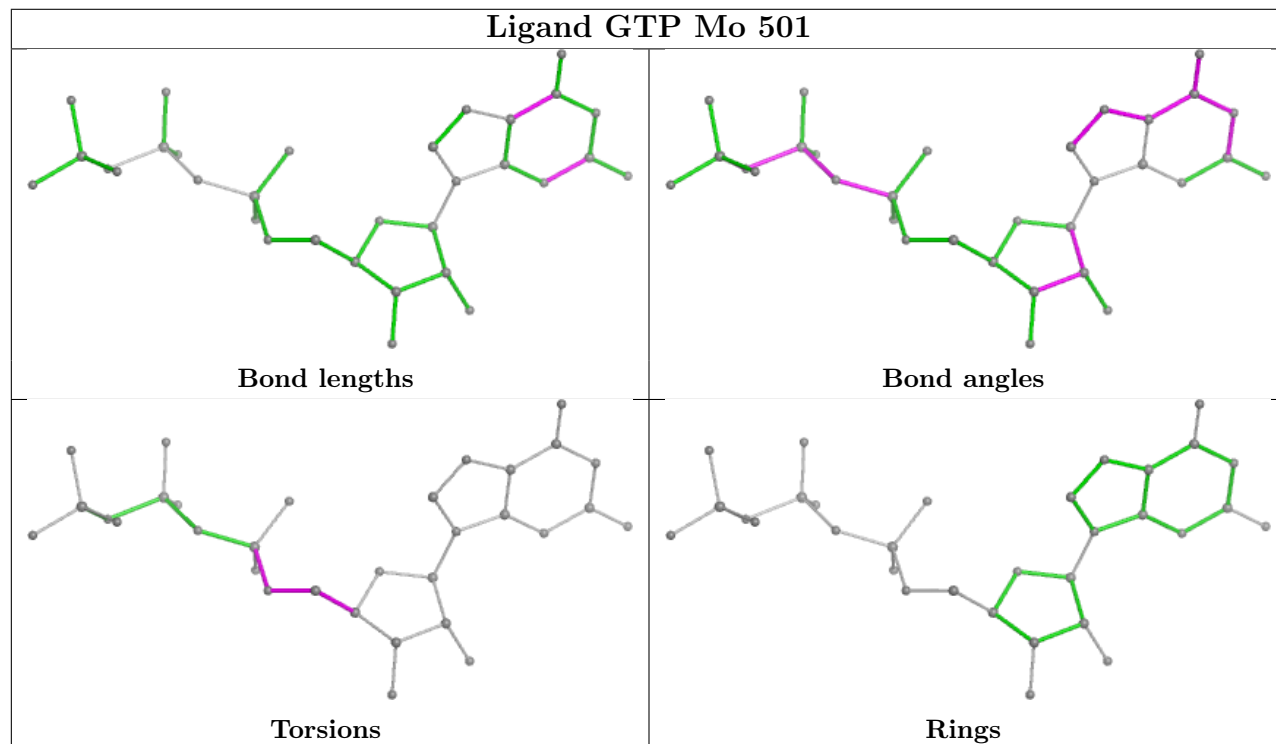
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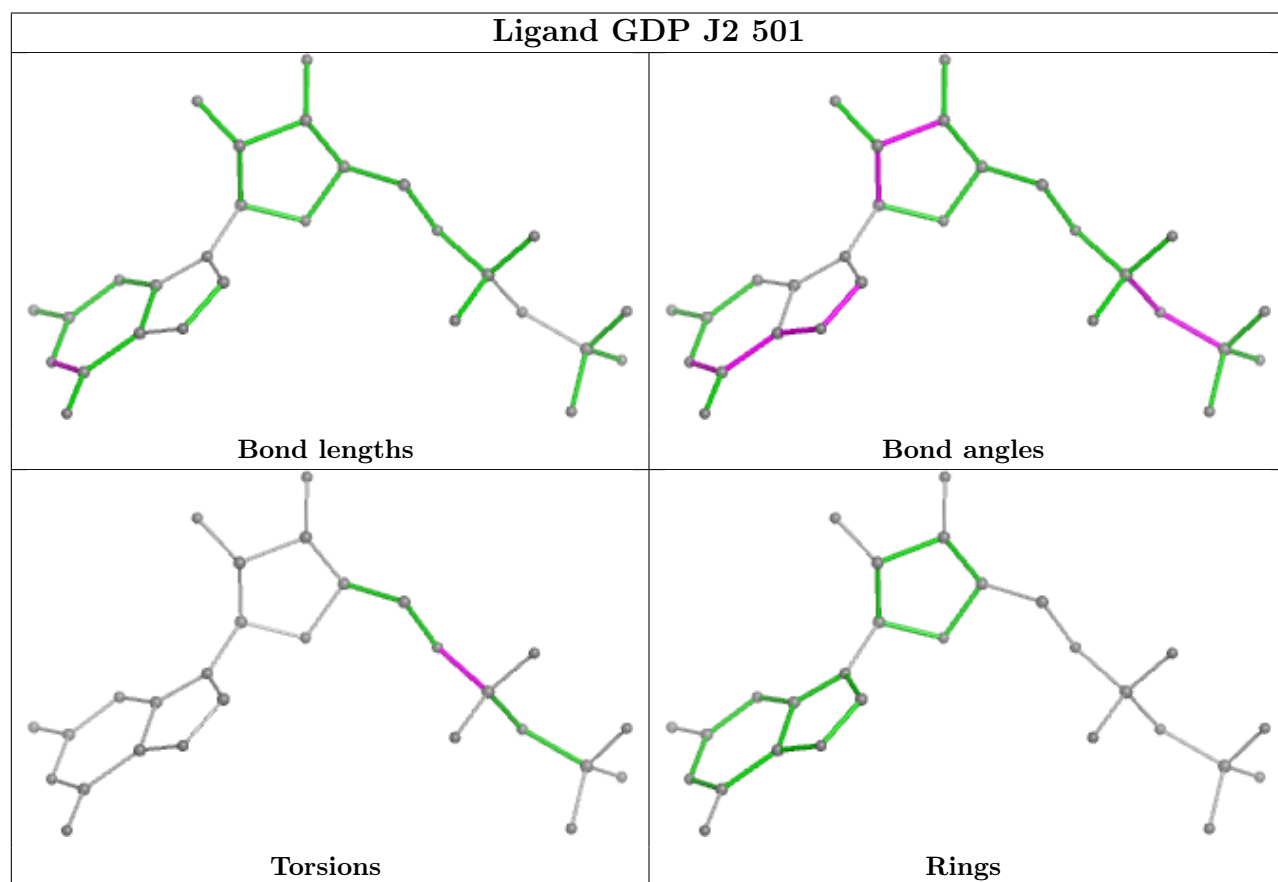
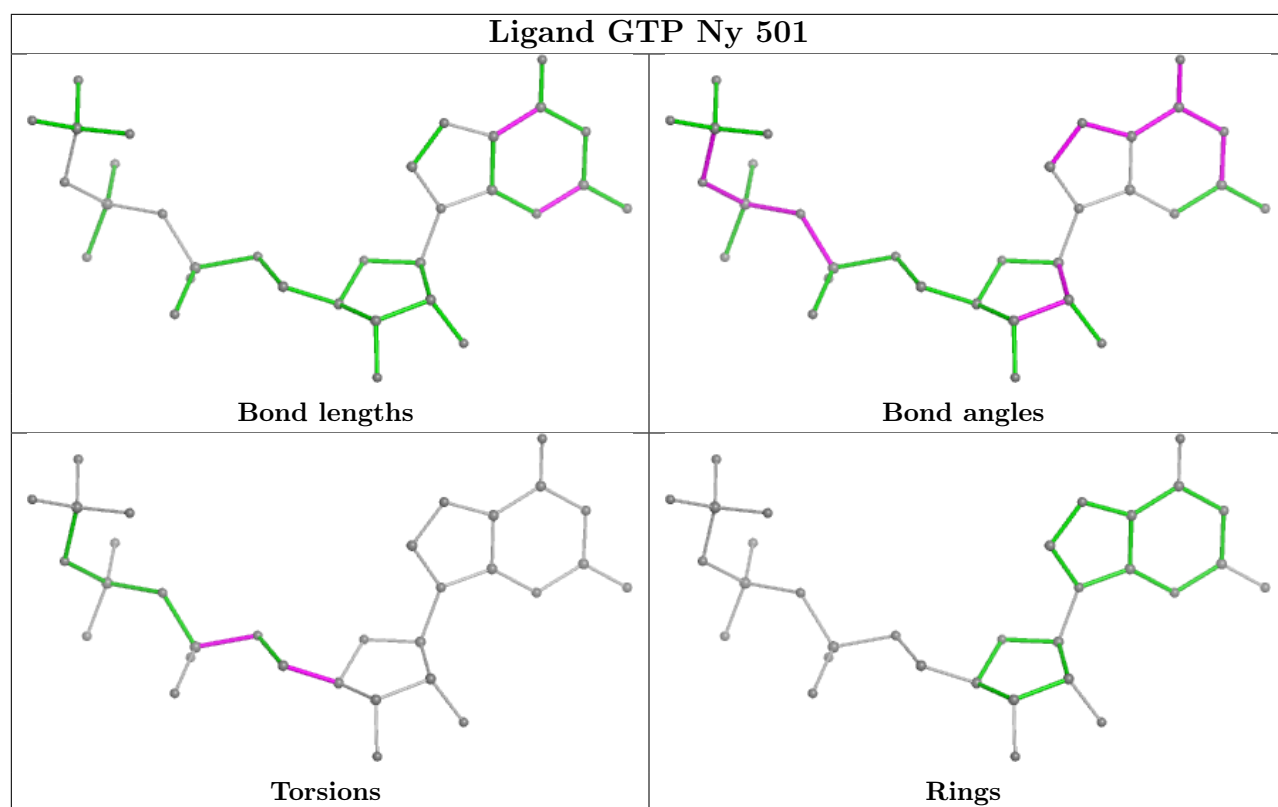


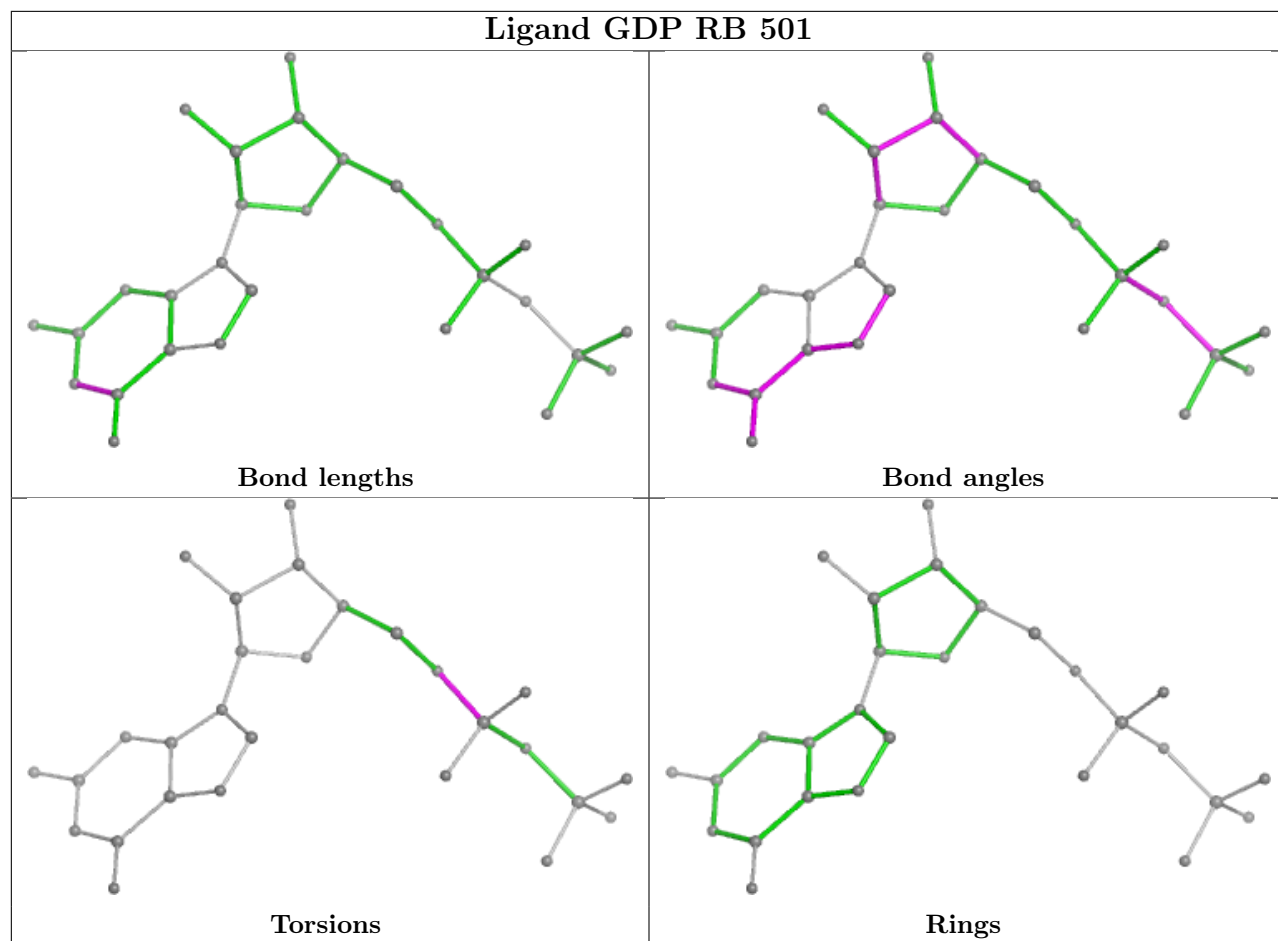
## Ligand GDP UL 501

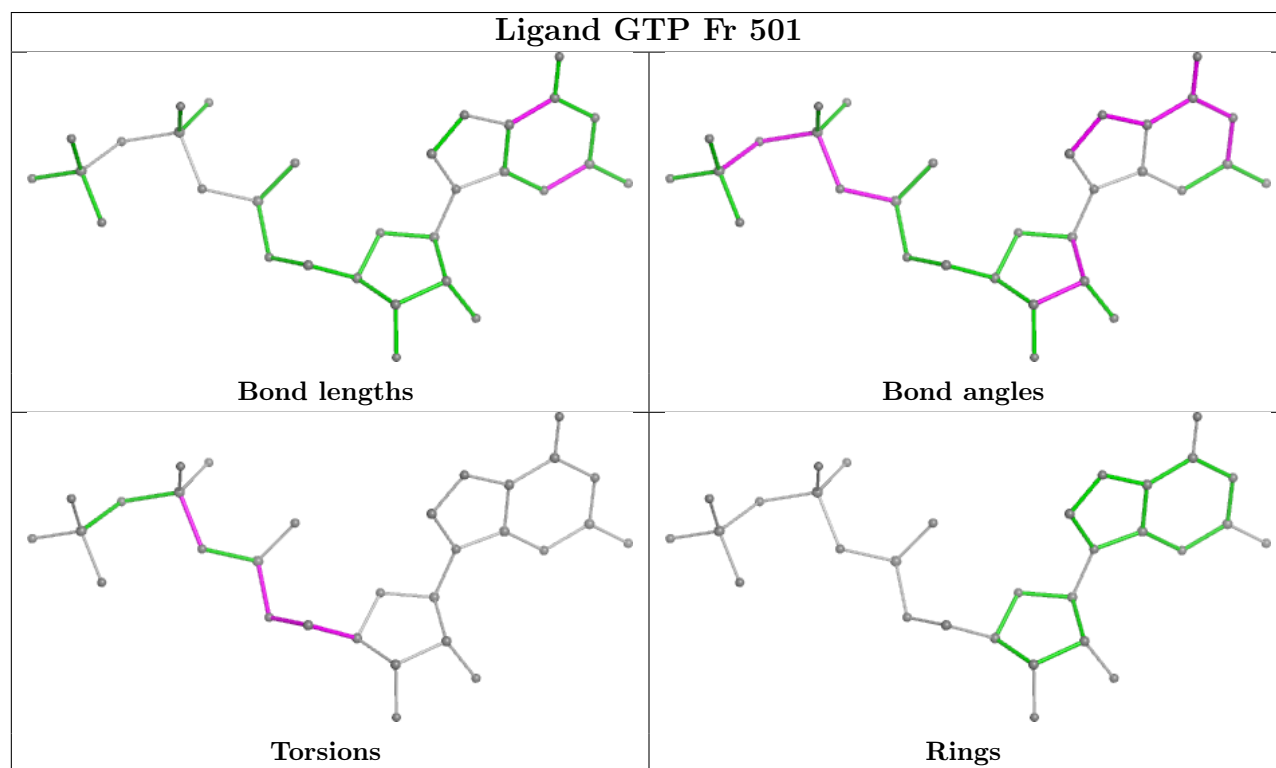
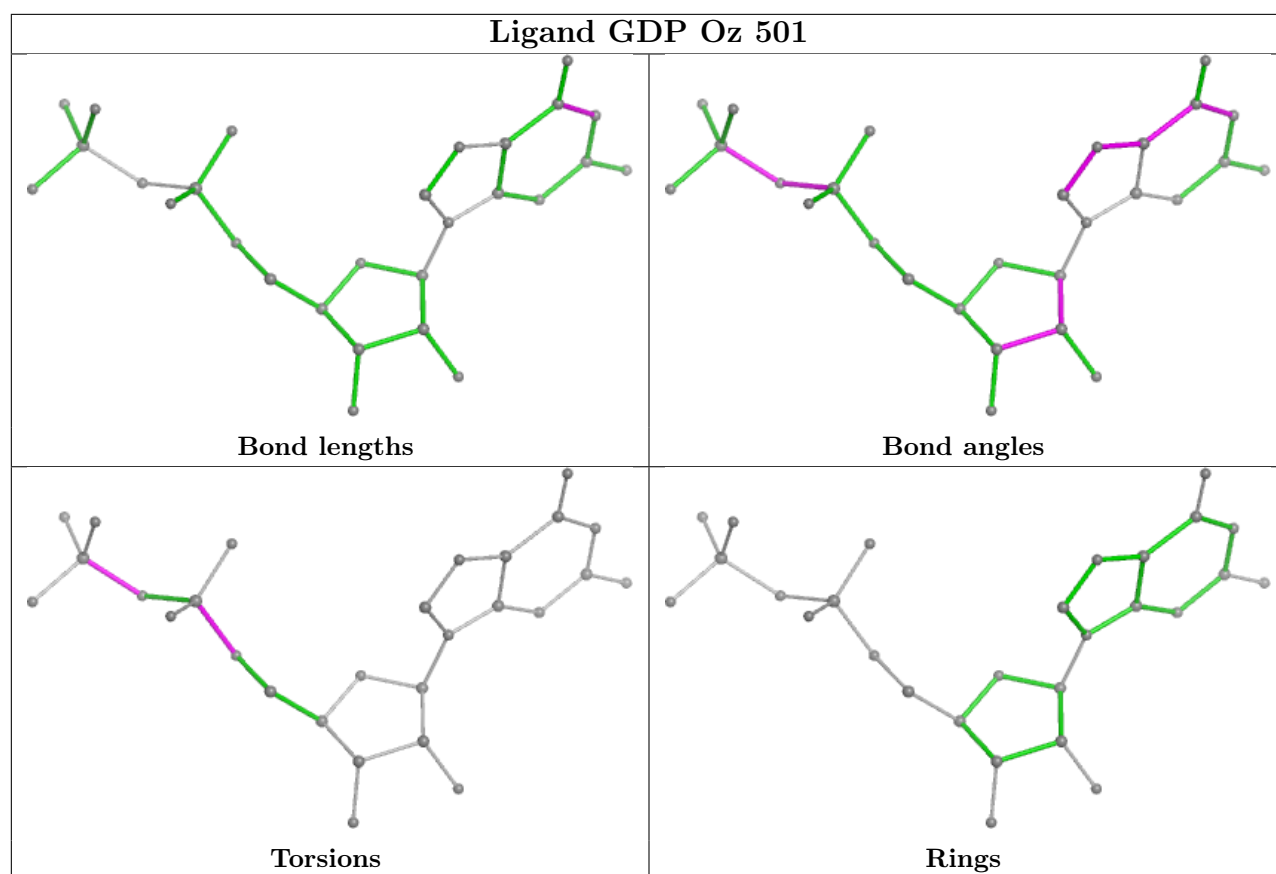


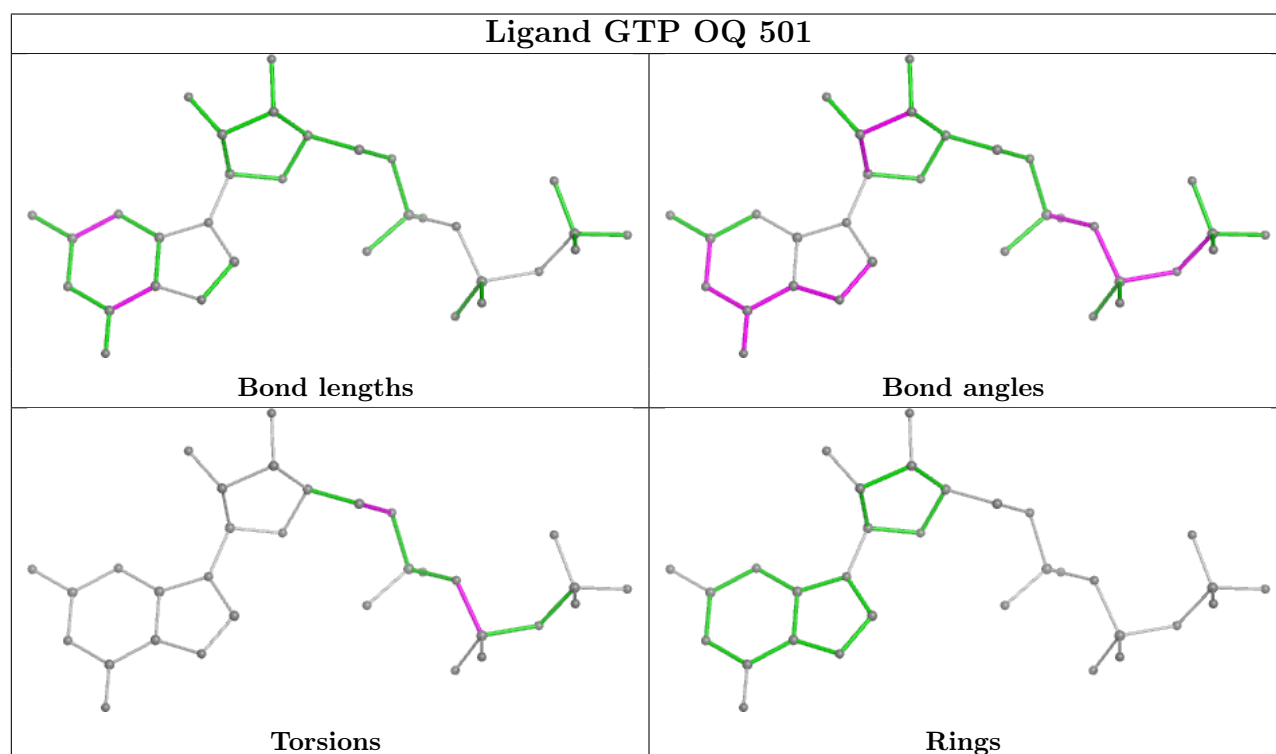
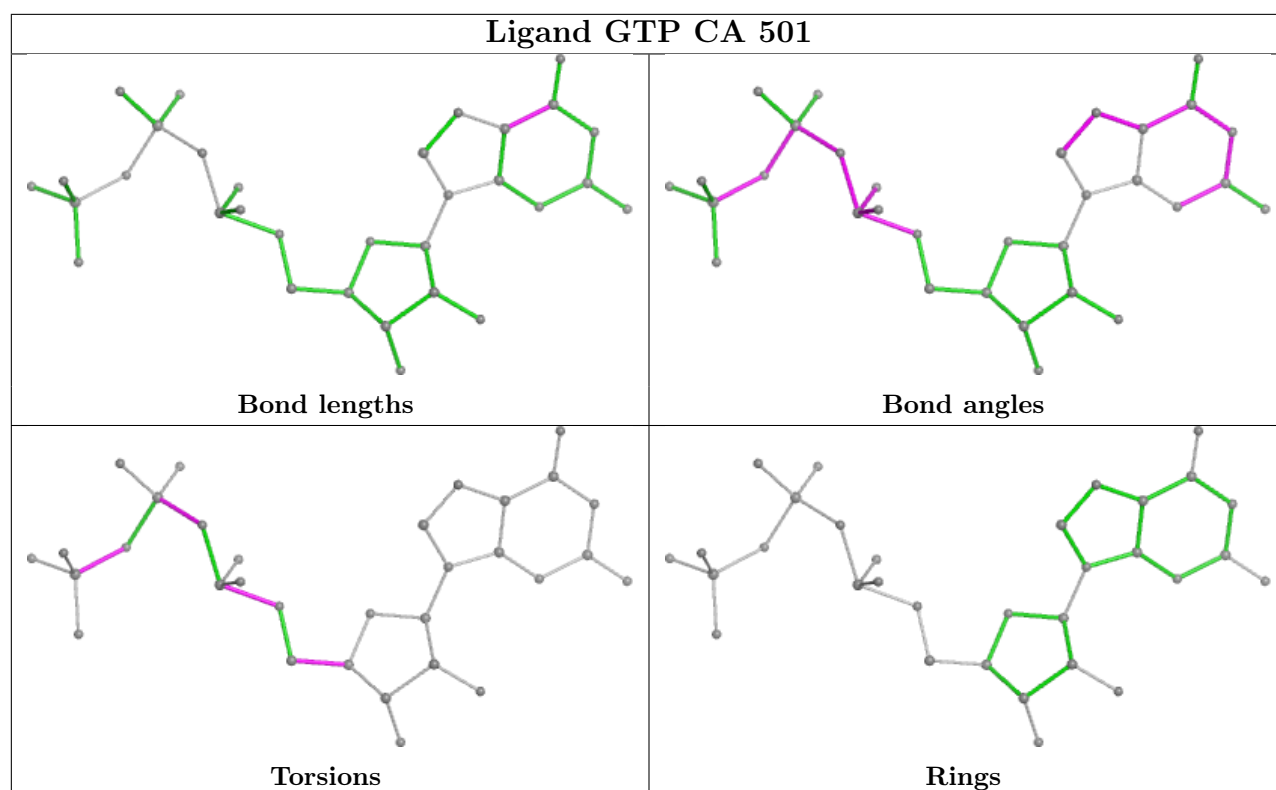
## Ligand GTP Mo 501



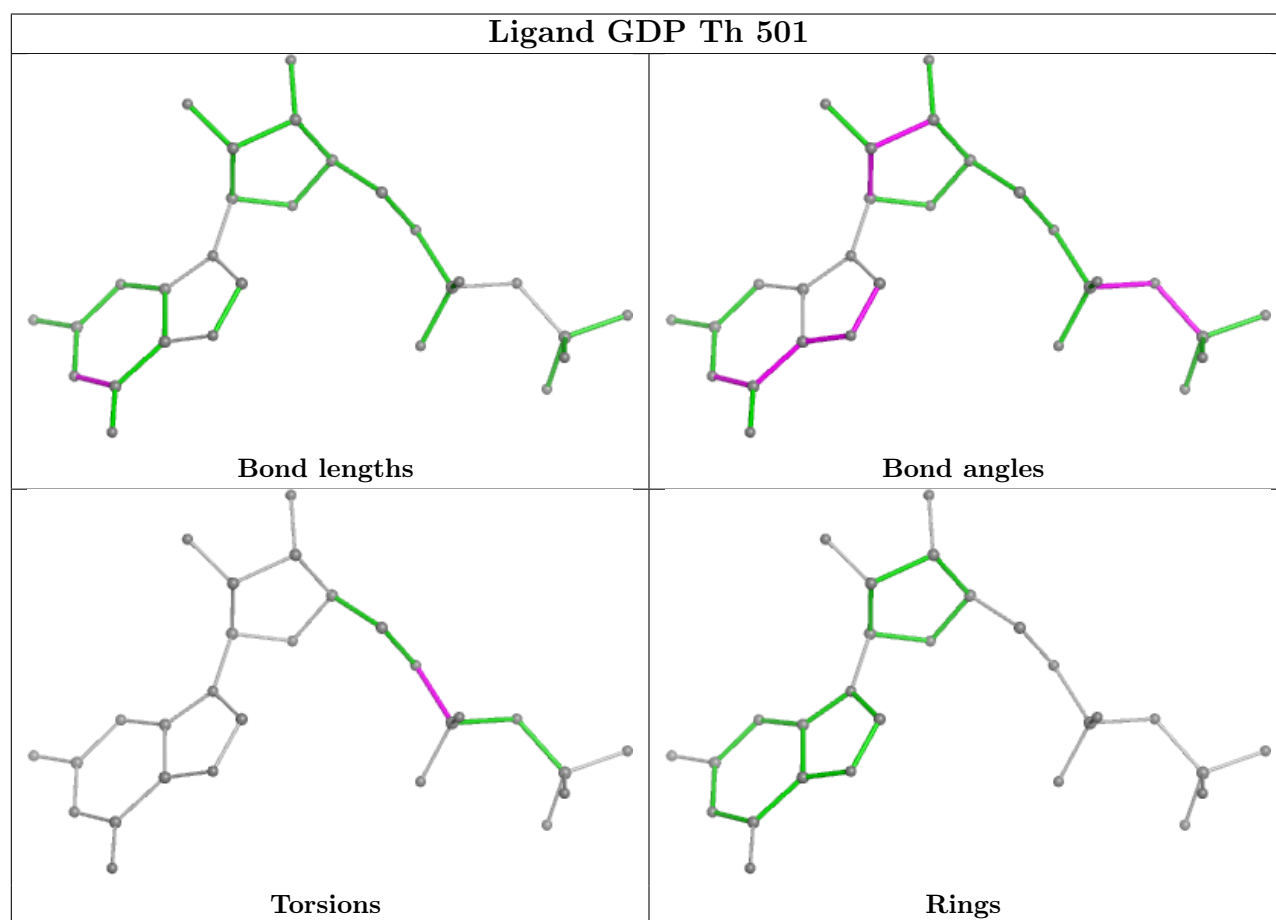
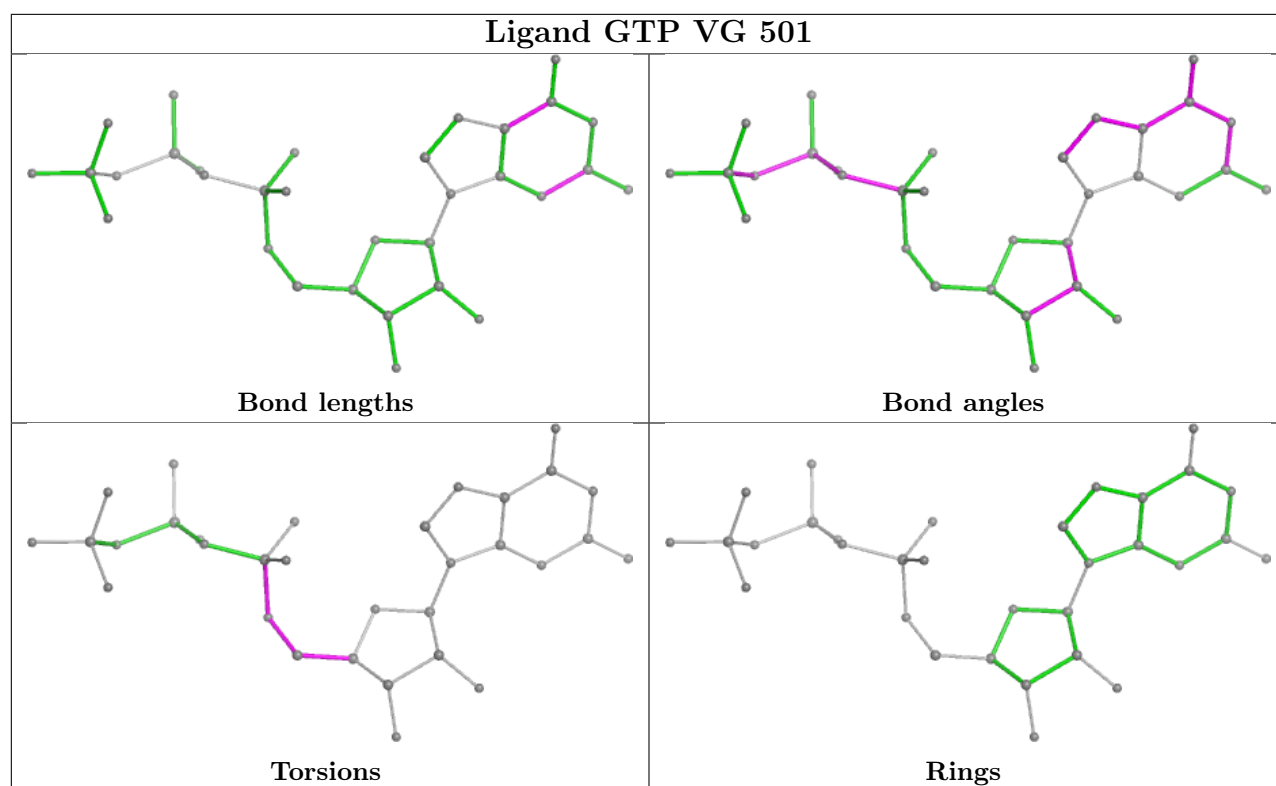


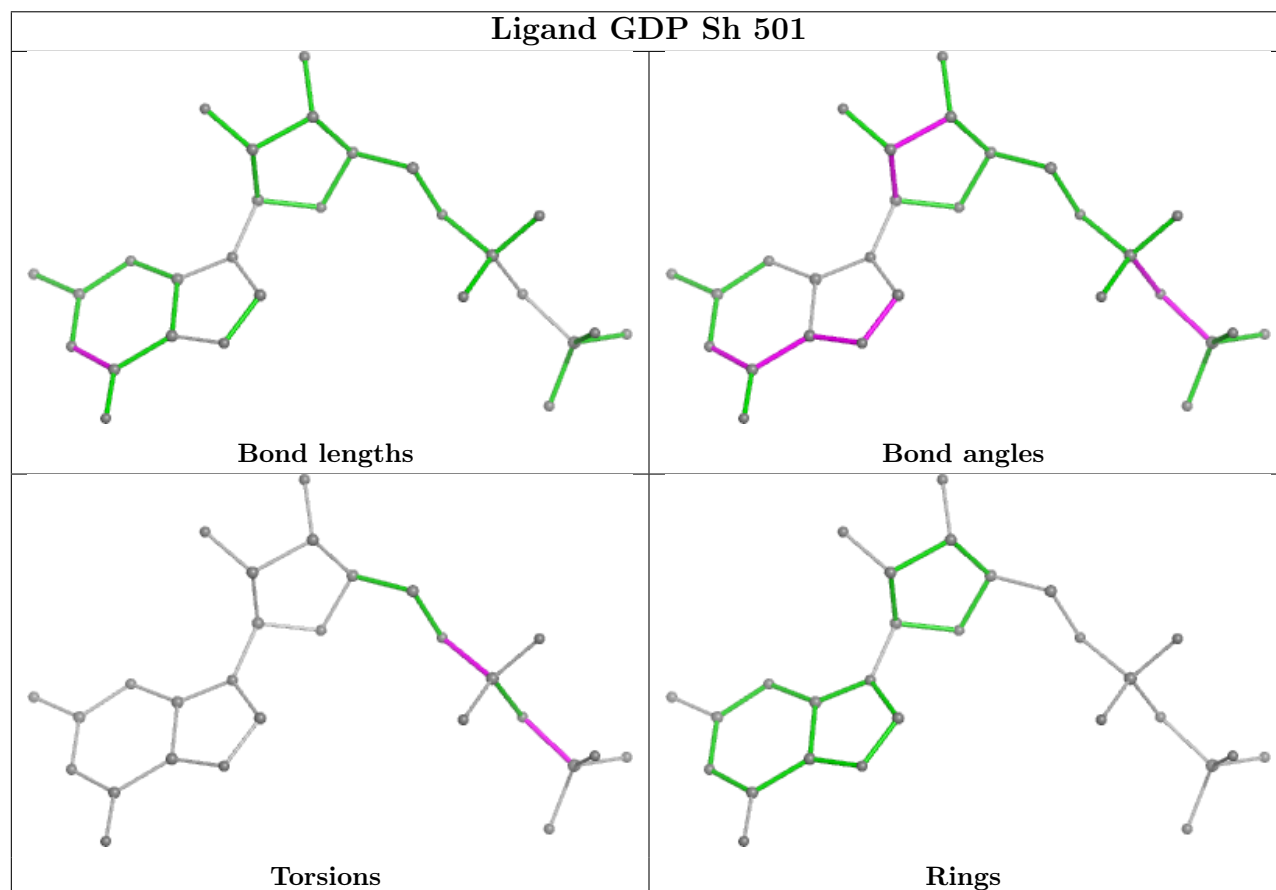
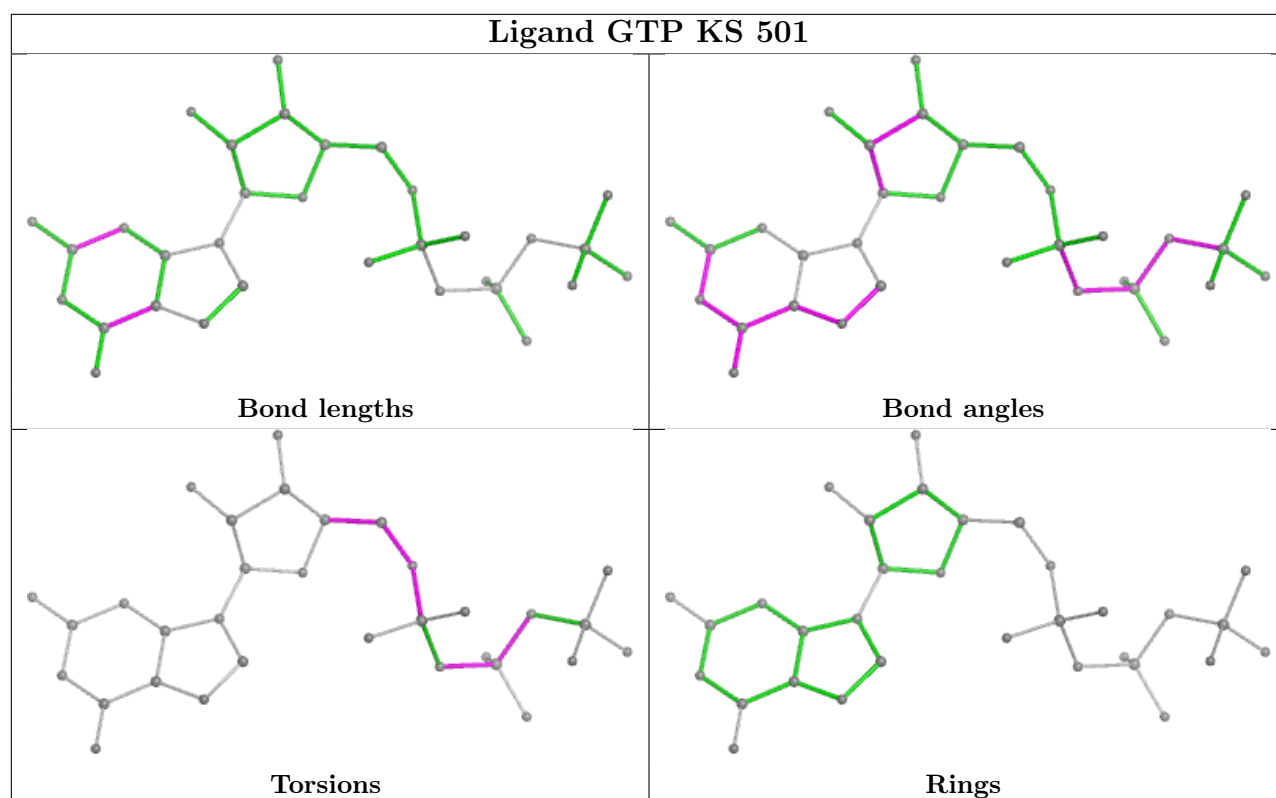


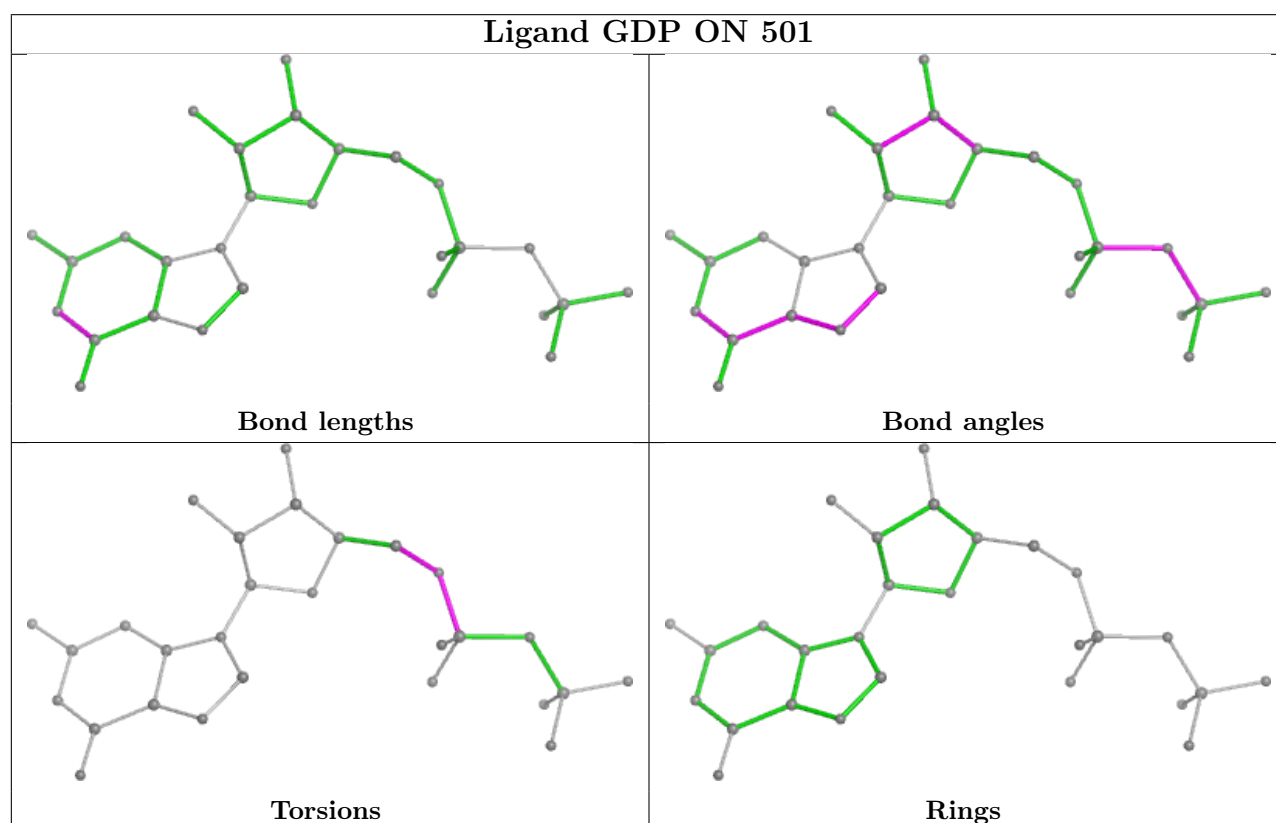
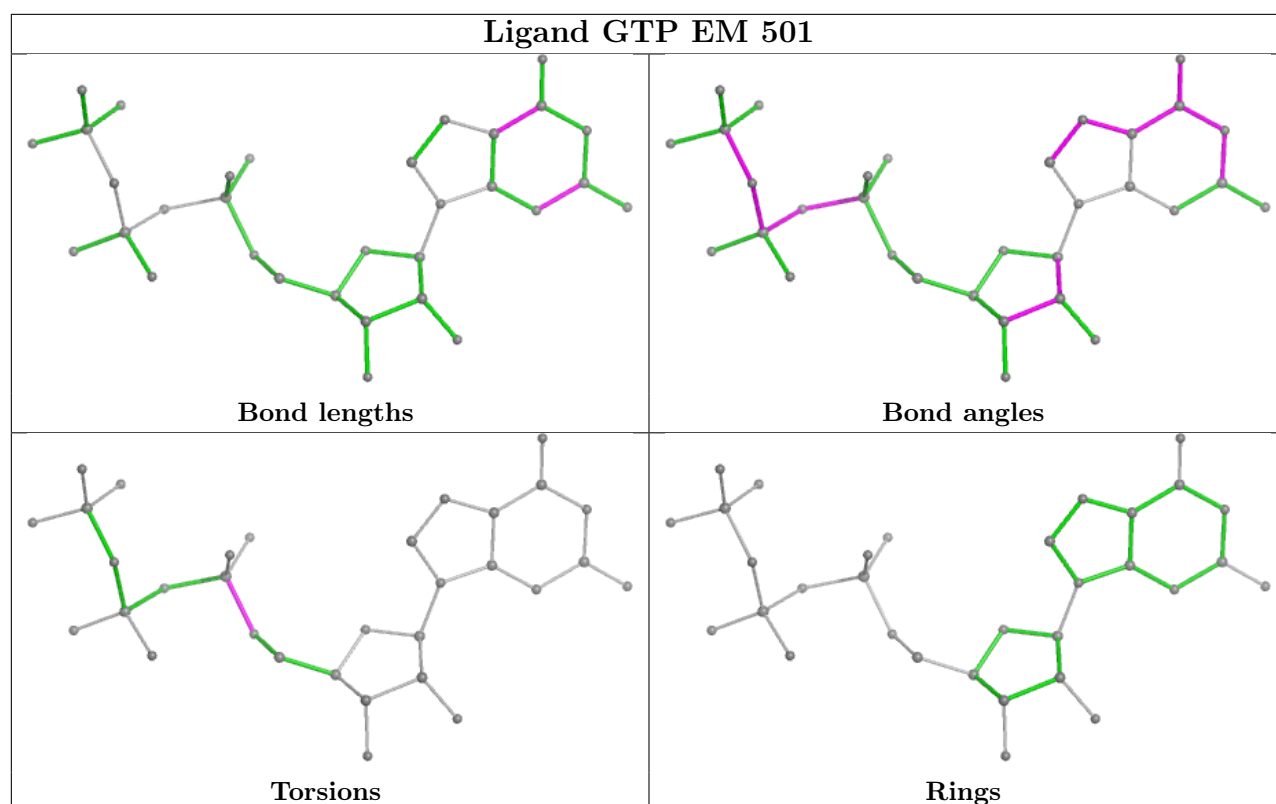




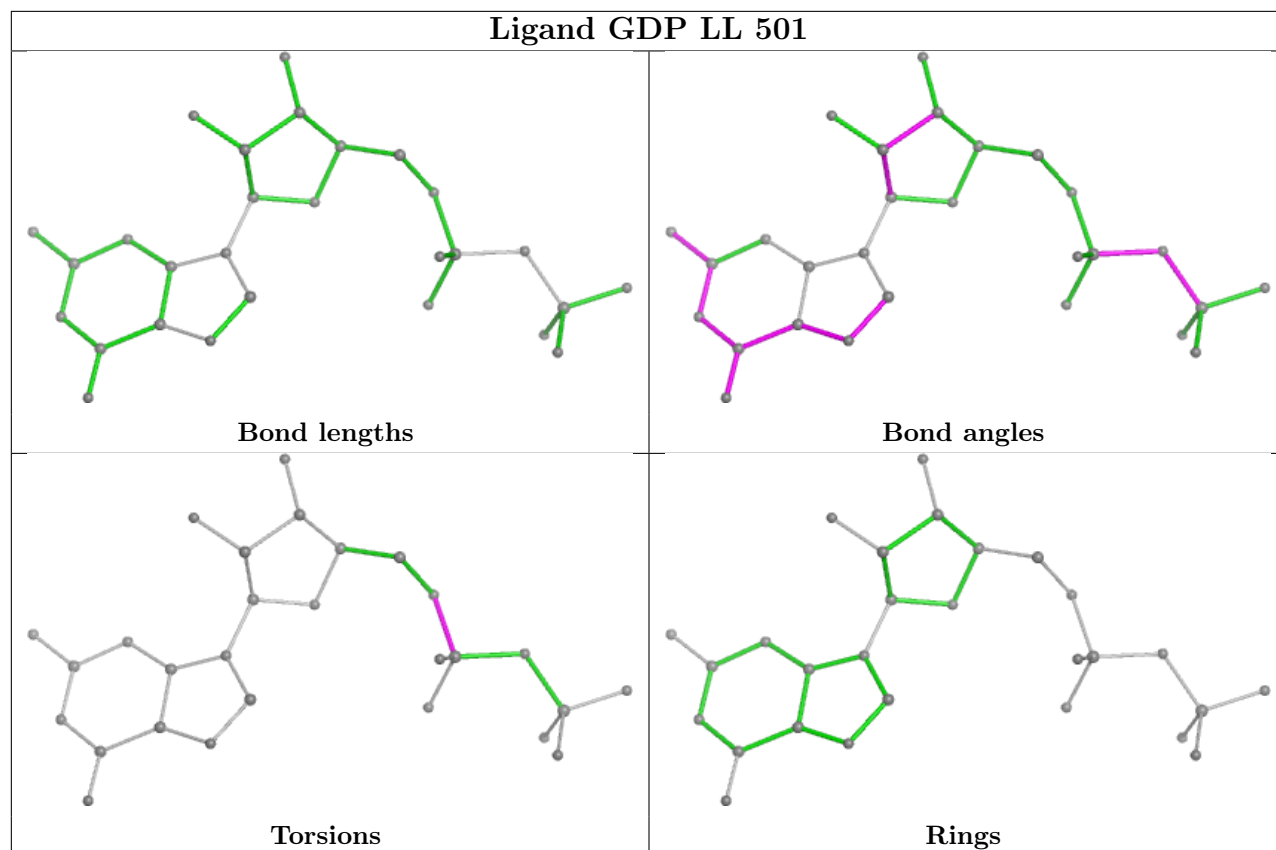




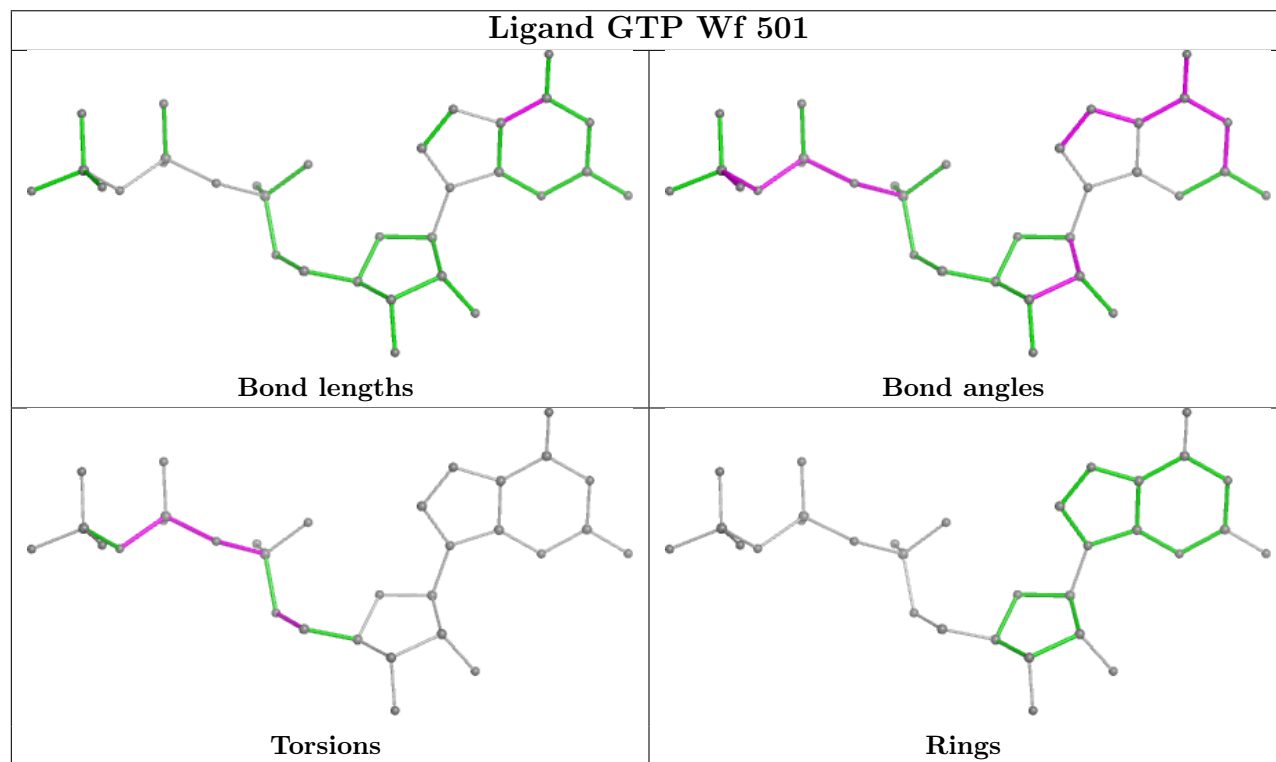




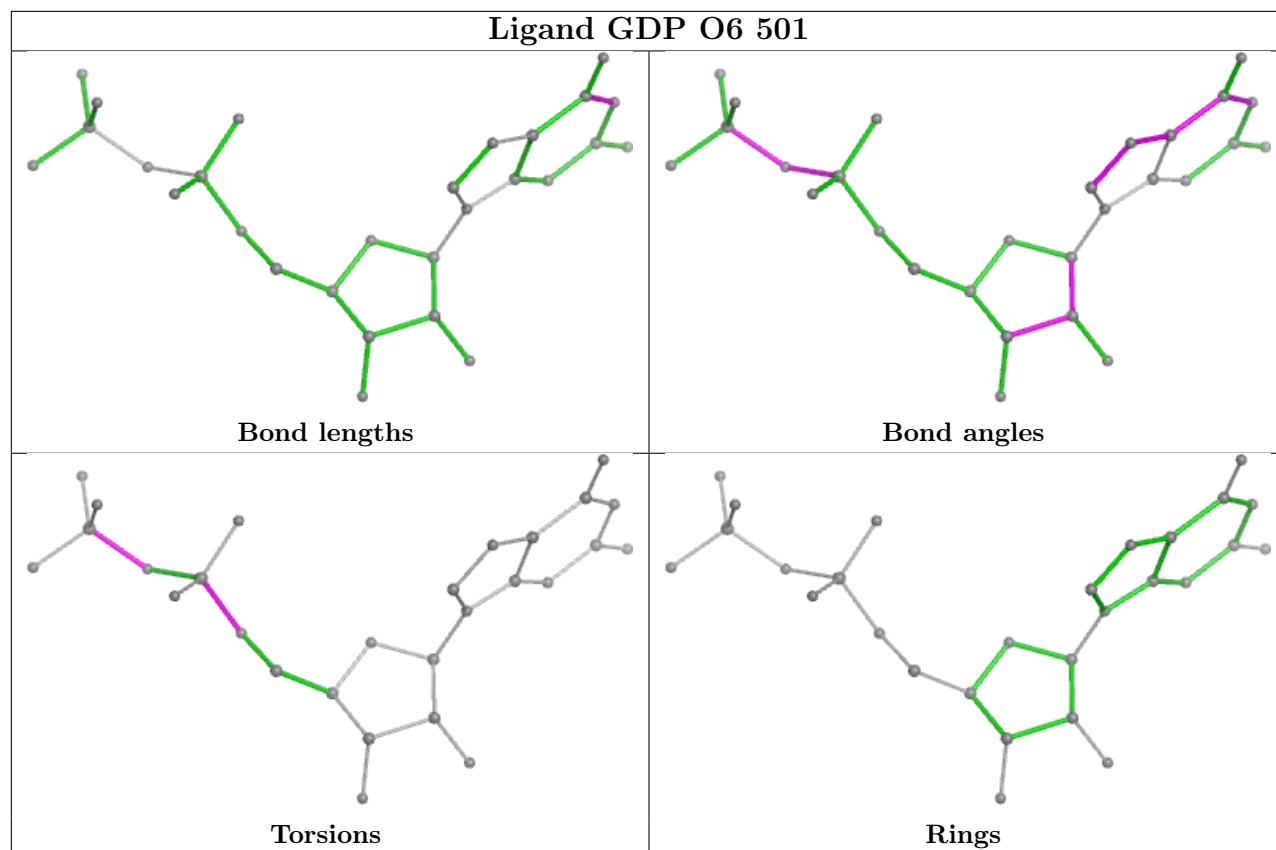
## Ligand GDP LL 501



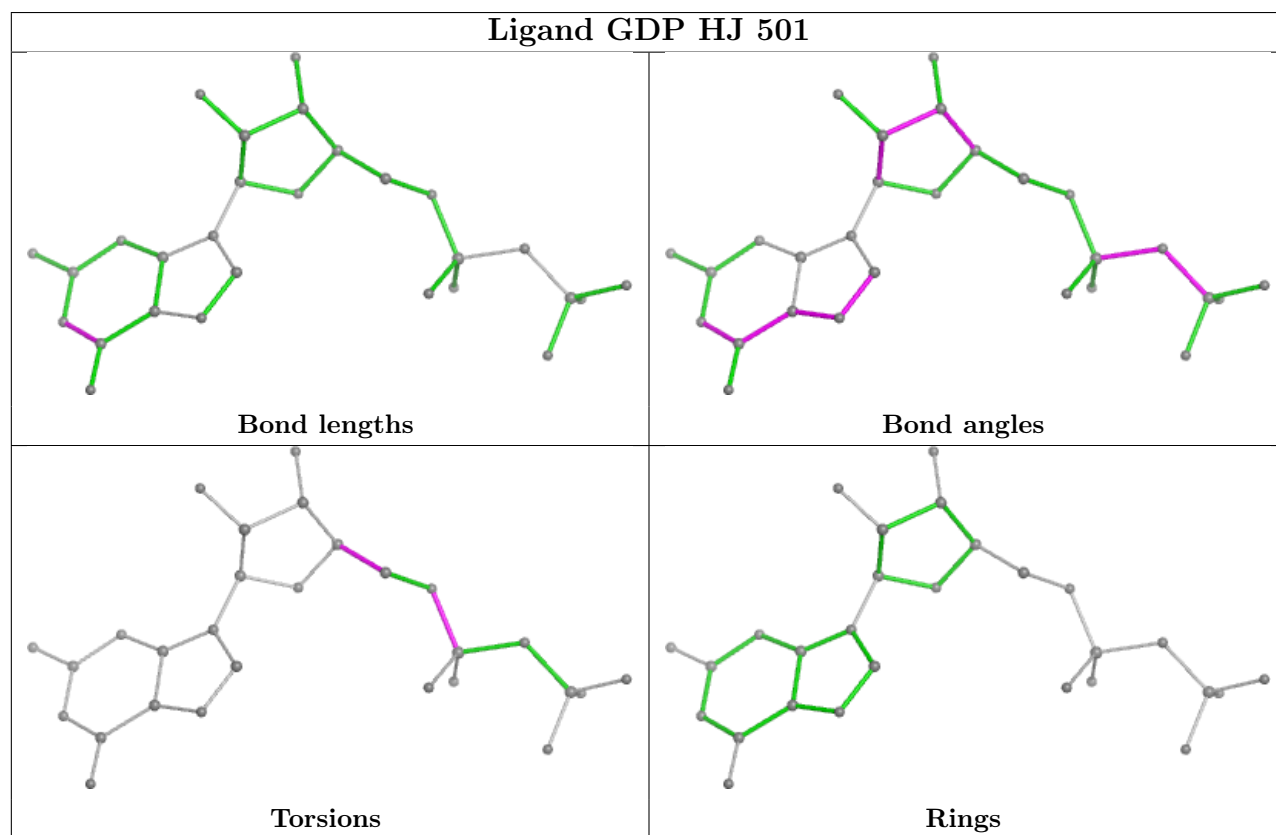
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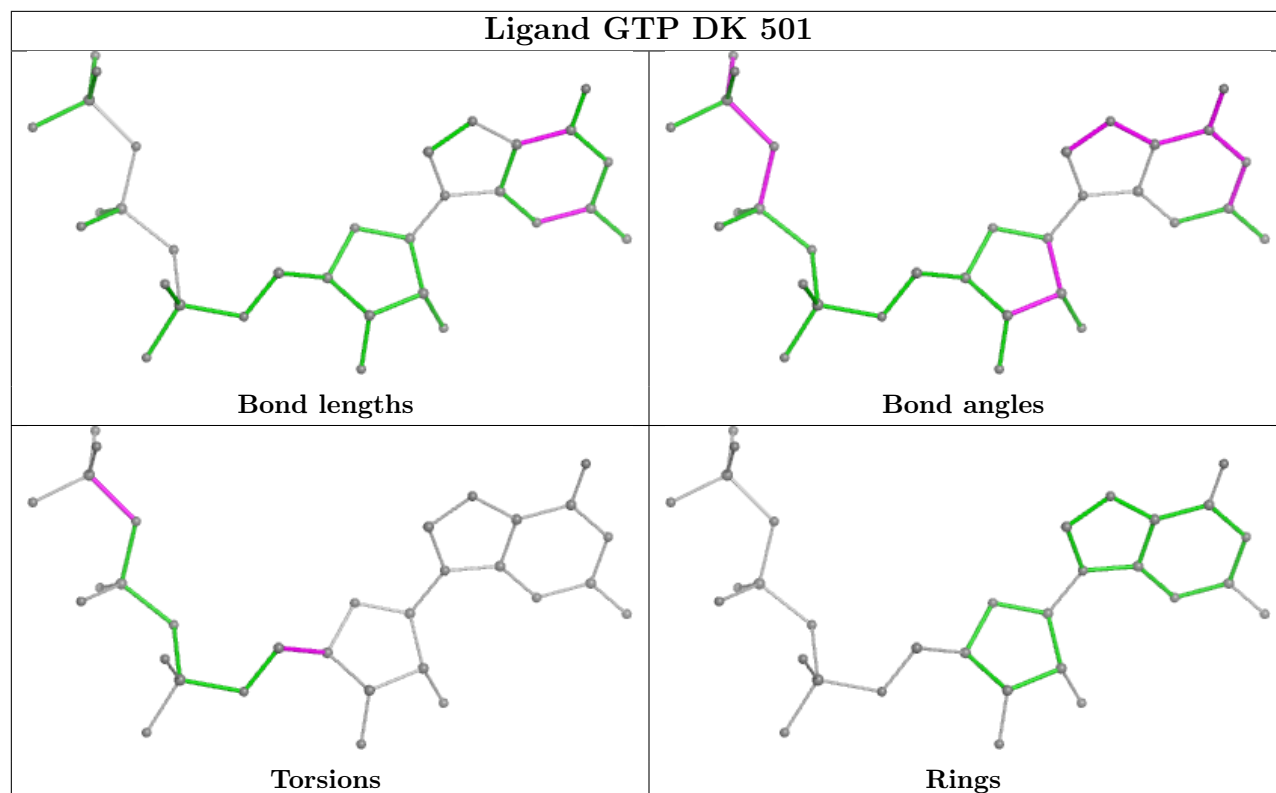
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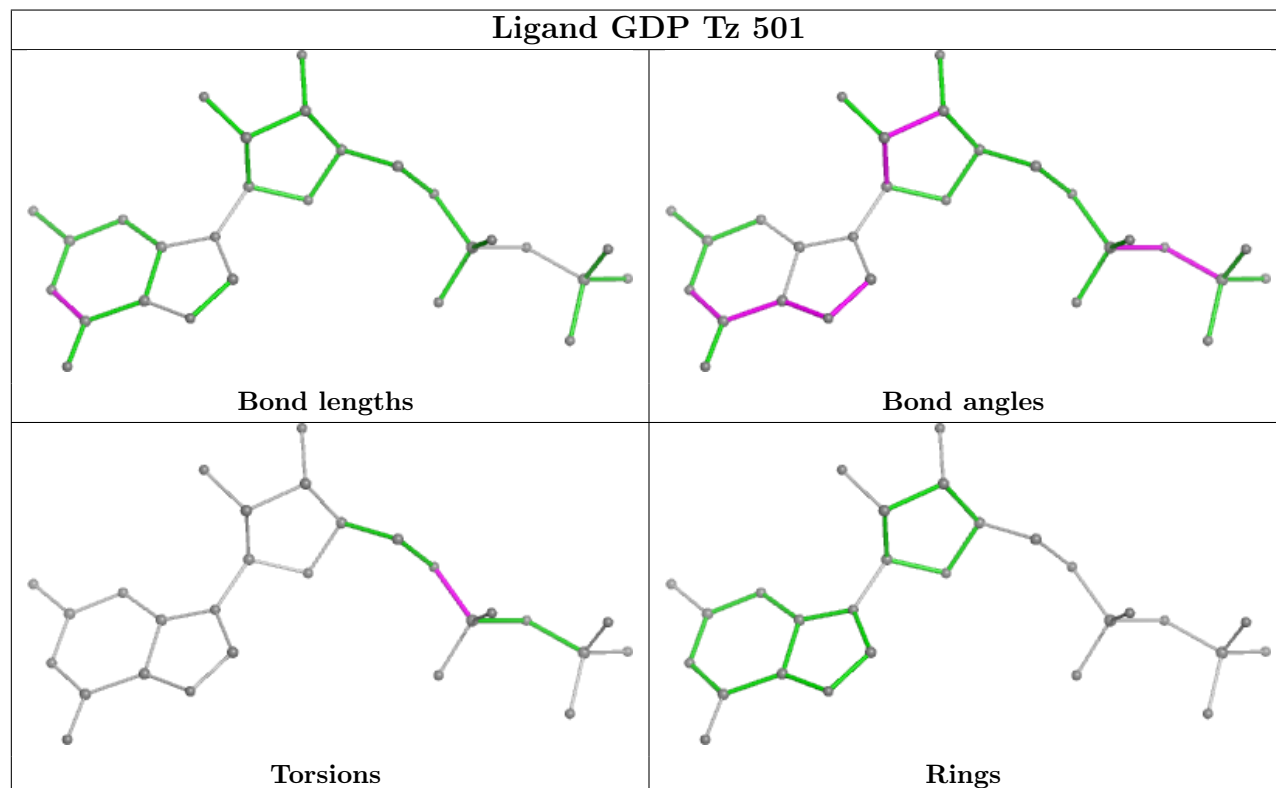
## Ligand GDP HJ 501



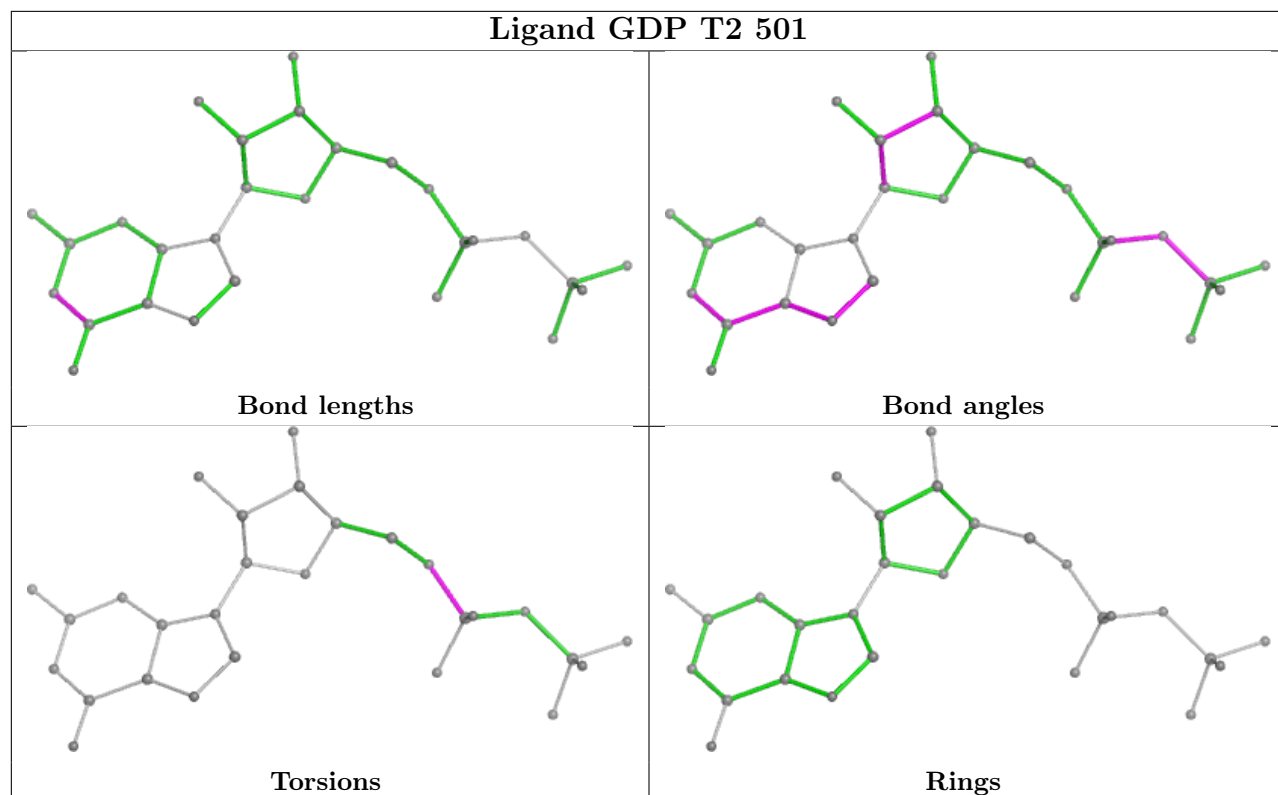
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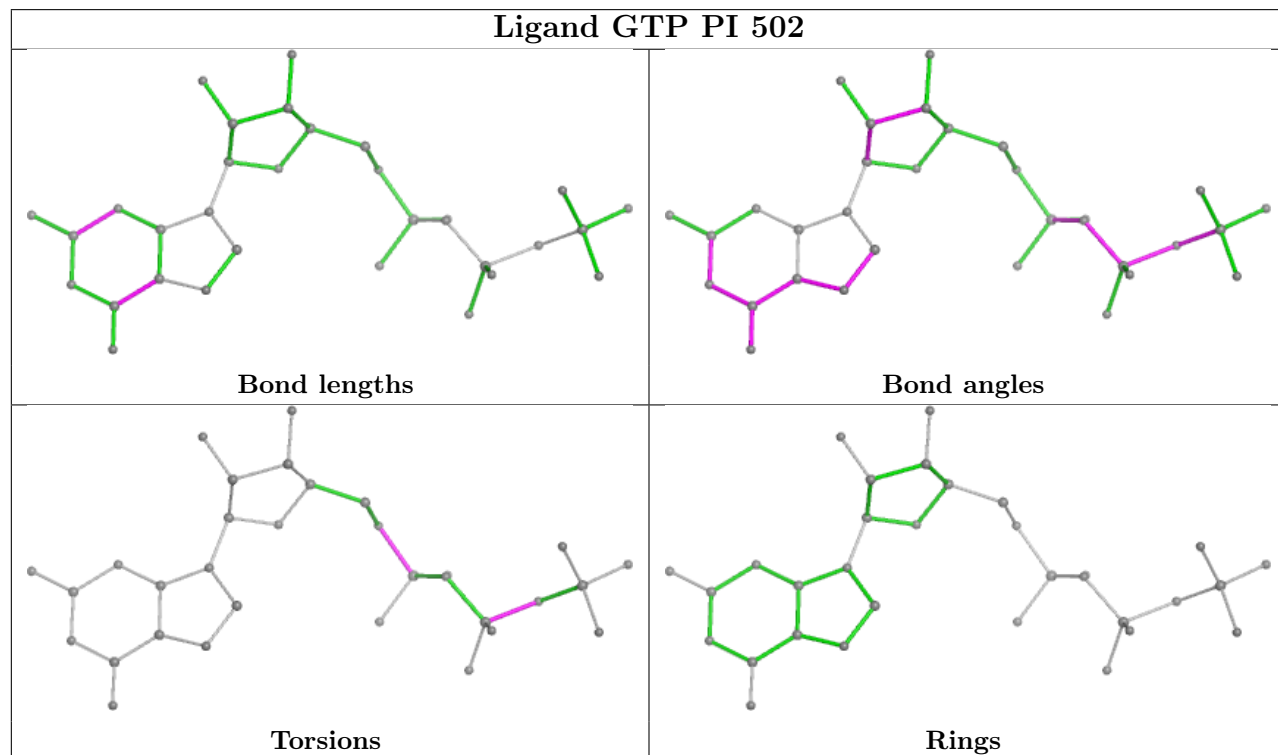
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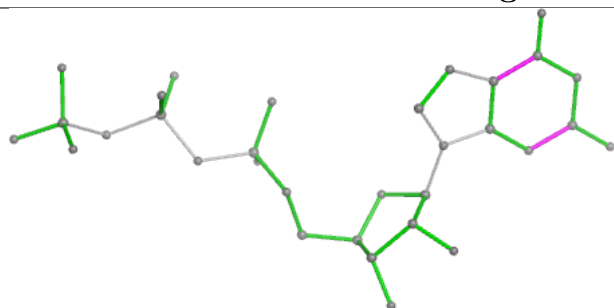
## Ligand GDP T2 501



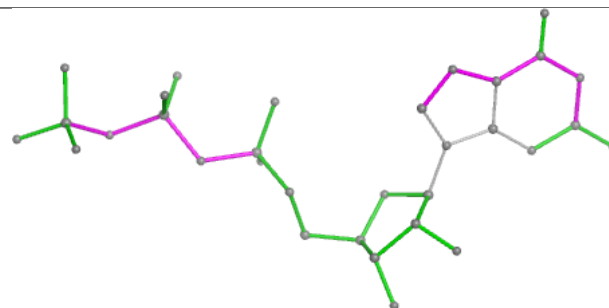
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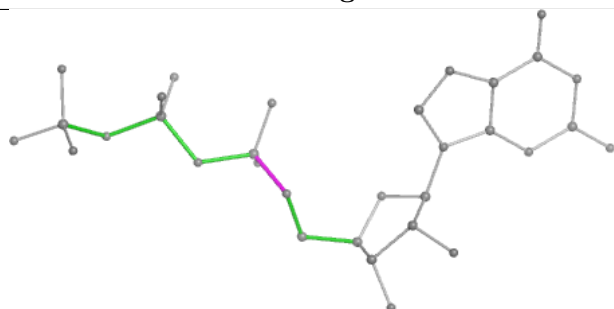
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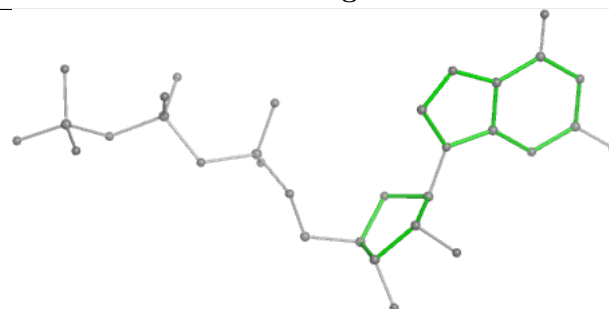
Bond lengths



Bond angles

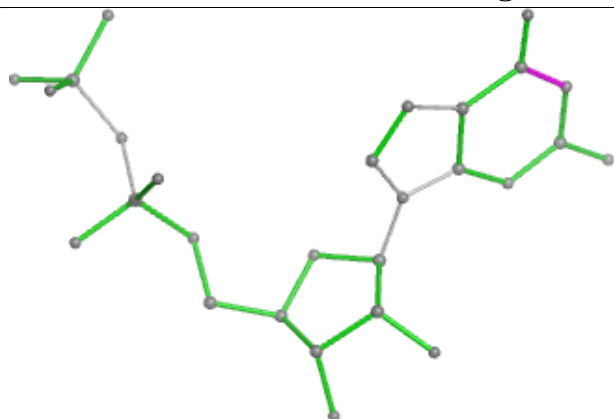


Torsions

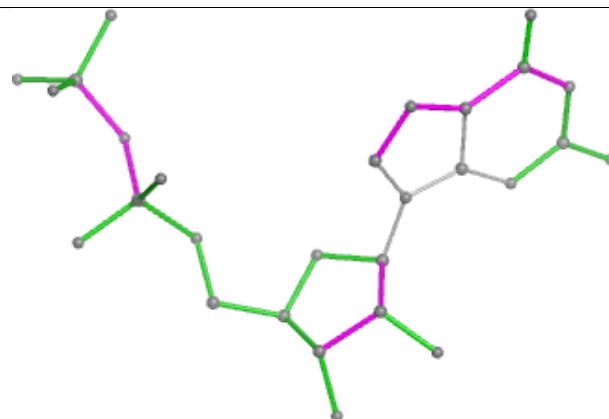


Rings

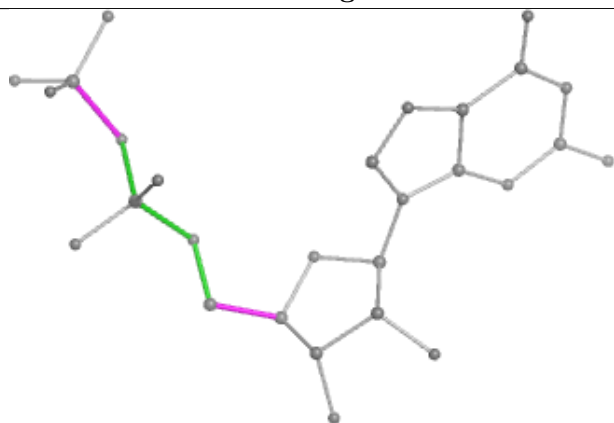
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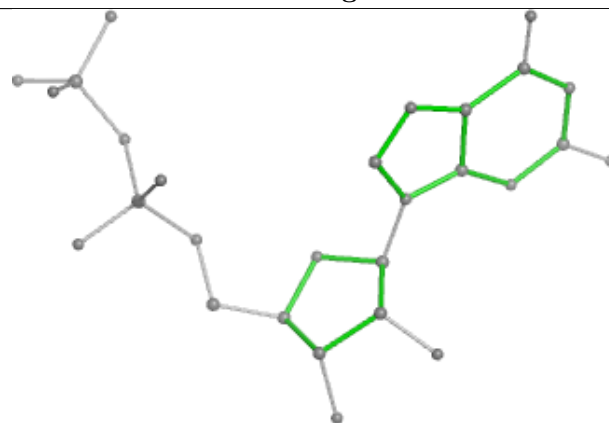
Bond lengths



Bond angles



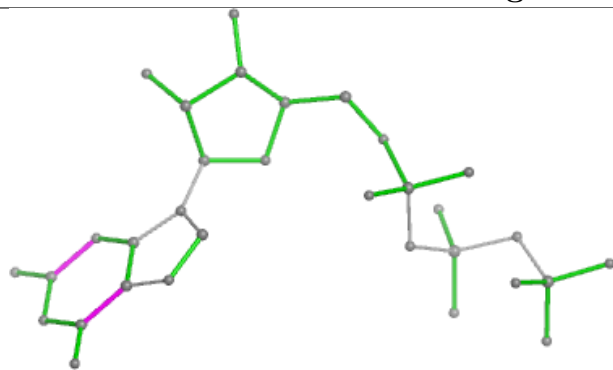
Torsions



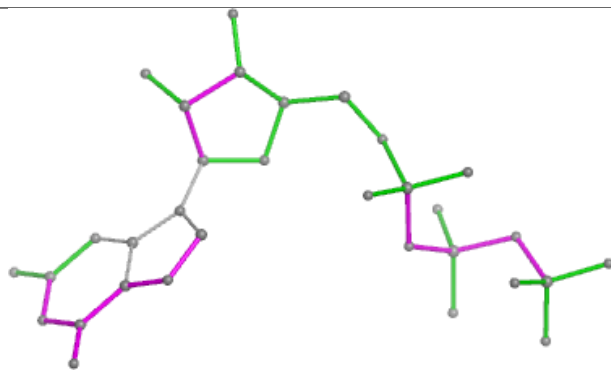
Rings



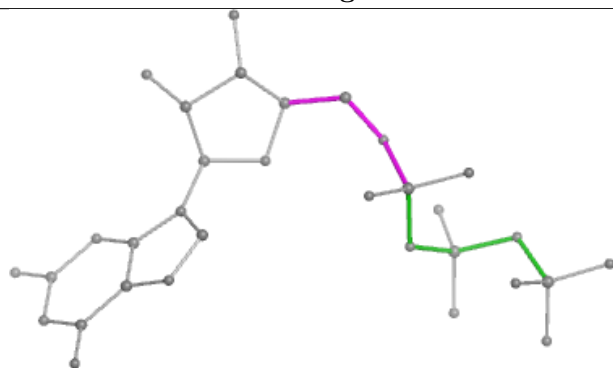
## Ligand GTP Vr 501



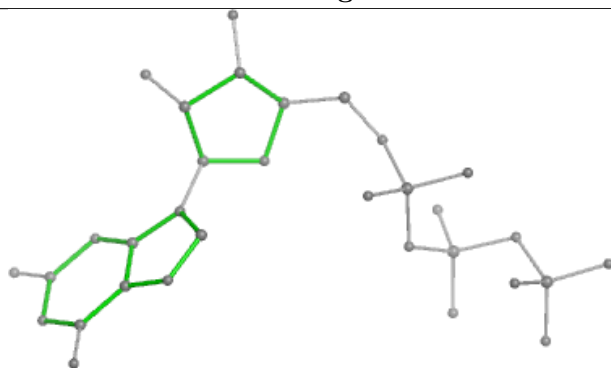
Bond lengths



Bond angles

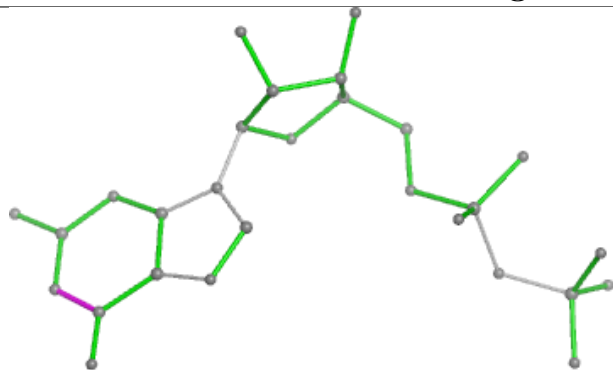


Torsions

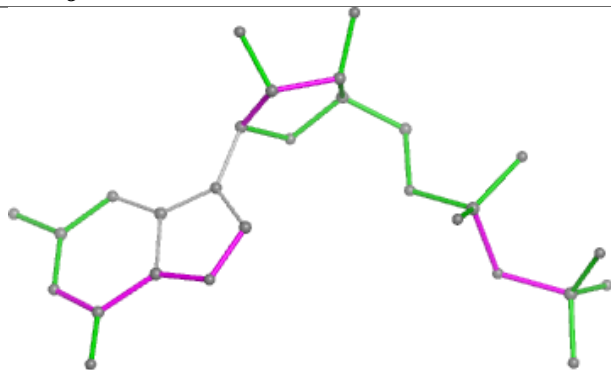


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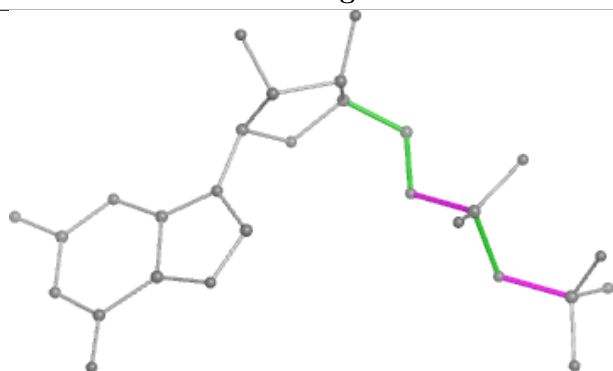
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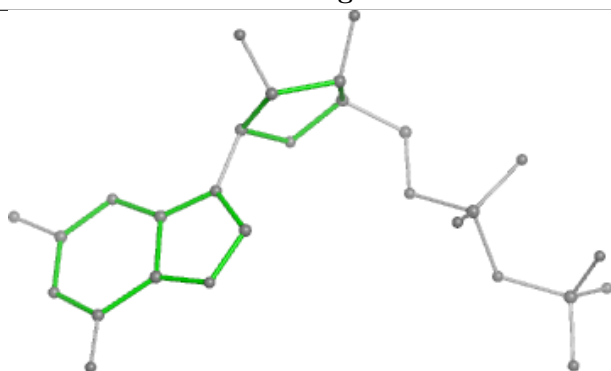
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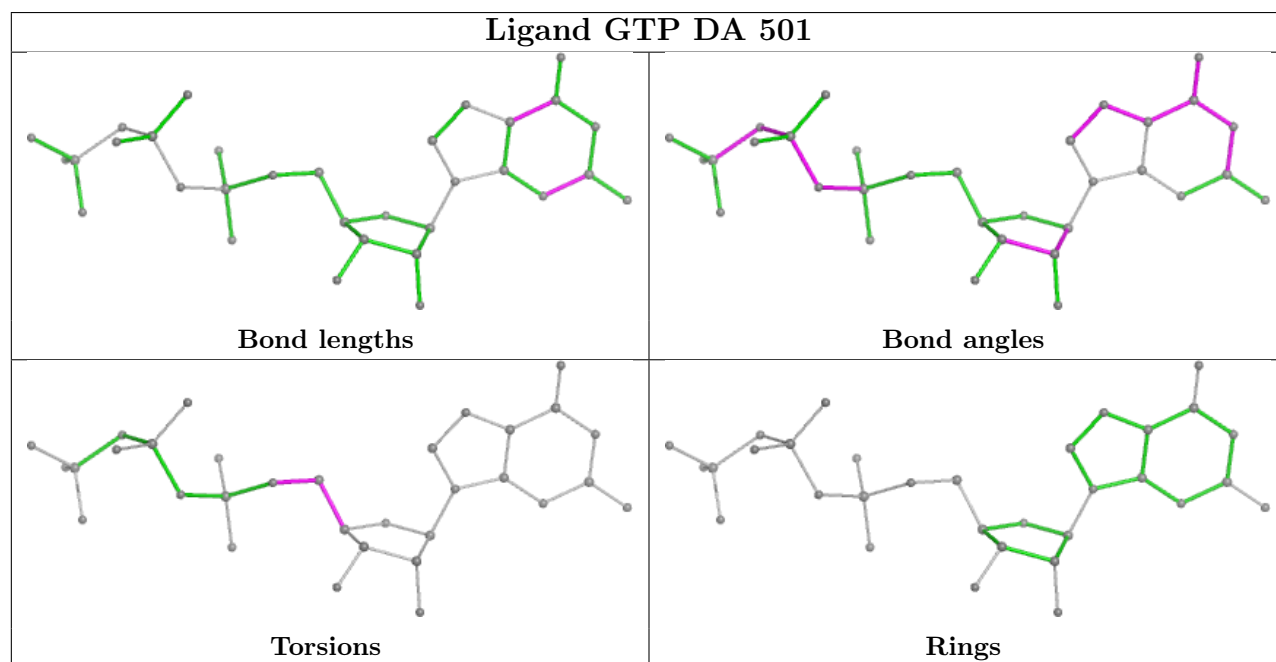
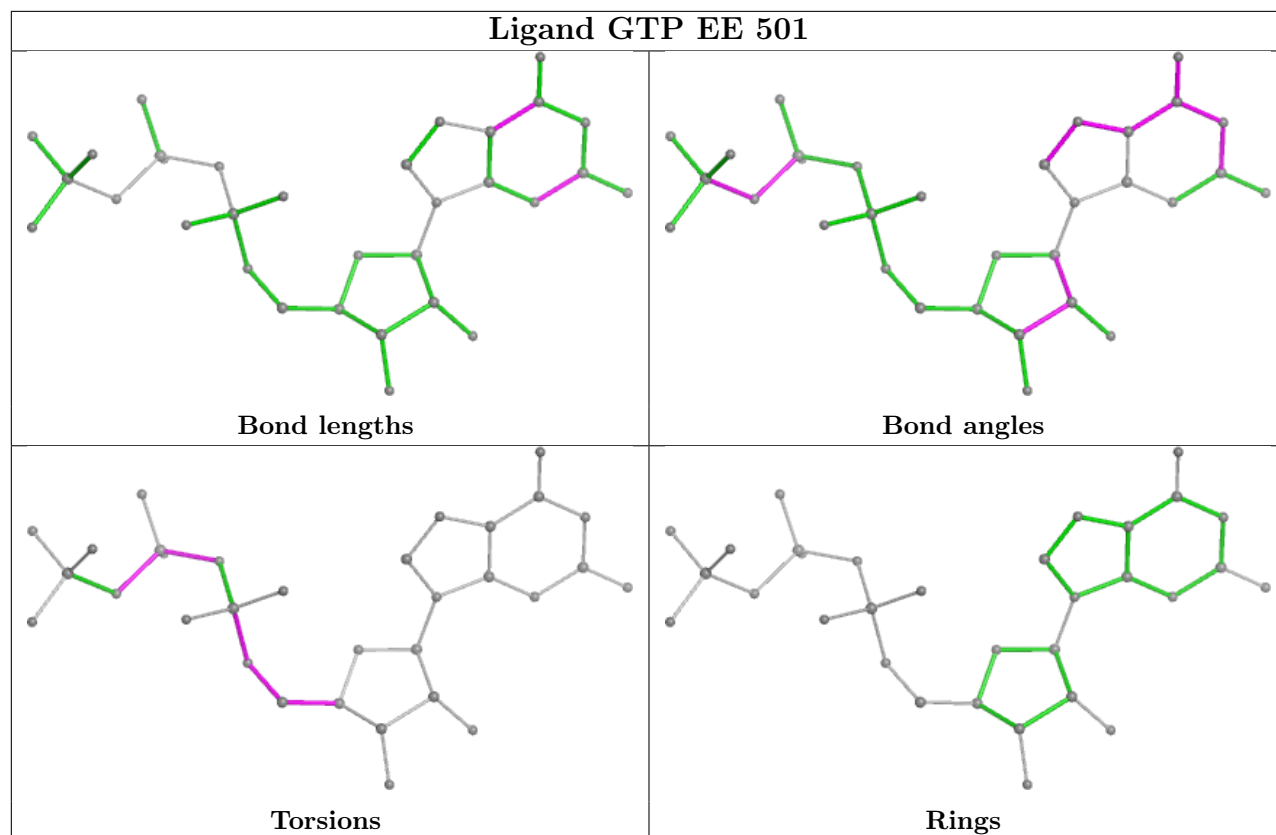
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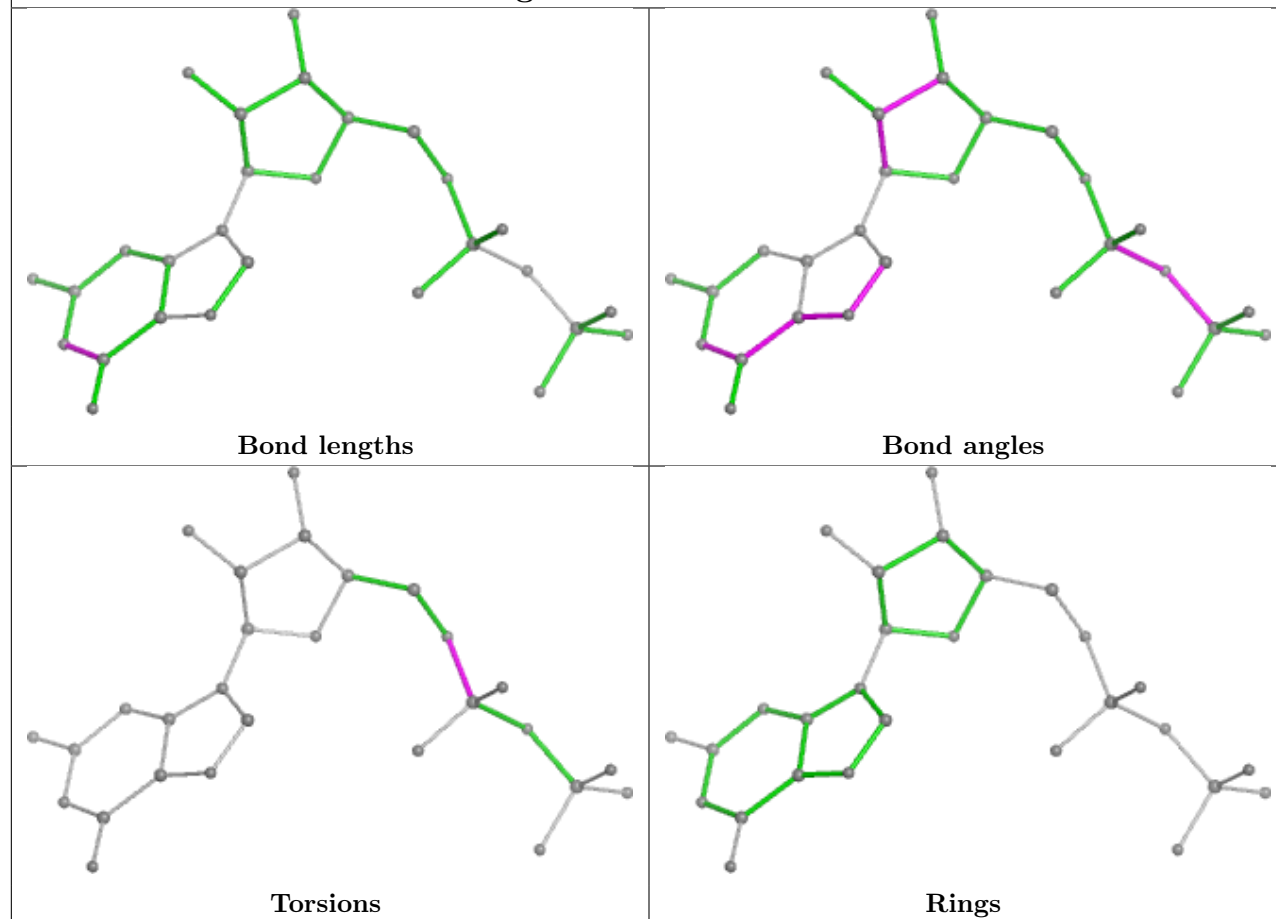
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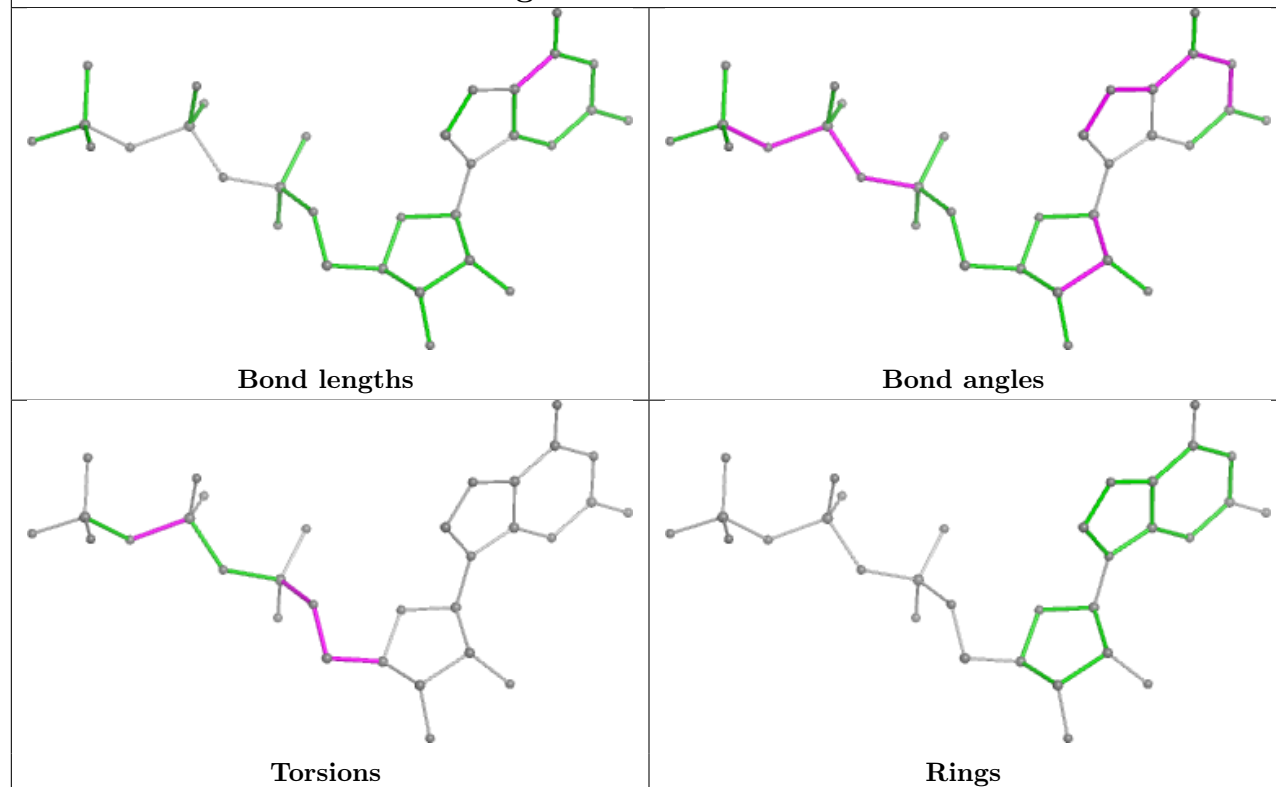
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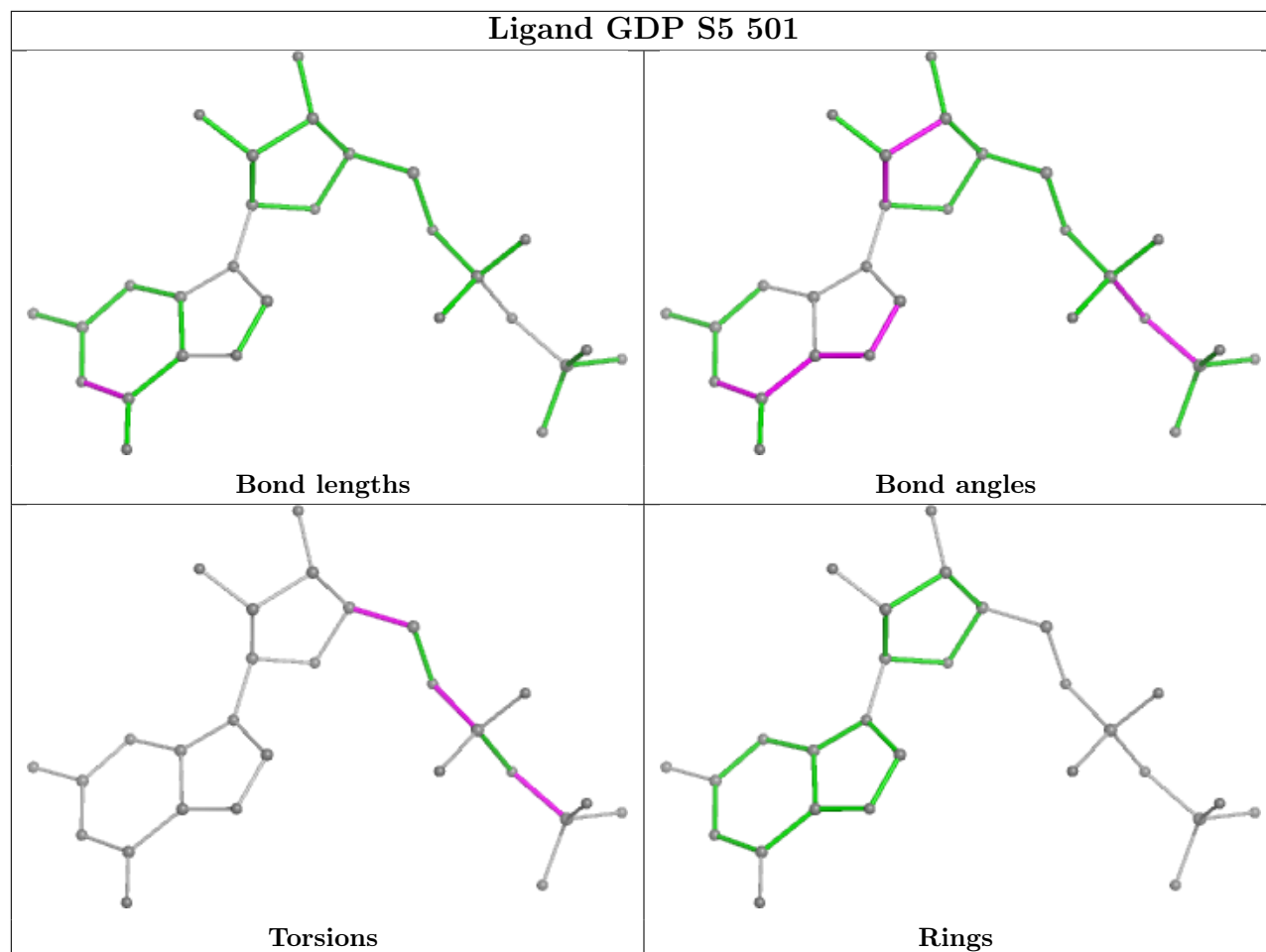
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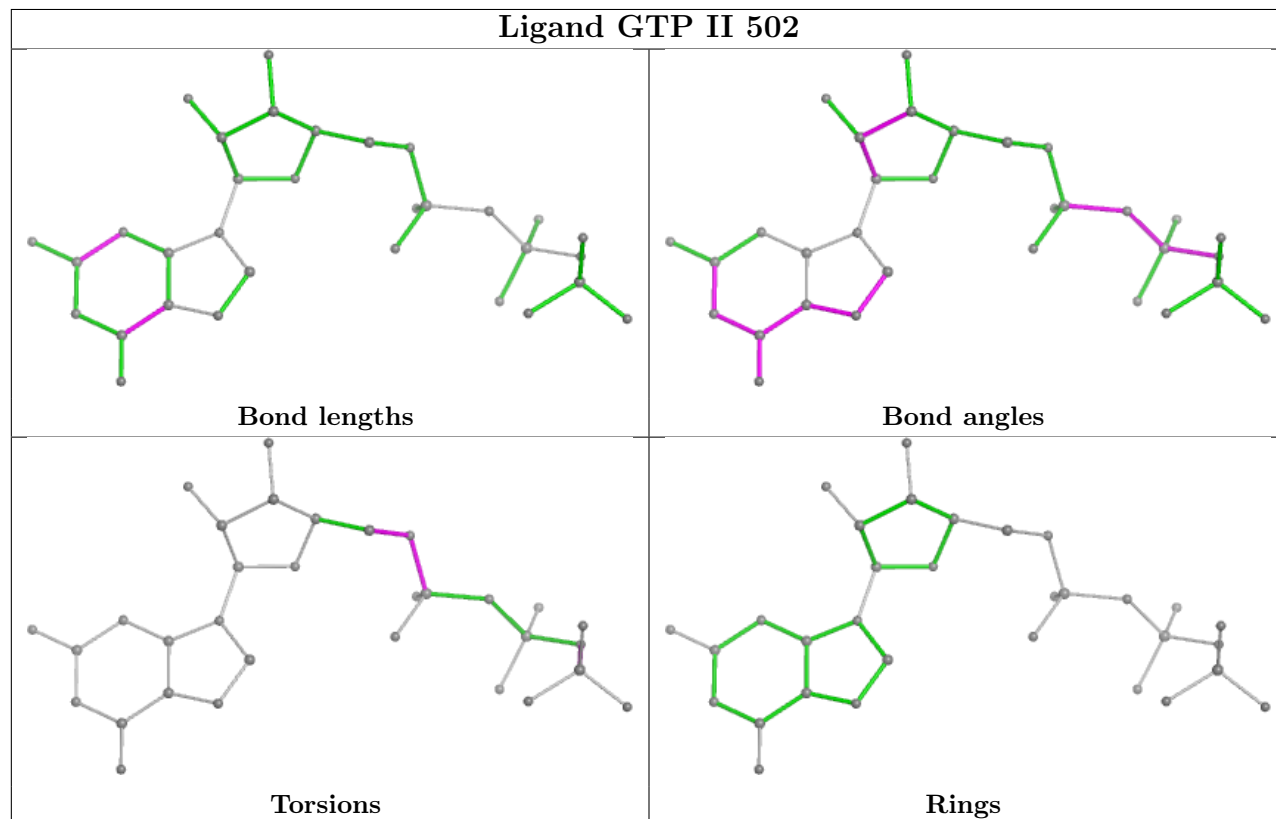
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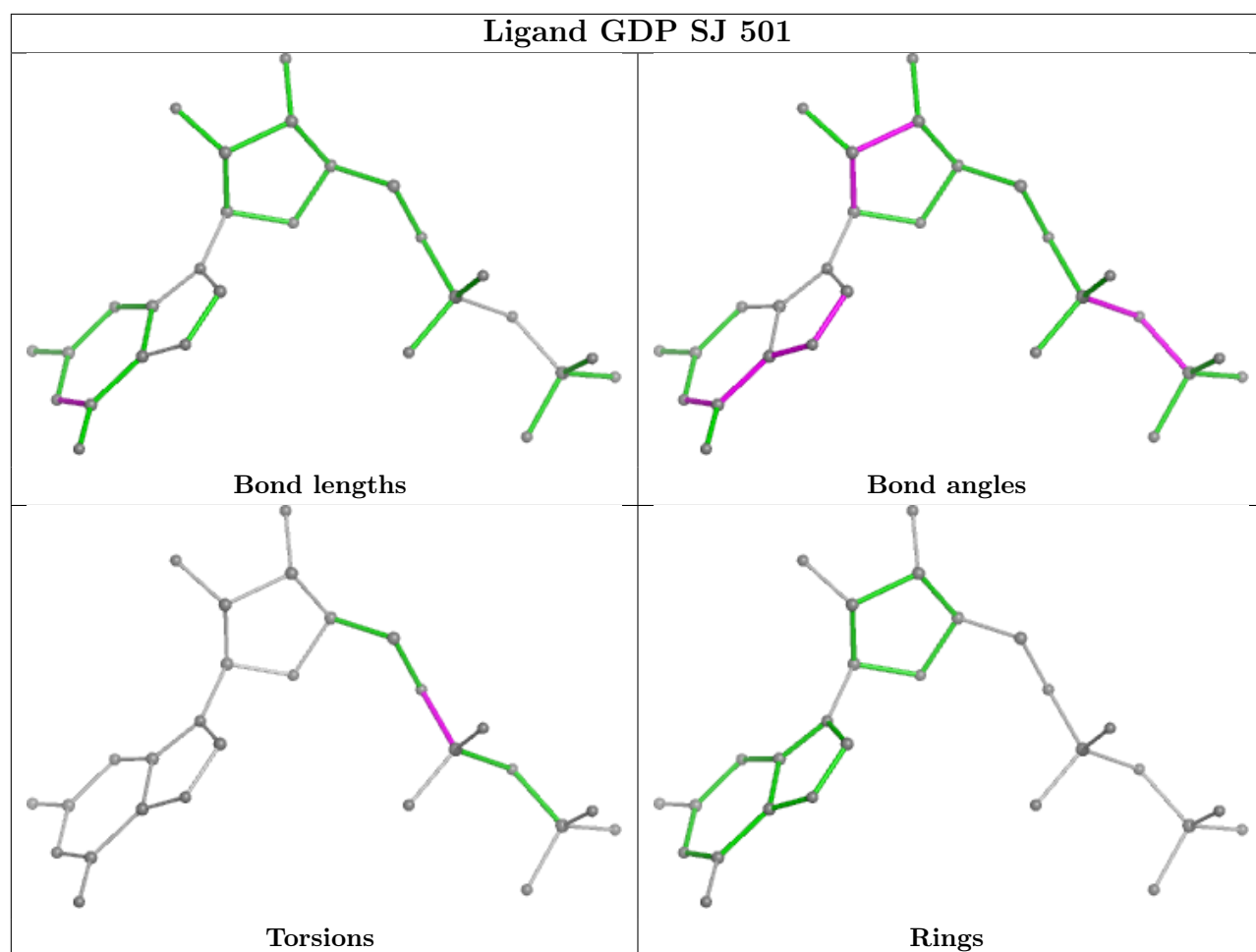


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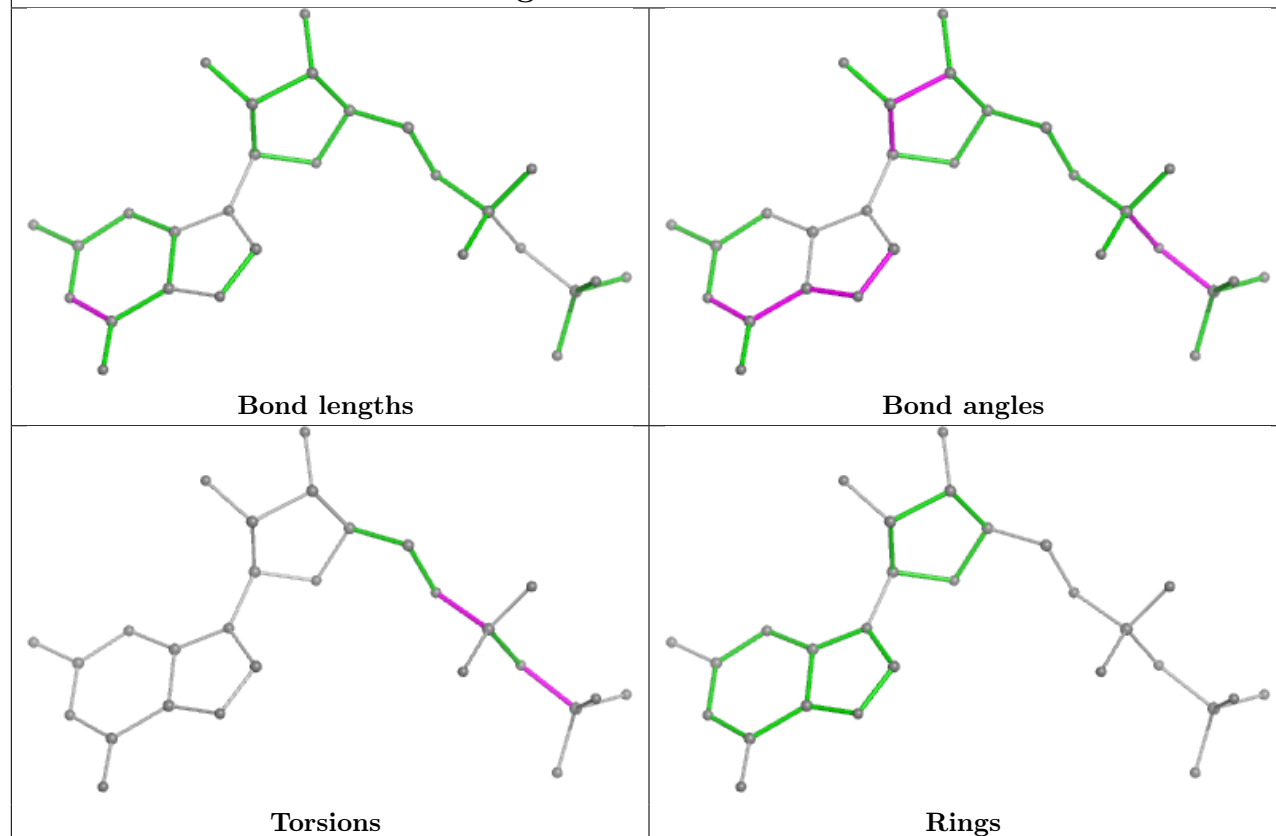


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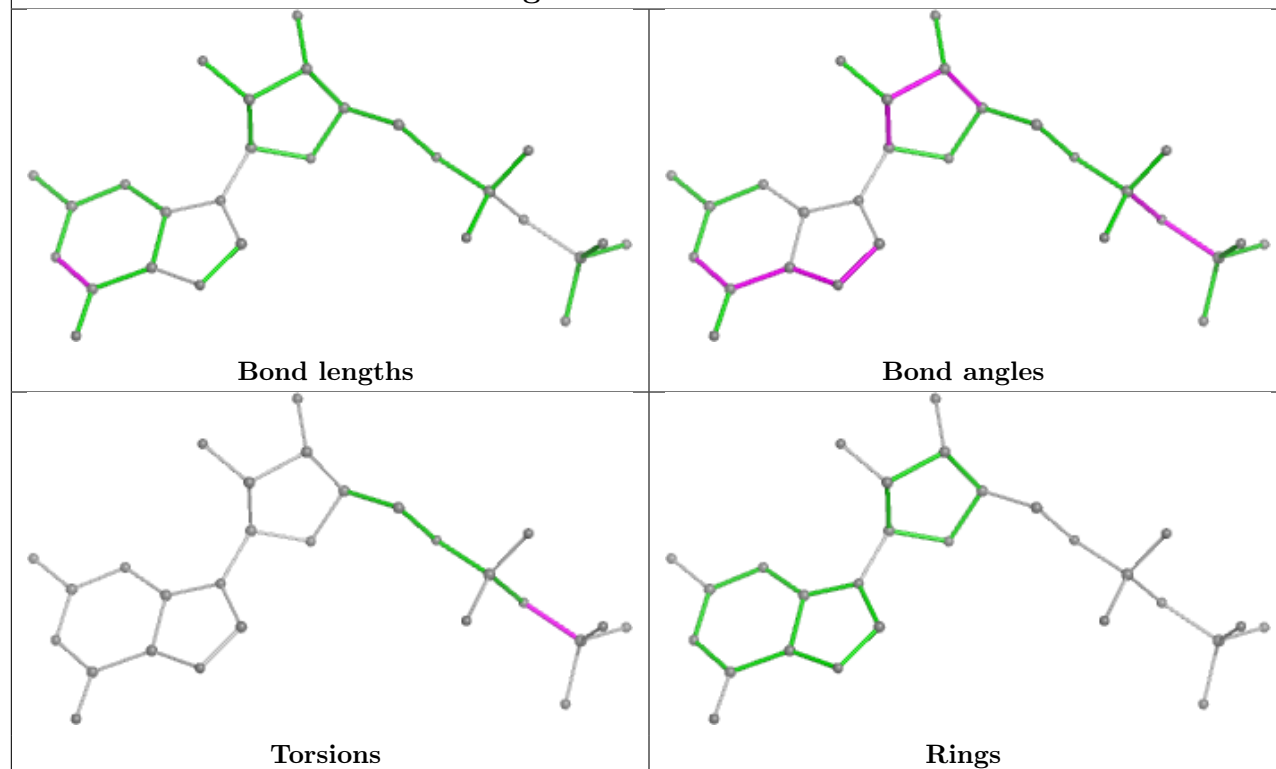


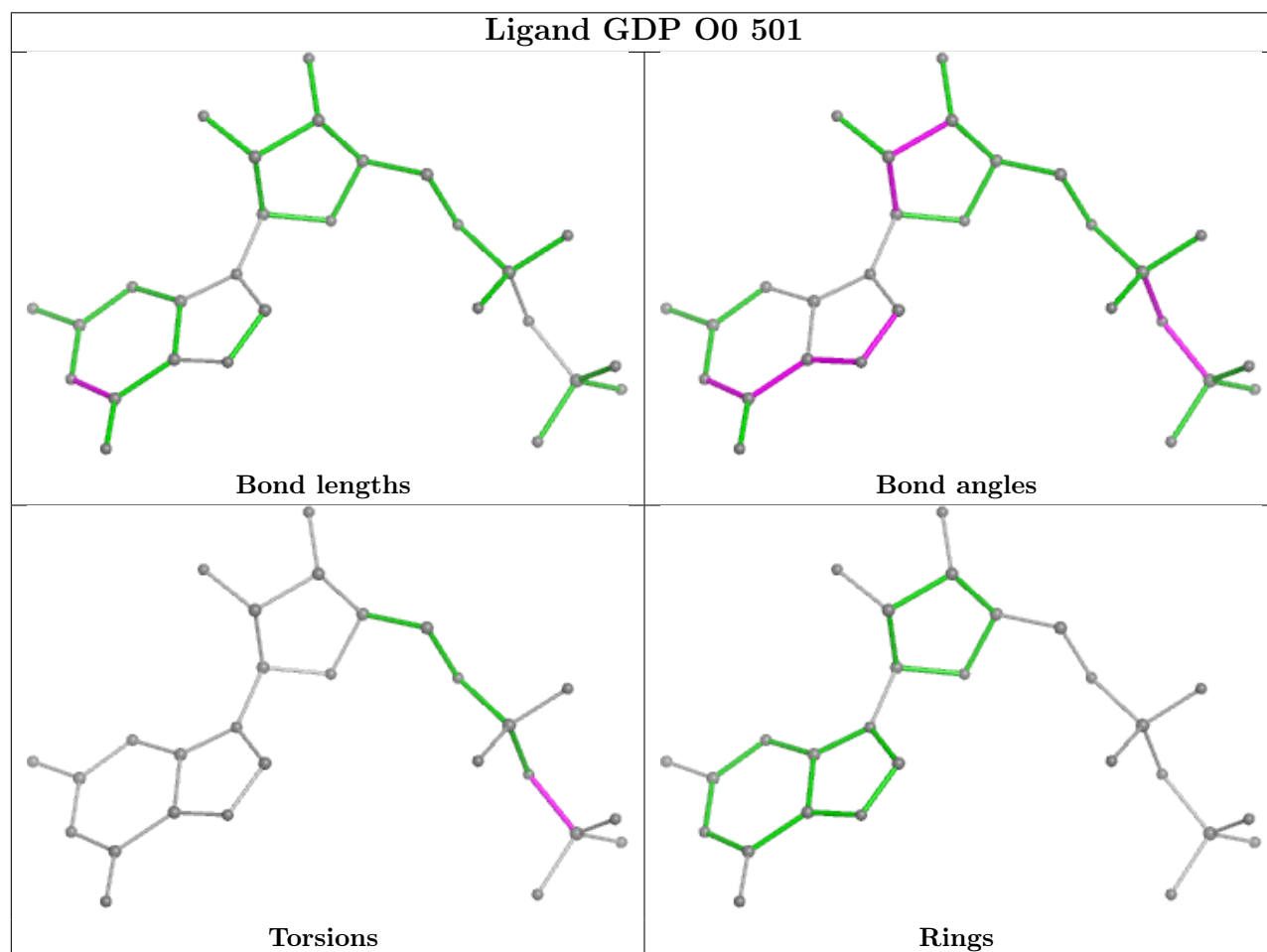
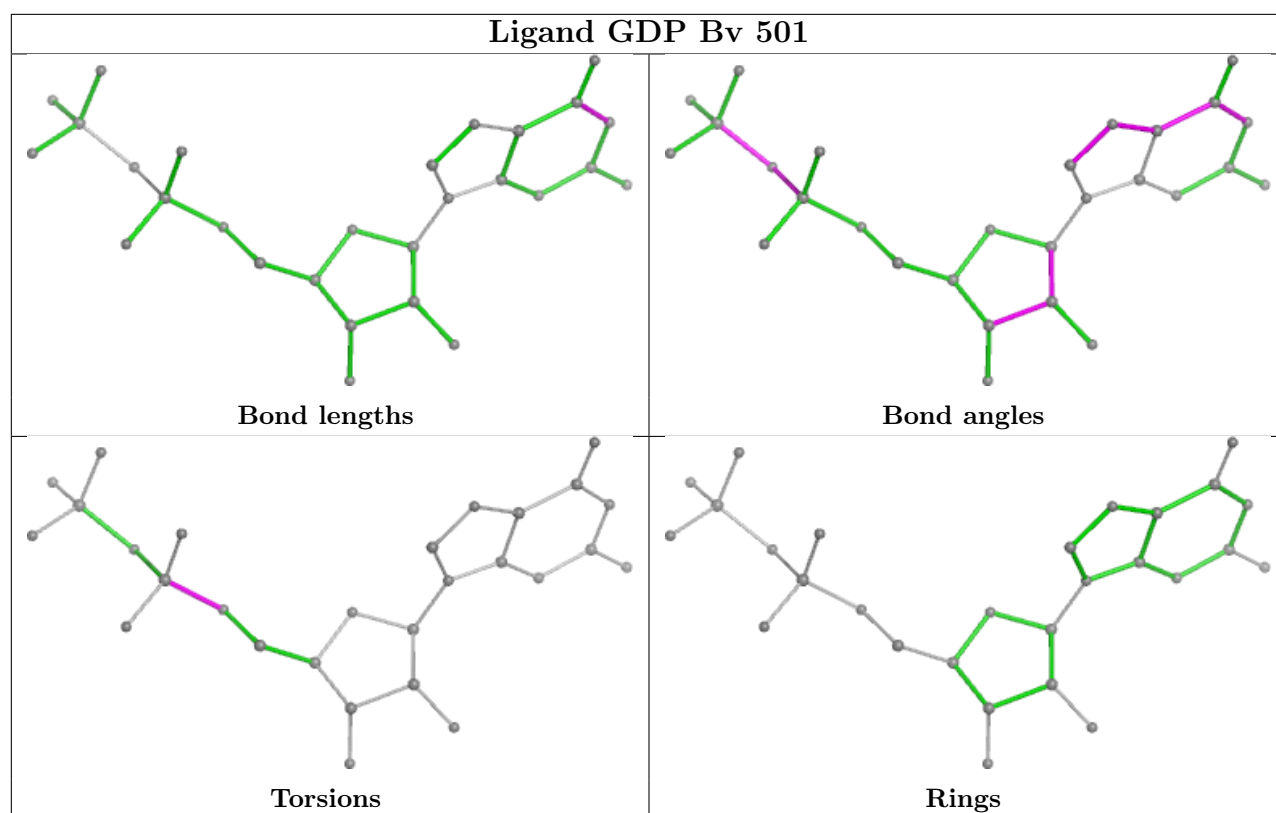


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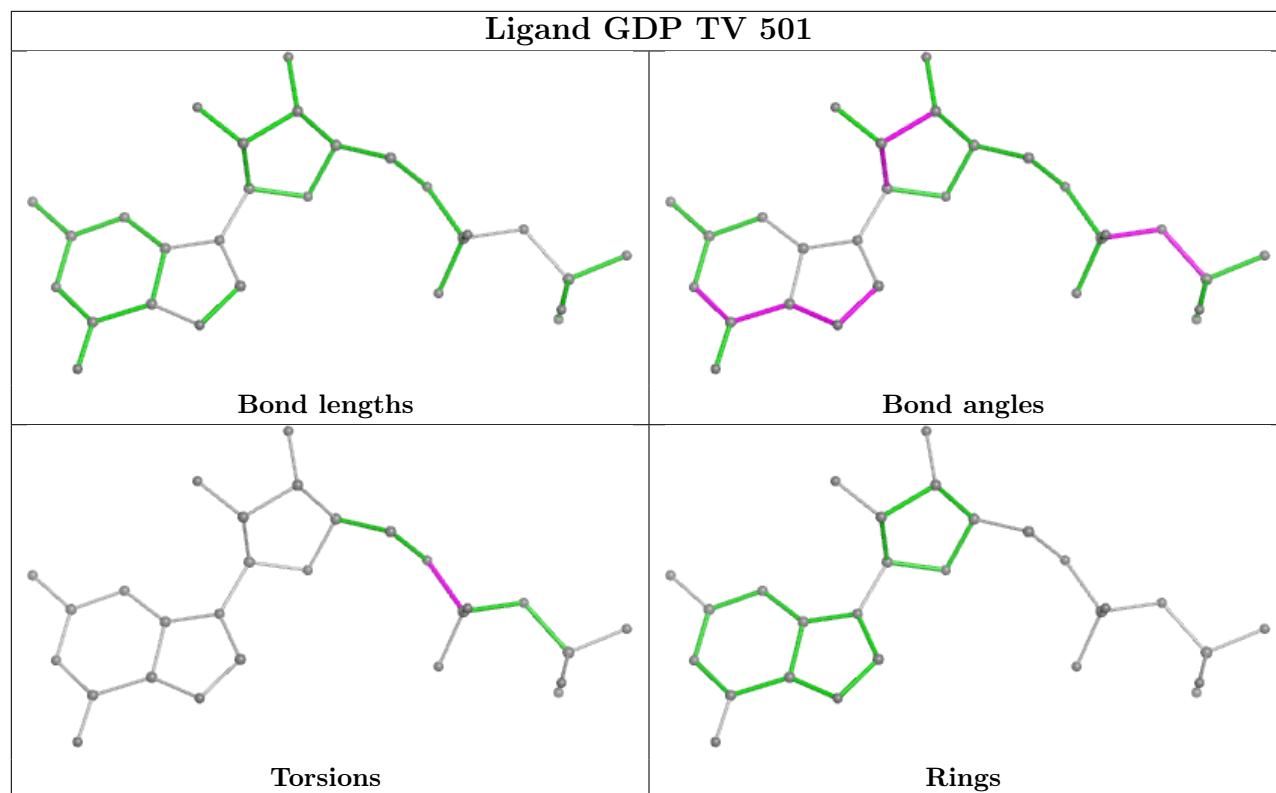


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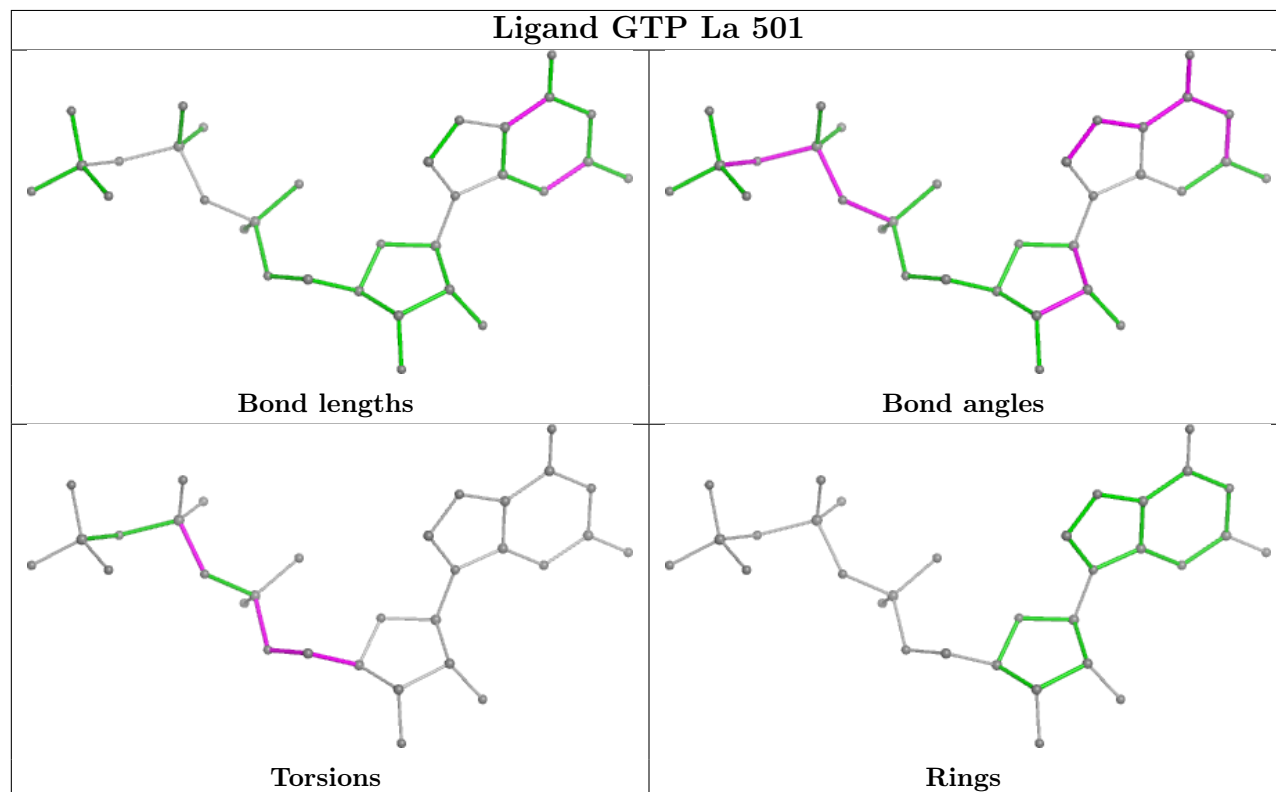




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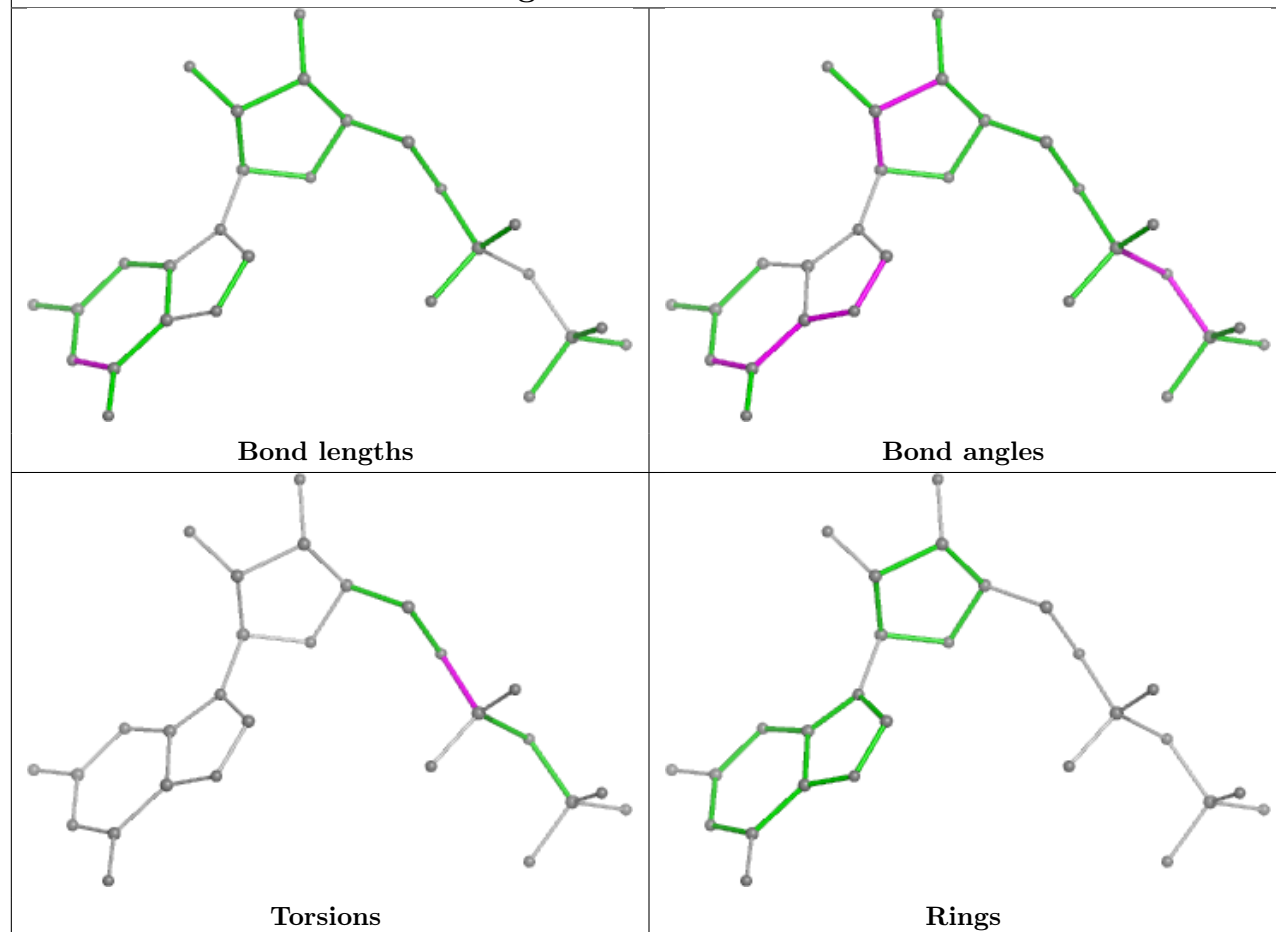


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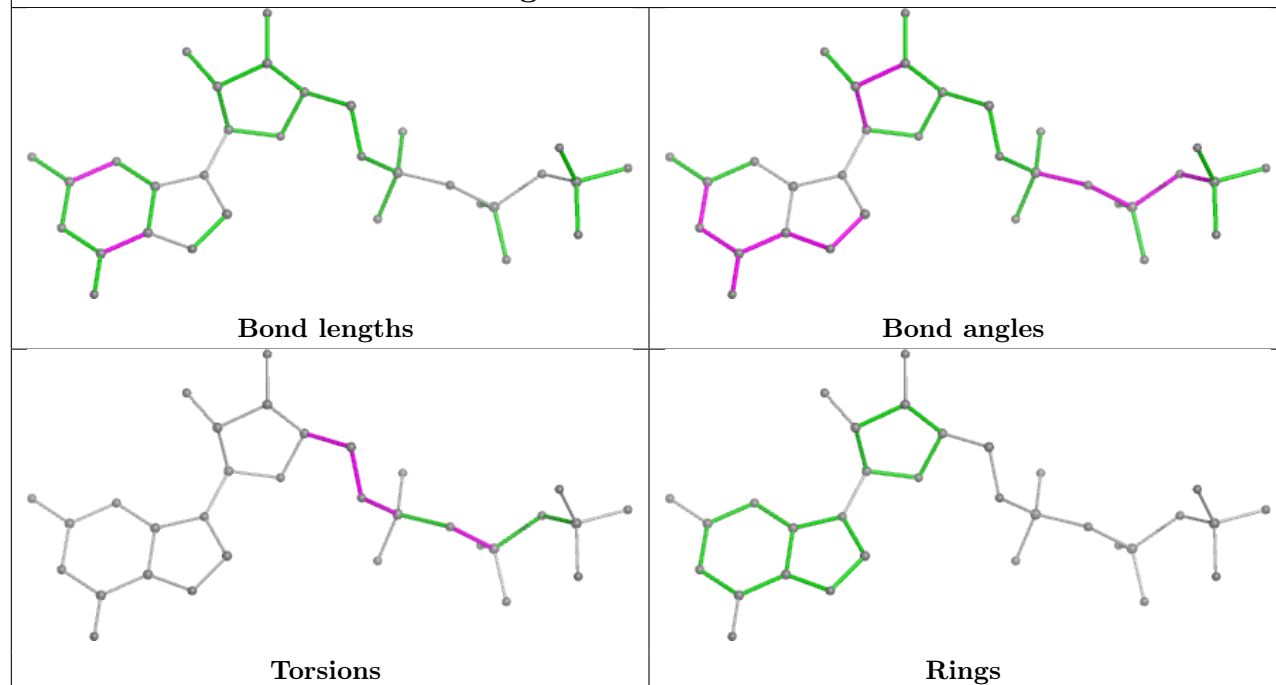


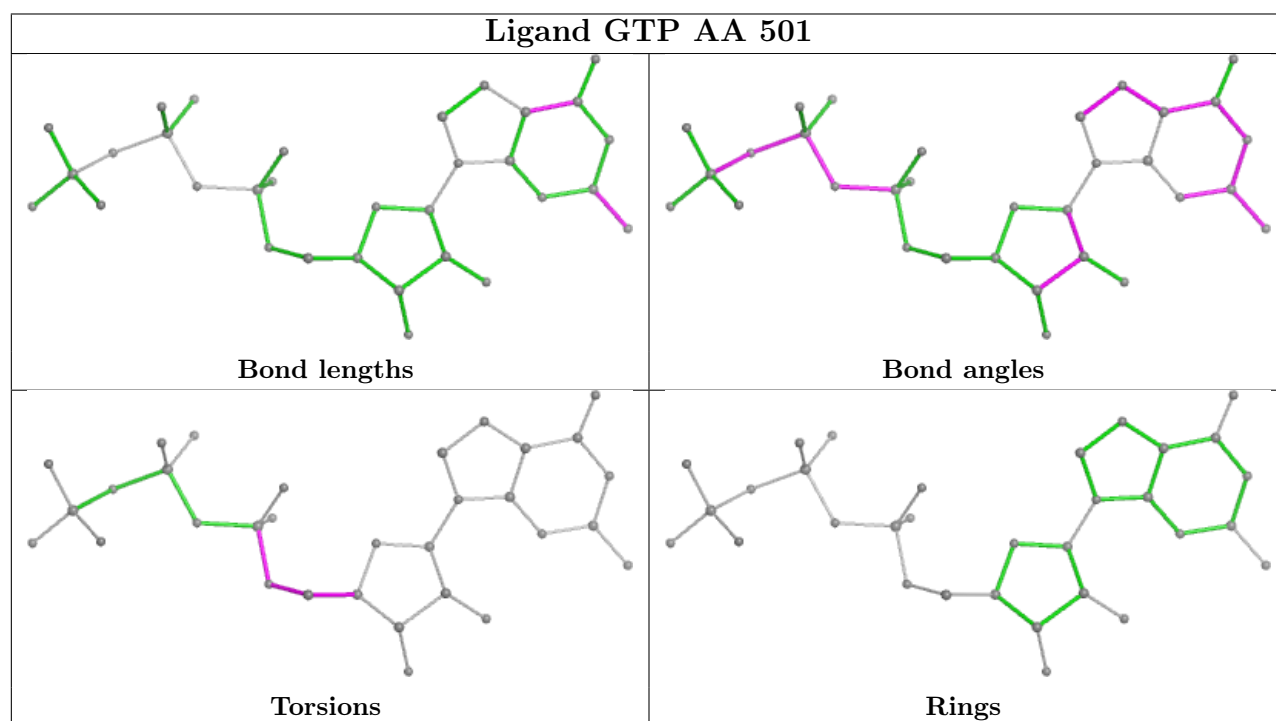
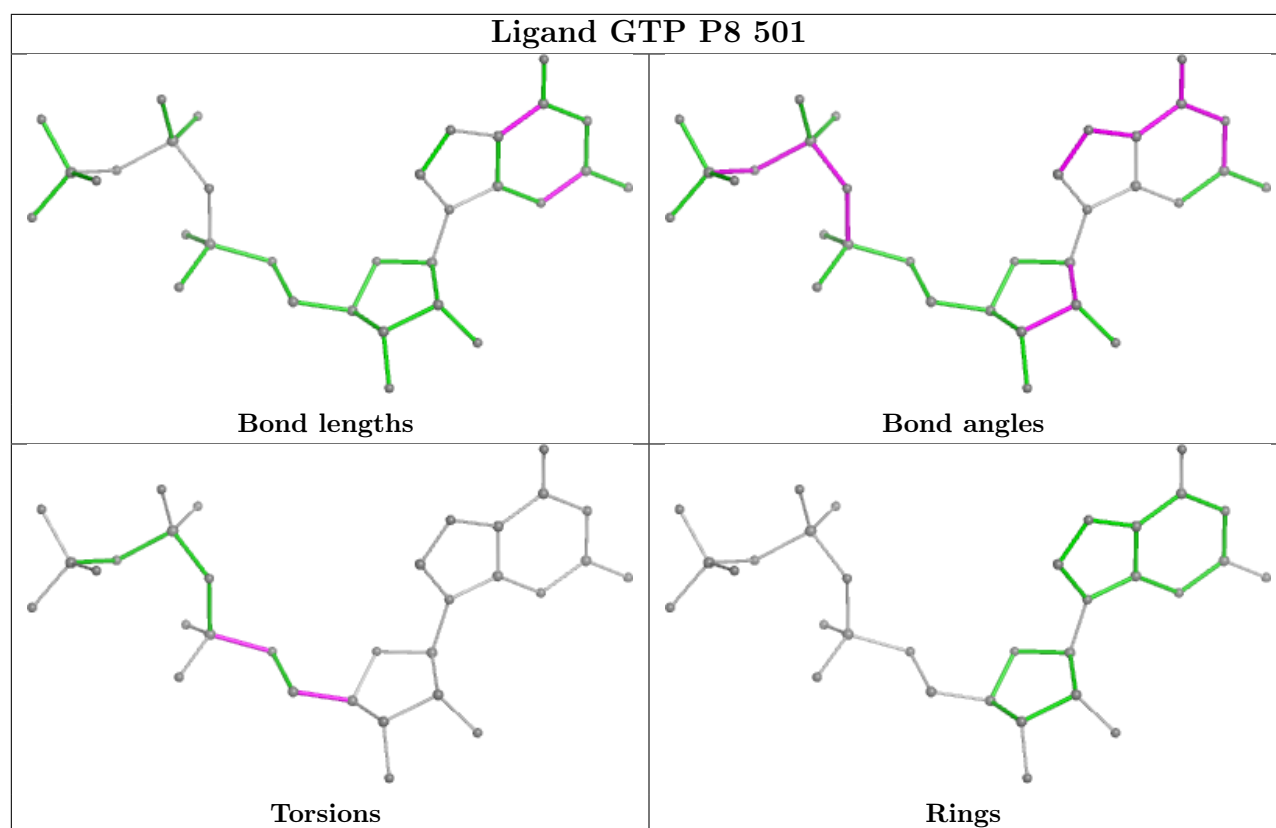


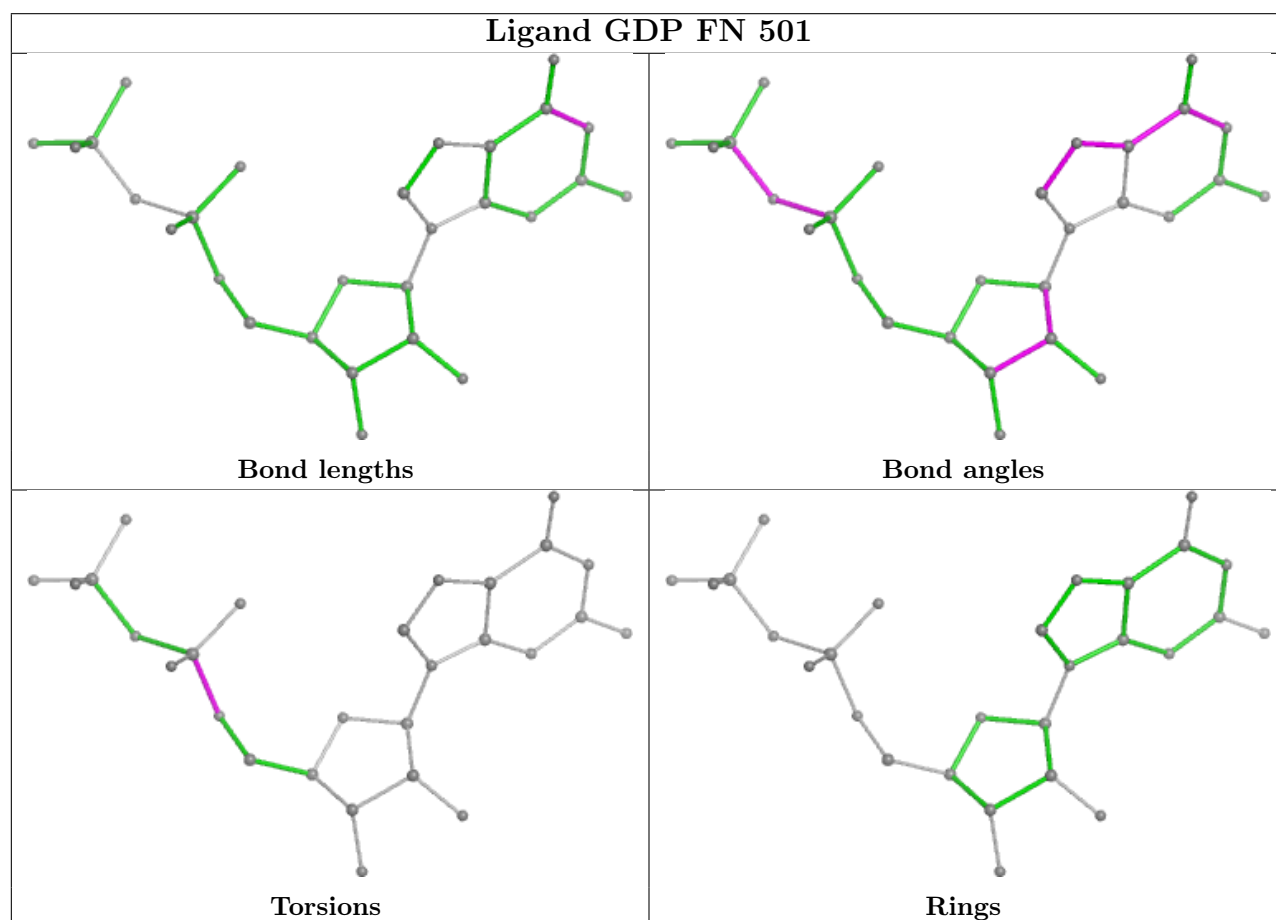
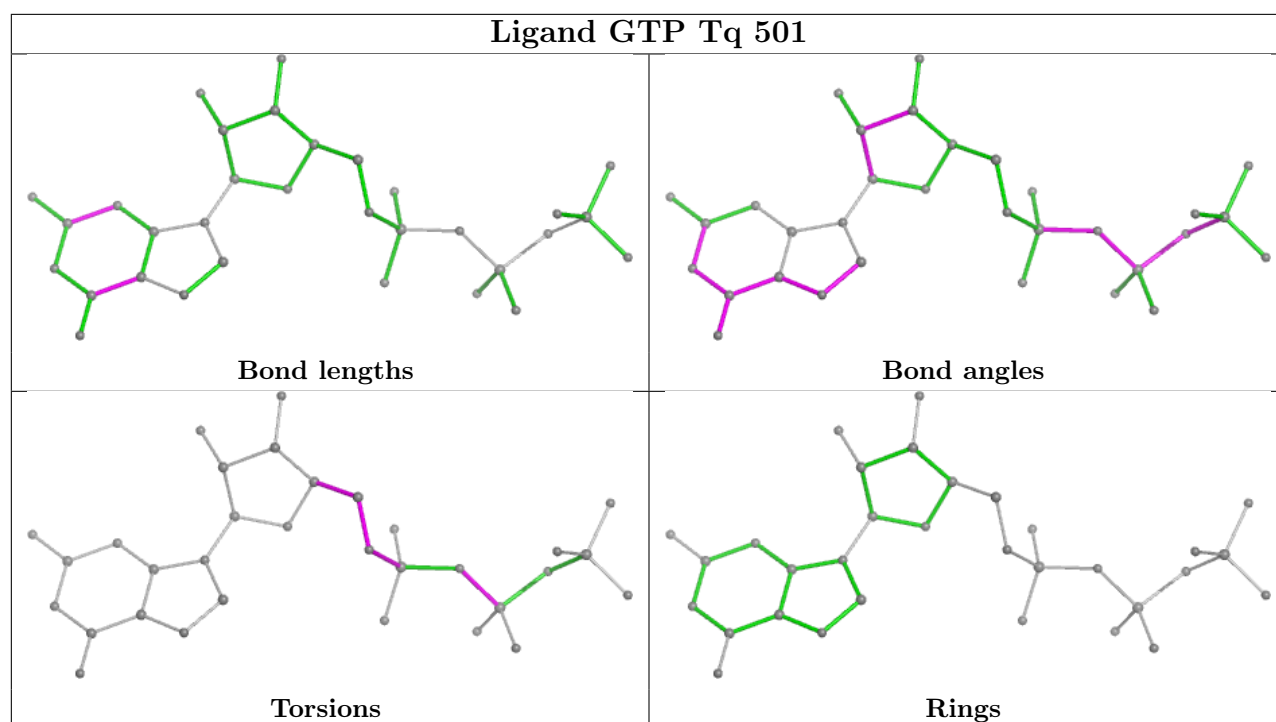
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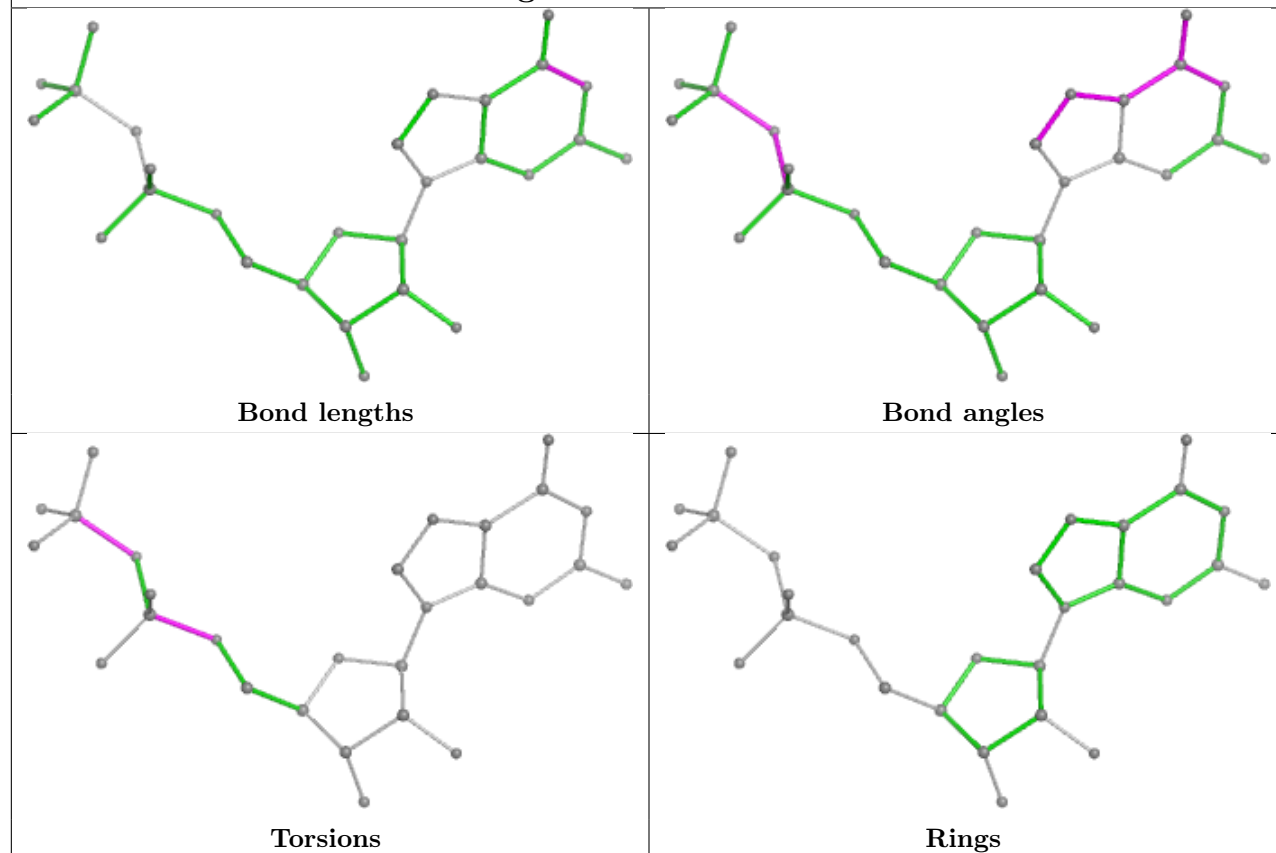
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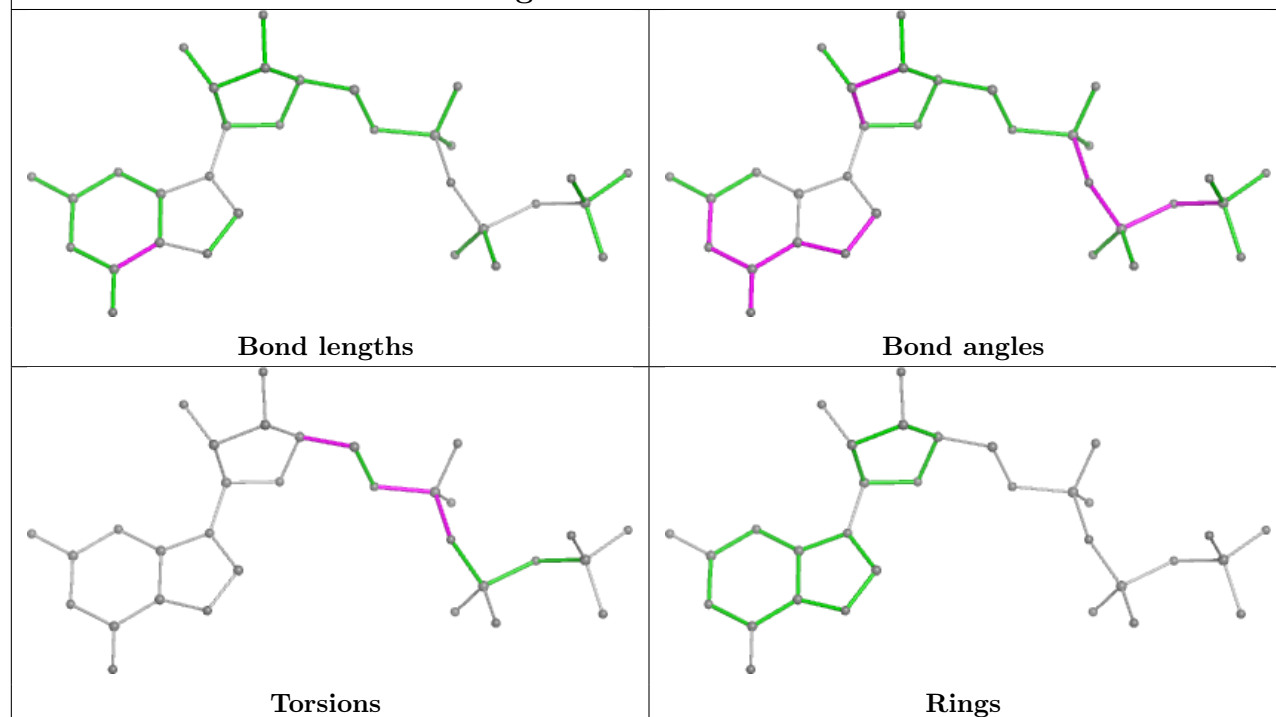




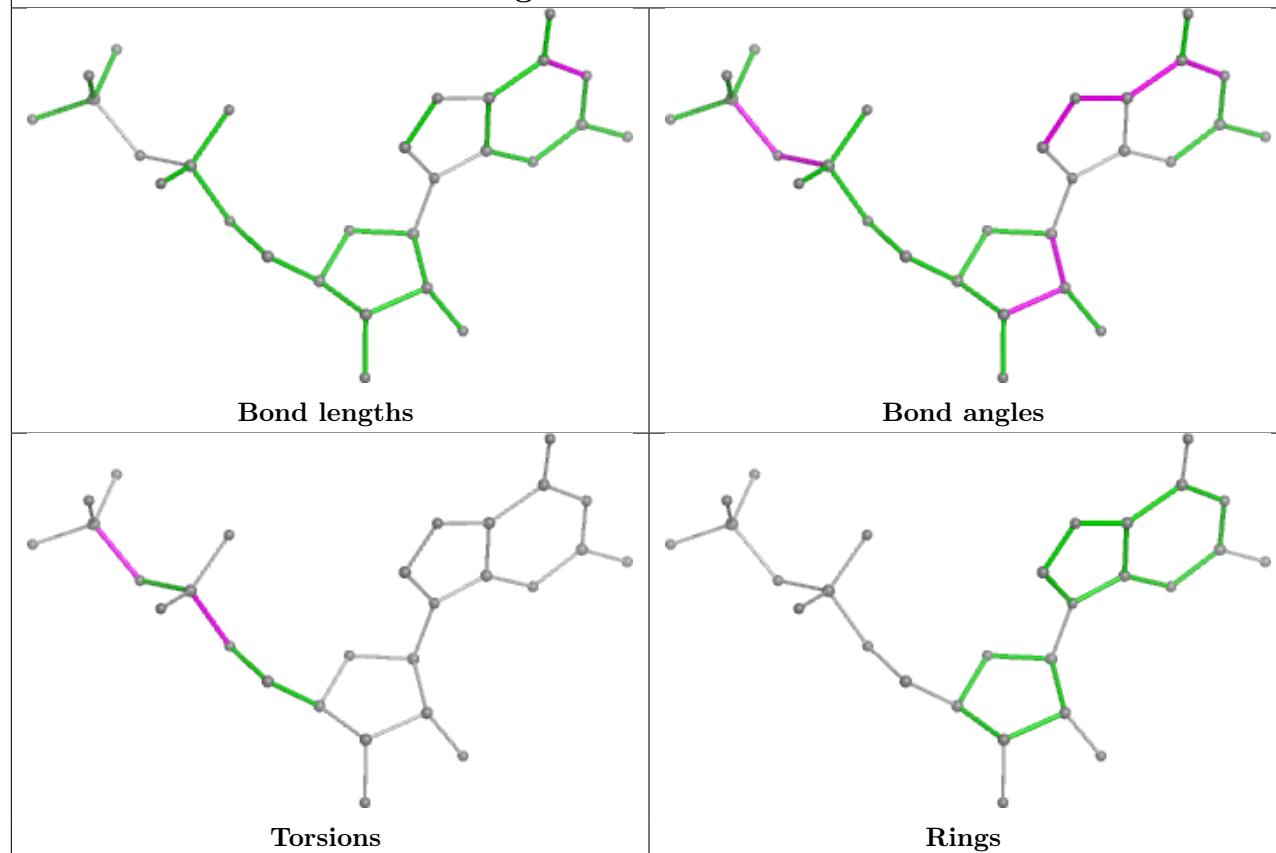
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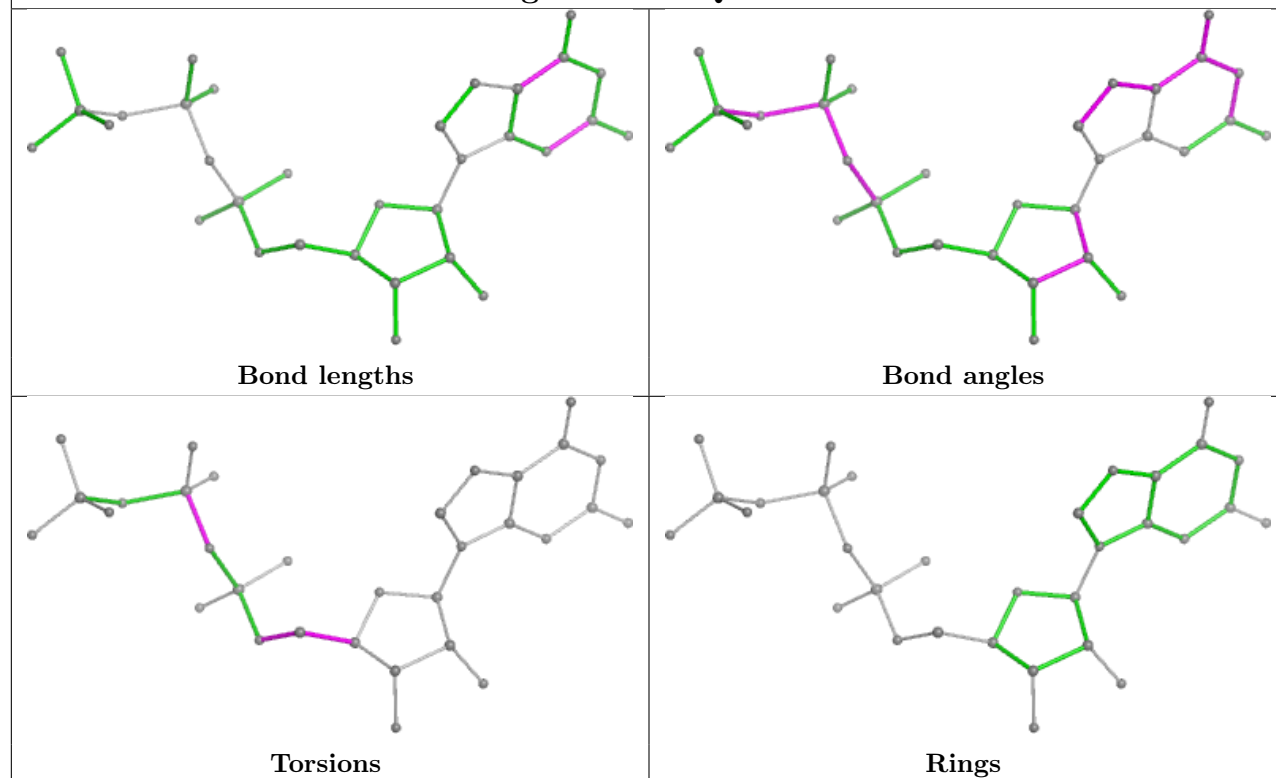
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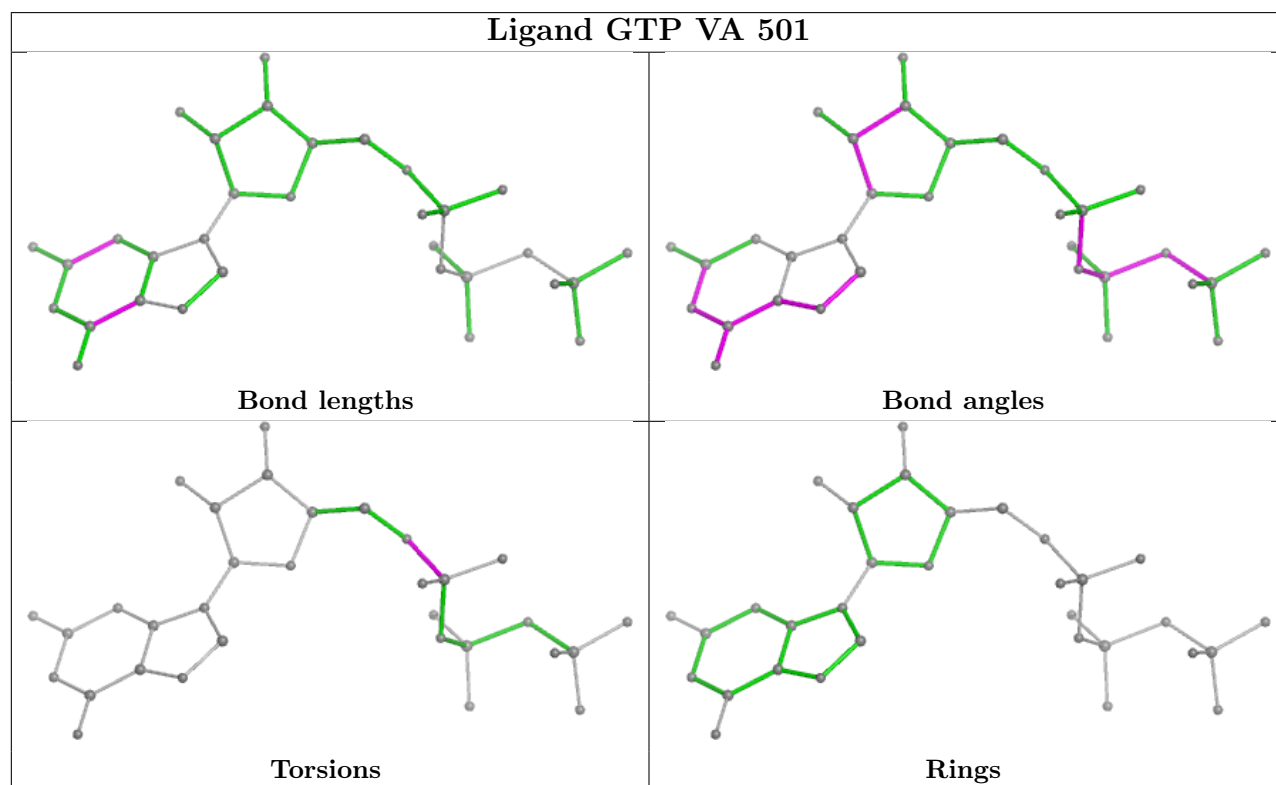
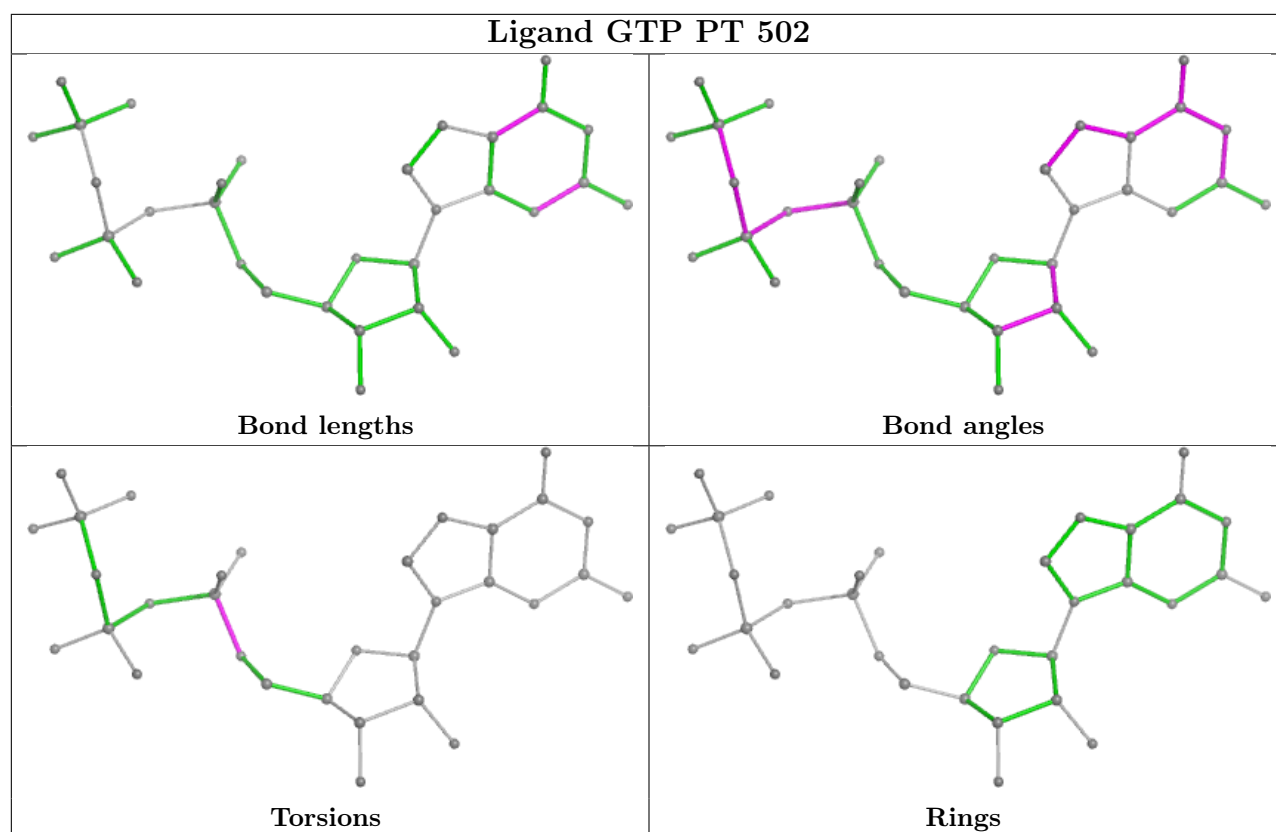


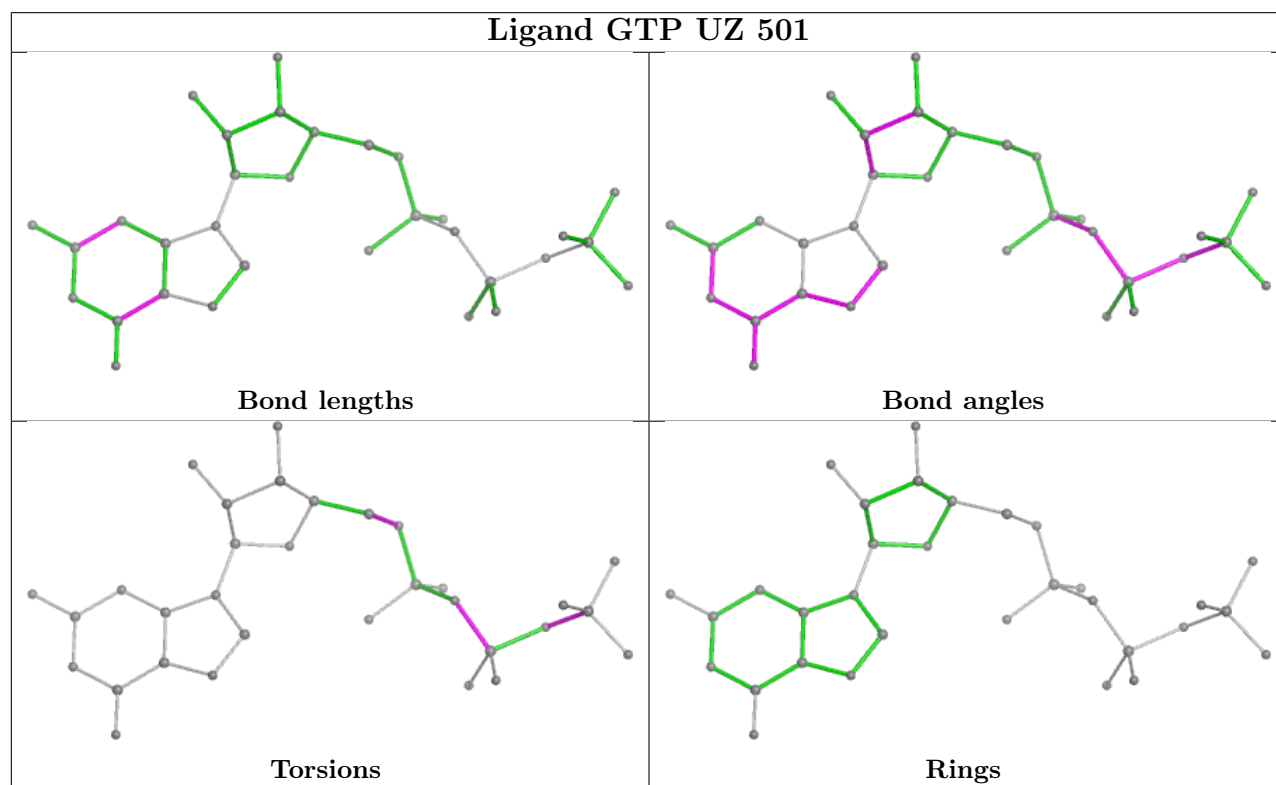
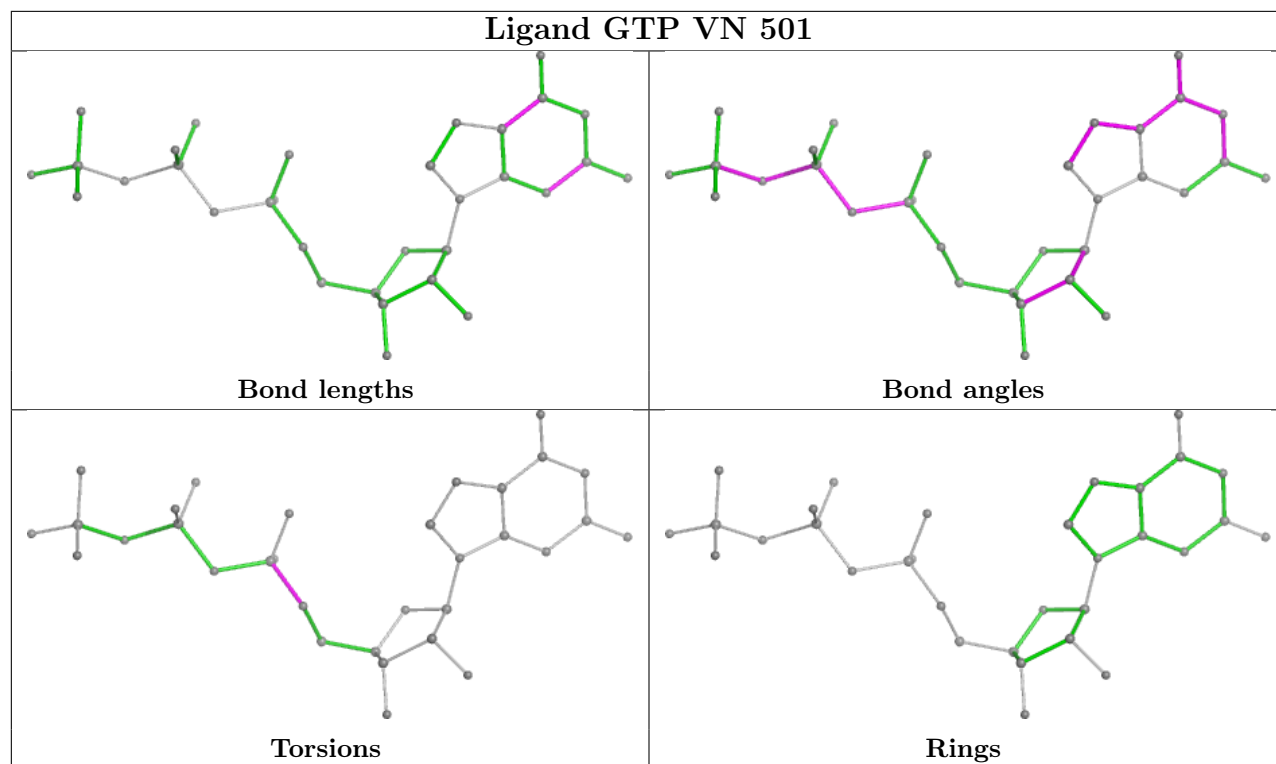
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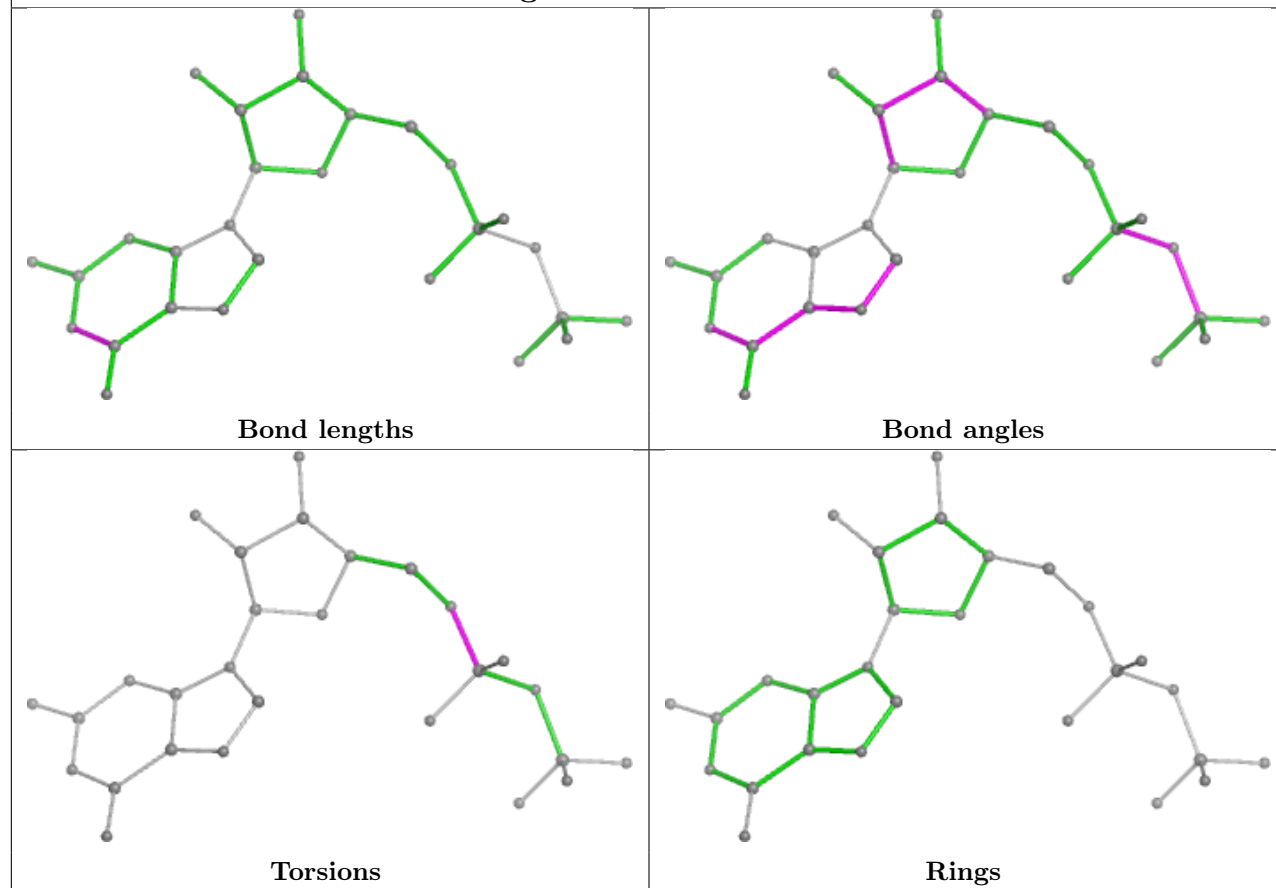
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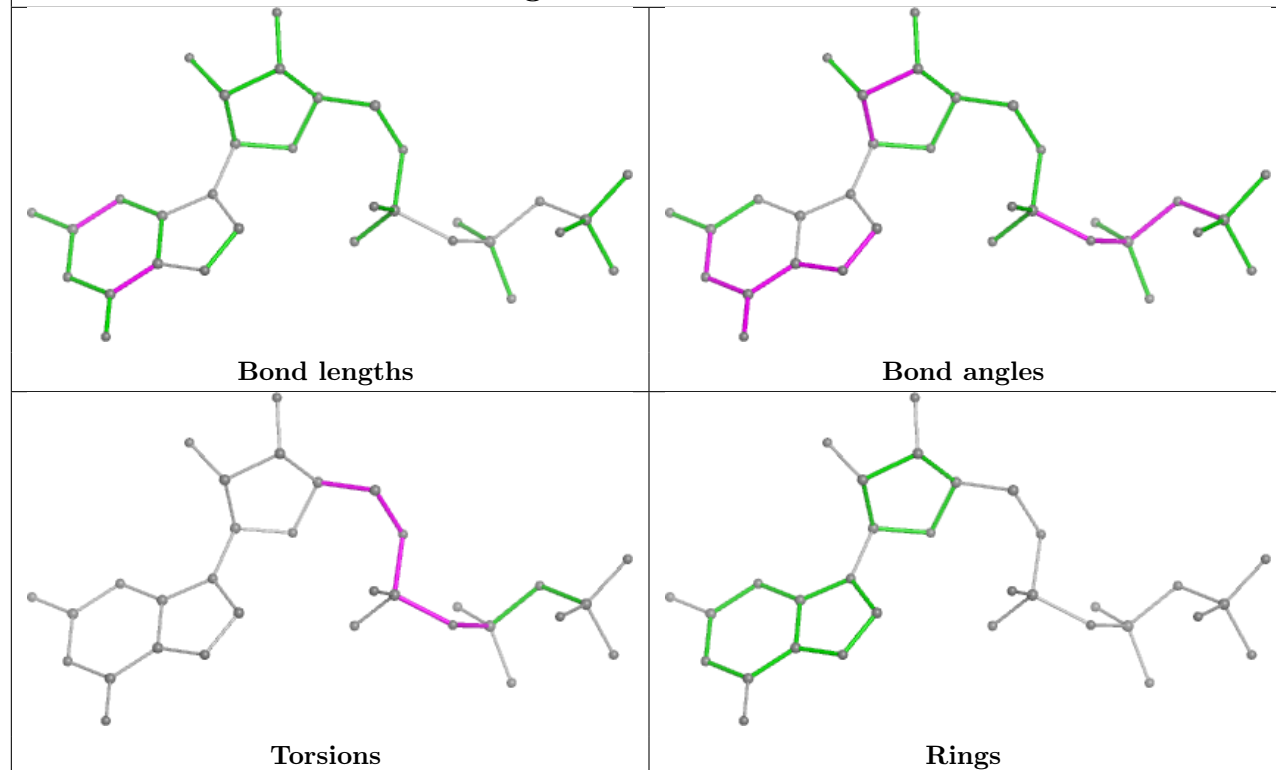




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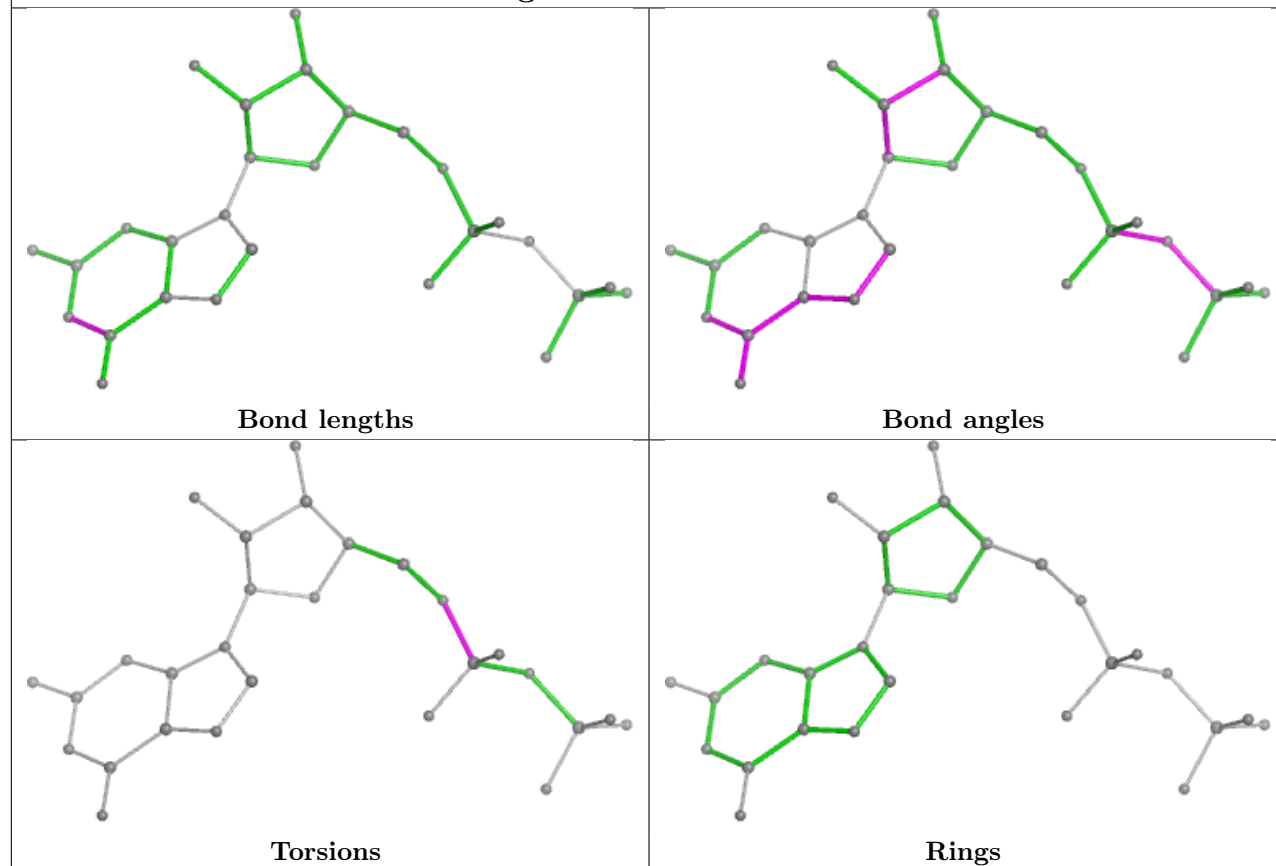


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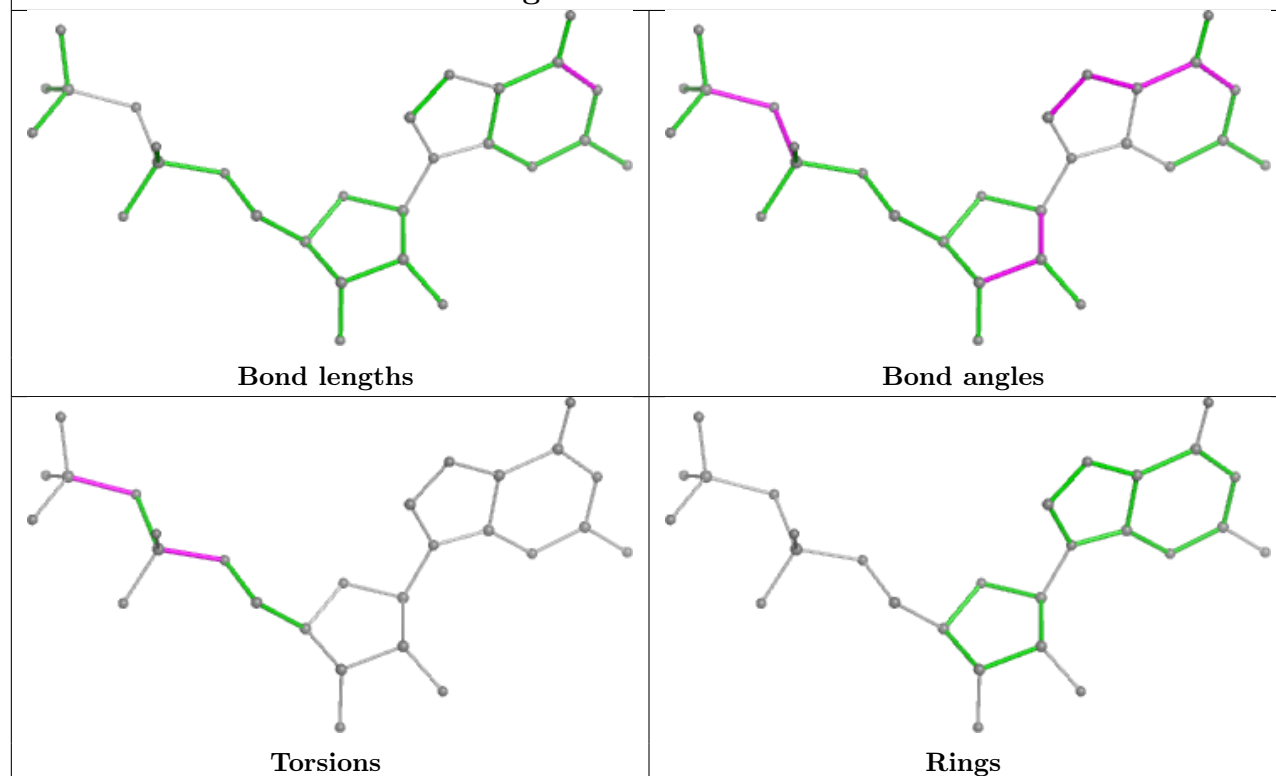




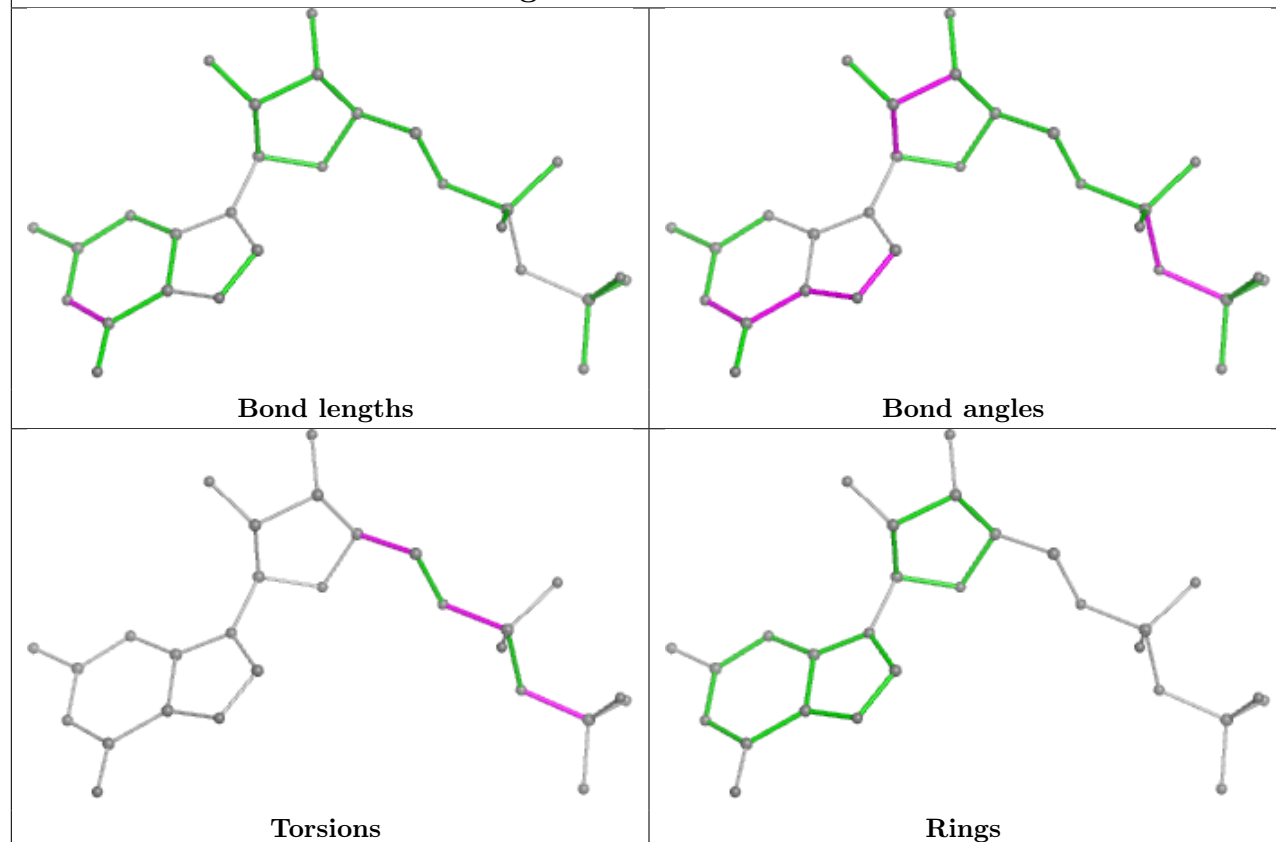
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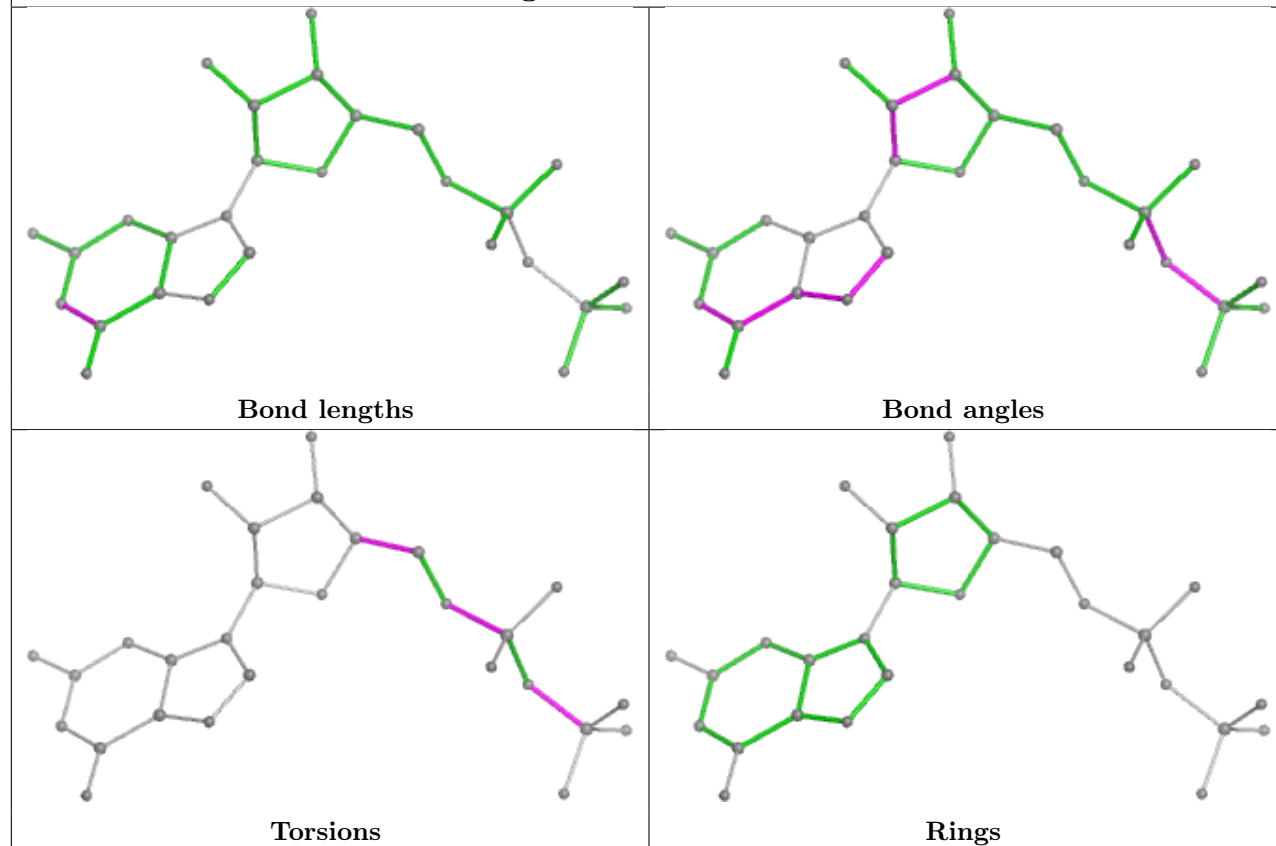
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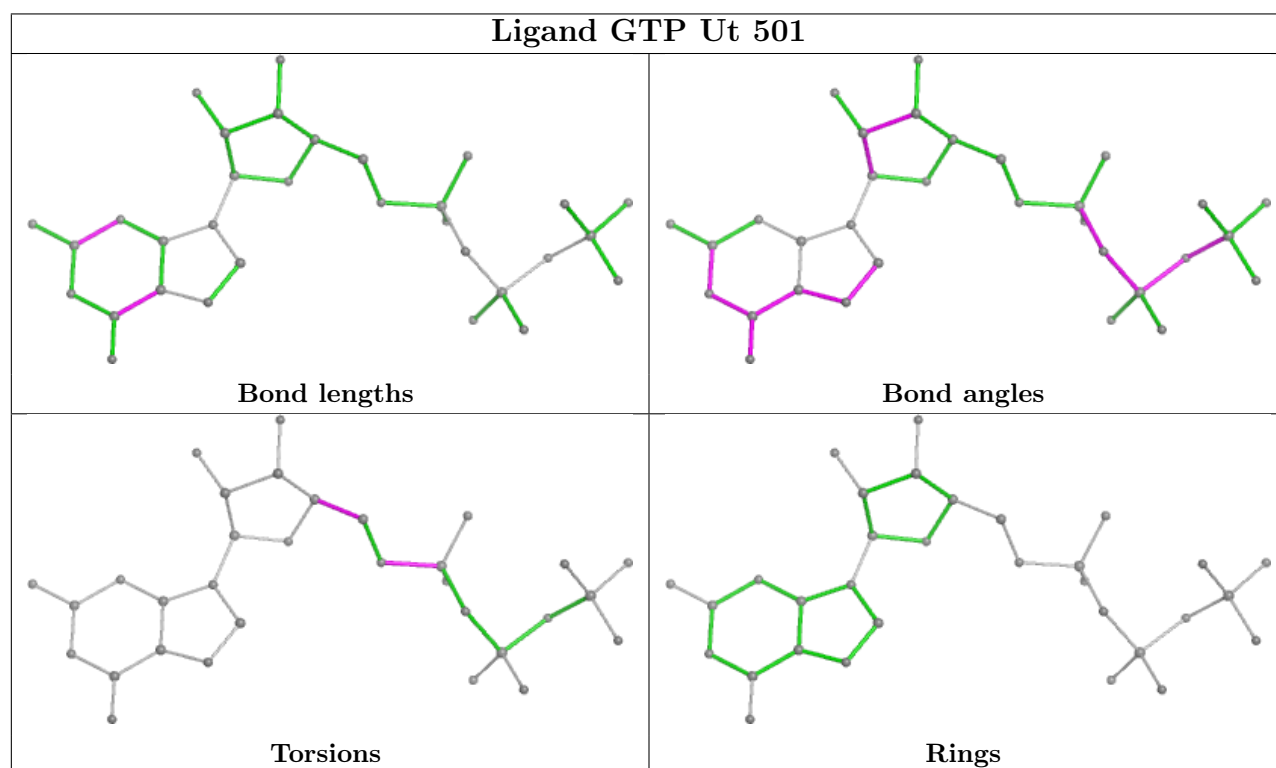
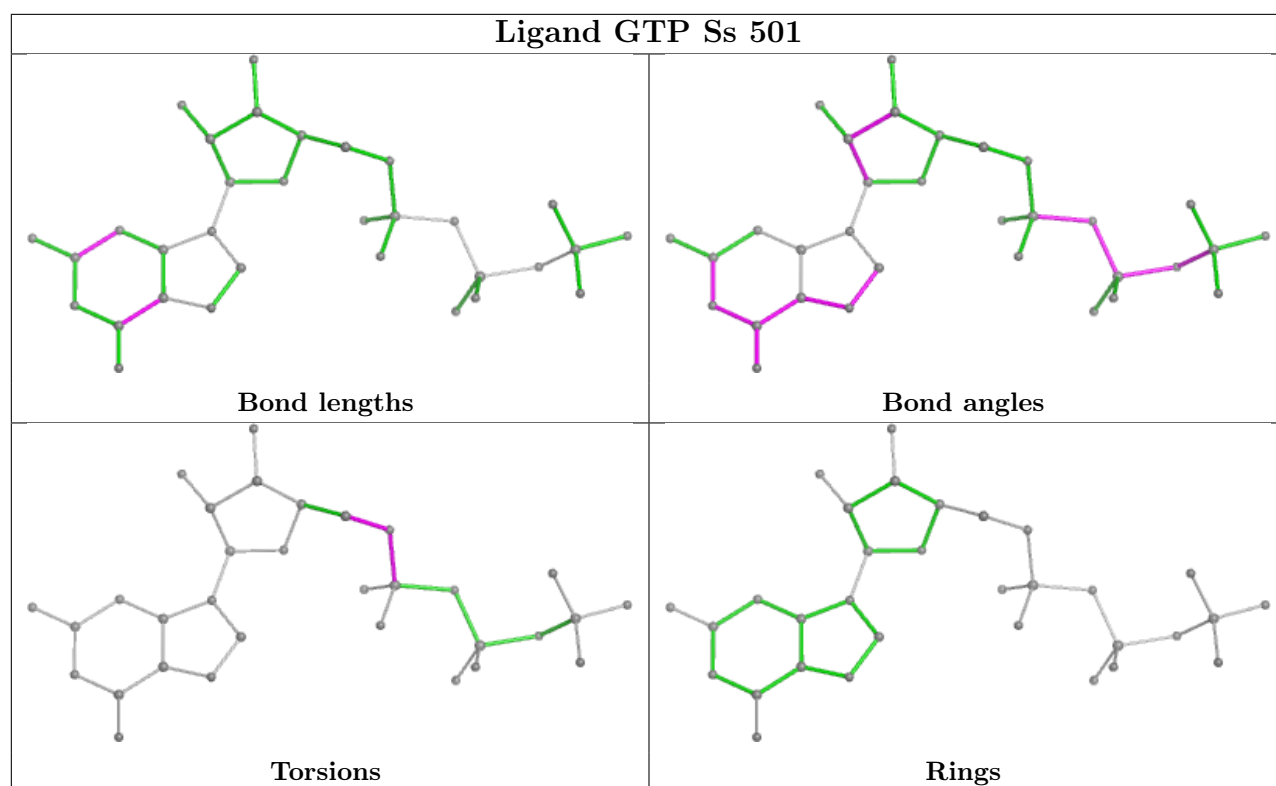


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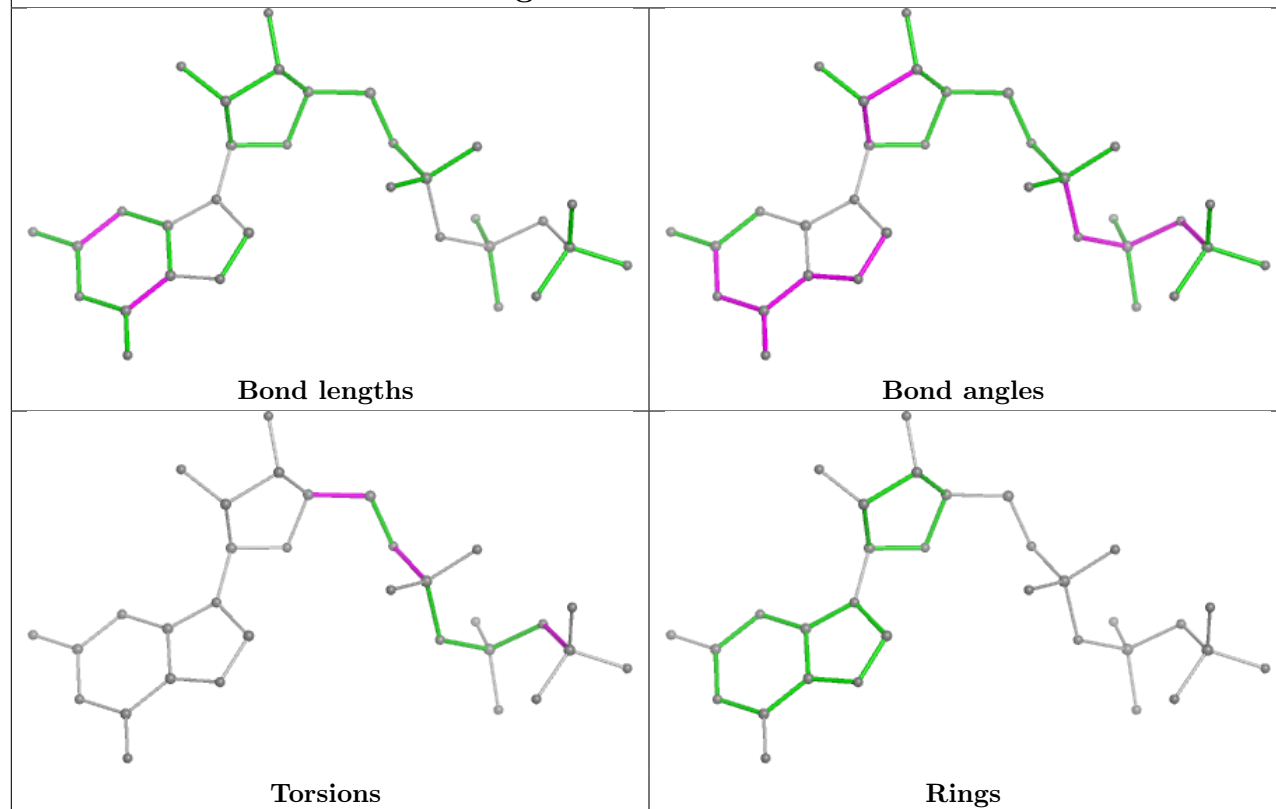


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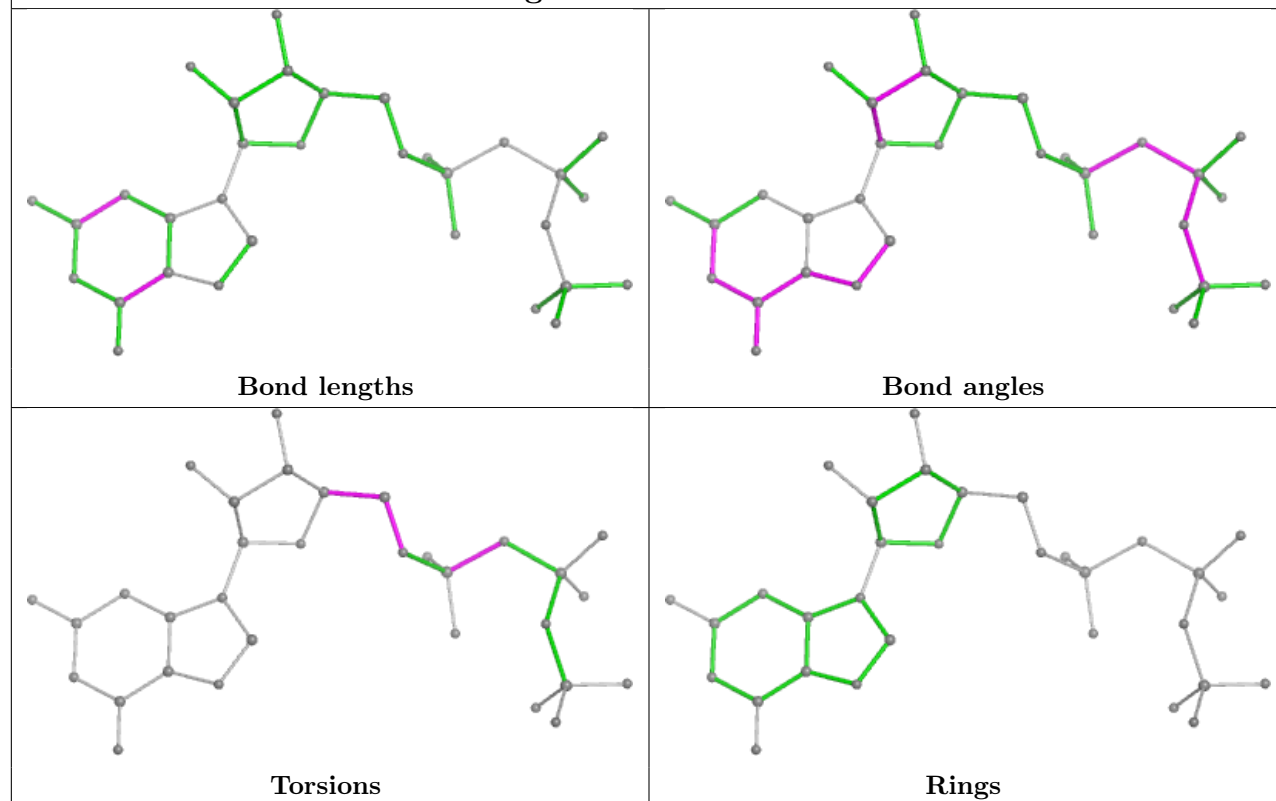




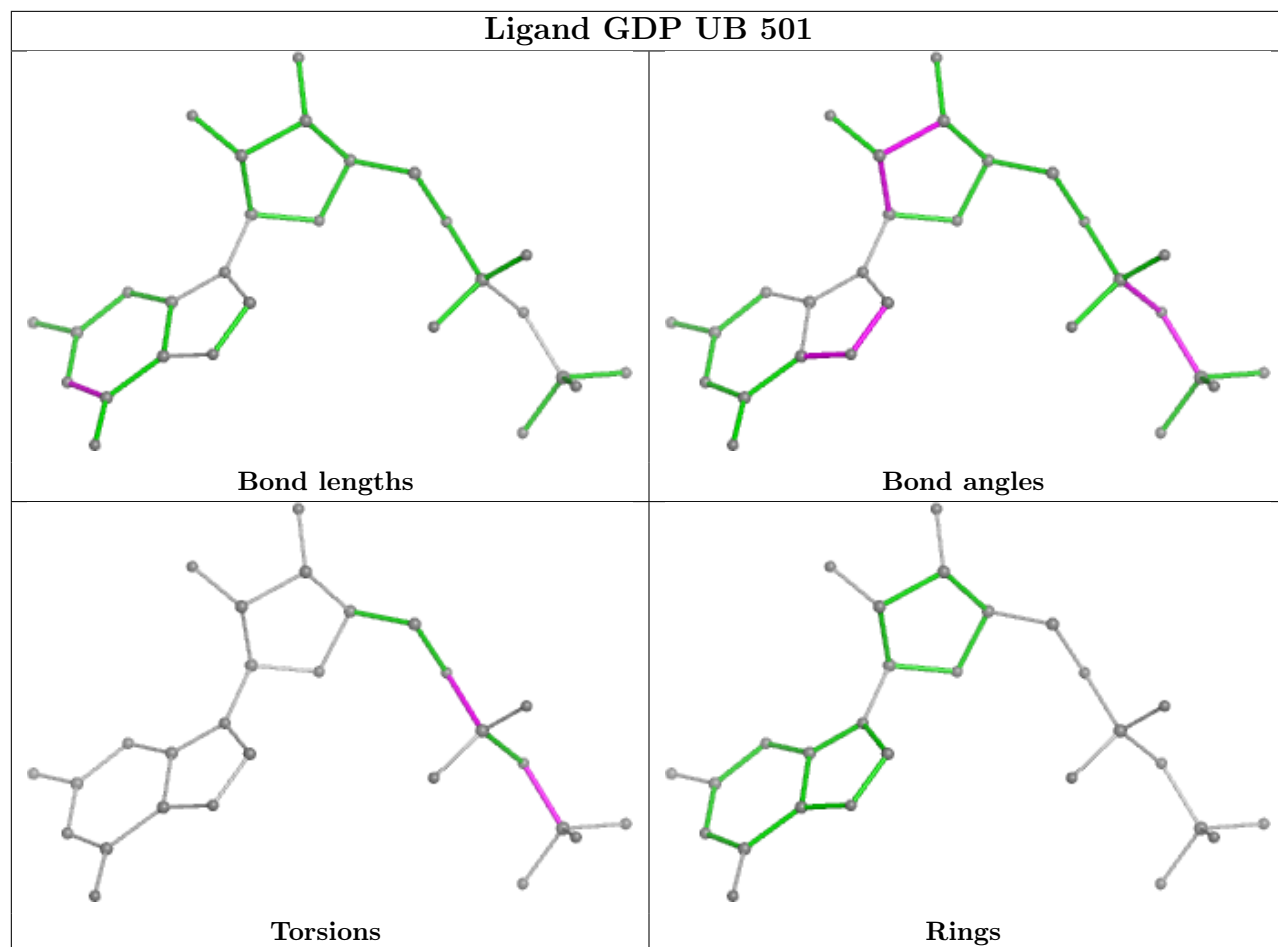
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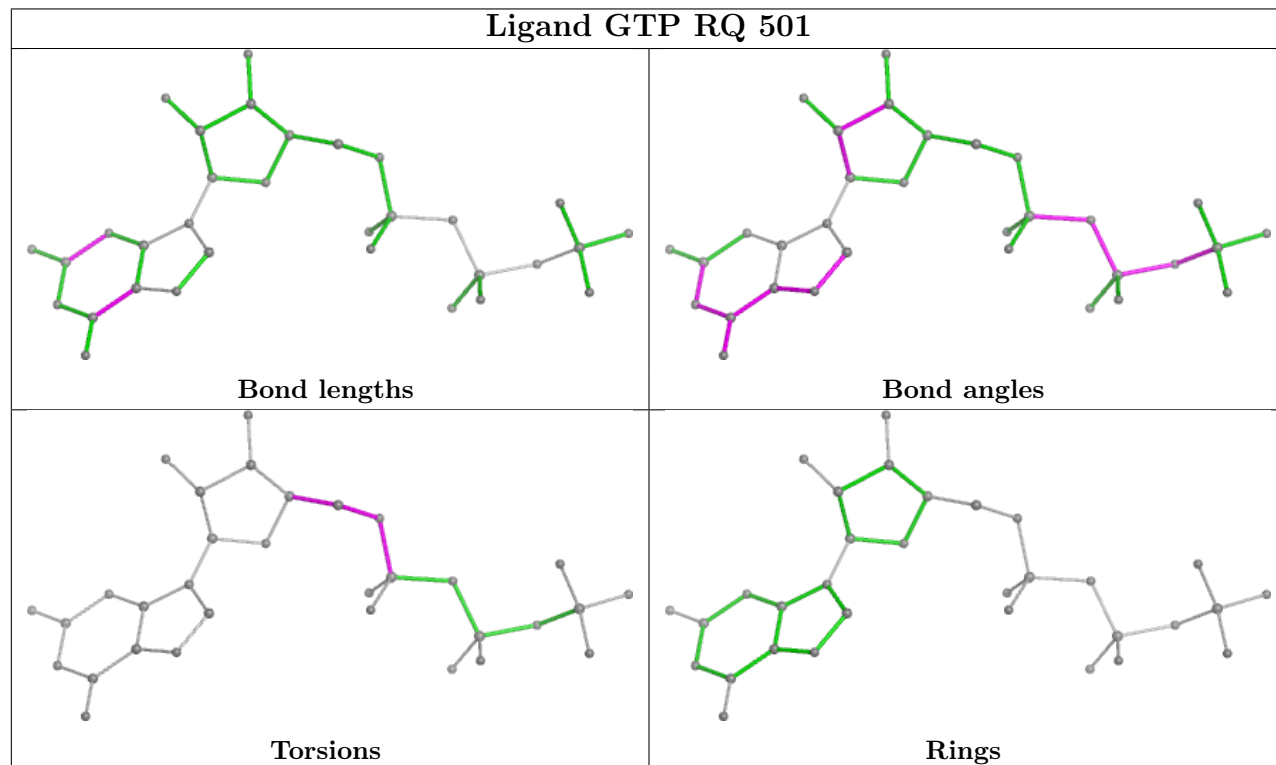
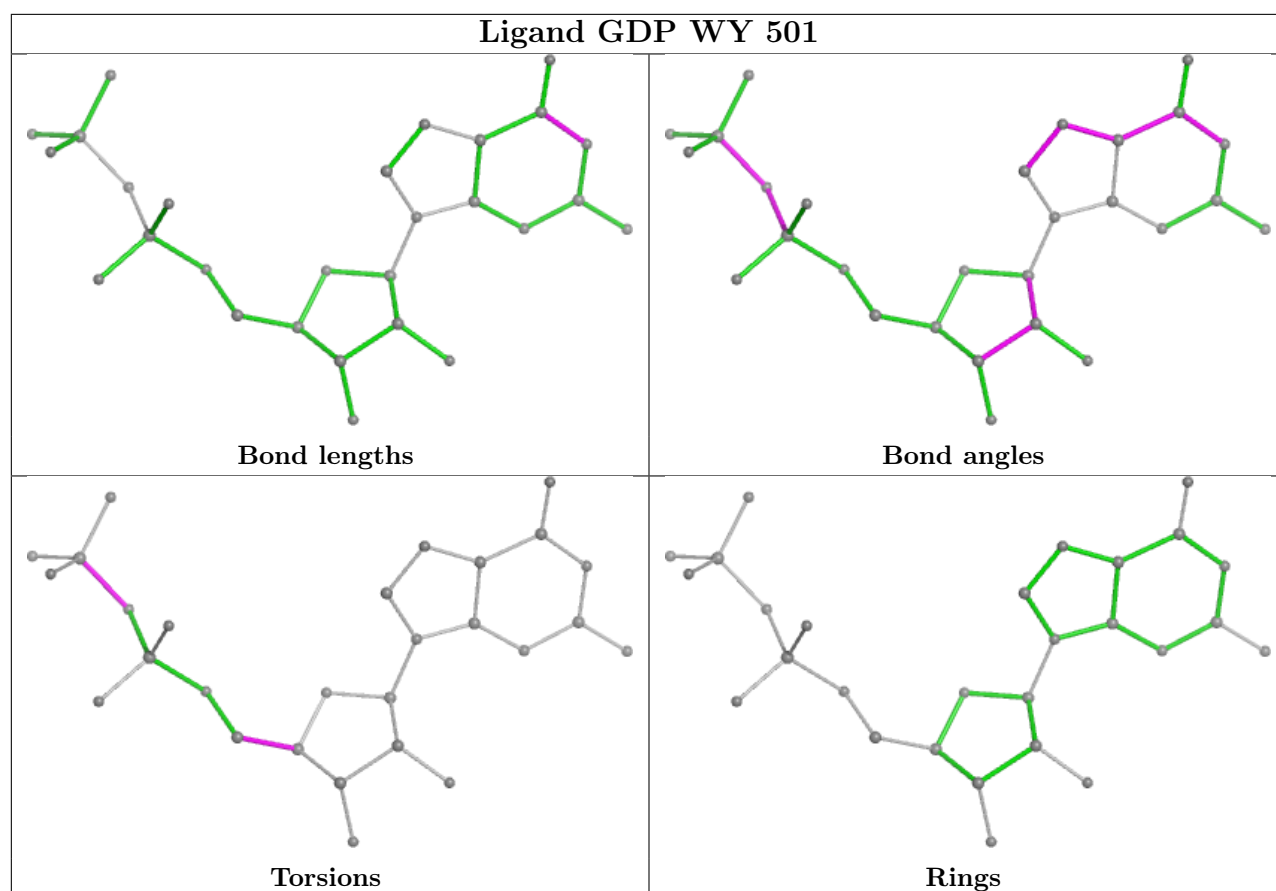


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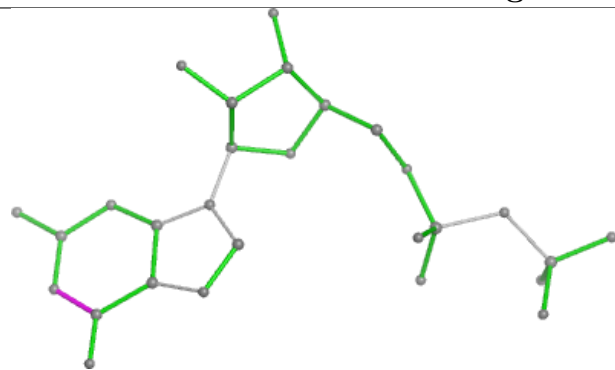


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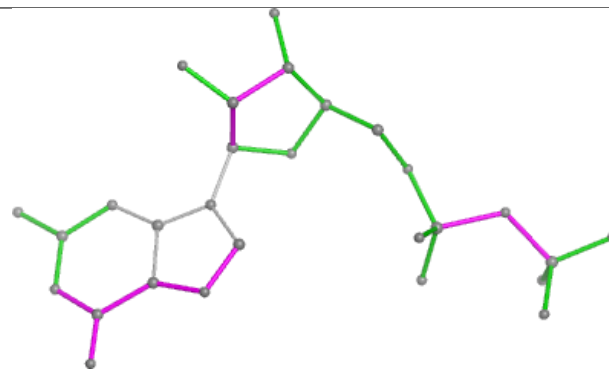




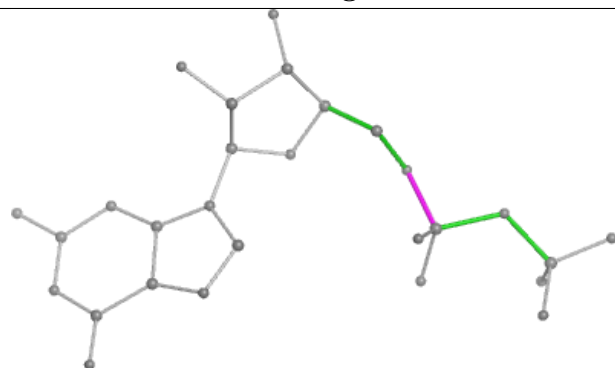
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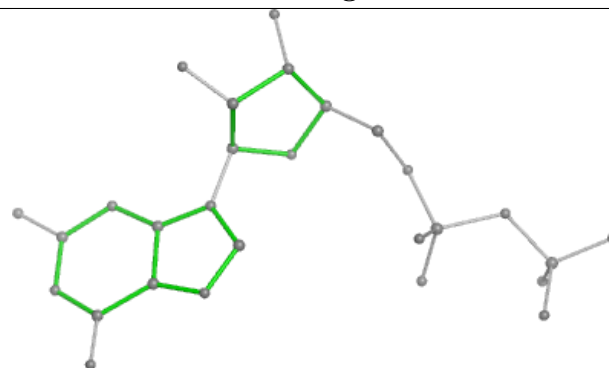
Bond lengths



Bond angles

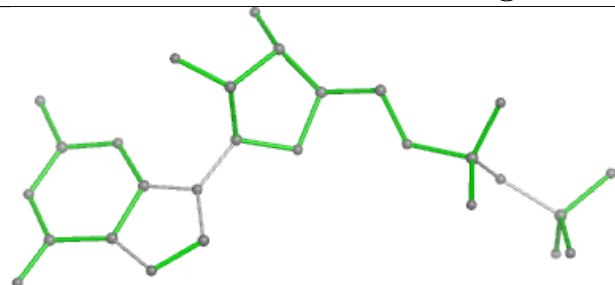


Torsions

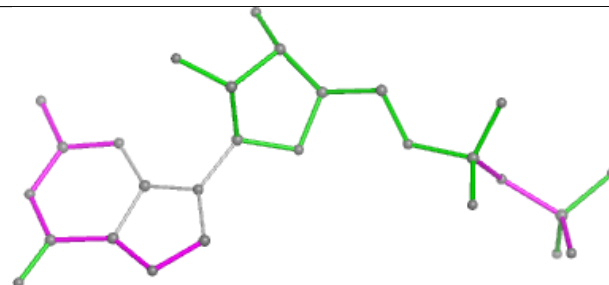


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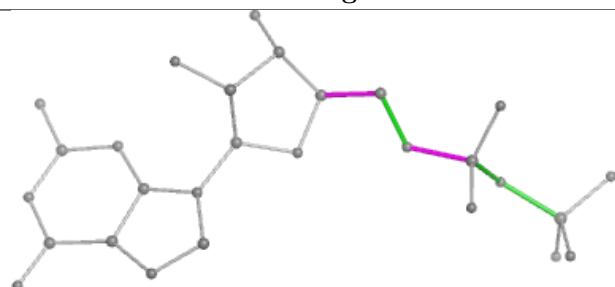
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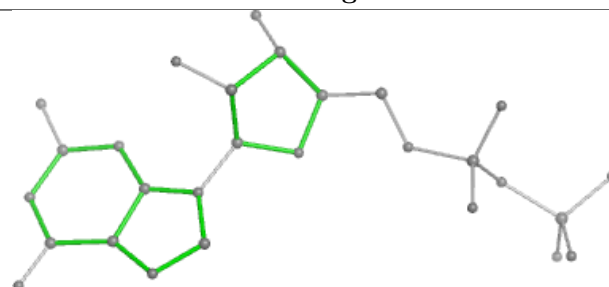
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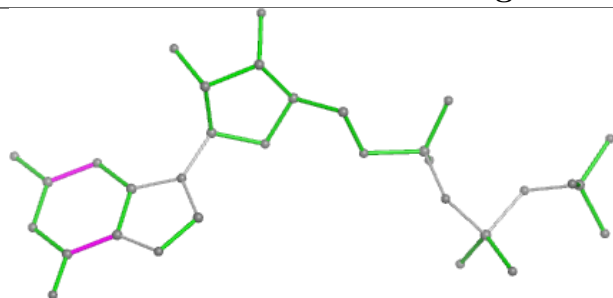


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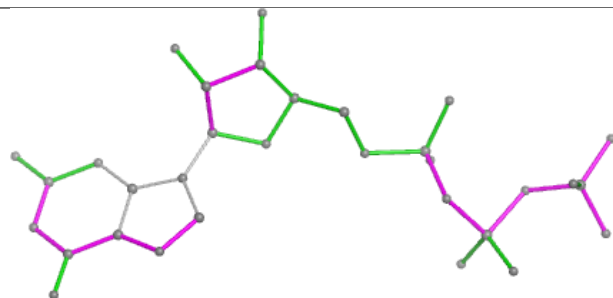


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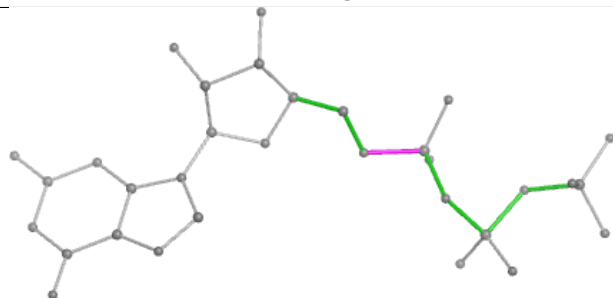
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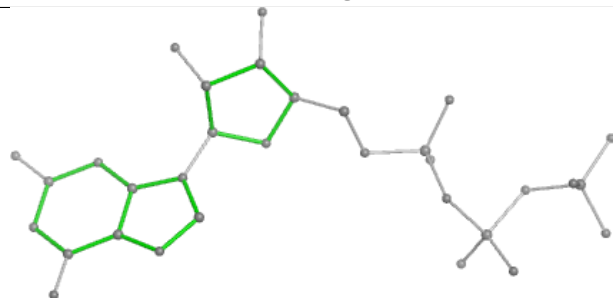
Bond lengths



Bond angles

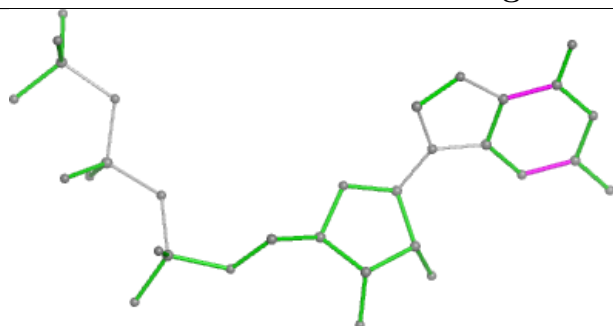


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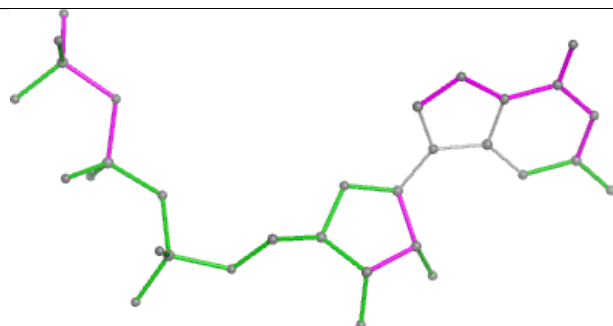


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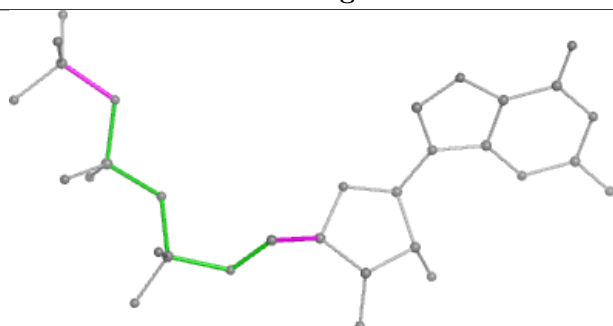
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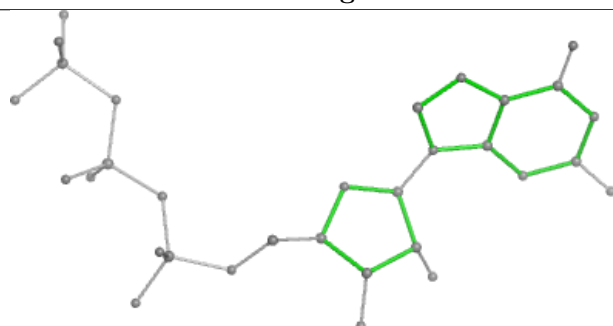
Bond lengths



Bond angles

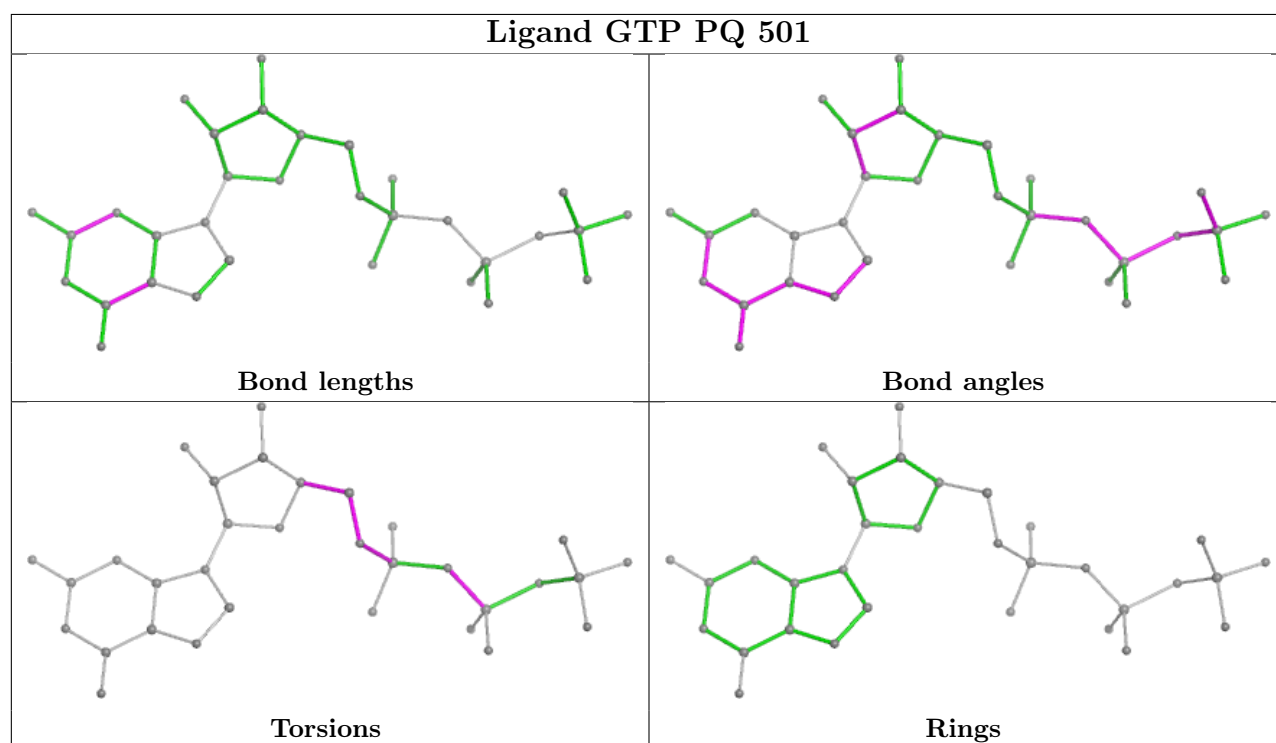
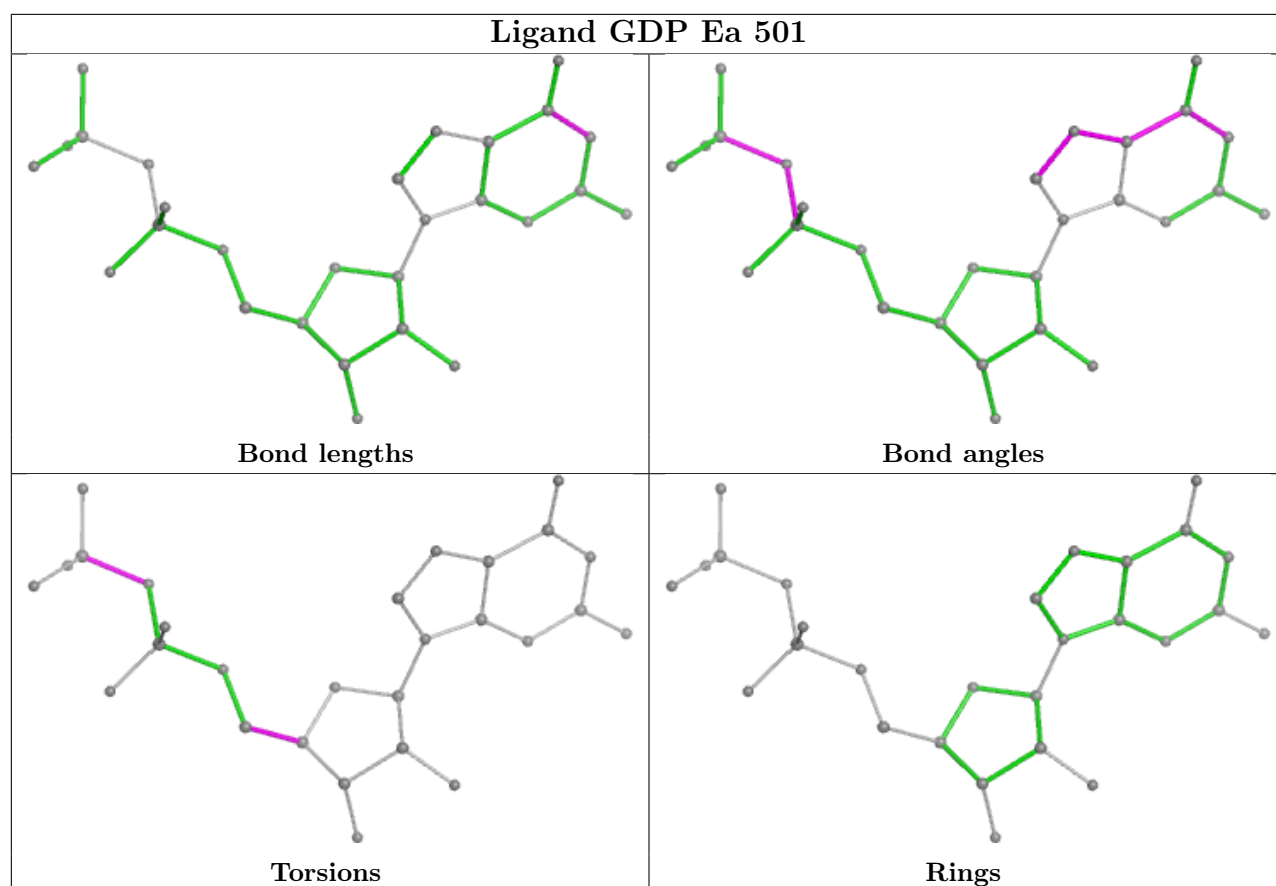


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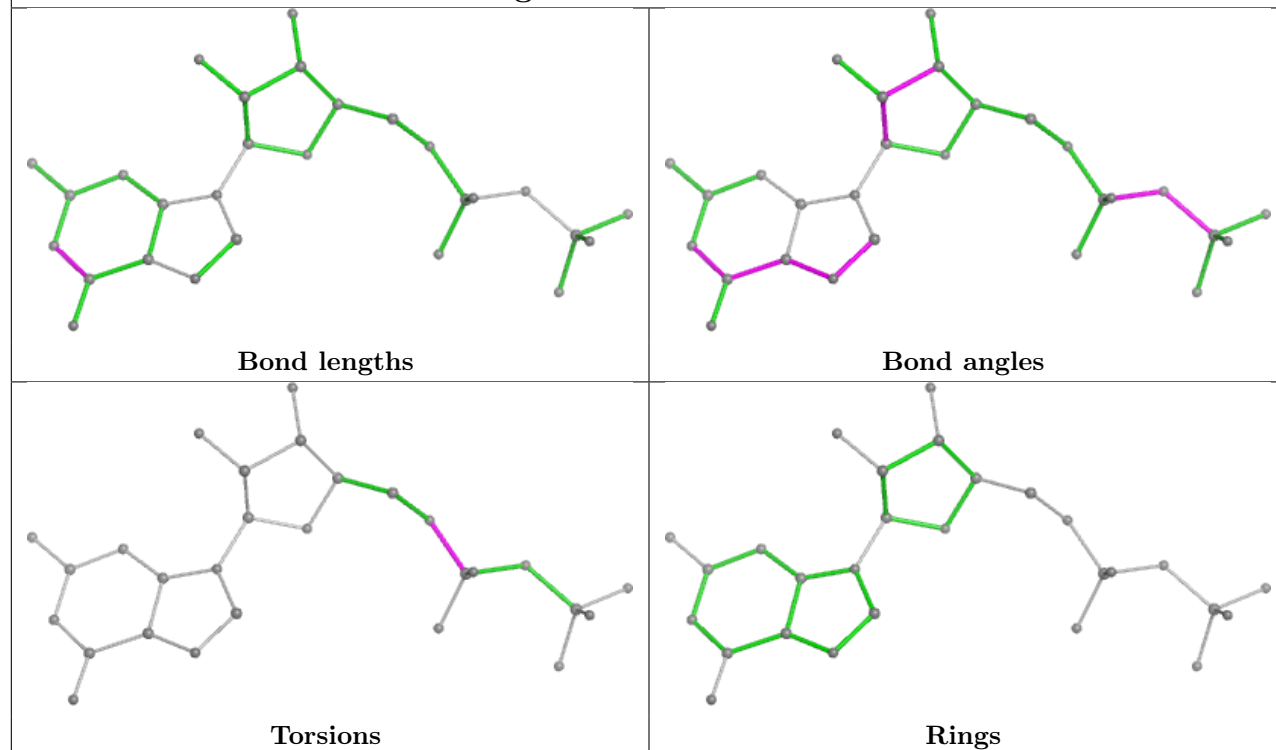


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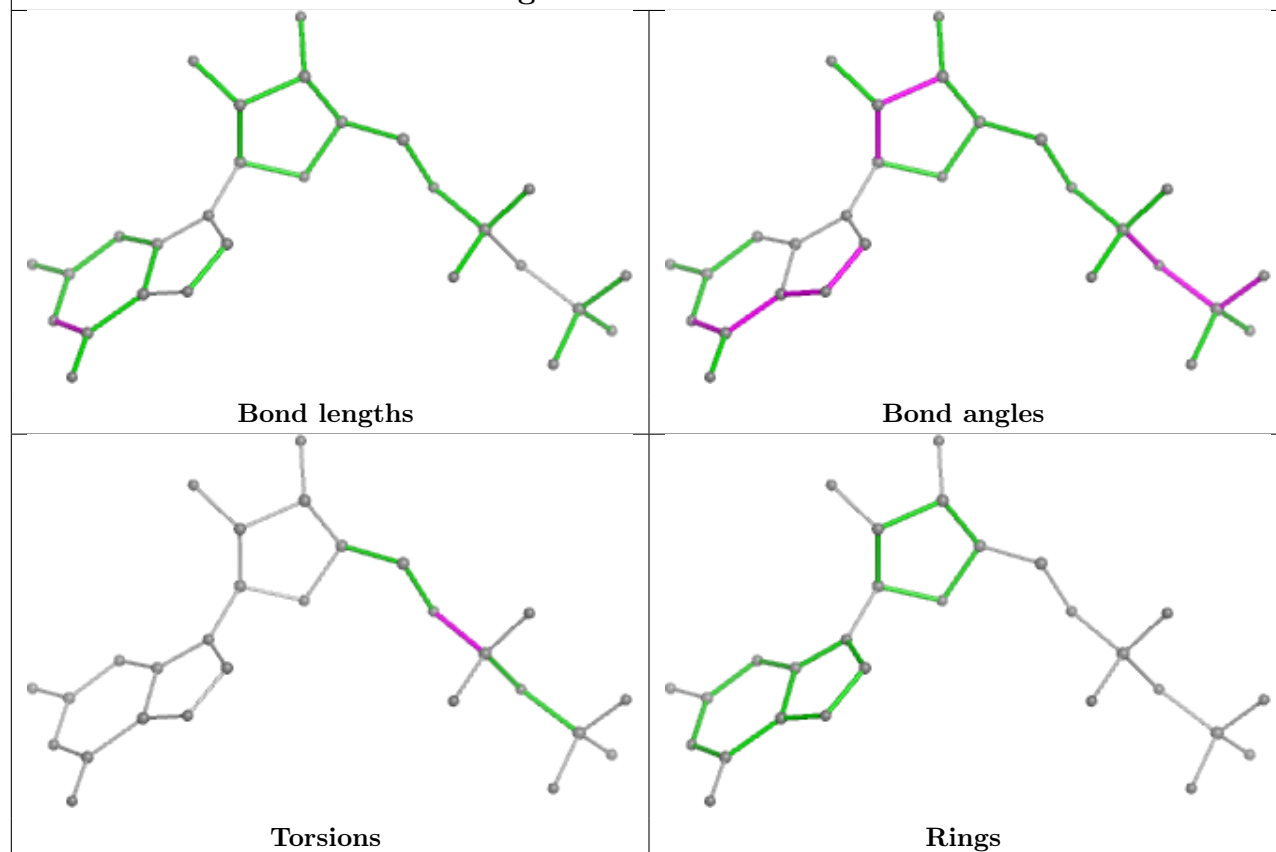


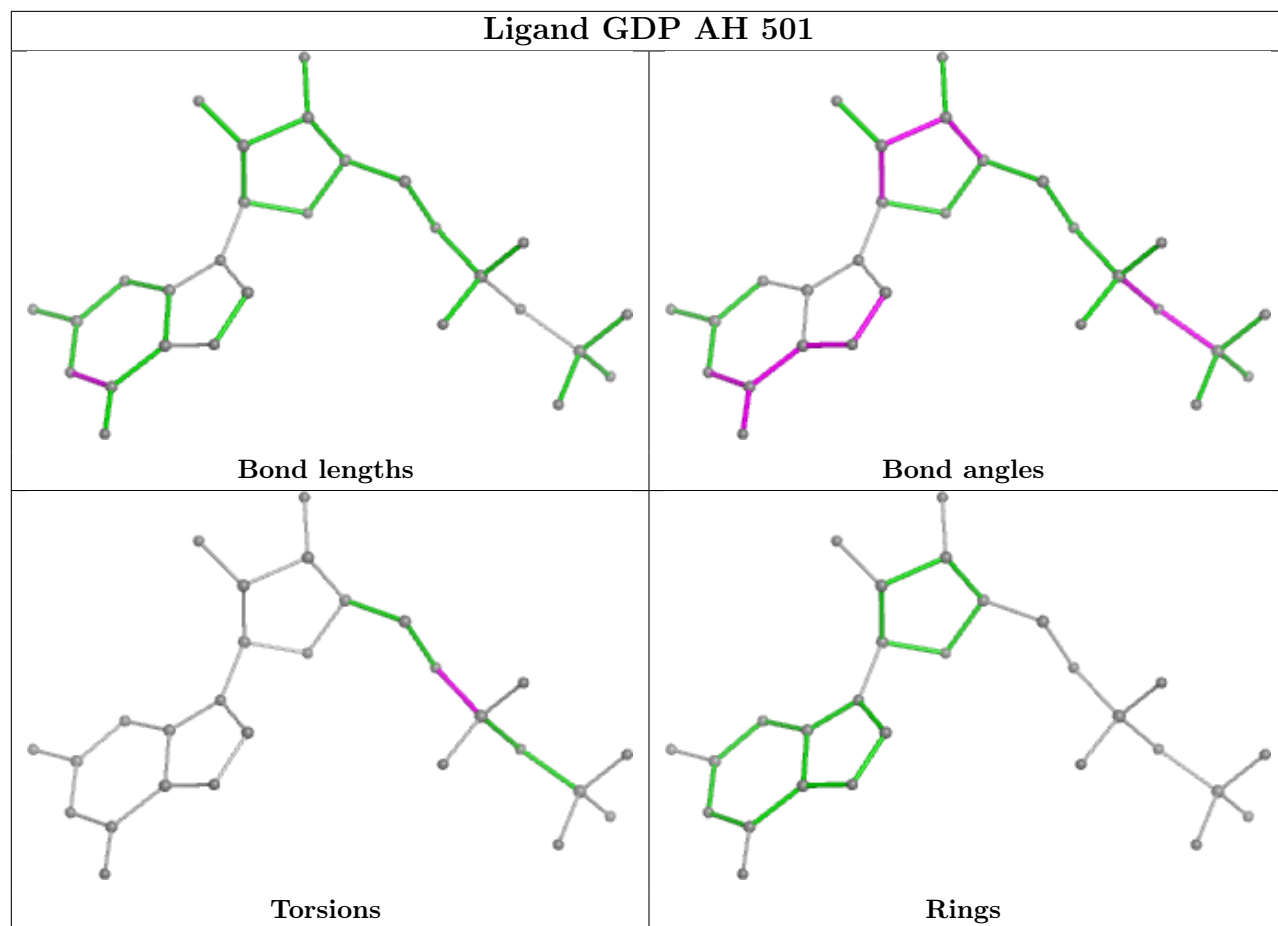


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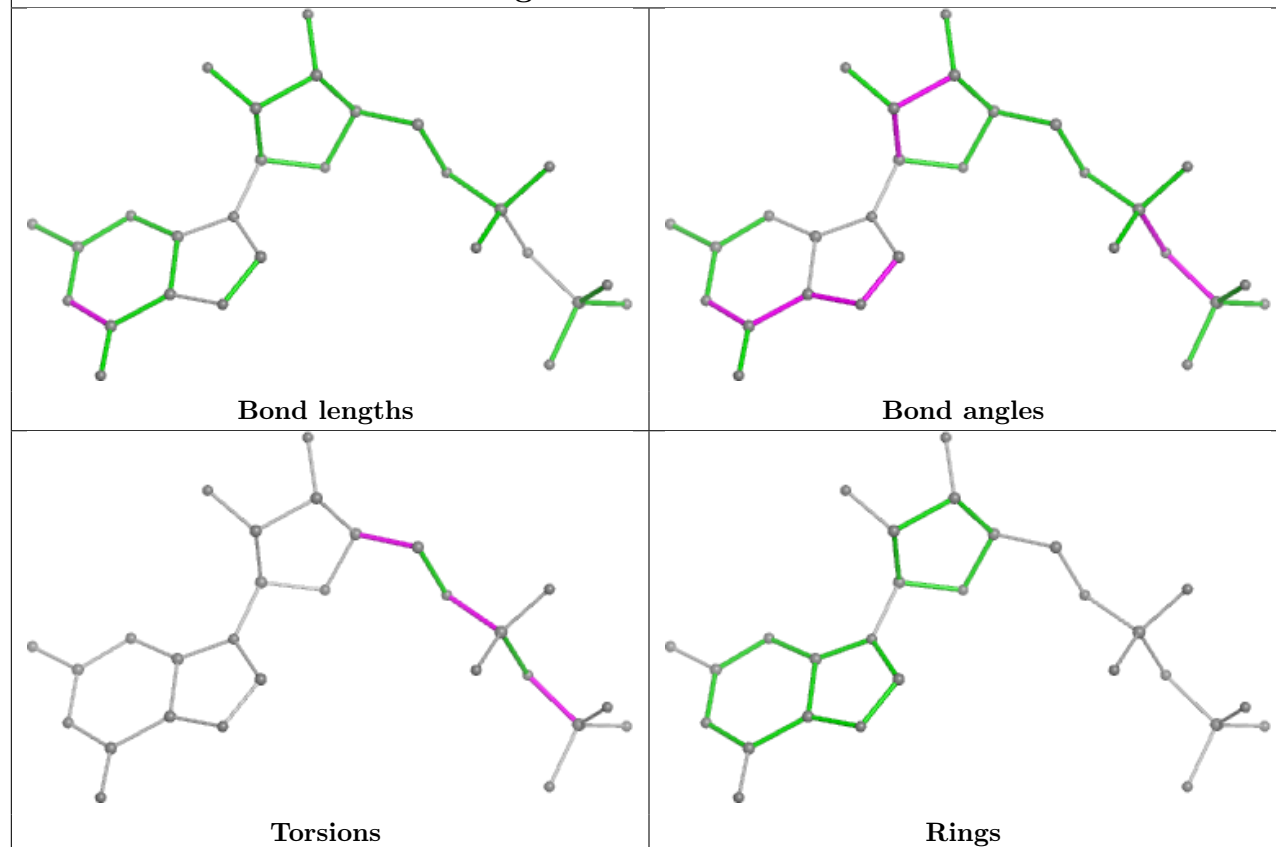


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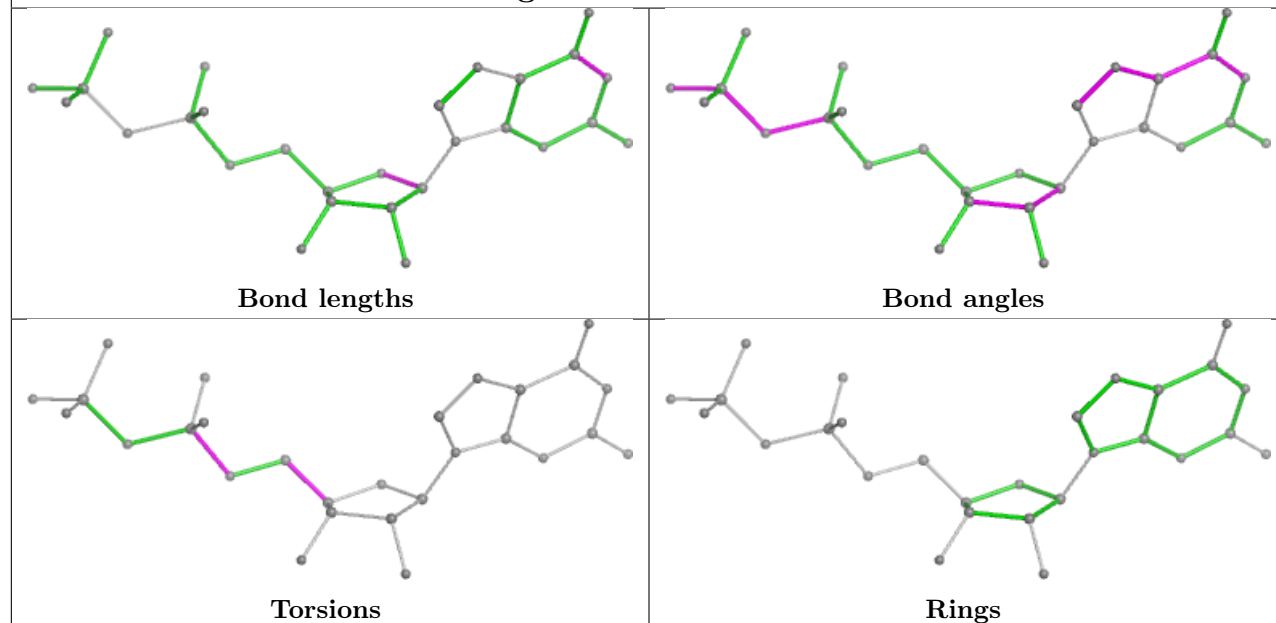


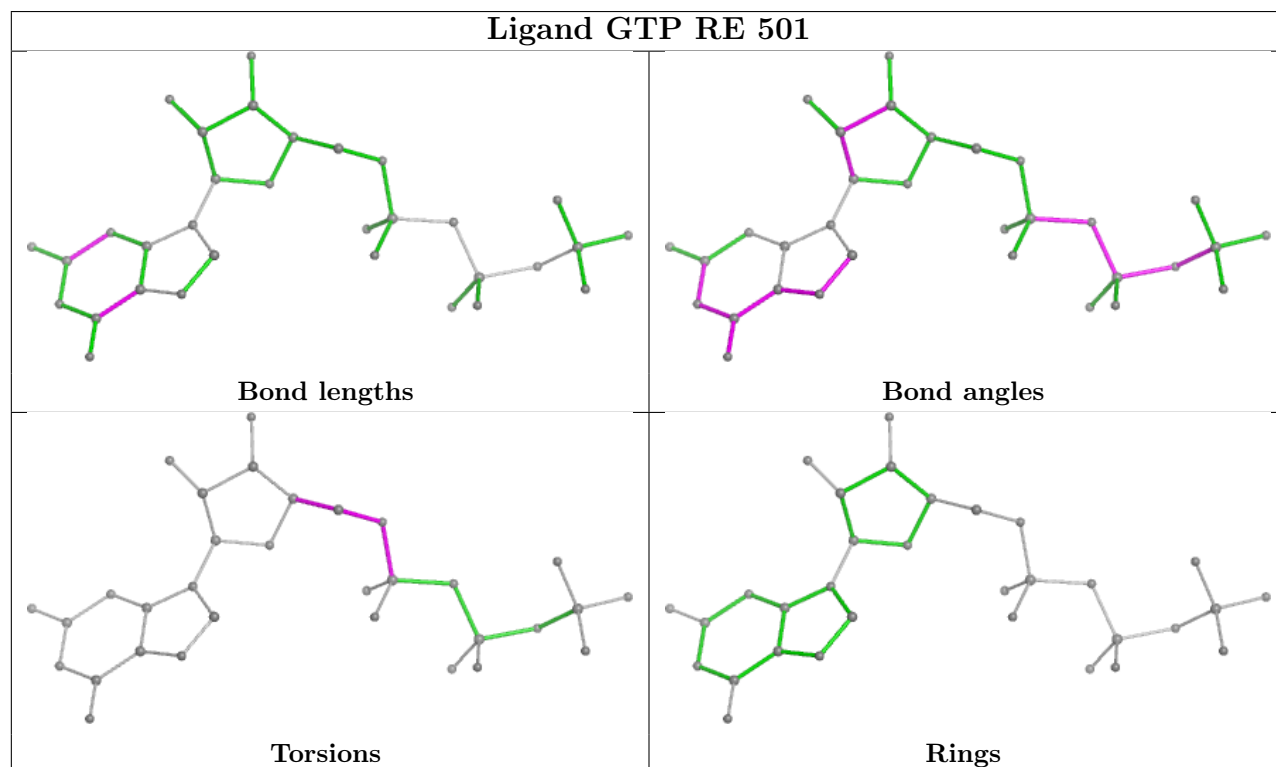
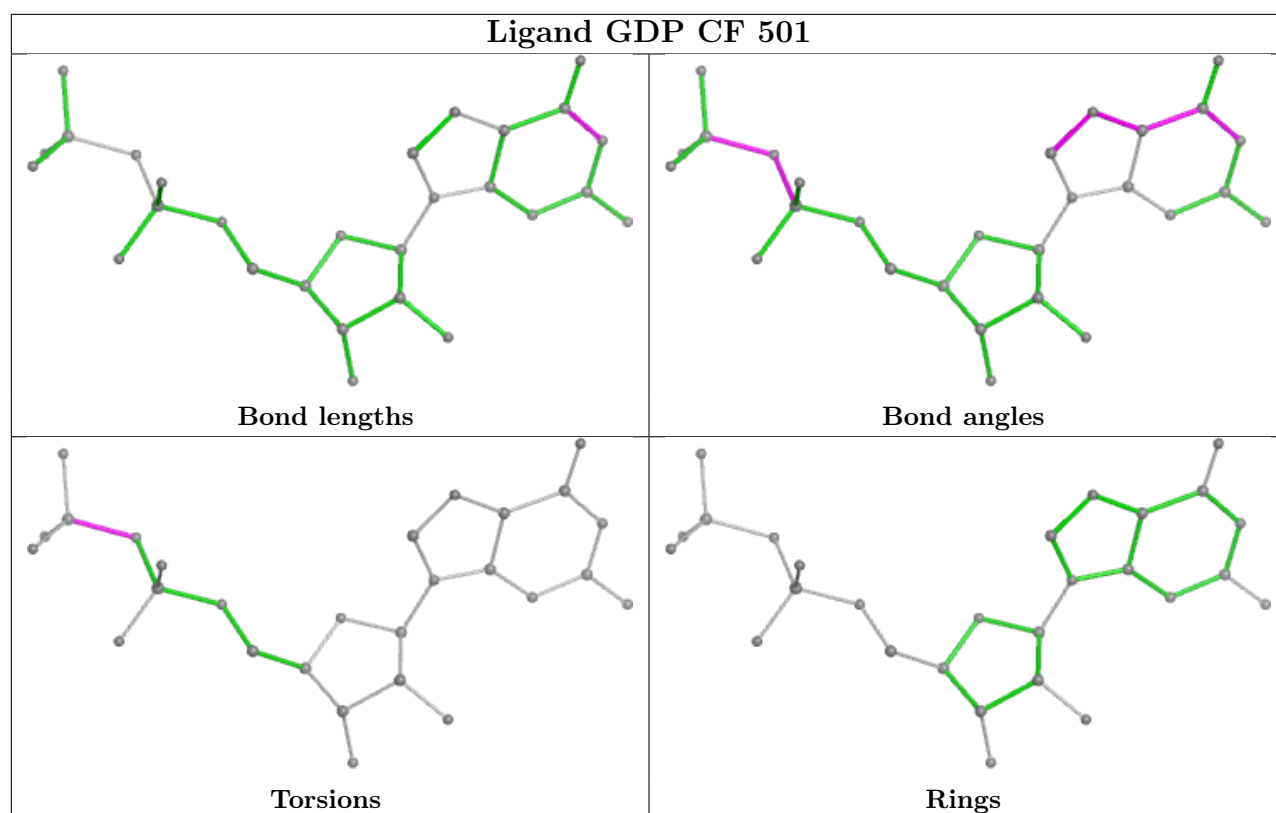


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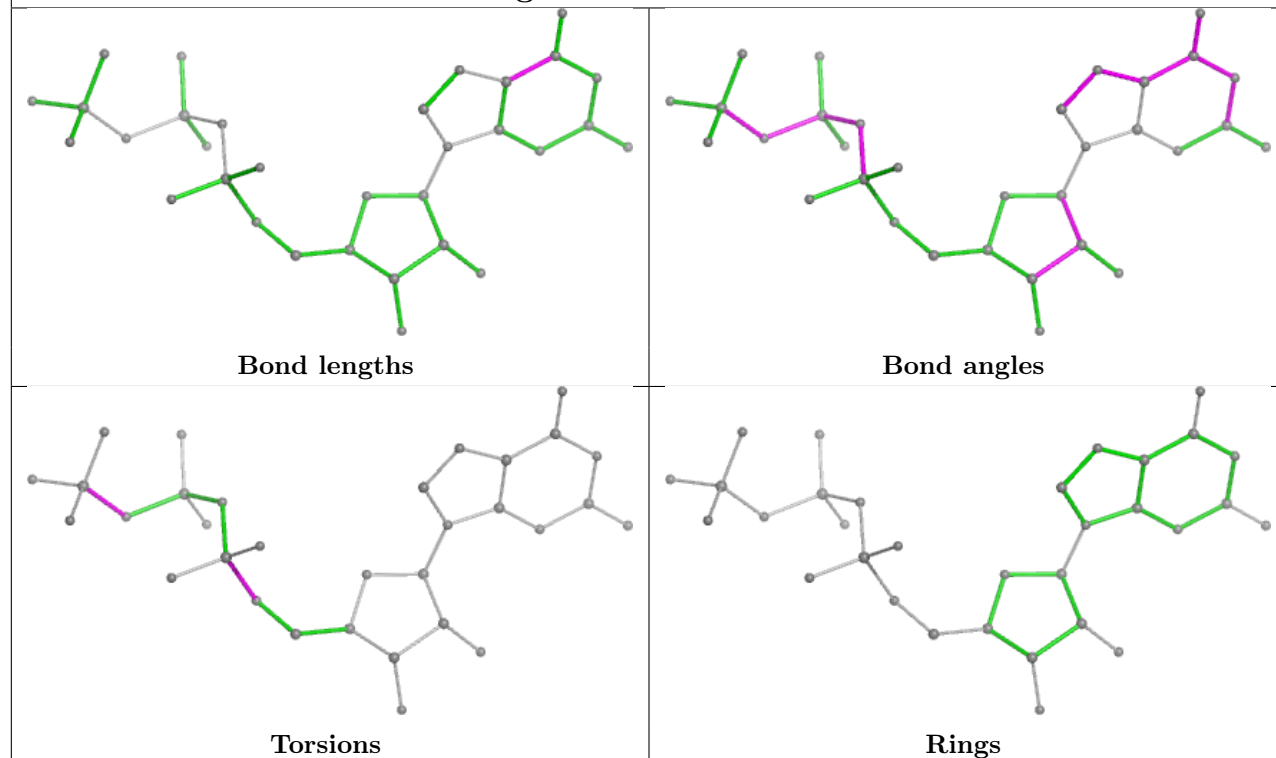


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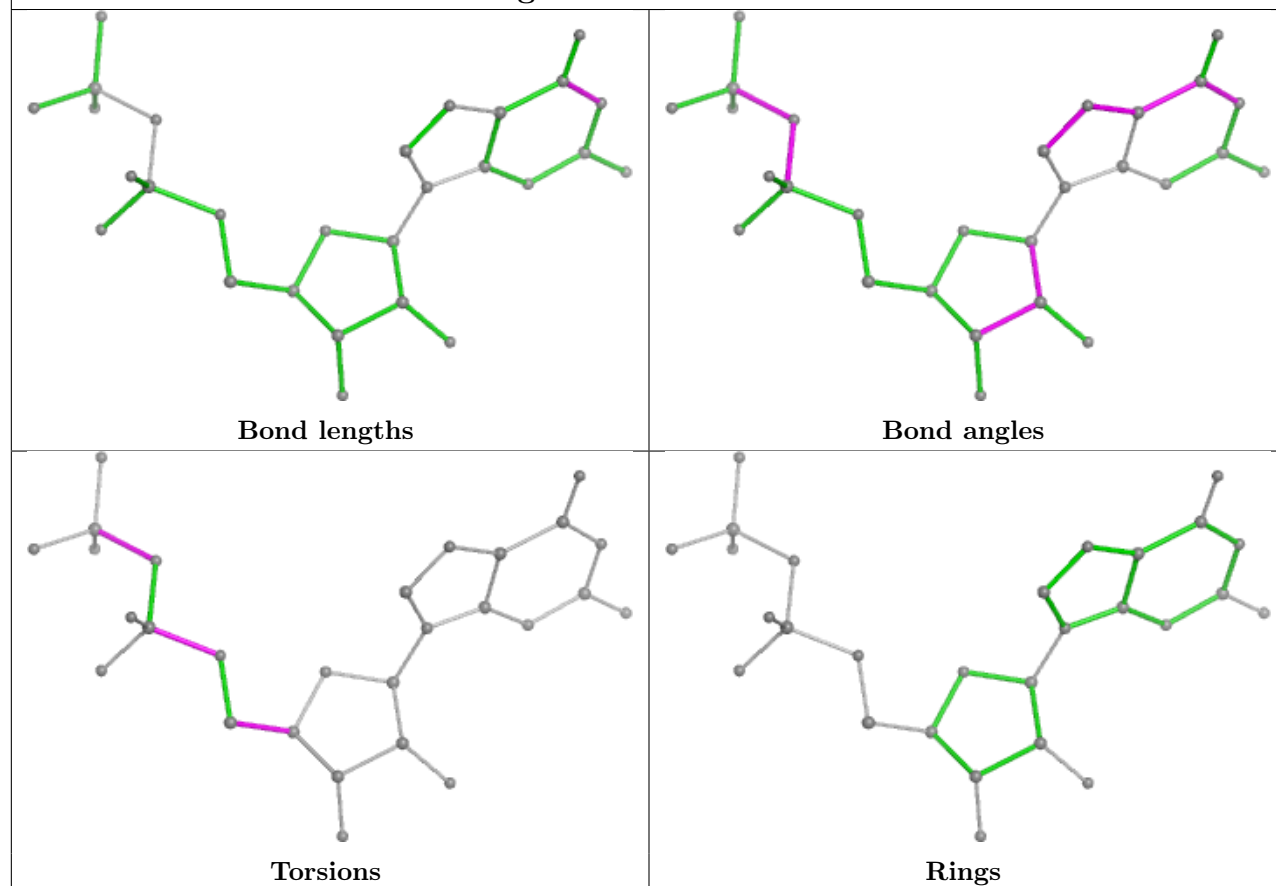




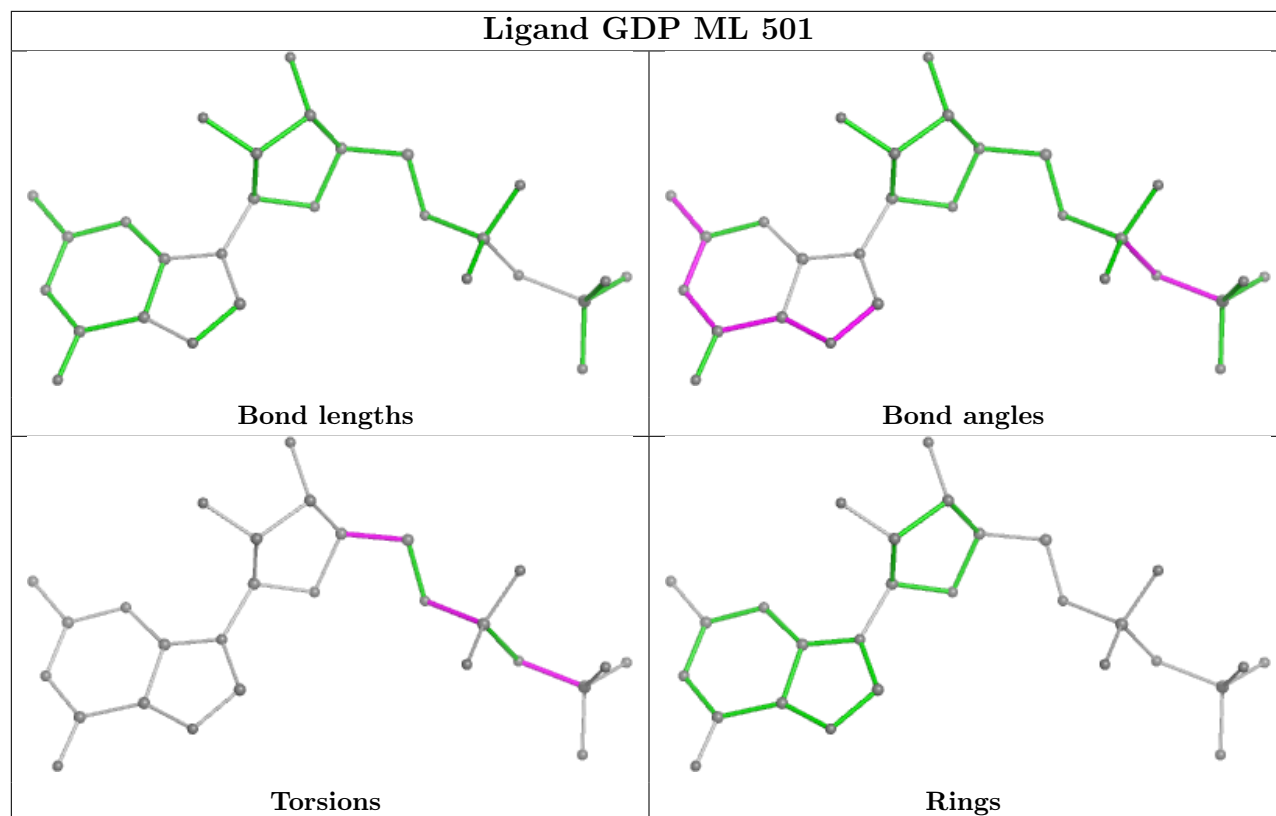
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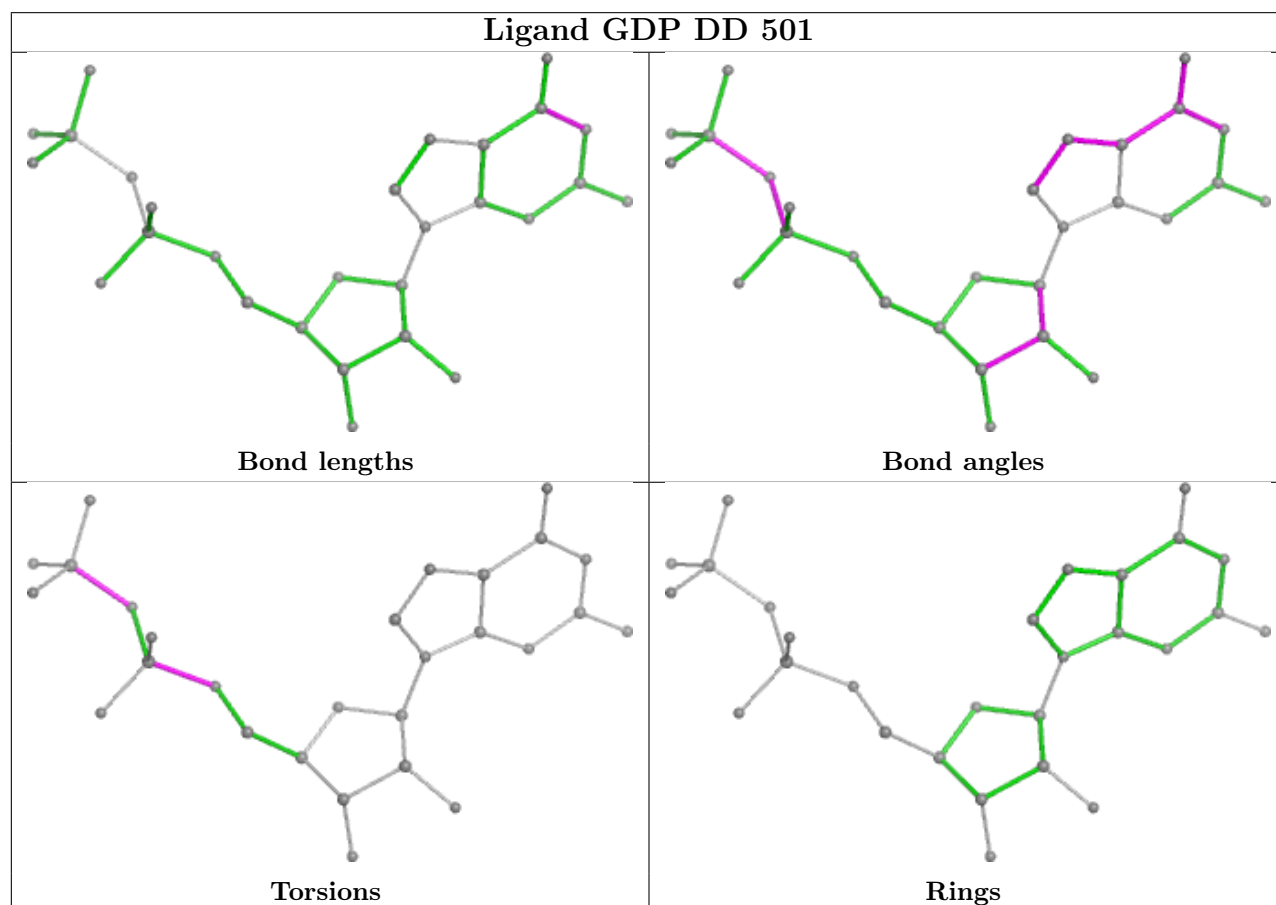
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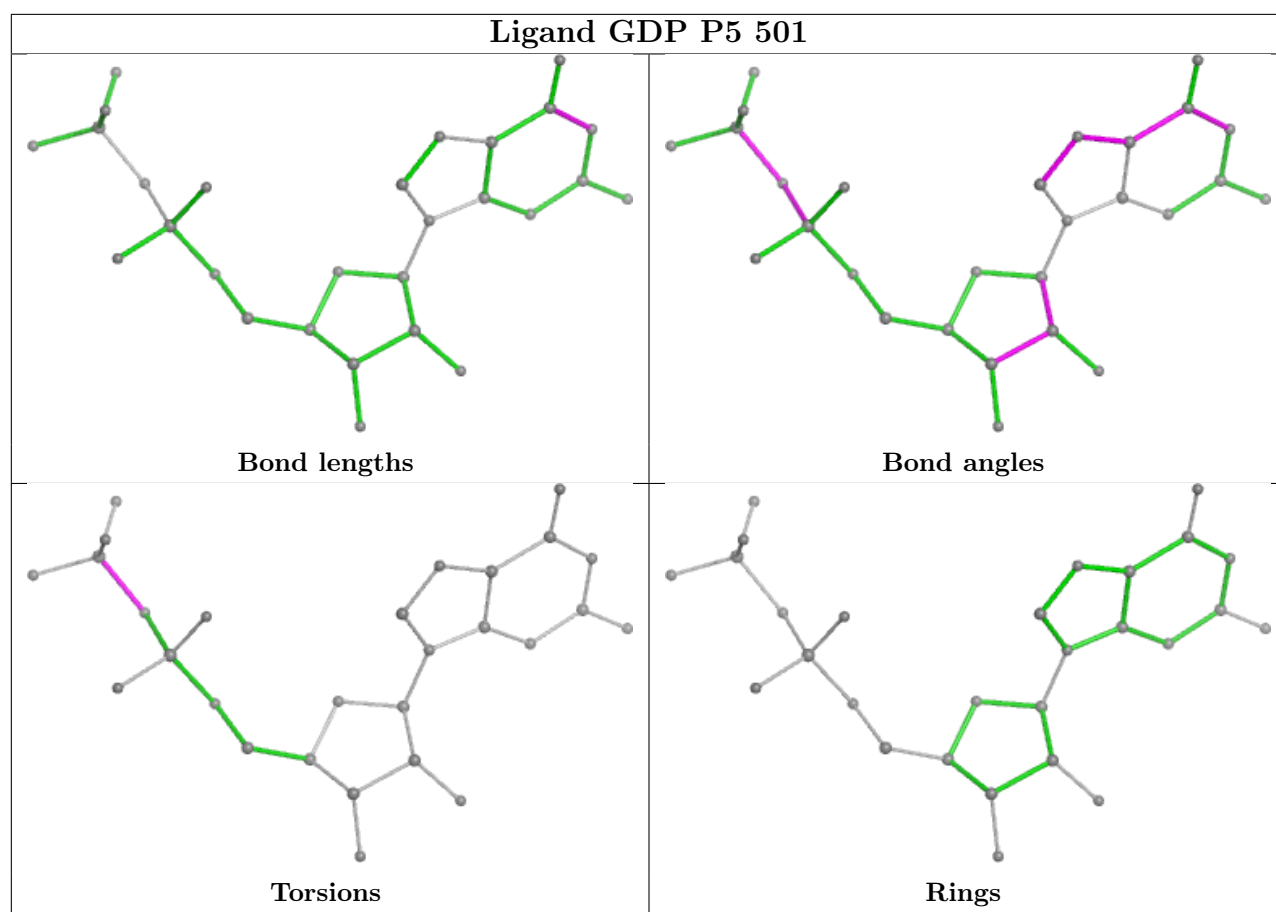


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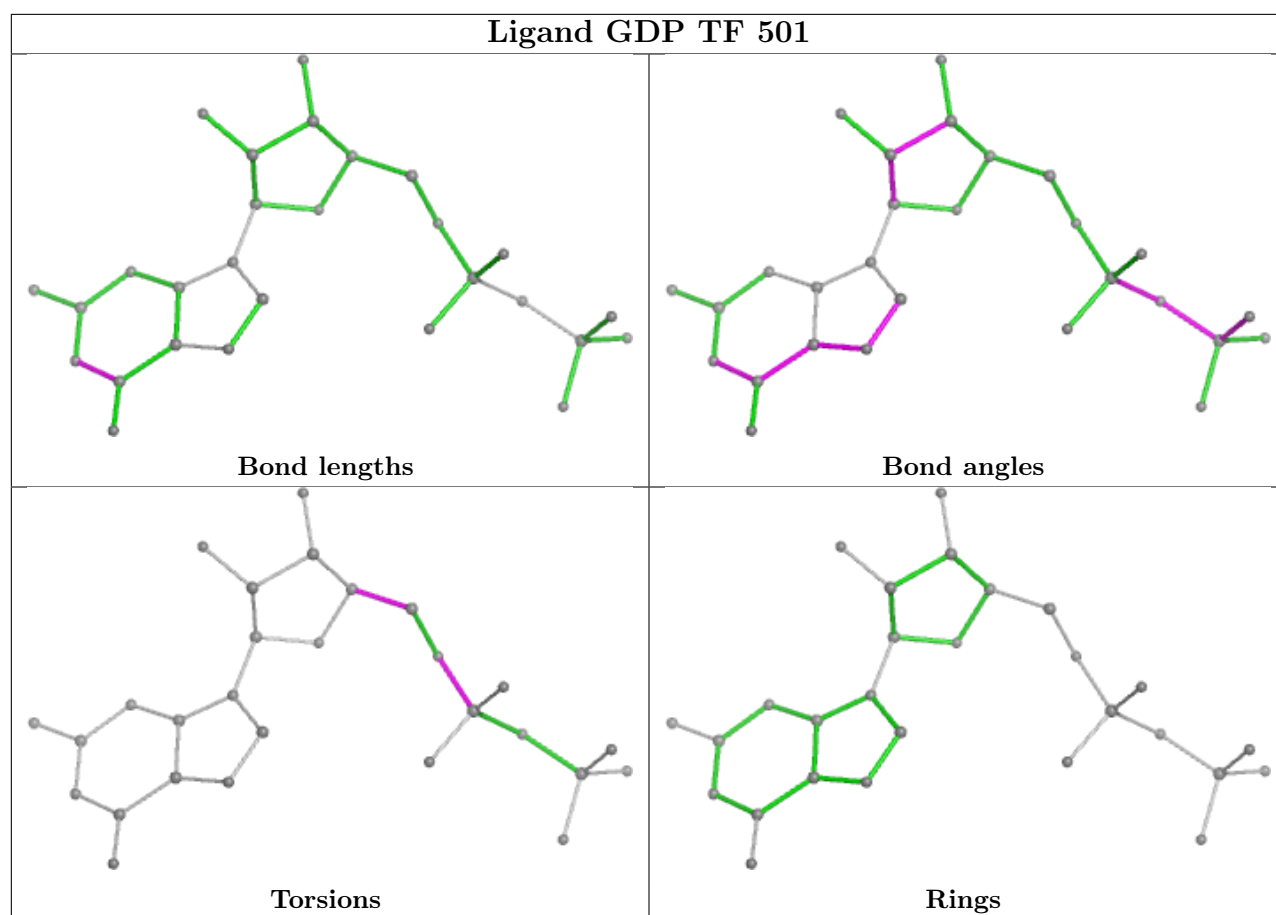


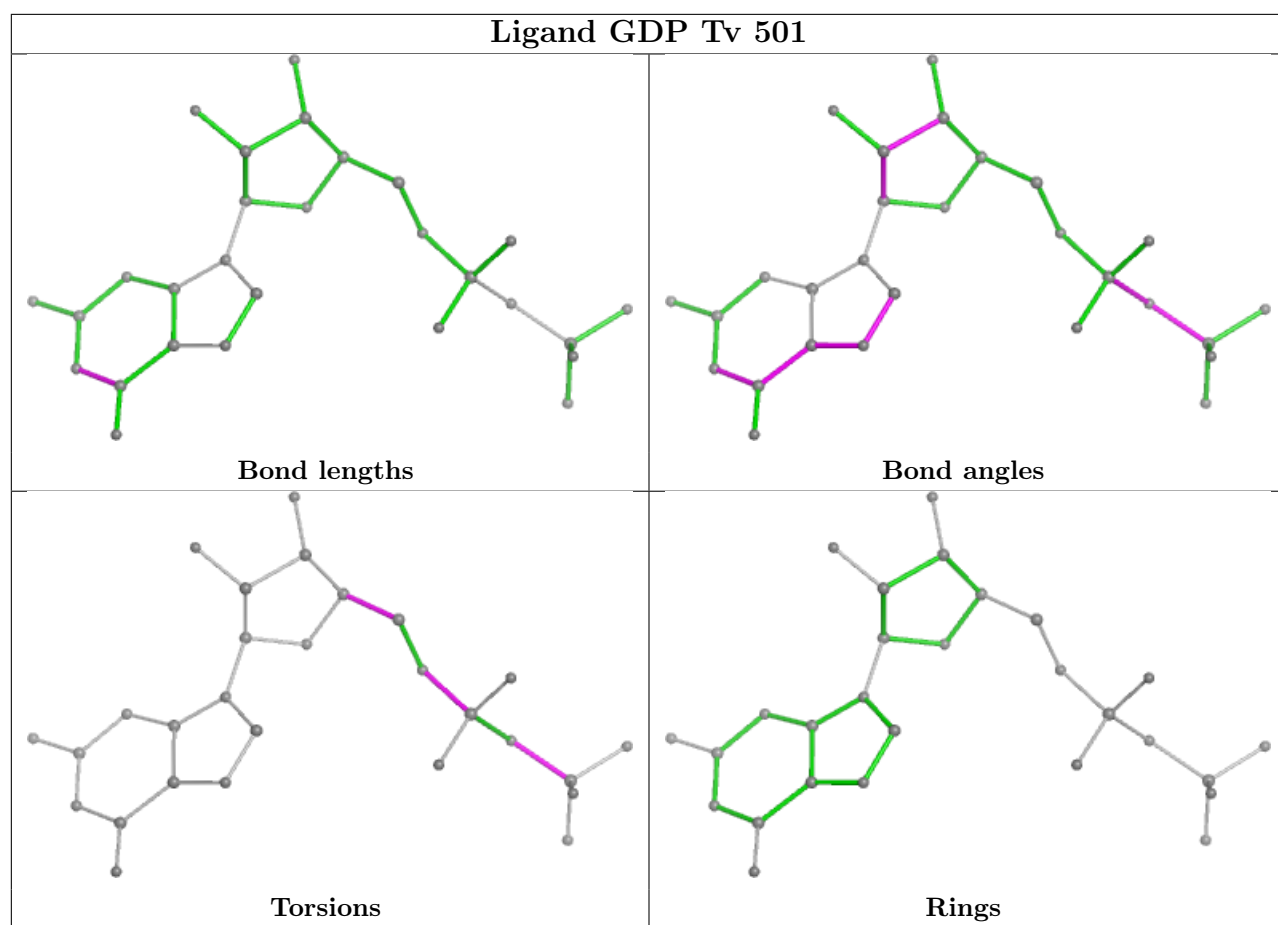
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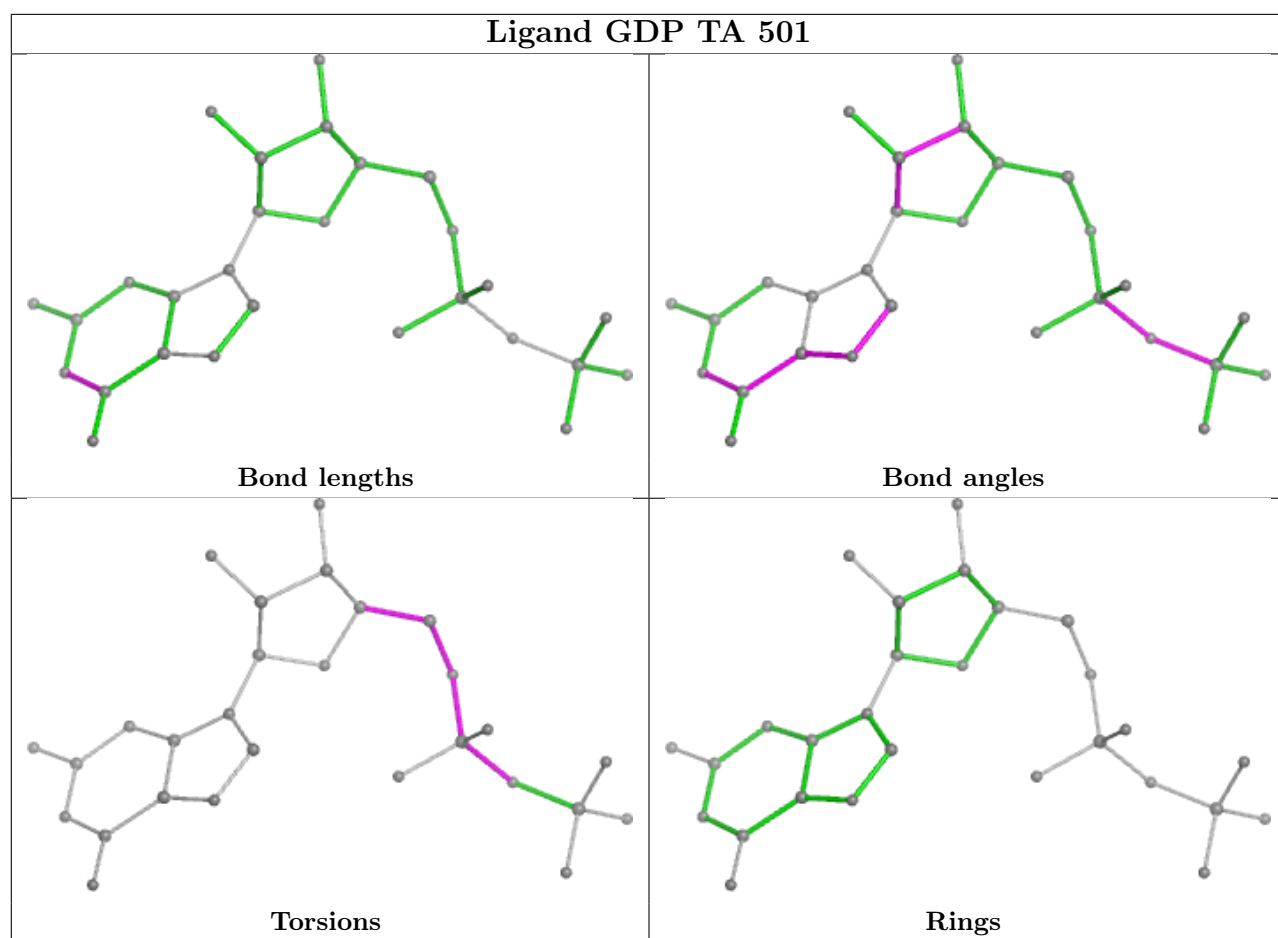




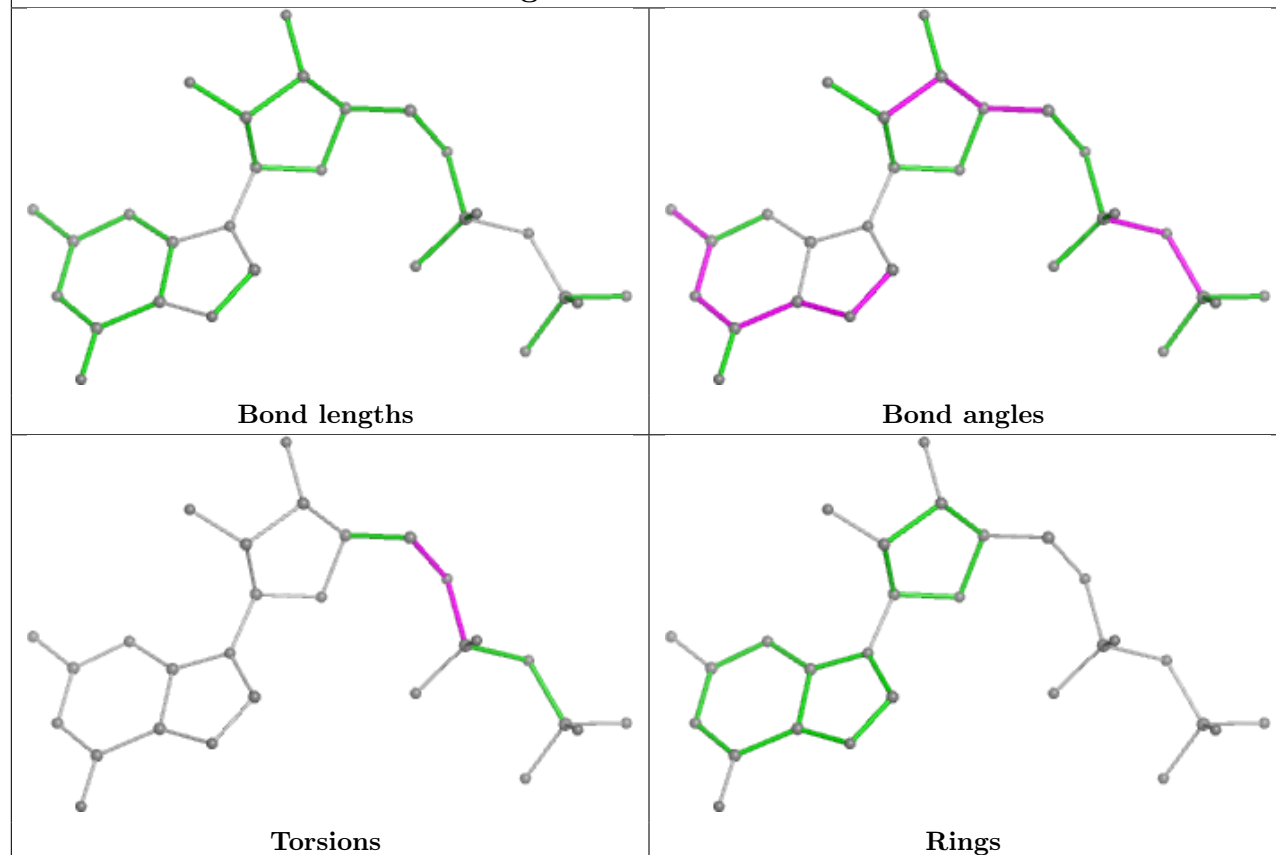




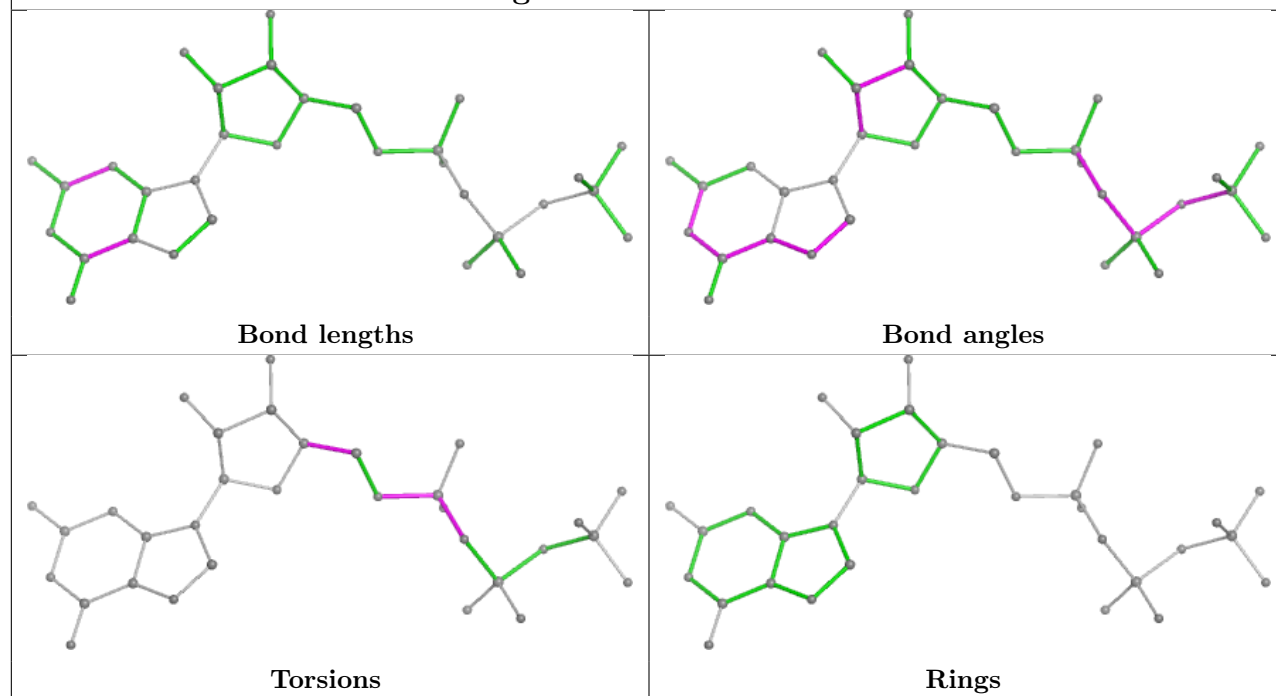


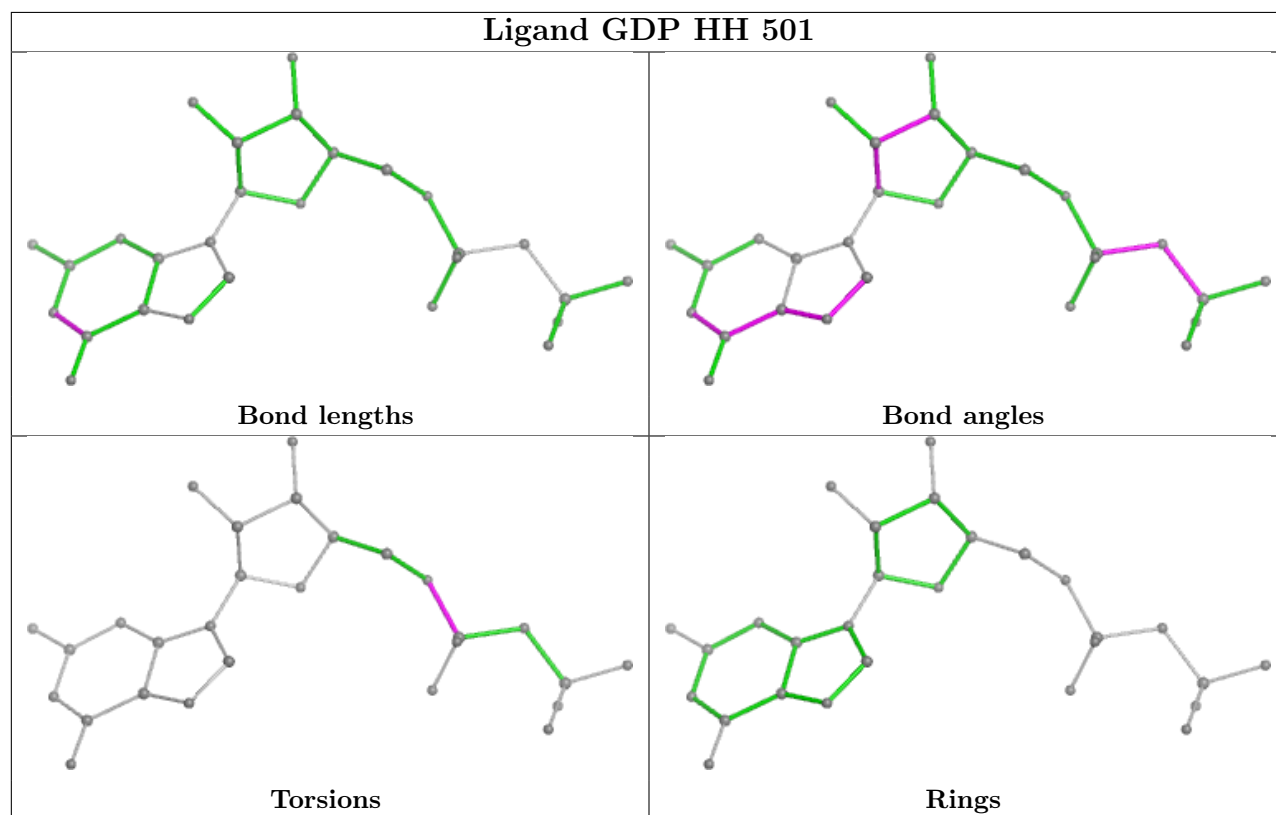
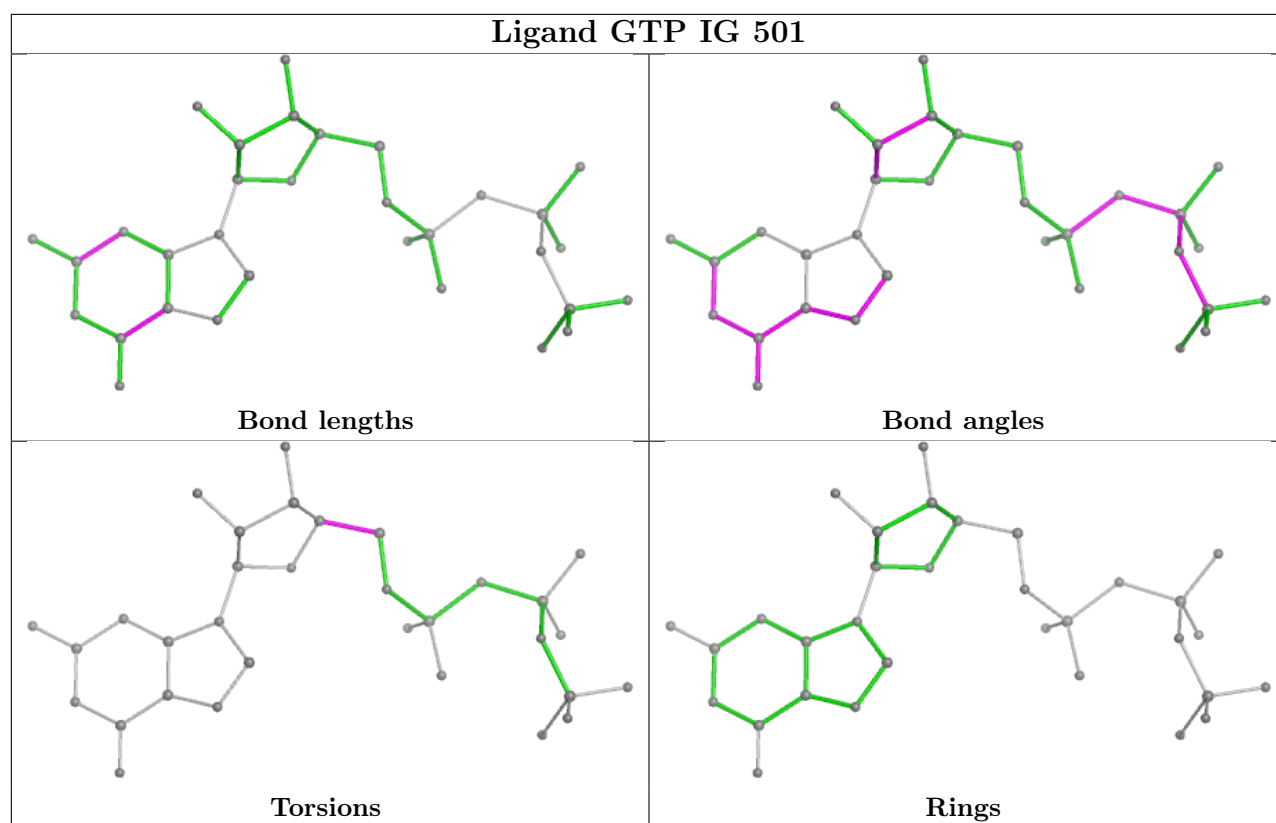


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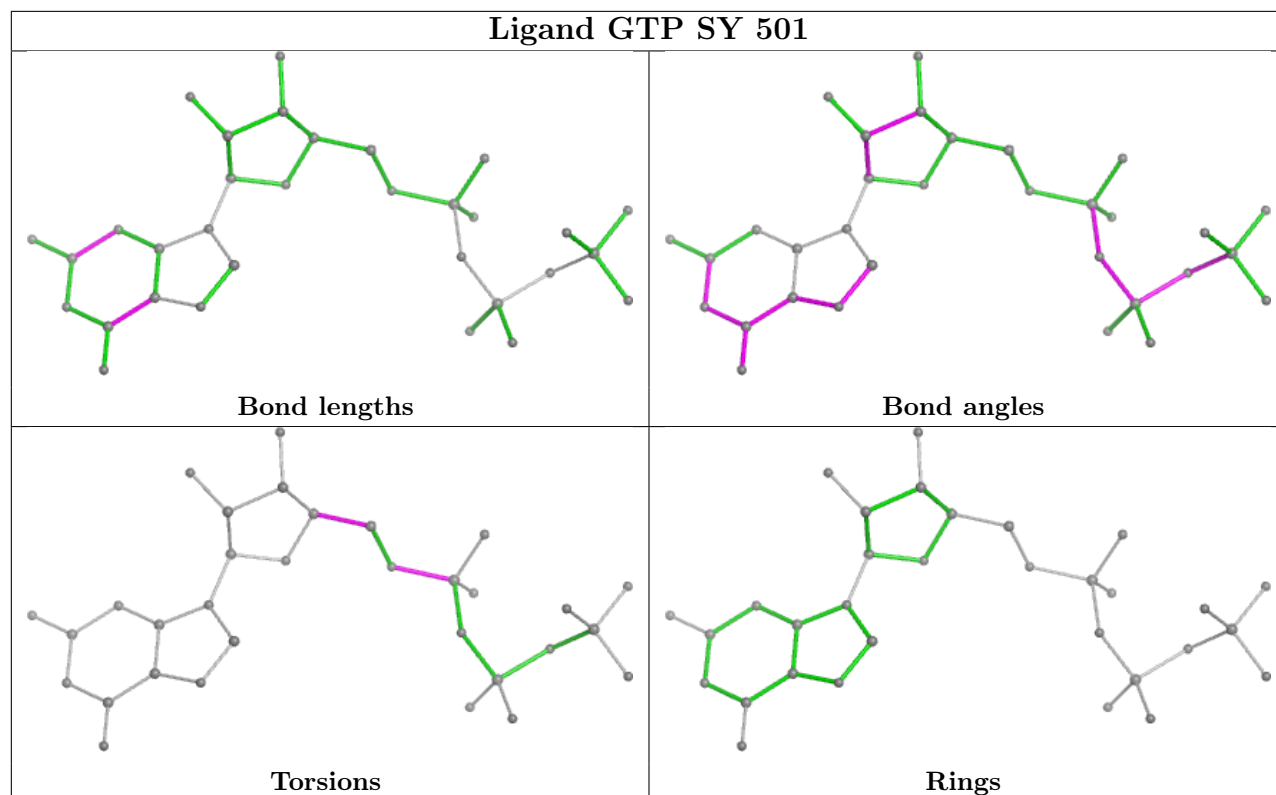


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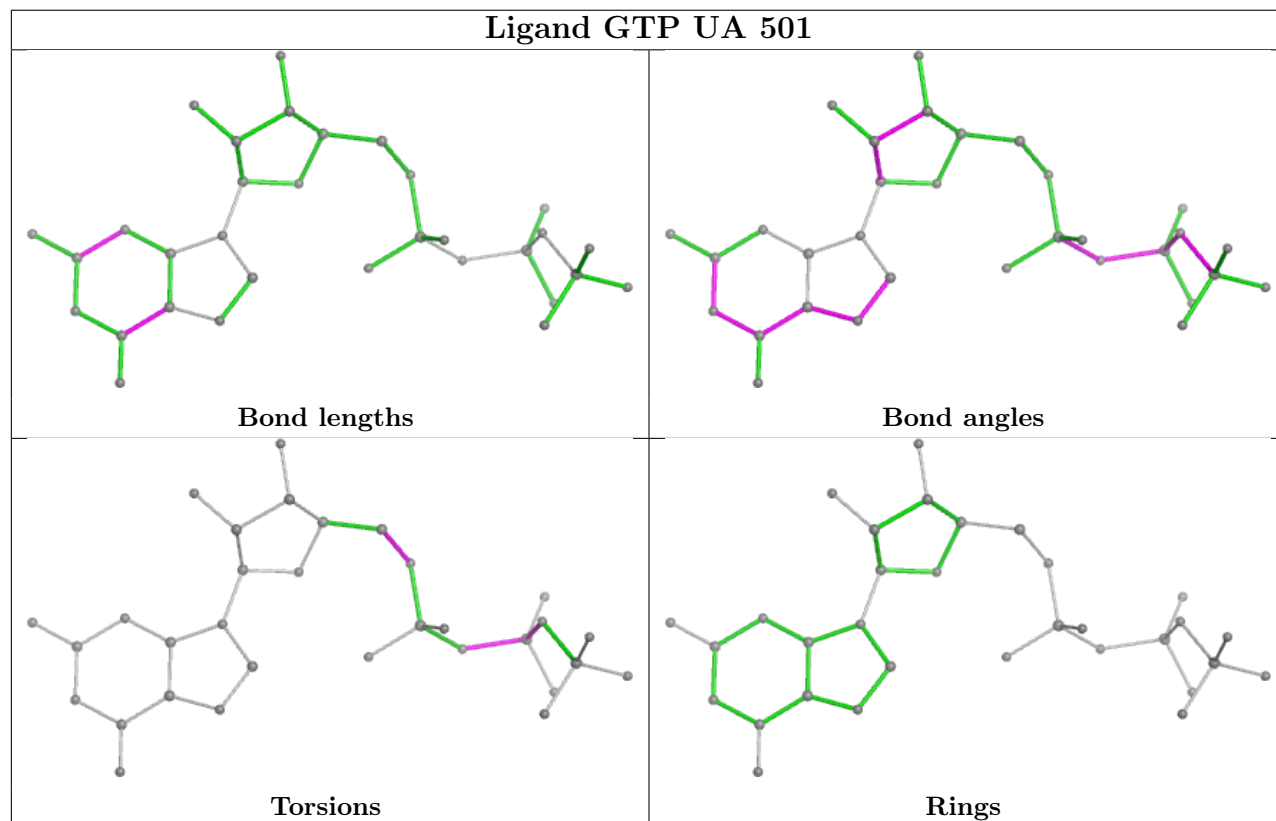




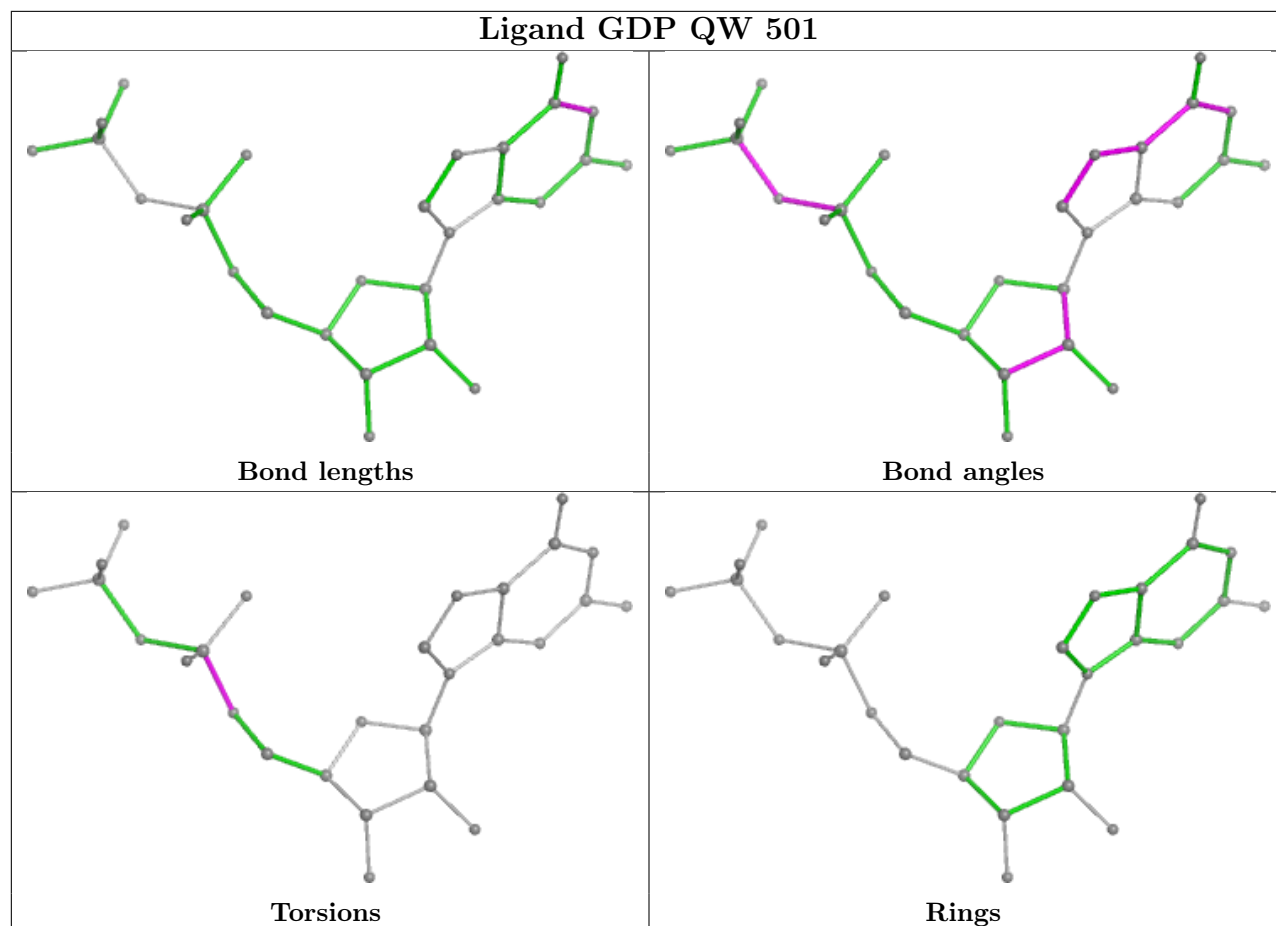
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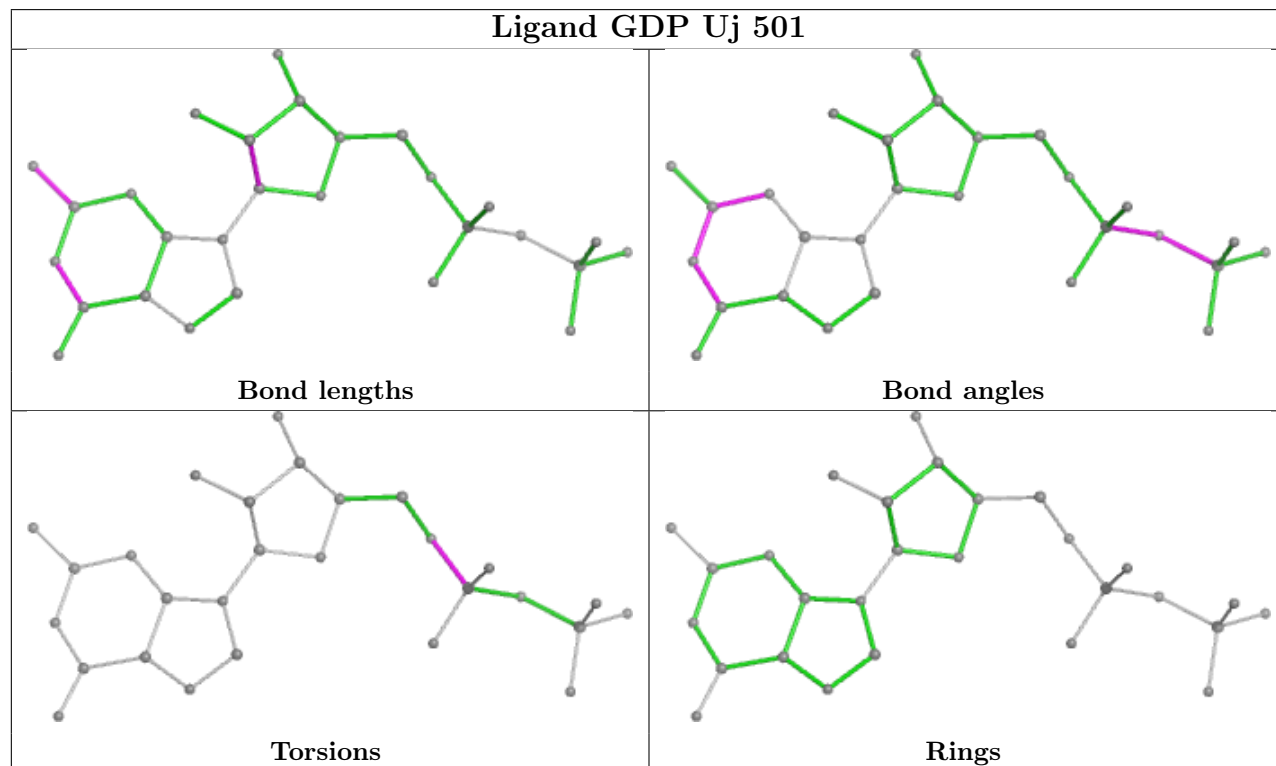
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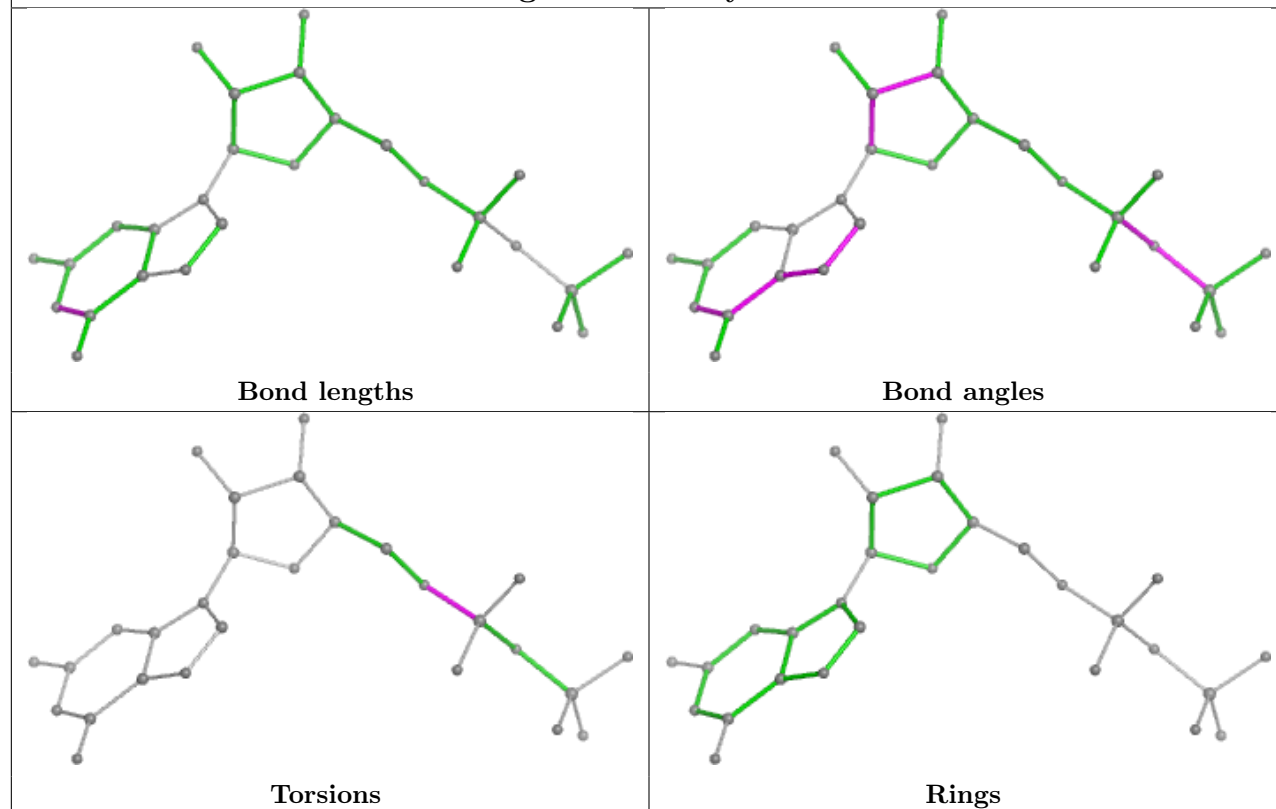
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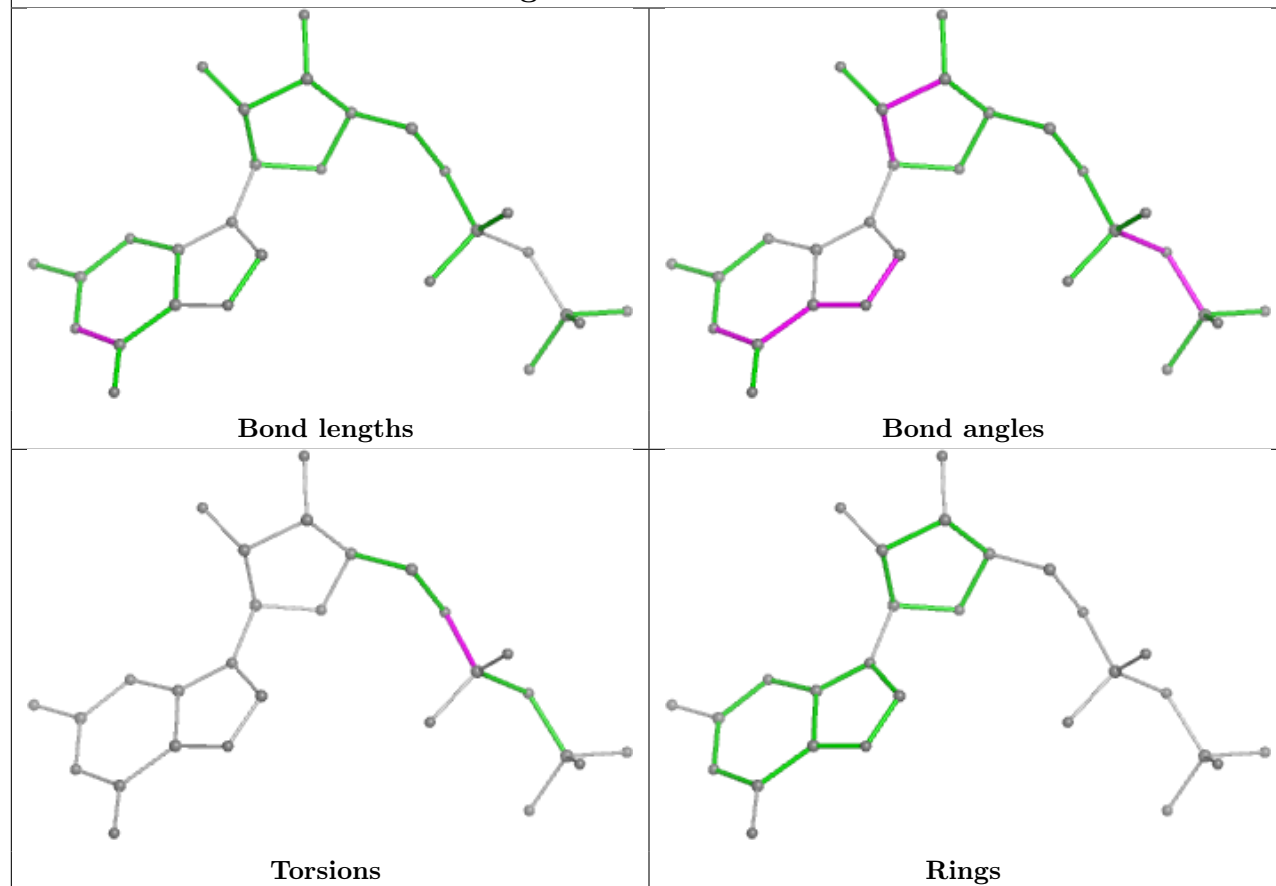
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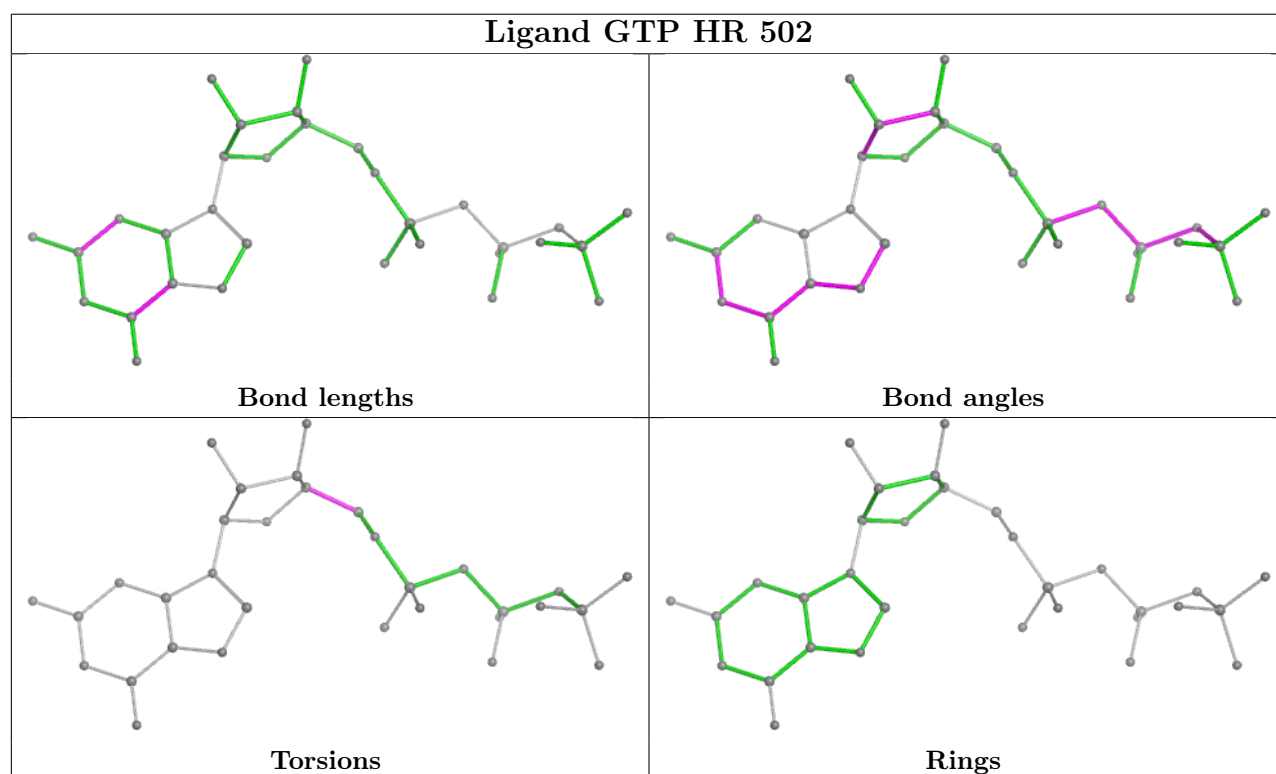
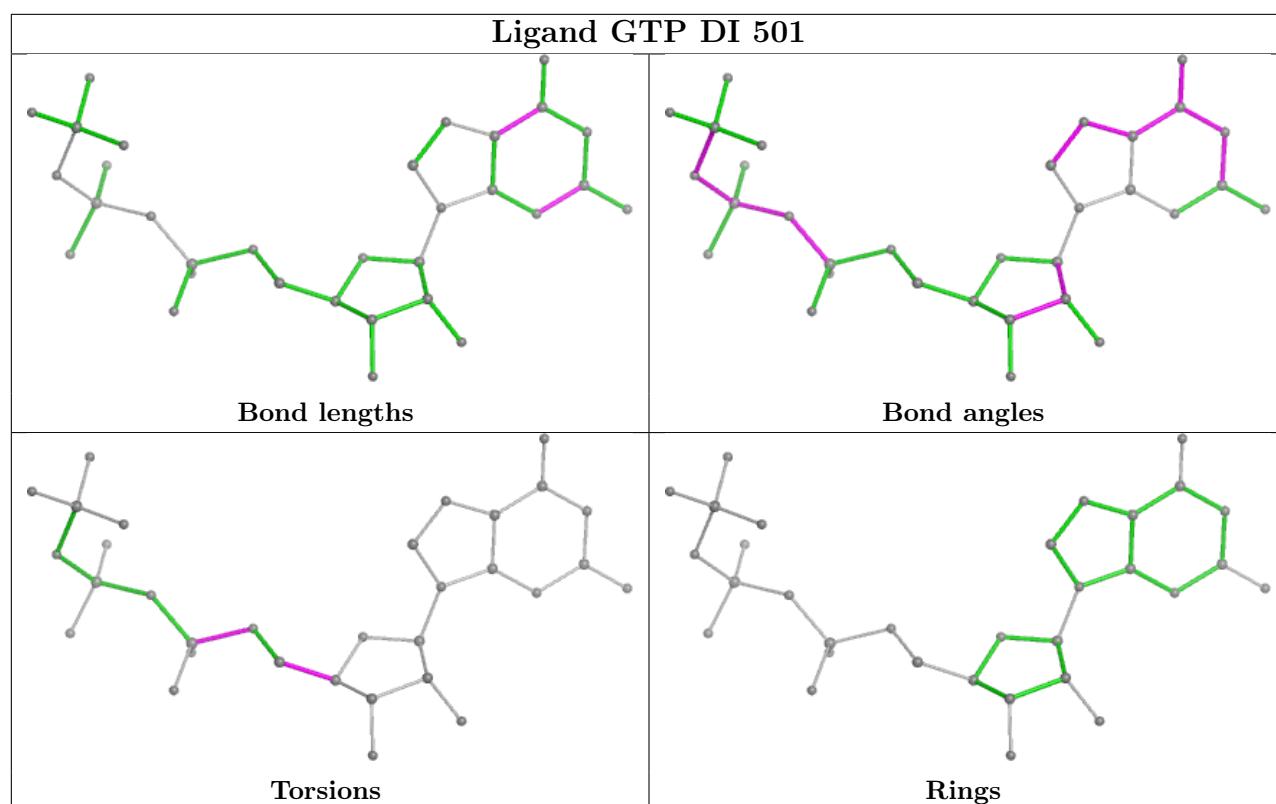
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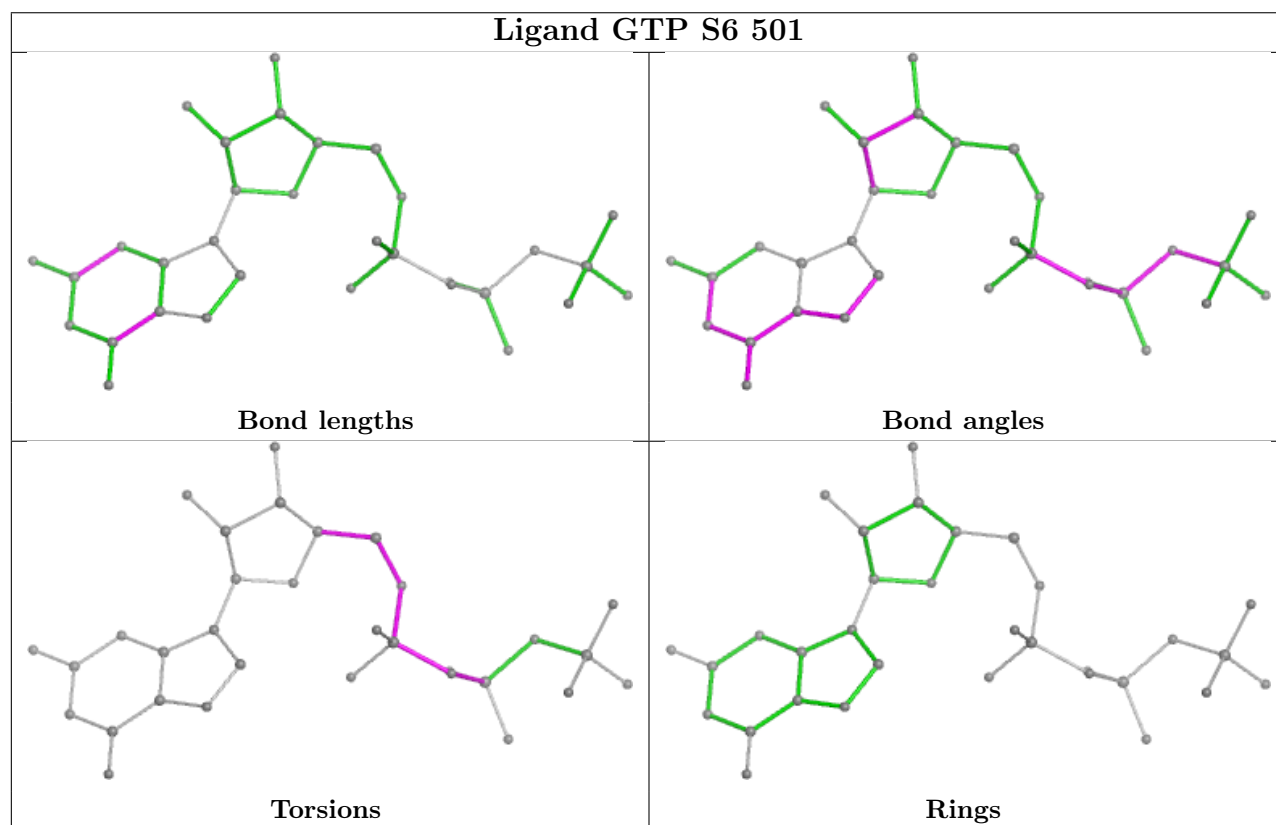
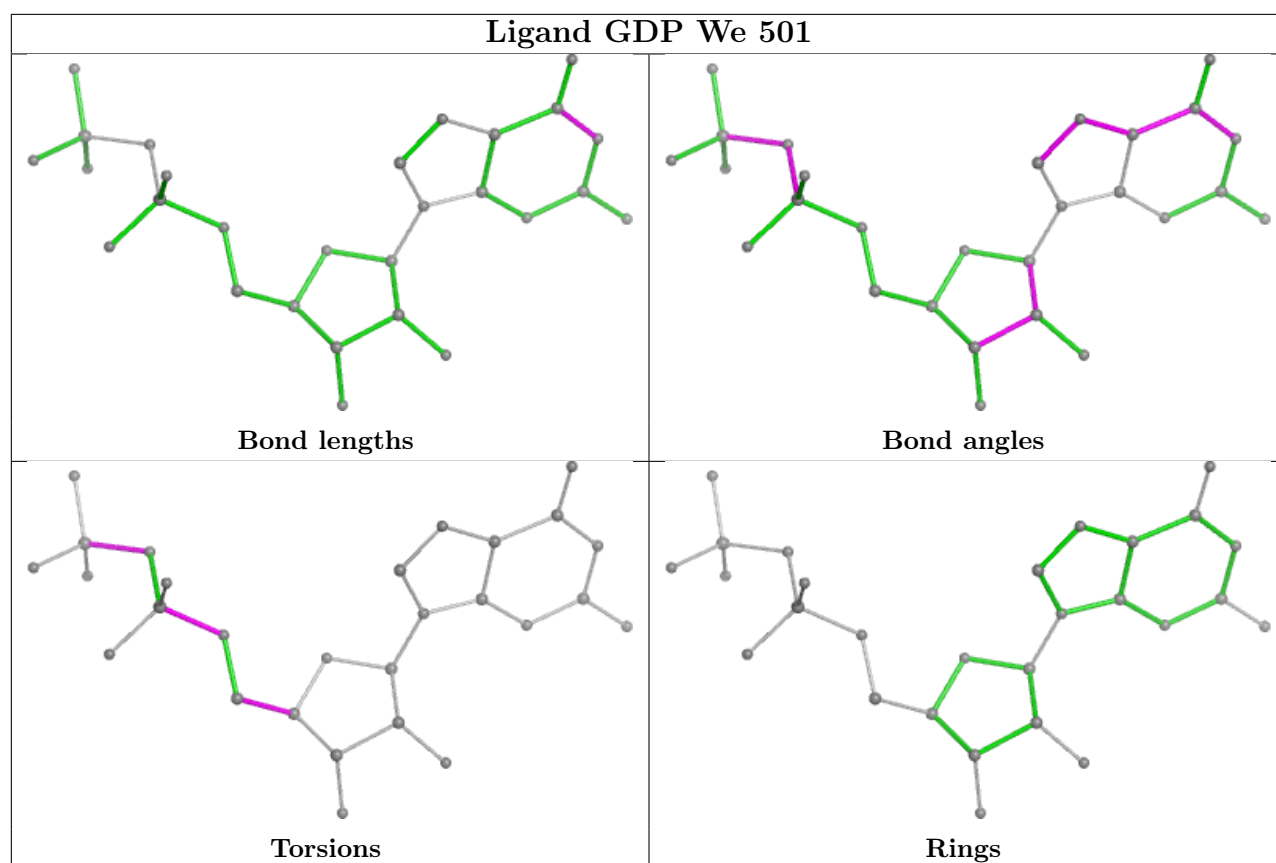


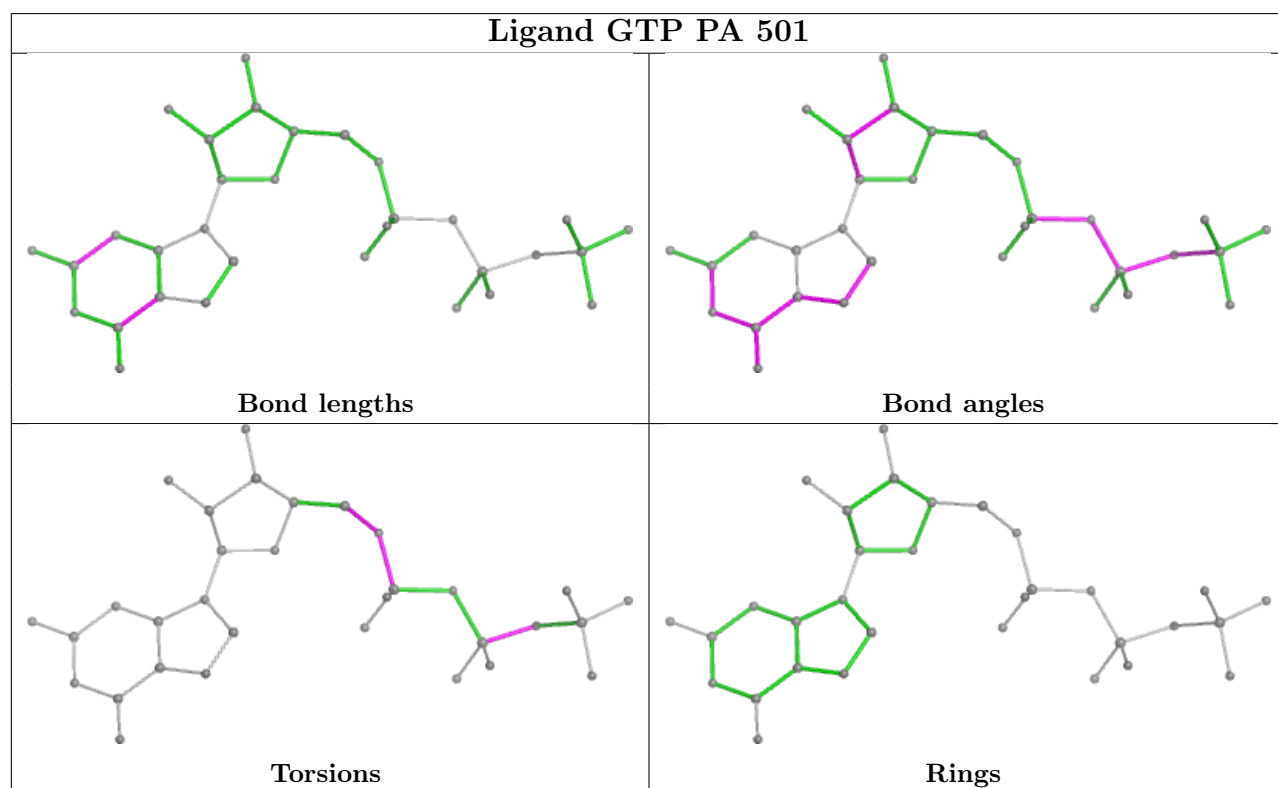
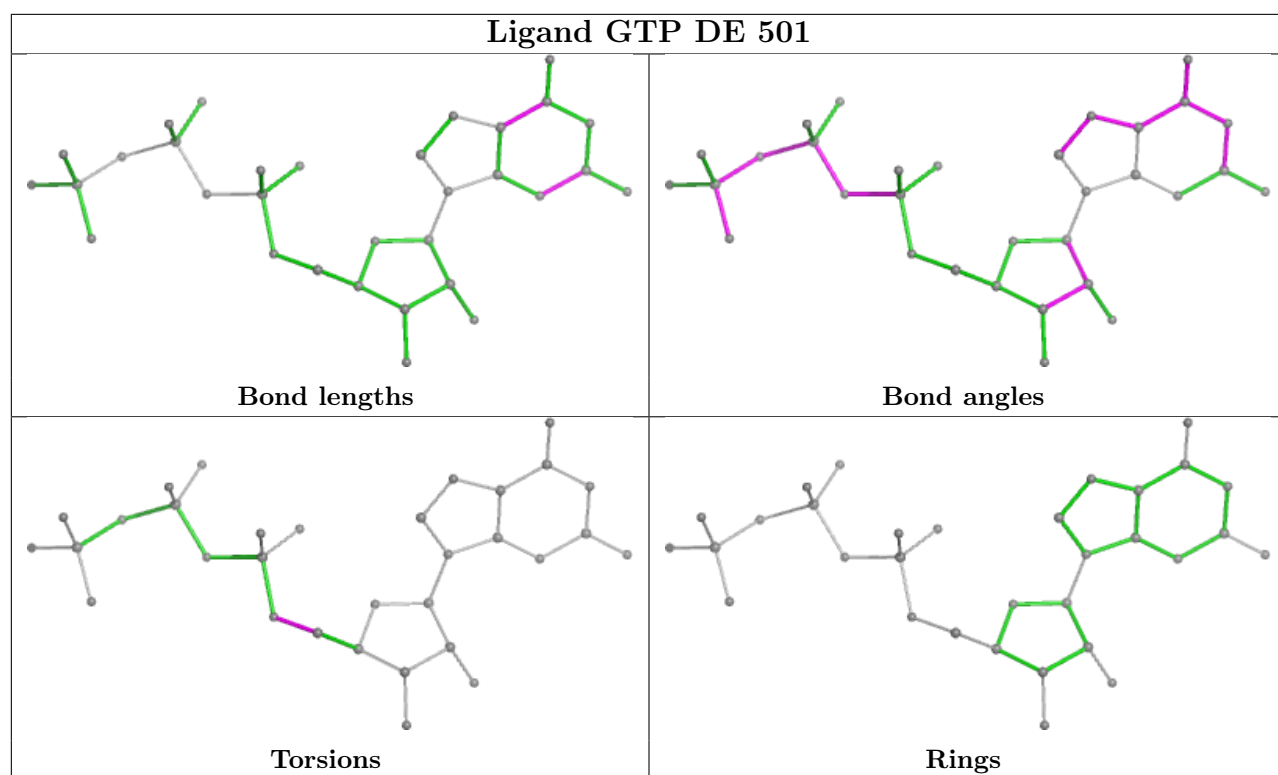
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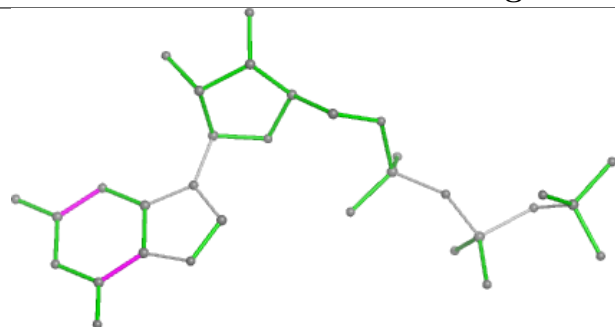




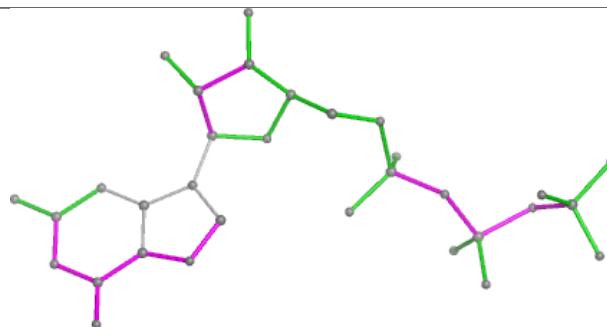




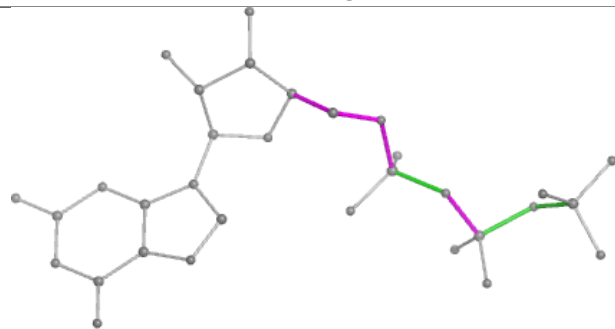
## Ligand GTP LE 501



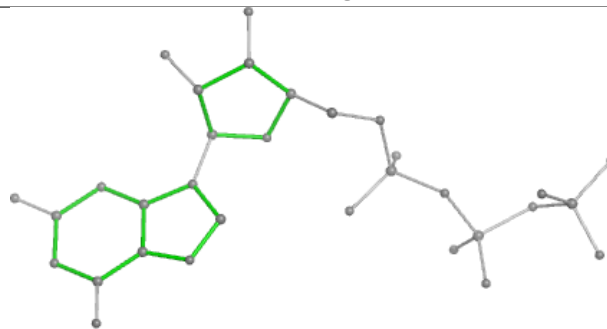
Bond lengths



Bond angles

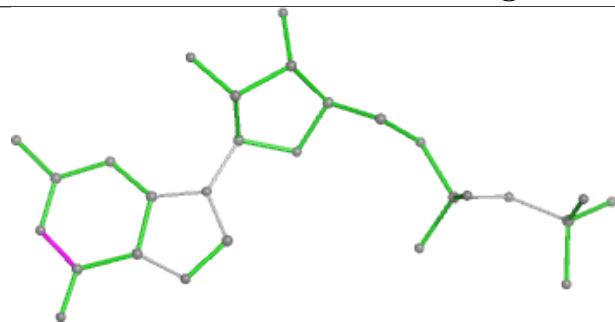


Torsions

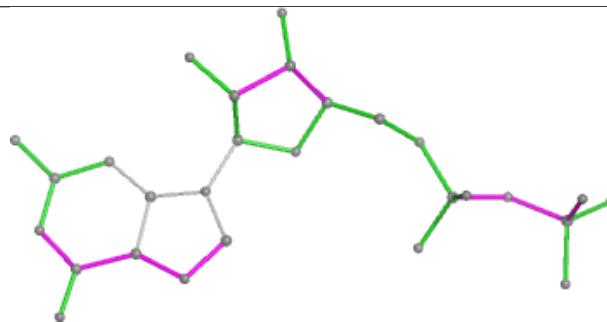


Rings

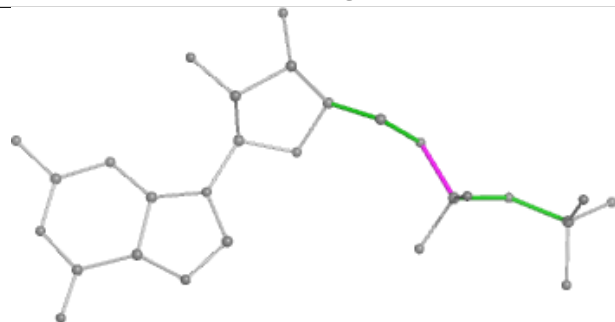
## Ligand GDP PD 501



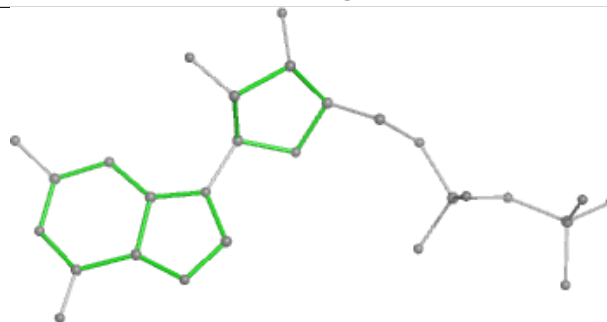
Bond lengths



Bond angles

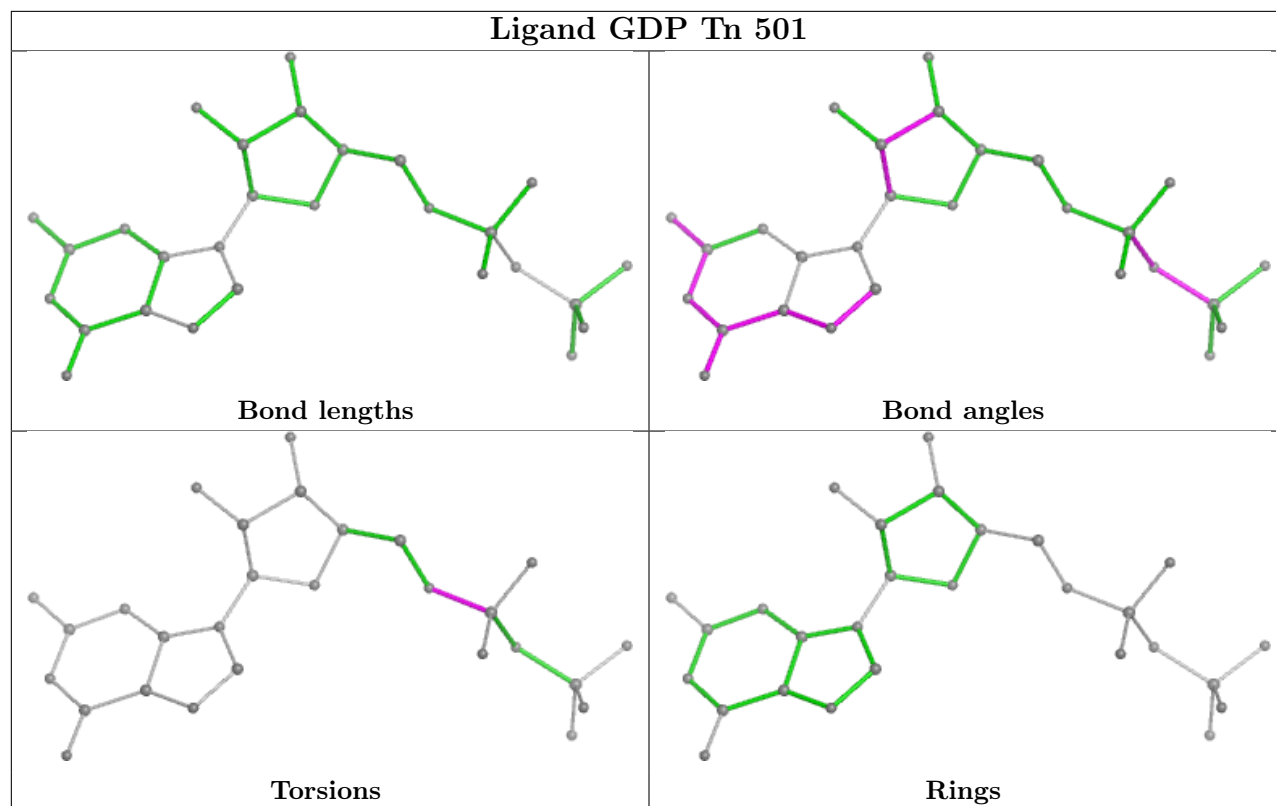


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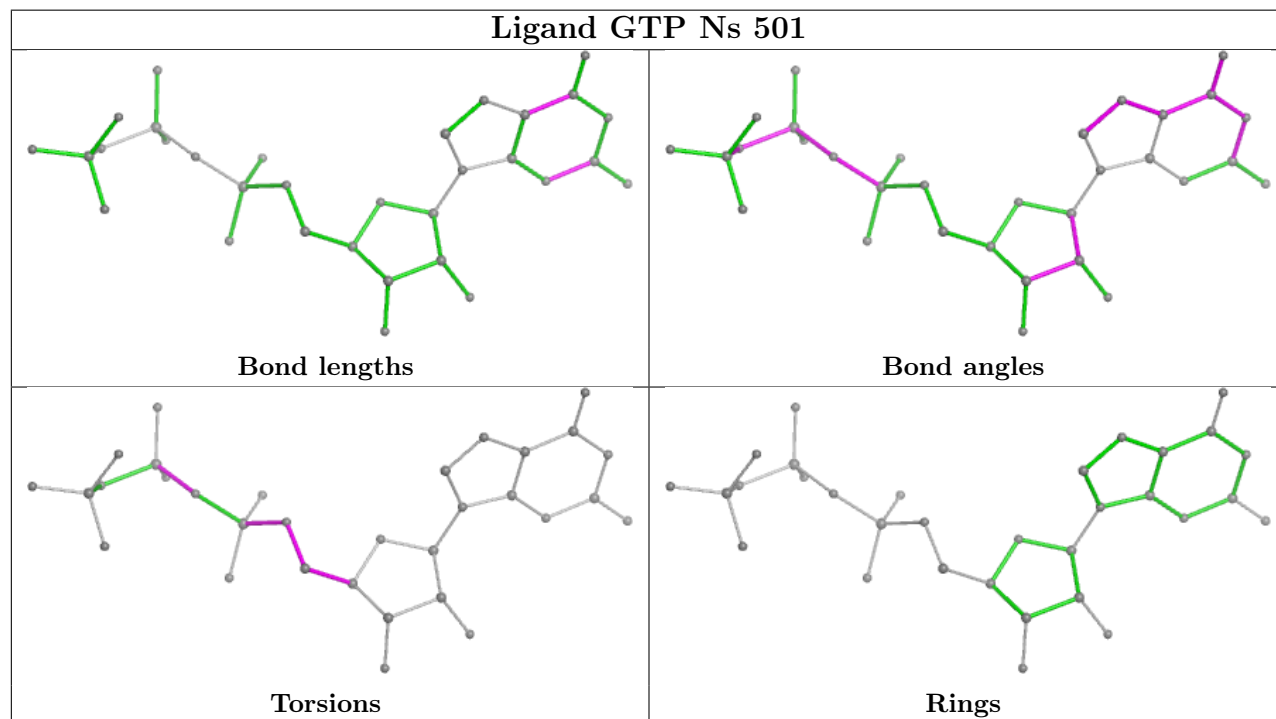


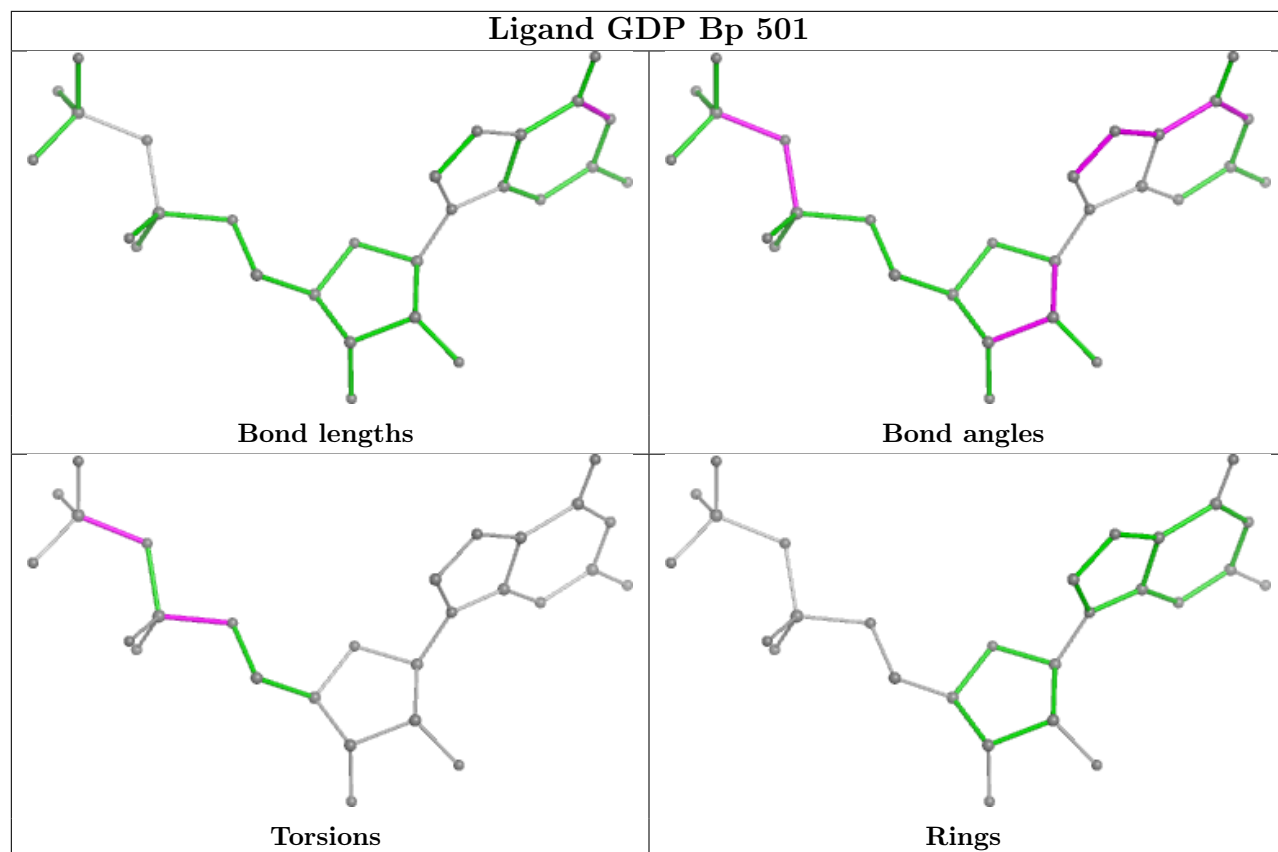
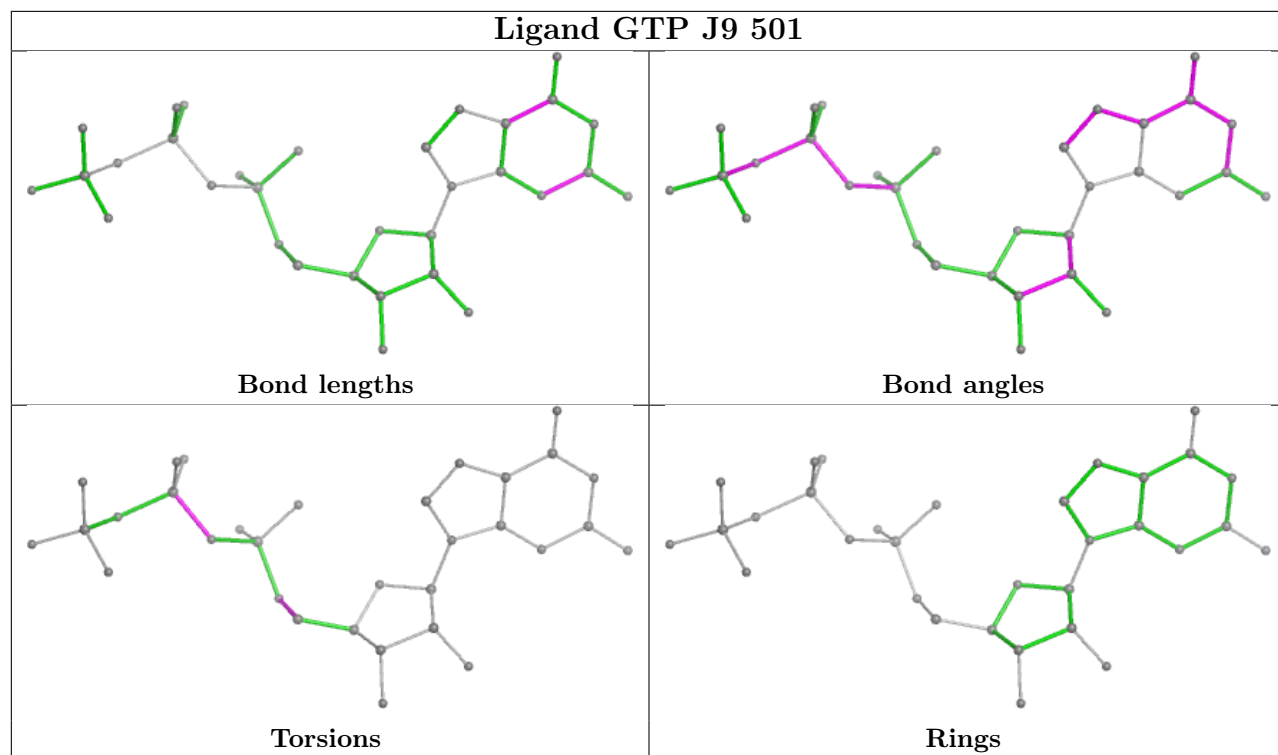
Rings

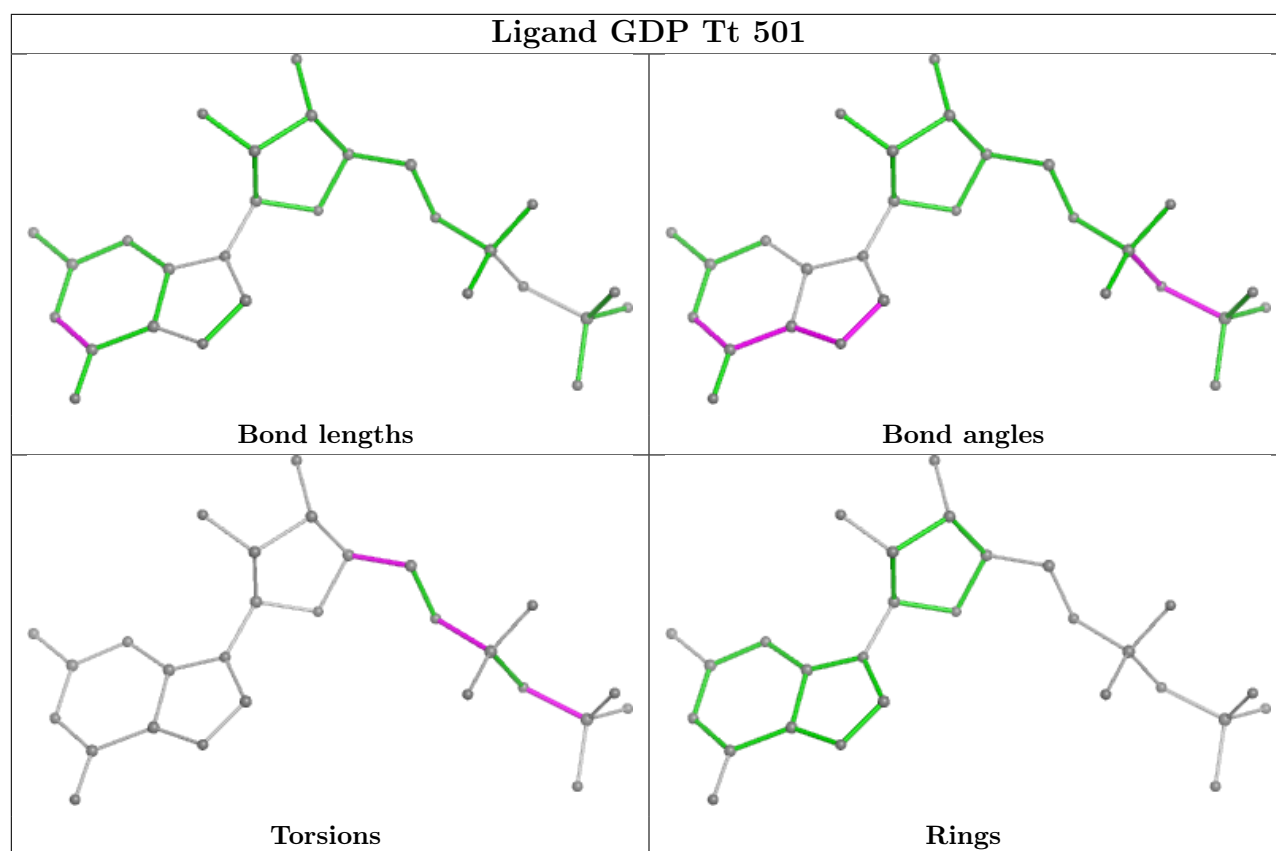
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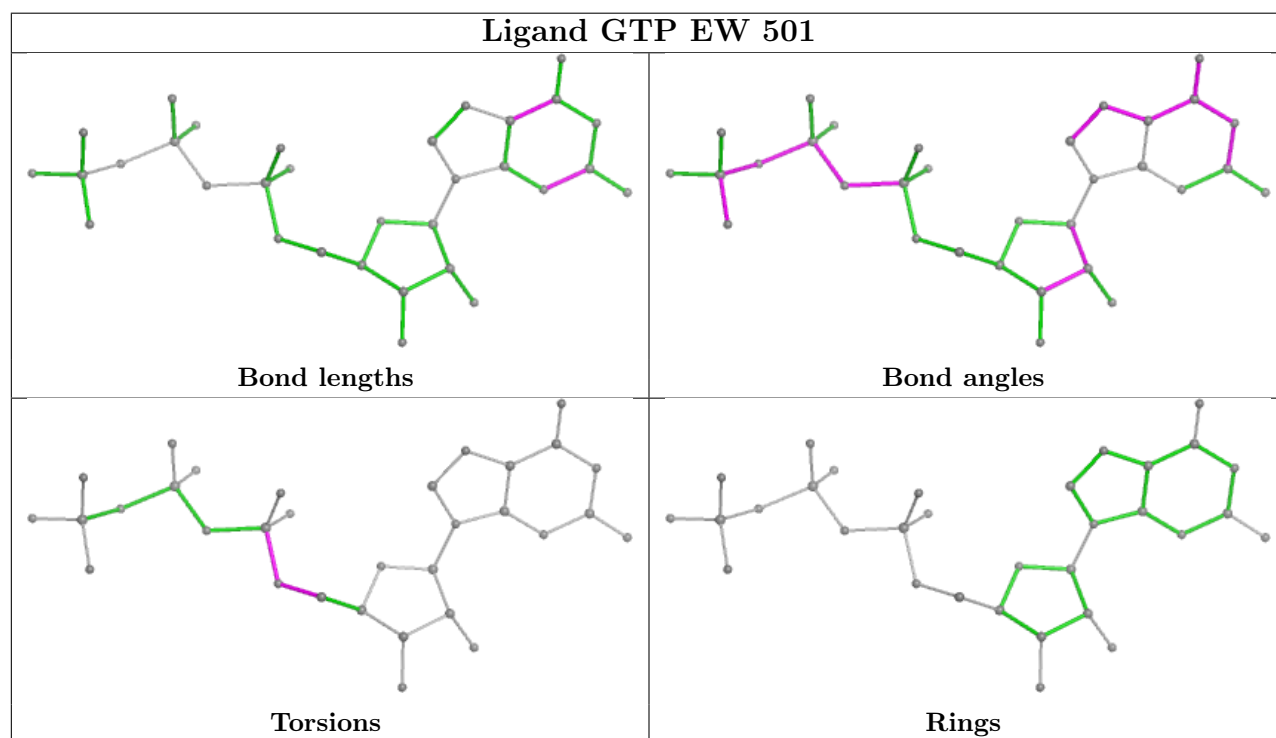
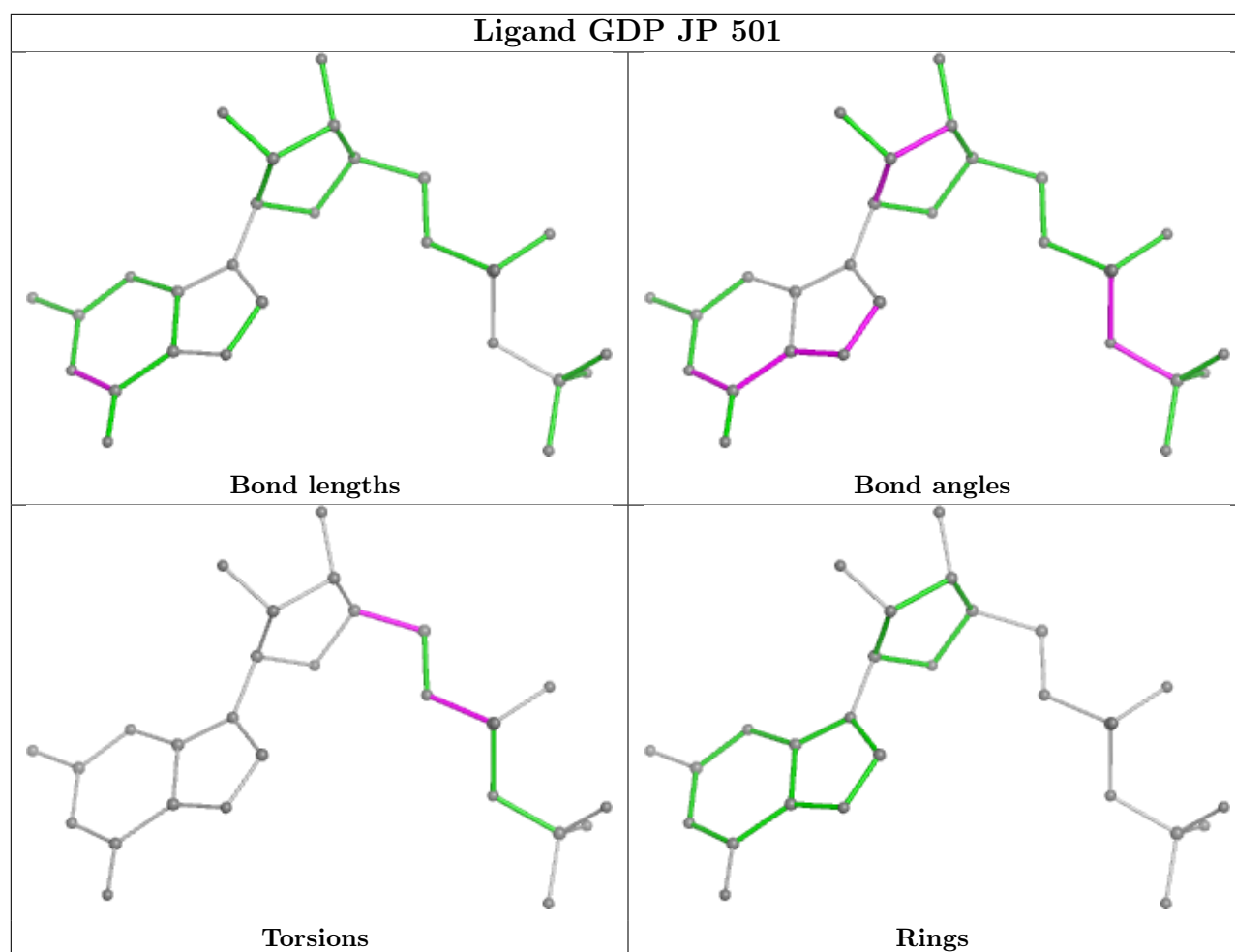


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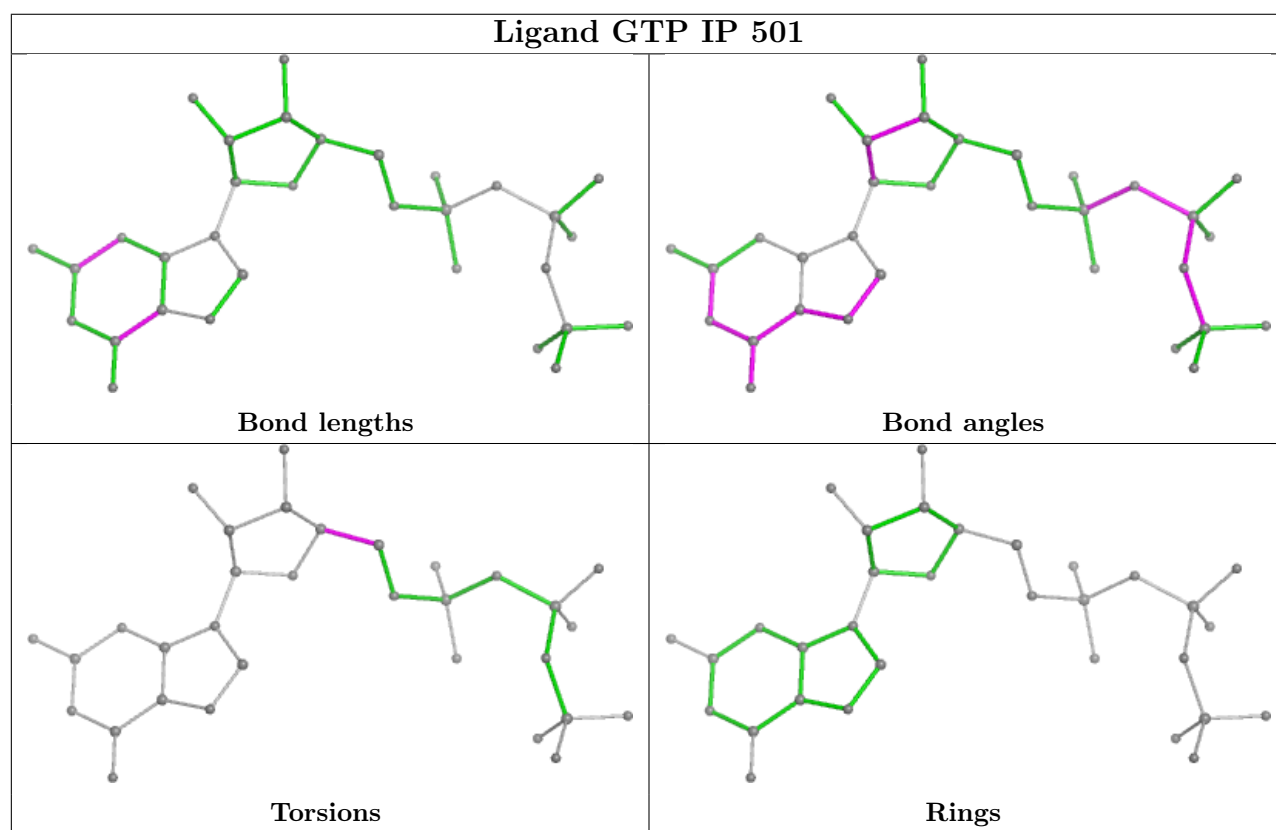
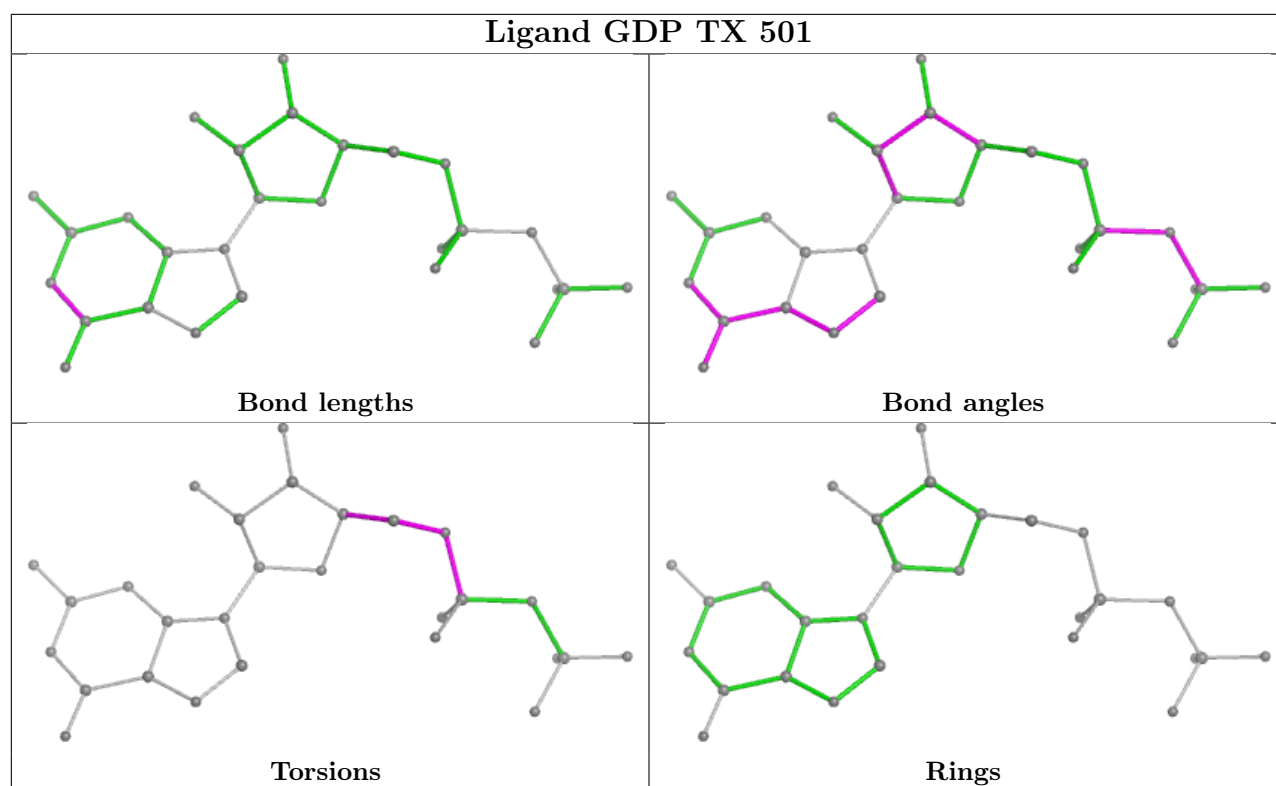




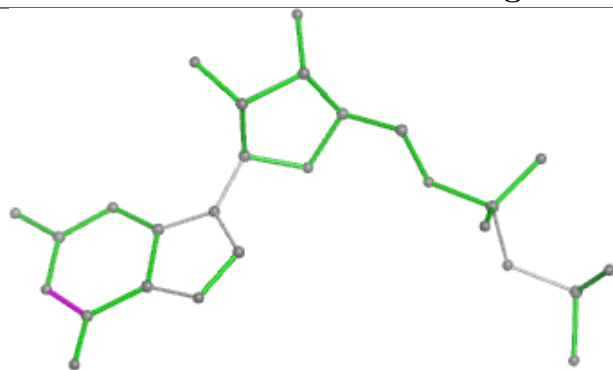




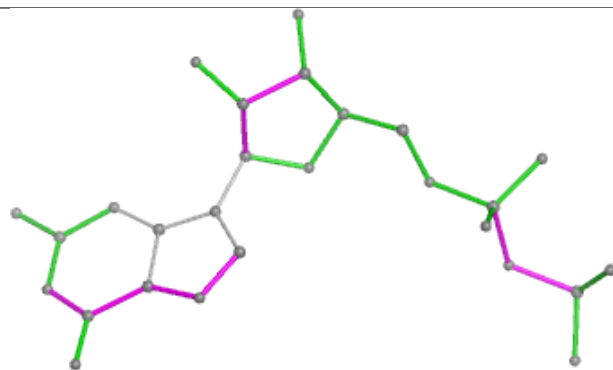




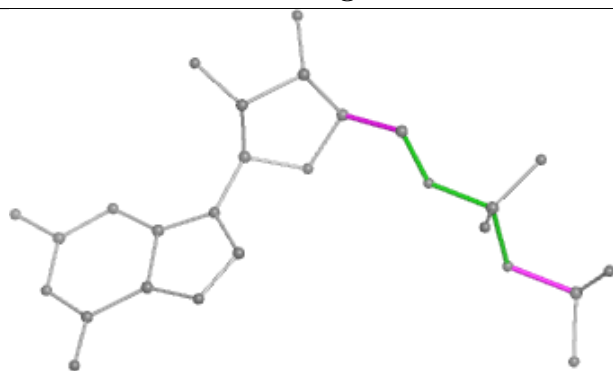
## Ligand GDP JF 501



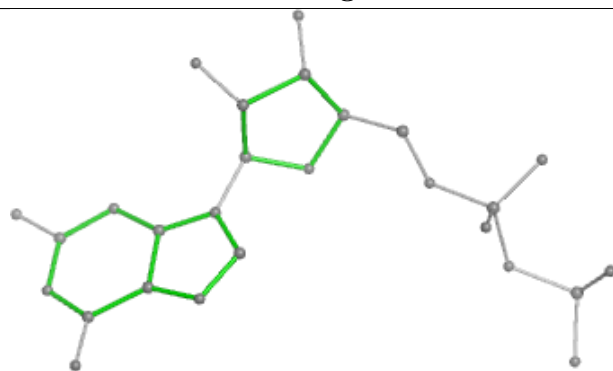
Bond lengths



Bond angles

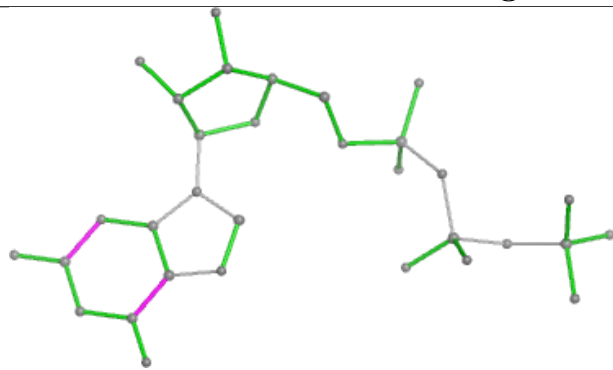


Torsions

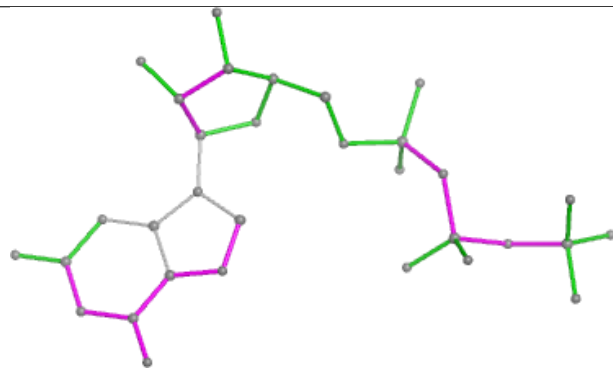


Rings

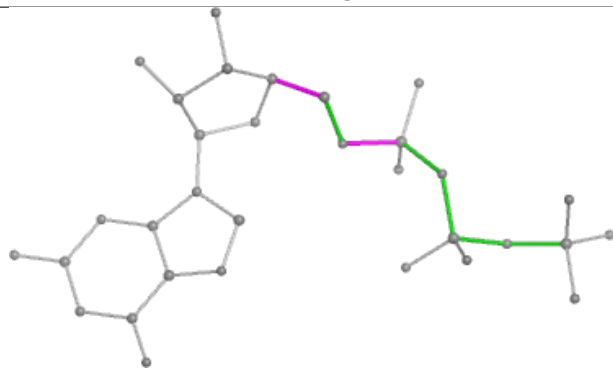
## Ligand GTP PO 502



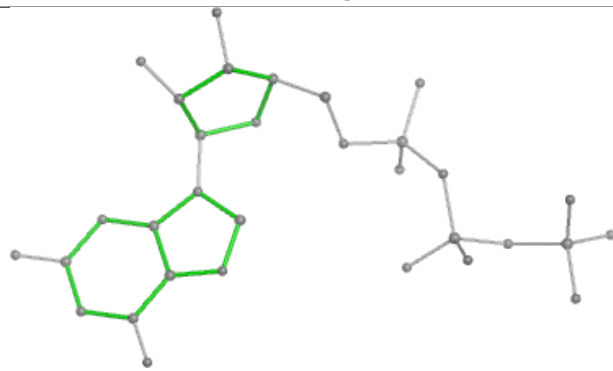
Bond lengths



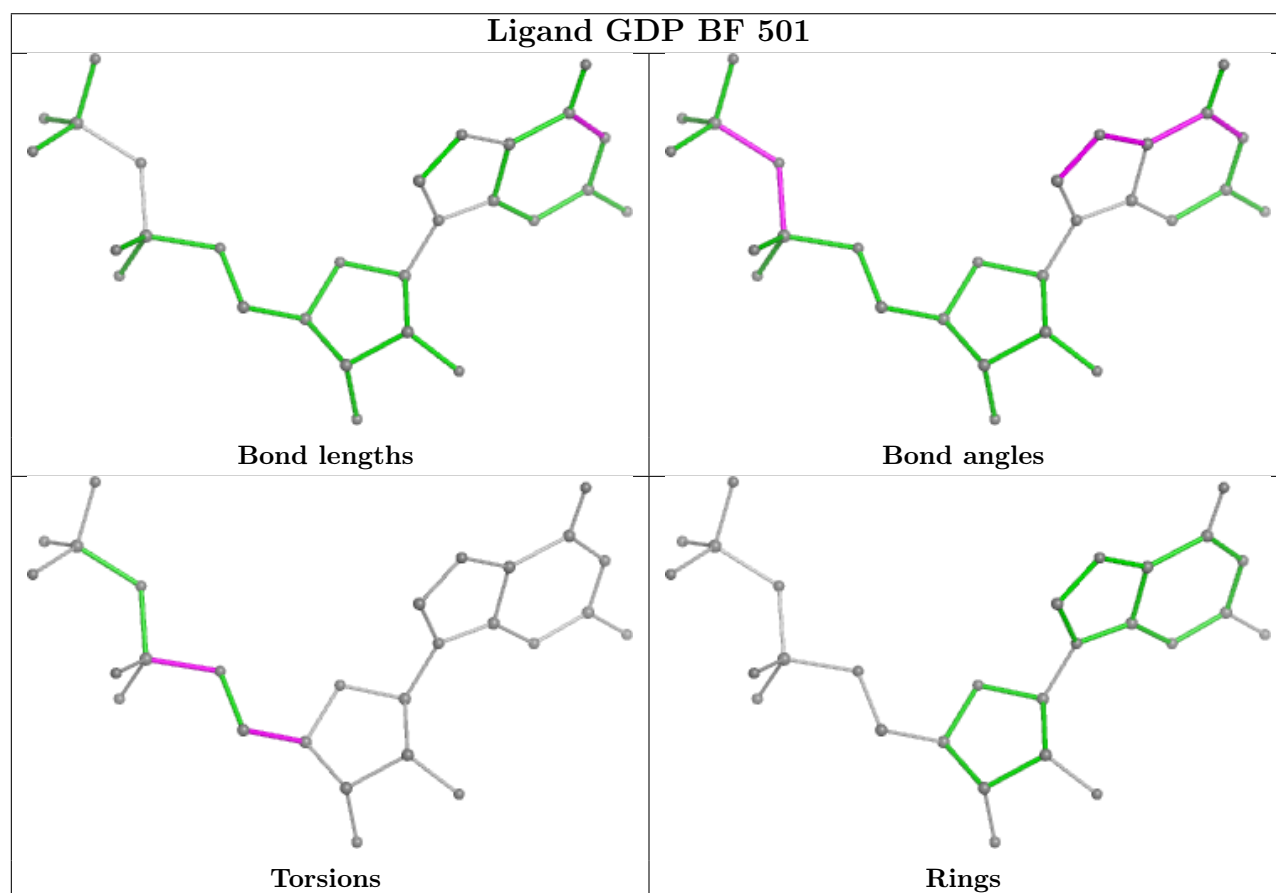
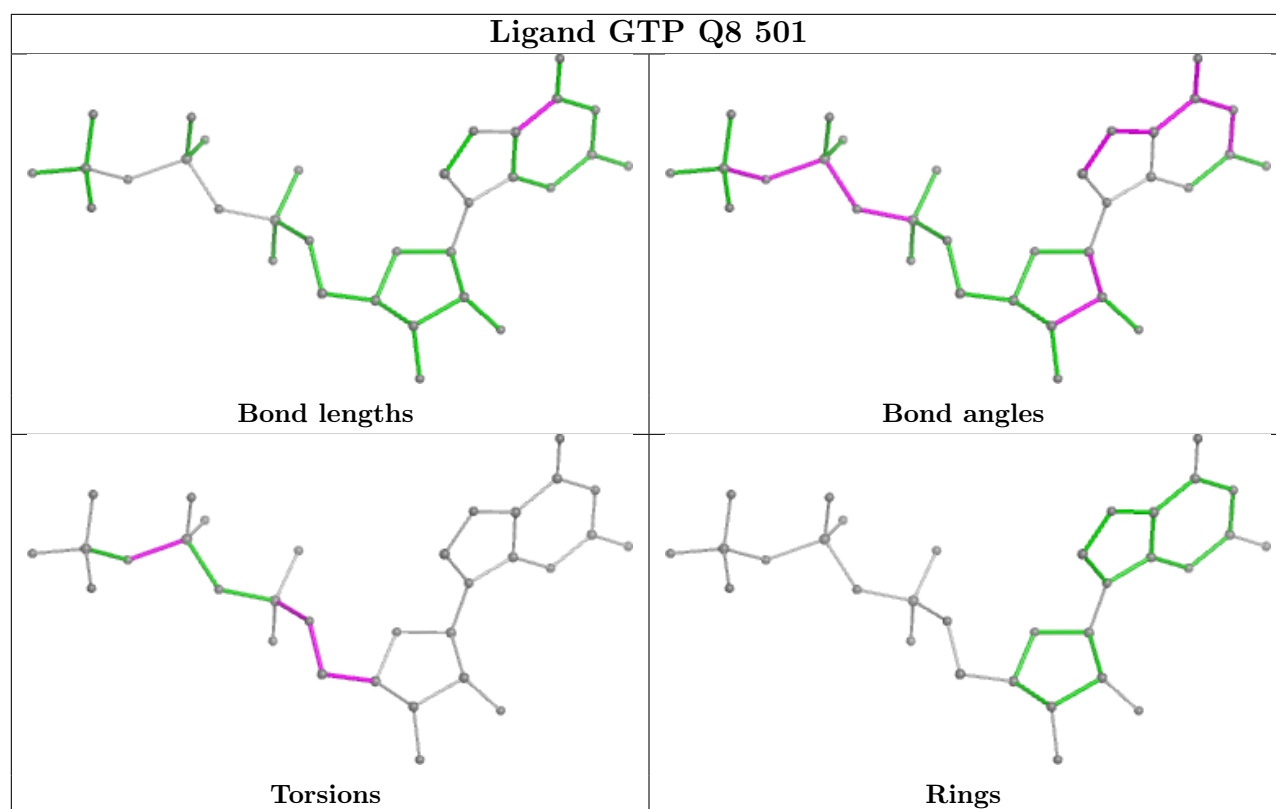
Bond angles

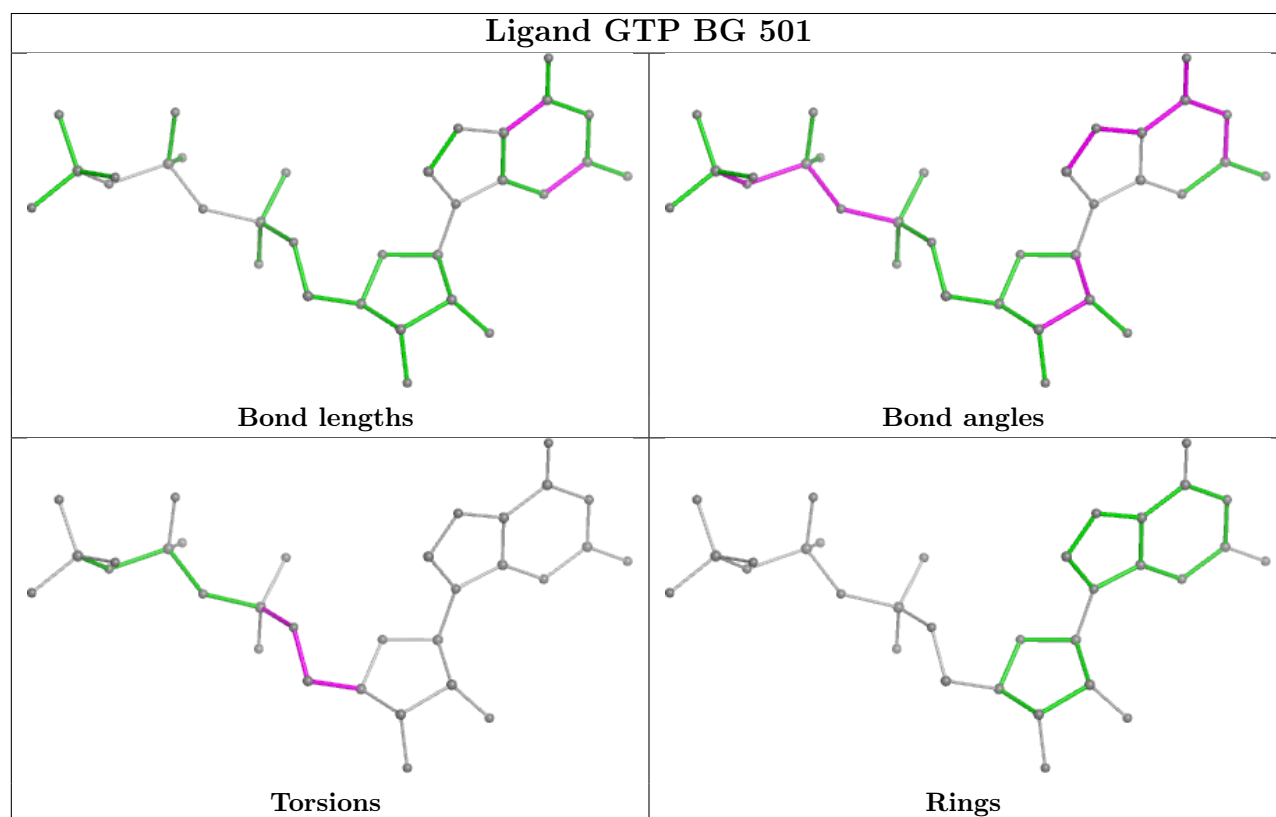
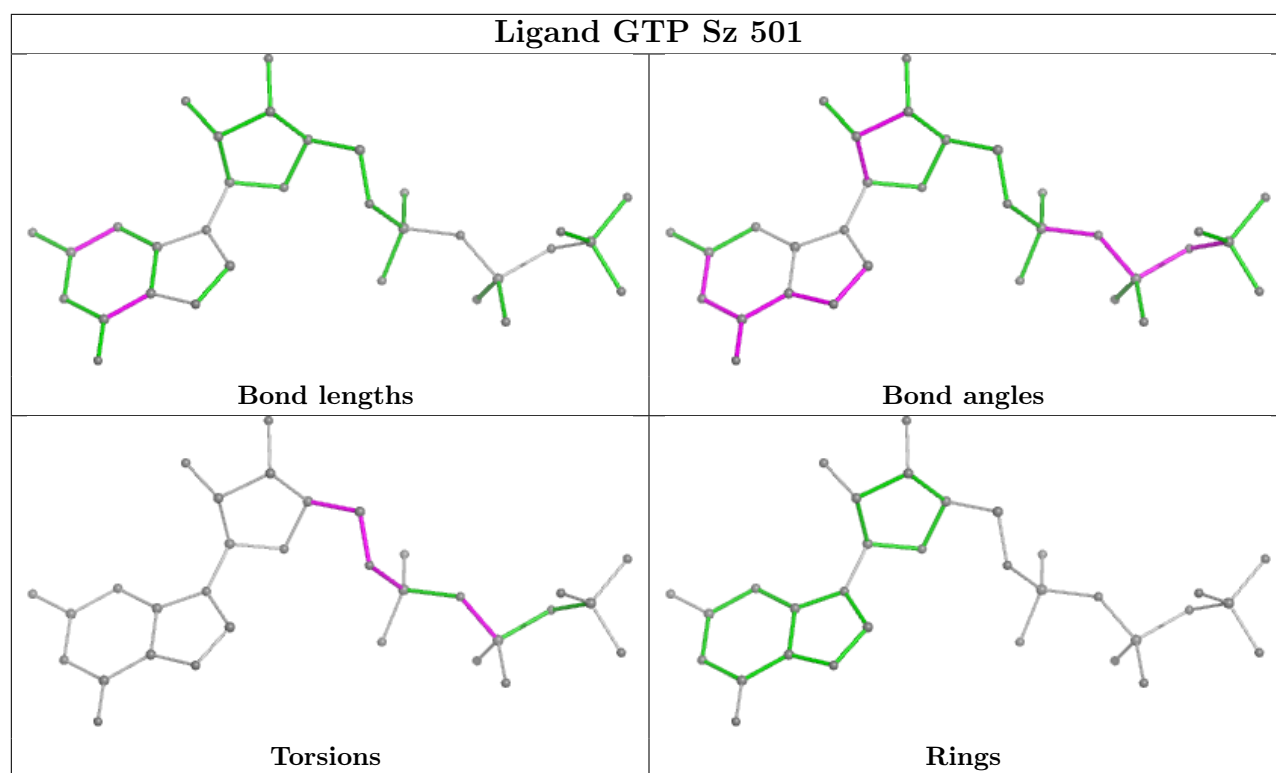


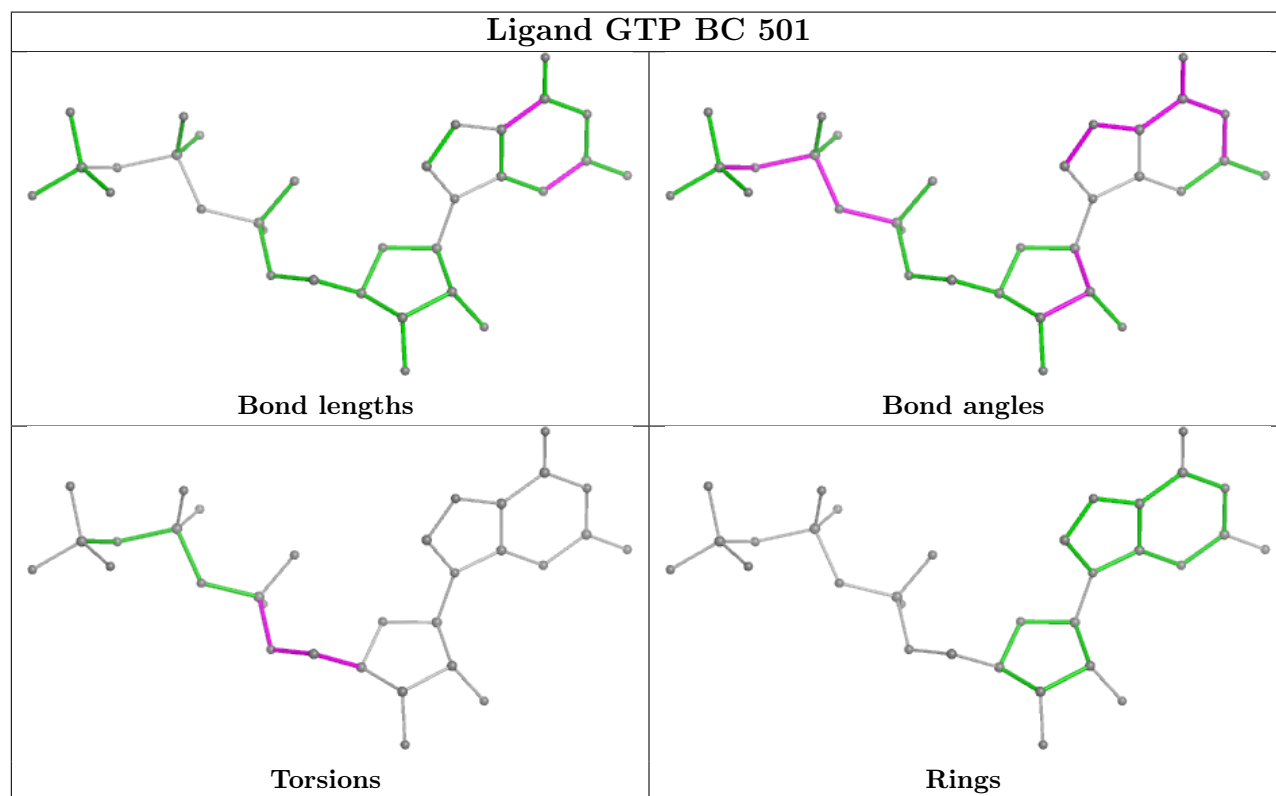
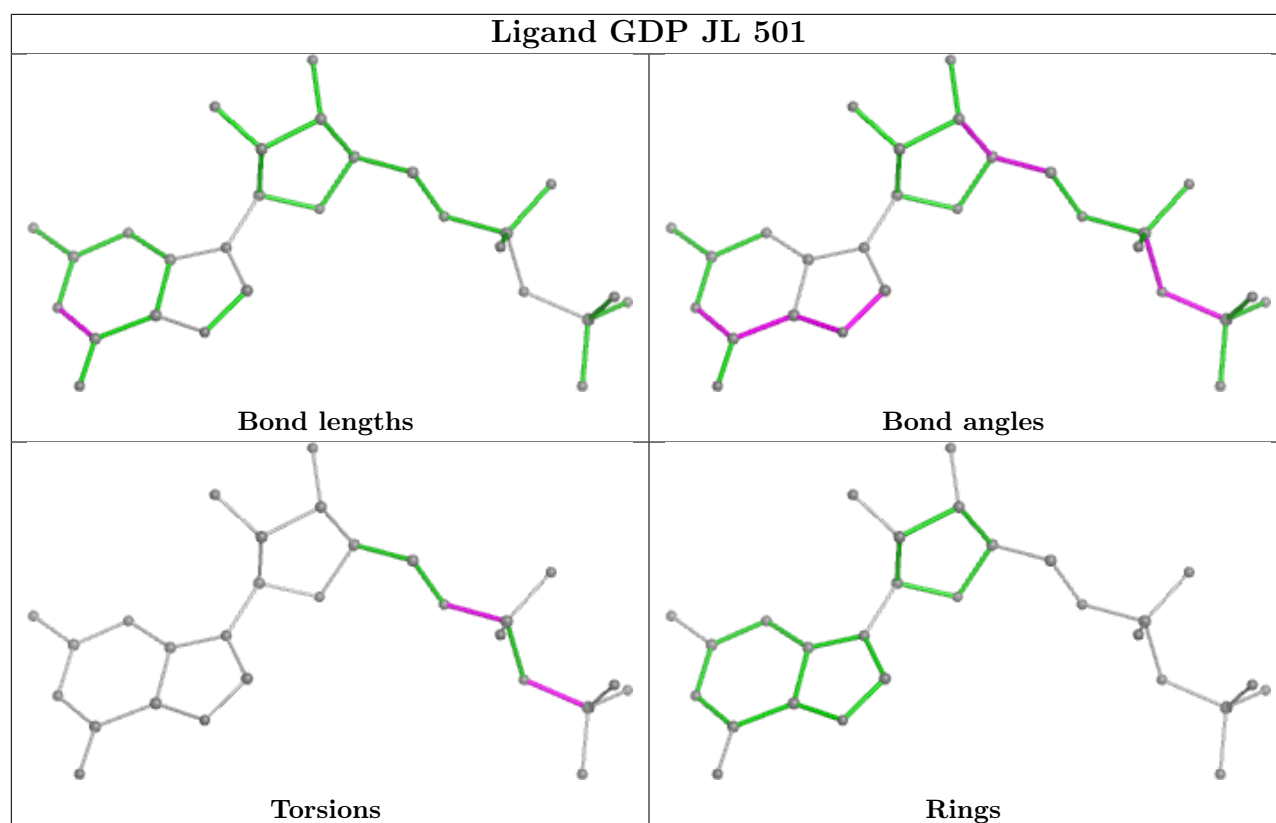
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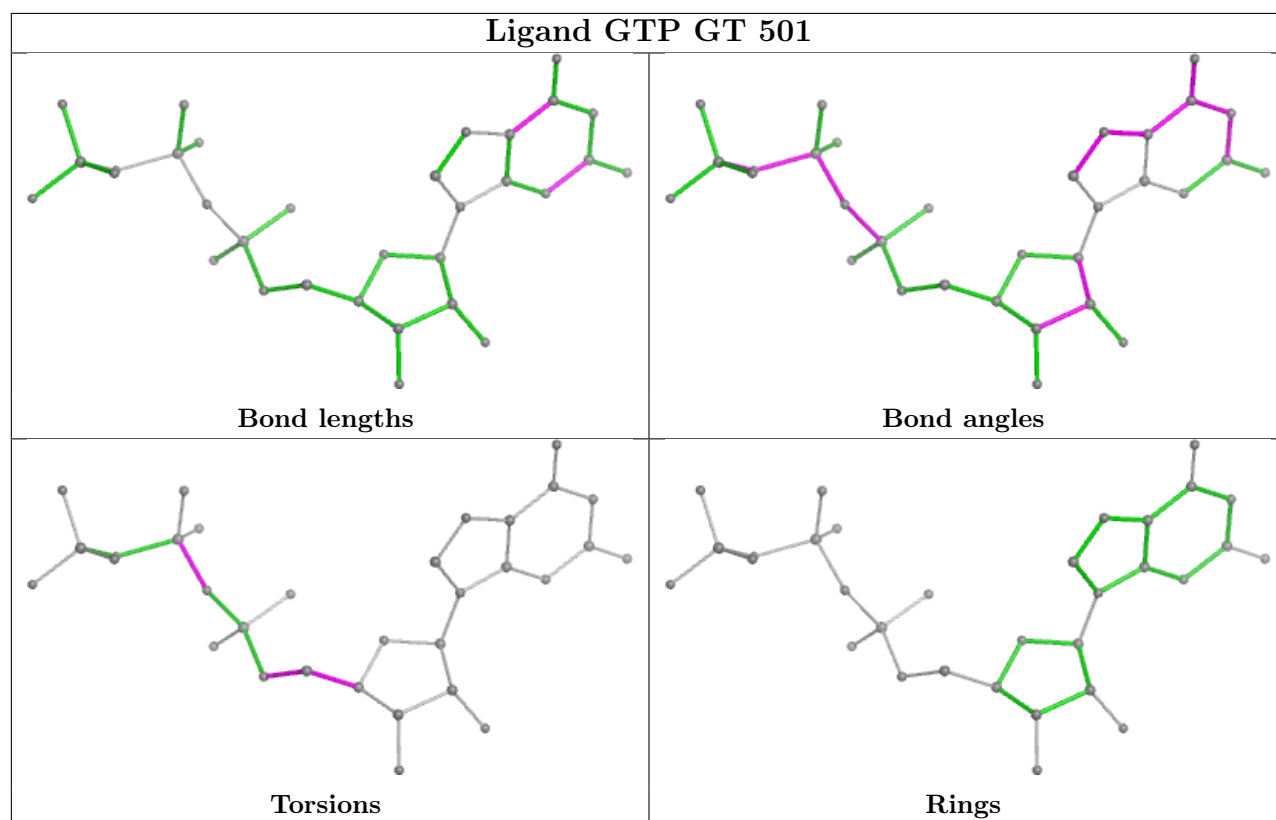
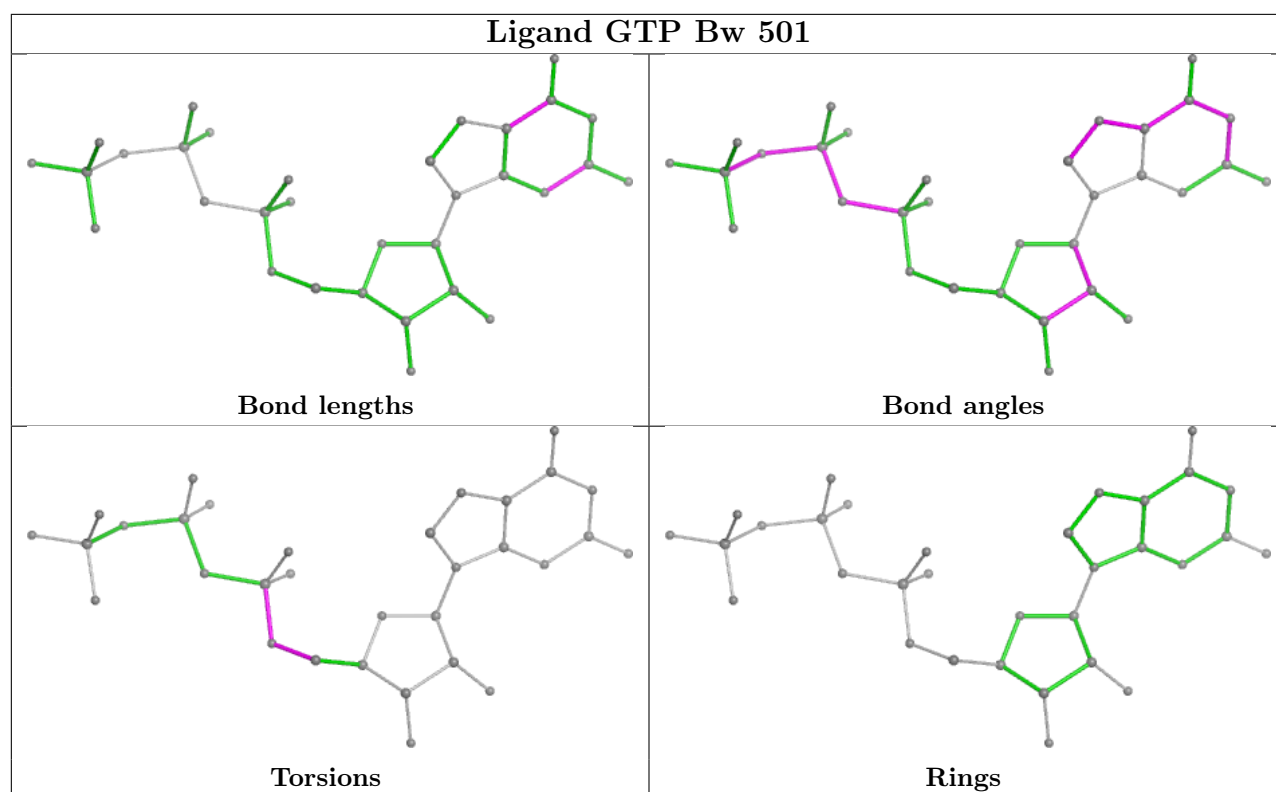


Rings

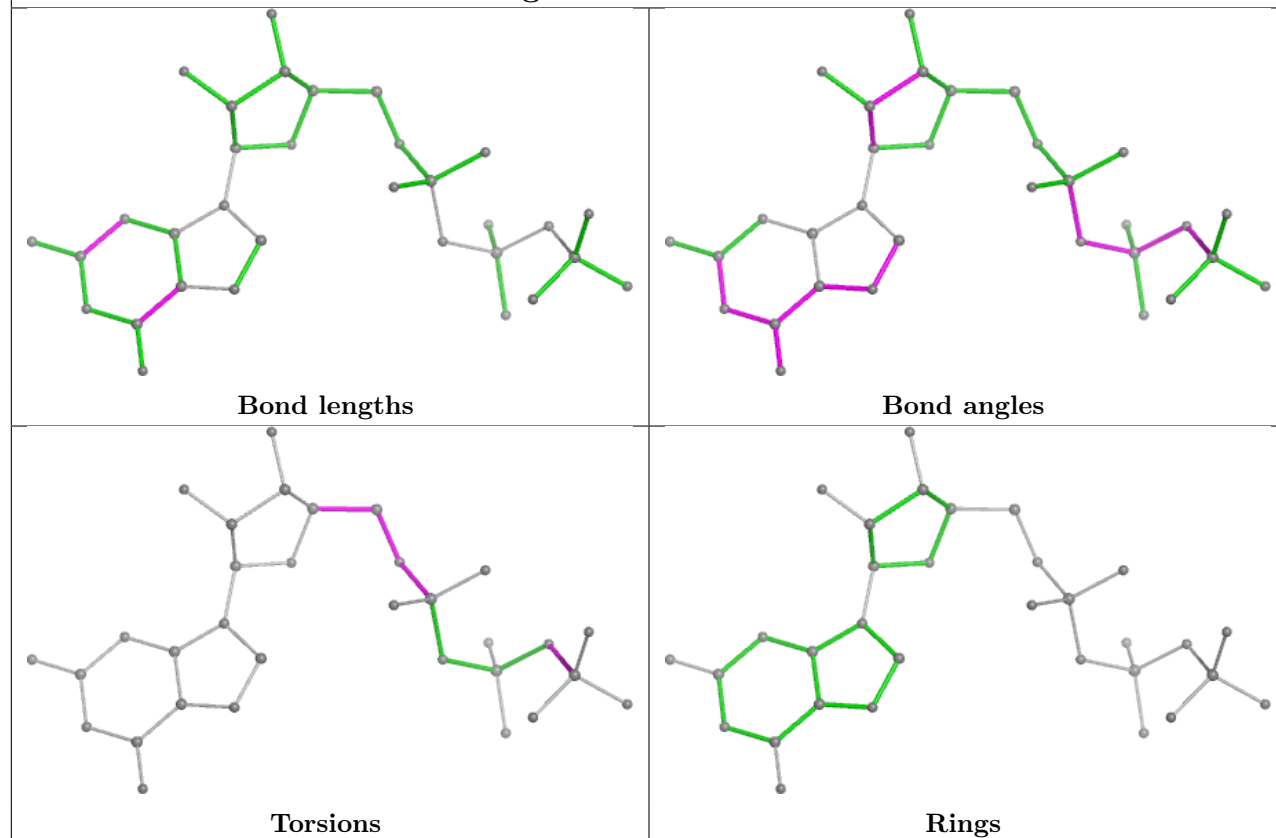




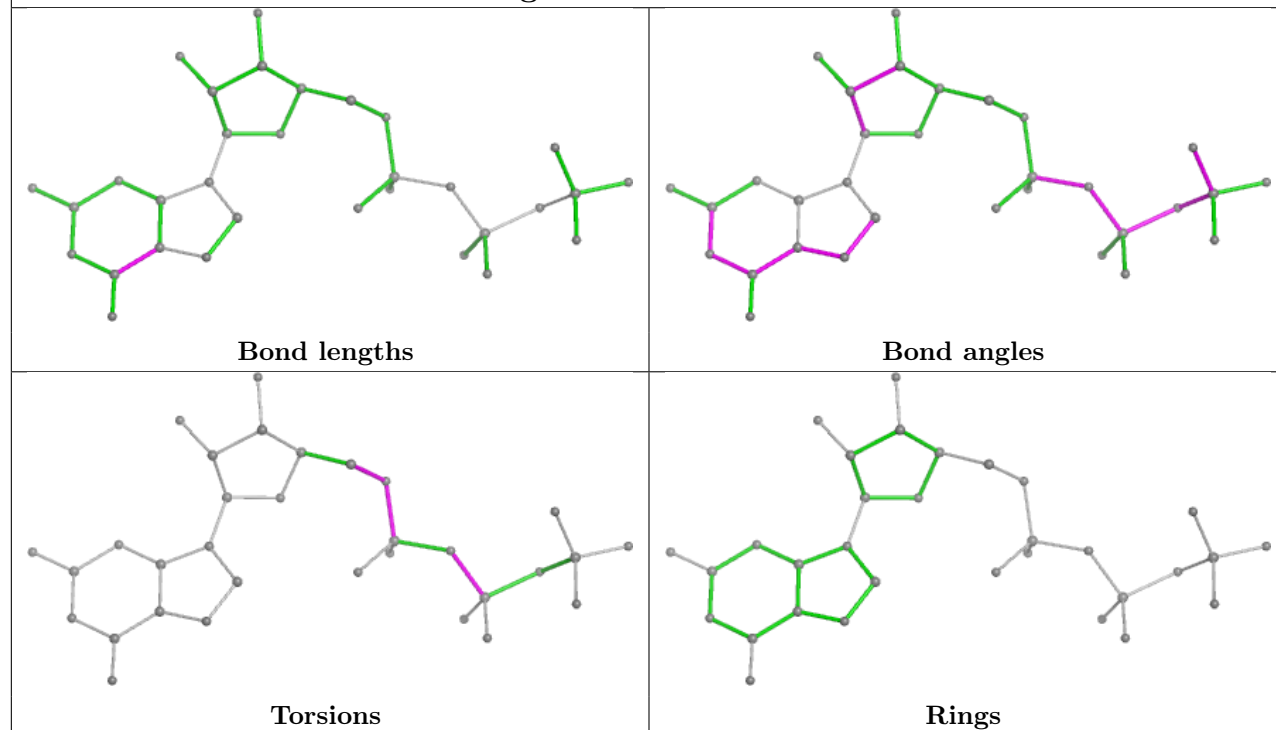


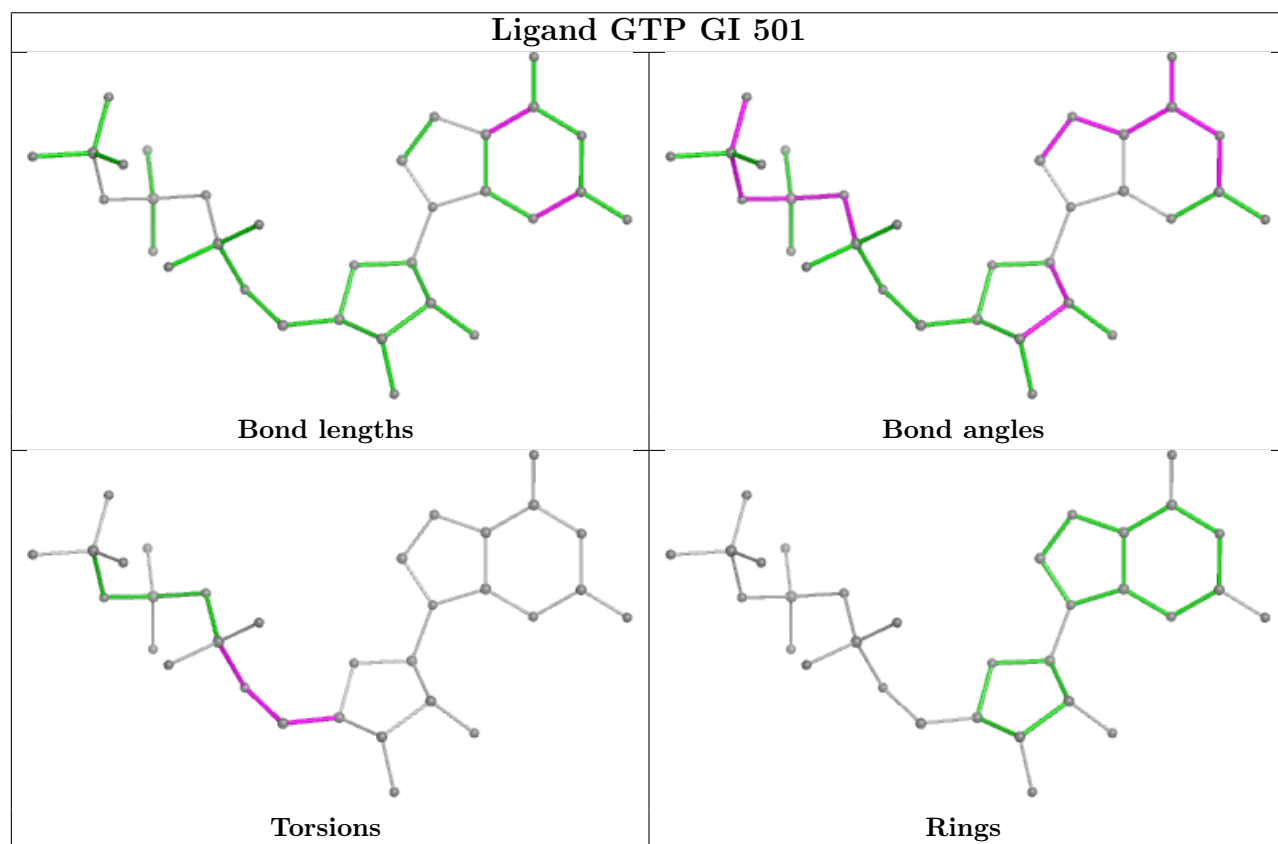
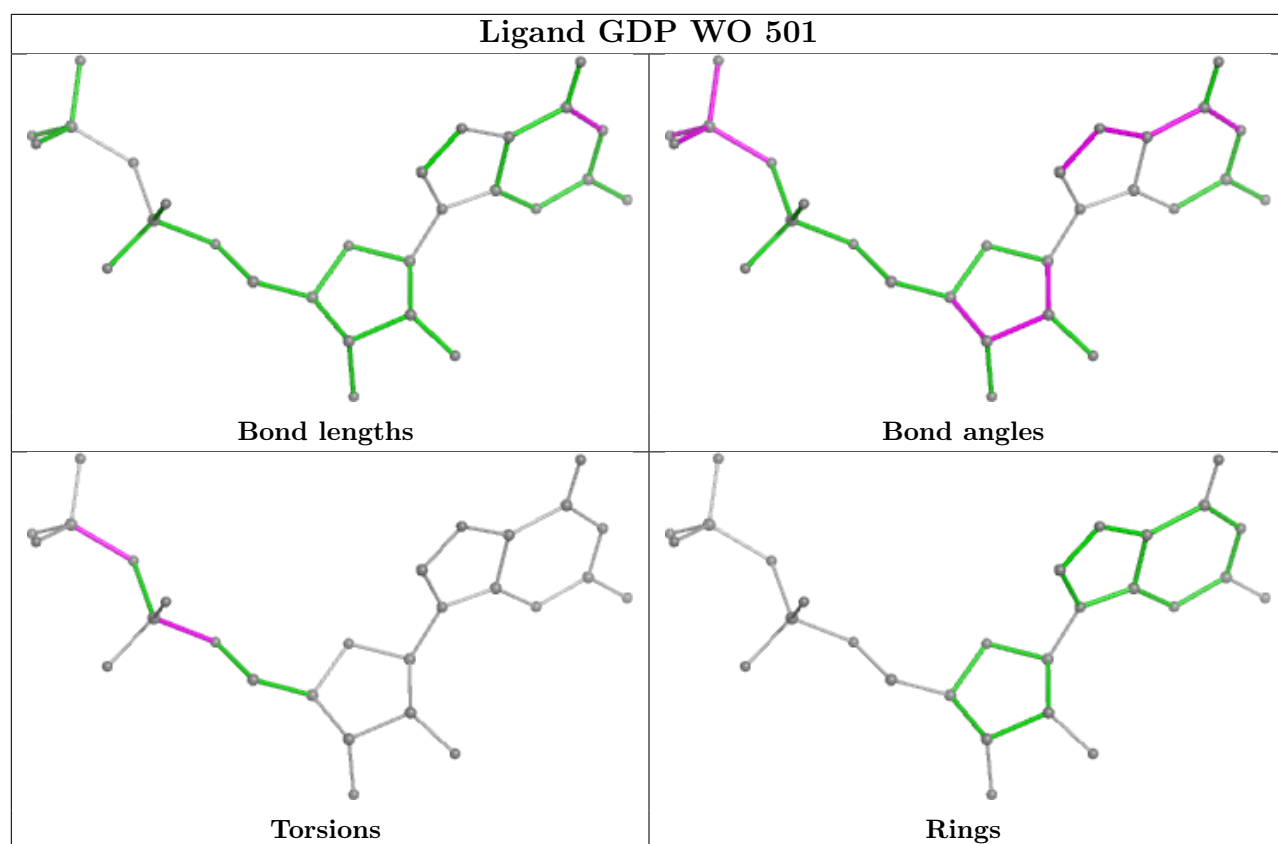


## Ligand GTP T5 501

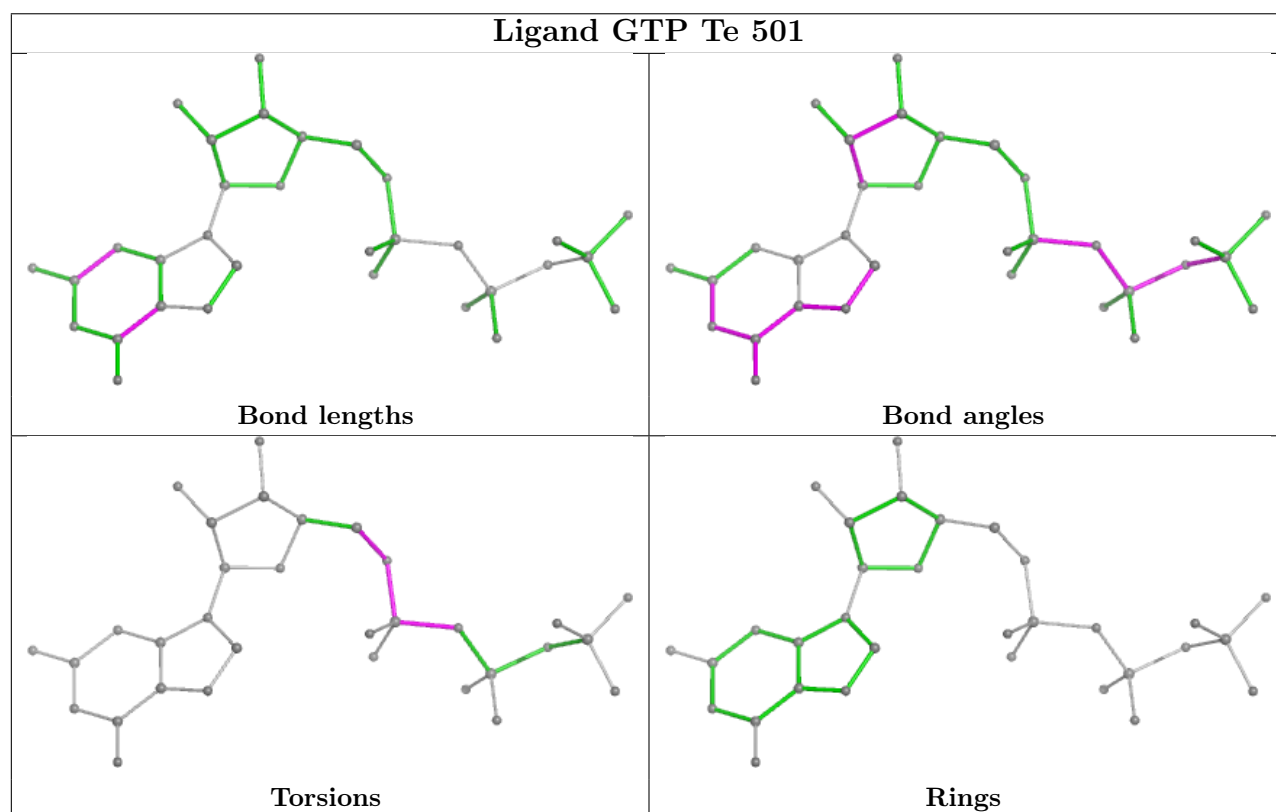
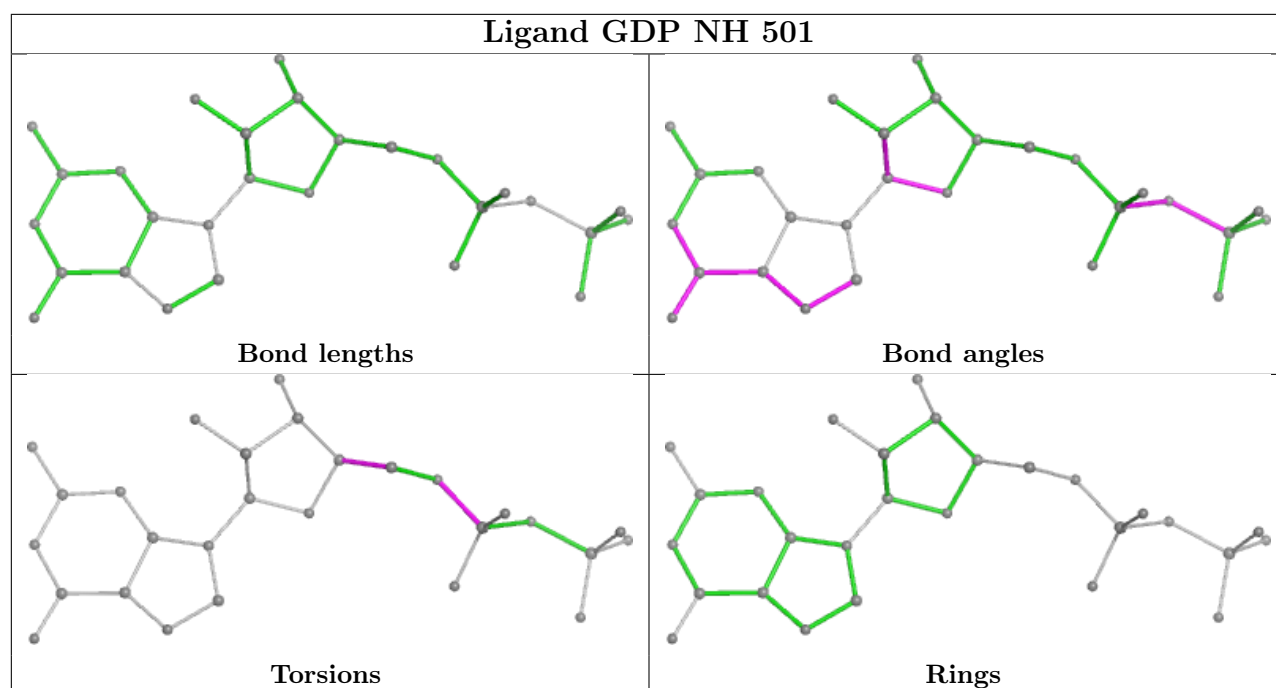


## Ligand GTP SV 501

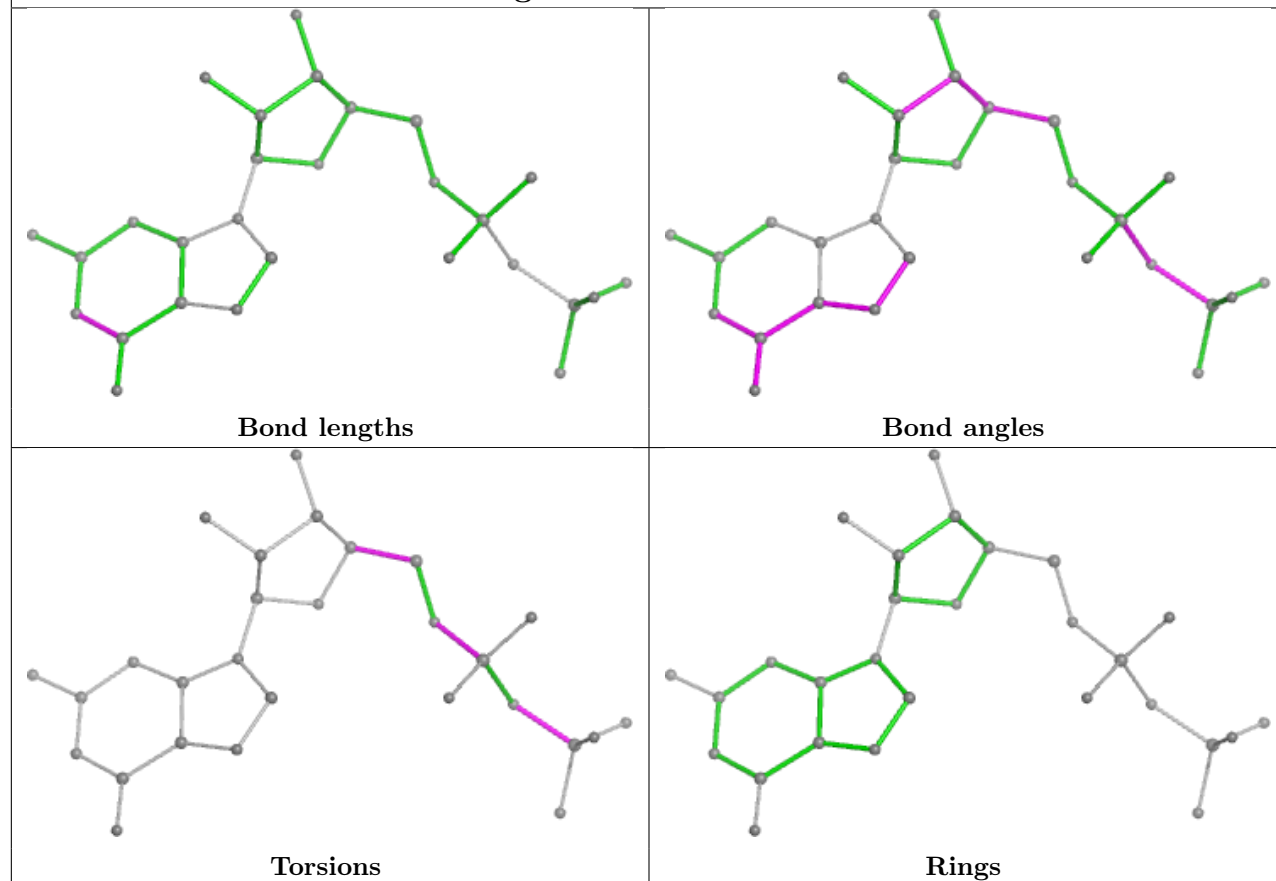




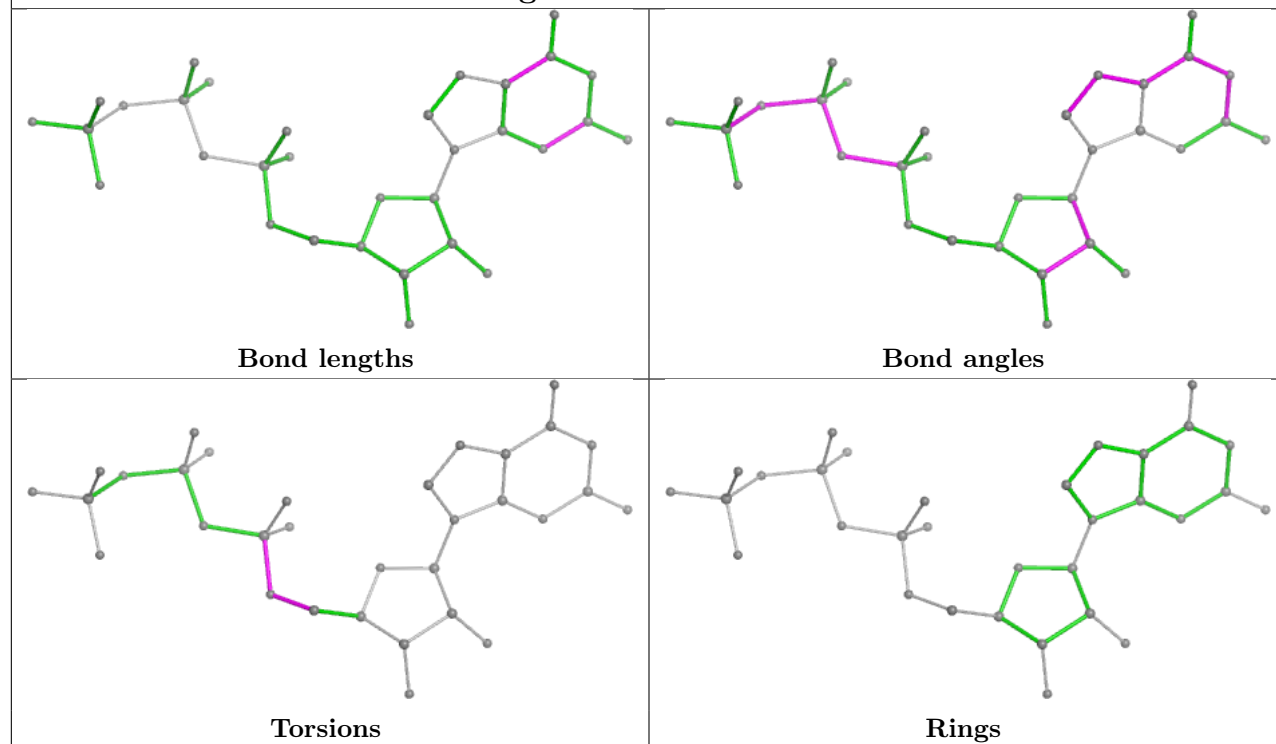




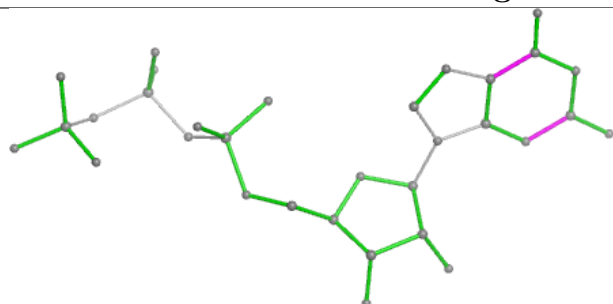
## Ligand GDP KH 501



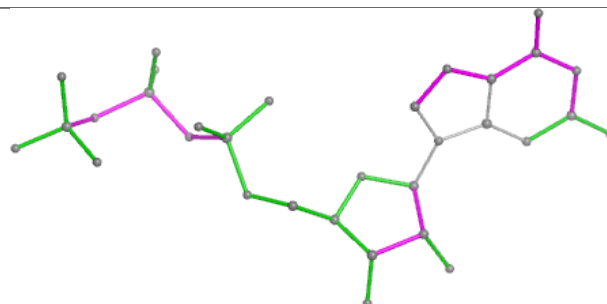
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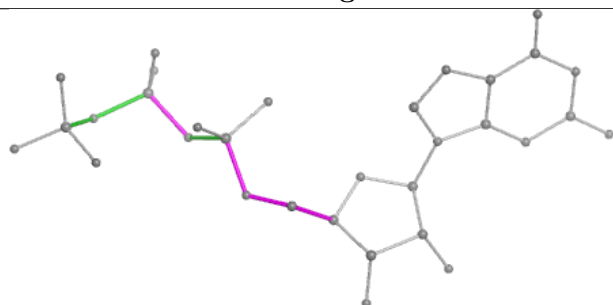
## Ligand GTP WG 501



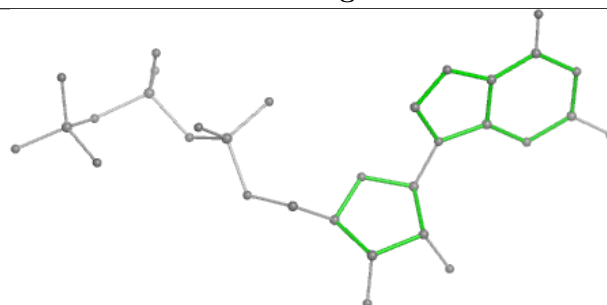
Bond lengths



Bond angles

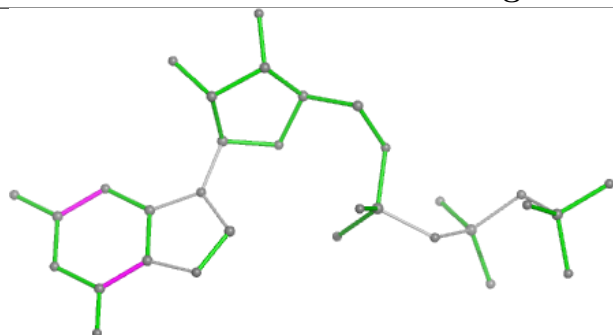


Torsions

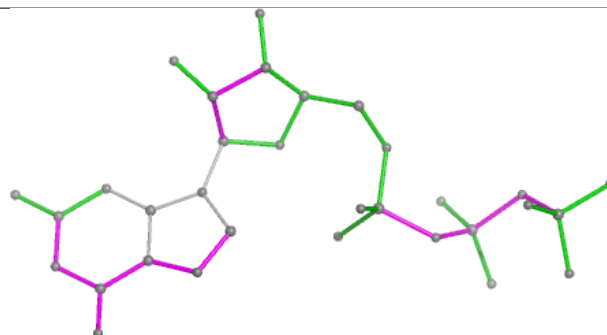


Rings

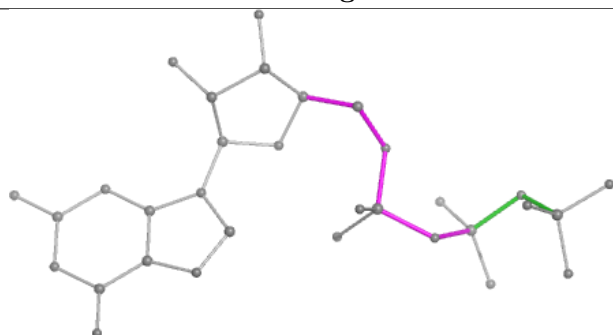
## Ligand GTP U5 501



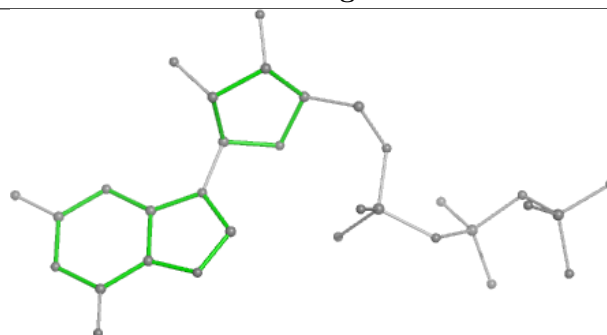
Bond lengths



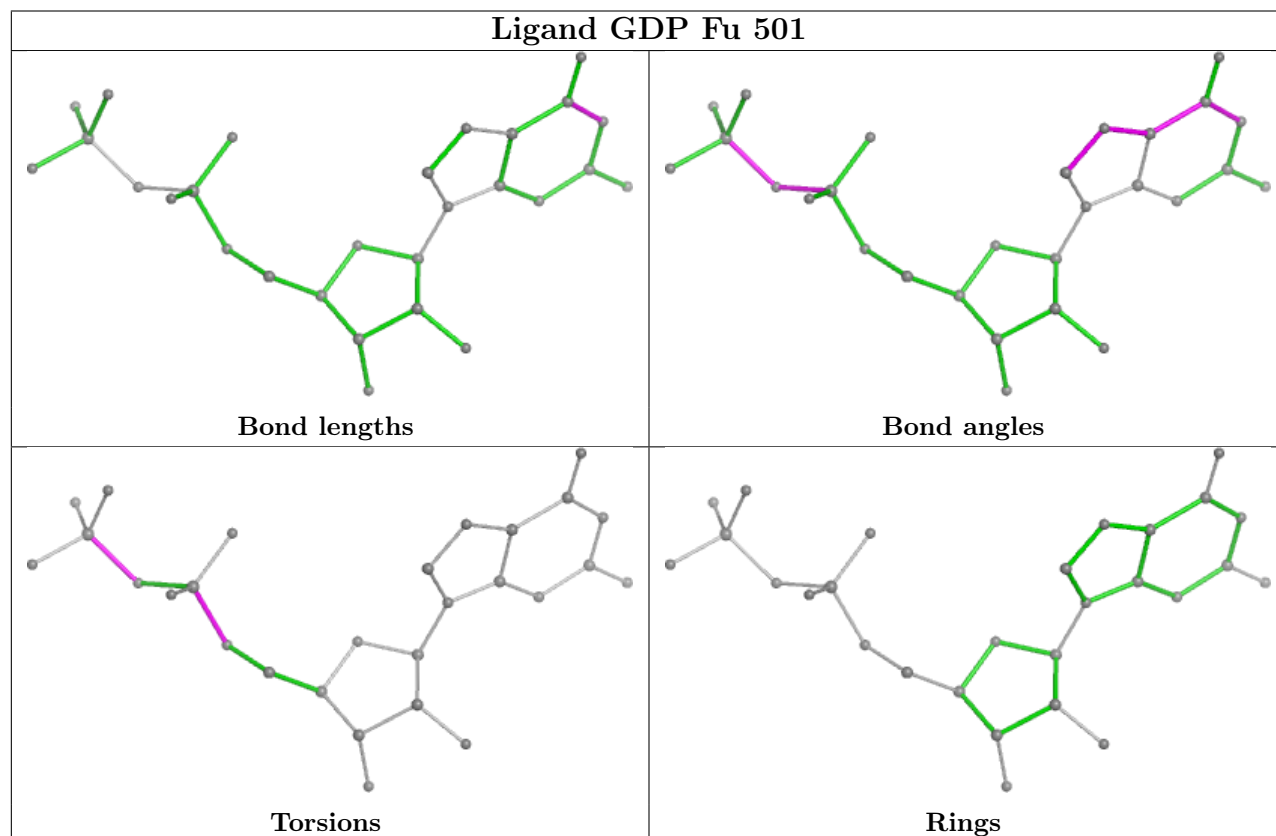
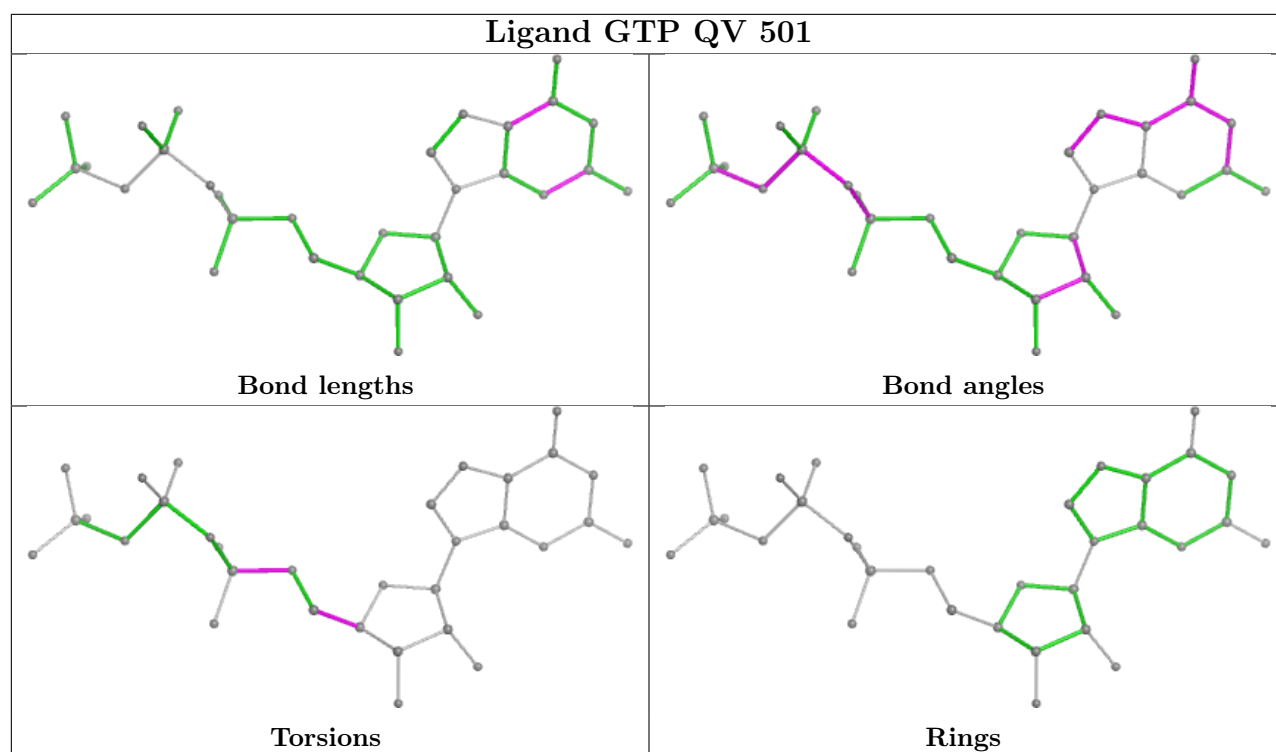
Bond angles

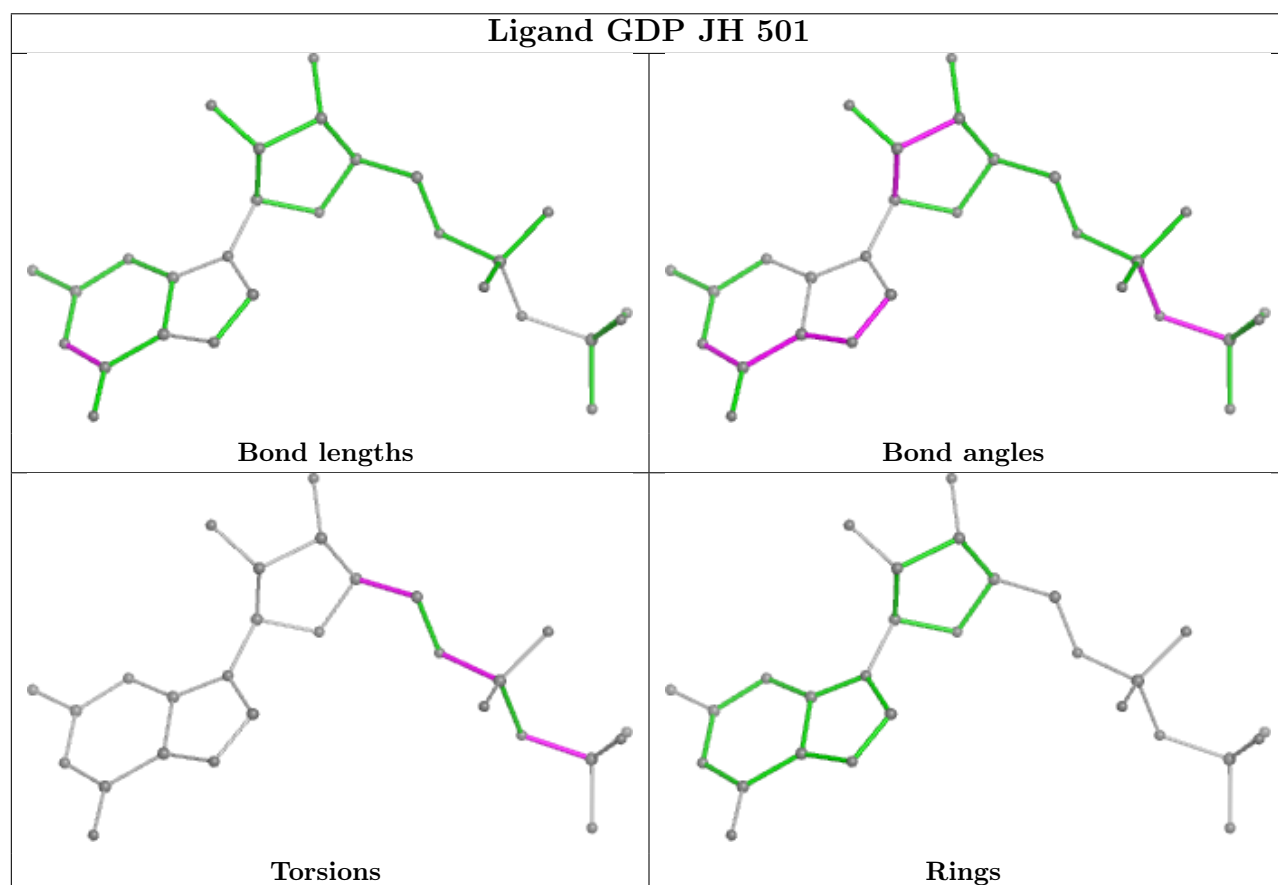
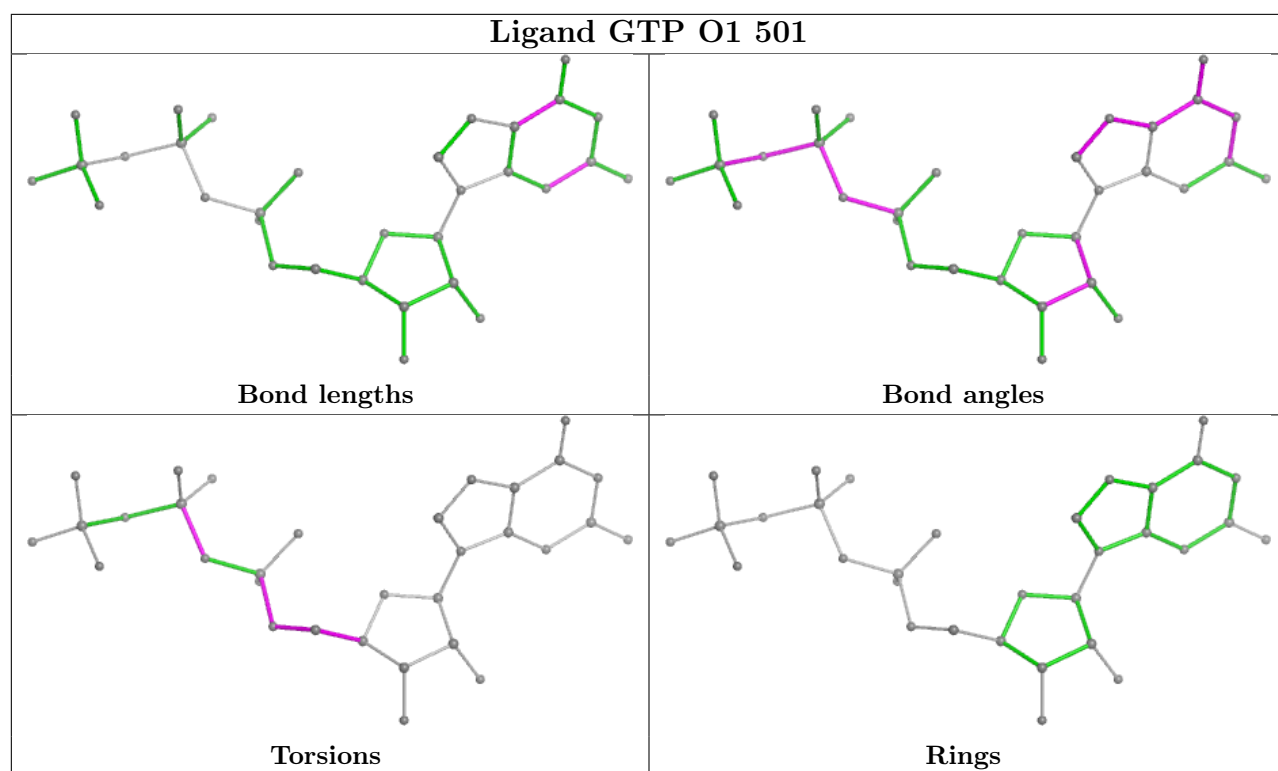


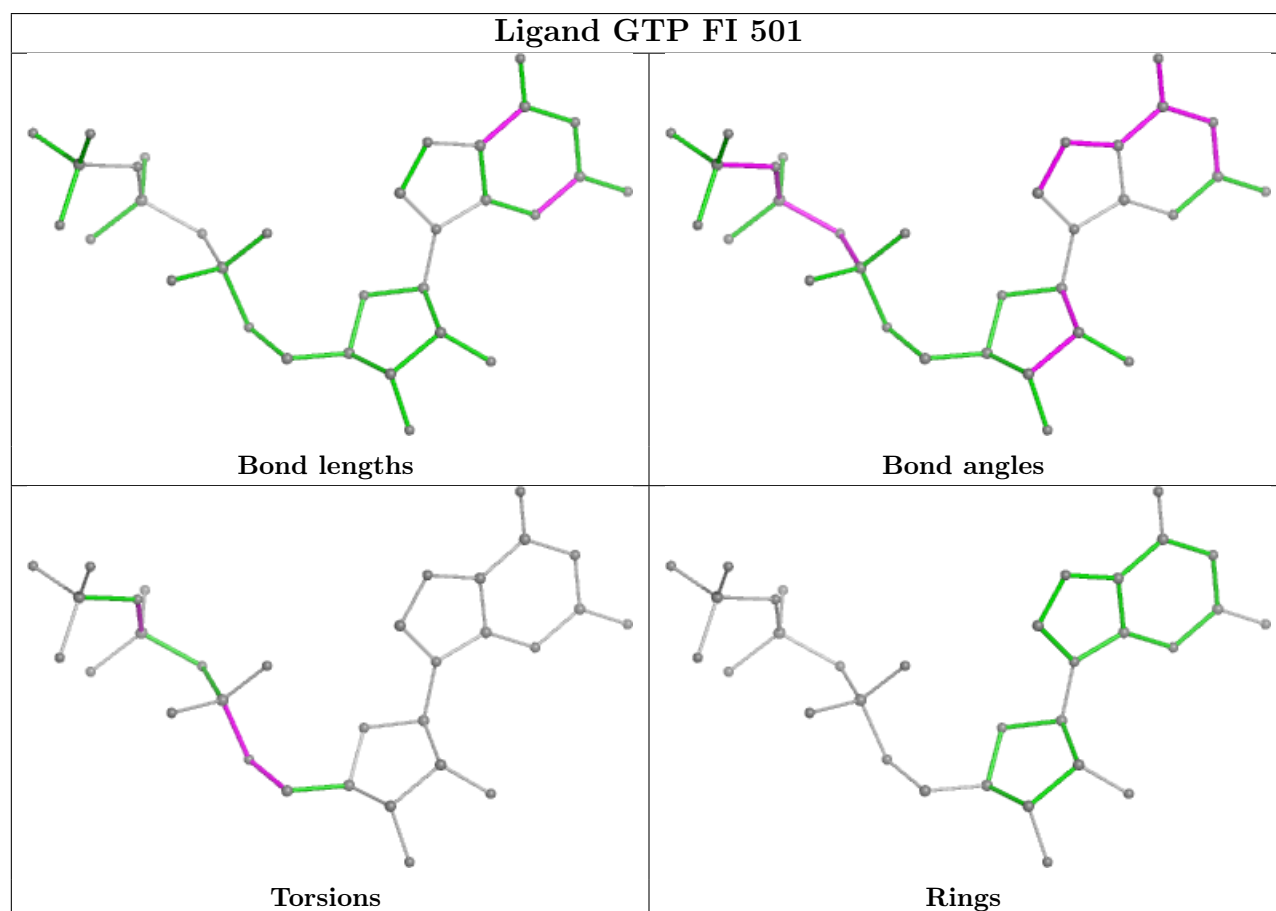
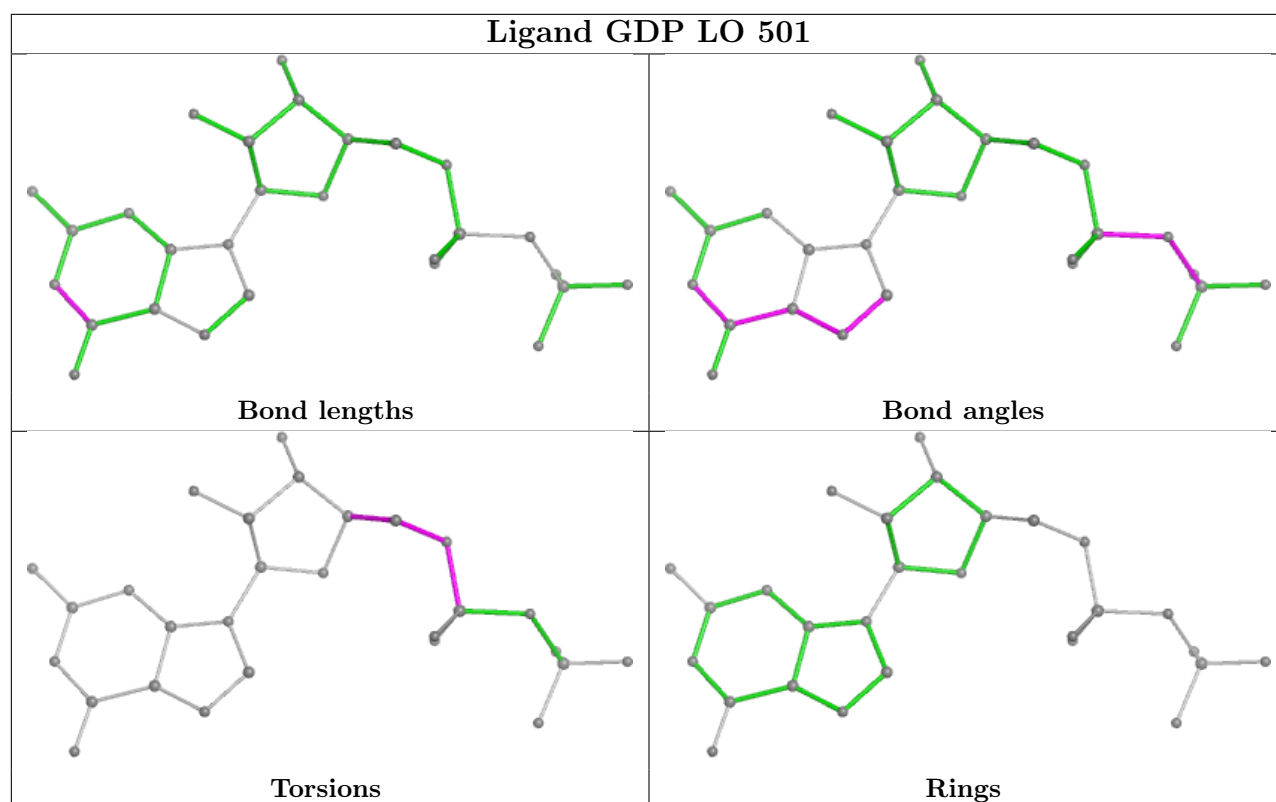
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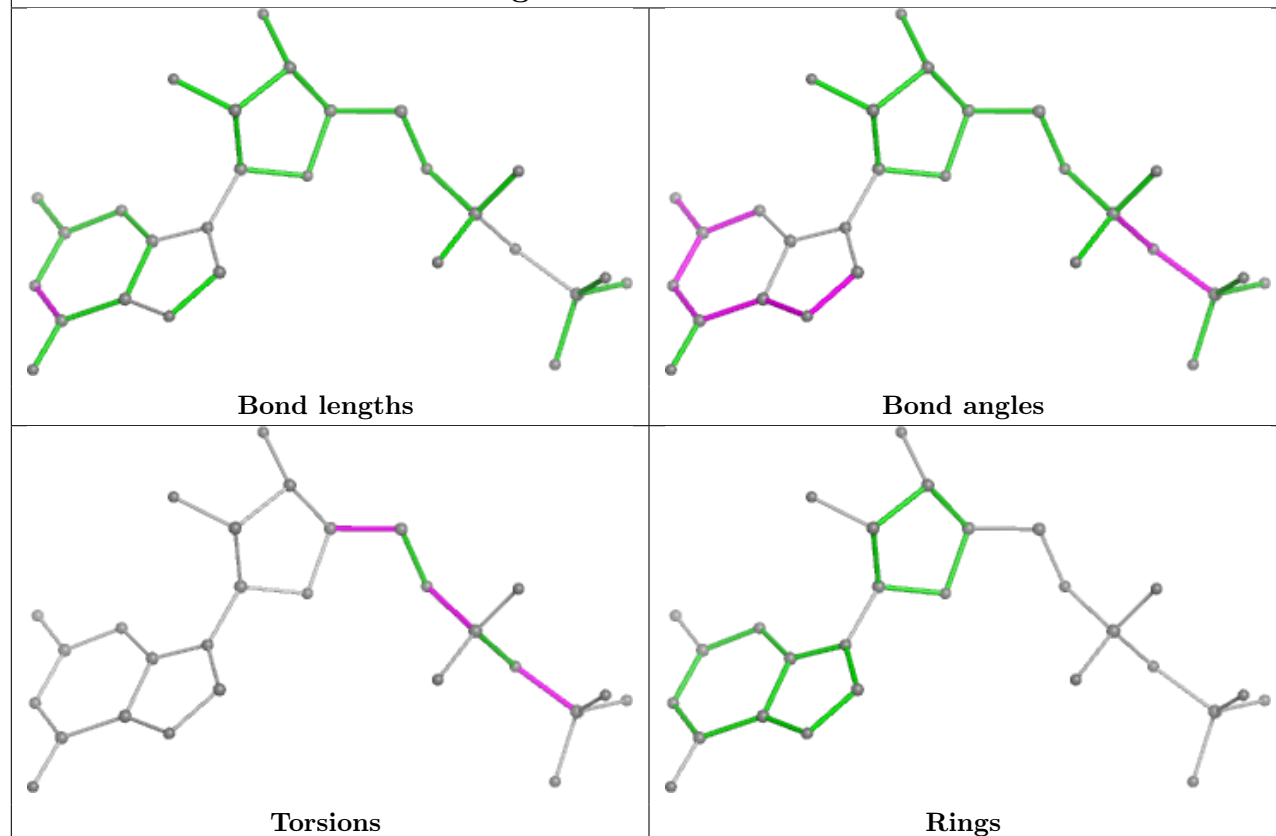
Rings



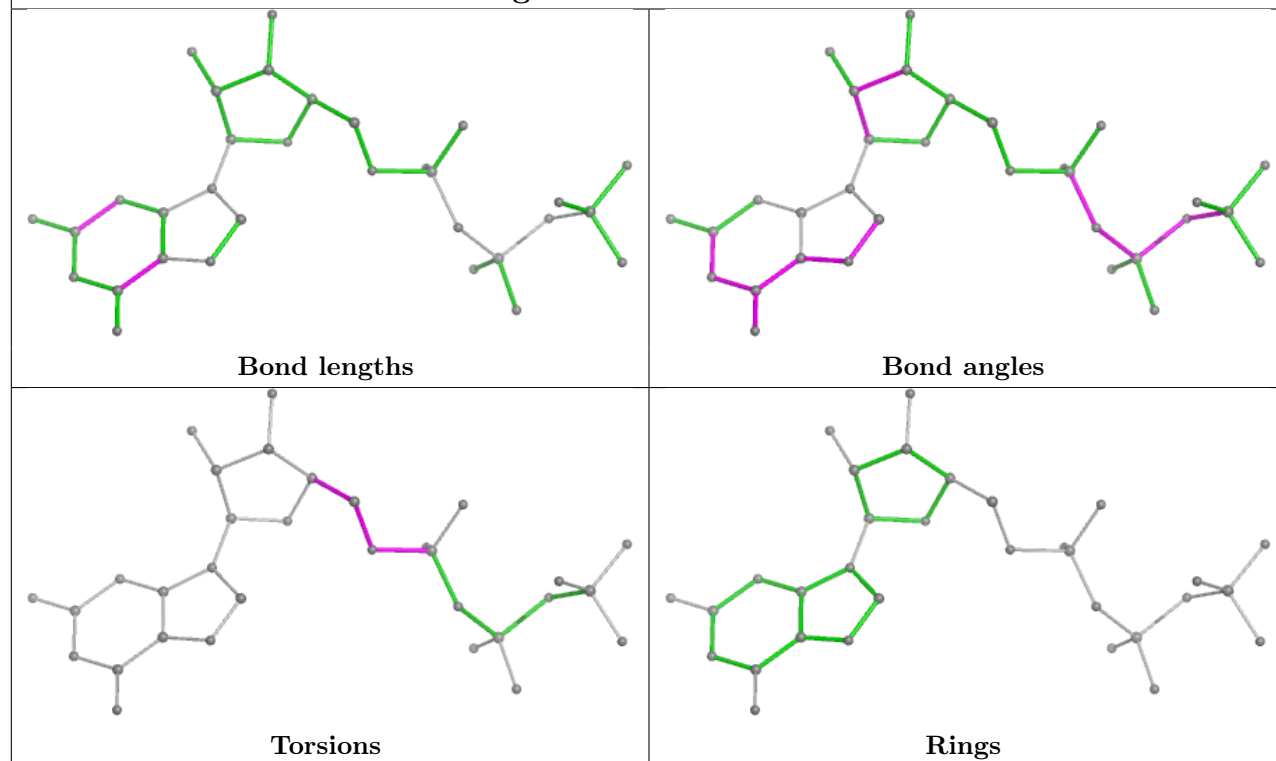


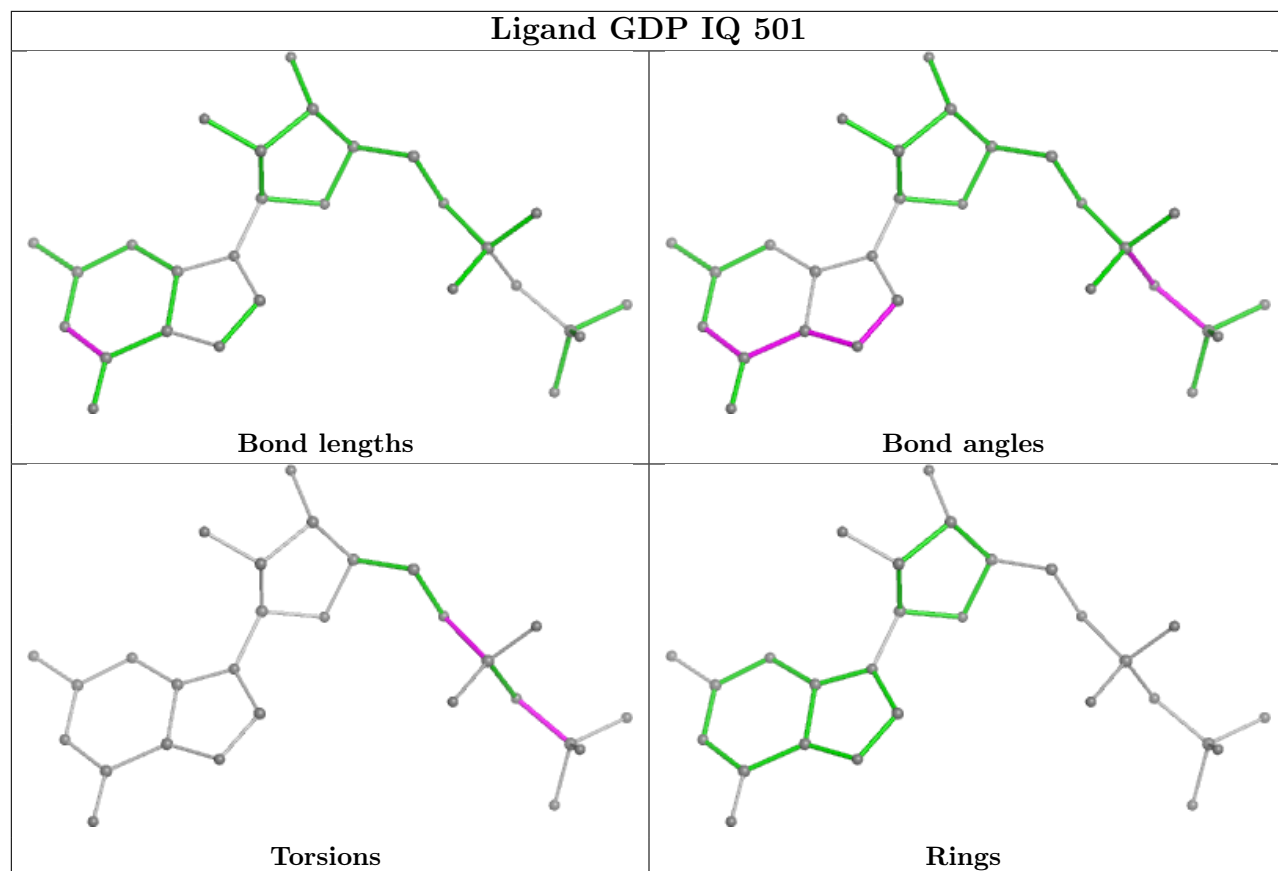


## Ligand GDP MD 501



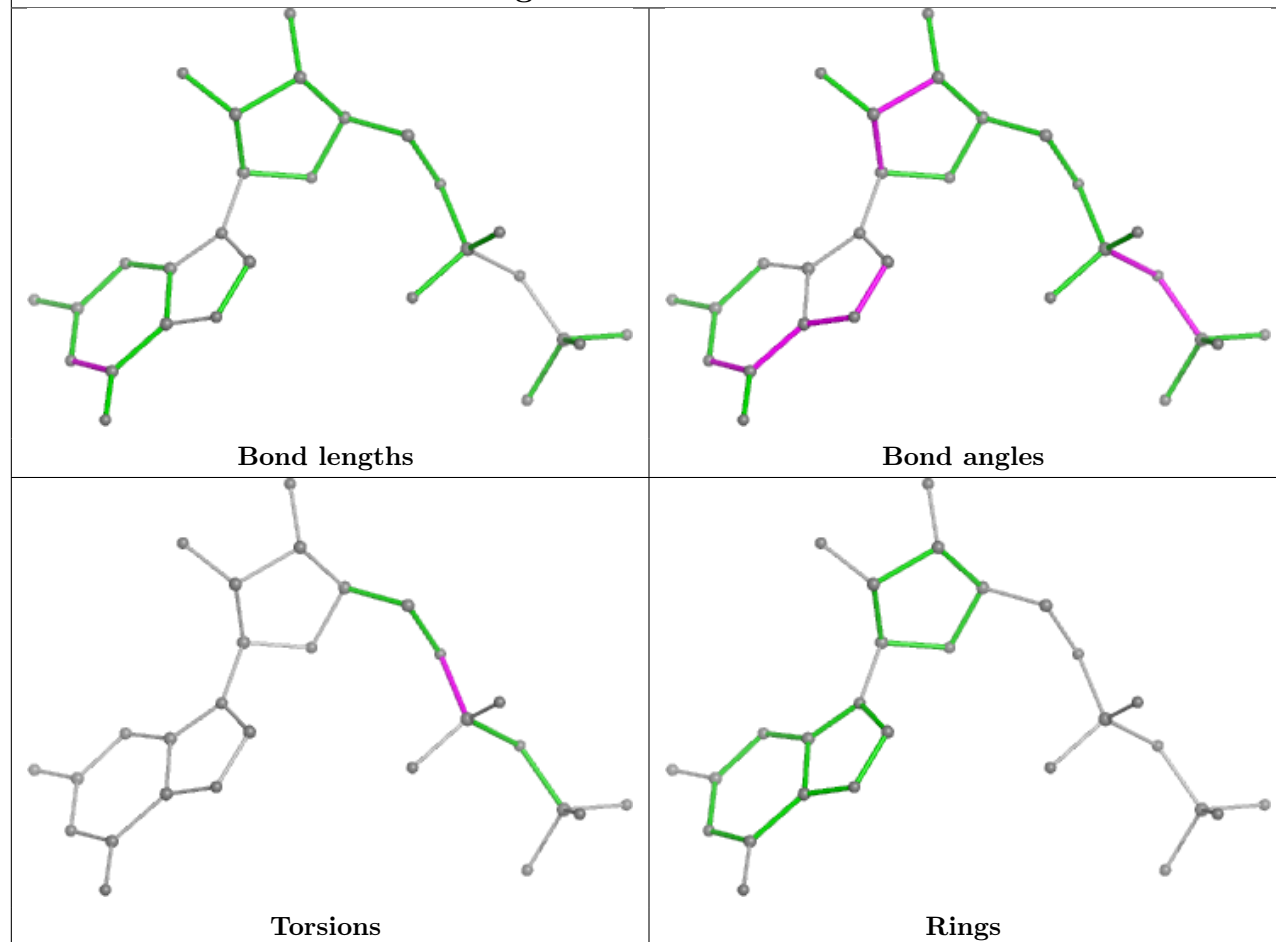
## Ligand GTP MN 501



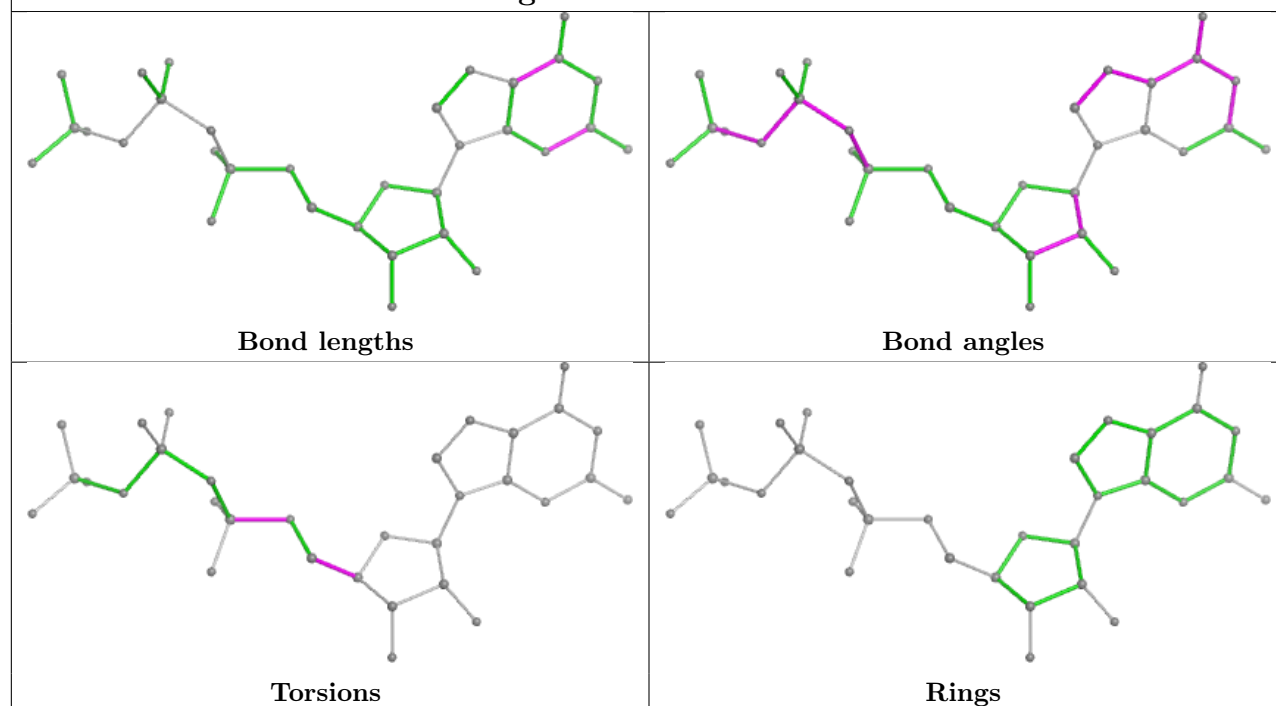




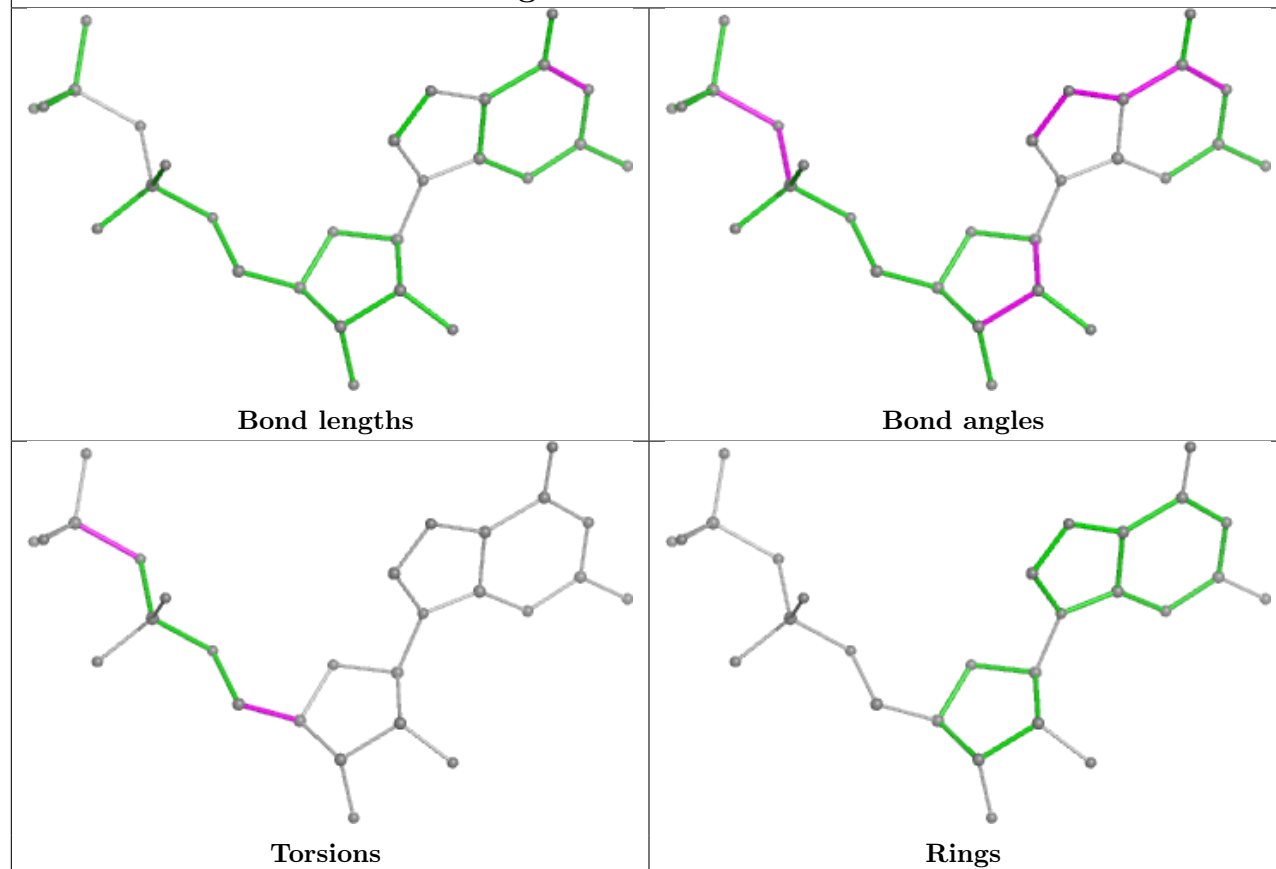
## Ligand GDP SM 501



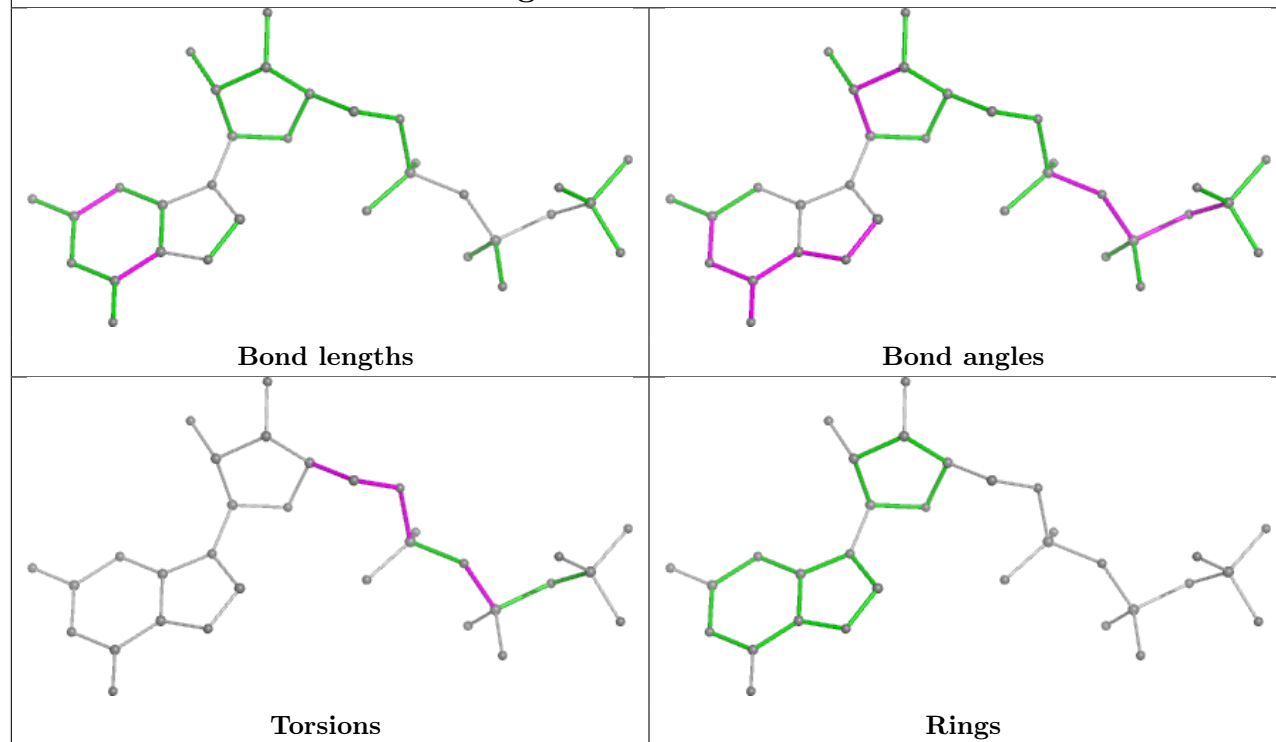
## Ligand GTP FK 501



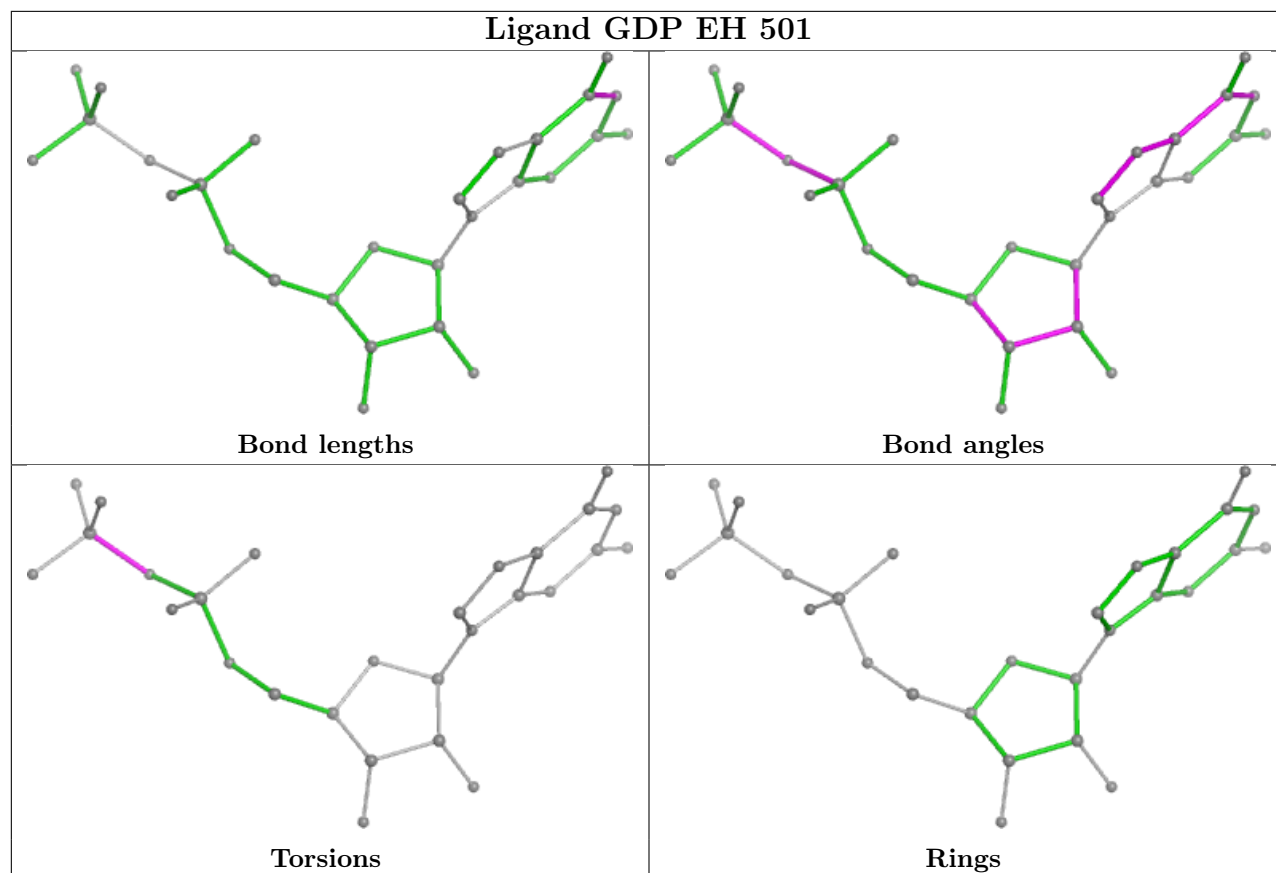
## Ligand GDP Ws 501



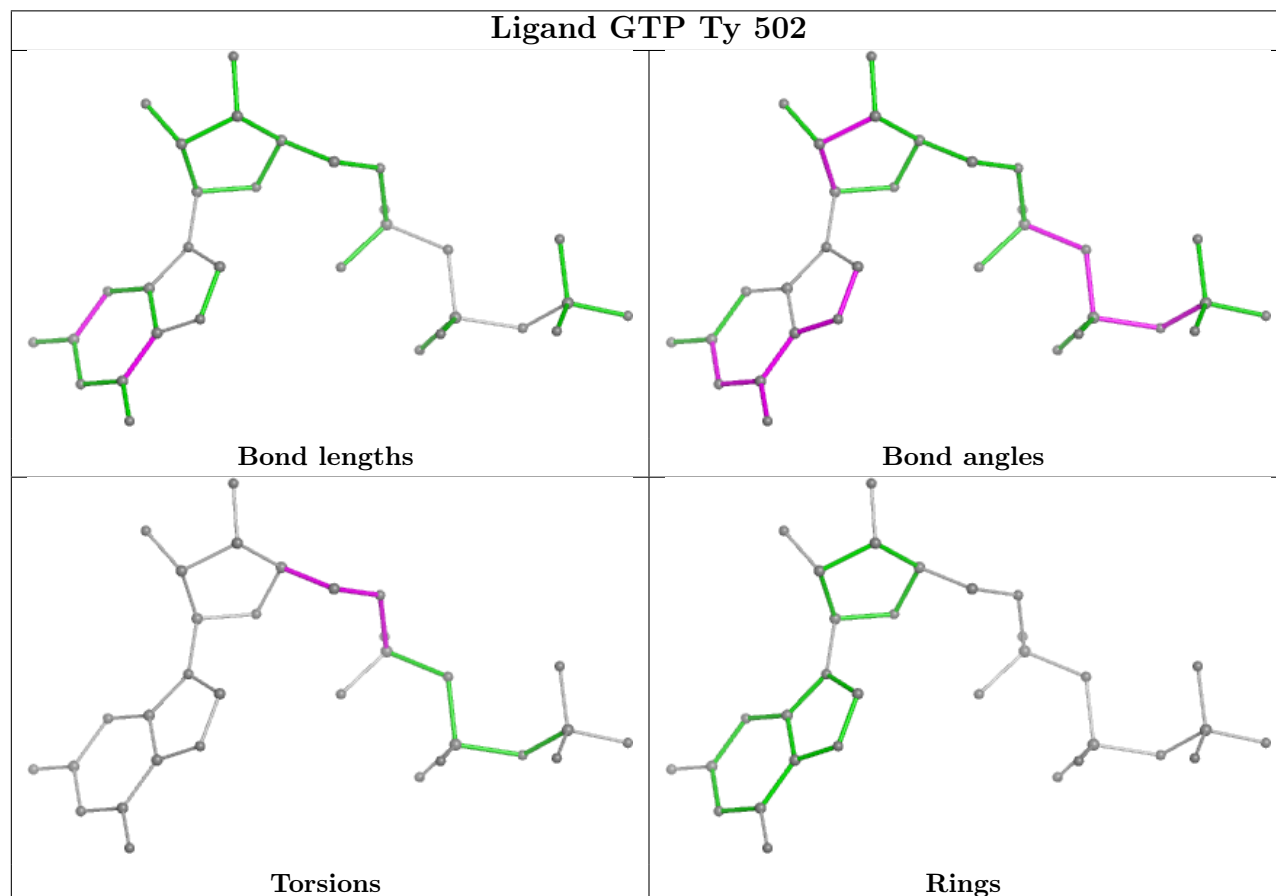
## Ligand GTP TY 501

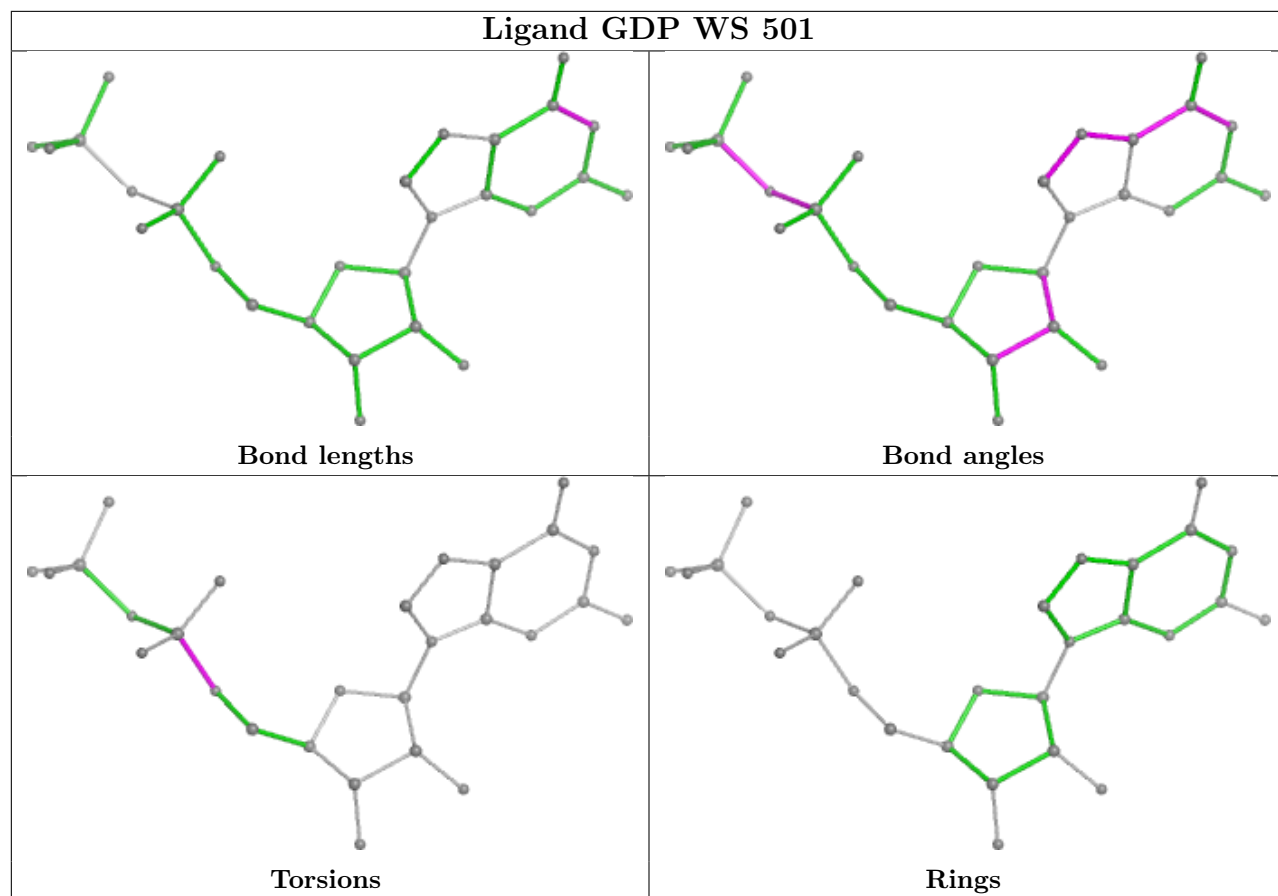


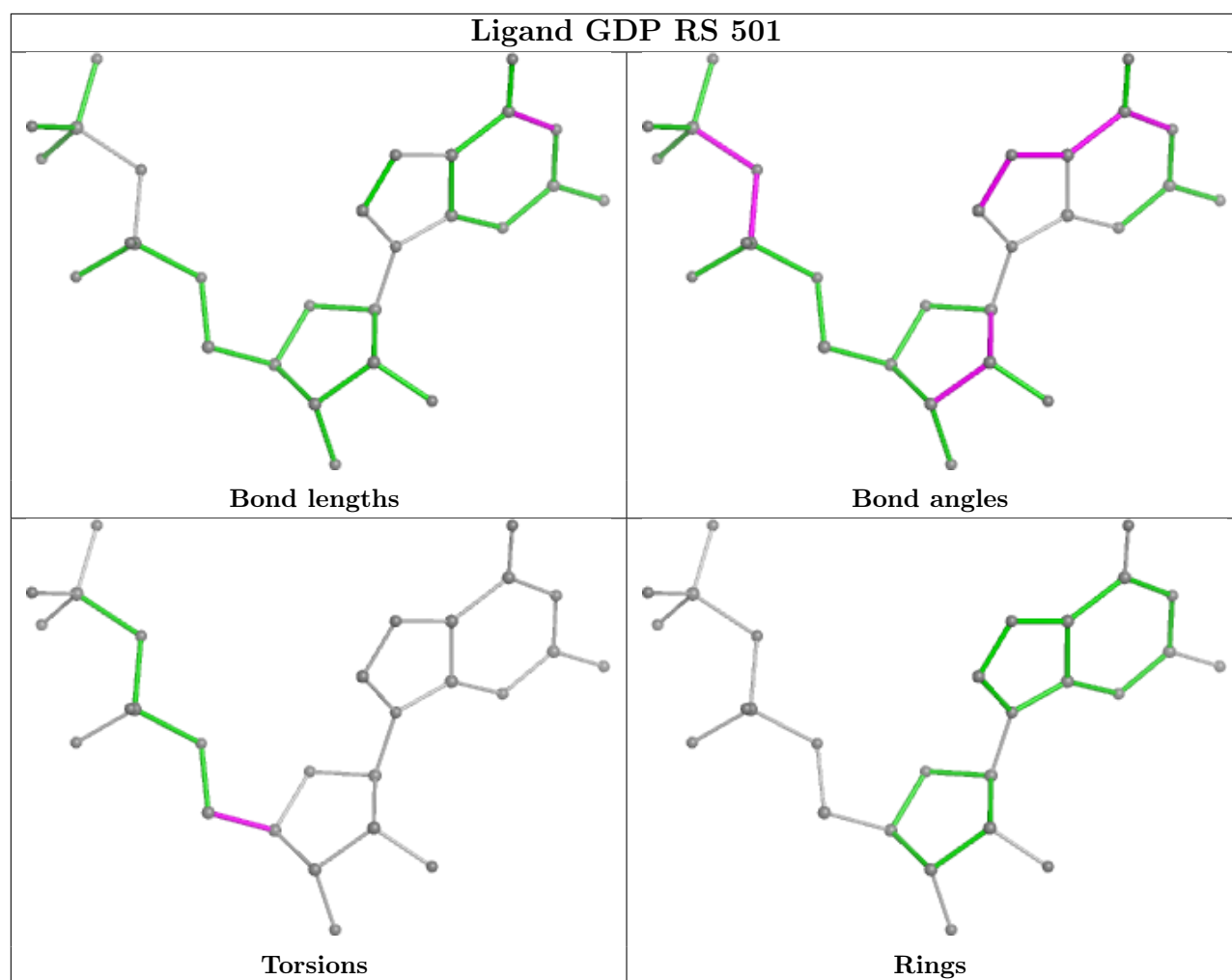
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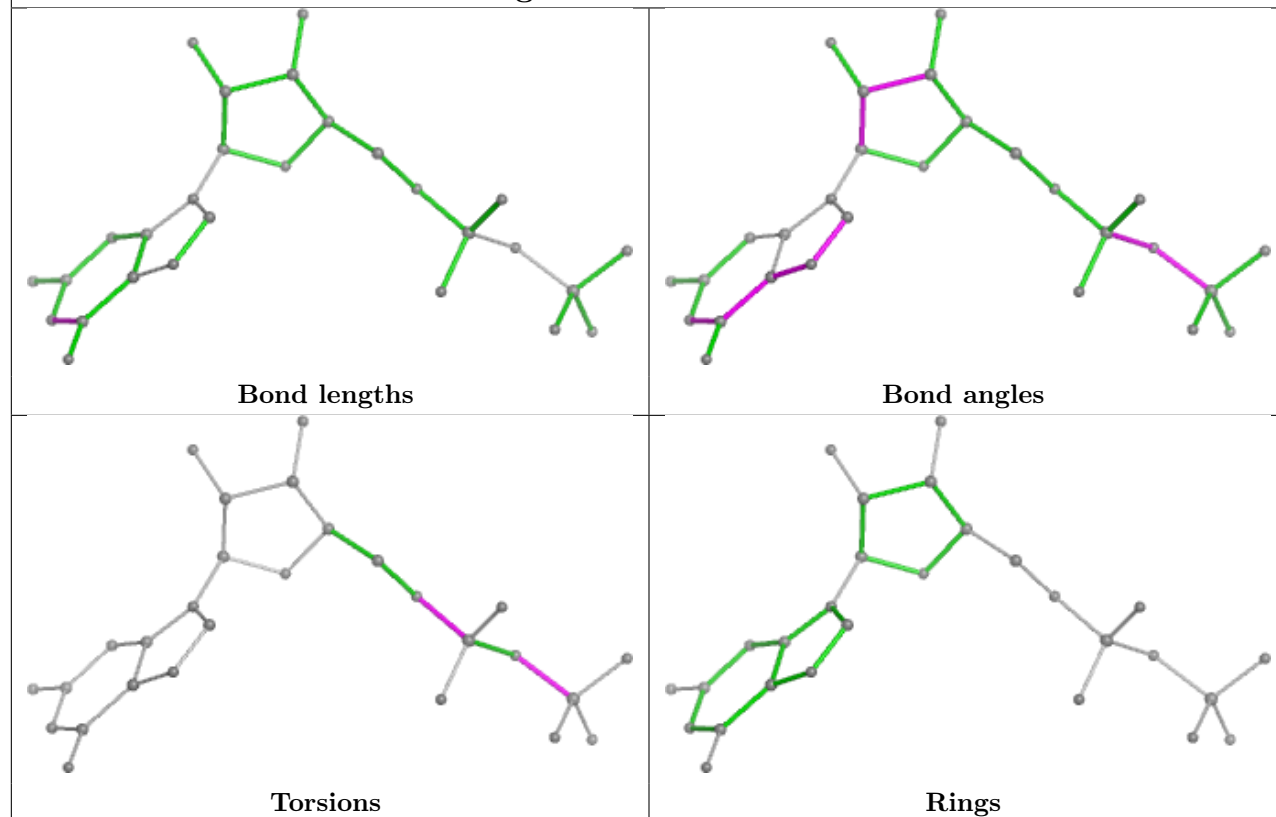
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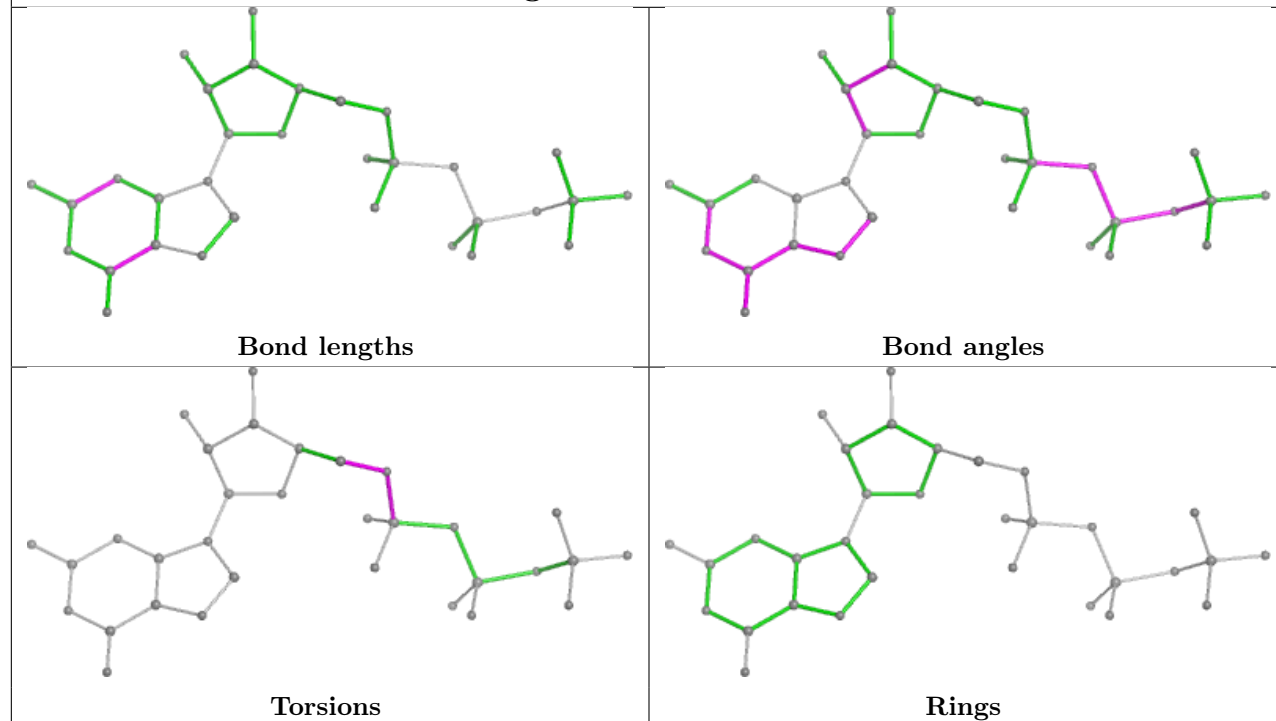




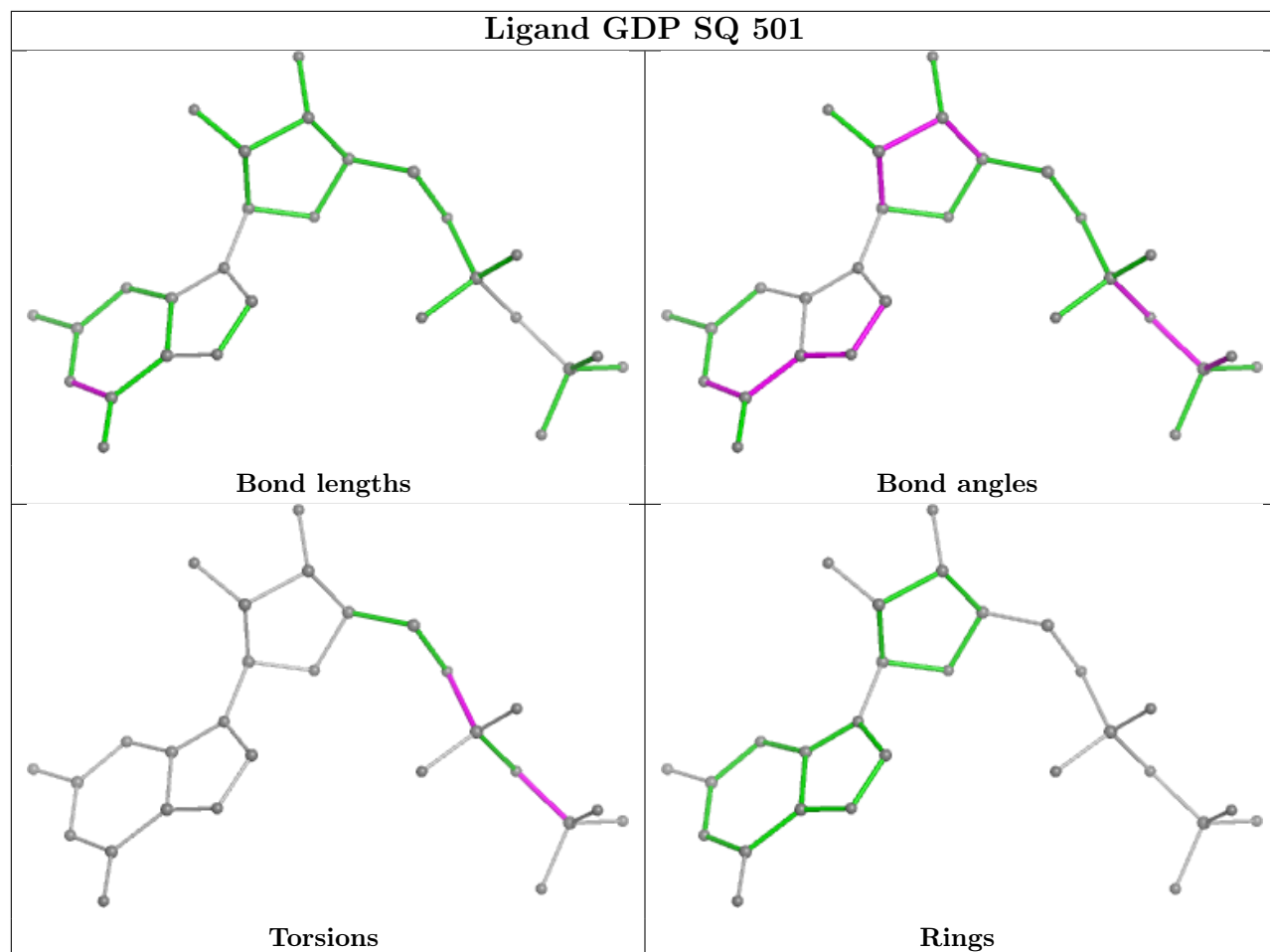
## Ligand GDP Uw 501



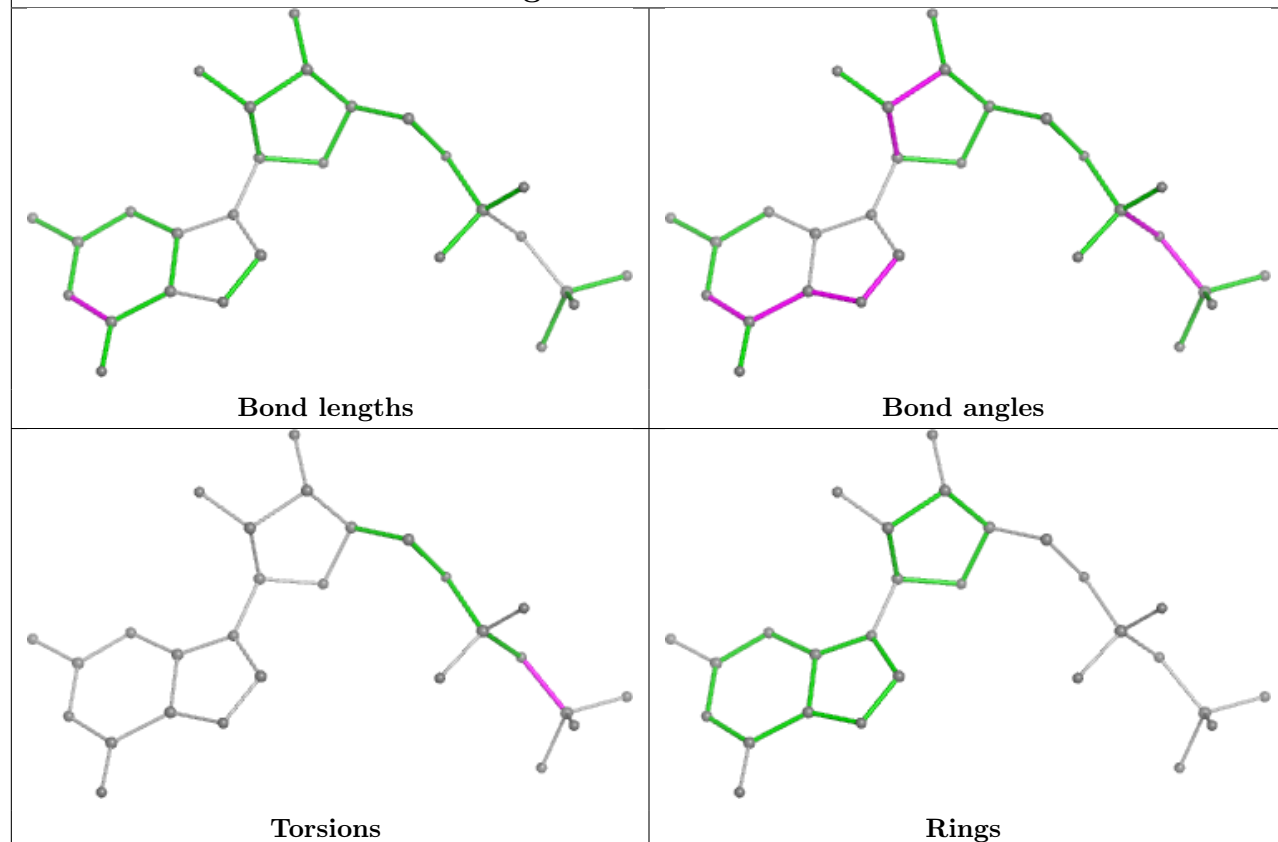
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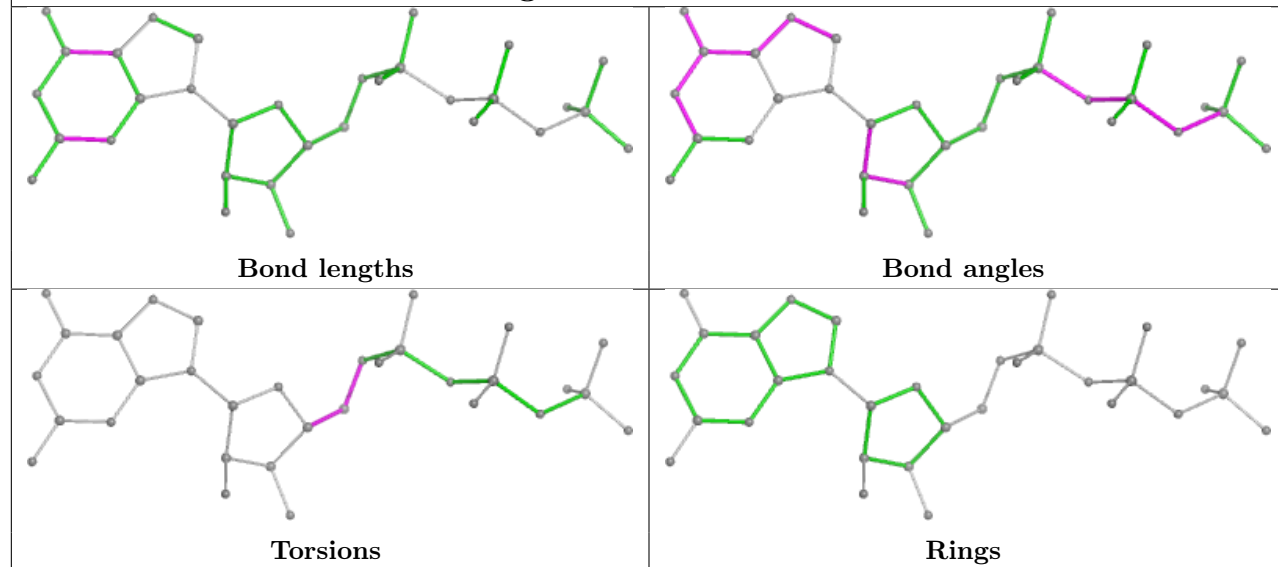
## Ligand GDP SQ 501



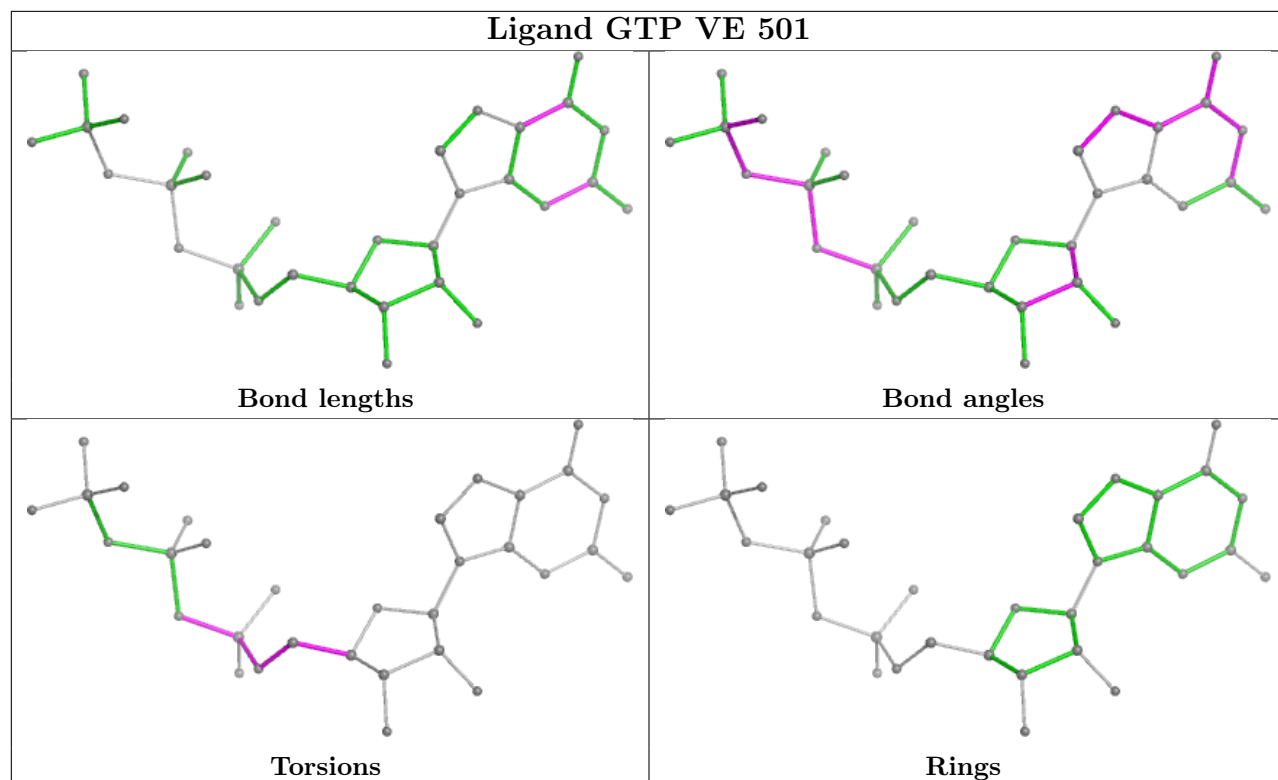
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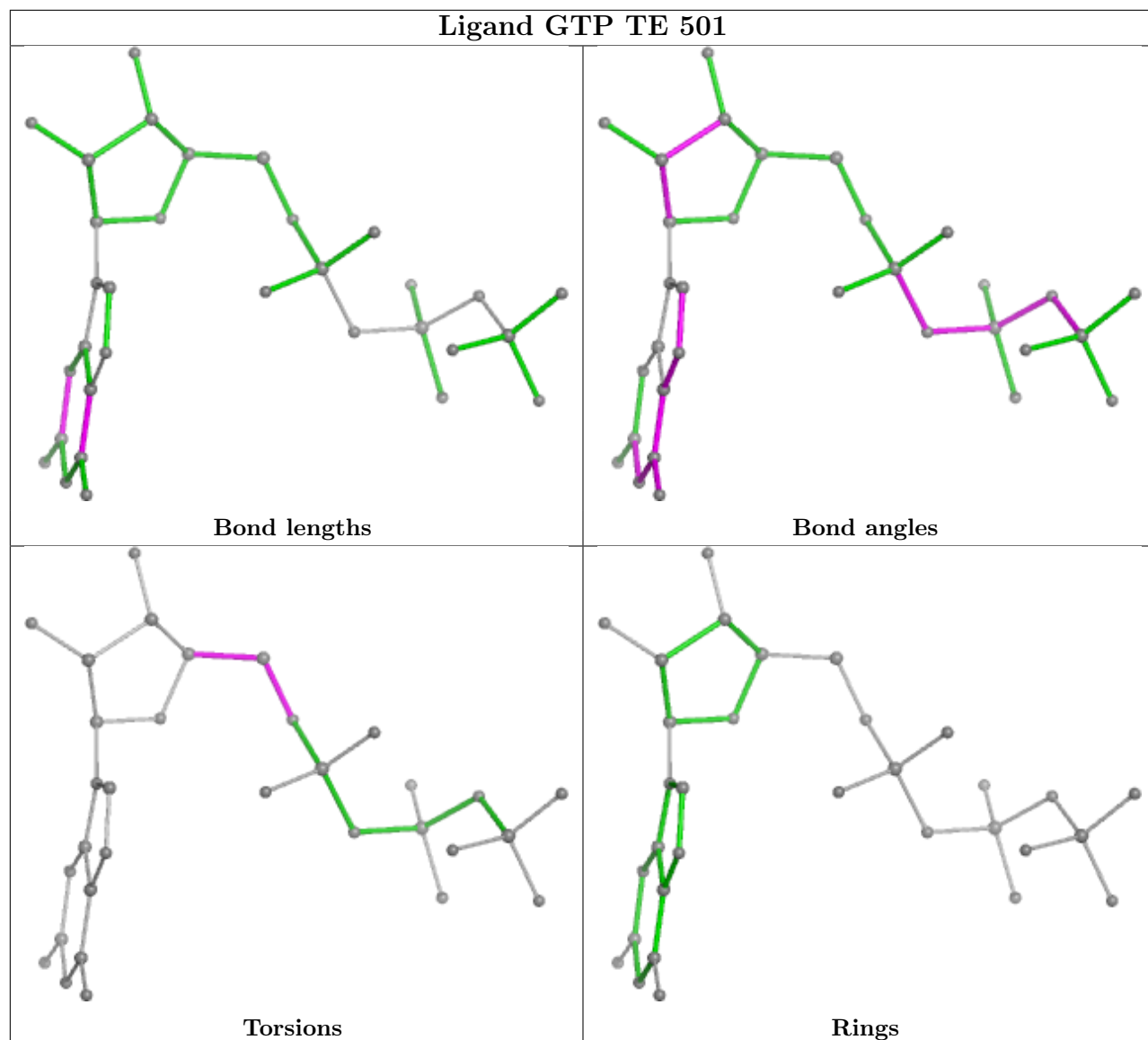
## Ligand GTP FG 501



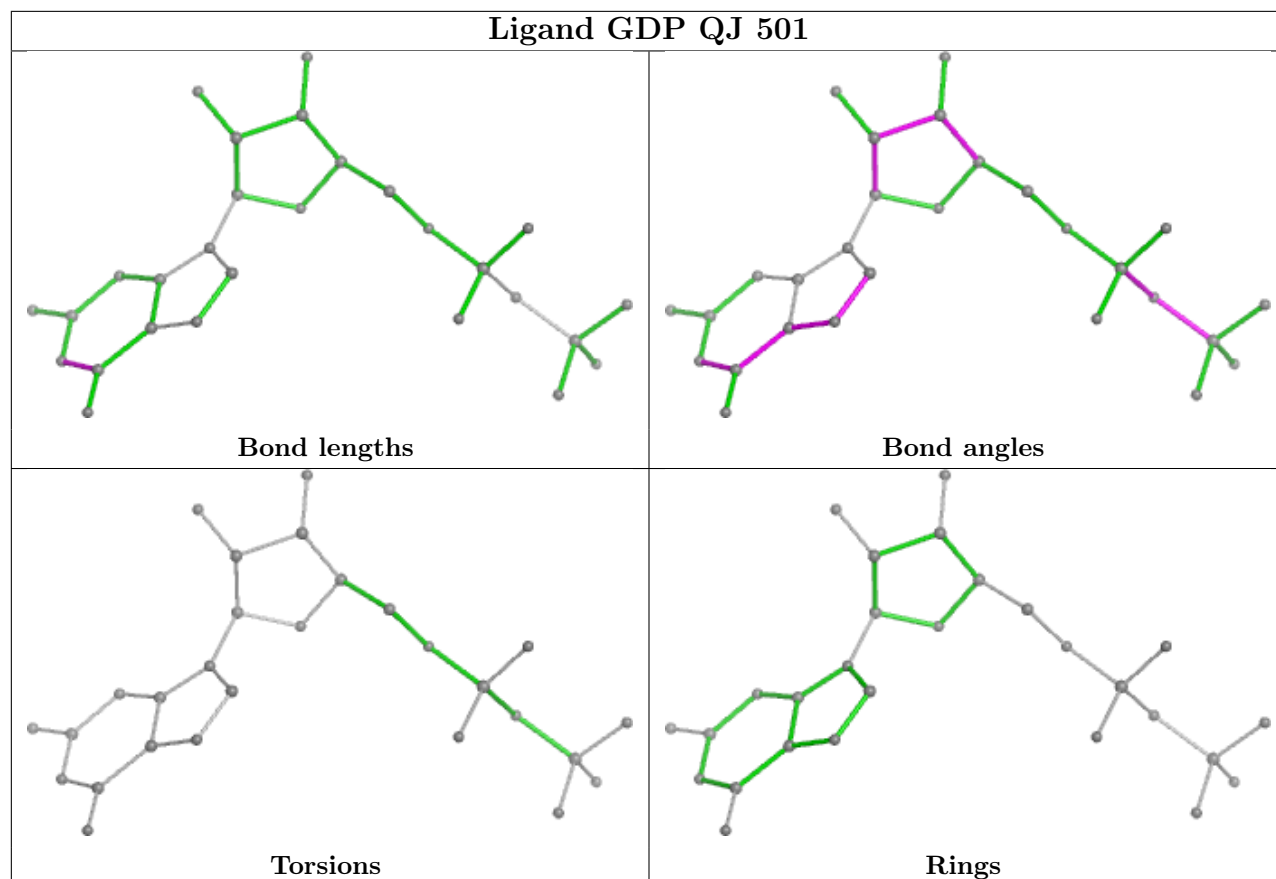




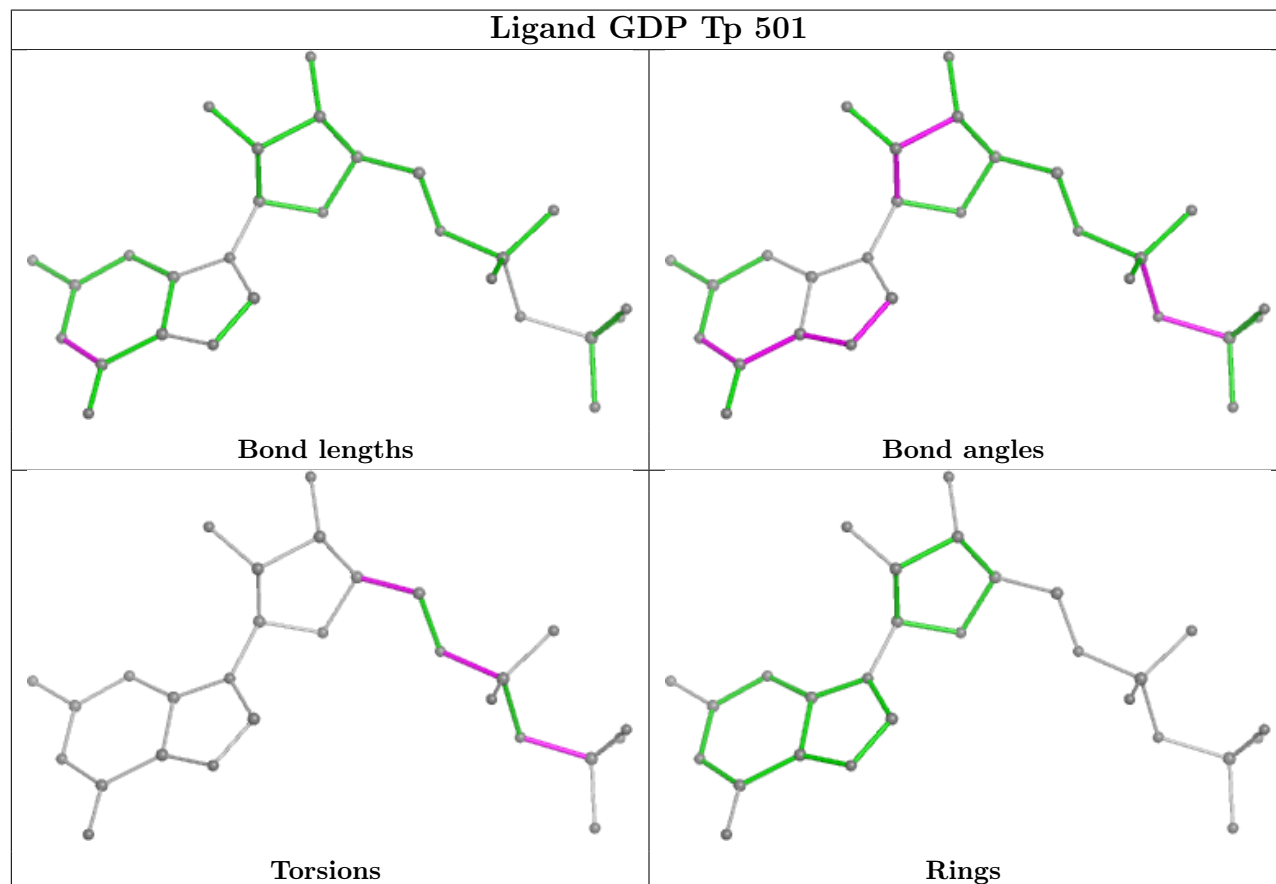
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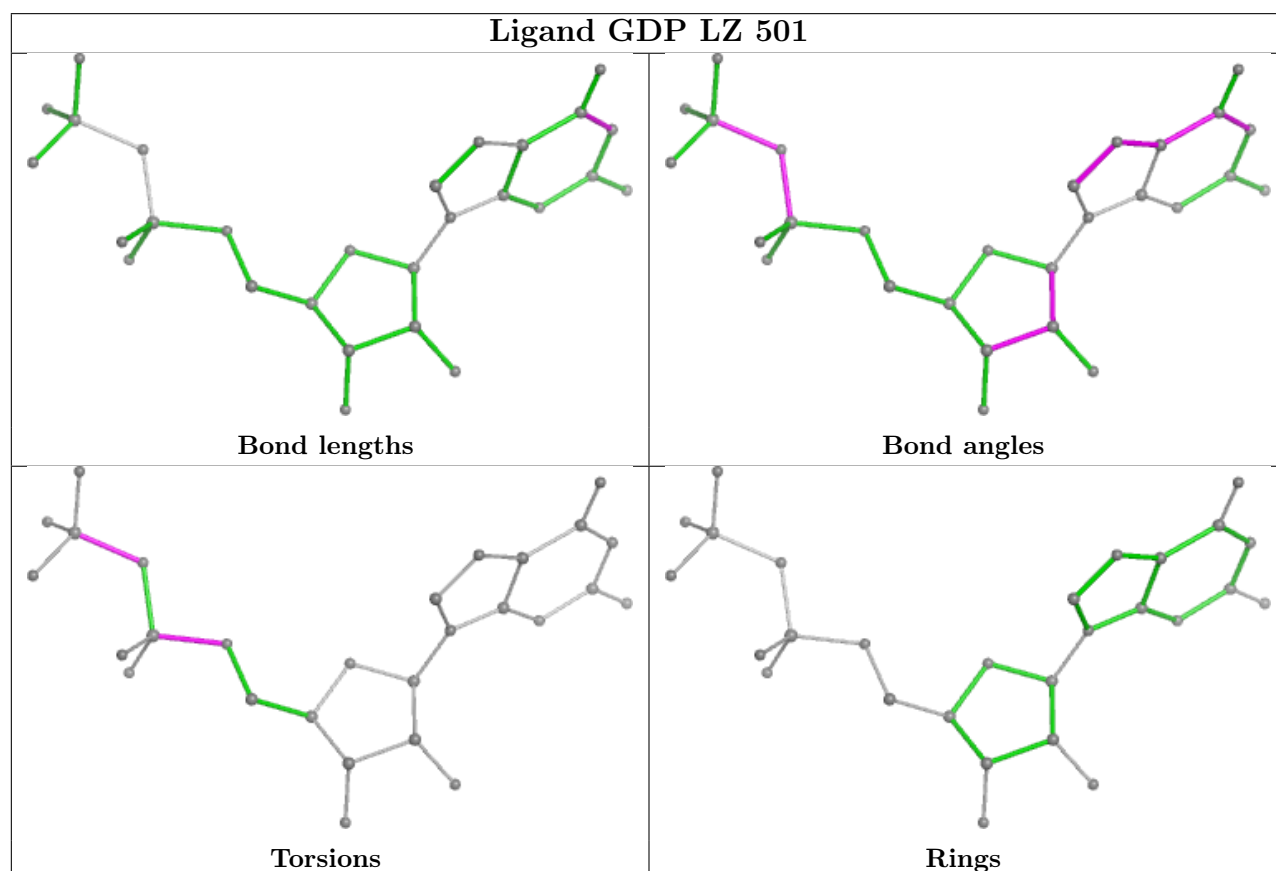
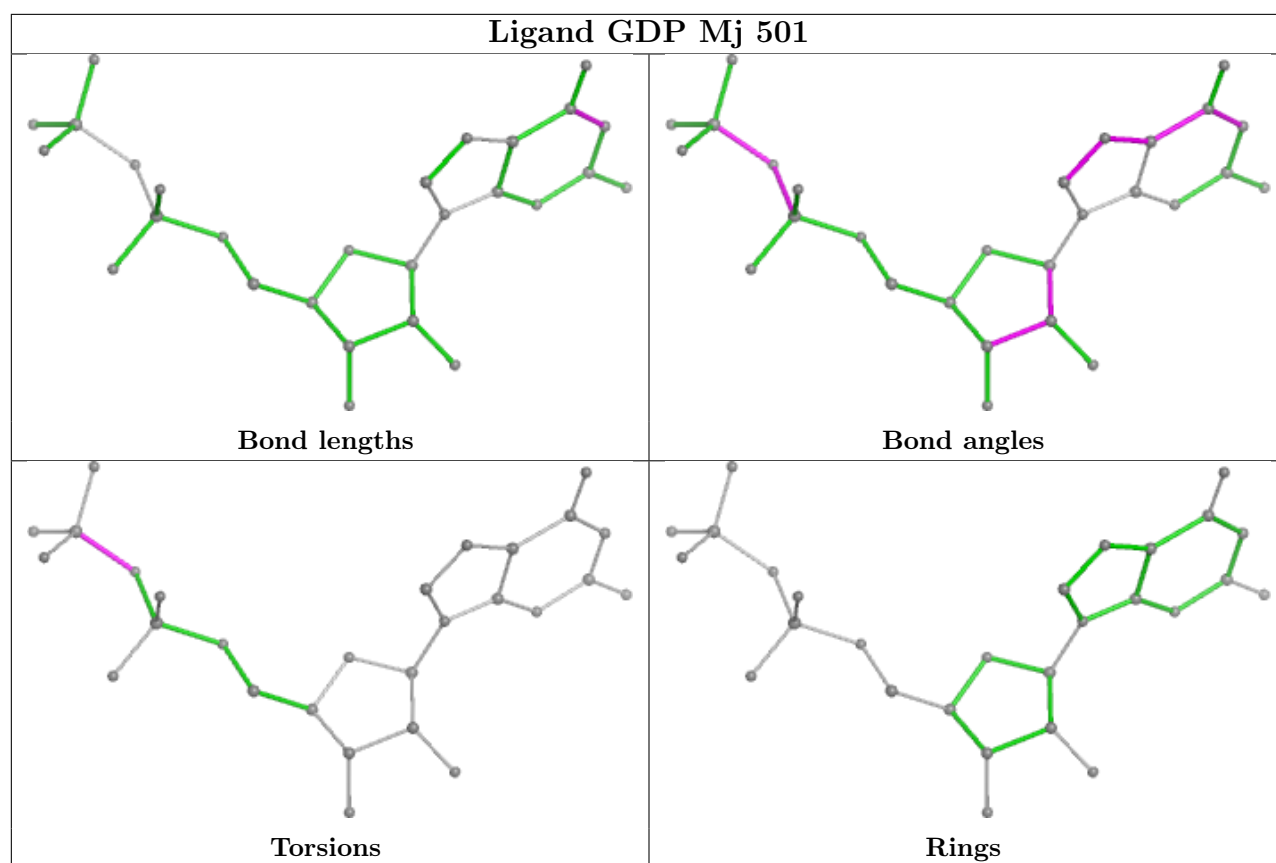


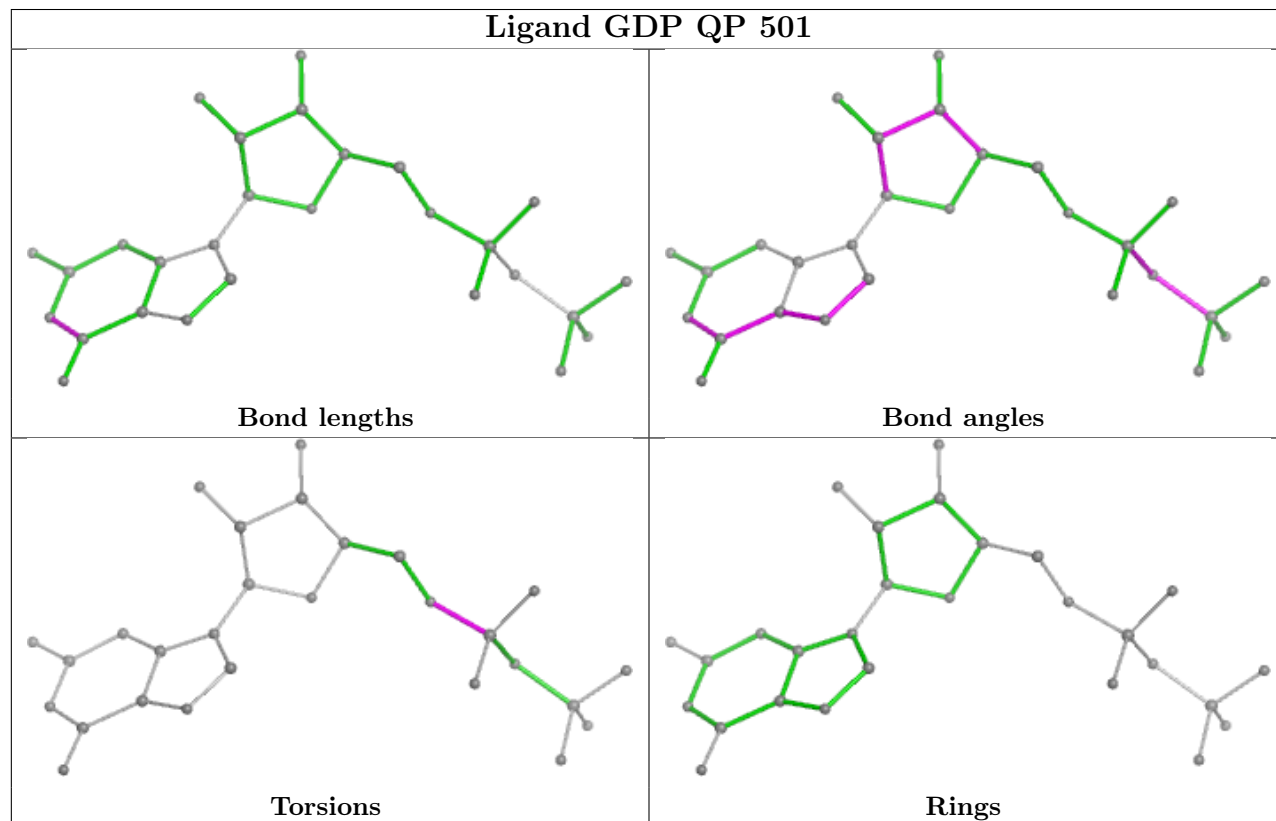
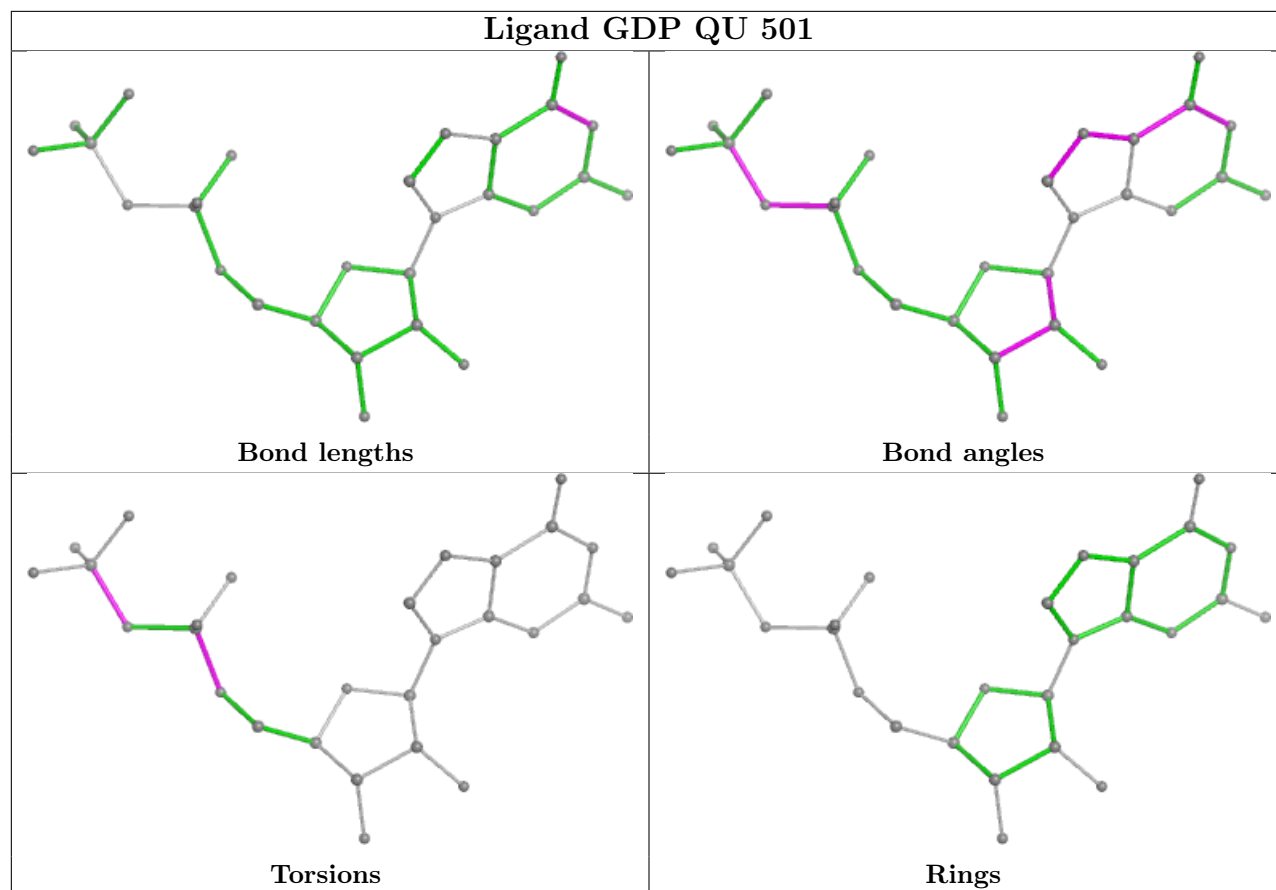
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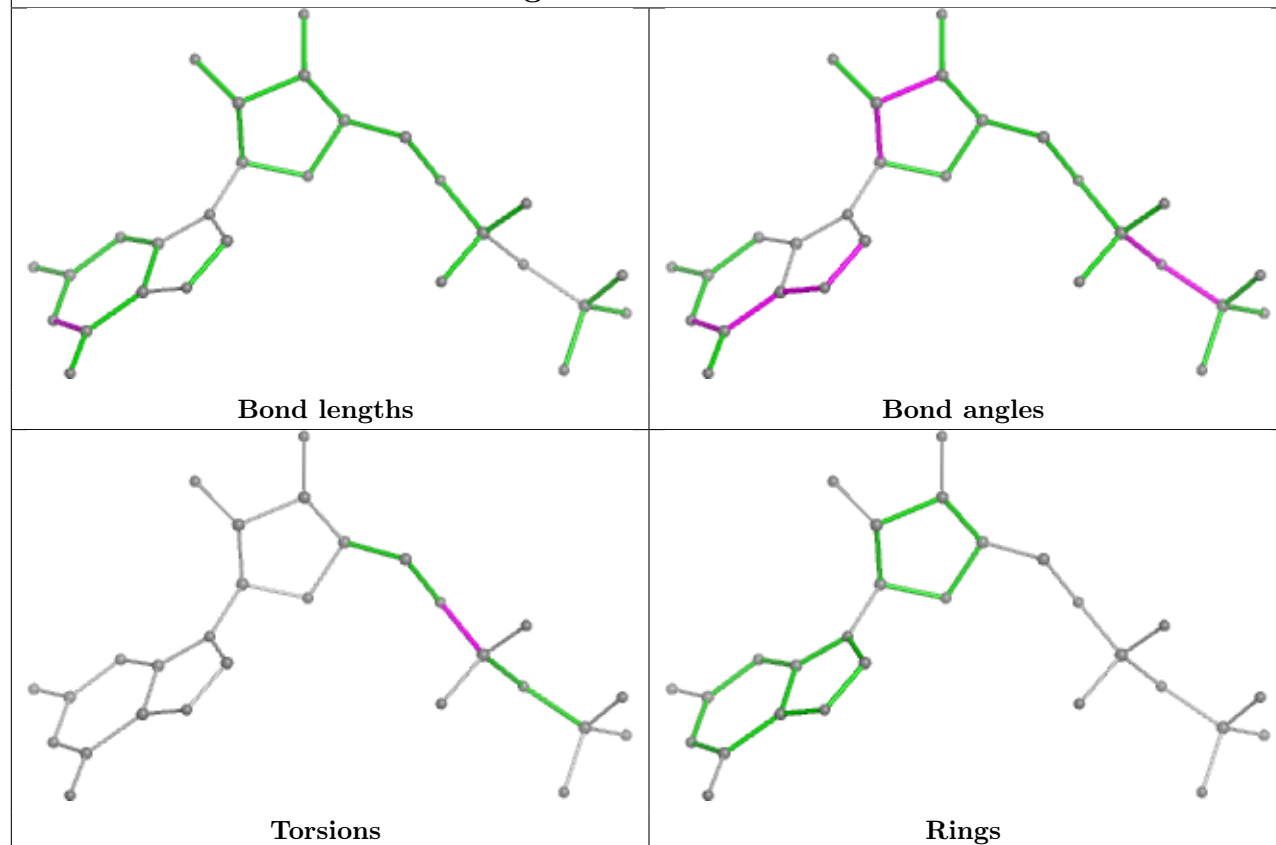
## Ligand GDP Tp 501



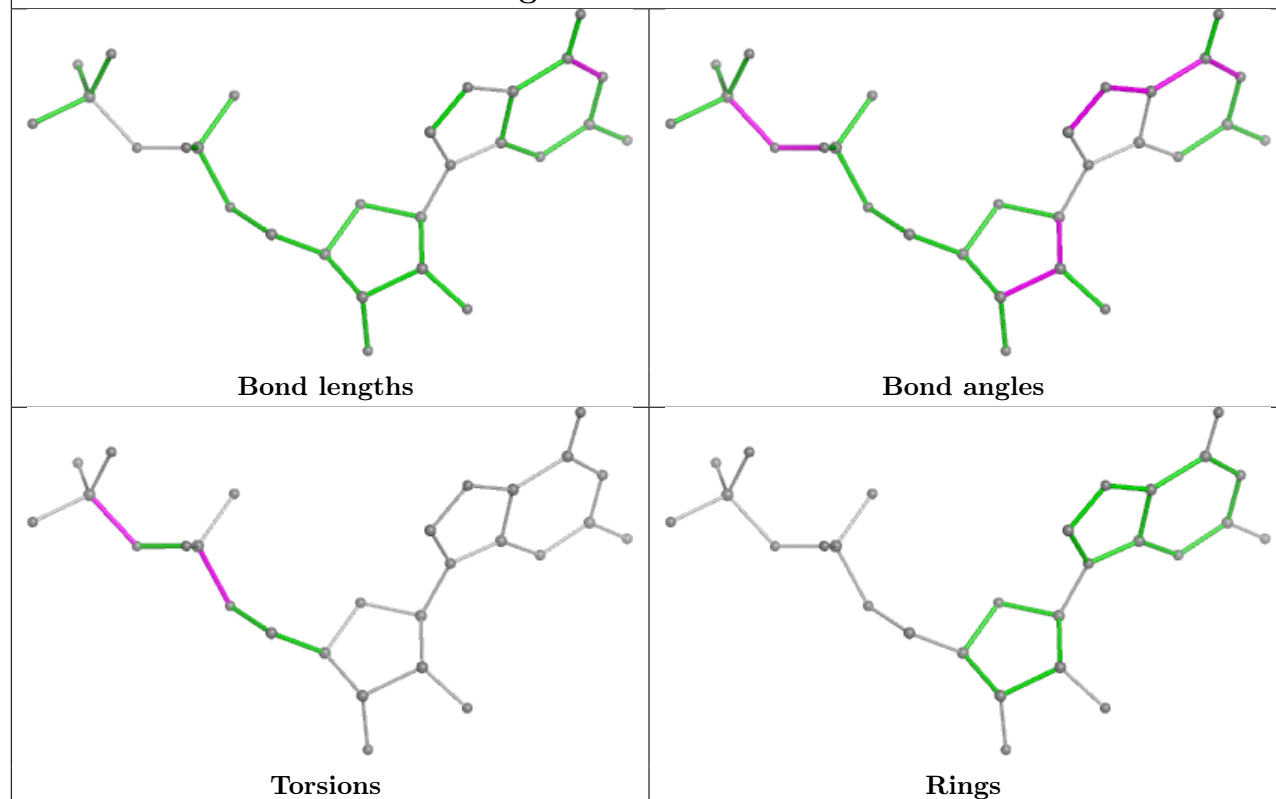


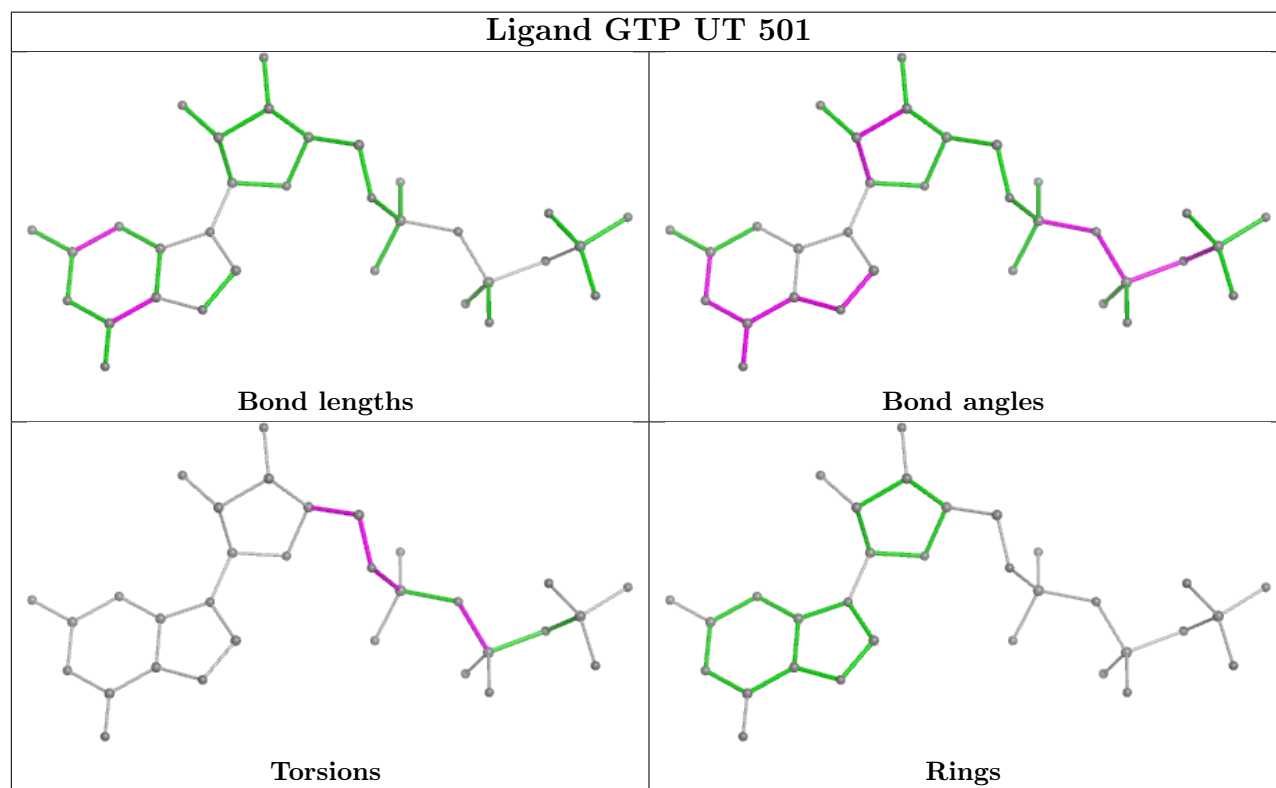
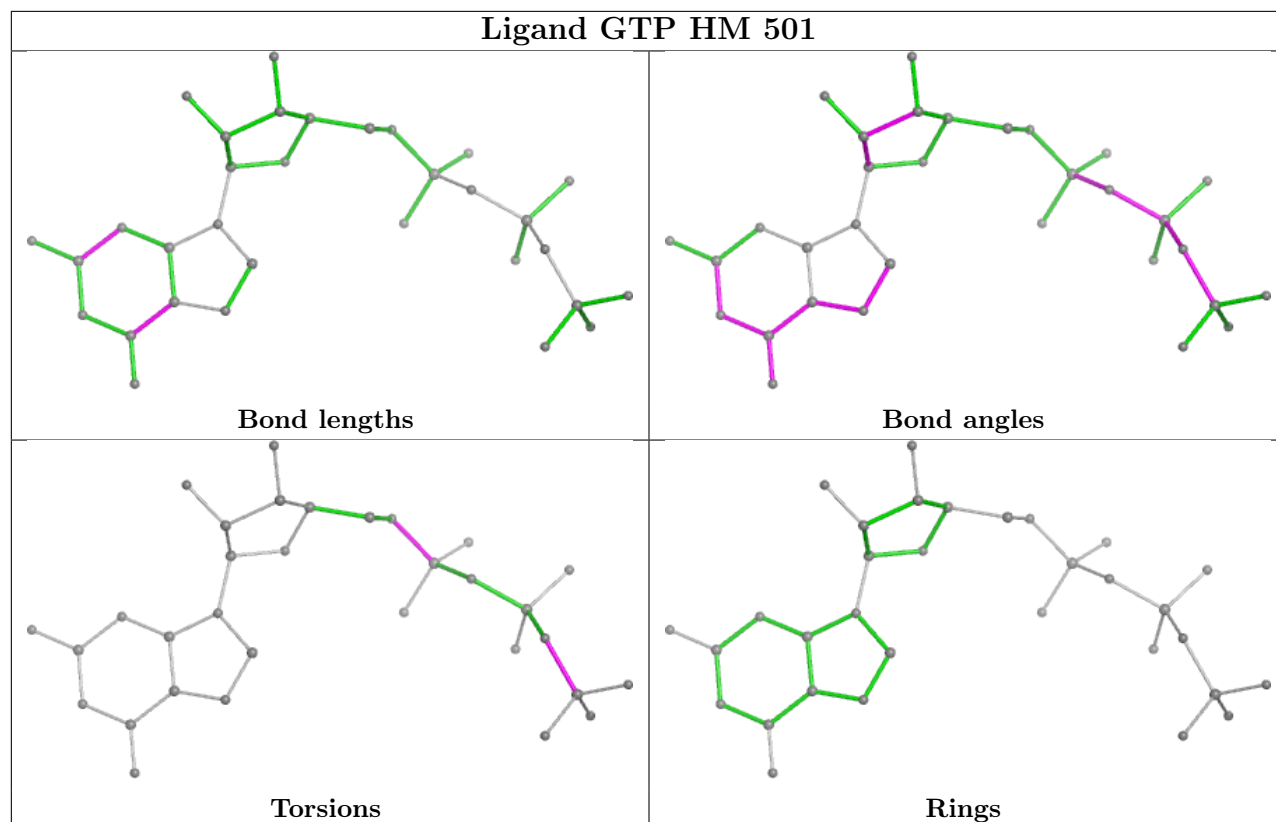


## Ligand GDP J8 501

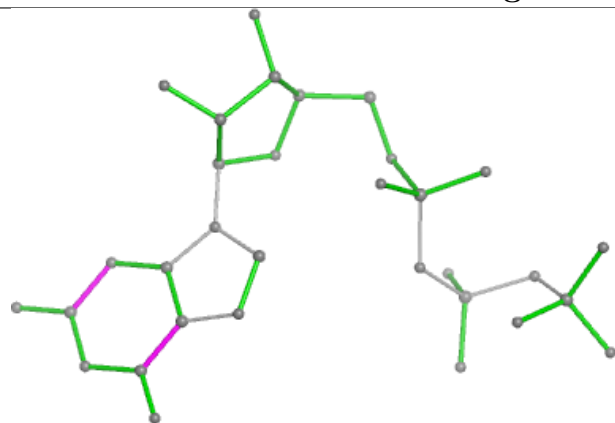


## Ligand GDP EF 501

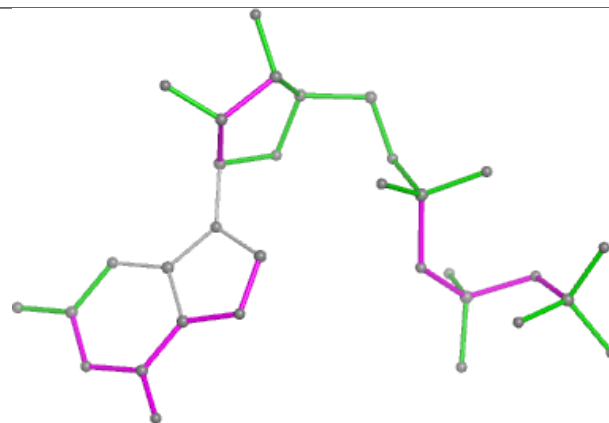




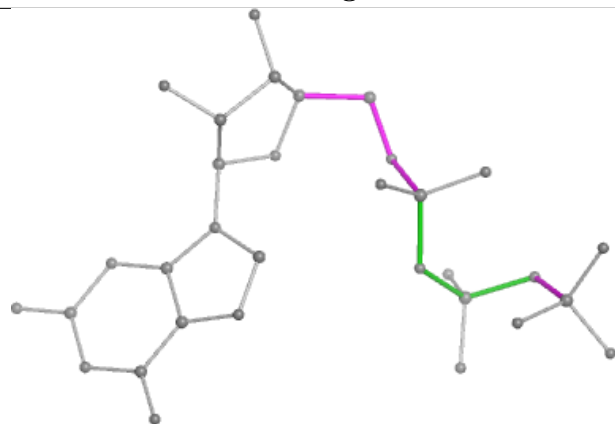
## Ligand GTP SG 501



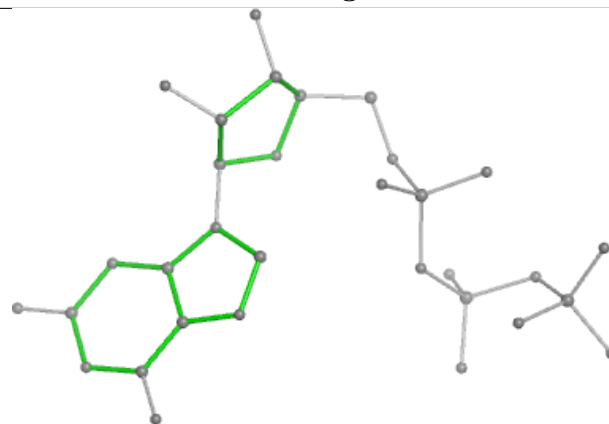
Bond lengths



Bond angles

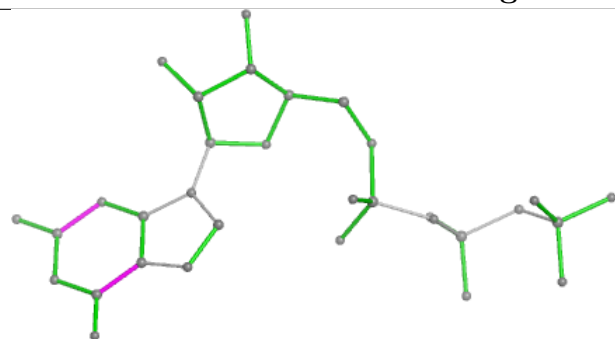


Torsions

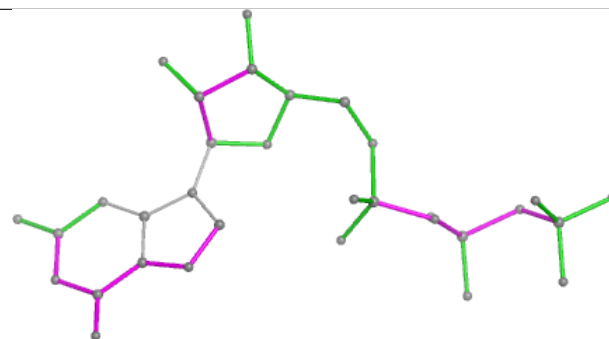


Rings

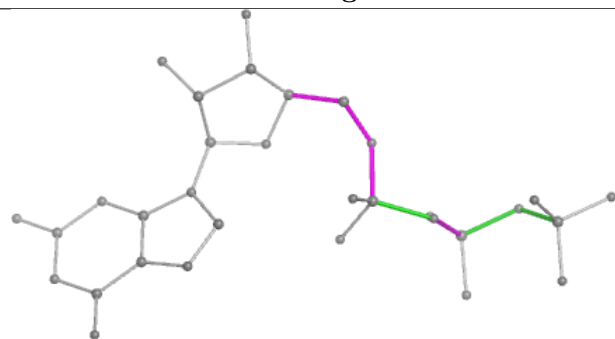
## Ligand GTP LM 502



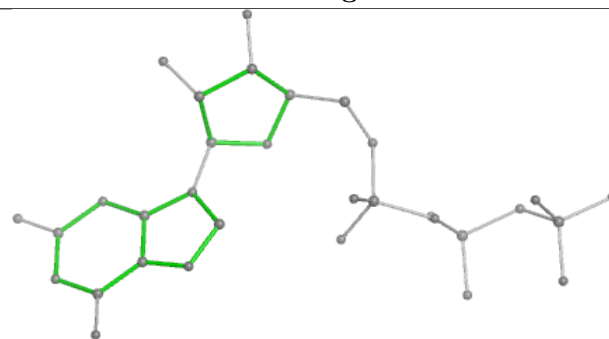
Bond lengths



Bond angles



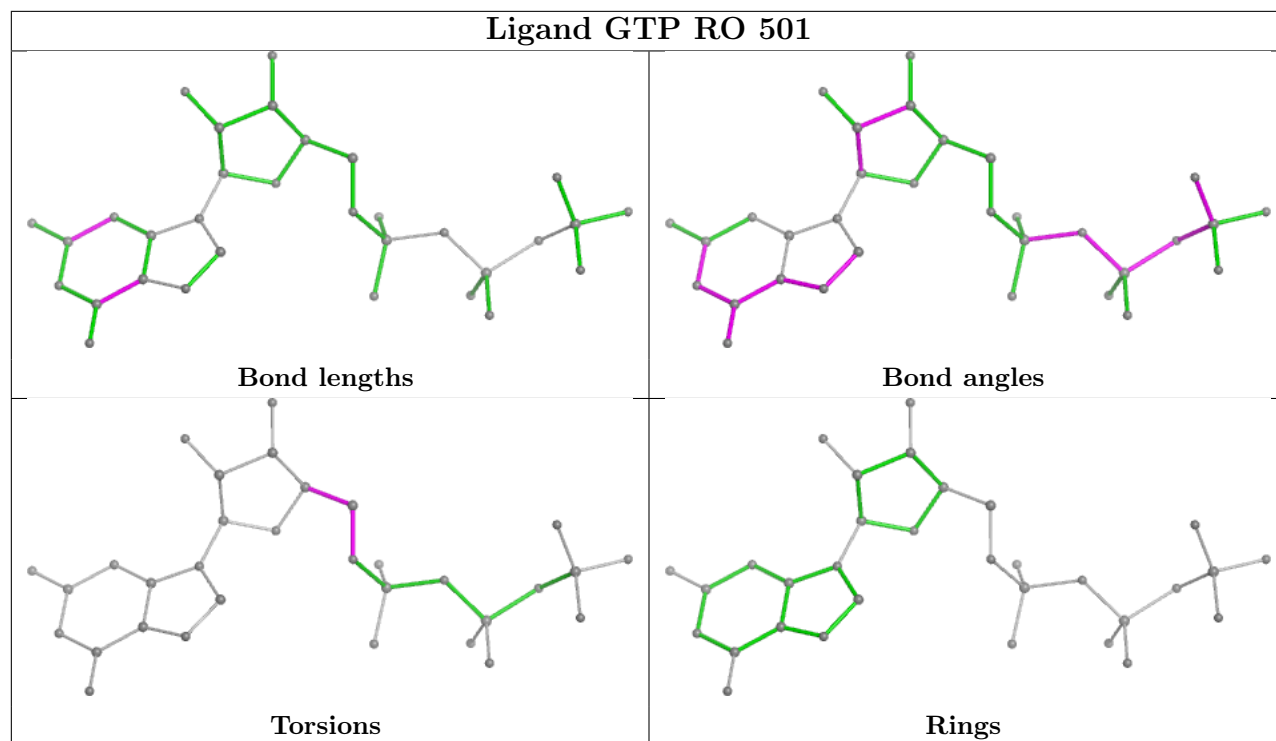
Torsions



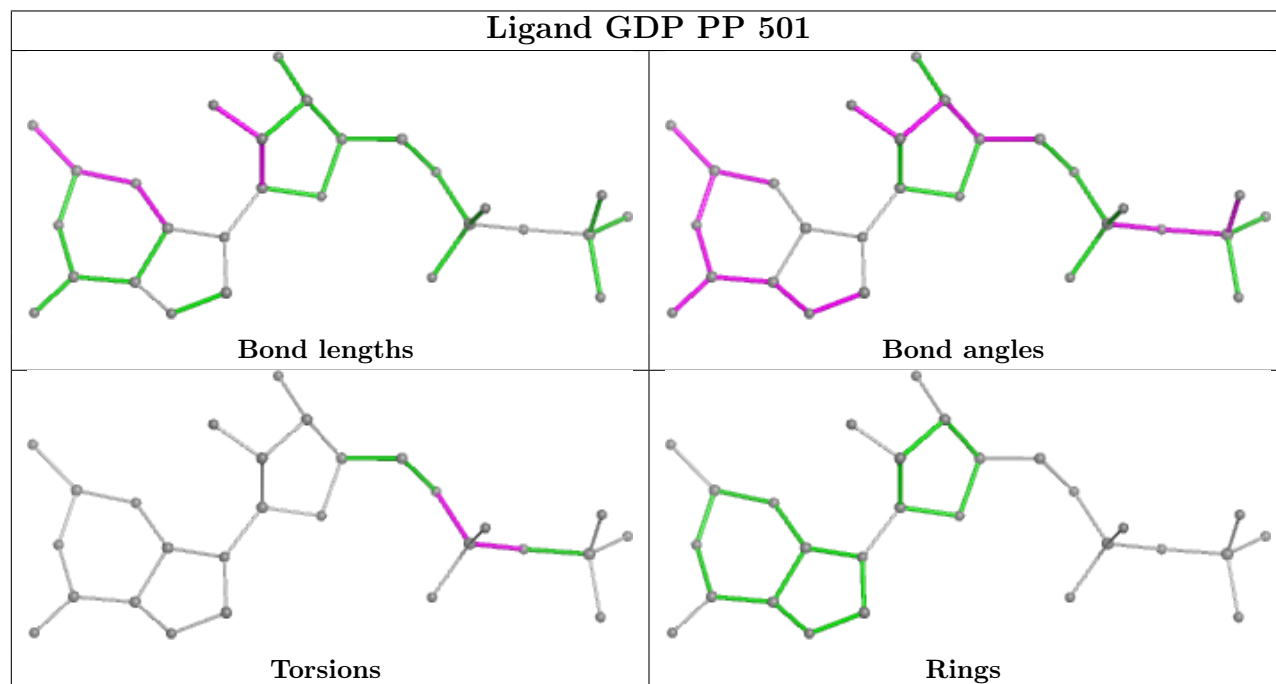
Rings

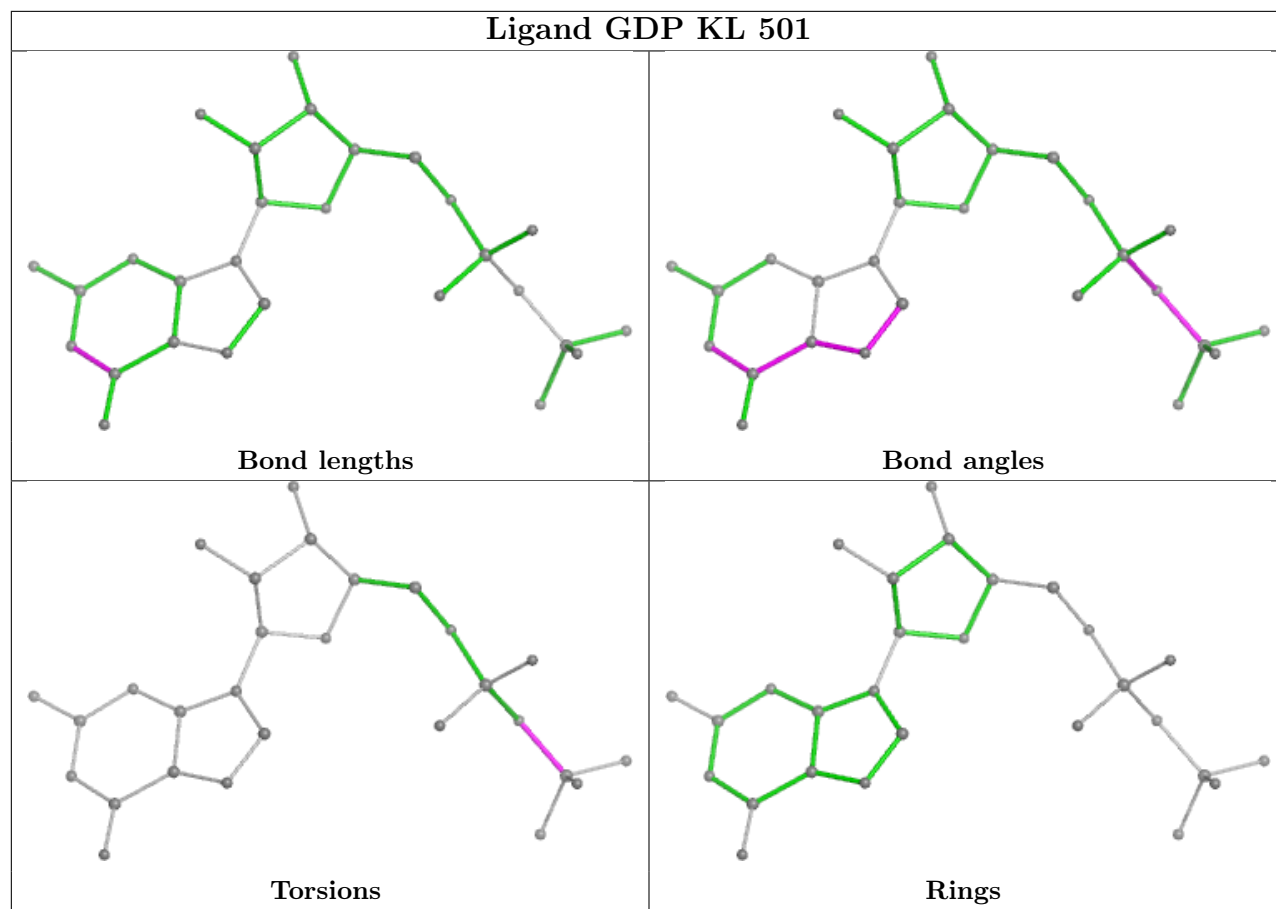


## Ligand GTP RO 501

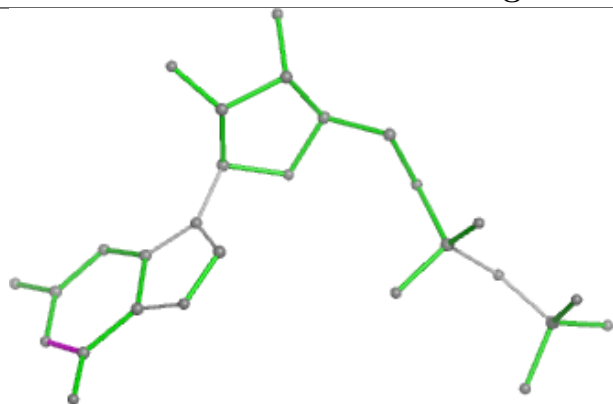


## Ligand GDP PP 501

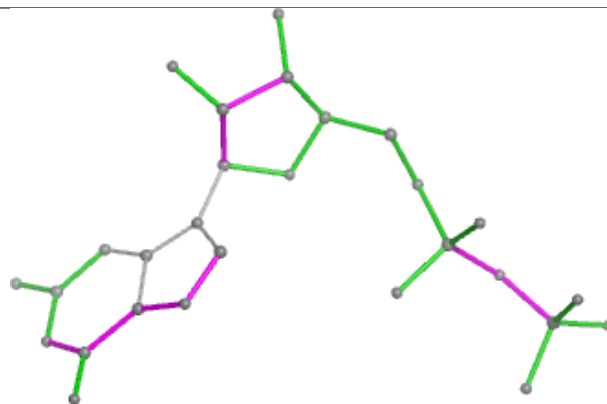




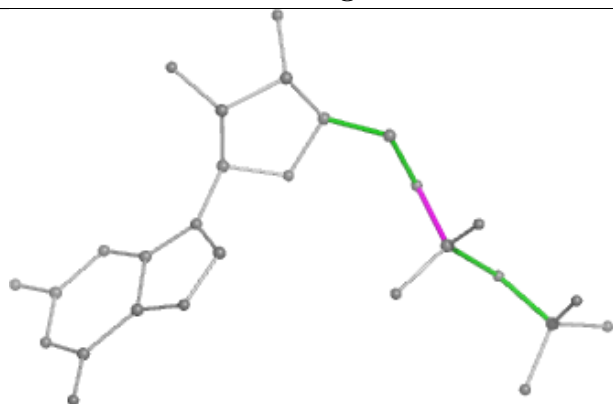
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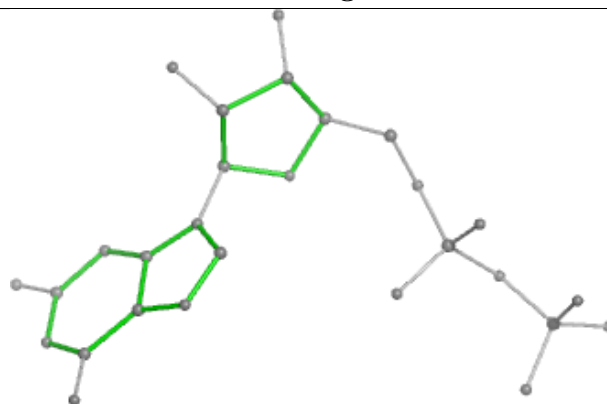
Bond lengths



Bond angles

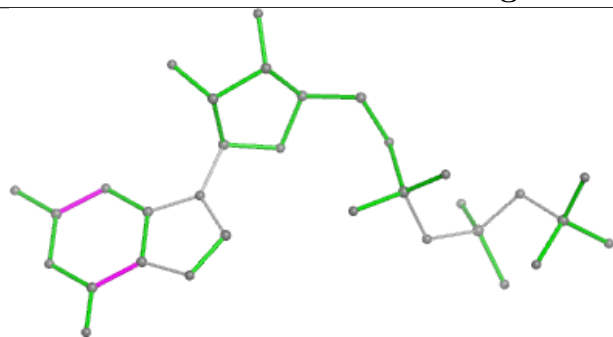


Torsions

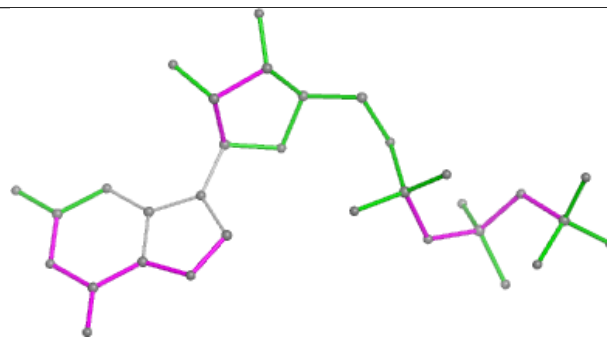


Rings

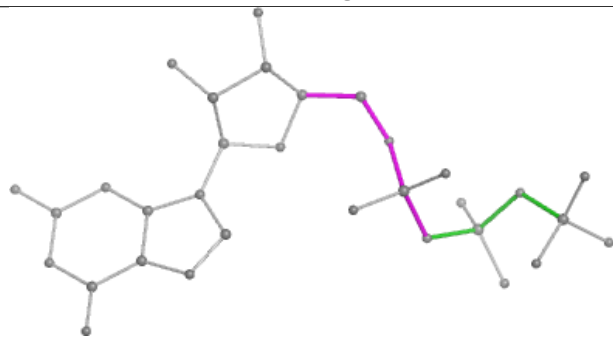
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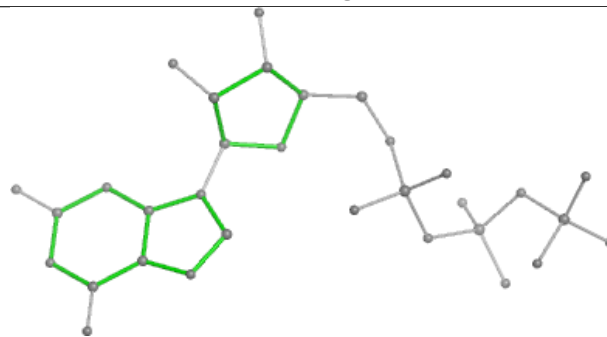
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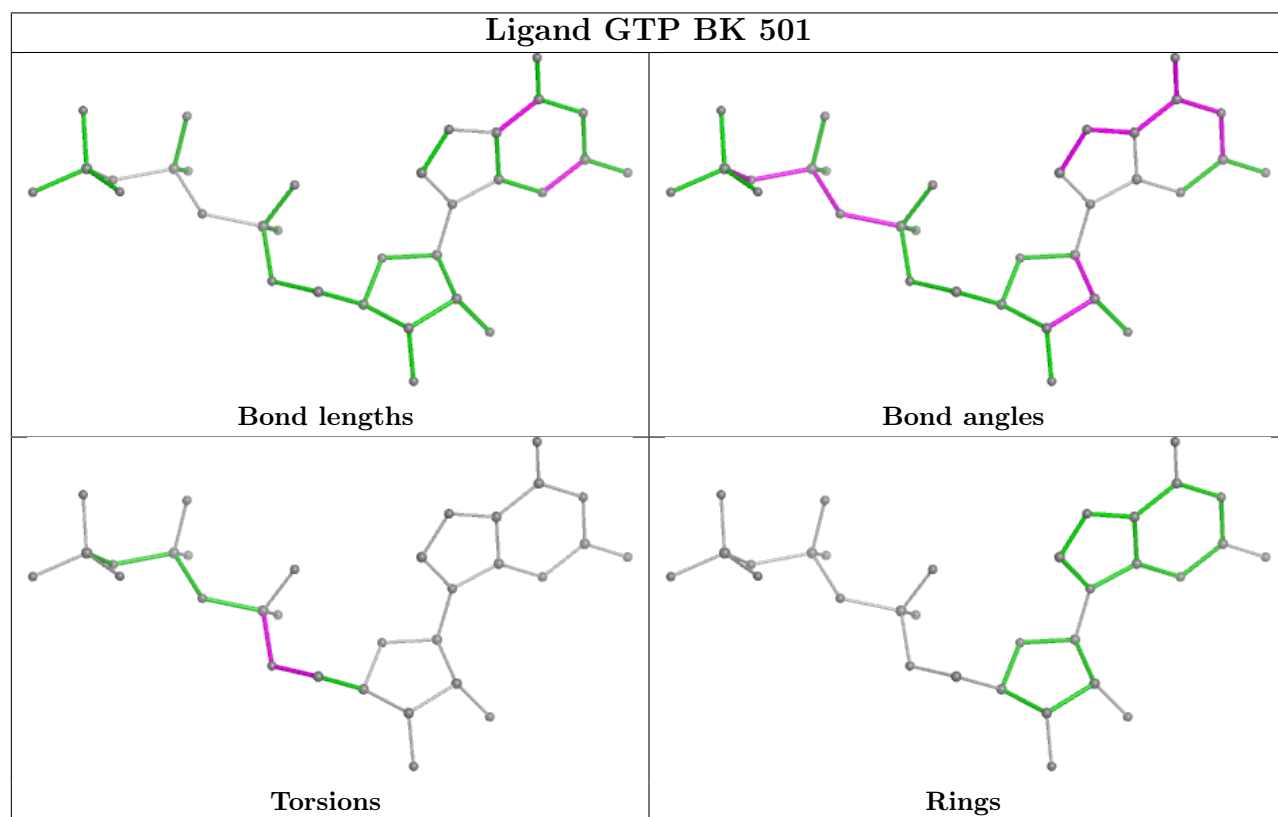
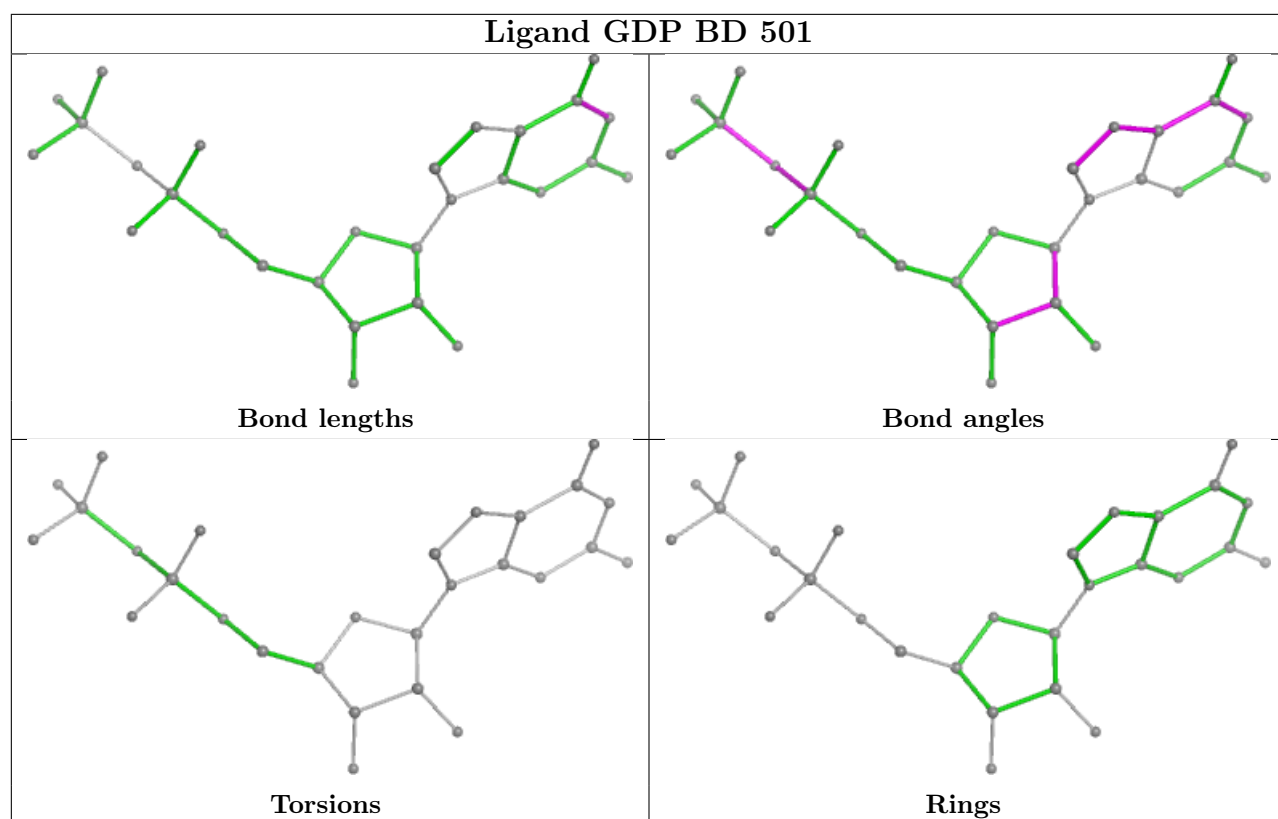
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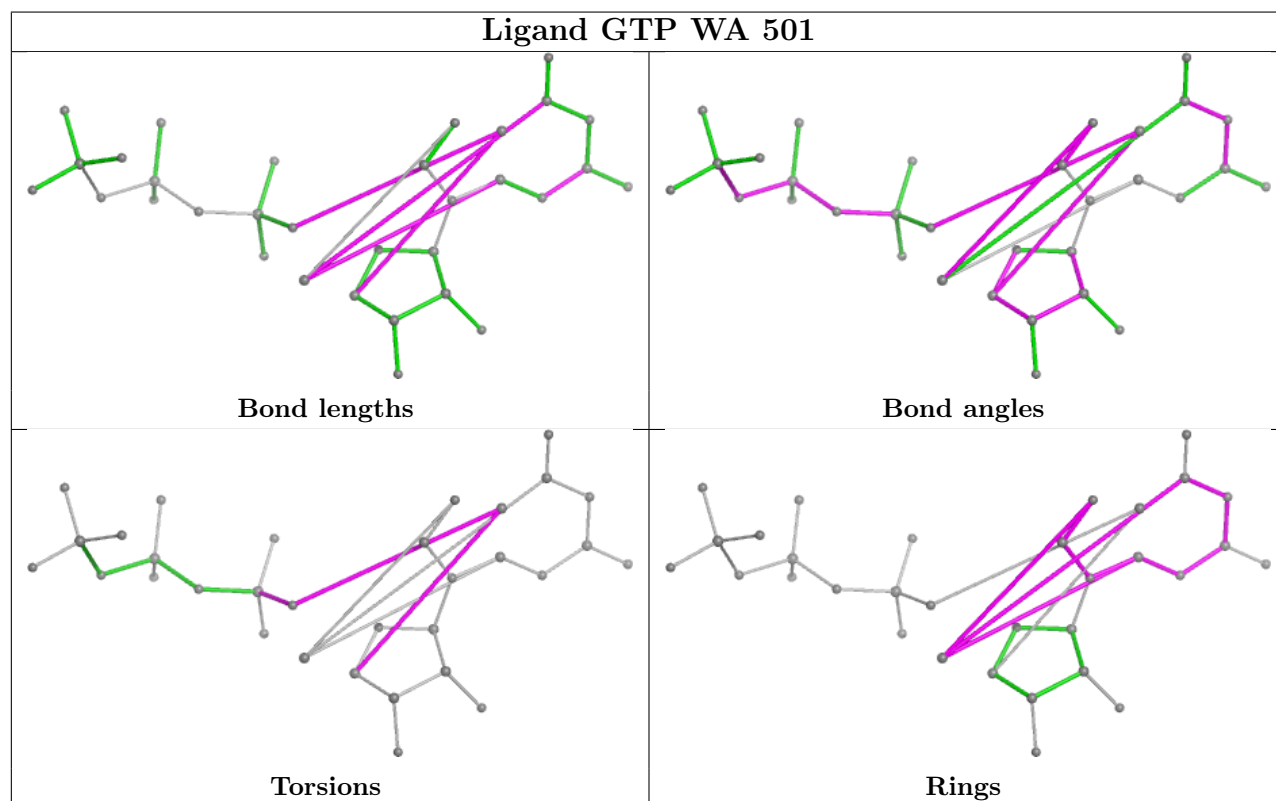
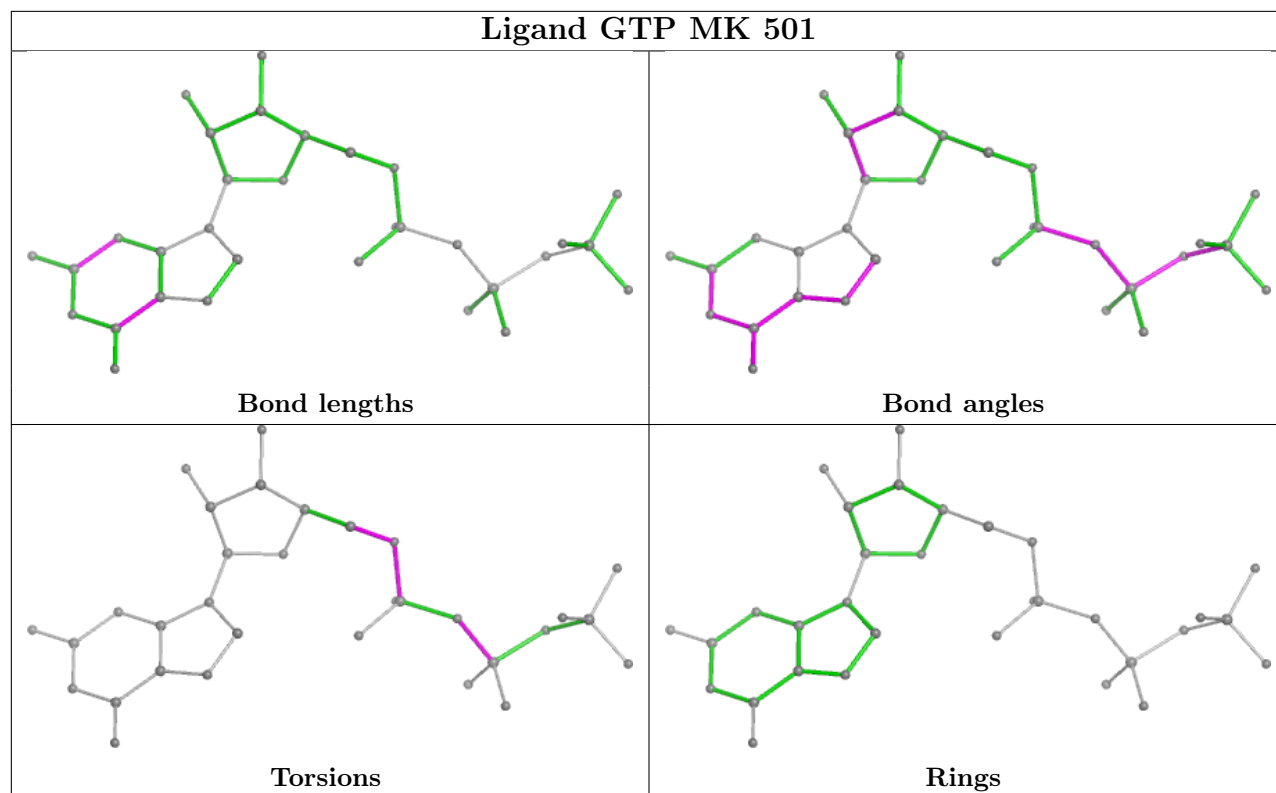


Torsions

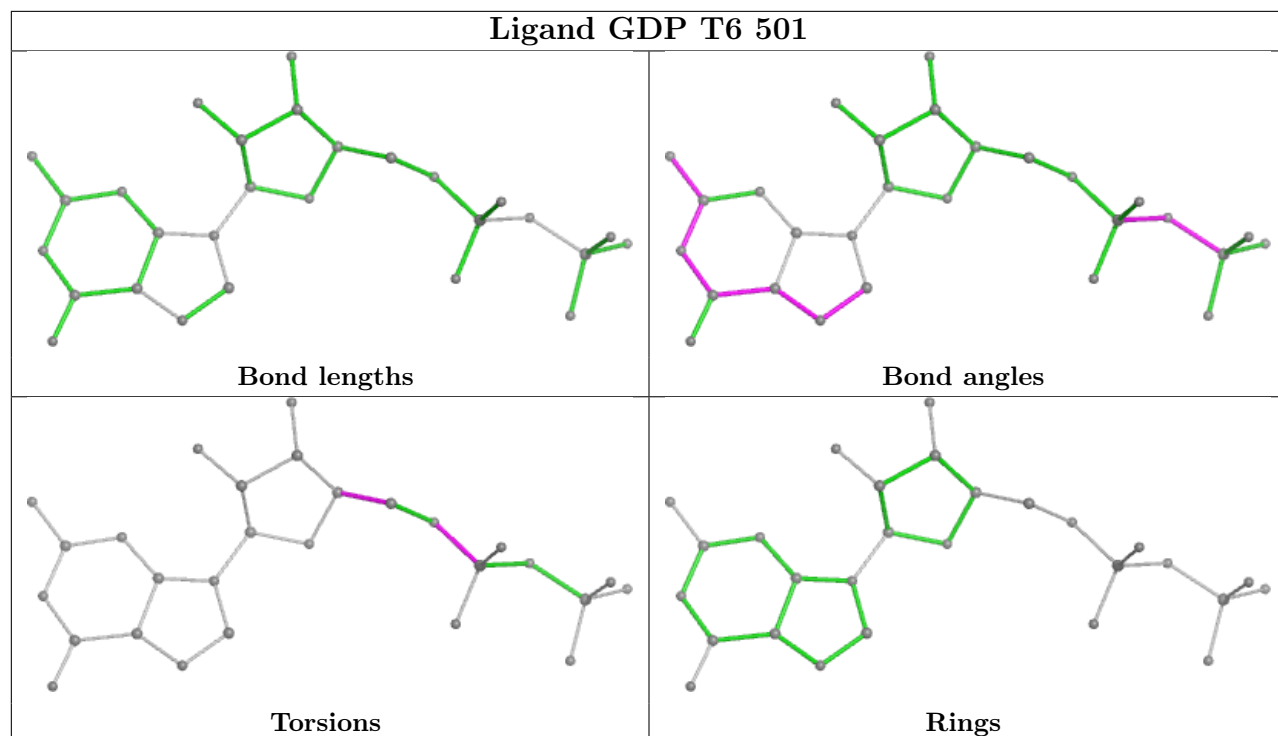


Rings

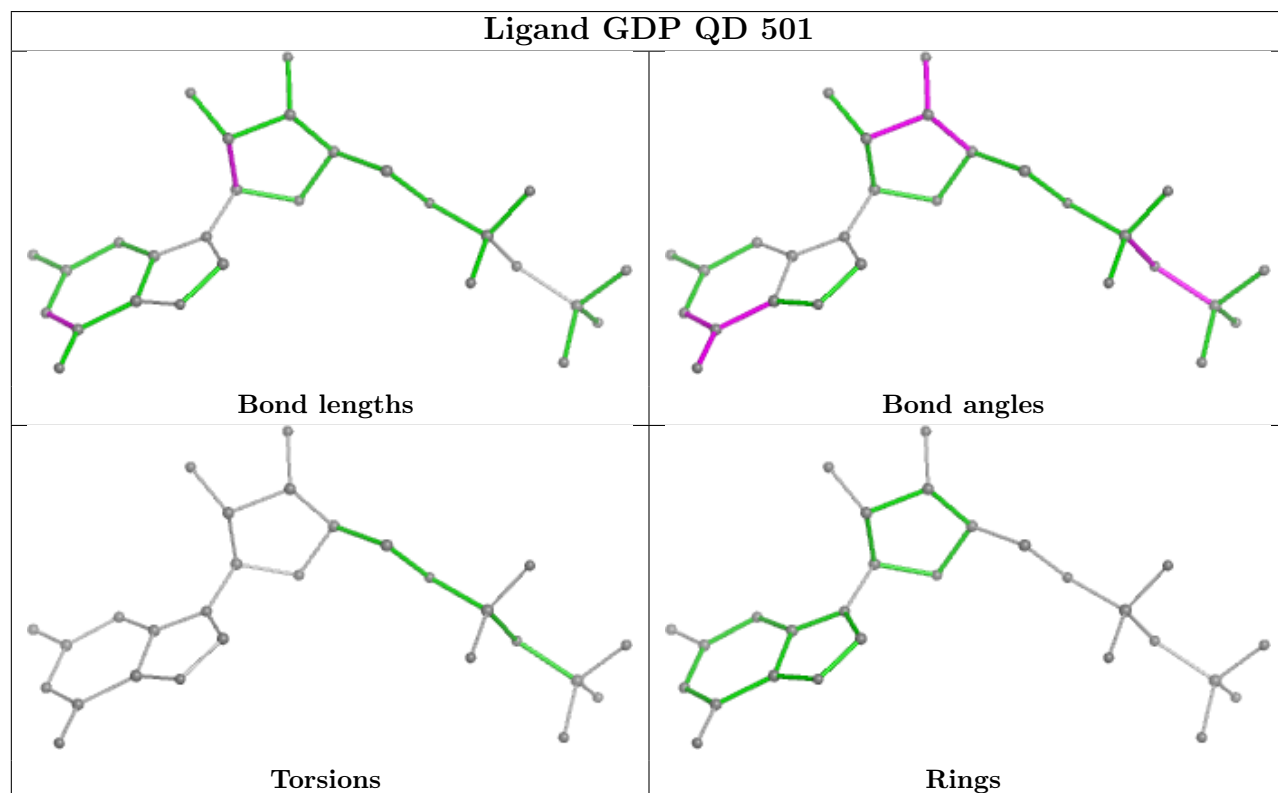


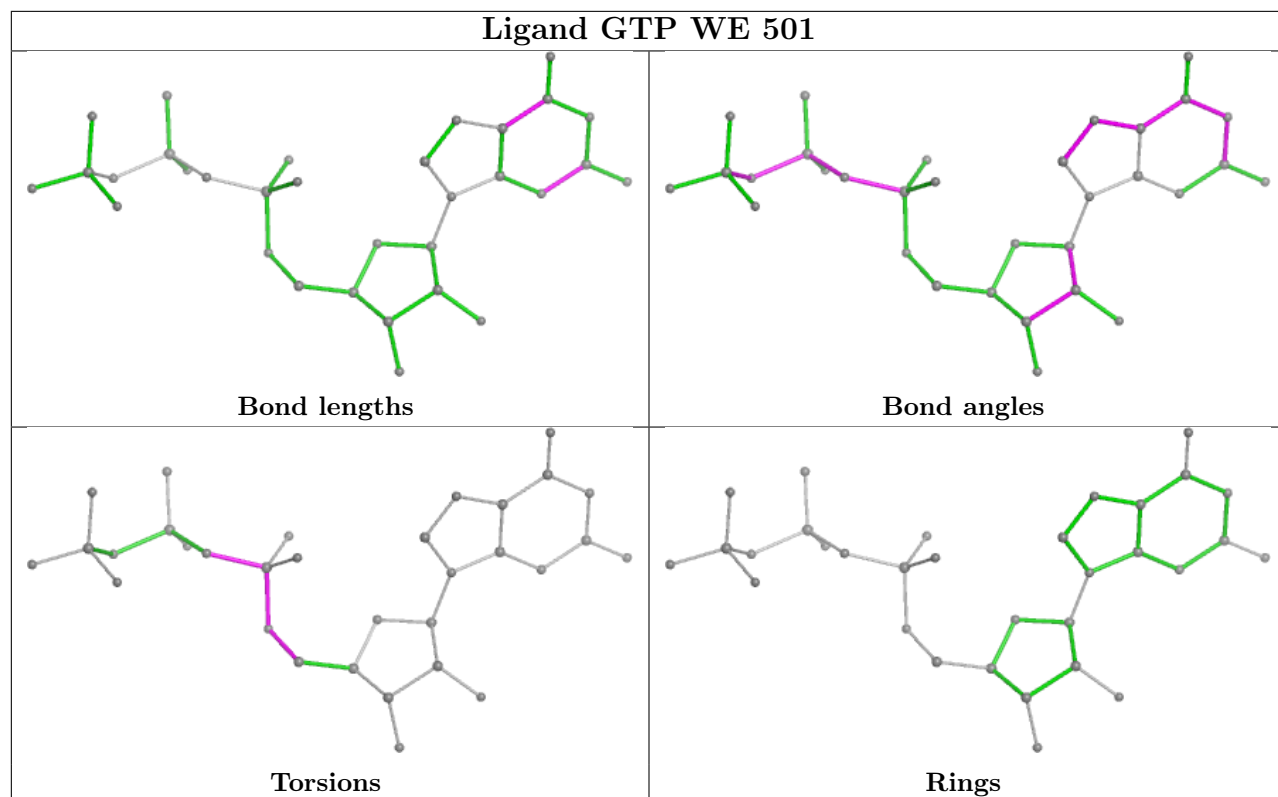


## Ligand GDP T6 501

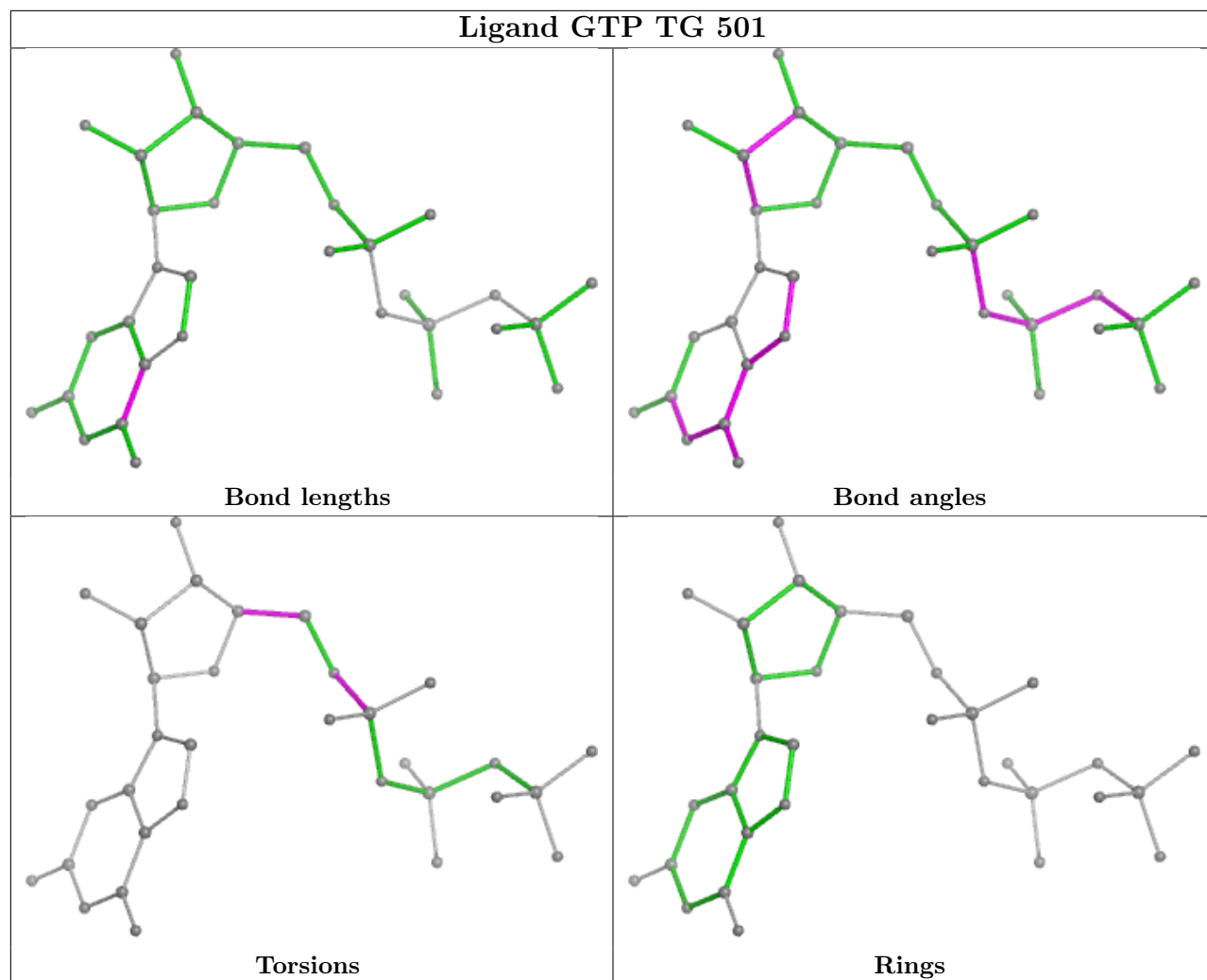


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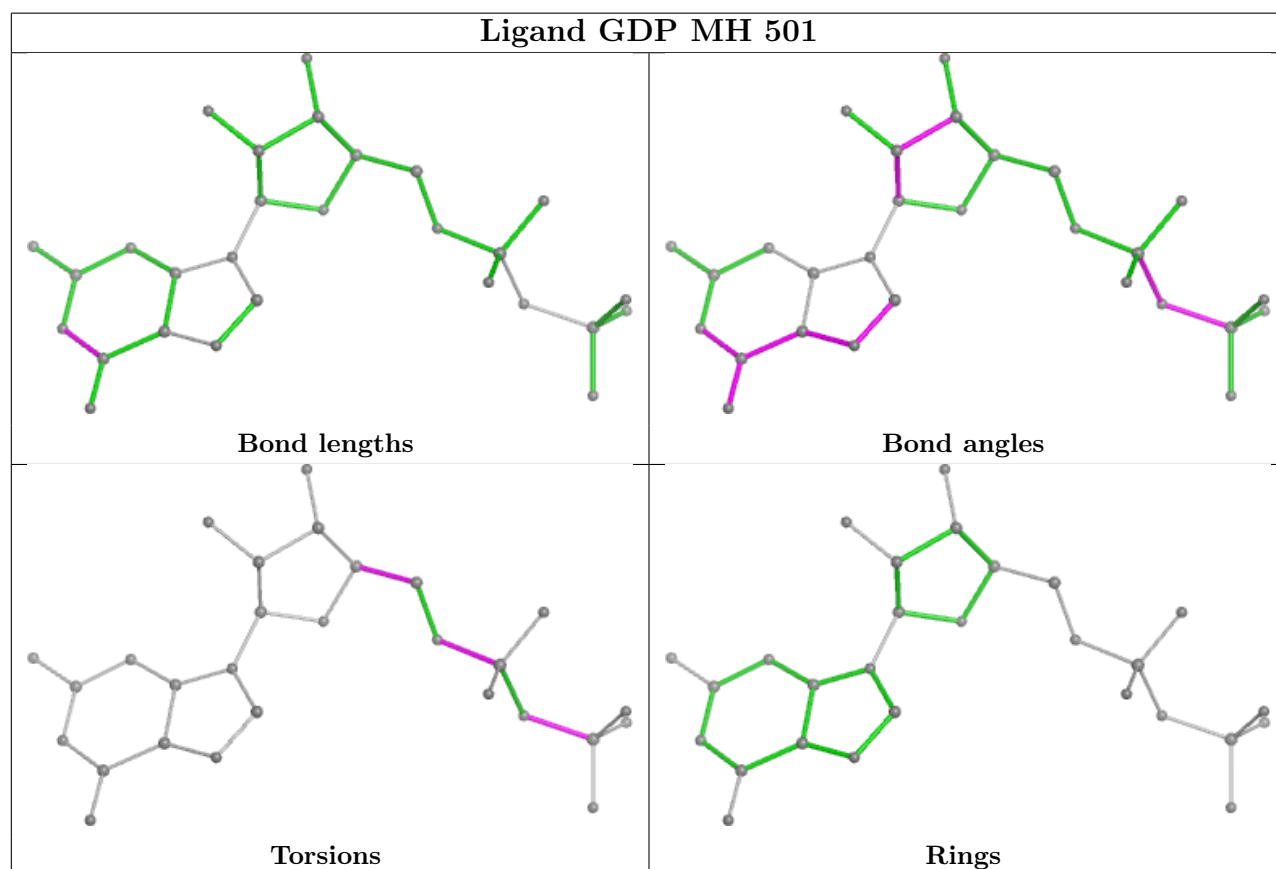
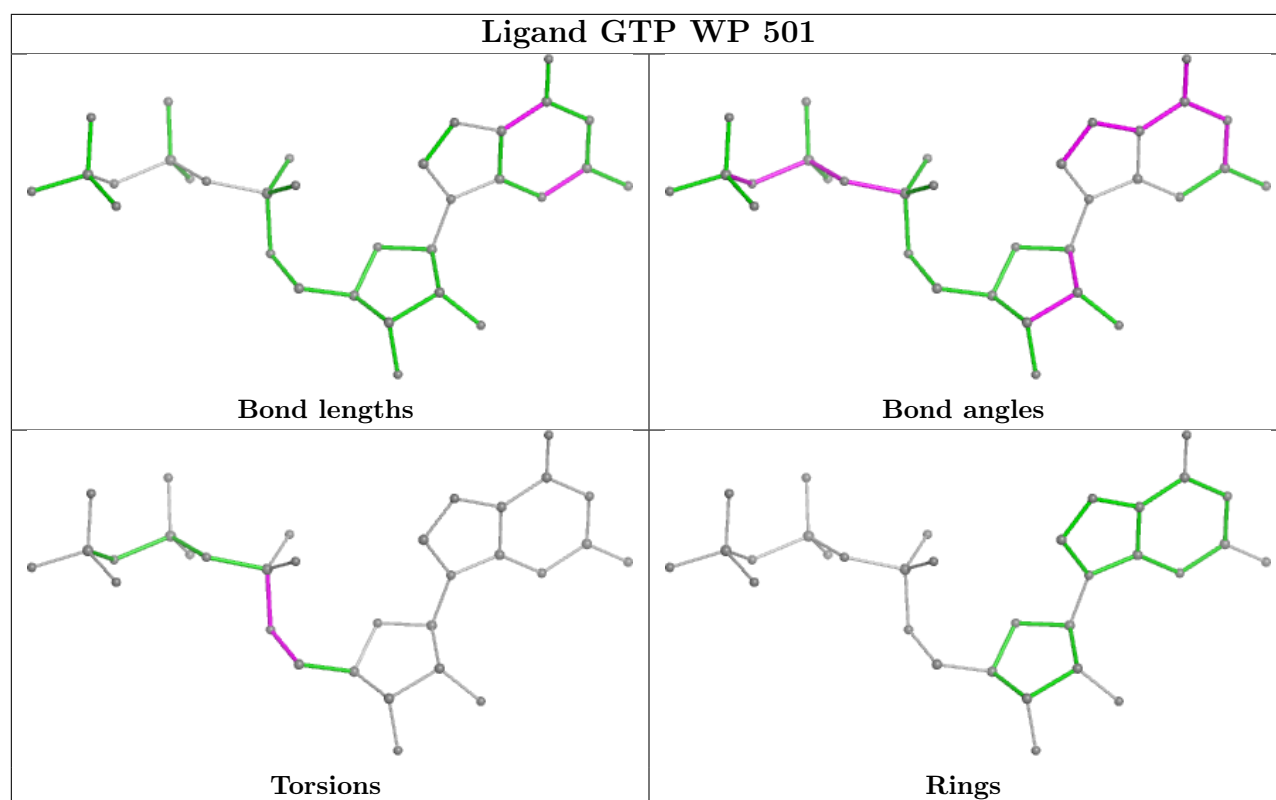


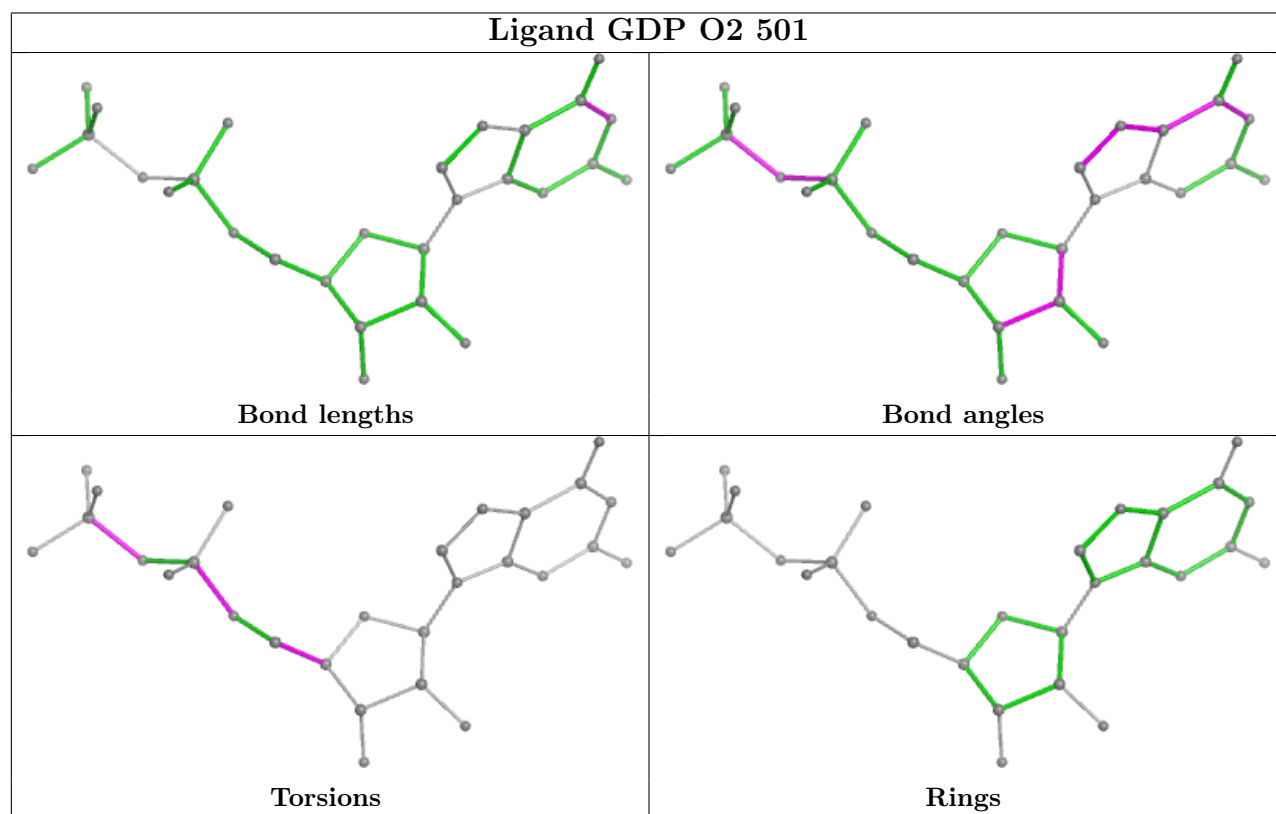
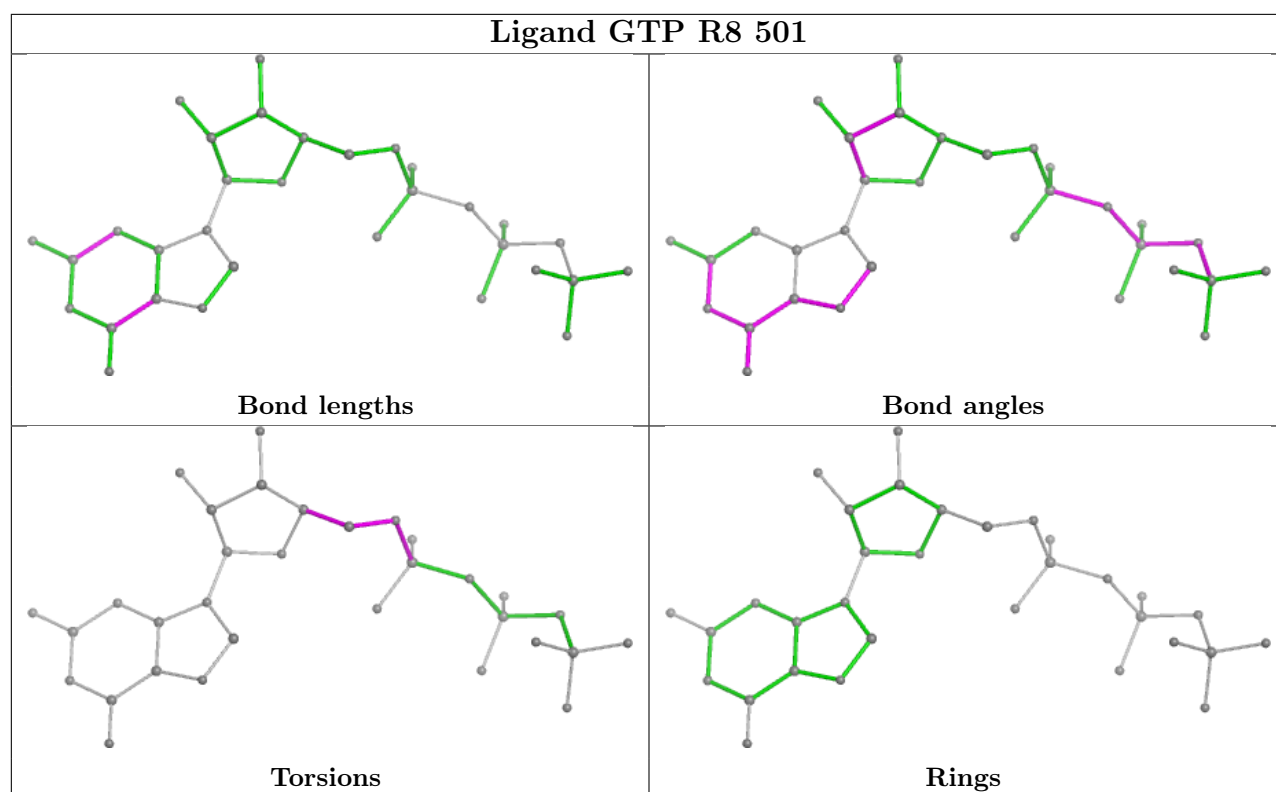


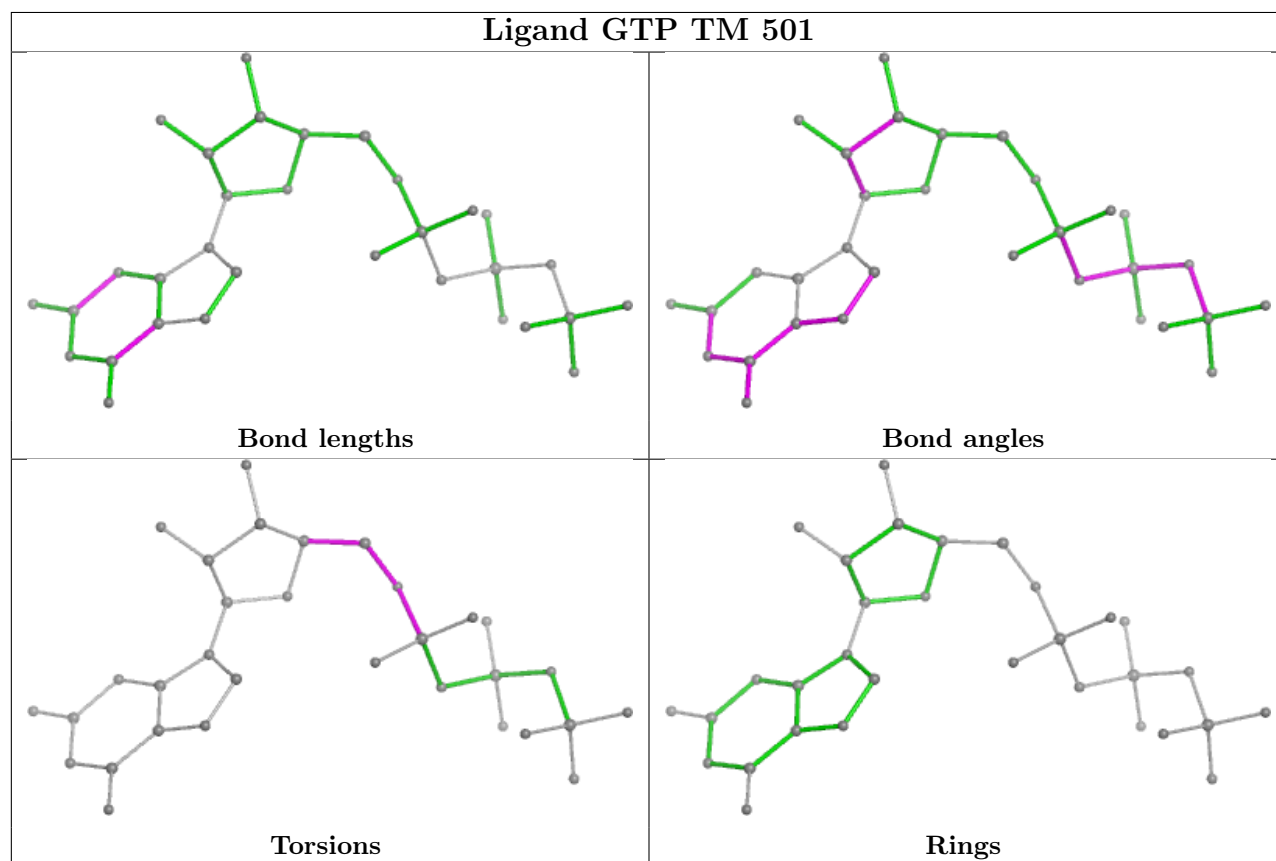
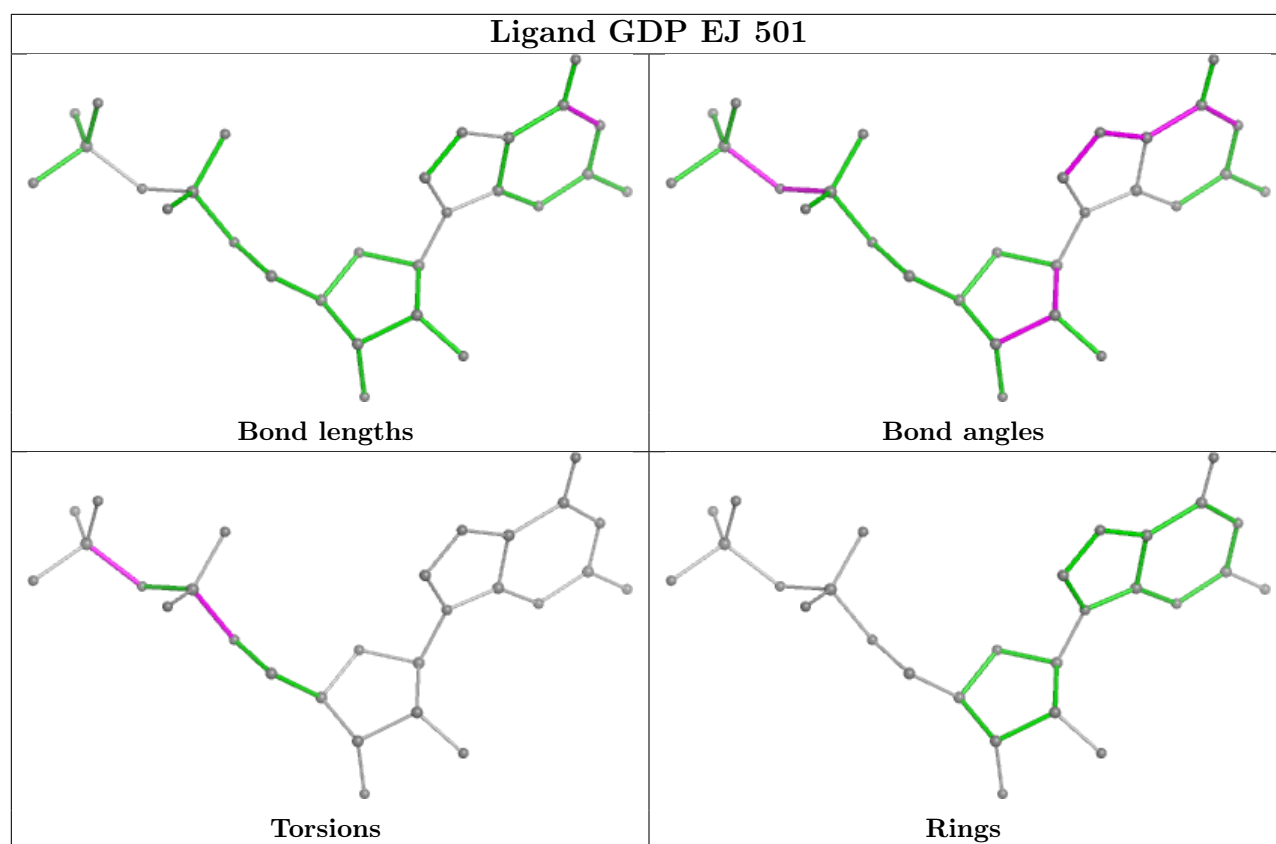
## Ligand GTP TG 501



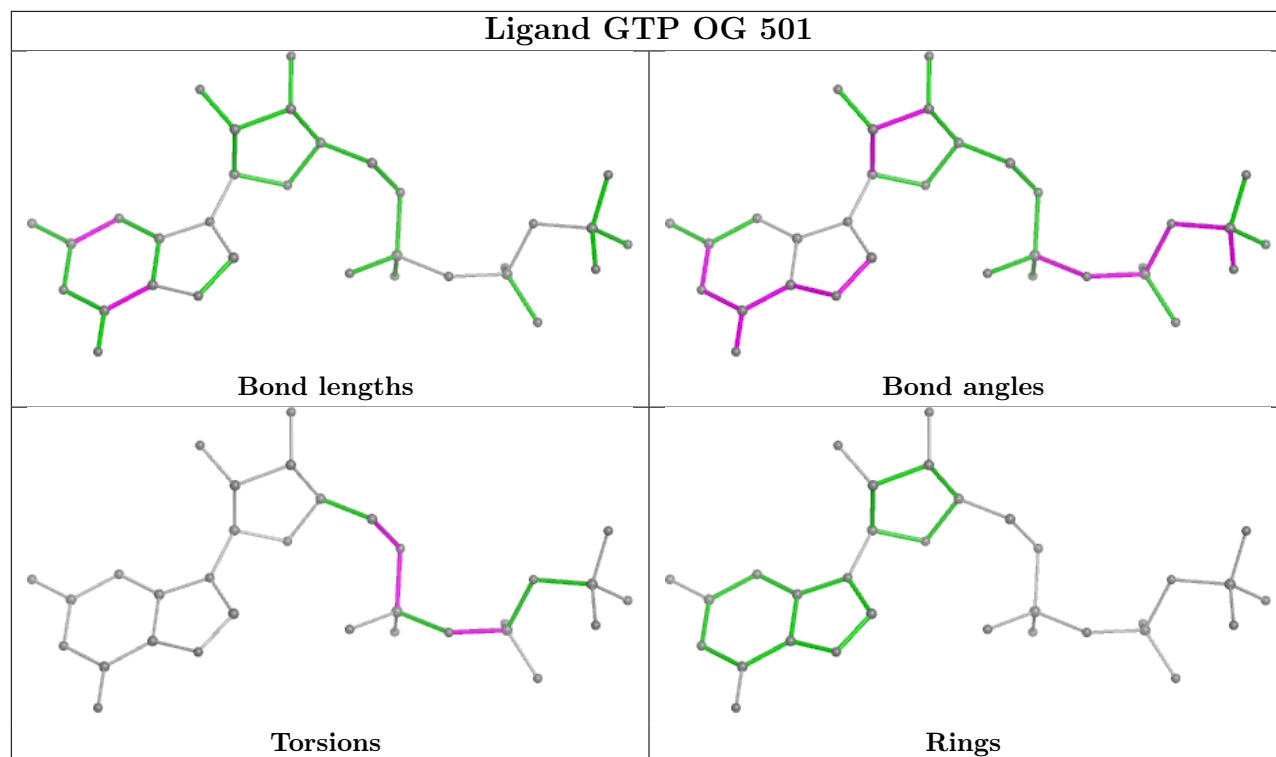




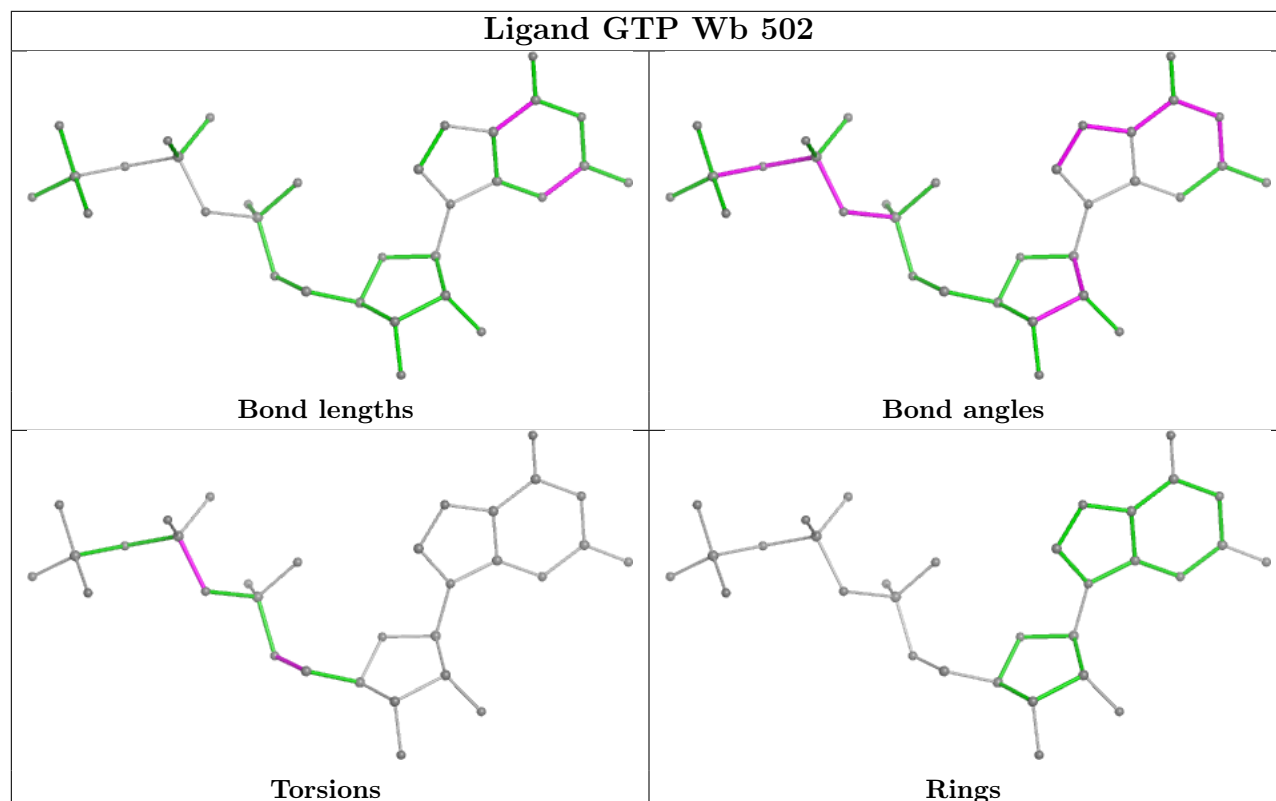


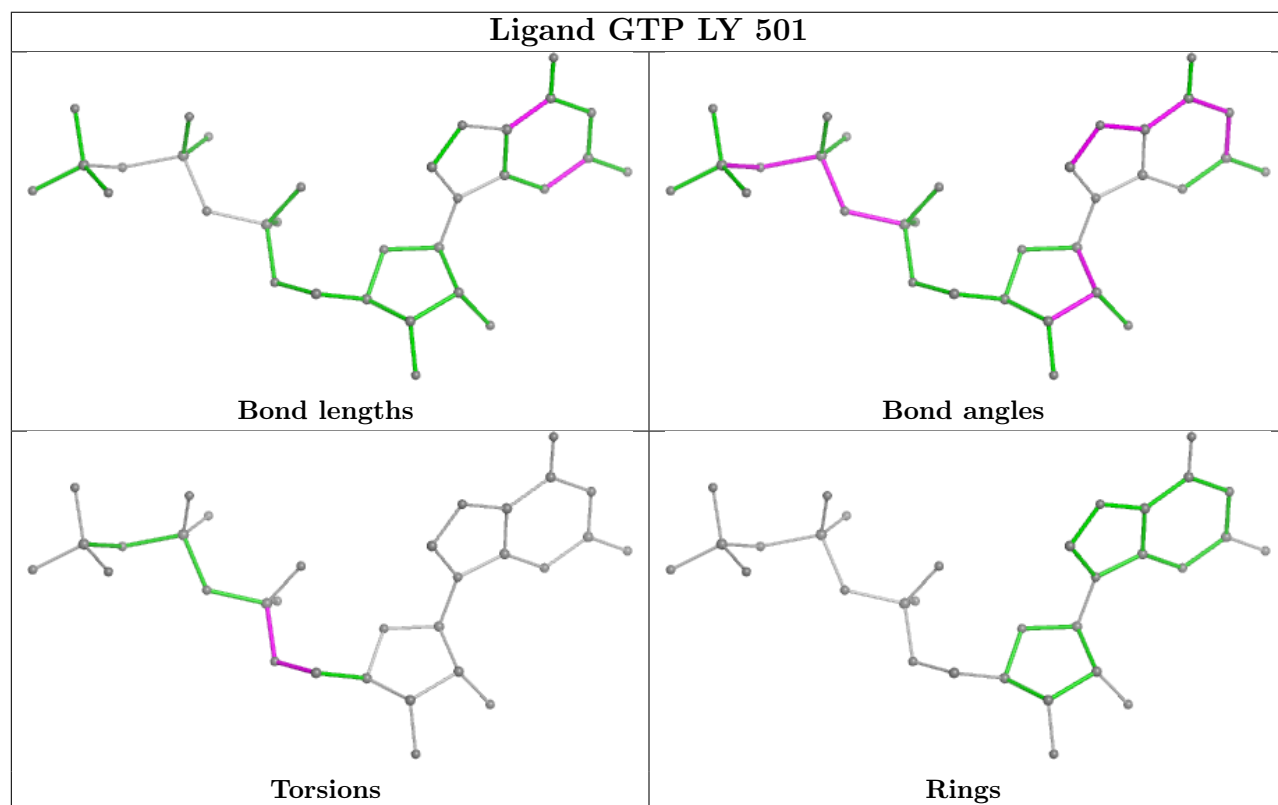
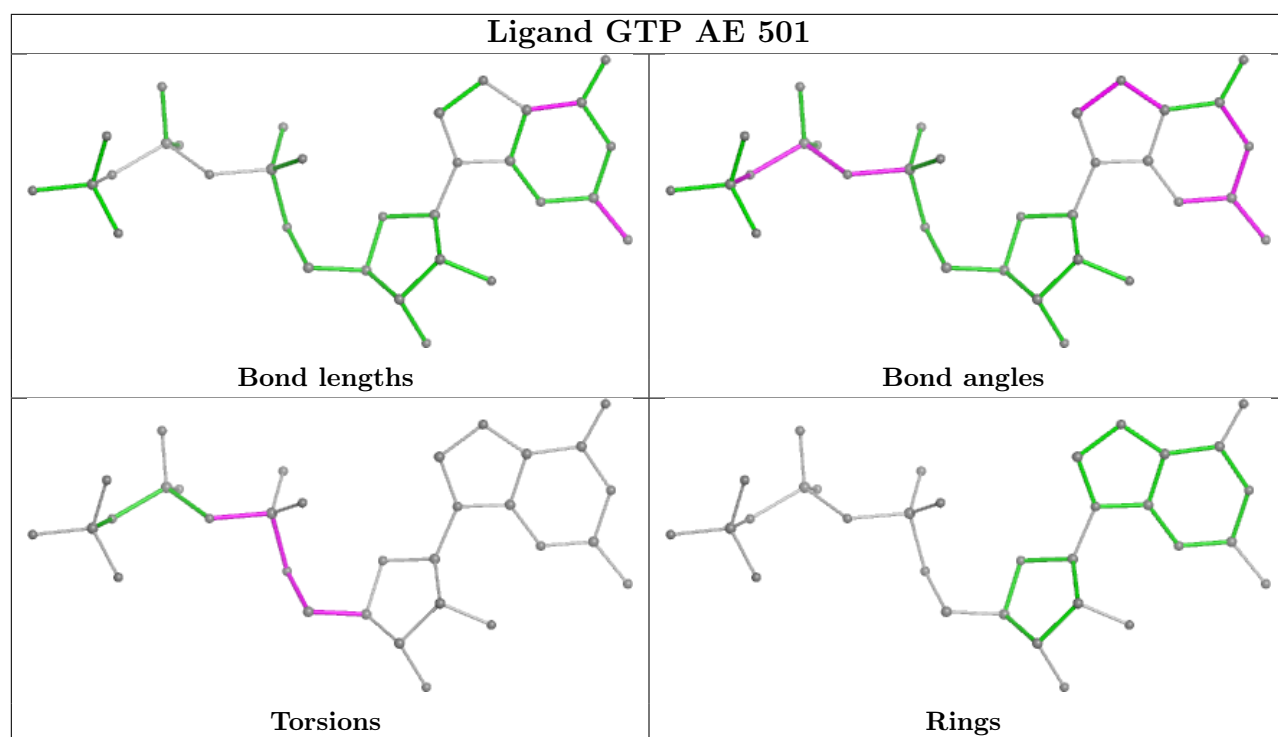


## Ligand GTP OG 501

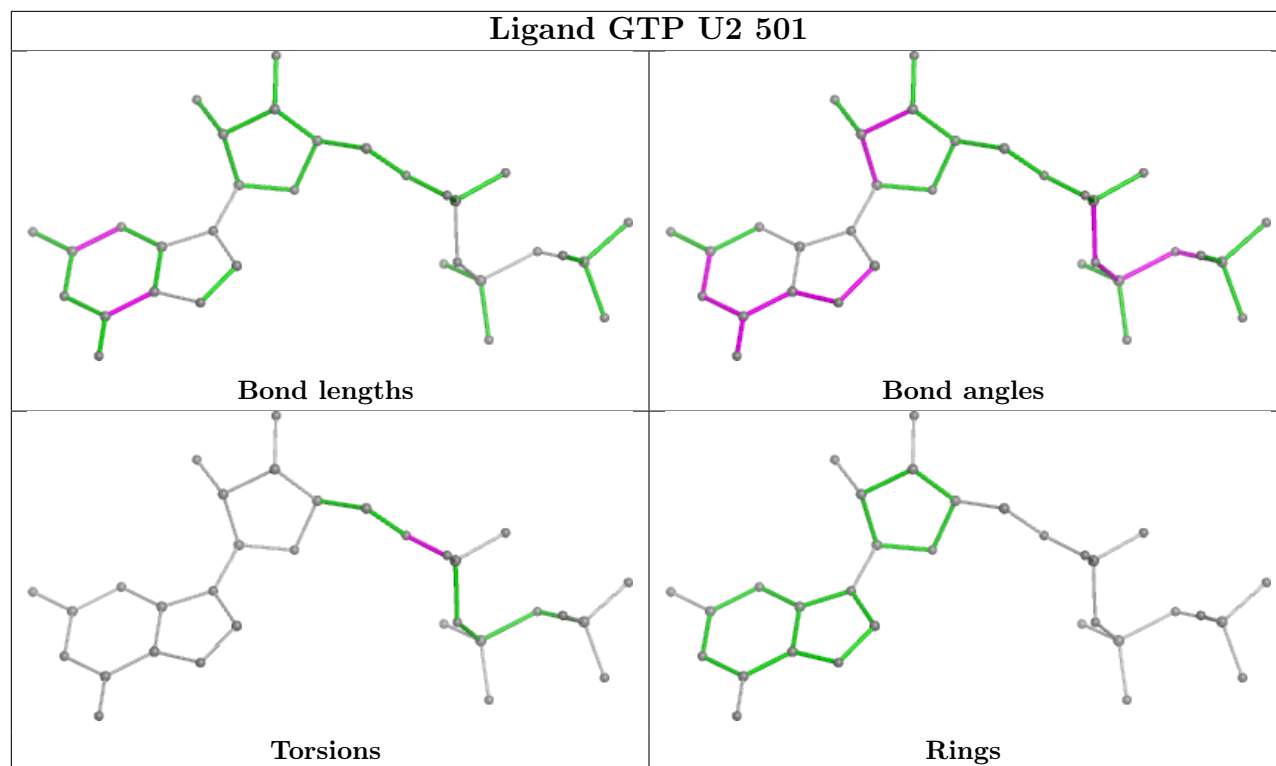


## Ligand GTP Wb 502

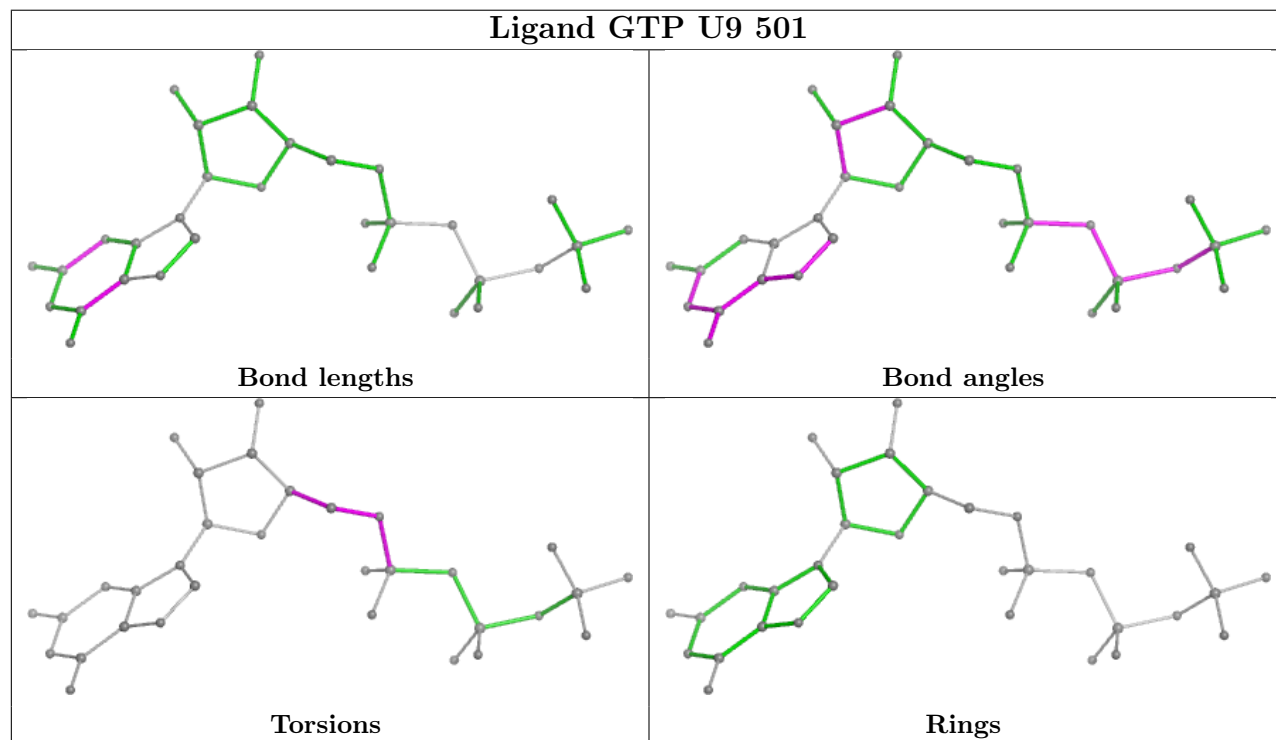


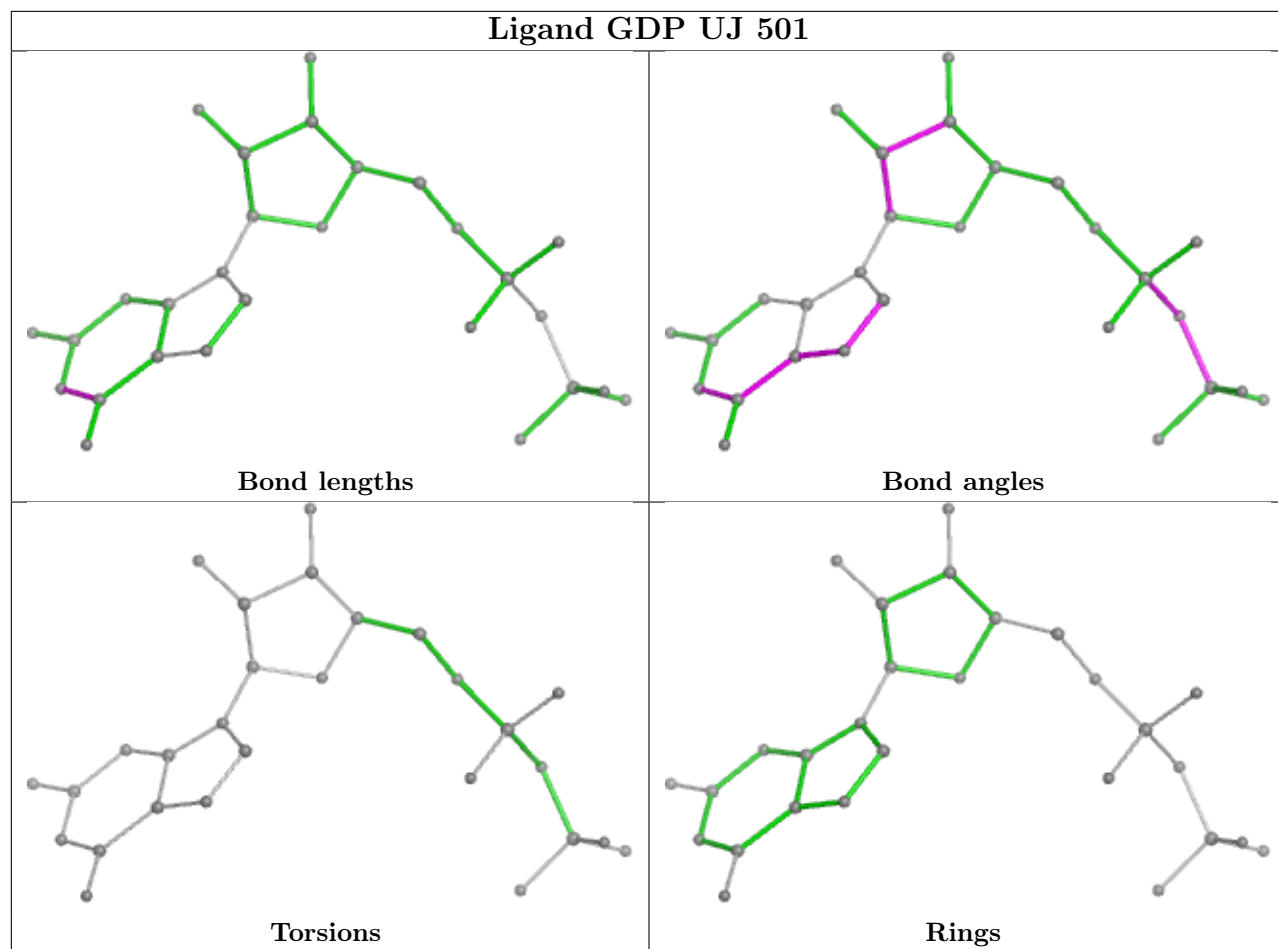


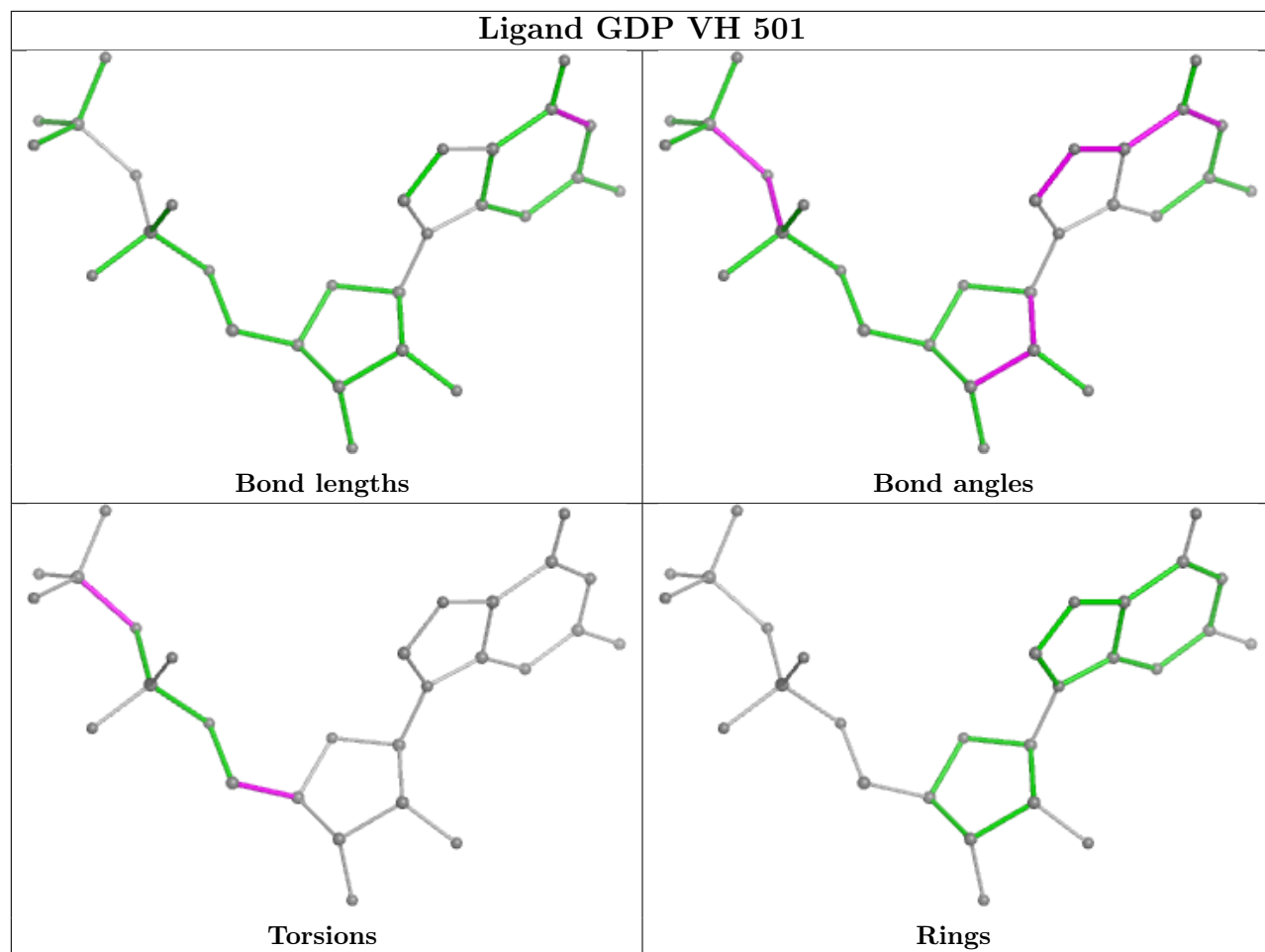
## Ligand GTP U2 501



## Ligand GTP U9 501

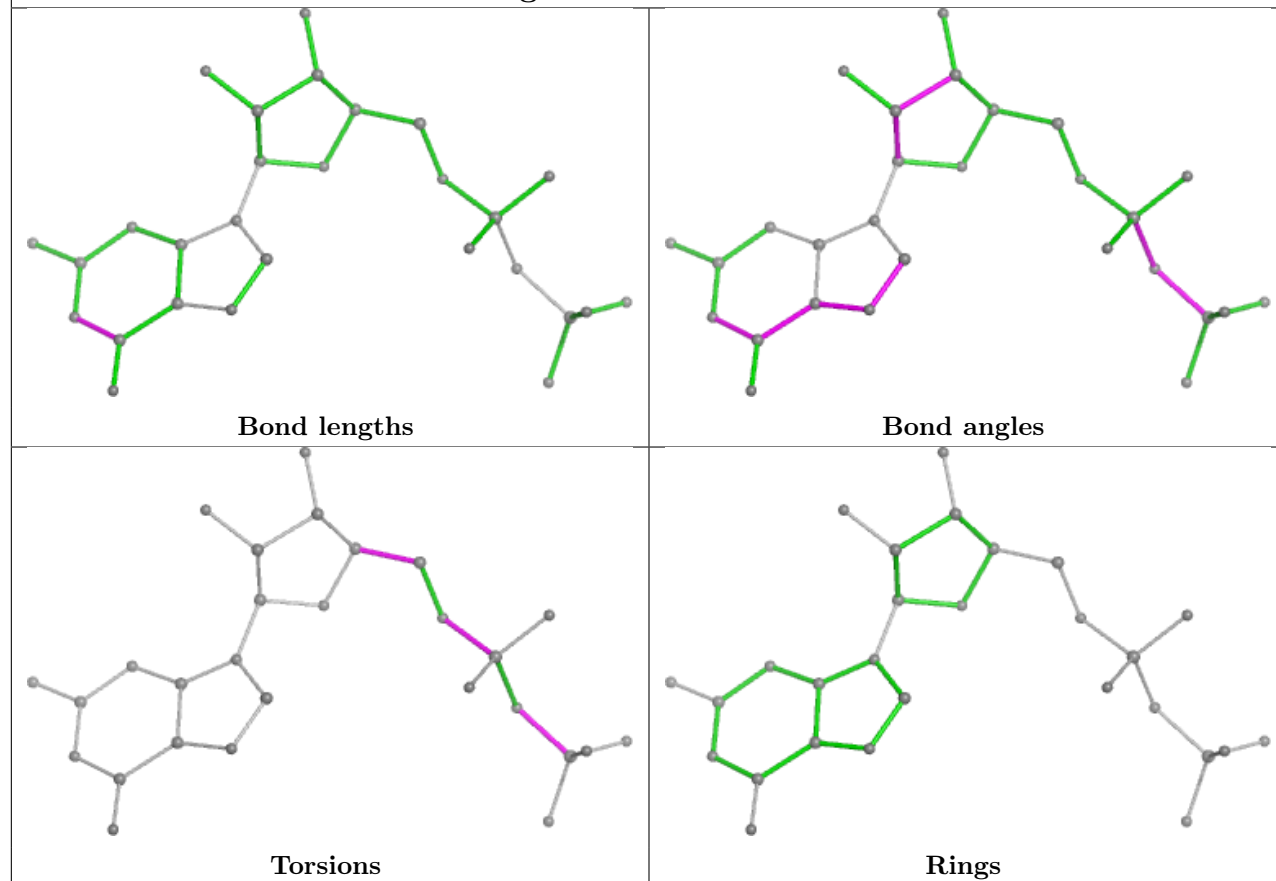




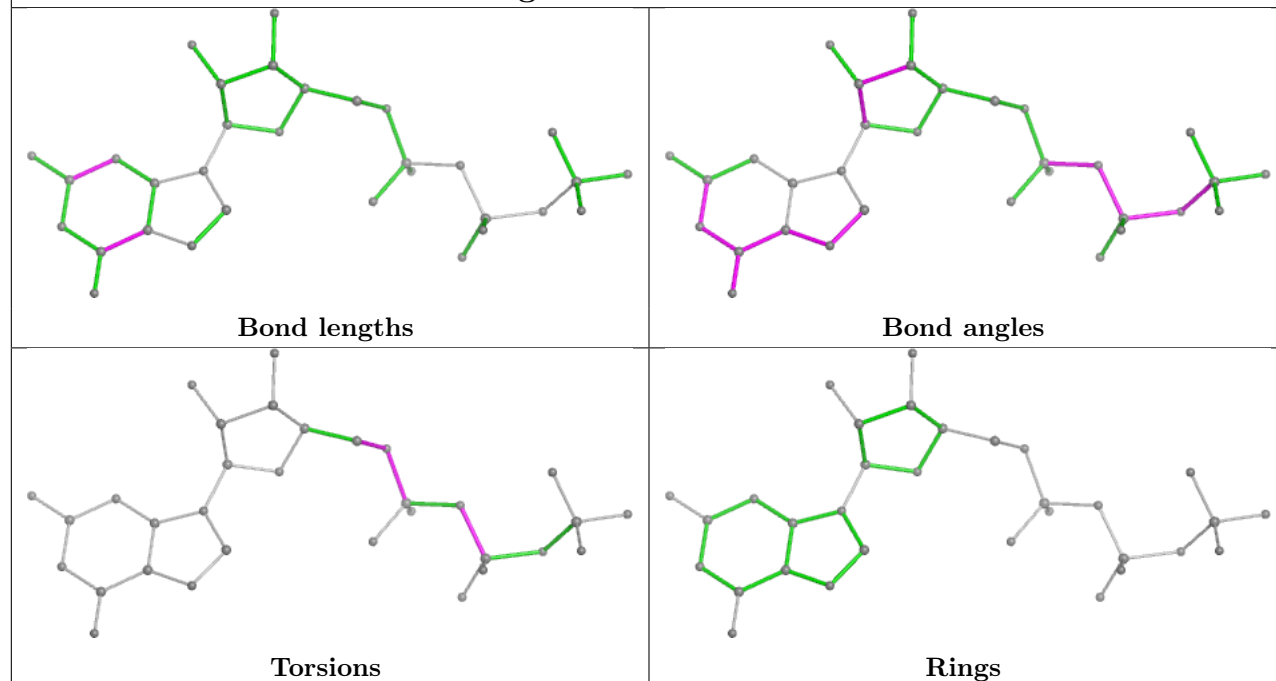


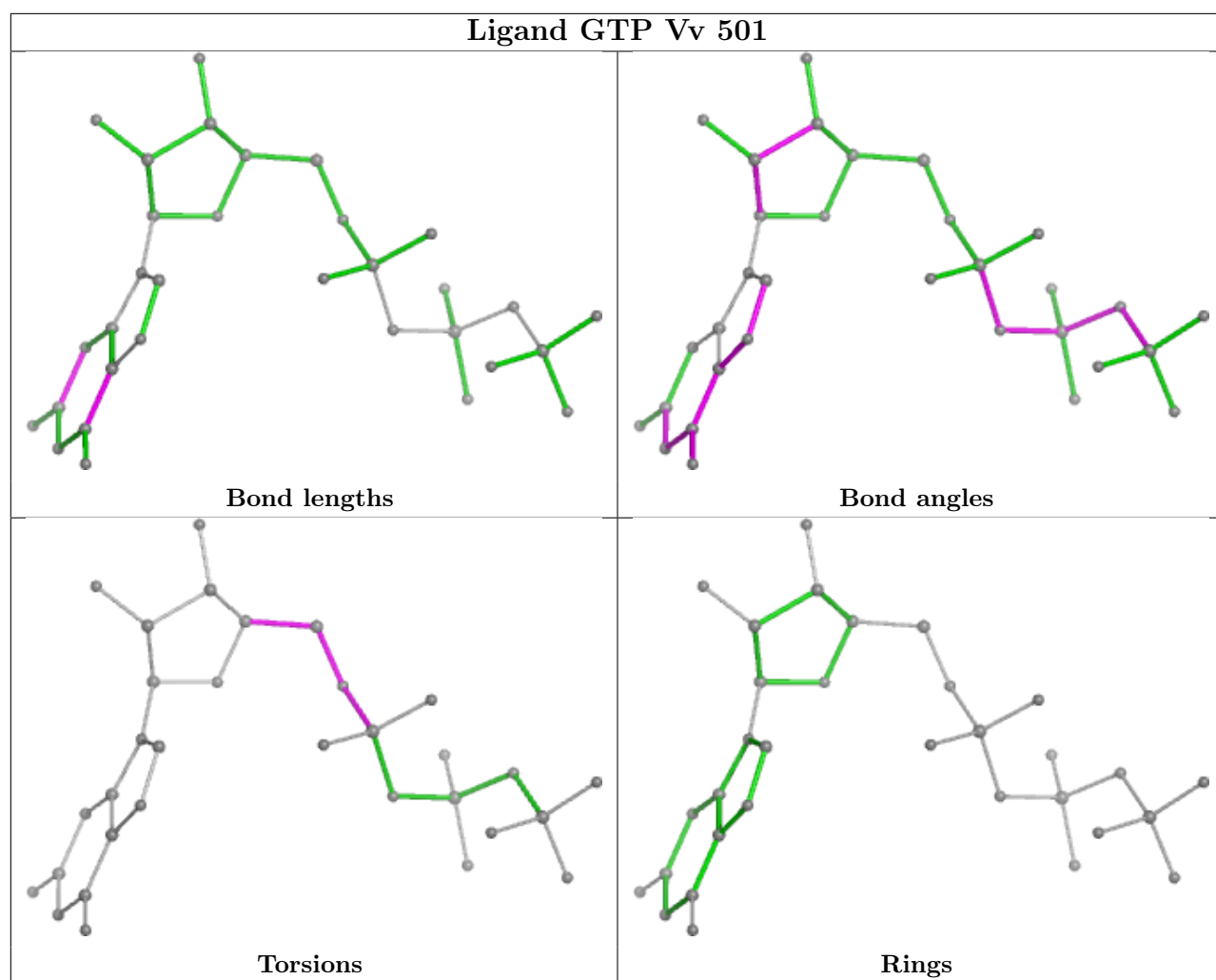


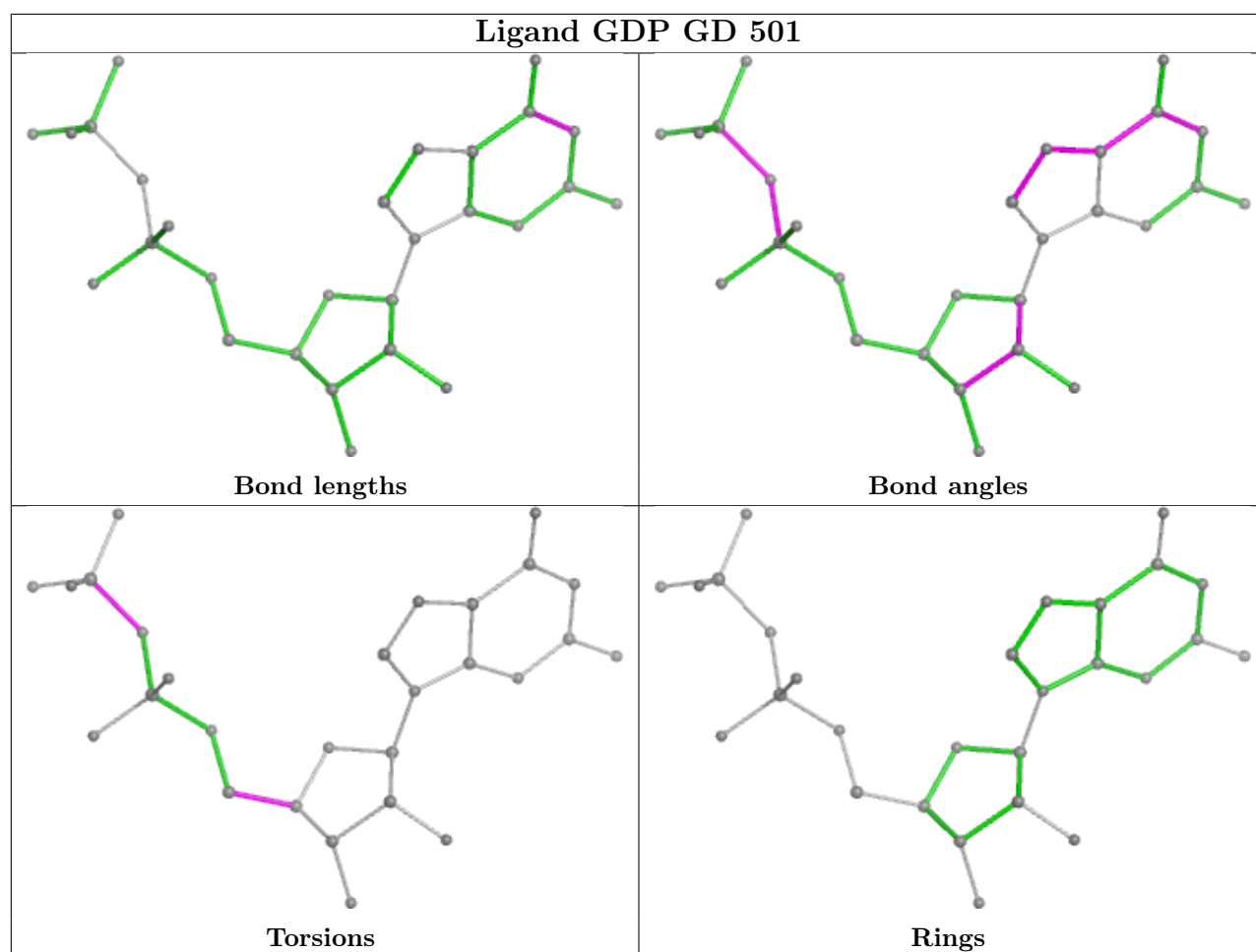
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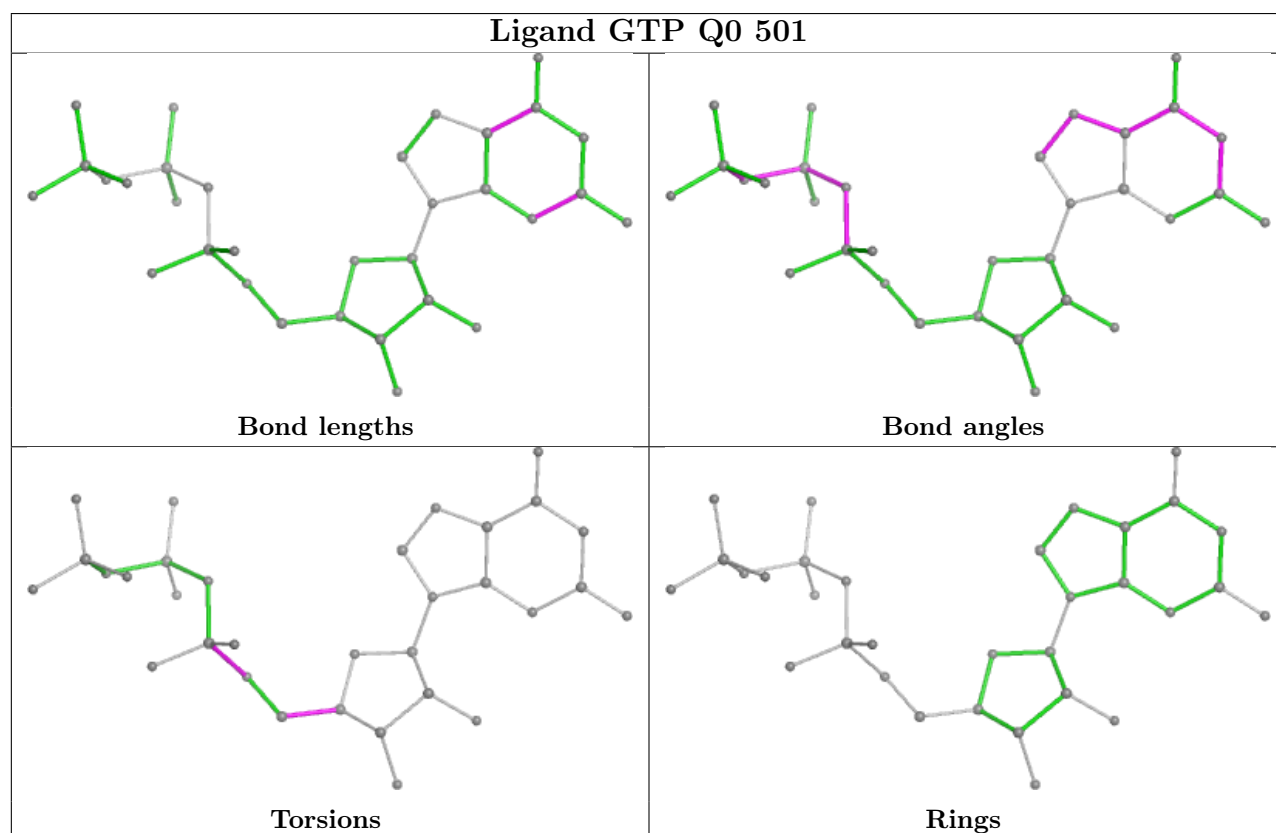
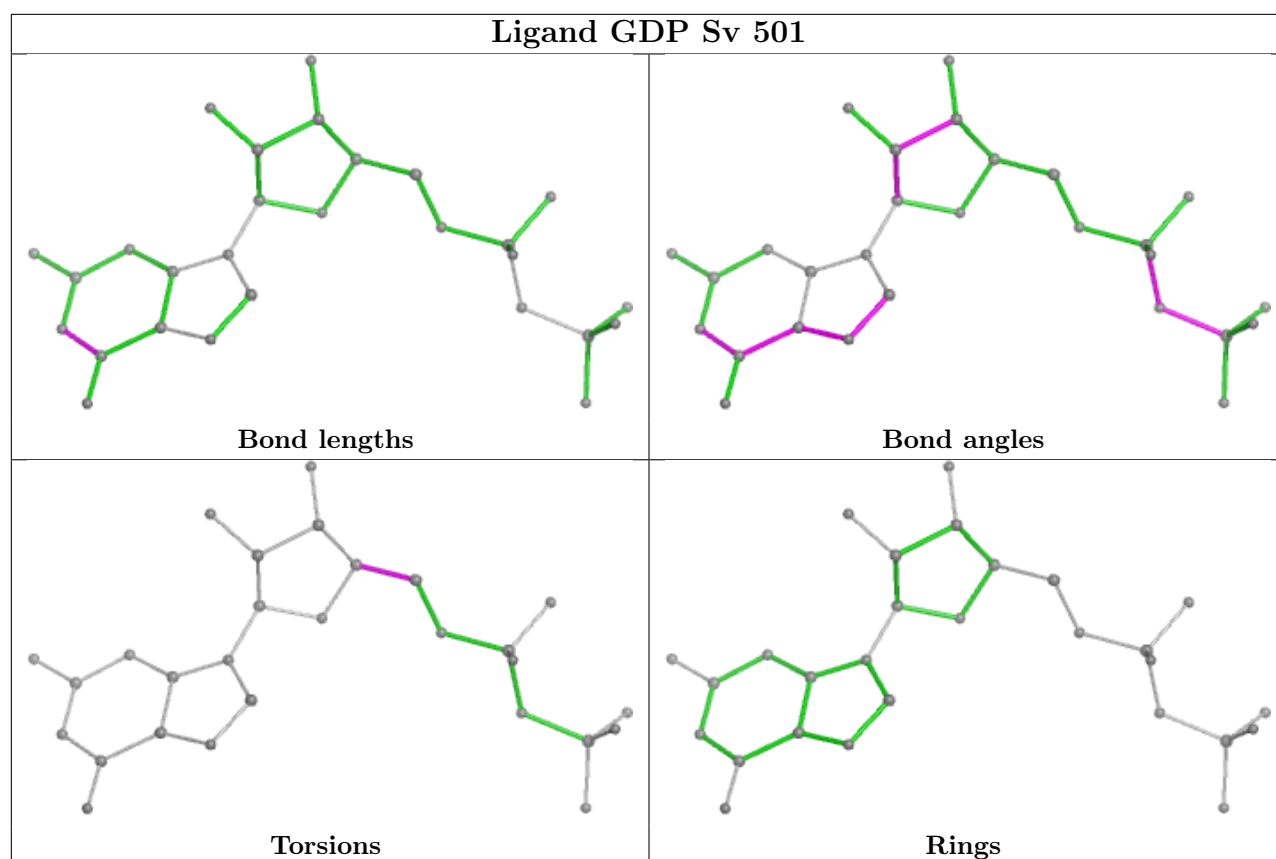


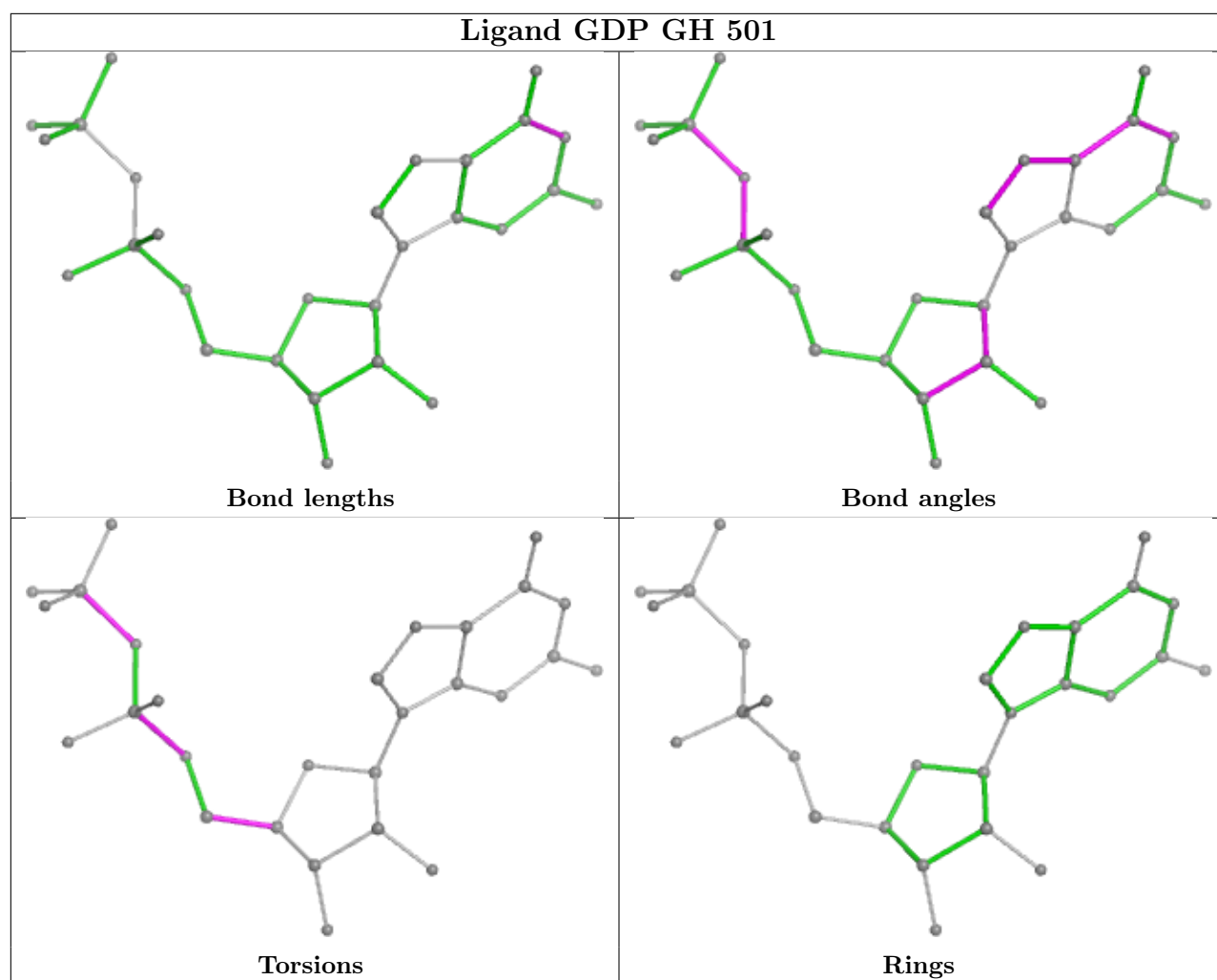
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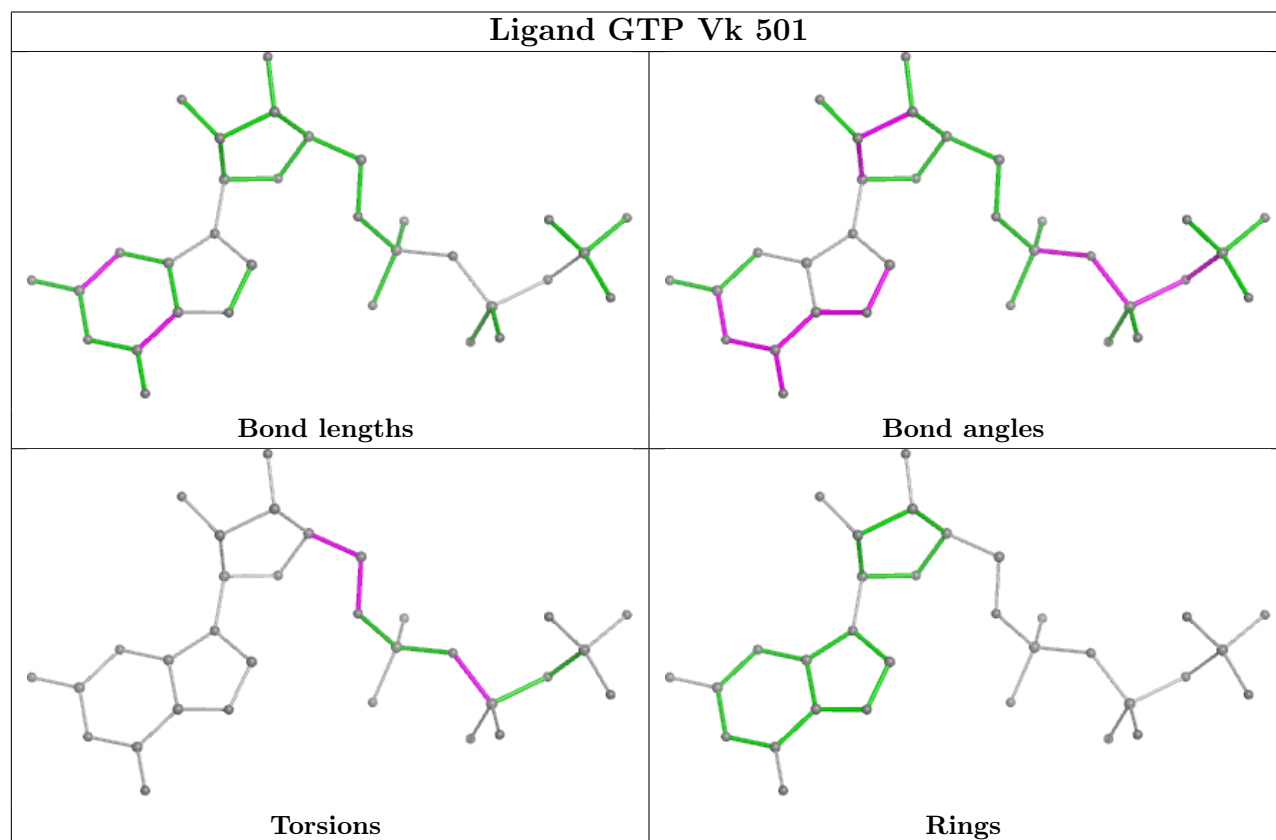
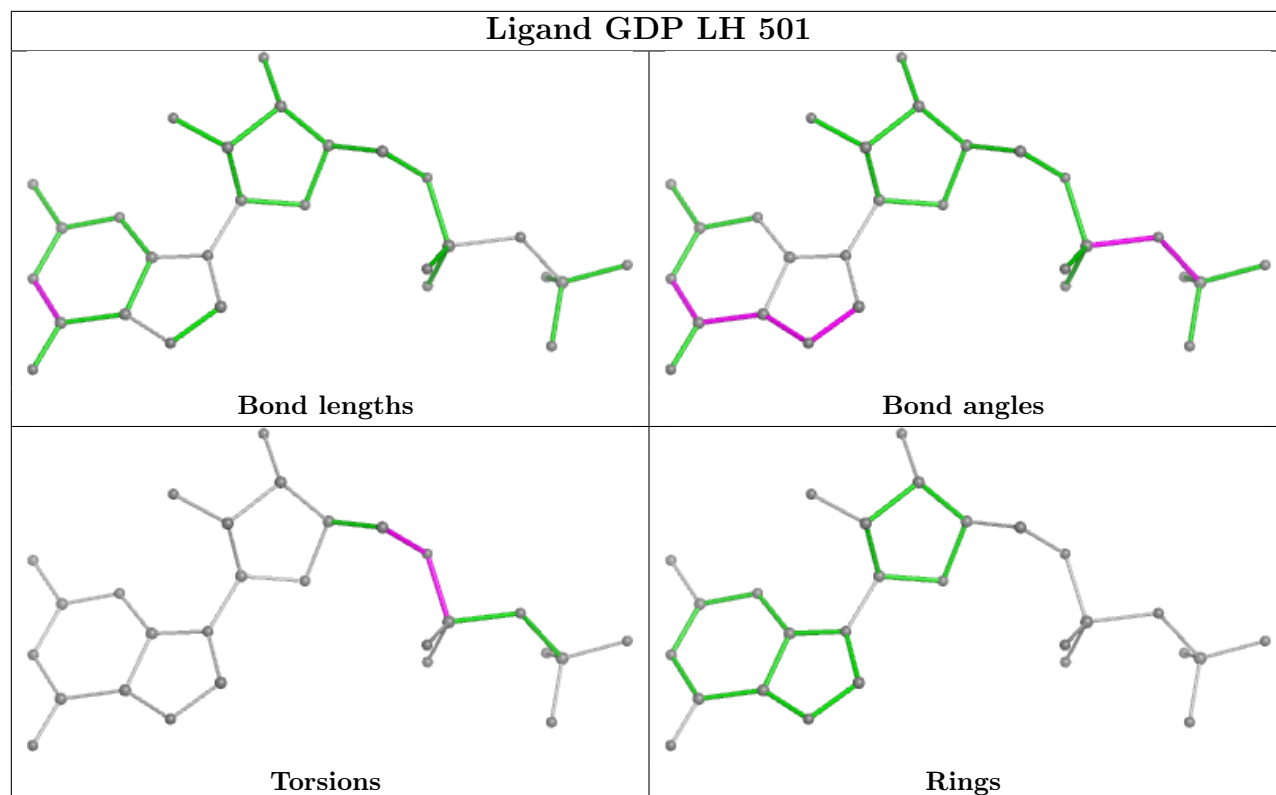


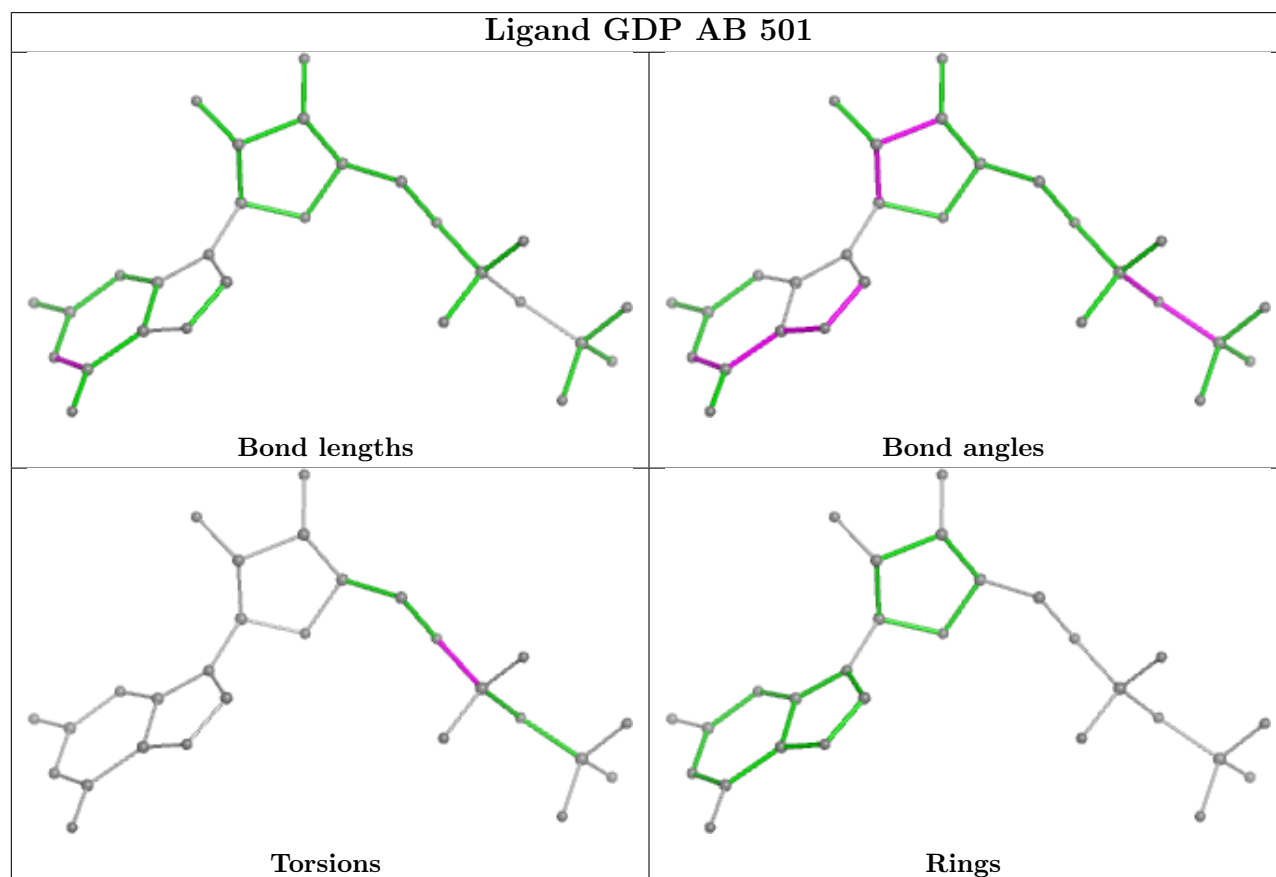
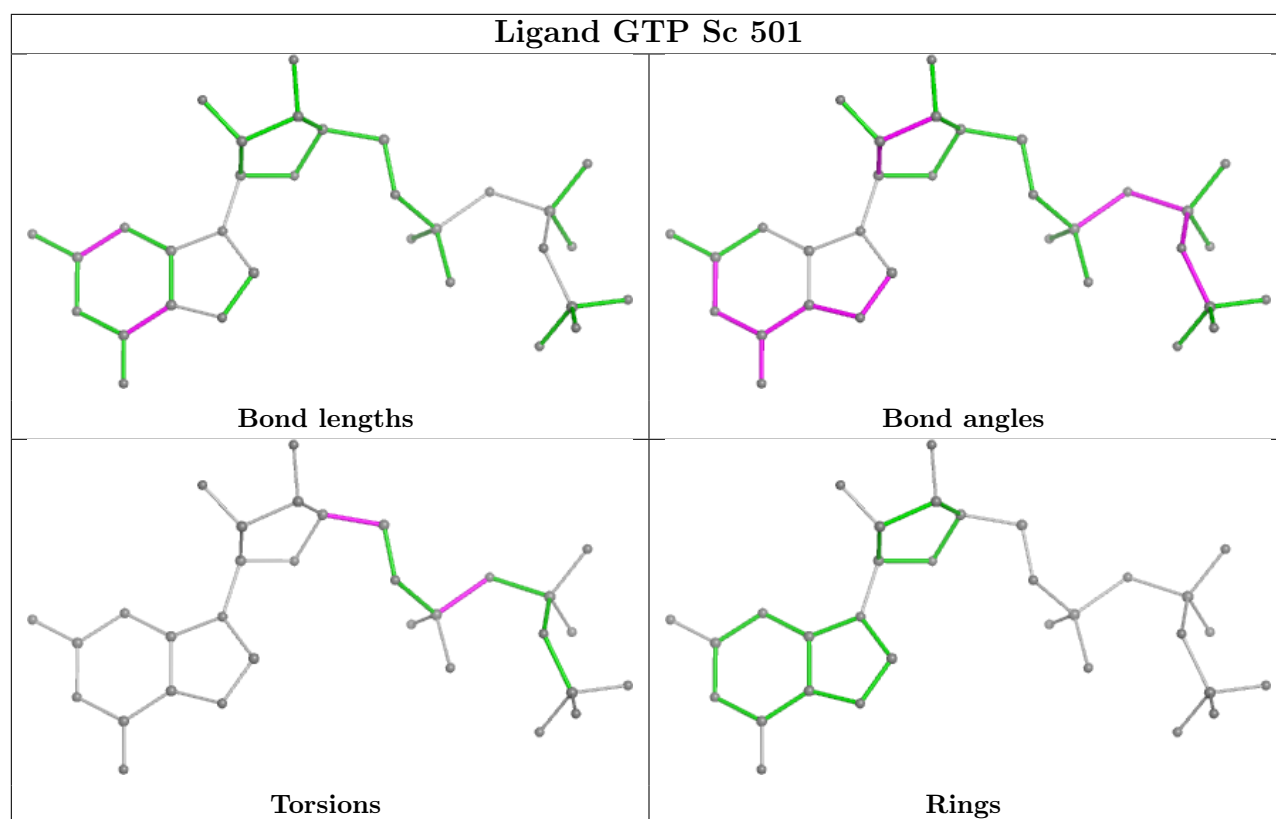




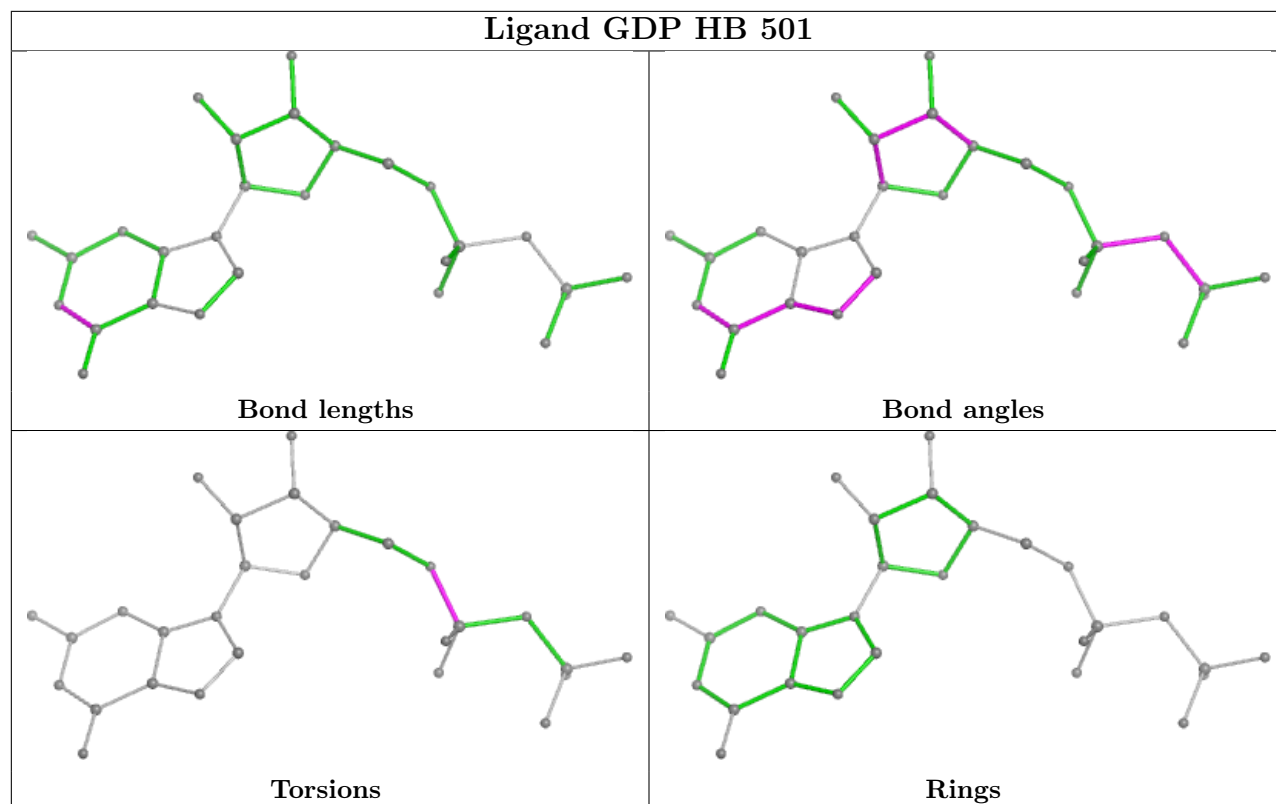




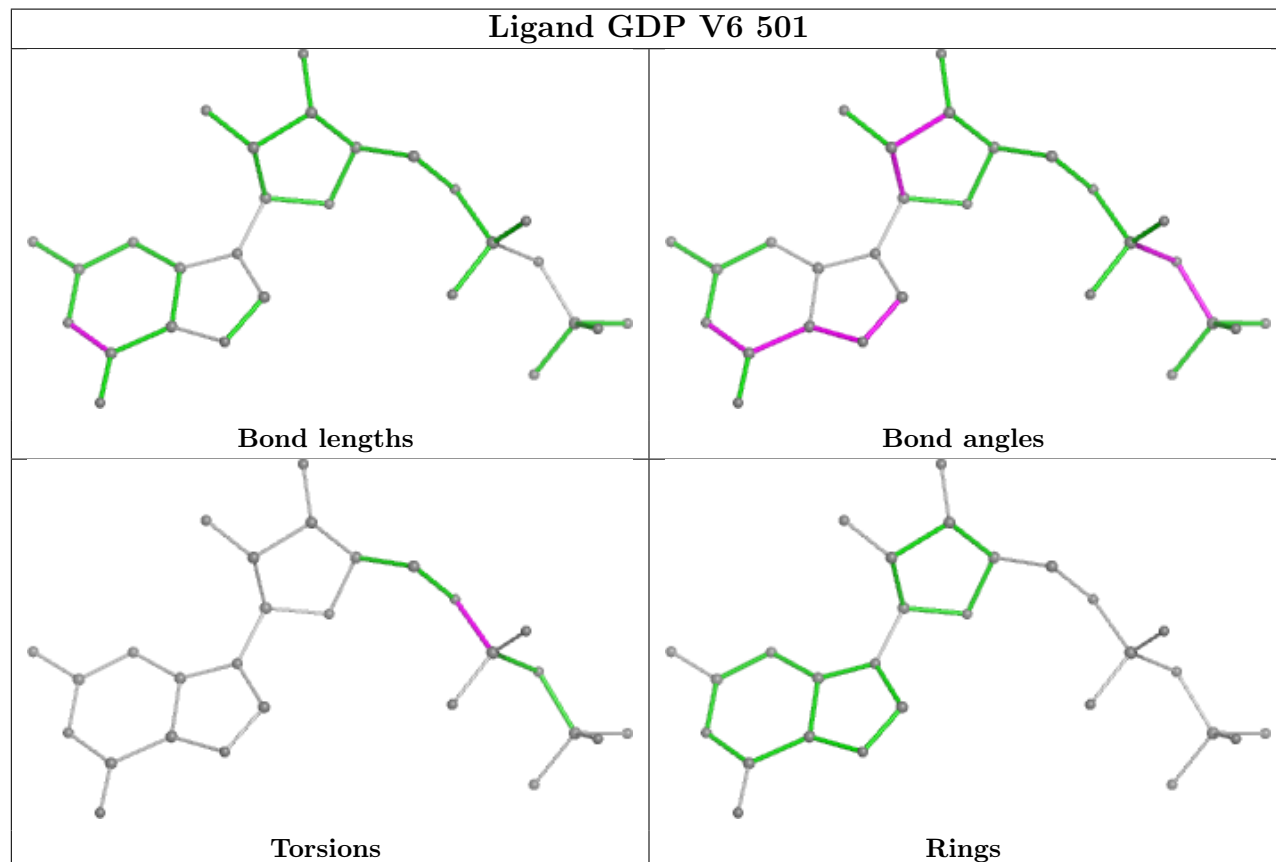




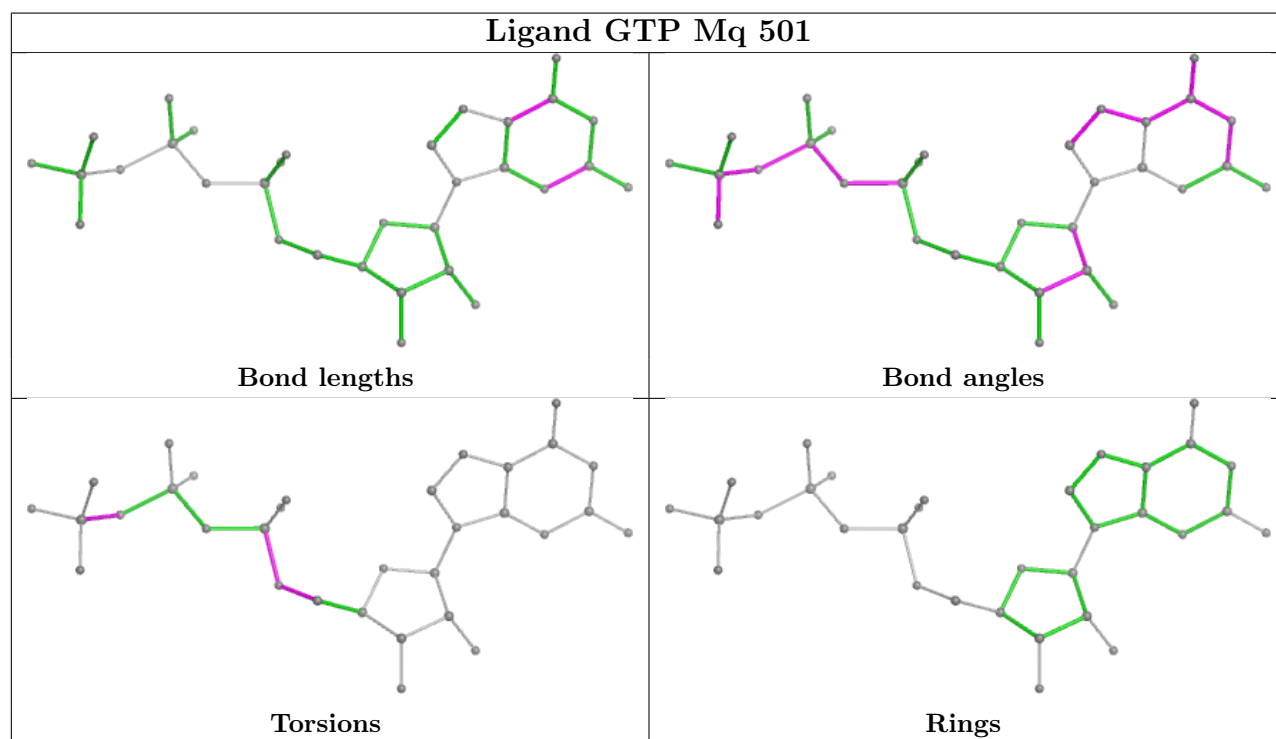
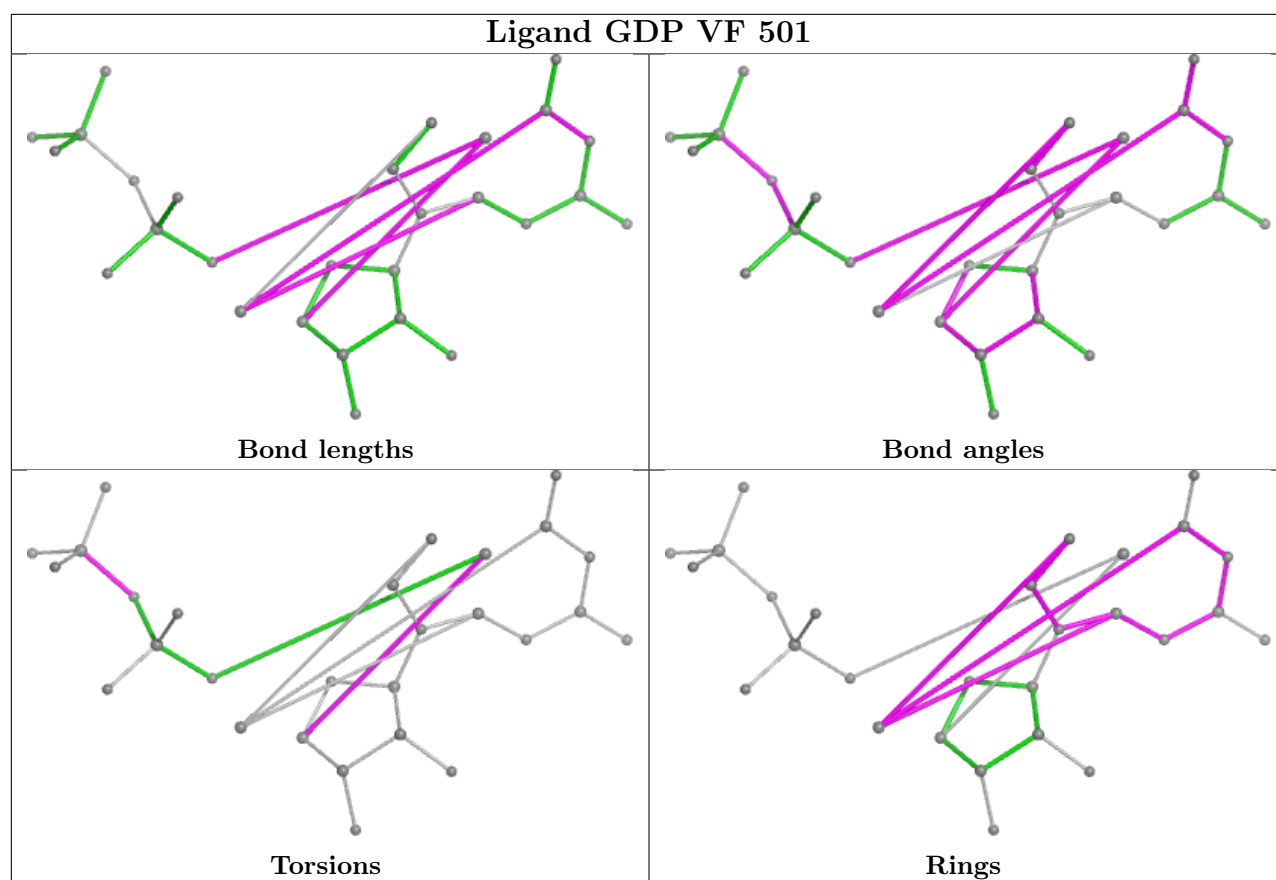
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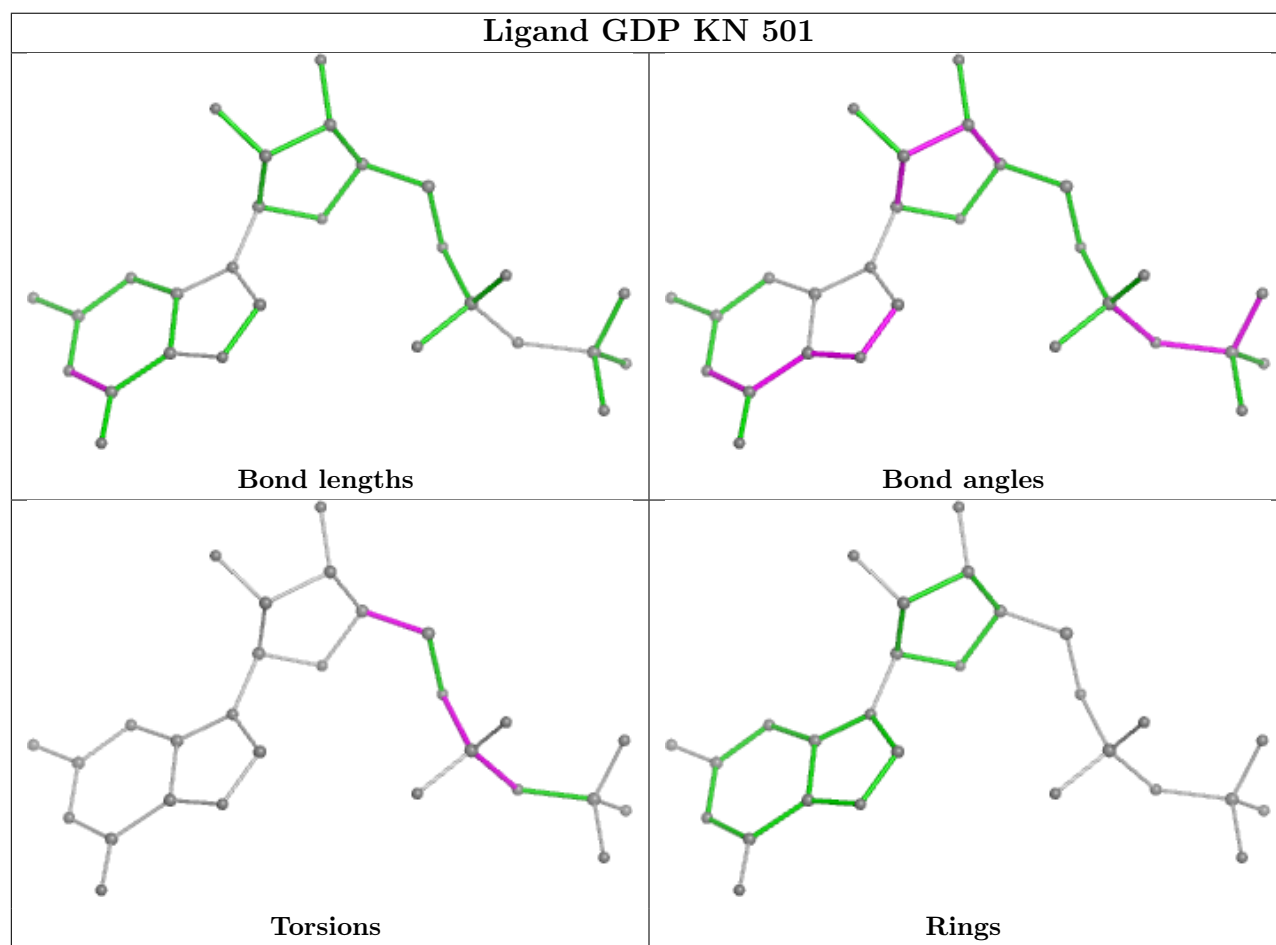
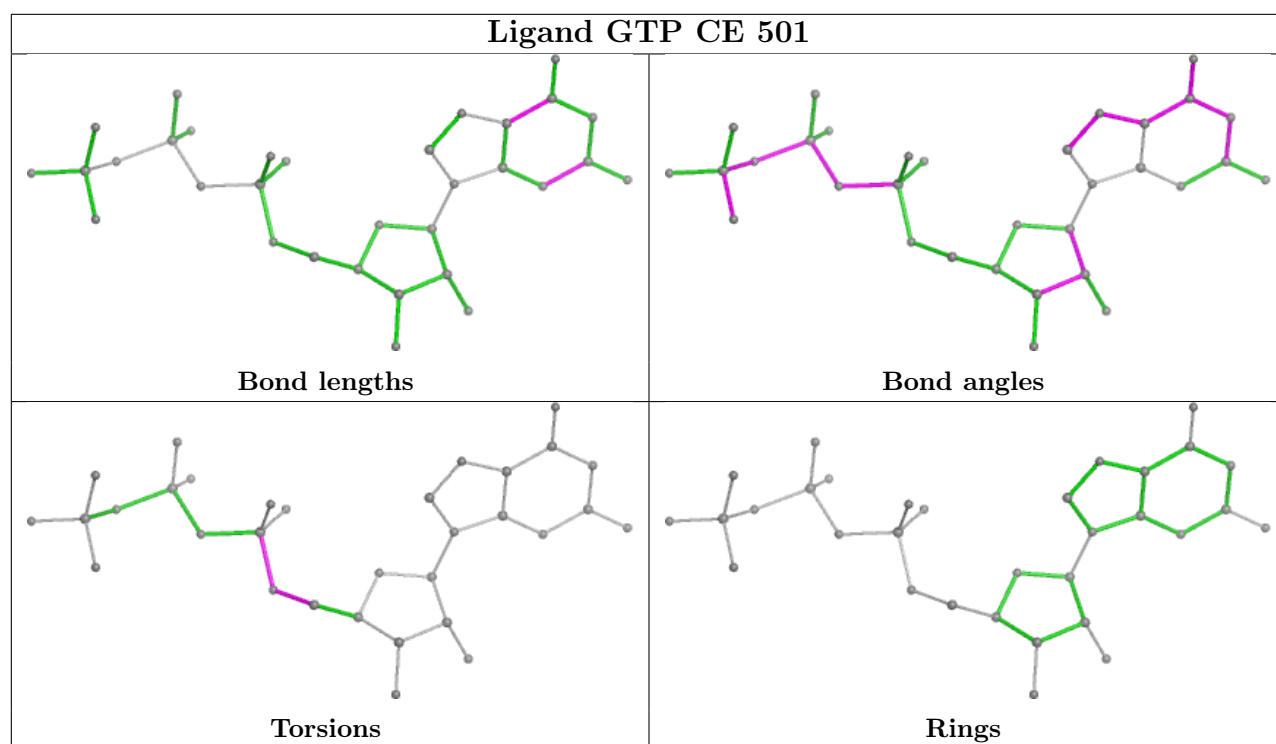


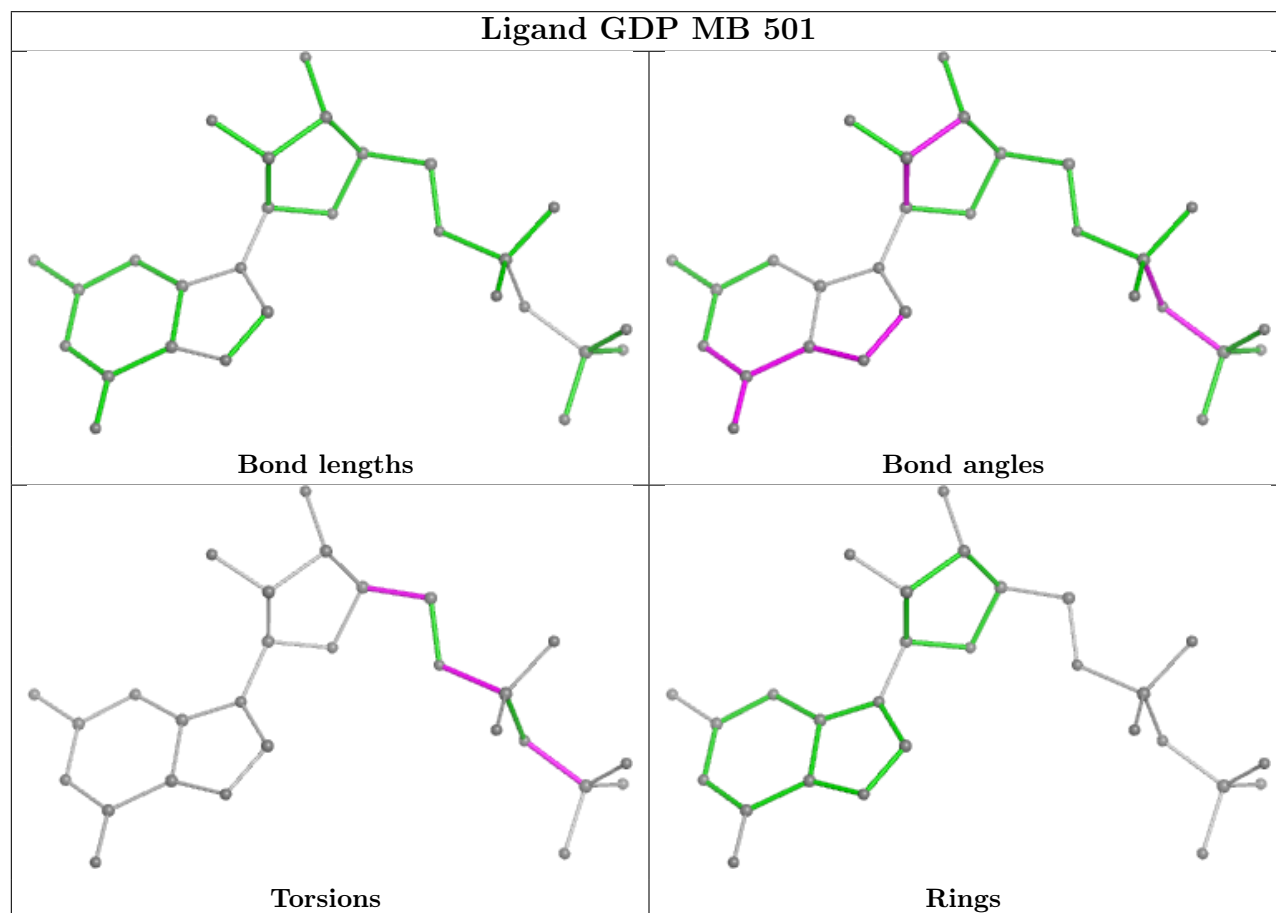
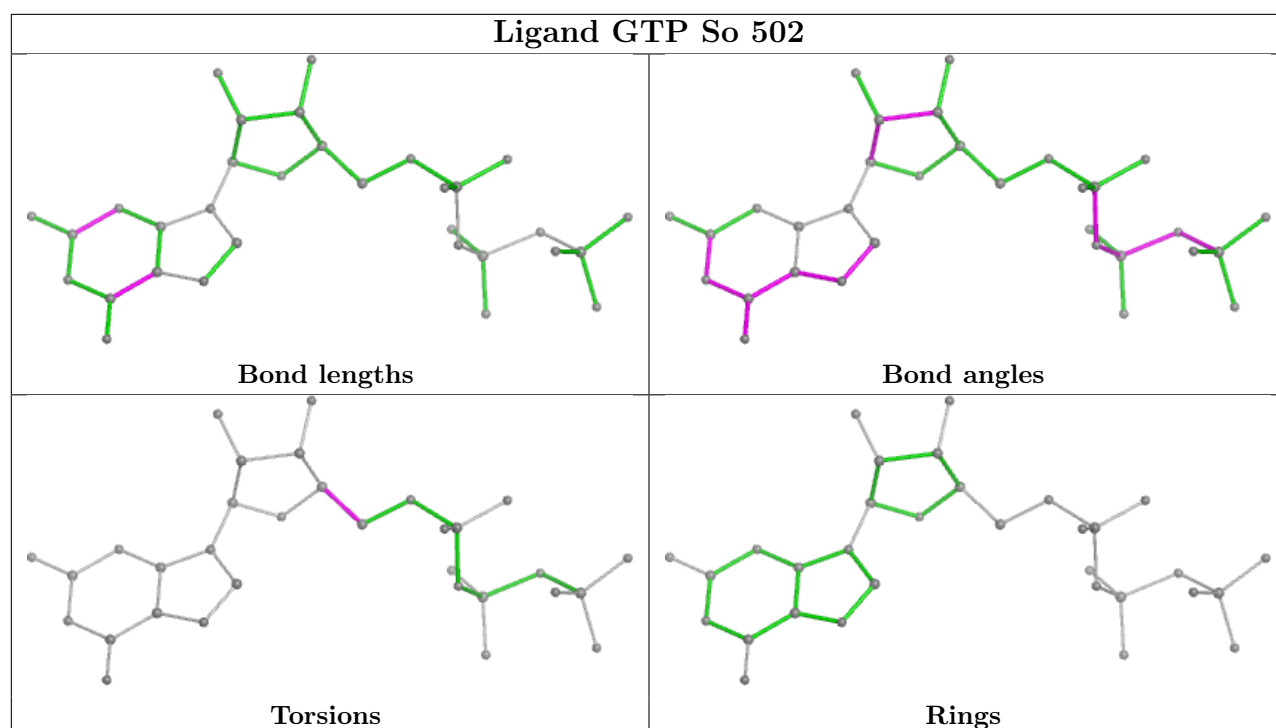
## Ligand GDP V6 501



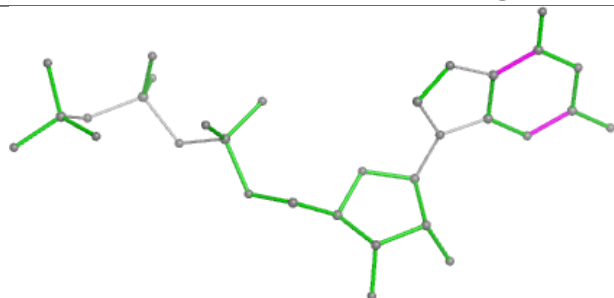




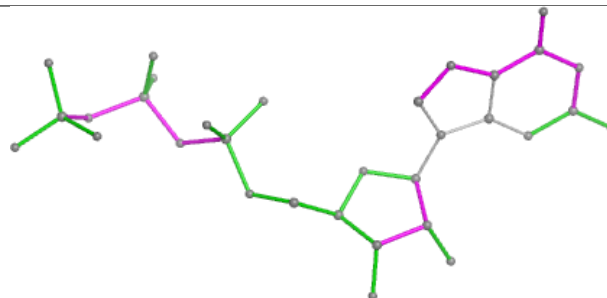




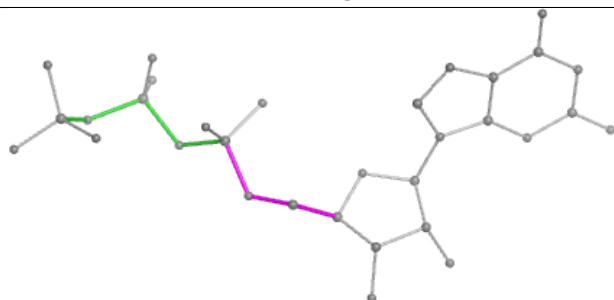
## Ligand GTP WR 501



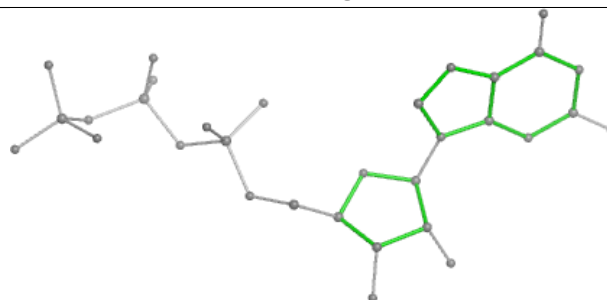
Bond lengths



Bond angles

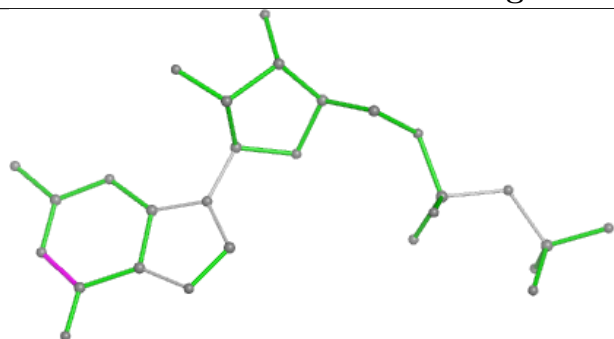


Torsions

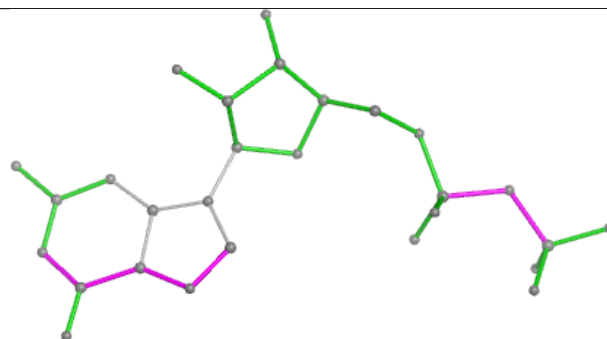


Rings

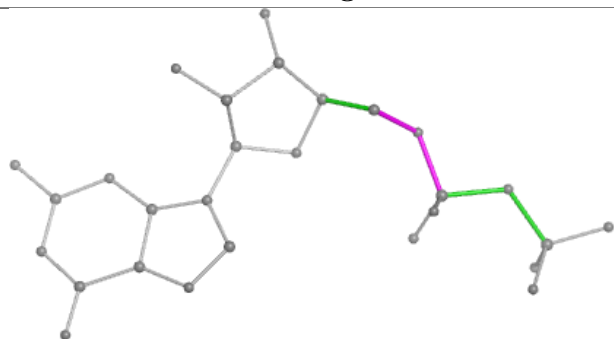
## Ligand GDP Tf 501



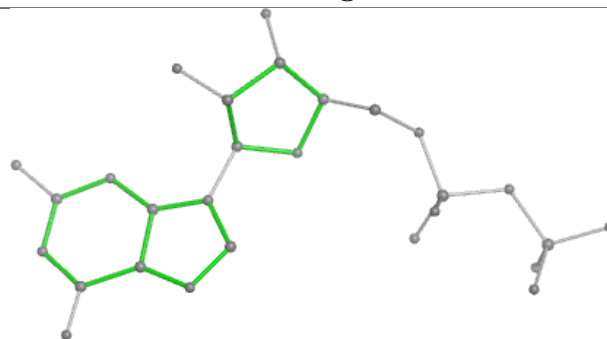
Bond lengths



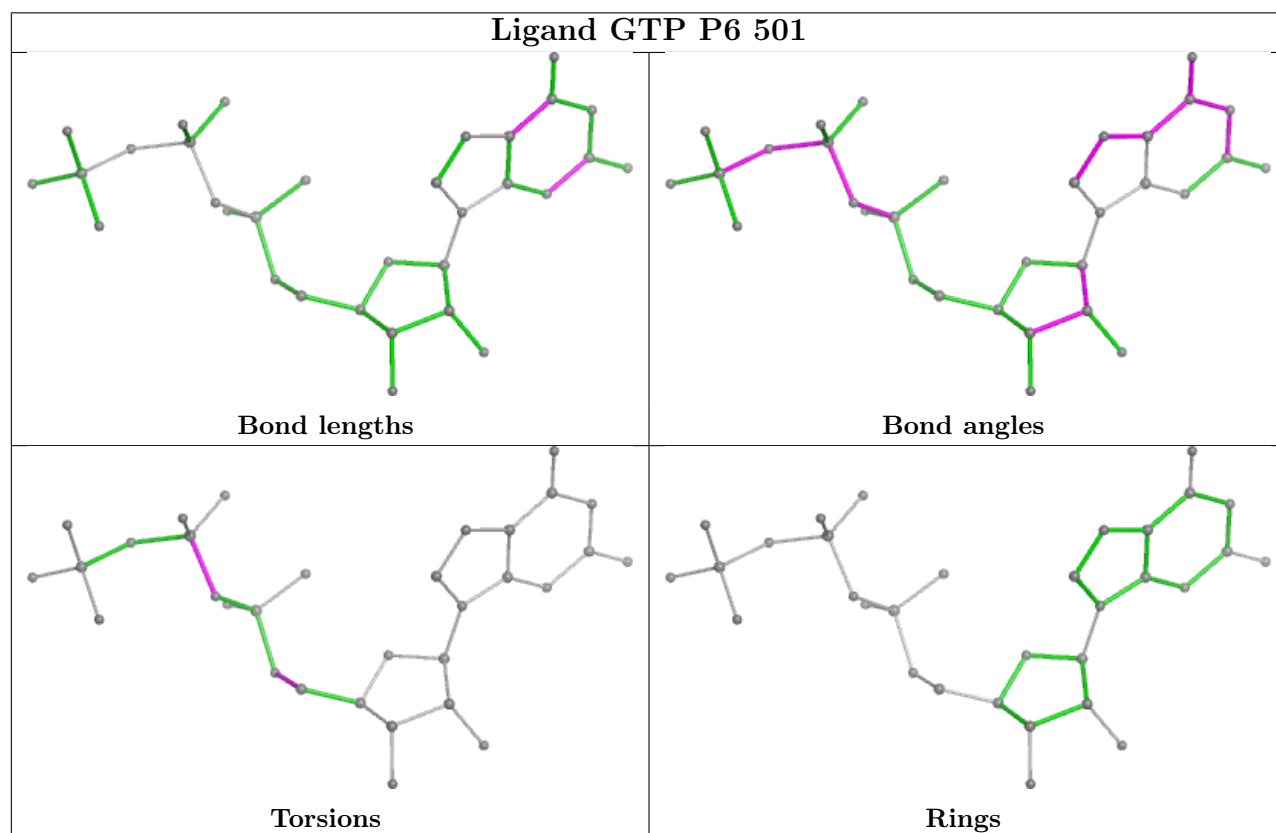
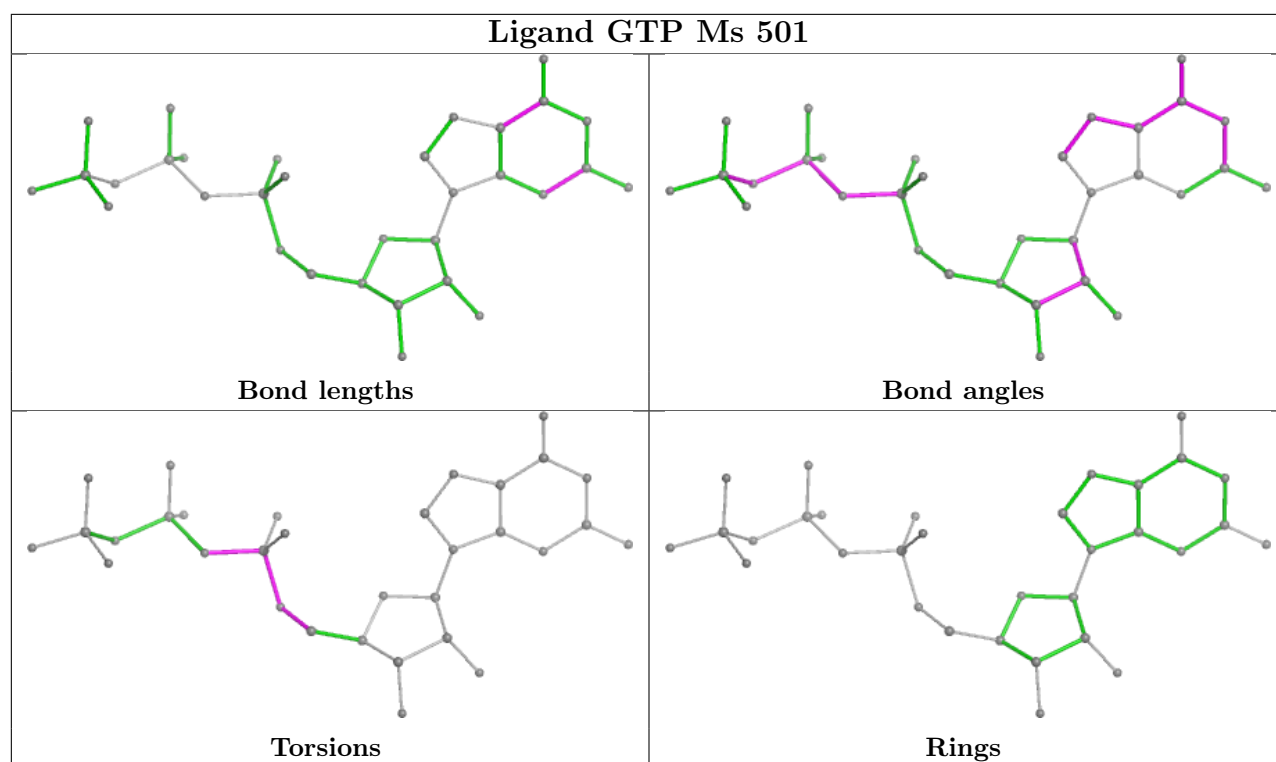
Bond angles



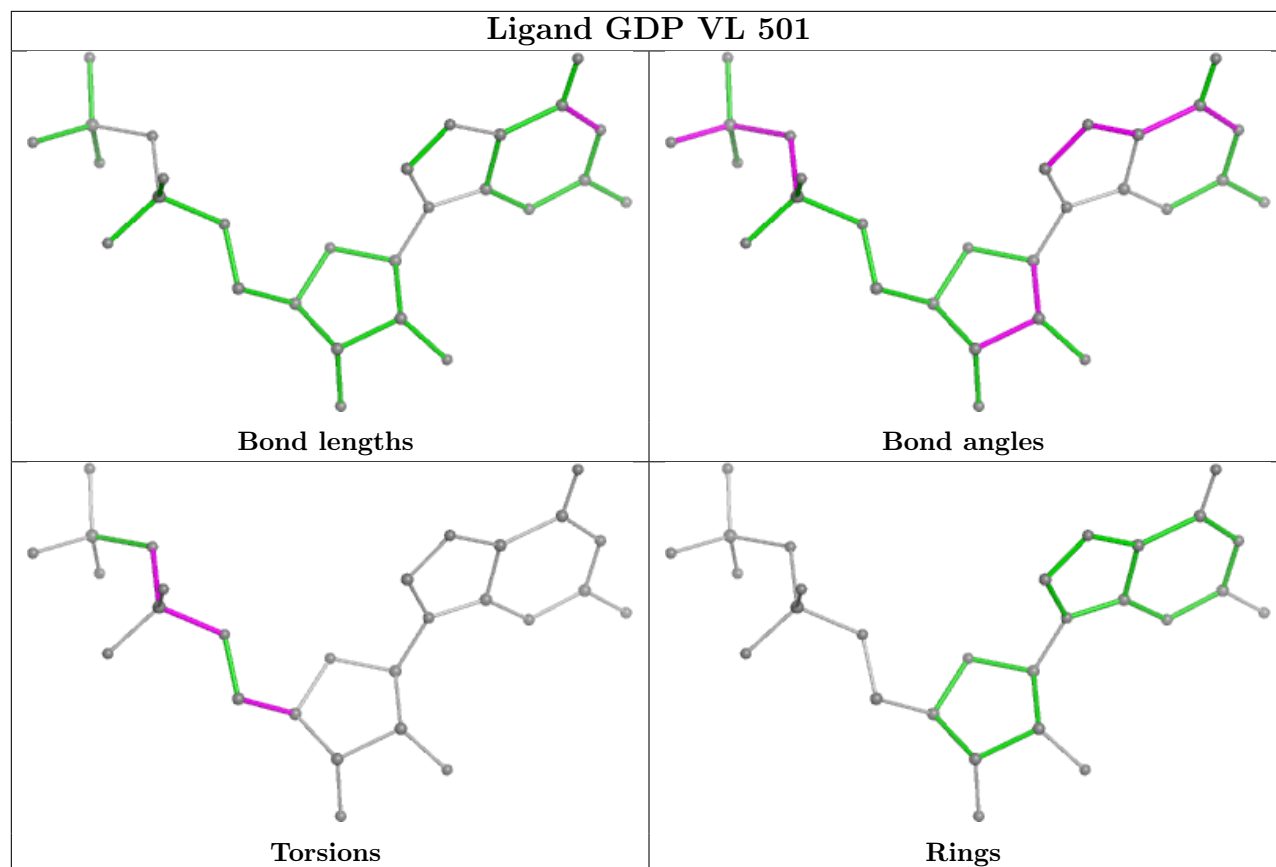
Torsions



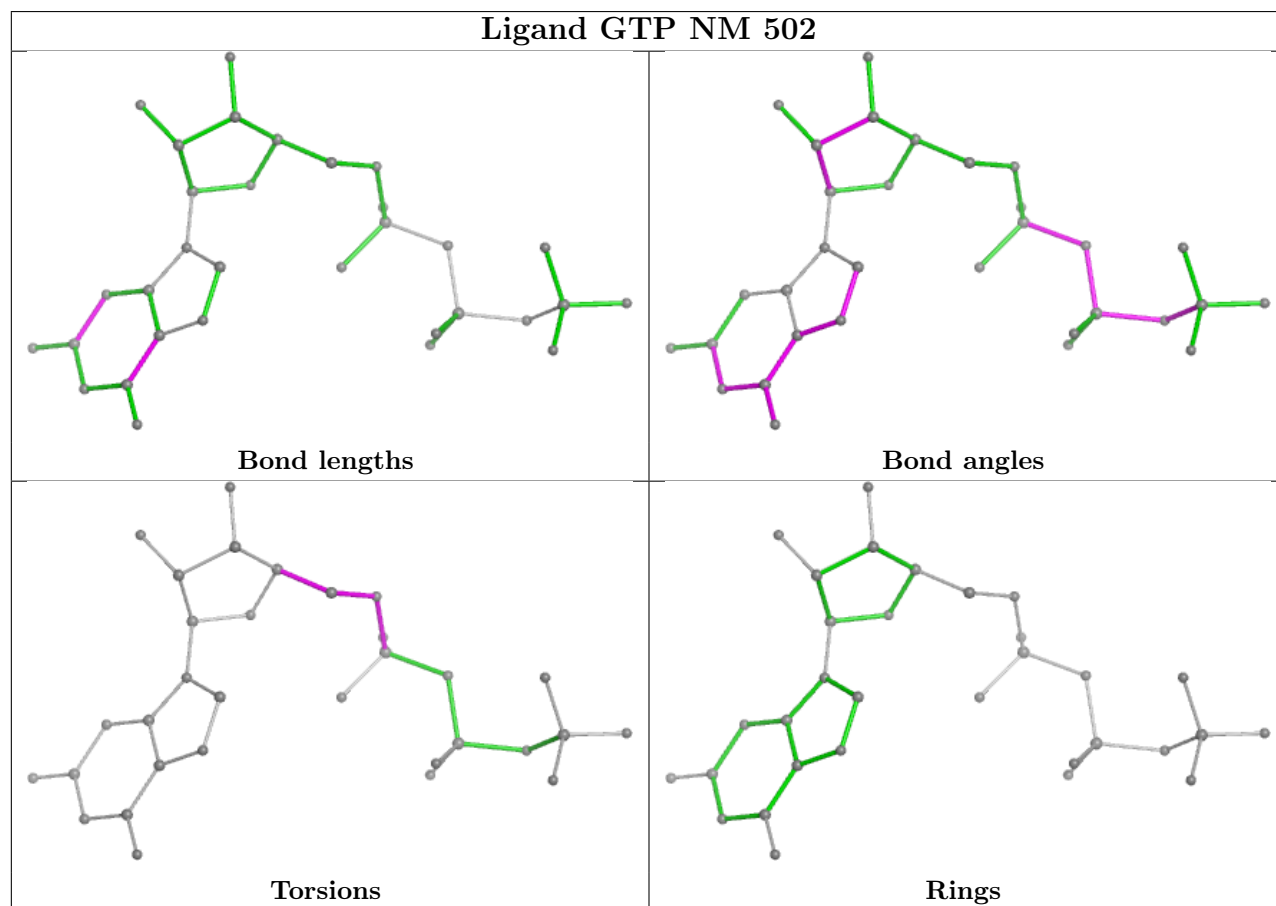
Rings

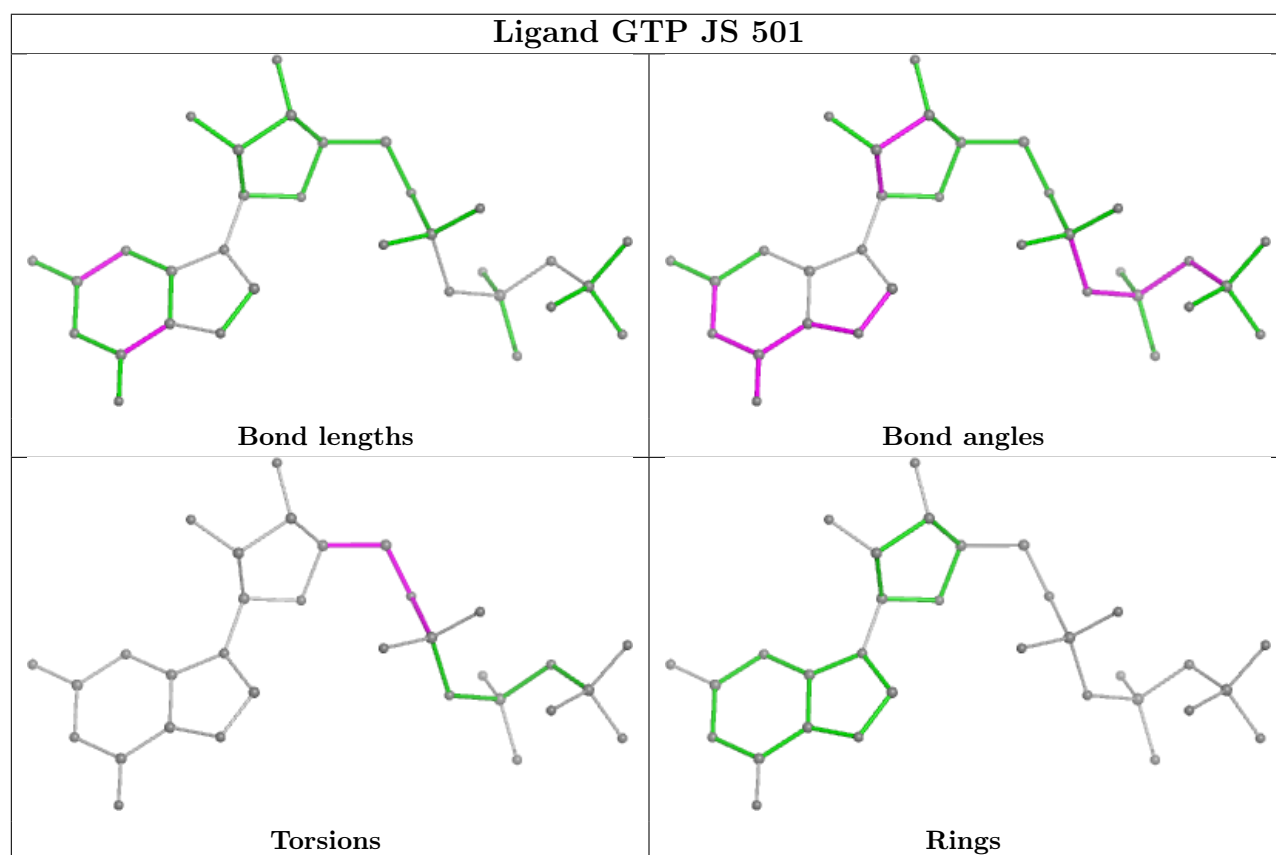
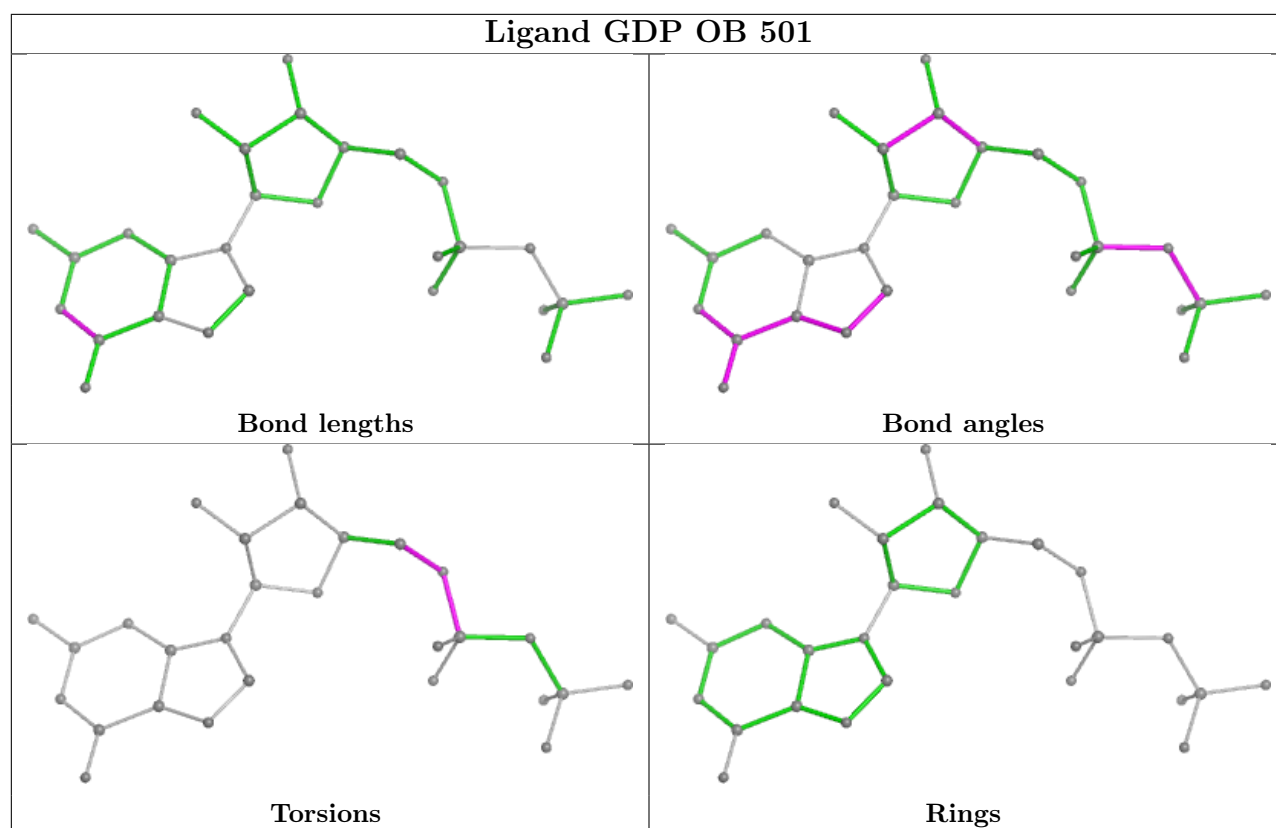


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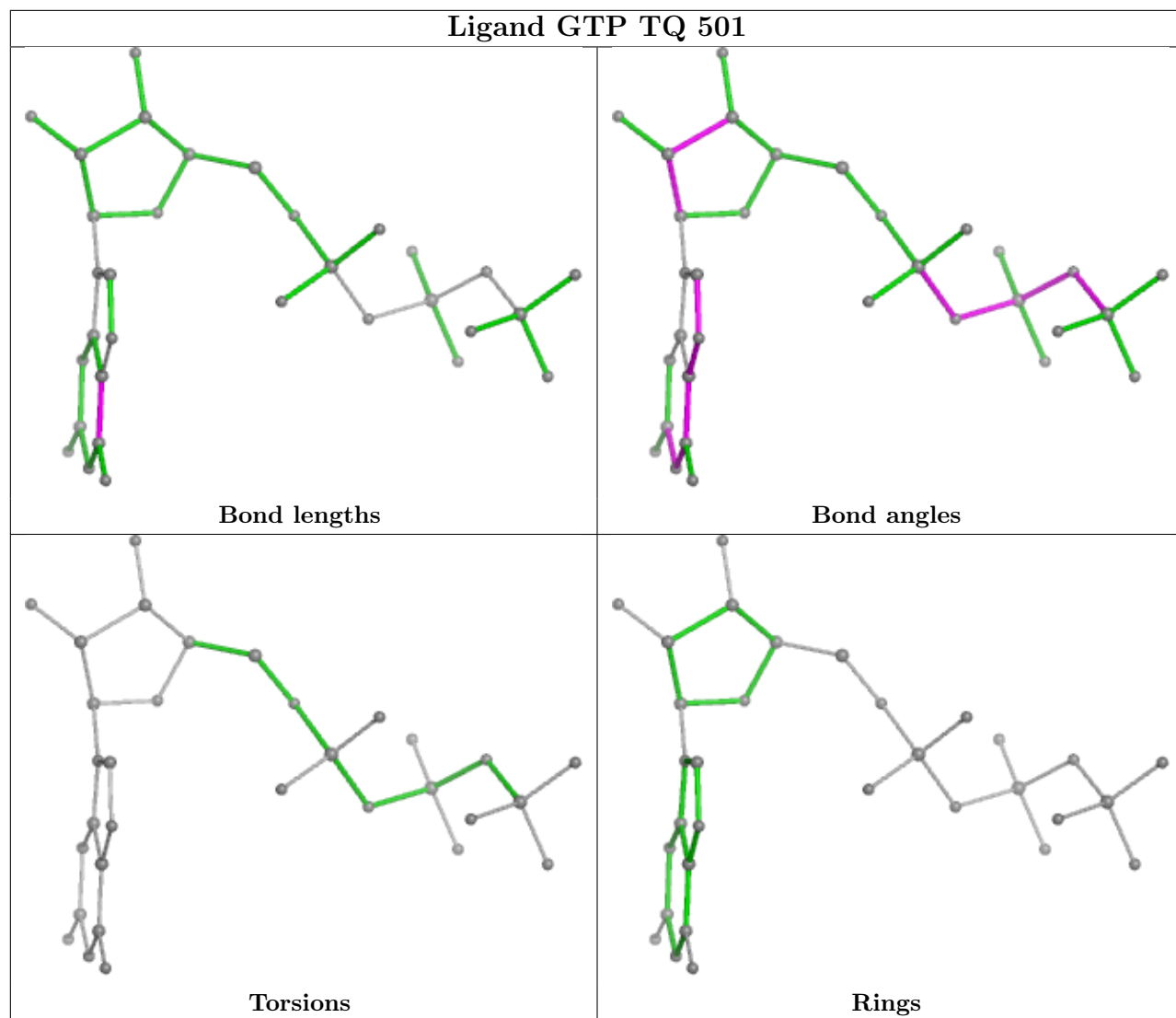


## Ligand GTP NM 502

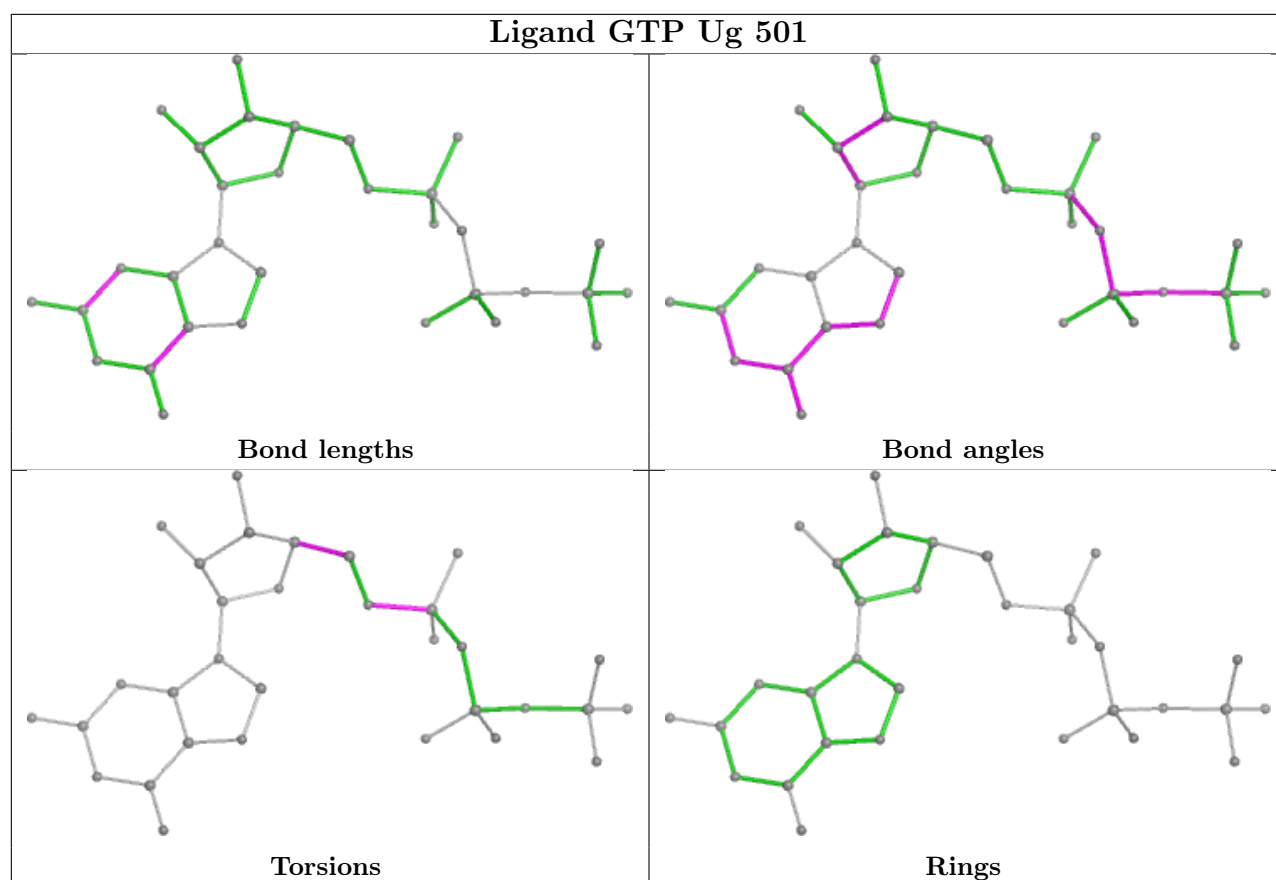


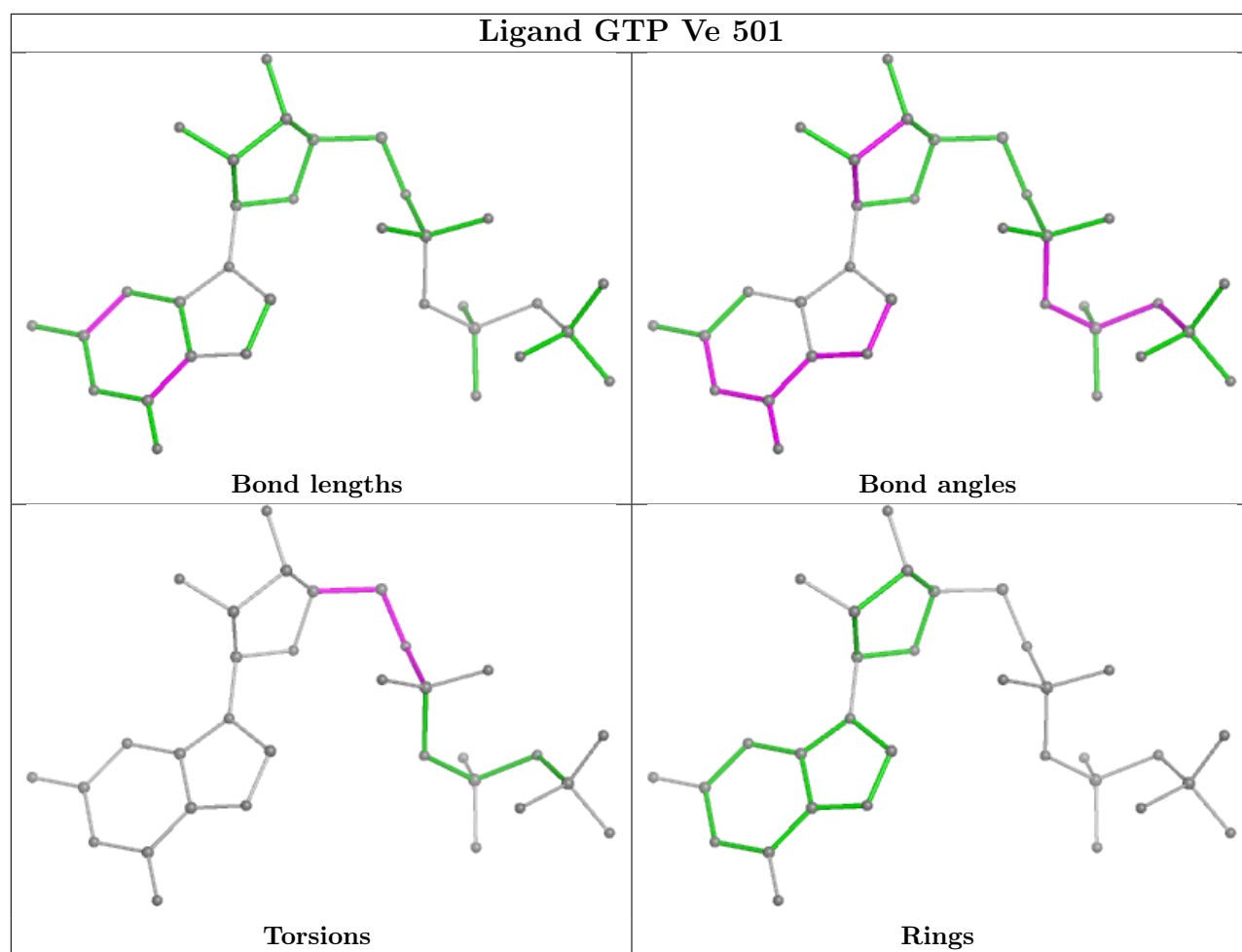


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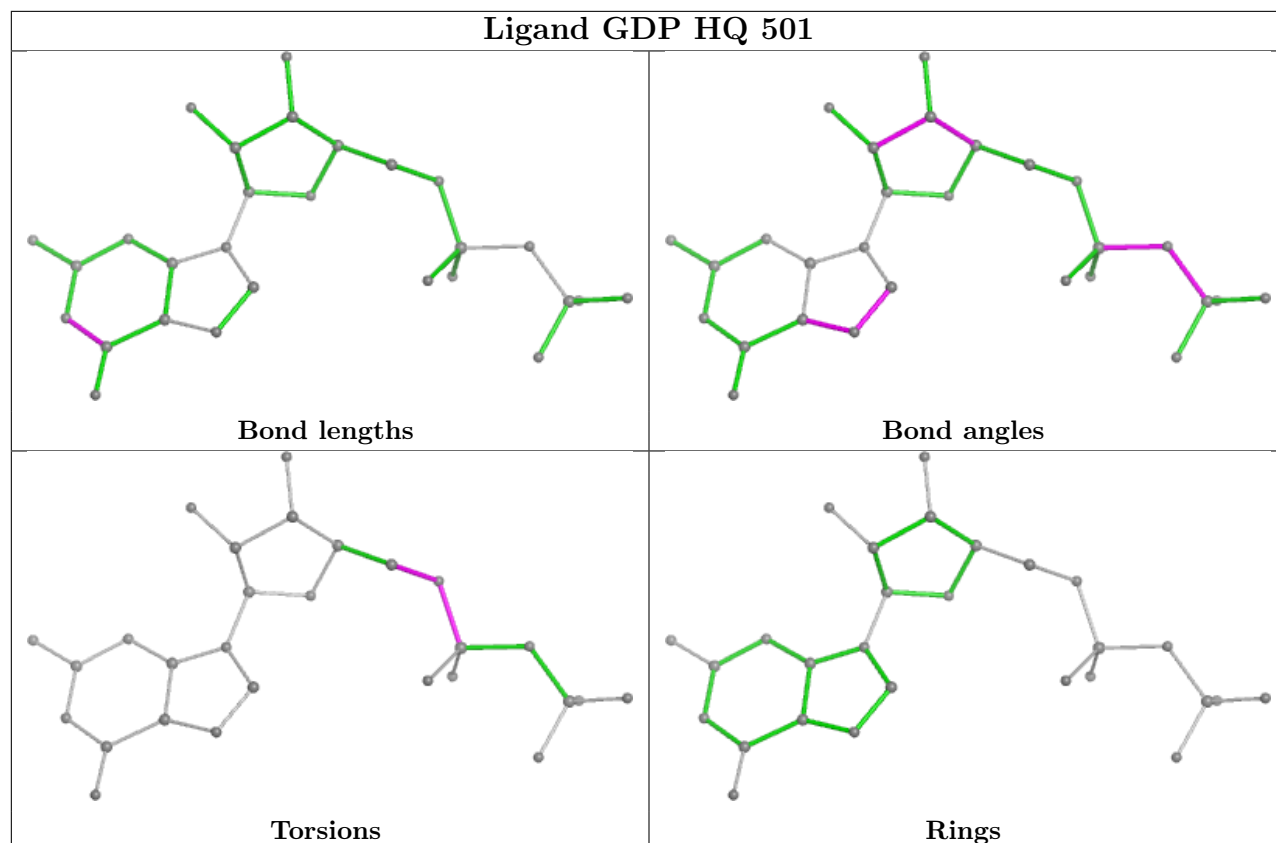




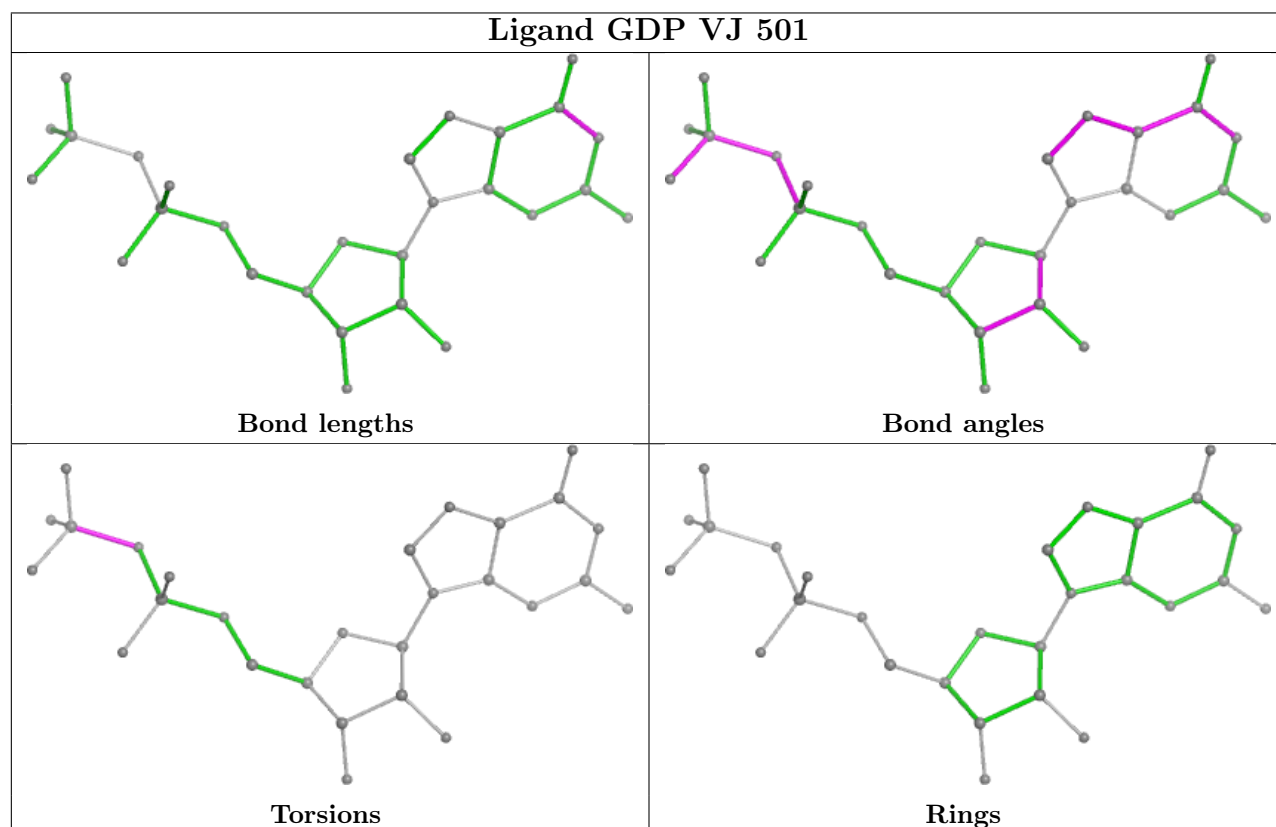


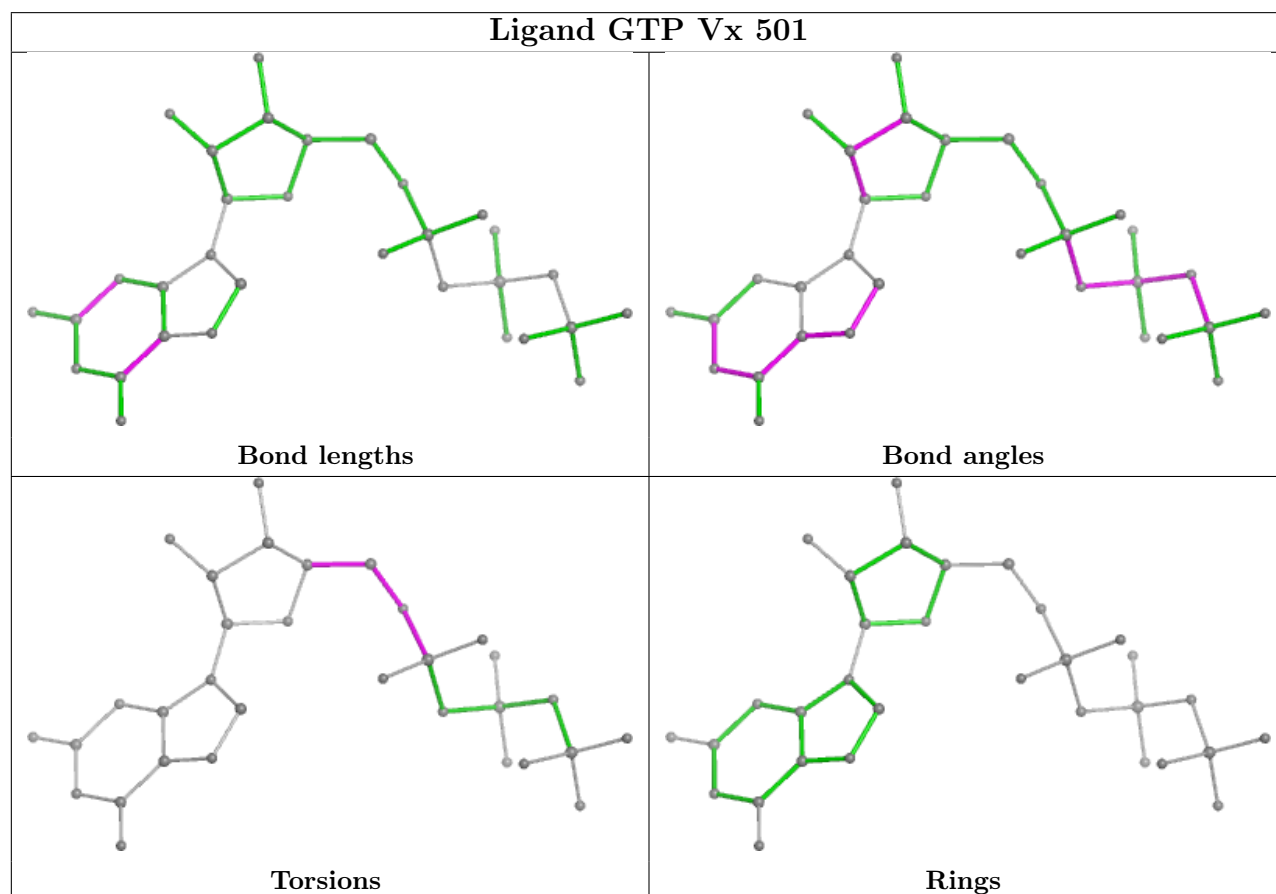
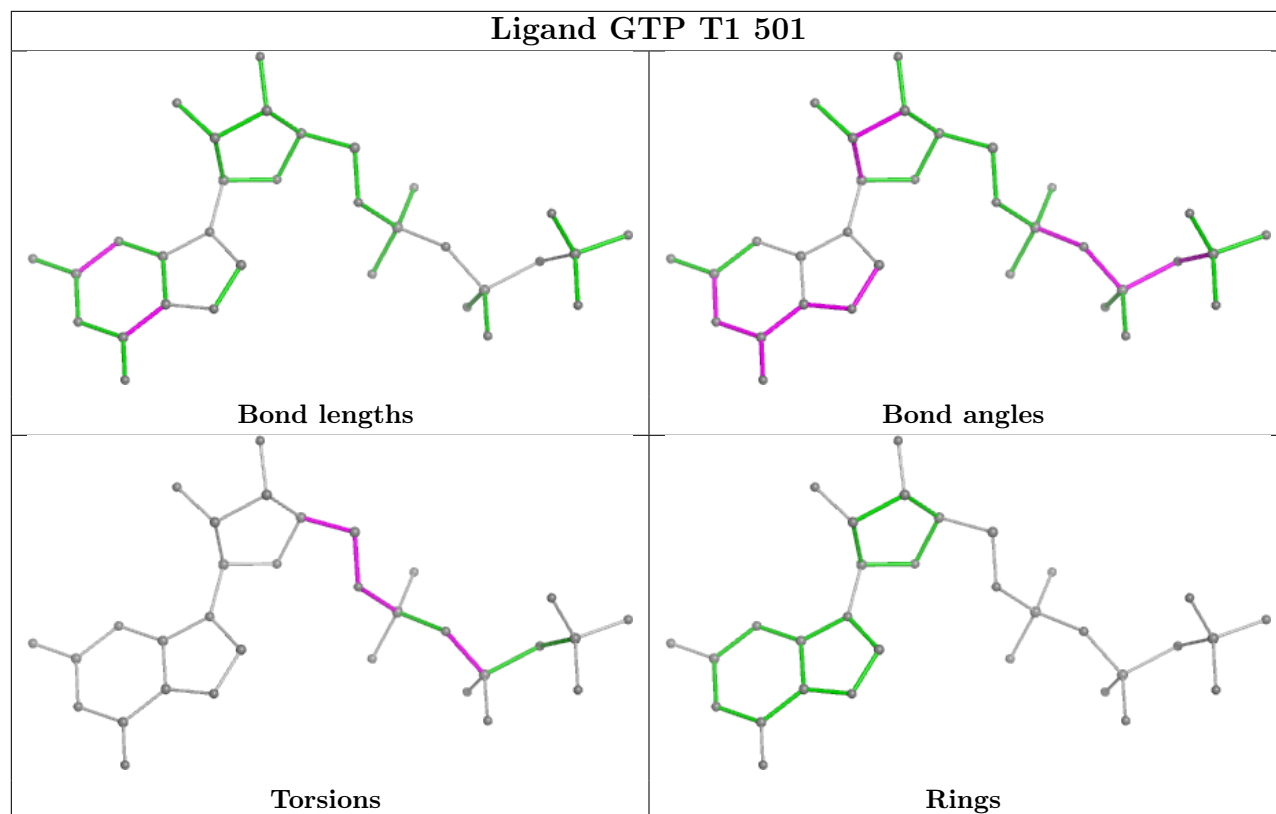


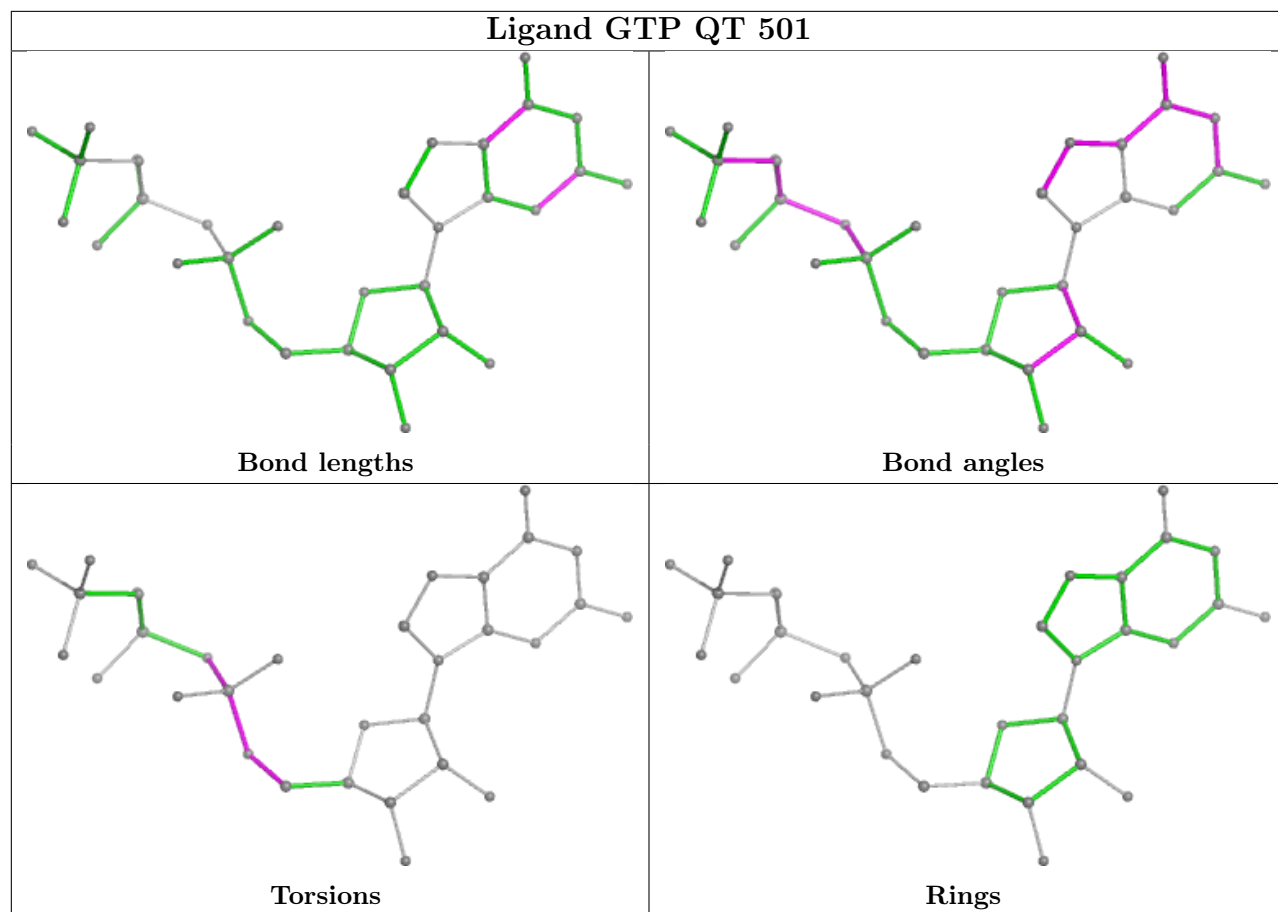
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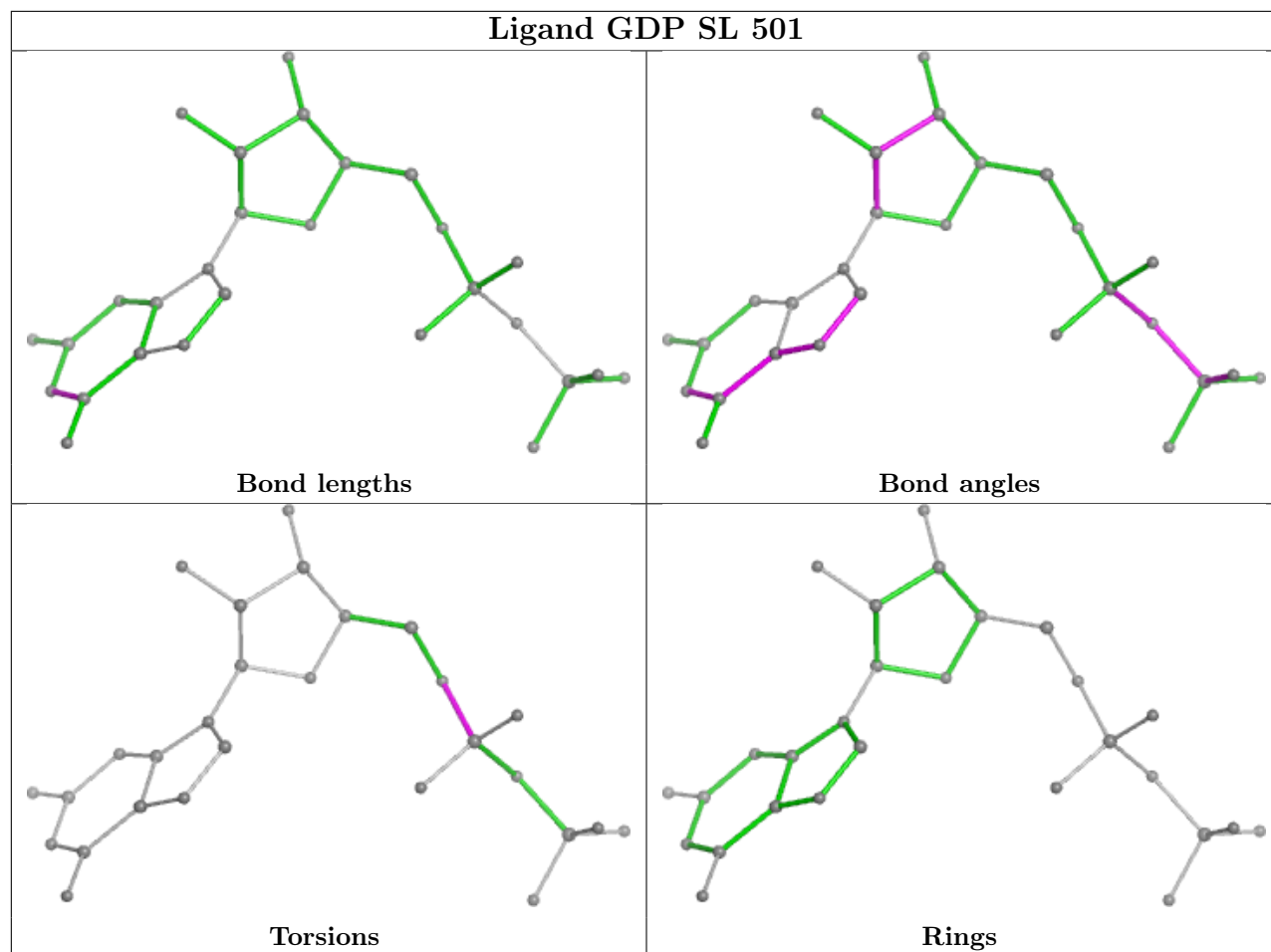


## Ligand GDP VJ 501

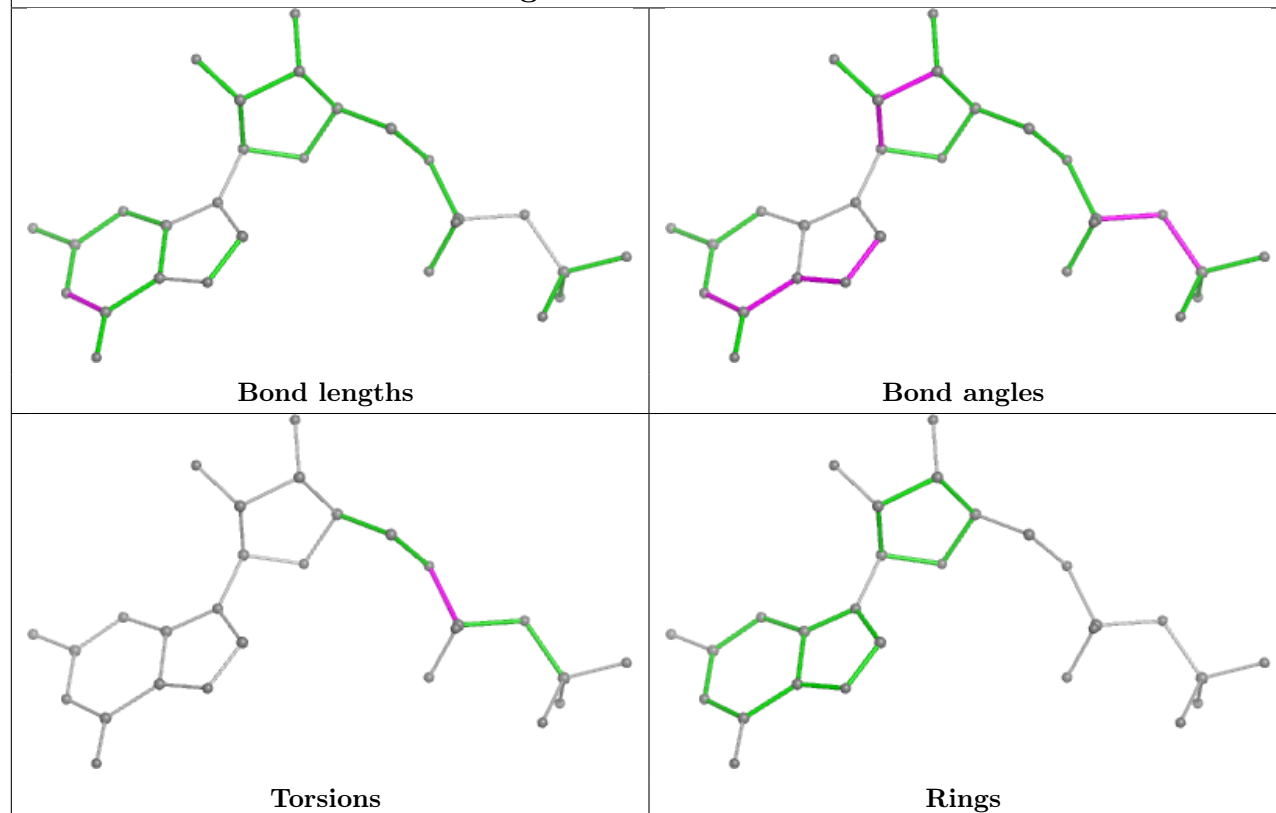




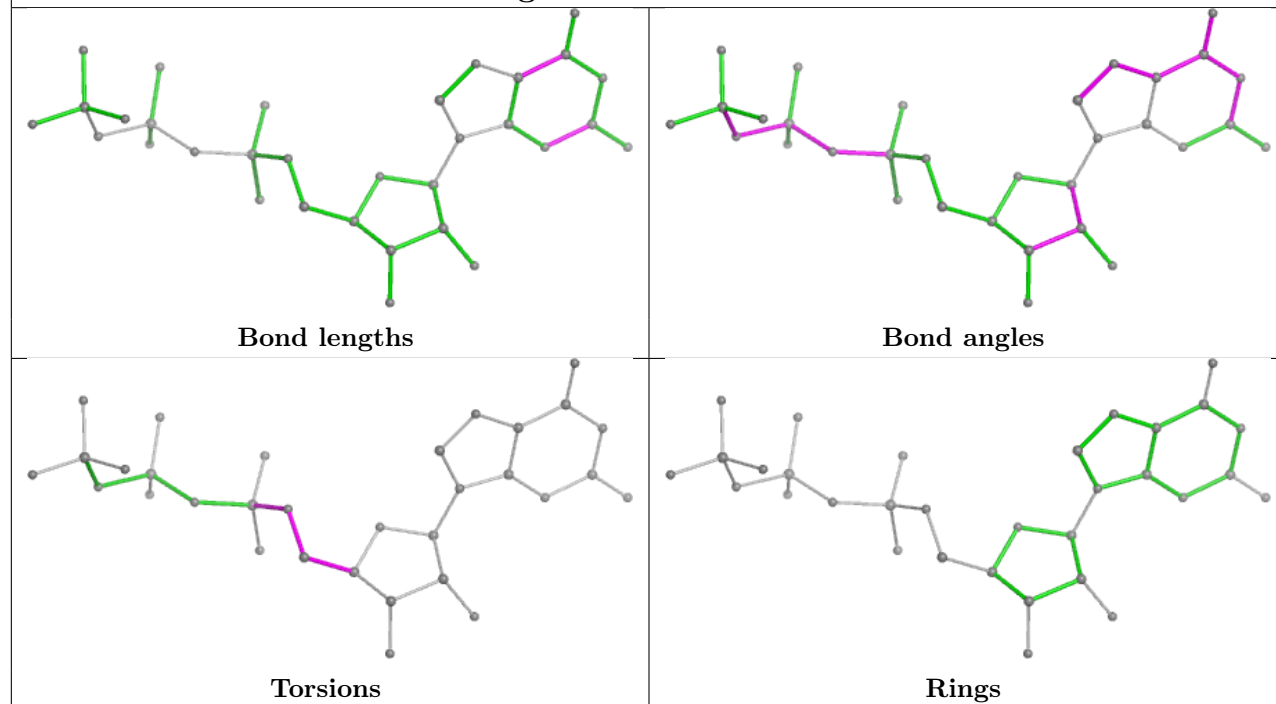


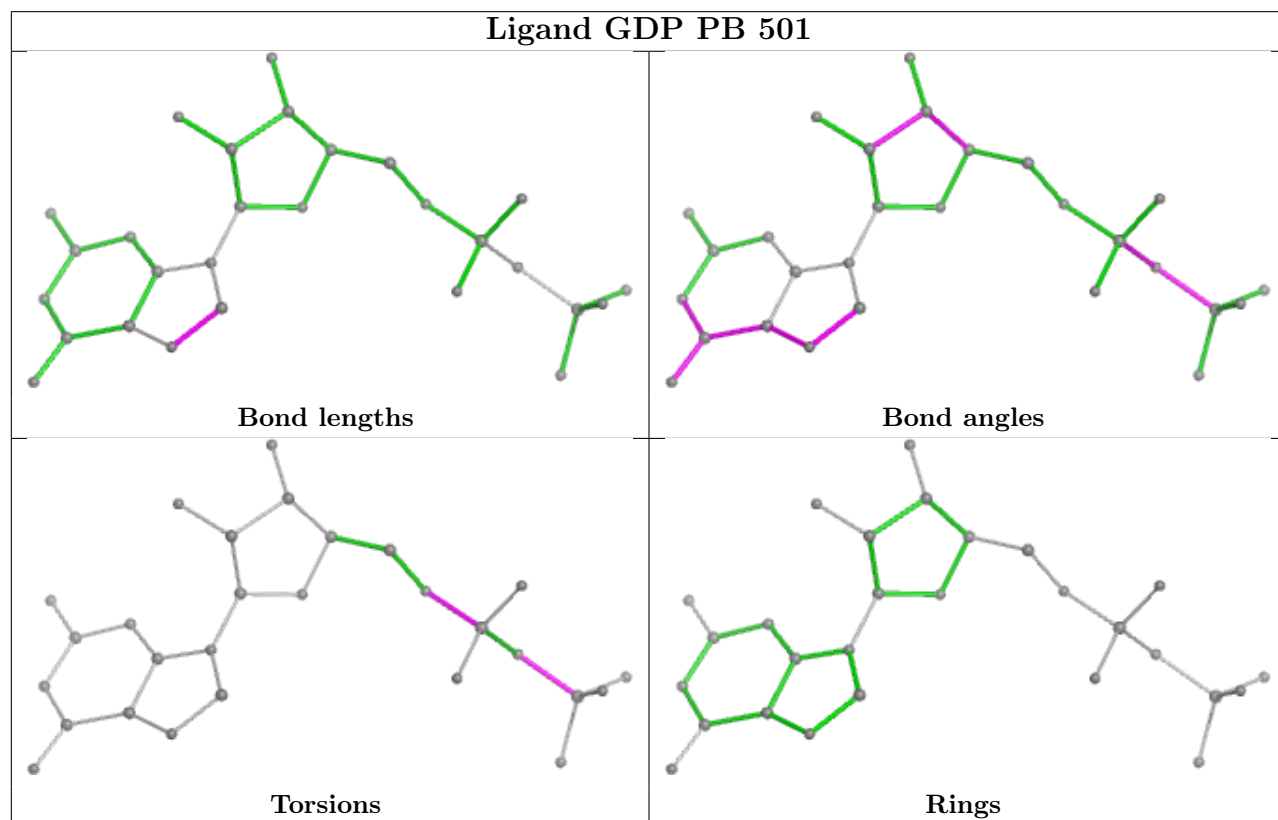
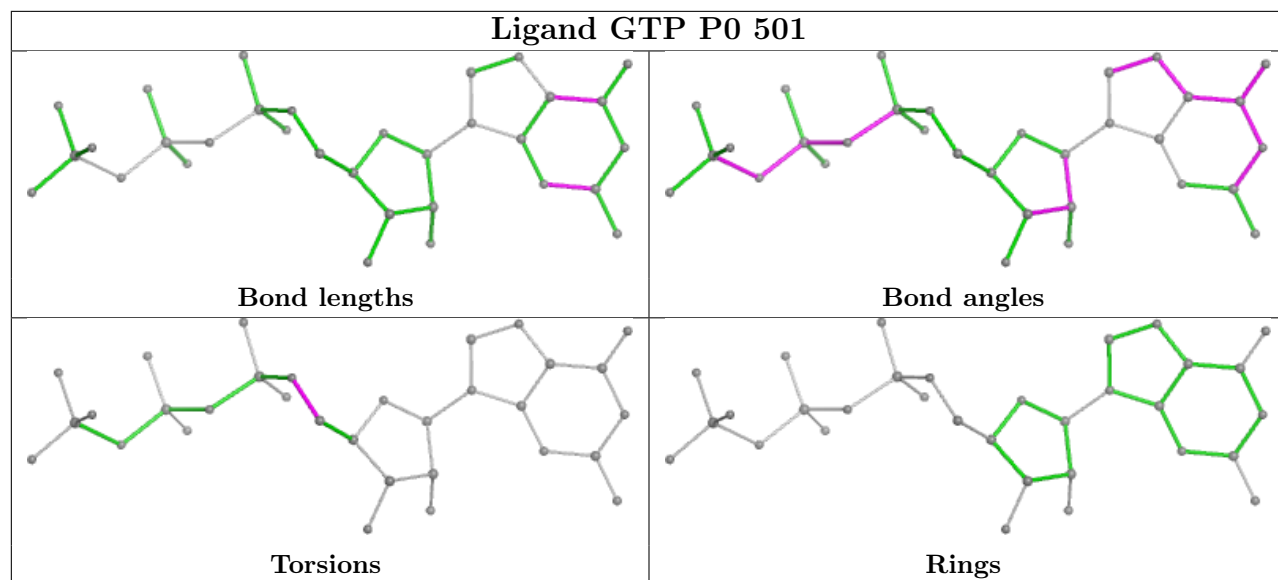


## Ligand GDP R1 501



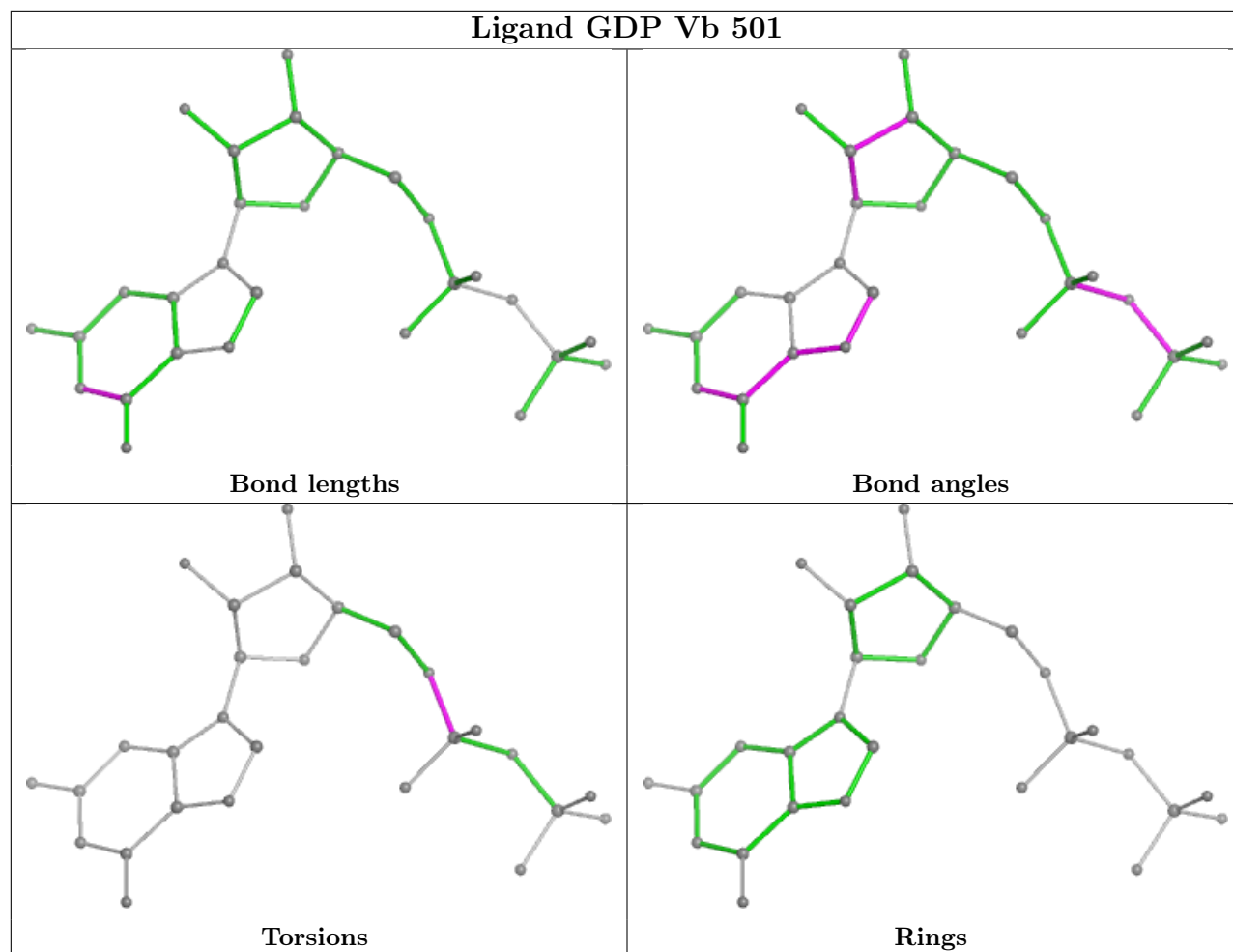
## Ligand GTP UE 501



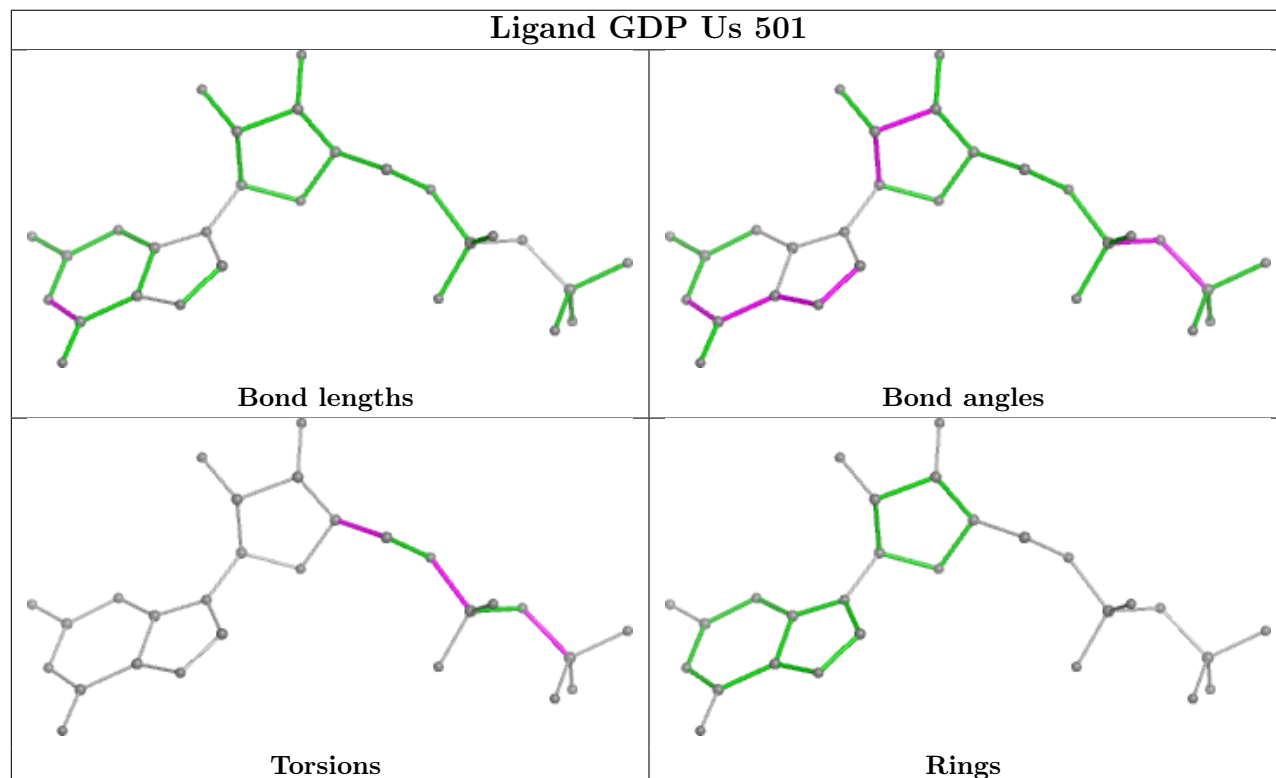


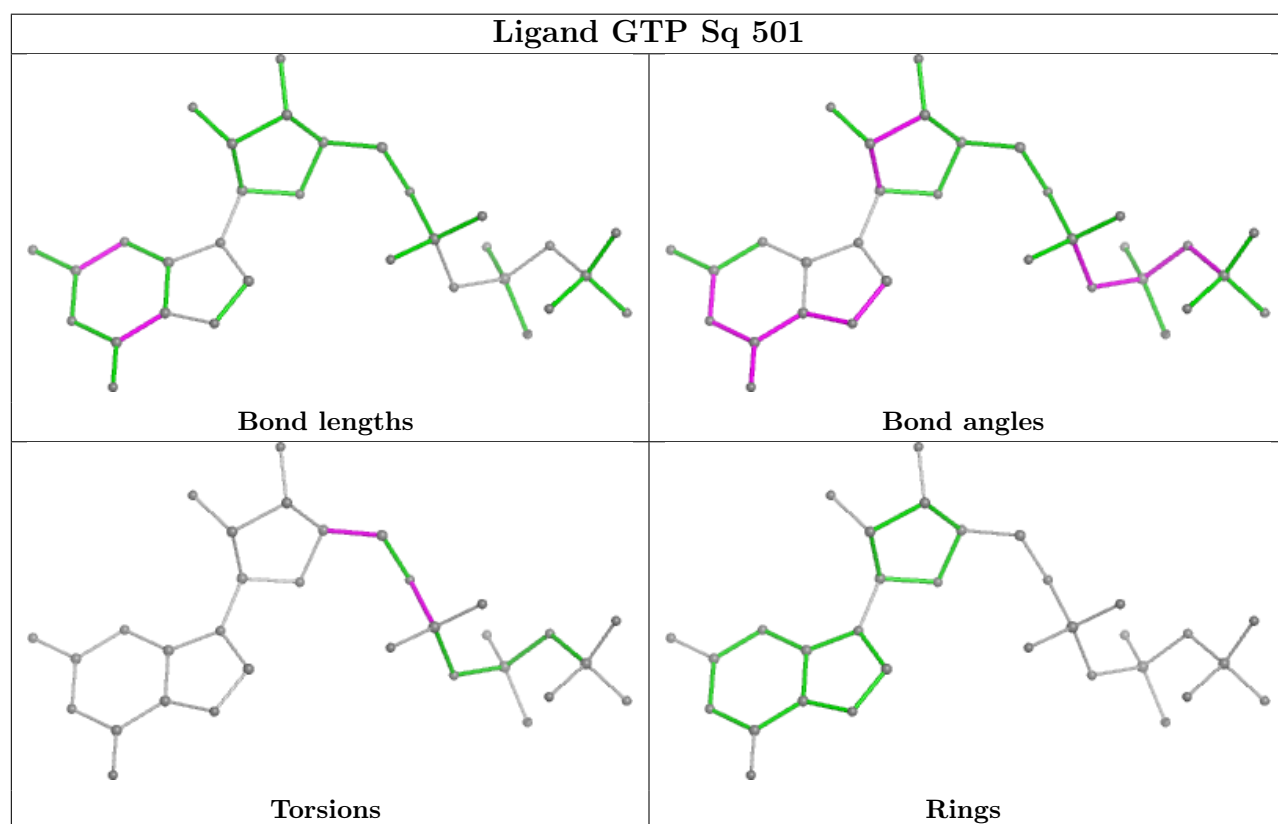
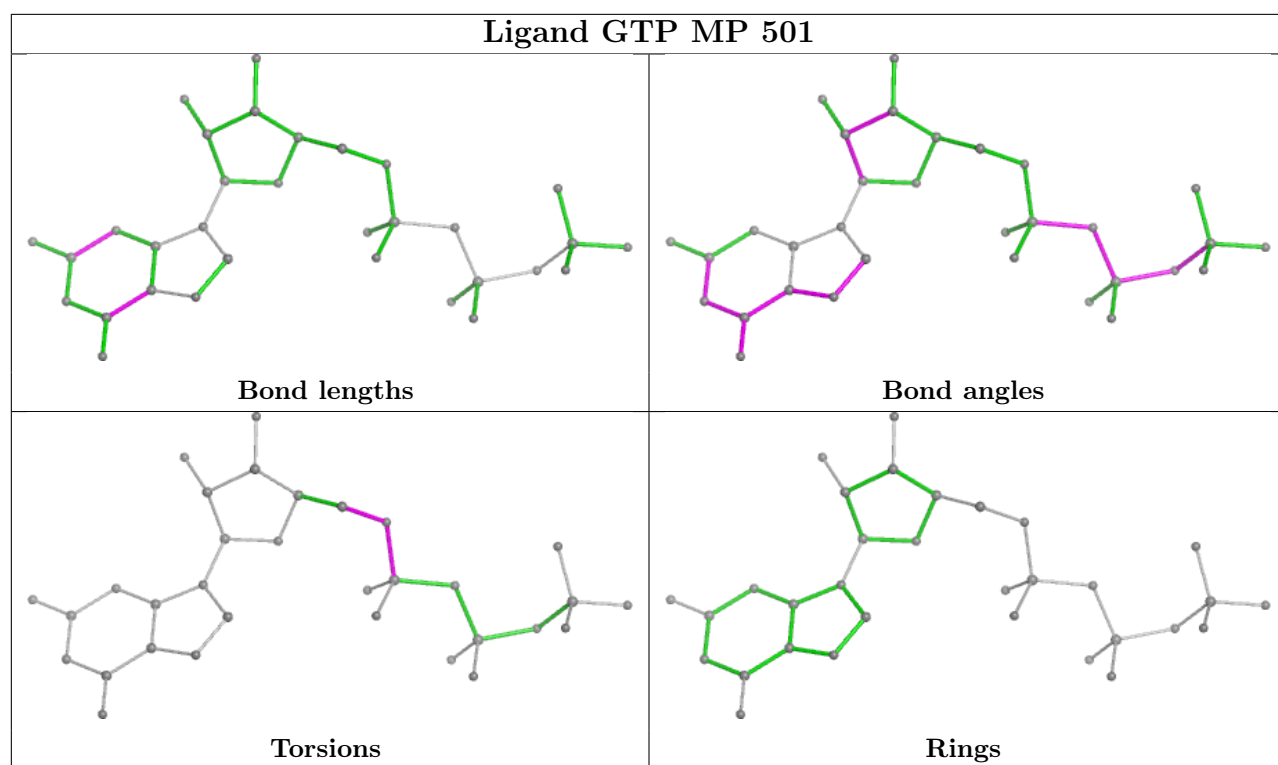


## Ligand GDP Vb 501

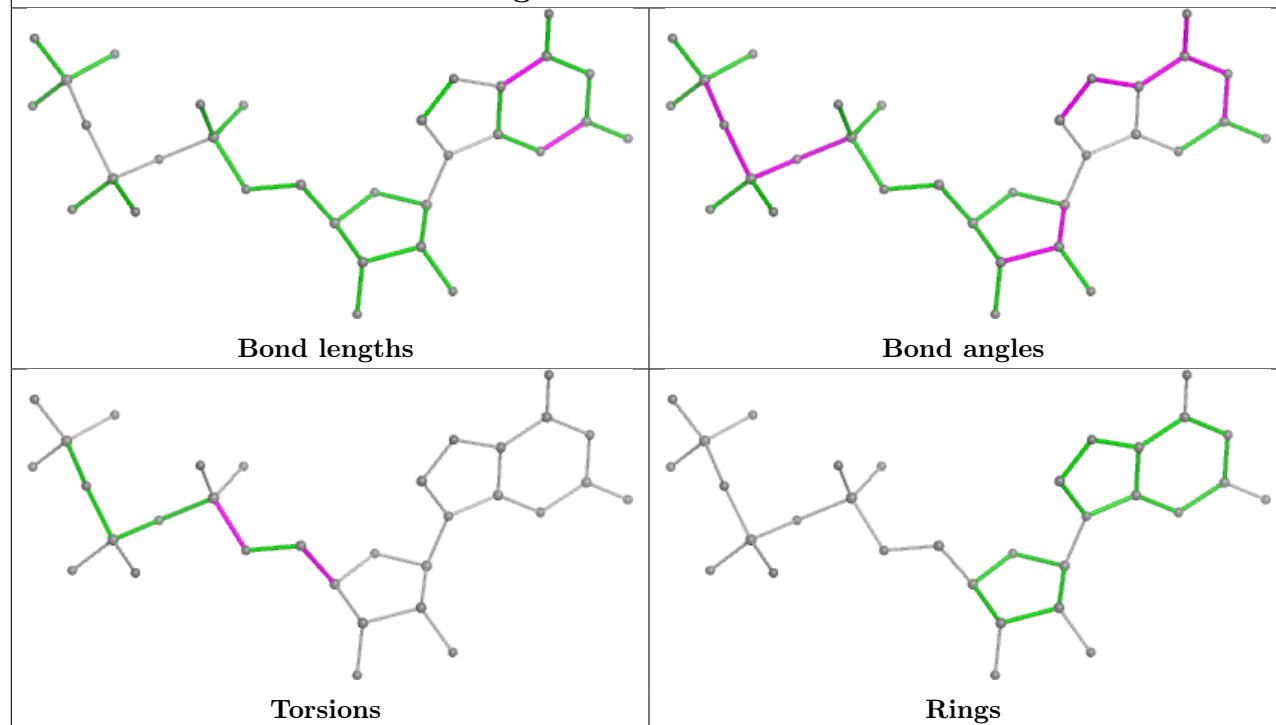


## Ligand GDP Us 501

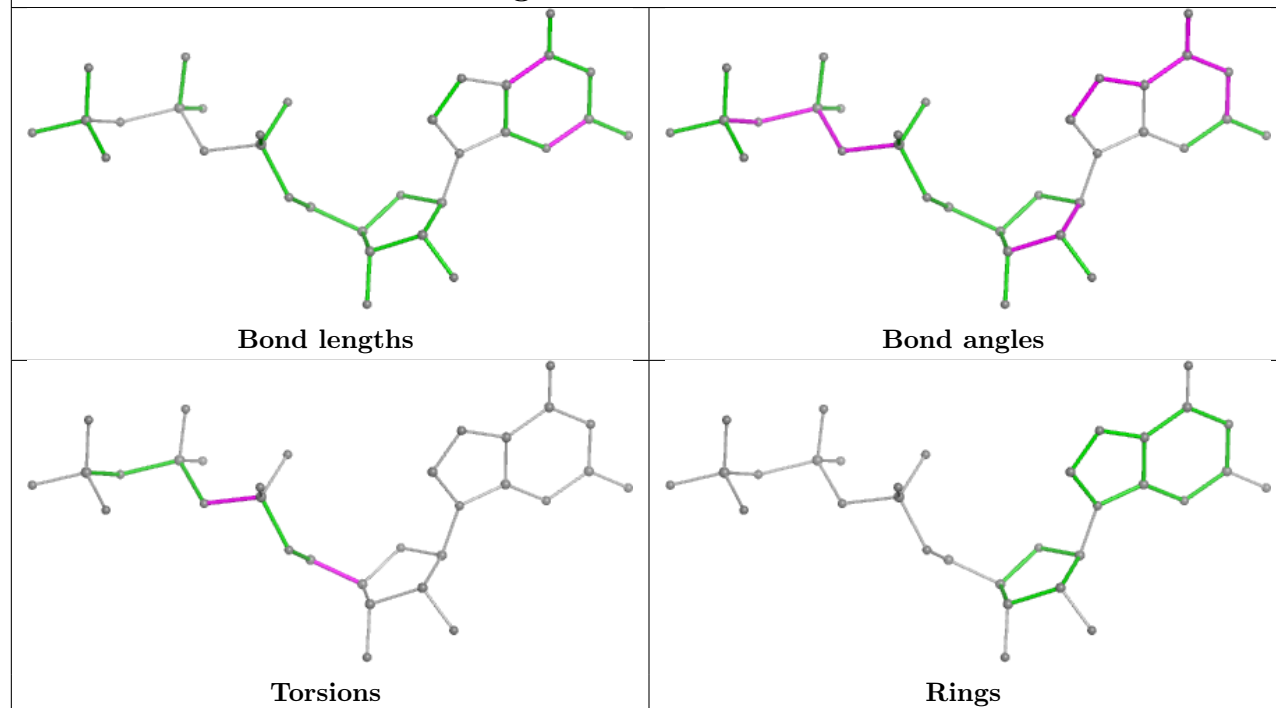




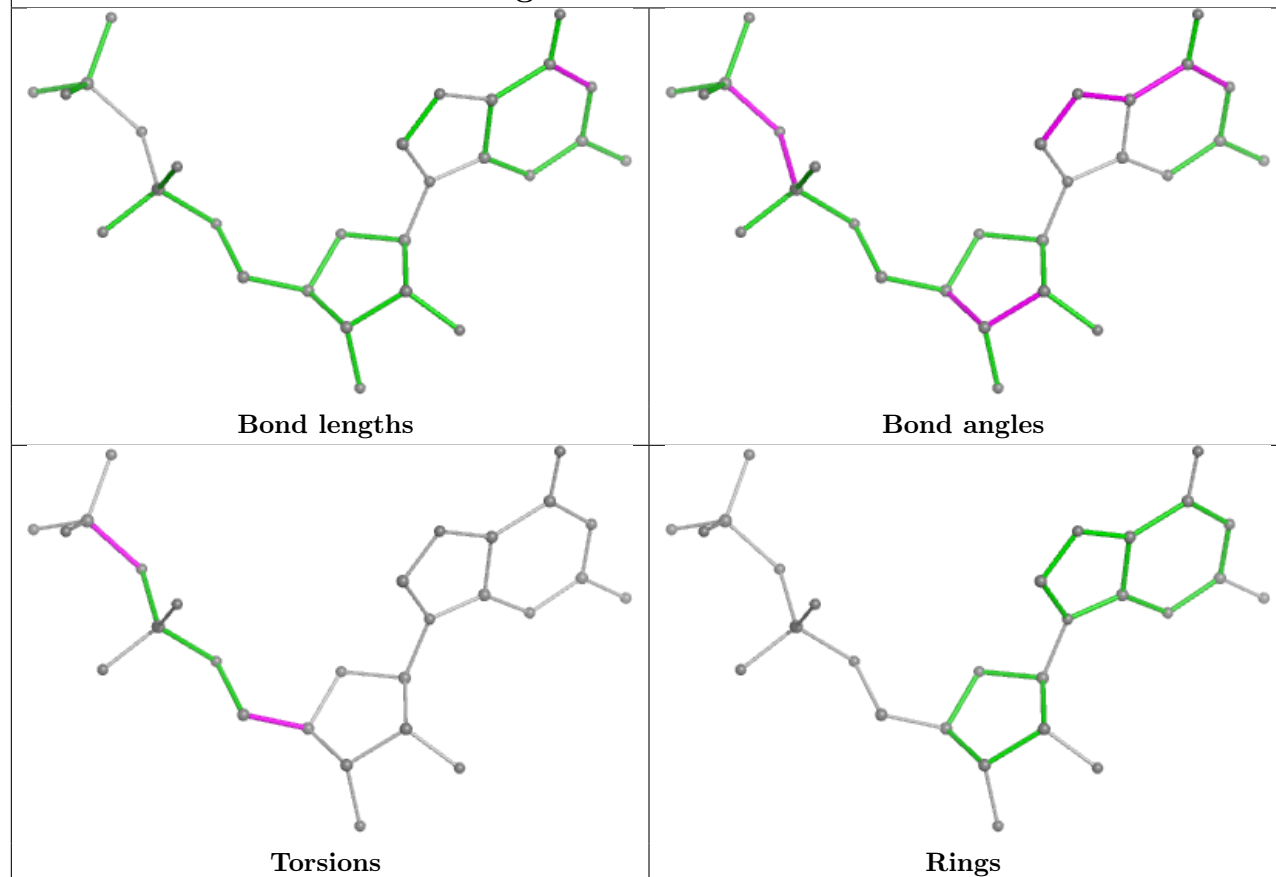
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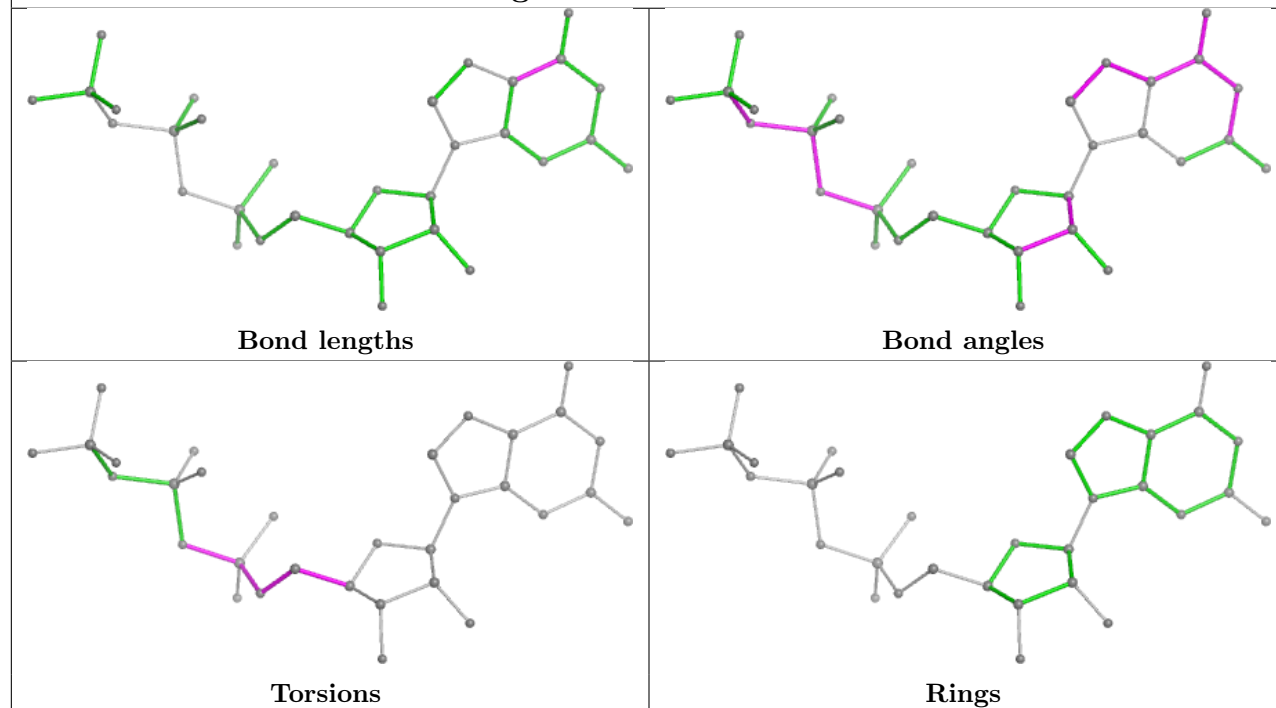
## Ligand GTP WC 501



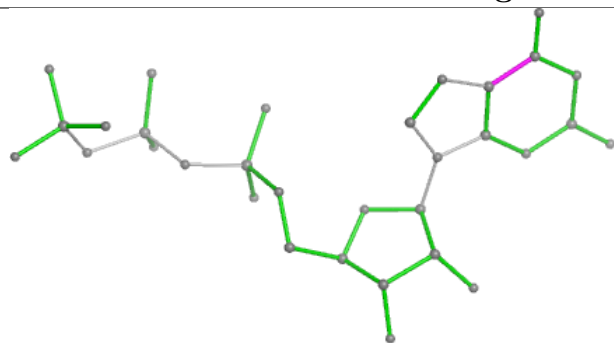
## Ligand GDP VB 501



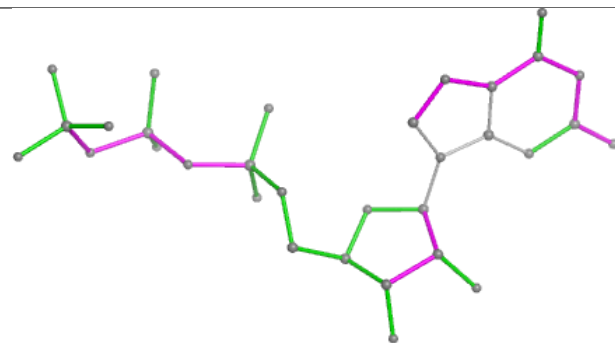
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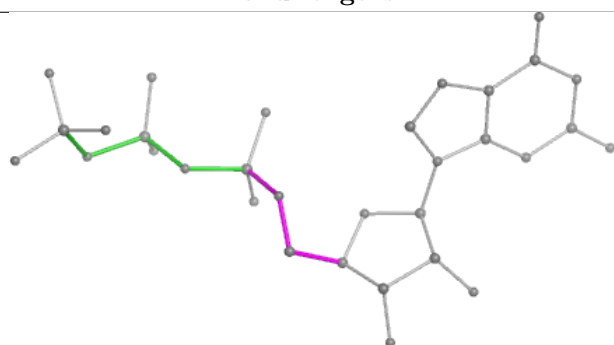
## Ligand GTP UM 502



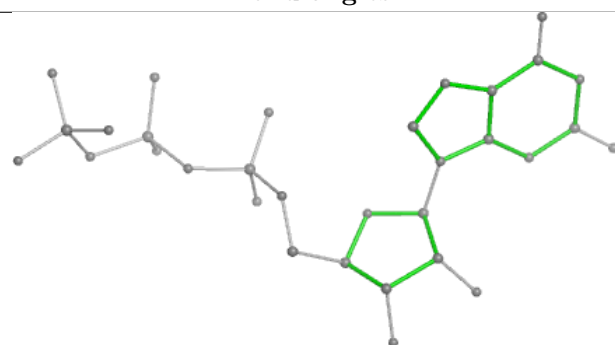
Bond lengths



Bond angles

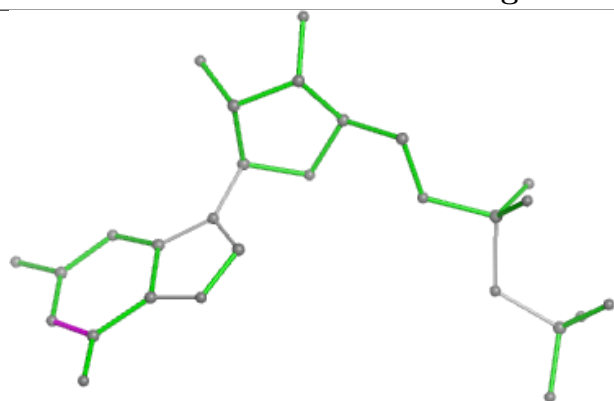


Torsions

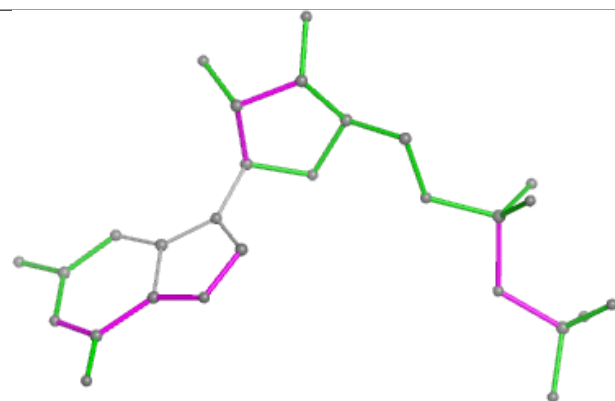


Rings

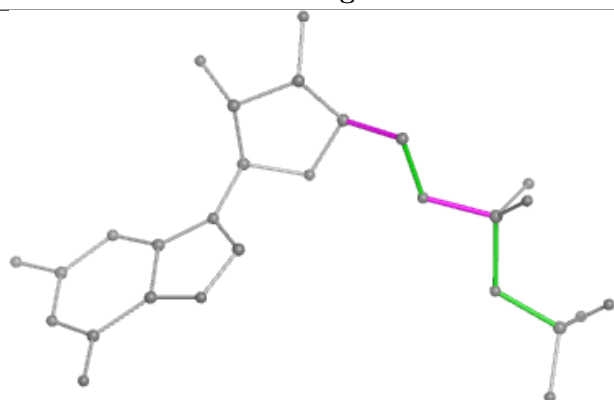
## Ligand GDP SX 501



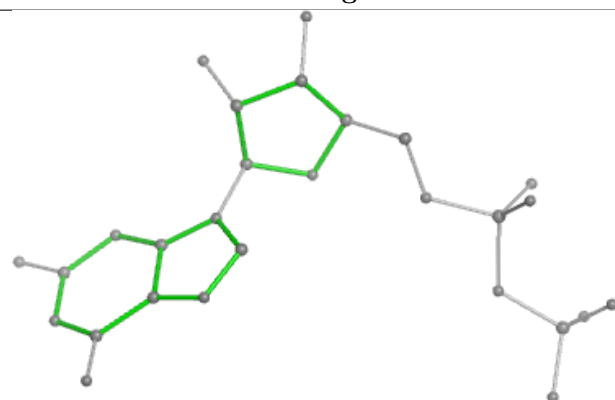
Bond lengths



Bond angles

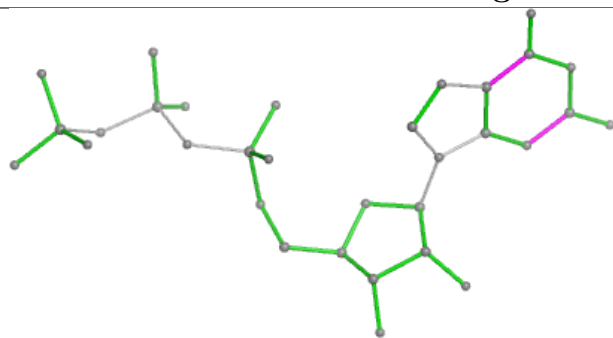


Torsions

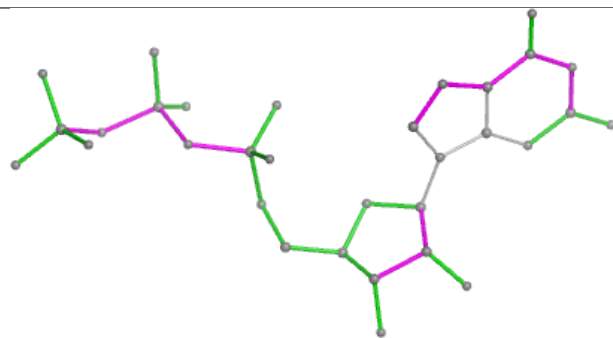


Rings

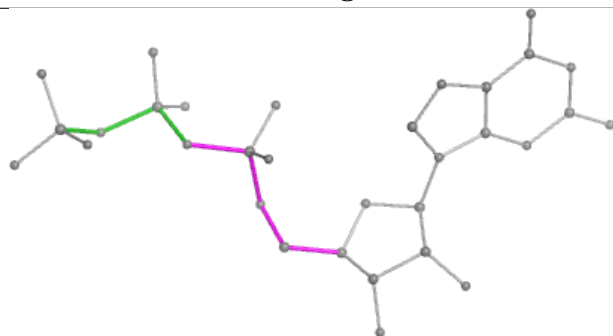
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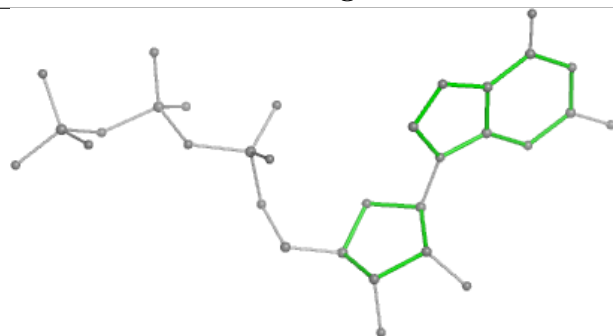
Bond lengths



Bond angles

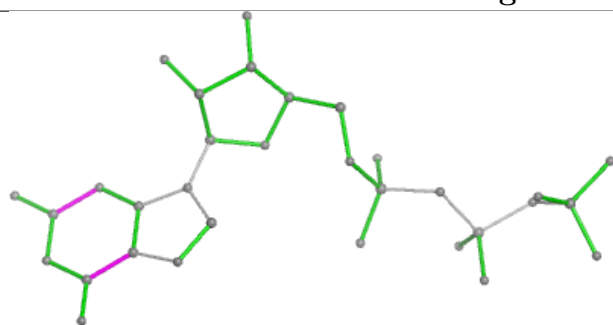


Torsions

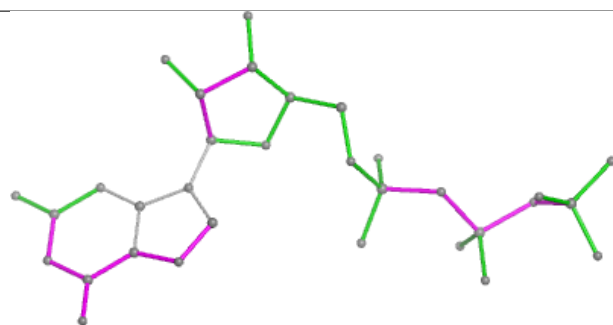


Rings

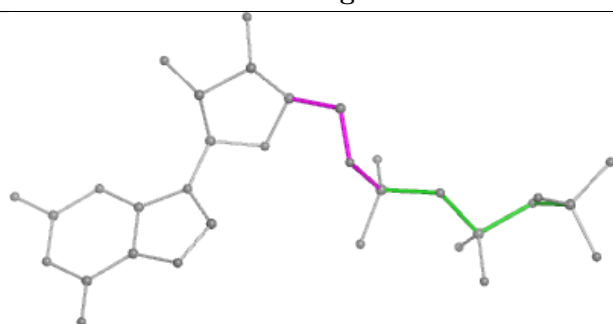
## Ligand GTP KC 501



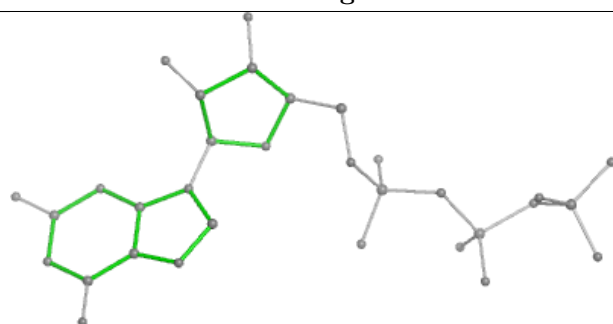
Bond lengths



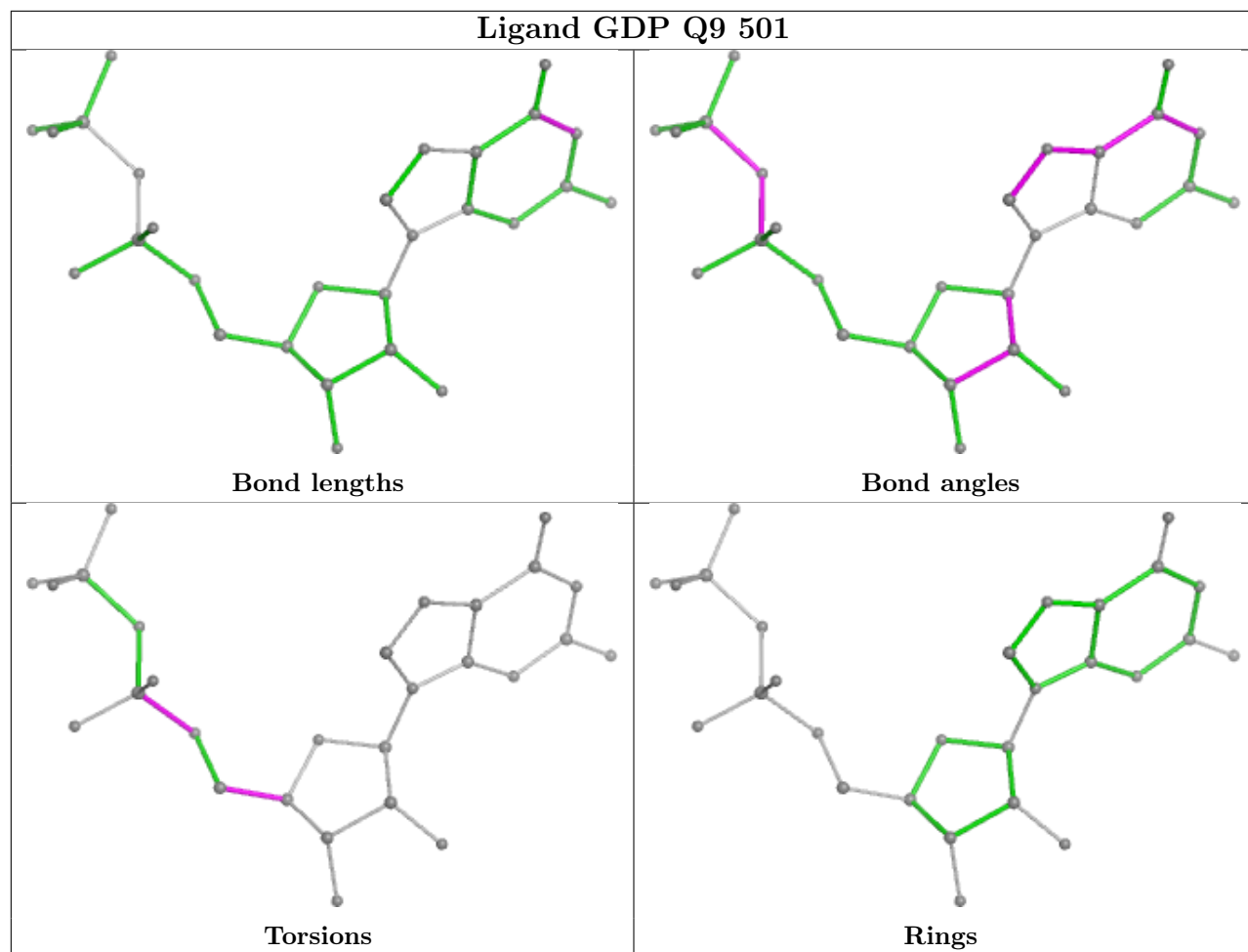
Bond angles

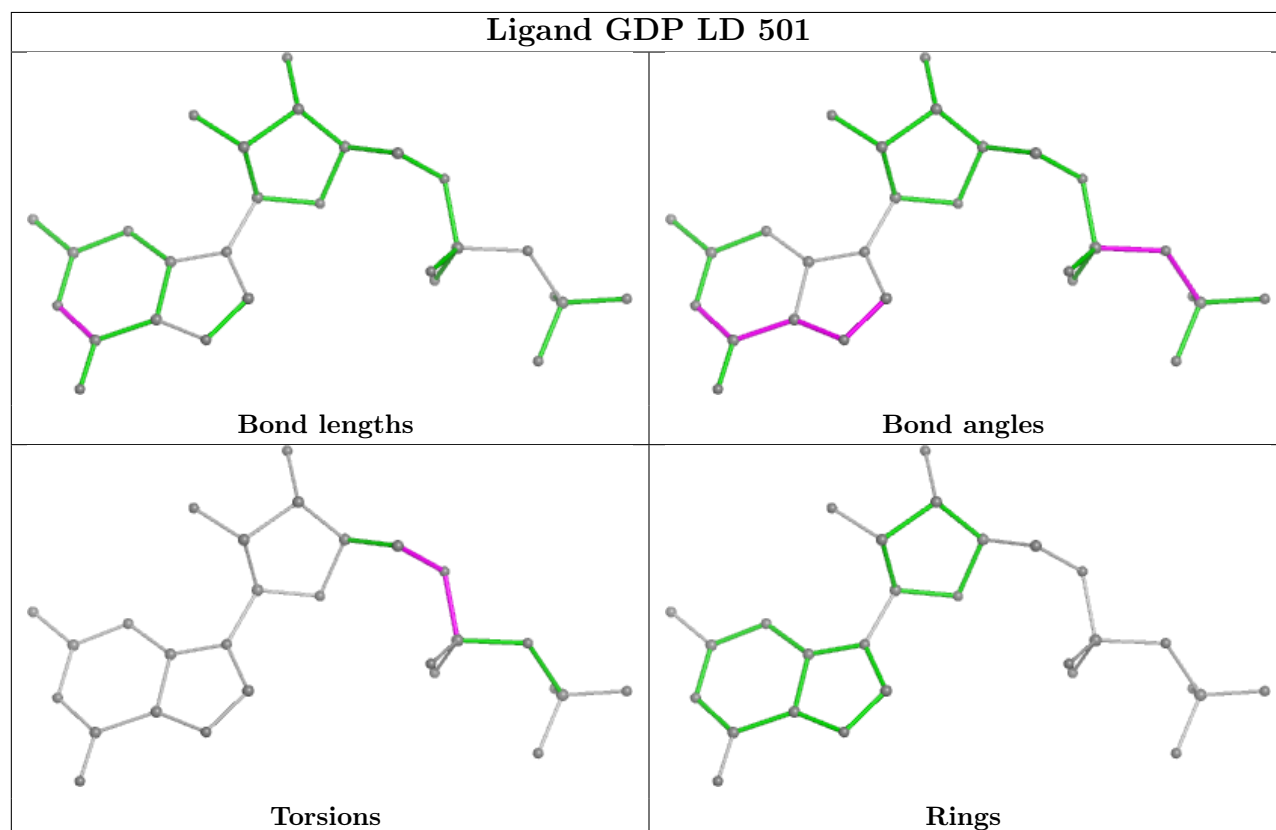
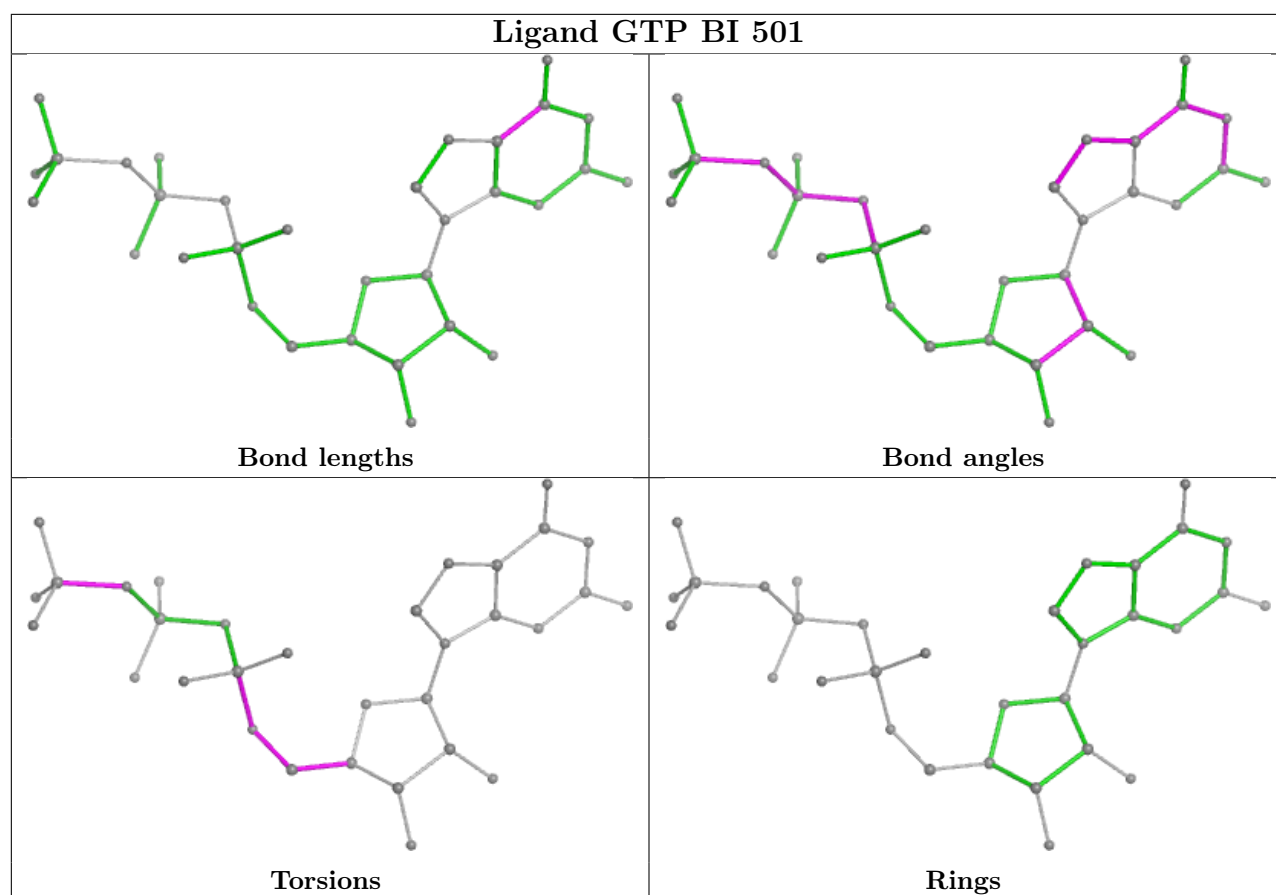


Torsions

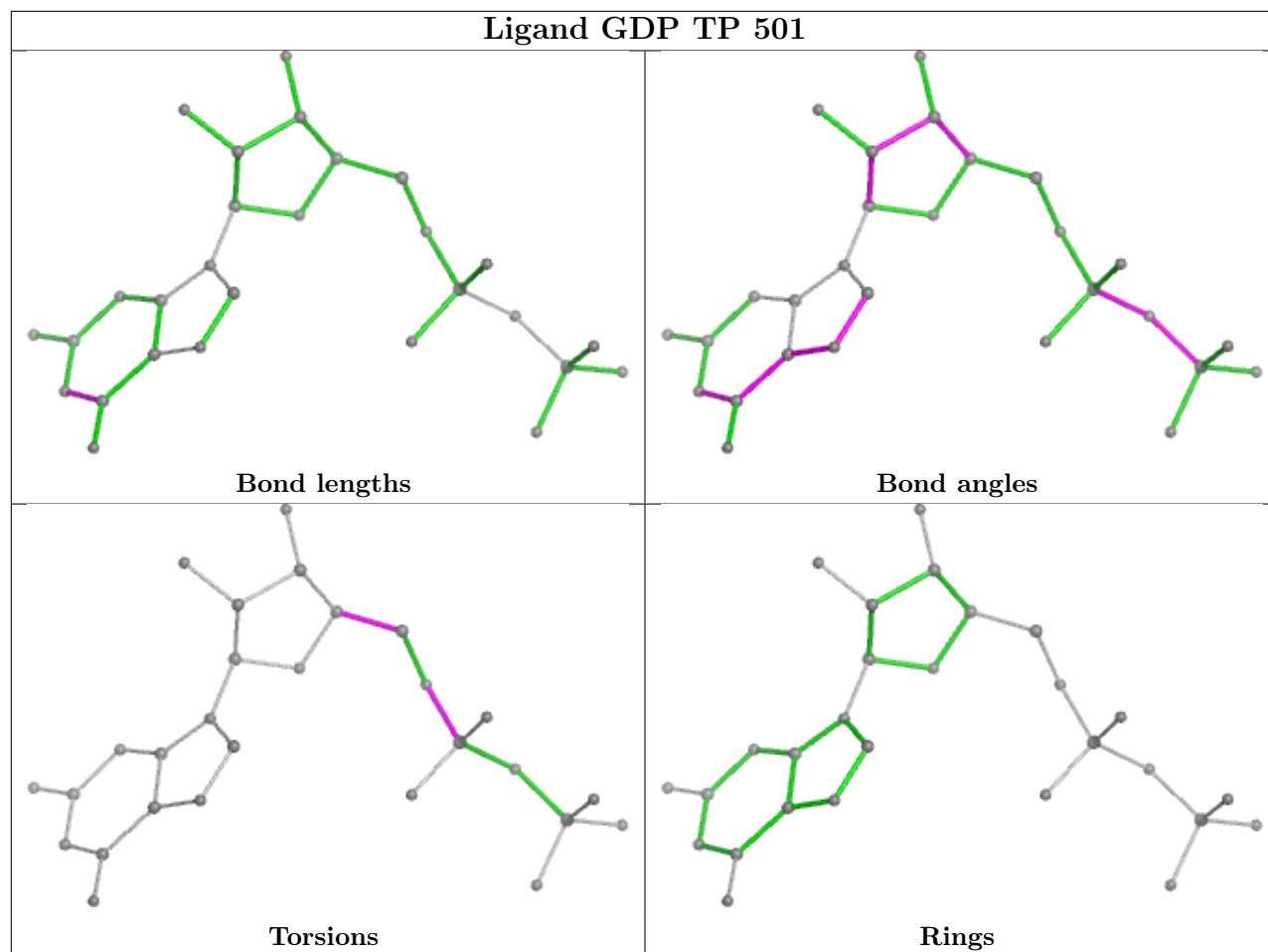


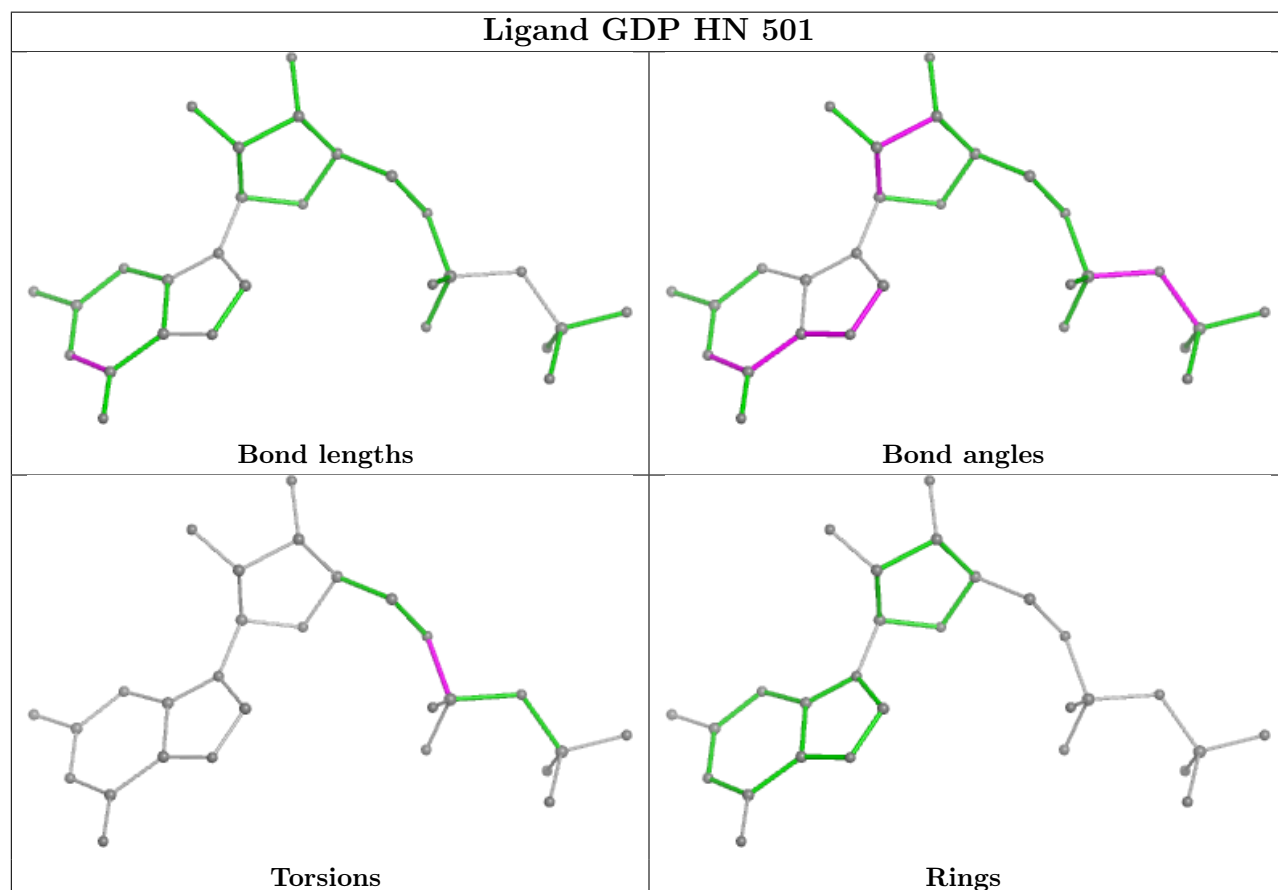
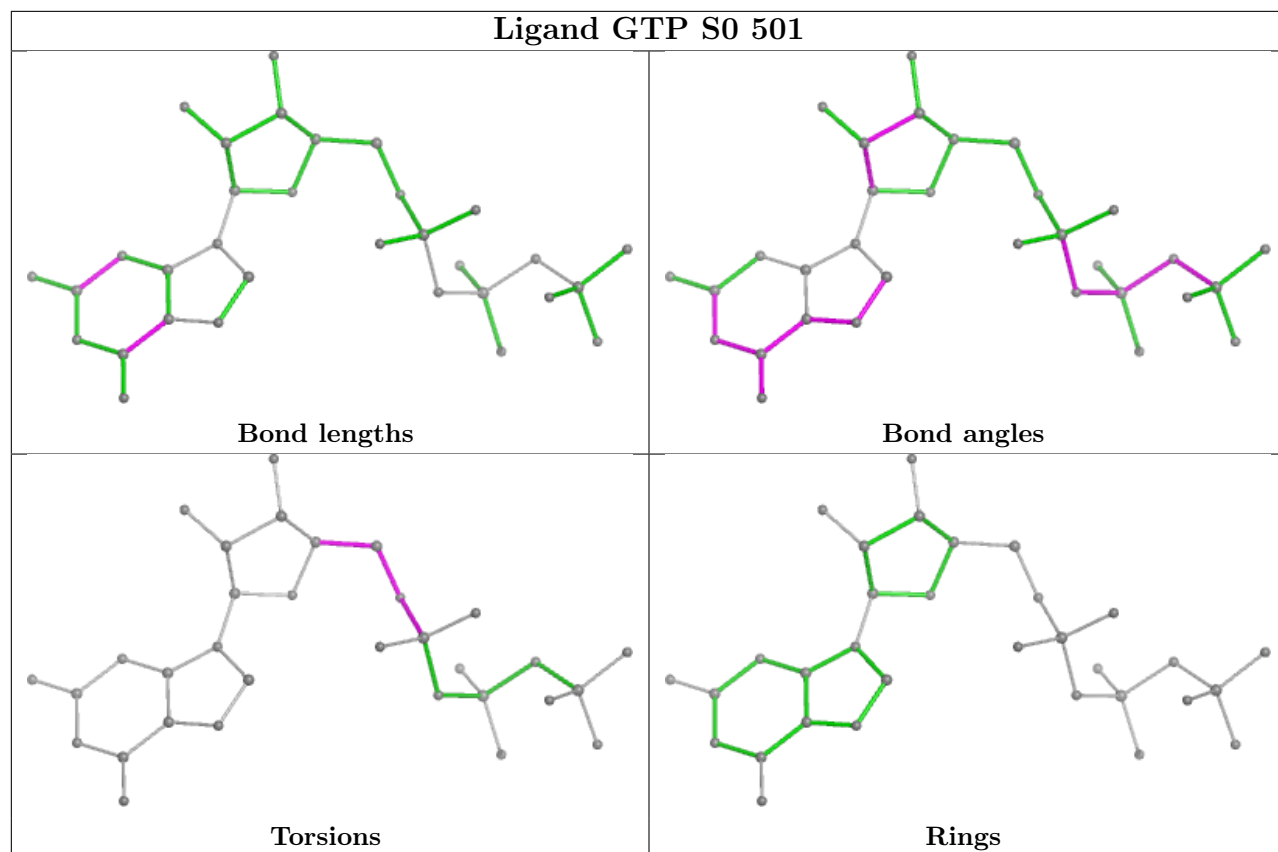
Rings



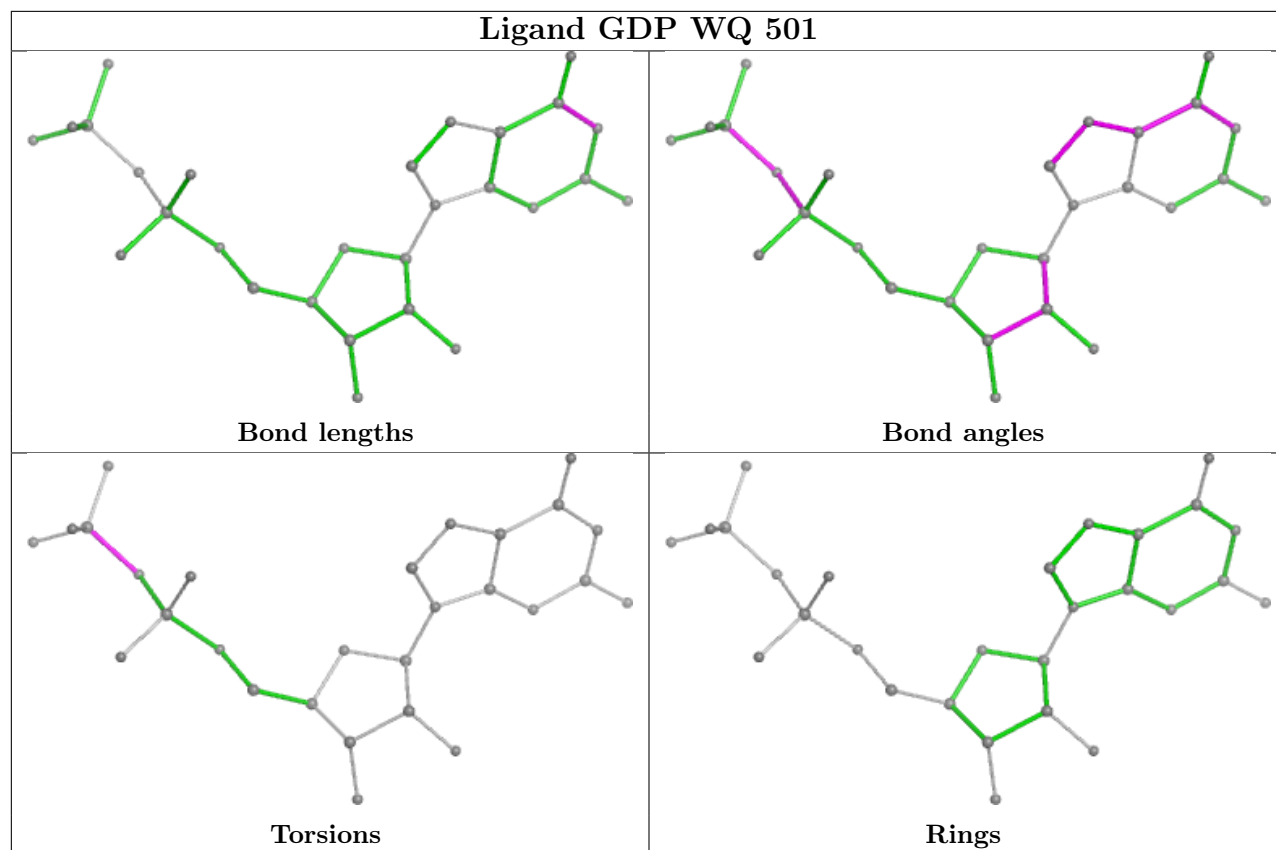




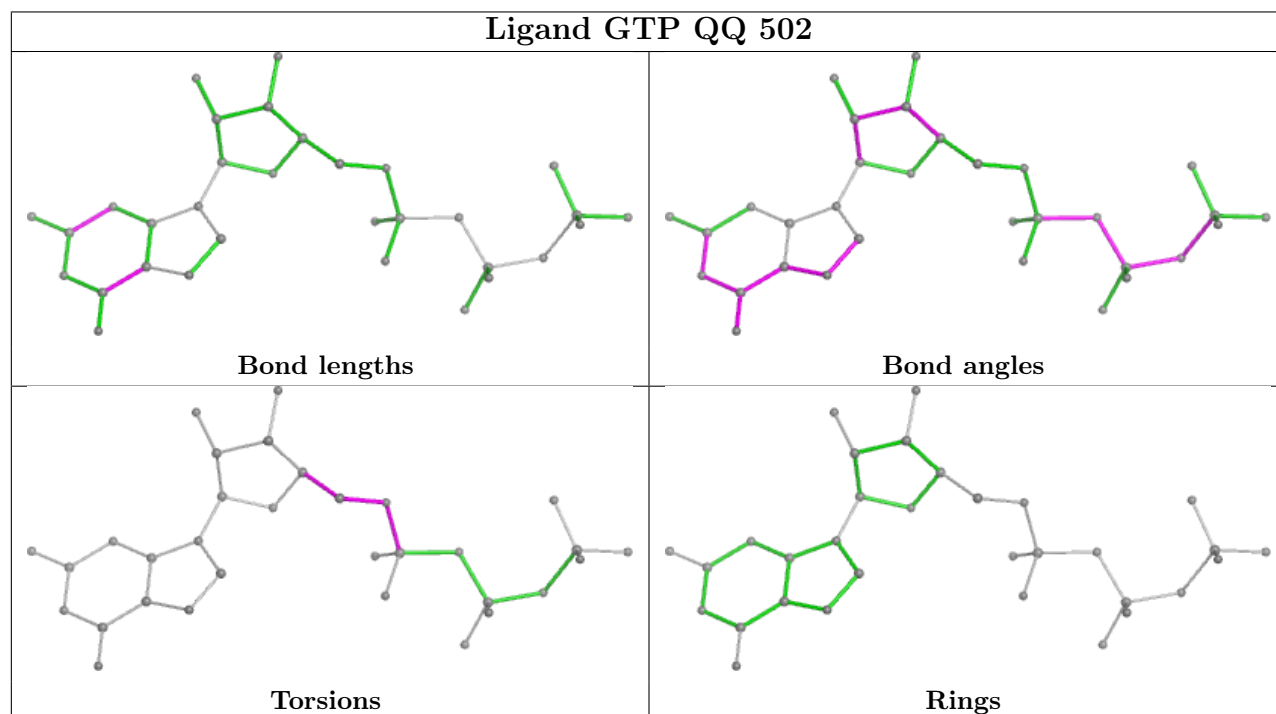




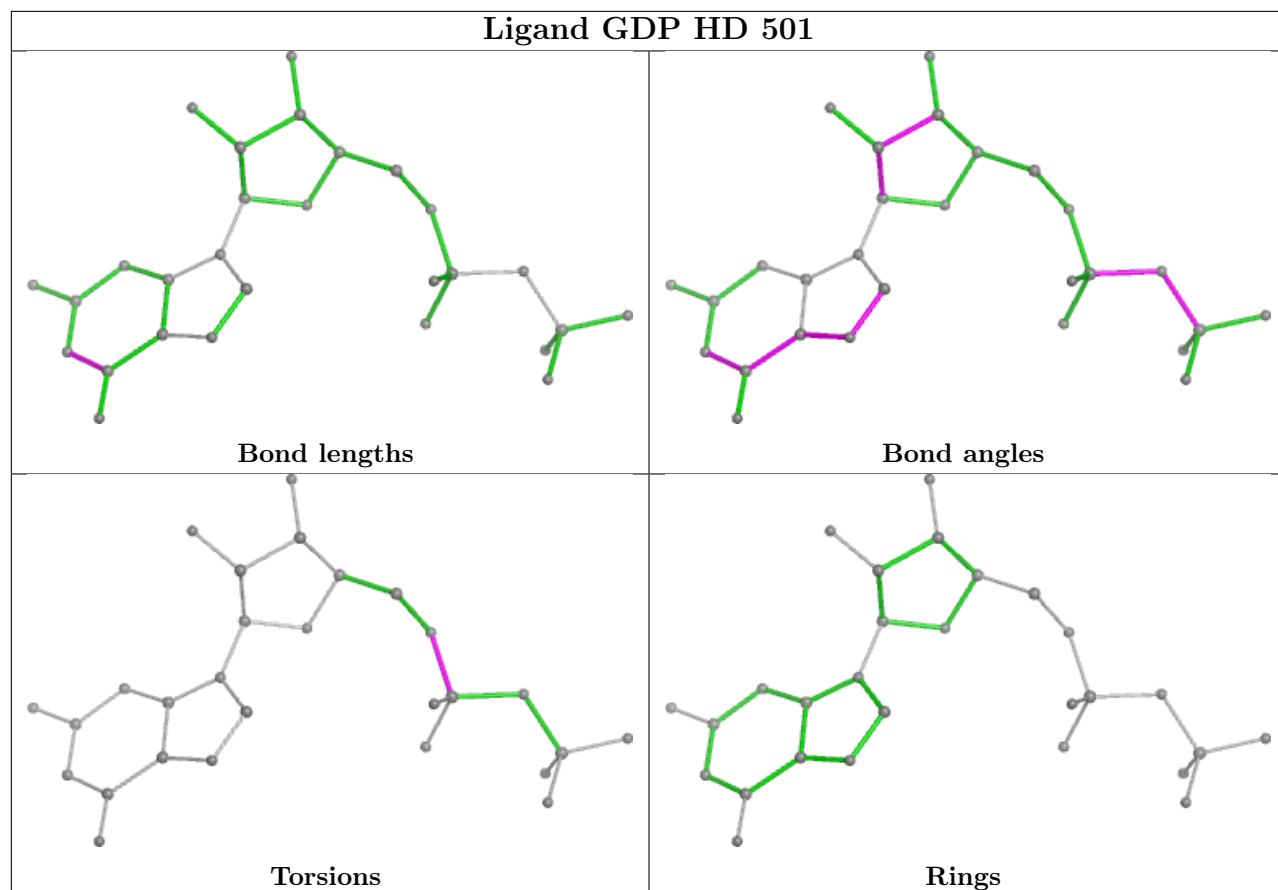
## Ligand GDP WQ 501



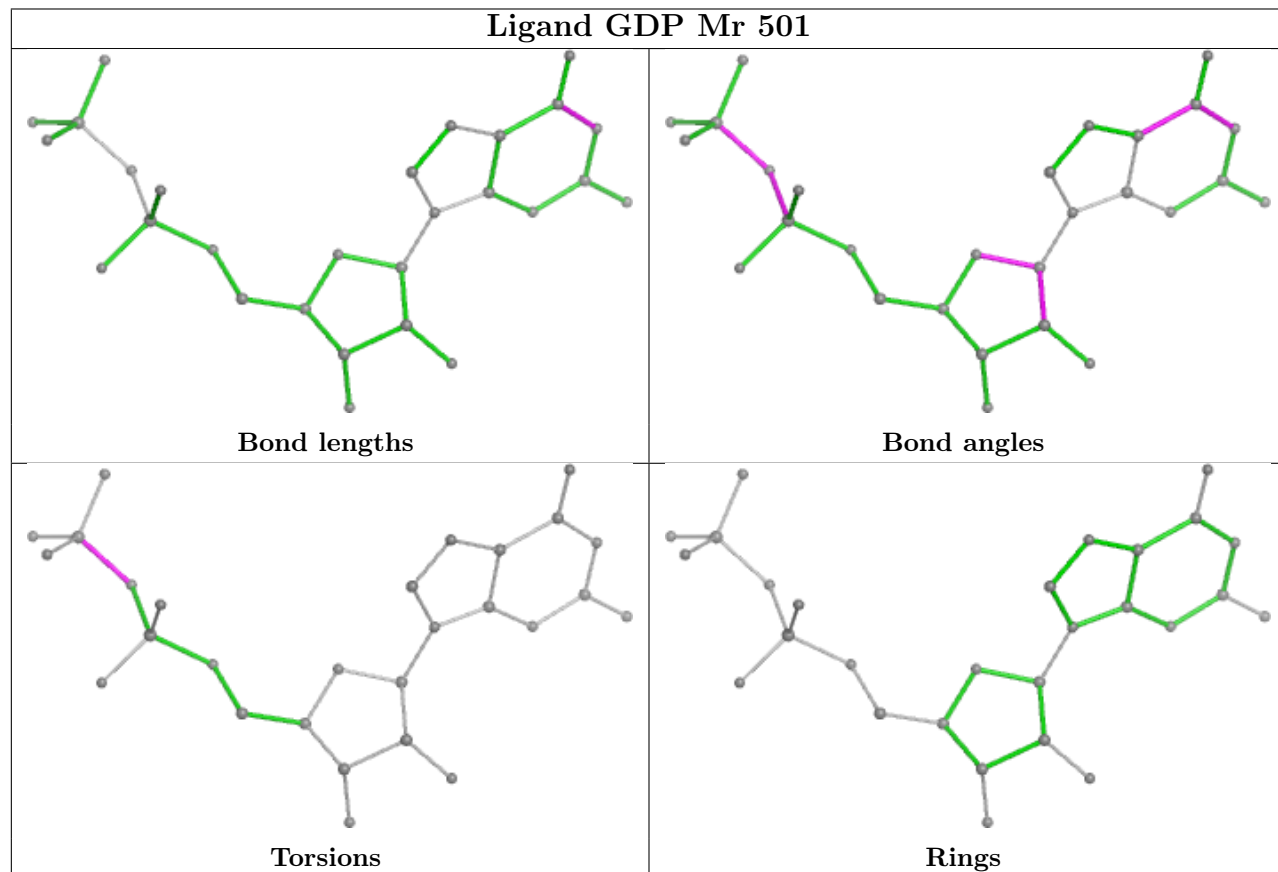
## Ligand GTP QQ 502

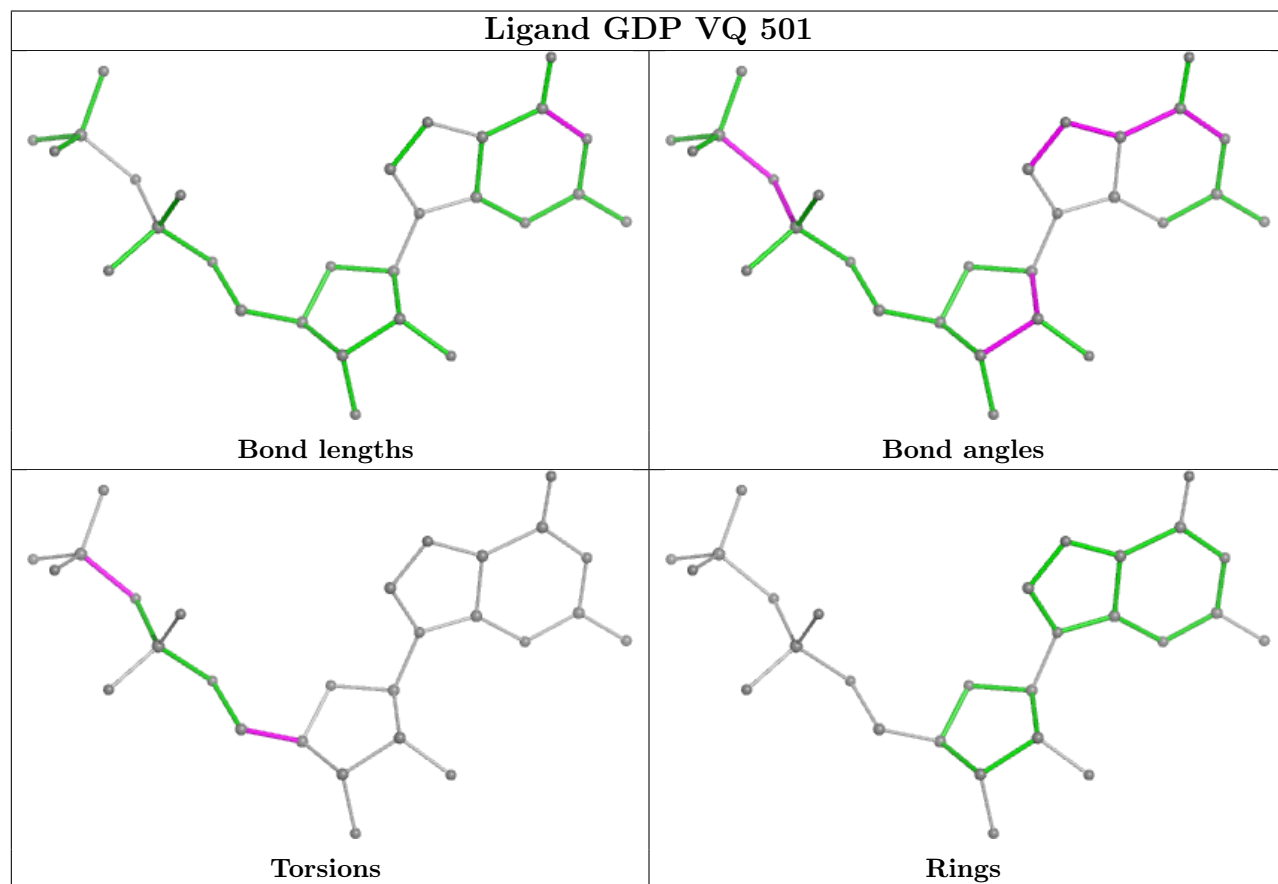
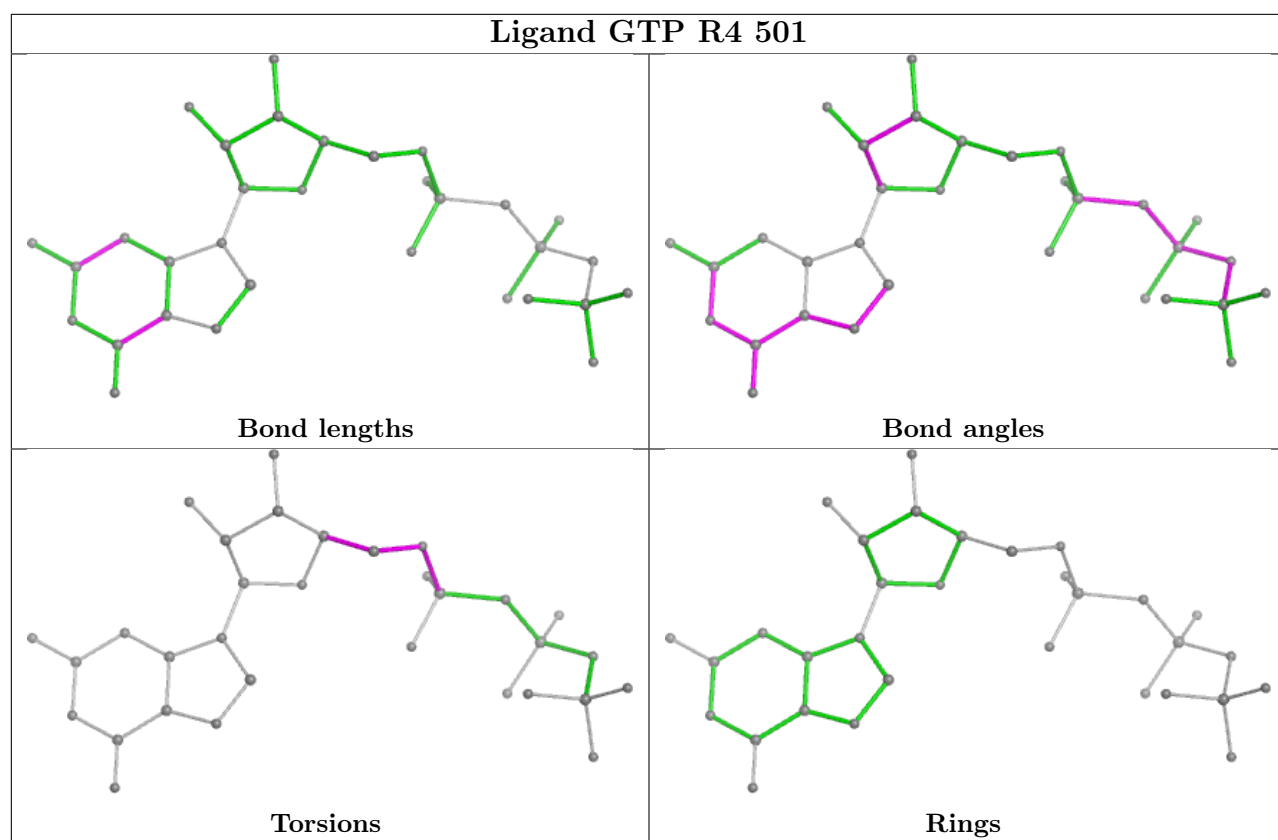


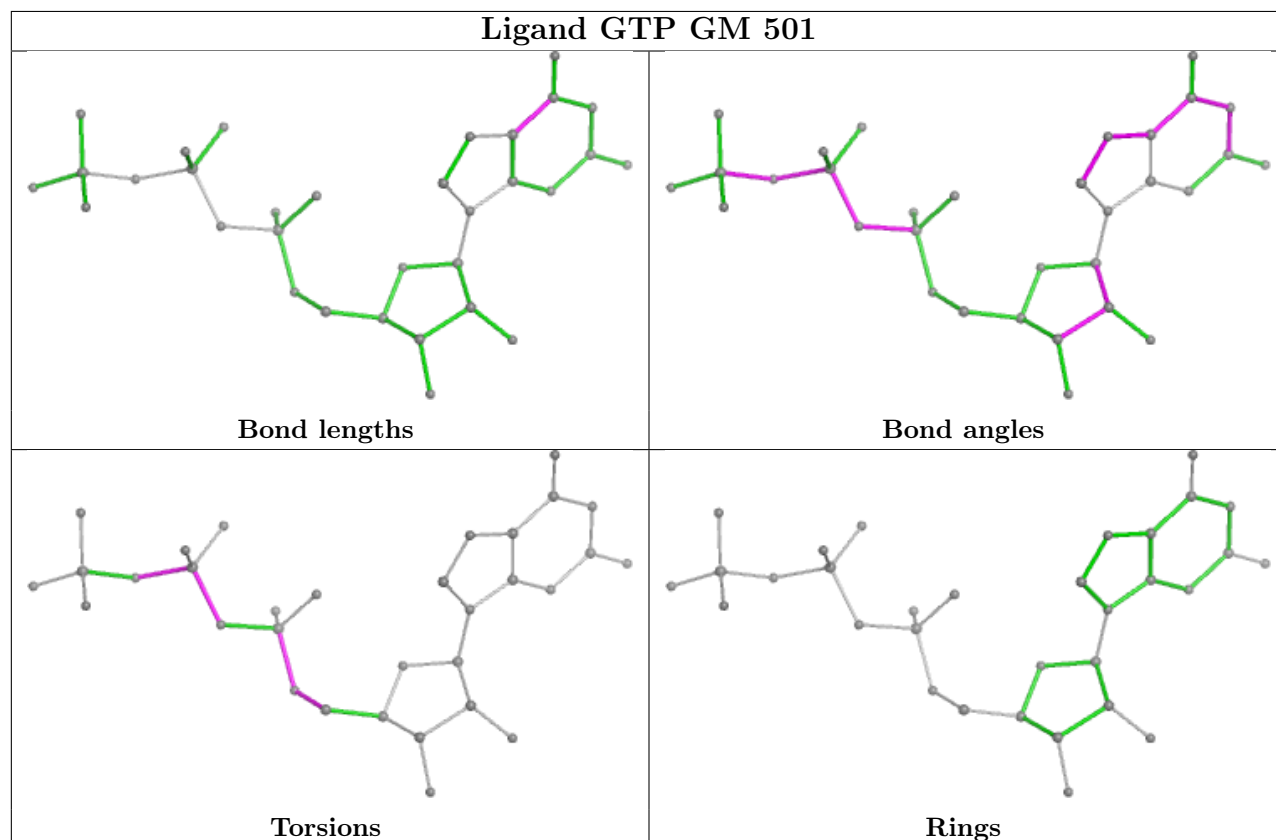
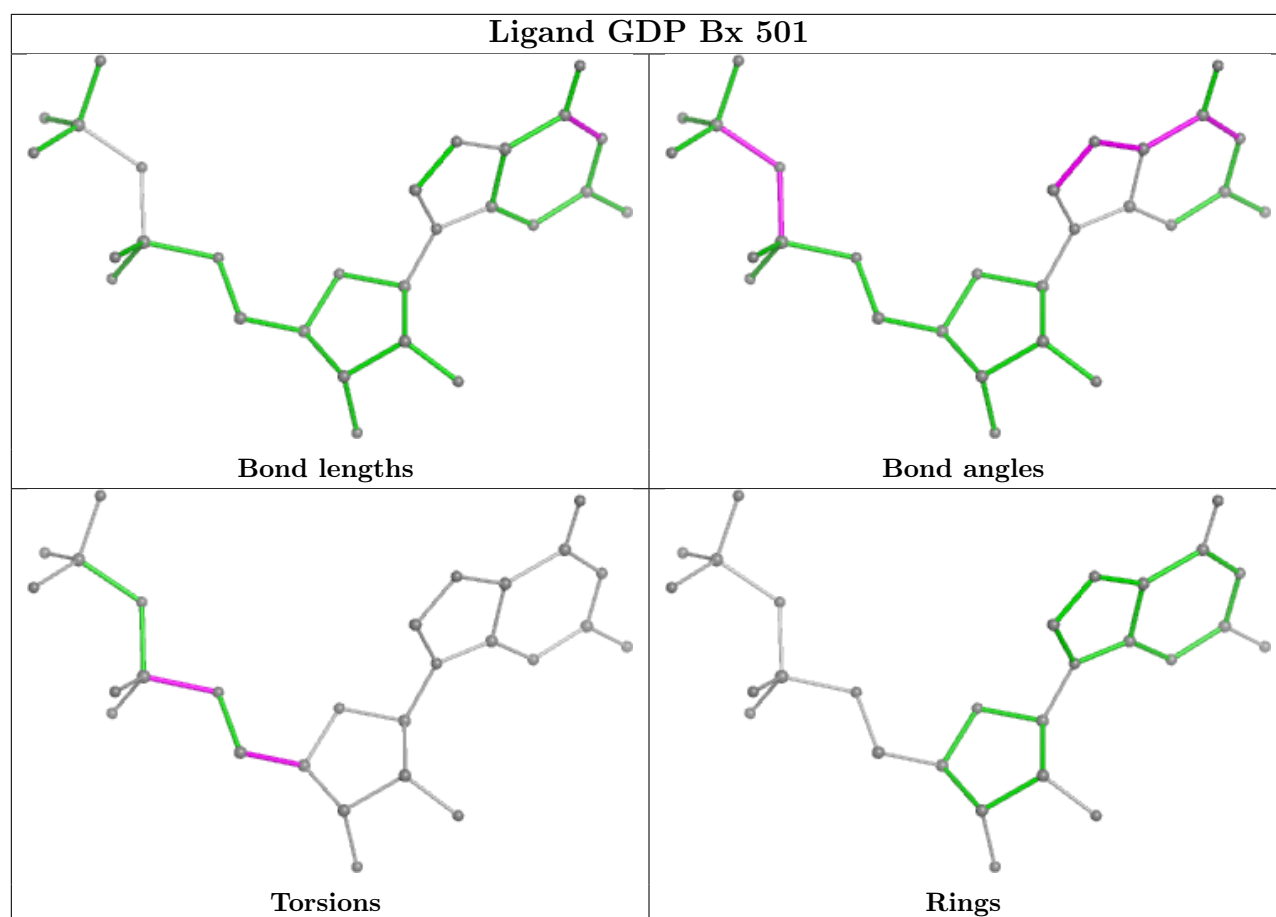
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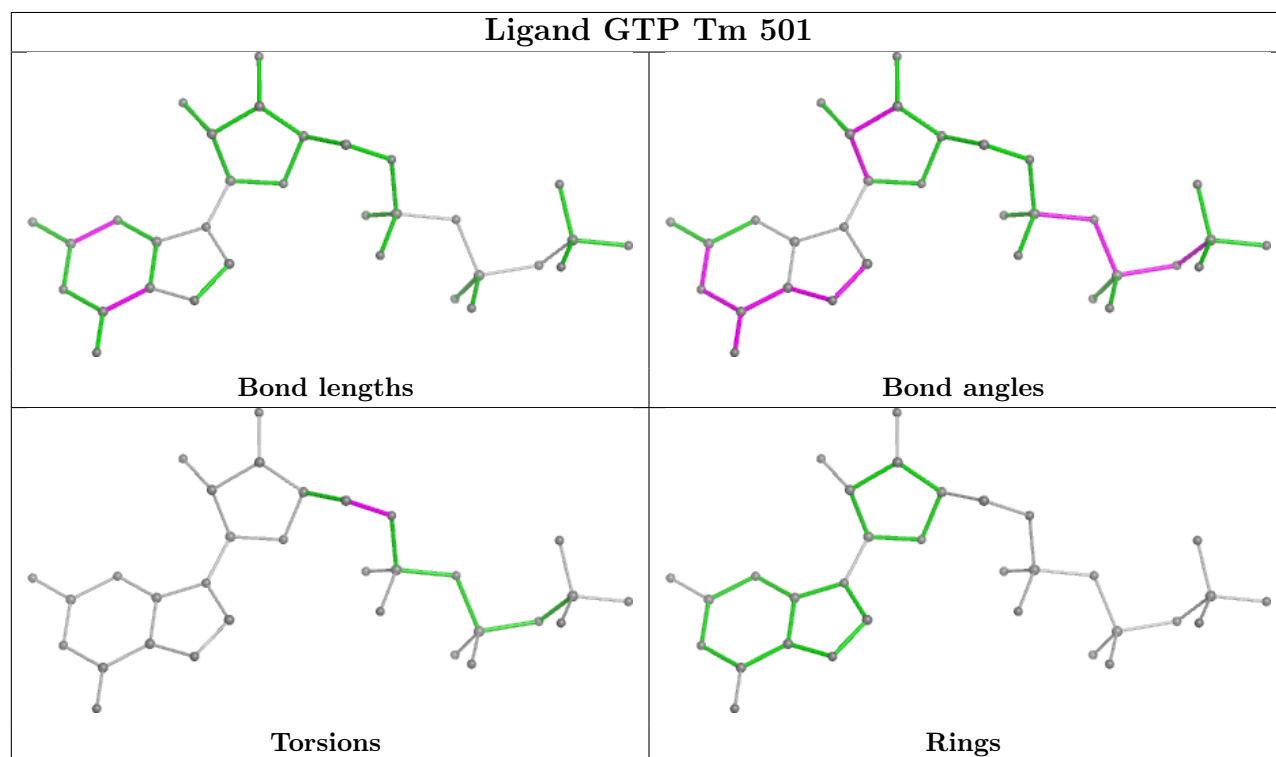
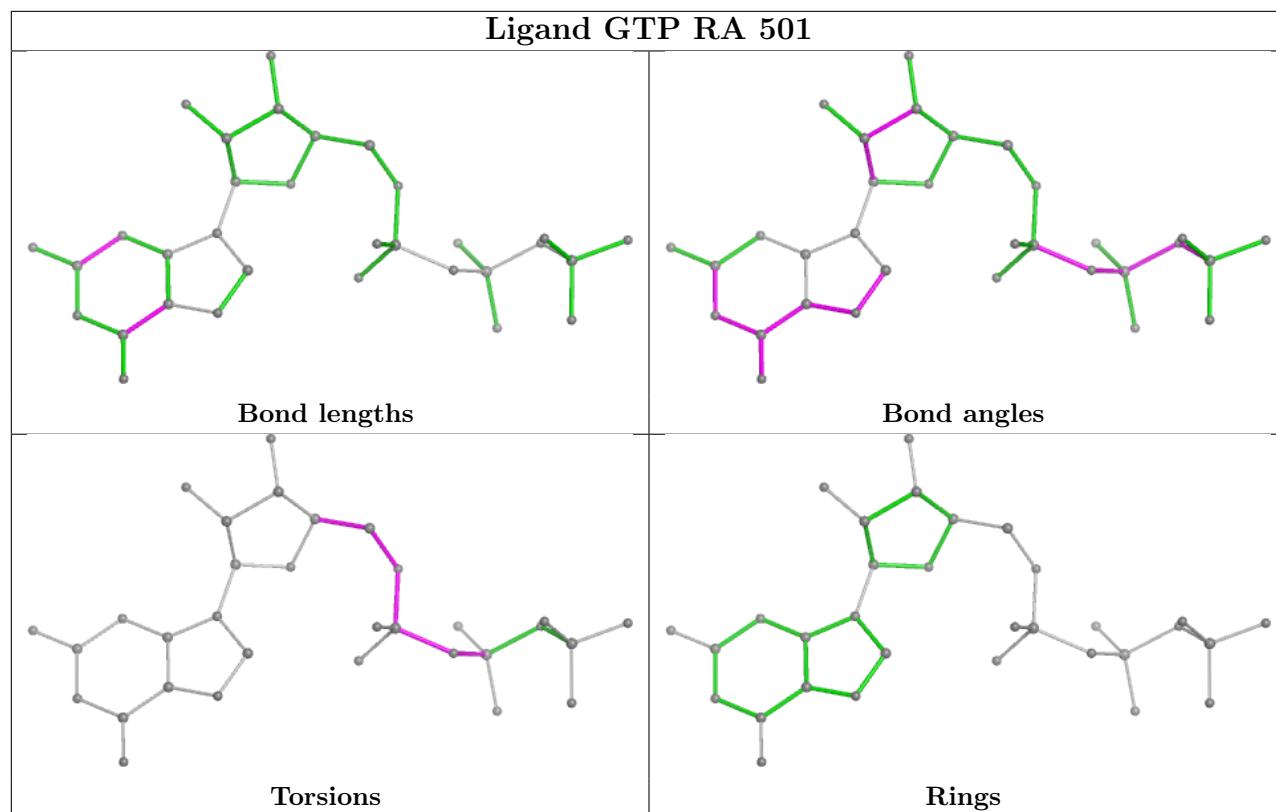


## Ligand GDP Mr 501

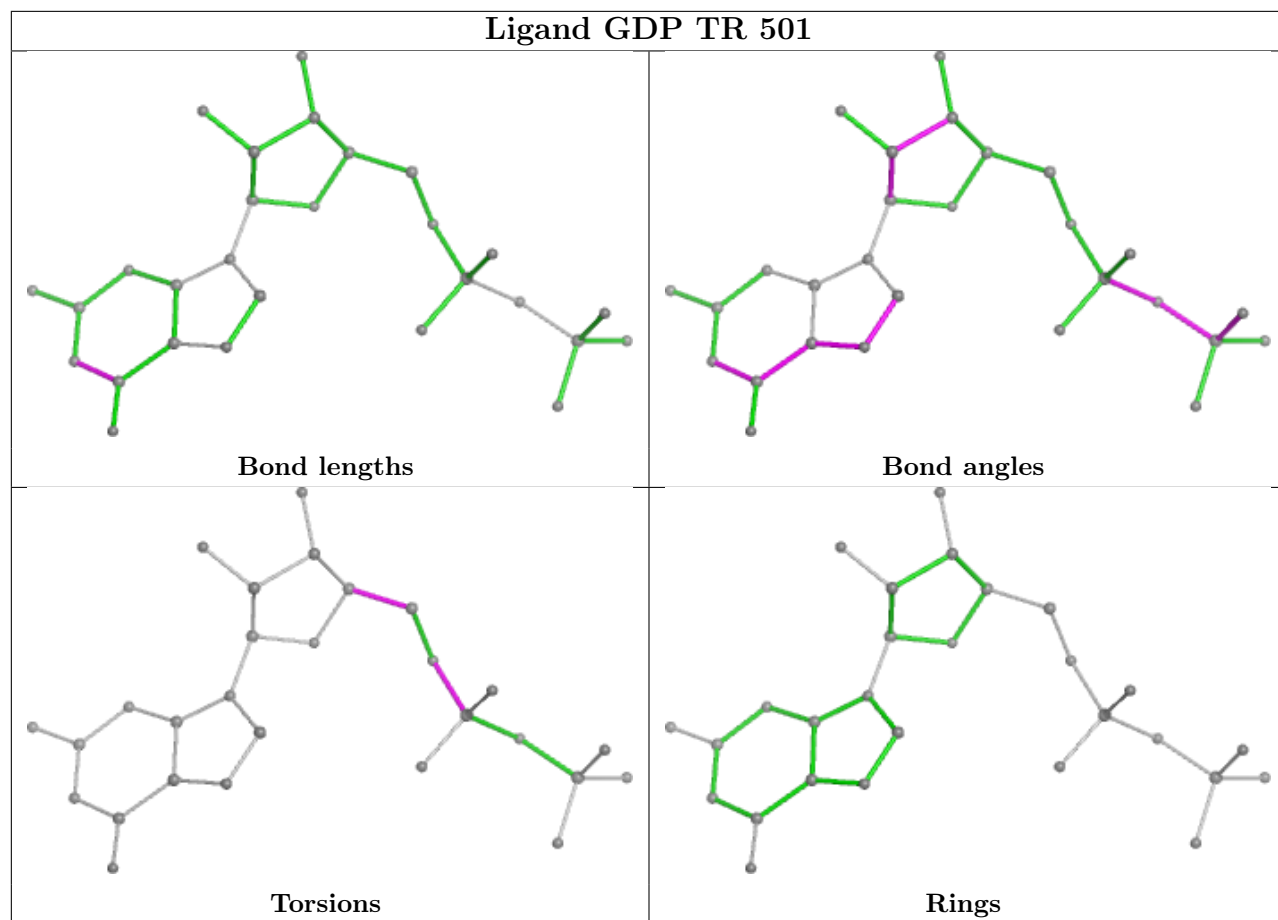




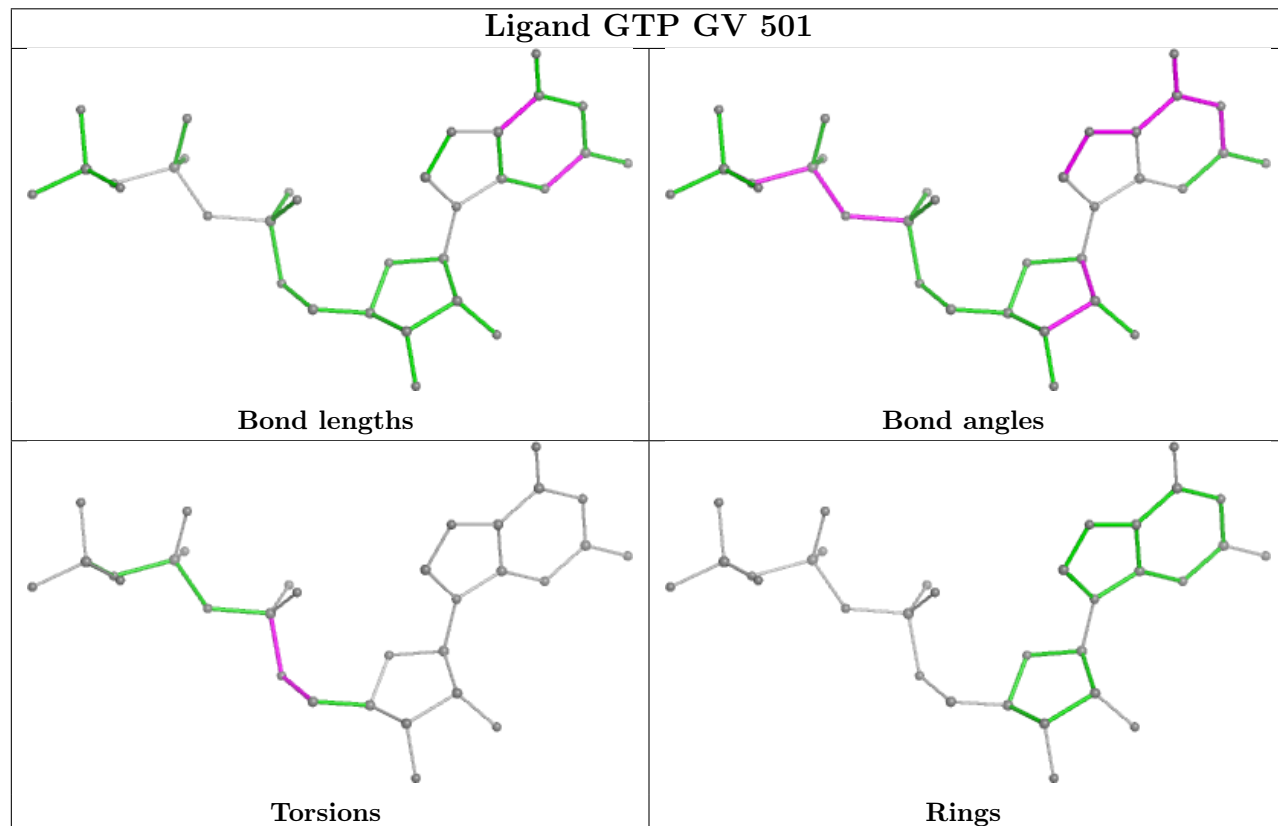




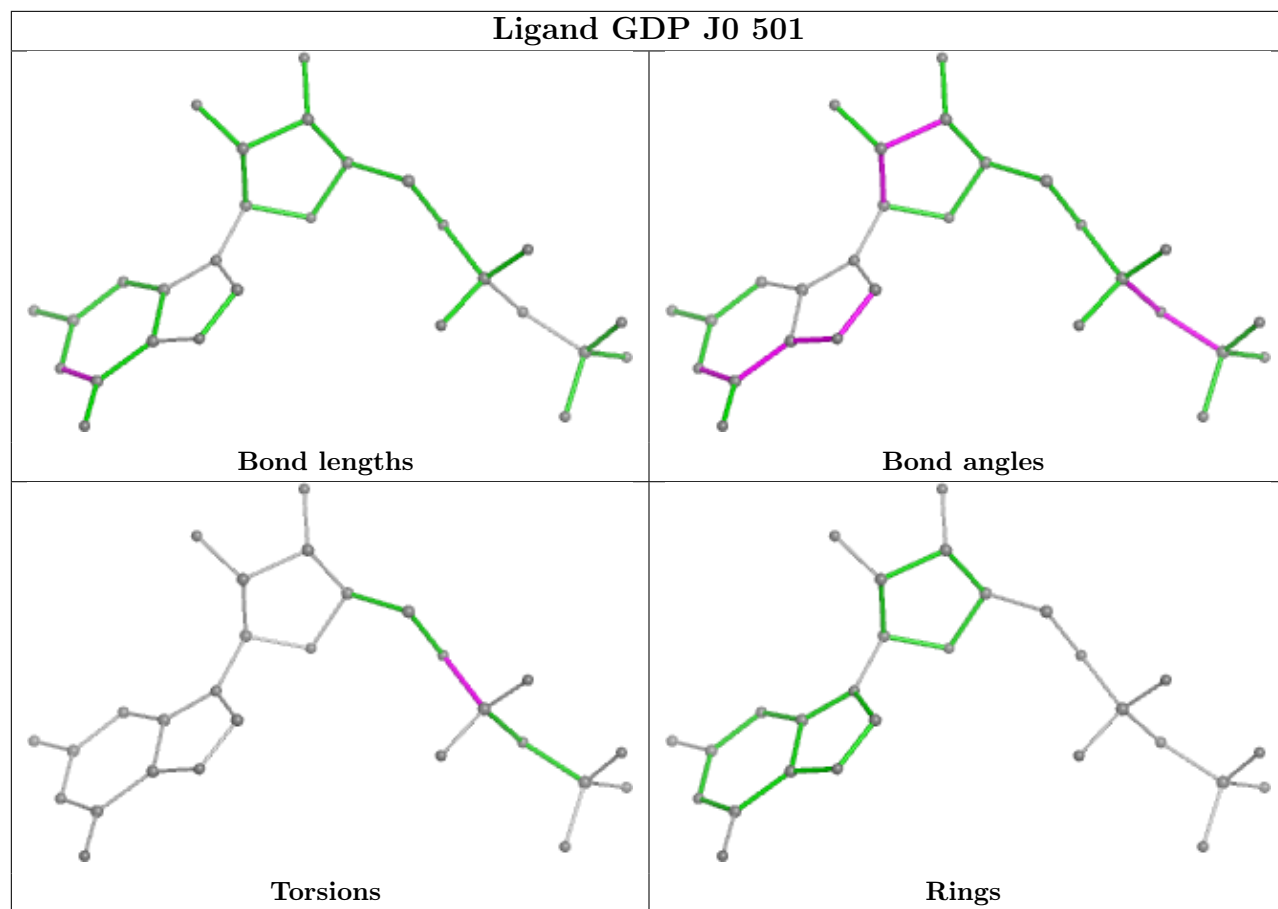
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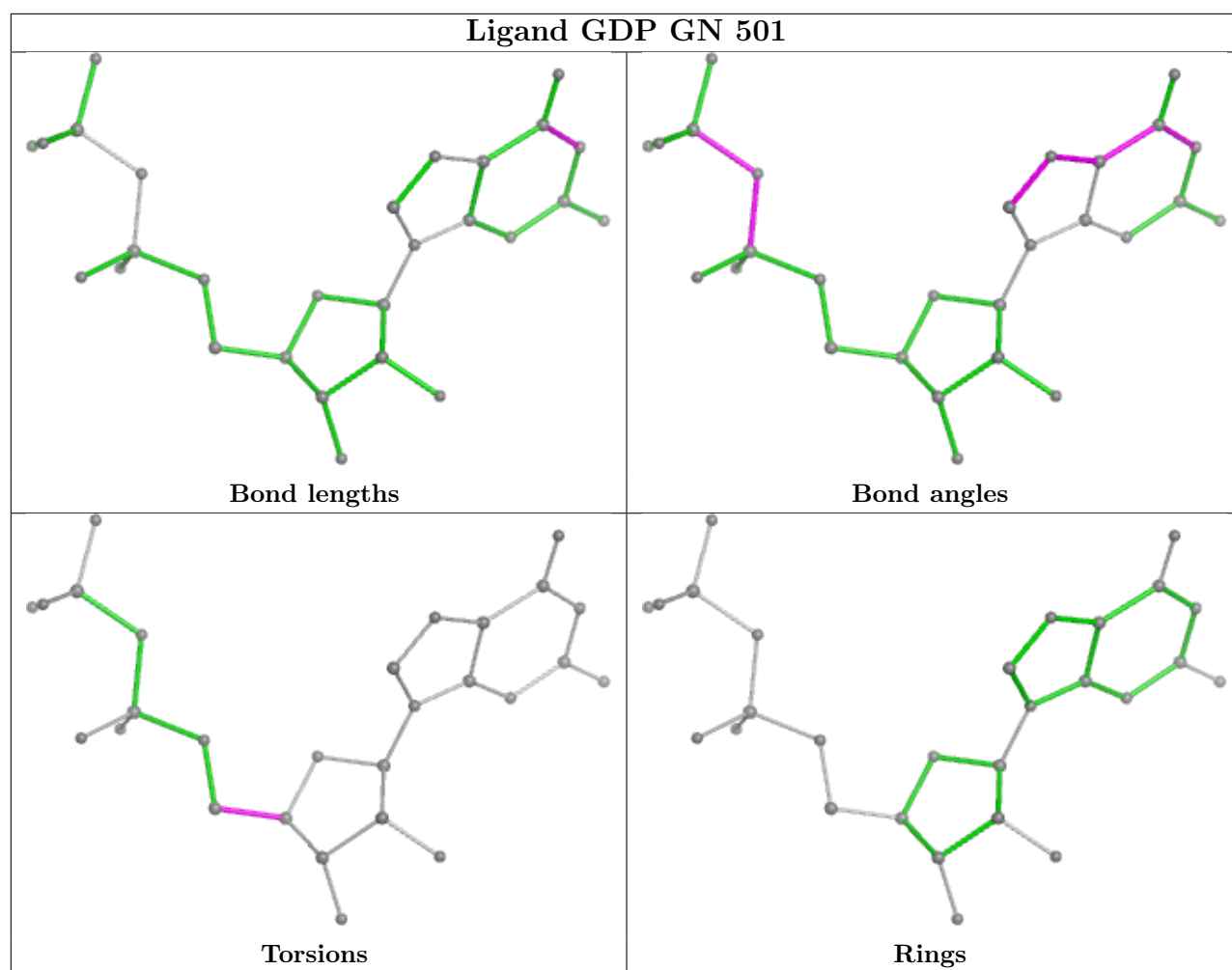


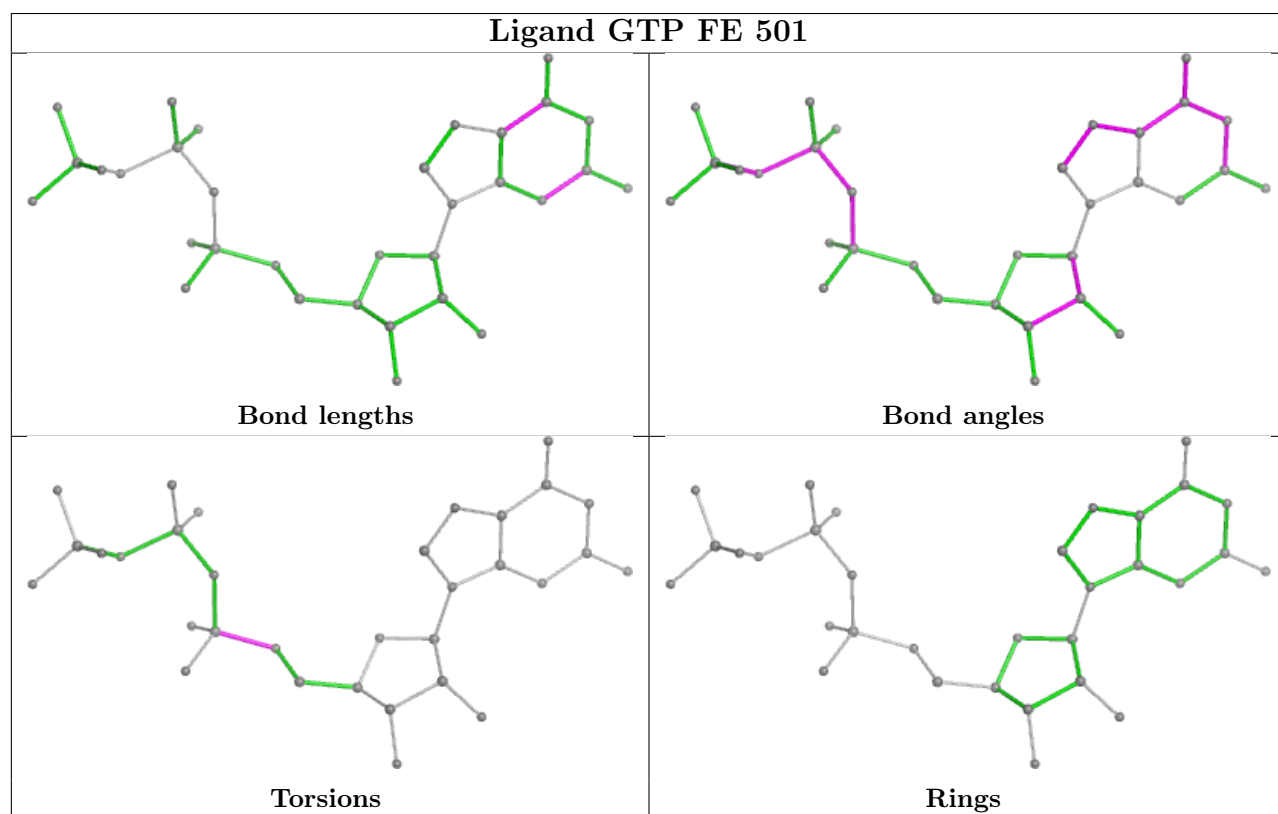
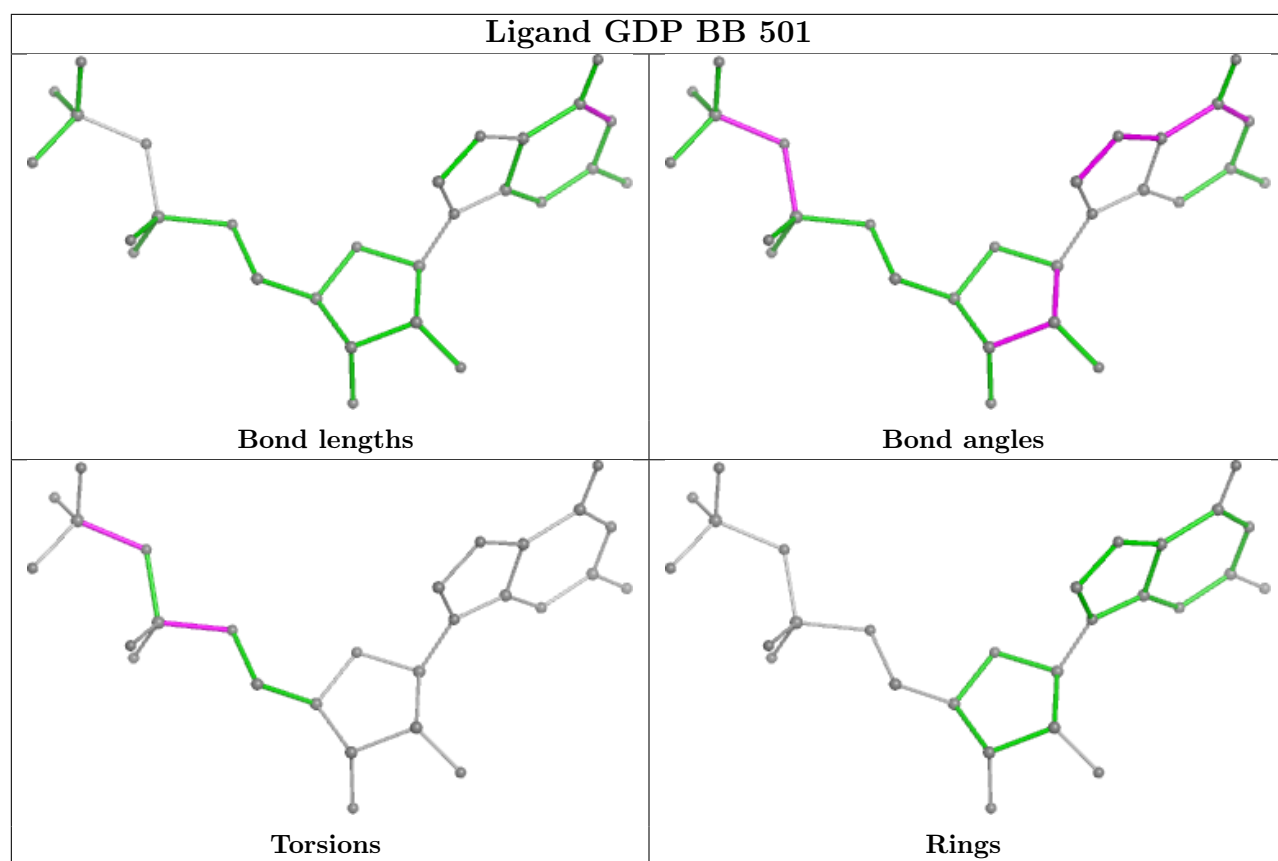
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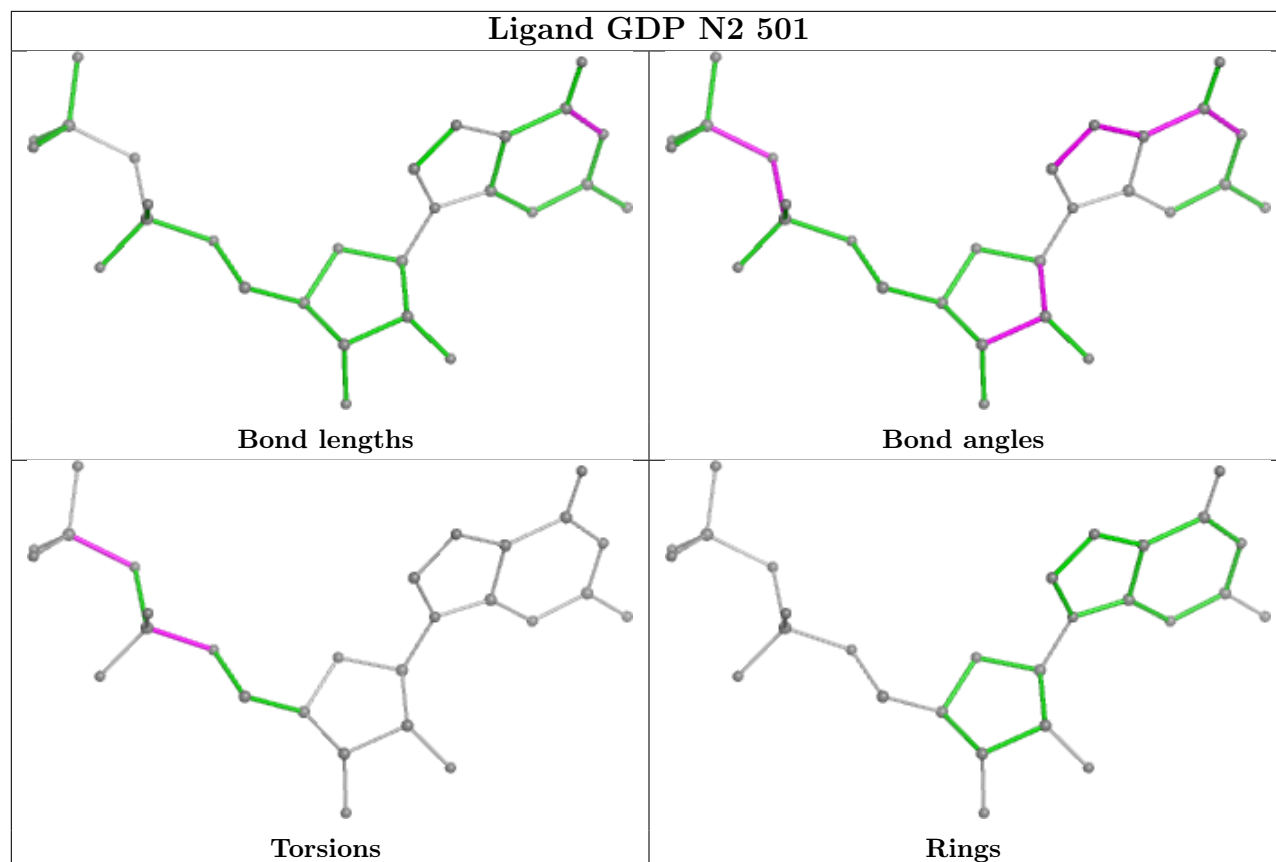




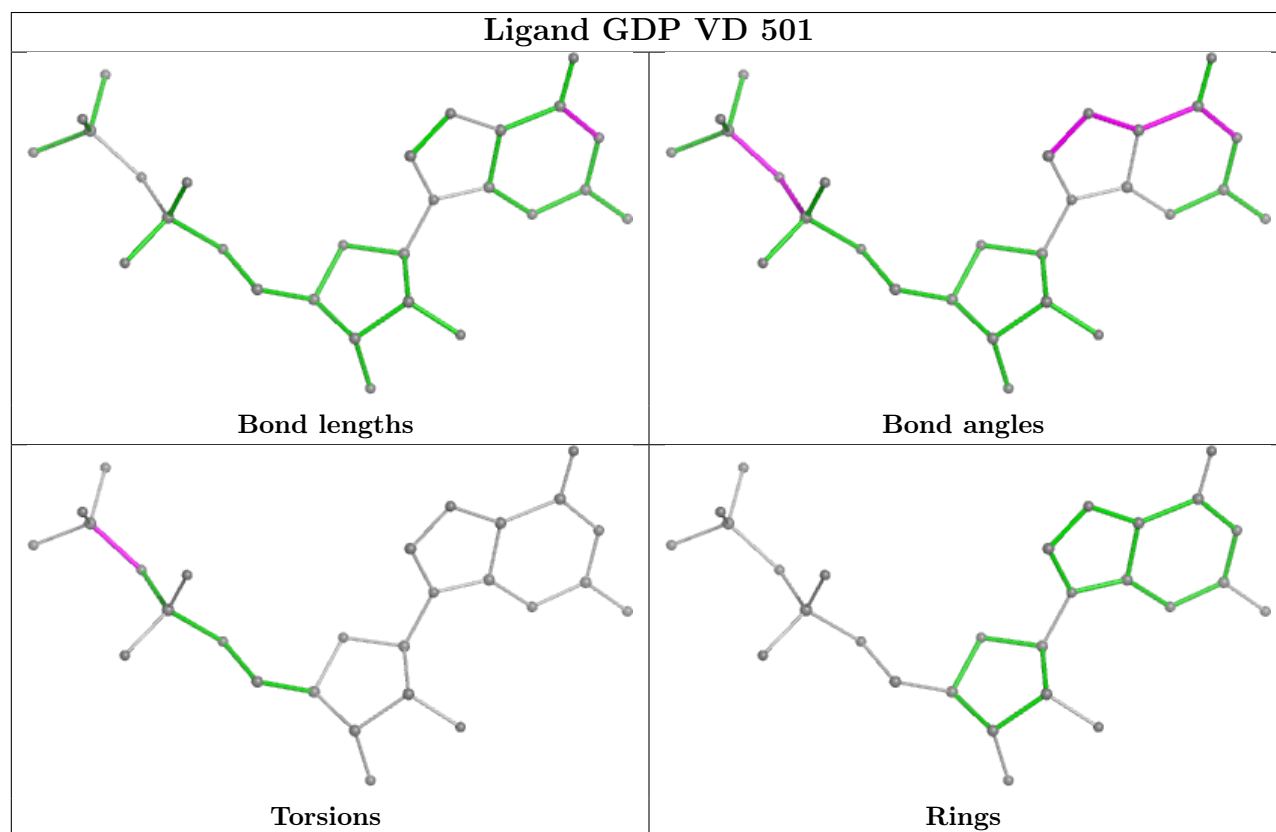




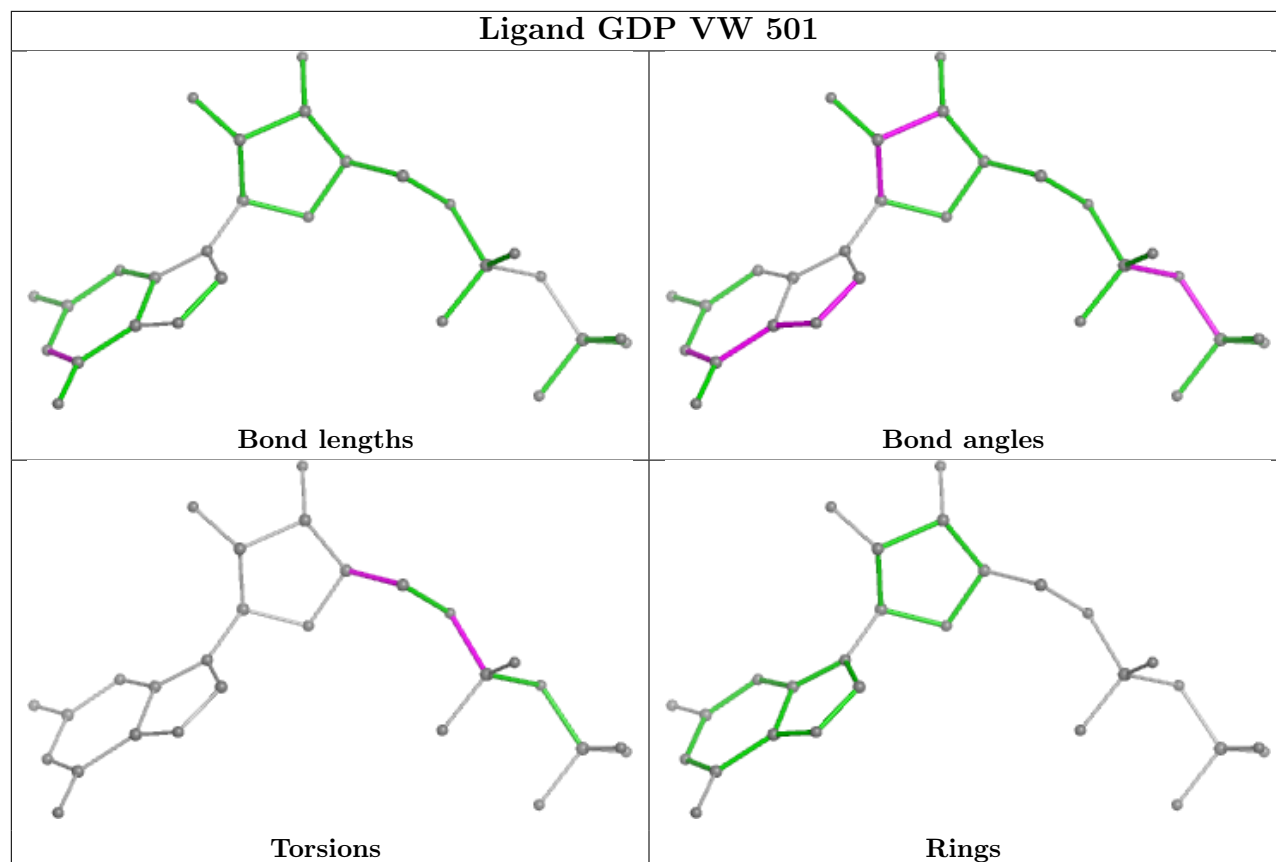
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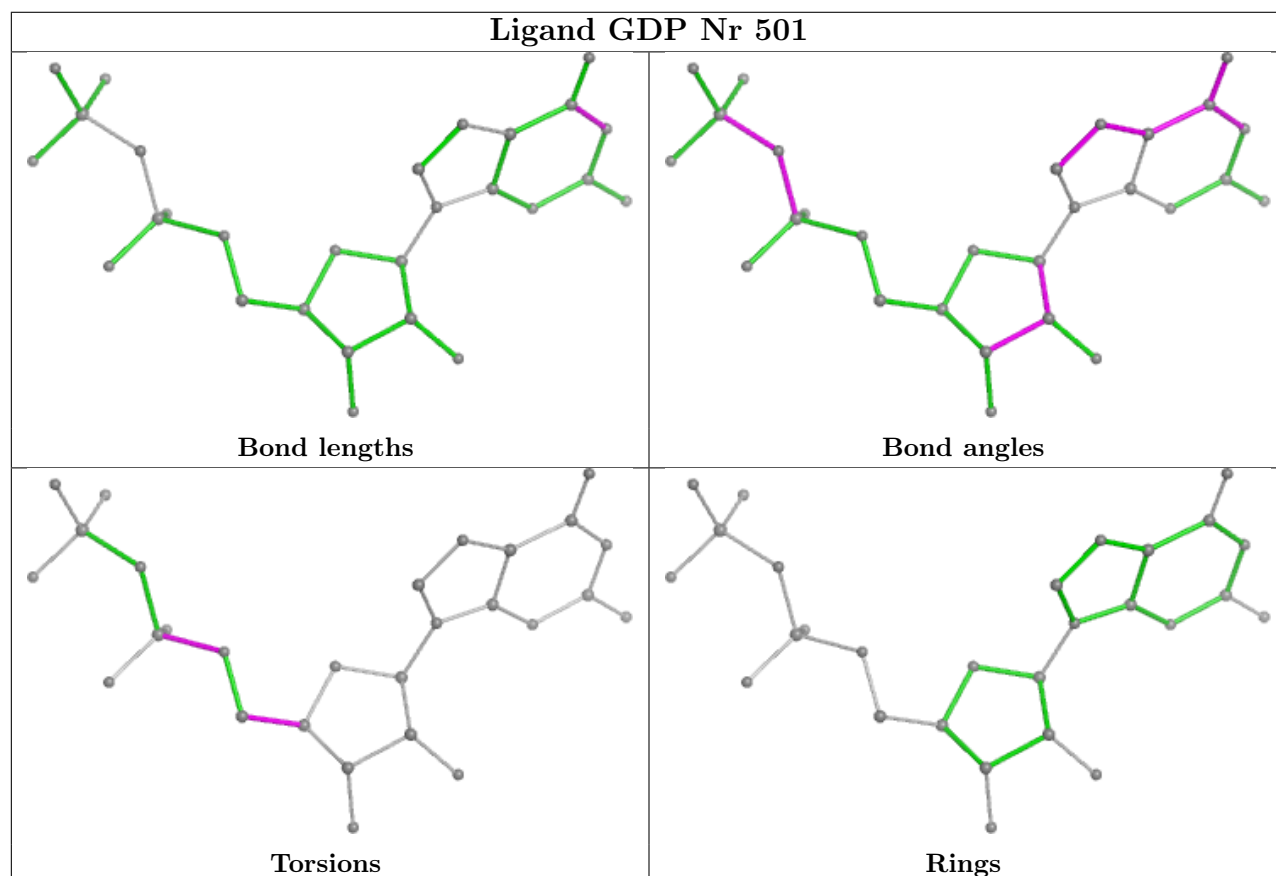
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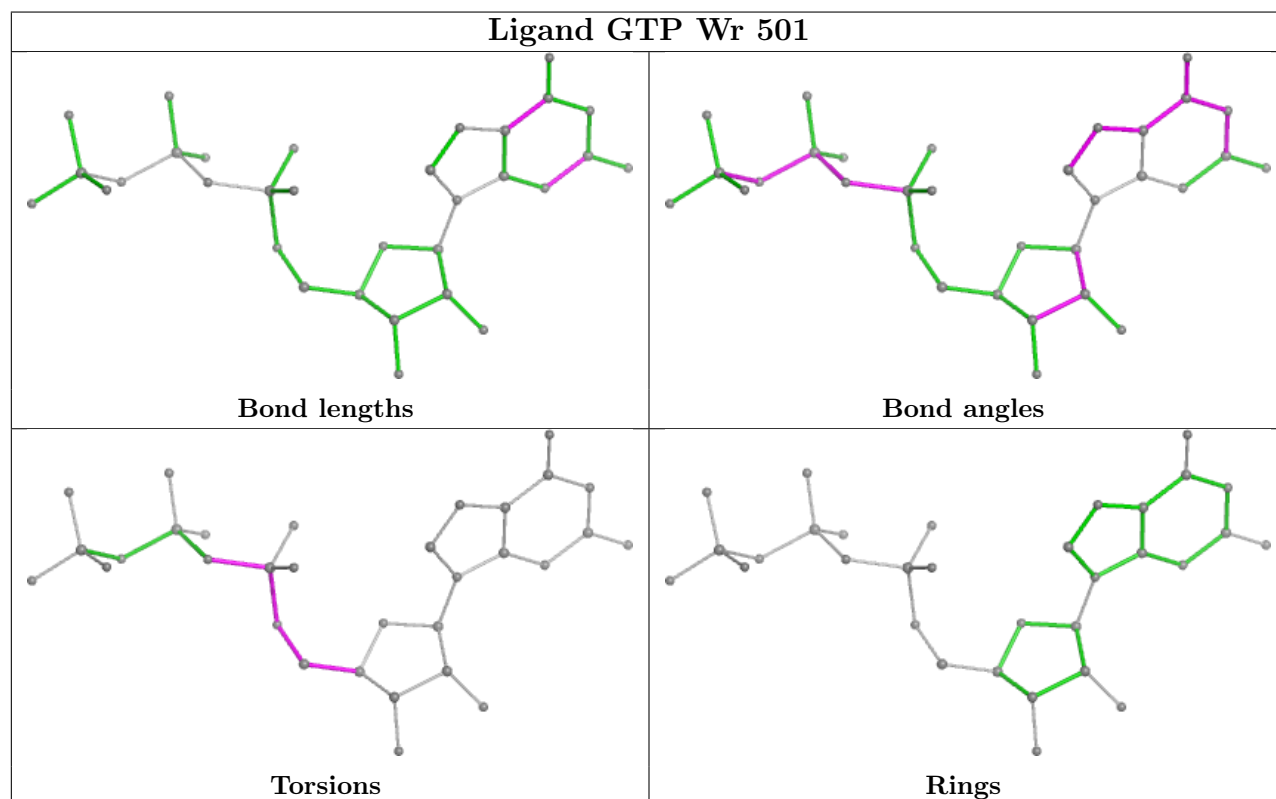
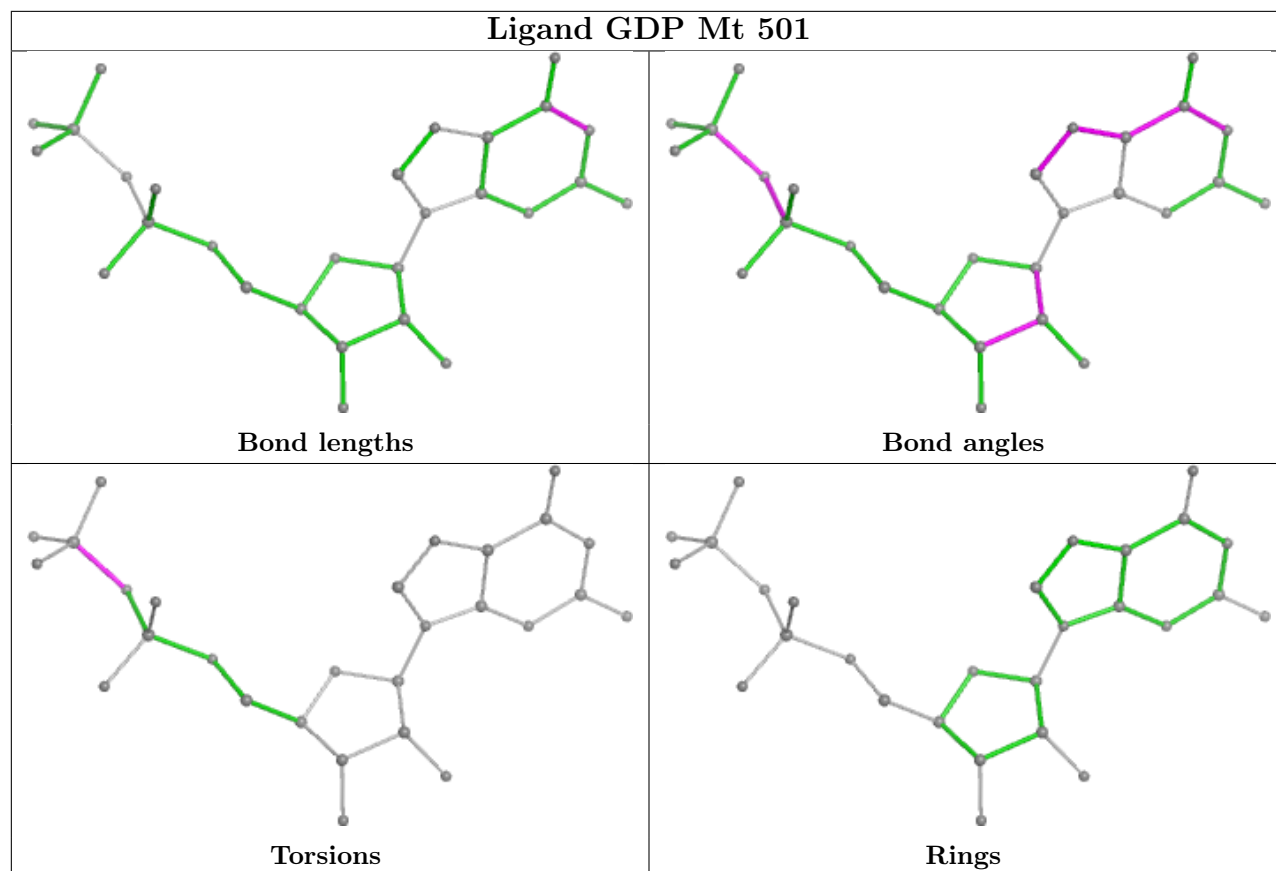


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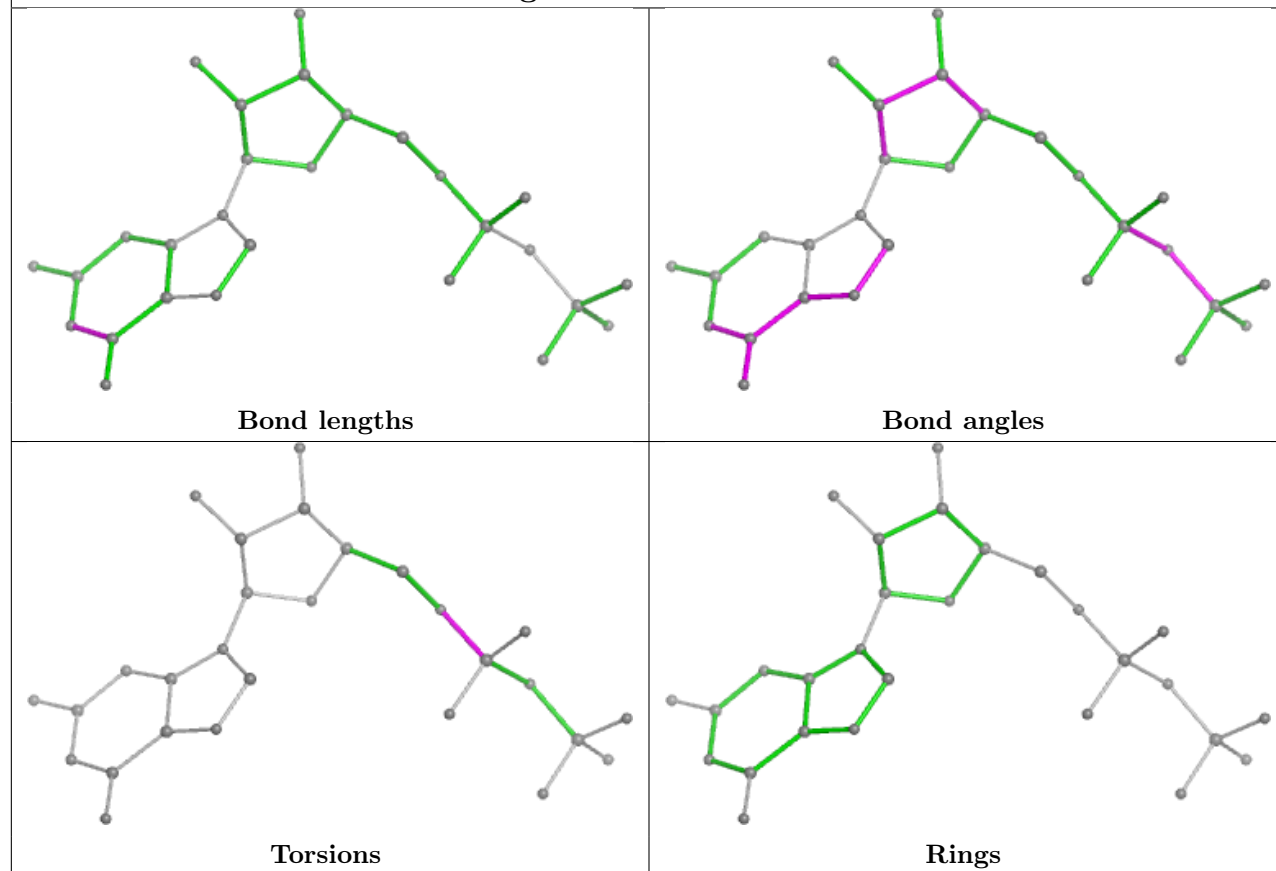


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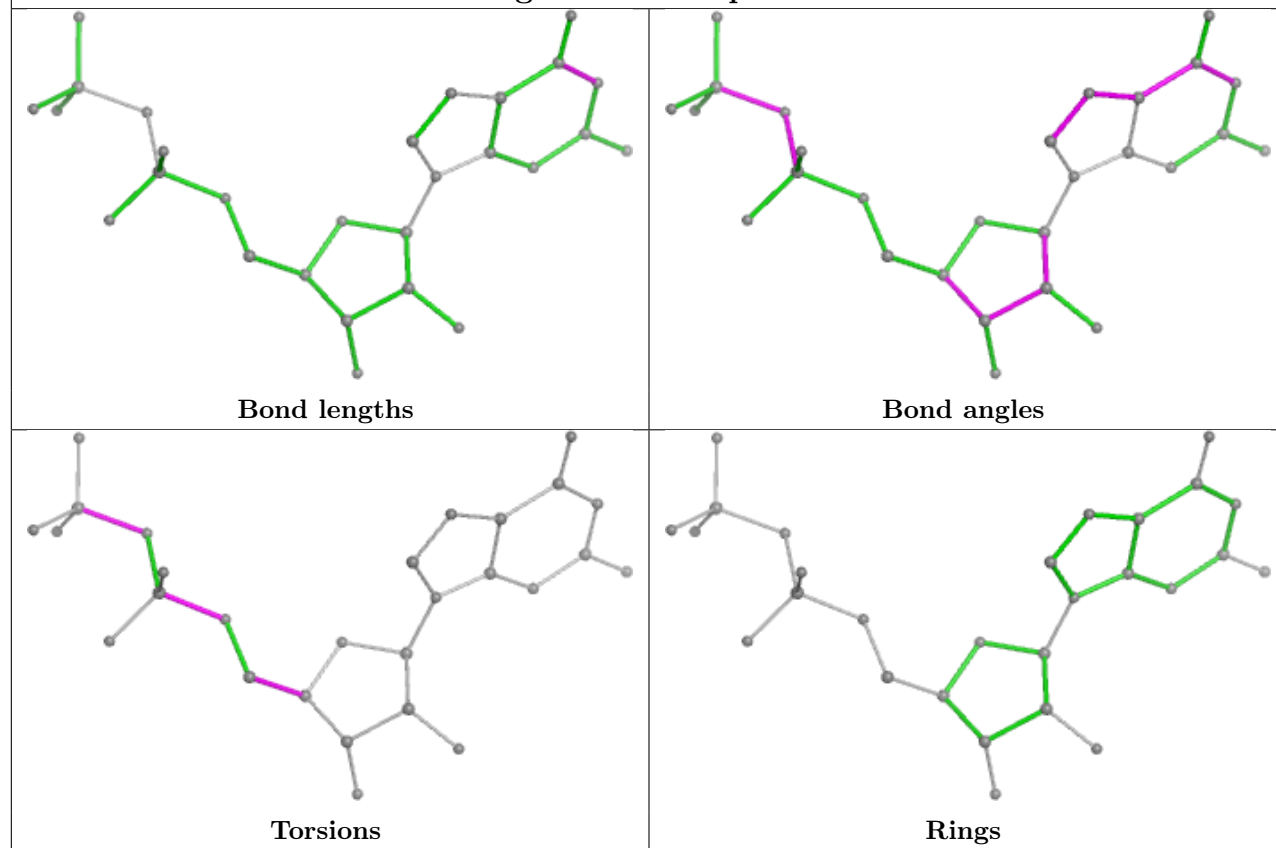


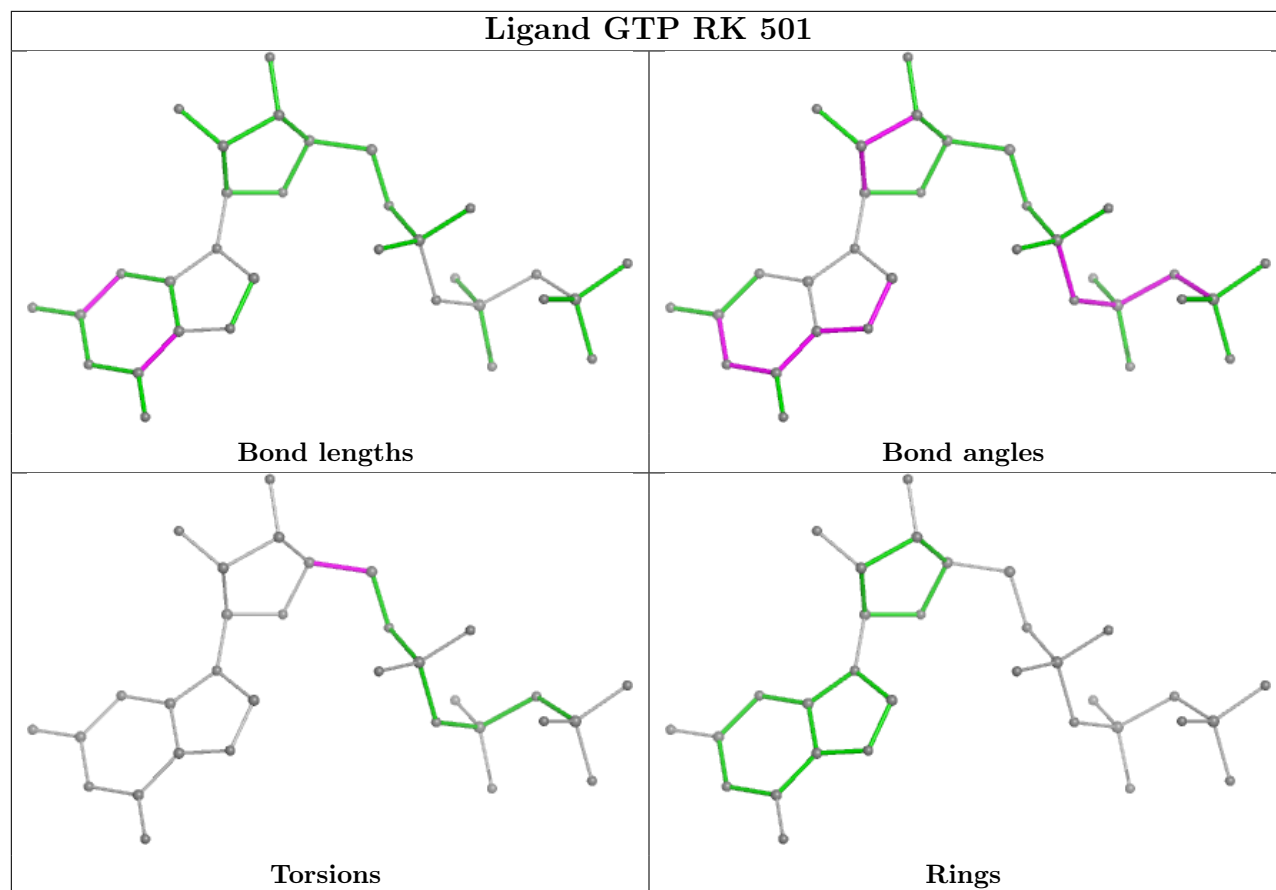


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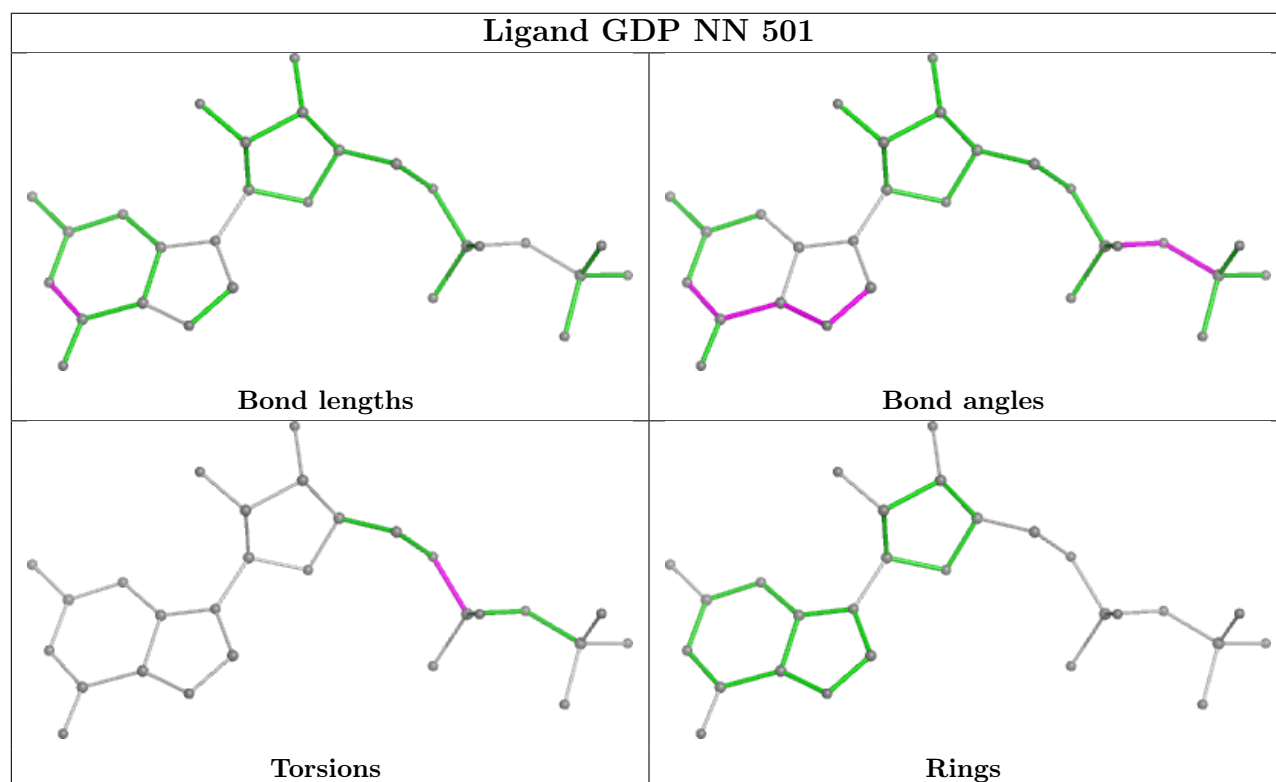
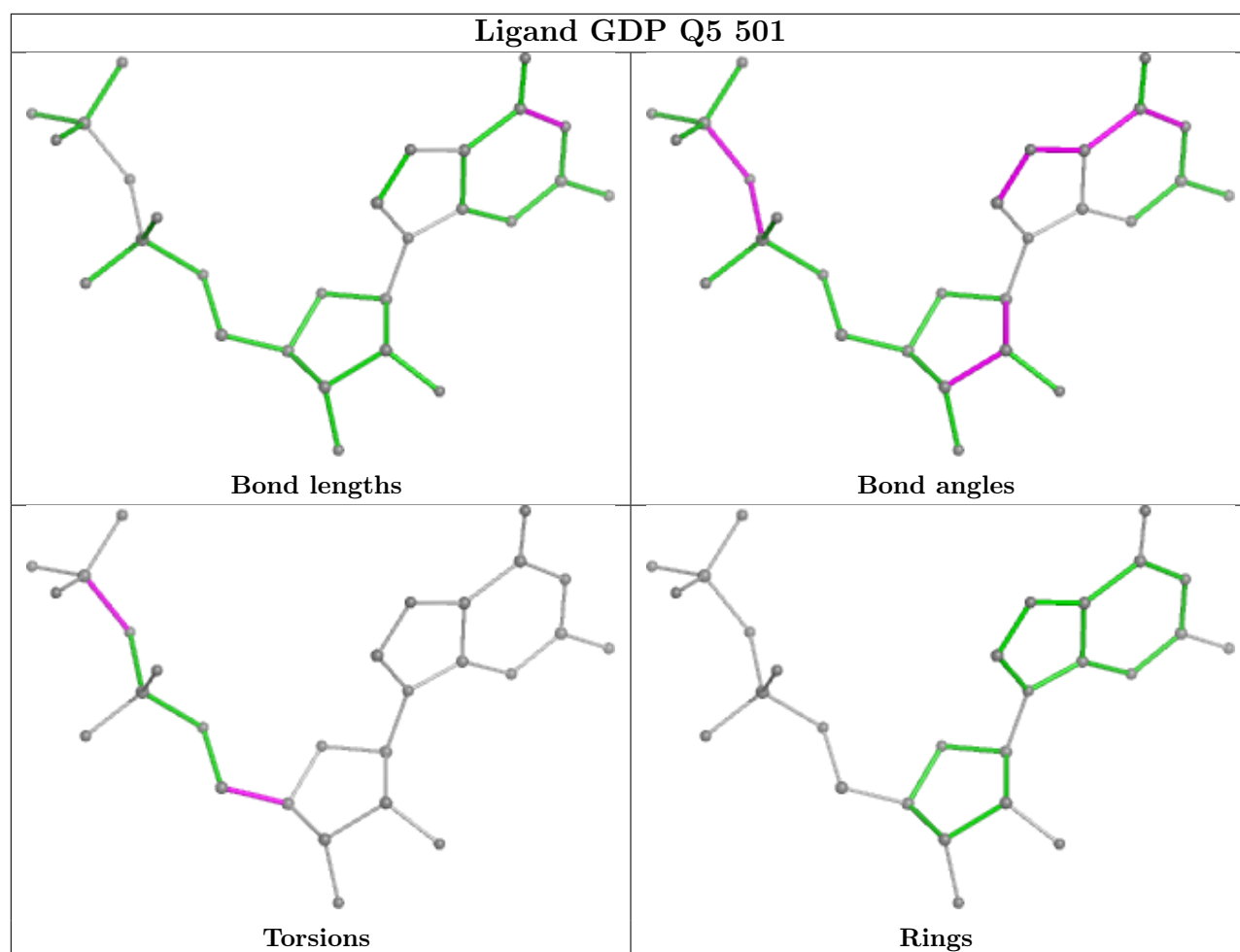


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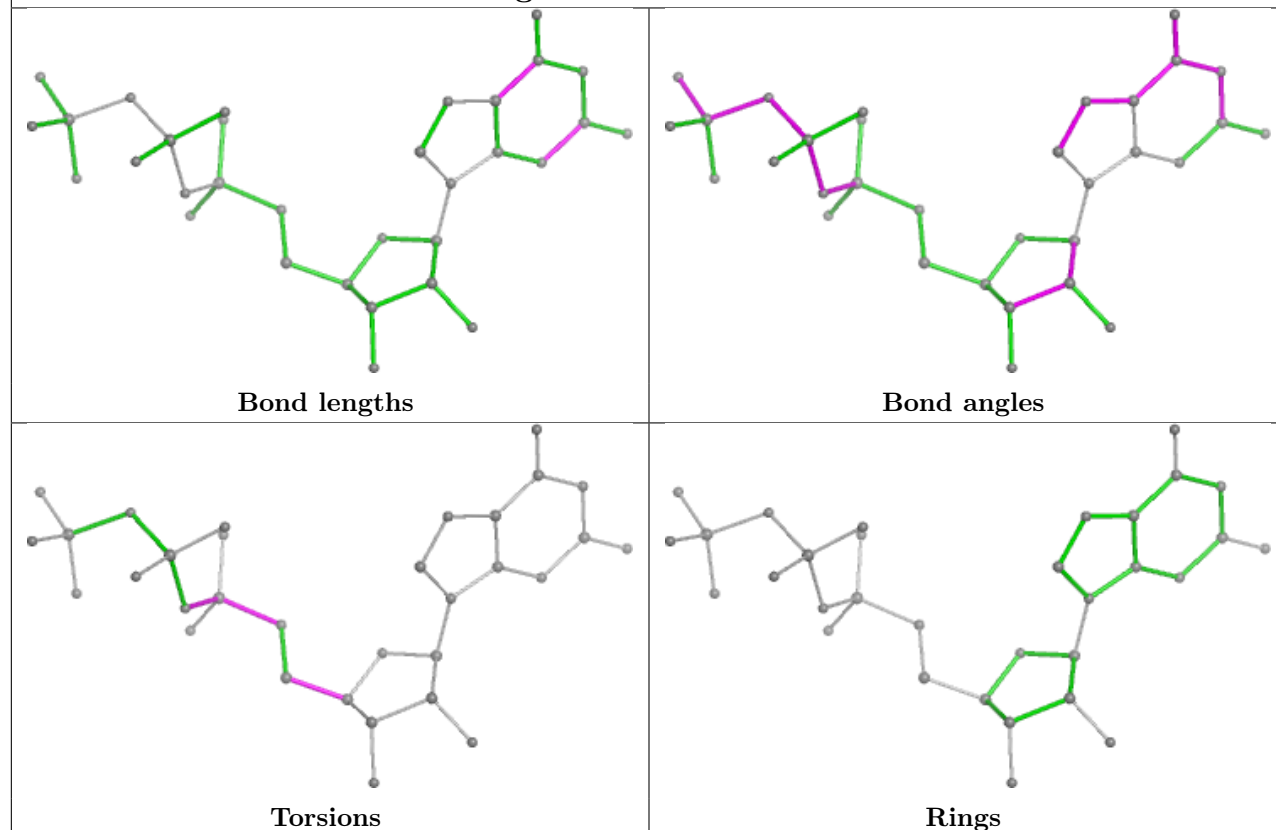




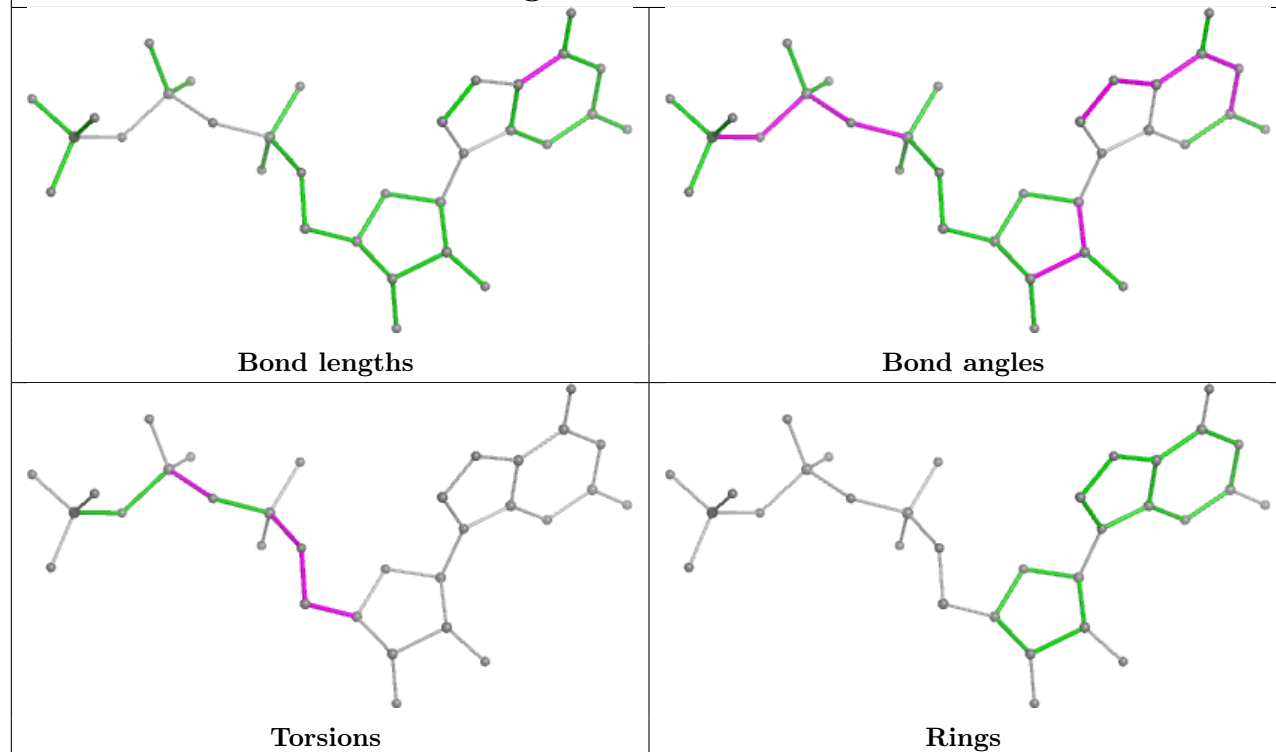


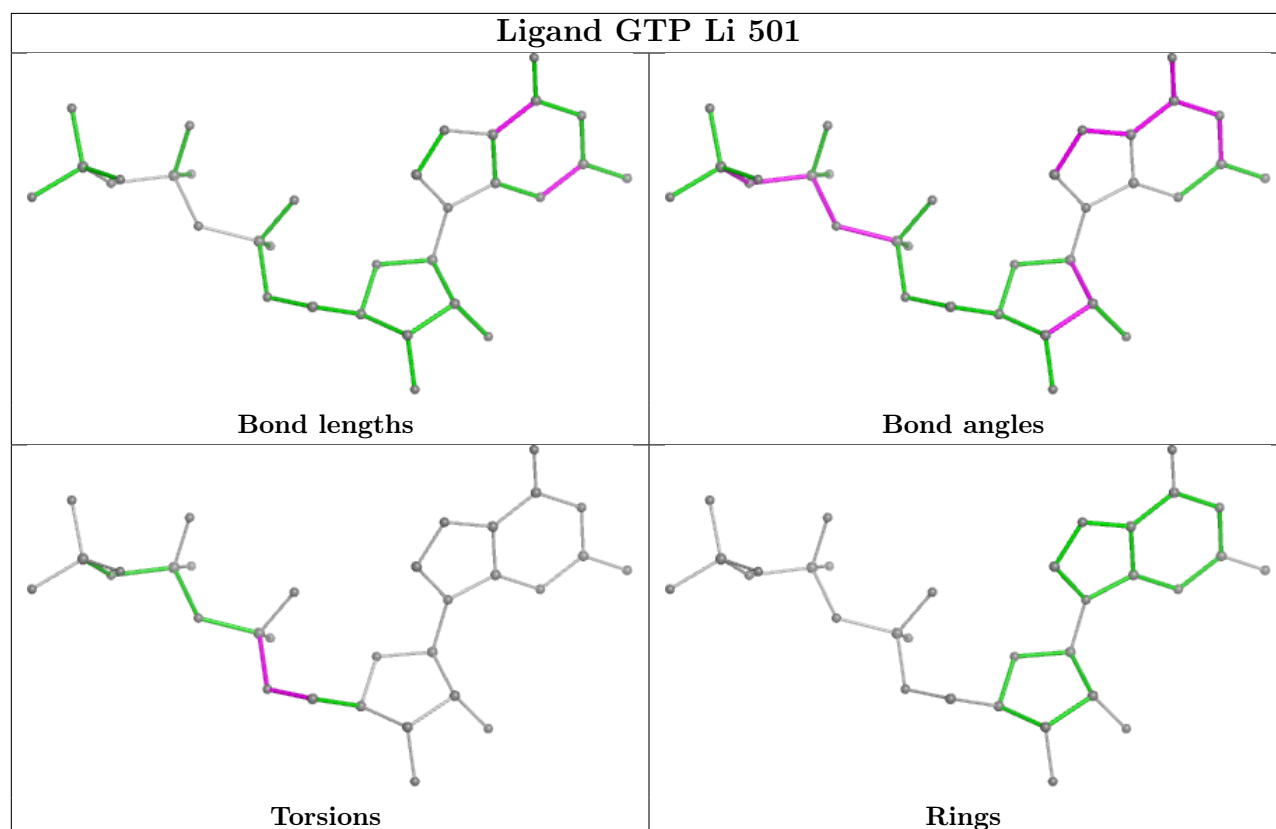
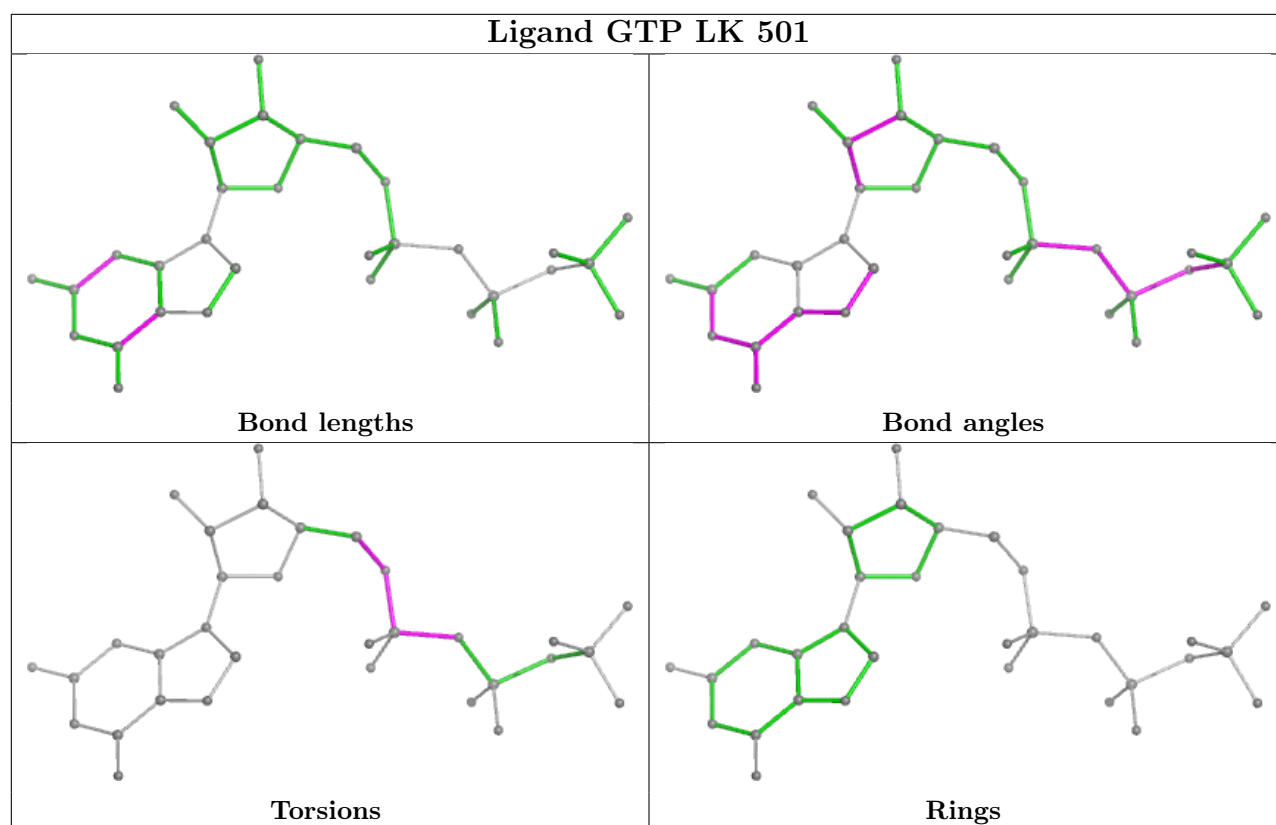


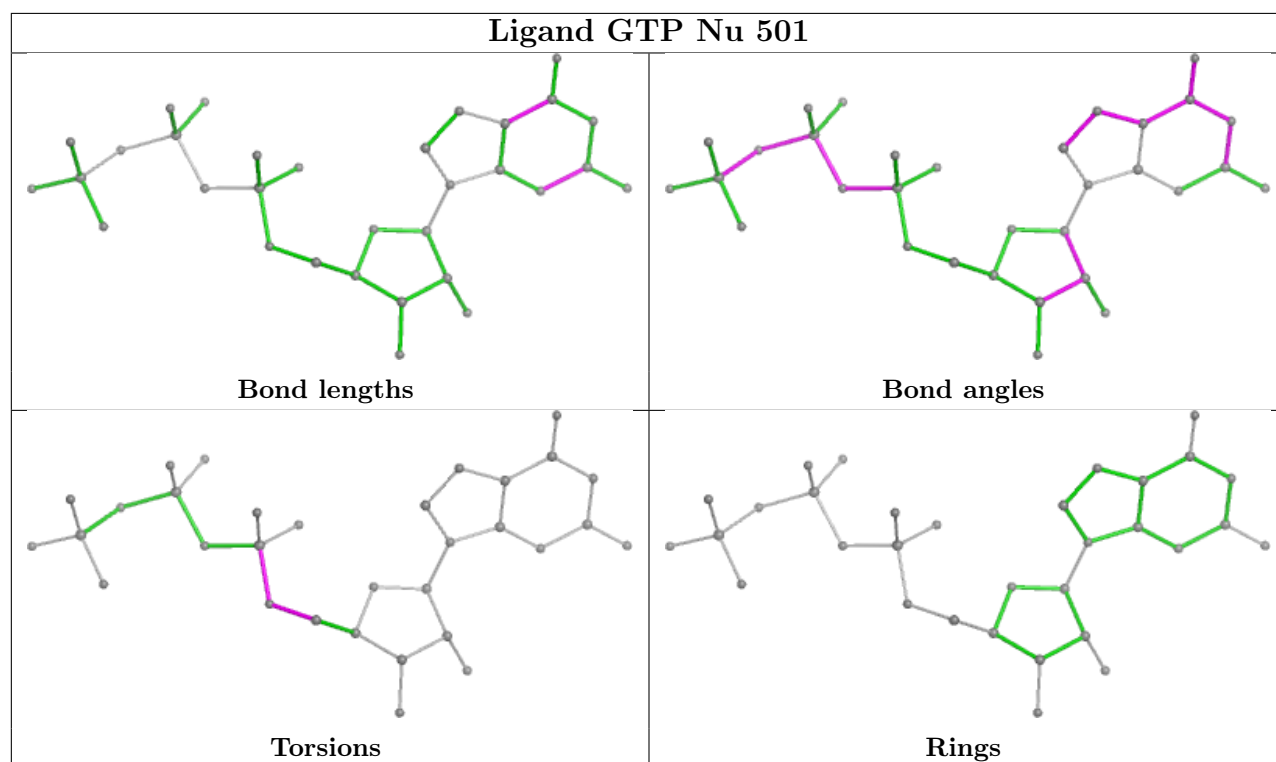
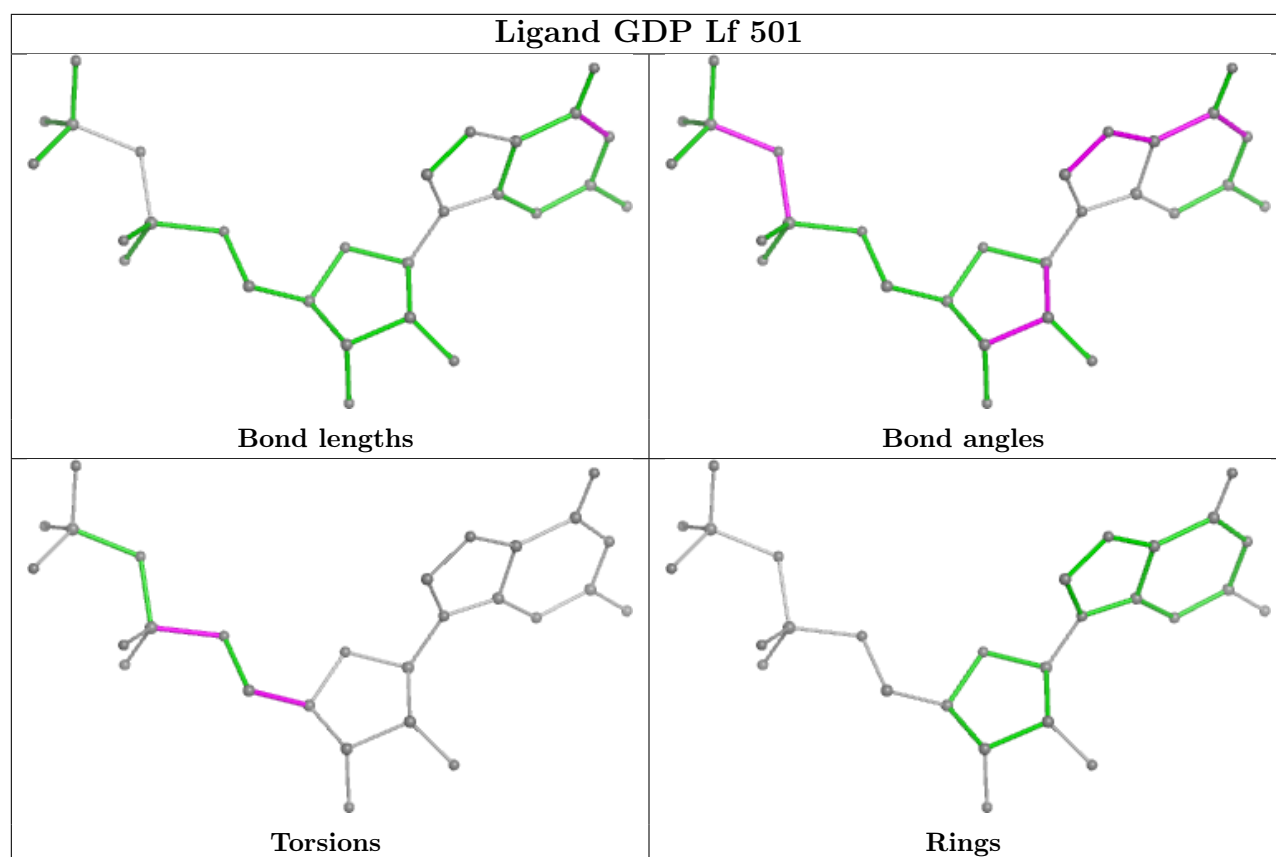
## Ligand GTP FM 501

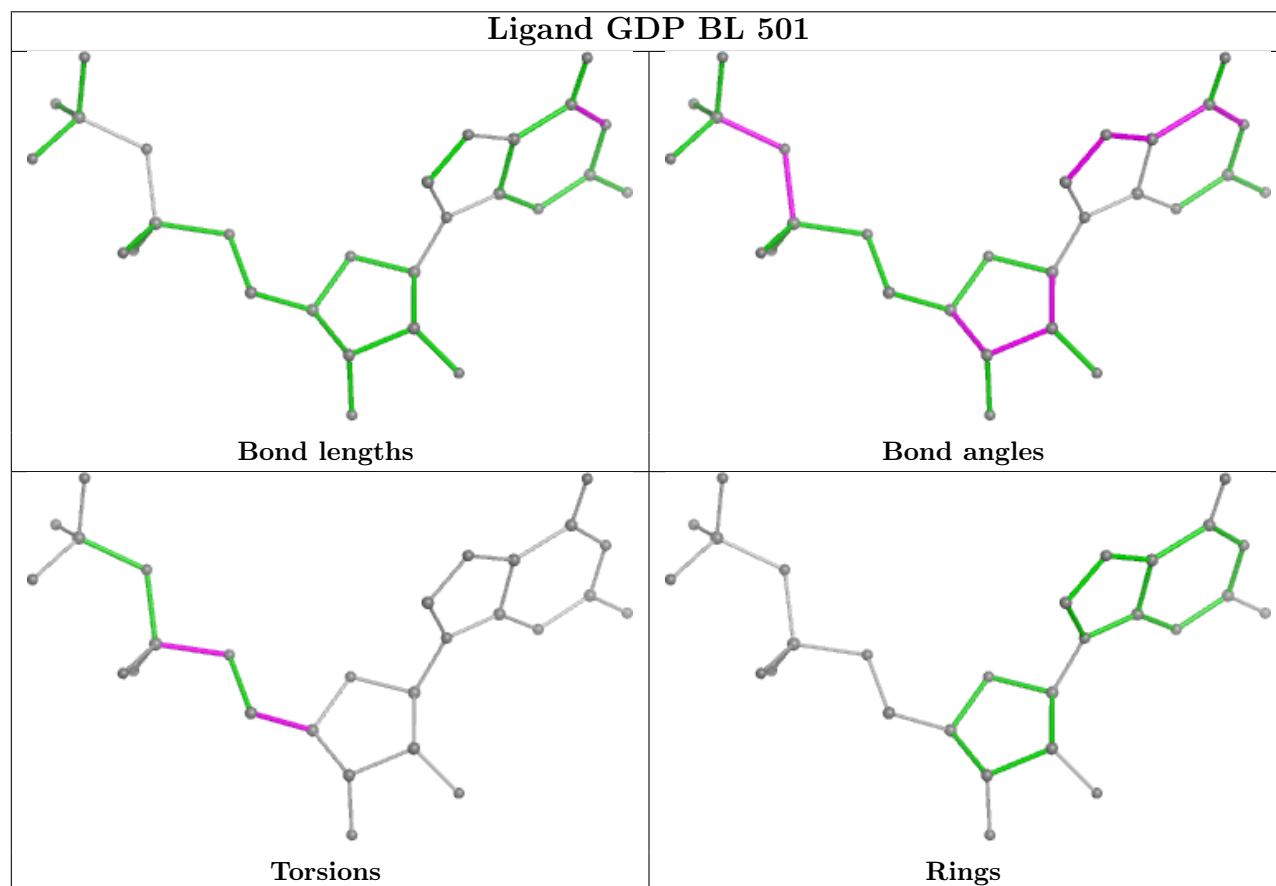
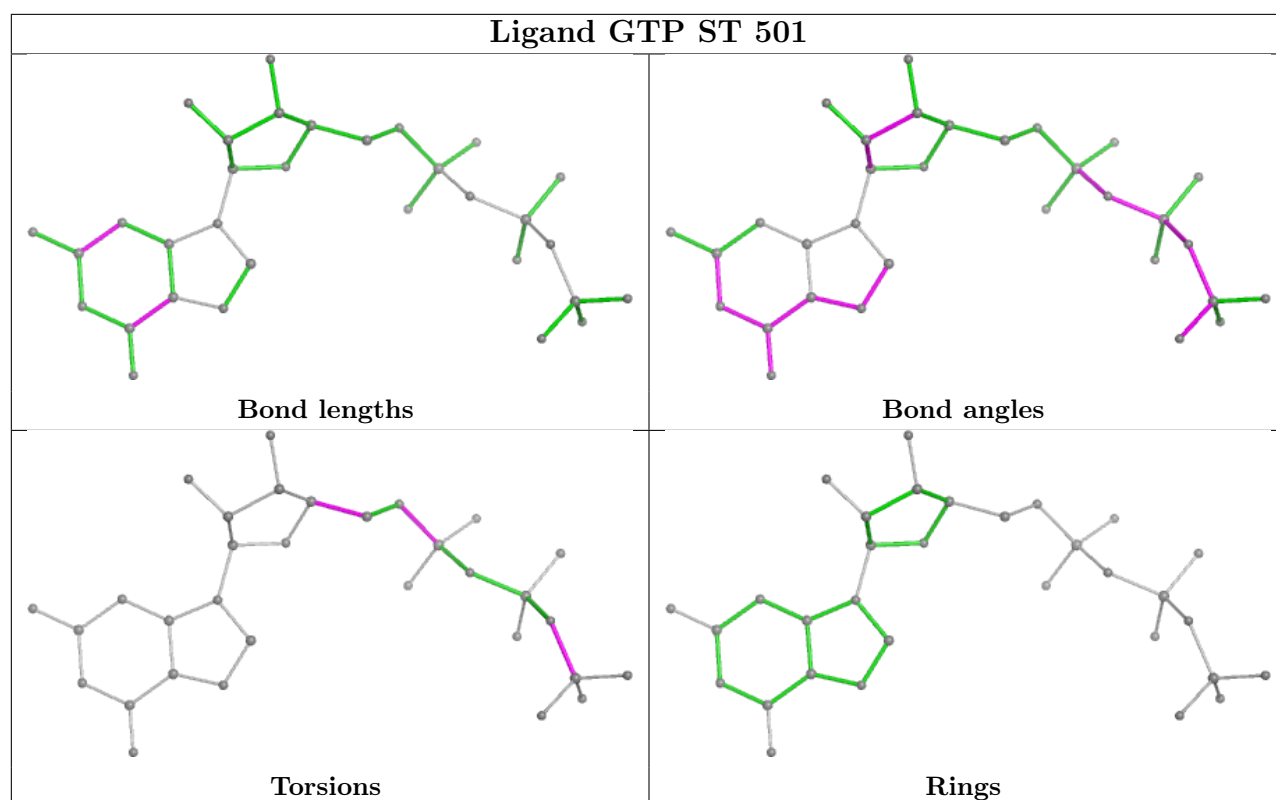


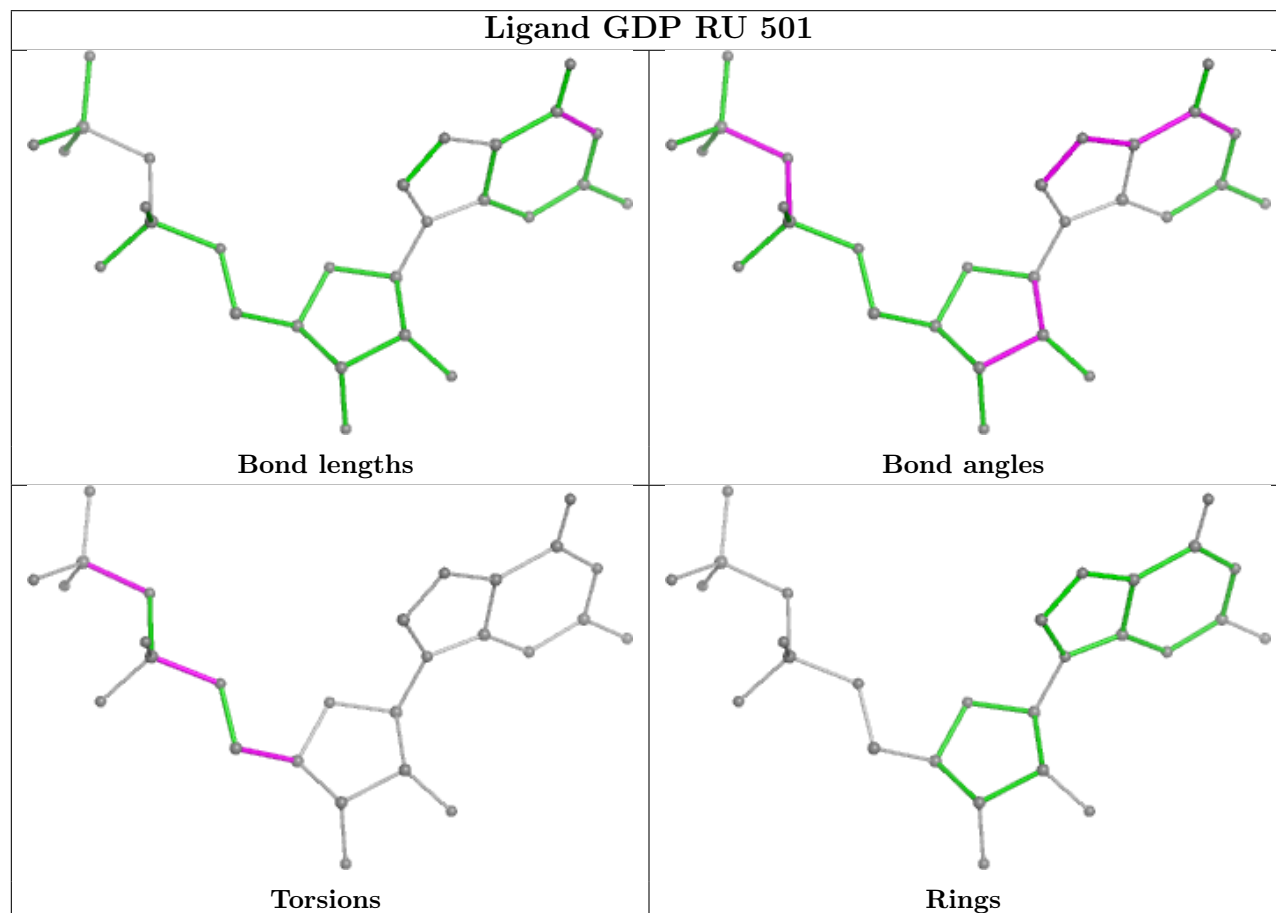
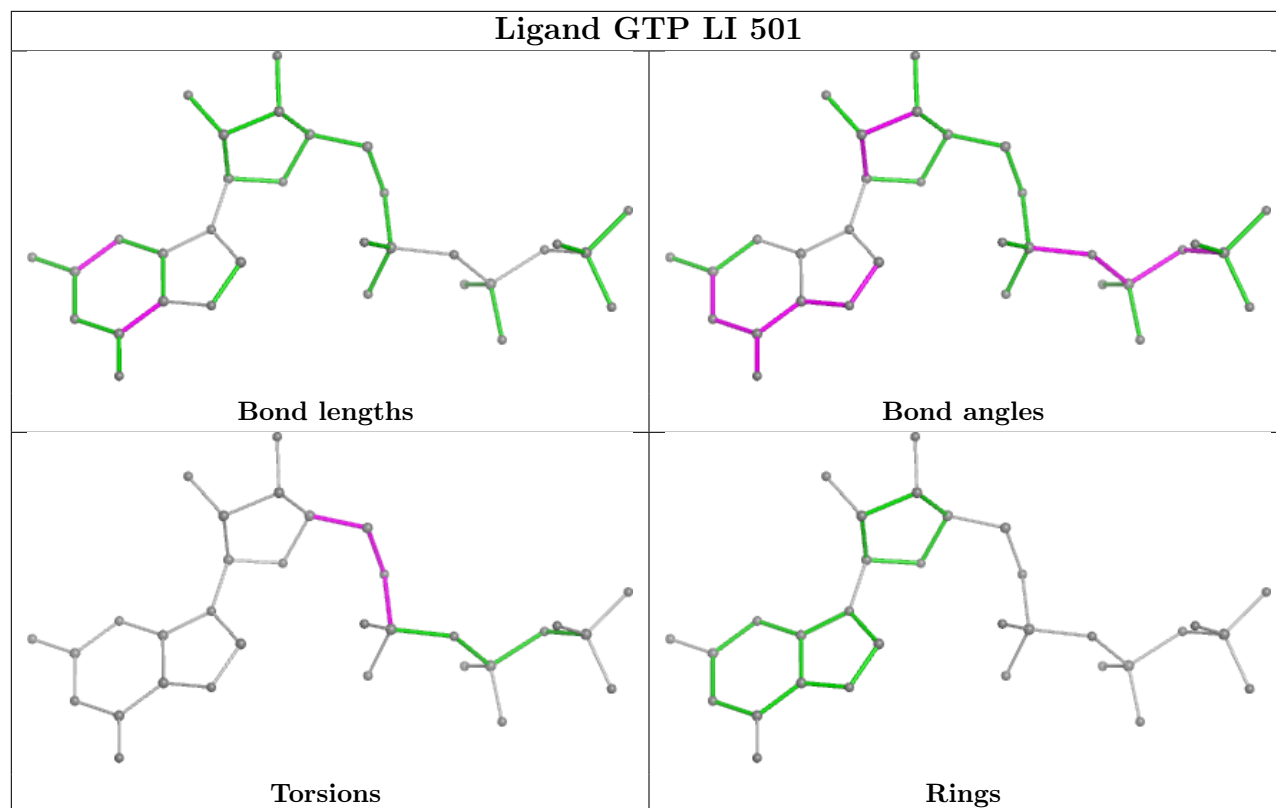
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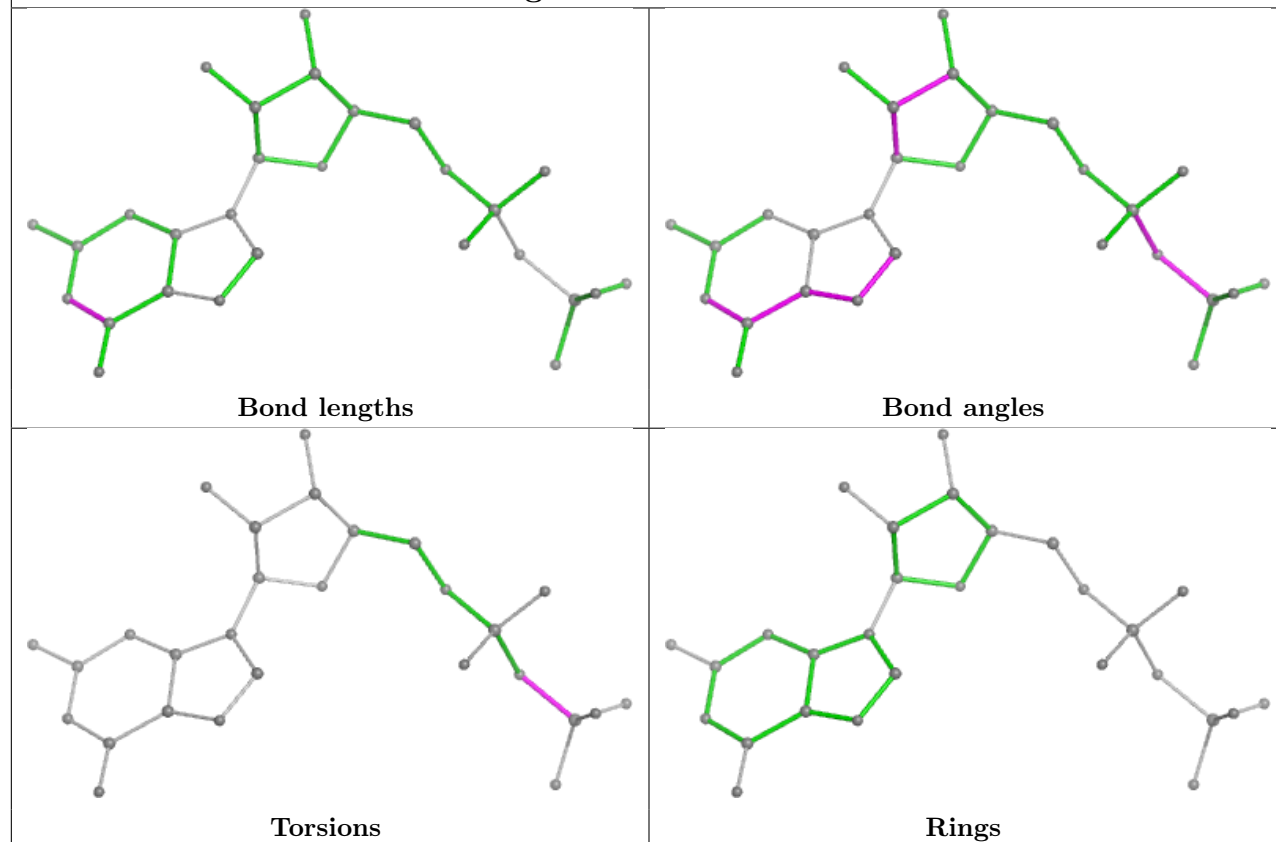




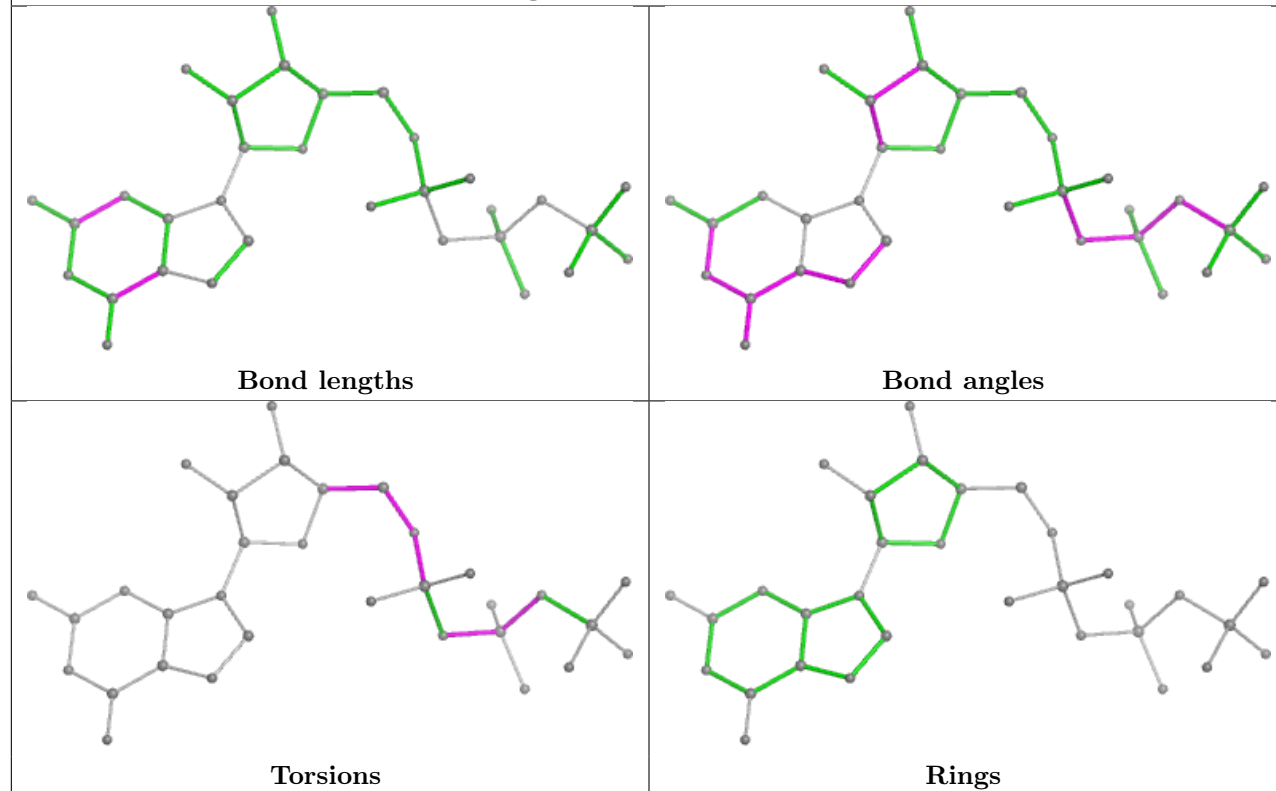




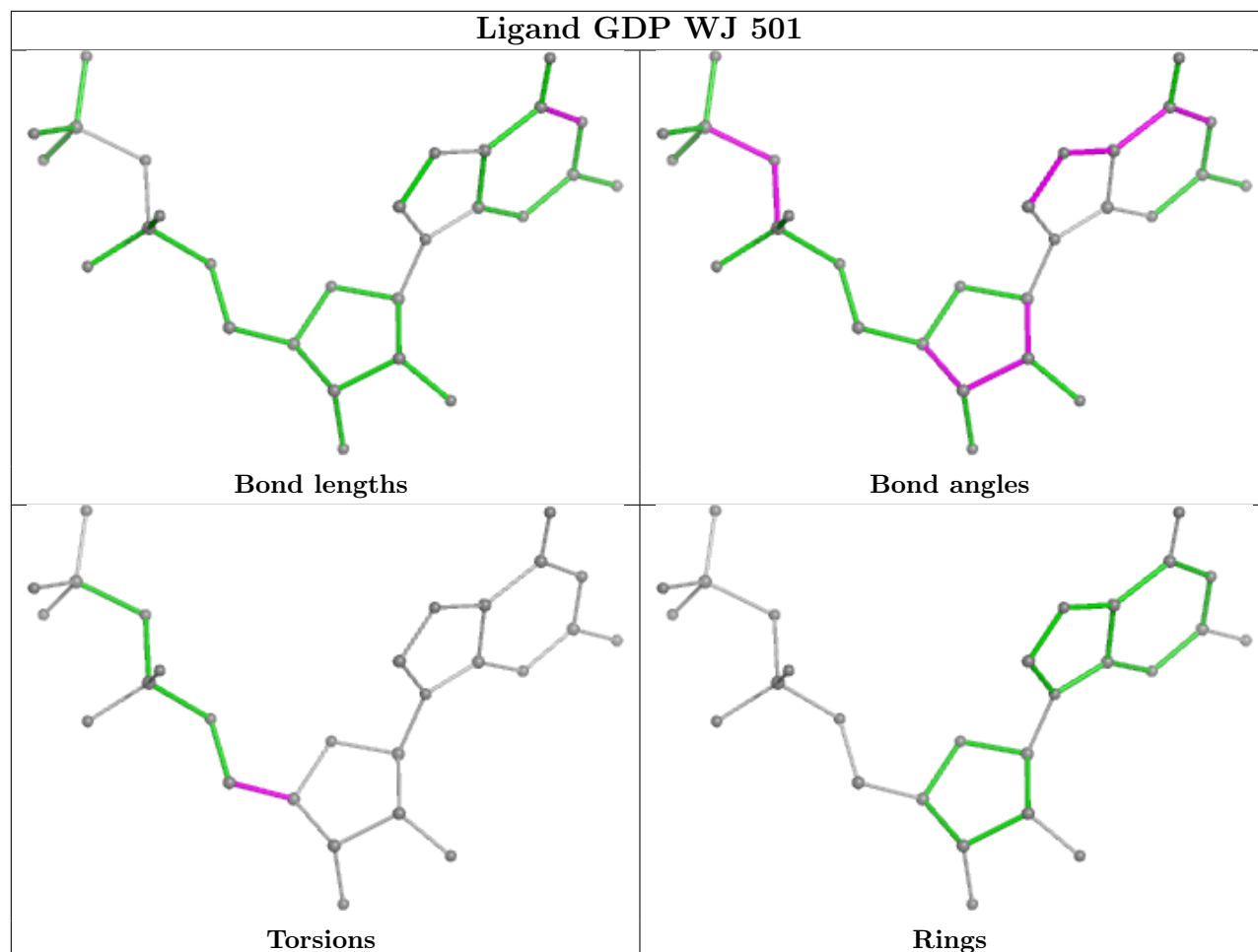
## Ligand GDP IL 501



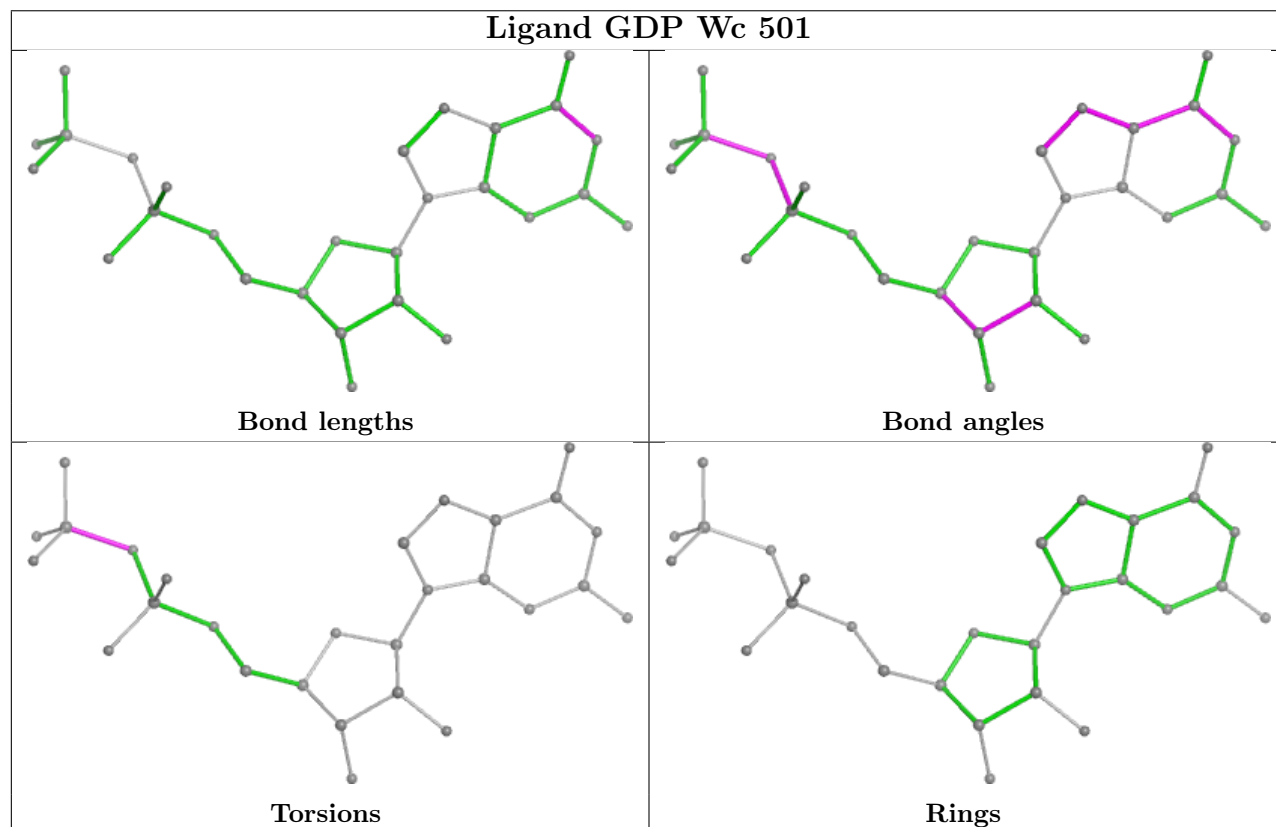
## Ligand GTP S2 501



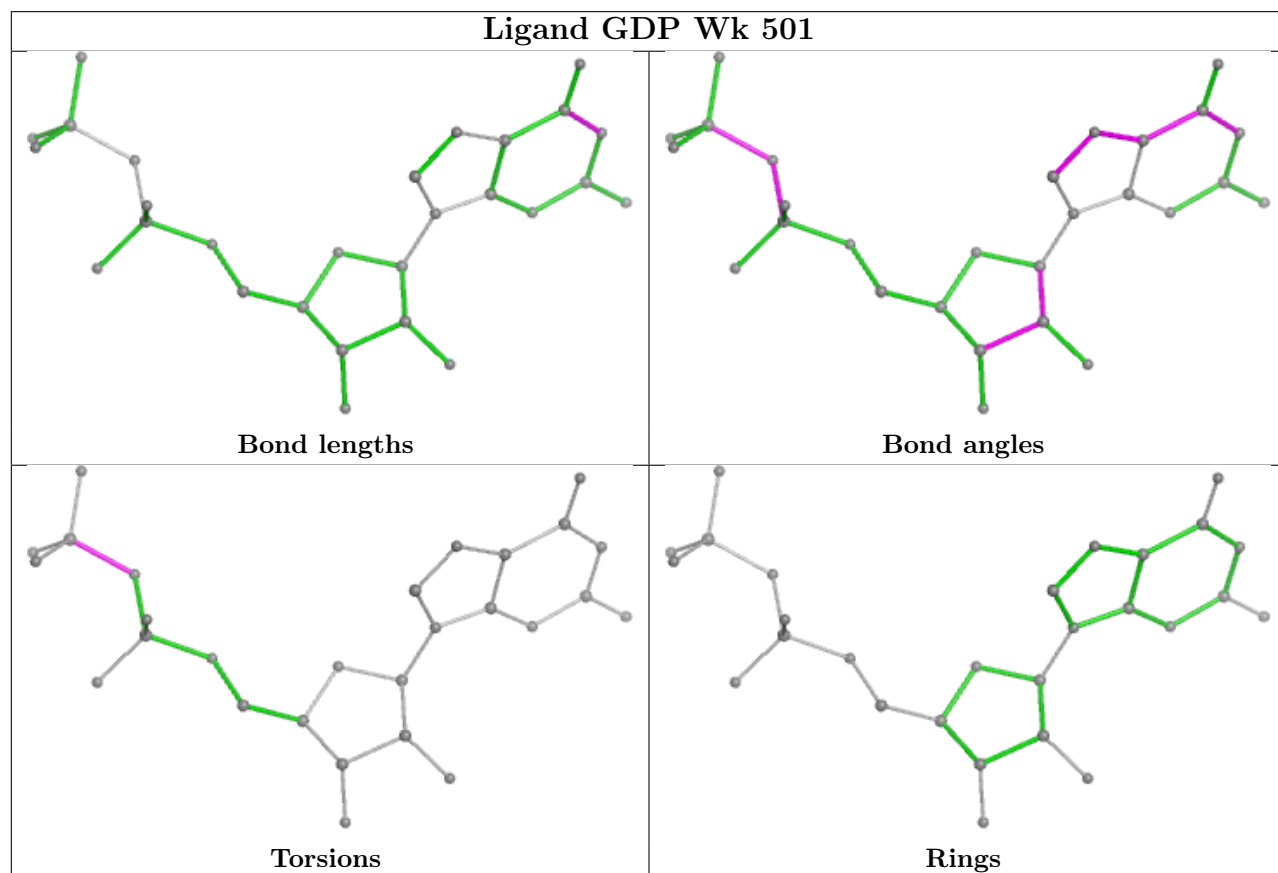
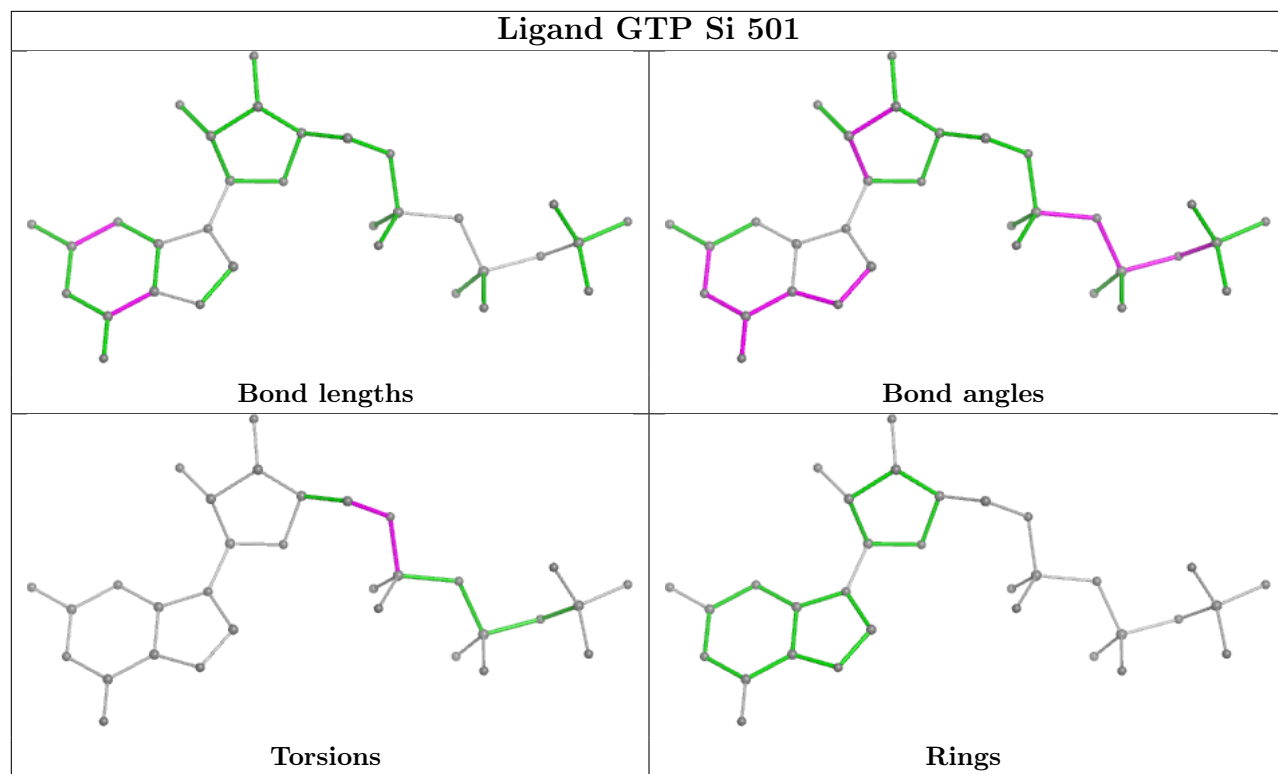
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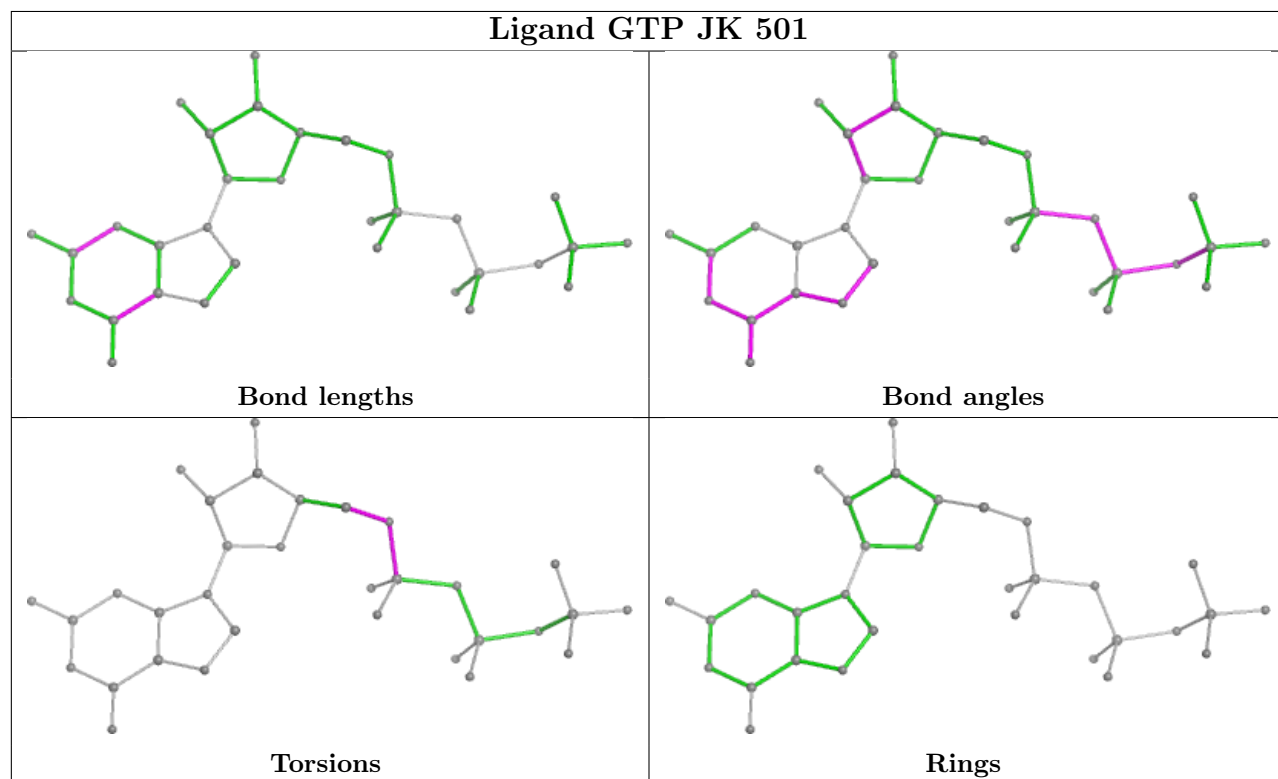
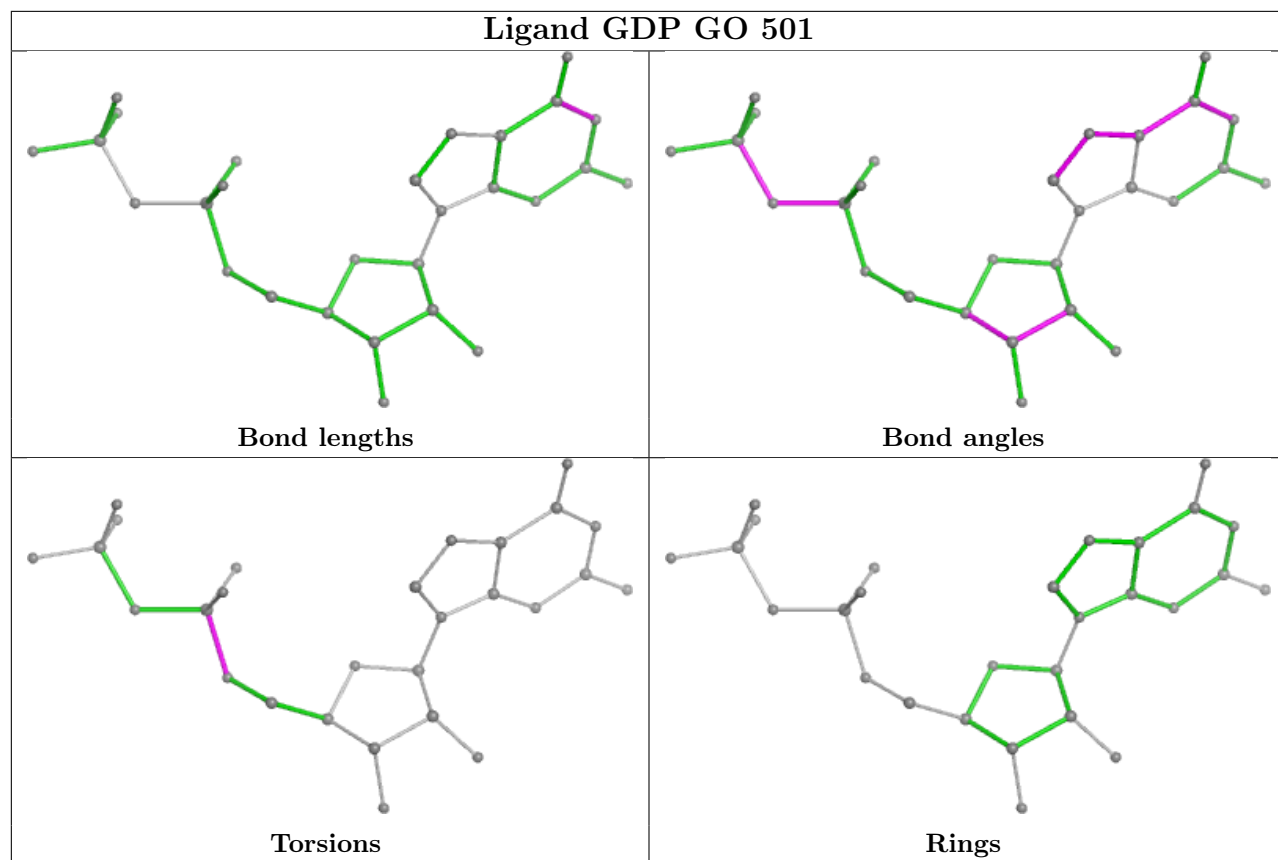


## Ligand GDP Wc 501

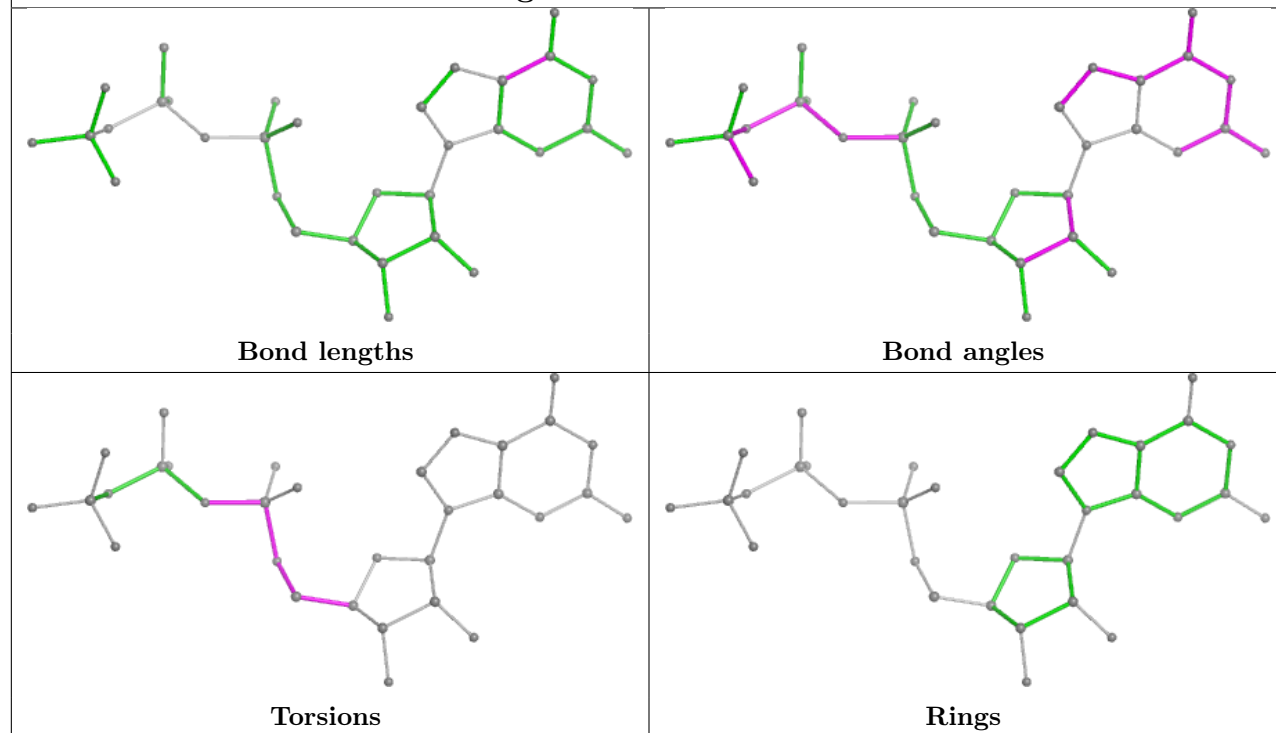




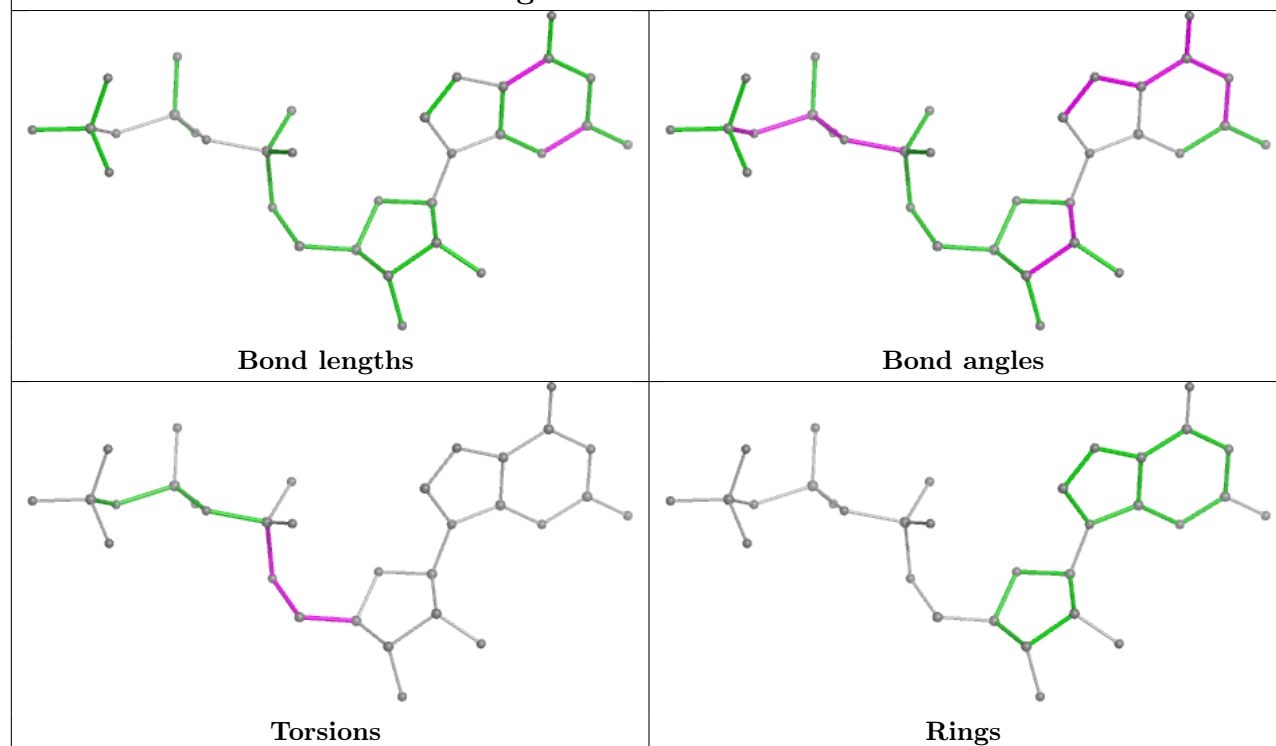


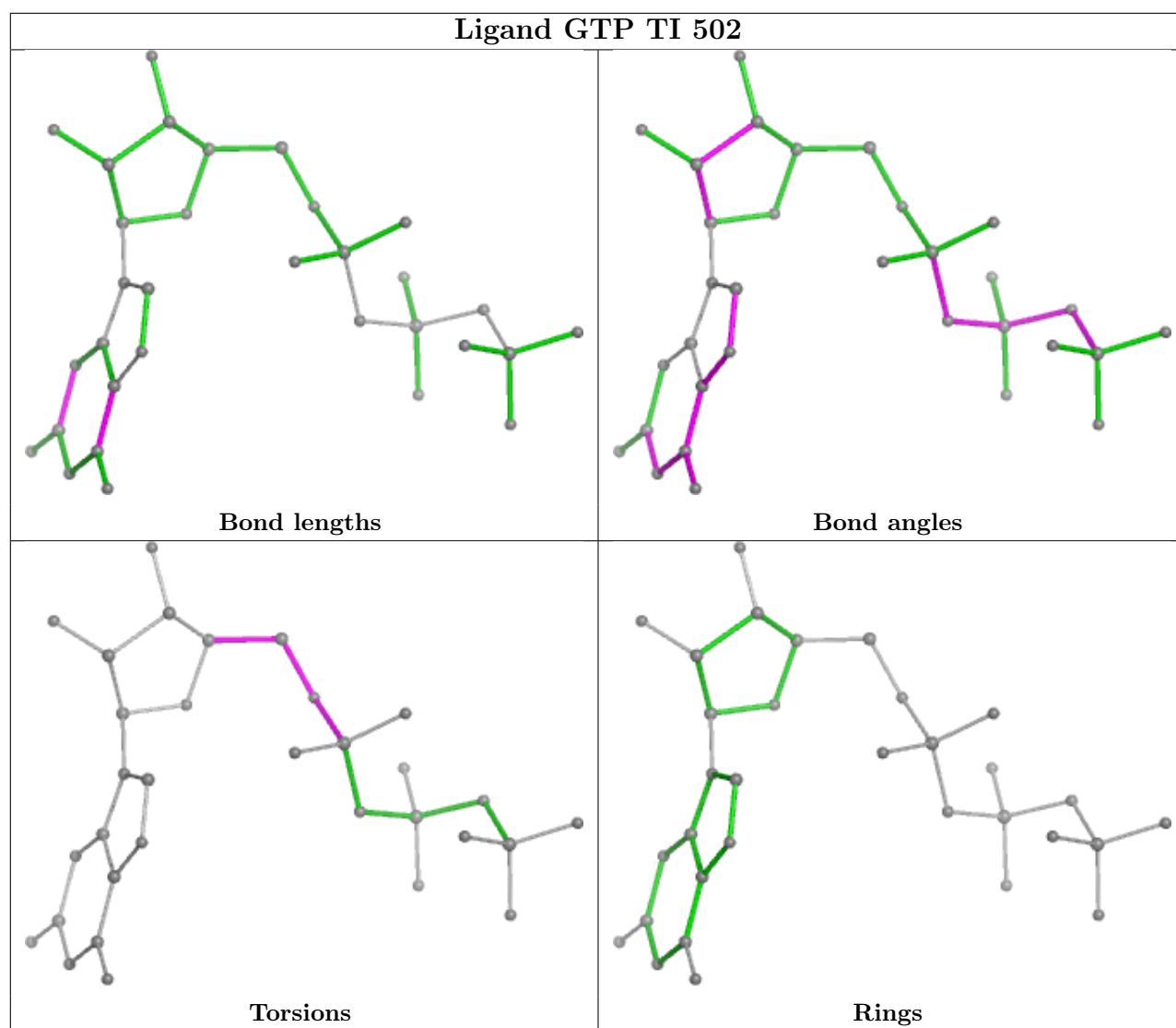


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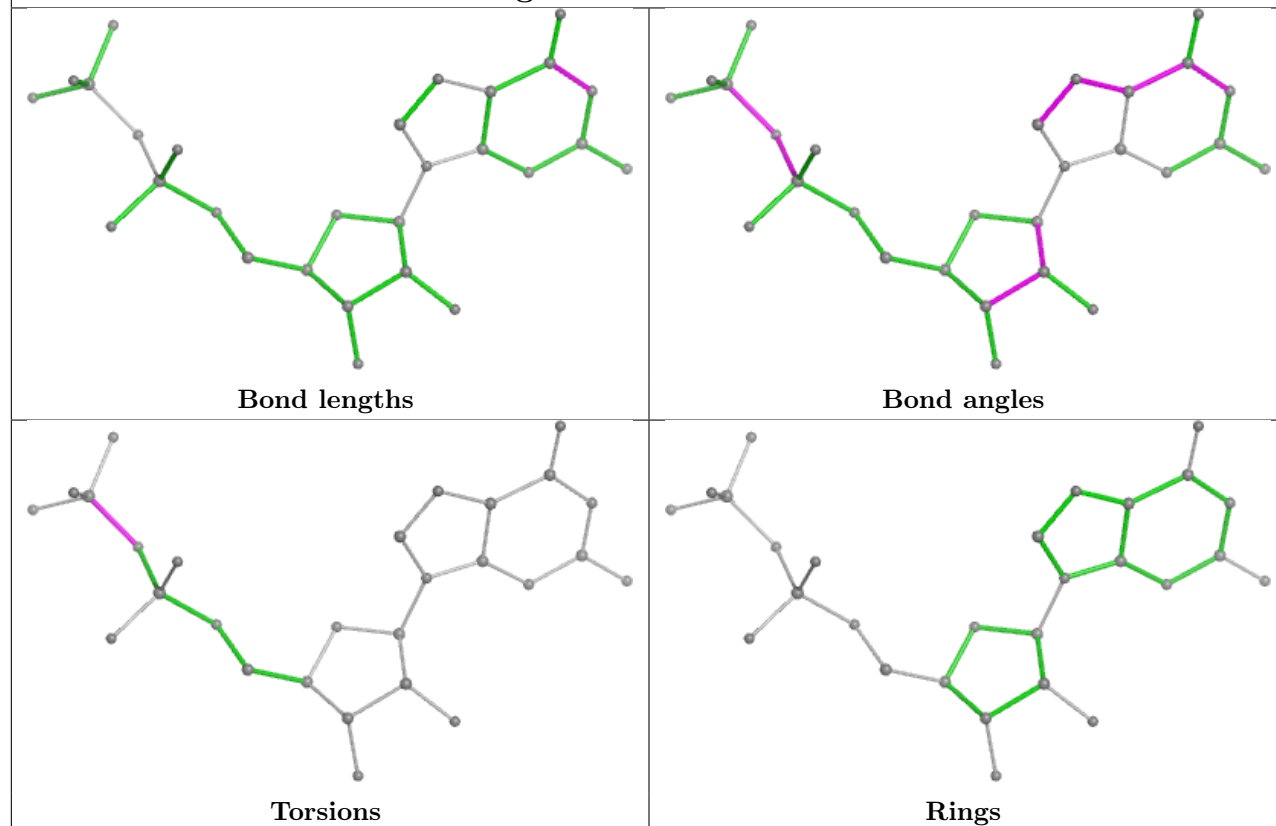


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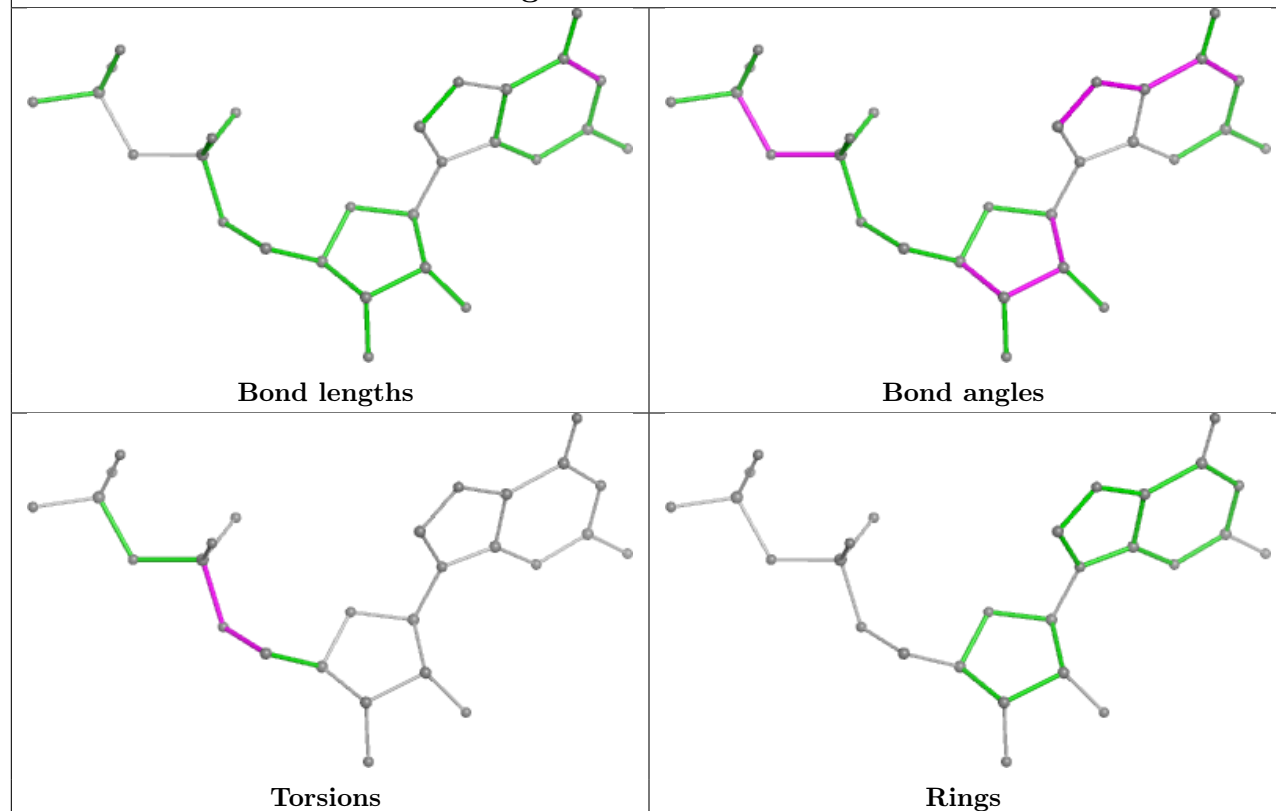


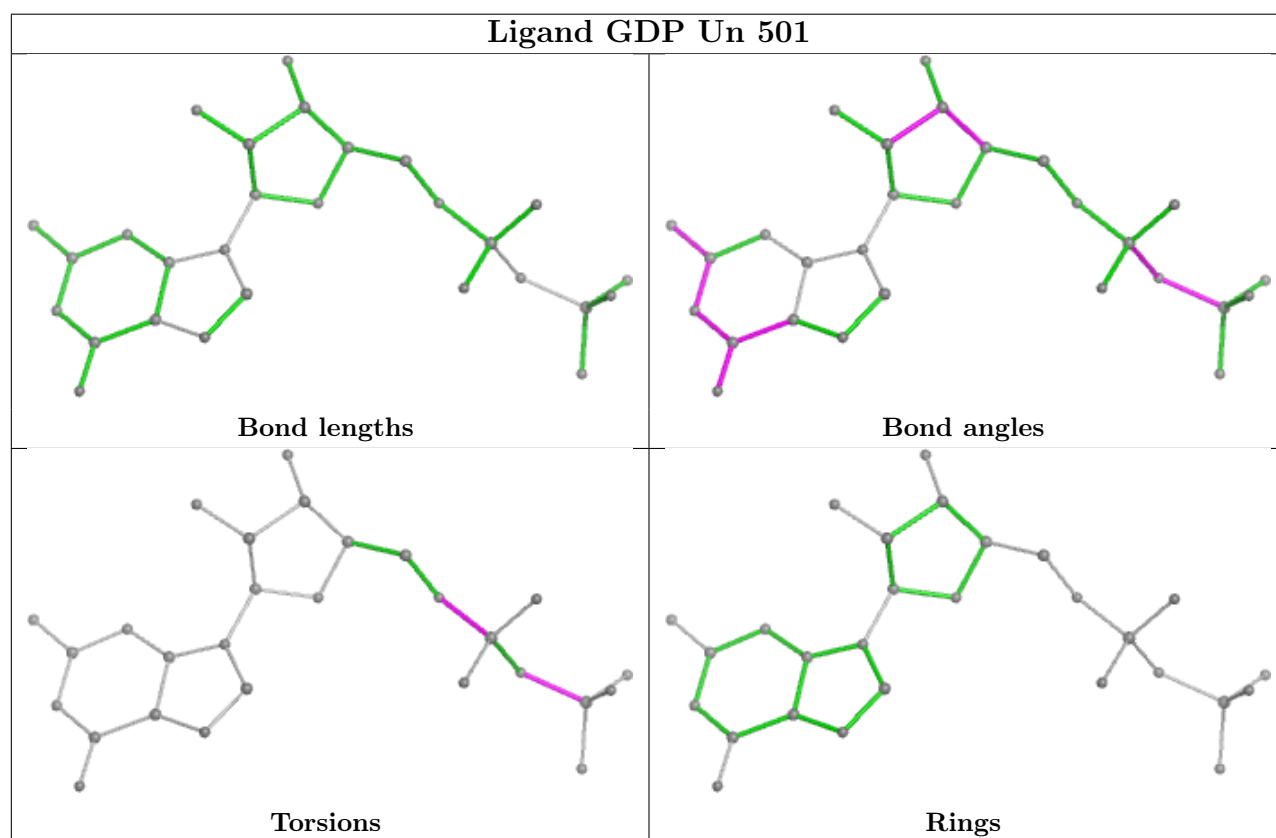
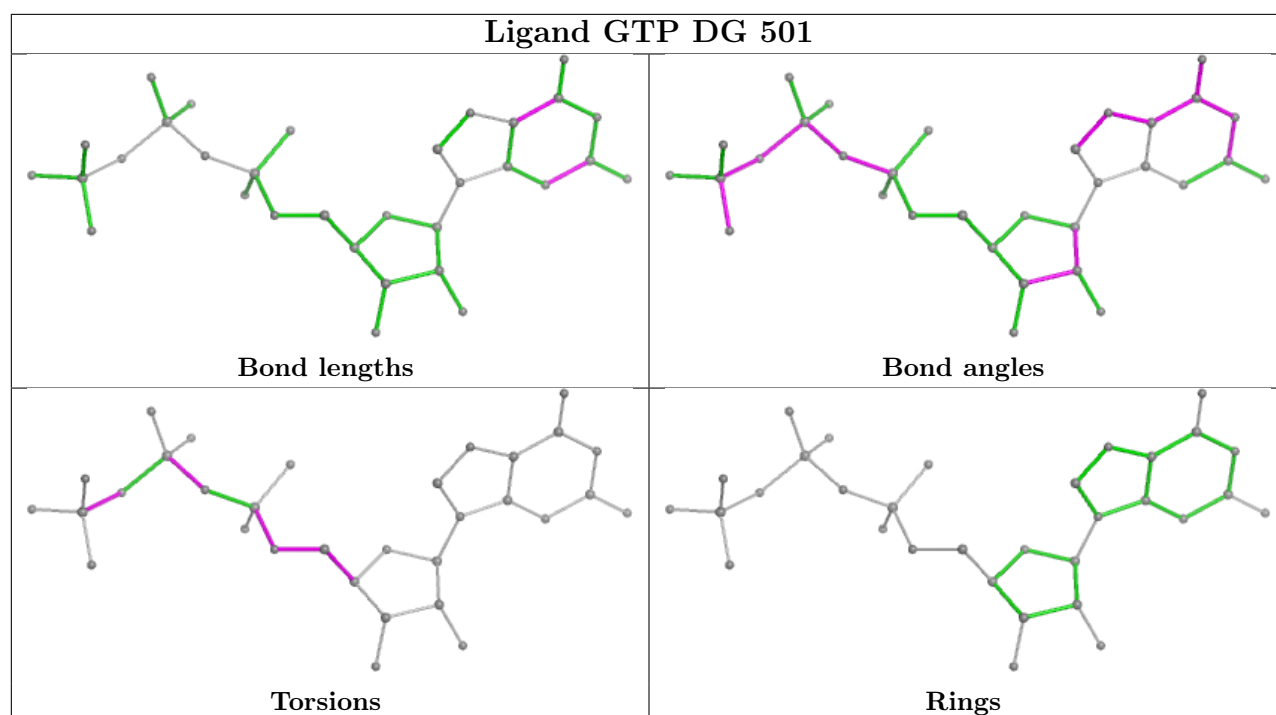


## Ligand GDP VO 501

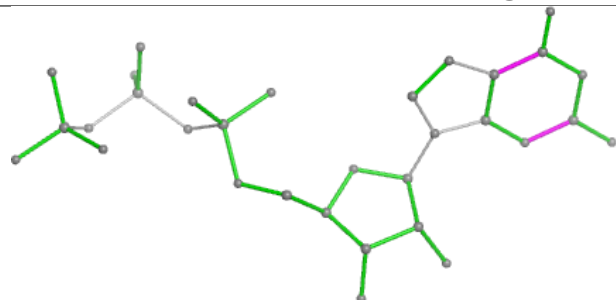


## Ligand GDP P7 501

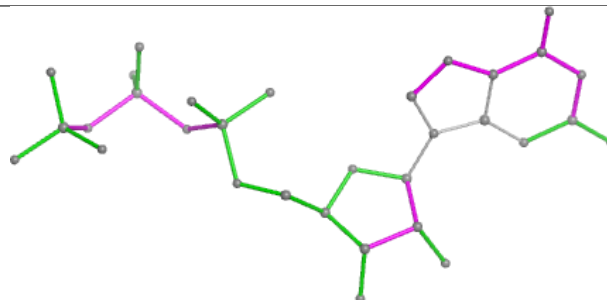




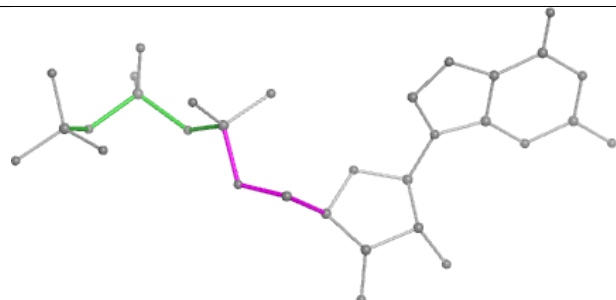
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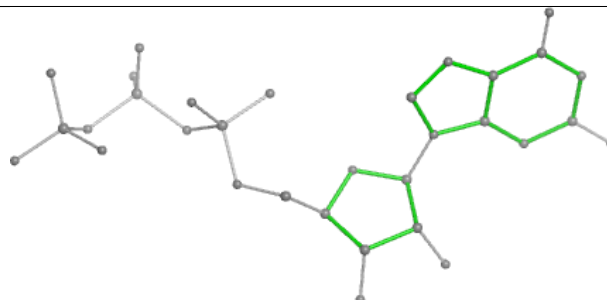
Bond lengths



Bond angles

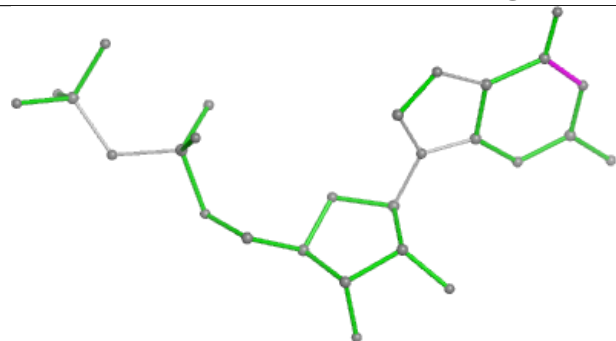


Torsions

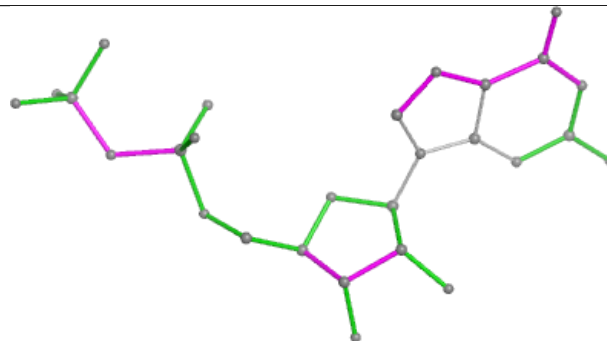


Rings

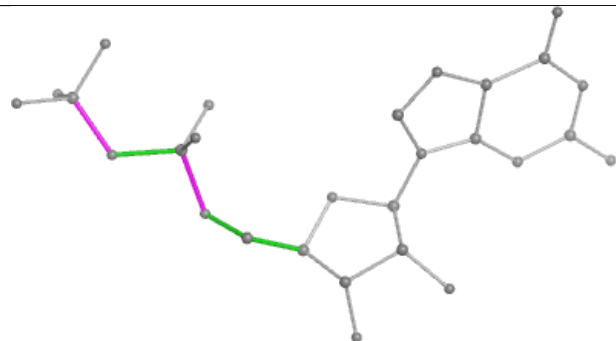
## Ligand GDP FF 501



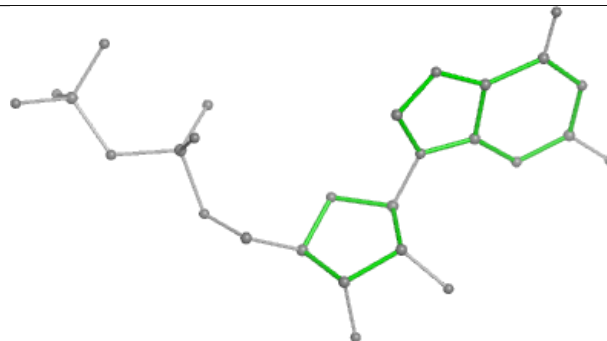
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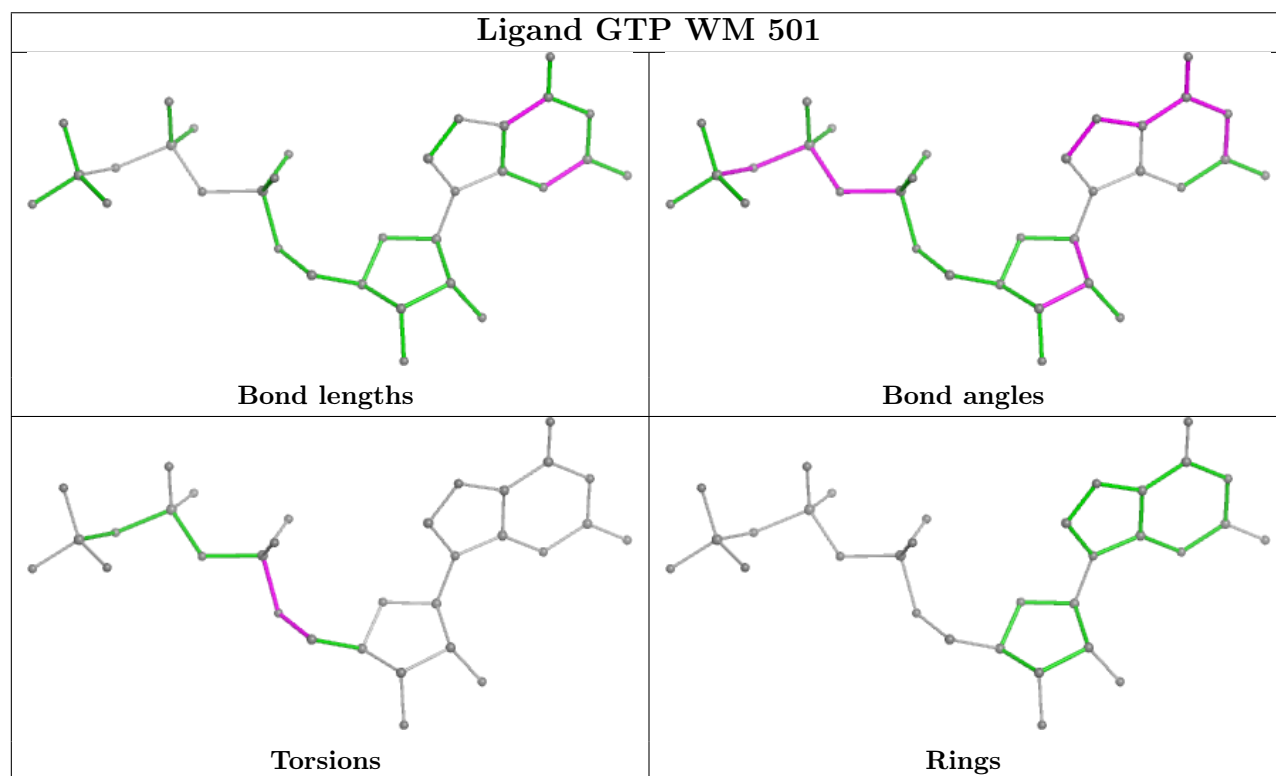
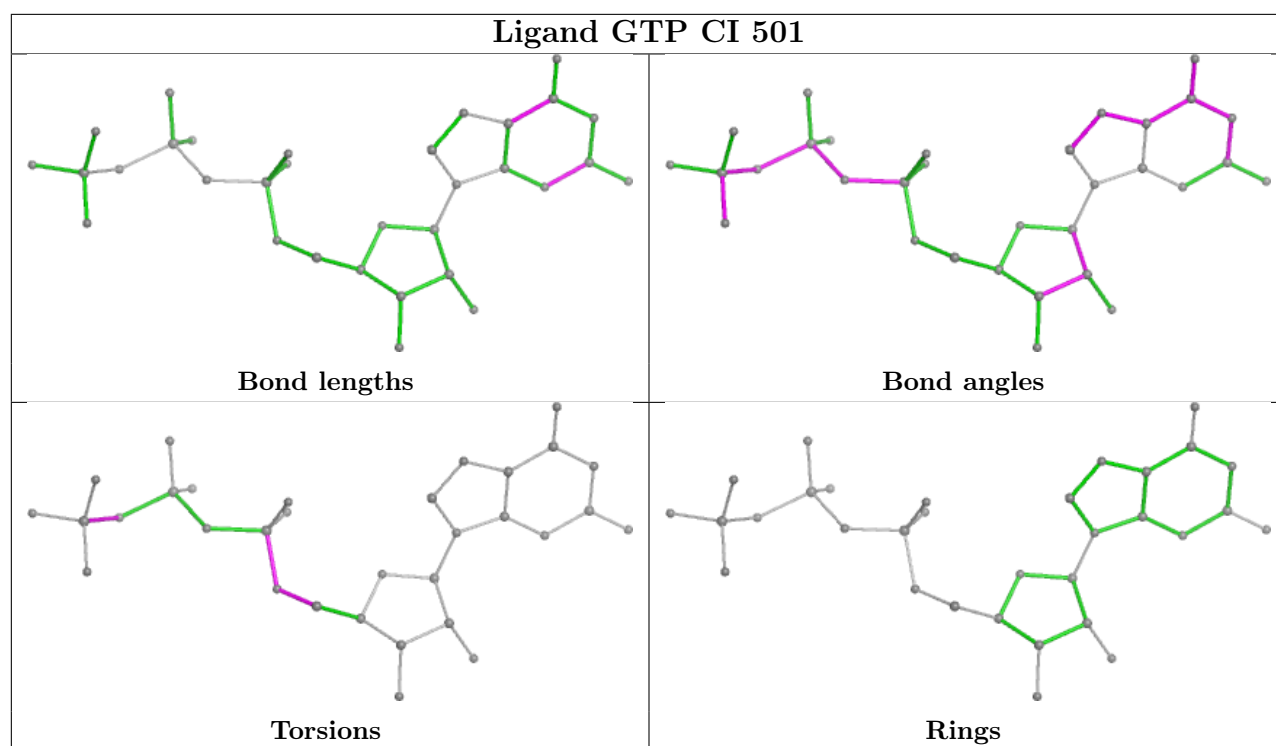
Bond angles



Torsions

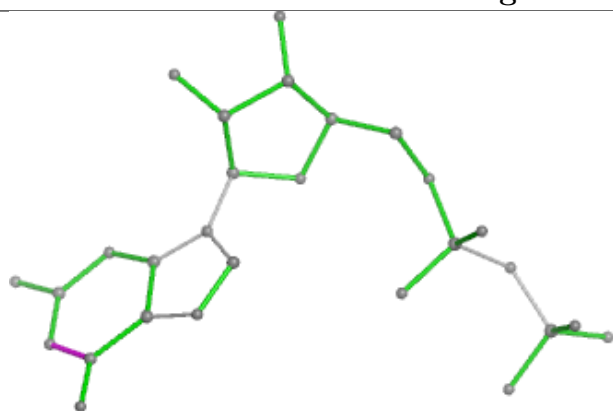


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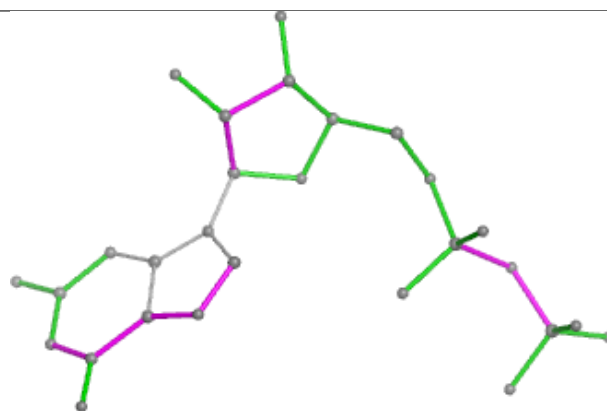




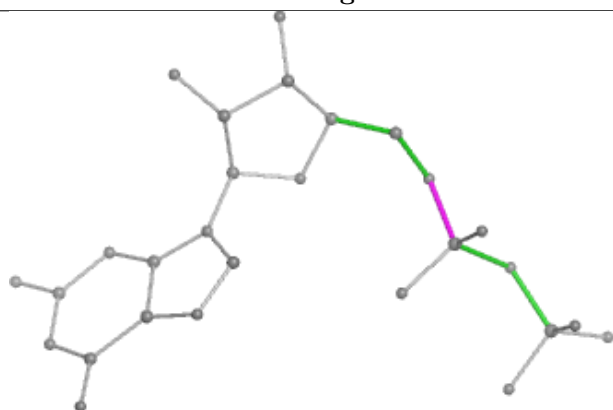
## Ligand GDP Vw 501



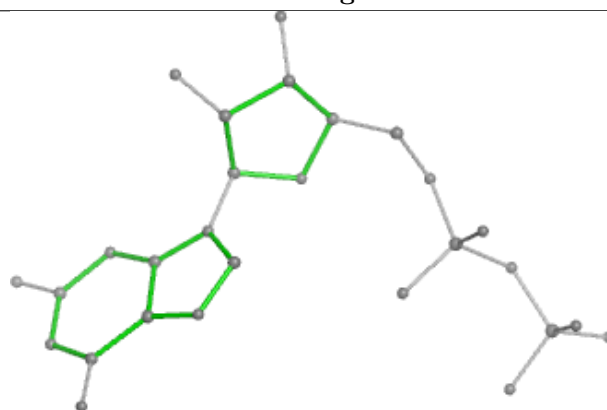
Bond lengths



Bond angles

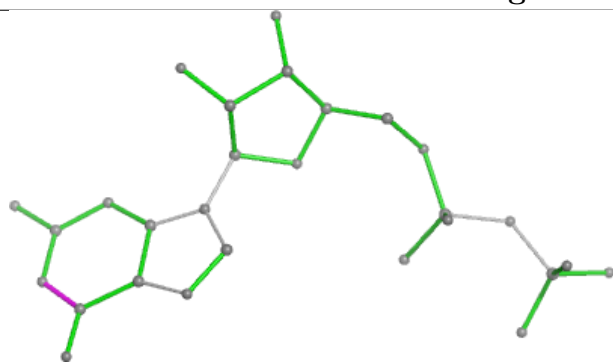


Torsions

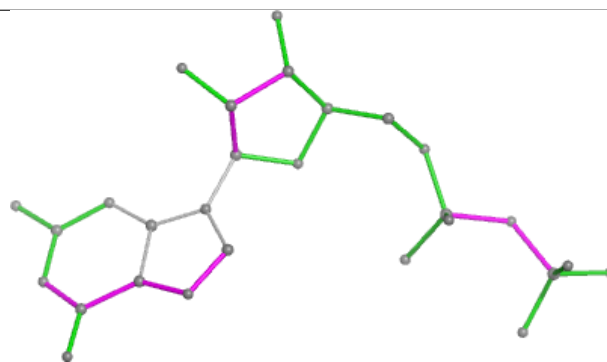


Rings

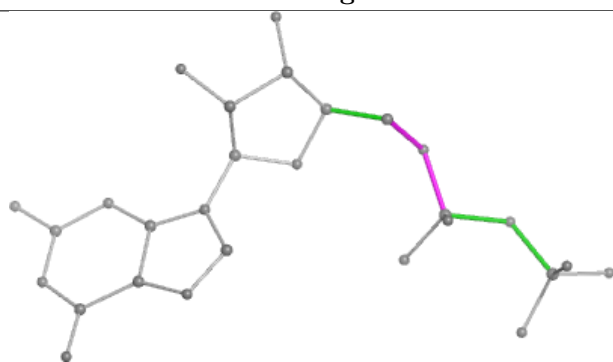
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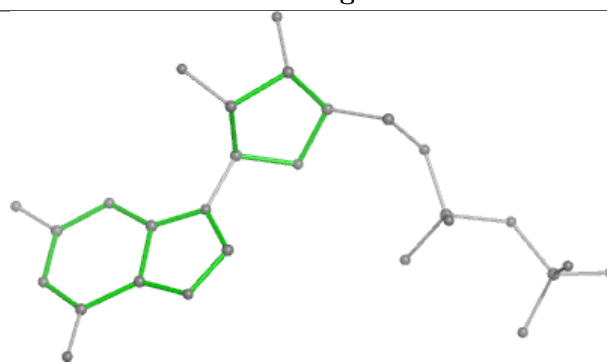
Bond lengths



Bond angles

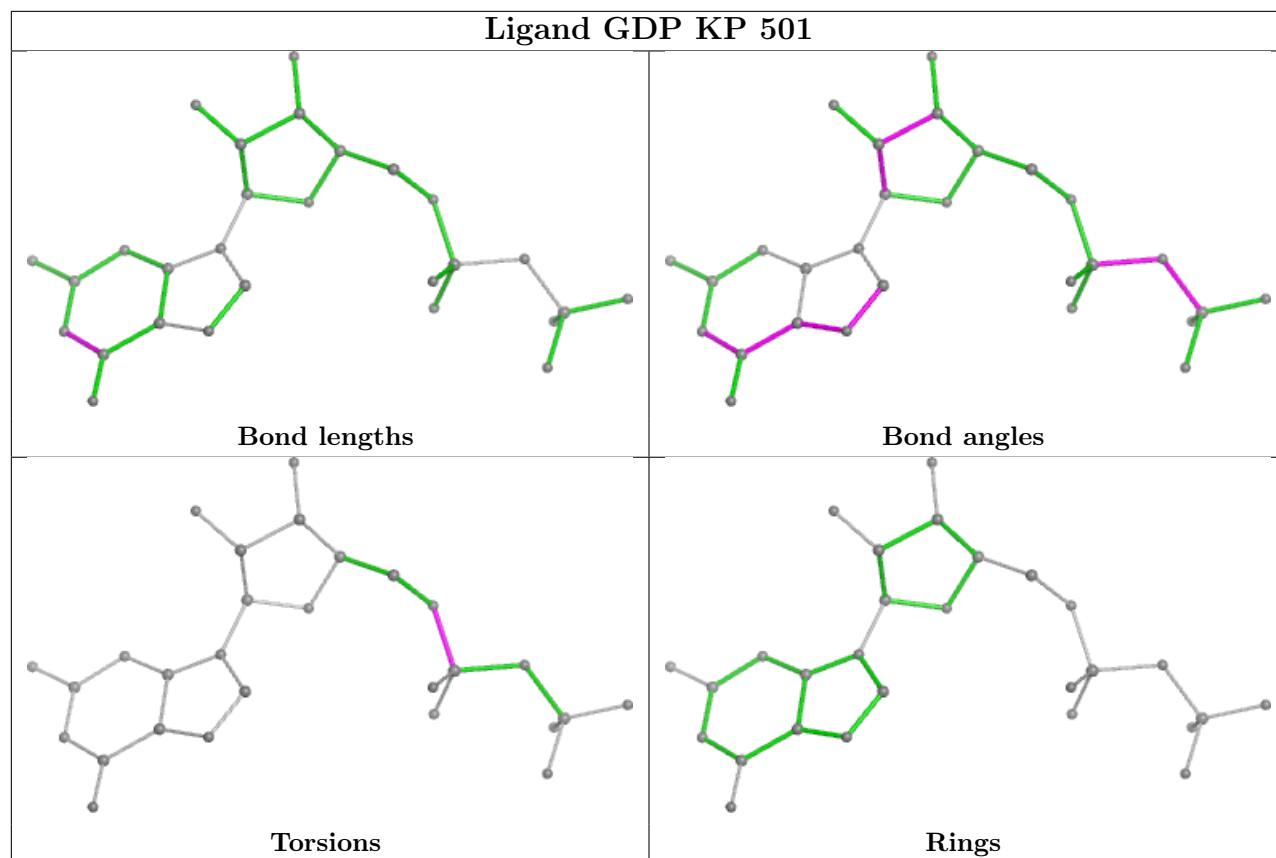


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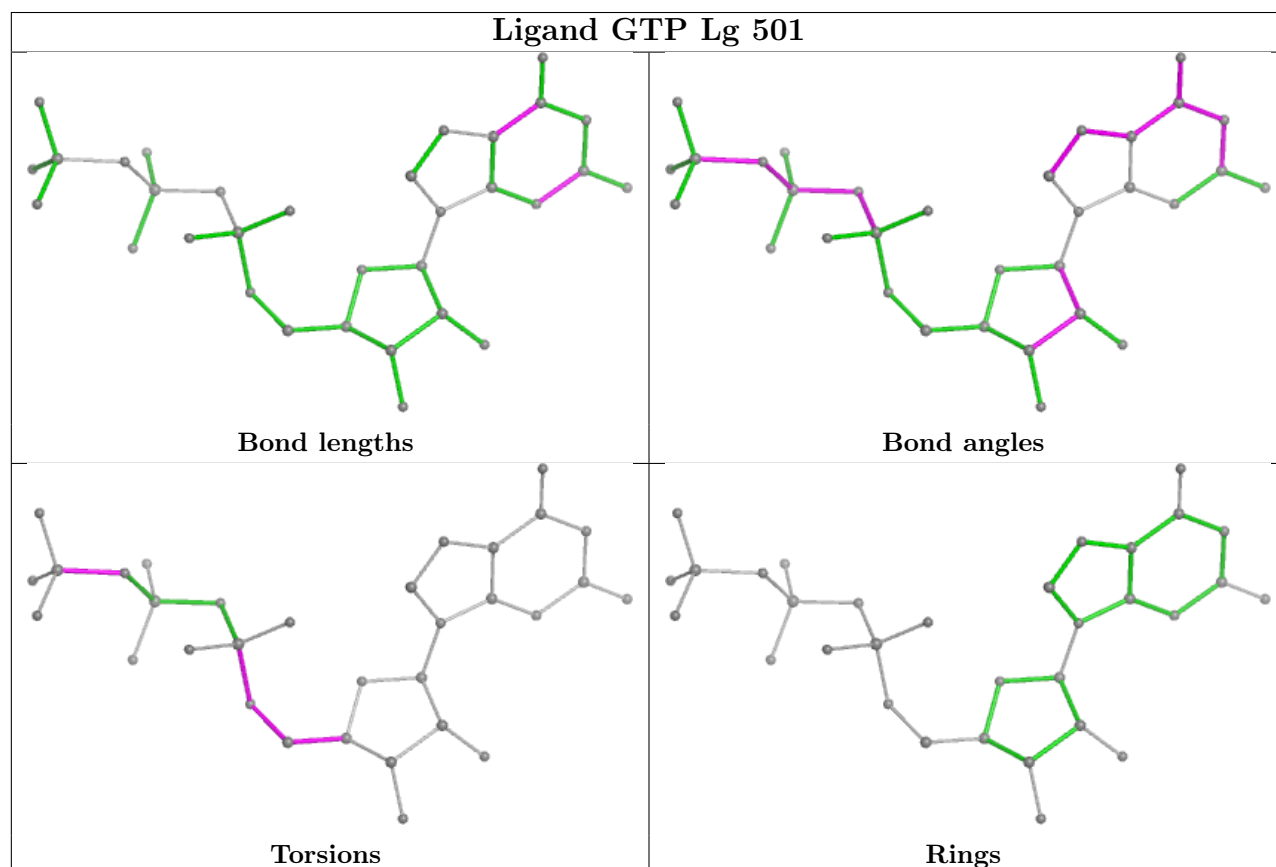


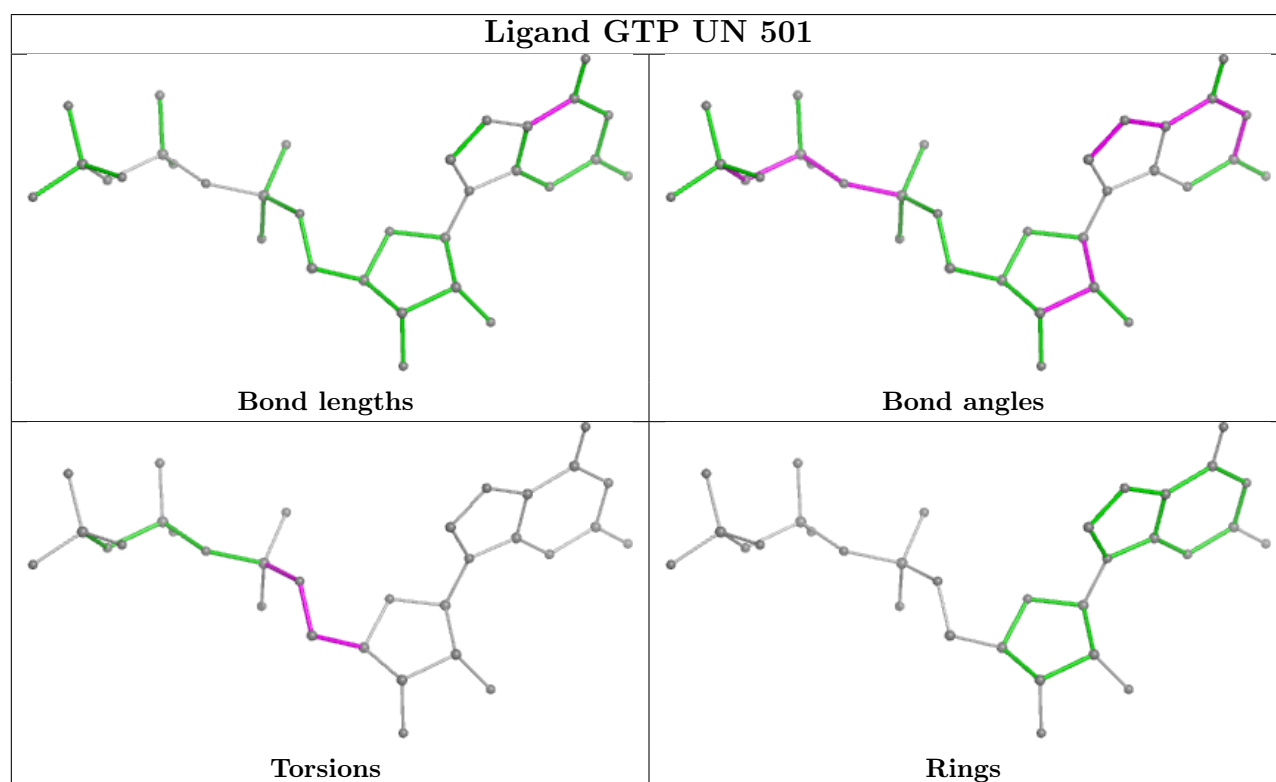
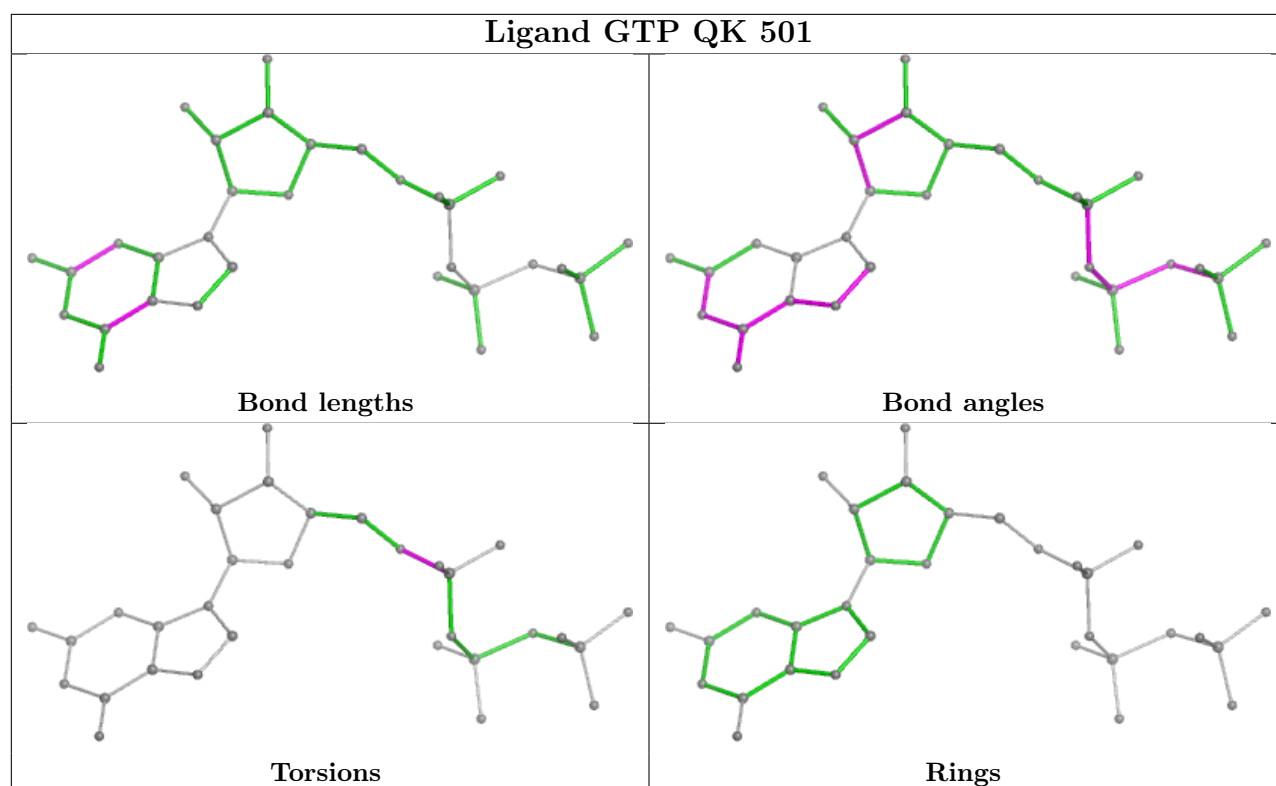
Rings

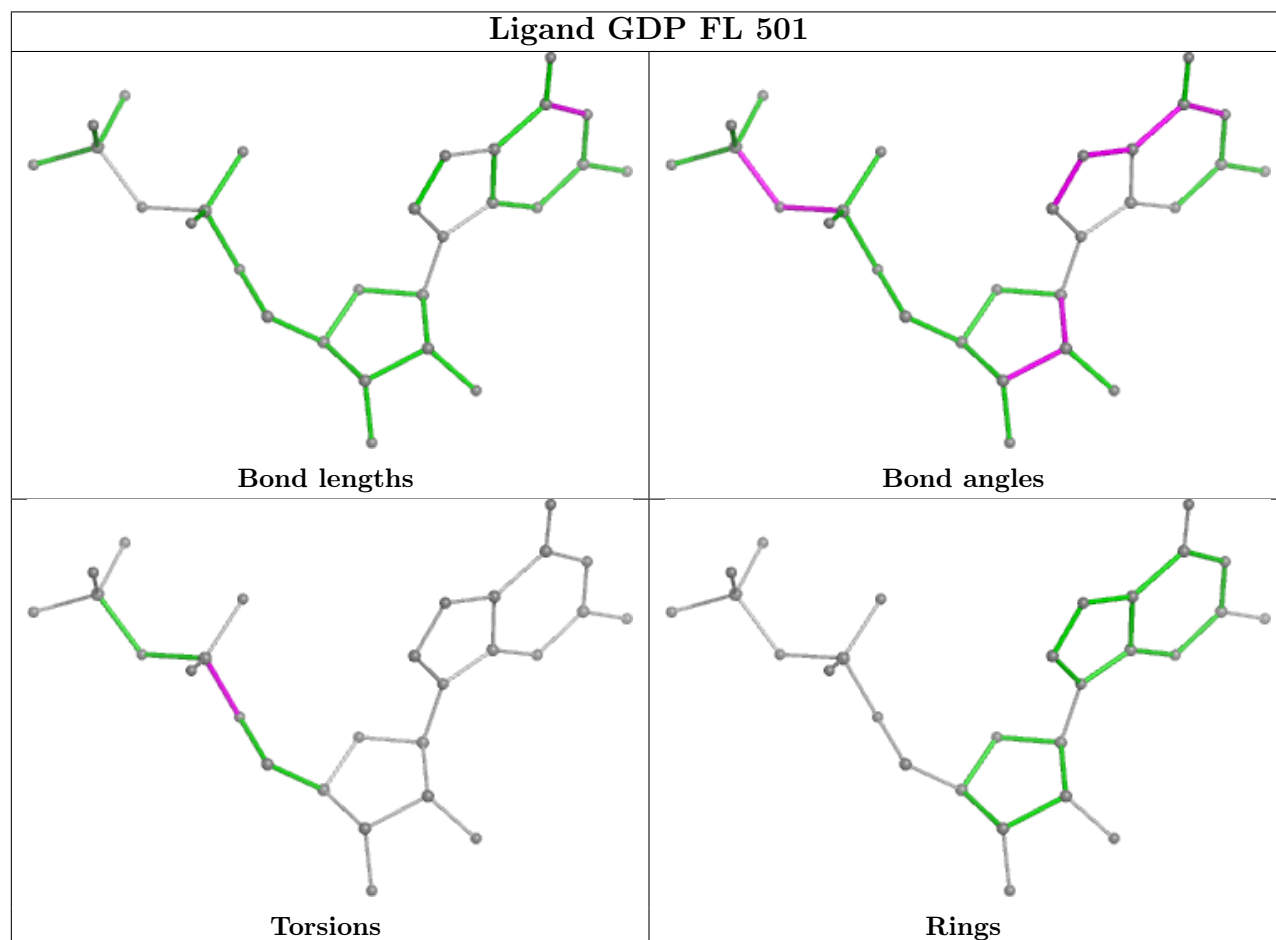
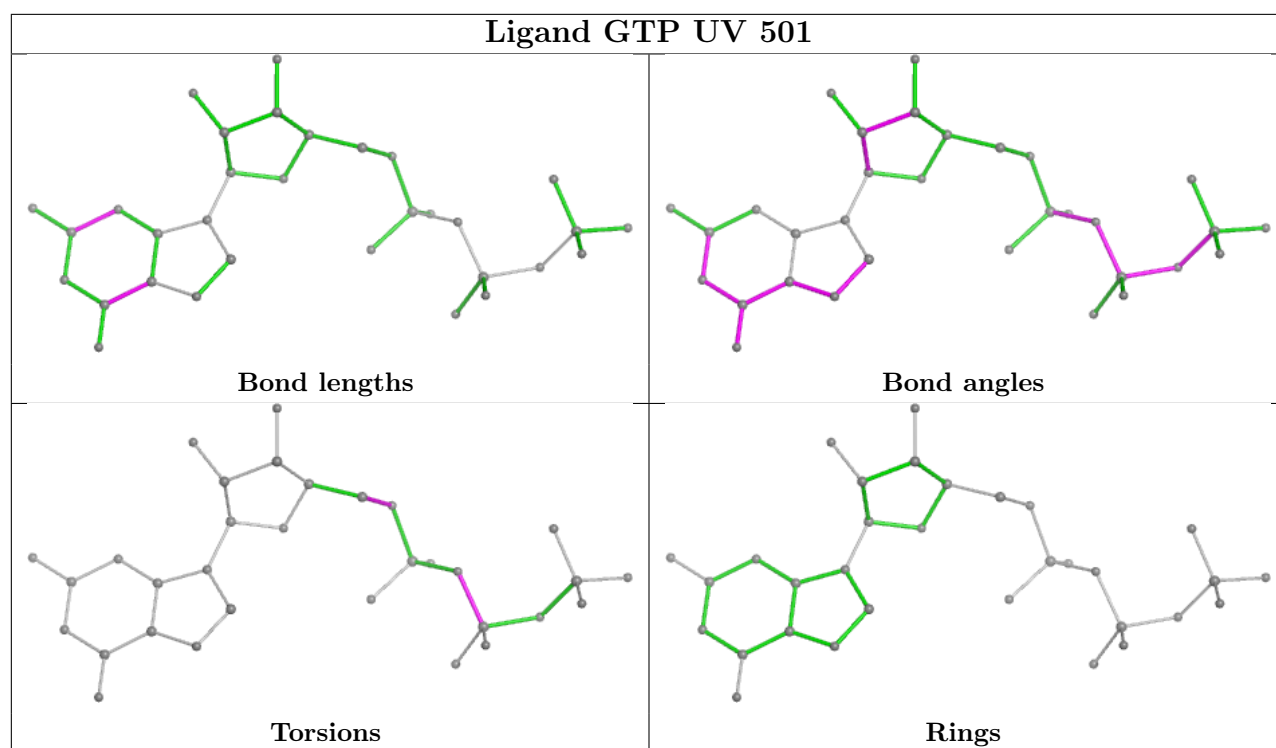
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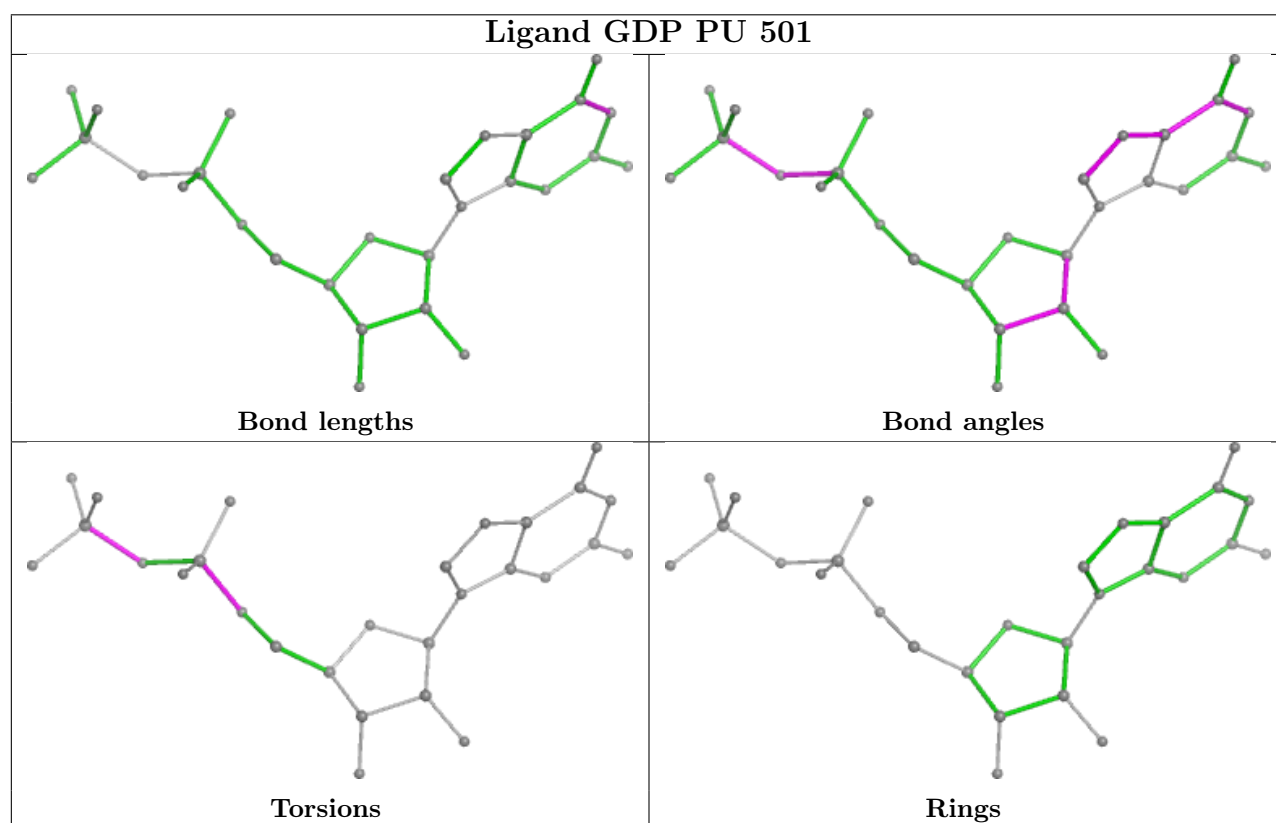
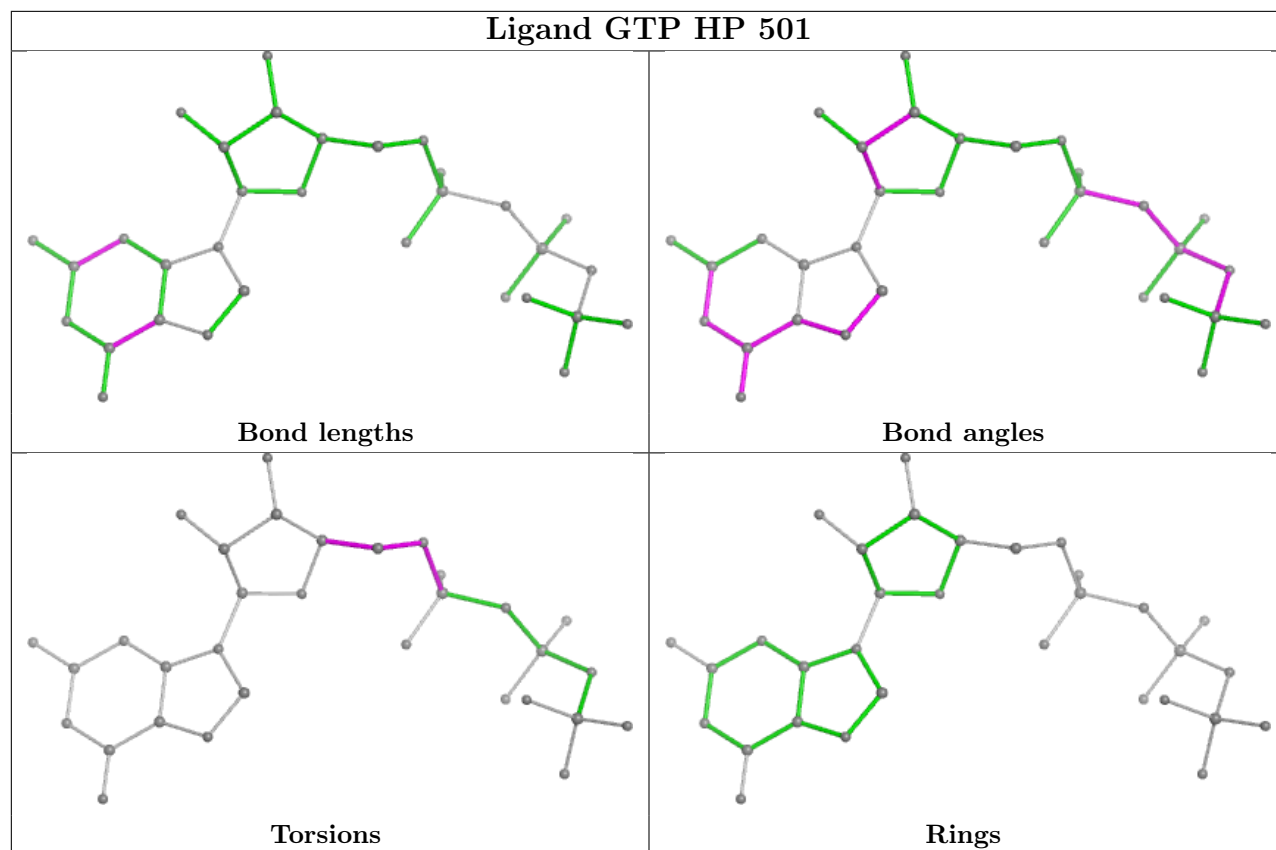


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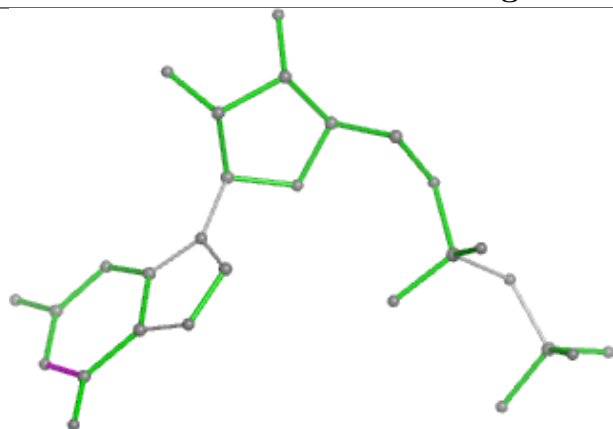




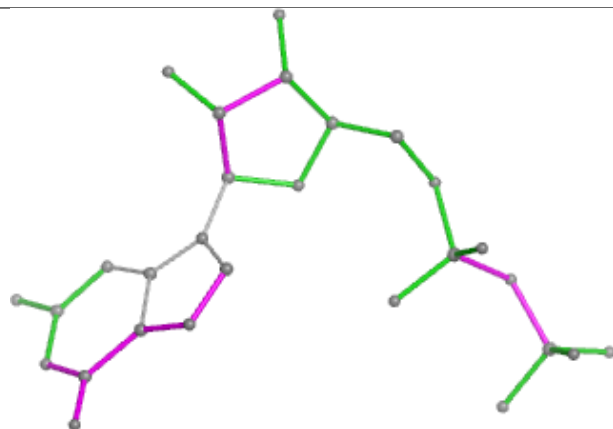




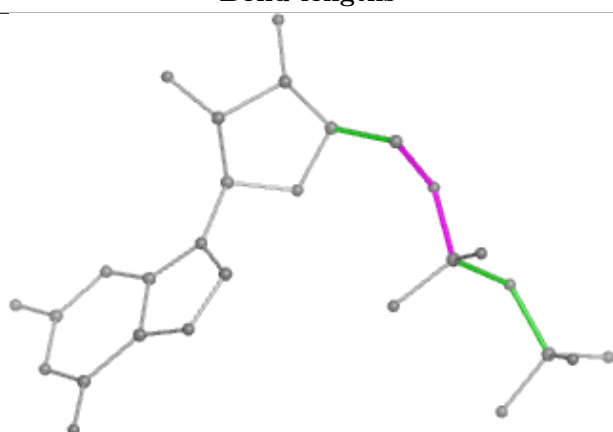
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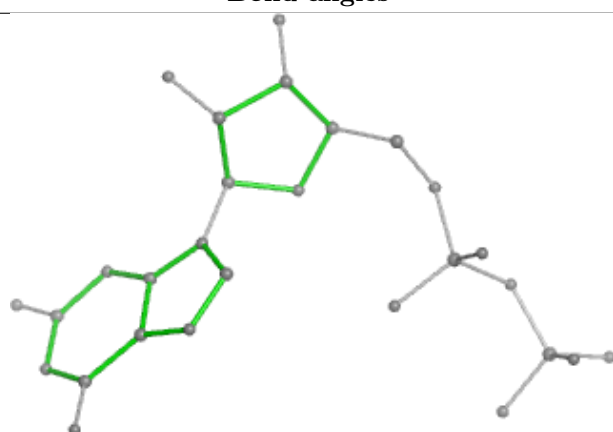
Bond lengths



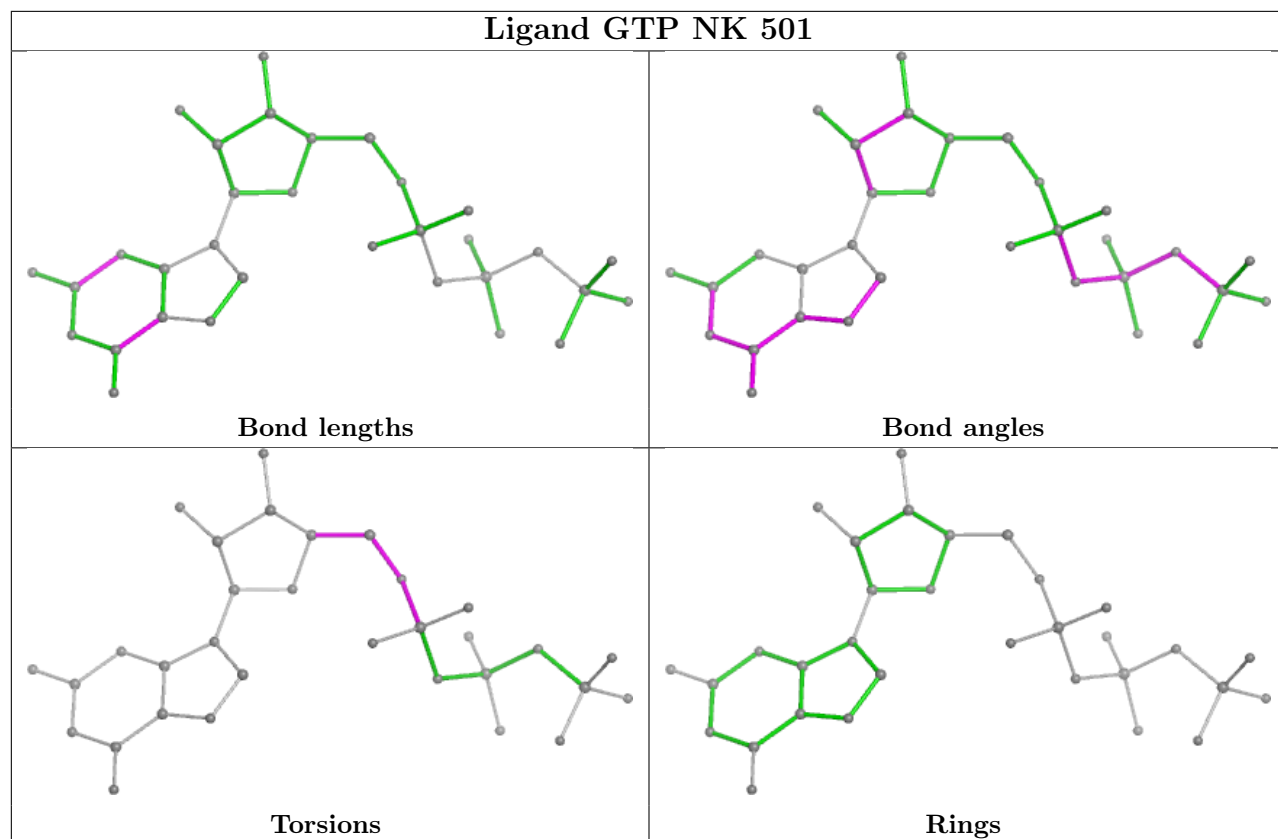
Bond angles

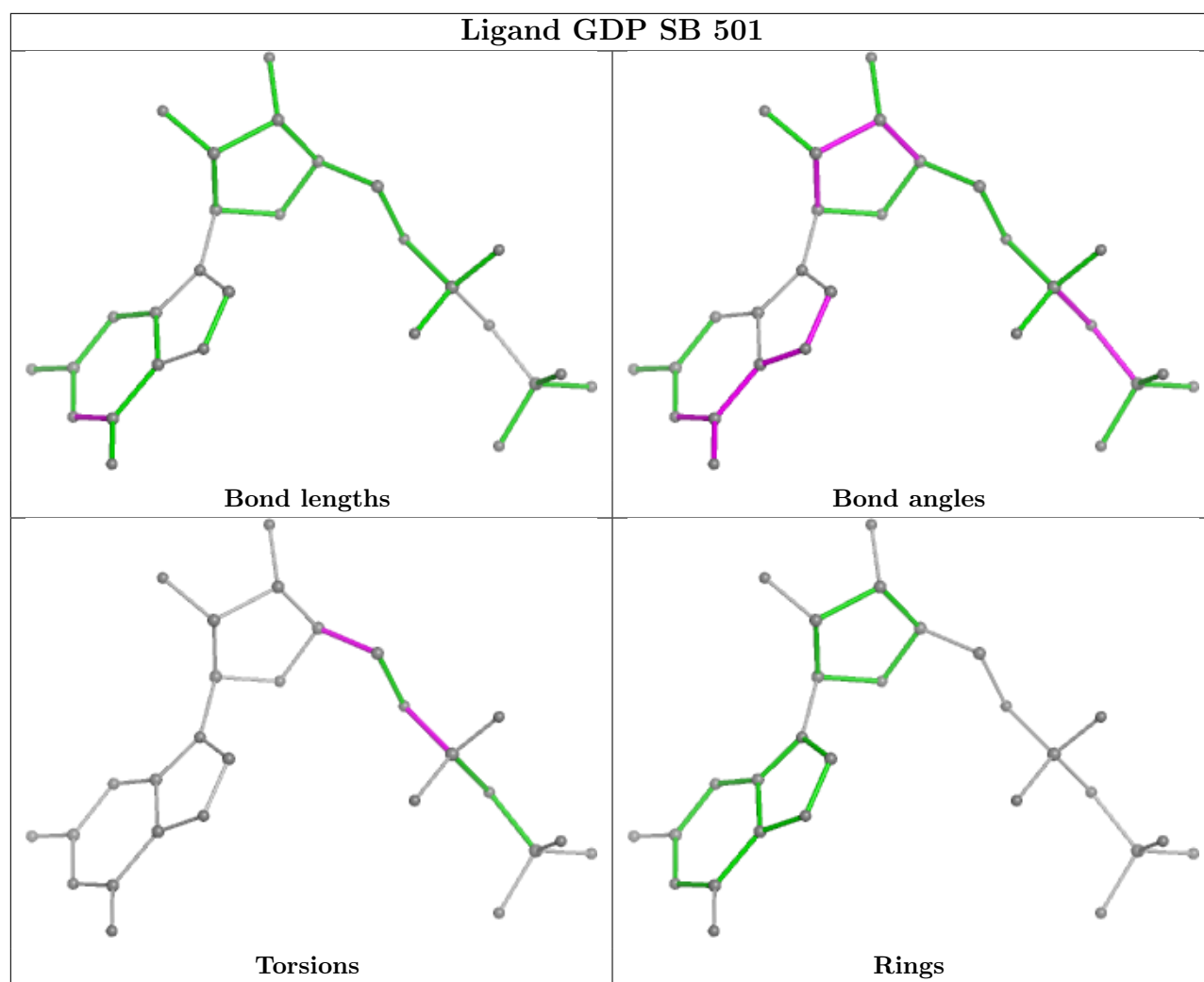


Torsions

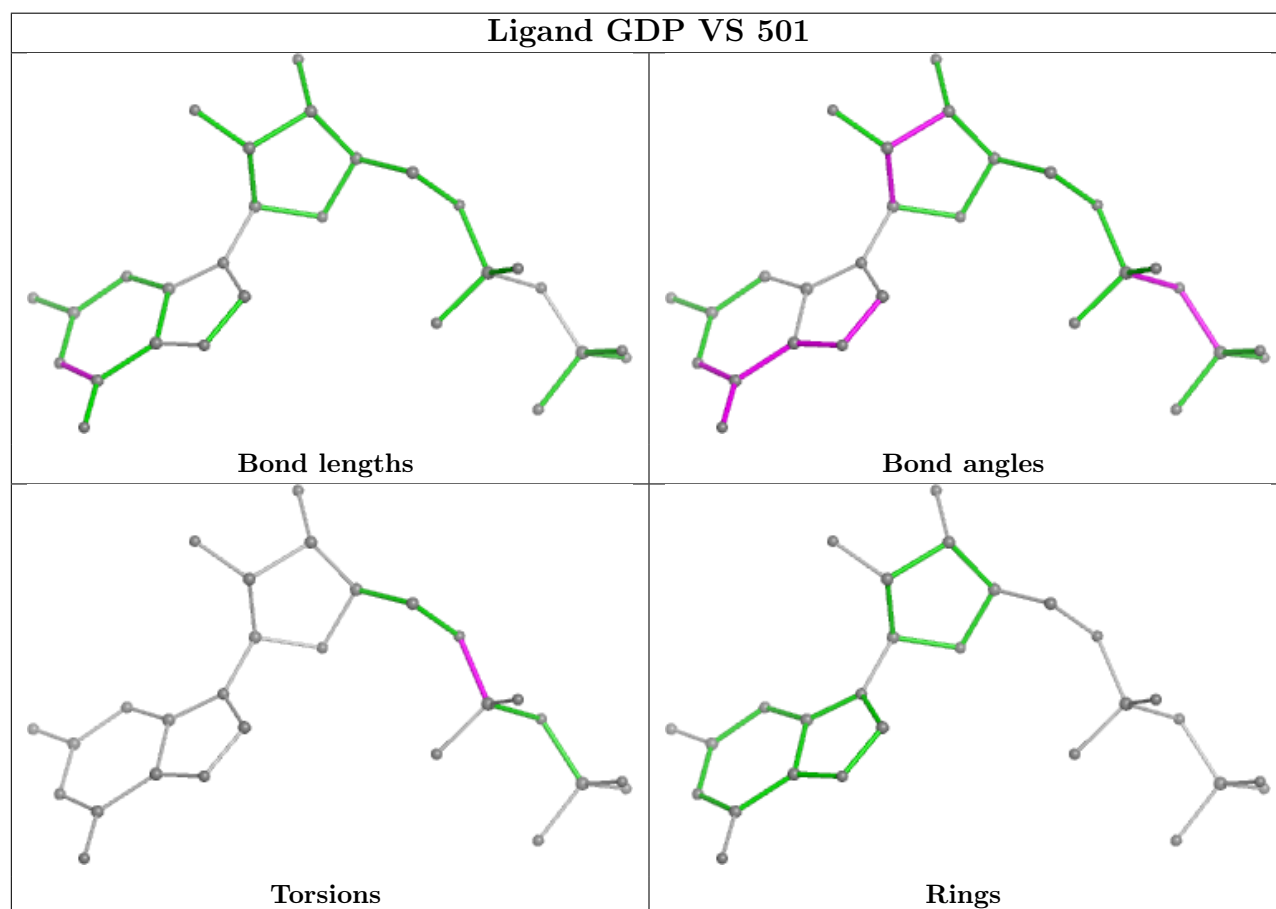
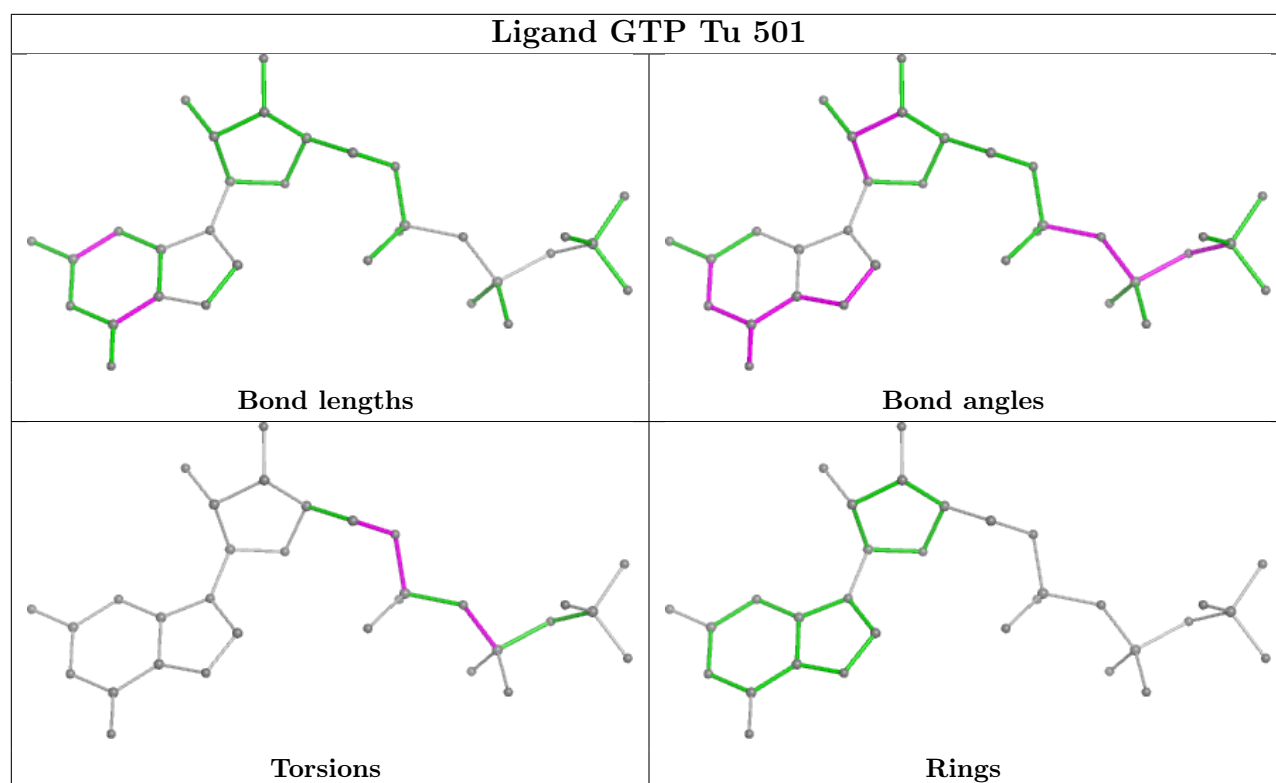


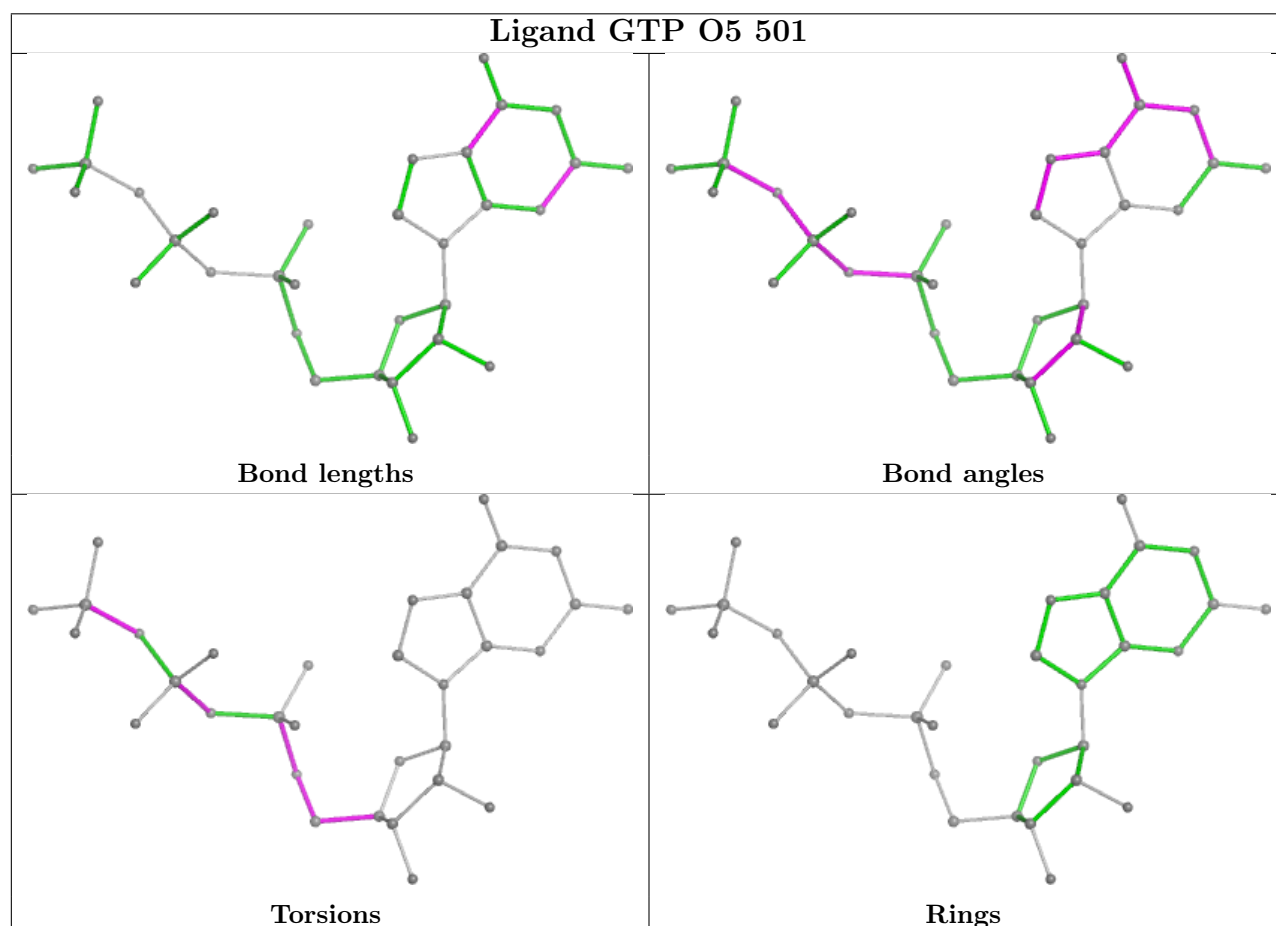
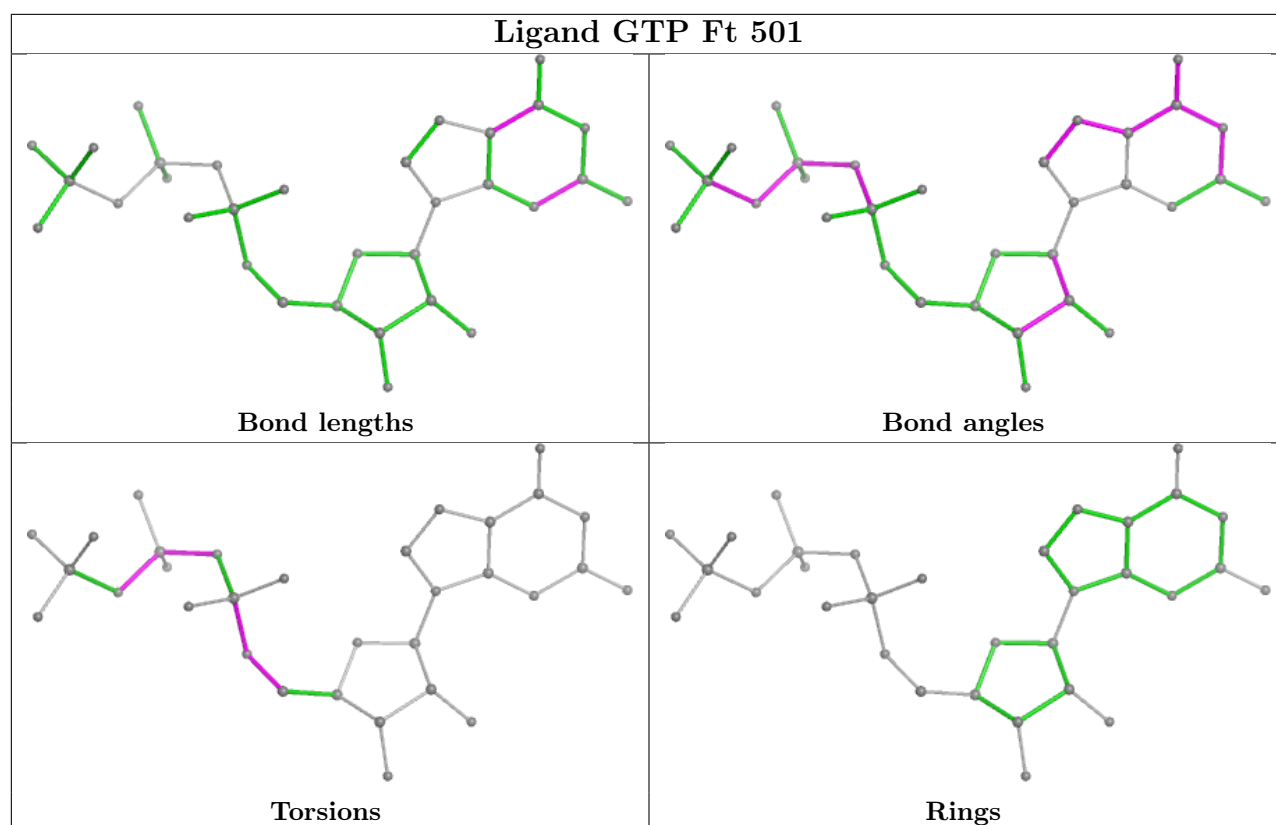
Rings

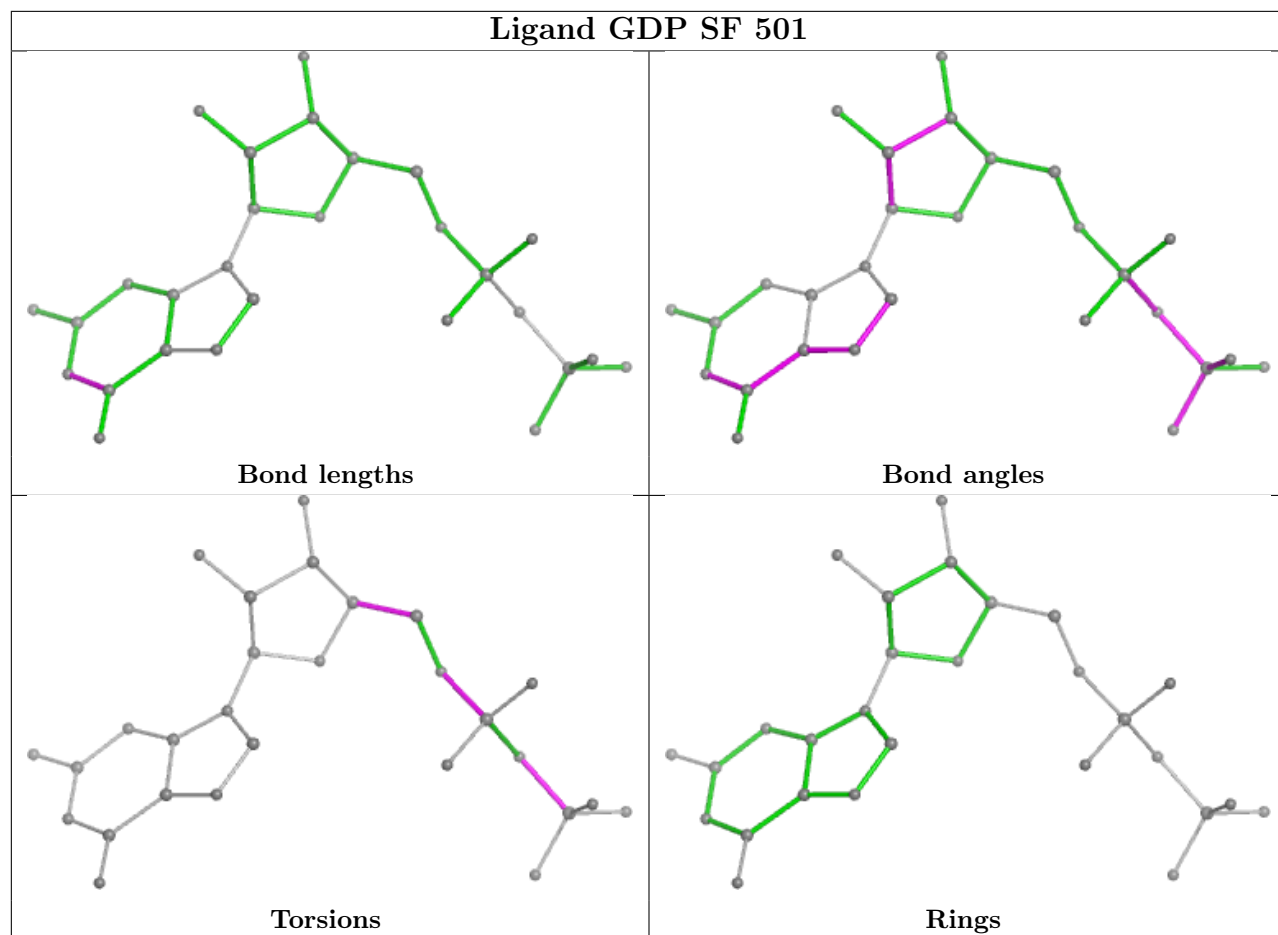


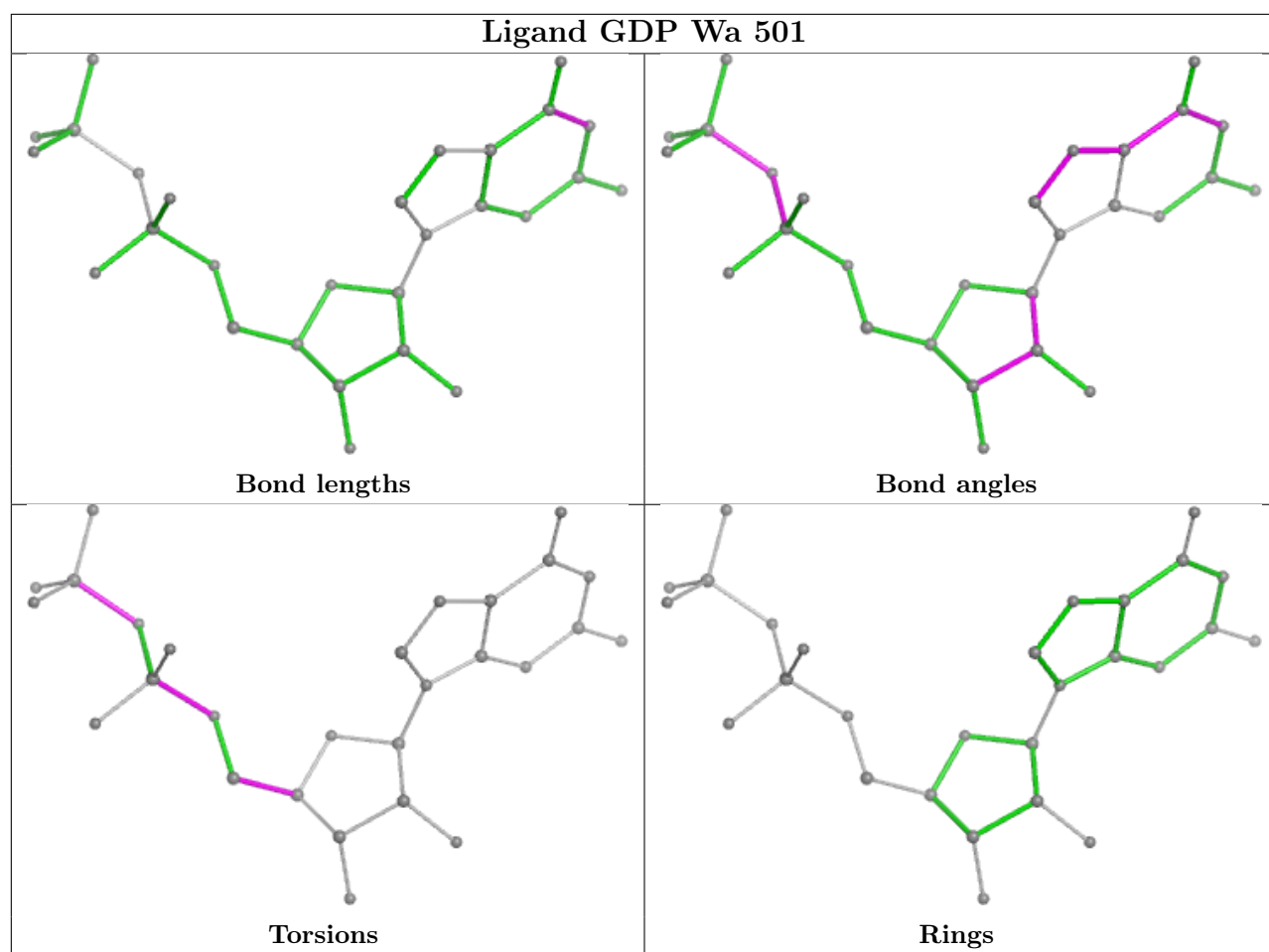


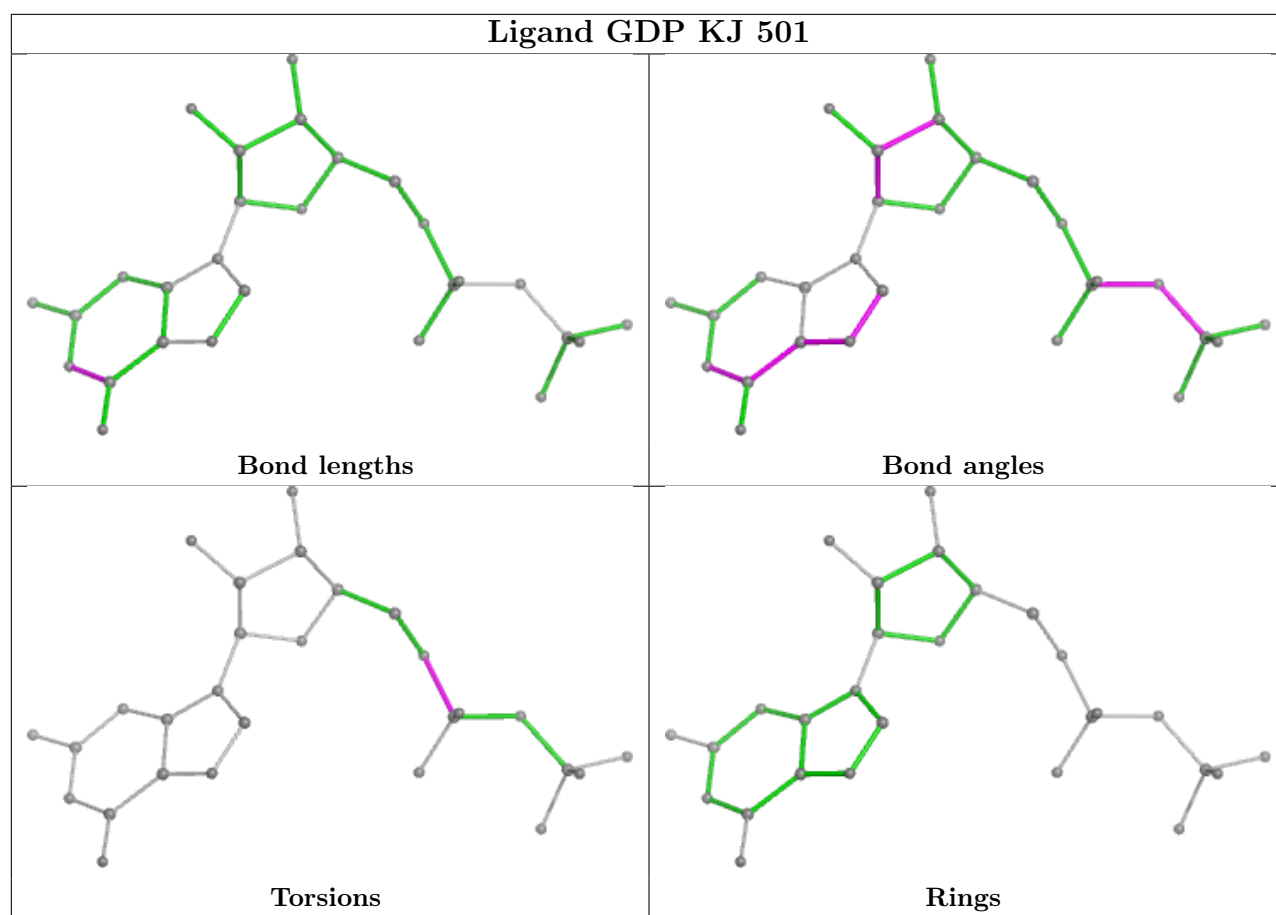




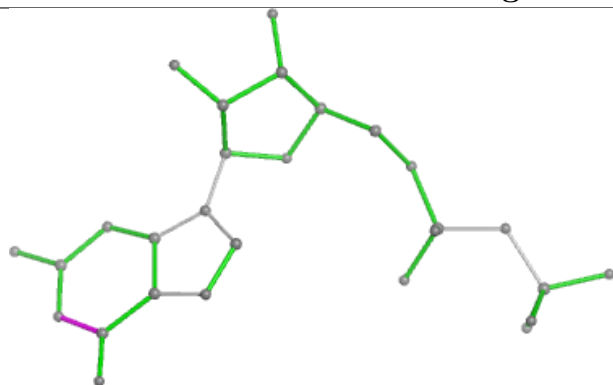




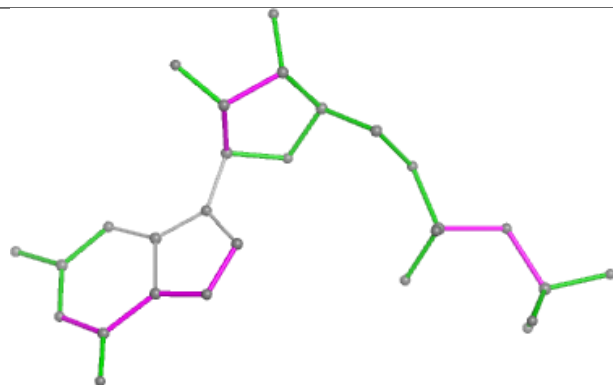




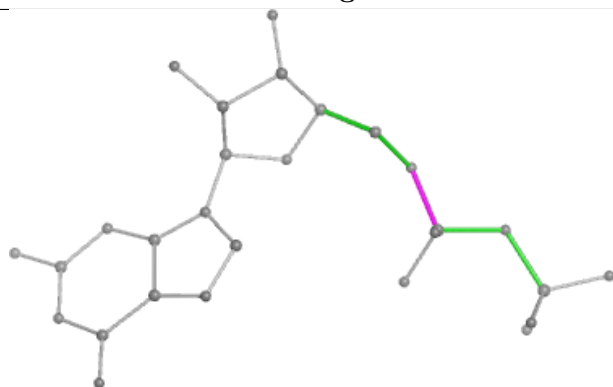
## Ligand GDP R3 501



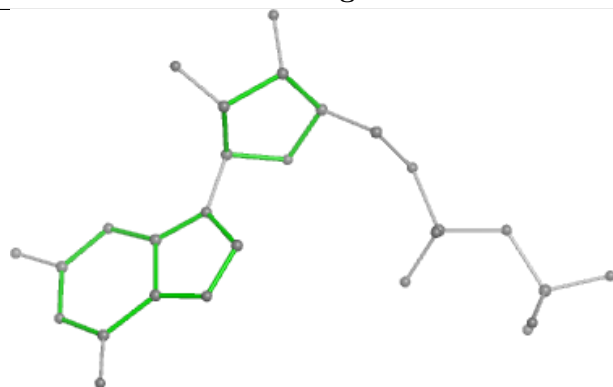
Bond lengths



Bond angles

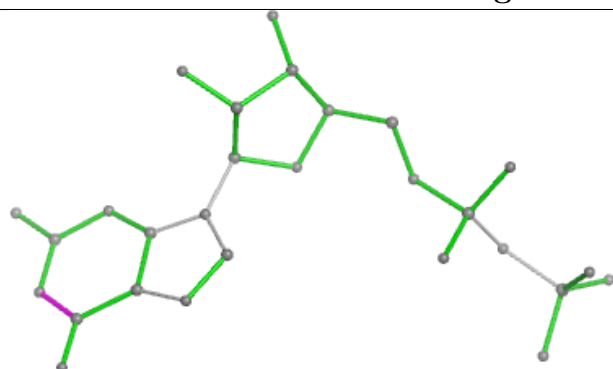


Torsions

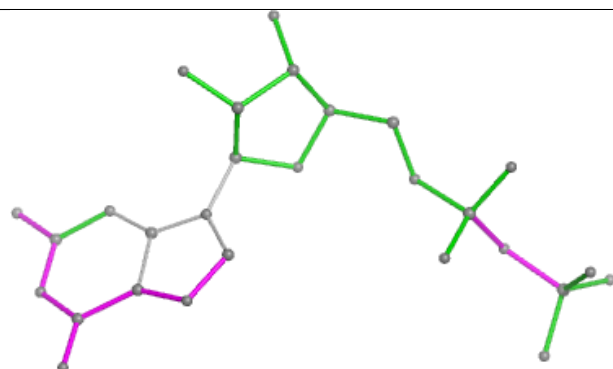


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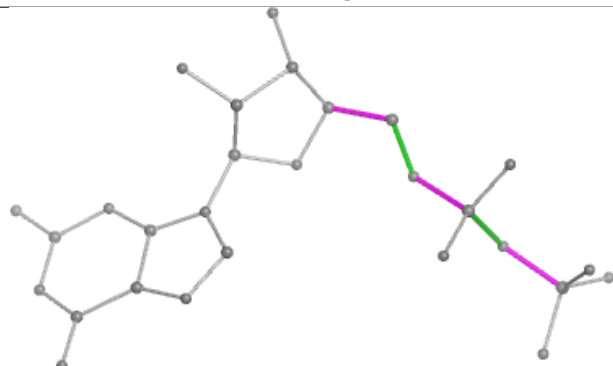
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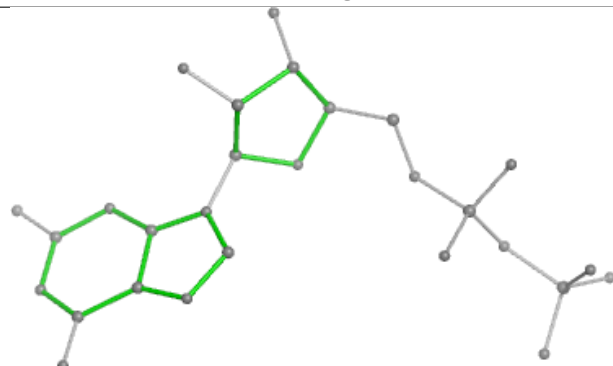
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Bond angles

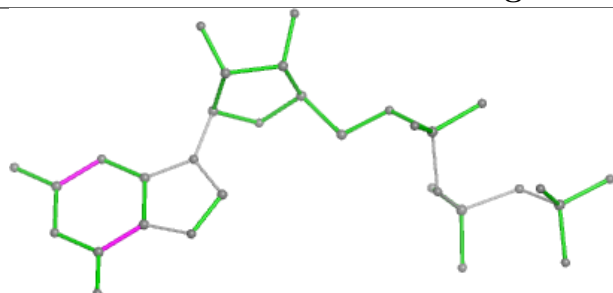


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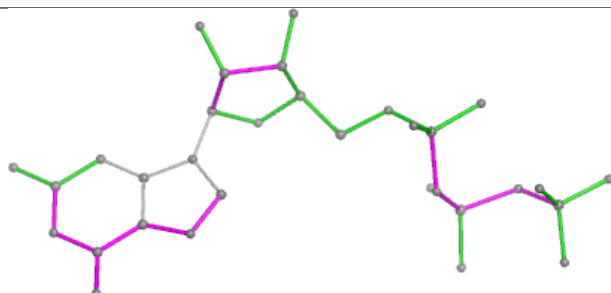


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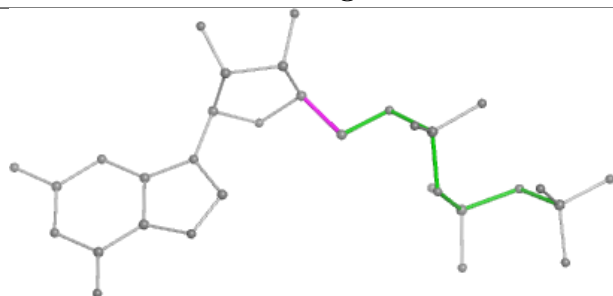
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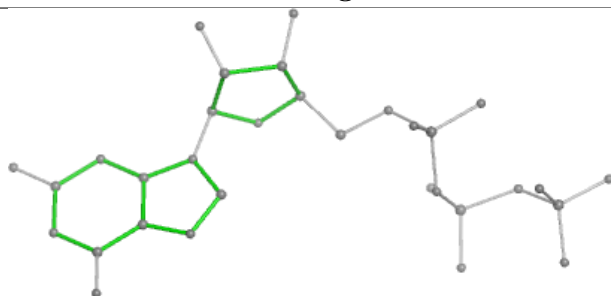
Bond lengths



Bond angles

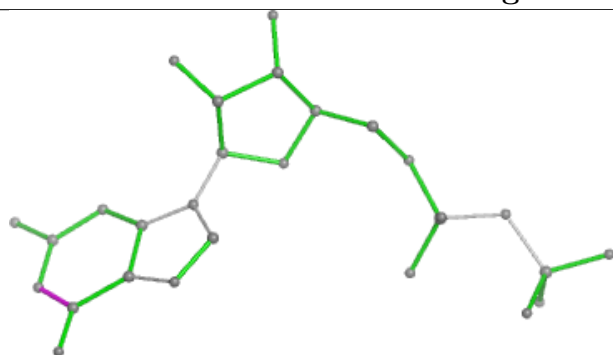


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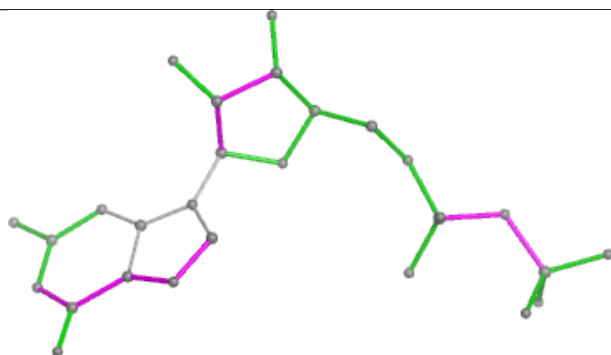


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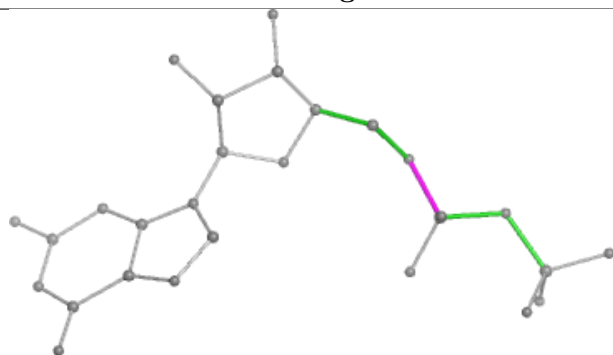
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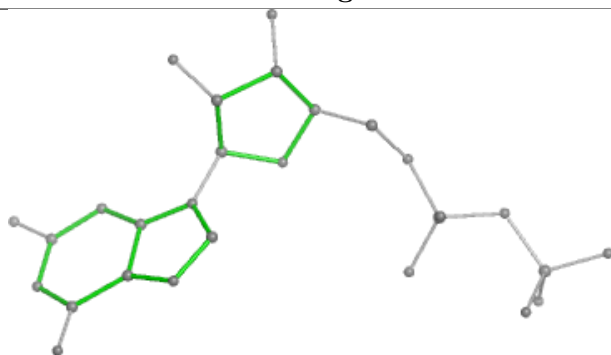
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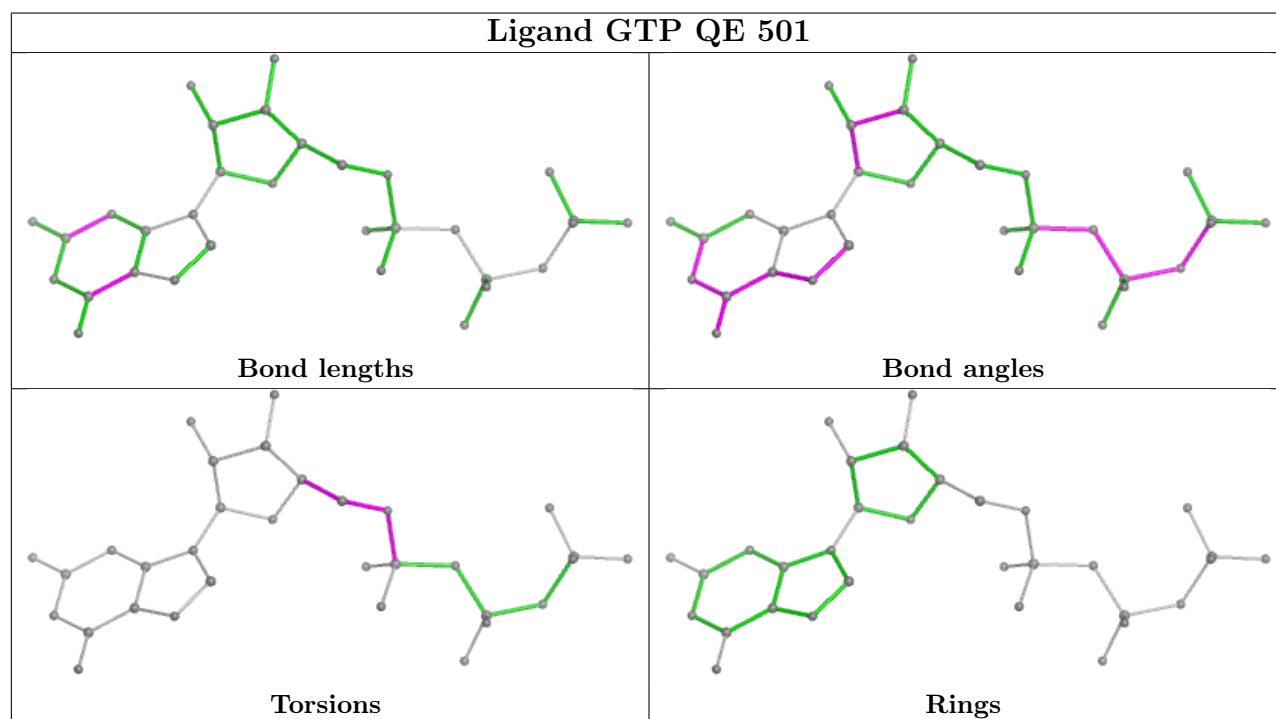
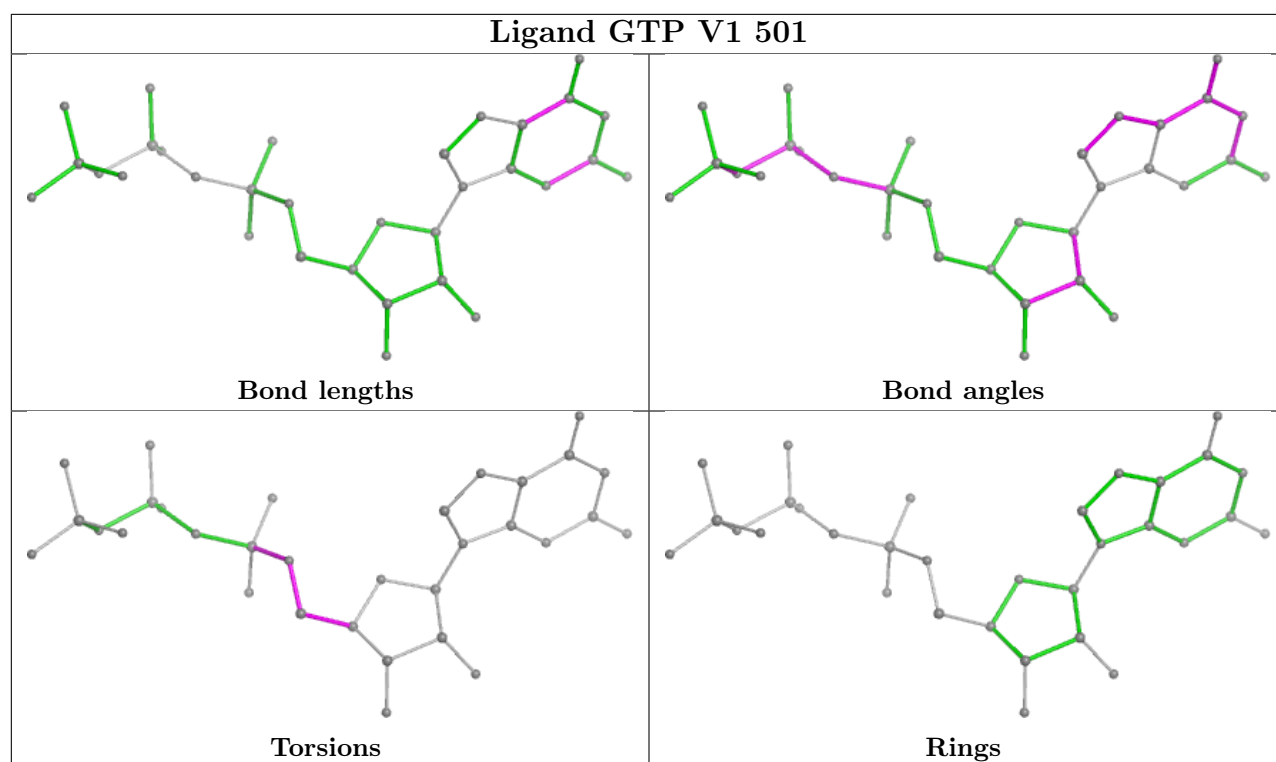
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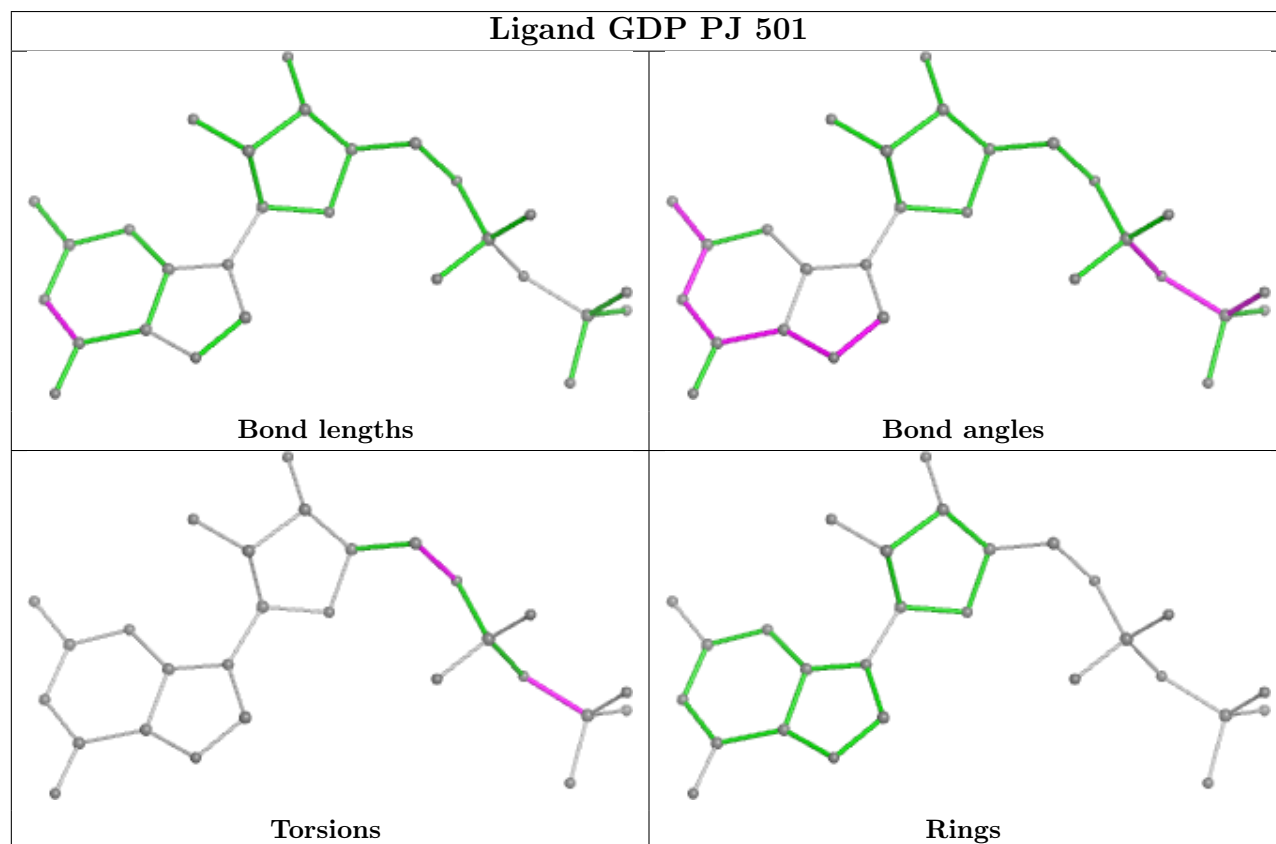
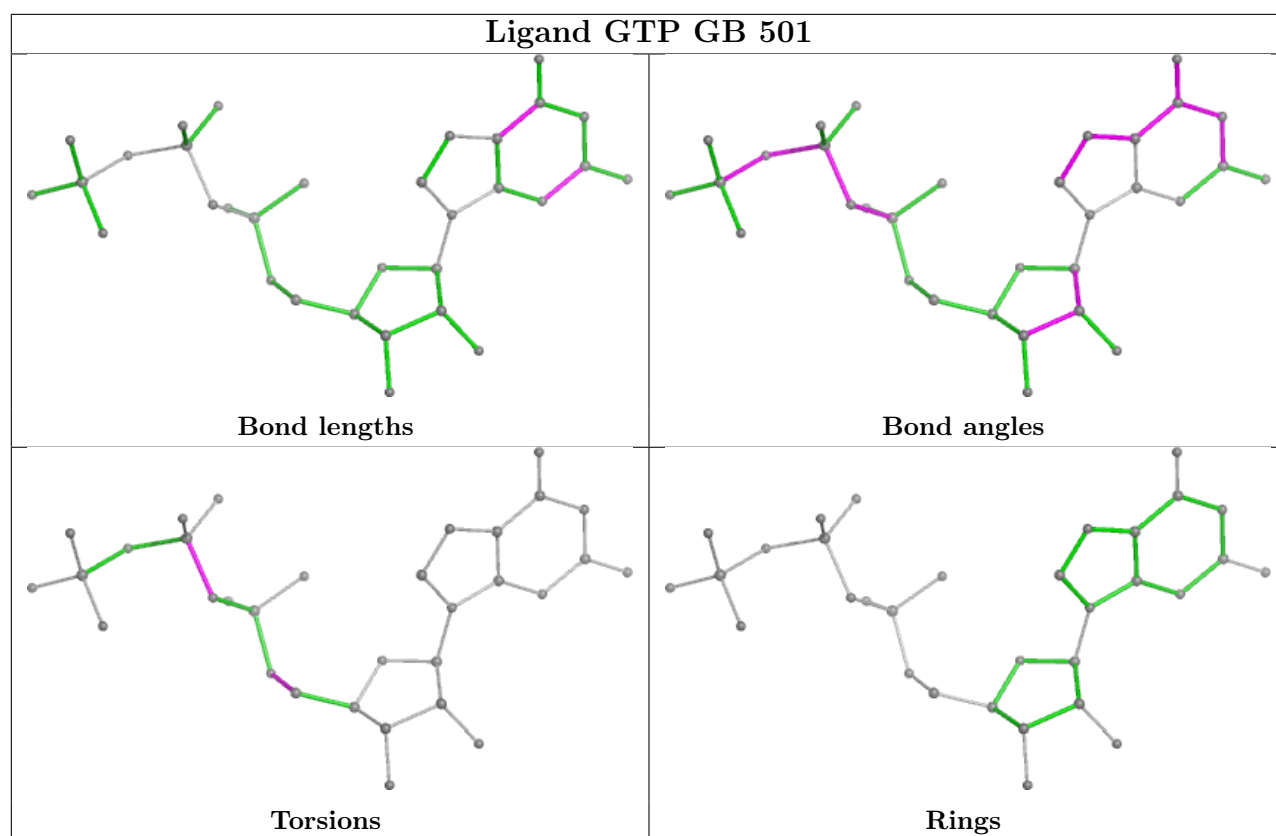
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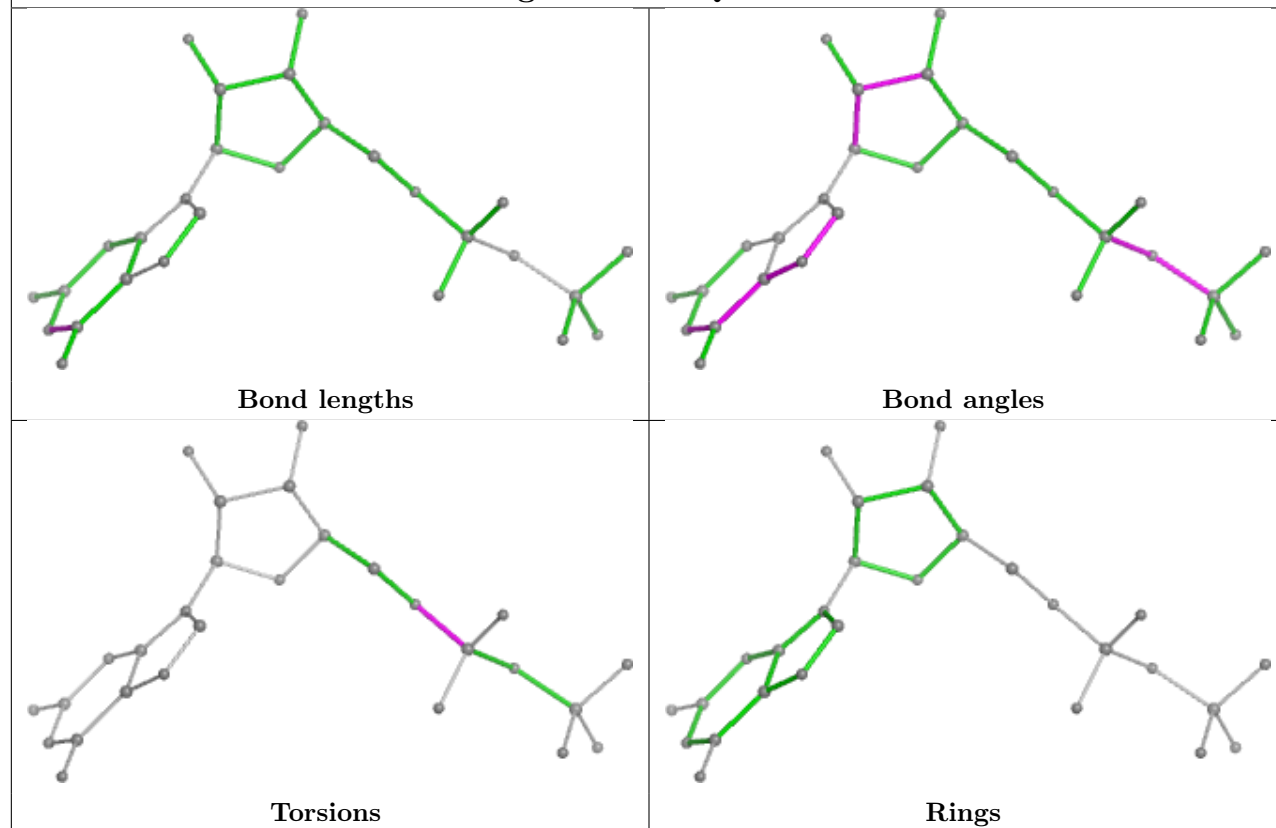
Rings



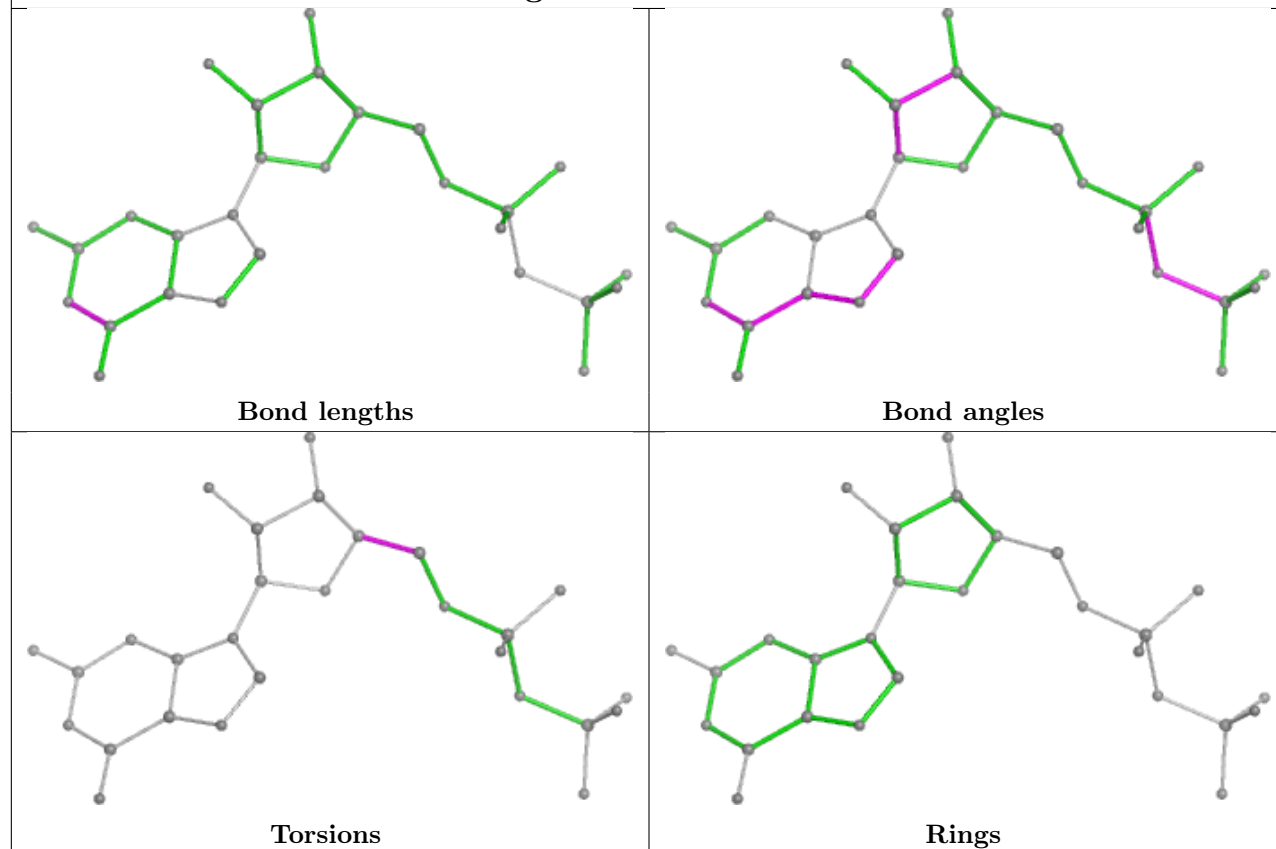


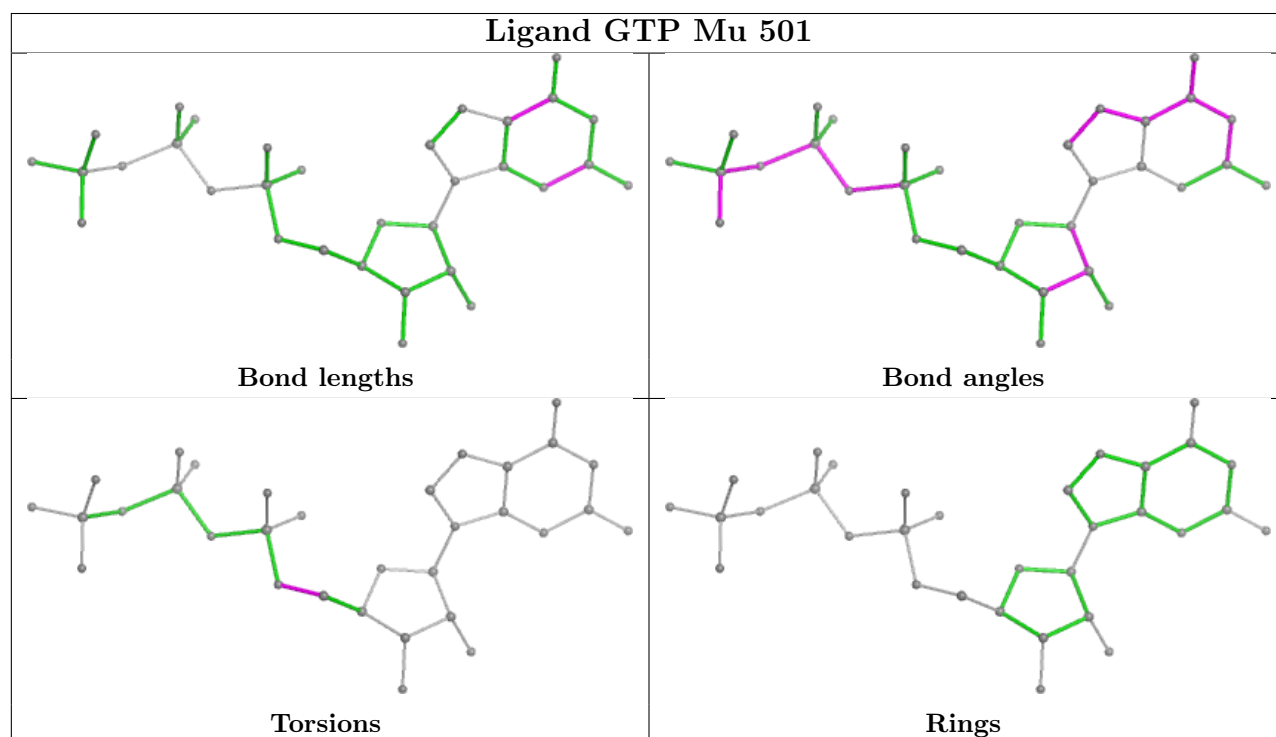
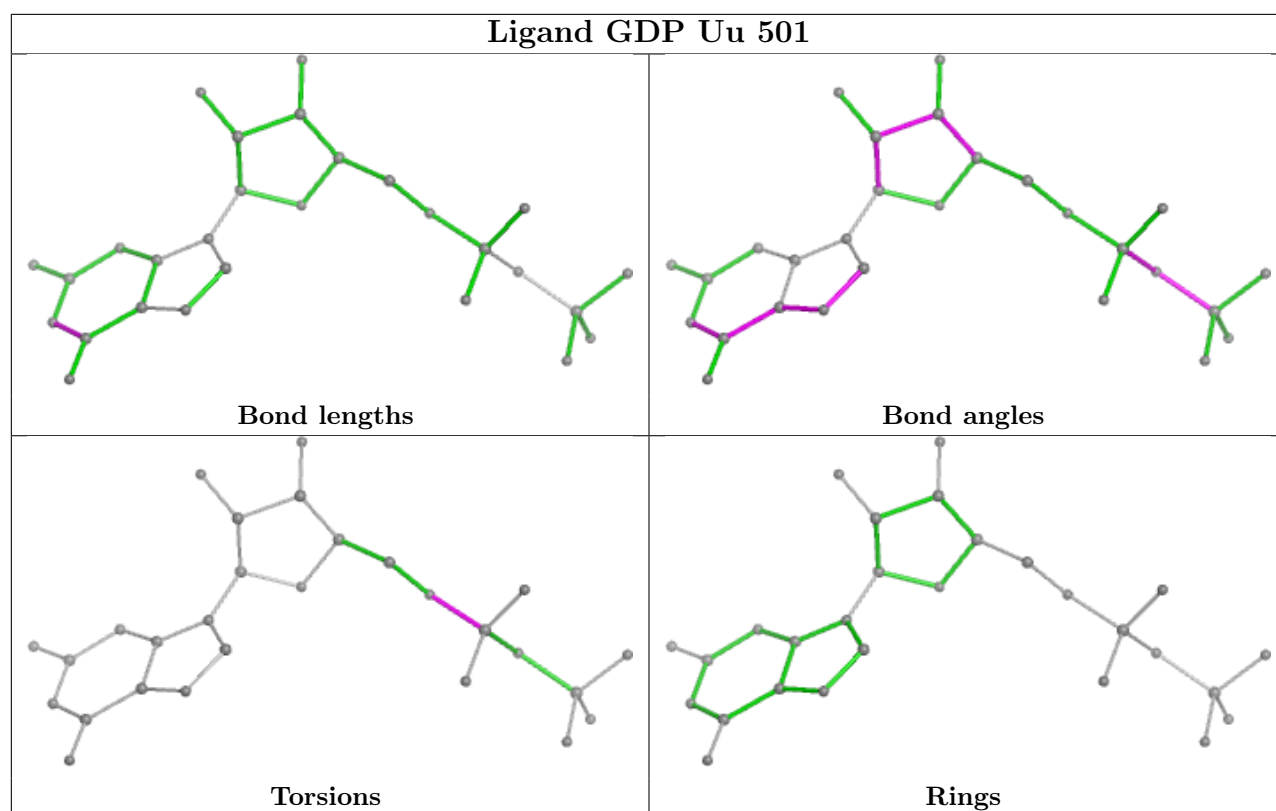


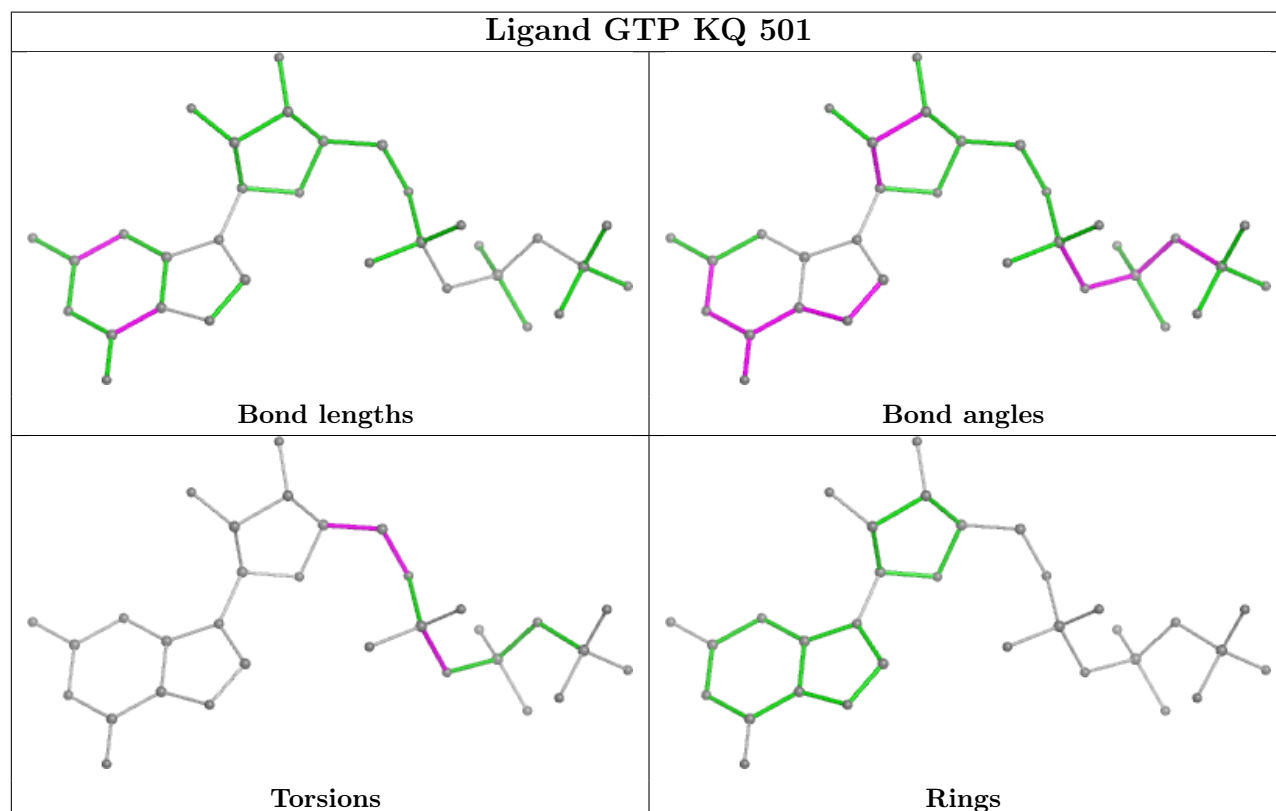
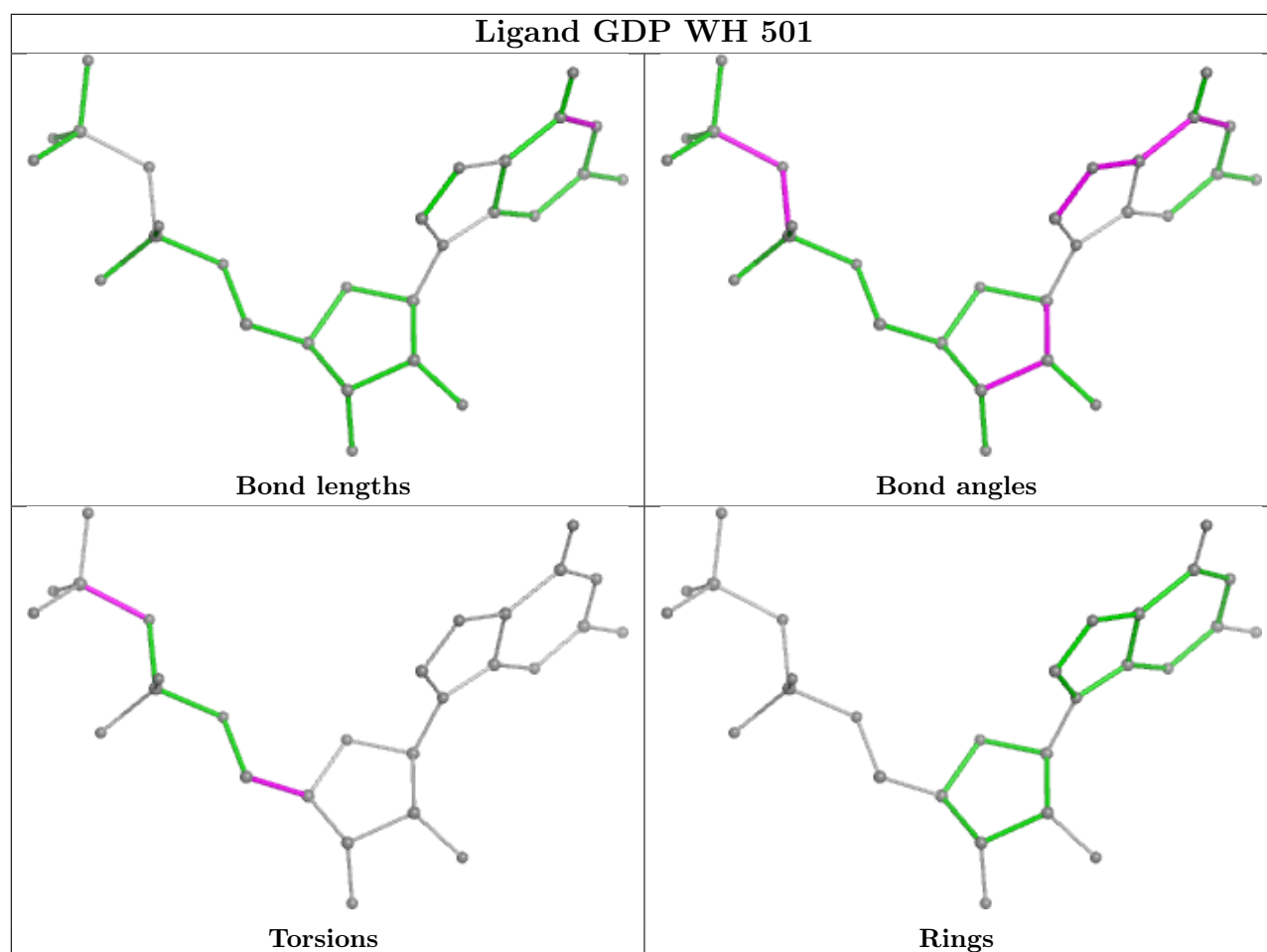
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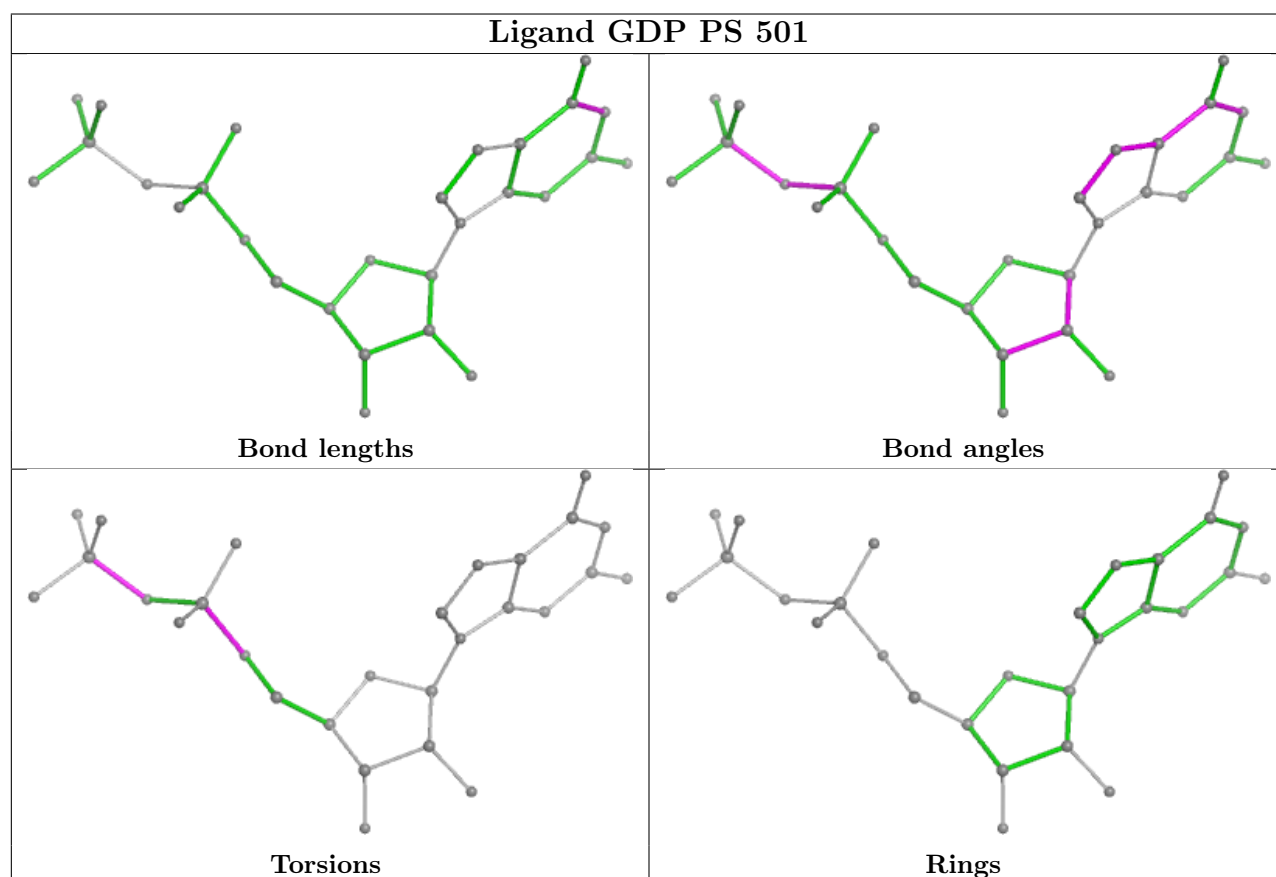
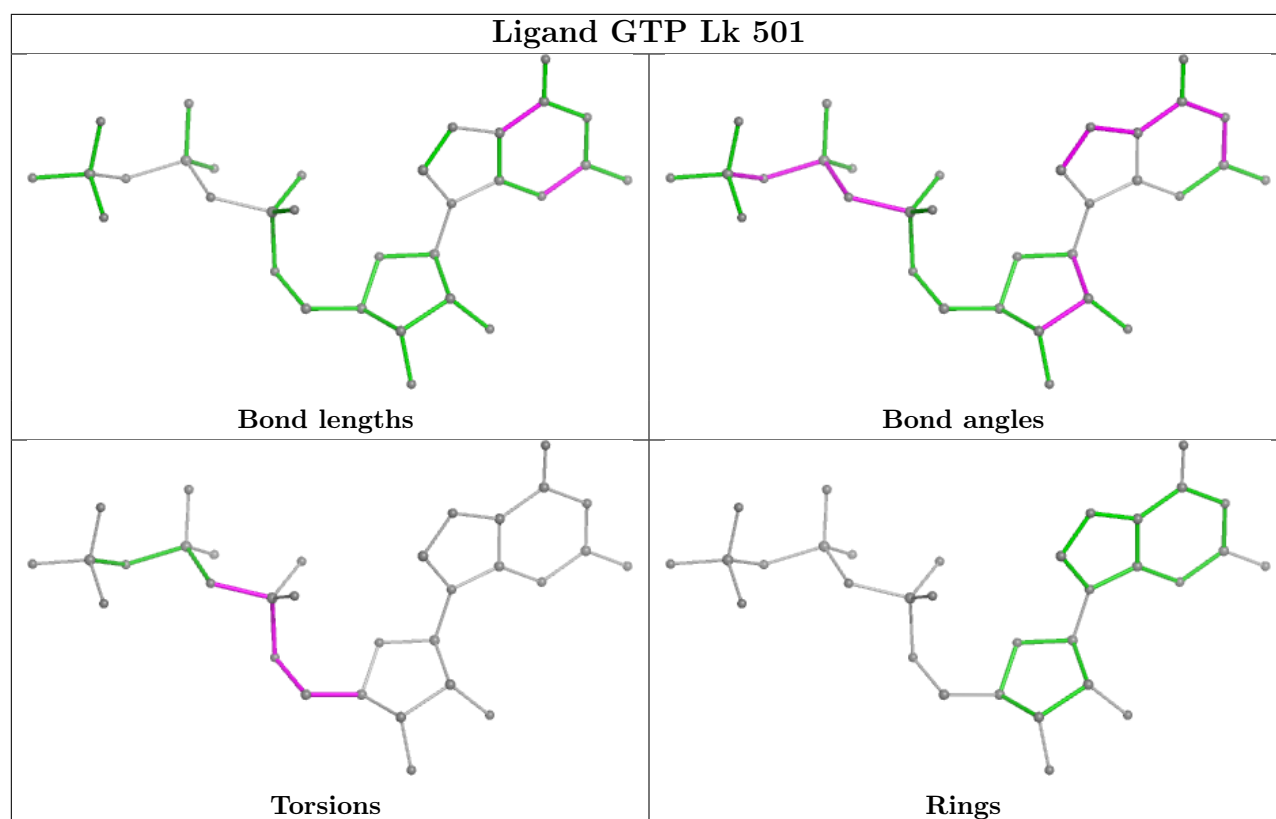


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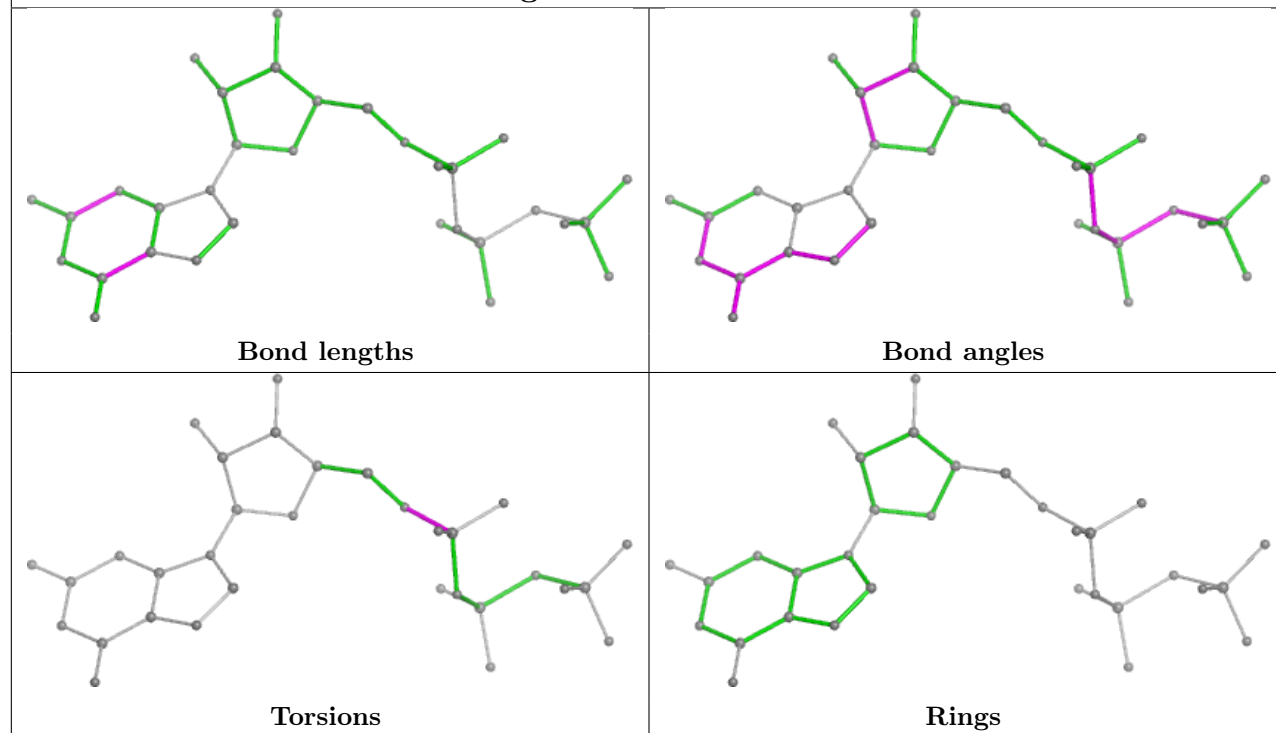




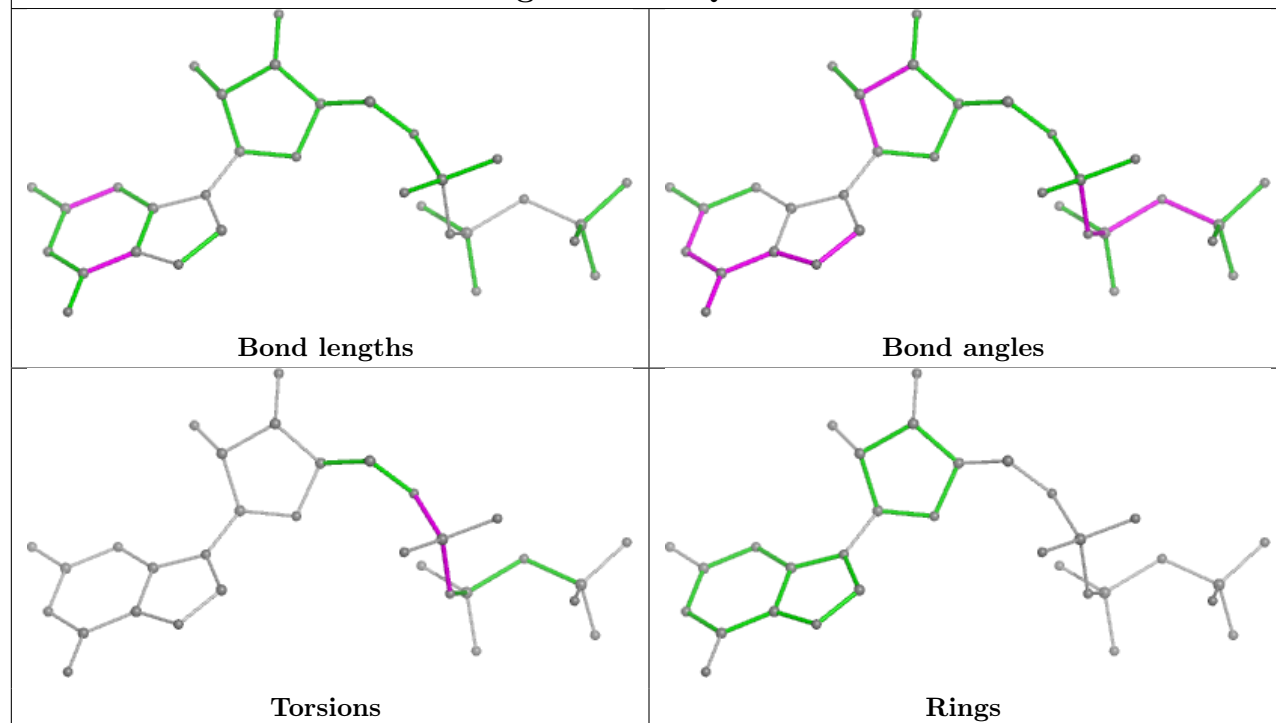




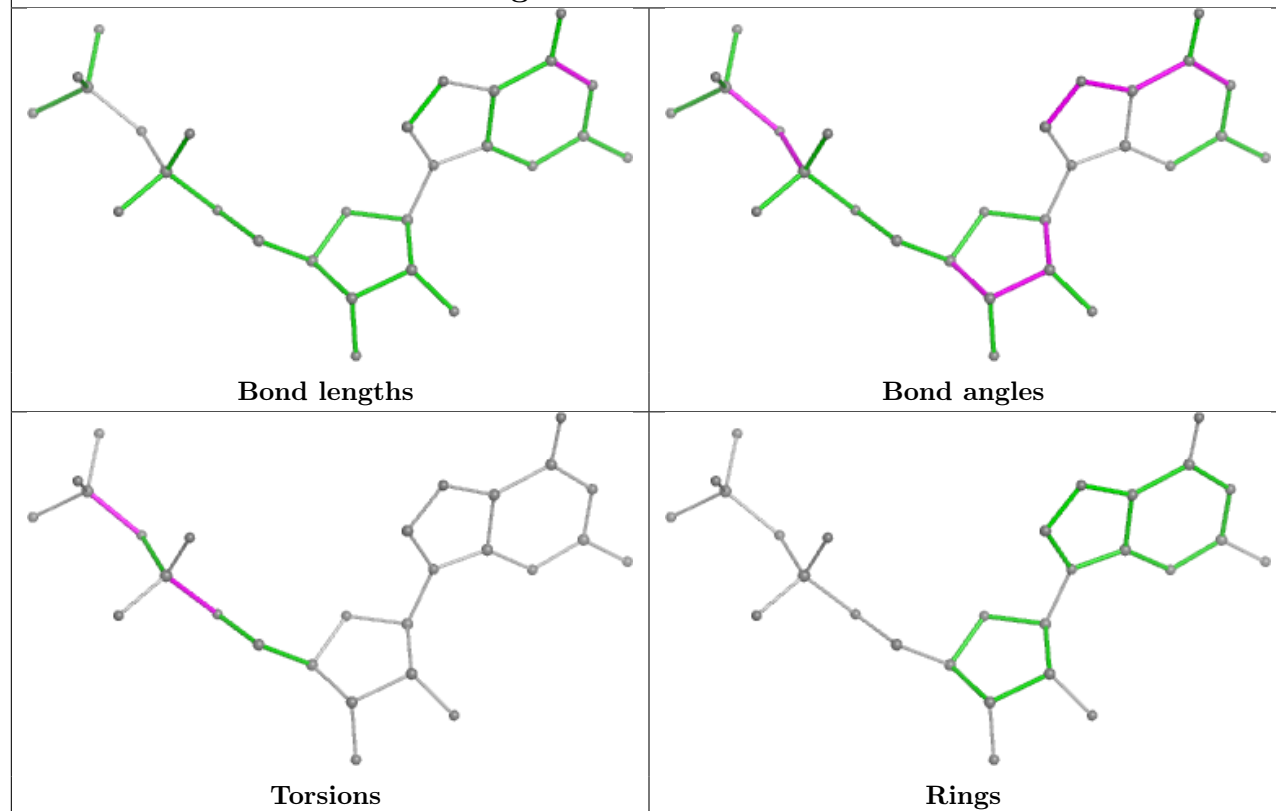
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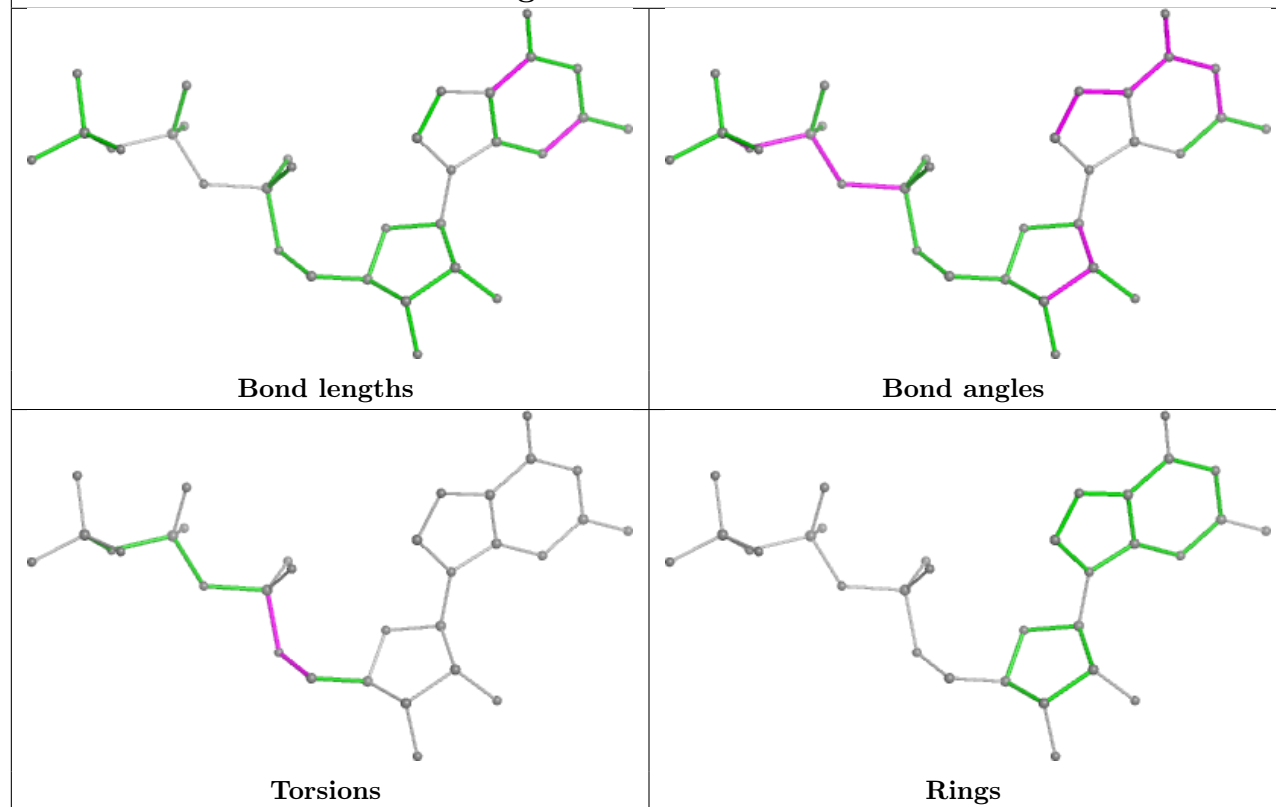
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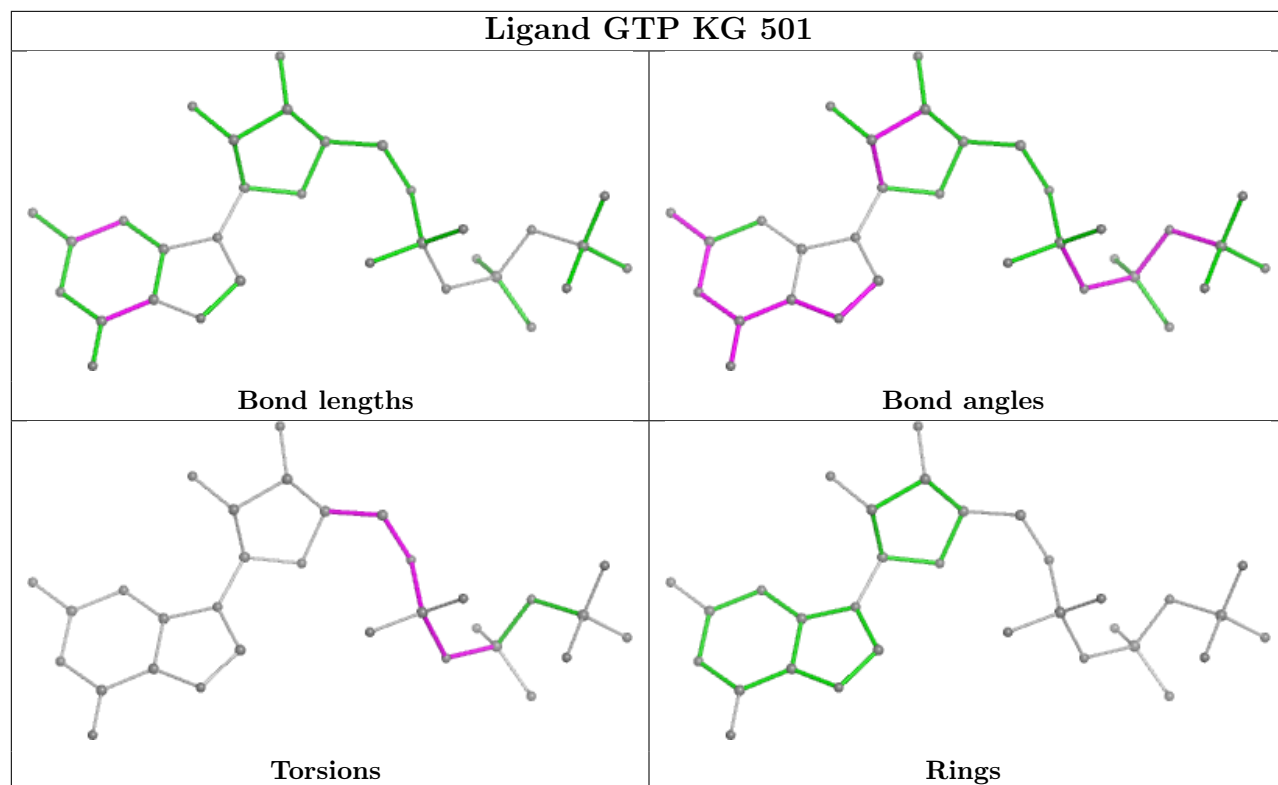
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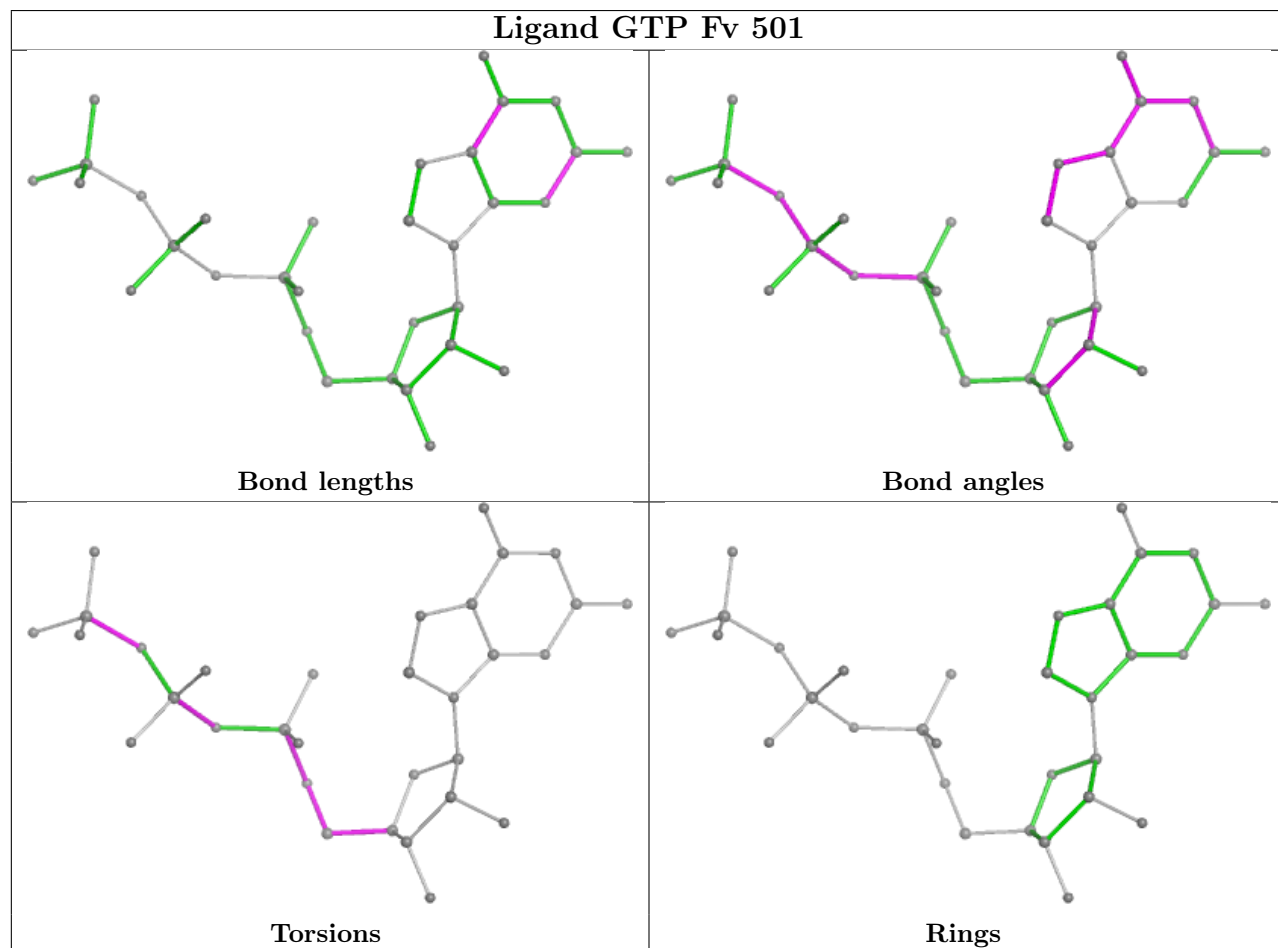
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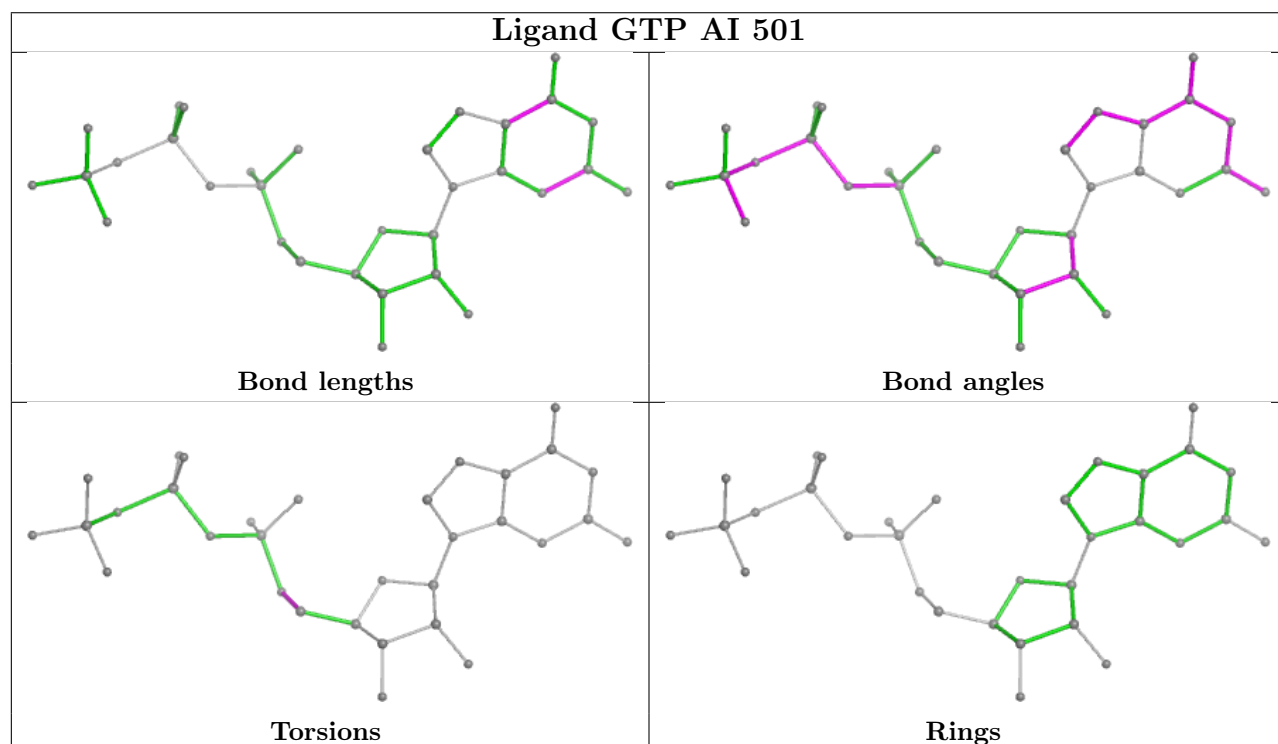
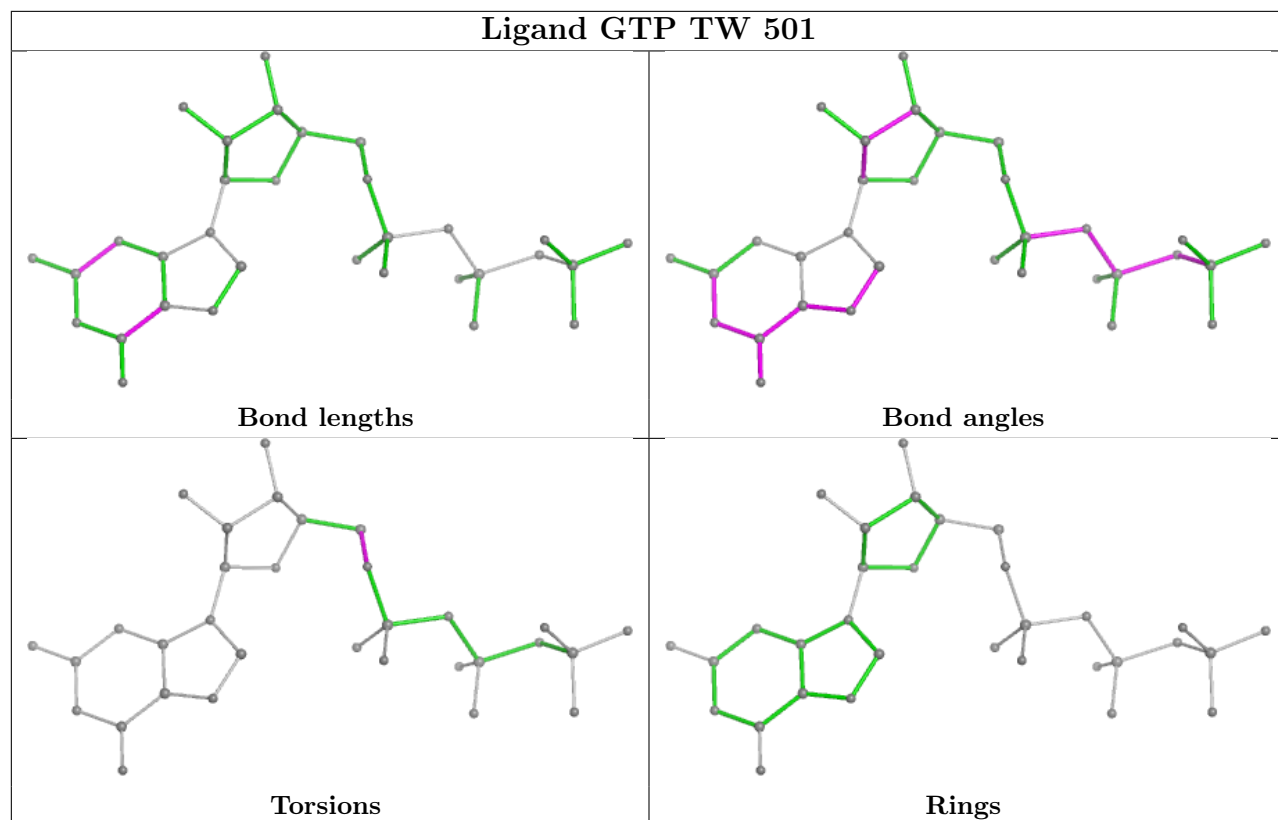
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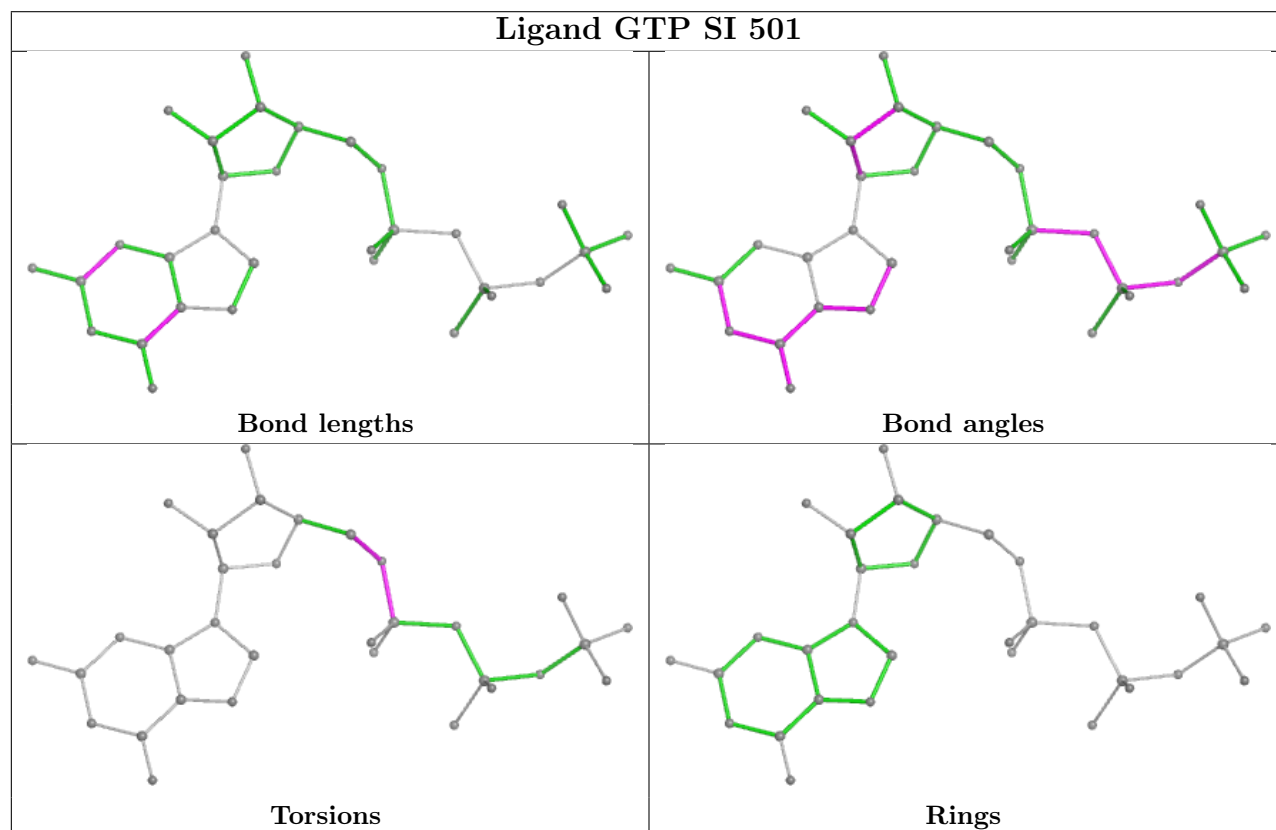
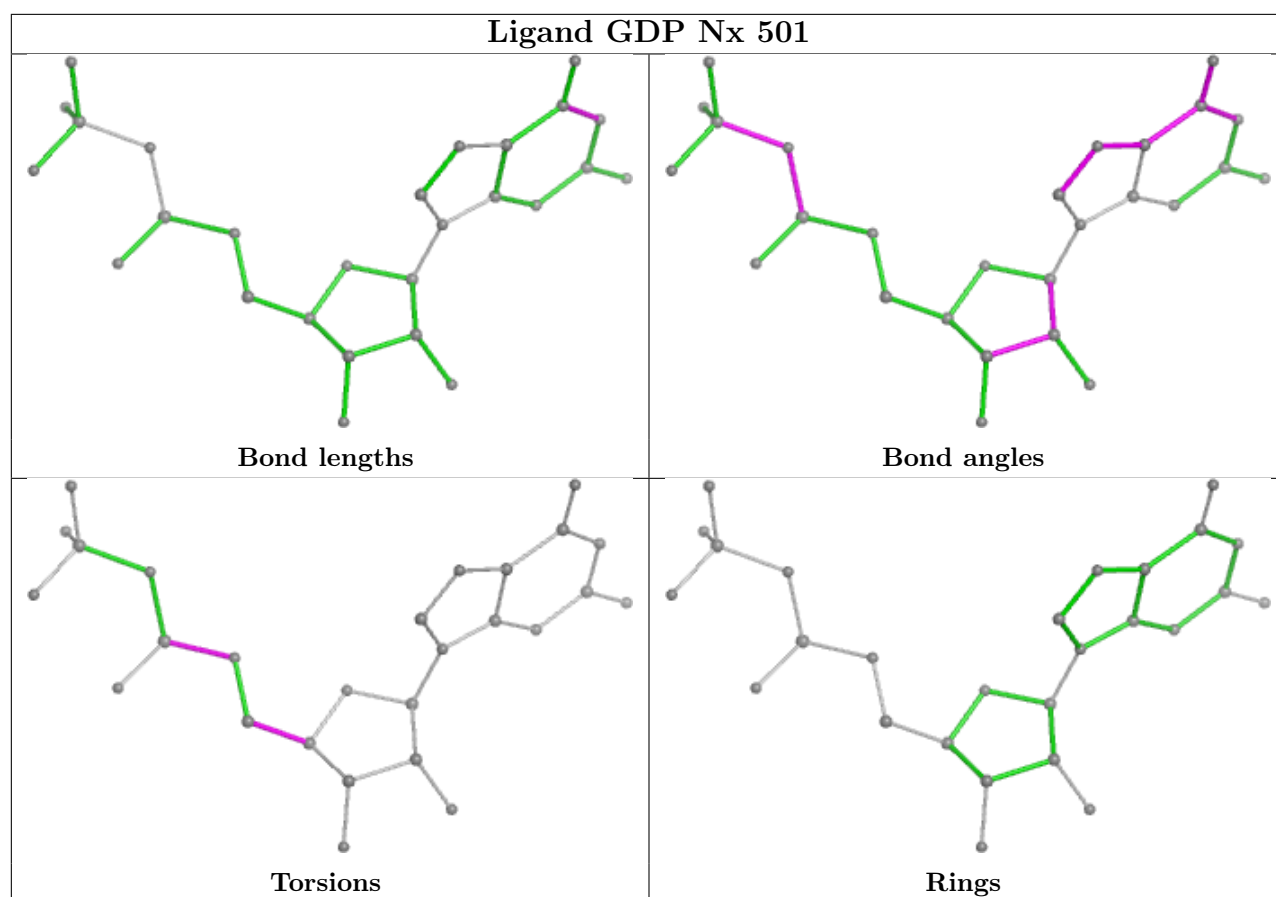


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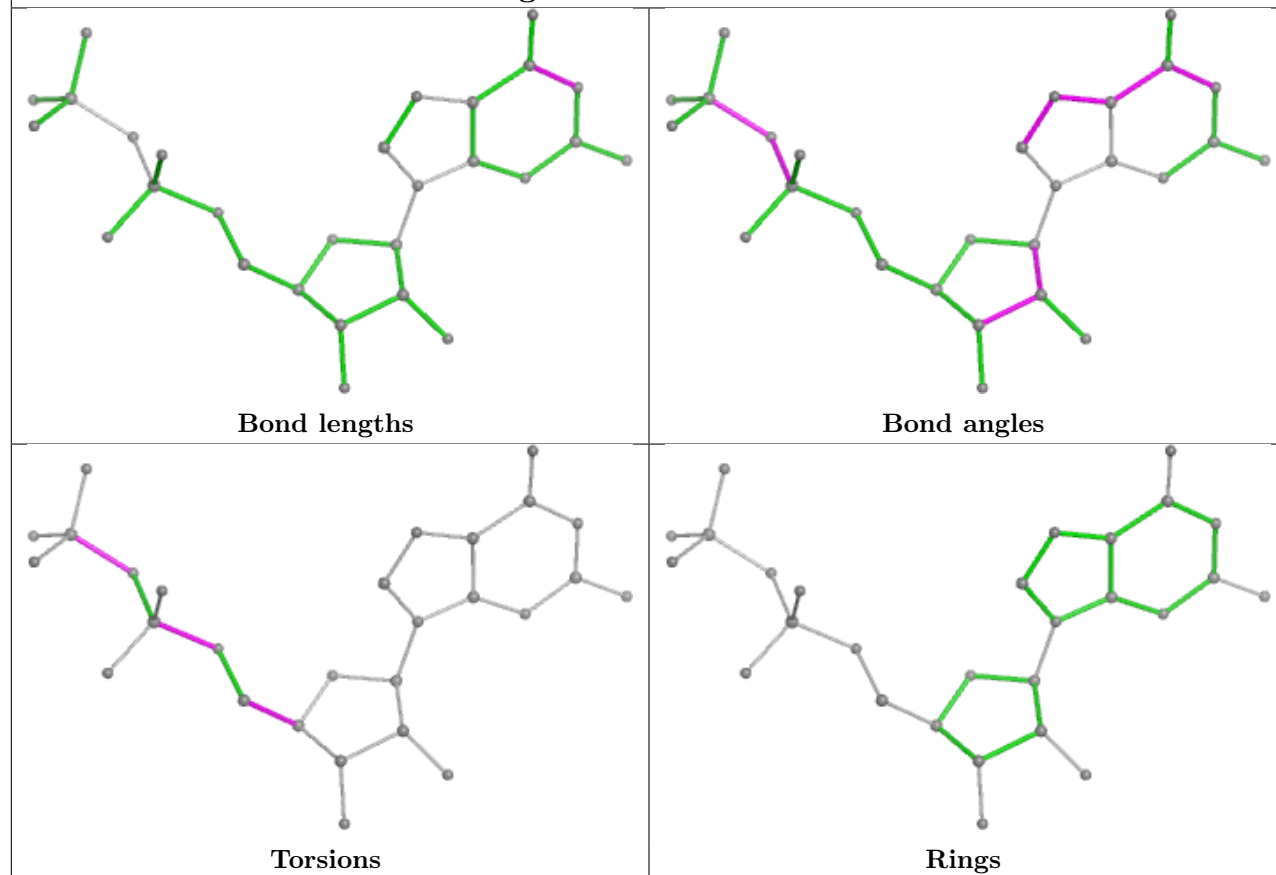




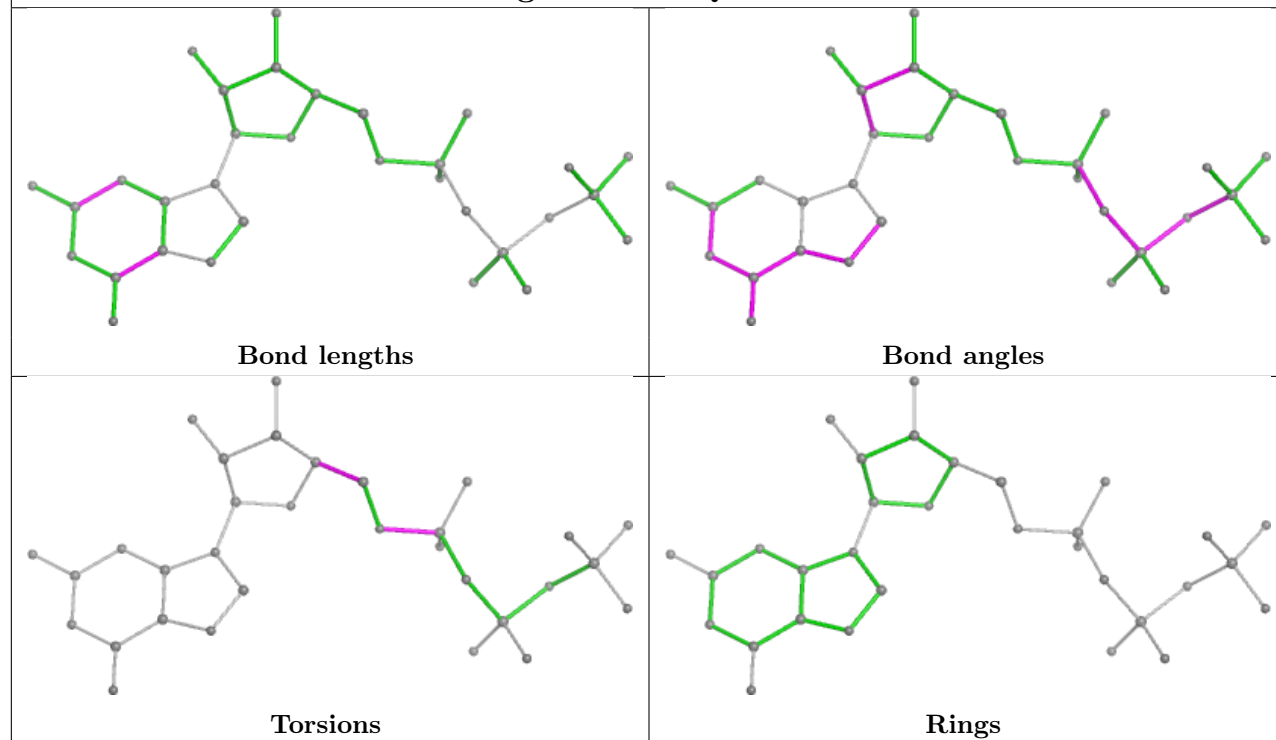




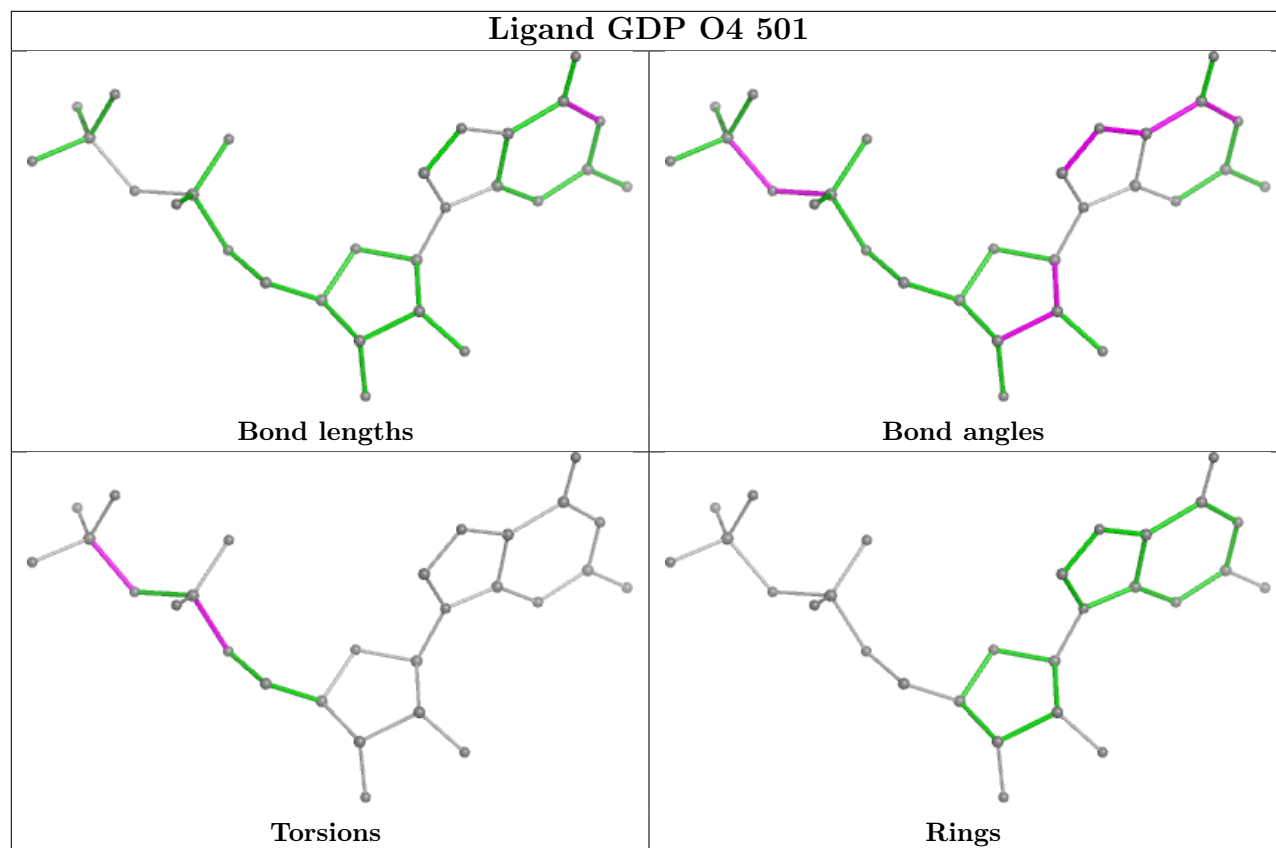
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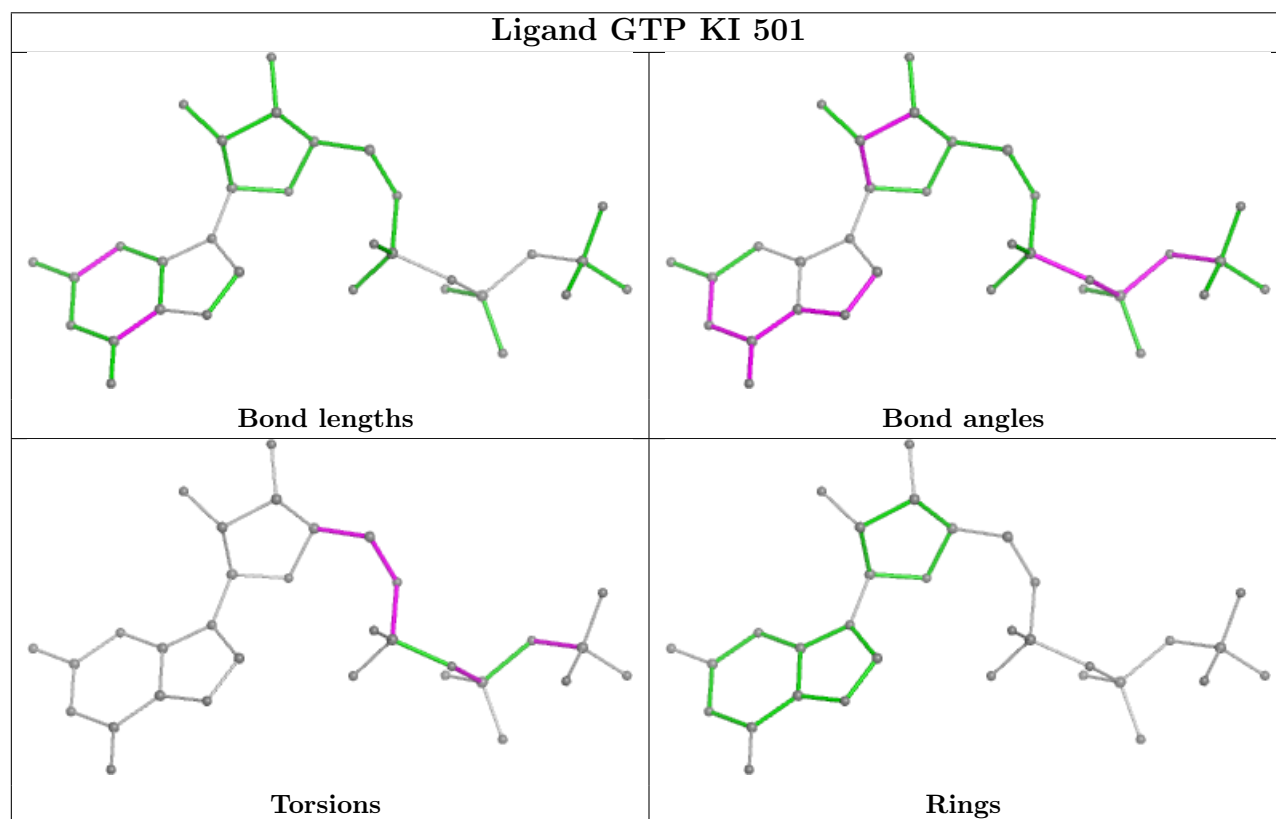
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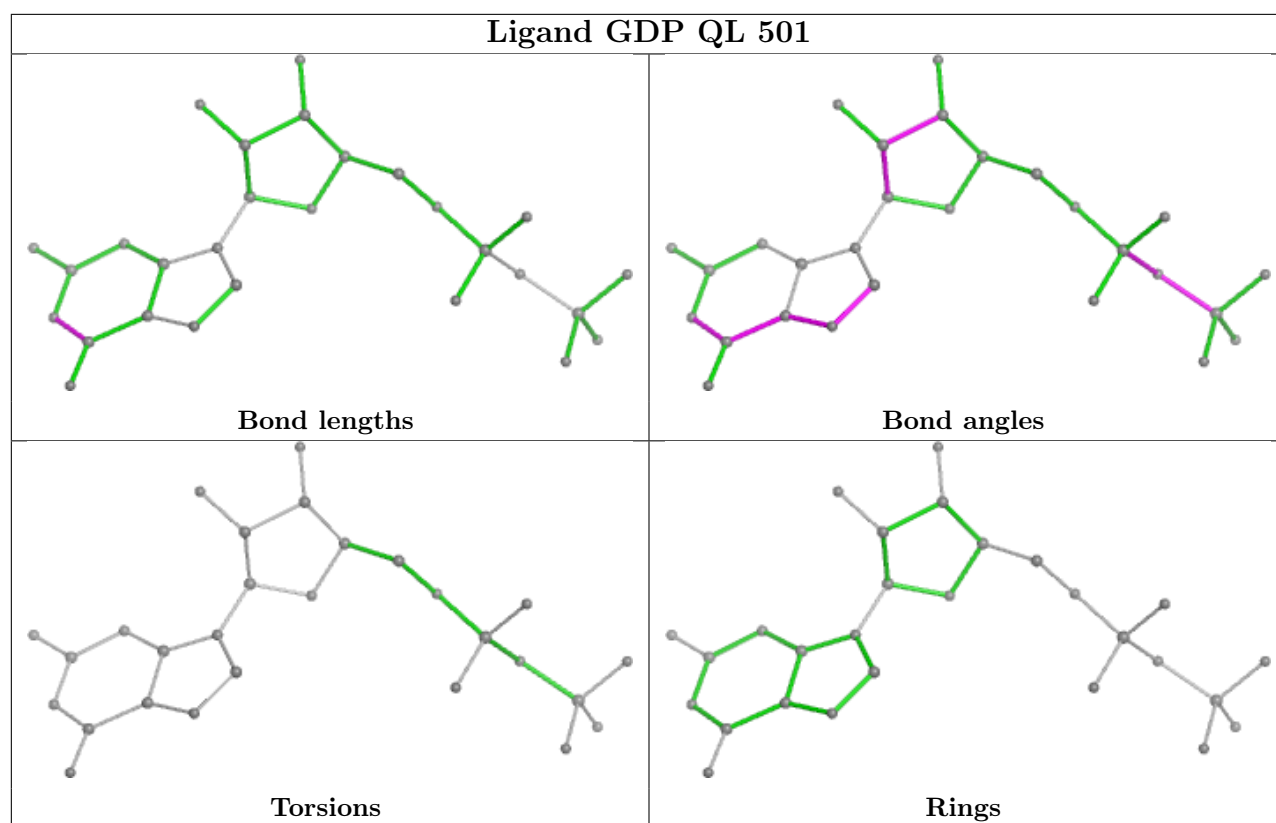


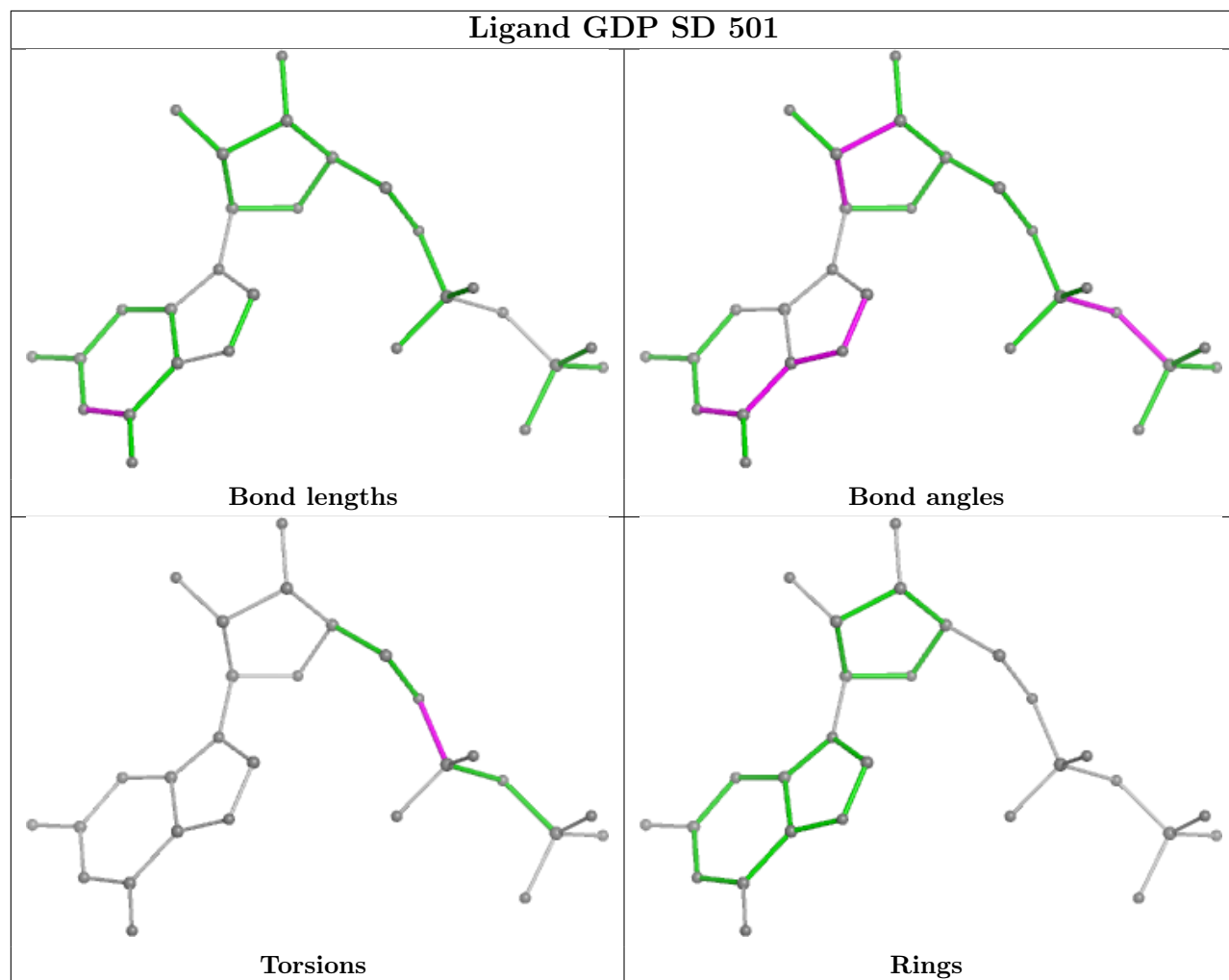
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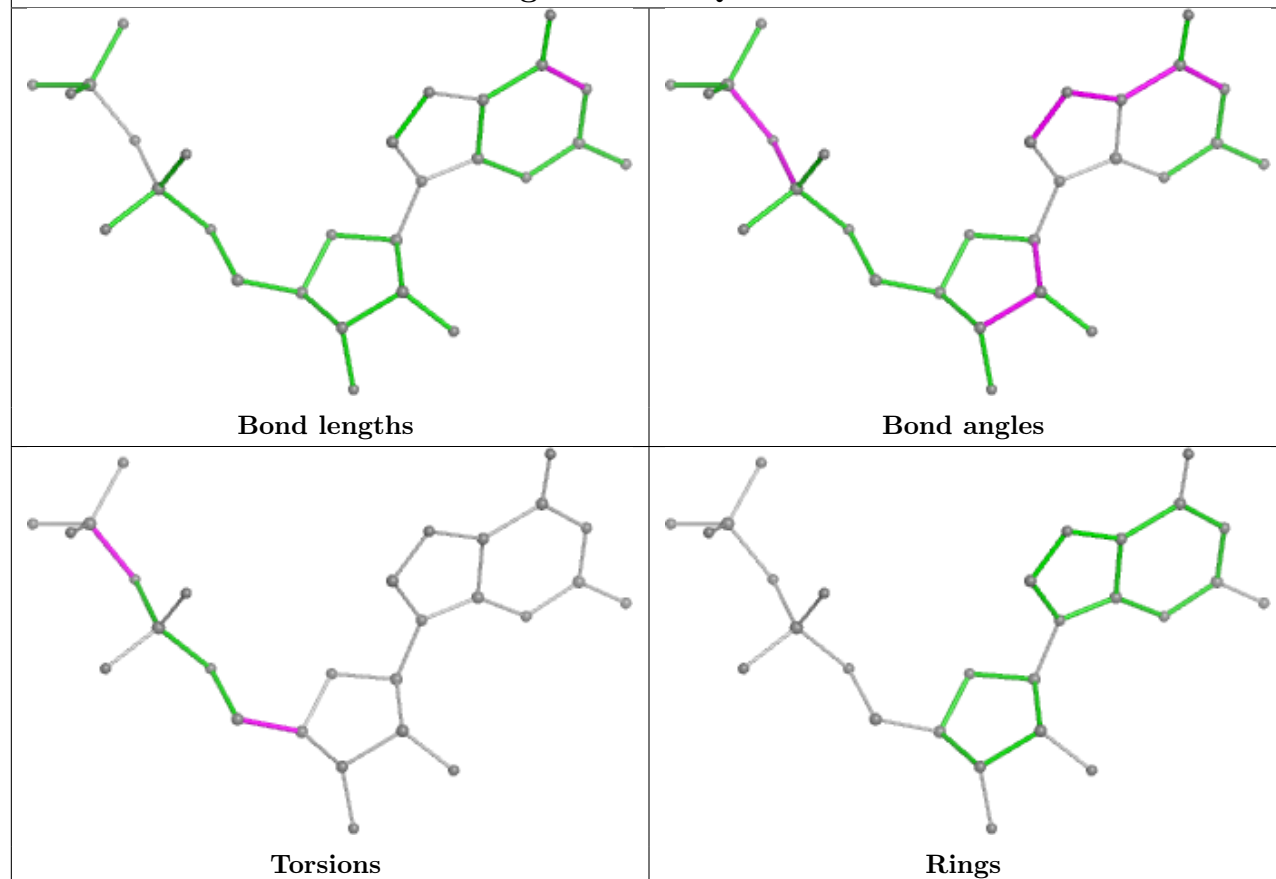
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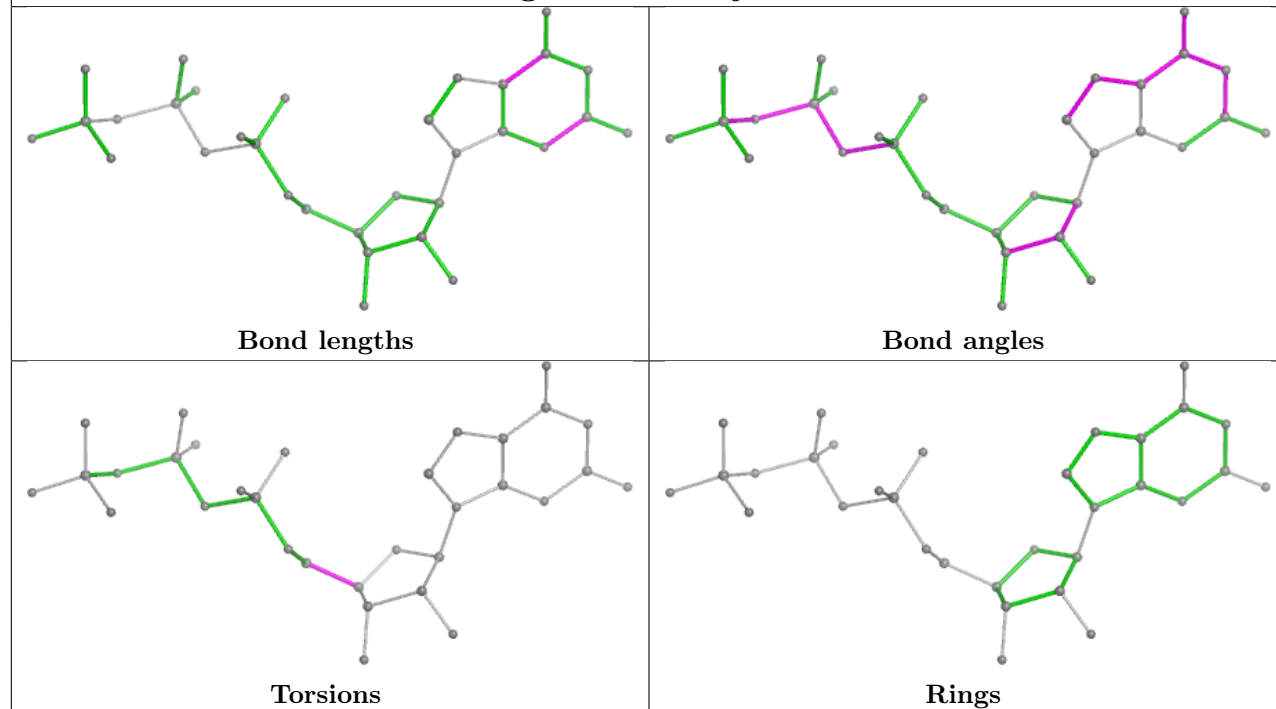


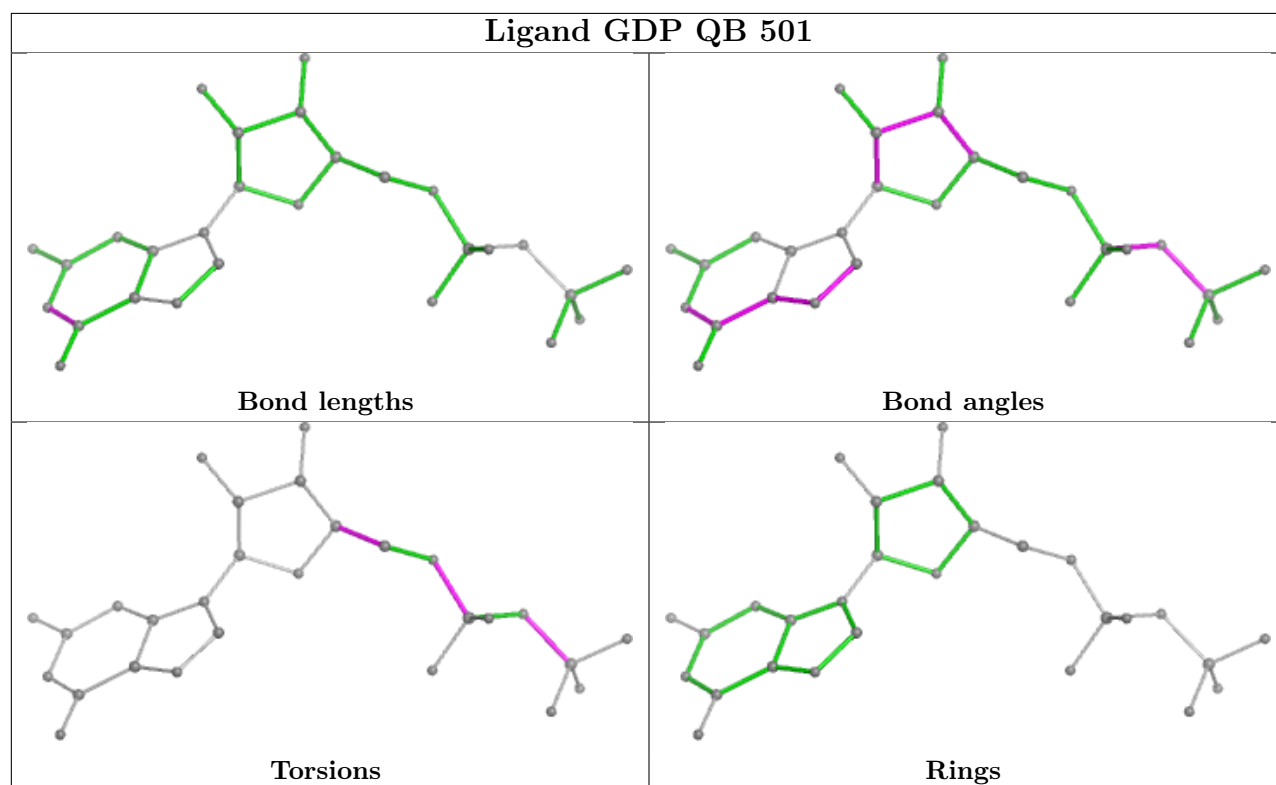
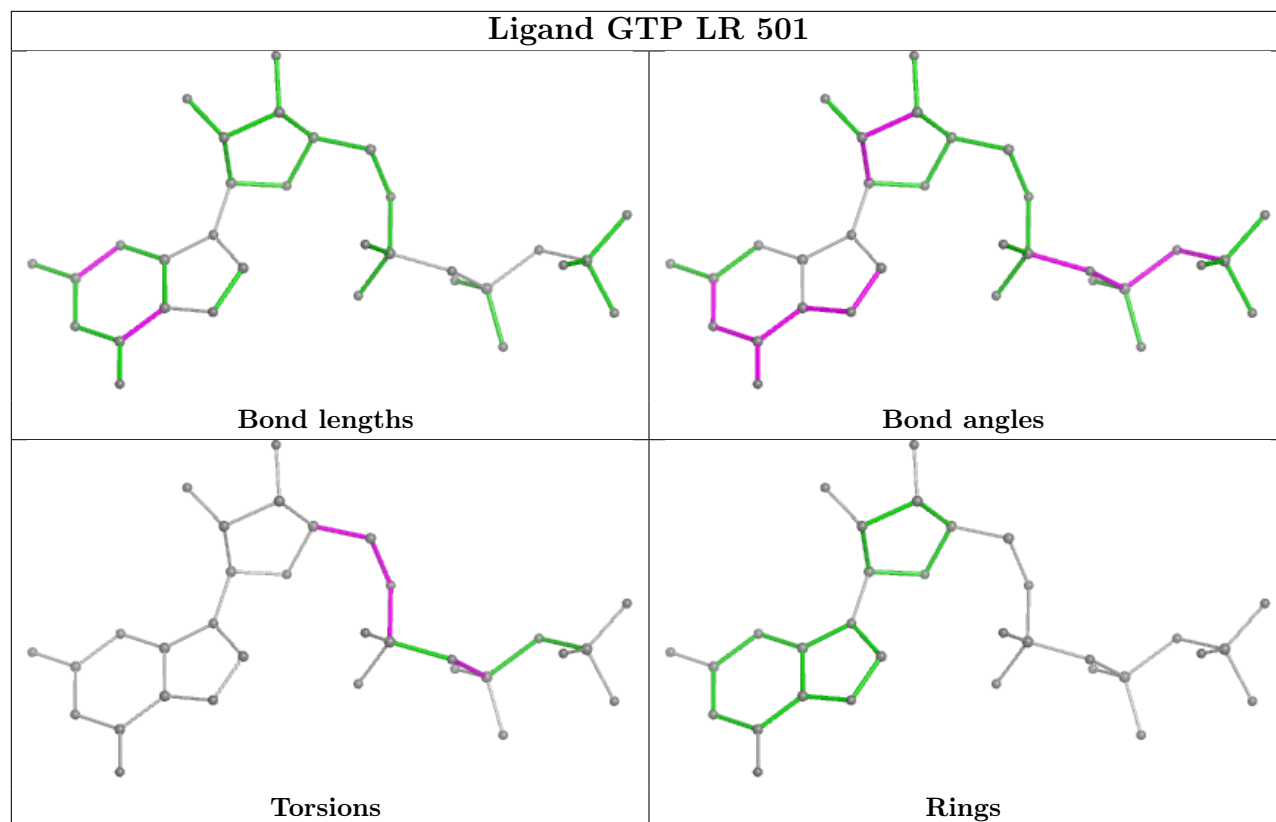


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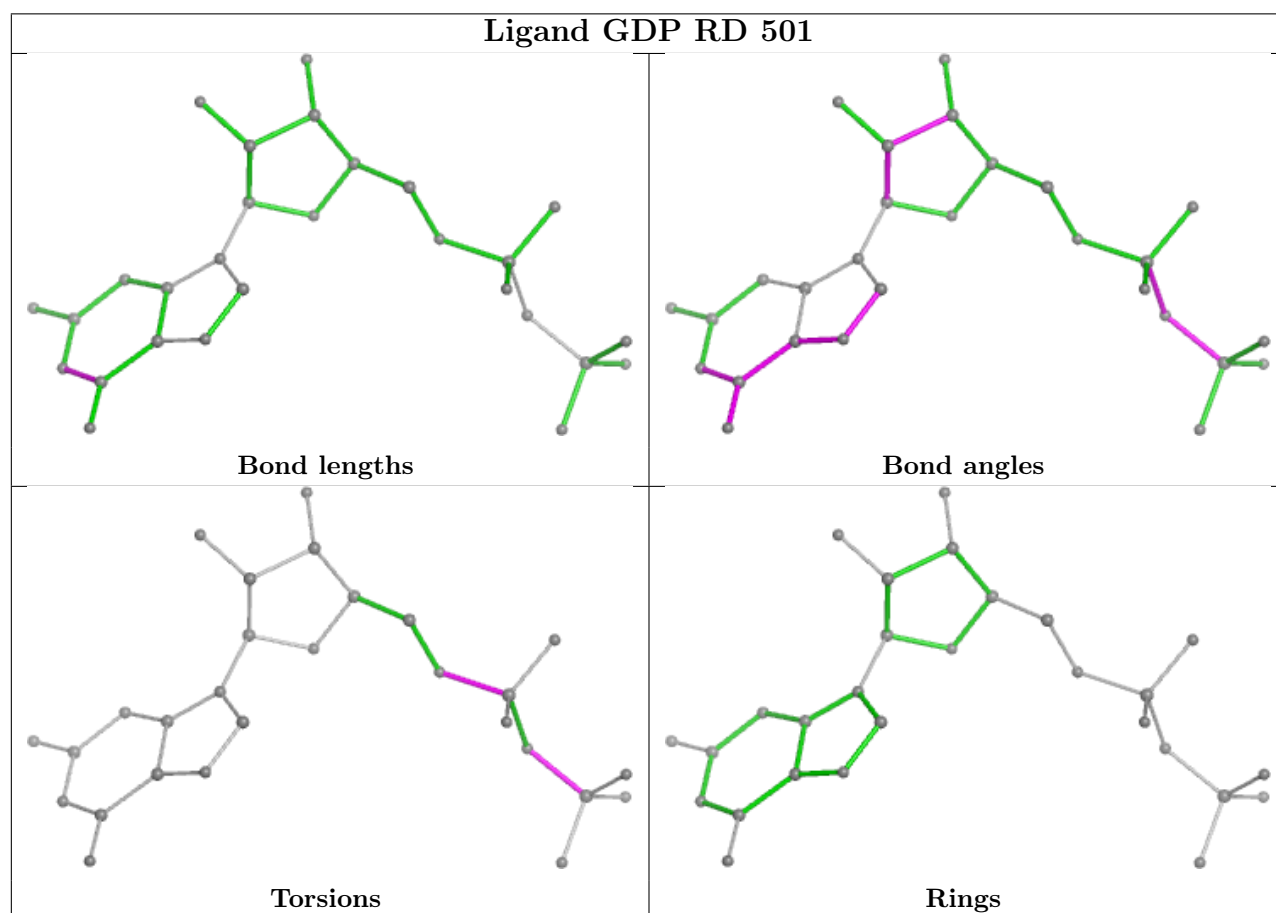
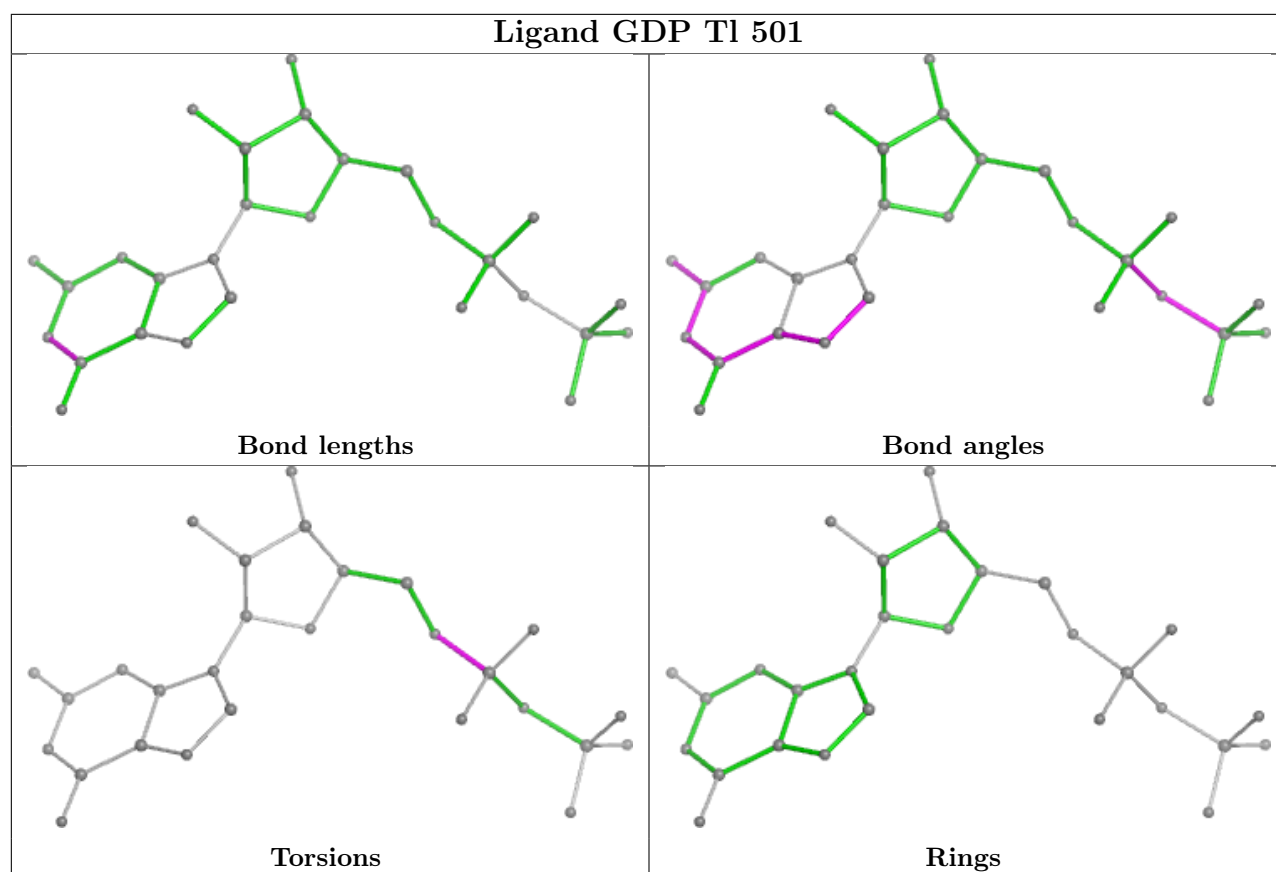


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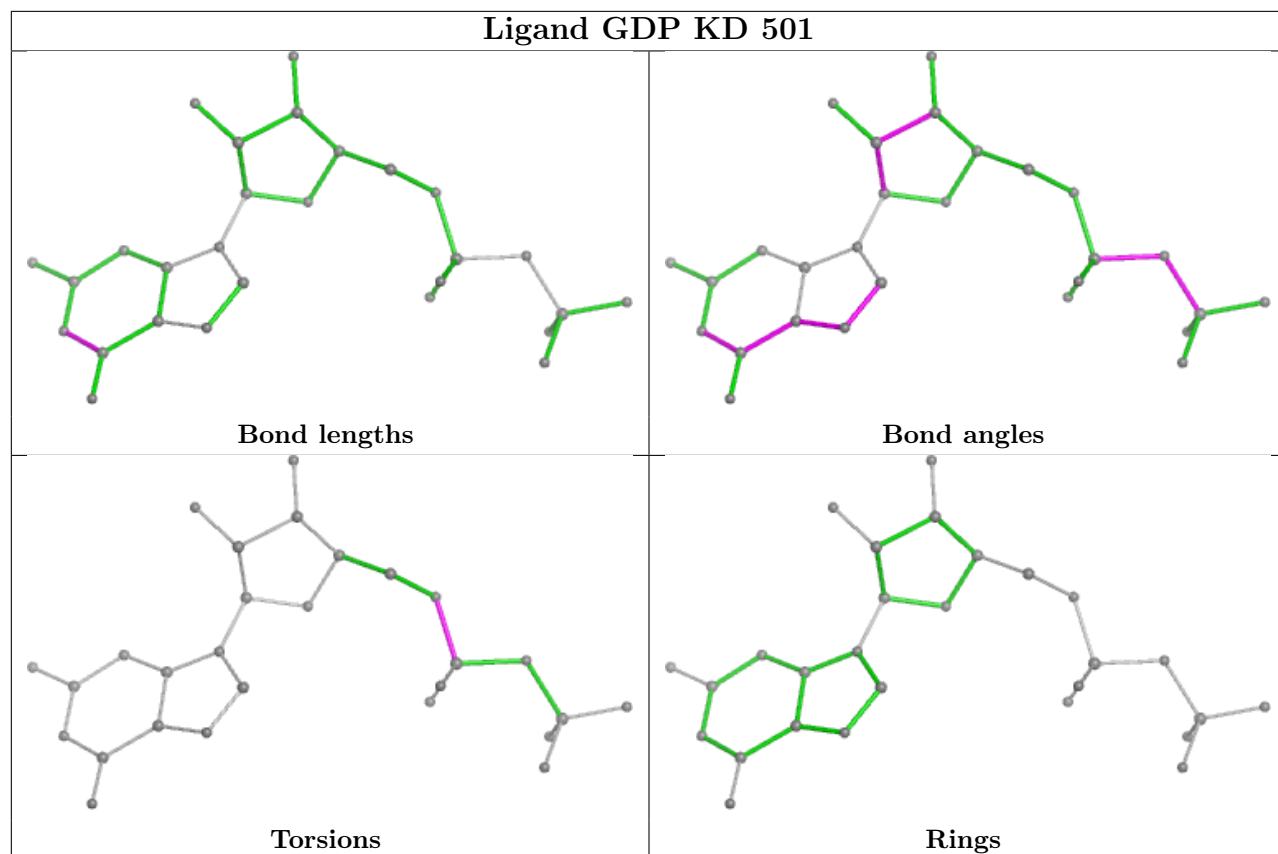




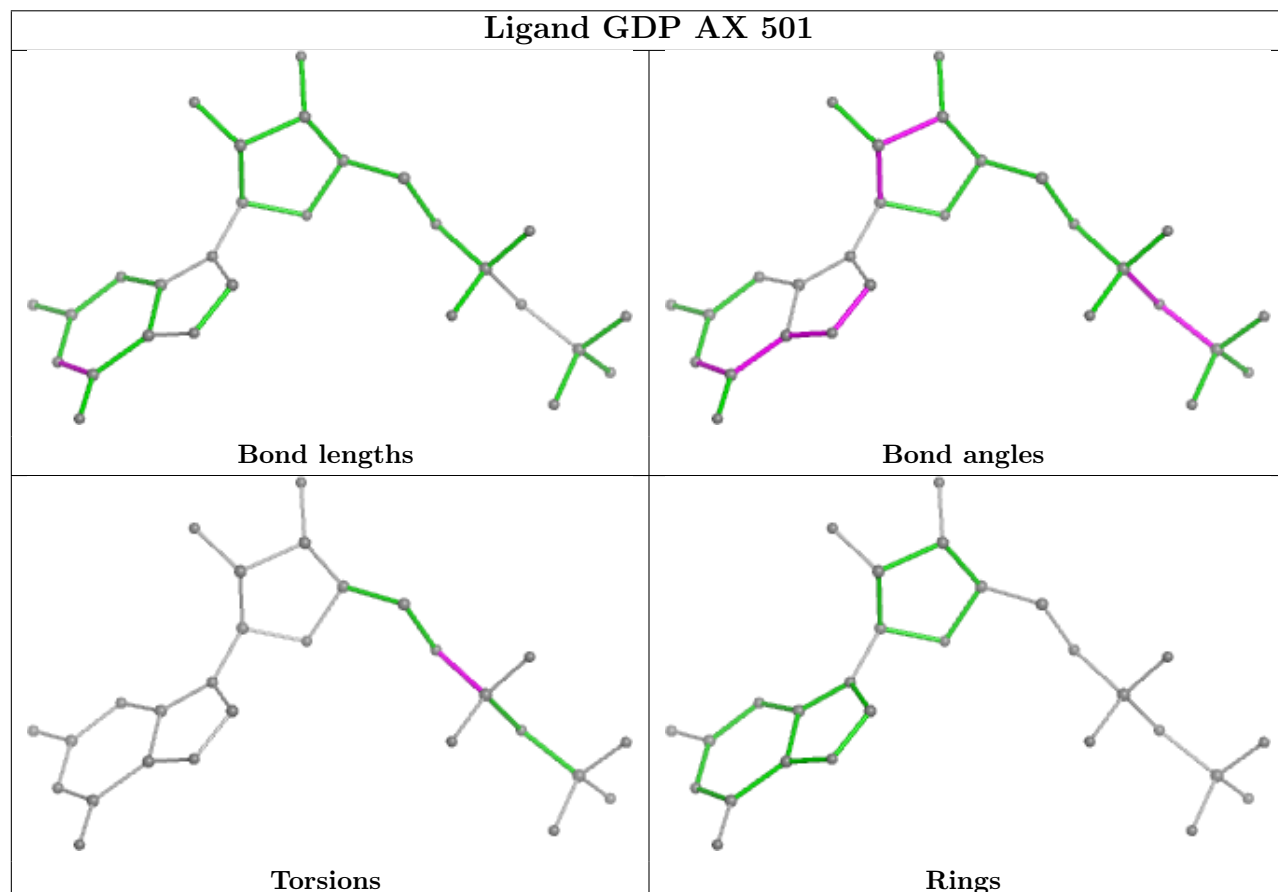




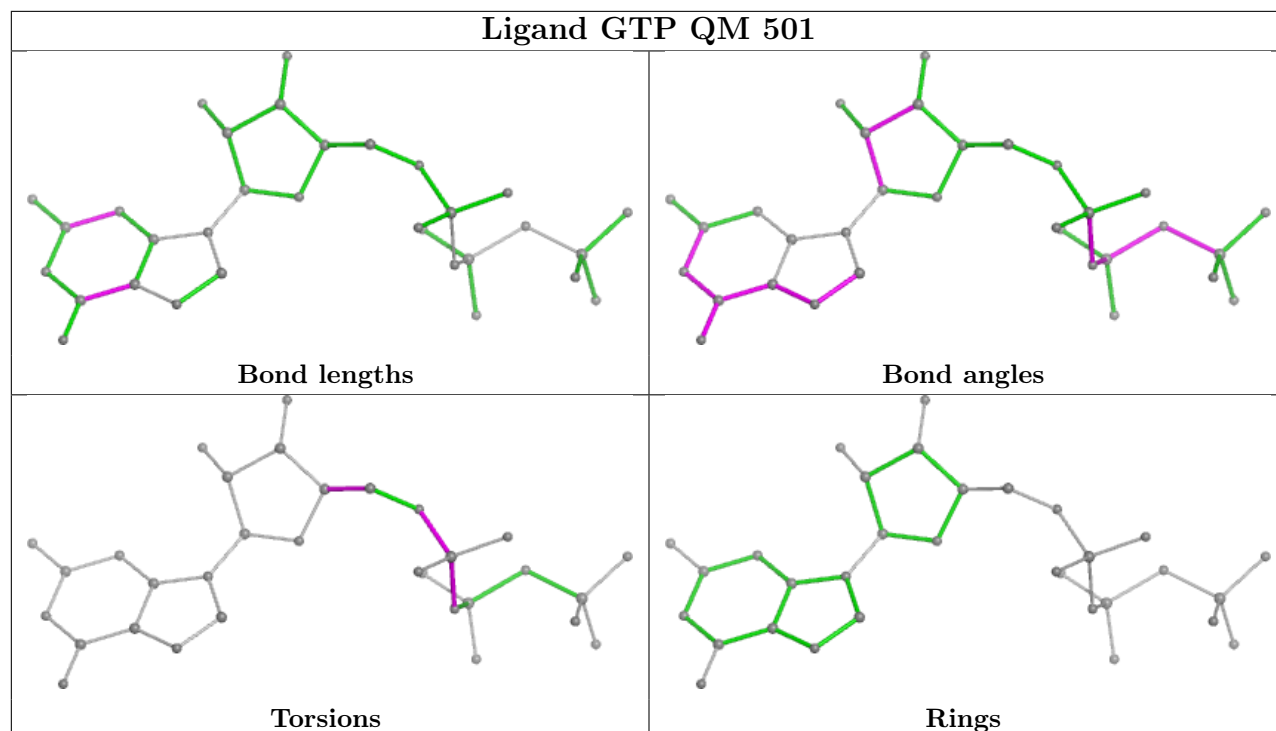
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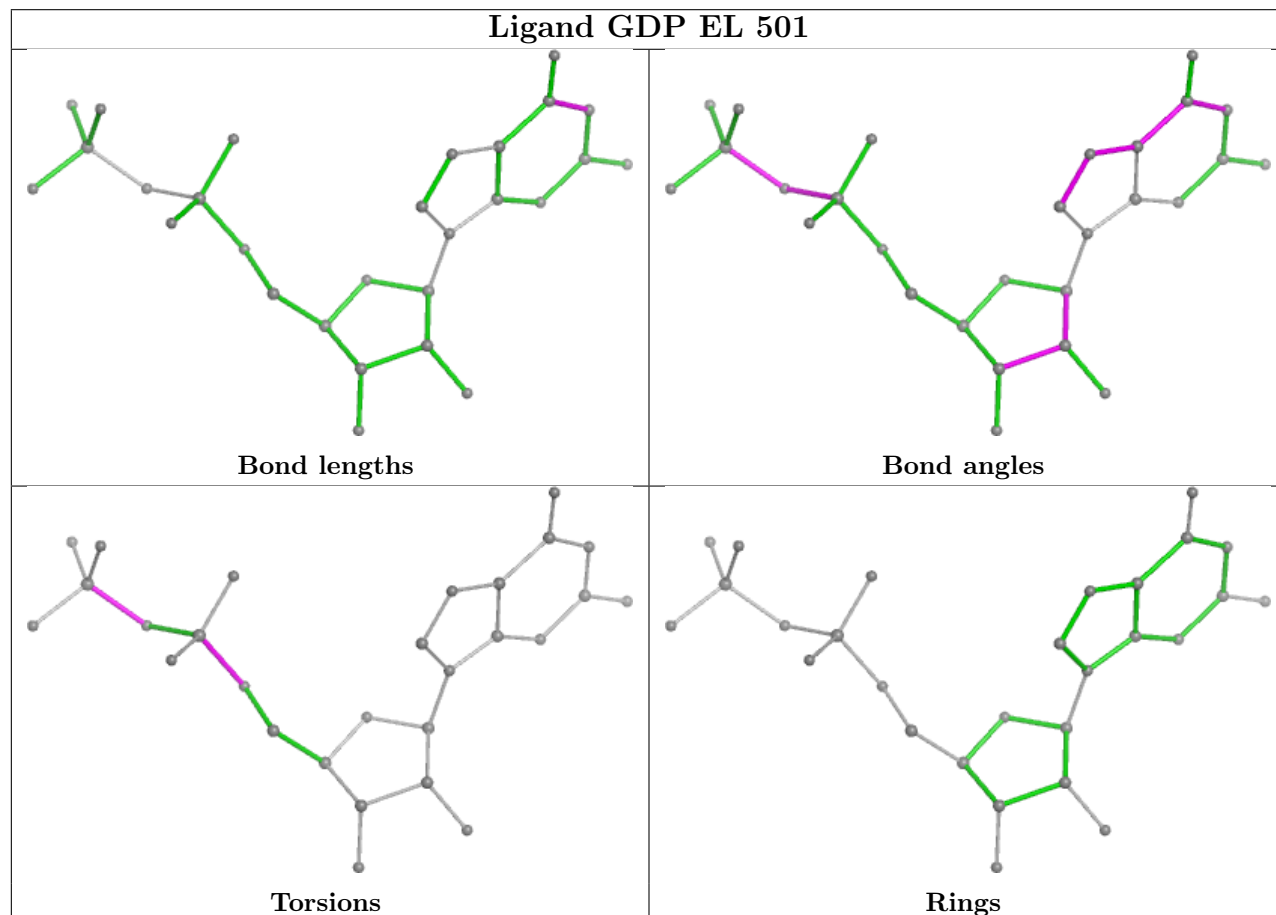
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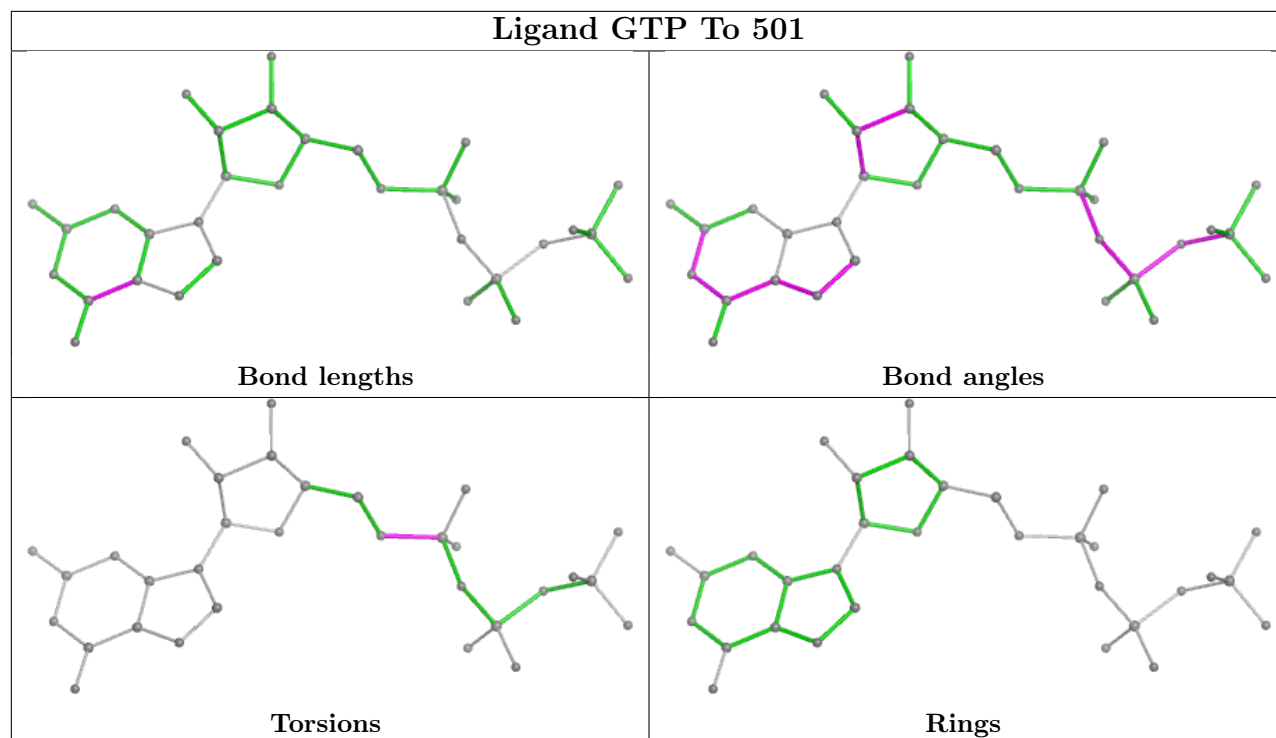
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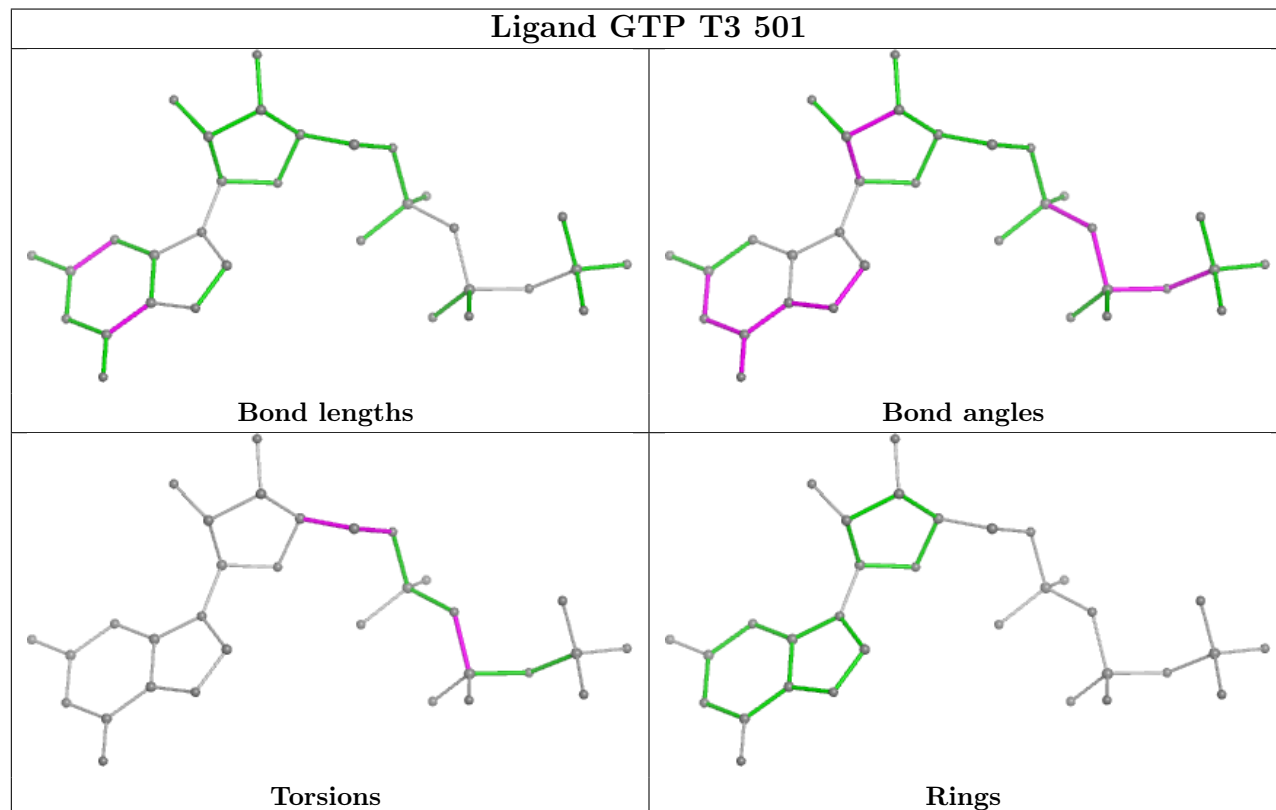
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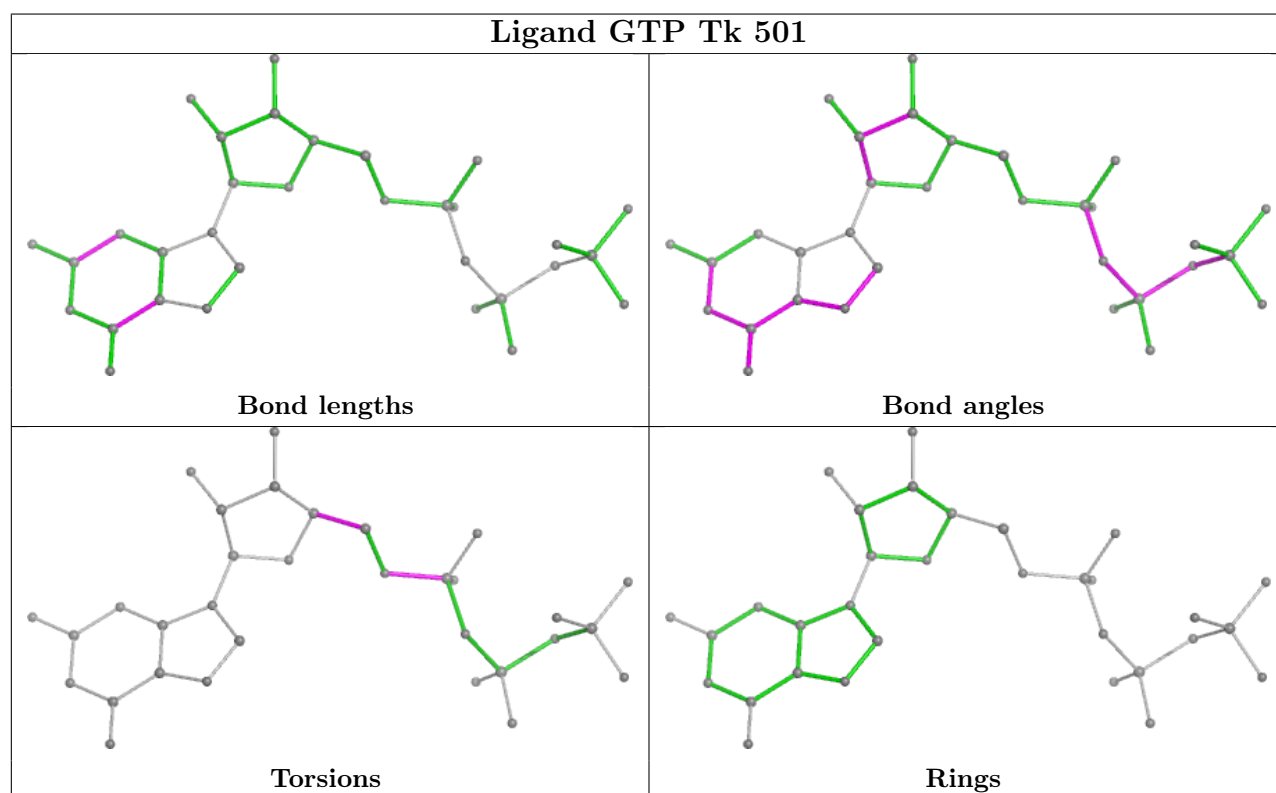
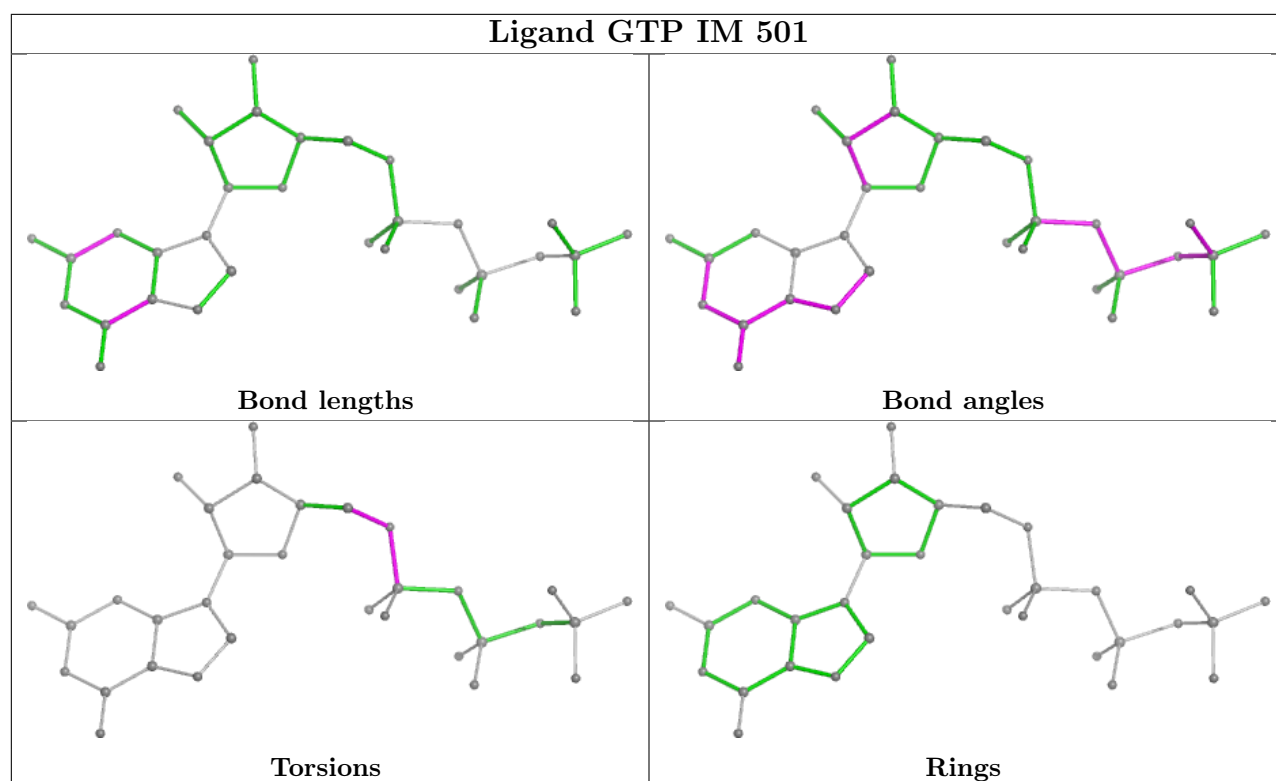


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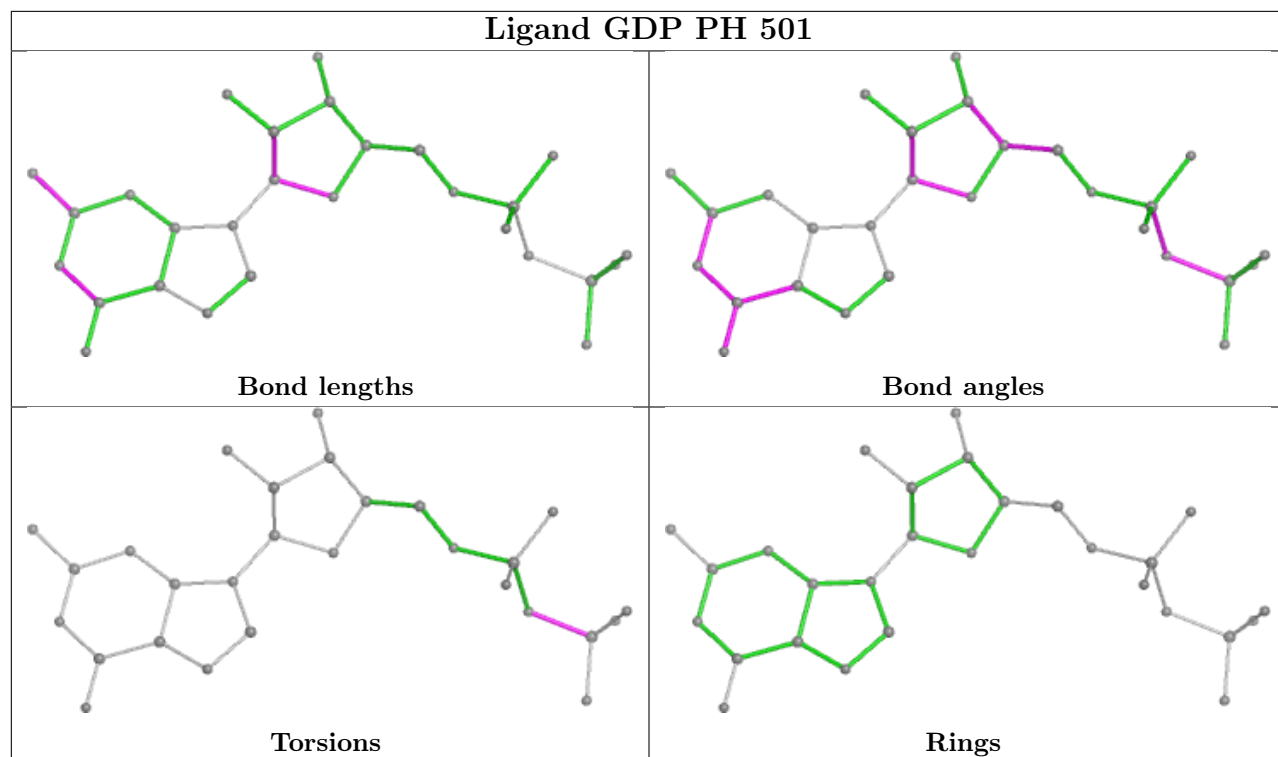


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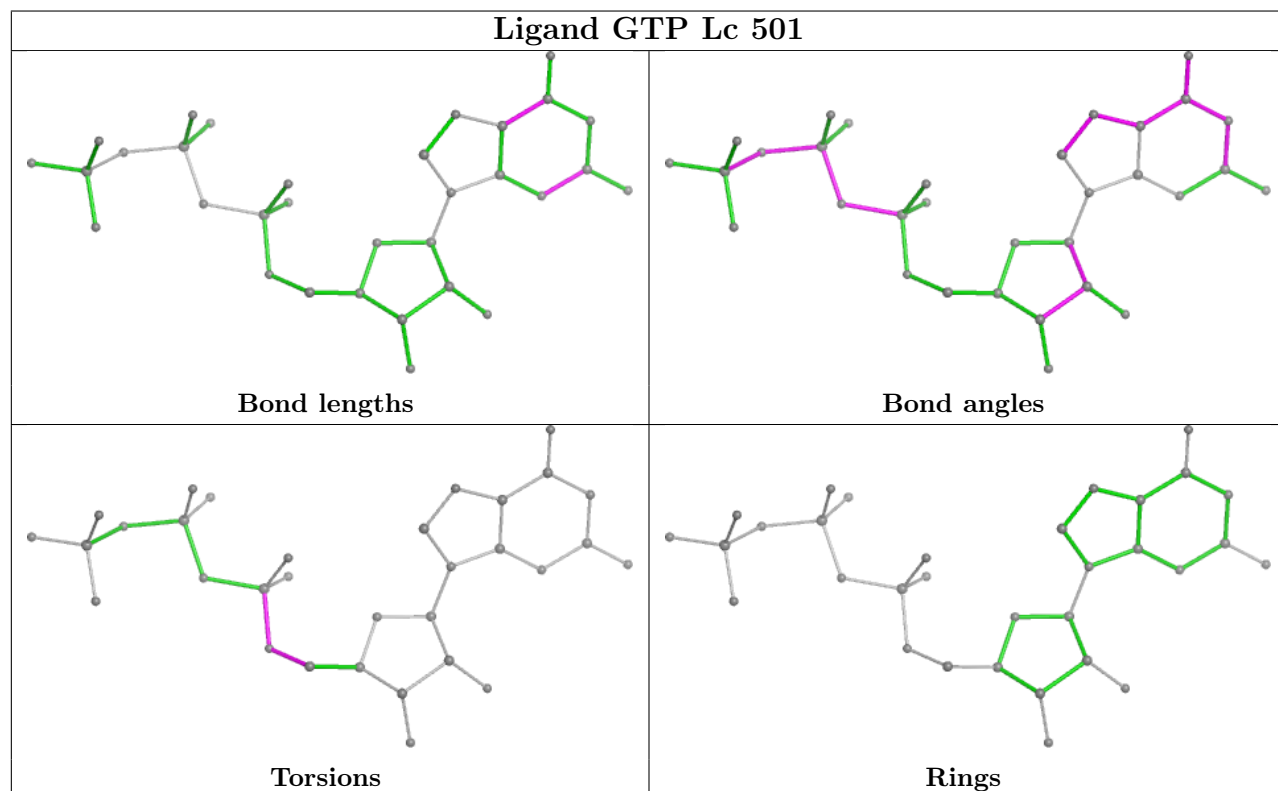




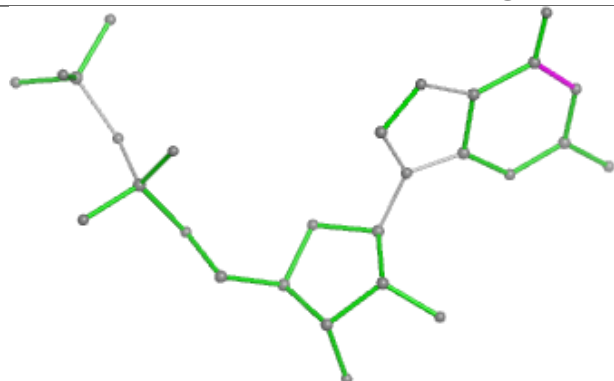
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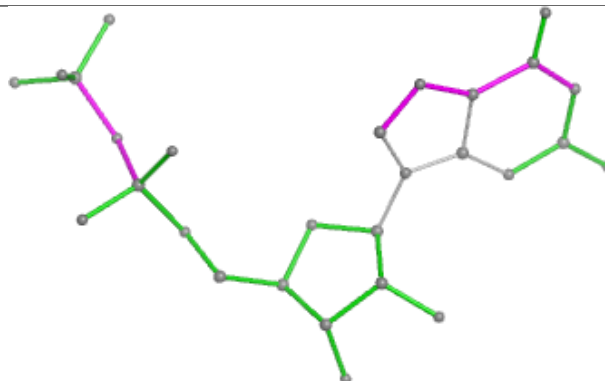
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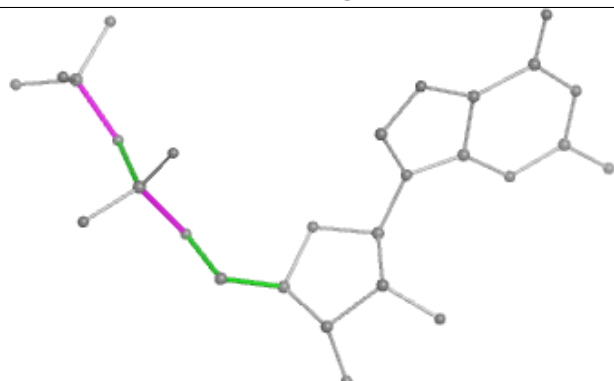
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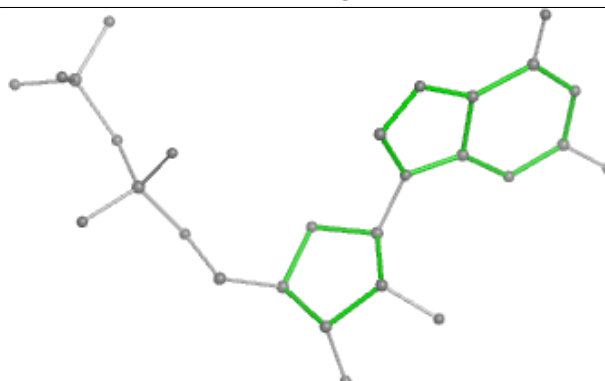
Bond lengths



Bond angles

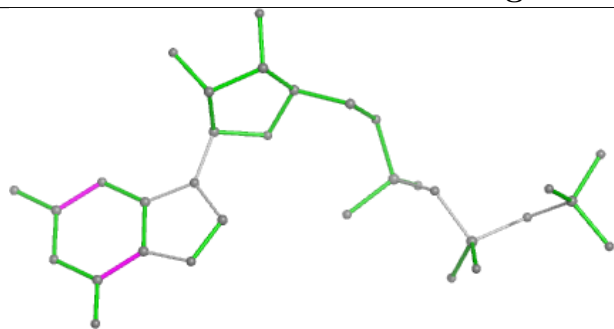


Torsions

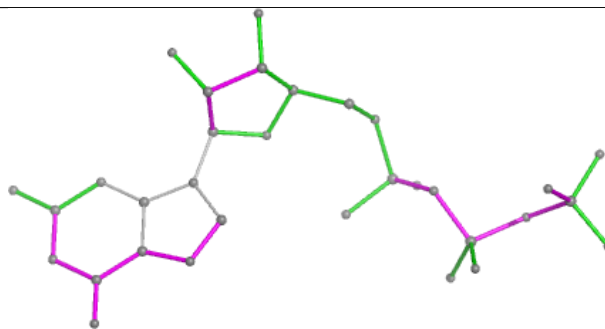


Rings

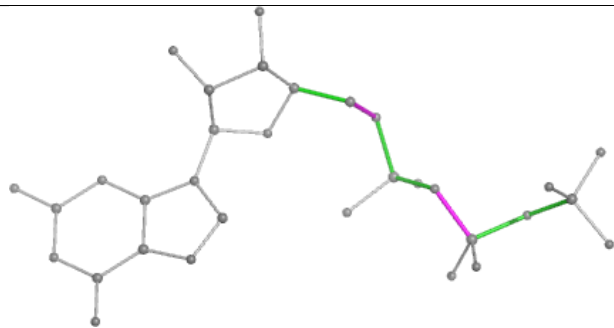
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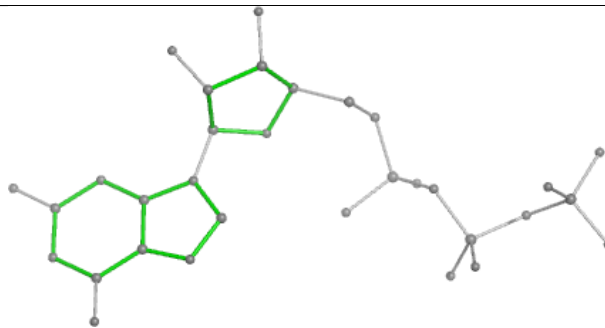
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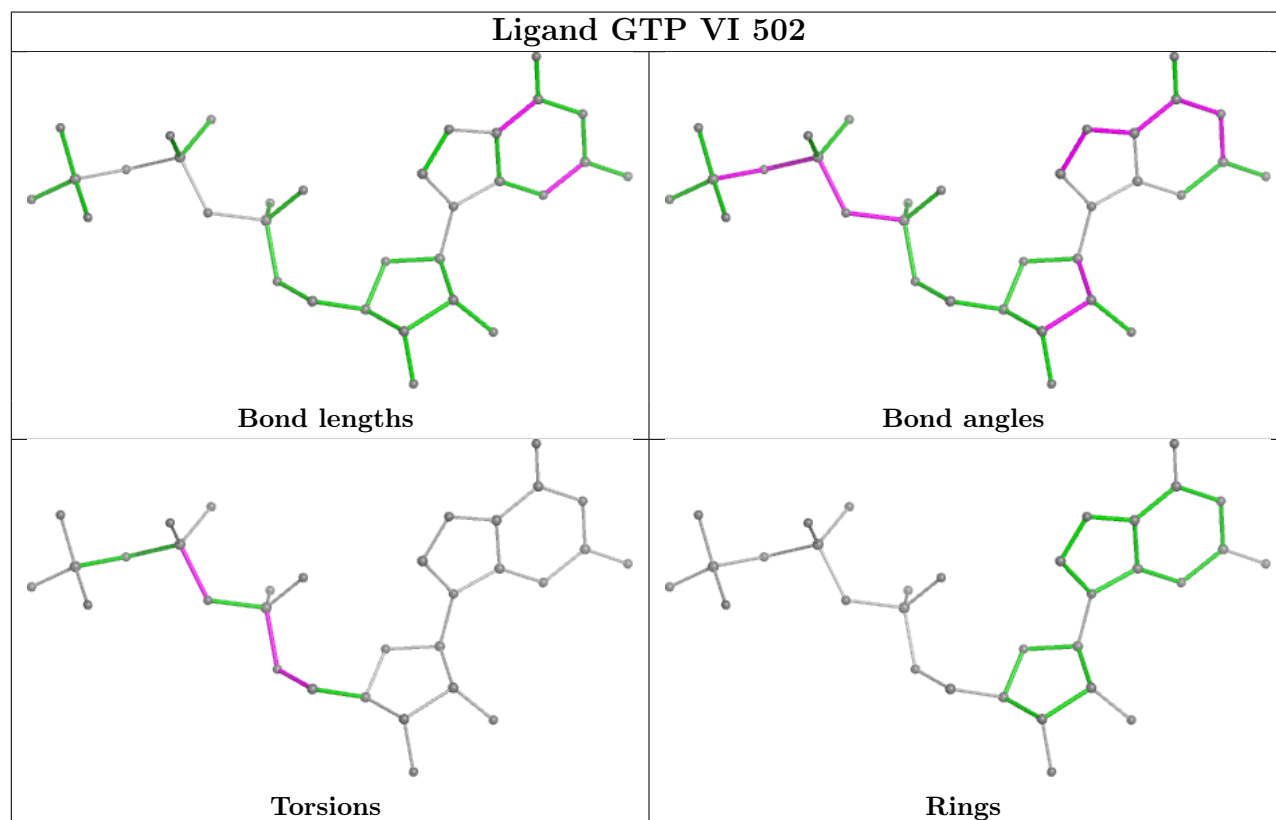
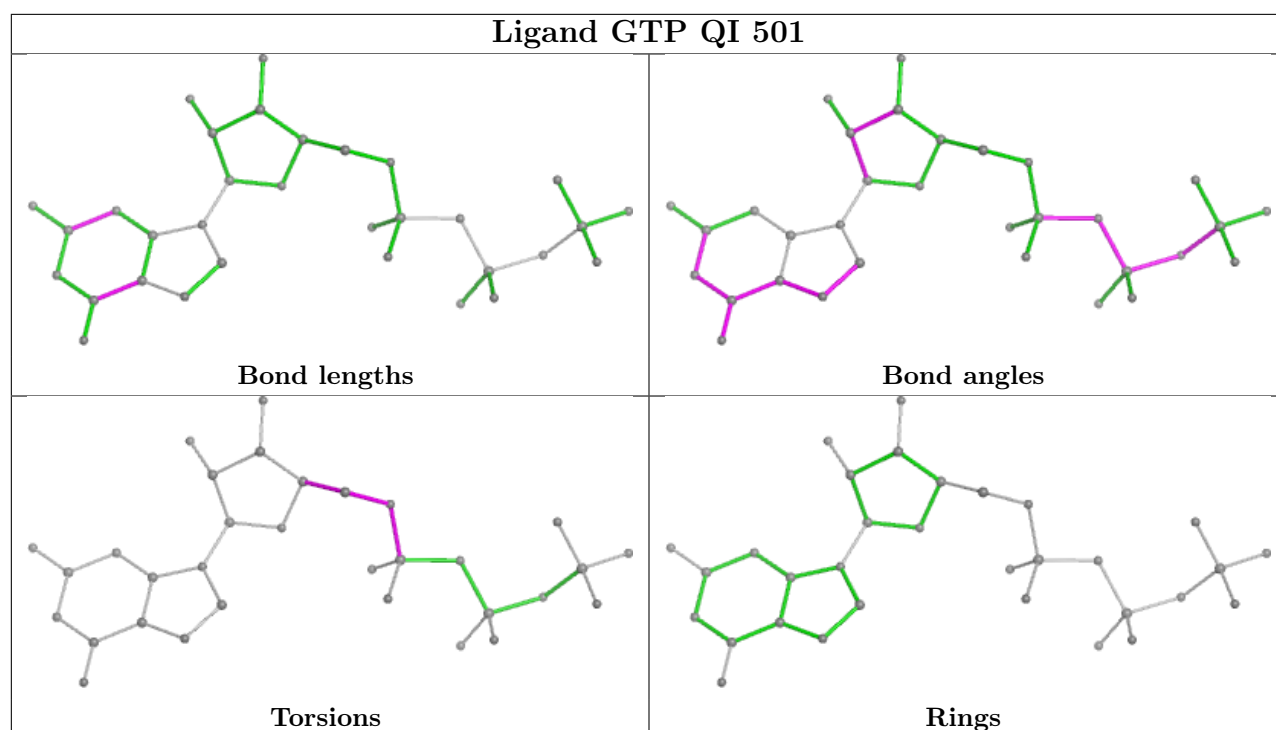
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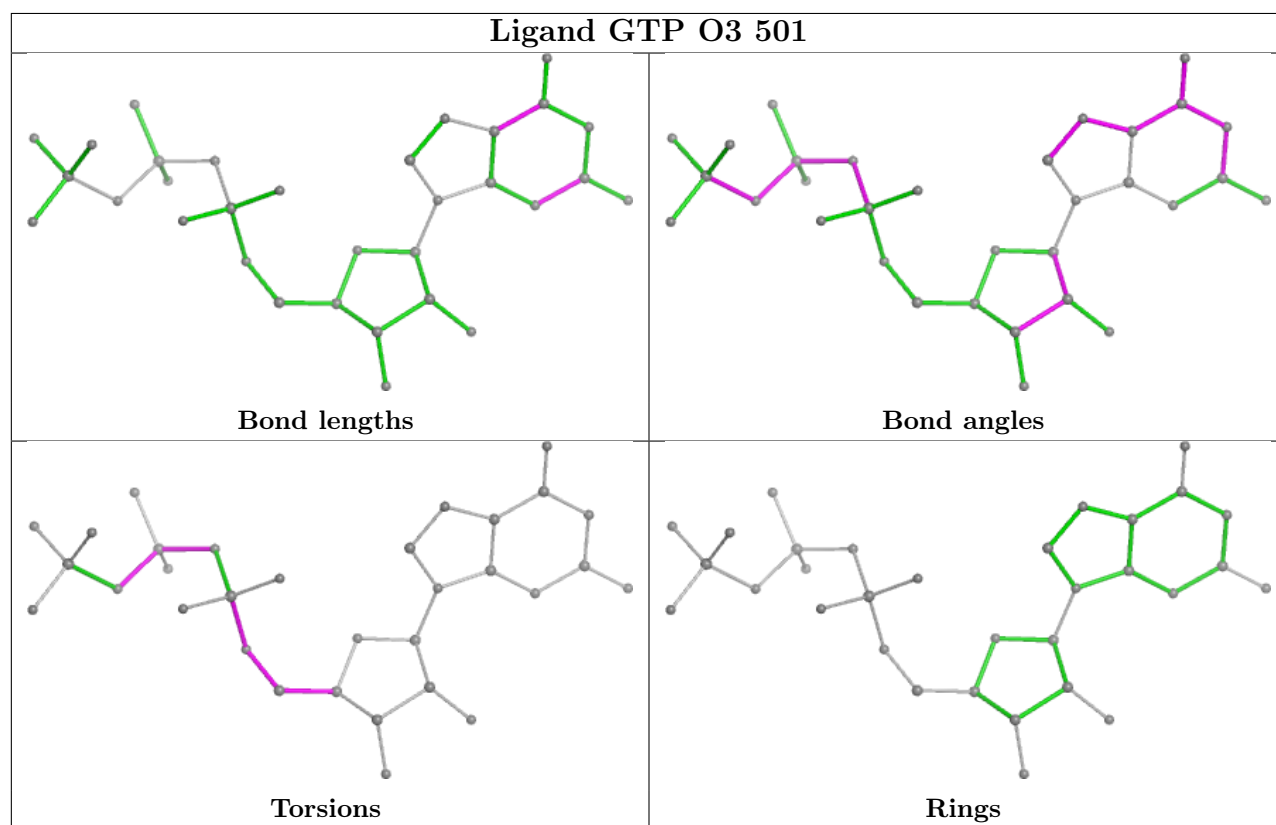
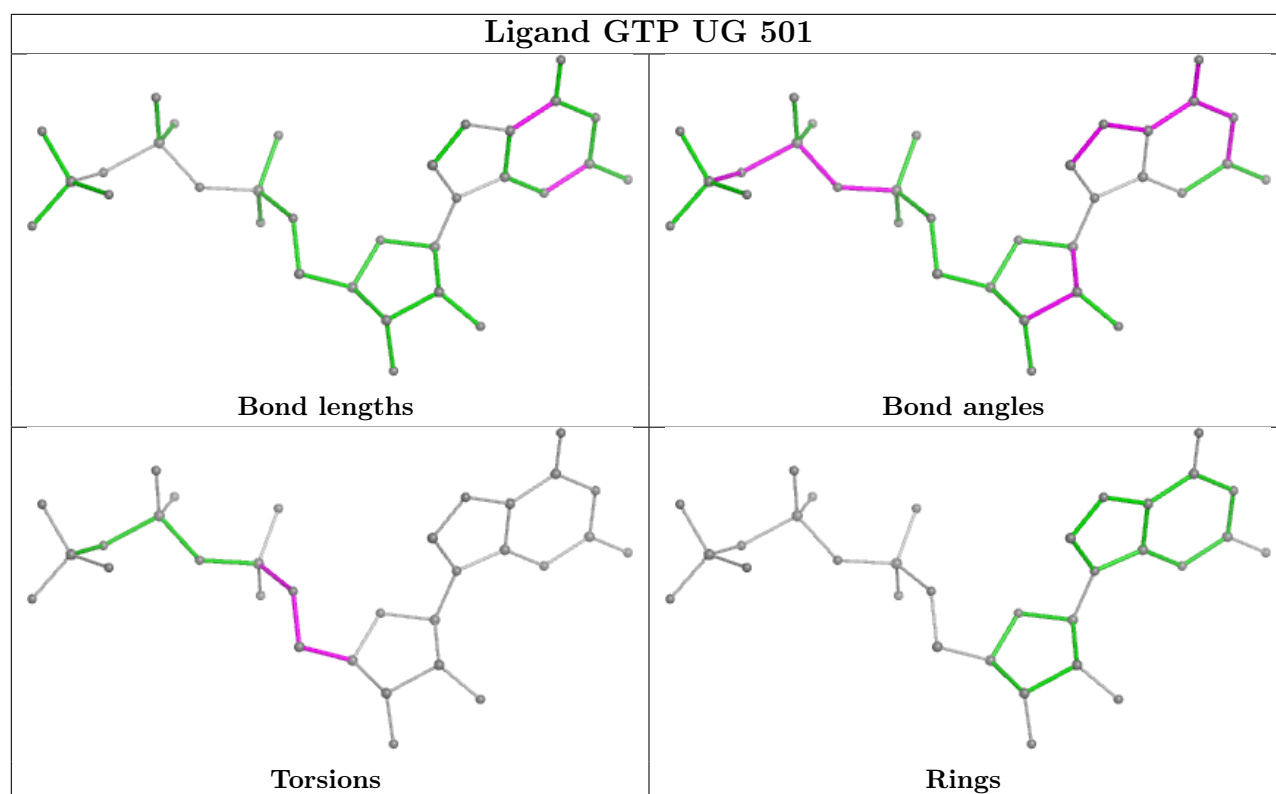
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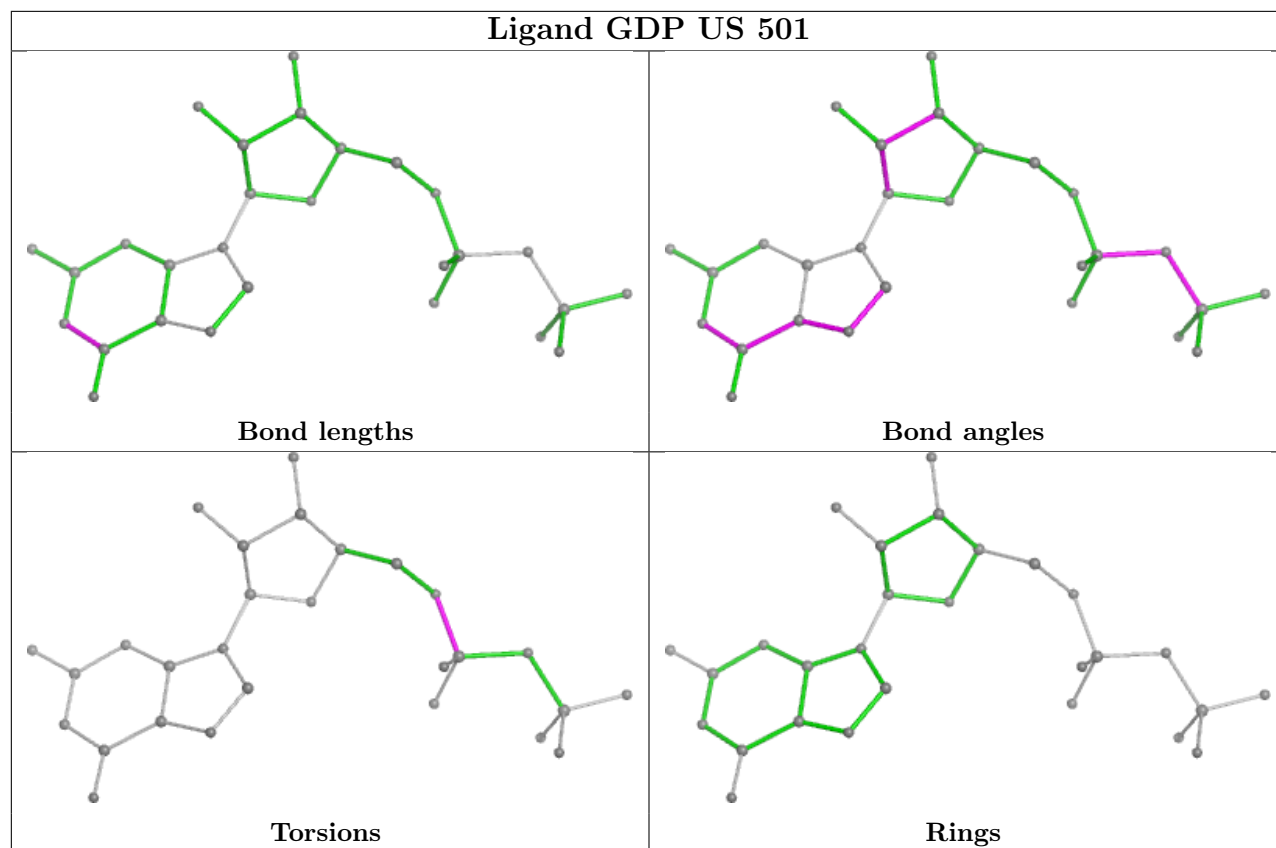
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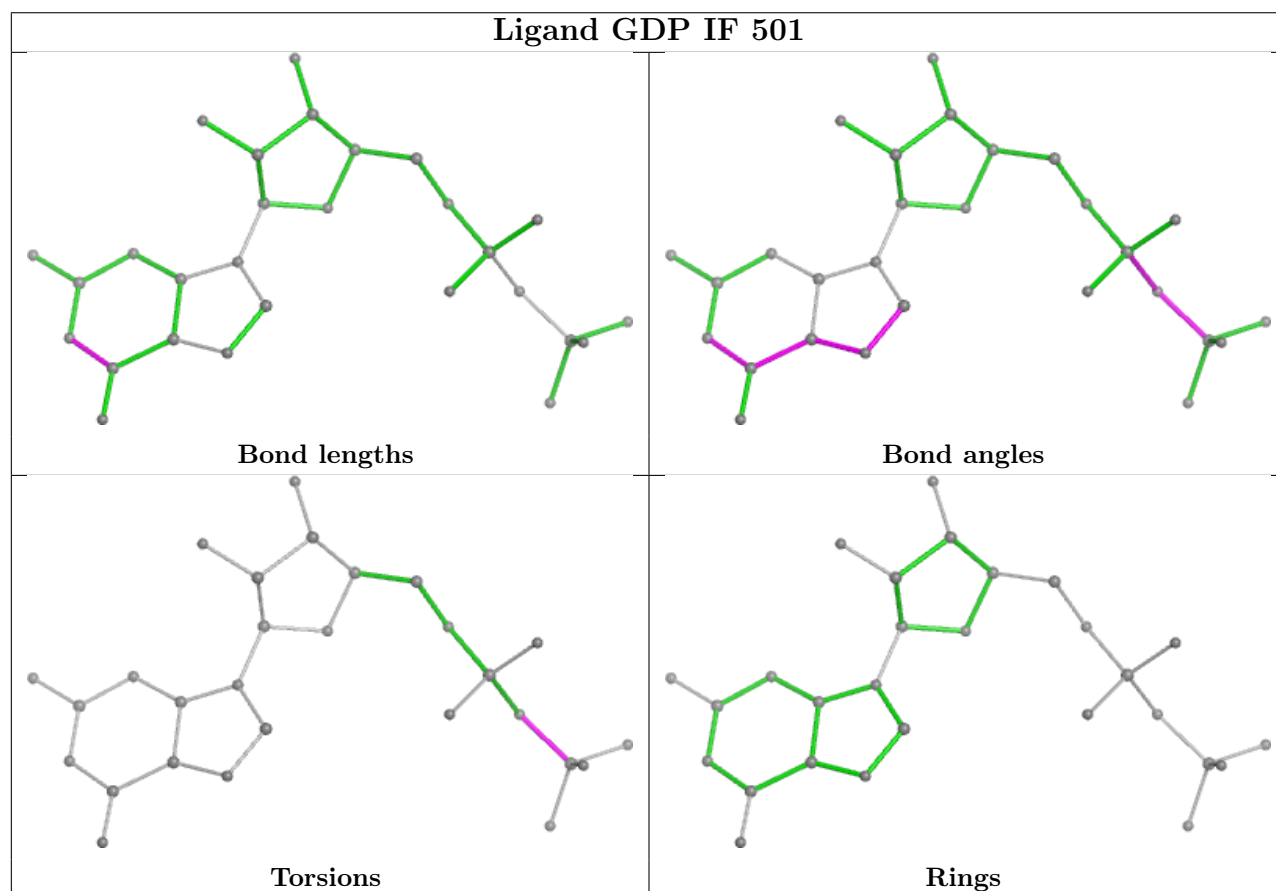




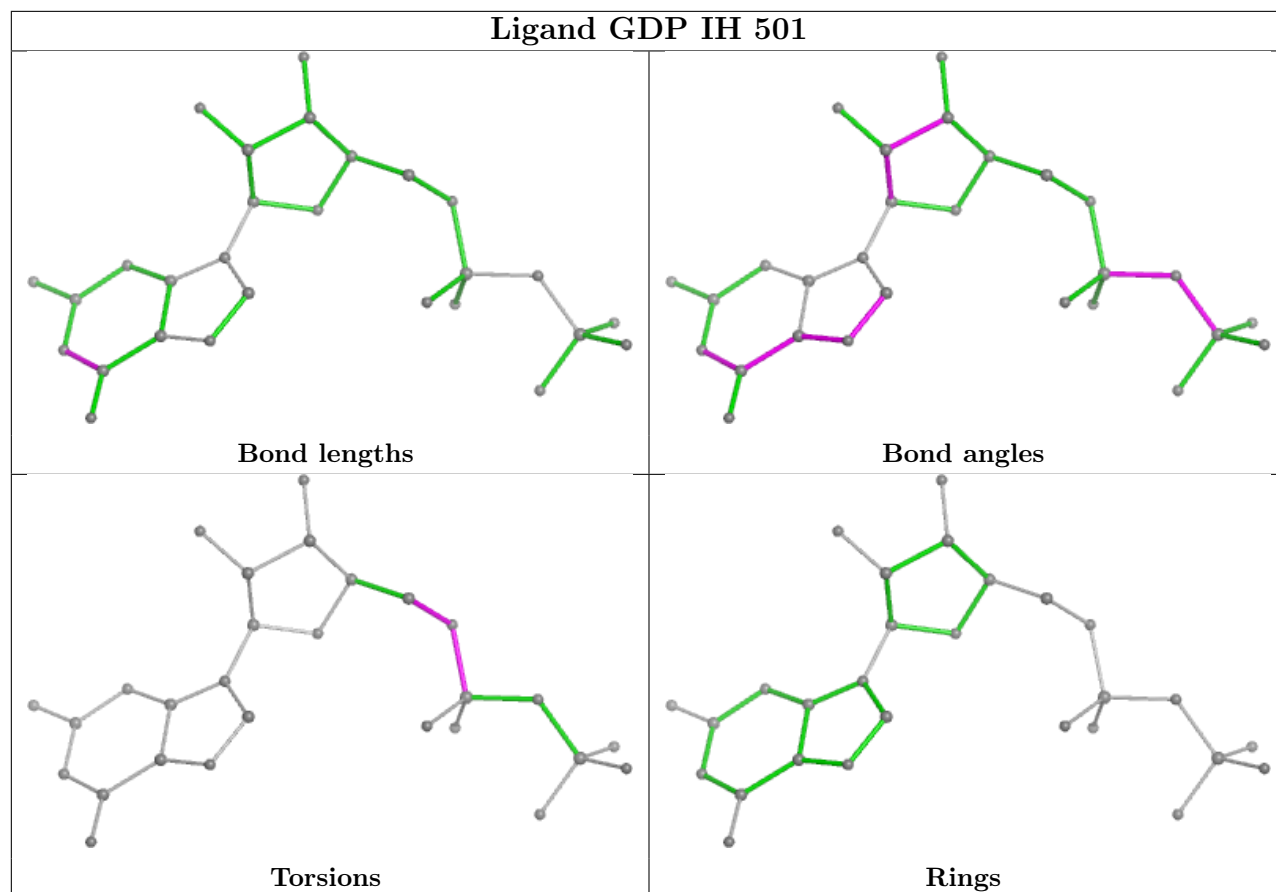
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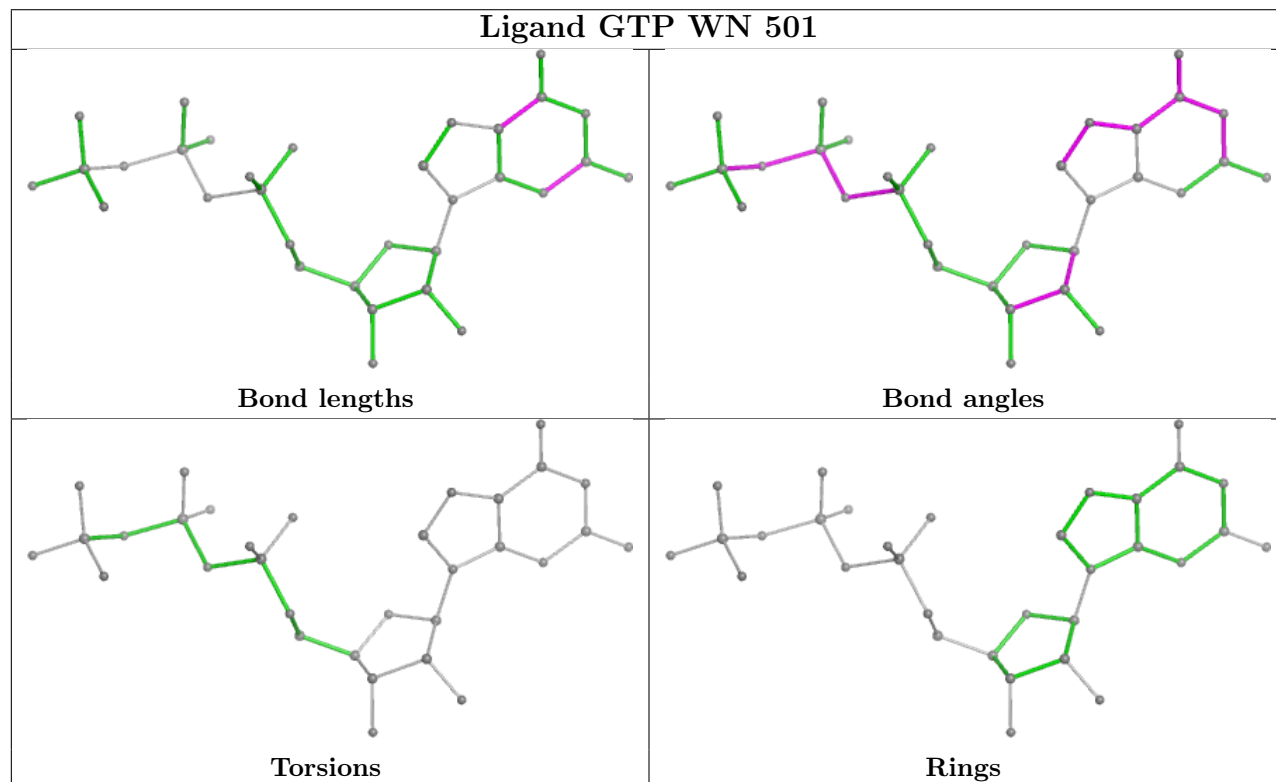
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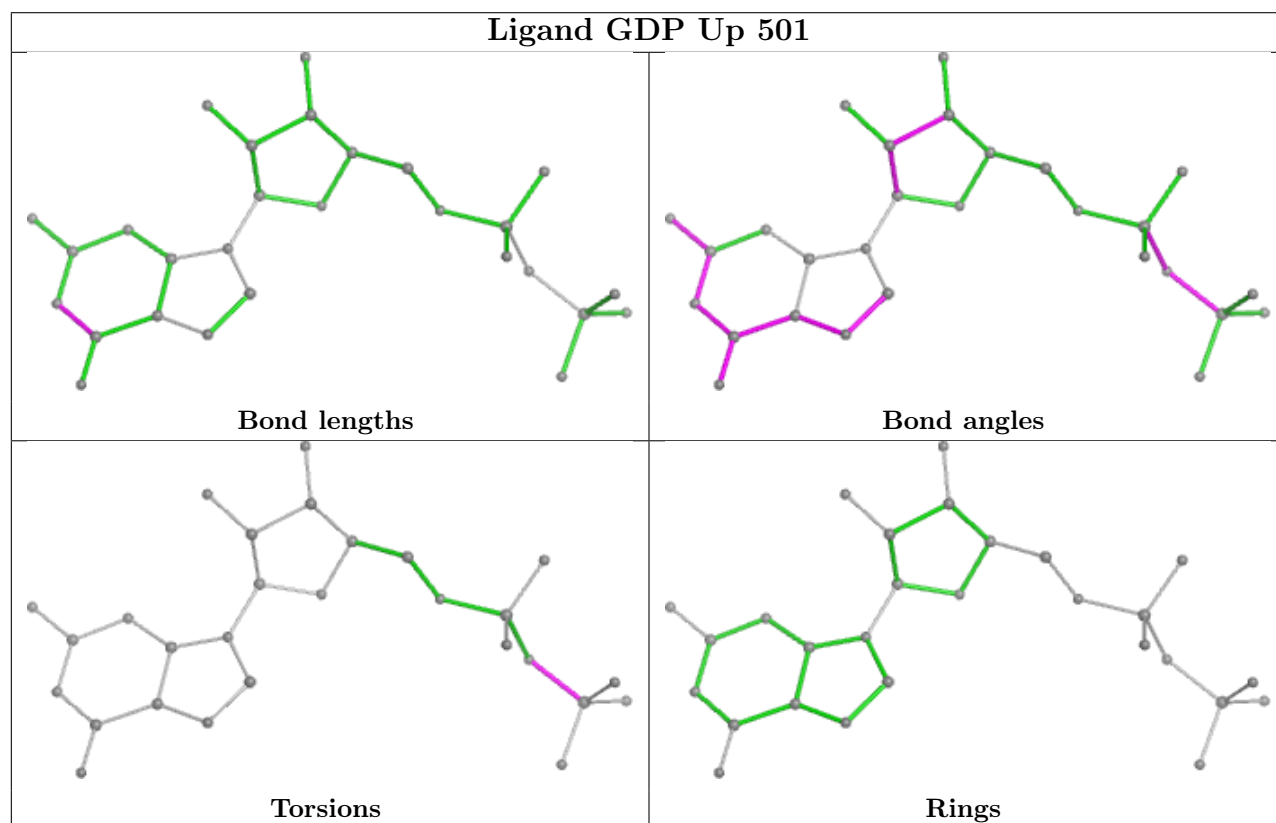
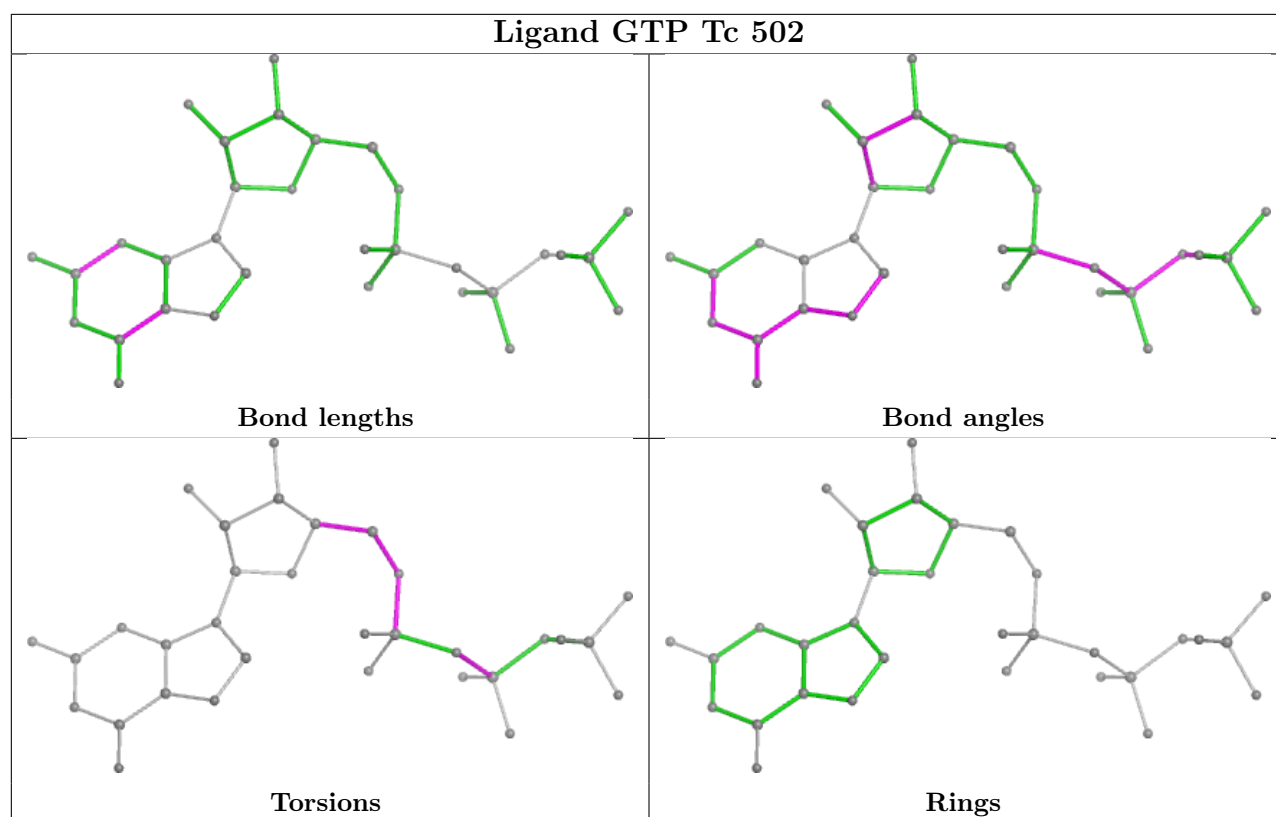


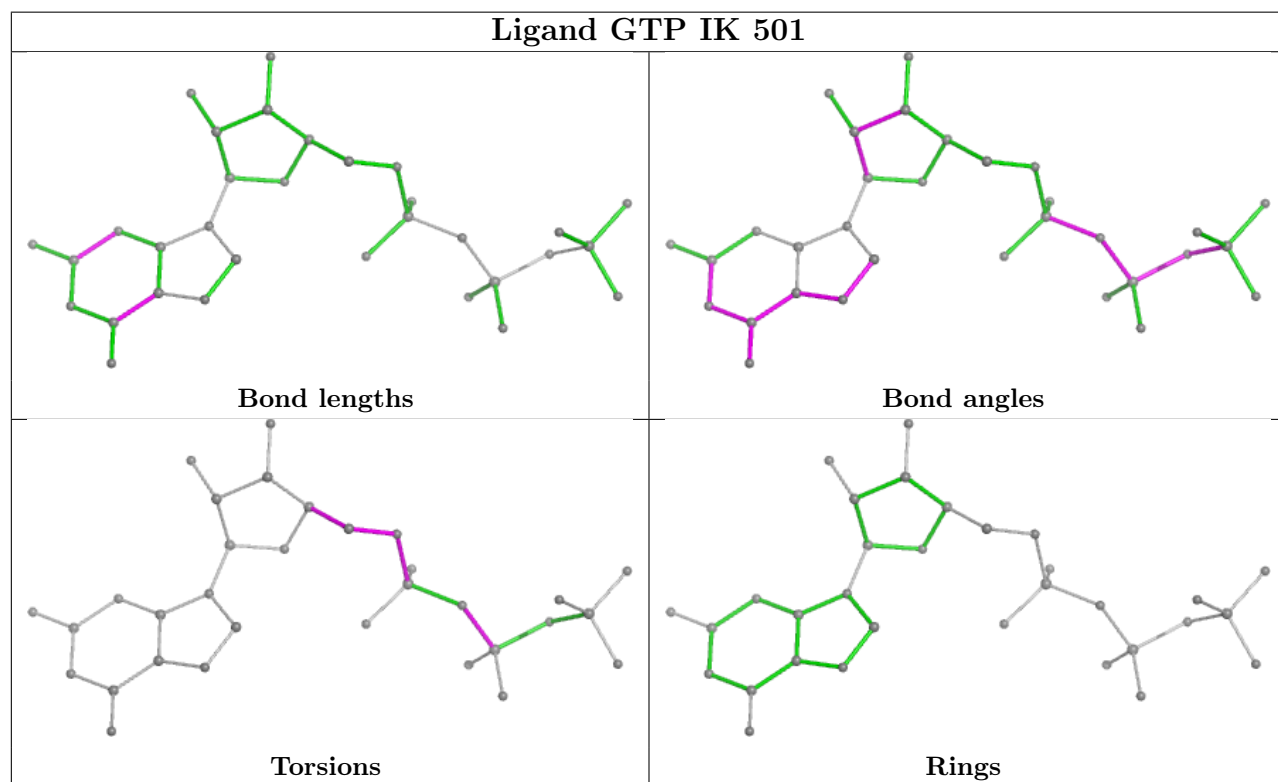
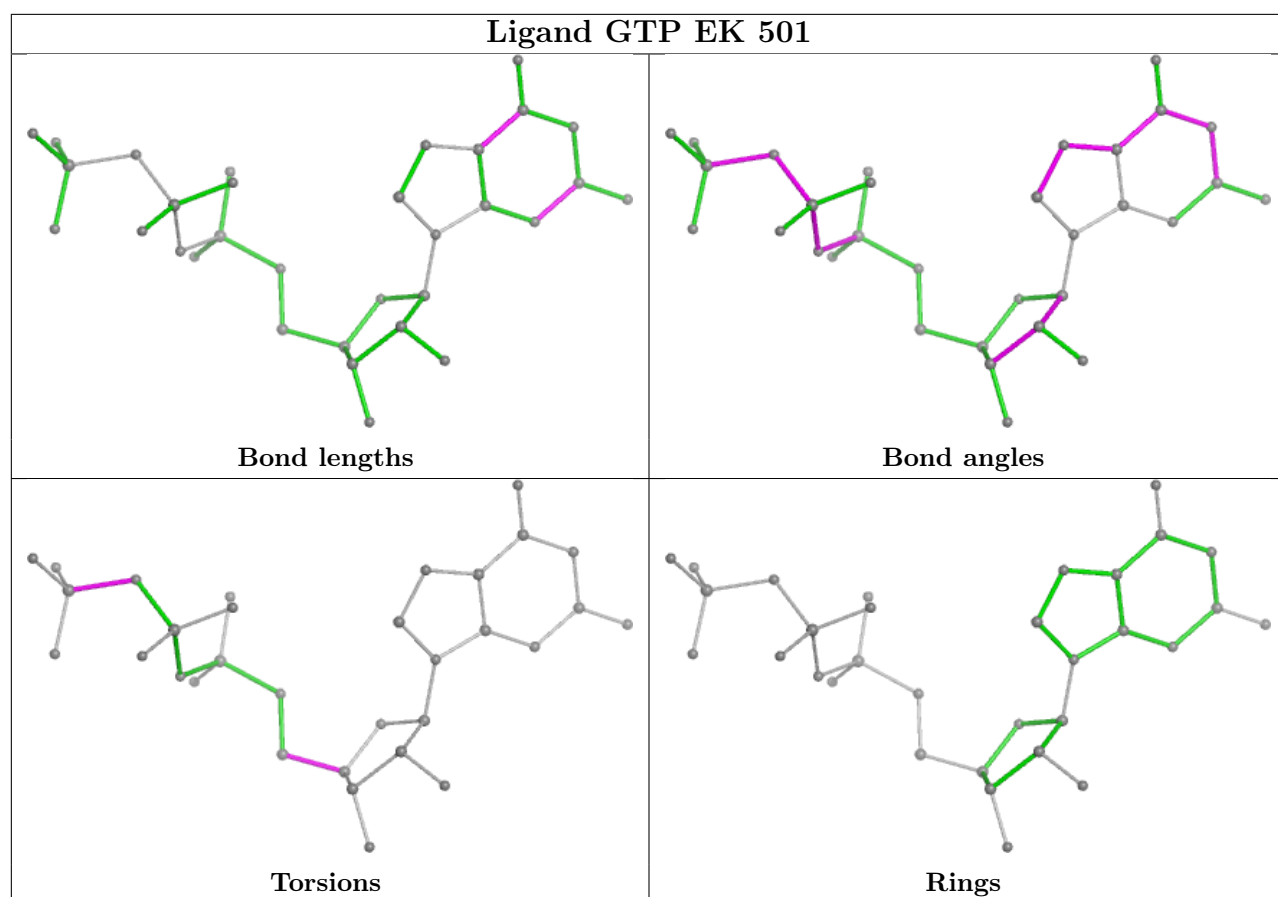
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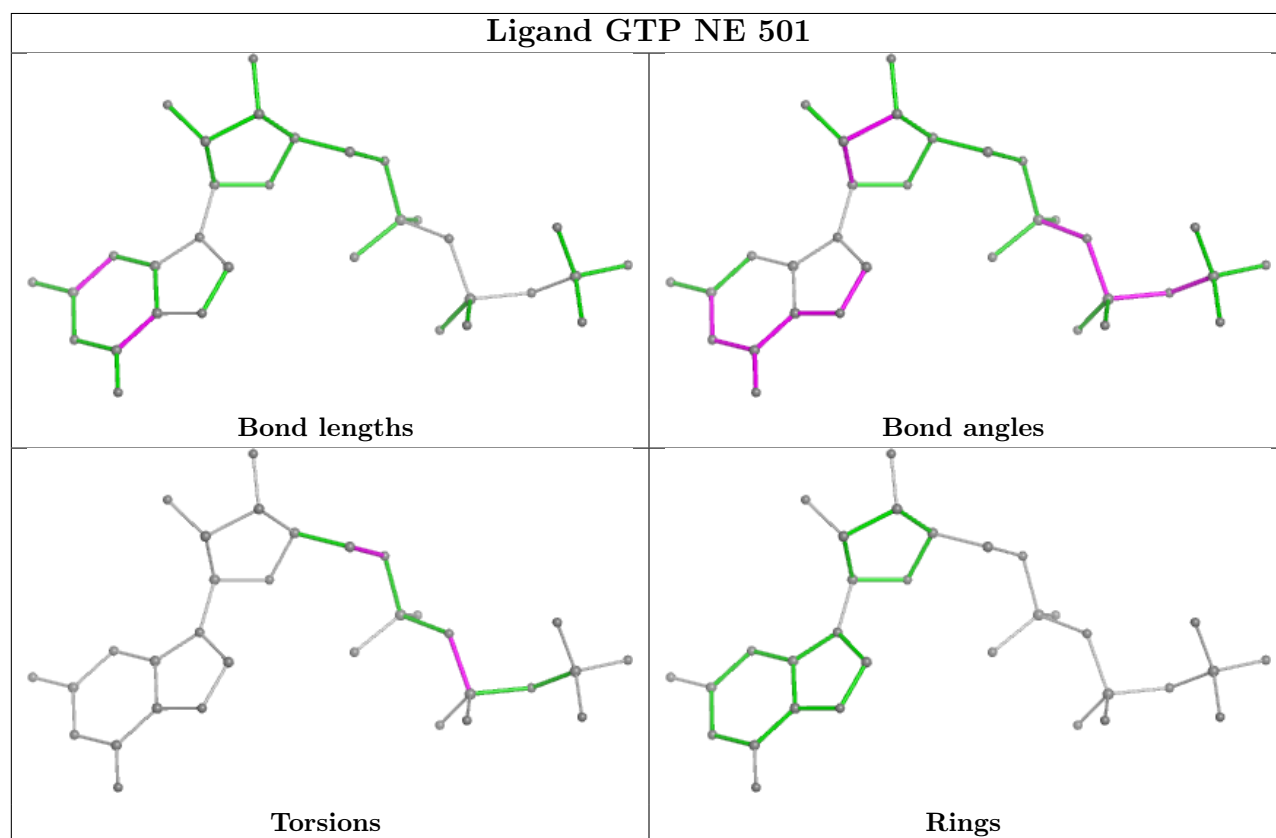
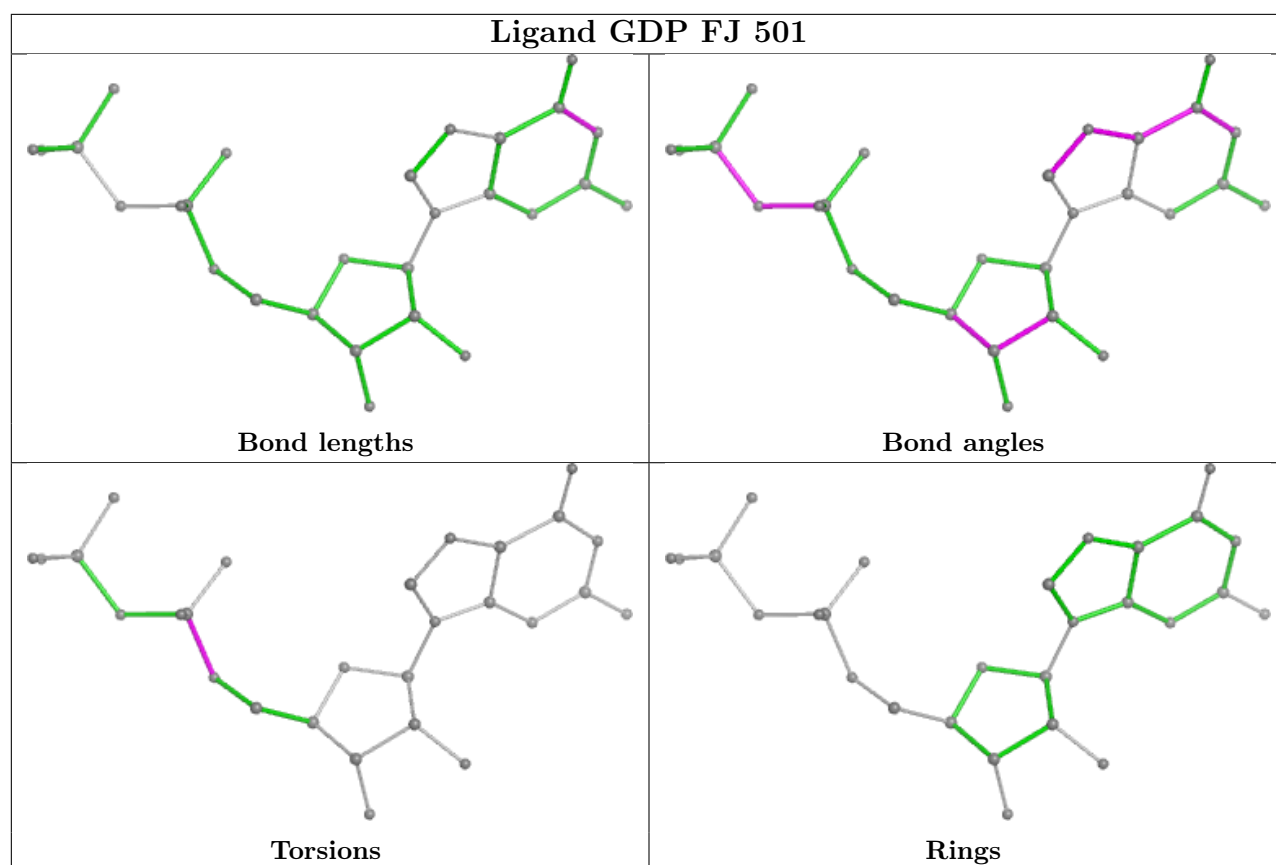


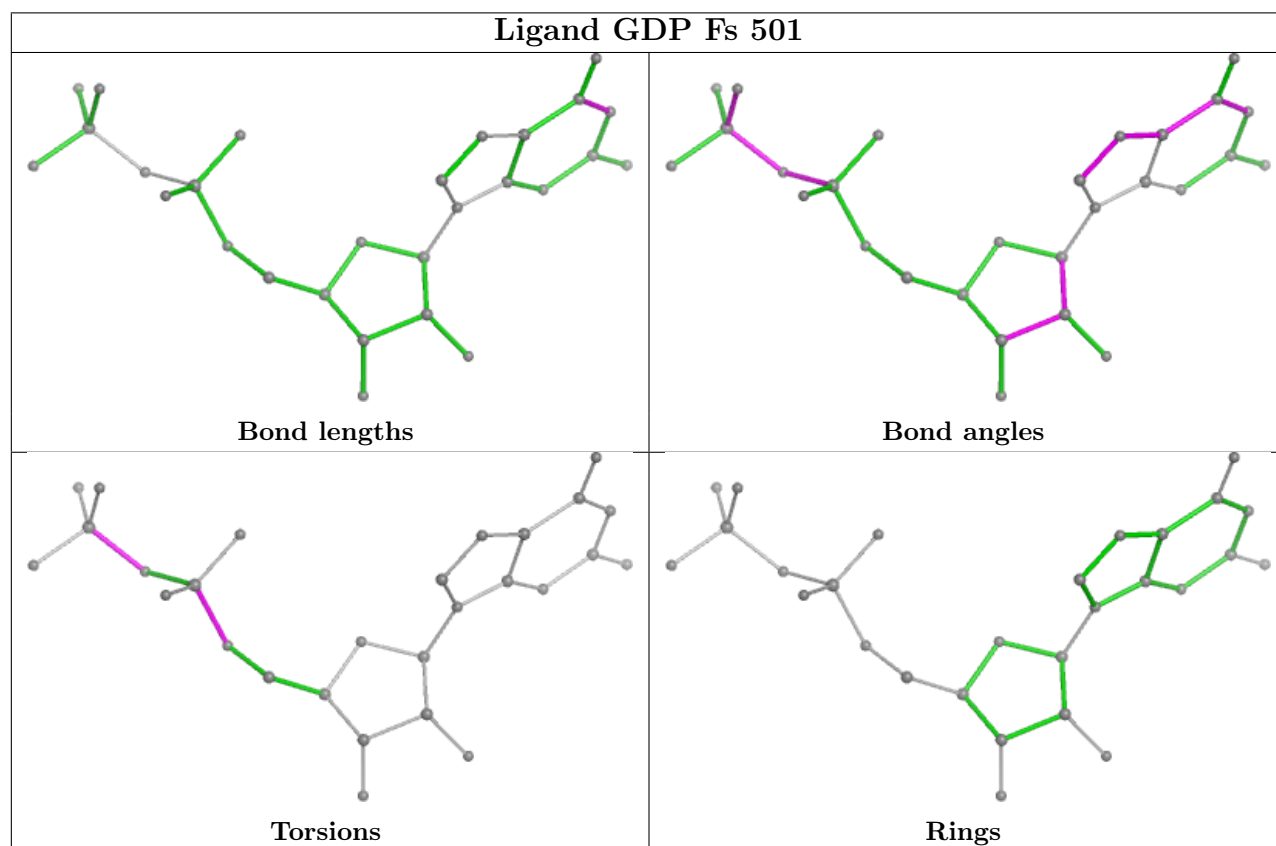
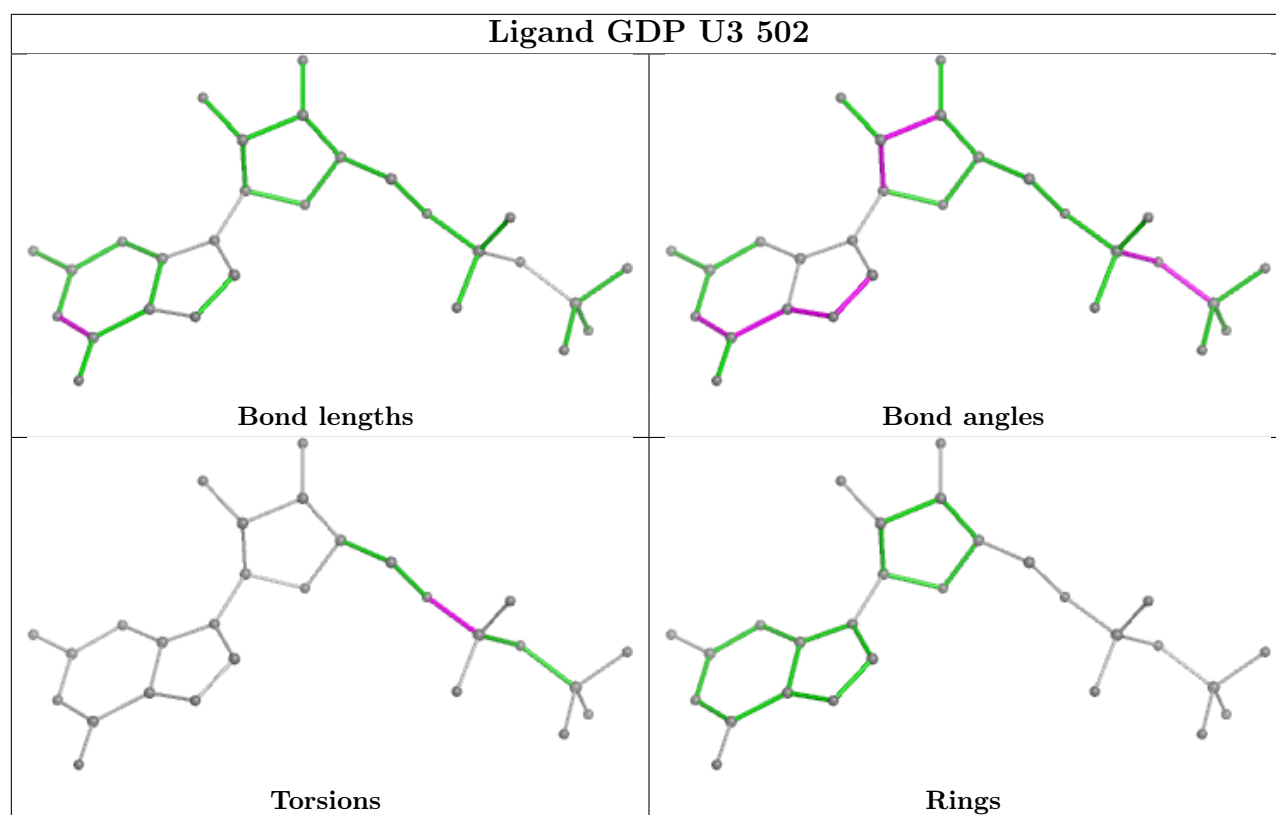
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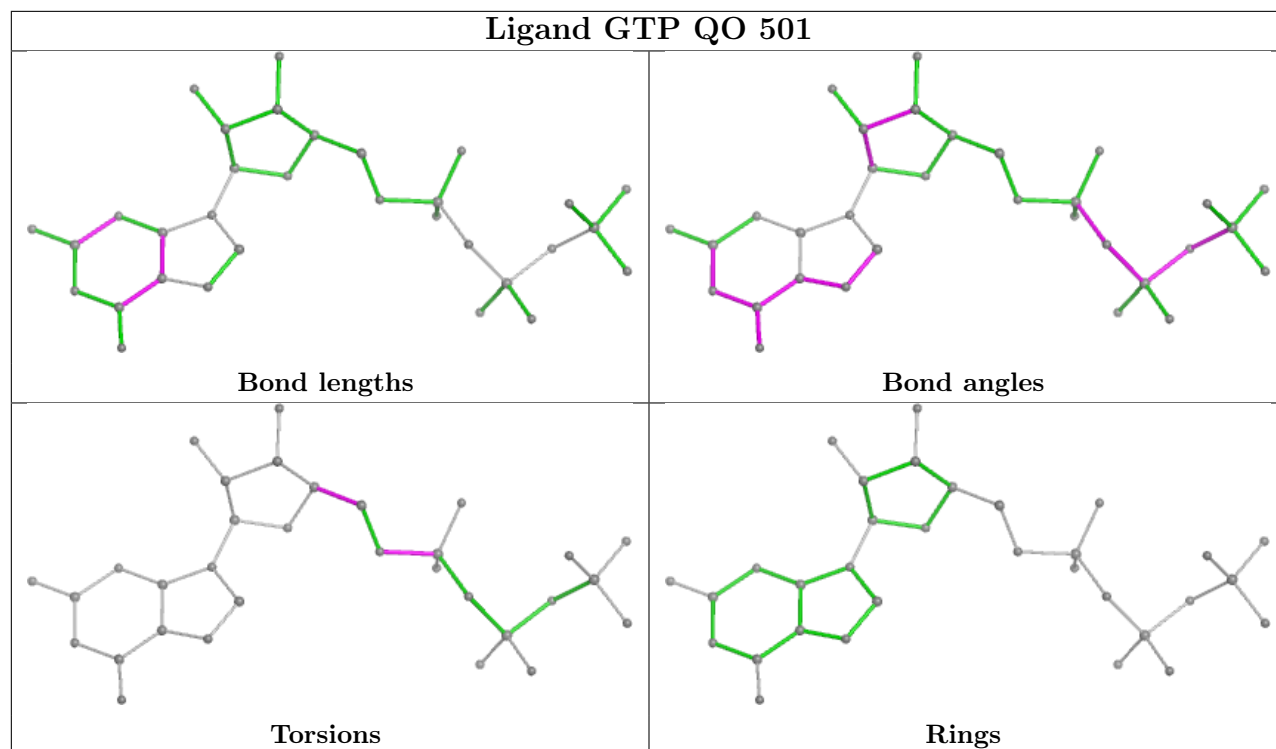




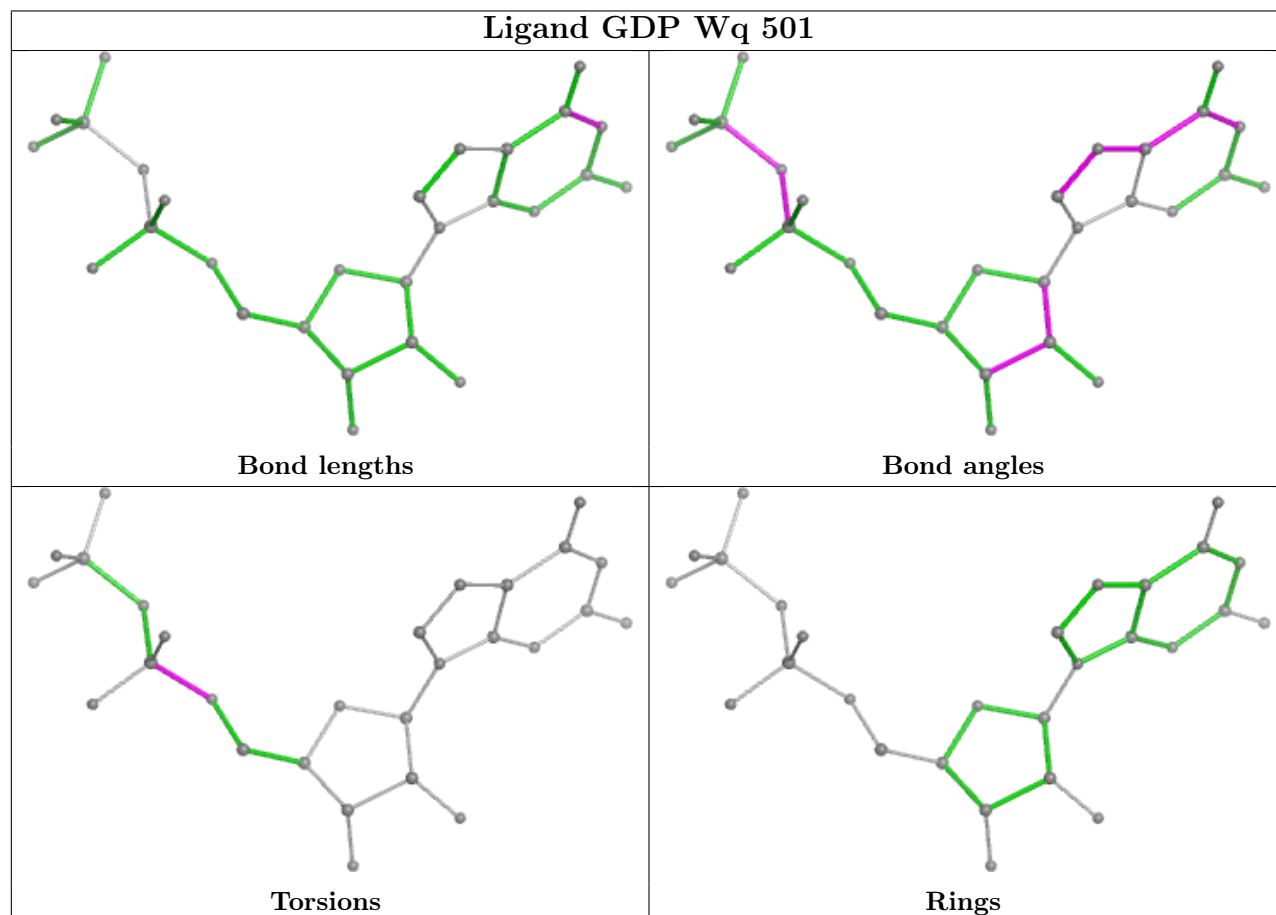




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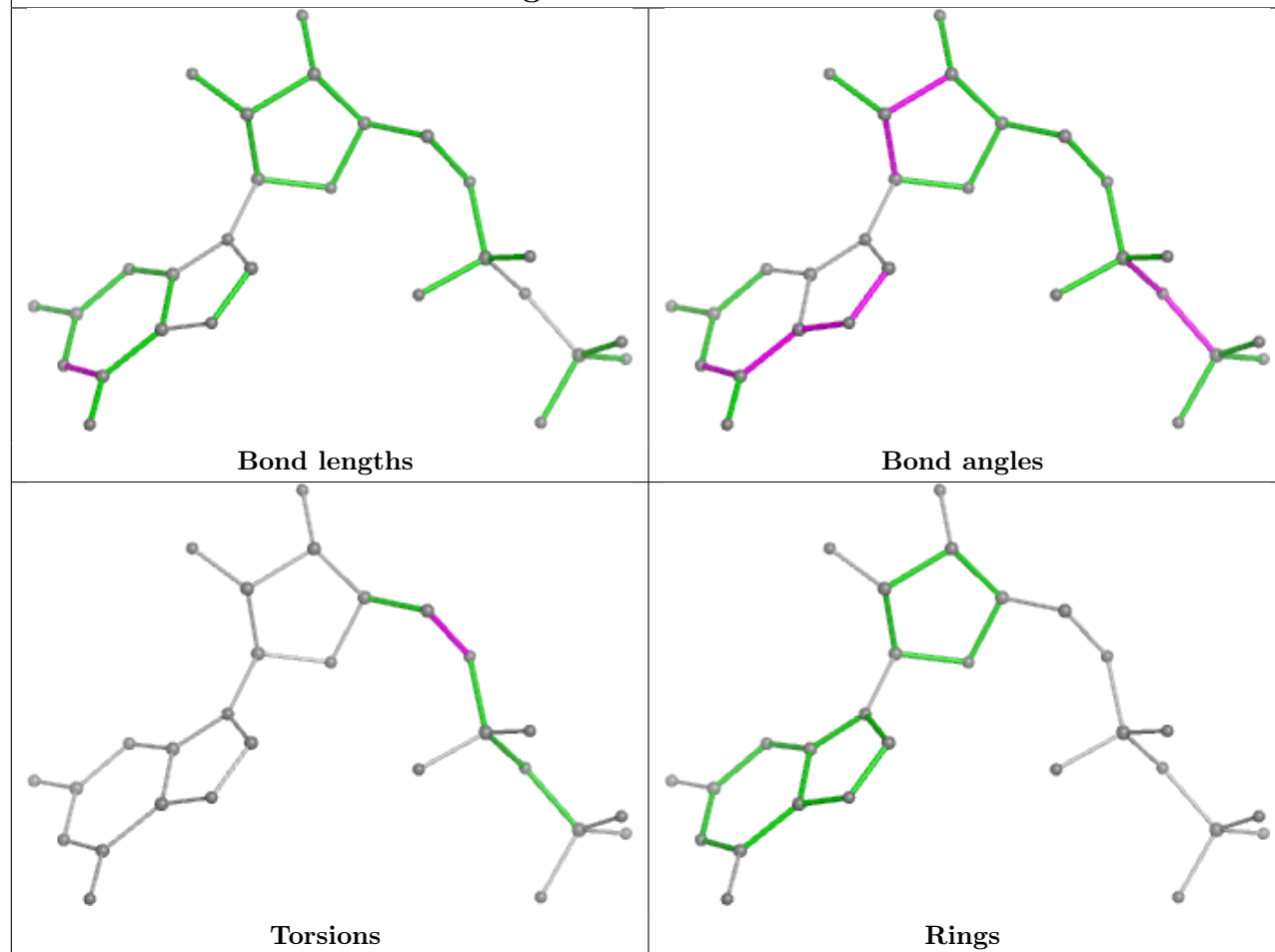


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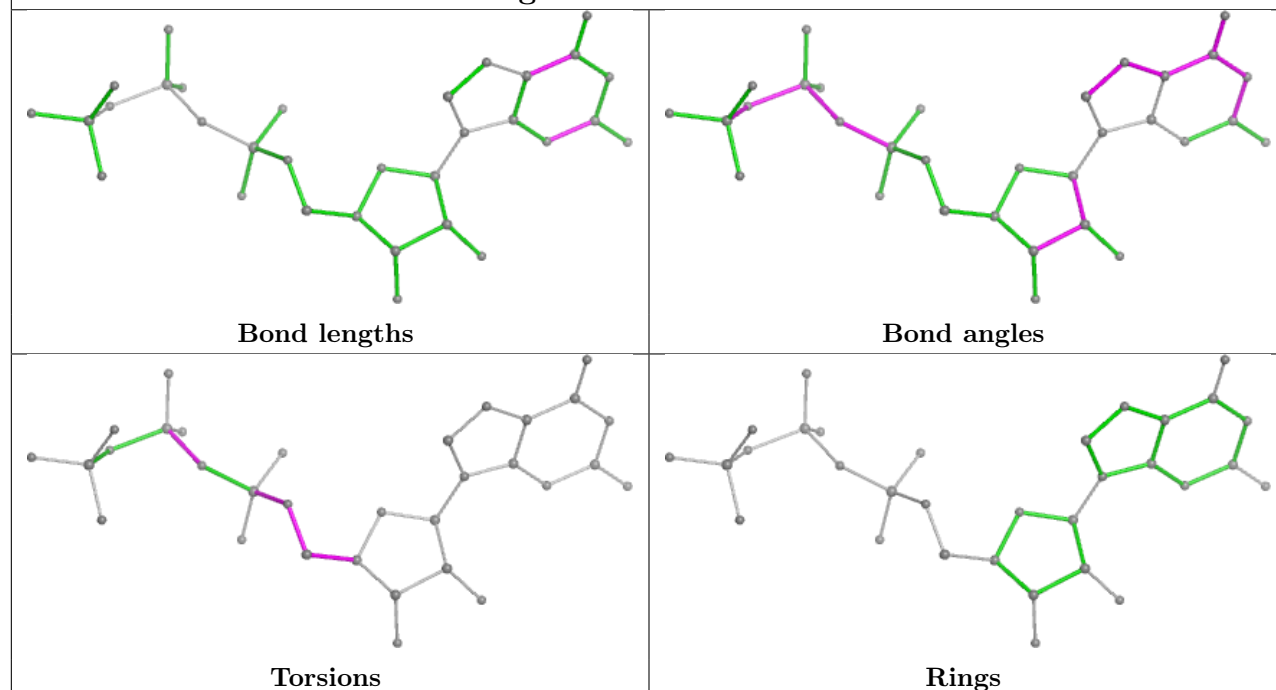




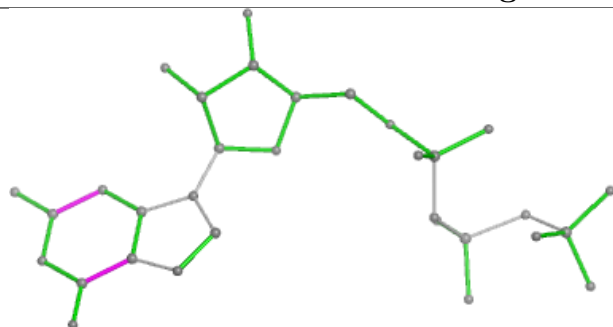
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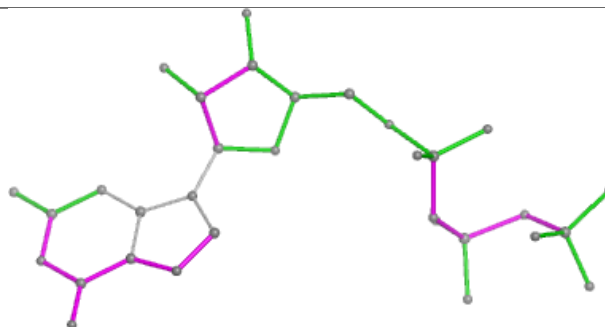
## Ligand GTP FU 501



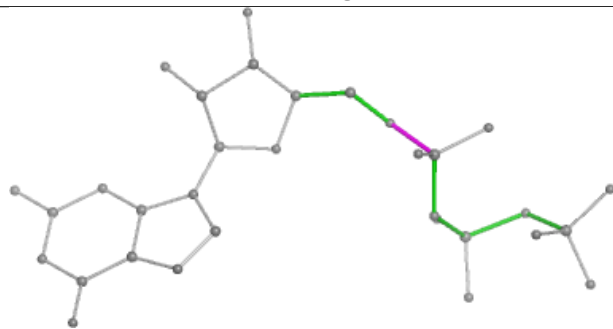
## Ligand GTP PK 501



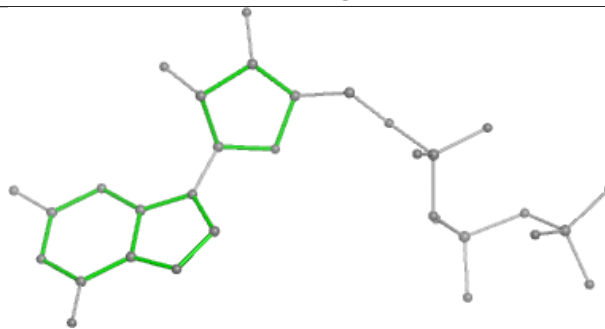
Bond lengths



Bond angles

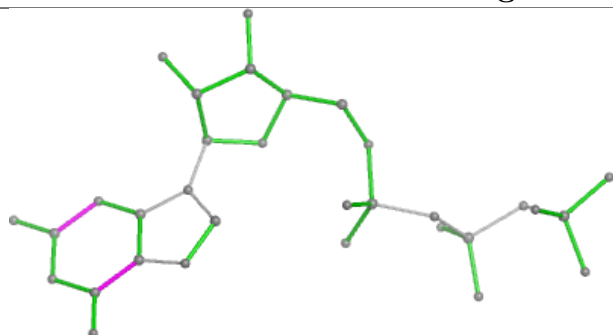


Torsions

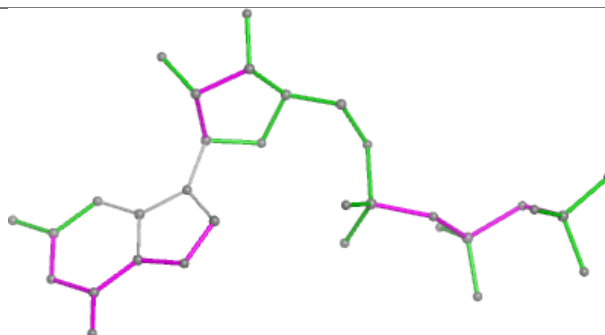


Rings

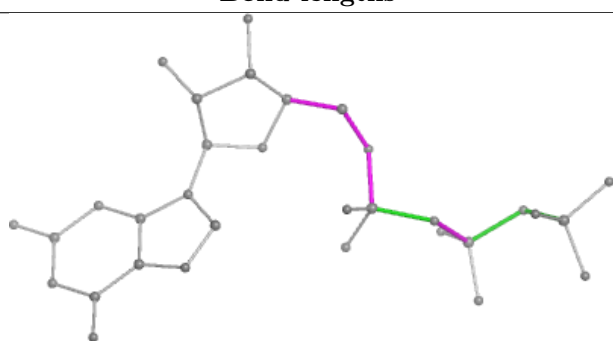
## Ligand GTP KK 502



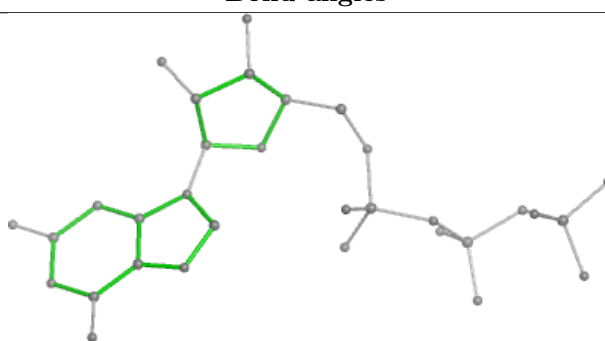
Bond lengths



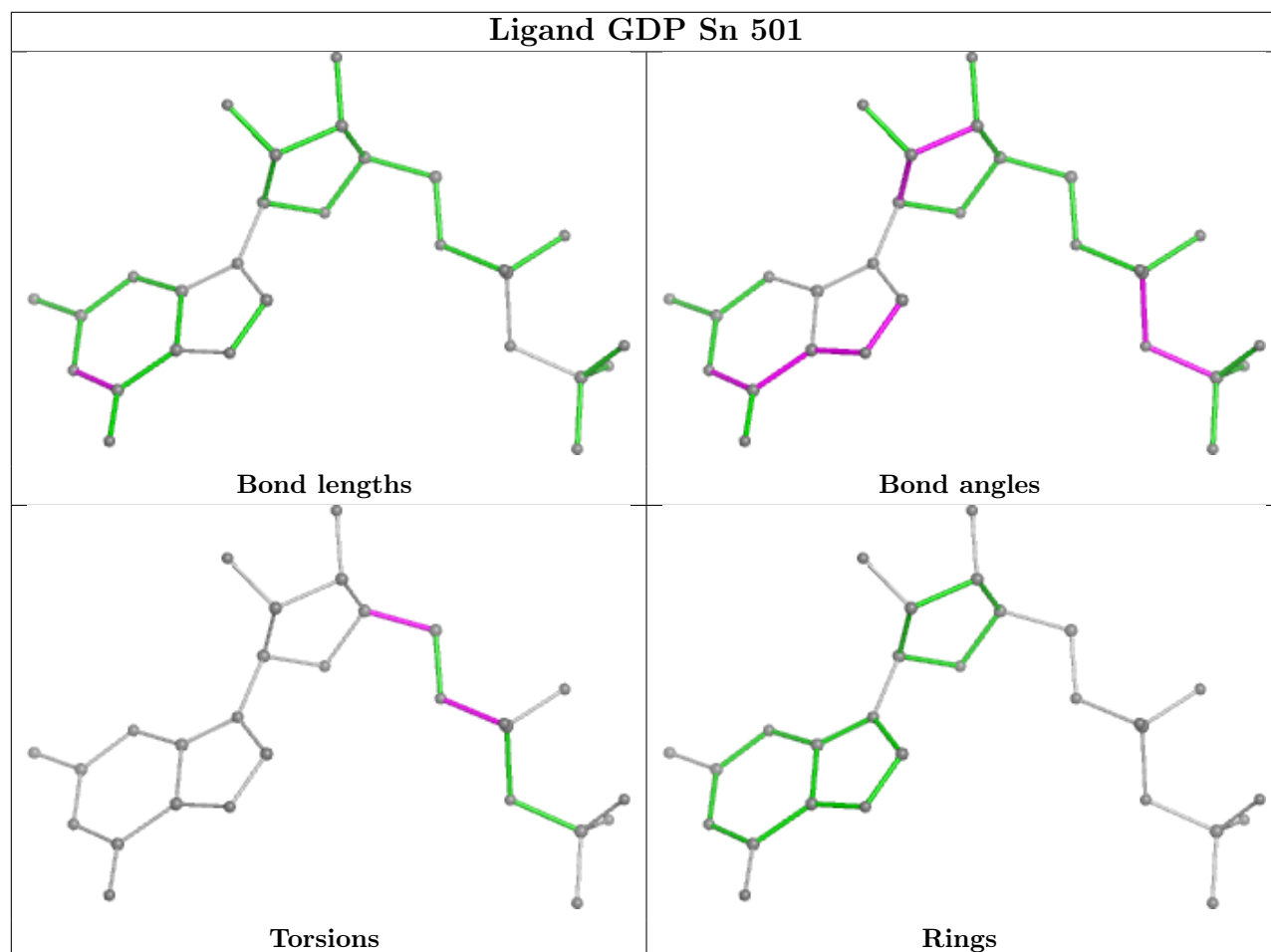
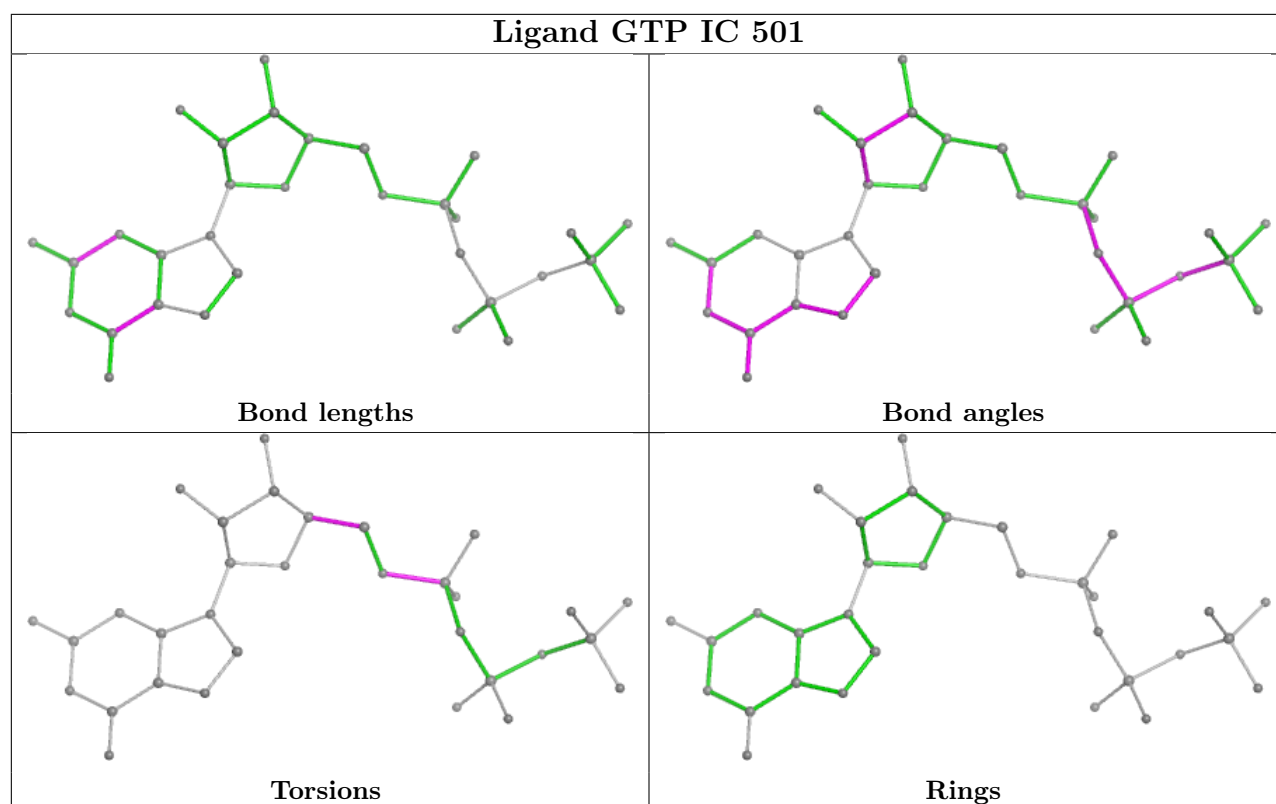
Bond angles

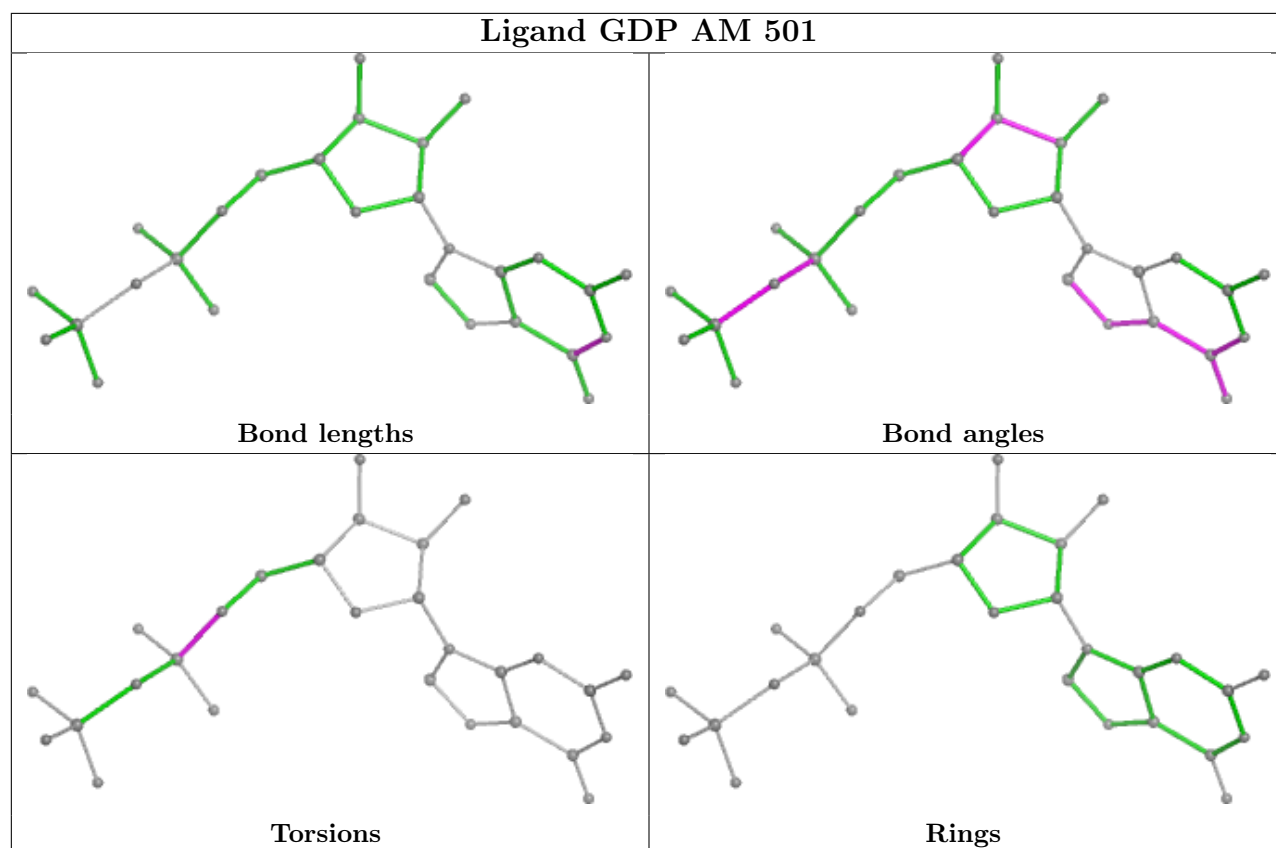
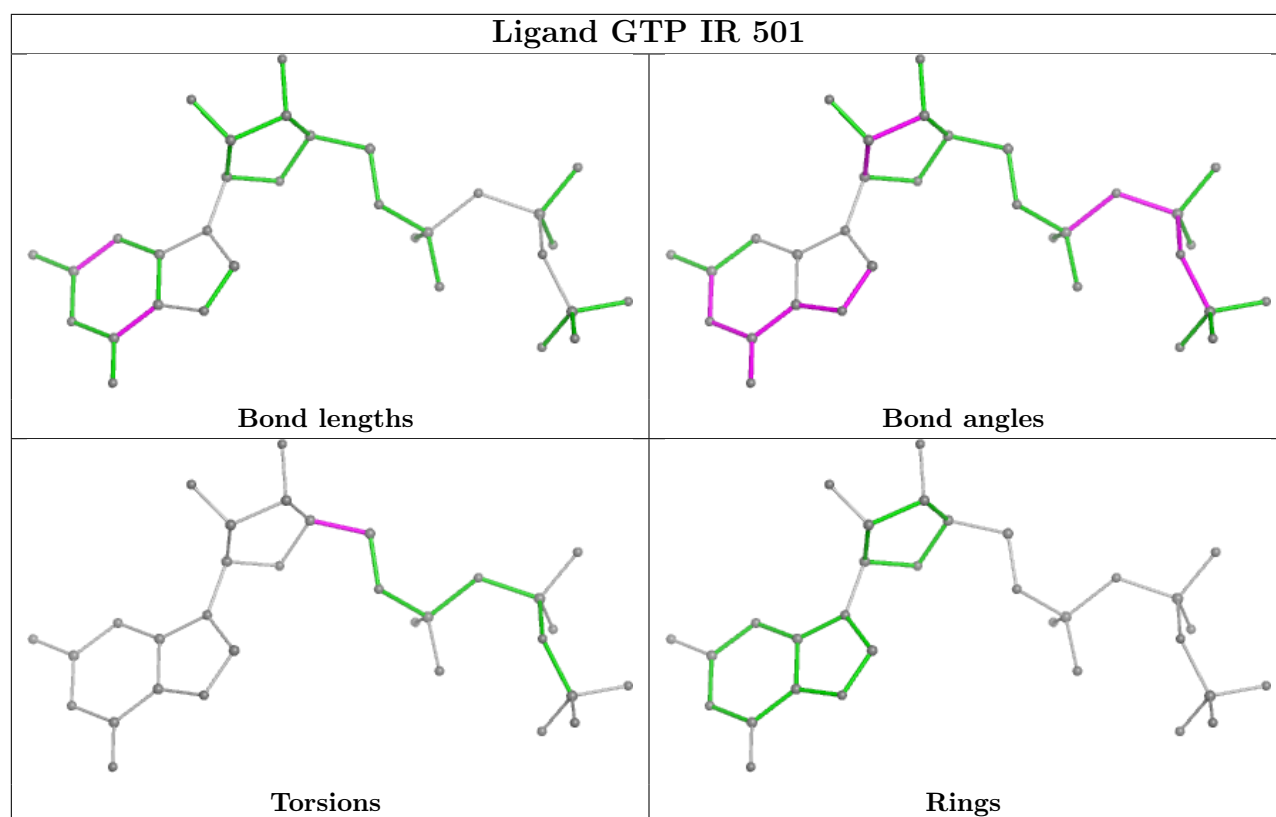


Torsions

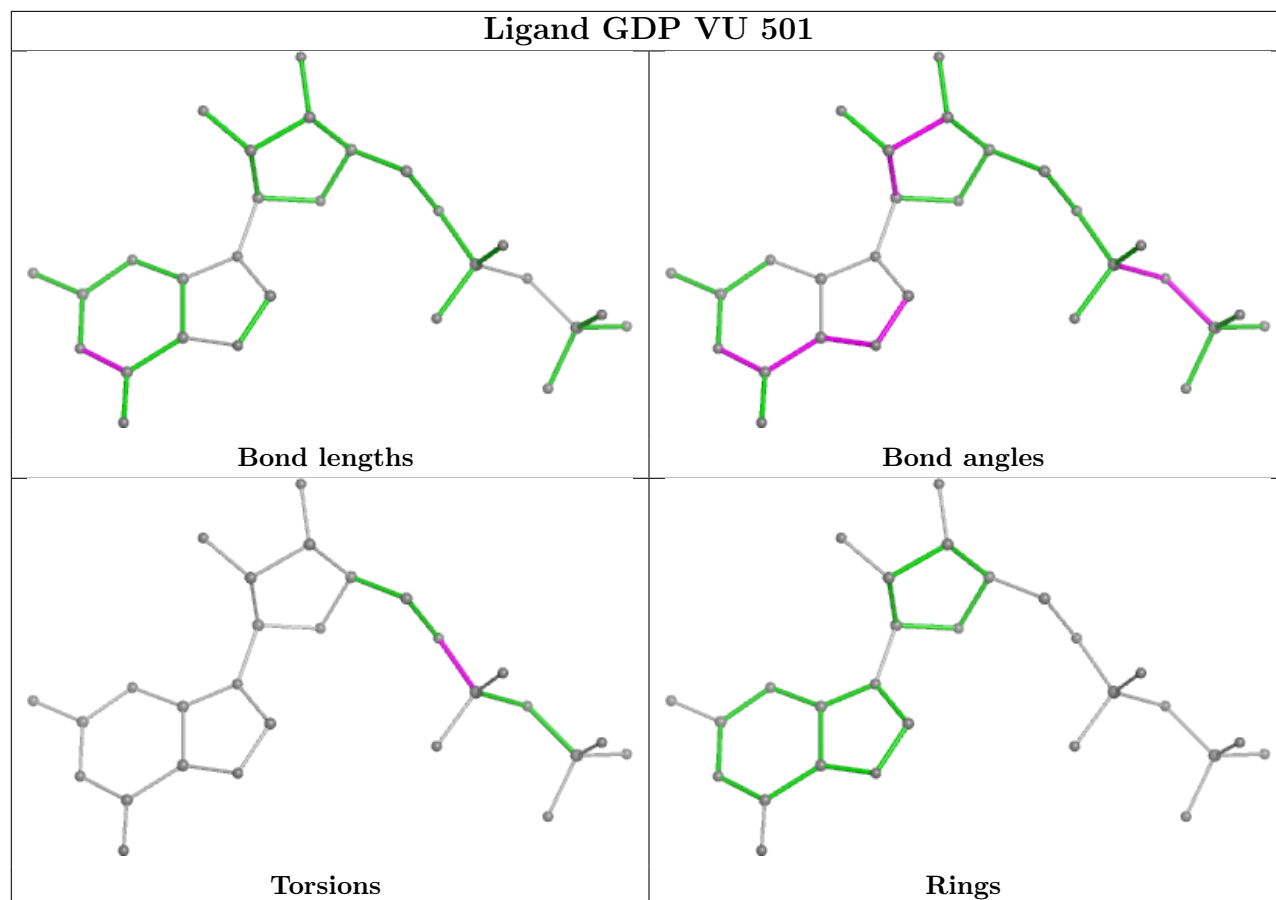


Rings

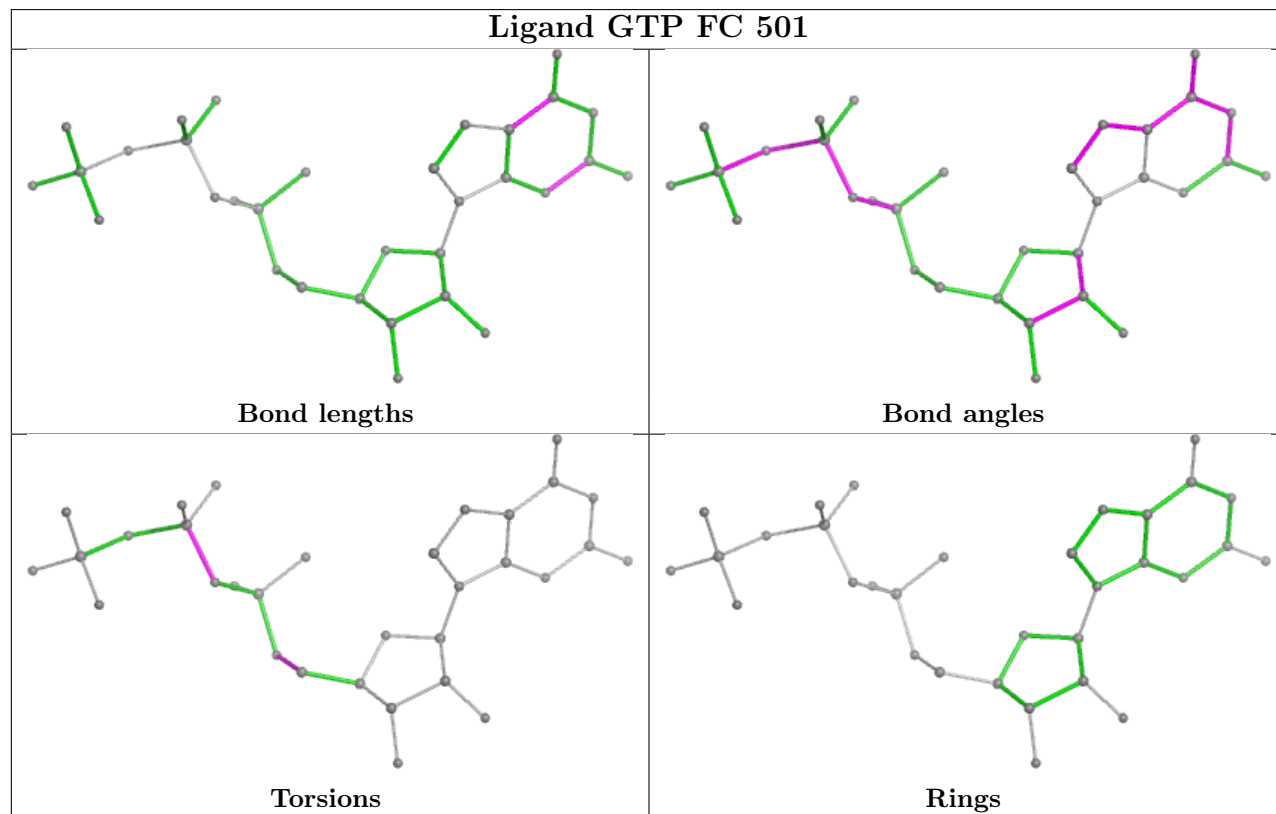


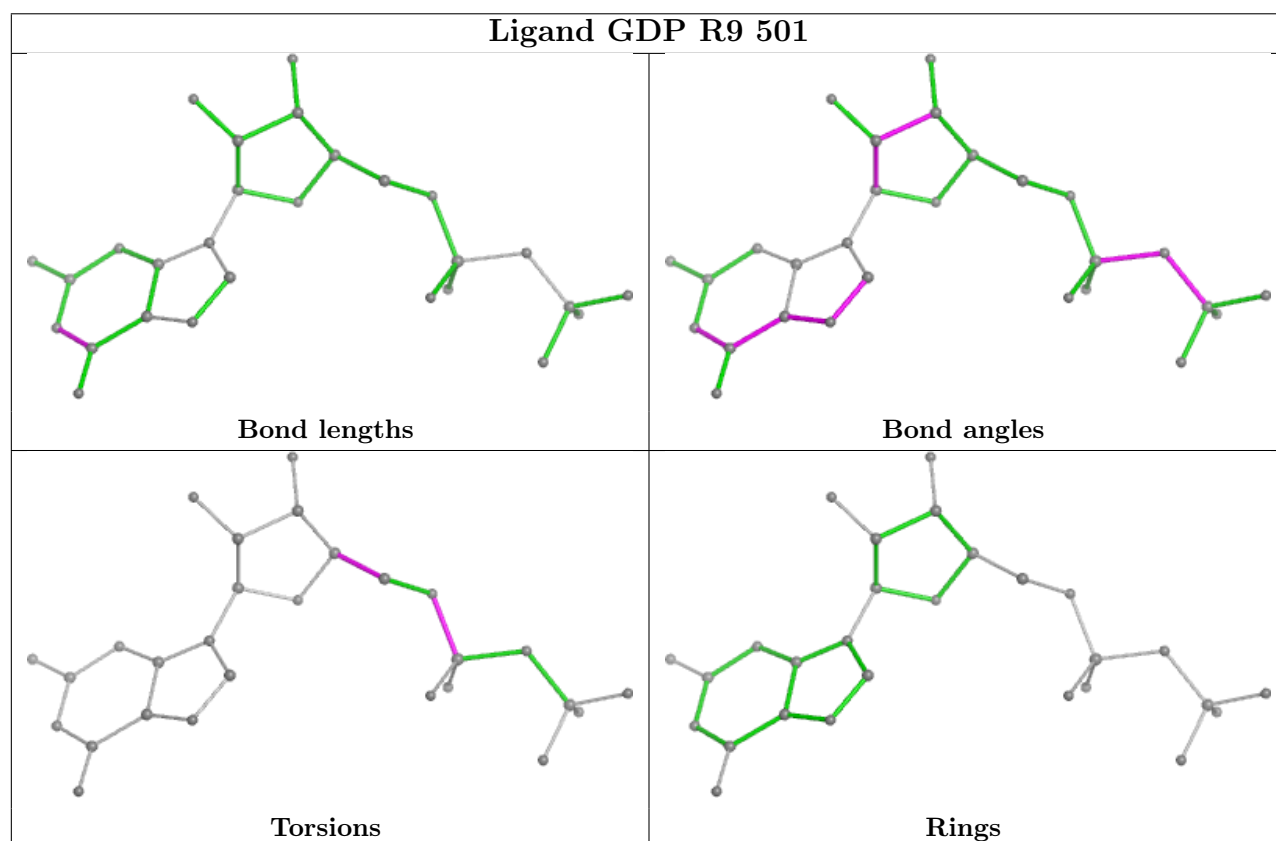
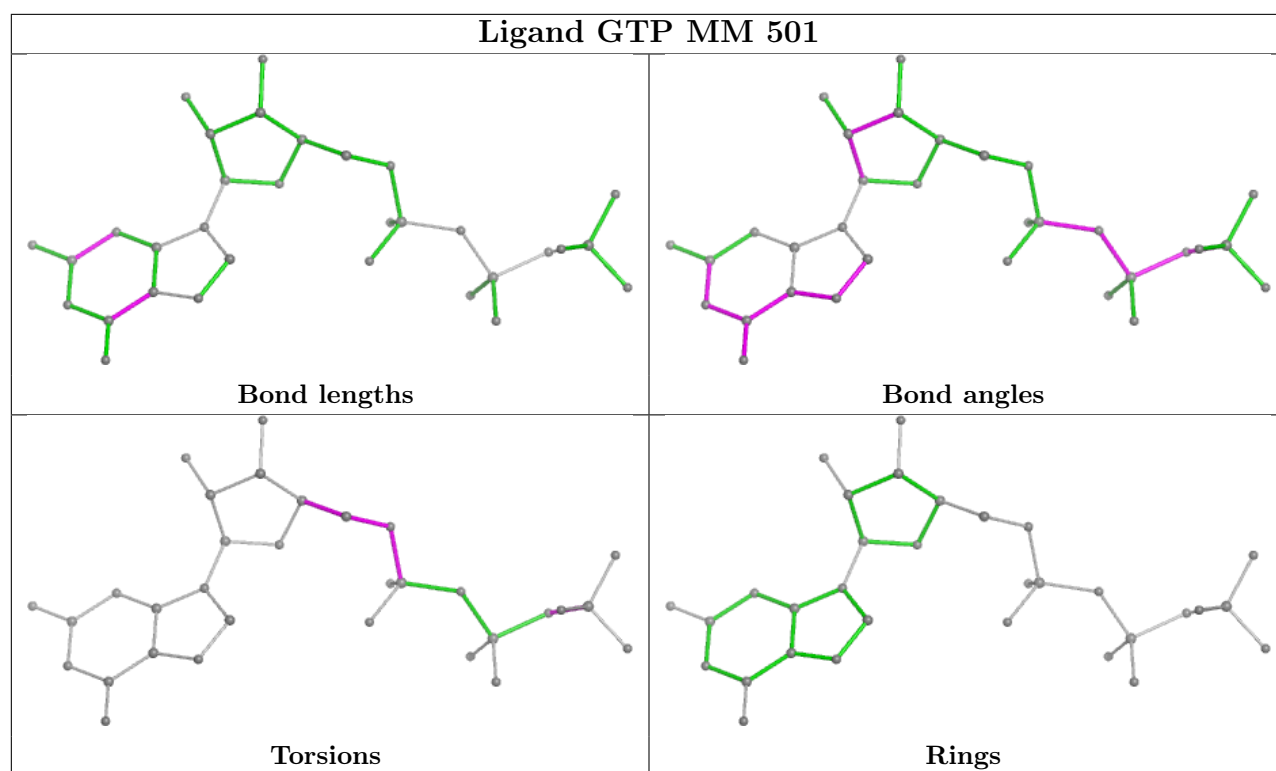


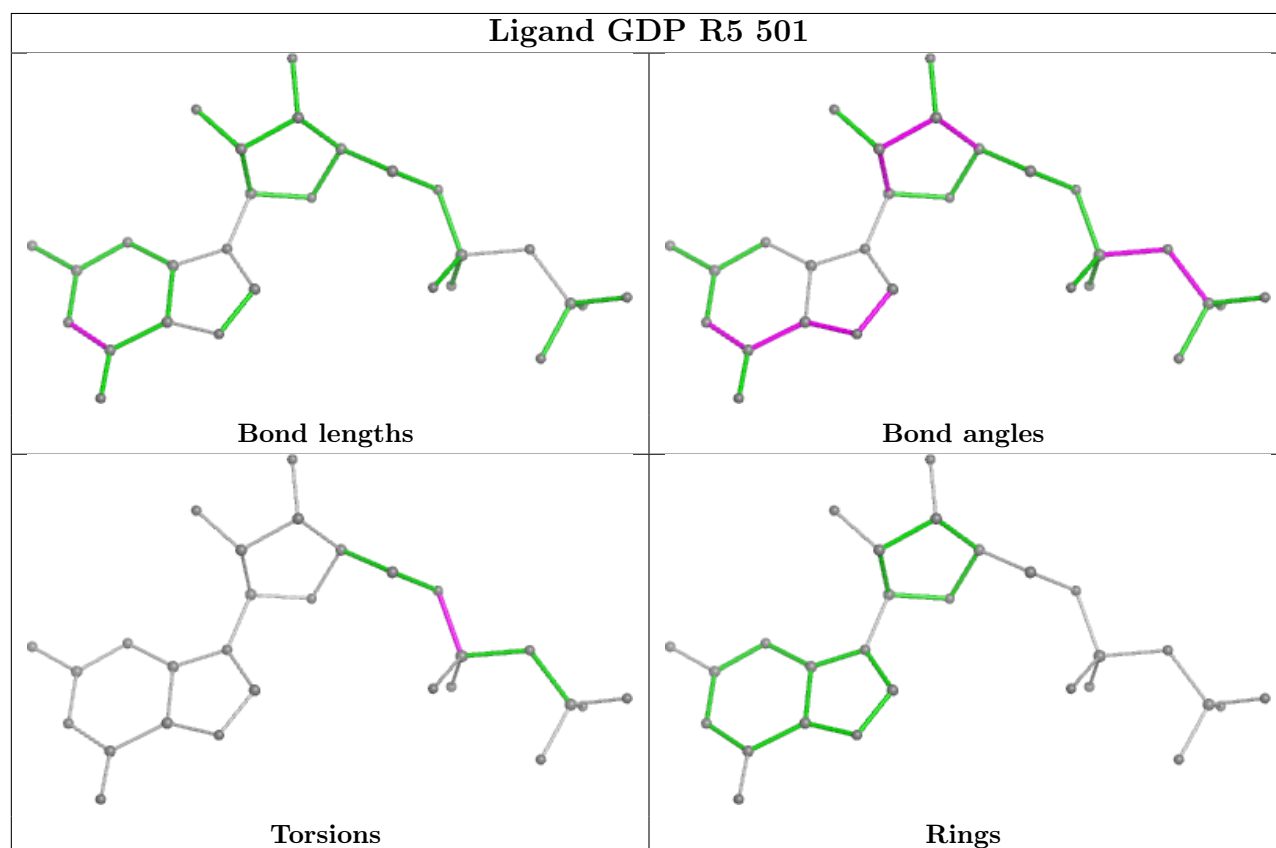
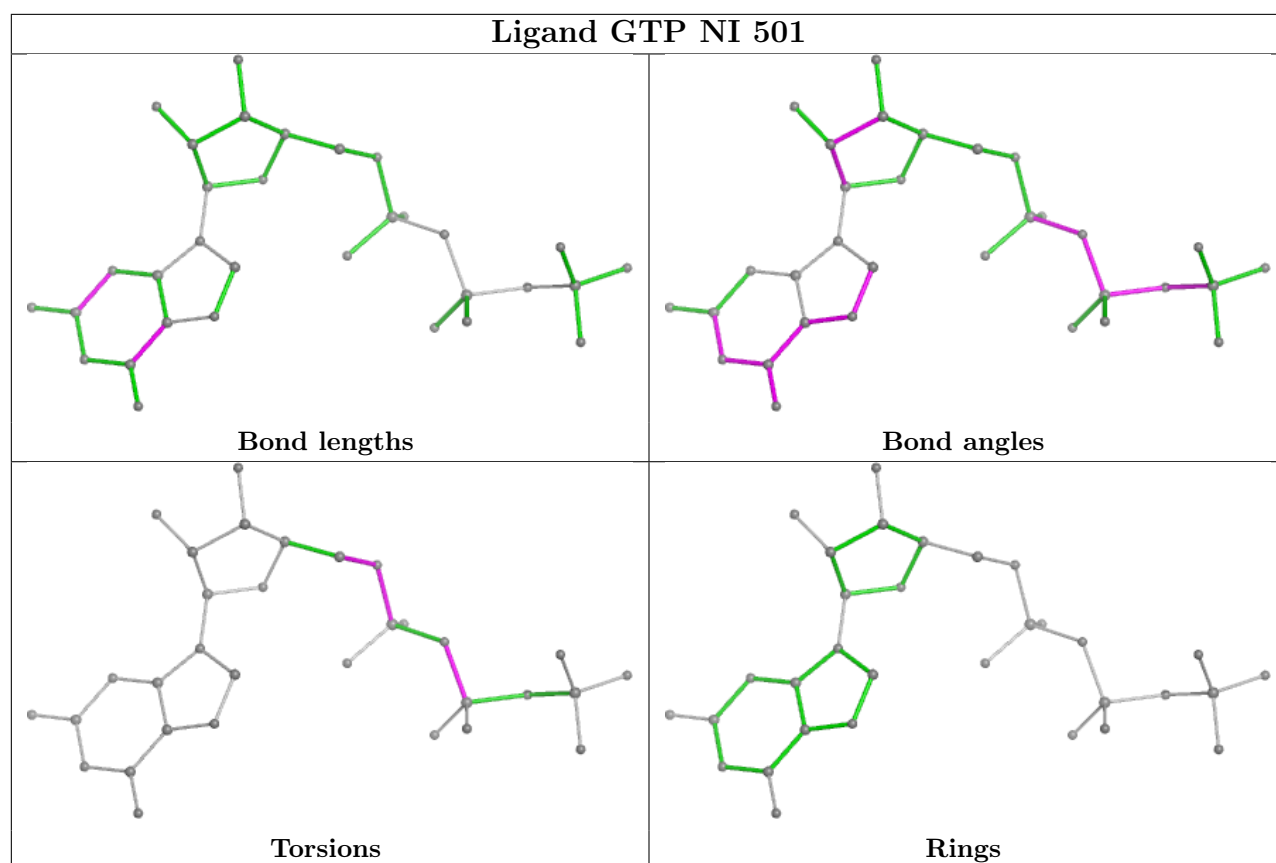
## Ligand GDP VU 501



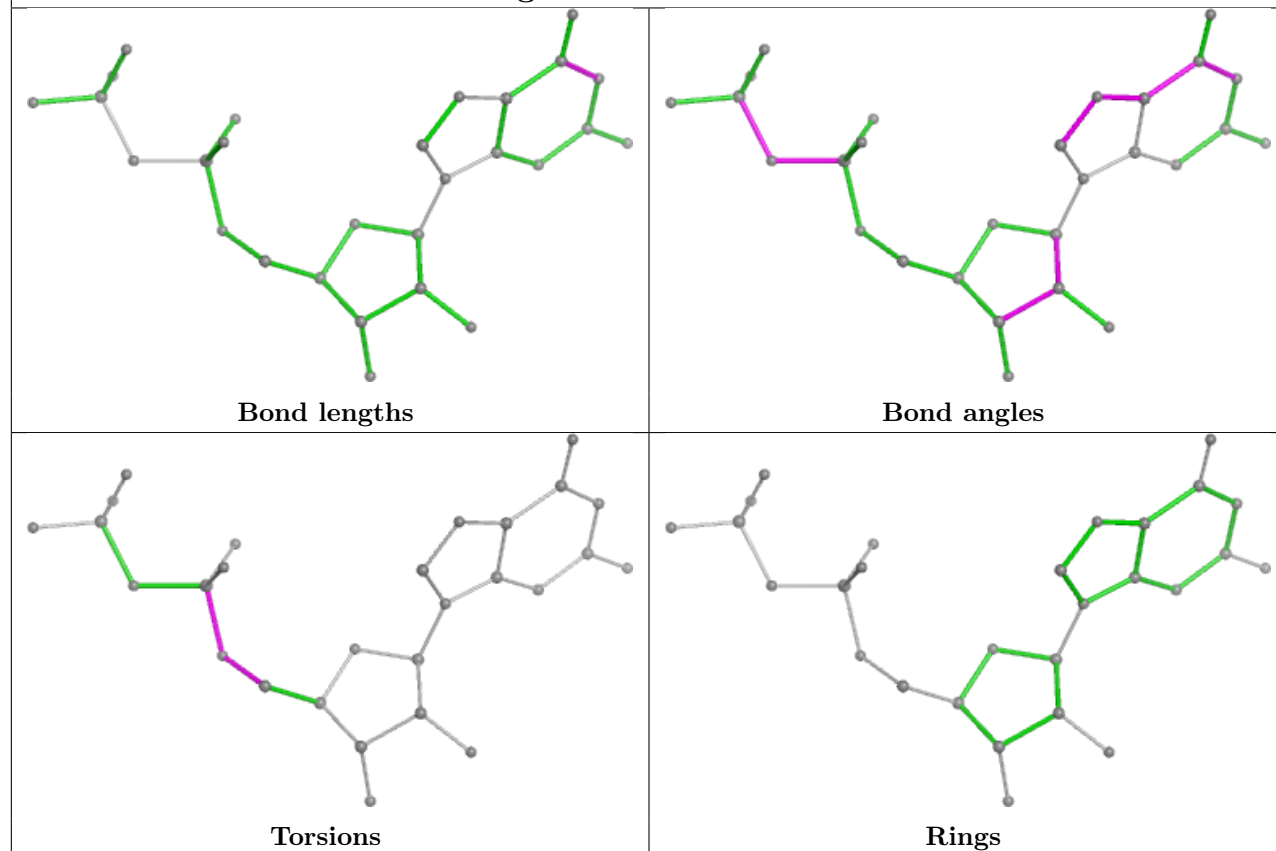
## Ligand GTP FC 501



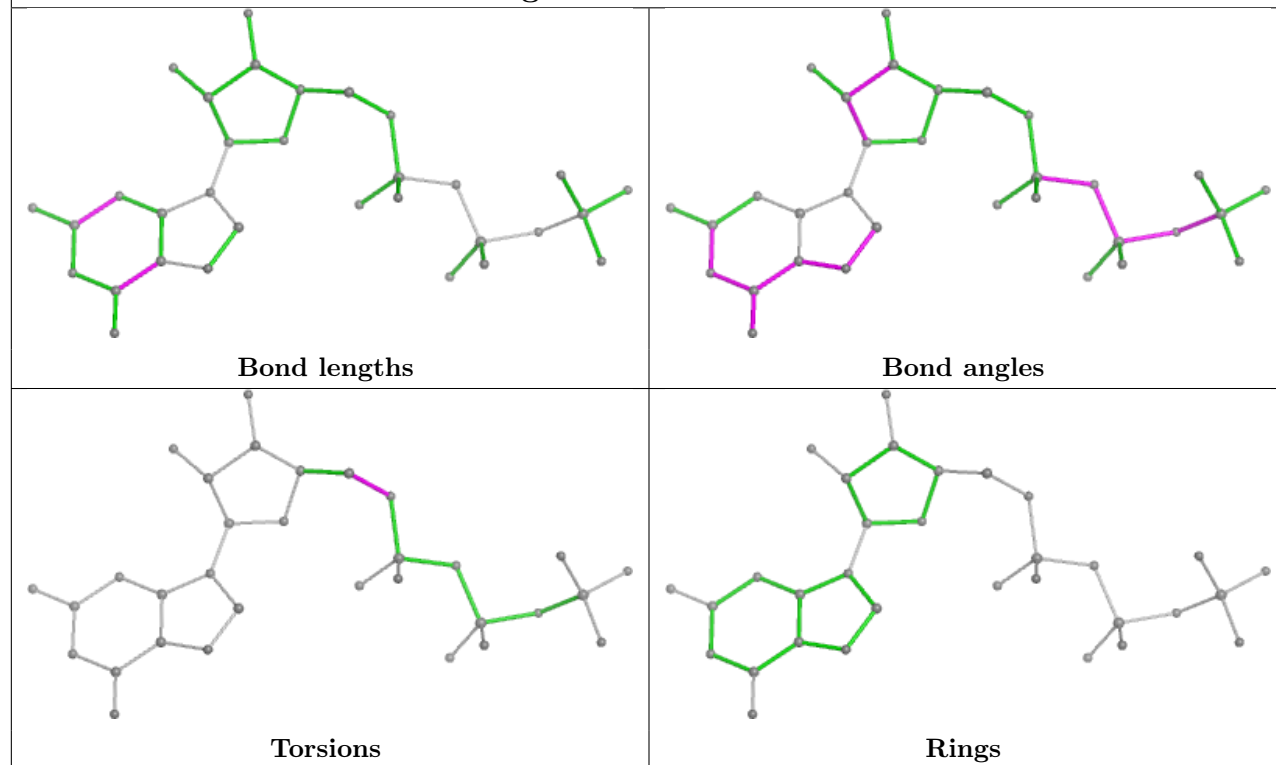




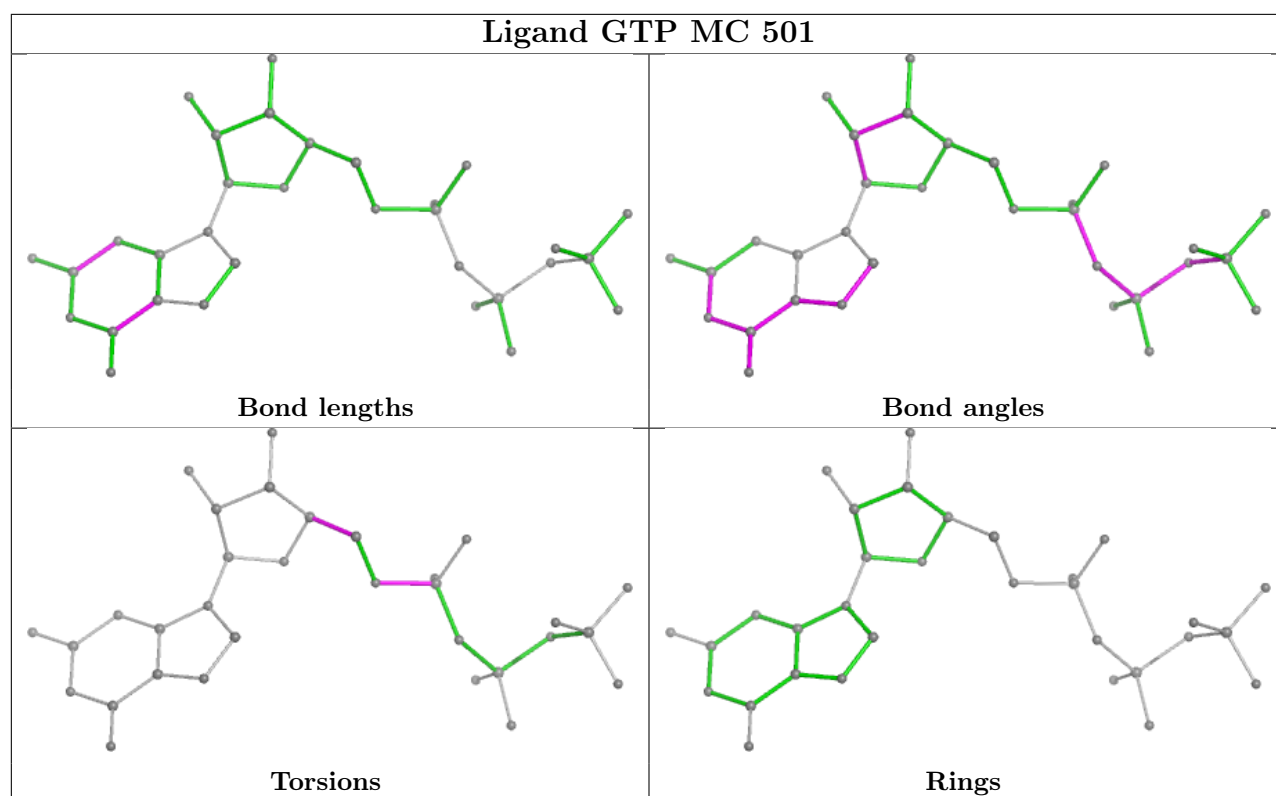
## Ligand GDP FD 501



## Ligand GTP Ue 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
94	H1	4
119	K2	4
40	G2	2
40	D0	2
57	Qw	1
136	Qu	1
135	Qt	1
101	I3	1
101	X4	1
142	X1	1

The worst 5 of 18 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Qw	140:ARG	C	141:ASP	N	5.39
1	Qu	90:ARG	C	91:VAL	N	3.90
1	Hl	3668:THR	C	3669:VAL	N	3.69
1	K2	2535:TYR	C	2536:VAL	N	3.48
1	G2	2552:THR	C	2553:PHE	N	3.47

## 5 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-50664. 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](#)

This section was not generated.

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

This section was not generated.

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

This section was not generated.

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

This section was not generated.

### 5.5 Orthogonal surface views [i](#)

This section was not generated.

### 5.6 Mask visualisation [i](#)

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

## 6 Map analysis ⓘ

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

### 6.1 Map-value distribution ⓘ

This section was not generated.

### 6.2 Volume estimate versus contour level ⓘ

This section was not generated.

### 6.3 Rotationally averaged power spectrum ⓘ

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

## 7 Fourier-Shell correlation ⓘ

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

## 8 Map-model fit

This section was not generated.