



Full wwPDB EM Validation Report ⓘ

Mar 28, 2026 – 04:14 AM UTC

PDB ID : 7SQC / pdb_00007sqc
EMDB ID : EMD-25381
Title : Ciliary C1 central pair apparatus isolated from *Chlamydomonas reinhardtii*
Authors : Gui, M.; Wang, X.; Dutcher, S.K.; Brown, A.; Zhang, R.
Deposited on : 2021-11-05
Resolution : 3.80 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

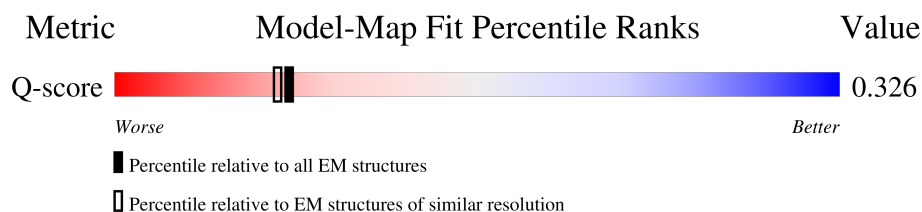
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 Å.

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



Metric	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Q-score	25397	10198 (3.30 - 4.30)

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

2 Entry composition [i](#)

There are 46 unique types of molecules in this entry. The entry contains 1218816 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 Flagellar associated protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	0A	58	Total	C	N	O	0	0
			287	171	58	58		
1	0B	63	Total	C	N	O	0	0
			312	186	63	63		
1	0C	58	Total	C	N	O	0	0
			287	171	58	58		
1	0D	63	Total	C	N	O	0	0
			312	186	63	63		
1	0E	58	Total	C	N	O	0	0
			287	171	58	58		
1	0F	63	Total	C	N	O	0	0
			312	186	63	63		
1	0G	58	Total	C	N	O	0	0
			287	171	58	58		
1	0H	63	Total	C	N	O	0	0
			312	186	63	63		
1	0I	62	Total	C	N	O	0	0
			308	184	62	62		
1	0J	56	Total	C	N	O	0	0
			278	166	56	56		
1	0K	63	Total	C	N	O	0	0
			312	186	63	63		
1	0L	54	Total	C	N	O	0	0
			268	160	54	54		

- Molecule 2 is a protein called FAP42.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1A	1639	Total	C	N	O	S	0	0
			10474	6458	1958	2021	37		
2	1B	1660	Total	C	N	O	S	0	0
			10580	6522	1979	2042	37		
2	1C	1700	Total	C	N	O	S	0	0
			10775	6637	2019	2082	37		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	1D	1686	Total	C	N	O	S	0	0
			10707	6597	2005	2068	37		

- Molecule 3 is a protein called FAP7.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	1F	224	Total	C	N	O	0	0
			1110	662	224	224		
3	1G	162	Total	C	N	O	0	0
			800	476	162	162		
3	1H	181	Total	C	N	O	0	0
			898	536	181	181		
3	1I	99	Total	C	N	O	0	0
			489	291	99	99		
3	1J	338	Total	C	N	O	0	0
			1673	997	338	338		
3	1K	344	Total	C	N	O	0	0
			1704	1016	344	344		
3	1L	338	Total	C	N	O	0	0
			1673	997	338	338		
3	1M	344	Total	C	N	O	0	0
			1704	1016	344	344		
3	1N	338	Total	C	N	O	0	0
			1673	997	338	338		
3	1O	344	Total	C	N	O	0	0
			1704	1016	344	344		
3	1P	338	Total	C	N	O	0	0
			1673	997	338	338		
3	1Q	344	Total	C	N	O	0	0
			1704	1016	344	344		
3	1R	338	Total	C	N	O	0	0
			1673	997	338	338		
3	1S	344	Total	C	N	O	0	0
			1704	1016	344	344		
3	1T	338	Total	C	N	O	0	0
			1673	997	338	338		
3	1U	344	Total	C	N	O	0	0
			1704	1016	344	344		
3	1V	218	Total	C	N	O	0	0
			1078	642	218	218		
3	1W	266	Total	C	N	O	0	0
			1320	788	266	266		

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Mol	Chain	Residues	Atoms				AltConf	Trace
3	1X	229	Total	C	N	O	0	0
			1133	675	229	229		
3	1Y	263	Total	C	N	O	0	0
			1305	779	263	263		

- Molecule 4 is a protein called FAP81.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	2A	744	Total	C	N	O	S	0	0
			4347	2640	859	838	10		
4	2B	754	Total	C	N	O	S	0	0
			4428	2692	874	852	10		

- Molecule 5 is a protein called FAP216.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	2E	231	Total	C	N	O	0	0
			1144	682	231	231		
5	2F	233	Total	C	N	O	0	0
			1154	688	233	233		

- Molecule 6 is a protein called FAP297.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	2H	408	Total	C	N	O	0	0
			2015	1199	408	408		
6	2I	408	Total	C	N	O	0	0
			2015	1199	408	408		

- Molecule 7 is a protein called FAP114.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	2K	248	Total	C	N	O	0	0
			1232	736	248	248		
7	2L	257	Total	C	N	O	0	0
			1277	763	257	257		
7	2M	256	Total	C	N	O	0	0
			1272	760	256	256		
7	2N	262	Total	C	N	O	0	0
			1302	778	262	262		
7	2O	251	Total	C	N	O	0	0
			1247	745	251	251		

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Mol	Chain	Residues	Atoms				AltConf	Trace
7	2P	185	Total	C	N	O	0	0
			917	547	185	185		
7	2Q	40	Total	C	N	O	0	0
			200	120	40	40		

- Molecule 8 is a protein called FAP305.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	3A	175	Total	C	N	O	0	0
			869	519	175	175		
8	3B	175	Total	C	N	O	0	0
			869	519	175	175		
8	3C	175	Total	C	N	O	0	0
			869	519	175	175		
8	3D	167	Total	C	N	O	0	0
			830	496	167	167		

- Molecule 9 is a protein called FAP119.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	3K	256	Total	C	N	O	0	0
			1274	762	256	256		
9	3L	241	Total	C	N	O	0	0
			1199	717	241	241		
9	3M	254	Total	C	N	O	0	0
			1264	756	254	254		
9	3N	244	Total	C	N	O	0	0
			1214	726	244	244		
9	3O	258	Total	C	N	O	0	0
			1284	768	258	258		
9	3P	254	Total	C	N	O	0	0
			1264	756	254	254		

- Molecule 10 is a protein called Calmodulin.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	4A	143	Total	C	N	O	0	0
			704	418	143	143		
10	4B	143	Total	C	N	O	0	0
			704	418	143	143		
10	4C	143	Total	C	N	O	0	0
			704	418	143	143		

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Mol	Chain	Residues	Atoms				AltConf	Trace
10	4D	143	Total 704	C 418	N 143	O 143	0	0
10	4E	143	Total 704	C 418	N 143	O 143	0	0
10	4F	143	Total 704	C 418	N 143	O 143	0	0
10	4G	143	Total 704	C 418	N 143	O 143	0	0
10	4H	143	Total 704	C 418	N 143	O 143	0	0
10	4I	143	Total 704	C 418	N 143	O 143	0	0
10	4J	143	Total 704	C 418	N 143	O 143	0	0
10	4K	143	Total 704	C 418	N 143	O 143	0	0
10	4L	143	Total 704	C 418	N 143	O 143	0	0

- Molecule 11 is a protein called FAP101.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	5A	551	Total 2713	C 1610	N 551	O 552	0	0
11	5B	551	Total 2713	C 1610	N 551	O 552	0	0
11	5C	551	Total 2713	C 1610	N 551	O 552	0	0
11	5D	551	Total 2713	C 1610	N 551	O 552	0	0

- Molecule 12 is a protein called FAP15.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	6A	291	Total 1435	C 853	N 291	O 291	0	0
12	6B	291	Total 1435	C 853	N 291	O 291	0	0
12	6C	253	Total 1250	C 744	N 253	O 253	0	0
12	6D	253	Total 1250	C 744	N 253	O 253	0	0

- Molecule 13 is a protein called FAP227.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	7A	119	Total	C	N	O	0	0
			574	336	119	119		
13	7B	132	Total	C	N	O	0	0
			637	373	132	132		
13	7C	118	Total	C	N	O	0	0
			567	331	118	118		
13	7D	102	Total	C	N	O	0	0
			491	287	102	102		
13	7E	113	Total	C	N	O	0	0
			544	318	113	113		
13	7F	103	Total	C	N	O	0	0
			496	290	103	103		
13	7G	119	Total	C	N	O	0	0
			574	336	119	119		
13	7H	132	Total	C	N	O	0	0
			637	373	132	132		
13	7I	120	Total	C	N	O	0	0
			579	339	120	120		
13	7J	132	Total	C	N	O	0	0
			637	373	132	132		
13	7K	119	Total	C	N	O	0	0
			574	336	119	119		
13	7L	117	Total	C	N	O	0	0
			564	330	117	117		

- Molecule 14 is a protein called FAP105.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	8A	250	Total	C	N	O	S	0	0
			1945	1180	385	374	6		
14	8B	134	Total	C	N	O	S	0	0
			1010	614	195	196	5		
14	8C	270	Total	C	N	O	S	0	0
			2082	1262	411	401	8		
14	8D	134	Total	C	N	O	S	0	0
			1010	614	195	196	5		

- Molecule 15 is a protein called PF6.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	9A	827	Total	C	N	O	0	0
			4075	2421	827	827		

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Mol	Chain	Residues	Atoms				AltConf	Trace
15	9B	827	Total	C	N	O	0	0
			4075	2421	827	827		
15	9C	827	Total	C	N	O	0	0
			4075	2421	827	827		
15	9D	827	Total	C	N	O	0	0
			4075	2421	827	827		
15	9E	681	Total	C	N	O	0	0
			3354	1992	681	681		
15	9F	679	Total	C	N	O	0	0
			3344	1986	679	679		

- Molecule 16 is a protein called FAP219.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	A0	135	Total	C	N	O		0	0
			1004	613	194	197			
16	A1	173	Total	C	N	O	S	0	0
			1295	796	248	250	1		
16	A2	173	Total	C	N	O	S	0	0
			1295	796	248	250	1		
16	A3	173	Total	C	N	O	S	0	0
			1295	796	248	250	1		
16	A4	37	Total	C	N	O	S	0	0
			284	178	53	52	1		

- Molecule 17 is a protein called FAP99.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	B0	242	Total	C	N	O	S	0	0
			1932	1159	396	373	4		
17	B1	468	Total	C	N	O	S	0	0
			3751	2269	761	713	8		
17	B2	243	Total	C	N	O	S	0	0
			1933	1166	395	368	4		

- Molecule 18 is a protein called CPC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	C0	1184	Total	C	N	O	S	0	0
			9027	5645	1643	1704	35		
18	C1	1322	Total	C	N	O	S	0	0
			10128	6312	1863	1912	41		

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Mol	Chain	Residues	Atoms					AltConf	Trace
18	C2	1498	Total	C	N	O	S	0	0
			11519	7179	2117	2177	46		
18	C3	1485	Total	C	N	O	S	0	0
			11424	7121	2099	2158	46		
18	C4	281	Total	C	N	O	S	0	0
			2245	1385	425	425	10		

- Molecule 19 is a protein called PF16.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	D0	465	Total	C	N	O	S	0	0
			3315	2083	581	640	11		
19	D1	465	Total	C	N	O	S	0	0
			3312	2082	581	638	11		
19	D2	468	Total	C	N	O	S	0	0
			3330	2092	584	643	11		
19	D3	468	Total	C	N	O	S	0	0
			3327	2091	584	641	11		
19	D4	465	Total	C	N	O	S	0	0
			3315	2083	581	640	11		
19	D5	468	Total	C	N	O	S	0	0
			3327	2091	584	641	11		
19	D6	468	Total	C	N	O	S	0	0
			3330	2092	584	643	11		
19	D7	468	Total	C	N	O	S	0	0
			3327	2091	584	641	11		
19	G0	464	Total	C	N	O	S	0	0
			3309	2080	580	638	11		
19	G1	466	Total	C	N	O	S	0	0
			3317	2085	582	639	11		
19	G2	467	Total	C	N	O	S	0	0
			3324	2089	583	641	11		
19	G3	466	Total	C	N	O	S	0	0
			3317	2085	582	639	11		
19	G4	467	Total	C	N	O	S	0	0
			3324	2089	583	641	11		
19	G5	466	Total	C	N	O	S	0	0
			3317	2085	582	639	11		
19	H0	463	Total	C	N	O	S	0	0
			3301	2076	579	635	11		
19	H1	445	Total	C	N	O	S	0	0
			3204	2018	558	617	11		

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Mol	Chain	Residues	Atoms					AltConf	Trace
19	H2	456	Total	C	N	O	S	0	0
			3232	2032	565	624	11		
19	H3	461	Total	C	N	O	S	0	0
			3281	2064	574	632	11		
19	H4	466	Total	C	N	O	S	0	0
			3316	2085	582	638	11		
19	H5	462	Total	C	N	O	S	0	0
			3288	2069	575	633	11		
19	H6	454	Total	C	N	O	S	0	0
			3214	2020	563	620	11		
19	H7	455	Total	C	N	O	S	0	0
			3244	2041	567	625	11		
19	I0	459	Total	C	N	O	S	0	0
			3274	2061	572	630	11		
19	I1	466	Total	C	N	O	S	0	0
			3316	2085	582	638	11		
19	J0	453	Total	C	N	O	S	0	0
			3253	2047	569	626	11		
19	J1	466	Total	C	N	O	S	0	0
			3317	2085	582	639	11		
19	J2	464	Total	C	N	O	S	0	0
			3306	2079	580	636	11		
19	J3	461	Total	C	N	O	S	0	0
			3292	2070	577	634	11		
19	K0	467	Total	C	N	O	S	0	0
			3322	2088	583	640	11		
19	K1	467	Total	C	N	O	S	0	0
			3322	2088	583	640	11		
19	K2	467	Total	C	N	O	S	0	0
			3322	2088	583	640	11		
19	K3	461	Total	C	N	O	S	0	0
			3292	2071	577	633	11		
19	L0	468	Total	C	N	O	S	0	0
			3531	2231	606	679	15		
19	L1	465	Total	C	N	O	S	0	0
			3511	2219	602	675	15		
19	L2	465	Total	C	N	O	S	0	0
			3511	2219	602	675	15		
19	L3	468	Total	C	N	O	S	0	0
			3531	2231	606	679	15		

- Molecule 20 is a protein called FAP108.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	E0	236	Total	C	N	O	S	0	0
			1864	1181	330	347	6		
20	E1	243	Total	C	N	O	S	0	0
			1903	1209	331	357	6		
20	E2	234	Total	C	N	O	S	0	0
			1842	1169	322	345	6		
20	E3	244	Total	C	N	O	S	0	0
			1910	1214	332	358	6		

- Molecule 21 is a protein called Hydin.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	F0	308	Total	C	N	O	S	0	0
			1524	908	308	308			
21	F1	482	Total	C	N	O	S	0	0
			2924	1794	554	571	5		
21	F2	482	Total	C	N	O	S	0	0
			2924	1794	554	571	5		
21	F3	482	Total	C	N	O	S	0	0
			2924	1794	554	571	5		

- Molecule 22 is a protein called FAP221.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	M0	231	Total	C	N	O	S	0	0
			1761	1105	308	342	6		
22	M1	564	Total	C	N	O	S	0	0
			4307	2709	769	811	18		

- Molecule 23 is a protein called FAP194.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	N0	495	Total	C	N	O	S	0	0
			2737	1656	525	548	8		
23	N1	507	Total	C	N	O	S	0	0
			2815	1705	538	564	8		
23	N2	495	Total	C	N	O	S	0	0
			2737	1656	525	548	8		
23	N3	509	Total	C	N	O	S	0	0
			2829	1714	540	567	8		

- Molecule 24 is a protein called Tubulin alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	NB	430	Total	C	N	O	S	0	0
			3341	2116	568	635	22		
24	ND	430	Total	C	N	O	S	0	0
			3341	2116	568	635	22		
24	NF	430	Total	C	N	O	S	0	0
			3341	2116	568	635	22		
24	NH	430	Total	C	N	O	S	0	0
			3341	2116	568	635	22		
24	NJ	430	Total	C	N	O	S	0	0
			3341	2116	568	635	22		
24	NL	430	Total	C	N	O	S	0	0
			3341	2116	568	635	22		
24	NN	430	Total	C	N	O	S	0	0
			3341	2116	568	635	22		
24	OD	430	Total	C	N	O	S	0	0
			3341	2116	568	635	22		
24	OF	430	Total	C	N	O	S	0	0
			3341	2116	568	635	22		
24	OH	430	Total	C	N	O	S	0	0
			3341	2116	568	635	22		
24	OJ	430	Total	C	N	O	S	0	0
			3341	2116	568	635	22		
24	OL	430	Total	C	N	O	S	0	0
			3341	2116	568	635	22		
24	ON	430	Total	C	N	O	S	0	0
			3341	2116	568	635	22		
24	OP	430	Total	C	N	O	S	0	0
			3341	2116	568	635	22		
24	PD	429	Total	C	N	O	S	0	0
			3335	2113	567	633	22		
24	PF	430	Total	C	N	O	S	0	0
			3341	2116	568	635	22		
24	PH	430	Total	C	N	O	S	0	0
			3341	2116	568	635	22		
24	PJ	430	Total	C	N	O	S	0	0
			3341	2116	568	635	22		
24	PL	429	Total	C	N	O	S	0	0
			3335	2113	567	633	22		
24	PN	430	Total	C	N	O	S	0	0
			3341	2116	568	635	22		
24	PP	430	Total	C	N	O	S	0	0
			3341	2116	568	635	22		
24	QD	430	Total	C	N	O	S	0	0
			3341	2116	568	635	22		

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Mol	Chain	Residues	Atoms					AltConf	Trace
24	QF	430	Total 3341	C 2116	N 568	O 635	S 22	0	0
24	QH	439	Total 3399	C 2149	N 578	O 650	S 22	0	0
24	QJ	430	Total 3341	C 2116	N 568	O 635	S 22	0	0
24	QL	430	Total 3341	C 2116	N 568	O 635	S 22	0	0
24	QN	429	Total 3335	C 2113	N 567	O 633	S 22	0	0
24	QP	439	Total 3399	C 2149	N 578	O 650	S 22	0	0
24	RD	430	Total 3341	C 2116	N 568	O 635	S 22	0	0
24	RF	430	Total 3341	C 2116	N 568	O 635	S 22	0	0
24	RH	430	Total 3341	C 2116	N 568	O 635	S 22	0	0
24	RJ	430	Total 3341	C 2116	N 568	O 635	S 22	0	0
24	RL	430	Total 3341	C 2116	N 568	O 635	S 22	0	0
24	RN	430	Total 3341	C 2116	N 568	O 635	S 22	0	0
24	RP	430	Total 3341	C 2116	N 568	O 635	S 22	0	0
24	SB	430	Total 3341	C 2116	N 568	O 635	S 22	0	0
24	SD	430	Total 3341	C 2116	N 568	O 635	S 22	0	0
24	SF	430	Total 3341	C 2116	N 568	O 635	S 22	0	0
24	SH	433	Total 3363	C 2127	N 571	O 643	S 22	0	0
24	SJ	430	Total 3341	C 2116	N 568	O 635	S 22	0	0
24	SL	430	Total 3341	C 2116	N 568	O 635	S 22	0	0
24	SN	430	Total 3341	C 2116	N 568	O 635	S 22	0	0
24	SP	433	Total 3363	C 2127	N 571	O 643	S 22	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
24	TB	430	Total 3341	C 2116	N 568	O 635	S 22	0	0
24	TD	430	Total 3341	C 2116	N 568	O 635	S 22	0	0
24	TF	430	Total 3341	C 2116	N 568	O 635	S 22	0	0
24	TH	433	Total 3363	C 2127	N 571	O 643	S 22	0	0
24	TJ	430	Total 3341	C 2116	N 568	O 635	S 22	0	0
24	TL	430	Total 3341	C 2116	N 568	O 635	S 22	0	0
24	TN	430	Total 3341	C 2116	N 568	O 635	S 22	0	0
24	TP	433	Total 3363	C 2127	N 571	O 643	S 22	0	0
24	UB	438	Total 3393	C 2146	N 577	O 648	S 22	0	0
24	UD	432	Total 3355	C 2123	N 570	O 640	S 22	0	0
24	UF	439	Total 3399	C 2149	N 578	O 650	S 22	0	0
24	UH	433	Total 3359	C 2125	N 571	O 641	S 22	0	0
24	UJ	439	Total 3399	C 2149	N 578	O 650	S 22	0	0
24	UL	432	Total 3353	C 2122	N 570	O 639	S 22	0	0
24	UN	439	Total 3399	C 2149	N 578	O 650	S 22	0	0
24	UP	431	Total 3349	C 2120	N 569	O 638	S 22	0	0
24	VB	430	Total 3341	C 2116	N 568	O 635	S 22	0	0
24	VD	430	Total 3341	C 2116	N 568	O 635	S 22	0	0
24	VF	430	Total 3341	C 2116	N 568	O 635	S 22	0	0
24	VH	433	Total 3363	C 2127	N 571	O 643	S 22	0	0
24	VJ	430	Total 3341	C 2116	N 568	O 635	S 22	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
24	VL	430	Total 3341	C 2116	N 568	O 635	S 22	0	0
24	VN	430	Total 3341	C 2116	N 568	O 635	S 22	0	0
24	VP	430	Total 3341	C 2116	N 568	O 635	S 22	0	0
24	WB	439	Total 3399	C 2149	N 578	O 650	S 22	0	0
24	WD	430	Total 3343	C 2117	N 568	O 636	S 22	0	0
24	WF	439	Total 3399	C 2149	N 578	O 650	S 22	0	0
24	WH	434	Total 3367	C 2129	N 572	O 644	S 22	0	0
24	WJ	438	Total 3393	C 2146	N 577	O 648	S 22	0	0
24	WL	431	Total 3349	C 2120	N 569	O 638	S 22	0	0
24	WN	439	Total 3399	C 2149	N 578	O 650	S 22	0	0
24	XB	430	Total 3341	C 2116	N 568	O 635	S 22	0	0
24	XD	430	Total 3341	C 2116	N 568	O 635	S 22	0	0
24	XF	430	Total 3341	C 2116	N 568	O 635	S 22	0	0
24	XH	430	Total 3341	C 2116	N 568	O 635	S 22	0	0
24	XJ	430	Total 3341	C 2116	N 568	O 635	S 22	0	0
24	XL	430	Total 3341	C 2116	N 568	O 635	S 22	0	0
24	XN	430	Total 3341	C 2116	N 568	O 635	S 22	0	0
24	YB	430	Total 3341	C 2116	N 568	O 635	S 22	0	0
24	YD	429	Total 3335	C 2113	N 567	O 633	S 22	0	0
24	YF	430	Total 3341	C 2116	N 568	O 635	S 22	0	0
24	YH	430	Total 3341	C 2116	N 568	O 635	S 22	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
24	YJ	430	Total 3341	C 2116	N 568	O 635	S 22	0	0
24	YL	430	Total 3341	C 2116	N 568	O 635	S 22	0	0
24	YN	430	Total 3341	C 2116	N 568	O 635	S 22	0	0
24	YP	430	Total 3341	C 2116	N 568	O 635	S 22	0	0
24	ZB	429	Total 3333	C 2112	N 567	O 632	S 22	0	0
24	ZD	429	Total 3333	C 2112	N 567	O 632	S 22	0	0
24	ZF	430	Total 3341	C 2116	N 568	O 635	S 22	0	0
24	ZH	430	Total 3341	C 2116	N 568	O 635	S 22	0	0
24	ZJ	430	Total 3341	C 2116	N 568	O 635	S 22	0	0
24	ZL	430	Total 3341	C 2116	N 568	O 635	S 22	0	0
24	ZN	430	Total 3341	C 2116	N 568	O 635	S 22	0	0
24	ZP	430	Total 3341	C 2116	N 568	O 635	S 22	0	0

- Molecule 25 is a protein called Tubulin beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	NC	427	Total 3354	C 2107	N 575	O 642	S 30	0	0
25	NE	427	Total 3354	C 2107	N 575	O 642	S 30	0	0
25	NG	427	Total 3354	C 2107	N 575	O 642	S 30	0	0
25	NI	427	Total 3354	C 2107	N 575	O 642	S 30	0	0
25	NK	427	Total 3354	C 2107	N 575	O 642	S 30	0	0
25	NM	427	Total 3354	C 2107	N 575	O 642	S 30	0	0
25	NO	427	Total 3354	C 2107	N 575	O 642	S 30	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
25	OC	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
25	OE	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
25	OG	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
25	OI	429	Total	C	N	O	S	0	0
			3365	2113	577	645	30		
25	OK	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
25	OM	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
25	OO	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
25	OQ	429	Total	C	N	O	S	0	0
			3365	2113	577	645	30		
25	PC	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
25	PE	429	Total	C	N	O	S	0	0
			3365	2113	577	645	30		
25	PG	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
25	PI	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
25	PK	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
25	PM	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
25	PO	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
25	PQ	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
25	QC	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
25	QE	429	Total	C	N	O	S	0	0
			3365	2113	577	645	30		
25	QG	428	Total	C	N	O	S	0	0
			3359	2110	576	643	30		
25	QI	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
25	QK	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		

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Mol	Chain	Residues	Atoms					AltConf	Trace
25	QM	429	Total	C	N	O	S	0	0
			3365	2113	577	645	30		
25	QO	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
25	QQ	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
25	RC	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
25	RE	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
25	RG	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
25	RI	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
25	RK	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
25	RM	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
25	RO	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
25	SC	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
25	SE	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
25	SG	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
25	SI	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
25	SK	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
25	SM	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
25	SO	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
25	TC	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
25	TE	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
25	TG	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
25	TI	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		

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Mol	Chain	Residues	Atoms					AltConf	Trace
25	TK	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
25	TM	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
25	TO	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
25	UC	432	Total	C	N	O	S	0	0
			3388	2126	580	652	30		
25	UE	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
25	UG	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
25	UI	431	Total	C	N	O	S	0	0
			3379	2121	579	649	30		
25	UK	432	Total	C	N	O	S	0	0
			3388	2126	580	652	30		
25	UM	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
25	UO	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
25	VC	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
25	VE	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
25	VG	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
25	VI	431	Total	C	N	O	S	0	0
			3379	2121	579	649	30		
25	VK	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
25	VM	428	Total	C	N	O	S	0	0
			3359	2110	576	643	30		
25	VO	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
25	WA	430	Total	C	N	O	S	0	0
			3370	2116	578	646	30		
25	WC	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
25	WE	430	Total	C	N	O	S	0	0
			3370	2116	578	646	30		
25	WG	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		

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Mol	Chain	Residues	Atoms					AltConf	Trace
25	WI	430	Total	C	N	O	S	0	0
			3370	2116	578	646	30		
25	WK	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
25	WM	430	Total	C	N	O	S	0	0
			3370	2116	578	646	30		
25	WO	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
25	XA	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
25	XC	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
25	XE	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
25	XG	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
25	XI	428	Total	C	N	O	S	0	0
			3359	2110	576	643	30		
25	XK	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
25	XM	428	Total	C	N	O	S	0	0
			3359	2110	576	643	30		
25	XO	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
25	YC	428	Total	C	N	O	S	0	0
			3359	2110	576	643	30		
25	YE	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
25	YG	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
25	YI	430	Total	C	N	O	S	0	0
			3370	2116	578	646	30		
25	YK	428	Total	C	N	O	S	0	0
			3359	2110	576	643	30		
25	YM	428	Total	C	N	O	S	0	0
			3359	2110	576	643	30		
25	YO	428	Total	C	N	O	S	0	0
			3359	2110	576	643	30		
25	ZC	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
25	ZE	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		

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Mol	Chain	Residues	Atoms					AltConf	Trace
25	ZG	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
25	ZI	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
25	ZK	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
25	ZM	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
25	ZO	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		

- Molecule 26 is a protein called FAP74.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	O0	1140	Total	C	N	O	S	0	0
			6206	3699	1262	1239	6		
26	O1	673	Total	C	N	O	S	0	0
			4290	2588	851	843	8		
26	O2	130	Total	C	N	O	S	0	0
			1002	615	185	200	2		

- Molecule 27 is a protein called FAP69.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	P0	355	Total	C	N	O	0	0
			1751	1041	355	355		
27	P1	722	Total	C	N	O	0	0
			3561	2117	722	722		
27	P2	732	Total	C	N	O	0	0
			3610	2146	732	732		
27	P3	732	Total	C	N	O	0	0
			3610	2146	732	732		

- Molecule 28 is a protein called FAP54.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Q0	2393	Total	C	N	O	S	0	0
			17935	11345	3284	3228	78		
28	Q1	2395	Total	C	N	O	S	0	0
			17945	11351	3286	3230	78		

- Molecule 29 is a protein called FAP46.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	R0	2070	Total	C	N	O	S	0	0
			10914	6558	2179	2171	6		
29	R1	2080	Total	C	N	O	S	0	0
			10963	6587	2189	2181	6		

- Molecule 30 is a protein called FAP275.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	S0	156	Total	C	N	O	S	0	0
			1191	736	229	222	4		
30	S1	156	Total	C	N	O	S	0	0
			1191	736	229	222	4		
30	S2	156	Total	C	N	O	S	0	0
			1191	736	229	222	4		
30	S3	153	Total	C	N	O	S	0	0
			1166	719	225	218	4		

- Molecule 31 is a protein called Unknown protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	S5	38	Total	C	N	O	0	0
			190	114	38	38		

- Molecule 32 is a protein called FAP47.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	T0	542	Total	C	N	O	S	0	0
			3339	2041	634	653	11		
32	T1	562	Total	C	N	O	S	0	0
			3434	2096	654	673	11		
32	T2	545	Total	C	N	O	S	0	0
			3355	2051	637	656	11		
32	T3	313	Total	C	N	O		0	0
			1541	915	313	313			

- Molecule 33 is a protein called FAP279.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	U0	201	Total	C	N	O	S	0	0
			1643	1048	289	300	6		
33	U1	201	Total	C	N	O	S	0	0
			1643	1048	289	300	6		

- Molecule 34 is a protein called FAP266.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	V0	198	Total	C	N	O	0	0
			956	560	198	198		
34	V1	191	Total	C	N	O	0	0
			921	539	191	191		

- Molecule 35 is a protein called FAP76.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	W0	1056	Total	C	N	O	0	0
			5224	3112	1056	1056		
35	W1	962	Total	C	N	O	0	0
			4758	2834	962	962		

- Molecule 36 is a protein called Unknown protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	W3	68	Total	C	N	O	0	0
			340	204	68	68		
36	W4	68	Total	C	N	O	0	0
			340	204	68	68		
36	W5	68	Total	C	N	O	0	0
			340	204	68	68		
36	W6	68	Total	C	N	O	0	0
			340	204	68	68		

- Molecule 37 is a protein called Unknown protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
37	W7	149	Total	C	N	O	0	0
			745	447	149	149		
37	W9	149	Total	C	N	O	0	0
			745	447	149	149		

- Molecule 38 is a protein called Unknown protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
38	W8	51	Total	C	N	O	0	0
			255	153	51	51		

- Molecule 39 is a protein called FAP246.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	X0	813	Total	C	N	O	S	0	0
			5308	3304	1010	981	13		
39	X1	813	Total	C	N	O	S	0	0
			5308	3304	1010	981	13		
39	X2	813	Total	C	N	O	S	0	0
			5308	3304	1010	981	13		
39	X3	813	Total	C	N	O	S	0	0
			5308	3304	1010	981	13		

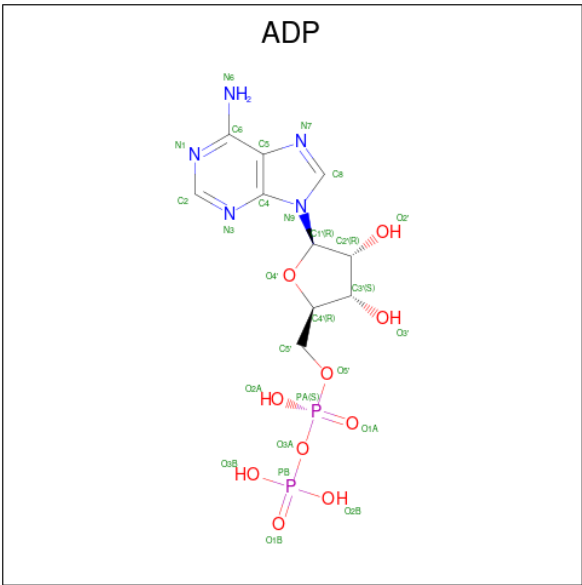
- Molecule 40 is a protein called Phosphopyruvate hydratase.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	Y0	476	Total	C	N	O	S	0	0
			3607	2262	615	708	22		
40	Y1	476	Total	C	N	O	S	0	0
			3607	2262	615	708	22		
40	Y2	476	Total	C	N	O	S	0	0
			3607	2262	615	708	22		
40	Y3	476	Total	C	N	O	S	0	0
			3607	2262	615	708	22		
40	Y4	476	Total	C	N	O	S	0	0
			3607	2262	615	708	22		
40	Y5	476	Total	C	N	O	S	0	0
			3607	2262	615	708	22		
40	Y6	476	Total	C	N	O	S	0	0
			3607	2262	615	708	22		
40	Y7	476	Total	C	N	O	S	0	0
			3607	2262	615	708	22		

- Molecule 41 is a protein called Heat shock protein 70A.

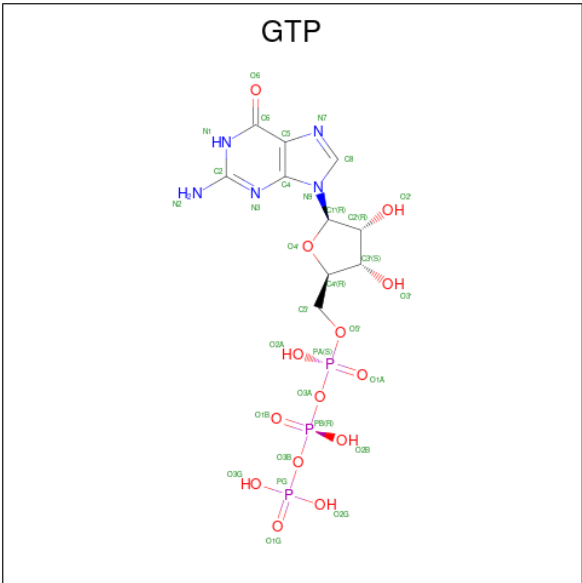
Mol	Chain	Residues	Atoms					AltConf	Trace
41	Z0	592	Total	C	N	O	S	0	0
			4599	2881	798	900	20		
41	Z1	592	Total	C	N	O	S	0	0
			4599	2881	798	900	20		
41	Z2	592	Total	C	N	O	S	0	0
			4599	2881	798	900	20		
41	Z3	592	Total	C	N	O	S	0	0
			4599	2881	798	900	20		

- Molecule 42 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



Mol	Chain	Residues	Atoms					AltConf
43	1A	1	Total	C	N	O	P	0
			31	10	6	12	3	
43	1B	1	Total	C	N	O	P	0
			31	10	6	12	3	
43	1C	1	Total	C	N	O	P	0
			31	10	6	12	3	
43	1D	1	Total	C	N	O	P	0
			31	10	6	12	3	
43	C0	1	Total	C	N	O	P	0
			31	10	6	12	3	
43	C1	1	Total	C	N	O	P	0
			31	10	6	12	3	
43	C2	1	Total	C	N	O	P	0
			31	10	6	12	3	
43	C3	1	Total	C	N	O	P	0
			31	10	6	12	3	

- Molecule 44 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



Mol	Chain	Residues	Atoms					AltConf
44	NB	1	Total	C	N	O	P	0
			32	10	5	14	3	
44	ND	1	Total	C	N	O	P	0
			32	10	5	14	3	
44	NF	1	Total	C	N	O	P	0
			32	10	5	14	3	
44	NH	1	Total	C	N	O	P	0
			32	10	5	14	3	

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
44	NJ	1	32	10	5	14	3	0
44	NL	1	32	10	5	14	3	0
44	NN	1	32	10	5	14	3	0
44	OD	1	32	10	5	14	3	0
44	OF	1	32	10	5	14	3	0
44	OH	1	32	10	5	14	3	0
44	OJ	1	32	10	5	14	3	0
44	OL	1	32	10	5	14	3	0
44	ON	1	32	10	5	14	3	0
44	OP	1	32	10	5	14	3	0
44	PD	1	32	10	5	14	3	0
44	PF	1	32	10	5	14	3	0
44	PH	1	32	10	5	14	3	0
44	PJ	1	32	10	5	14	3	0
44	PL	1	32	10	5	14	3	0
44	PN	1	32	10	5	14	3	0
44	PP	1	32	10	5	14	3	0
44	QD	1	32	10	5	14	3	0
44	QF	1	32	10	5	14	3	0
44	QH	1	32	10	5	14	3	0
44	QJ	1	32	10	5	14	3	0

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Mol	Chain	Residues	Atoms					AltConf
44	QL	1	Total 32	C 10	N 5	O 14	P 3	0
44	QN	1	Total 32	C 10	N 5	O 14	P 3	0
44	QP	1	Total 32	C 10	N 5	O 14	P 3	0
44	RD	1	Total 32	C 10	N 5	O 14	P 3	0
44	RF	1	Total 32	C 10	N 5	O 14	P 3	0
44	RH	1	Total 32	C 10	N 5	O 14	P 3	0
44	RJ	1	Total 32	C 10	N 5	O 14	P 3	0
44	RL	1	Total 32	C 10	N 5	O 14	P 3	0
44	RN	1	Total 32	C 10	N 5	O 14	P 3	0
44	RP	1	Total 32	C 10	N 5	O 14	P 3	0
44	SB	1	Total 32	C 10	N 5	O 14	P 3	0
44	SD	1	Total 32	C 10	N 5	O 14	P 3	0
44	SF	1	Total 32	C 10	N 5	O 14	P 3	0
44	SH	1	Total 32	C 10	N 5	O 14	P 3	0
44	SJ	1	Total 32	C 10	N 5	O 14	P 3	0
44	SL	1	Total 32	C 10	N 5	O 14	P 3	0
44	SN	1	Total 32	C 10	N 5	O 14	P 3	0
44	SP	1	Total 32	C 10	N 5	O 14	P 3	0
44	TB	1	Total 32	C 10	N 5	O 14	P 3	0
44	TD	1	Total 32	C 10	N 5	O 14	P 3	0
44	TF	1	Total 32	C 10	N 5	O 14	P 3	0

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Mol	Chain	Residues	Atoms					AltConf
44	TH	1	Total 32	C 10	N 5	O 14	P 3	0
44	TJ	1	Total 32	C 10	N 5	O 14	P 3	0
44	TL	1	Total 32	C 10	N 5	O 14	P 3	0
44	TN	1	Total 32	C 10	N 5	O 14	P 3	0
44	TP	1	Total 32	C 10	N 5	O 14	P 3	0
44	UB	1	Total 32	C 10	N 5	O 14	P 3	0
44	UD	1	Total 32	C 10	N 5	O 14	P 3	0
44	UF	1	Total 32	C 10	N 5	O 14	P 3	0
44	UH	1	Total 32	C 10	N 5	O 14	P 3	0
44	UJ	1	Total 32	C 10	N 5	O 14	P 3	0
44	UL	1	Total 32	C 10	N 5	O 14	P 3	0
44	UN	1	Total 32	C 10	N 5	O 14	P 3	0
44	UP	1	Total 32	C 10	N 5	O 14	P 3	0
44	VB	1	Total 32	C 10	N 5	O 14	P 3	0
44	VD	1	Total 32	C 10	N 5	O 14	P 3	0
44	VF	1	Total 32	C 10	N 5	O 14	P 3	0
44	VH	1	Total 32	C 10	N 5	O 14	P 3	0
44	VJ	1	Total 32	C 10	N 5	O 14	P 3	0
44	VL	1	Total 32	C 10	N 5	O 14	P 3	0
44	VN	1	Total 32	C 10	N 5	O 14	P 3	0
44	VP	1	Total 32	C 10	N 5	O 14	P 3	0

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Mol	Chain	Residues	Atoms					AltConf
44	WB	1	Total 32	C 10	N 5	O 14	P 3	0
44	WD	1	Total 32	C 10	N 5	O 14	P 3	0
44	WF	1	Total 32	C 10	N 5	O 14	P 3	0
44	WH	1	Total 32	C 10	N 5	O 14	P 3	0
44	WJ	1	Total 32	C 10	N 5	O 14	P 3	0
44	WL	1	Total 32	C 10	N 5	O 14	P 3	0
44	WN	1	Total 32	C 10	N 5	O 14	P 3	0
44	XB	1	Total 32	C 10	N 5	O 14	P 3	0
44	XD	1	Total 32	C 10	N 5	O 14	P 3	0
44	XF	1	Total 32	C 10	N 5	O 14	P 3	0
44	XH	1	Total 32	C 10	N 5	O 14	P 3	0
44	XJ	1	Total 32	C 10	N 5	O 14	P 3	0
44	XL	1	Total 32	C 10	N 5	O 14	P 3	0
44	XN	1	Total 32	C 10	N 5	O 14	P 3	0
44	YB	1	Total 32	C 10	N 5	O 14	P 3	0
44	YD	1	Total 32	C 10	N 5	O 14	P 3	0
44	YF	1	Total 32	C 10	N 5	O 14	P 3	0
44	YH	1	Total 32	C 10	N 5	O 14	P 3	0
44	YJ	1	Total 32	C 10	N 5	O 14	P 3	0
44	YL	1	Total 32	C 10	N 5	O 14	P 3	0
44	YN	1	Total 32	C 10	N 5	O 14	P 3	0

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Mol	Chain	Residues	Atoms					AltConf
44	YP	1	Total	C	N	O	P	0
			32	10	5	14	3	
44	ZB	1	Total	C	N	O	P	0
			32	10	5	14	3	
44	ZD	1	Total	C	N	O	P	0
			32	10	5	14	3	
44	ZF	1	Total	C	N	O	P	0
			32	10	5	14	3	
44	ZH	1	Total	C	N	O	P	0
			32	10	5	14	3	
44	ZJ	1	Total	C	N	O	P	0
			32	10	5	14	3	
44	ZL	1	Total	C	N	O	P	0
			32	10	5	14	3	
44	ZN	1	Total	C	N	O	P	0
			32	10	5	14	3	
44	ZP	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 45 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
45	NB	1	Total	Mg	0
			1	1	
45	ND	1	Total	Mg	0
			1	1	
45	NG	1	Total	Mg	0
			1	1	
45	NH	1	Total	Mg	0
			1	1	
45	NJ	1	Total	Mg	0
			1	1	
45	NL	1	Total	Mg	0
			1	1	
45	NN	1	Total	Mg	0
			1	1	
45	OD	1	Total	Mg	0
			1	1	
45	OF	1	Total	Mg	0
			1	1	
45	OH	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
45	OJ	1	Total 1	Mg 1	0
45	OL	1	Total 1	Mg 1	0
45	ON	1	Total 1	Mg 1	0
45	OP	1	Total 1	Mg 1	0
45	PD	1	Total 1	Mg 1	0
45	PF	1	Total 1	Mg 1	0
45	PI	1	Total 1	Mg 1	0
45	PJ	1	Total 1	Mg 1	0
45	PL	1	Total 1	Mg 1	0
45	PN	1	Total 1	Mg 1	0
45	PP	1	Total 1	Mg 1	0
45	QD	1	Total 1	Mg 1	0
45	QF	1	Total 1	Mg 1	0
45	QH	1	Total 1	Mg 1	0
45	QJ	1	Total 1	Mg 1	0
45	QL	1	Total 1	Mg 1	0
45	QN	1	Total 1	Mg 1	0
45	QP	1	Total 1	Mg 1	0
45	RD	1	Total 1	Mg 1	0
45	RF	1	Total 1	Mg 1	0
45	RI	1	Total 1	Mg 1	0

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Mol	Chain	Residues	Atoms		AltConf
45	RJ	1	Total 1	Mg 1	0
45	RL	1	Total 1	Mg 1	0
45	RN	1	Total 1	Mg 1	0
45	RP	1	Total 1	Mg 1	0
45	SC	1	Total 1	Mg 1	0
45	SD	1	Total 1	Mg 1	0
45	SG	1	Total 1	Mg 1	0
45	SH	1	Total 1	Mg 1	0
45	SJ	1	Total 1	Mg 1	0
45	SL	1	Total 1	Mg 1	0
45	SO	1	Total 1	Mg 1	0
45	SP	1	Total 1	Mg 1	0
45	TB	1	Total 1	Mg 1	0
45	TD	1	Total 1	Mg 1	0
45	TG	1	Total 1	Mg 1	0
45	TH	1	Total 1	Mg 1	0
45	TJ	1	Total 1	Mg 1	0
45	TM	1	Total 1	Mg 1	0
45	TN	1	Total 1	Mg 1	0
45	TP	1	Total 1	Mg 1	0
45	UB	1	Total 1	Mg 1	0

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Mol	Chain	Residues	Atoms		AltConf
45	UD	1	Total 1	Mg 1	0
45	UF	1	Total 1	Mg 1	0
45	UH	1	Total 1	Mg 1	0
45	UJ	1	Total 1	Mg 1	0
45	UL	1	Total 1	Mg 1	0
45	UN	1	Total 1	Mg 1	0
45	UP	1	Total 1	Mg 1	0
45	VB	1	Total 1	Mg 1	0
45	VD	1	Total 1	Mg 1	0
45	VF	1	Total 1	Mg 1	0
45	VH	1	Total 1	Mg 1	0
45	VJ	1	Total 1	Mg 1	0
45	VL	1	Total 1	Mg 1	0
45	VN	1	Total 1	Mg 1	0
45	VP	1	Total 1	Mg 1	0
45	WB	1	Total 1	Mg 1	0
45	WD	1	Total 1	Mg 1	0
45	WG	1	Total 1	Mg 1	0
45	WH	1	Total 1	Mg 1	0
45	WJ	1	Total 1	Mg 1	0
45	WL	1	Total 1	Mg 1	0

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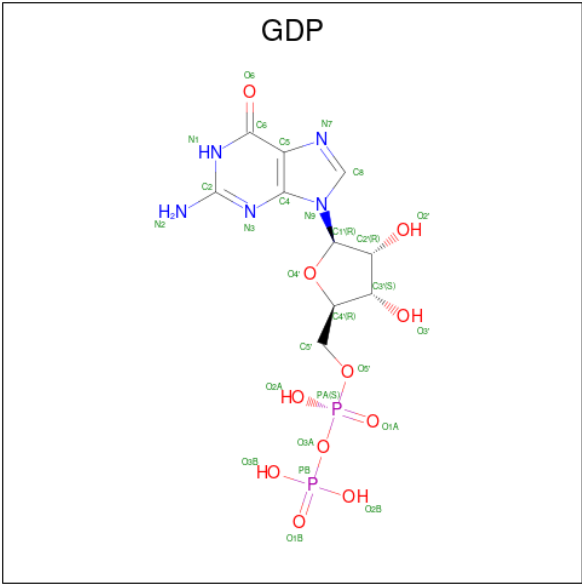
Mol	Chain	Residues	Atoms		AltConf
45	WN	1	Total 1	Mg 1	0
45	XB	1	Total 1	Mg 1	0
45	XD	1	Total 1	Mg 1	0
45	XF	1	Total 1	Mg 1	0
45	XH	1	Total 1	Mg 1	0
45	XJ	1	Total 1	Mg 1	0
45	XM	1	Total 1	Mg 1	0
45	XN	1	Total 1	Mg 1	0
45	YB	1	Total 1	Mg 1	0
45	YD	1	Total 1	Mg 1	0
45	YF	1	Total 1	Mg 1	0
45	YH	1	Total 1	Mg 1	0
45	YJ	1	Total 1	Mg 1	0
45	YL	1	Total 1	Mg 1	0
45	YN	1	Total 1	Mg 1	0
45	YP	1	Total 1	Mg 1	0
45	ZB	1	Total 1	Mg 1	0
45	ZD	1	Total 1	Mg 1	0
45	ZF	1	Total 1	Mg 1	0
45	ZH	1	Total 1	Mg 1	0
45	ZJ	1	Total 1	Mg 1	0

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Mol	Chain	Residues	Atoms		AltConf
45	ZL	1	Total	Mg	0
			1	1	
45	ZN	1	Total	Mg	0
			1	1	
45	ZP	1	Total	Mg	0
			1	1	

- Molecule 46 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
46	OE	1	28	10	5	11	2	0
46	OG	1	28	10	5	11	2	0
46	OI	1	28	10	5	11	2	0
46	OK	1	28	10	5	11	2	0
46	OM	1	28	10	5	11	2	0
46	OO	1	28	10	5	11	2	0
46	OQ	1	28	10	5	11	2	0
46	PC	1	28	10	5	11	2	0
46	PE	1	28	10	5	11	2	0
46	PG	1	28	10	5	11	2	0
46	PI	1	28	10	5	11	2	0
46	PK	1	28	10	5	11	2	0
46	PM	1	28	10	5	11	2	0
46	PO	1	28	10	5	11	2	0
46	PQ	1	28	10	5	11	2	0
46	QC	1	28	10	5	11	2	0
46	QE	1	28	10	5	11	2	0
46	QG	1	28	10	5	11	2	0
46	QI	1	28	10	5	11	2	0
46	QK	1	28	10	5	11	2	0
46	QM	1	28	10	5	11	2	0

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Mol	Chain	Residues	Atoms					AltConf
46	QO	1	Total 28	C 10	N 5	O 11	P 2	0
46	QQ	1	Total 28	C 10	N 5	O 11	P 2	0
46	RC	1	Total 28	C 10	N 5	O 11	P 2	0
46	RE	1	Total 28	C 10	N 5	O 11	P 2	0
46	RG	1	Total 28	C 10	N 5	O 11	P 2	0
46	RI	1	Total 28	C 10	N 5	O 11	P 2	0
46	RK	1	Total 28	C 10	N 5	O 11	P 2	0
46	RM	1	Total 28	C 10	N 5	O 11	P 2	0
46	RO	1	Total 28	C 10	N 5	O 11	P 2	0
46	SC	1	Total 28	C 10	N 5	O 11	P 2	0
46	SE	1	Total 28	C 10	N 5	O 11	P 2	0
46	SG	1	Total 28	C 10	N 5	O 11	P 2	0
46	SI	1	Total 28	C 10	N 5	O 11	P 2	0
46	SK	1	Total 28	C 10	N 5	O 11	P 2	0
46	SM	1	Total 28	C 10	N 5	O 11	P 2	0
46	SO	1	Total 28	C 10	N 5	O 11	P 2	0
46	TC	1	Total 28	C 10	N 5	O 11	P 2	0
46	TE	1	Total 28	C 10	N 5	O 11	P 2	0
46	TG	1	Total 28	C 10	N 5	O 11	P 2	0
46	TI	1	Total 28	C 10	N 5	O 11	P 2	0
46	TK	1	Total 28	C 10	N 5	O 11	P 2	0

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Mol	Chain	Residues	Atoms					AltConf
46	TM	1	Total 28	C 10	N 5	O 11	P 2	0
46	TO	1	Total 28	C 10	N 5	O 11	P 2	0
46	UC	1	Total 28	C 10	N 5	O 11	P 2	0
46	UE	1	Total 28	C 10	N 5	O 11	P 2	0
46	UG	1	Total 28	C 10	N 5	O 11	P 2	0
46	UI	1	Total 28	C 10	N 5	O 11	P 2	0
46	UK	1	Total 28	C 10	N 5	O 11	P 2	0
46	UM	1	Total 28	C 10	N 5	O 11	P 2	0
46	UO	1	Total 28	C 10	N 5	O 11	P 2	0
46	VC	1	Total 28	C 10	N 5	O 11	P 2	0
46	VE	1	Total 28	C 10	N 5	O 11	P 2	0
46	VG	1	Total 28	C 10	N 5	O 11	P 2	0
46	VI	1	Total 28	C 10	N 5	O 11	P 2	0
46	VK	1	Total 28	C 10	N 5	O 11	P 2	0
46	VM	1	Total 28	C 10	N 5	O 11	P 2	0
46	VO	1	Total 28	C 10	N 5	O 11	P 2	0
46	WA	1	Total 28	C 10	N 5	O 11	P 2	0
46	WC	1	Total 28	C 10	N 5	O 11	P 2	0
46	WE	1	Total 28	C 10	N 5	O 11	P 2	0
46	WG	1	Total 28	C 10	N 5	O 11	P 2	0
46	WI	1	Total 28	C 10	N 5	O 11	P 2	0

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Mol	Chain	Residues	Atoms					AltConf
46	WK	1	Total 28	C 10	N 5	O 11	P 2	0
46	WM	1	Total 28	C 10	N 5	O 11	P 2	0
46	WO	1	Total 28	C 10	N 5	O 11	P 2	0
46	XA	1	Total 28	C 10	N 5	O 11	P 2	0
46	XC	1	Total 28	C 10	N 5	O 11	P 2	0
46	XE	1	Total 28	C 10	N 5	O 11	P 2	0
46	XG	1	Total 28	C 10	N 5	O 11	P 2	0
46	XI	1	Total 28	C 10	N 5	O 11	P 2	0
46	XK	1	Total 28	C 10	N 5	O 11	P 2	0
46	XM	1	Total 28	C 10	N 5	O 11	P 2	0
46	XO	1	Total 28	C 10	N 5	O 11	P 2	0
46	YC	1	Total 28	C 10	N 5	O 11	P 2	0
46	YE	1	Total 28	C 10	N 5	O 11	P 2	0
46	YG	1	Total 28	C 10	N 5	O 11	P 2	0
46	YI	1	Total 28	C 10	N 5	O 11	P 2	0
46	YK	1	Total 28	C 10	N 5	O 11	P 2	0
46	YM	1	Total 28	C 10	N 5	O 11	P 2	0
46	YO	1	Total 28	C 10	N 5	O 11	P 2	0
46	ZC	1	Total 28	C 10	N 5	O 11	P 2	0
46	ZE	1	Total 28	C 10	N 5	O 11	P 2	0
46	ZG	1	Total 28	C 10	N 5	O 11	P 2	0

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Mol	Chain	Residues	Atoms					AltConf
46	ZI	1	Total	C	N	O	P	0
			28	10	5	11	2	
46	ZK	1	Total	C	N	O	P	0
			28	10	5	11	2	
46	ZM	1	Total	C	N	O	P	0
			28	10	5	11	2	
46	ZO	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	80007	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 ($e^-/\text{\AA}^2$)	39.6	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.073	Depositor
Minimum map value	0.000	Depositor
Average map value	0.007	Depositor
Map value standard deviation	0.053	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	889.6, 889.6, 889.6	wwPDB
Map dimensions	640, 640, 640	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.39, 1.39, 1.39	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 302 ligands modelled in this entry, 97 are monoatomic - leaving 205 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
44	GTP	ZP	501	45	33,34,34	0.94	1 (3%)	50,54,54	1.56	9 (18%)
44	GTP	ZB	501	45	33,34,34	0.94	1 (3%)	50,54,54	1.54	9 (18%)
44	GTP	OH	501	45	33,34,34	0.91	1 (3%)	50,54,54	1.55	9 (18%)
46	GDP	RI	502	-	29,30,30	1.14	3 (10%)	45,47,47	1.79	7 (15%)
46	GDP	VM	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.74	6 (13%)
46	GDP	XA	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.70	6 (13%)
46	GDP	WM	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	6 (13%)
44	GTP	NF	501	45	33,34,34	0.88	1 (3%)	50,54,54	1.58	8 (16%)
44	GTP	OD	501	45	33,34,34	0.90	1 (3%)	50,54,54	1.57	8 (16%)
44	GTP	NB	501	45	33,34,34	0.90	1 (3%)	50,54,54	1.61	9 (18%)
46	GDP	TK	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.77	6 (13%)
44	GTP	OP	501	45	33,34,34	0.91	1 (3%)	50,54,54	1.58	8 (16%)
46	GDP	WE	501	-	29,30,30	1.13	2 (6%)	45,47,47	1.75	6 (13%)
44	GTP	RH	501	45	33,34,34	0.94	1 (3%)	50,54,54	1.62	10 (20%)
44	GTP	UJ	501	45	33,34,34	0.95	1 (3%)	50,54,54	1.59	9 (18%)
46	GDP	UK	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.71	6 (13%)
43	ANP	C3	2001	-	33,33,33	1.03	4 (12%)	45,52,52	0.93	2 (4%)
46	GDP	WA	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.74	6 (13%)
46	GDP	WI	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.72	6 (13%)
46	GDP	ZK	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)
43	ANP	1C	2602	-	33,33,33	0.92	4 (12%)	45,52,52	0.84	2 (4%)
46	GDP	NM	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.74	6 (13%)
46	GDP	QK	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.77	6 (13%)
46	GDP	ZE	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.76	6 (13%)
44	GTP	NL	501	45	33,34,34	0.91	1 (3%)	50,54,54	1.58	9 (18%)
44	GTP	RJ	501	45	33,34,34	0.91	1 (3%)	50,54,54	1.55	8 (16%)
46	GDP	RC	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.76	7 (15%)
44	GTP	VF	501	45	33,34,34	0.90	1 (3%)	50,54,54	1.54	8 (16%)
43	ANP	C0	2001	-	33,33,33	0.95	4 (12%)	45,52,52	0.64	0
46	GDP	SK	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)
46	GDP	QO	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.75	6 (13%)
46	GDP	QG	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.77	7 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
46	GDP	SE	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.77	7 (15%)
44	GTP	PF	501	45	33,34,34	0.90	1 (3%)	50,54,54	1.60	10 (20%)
42	ADP	1A	2601	-	28,29,29	1.66	4 (14%)	43,45,45	2.39	11 (25%)
44	GTP	PL	501	45	33,34,34	0.90	1 (3%)	50,54,54	1.57	8 (16%)
44	GTP	VJ	501	45	33,34,34	0.93	1 (3%)	50,54,54	1.58	9 (18%)
46	GDP	PK	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.75	6 (13%)
46	GDP	ZM	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.74	7 (15%)
46	GDP	OC	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)
46	GDP	PG	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.75	7 (15%)
44	GTP	YB	501	45	33,34,34	0.94	1 (3%)	50,54,54	1.57	9 (18%)
46	GDP	RK	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.75	6 (13%)
46	GDP	XE	501	-	29,30,30	1.15	2 (6%)	45,47,47	1.78	6 (13%)
46	GDP	OE	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	6 (13%)
46	GDP	YC	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.78	7 (15%)
46	GDP	UE	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.76	6 (13%)
44	GTP	VH	501	45	33,34,34	0.95	1 (3%)	50,54,54	1.60	8 (16%)
46	GDP	YO	501	-	29,30,30	1.14	4 (13%)	45,47,47	1.70	6 (13%)
46	GDP	YI	501	-	29,30,30	1.14	2 (6%)	45,47,47	1.74	5 (11%)
44	GTP	YH	501	45	33,34,34	0.92	1 (3%)	50,54,54	1.61	10 (20%)
44	GTP	ZF	501	45	33,34,34	0.94	1 (3%)	50,54,54	1.53	9 (18%)
44	GTP	ON	501	45	33,34,34	0.93	1 (3%)	50,54,54	1.59	9 (18%)
46	GDP	QM	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	8 (17%)
46	GDP	UG	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.77	7 (15%)
46	GDP	XM	502	-	29,30,30	1.16	3 (10%)	45,47,47	1.76	6 (13%)
46	GDP	PM	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.70	5 (11%)
43	ANP	1D	2602	-	33,33,33	0.92	4 (12%)	45,52,52	0.74	0
43	ANP	1A	2602	-	33,33,33	0.88	3 (9%)	45,52,52	0.70	0
44	GTP	WJ	501	45	33,34,34	0.90	1 (3%)	50,54,54	1.60	11 (22%)
44	GTP	WB	501	45	33,34,34	0.94	1 (3%)	50,54,54	1.57	8 (16%)
44	GTP	QH	501	45	33,34,34	0.90	1 (3%)	50,54,54	1.58	9 (18%)
46	GDP	NC	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.72	6 (13%)
46	GDP	RG	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.74	6 (13%)
44	GTP	PN	501	45	33,34,34	0.90	1 (3%)	50,54,54	1.58	8 (16%)
44	GTP	XB	501	45	33,34,34	0.95	1 (3%)	50,54,54	1.57	8 (16%)
46	GDP	ZG	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.72	6 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
44	GTP	PH	501	45	33,34,34	0.93	1 (3%)	50,54,54	1.59	9 (18%)
46	GDP	XG	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.73	6 (13%)
46	GDP	PE	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.75	7 (15%)
46	GDP	ZO	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)
46	GDP	XO	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.75	6 (13%)
44	GTP	SL	501	45	33,34,34	0.92	1 (3%)	50,54,54	1.57	9 (18%)
44	GTP	QF	501	45	33,34,34	0.91	1 (3%)	50,54,54	1.58	9 (18%)
46	GDP	WO	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	7 (15%)
44	GTP	RN	501	45	33,34,34	0.94	1 (3%)	50,54,54	1.59	9 (18%)
44	GTP	VN	501	45	33,34,34	0.93	1 (3%)	50,54,54	1.55	8 (16%)
46	GDP	ZI	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.75	6 (13%)
44	GTP	QN	501	45	33,34,34	0.94	1 (3%)	50,54,54	1.61	10 (20%)
44	GTP	XL	501	45	33,34,34	0.92	1 (3%)	50,54,54	1.59	9 (18%)
44	GTP	UL	501	45	33,34,34	0.90	1 (3%)	50,54,54	1.56	9 (18%)
43	ANP	1B	2602	-	33,33,33	0.94	4 (12%)	45,52,52	0.76	1 (2%)
44	GTP	SB	501	45	33,34,34	0.94	1 (3%)	50,54,54	1.57	9 (18%)
43	ANP	C2	2001	-	33,33,33	0.94	4 (12%)	45,52,52	0.79	2 (4%)
44	GTP	PJ	501	45	33,34,34	0.94	1 (3%)	50,54,54	1.62	10 (20%)
44	GTP	YF	501	45	33,34,34	0.93	1 (3%)	50,54,54	1.57	9 (18%)
46	GDP	SO	502	-	29,30,30	1.14	4 (13%)	45,47,47	1.68	6 (13%)
46	GDP	TI	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.74	6 (13%)
44	GTP	UN	501	45	33,34,34	0.92	1 (3%)	50,54,54	1.62	10 (20%)
46	GDP	OO	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.74	6 (13%)
44	GTP	RL	501	45	33,34,34	0.92	1 (3%)	50,54,54	1.60	8 (16%)
46	GDP	UO	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	6 (13%)
46	GDP	XI	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.74	6 (13%)
46	GDP	ZC	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.73	7 (15%)
44	GTP	ND	501	45	33,34,34	0.93	1 (3%)	50,54,54	1.57	9 (18%)
44	GTP	UH	501	45	33,34,34	0.94	1 (3%)	50,54,54	1.60	9 (18%)
46	GDP	VG	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.78	7 (15%)
44	GTP	XJ	501	45	33,34,34	0.93	1 (3%)	50,54,54	1.56	8 (16%)
46	GDP	PC	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.78	7 (15%)
46	GDP	RE	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.75	6 (13%)
46	GDP	YM	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.76	6 (13%)
44	GTP	UB	501	45	33,34,34	0.91	1 (3%)	50,54,54	1.57	8 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
44	GTP	VD	501	45	33,34,34	0.95	1 (3%)	50,54,54	1.59	9 (18%)
46	GDP	OQ	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.78	7 (15%)
46	GDP	PO	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	7 (15%)
46	GDP	TC	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.79	7 (15%)
44	GTP	YL	501	45	33,34,34	0.93	0	50,54,54	1.58	9 (18%)
46	GDP	QC	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	7 (15%)
44	GTP	WH	501	45	33,34,34	0.92	1 (3%)	50,54,54	1.60	8 (16%)
46	GDP	OK	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	7 (15%)
46	GDP	XK	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.72	7 (15%)
44	GTP	OL	501	45	33,34,34	0.93	1 (3%)	50,54,54	1.62	10 (20%)
46	GDP	NG	502	-	29,30,30	1.17	3 (10%)	45,47,47	1.78	7 (15%)
44	GTP	ZL	501	45	33,34,34	0.92	1 (3%)	50,54,54	1.56	9 (18%)
44	GTP	NN	501	45	33,34,34	0.93	1 (3%)	50,54,54	1.58	9 (18%)
44	GTP	UF	501	45	33,34,34	0.93	1 (3%)	50,54,54	1.56	9 (18%)
46	GDP	QQ	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	7 (15%)
46	GDP	UM	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	6 (13%)
46	GDP	NE	501	-	29,30,30	1.16	2 (6%)	45,47,47	1.76	7 (15%)
44	GTP	ZN	501	45	33,34,34	0.91	1 (3%)	50,54,54	1.56	8 (16%)
44	GTP	PP	501	45	33,34,34	0.93	1 (3%)	50,54,54	1.58	9 (18%)
44	GTP	ZH	501	45	33,34,34	0.92	1 (3%)	50,54,54	1.59	9 (18%)
44	GTP	YJ	501	45	33,34,34	0.91	1 (3%)	50,54,54	1.58	8 (16%)
46	GDP	SC	502	-	29,30,30	1.15	3 (10%)	45,47,47	1.75	6 (13%)
46	GDP	TM	502	-	29,30,30	1.15	3 (10%)	45,47,47	1.78	7 (15%)
44	GTP	OJ	501	45	33,34,34	0.87	1 (3%)	50,54,54	1.59	9 (18%)
42	ADP	1D	2601	-	28,29,29	1.65	4 (14%)	43,45,45	2.41	14 (32%)
44	GTP	XN	501	45	33,34,34	0.93	1 (3%)	50,54,54	1.54	8 (16%)
44	GTP	TJ	501	45	33,34,34	0.94	1 (3%)	50,54,54	1.61	8 (16%)
46	GDP	OI	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.75	7 (15%)
44	GTP	ZJ	501	45	33,34,34	0.92	1 (3%)	50,54,54	1.58	9 (18%)
44	GTP	QP	501	45	33,34,34	0.94	1 (3%)	50,54,54	1.57	8 (16%)
46	GDP	WC	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.79	7 (15%)
44	GTP	WL	501	45	33,34,34	0.90	1 (3%)	50,54,54	1.61	9 (18%)
46	GDP	TG	502	-	29,30,30	1.14	3 (10%)	45,47,47	1.75	6 (13%)
46	GDP	VC	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)
44	GTP	QD	501	45	33,34,34	0.95	1 (3%)	50,54,54	1.62	11 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
44	GTP	RF	501	45	33,34,34	0.96	1 (3%)	50,54,54	1.63	9 (18%)
46	GDP	VO	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.76	7 (15%)
44	GTP	PD	501	45	33,34,34	0.92	1 (3%)	50,54,54	1.58	9 (18%)
44	GTP	ZD	501	45	33,34,34	0.94	1 (3%)	50,54,54	1.55	10 (20%)
44	GTP	NJ	501	45	33,34,34	0.96	2 (6%)	50,54,54	1.62	10 (20%)
46	GDP	RO	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.74	6 (13%)
46	GDP	WK	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.75	6 (13%)
46	GDP	OG	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.76	7 (15%)
44	GTP	WF	501	45	33,34,34	0.86	1 (3%)	50,54,54	1.60	8 (16%)
46	GDP	PQ	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	7 (15%)
46	GDP	YK	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.74	6 (13%)
46	GDP	VK	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.75	6 (13%)
44	GTP	SJ	501	45	33,34,34	0.88	1 (3%)	50,54,54	1.61	9 (18%)
44	GTP	OF	501	45	33,34,34	0.93	1 (3%)	50,54,54	1.58	8 (16%)
44	GTP	XF	501	45	33,34,34	0.92	1 (3%)	50,54,54	1.60	9 (18%)
44	GTP	TN	501	45	33,34,34	0.90	1 (3%)	50,54,54	1.58	9 (18%)
46	GDP	UI	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.72	7 (15%)
46	GDP	VE	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.71	6 (13%)
44	GTP	UP	501	45	33,34,34	0.95	1 (3%)	50,54,54	1.57	9 (18%)
46	GDP	WG	502	-	29,30,30	1.14	3 (10%)	45,47,47	1.74	6 (13%)
43	ANP	C1	2001	-	33,33,33	0.96	3 (9%)	45,52,52	0.76	0
46	GDP	QI	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	6 (13%)
44	GTP	YP	501	45	33,34,34	0.95	1 (3%)	50,54,54	1.61	10 (20%)
44	GTP	RP	501	45	33,34,34	0.94	1 (3%)	50,54,54	1.62	10 (20%)
44	GTP	SD	501	45	33,34,34	0.90	1 (3%)	50,54,54	1.59	8 (16%)
46	GDP	PI	502	-	29,30,30	1.14	3 (10%)	45,47,47	1.75	7 (15%)
44	GTP	SH	501	45	33,34,34	0.90	1 (3%)	50,54,54	1.61	10 (20%)
44	GTP	VB	501	45	33,34,34	0.93	1 (3%)	50,54,54	1.54	8 (16%)
46	GDP	XC	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.76	7 (15%)
44	GTP	TL	501	45	33,34,34	0.94	1 (3%)	50,54,54	1.56	9 (18%)
46	GDP	QE	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.78	7 (15%)
42	ADP	1C	2601	-	28,29,29	1.64	4 (14%)	43,45,45	2.39	11 (25%)
44	GTP	VL	501	45	33,34,34	0.95	1 (3%)	50,54,54	1.60	10 (20%)
44	GTP	VP	501	45	33,34,34	0.96	1 (3%)	50,54,54	1.55	8 (16%)
44	GTP	XD	501	45	33,34,34	0.95	1 (3%)	50,54,54	1.59	11 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
46	GDP	SI	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.72	7 (15%)
44	GTP	TF	501	45	33,34,34	0.93	1 (3%)	50,54,54	1.57	9 (18%)
46	GDP	NK	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.73	6 (13%)
46	GDP	TE	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)
46	GDP	OM	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	7 (15%)
44	GTP	YN	501	45	33,34,34	0.93	1 (3%)	50,54,54	1.56	10 (20%)
46	GDP	SM	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.77	7 (15%)
44	GTP	QL	501	45	33,34,34	0.90	1 (3%)	50,54,54	1.59	9 (18%)
44	GTP	NH	501	45	33,34,34	0.92	1 (3%)	50,54,54	1.63	9 (18%)
42	ADP	1B	2601	-	28,29,29	1.64	4 (14%)	43,45,45	2.50	15 (34%)
46	GDP	YE	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.76	6 (13%)
46	GDP	UC	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)
46	GDP	VI	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.72	6 (13%)
44	GTP	SN	501	45	33,34,34	0.91	1 (3%)	50,54,54	1.55	9 (18%)
44	GTP	SF	501	45	33,34,34	0.92	1 (3%)	50,54,54	1.59	9 (18%)
44	GTP	RD	501	45	33,34,34	0.94	1 (3%)	50,54,54	1.56	8 (16%)
46	GDP	RM	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.75	6 (13%)
44	GTP	SP	501	45	33,34,34	0.95	1 (3%)	50,54,54	1.60	9 (18%)
46	GDP	NO	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.78	7 (15%)
44	GTP	TD	501	45	33,34,34	0.93	1 (3%)	50,54,54	1.56	9 (18%)
44	GTP	TH	501	45	33,34,34	0.92	1 (3%)	50,54,54	1.61	9 (18%)
44	GTP	TP	501	45	33,34,34	0.96	1 (3%)	50,54,54	1.60	10 (20%)
44	GTP	WD	501	45	33,34,34	0.95	1 (3%)	50,54,54	1.56	9 (18%)
44	GTP	XH	501	45	33,34,34	0.94	1 (3%)	50,54,54	1.59	9 (18%)
46	GDP	NI	501	-	29,30,30	1.12	3 (10%)	45,47,47	1.71	6 (13%)
44	GTP	TB	501	45	33,34,34	0.90	1 (3%)	50,54,54	1.56	9 (18%)
44	GTP	UD	501	45	33,34,34	0.94	1 (3%)	50,54,54	1.60	8 (16%)
44	GTP	WN	501	45	33,34,34	0.94	1 (3%)	50,54,54	1.59	9 (18%)
46	GDP	SG	502	-	29,30,30	1.14	3 (10%)	45,47,47	1.74	6 (13%)
44	GTP	QJ	501	45	33,34,34	0.92	1 (3%)	50,54,54	1.58	9 (18%)
44	GTP	YD	501	45	33,34,34	0.94	1 (3%)	50,54,54	1.57	10 (20%)
46	GDP	YG	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	6 (13%)
46	GDP	TO	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	6 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
44	GTP	ZP	501	45	-	4/22/38/38	0/3/3/3
44	GTP	ZB	501	45	-	5/22/38/38	0/3/3/3
44	GTP	OH	501	45	-	4/22/38/38	0/3/3/3
46	GDP	RI	502	-	-	0/16/32/32	0/3/3/3
46	GDP	VM	501	-	-	4/16/32/32	0/3/3/3
46	GDP	XA	501	-	-	1/16/32/32	0/3/3/3
46	GDP	WM	501	-	-	0/16/32/32	0/3/3/3
44	GTP	NF	501	45	-	1/22/38/38	0/3/3/3
44	GTP	OD	501	45	-	8/22/38/38	0/3/3/3
44	GTP	NB	501	45	-	7/22/38/38	0/3/3/3
46	GDP	TK	501	-	-	2/16/32/32	0/3/3/3
44	GTP	OP	501	45	-	3/22/38/38	0/3/3/3
46	GDP	WE	501	-	-	2/16/32/32	0/3/3/3
44	GTP	RH	501	45	-	6/22/38/38	0/3/3/3
44	GTP	UJ	501	45	-	3/22/38/38	0/3/3/3
46	GDP	UK	501	-	-	1/16/32/32	0/3/3/3
43	ANP	C3	2001	-	-	5/18/38/38	0/3/3/3
46	GDP	WA	501	-	-	2/16/32/32	0/3/3/3
46	GDP	WI	501	-	-	0/16/32/32	0/3/3/3
46	GDP	ZK	501	-	-	1/16/32/32	0/3/3/3
43	ANP	1C	2602	-	-	10/18/38/38	0/3/3/3
46	GDP	NM	501	-	-	1/16/32/32	0/3/3/3
46	GDP	QK	501	-	-	0/16/32/32	0/3/3/3
46	GDP	ZE	501	-	-	2/16/32/32	0/3/3/3
44	GTP	NL	501	45	-	5/22/38/38	0/3/3/3
44	GTP	RJ	501	45	-	7/22/38/38	0/3/3/3
46	GDP	RC	501	-	-	0/16/32/32	0/3/3/3
44	GTP	VF	501	45	-	3/22/38/38	0/3/3/3
43	ANP	C0	2001	-	-	3/18/38/38	0/3/3/3
46	GDP	SK	501	-	-	1/16/32/32	0/3/3/3
46	GDP	QO	501	-	-	1/16/32/32	0/3/3/3
46	GDP	QG	501	-	-	1/16/32/32	0/3/3/3
46	GDP	SE	501	-	-	1/16/32/32	0/3/3/3
44	GTP	PF	501	45	-	5/22/38/38	0/3/3/3
42	ADP	1A	2601	-	-	7/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
44	GTP	PL	501	45	-	3/22/38/38	0/3/3/3
44	GTP	VJ	501	45	-	6/22/38/38	0/3/3/3
46	GDP	PK	501	-	-	3/16/32/32	0/3/3/3
46	GDP	ZM	501	-	-	1/16/32/32	0/3/3/3
46	GDP	OC	501	-	-	2/16/32/32	0/3/3/3
46	GDP	PG	501	-	-	0/16/32/32	0/3/3/3
44	GTP	YB	501	45	-	7/22/38/38	0/3/3/3
46	GDP	RK	501	-	-	1/16/32/32	0/3/3/3
46	GDP	XE	501	-	-	1/16/32/32	0/3/3/3
46	GDP	OE	501	-	-	2/16/32/32	0/3/3/3
46	GDP	YC	501	-	-	3/16/32/32	0/3/3/3
46	GDP	UE	501	-	-	1/16/32/32	0/3/3/3
44	GTP	VH	501	45	-	4/22/38/38	0/3/3/3
46	GDP	YO	501	-	-	2/16/32/32	0/3/3/3
46	GDP	YI	501	-	-	2/16/32/32	0/3/3/3
44	GTP	YH	501	45	-	4/22/38/38	0/3/3/3
44	GTP	ZF	501	45	-	5/22/38/38	0/3/3/3
44	GTP	ON	501	45	-	3/22/38/38	0/3/3/3
46	GDP	QM	501	-	-	2/16/32/32	0/3/3/3
46	GDP	UG	501	-	-	0/16/32/32	0/3/3/3
46	GDP	XM	502	-	-	2/16/32/32	0/3/3/3
46	GDP	PM	501	-	-	0/16/32/32	0/3/3/3
43	ANP	1D	2602	-	-	13/18/38/38	0/3/3/3
43	ANP	1A	2602	-	-	14/18/38/38	0/3/3/3
44	GTP	WJ	501	45	-	7/22/38/38	0/3/3/3
44	GTP	WB	501	45	-	3/22/38/38	0/3/3/3
44	GTP	QH	501	45	-	5/22/38/38	0/3/3/3
46	GDP	NC	501	-	-	2/16/32/32	0/3/3/3
46	GDP	RG	501	-	-	2/16/32/32	0/3/3/3
44	GTP	PN	501	45	-	4/22/38/38	0/3/3/3
44	GTP	XB	501	45	-	3/22/38/38	0/3/3/3
46	GDP	ZG	501	-	-	2/16/32/32	0/3/3/3
44	GTP	PH	501	45	-	9/22/38/38	0/3/3/3
46	GDP	XG	501	-	-	2/16/32/32	0/3/3/3
46	GDP	PE	501	-	-	2/16/32/32	0/3/3/3
46	GDP	ZO	501	-	-	1/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
46	GDP	XO	501	-	-	2/16/32/32	0/3/3/3
44	GTP	SL	501	45	-	2/22/38/38	0/3/3/3
44	GTP	QF	501	45	-	3/22/38/38	0/3/3/3
46	GDP	WO	501	-	-	0/16/32/32	0/3/3/3
44	GTP	RN	501	45	-	4/22/38/38	0/3/3/3
44	GTP	VN	501	45	-	2/22/38/38	0/3/3/3
46	GDP	ZI	501	-	-	0/16/32/32	0/3/3/3
44	GTP	QN	501	45	-	7/22/38/38	0/3/3/3
44	GTP	XL	501	45	-	6/22/38/38	0/3/3/3
44	GTP	UL	501	45	-	8/22/38/38	0/3/3/3
43	ANP	1B	2602	-	-	12/18/38/38	0/3/3/3
44	GTP	SB	501	45	-	4/22/38/38	0/3/3/3
43	ANP	C2	2001	-	-	2/18/38/38	0/3/3/3
44	GTP	PJ	501	45	-	4/22/38/38	0/3/3/3
44	GTP	YF	501	45	-	4/22/38/38	0/3/3/3
46	GDP	SO	502	-	-	2/16/32/32	0/3/3/3
46	GDP	TI	501	-	-	2/16/32/32	0/3/3/3
44	GTP	UN	501	45	-	4/22/38/38	0/3/3/3
46	GDP	OO	501	-	-	2/16/32/32	0/3/3/3
44	GTP	RL	501	45	-	4/22/38/38	0/3/3/3
46	GDP	UO	501	-	-	2/16/32/32	0/3/3/3
46	GDP	XI	501	-	-	1/16/32/32	0/3/3/3
46	GDP	ZC	501	-	-	0/16/32/32	0/3/3/3
44	GTP	ND	501	45	-	7/22/38/38	0/3/3/3
44	GTP	UH	501	45	-	4/22/38/38	0/3/3/3
46	GDP	VG	501	-	-	1/16/32/32	0/3/3/3
44	GTP	XJ	501	45	-	3/22/38/38	0/3/3/3
46	GDP	PC	501	-	-	1/16/32/32	0/3/3/3
46	GDP	RE	501	-	-	3/16/32/32	0/3/3/3
46	GDP	YM	501	-	-	2/16/32/32	0/3/3/3
44	GTP	UB	501	45	-	3/22/38/38	0/3/3/3
44	GTP	VD	501	45	-	3/22/38/38	0/3/3/3
46	GDP	OQ	501	-	-	1/16/32/32	0/3/3/3
46	GDP	PO	501	-	-	1/16/32/32	0/3/3/3
46	GDP	TC	501	-	-	1/16/32/32	0/3/3/3
44	GTP	YL	501	45	-	4/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
46	GDP	QC	501	-	-	0/16/32/32	0/3/3/3
44	GTP	WH	501	45	-	7/22/38/38	0/3/3/3
46	GDP	OK	501	-	-	2/16/32/32	0/3/3/3
46	GDP	XK	501	-	-	1/16/32/32	0/3/3/3
44	GTP	OL	501	45	-	7/22/38/38	0/3/3/3
46	GDP	NG	502	-	-	2/16/32/32	0/3/3/3
44	GTP	ZL	501	45	-	1/22/38/38	0/3/3/3
44	GTP	NN	501	45	-	5/22/38/38	0/3/3/3
44	GTP	UF	501	45	-	4/22/38/38	0/3/3/3
46	GDP	QQ	501	-	-	1/16/32/32	0/3/3/3
46	GDP	UM	501	-	-	0/16/32/32	0/3/3/3
46	GDP	NE	501	-	-	1/16/32/32	0/3/3/3
44	GTP	ZN	501	45	-	7/22/38/38	0/3/3/3
44	GTP	PP	501	45	-	9/22/38/38	0/3/3/3
44	GTP	ZH	501	45	-	4/22/38/38	0/3/3/3
44	GTP	YJ	501	45	-	5/22/38/38	0/3/3/3
46	GDP	SC	502	-	-	2/16/32/32	0/3/3/3
46	GDP	TM	502	-	-	0/16/32/32	0/3/3/3
44	GTP	OJ	501	45	-	4/22/38/38	0/3/3/3
42	ADP	1D	2601	-	-	6/16/32/32	0/3/3/3
44	GTP	XN	501	45	-	2/22/38/38	0/3/3/3
44	GTP	TJ	501	45	-	5/22/38/38	0/3/3/3
46	GDP	OI	501	-	-	2/16/32/32	0/3/3/3
44	GTP	ZJ	501	45	-	5/22/38/38	0/3/3/3
44	GTP	QP	501	45	-	7/22/38/38	0/3/3/3
46	GDP	WC	501	-	-	4/16/32/32	0/3/3/3
44	GTP	WL	501	45	-	6/22/38/38	0/3/3/3
46	GDP	TG	502	-	-	0/16/32/32	0/3/3/3
46	GDP	VC	501	-	-	0/16/32/32	0/3/3/3
44	GTP	QD	501	45	-	4/22/38/38	0/3/3/3
44	GTP	RF	501	45	-	4/22/38/38	0/3/3/3
46	GDP	VO	501	-	-	2/16/32/32	0/3/3/3
44	GTP	PD	501	45	-	3/22/38/38	0/3/3/3
44	GTP	ZD	501	45	-	4/22/38/38	0/3/3/3
44	GTP	NJ	501	45	-	7/22/38/38	0/3/3/3
46	GDP	RO	501	-	-	2/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
46	GDP	WK	501	-	-	0/16/32/32	0/3/3/3
46	GDP	OG	501	-	-	0/16/32/32	0/3/3/3
44	GTP	WF	501	45	-	3/22/38/38	0/3/3/3
46	GDP	PQ	501	-	-	1/16/32/32	0/3/3/3
46	GDP	YK	501	-	-	0/16/32/32	0/3/3/3
46	GDP	VK	501	-	-	0/16/32/32	0/3/3/3
44	GTP	SJ	501	45	-	0/22/38/38	0/3/3/3
44	GTP	OF	501	45	-	3/22/38/38	0/3/3/3
44	GTP	XF	501	45	-	4/22/38/38	0/3/3/3
44	GTP	TN	501	45	-	2/22/38/38	0/3/3/3
46	GDP	UI	501	-	-	0/16/32/32	0/3/3/3
46	GDP	VE	501	-	-	0/16/32/32	0/3/3/3
44	GTP	UP	501	45	-	4/22/38/38	0/3/3/3
46	GDP	WG	502	-	-	0/16/32/32	0/3/3/3
43	ANP	C1	2001	-	-	2/18/38/38	0/3/3/3
46	GDP	QI	501	-	-	0/16/32/32	0/3/3/3
44	GTP	YP	501	45	-	4/22/38/38	0/3/3/3
44	GTP	RP	501	45	-	5/22/38/38	0/3/3/3
44	GTP	SD	501	45	-	7/22/38/38	0/3/3/3
46	GDP	PI	502	-	-	0/16/32/32	0/3/3/3
44	GTP	SH	501	45	-	7/22/38/38	0/3/3/3
44	GTP	VB	501	45	-	4/22/38/38	0/3/3/3
46	GDP	XC	501	-	-	2/16/32/32	0/3/3/3
44	GTP	TL	501	45	-	4/22/38/38	0/3/3/3
46	GDP	QE	501	-	-	1/16/32/32	0/3/3/3
42	ADP	1C	2601	-	-	7/16/32/32	0/3/3/3
44	GTP	VL	501	45	-	4/22/38/38	0/3/3/3
44	GTP	VP	501	45	-	3/22/38/38	0/3/3/3
44	GTP	XD	501	45	-	1/22/38/38	0/3/3/3
46	GDP	SI	501	-	-	0/16/32/32	0/3/3/3
44	GTP	TF	501	45	-	3/22/38/38	0/3/3/3
46	GDP	NK	501	-	-	1/16/32/32	0/3/3/3
46	GDP	TE	501	-	-	1/16/32/32	0/3/3/3
46	GDP	OM	501	-	-	2/16/32/32	0/3/3/3
44	GTP	YN	501	45	-	3/22/38/38	0/3/3/3
46	GDP	SM	501	-	-	0/16/32/32	0/3/3/3
44	GTP	QL	501	45	-	4/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
44	GTP	NH	501	45	-	6/22/38/38	0/3/3/3
42	ADP	1B	2601	-	-	7/16/32/32	0/3/3/3
46	GDP	YE	501	-	-	2/16/32/32	0/3/3/3
46	GDP	UC	501	-	-	1/16/32/32	0/3/3/3
46	GDP	VI	501	-	-	4/16/32/32	0/3/3/3
44	GTP	SN	501	45	-	3/22/38/38	0/3/3/3
44	GTP	SF	501	45	-	5/22/38/38	0/3/3/3
44	GTP	RD	501	45	-	4/22/38/38	0/3/3/3
46	GDP	RM	501	-	-	2/16/32/32	0/3/3/3
44	GTP	SP	501	45	-	1/22/38/38	0/3/3/3
46	GDP	NO	501	-	-	1/16/32/32	0/3/3/3
44	GTP	TD	501	45	-	4/22/38/38	0/3/3/3
44	GTP	TH	501	45	-	6/22/38/38	0/3/3/3
44	GTP	TP	501	45	-	4/22/38/38	0/3/3/3
44	GTP	WD	501	45	-	5/22/38/38	0/3/3/3
44	GTP	XH	501	45	-	8/22/38/38	0/3/3/3
46	GDP	NI	501	-	-	1/16/32/32	0/3/3/3
44	GTP	TB	501	45	-	4/22/38/38	0/3/3/3
44	GTP	UD	501	45	-	4/22/38/38	0/3/3/3
44	GTP	WN	501	45	-	7/22/38/38	0/3/3/3
46	GDP	SG	502	-	-	2/16/32/32	0/3/3/3
44	GTP	QJ	501	45	-	2/22/38/38	0/3/3/3
44	GTP	YD	501	45	-	2/22/38/38	0/3/3/3
46	GDP	YG	501	-	-	1/16/32/32	0/3/3/3
46	GDP	TO	501	-	-	0/16/32/32	0/3/3/3

All (429) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	1A	2601	ADP	C5-C4	5.82	1.49	1.39
42	1C	2601	ADP	C5-C4	5.74	1.49	1.39
42	1D	2601	ADP	C5-C4	5.72	1.49	1.39
42	1B	2601	ADP	C5-C4	5.64	1.49	1.39
42	1B	2601	ADP	C5-C6	4.27	1.52	1.41
42	1D	2601	ADP	C5-C6	4.20	1.52	1.41
42	1A	2601	ADP	C5-C6	4.13	1.52	1.41
42	1C	2601	ADP	C5-C6	4.04	1.52	1.41
46	XE	501	GDP	C5-C4	3.13	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	YC	501	GDP	C5-C4	3.12	1.47	1.38
46	ZE	501	GDP	C5-C4	3.12	1.47	1.38
46	XM	502	GDP	C5-C4	3.10	1.47	1.38
46	XC	501	GDP	C5-C4	3.09	1.47	1.38
46	TC	501	GDP	C5-C4	3.09	1.47	1.38
46	OE	501	GDP	C5-C4	3.09	1.47	1.38
46	QG	501	GDP	C5-C4	3.09	1.47	1.38
46	SE	501	GDP	C5-C4	3.09	1.47	1.38
46	UE	501	GDP	C5-C4	3.09	1.47	1.38
46	TE	501	GDP	C5-C4	3.08	1.47	1.38
46	VC	501	GDP	C5-C4	3.08	1.47	1.38
46	NO	501	GDP	C5-C4	3.08	1.47	1.38
46	ZO	501	GDP	C5-C4	3.08	1.47	1.38
46	YE	501	GDP	C5-C4	3.08	1.47	1.38
46	PE	501	GDP	C5-C4	3.08	1.47	1.38
46	WK	501	GDP	C5-C4	3.07	1.47	1.38
46	PQ	501	GDP	C5-C4	3.07	1.47	1.38
46	OQ	501	GDP	C5-C4	3.07	1.47	1.38
46	NG	502	GDP	C5-C4	3.07	1.47	1.38
46	UM	501	GDP	C5-C4	3.07	1.47	1.38
46	SC	502	GDP	C5-C4	3.07	1.47	1.38
46	TM	502	GDP	C5-C4	3.07	1.47	1.38
46	PG	501	GDP	C5-C4	3.06	1.47	1.38
46	TO	501	GDP	C5-C4	3.06	1.47	1.38
46	WO	501	GDP	C5-C4	3.06	1.47	1.38
46	NK	501	GDP	C5-C4	3.06	1.47	1.38
46	QC	501	GDP	C5-C4	3.06	1.47	1.38
46	QE	501	GDP	C5-C4	3.05	1.47	1.38
46	RC	501	GDP	C5-C4	3.05	1.47	1.38
46	ZK	501	GDP	C5-C4	3.05	1.47	1.38
46	NC	501	GDP	C5-C4	3.05	1.47	1.38
46	WC	501	GDP	C5-C4	3.05	1.47	1.38
46	PI	502	GDP	C5-C4	3.05	1.47	1.38
46	YG	501	GDP	C5-C4	3.05	1.47	1.38
46	OC	501	GDP	C5-C4	3.05	1.47	1.38
46	WM	501	GDP	C5-C4	3.04	1.47	1.38
46	ZM	501	GDP	C5-C4	3.04	1.47	1.38
46	SK	501	GDP	C5-C4	3.04	1.47	1.38
46	RO	501	GDP	C5-C4	3.04	1.47	1.38
46	VK	501	GDP	C5-C4	3.03	1.47	1.38
46	PC	501	GDP	C5-C4	3.03	1.47	1.38
46	UO	501	GDP	C5-C4	3.03	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	VM	501	GDP	C5-C4	3.03	1.47	1.38
46	QO	501	GDP	C5-C4	3.03	1.47	1.38
46	PO	501	GDP	C5-C4	3.03	1.47	1.38
46	QQ	501	GDP	C5-C4	3.03	1.47	1.38
46	PK	501	GDP	C5-C4	3.02	1.47	1.38
46	OI	501	GDP	C5-C4	3.02	1.47	1.38
46	SM	501	GDP	C5-C4	3.02	1.47	1.38
46	WE	501	GDP	C5-C4	3.02	1.47	1.38
46	ZC	501	GDP	C5-C4	3.02	1.47	1.38
46	ZI	501	GDP	C5-C4	3.02	1.47	1.38
46	RG	501	GDP	C5-C4	3.02	1.47	1.38
46	RM	501	GDP	C5-C4	3.02	1.47	1.38
46	WA	501	GDP	C5-C4	3.02	1.47	1.38
46	OM	501	GDP	C5-C4	3.02	1.47	1.38
46	NE	501	GDP	C5-C4	3.01	1.47	1.38
46	YK	501	GDP	C5-C4	3.01	1.47	1.38
46	QM	501	GDP	C5-C4	3.01	1.47	1.38
46	RI	502	GDP	C5-C4	3.01	1.47	1.38
46	WI	501	GDP	C5-C4	3.01	1.47	1.38
46	TI	501	GDP	C5-C4	3.01	1.47	1.38
46	YI	501	GDP	C5-C4	3.01	1.47	1.38
46	VE	501	GDP	C5-C4	3.00	1.47	1.38
46	RE	501	GDP	C5-C4	3.00	1.47	1.38
46	NM	501	GDP	C5-C4	3.00	1.47	1.38
46	VO	501	GDP	C5-C4	3.00	1.47	1.38
46	QI	501	GDP	C5-C4	3.00	1.47	1.38
46	UG	501	GDP	C5-C4	3.00	1.47	1.38
46	ZG	501	GDP	C5-C4	3.00	1.47	1.38
46	XG	501	GDP	C5-C4	2.99	1.46	1.38
46	XO	501	GDP	C5-C4	2.99	1.46	1.38
46	XA	501	GDP	C5-C4	2.99	1.46	1.38
46	XI	501	GDP	C5-C4	2.99	1.46	1.38
46	YM	501	GDP	C5-C4	2.98	1.46	1.38
46	NI	501	GDP	C5-C4	2.98	1.46	1.38
46	SG	502	GDP	C5-C4	2.98	1.46	1.38
46	QK	501	GDP	C5-C4	2.98	1.46	1.38
46	OK	501	GDP	C5-C4	2.98	1.46	1.38
46	WG	502	GDP	C5-C4	2.97	1.46	1.38
46	RK	501	GDP	C5-C4	2.97	1.46	1.38
46	TK	501	GDP	C5-C4	2.97	1.46	1.38
46	UK	501	GDP	C5-C4	2.97	1.46	1.38
46	OG	501	GDP	C5-C4	2.96	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	SI	501	GDP	C5-C4	2.95	1.46	1.38
46	TG	502	GDP	C5-C4	2.95	1.46	1.38
46	UC	501	GDP	C5-C4	2.95	1.46	1.38
46	VG	501	GDP	C5-C4	2.94	1.46	1.38
46	UI	501	GDP	C5-C4	2.94	1.46	1.38
46	PM	501	GDP	C5-C4	2.94	1.46	1.38
46	SO	502	GDP	C5-C4	2.93	1.46	1.38
46	OO	501	GDP	C5-C4	2.92	1.46	1.38
46	VI	501	GDP	C5-C4	2.92	1.46	1.38
46	YO	501	GDP	C5-C4	2.90	1.46	1.38
46	XK	501	GDP	C5-C4	2.88	1.46	1.38
46	OK	501	GDP	C6-N1	-2.63	1.33	1.38
46	QK	501	GDP	C6-N1	-2.61	1.34	1.38
43	C1	2001	ANP	PG-O1G	2.61	1.50	1.46
46	TK	501	GDP	C6-N1	-2.61	1.34	1.38
46	VG	501	GDP	C6-N1	-2.61	1.34	1.38
46	OC	501	GDP	C6-N1	-2.59	1.34	1.38
46	TG	502	GDP	C6-N1	-2.59	1.34	1.38
46	WM	501	GDP	C6-N1	-2.58	1.34	1.38
46	YG	501	GDP	C6-N1	-2.58	1.34	1.38
46	ZI	501	GDP	C6-N1	-2.57	1.34	1.38
46	PC	501	GDP	C6-N1	-2.57	1.34	1.38
46	PK	501	GDP	C6-N1	-2.57	1.34	1.38
46	TM	502	GDP	C6-N1	-2.56	1.34	1.38
46	QI	501	GDP	C6-N1	-2.56	1.34	1.38
46	NK	501	GDP	C6-N1	-2.56	1.34	1.38
46	SK	501	GDP	C6-N1	-2.55	1.34	1.38
46	XM	502	GDP	C6-N1	-2.55	1.34	1.38
46	UG	501	GDP	C6-N1	-2.55	1.34	1.38
46	OG	501	GDP	C6-N1	-2.55	1.34	1.38
46	NG	502	GDP	C6-N1	-2.55	1.34	1.38
46	WK	501	GDP	C6-N1	-2.55	1.34	1.38
43	C0	2001	ANP	PG-O1G	2.54	1.50	1.46
46	SM	501	GDP	C6-N1	-2.54	1.34	1.38
46	PM	501	GDP	C6-N1	-2.54	1.34	1.38
46	SI	501	GDP	C6-N1	-2.54	1.34	1.38
46	VO	501	GDP	C6-N1	-2.54	1.34	1.38
46	VM	501	GDP	C6-N1	-2.54	1.34	1.38
46	PG	501	GDP	C6-N1	-2.54	1.34	1.38
46	YI	501	GDP	C6-N1	-2.54	1.34	1.38
46	ZG	501	GDP	C6-N1	-2.54	1.34	1.38
46	WI	501	GDP	C6-N1	-2.53	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	SE	501	GDP	C6-N1	-2.53	1.34	1.38
46	UO	501	GDP	C6-N1	-2.53	1.34	1.38
46	UE	501	GDP	C6-N1	-2.53	1.34	1.38
46	QO	501	GDP	C6-N1	-2.53	1.34	1.38
46	RC	501	GDP	C6-N1	-2.53	1.34	1.38
46	QQ	501	GDP	C6-N1	-2.53	1.34	1.38
46	TC	501	GDP	C6-N1	-2.53	1.34	1.38
46	OI	501	GDP	C6-N1	-2.52	1.34	1.38
46	WO	501	GDP	C6-N1	-2.52	1.34	1.38
46	PQ	501	GDP	C6-N1	-2.52	1.34	1.38
46	RI	502	GDP	C6-N1	-2.52	1.34	1.38
46	WG	502	GDP	C6-N1	-2.52	1.34	1.38
46	QC	501	GDP	C6-N1	-2.52	1.34	1.38
46	ZE	501	GDP	C6-N1	-2.52	1.34	1.38
46	ZO	501	GDP	C6-N1	-2.52	1.34	1.38
46	ZM	501	GDP	C6-N1	-2.51	1.34	1.38
46	UM	501	GDP	C6-N1	-2.51	1.34	1.38
43	C0	2001	ANP	PB-O3A	-2.51	1.56	1.59
46	YK	501	GDP	C6-N1	-2.51	1.34	1.38
43	C3	2001	ANP	PG-O1G	2.51	1.50	1.46
46	WC	501	GDP	C6-N1	-2.51	1.34	1.38
46	QG	501	GDP	C6-N1	-2.51	1.34	1.38
46	ZK	501	GDP	C6-N1	-2.50	1.34	1.38
46	YM	501	GDP	C6-N1	-2.50	1.34	1.38
46	YO	501	GDP	C6-N1	-2.50	1.34	1.38
46	PO	501	GDP	C6-N1	-2.50	1.34	1.38
46	XI	501	GDP	C6-N1	-2.50	1.34	1.38
46	TI	501	GDP	C6-N1	-2.50	1.34	1.38
43	C1	2001	ANP	PG-N3B	2.49	1.69	1.63
46	RK	501	GDP	C6-N1	-2.49	1.34	1.38
43	C2	2001	ANP	PG-O1G	2.49	1.50	1.46
46	SC	502	GDP	C6-N1	-2.49	1.34	1.38
46	RE	501	GDP	C6-N1	-2.49	1.34	1.38
46	OQ	501	GDP	C6-N1	-2.49	1.34	1.38
46	XA	501	GDP	C6-N1	-2.49	1.34	1.38
46	TO	501	GDP	C6-N1	-2.48	1.34	1.38
46	SG	502	GDP	C6-N1	-2.48	1.34	1.38
46	VC	501	GDP	C6-N1	-2.48	1.34	1.38
43	C3	2001	ANP	PG-N3B	2.48	1.69	1.63
46	UI	501	GDP	C6-N1	-2.48	1.34	1.38
46	ZC	501	GDP	C6-N1	-2.48	1.34	1.38
46	XE	501	GDP	C6-N1	-2.48	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	VE	501	GDP	C6-N1	-2.48	1.34	1.38
46	WA	501	GDP	C6-N1	-2.48	1.34	1.38
46	XO	501	GDP	C6-N1	-2.48	1.34	1.38
46	RG	501	GDP	C6-N1	-2.47	1.34	1.38
46	UC	501	GDP	C6-N1	-2.47	1.34	1.38
46	NO	501	GDP	C6-N1	-2.47	1.34	1.38
46	XG	501	GDP	C6-N1	-2.47	1.34	1.38
46	QM	501	GDP	C6-N1	-2.47	1.34	1.38
46	VK	501	GDP	C6-N1	-2.47	1.34	1.38
46	XC	501	GDP	C6-N1	-2.46	1.34	1.38
46	YE	501	GDP	C6-N1	-2.46	1.34	1.38
46	YC	501	GDP	C6-N1	-2.46	1.34	1.38
46	RM	501	GDP	C6-N1	-2.46	1.34	1.38
46	OM	501	GDP	C6-N1	-2.46	1.34	1.38
43	1C	2602	ANP	PG-N3B	2.46	1.69	1.63
43	1B	2602	ANP	PG-O1G	2.45	1.49	1.46
46	QE	501	GDP	C6-N1	-2.45	1.34	1.38
46	SO	502	GDP	C6-N1	-2.45	1.34	1.38
46	UK	501	GDP	C6-N1	-2.45	1.34	1.38
46	PE	501	GDP	C6-N1	-2.45	1.34	1.38
43	C1	2001	ANP	PB-O1B	2.45	1.49	1.46
43	C0	2001	ANP	PG-N3B	2.44	1.69	1.63
43	1D	2602	ANP	PG-O1G	2.44	1.49	1.46
46	OE	501	GDP	C6-N1	-2.44	1.34	1.38
46	TE	501	GDP	C6-N1	-2.43	1.34	1.38
46	OO	501	GDP	C6-N1	-2.43	1.34	1.38
46	NE	501	GDP	C6-N1	-2.43	1.34	1.38
46	RO	501	GDP	C6-N1	-2.43	1.34	1.38
43	1B	2602	ANP	PG-N3B	2.43	1.69	1.63
43	1A	2602	ANP	PG-O1G	2.42	1.49	1.46
43	1C	2602	ANP	PB-O1B	2.42	1.49	1.46
46	NC	501	GDP	C6-N1	-2.42	1.34	1.38
46	VI	501	GDP	C6-N1	-2.42	1.34	1.38
46	NM	501	GDP	C6-N1	-2.41	1.34	1.38
46	WE	501	GDP	C6-N1	-2.41	1.34	1.38
46	NI	501	GDP	C6-N1	-2.40	1.34	1.38
46	PI	502	GDP	C6-N1	-2.40	1.34	1.38
43	1A	2602	ANP	PB-O1B	2.38	1.49	1.46
46	XK	501	GDP	C6-N1	-2.38	1.34	1.38
43	1D	2602	ANP	PG-N3B	2.35	1.69	1.63
43	1A	2602	ANP	PG-N3B	2.33	1.69	1.63
43	1D	2602	ANP	PB-O3A	-2.33	1.56	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	1D	2602	ANP	PB-O1B	2.33	1.49	1.46
43	C2	2001	ANP	PG-N3B	2.32	1.69	1.63
43	C0	2001	ANP	PB-O1B	2.32	1.49	1.46
43	C2	2001	ANP	PB-O1B	2.32	1.49	1.46
43	C3	2001	ANP	PB-O1B	2.31	1.49	1.46
46	VG	501	GDP	C5-N7	-2.31	1.34	1.39
42	1D	2601	ADP	C8-N7	2.29	1.36	1.31
43	1B	2602	ANP	PA-O3A	2.28	1.62	1.59
43	C2	2001	ANP	PB-O3A	-2.27	1.56	1.59
42	1B	2601	ADP	C8-N7	2.26	1.36	1.31
46	SO	502	GDP	C4-N9	-2.24	1.32	1.38
42	1A	2601	ADP	C8-N7	2.23	1.36	1.31
46	XK	501	GDP	C4-N9	-2.22	1.32	1.38
44	YB	501	GTP	C2-N3	2.22	1.38	1.33
44	SJ	501	GTP	C2-N3	2.21	1.38	1.33
44	QD	501	GTP	C2-N3	2.20	1.38	1.33
44	RF	501	GTP	C2-N3	2.20	1.38	1.33
43	1C	2602	ANP	PB-O3A	-2.20	1.56	1.59
46	SI	501	GDP	C5-N7	-2.20	1.34	1.39
44	NB	501	GTP	C2-N3	2.19	1.38	1.33
44	UB	501	GTP	C2-N3	2.19	1.38	1.33
44	PP	501	GTP	C2-N3	2.19	1.38	1.33
44	NN	501	GTP	C2-N3	2.19	1.38	1.33
44	SP	501	GTP	C2-N3	2.19	1.38	1.33
43	1B	2602	ANP	PB-O1B	2.19	1.49	1.46
44	OH	501	GTP	C2-N3	2.19	1.38	1.33
44	ND	501	GTP	C2-N3	2.18	1.38	1.33
44	TL	501	GTP	C2-N3	2.18	1.38	1.33
44	UF	501	GTP	C2-N3	2.18	1.38	1.33
44	XB	501	GTP	C2-N3	2.18	1.38	1.33
44	ZB	501	GTP	C2-N3	2.18	1.38	1.33
44	UH	501	GTP	C2-N3	2.18	1.38	1.33
46	VI	501	GDP	C5-N7	-2.18	1.34	1.39
44	QN	501	GTP	C2-N3	2.18	1.38	1.33
44	NL	501	GTP	C2-N3	2.18	1.38	1.33
44	OL	501	GTP	C2-N3	2.18	1.38	1.33
44	YF	501	GTP	C2-N3	2.18	1.38	1.33
44	SB	501	GTP	C2-N3	2.17	1.38	1.33
44	WB	501	GTP	C2-N3	2.17	1.38	1.33
46	QE	501	GDP	C5-N7	-2.17	1.34	1.39
46	QO	501	GDP	C5-N7	-2.17	1.34	1.39
44	RL	501	GTP	C2-N3	2.17	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	QL	501	GTP	C2-N3	2.17	1.38	1.33
44	YN	501	GTP	C2-N3	2.17	1.38	1.33
44	WH	501	GTP	C2-N3	2.17	1.38	1.33
44	WN	501	GTP	C2-N3	2.16	1.38	1.33
44	XN	501	GTP	C2-N3	2.16	1.38	1.33
44	WJ	501	GTP	C2-N3	2.16	1.38	1.33
44	TN	501	GTP	C2-N3	2.16	1.38	1.33
46	WG	502	GDP	C5-N7	-2.16	1.34	1.39
44	PJ	501	GTP	C2-N3	2.16	1.38	1.33
44	SN	501	GTP	C2-N3	2.16	1.38	1.33
46	PO	501	GDP	C5-N7	-2.16	1.34	1.39
44	TB	501	GTP	C2-N3	2.16	1.38	1.33
42	1C	2601	ADP	C8-N7	2.16	1.35	1.31
46	WC	501	GDP	C5-N7	-2.16	1.34	1.39
44	SF	501	GTP	C2-N3	2.16	1.38	1.33
44	TF	501	GTP	C2-N3	2.16	1.38	1.33
44	QJ	501	GTP	C2-N3	2.16	1.38	1.33
44	YD	501	GTP	C2-N3	2.16	1.38	1.33
44	NH	501	GTP	C2-N3	2.15	1.38	1.33
44	SH	501	GTP	C2-N3	2.15	1.38	1.33
44	TJ	501	GTP	C2-N3	2.15	1.38	1.33
46	NG	502	GDP	C5-N7	-2.15	1.34	1.39
44	UP	501	GTP	C2-N3	2.15	1.38	1.33
46	ZG	501	GDP	C5-N7	-2.15	1.34	1.39
43	1C	2602	ANP	PG-O1G	2.15	1.49	1.46
44	OP	501	GTP	C2-N3	2.15	1.38	1.33
46	QK	501	GDP	C5-N7	-2.15	1.34	1.39
44	WL	501	GTP	C2-N3	2.15	1.38	1.33
44	UJ	501	GTP	C2-N3	2.15	1.38	1.33
44	XD	501	GTP	C2-N3	2.15	1.38	1.33
44	UD	501	GTP	C2-N3	2.15	1.38	1.33
44	NF	501	GTP	C2-N3	2.15	1.38	1.33
44	PD	501	GTP	C2-N3	2.14	1.38	1.33
44	UN	501	GTP	C2-N3	2.14	1.38	1.33
44	ON	501	GTP	C2-N3	2.14	1.38	1.33
44	TD	501	GTP	C2-N3	2.14	1.38	1.33
46	QM	501	GDP	C5-N7	-2.14	1.34	1.39
46	UM	501	GDP	C5-N7	-2.14	1.34	1.39
44	SL	501	GTP	C2-N3	2.14	1.38	1.33
44	QH	501	GTP	C2-N3	2.14	1.38	1.33
44	ZJ	501	GTP	C2-N3	2.14	1.38	1.33
46	QC	501	GDP	C5-N7	-2.14	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	OD	501	GTP	C2-N3	2.13	1.38	1.33
44	QP	501	GTP	C2-N3	2.13	1.38	1.33
44	PN	501	GTP	C2-N3	2.13	1.38	1.33
44	VD	501	GTP	C2-N3	2.13	1.38	1.33
44	YP	501	GTP	C2-N3	2.13	1.38	1.33
46	YC	501	GDP	C5-N7	-2.13	1.34	1.39
44	RH	501	GTP	C2-N3	2.13	1.38	1.33
44	XF	501	GTP	C2-N3	2.13	1.38	1.33
42	1C	2601	ADP	C8-N9	-2.12	1.33	1.37
44	VF	501	GTP	C2-N3	2.12	1.38	1.33
44	XH	501	GTP	C2-N3	2.12	1.38	1.33
44	WD	501	GTP	C2-N3	2.12	1.38	1.33
46	XG	501	GDP	C5-N7	-2.12	1.34	1.39
44	VJ	501	GTP	C2-N3	2.12	1.38	1.33
44	PH	501	GTP	C2-N3	2.12	1.38	1.33
46	PC	501	GDP	C5-N7	-2.12	1.34	1.39
44	VL	501	GTP	C2-N3	2.12	1.38	1.33
46	QI	501	GDP	C5-N7	-2.12	1.34	1.39
44	XL	501	GTP	C2-N3	2.12	1.38	1.33
44	YJ	501	GTP	C2-N3	2.12	1.38	1.33
44	PF	501	GTP	C2-N3	2.12	1.38	1.33
46	VO	501	GDP	C5-N7	-2.12	1.34	1.39
44	SD	501	GTP	C2-N3	2.12	1.38	1.33
46	ZO	501	GDP	C5-N7	-2.11	1.34	1.39
44	OJ	501	GTP	C2-N3	2.11	1.38	1.33
44	RD	501	GTP	C2-N3	2.11	1.38	1.33
46	VK	501	GDP	C5-N7	-2.11	1.34	1.39
46	OI	501	GDP	C5-N7	-2.11	1.34	1.39
44	VH	501	GTP	C2-N3	2.11	1.38	1.33
46	NK	501	GDP	C5-N7	-2.11	1.34	1.39
46	SC	502	GDP	C5-N7	-2.11	1.34	1.39
44	QF	501	GTP	C2-N3	2.11	1.38	1.33
46	WK	501	GDP	C5-N7	-2.11	1.34	1.39
42	1A	2601	ADP	C8-N9	-2.11	1.34	1.37
44	PL	501	GTP	C2-N3	2.11	1.38	1.33
44	VB	501	GTP	C2-N3	2.11	1.38	1.33
44	YH	501	GTP	C2-N3	2.11	1.38	1.33
44	ZP	501	GTP	C2-N3	2.11	1.38	1.33
46	OC	501	GDP	C5-N7	-2.11	1.34	1.39
44	TP	501	GTP	C2-N3	2.11	1.38	1.33
46	RC	501	GDP	C5-N7	-2.11	1.34	1.39
46	OK	501	GDP	C5-N7	-2.10	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	OO	501	GDP	C5-N7	-2.10	1.34	1.39
44	ZN	501	GTP	C2-N3	2.10	1.38	1.33
46	SE	501	GDP	C5-N7	-2.10	1.34	1.39
46	ZC	501	GDP	C5-N7	-2.10	1.34	1.39
46	PQ	501	GDP	C5-N7	-2.10	1.34	1.39
46	XM	502	GDP	C5-N7	-2.10	1.34	1.39
46	NO	501	GDP	C5-N7	-2.10	1.34	1.39
46	TI	501	GDP	C5-N7	-2.10	1.34	1.39
46	ZK	501	GDP	C5-N7	-2.10	1.34	1.39
42	1B	2601	ADP	C8-N9	-2.10	1.34	1.37
44	RN	501	GTP	C2-N3	2.10	1.38	1.33
44	ZF	501	GTP	C2-N3	2.10	1.38	1.33
46	SK	501	GDP	C5-N7	-2.10	1.34	1.39
46	UO	501	GDP	C5-N7	-2.10	1.34	1.39
46	ZI	501	GDP	C5-N7	-2.10	1.34	1.39
44	RP	501	GTP	C2-N3	2.10	1.38	1.33
46	UC	501	GDP	C5-N7	-2.10	1.34	1.39
44	OF	501	GTP	C2-N3	2.09	1.38	1.33
46	NM	501	GDP	C5-N7	-2.09	1.34	1.39
46	WI	501	GDP	C5-N7	-2.09	1.34	1.39
46	OQ	501	GDP	C5-N7	-2.09	1.34	1.39
46	OM	501	GDP	C5-N7	-2.09	1.34	1.39
46	PG	501	GDP	C5-N7	-2.09	1.34	1.39
46	PI	502	GDP	C5-N7	-2.09	1.34	1.39
46	YG	501	GDP	C5-N7	-2.09	1.34	1.39
44	UL	501	GTP	C2-N3	2.09	1.38	1.33
44	WF	501	GTP	C2-N3	2.09	1.38	1.33
46	TC	501	GDP	C5-N7	-2.09	1.34	1.39
46	WO	501	GDP	C5-N7	-2.09	1.34	1.39
44	ZL	501	GTP	C2-N3	2.09	1.38	1.33
44	XJ	501	GTP	C2-N3	2.09	1.38	1.33
46	UG	501	GDP	C5-N7	-2.09	1.34	1.39
44	TH	501	GTP	C2-N3	2.08	1.38	1.33
46	SG	502	GDP	C5-N7	-2.08	1.34	1.39
46	SM	501	GDP	C5-N7	-2.08	1.34	1.39
46	WA	501	GDP	C5-N7	-2.08	1.34	1.39
46	PK	501	GDP	C5-N7	-2.08	1.34	1.39
46	PE	501	GDP	C5-N7	-2.08	1.34	1.39
46	TO	501	GDP	C5-N7	-2.08	1.34	1.39
44	VN	501	GTP	C2-N3	2.08	1.38	1.33
46	XA	501	GDP	C5-N7	-2.07	1.34	1.39
46	TE	501	GDP	C5-N7	-2.07	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	RI	502	GDP	C5-N7	-2.07	1.34	1.39
46	ZE	501	GDP	C5-N7	-2.06	1.34	1.39
44	ZD	501	GTP	C2-N3	2.06	1.38	1.33
42	1D	2601	ADP	C8-N9	-2.06	1.34	1.37
46	XC	501	GDP	C5-N7	-2.06	1.34	1.39
46	YO	501	GDP	C5-N7	-2.06	1.34	1.39
46	XI	501	GDP	C5-N7	-2.06	1.34	1.39
46	YE	501	GDP	C5-N7	-2.06	1.34	1.39
46	RK	501	GDP	C5-N7	-2.06	1.34	1.39
46	OE	501	GDP	C5-N7	-2.06	1.34	1.39
46	VC	501	GDP	C5-N7	-2.06	1.34	1.39
46	QQ	501	GDP	C5-N7	-2.06	1.35	1.39
46	WM	501	GDP	C5-N7	-2.06	1.35	1.39
43	C3	2001	ANP	PB-O3A	-2.05	1.56	1.59
46	NC	501	GDP	C5-N7	-2.05	1.35	1.39
46	UK	501	GDP	C5-N7	-2.05	1.35	1.39
46	OG	501	GDP	C5-N7	-2.05	1.35	1.39
46	QG	501	GDP	C5-N7	-2.05	1.35	1.39
44	NJ	501	GTP	C2-N3	2.05	1.38	1.33
46	RO	501	GDP	C5-N7	-2.05	1.35	1.39
46	SO	502	GDP	C5-N7	-2.05	1.35	1.39
46	XO	501	GDP	C5-N7	-2.05	1.35	1.39
46	YK	501	GDP	C5-N7	-2.05	1.35	1.39
46	ZM	501	GDP	C5-N7	-2.04	1.35	1.39
44	ZH	501	GTP	C2-N3	2.04	1.38	1.33
46	TK	501	GDP	C5-N7	-2.04	1.35	1.39
46	VE	501	GDP	C5-N7	-2.04	1.35	1.39
44	NJ	501	GTP	PB-O3B	2.03	1.61	1.59
44	RJ	501	GTP	C2-N3	2.03	1.38	1.33
46	RG	501	GDP	C5-N7	-2.03	1.35	1.39
46	UI	501	GDP	C5-N7	-2.03	1.35	1.39
46	YO	501	GDP	C4-N9	-2.03	1.32	1.38
46	YM	501	GDP	C5-N7	-2.03	1.35	1.39
46	TM	502	GDP	C5-N7	-2.02	1.35	1.39
46	UE	501	GDP	C5-N7	-2.02	1.35	1.39
46	VM	501	GDP	C5-N7	-2.02	1.35	1.39
46	RE	501	GDP	C5-N7	-2.02	1.35	1.39
44	VP	501	GTP	C2-N3	2.01	1.38	1.33
46	RM	501	GDP	C5-N7	-2.01	1.35	1.39
46	PM	501	GDP	C5-N7	-2.01	1.35	1.39
46	NI	501	GDP	C5-N7	-2.01	1.35	1.39
46	TG	502	GDP	C5-N7	-2.00	1.35	1.39

All (1545) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	1B	2601	ADP	C4-C5-N7	-7.74	101.73	110.58
42	1A	2601	ADP	C4-C5-N7	-7.37	102.15	110.58
42	1D	2601	ADP	C4-C5-N7	-7.37	102.15	110.58
42	1C	2601	ADP	C4-C5-N7	-7.35	102.18	110.58
46	RI	502	GDP	C5-C4-N3	-6.28	118.40	128.39
46	XE	501	GDP	C5-C4-N3	-6.26	118.43	128.39
46	YC	501	GDP	C5-C4-N3	-6.24	118.45	128.39
46	ZE	501	GDP	C5-C4-N3	-6.24	118.45	128.39
46	UG	501	GDP	C5-C4-N3	-6.21	118.51	128.39
42	1B	2601	ADP	C6-C5-N7	6.21	144.05	132.09
46	OK	501	GDP	C5-C4-N3	-6.20	118.52	128.39
46	YG	501	GDP	C5-C4-N3	-6.20	118.52	128.39
46	QG	501	GDP	C5-C4-N3	-6.20	118.53	128.39
46	VG	501	GDP	C5-C4-N3	-6.19	118.54	128.39
46	TC	501	GDP	C5-C4-N3	-6.19	118.54	128.39
46	WM	501	GDP	C5-C4-N3	-6.19	118.55	128.39
46	ZO	501	GDP	C5-C4-N3	-6.18	118.55	128.39
46	QO	501	GDP	C5-C4-N3	-6.18	118.56	128.39
46	WO	501	GDP	C5-C4-N3	-6.18	118.56	128.39
46	NG	502	GDP	C5-C4-N3	-6.17	118.57	128.39
46	TK	501	GDP	C5-C4-N3	-6.17	118.57	128.39
46	QK	501	GDP	C5-C4-N3	-6.17	118.57	128.39
46	QC	501	GDP	C5-C4-N3	-6.16	118.58	128.39
46	TO	501	GDP	C5-C4-N3	-6.16	118.59	128.39
46	NO	501	GDP	C5-C4-N3	-6.16	118.59	128.39
46	WC	501	GDP	C5-C4-N3	-6.16	118.59	128.39
46	SG	502	GDP	C5-C4-N3	-6.16	118.59	128.39
46	PQ	501	GDP	C5-C4-N3	-6.15	118.60	128.39
46	PC	501	GDP	C5-C4-N3	-6.15	118.60	128.39
46	UM	501	GDP	C5-C4-N3	-6.15	118.60	128.39
46	PO	501	GDP	C5-C4-N3	-6.15	118.61	128.39
46	QE	501	GDP	C5-C4-N3	-6.14	118.62	128.39
46	XC	501	GDP	C5-C4-N3	-6.14	118.62	128.39
46	VC	501	GDP	C5-C4-N3	-6.13	118.63	128.39
46	SK	501	GDP	C5-C4-N3	-6.13	118.64	128.39
46	OG	501	GDP	C5-C4-N3	-6.12	118.65	128.39
46	SE	501	GDP	C5-C4-N3	-6.11	118.67	128.39
46	XM	502	GDP	C5-C4-N3	-6.11	118.67	128.39
46	RC	501	GDP	C5-C4-N3	-6.09	118.69	128.39
46	WK	501	GDP	C5-C4-N3	-6.09	118.70	128.39
46	OC	501	GDP	C5-C4-N3	-6.09	118.70	128.39
46	WG	502	GDP	C5-C4-N3	-6.09	118.70	128.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	ZK	501	GDP	C5-C4-N3	-6.09	118.70	128.39
46	YE	501	GDP	C5-C4-N3	-6.08	118.71	128.39
46	YK	501	GDP	C5-C4-N3	-6.08	118.72	128.39
46	TE	501	GDP	C5-C4-N3	-6.07	118.72	128.39
46	OM	501	GDP	C5-C4-N3	-6.07	118.73	128.39
46	RM	501	GDP	C5-C4-N3	-6.07	118.73	128.39
46	WI	501	GDP	C5-C4-N3	-6.07	118.73	128.39
46	UE	501	GDP	C5-C4-N3	-6.07	118.73	128.39
46	ZI	501	GDP	C5-C4-N3	-6.07	118.73	128.39
46	SC	502	GDP	C5-C4-N3	-6.06	118.74	128.39
46	UO	501	GDP	C5-C4-N3	-6.06	118.75	128.39
46	XI	501	GDP	C5-C4-N3	-6.06	118.75	128.39
46	VO	501	GDP	C5-C4-N3	-6.06	118.75	128.39
46	QQ	501	GDP	C5-C4-N3	-6.06	118.75	128.39
46	PG	501	GDP	C5-C4-N3	-6.05	118.75	128.39
46	OI	501	GDP	C5-C4-N3	-6.05	118.76	128.39
46	PE	501	GDP	C5-C4-N3	-6.05	118.77	128.39
46	OE	501	GDP	C5-C4-N3	-6.04	118.77	128.39
46	ZG	501	GDP	C5-C4-N3	-6.04	118.77	128.39
46	OQ	501	GDP	C5-C4-N3	-6.04	118.78	128.39
42	1D	2601	ADP	C6-C5-N7	6.04	143.73	132.09
46	QI	501	GDP	C5-C4-N3	-6.03	118.80	128.39
46	RG	501	GDP	C5-C4-N3	-6.02	118.81	128.39
46	SM	501	GDP	C5-C4-N3	-6.01	118.82	128.39
46	TI	501	GDP	C5-C4-N3	-6.01	118.83	128.39
46	PI	502	GDP	C5-C4-N3	-6.00	118.84	128.39
46	WA	501	GDP	C5-C4-N3	-5.99	118.85	128.39
46	RE	501	GDP	C5-C4-N3	-5.99	118.86	128.39
46	VK	501	GDP	C5-C4-N3	-5.98	118.87	128.39
46	RO	501	GDP	C5-C4-N3	-5.98	118.88	128.39
46	TM	502	GDP	C5-C4-N3	-5.98	118.88	128.39
46	UC	501	GDP	C5-C4-N3	-5.97	118.88	128.39
46	NK	501	GDP	C5-C4-N3	-5.97	118.89	128.39
46	QM	501	GDP	C5-C4-N3	-5.97	118.89	128.39
46	VM	501	GDP	C5-C4-N3	-5.96	118.90	128.39
46	XG	501	GDP	C5-C4-N3	-5.95	118.92	128.39
46	RK	501	GDP	C5-C4-N3	-5.94	118.93	128.39
46	YM	501	GDP	C5-C4-N3	-5.94	118.94	128.39
46	PK	501	GDP	C5-C4-N3	-5.93	118.95	128.39
46	TG	502	GDP	C5-C4-N3	-5.89	119.02	128.39
46	UI	501	GDP	C5-C4-N3	-5.89	119.02	128.39
46	NC	501	GDP	C5-C4-N3	-5.89	119.02	128.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	SI	501	GDP	C5-C4-N3	-5.87	119.04	128.39
46	NM	501	GDP	C5-C4-N3	-5.87	119.05	128.39
42	1A	2601	ADP	C6-C5-N7	5.87	143.40	132.09
46	XO	501	GDP	C5-C4-N3	-5.86	119.07	128.39
42	1C	2601	ADP	C6-C5-N7	5.86	143.38	132.09
46	ZM	501	GDP	C5-C4-N3	-5.83	119.11	128.39
46	YI	501	GDP	C5-C4-N3	-5.83	119.11	128.39
46	NI	501	GDP	C5-C4-N3	-5.83	119.12	128.39
46	NE	501	GDP	C5-C4-N3	-5.81	119.15	128.39
46	XA	501	GDP	C5-C4-N3	-5.78	119.19	128.39
46	WE	501	GDP	C5-C4-N3	-5.78	119.19	128.39
46	OO	501	GDP	C5-C4-N3	-5.77	119.20	128.39
46	ZC	501	GDP	C5-C4-N3	-5.77	119.21	128.39
46	VI	501	GDP	C5-C4-N3	-5.75	119.23	128.39
46	YO	501	GDP	C5-C4-N3	-5.74	119.26	128.39
46	UK	501	GDP	C5-C4-N3	-5.74	119.26	128.39
46	VE	501	GDP	C5-C4-N3	-5.68	119.36	128.39
46	PM	501	GDP	C5-C4-N3	-5.62	119.44	128.39
46	XK	501	GDP	C5-C4-N3	-5.26	120.02	128.39
44	NH	501	GTP	C5-C4-N3	-5.26	120.02	128.39
46	SO	502	GDP	C5-C4-N3	-5.24	120.05	128.39
44	NB	501	GTP	C5-C4-N3	-5.20	120.12	128.39
44	TL	501	GTP	C5-C4-N3	-5.15	120.19	128.39
44	UH	501	GTP	C5-C4-N3	-5.15	120.20	128.39
44	SH	501	GTP	C5-C4-N3	-5.14	120.20	128.39
42	1B	2601	ADP	C5-N7-C8	5.14	111.53	103.45
44	PP	501	GTP	C5-C4-N3	-5.14	120.20	128.39
44	NN	501	GTP	C5-C4-N3	-5.14	120.21	128.39
44	WL	501	GTP	C5-C4-N3	-5.14	120.21	128.39
44	SP	501	GTP	C5-C4-N3	-5.14	120.22	128.39
44	PH	501	GTP	C5-C4-N3	-5.13	120.22	128.39
44	NJ	501	GTP	C5-C4-N3	-5.12	120.24	128.39
46	RI	502	GDP	C2-N3-C4	5.12	121.11	112.30
44	UN	501	GTP	C5-C4-N3	-5.11	120.25	128.39
46	XE	501	GDP	C2-N3-C4	5.11	121.11	112.30
44	QD	501	GTP	C5-C4-N3	-5.11	120.26	128.39
44	QN	501	GTP	C5-C4-N3	-5.11	120.26	128.39
44	VL	501	GTP	C5-C4-N3	-5.11	120.26	128.39
44	ON	501	GTP	C5-C4-N3	-5.11	120.27	128.39
44	SF	501	GTP	C5-C4-N3	-5.10	120.27	128.39
44	ND	501	GTP	C5-C4-N3	-5.10	120.27	128.39
46	UG	501	GDP	C2-N3-C4	5.10	121.09	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	SJ	501	GTP	C5-C4-N3	-5.09	120.28	128.39
44	OL	501	GTP	C5-C4-N3	-5.09	120.29	128.39
46	QK	501	GDP	C2-N3-C4	5.09	121.06	112.30
44	WN	501	GTP	C5-C4-N3	-5.08	120.30	128.39
44	UJ	501	GTP	C5-C4-N3	-5.08	120.30	128.39
46	OG	501	GDP	C2-N3-C4	5.08	121.05	112.30
46	QO	501	GDP	C2-N3-C4	5.08	121.05	112.30
44	QF	501	GTP	C5-C4-N3	-5.08	120.31	128.39
44	QL	501	GTP	C5-C4-N3	-5.08	120.31	128.39
44	NL	501	GTP	C5-C4-N3	-5.08	120.31	128.39
44	XH	501	GTP	C5-C4-N3	-5.08	120.31	128.39
46	UM	501	GDP	C2-N3-C4	5.07	121.04	112.30
44	WJ	501	GTP	C5-C4-N3	-5.07	120.32	128.39
44	OP	501	GTP	C5-C4-N3	-5.07	120.32	128.39
44	WH	501	GTP	C5-C4-N3	-5.07	120.32	128.39
46	TC	501	GDP	C2-N3-C4	5.07	121.03	112.30
44	WF	501	GTP	C5-C4-N3	-5.07	120.33	128.39
44	ZJ	501	GTP	C5-C4-N3	-5.07	120.33	128.39
44	SB	501	GTP	C5-C4-N3	-5.07	120.33	128.39
42	1C	2601	ADP	C5-N7-C8	5.07	111.41	103.45
46	OK	501	GDP	C2-N3-C4	5.07	121.03	112.30
46	XI	501	GDP	C2-N3-C4	5.06	121.02	112.30
46	YC	501	GDP	C2-N3-C4	5.06	121.02	112.30
46	QC	501	GDP	C2-N3-C4	5.06	121.02	112.30
44	TJ	501	GTP	C5-C4-N3	-5.06	120.33	128.39
44	RF	501	GTP	C5-C4-N3	-5.06	120.34	128.39
44	YP	501	GTP	C5-C4-N3	-5.06	120.34	128.39
46	WM	501	GDP	C2-N3-C4	5.05	121.00	112.30
46	WK	501	GDP	C2-N3-C4	5.05	121.00	112.30
46	NO	501	GDP	C2-N3-C4	5.05	121.00	112.30
46	ZE	501	GDP	C2-N3-C4	5.05	121.00	112.30
46	TO	501	GDP	C2-N3-C4	5.05	120.99	112.30
46	PO	501	GDP	C2-N3-C4	5.04	120.98	112.30
46	XM	502	GDP	C2-N3-C4	5.04	120.98	112.30
46	RM	501	GDP	C2-N3-C4	5.04	120.98	112.30
46	RE	501	GDP	C2-N3-C4	5.04	120.98	112.30
46	SG	502	GDP	C2-N3-C4	5.04	120.98	112.30
44	QJ	501	GTP	C5-C4-N3	-5.04	120.37	128.39
44	VD	501	GTP	C5-C4-N3	-5.04	120.37	128.39
42	1A	2601	ADP	C5-N7-C8	5.04	111.37	103.45
44	YH	501	GTP	C5-C4-N3	-5.04	120.37	128.39
44	YD	501	GTP	C5-C4-N3	-5.04	120.38	128.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	YG	501	GDP	C2-N3-C4	5.03	120.97	112.30
44	PD	501	GTP	C5-C4-N3	-5.03	120.38	128.39
44	VJ	501	GTP	C5-C4-N3	-5.03	120.38	128.39
46	SE	501	GDP	C2-N3-C4	5.03	120.96	112.30
44	PN	501	GTP	C5-C4-N3	-5.03	120.39	128.39
46	UO	501	GDP	C2-N3-C4	5.03	120.96	112.30
44	XB	501	GTP	C5-C4-N3	-5.03	120.39	128.39
46	PQ	501	GDP	C2-N3-C4	5.03	120.96	112.30
46	XC	501	GDP	C2-N3-C4	5.03	120.96	112.30
46	QG	501	GDP	C2-N3-C4	5.02	120.95	112.30
44	NF	501	GTP	C5-C4-N3	-5.02	120.40	128.39
46	RK	501	GDP	C2-N3-C4	5.02	120.95	112.30
46	TE	501	GDP	C2-N3-C4	5.02	120.95	112.30
44	YB	501	GTP	C5-C4-N3	-5.02	120.40	128.39
46	WO	501	GDP	C2-N3-C4	5.02	120.95	112.30
46	YK	501	GDP	C2-N3-C4	5.02	120.95	112.30
46	OE	501	GDP	C2-N3-C4	5.02	120.95	112.30
46	WC	501	GDP	C2-N3-C4	5.02	120.95	112.30
46	OM	501	GDP	C2-N3-C4	5.02	120.94	112.30
46	YE	501	GDP	C2-N3-C4	5.02	120.94	112.30
44	SL	501	GTP	C5-C4-N3	-5.02	120.40	128.39
44	WD	501	GTP	C5-C4-N3	-5.02	120.40	128.39
46	RC	501	GDP	C2-N3-C4	5.02	120.94	112.30
46	ZI	501	GDP	C2-N3-C4	5.02	120.94	112.30
44	SD	501	GTP	C5-C4-N3	-5.02	120.41	128.39
46	OQ	501	GDP	C2-N3-C4	5.02	120.94	112.30
46	SK	501	GDP	C2-N3-C4	5.02	120.94	112.30
44	XF	501	GTP	C5-C4-N3	-5.02	120.41	128.39
46	RG	501	GDP	C2-N3-C4	5.01	120.94	112.30
46	PE	501	GDP	C2-N3-C4	5.01	120.93	112.30
46	UE	501	GDP	C2-N3-C4	5.01	120.93	112.30
46	ZO	501	GDP	C2-N3-C4	5.01	120.93	112.30
46	ZK	501	GDP	C2-N3-C4	5.01	120.93	112.30
46	VM	501	GDP	C2-N3-C4	5.01	120.93	112.30
46	SC	502	GDP	C2-N3-C4	5.01	120.93	112.30
46	TK	501	GDP	C2-N3-C4	5.01	120.93	112.30
44	PJ	501	GTP	C5-C4-N3	-5.01	120.42	128.39
44	WB	501	GTP	C5-C4-N3	-5.01	120.42	128.39
46	VC	501	GDP	C2-N3-C4	5.01	120.93	112.30
44	UP	501	GTP	C5-C4-N3	-5.01	120.42	128.39
46	QQ	501	GDP	C2-N3-C4	5.01	120.92	112.30
44	TB	501	GTP	C5-C4-N3	-5.01	120.42	128.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	SM	501	GDP	C2-N3-C4	5.00	120.92	112.30
46	PC	501	GDP	C2-N3-C4	5.00	120.92	112.30
46	UI	501	GDP	C2-N3-C4	5.00	120.92	112.30
46	UC	501	GDP	C2-N3-C4	5.00	120.91	112.30
46	XO	501	GDP	C2-N3-C4	5.00	120.91	112.30
46	OI	501	GDP	C2-N3-C4	5.00	120.91	112.30
46	NG	502	GDP	C2-N3-C4	5.00	120.91	112.30
44	XL	501	GTP	C5-C4-N3	-5.00	120.44	128.39
46	RO	501	GDP	C2-N3-C4	5.00	120.91	112.30
46	WA	501	GDP	C2-N3-C4	4.99	120.90	112.30
46	QI	501	GDP	C2-N3-C4	4.99	120.90	112.30
44	TN	501	GTP	C5-C4-N3	-4.99	120.44	128.39
44	TF	501	GTP	C5-C4-N3	-4.99	120.45	128.39
46	YI	501	GDP	C2-N3-C4	4.99	120.89	112.30
44	VH	501	GTP	C5-C4-N3	-4.99	120.45	128.39
44	YF	501	GTP	C5-C4-N3	-4.99	120.45	128.39
46	VK	501	GDP	C2-N3-C4	4.98	120.89	112.30
44	RL	501	GTP	C5-C4-N3	-4.98	120.46	128.39
46	PG	501	GDP	C2-N3-C4	4.98	120.88	112.30
44	UD	501	GTP	C5-C4-N3	-4.98	120.47	128.39
46	QM	501	GDP	C2-N3-C4	4.98	120.87	112.30
44	XD	501	GTP	C5-C4-N3	-4.98	120.47	128.39
46	PI	502	GDP	C2-N3-C4	4.98	120.87	112.30
42	1D	2601	ADP	C5-N7-C8	4.98	111.27	103.45
46	XG	501	GDP	C2-N3-C4	4.98	120.87	112.30
46	VO	501	GDP	C2-N3-C4	4.97	120.87	112.30
46	TM	502	GDP	C2-N3-C4	4.97	120.87	112.30
46	OC	501	GDP	C2-N3-C4	4.97	120.86	112.30
44	UB	501	GTP	C5-C4-N3	-4.97	120.48	128.39
46	PK	501	GDP	C2-N3-C4	4.97	120.86	112.30
46	WI	501	GDP	C2-N3-C4	4.97	120.86	112.30
44	QH	501	GTP	C5-C4-N3	-4.97	120.49	128.39
44	ZN	501	GTP	C5-C4-N3	-4.96	120.49	128.39
44	TD	501	GTP	C5-C4-N3	-4.96	120.49	128.39
44	SN	501	GTP	C5-C4-N3	-4.96	120.50	128.39
44	YN	501	GTP	C5-C4-N3	-4.96	120.50	128.39
44	TP	501	GTP	C5-C4-N3	-4.96	120.50	128.39
44	PF	501	GTP	C5-C4-N3	-4.95	120.50	128.39
44	OD	501	GTP	C5-C4-N3	-4.95	120.51	128.39
46	TG	502	GDP	C2-N3-C4	4.95	120.83	112.30
44	ZL	501	GTP	C5-C4-N3	-4.95	120.51	128.39
46	QE	501	GDP	C2-N3-C4	4.95	120.83	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	UF	501	GTP	C5-C4-N3	-4.95	120.51	128.39
44	RN	501	GTP	C5-C4-N3	-4.95	120.52	128.39
46	VG	501	GDP	C2-N3-C4	4.95	120.82	112.30
46	WG	502	GDP	C2-N3-C4	4.95	120.82	112.30
46	TI	501	GDP	C2-N3-C4	4.94	120.81	112.30
44	QP	501	GTP	C5-C4-N3	-4.94	120.53	128.39
44	TH	501	GTP	C5-C4-N3	-4.94	120.53	128.39
44	RP	501	GTP	C5-C4-N3	-4.94	120.53	128.39
46	PM	501	GDP	C2-N3-C4	4.94	120.81	112.30
44	OJ	501	GTP	C5-C4-N3	-4.94	120.53	128.39
44	XN	501	GTP	C5-C4-N3	-4.93	120.55	128.39
46	YM	501	GDP	C2-N3-C4	4.93	120.79	112.30
46	WE	501	GDP	C2-N3-C4	4.92	120.78	112.30
46	NM	501	GDP	C2-N3-C4	4.92	120.77	112.30
46	ZG	501	GDP	C2-N3-C4	4.92	120.77	112.30
46	NC	501	GDP	C2-N3-C4	4.92	120.77	112.30
46	NI	501	GDP	C2-N3-C4	4.91	120.77	112.30
44	RH	501	GTP	C5-C4-N3	-4.91	120.58	128.39
46	OO	501	GDP	C2-N3-C4	4.91	120.75	112.30
44	OF	501	GTP	C5-C4-N3	-4.90	120.59	128.39
44	VF	501	GTP	C5-C4-N3	-4.90	120.59	128.39
44	ZP	501	GTP	C5-C4-N3	-4.90	120.59	128.39
44	ZB	501	GTP	C5-C4-N3	-4.90	120.60	128.39
46	NK	501	GDP	C2-N3-C4	4.90	120.73	112.30
46	ZM	501	GDP	C2-N3-C4	4.89	120.72	112.30
44	VN	501	GTP	C5-C4-N3	-4.89	120.61	128.39
44	RD	501	GTP	C5-C4-N3	-4.88	120.62	128.39
44	VB	501	GTP	C5-C4-N3	-4.88	120.62	128.39
46	NE	501	GDP	C2-N3-C4	4.88	120.70	112.30
46	VI	501	GDP	C2-N3-C4	4.88	120.70	112.30
44	YJ	501	GTP	C5-C4-N3	-4.88	120.63	128.39
44	PL	501	GTP	C5-C4-N3	-4.87	120.64	128.39
44	XJ	501	GTP	C5-C4-N3	-4.87	120.64	128.39
44	OH	501	GTP	C5-C4-N3	-4.86	120.65	128.39
46	VE	501	GDP	C2-N3-C4	4.85	120.66	112.30
44	ZD	501	GTP	C5-C4-N3	-4.85	120.67	128.39
44	UL	501	GTP	C5-C4-N3	-4.85	120.68	128.39
44	RJ	501	GTP	C5-C4-N3	-4.84	120.68	128.39
46	XA	501	GDP	C2-N3-C4	4.83	120.62	112.30
46	SI	501	GDP	C2-N3-C4	4.83	120.62	112.30
46	ZC	501	GDP	C2-N3-C4	4.82	120.61	112.30
44	NH	501	GTP	C2-N3-C4	4.82	120.61	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	ZF	501	GTP	C5-C4-N3	-4.82	120.72	128.39
44	YL	501	GTP	C5-C4-N3	-4.82	120.72	128.39
46	UK	501	GDP	C2-N3-C4	4.80	120.57	112.30
44	ZH	501	GTP	C5-C4-N3	-4.80	120.75	128.39
46	YO	501	GDP	C2-N3-C4	4.80	120.57	112.30
46	OK	501	GDP	N9-C4-N3	4.75	135.45	125.95
46	PC	501	GDP	N9-C4-N3	4.74	135.43	125.95
46	XK	501	GDP	C2-N3-C4	4.72	120.44	112.30
46	UC	501	GDP	N9-C4-N3	4.72	135.40	125.95
44	SF	501	GTP	C2-N3-C4	4.72	120.43	112.30
44	VP	501	GTP	C5-C4-N3	-4.72	120.88	128.39
44	UJ	501	GTP	C2-N3-C4	4.71	120.41	112.30
46	VG	501	GDP	N9-C4-N3	4.70	135.36	125.95
44	SJ	501	GTP	C2-N3-C4	4.70	120.39	112.30
44	UN	501	GTP	C2-N3-C4	4.69	120.38	112.30
44	QF	501	GTP	C2-N3-C4	4.69	120.37	112.30
44	SP	501	GTP	C2-N3-C4	4.68	120.37	112.30
44	UH	501	GTP	C2-N3-C4	4.68	120.37	112.30
44	PJ	501	GTP	C2-N3-C4	4.68	120.36	112.30
44	RP	501	GTP	C2-N3-C4	4.67	120.35	112.30
44	NJ	501	GTP	C2-N3-C4	4.67	120.35	112.30
46	OM	501	GDP	N9-C4-N3	4.67	135.29	125.95
44	TP	501	GTP	C2-N3-C4	4.67	120.34	112.30
44	SH	501	GTP	C2-N3-C4	4.67	120.34	112.30
44	RN	501	GTP	C2-N3-C4	4.67	120.34	112.30
46	ZE	501	GDP	N9-C4-N3	4.67	135.28	125.95
44	WF	501	GTP	C2-N3-C4	4.66	120.33	112.30
44	WL	501	GTP	C2-N3-C4	4.66	120.32	112.30
46	RI	502	GDP	N9-C4-N3	4.66	135.26	125.95
44	QD	501	GTP	C2-N3-C4	4.66	120.32	112.30
46	UG	501	GDP	N9-C4-N3	4.65	135.25	125.95
44	XF	501	GTP	C2-N3-C4	4.65	120.31	112.30
44	ZJ	501	GTP	C2-N3-C4	4.65	120.31	112.30
44	WH	501	GTP	C2-N3-C4	4.65	120.31	112.30
44	VL	501	GTP	C2-N3-C4	4.65	120.30	112.30
44	OP	501	GTP	C2-N3-C4	4.64	120.30	112.30
44	RL	501	GTP	C2-N3-C4	4.64	120.29	112.30
44	YH	501	GTP	C2-N3-C4	4.64	120.29	112.30
44	PD	501	GTP	C2-N3-C4	4.64	120.29	112.30
44	TN	501	GTP	C2-N3-C4	4.64	120.29	112.30
46	NE	501	GDP	N9-C4-N3	4.64	135.23	125.95
44	TJ	501	GTP	C2-N3-C4	4.64	120.29	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	WJ	501	GTP	C2-N3-C4	4.63	120.28	112.30
44	QL	501	GTP	C2-N3-C4	4.63	120.28	112.30
44	RF	501	GTP	C2-N3-C4	4.63	120.28	112.30
44	YP	501	GTP	C2-N3-C4	4.63	120.28	112.30
44	XL	501	GTP	C2-N3-C4	4.63	120.28	112.30
44	NB	501	GTP	C2-N3-C4	4.63	120.28	112.30
44	TH	501	GTP	C2-N3-C4	4.63	120.28	112.30
44	WD	501	GTP	C2-N3-C4	4.63	120.27	112.30
46	PO	501	GDP	N9-C4-N3	4.63	135.20	125.95
46	SG	502	GDP	N9-C4-N3	4.62	135.20	125.95
44	UD	501	GTP	C2-N3-C4	4.62	120.26	112.30
44	NF	501	GTP	C2-N3-C4	4.62	120.26	112.30
44	PL	501	GTP	C2-N3-C4	4.62	120.26	112.30
44	SL	501	GTP	C2-N3-C4	4.62	120.26	112.30
44	TB	501	GTP	C2-N3-C4	4.62	120.26	112.30
44	WN	501	GTP	C2-N3-C4	4.62	120.26	112.30
46	YC	501	GDP	N9-C4-N3	4.62	135.19	125.95
44	ND	501	GTP	C2-N3-C4	4.62	120.26	112.30
44	PP	501	GTP	C2-N3-C4	4.62	120.26	112.30
44	QH	501	GTP	C2-N3-C4	4.62	120.26	112.30
44	PN	501	GTP	C2-N3-C4	4.62	120.25	112.30
44	NN	501	GTP	C2-N3-C4	4.62	120.25	112.30
44	ZH	501	GTP	C2-N3-C4	4.62	120.25	112.30
44	ZN	501	GTP	C2-N3-C4	4.61	120.25	112.30
44	XH	501	GTP	C2-N3-C4	4.61	120.24	112.30
44	QN	501	GTP	C2-N3-C4	4.61	120.24	112.30
44	UF	501	GTP	C2-N3-C4	4.61	120.24	112.30
46	XM	502	GDP	N9-C4-N3	4.61	135.17	125.95
46	ZO	501	GDP	N9-C4-N3	4.61	135.16	125.95
44	ON	501	GTP	C2-N3-C4	4.61	120.23	112.30
46	TK	501	GDP	N9-C4-N3	4.61	135.16	125.95
44	OL	501	GTP	C2-N3-C4	4.61	120.23	112.30
46	YM	501	GDP	N9-C4-N3	4.60	135.16	125.95
44	TF	501	GTP	C2-N3-C4	4.60	120.23	112.30
44	QP	501	GTP	C2-N3-C4	4.60	120.23	112.30
44	YB	501	GTP	C2-N3-C4	4.60	120.23	112.30
44	UP	501	GTP	C2-N3-C4	4.60	120.23	112.30
44	QJ	501	GTP	C2-N3-C4	4.60	120.23	112.30
44	SB	501	GTP	C2-N3-C4	4.60	120.22	112.30
44	OF	501	GTP	C2-N3-C4	4.60	120.22	112.30
44	XB	501	GTP	C2-N3-C4	4.60	120.22	112.30
44	RH	501	GTP	C2-N3-C4	4.60	120.22	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	TL	501	GTP	C2-N3-C4	4.59	120.21	112.30
44	VD	501	GTP	C2-N3-C4	4.59	120.21	112.30
46	QE	501	GDP	N9-C4-N3	4.59	135.14	125.95
44	YN	501	GTP	C2-N3-C4	4.59	120.21	112.30
46	XE	501	GDP	N9-C4-N3	4.59	135.13	125.95
44	UB	501	GTP	C2-N3-C4	4.59	120.21	112.30
44	YF	501	GTP	C2-N3-C4	4.59	120.21	112.30
44	PH	501	GTP	C2-N3-C4	4.59	120.21	112.30
44	PF	501	GTP	C2-N3-C4	4.59	120.20	112.30
44	XD	501	GTP	C2-N3-C4	4.59	120.20	112.30
44	SD	501	GTP	C2-N3-C4	4.59	120.20	112.30
46	YG	501	GDP	N9-C4-N3	4.58	135.12	125.95
44	OJ	501	GTP	C2-N3-C4	4.58	120.20	112.30
44	VH	501	GTP	C2-N3-C4	4.58	120.20	112.30
46	NO	501	GDP	N9-C4-N3	4.58	135.12	125.95
44	NL	501	GTP	C2-N3-C4	4.58	120.19	112.30
46	NG	502	GDP	N9-C4-N3	4.58	135.11	125.95
44	WB	501	GTP	C2-N3-C4	4.58	120.19	112.30
44	YD	501	GTP	C2-N3-C4	4.58	120.19	112.30
44	YJ	501	GTP	C2-N3-C4	4.58	120.19	112.30
44	OD	501	GTP	C2-N3-C4	4.58	120.19	112.30
44	VP	501	GTP	C2-N3-C4	4.58	120.19	112.30
44	TD	501	GTP	C2-N3-C4	4.58	120.18	112.30
44	VN	501	GTP	C2-N3-C4	4.57	120.18	112.30
46	VO	501	GDP	N9-C4-N3	4.57	135.10	125.95
46	UM	501	GDP	N9-C4-N3	4.57	135.09	125.95
44	ZL	501	GTP	C2-N3-C4	4.57	120.17	112.30
46	SO	502	GDP	C2-N3-C4	4.57	120.17	112.30
44	ZD	501	GTP	C2-N3-C4	4.57	120.17	112.30
46	WC	501	GDP	N9-C4-N3	4.57	135.09	125.95
44	XN	501	GTP	C2-N3-C4	4.57	120.17	112.30
44	RD	501	GTP	C2-N3-C4	4.57	120.17	112.30
46	TC	501	GDP	N9-C4-N3	4.57	135.09	125.95
44	VJ	501	GTP	C2-N3-C4	4.57	120.17	112.30
46	SE	501	GDP	N9-C4-N3	4.56	135.07	125.95
46	QK	501	GDP	N9-C4-N3	4.56	135.07	125.95
46	SK	501	GDP	N9-C4-N3	4.56	135.07	125.95
44	XJ	501	GTP	C2-N3-C4	4.56	120.15	112.30
46	PQ	501	GDP	N9-C4-N3	4.56	135.06	125.95
44	VF	501	GTP	C2-N3-C4	4.55	120.14	112.30
44	SN	501	GTP	C2-N3-C4	4.55	120.13	112.30
44	UL	501	GTP	C2-N3-C4	4.55	120.13	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	OQ	501	GDP	N9-C4-N3	4.55	135.04	125.95
46	WM	501	GDP	N9-C4-N3	4.54	135.03	125.95
46	UO	501	GDP	N9-C4-N3	4.54	135.03	125.95
46	WO	501	GDP	N9-C4-N3	4.53	135.02	125.95
44	ZF	501	GTP	C2-N3-C4	4.53	120.11	112.30
46	TO	501	GDP	N9-C4-N3	4.53	135.01	125.95
46	QC	501	GDP	N9-C4-N3	4.53	135.01	125.95
46	ZG	501	GDP	N9-C4-N3	4.53	135.01	125.95
46	YE	501	GDP	N9-C4-N3	4.53	135.00	125.95
46	SI	501	GDP	N9-C4-N3	4.52	135.00	125.95
46	QO	501	GDP	N9-C4-N3	4.52	135.00	125.95
46	QQ	501	GDP	N9-C4-N3	4.52	135.00	125.95
46	WG	502	GDP	N9-C4-N3	4.52	134.99	125.95
46	OG	501	GDP	N9-C4-N3	4.52	134.99	125.95
44	YL	501	GTP	C2-N3-C4	4.52	120.08	112.30
46	OC	501	GDP	N9-C4-N3	4.52	134.98	125.95
46	ZK	501	GDP	N9-C4-N3	4.52	134.98	125.95
46	WI	501	GDP	N9-C4-N3	4.51	134.98	125.95
44	RJ	501	GTP	C2-N3-C4	4.51	120.07	112.30
44	ZB	501	GTP	C2-N3-C4	4.51	120.07	112.30
46	VC	501	GDP	N9-C4-N3	4.51	134.97	125.95
44	ZP	501	GTP	C2-N3-C4	4.51	120.06	112.30
42	1B	2601	ADP	N3-C2-N1	-4.51	121.76	128.58
46	QM	501	GDP	N9-C4-N3	4.51	134.96	125.95
46	OI	501	GDP	N9-C4-N3	4.50	134.96	125.95
44	OH	501	GTP	C2-N3-C4	4.50	120.06	112.30
46	XC	501	GDP	N9-C4-N3	4.50	134.95	125.95
44	VB	501	GTP	C2-N3-C4	4.50	120.05	112.30
46	SC	502	GDP	N9-C4-N3	4.50	134.94	125.95
46	WA	501	GDP	N9-C4-N3	4.49	134.93	125.95
46	UE	501	GDP	N9-C4-N3	4.49	134.93	125.95
46	PE	501	GDP	N9-C4-N3	4.49	134.93	125.95
46	RC	501	GDP	N9-C4-N3	4.49	134.93	125.95
46	QG	501	GDP	N9-C4-N3	4.48	134.91	125.95
46	OE	501	GDP	N9-C4-N3	4.48	134.90	125.95
46	QI	501	GDP	N9-C4-N3	4.47	134.89	125.95
46	YK	501	GDP	N9-C4-N3	4.46	134.88	125.95
46	ZI	501	GDP	N9-C4-N3	4.46	134.88	125.95
42	1B	2601	ADP	C5-C4-N3	-4.46	120.57	126.72
46	WK	501	GDP	N9-C4-N3	4.45	134.86	125.95
46	TM	502	GDP	N9-C4-N3	4.45	134.85	125.95
46	VK	501	GDP	N9-C4-N3	4.45	134.84	125.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	ZC	501	GDP	N9-C4-N3	4.45	134.84	125.95
46	TE	501	GDP	N9-C4-N3	4.44	134.84	125.95
46	SM	501	GDP	N9-C4-N3	4.44	134.83	125.95
46	XG	501	GDP	N9-C4-N3	4.44	134.83	125.95
46	NK	501	GDP	N9-C4-N3	4.42	134.80	125.95
46	TG	502	GDP	N9-C4-N3	4.42	134.79	125.95
46	TI	501	GDP	N9-C4-N3	4.42	134.79	125.95
46	PG	501	GDP	N9-C4-N3	4.42	134.78	125.95
46	PI	502	GDP	N9-C4-N3	4.40	134.76	125.95
46	NM	501	GDP	N9-C4-N3	4.40	134.75	125.95
46	OO	501	GDP	N9-C4-N3	4.39	134.74	125.95
46	RM	501	GDP	N9-C4-N3	4.39	134.74	125.95
46	XI	501	GDP	N9-C4-N3	4.39	134.73	125.95
46	RG	501	GDP	N9-C4-N3	4.38	134.72	125.95
42	1C	2601	ADP	C5-C4-N3	-4.37	120.70	126.72
46	PK	501	GDP	N9-C4-N3	4.36	134.68	125.95
46	RK	501	GDP	N9-C4-N3	4.36	134.68	125.95
46	RE	501	GDP	N9-C4-N3	4.36	134.67	125.95
46	RO	501	GDP	N9-C4-N3	4.35	134.66	125.95
46	VI	501	GDP	N9-C4-N3	4.35	134.65	125.95
46	VM	501	GDP	N9-C4-N3	4.34	134.63	125.95
42	1B	2601	ADP	C2-N3-C4	4.32	122.38	111.83
42	1A	2601	ADP	C5-C4-N3	-4.30	120.79	126.72
46	UI	501	GDP	N9-C4-N3	4.30	134.56	125.95
46	XO	501	GDP	N9-C4-N3	4.28	134.51	125.95
42	1A	2601	ADP	N3-C2-N1	-4.27	122.12	128.58
46	ZM	501	GDP	N9-C4-N3	4.27	134.49	125.95
42	1C	2601	ADP	N3-C2-N1	-4.26	122.13	128.58
46	NI	501	GDP	N9-C4-N3	4.25	134.45	125.95
42	1D	2601	ADP	N3-C2-N1	-4.25	122.15	128.58
46	XA	501	GDP	N9-C4-N3	4.24	134.44	125.95
46	NC	501	GDP	N9-C4-N3	4.22	134.40	125.95
46	UK	501	GDP	N9-C4-N3	4.21	134.37	125.95
46	VE	501	GDP	N9-C4-N3	4.20	134.34	125.95
42	1D	2601	ADP	C5-C4-N3	-4.19	120.95	126.72
46	WE	501	GDP	N9-C4-N3	4.18	134.32	125.95
46	YI	501	GDP	N9-C4-N3	4.13	134.20	125.95
46	YO	501	GDP	N9-C4-N3	4.08	134.12	125.95
42	1C	2601	ADP	C2-N3-C4	4.07	121.78	111.83
42	1A	2601	ADP	C2-N3-C4	4.05	121.72	111.83
46	PM	501	GDP	N9-C4-N3	4.04	134.03	125.95
42	1D	2601	ADP	C2-N3-C4	4.00	121.59	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	SO	502	GDP	N9-C4-N3	4.00	133.94	125.95
46	XK	501	GDP	N9-C4-N3	3.92	133.78	125.95
46	YI	501	GDP	C6-C5-N7	3.78	137.17	130.29
46	PM	501	GDP	C6-C5-N7	3.68	136.99	130.29
46	XK	501	GDP	C6-C5-N7	3.59	136.83	130.29
46	SO	502	GDP	C6-C5-N7	3.54	136.73	130.29
46	WE	501	GDP	C6-C5-N7	3.52	136.70	130.29
46	UI	501	GDP	C6-C5-N7	3.49	136.65	130.29
46	YO	501	GDP	C6-C5-N7	3.49	136.63	130.29
46	XO	501	GDP	C6-C5-N7	3.46	136.59	130.29
46	NC	501	GDP	C6-C5-N7	3.45	136.57	130.29
44	PH	501	GTP	N9-C4-N3	3.45	132.85	125.95
44	NB	501	GTP	N9-C4-N3	3.45	132.85	125.95
46	RE	501	GDP	C6-C5-N7	3.44	136.55	130.29
42	1C	2601	ADP	N9-C8-N7	-3.44	109.06	113.94
42	1D	2601	ADP	N9-C8-N7	-3.44	109.06	113.94
46	ZM	501	GDP	C6-C5-N7	3.43	136.53	130.29
46	NI	501	GDP	C6-C5-N7	3.43	136.53	130.29
42	1B	2601	ADP	N9-C8-N7	-3.42	109.08	113.94
46	VE	501	GDP	C6-C5-N7	3.42	136.52	130.29
46	XA	501	GDP	C6-C5-N7	3.42	136.51	130.29
42	1A	2601	ADP	N9-C8-N7	-3.42	109.09	113.94
46	TG	502	GDP	C6-C5-N7	3.42	136.51	130.29
46	PK	501	GDP	C6-C5-N7	3.41	136.49	130.29
46	VM	501	GDP	C6-C5-N7	3.40	136.49	130.29
44	PP	501	GTP	N9-C4-N3	3.40	132.76	125.95
46	RM	501	GDP	C6-C5-N7	3.40	136.47	130.29
46	TM	502	GDP	C6-C5-N7	3.39	136.47	130.29
44	SJ	501	GTP	N9-C4-N3	3.39	132.72	125.95
46	RG	501	GDP	C6-C5-N7	3.38	136.45	130.29
44	NH	501	GTP	N9-C4-N3	3.38	132.71	125.95
44	TL	501	GTP	N9-C4-N3	3.38	132.71	125.95
46	RO	501	GDP	C6-C5-N7	3.38	136.44	130.29
46	UE	501	GDP	C6-C5-N7	3.38	136.44	130.29
44	UH	501	GTP	N9-C4-N3	3.37	132.69	125.95
46	XI	501	GDP	C6-C5-N7	3.37	136.42	130.29
46	UK	501	GDP	C6-C5-N7	3.36	136.41	130.29
46	WC	501	GDP	C6-C5-N7	3.36	136.41	130.29
46	RK	501	GDP	C6-C5-N7	3.35	136.38	130.29
44	RL	501	GTP	N9-C4-N3	3.35	132.64	125.95
46	OE	501	GDP	C6-C5-N7	3.33	136.35	130.29
46	WK	501	GDP	C6-C5-N7	3.33	136.34	130.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	NL	501	GTP	N9-C4-N3	3.32	132.60	125.95
46	SM	501	GDP	C6-C5-N7	3.32	136.34	130.29
46	WA	501	GDP	C6-C5-N7	3.32	136.33	130.29
44	SH	501	GTP	N9-C4-N3	3.32	132.59	125.95
44	WN	501	GTP	N9-C4-N3	3.32	132.59	125.95
44	ON	501	GTP	N9-C4-N3	3.31	132.58	125.95
46	QI	501	GDP	C6-C5-N7	3.31	136.32	130.29
44	NJ	501	GTP	N9-C4-N3	3.31	132.57	125.95
44	QD	501	GTP	N9-C4-N3	3.31	132.57	125.95
44	ND	501	GTP	N9-C4-N3	3.31	132.57	125.95
46	VK	501	GDP	C6-C5-N7	3.30	136.30	130.29
46	TI	501	GDP	C6-C5-N7	3.30	136.30	130.29
44	OP	501	GTP	N9-C4-N3	3.30	132.55	125.95
44	QL	501	GTP	N9-C4-N3	3.30	132.55	125.95
44	SP	501	GTP	N9-C4-N3	3.30	132.55	125.95
46	NM	501	GDP	C6-C5-N7	3.30	136.29	130.29
46	QK	501	GDP	C6-C5-N7	3.30	136.29	130.29
44	QJ	501	GTP	N9-C4-N3	3.29	132.54	125.95
46	XM	502	GDP	C6-C5-N7	3.29	136.28	130.29
46	YE	501	GDP	C6-C5-N7	3.29	136.28	130.29
44	XH	501	GTP	N9-C4-N3	3.29	132.53	125.95
46	ZI	501	GDP	C6-C5-N7	3.29	136.28	130.29
44	WB	501	GTP	N9-C4-N3	3.29	132.53	125.95
46	PE	501	GDP	C6-C5-N7	3.29	136.27	130.29
46	PG	501	GDP	C6-C5-N7	3.29	136.27	130.29
46	QQ	501	GDP	C6-C5-N7	3.29	136.27	130.29
46	XG	501	GDP	C6-C5-N7	3.29	136.27	130.29
46	NK	501	GDP	C6-C5-N7	3.28	136.27	130.29
44	QN	501	GTP	N9-C4-N3	3.28	132.52	125.95
44	XB	501	GTP	N9-C4-N3	3.28	132.52	125.95
44	OL	501	GTP	N9-C4-N3	3.28	132.51	125.95
44	SB	501	GTP	N9-C4-N3	3.28	132.51	125.95
46	OO	501	GDP	C6-C5-N7	3.28	136.26	130.29
44	WL	501	GTP	N9-C4-N3	3.28	132.51	125.95
44	TJ	501	GTP	N9-C4-N3	3.28	132.51	125.95
46	TE	501	GDP	C6-C5-N7	3.28	136.25	130.29
46	YK	501	GDP	C6-C5-N7	3.28	136.25	130.29
44	VL	501	GTP	N9-C4-N3	3.27	132.50	125.95
46	TC	501	GDP	C6-C5-N7	3.27	136.25	130.29
46	QO	501	GDP	C6-C5-N7	3.27	136.24	130.29
44	VH	501	GTP	N9-C4-N3	3.27	132.49	125.95
46	RC	501	GDP	C6-C5-N7	3.27	136.24	130.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	PJ	501	GTP	N9-C4-N3	3.27	132.49	125.95
44	YD	501	GTP	N9-C4-N3	3.27	132.48	125.95
44	VD	501	GTP	N9-C4-N3	3.26	132.48	125.95
44	VJ	501	GTP	N9-C4-N3	3.26	132.48	125.95
46	TK	501	GDP	C6-C5-N7	3.26	136.22	130.29
46	TO	501	GDP	C6-C5-N7	3.26	136.22	130.29
44	NN	501	GTP	N9-C4-N3	3.26	132.47	125.95
44	WH	501	GTP	N9-C4-N3	3.26	132.47	125.95
46	OG	501	GDP	C6-C5-N7	3.26	136.21	130.29
44	XF	501	GTP	N9-C4-N3	3.25	132.46	125.95
44	TB	501	GTP	N9-C4-N3	3.25	132.46	125.95
46	SC	502	GDP	C6-C5-N7	3.25	136.21	130.29
46	QG	501	GDP	C6-C5-N7	3.25	136.21	130.29
44	WJ	501	GTP	N9-C4-N3	3.25	132.45	125.95
44	XL	501	GTP	N9-C4-N3	3.25	132.45	125.95
46	VI	501	GDP	C6-C5-N7	3.25	136.20	130.29
46	UO	501	GDP	C6-C5-N7	3.25	136.20	130.29
44	PN	501	GTP	N9-C4-N3	3.25	132.44	125.95
44	PD	501	GTP	N9-C4-N3	3.24	132.44	125.95
44	YF	501	GTP	N9-C4-N3	3.24	132.44	125.95
44	XD	501	GTP	N9-C4-N3	3.24	132.44	125.95
44	SF	501	GTP	N9-C4-N3	3.24	132.43	125.95
46	WM	501	GDP	C6-C5-N7	3.24	136.19	130.29
46	WI	501	GDP	C6-C5-N7	3.24	136.19	130.29
44	YB	501	GTP	N9-C4-N3	3.24	132.43	125.95
44	YP	501	GTP	N9-C4-N3	3.24	132.43	125.95
46	PI	502	GDP	C6-C5-N7	3.24	136.18	130.29
46	ZK	501	GDP	C6-C5-N7	3.24	136.18	130.29
46	QC	501	GDP	C6-C5-N7	3.24	136.18	130.29
44	UN	501	GTP	N9-C4-N3	3.24	132.42	125.95
44	UD	501	GTP	N9-C4-N3	3.23	132.42	125.95
46	XC	501	GDP	C6-C5-N7	3.23	136.17	130.29
44	ZB	501	GTP	N9-C4-N3	3.23	132.42	125.95
46	YM	501	GDP	C6-C5-N7	3.23	136.17	130.29
46	SE	501	GDP	C6-C5-N7	3.23	136.17	130.29
46	UM	501	GDP	C6-C5-N7	3.23	136.17	130.29
44	ZP	501	GTP	N9-C4-N3	3.23	132.41	125.95
46	XE	501	GDP	C6-C5-N7	3.23	136.16	130.29
44	TN	501	GTP	N9-C4-N3	3.23	132.40	125.95
44	RF	501	GTP	N9-C4-N3	3.22	132.40	125.95
44	UB	501	GTP	N9-C4-N3	3.22	132.40	125.95
46	OQ	501	GDP	C6-C5-N7	3.22	136.15	130.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	PF	501	GTP	N9-C4-N3	3.22	132.39	125.95
44	SL	501	GTP	N9-C4-N3	3.22	132.39	125.95
44	TF	501	GTP	N9-C4-N3	3.22	132.39	125.95
44	YN	501	GTP	N9-C4-N3	3.22	132.39	125.95
44	ZJ	501	GTP	N9-C4-N3	3.22	132.39	125.95
46	WO	501	GDP	C6-C5-N7	3.22	136.15	130.29
46	ZE	501	GDP	C6-C5-N7	3.22	136.15	130.29
46	VC	501	GDP	C6-C5-N7	3.22	136.15	130.29
46	NG	502	GDP	C6-C5-N7	3.22	136.14	130.29
46	RI	502	GDP	C6-C5-N7	3.21	136.14	130.29
44	UJ	501	GTP	N9-C4-N3	3.21	132.38	125.95
44	SN	501	GTP	N9-C4-N3	3.21	132.37	125.95
46	SG	502	GDP	C6-C5-N7	3.21	136.13	130.29
44	QF	501	GTP	N9-C4-N3	3.21	132.37	125.95
46	NE	501	GDP	C6-C5-N7	3.21	136.13	130.29
46	NO	501	GDP	C6-C5-N7	3.21	136.12	130.29
46	OI	501	GDP	C6-C5-N7	3.20	136.12	130.29
44	UP	501	GTP	N9-C4-N3	3.20	132.36	125.95
46	OC	501	GDP	C6-C5-N7	3.20	136.12	130.29
46	WG	502	GDP	C6-C5-N7	3.20	136.12	130.29
44	WD	501	GTP	N9-C4-N3	3.20	132.35	125.95
46	ZG	501	GDP	C6-C5-N7	3.20	136.10	130.29
44	SD	501	GTP	N9-C4-N3	3.19	132.33	125.95
44	OD	501	GTP	N9-C4-N3	3.19	132.33	125.95
46	QM	501	GDP	C6-C5-N7	3.19	136.09	130.29
44	TP	501	GTP	N9-C4-N3	3.19	132.32	125.95
46	ZC	501	GDP	C6-C5-N7	3.18	136.09	130.29
44	ZN	501	GTP	N9-C4-N3	3.18	132.32	125.95
44	NF	501	GTP	N9-C4-N3	3.18	132.32	125.95
44	VB	501	GTP	N9-C4-N3	3.18	132.32	125.95
46	PQ	501	GDP	C6-C5-N7	3.18	136.08	130.29
44	YH	501	GTP	N9-C4-N3	3.18	132.31	125.95
44	QH	501	GTP	N9-C4-N3	3.18	132.31	125.95
44	VF	501	GTP	N9-C4-N3	3.18	132.31	125.95
46	VO	501	GDP	C6-C5-N7	3.17	136.06	130.29
44	VN	501	GTP	N9-C4-N3	3.16	132.28	125.95
46	YG	501	GDP	C6-C5-N7	3.16	136.04	130.29
46	SK	501	GDP	C6-C5-N7	3.15	136.03	130.29
44	UF	501	GTP	N9-C4-N3	3.15	132.26	125.95
44	TD	501	GTP	N9-C4-N3	3.15	132.25	125.95
46	ZO	501	GDP	C6-C5-N7	3.15	136.02	130.29
44	TH	501	GTP	N9-C4-N3	3.14	132.24	125.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	XN	501	GTP	N9-C4-N3	3.14	132.24	125.95
44	ZL	501	GTP	N9-C4-N3	3.14	132.23	125.95
44	RH	501	GTP	N9-C4-N3	3.14	132.23	125.95
46	YC	501	GDP	C6-C5-N7	3.13	135.99	130.29
46	PO	501	GDP	C6-C5-N7	3.13	135.99	130.29
44	WF	501	GTP	N9-C4-N3	3.13	132.21	125.95
44	UL	501	GTP	N9-C4-N3	3.12	132.20	125.95
42	1C	2601	ADP	C4-N9-C8	3.12	109.02	105.74
44	OJ	501	GTP	N9-C4-N3	3.12	132.19	125.95
42	1D	2601	ADP	C4-N9-C8	3.12	109.01	105.74
44	XJ	501	GTP	N9-C4-N3	3.12	132.18	125.95
46	OK	501	GDP	C6-C5-N7	3.10	135.94	130.29
42	1A	2601	ADP	C4-N9-C8	3.10	109.00	105.74
46	QE	501	GDP	C6-C5-N7	3.10	135.94	130.29
46	UG	501	GDP	C6-C5-N7	3.09	135.92	130.29
44	OH	501	GTP	N9-C4-N3	3.09	132.13	125.95
44	PL	501	GTP	N9-C4-N3	3.09	132.13	125.95
44	ZF	501	GTP	N9-C4-N3	3.09	132.12	125.95
46	OM	501	GDP	C6-C5-N7	3.08	135.90	130.29
44	WF	501	GTP	C2-N1-C6	-3.07	119.55	125.11
44	YJ	501	GTP	N9-C4-N3	3.07	132.09	125.95
44	NN	501	GTP	C2-N1-C6	-3.06	119.56	125.11
44	QP	501	GTP	N9-C4-N3	3.06	132.07	125.95
44	NH	501	GTP	C2-N1-C6	-3.06	119.57	125.11
46	PC	501	GDP	C6-C5-N7	3.05	135.85	130.29
46	SI	501	GDP	C6-C5-N7	3.05	135.85	130.29
44	ZD	501	GTP	N9-C4-N3	3.05	132.06	125.95
44	RN	501	GTP	N9-C4-N3	3.04	132.04	125.95
44	RD	501	GTP	N9-C4-N3	3.03	132.02	125.95
46	UC	501	GDP	C6-C5-N7	3.03	135.80	130.29
44	SJ	501	GTP	C2-N1-C6	-3.03	119.62	125.11
42	1D	2601	ADP	C6-C5-C4	-3.03	113.05	117.18
44	OP	501	GTP	C2-N1-C6	-3.03	119.62	125.11
44	VP	501	GTP	N9-C4-N3	3.02	132.00	125.95
44	RJ	501	GTP	N9-C4-N3	3.02	131.99	125.95
44	NB	501	GTP	C2-N1-C6	-3.02	119.64	125.11
44	UH	501	GTP	C2-N1-C6	-3.02	119.64	125.11
44	QN	501	GTP	C2-N1-C6	-3.01	119.65	125.11
44	OF	501	GTP	N9-C4-N3	3.01	131.97	125.95
44	TL	501	GTP	C2-N1-C6	-3.01	119.66	125.11
42	1B	2601	ADP	C6-C5-C4	-3.01	113.07	117.18
44	NJ	501	GTP	C2-N1-C6	-3.00	119.66	125.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	RP	501	GTP	N9-C4-N3	3.00	131.94	125.95
44	UD	501	GTP	C2-N1-C6	-2.99	119.69	125.11
44	VJ	501	GTP	C2-N1-C6	-2.99	119.69	125.11
44	QJ	501	GTP	C2-N1-C6	-2.99	119.69	125.11
44	SH	501	GTP	C2-N1-C6	-2.99	119.69	125.11
44	RF	501	GTP	C2-N1-C6	-2.99	119.70	125.11
44	UN	501	GTP	C2-N1-C6	-2.99	119.70	125.11
44	WL	501	GTP	C2-N1-C6	-2.99	119.70	125.11
44	VD	501	GTP	C2-N1-C6	-2.99	119.70	125.11
44	WH	501	GTP	C2-N1-C6	-2.98	119.70	125.11
44	PJ	501	GTP	C2-N1-C6	-2.98	119.70	125.11
44	ZH	501	GTP	N9-C4-N3	2.98	131.92	125.95
44	YL	501	GTP	N9-C4-N3	2.98	131.91	125.95
44	NF	501	GTP	C2-N1-C6	-2.98	119.71	125.11
44	PN	501	GTP	C2-N1-C6	-2.98	119.71	125.11
44	SP	501	GTP	C2-N1-C6	-2.98	119.71	125.11
44	QL	501	GTP	C2-N1-C6	-2.98	119.71	125.11
44	PP	501	GTP	C2-N1-C6	-2.97	119.72	125.11
44	YF	501	GTP	C2-N1-C6	-2.97	119.72	125.11
44	ND	501	GTP	C2-N1-C6	-2.97	119.72	125.11
46	VG	501	GDP	C6-C5-N7	2.97	135.70	130.29
44	RL	501	GTP	C2-N1-C6	-2.97	119.72	125.11
44	ZJ	501	GTP	C2-N1-C6	-2.97	119.72	125.11
44	QF	501	GTP	C2-N1-C6	-2.97	119.72	125.11
44	SL	501	GTP	C2-N1-C6	-2.97	119.73	125.11
44	RD	501	GTP	C2-N1-C6	-2.97	119.73	125.11
44	XH	501	GTP	C2-N1-C6	-2.97	119.73	125.11
44	NL	501	GTP	C2-N1-C6	-2.96	119.74	125.11
44	OF	501	GTP	C2-N1-C6	-2.96	119.74	125.11
44	OL	501	GTP	C2-N1-C6	-2.96	119.74	125.11
44	WN	501	GTP	C2-N1-C6	-2.96	119.75	125.11
44	SD	501	GTP	C2-N1-C6	-2.96	119.75	125.11
44	VH	501	GTP	C2-N1-C6	-2.96	119.75	125.11
44	ON	501	GTP	C2-N1-C6	-2.95	119.75	125.11
44	QH	501	GTP	C2-N1-C6	-2.95	119.75	125.11
44	YP	501	GTP	C2-N1-C6	-2.95	119.75	125.11
44	TH	501	GTP	C2-N1-C6	-2.95	119.75	125.11
44	WJ	501	GTP	C2-N1-C6	-2.95	119.76	125.11
44	UJ	501	GTP	C2-N1-C6	-2.94	119.77	125.11
44	TJ	501	GTP	C2-N1-C6	-2.94	119.77	125.11
44	UF	501	GTP	C2-N1-C6	-2.94	119.78	125.11
44	TD	501	GTP	C2-N1-C6	-2.94	119.78	125.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	QD	501	GTP	C2-N1-C6	-2.94	119.79	125.11
44	SB	501	GTP	C2-N1-C6	-2.93	119.79	125.11
44	QP	501	GTP	C2-N1-C6	-2.93	119.80	125.11
44	SF	501	GTP	C2-N1-C6	-2.93	119.80	125.11
44	XF	501	GTP	C2-N1-C6	-2.93	119.80	125.11
44	WD	501	GTP	C2-N1-C6	-2.93	119.80	125.11
44	VL	501	GTP	C2-N1-C6	-2.93	119.80	125.11
42	1D	2601	ADP	C2-N1-C6	2.93	123.54	118.73
44	PF	501	GTP	C2-N1-C6	-2.93	119.81	125.11
44	XB	501	GTP	C2-N1-C6	-2.93	119.81	125.11
44	YB	501	GTP	C2-N1-C6	-2.93	119.81	125.11
44	PD	501	GTP	C2-N1-C6	-2.92	119.81	125.11
44	RJ	501	GTP	C2-N1-C6	-2.92	119.81	125.11
44	XL	501	GTP	C2-N1-C6	-2.92	119.81	125.11
44	TN	501	GTP	C2-N1-C6	-2.92	119.81	125.11
44	YN	501	GTP	C2-N1-C6	-2.92	119.82	125.11
44	WB	501	GTP	C2-N1-C6	-2.92	119.82	125.11
44	RH	501	GTP	C2-N1-C6	-2.91	119.83	125.11
44	YD	501	GTP	C2-N1-C6	-2.91	119.84	125.11
44	RP	501	GTP	C2-N1-C6	-2.91	119.84	125.11
44	TP	501	GTP	C2-N1-C6	-2.91	119.84	125.11
44	XD	501	GTP	C2-N1-C6	-2.90	119.84	125.11
44	TB	501	GTP	C2-N1-C6	-2.90	119.85	125.11
44	YH	501	GTP	C2-N1-C6	-2.90	119.85	125.11
44	OJ	501	GTP	C2-N1-C6	-2.90	119.86	125.11
44	TF	501	GTP	C2-N1-C6	-2.90	119.86	125.11
44	YL	501	GTP	C2-N1-C6	-2.90	119.86	125.11
44	UB	501	GTP	C2-N1-C6	-2.88	119.89	125.11
44	UL	501	GTP	C2-N1-C6	-2.88	119.89	125.11
44	PH	501	GTP	C2-N1-C6	-2.88	119.89	125.11
44	ZL	501	GTP	C2-N1-C6	-2.87	119.90	125.11
44	VN	501	GTP	C2-N1-C6	-2.87	119.90	125.11
42	1B	2601	ADP	C2-N1-C6	2.87	123.44	118.73
44	ZH	501	GTP	C2-N1-C6	-2.87	119.91	125.11
44	ZN	501	GTP	C2-N1-C6	-2.87	119.91	125.11
42	1A	2601	ADP	C6-C5-C4	-2.86	113.27	117.18
46	YI	501	GDP	C4-C5-N7	-2.86	106.14	110.67
44	UP	501	GTP	C2-N1-C6	-2.86	119.93	125.11
44	YL	501	GTP	N9-C8-N7	-2.85	108.11	113.40
44	PL	501	GTP	C2-N1-C6	-2.85	119.95	125.11
44	SN	501	GTP	C2-N1-C6	-2.85	119.95	125.11
44	VF	501	GTP	C2-N1-C6	-2.84	119.95	125.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	OD	501	GTP	C2-N1-C6	-2.84	119.96	125.11
44	XN	501	GTP	C2-N1-C6	-2.84	119.96	125.11
44	YJ	501	GTP	C2-N1-C6	-2.83	119.97	125.11
42	1A	2601	ADP	C2-N1-C6	2.82	123.36	118.73
42	1C	2601	ADP	C6-C5-C4	-2.82	113.33	117.18
44	RL	501	GTP	N9-C8-N7	-2.82	108.17	113.40
44	XJ	501	GTP	C2-N1-C6	-2.81	120.01	125.11
46	WC	501	GDP	C4-C5-N7	-2.81	106.21	110.67
44	PL	501	GTP	N9-C8-N7	-2.80	108.20	113.40
44	RN	501	GTP	C2-N1-C6	-2.80	120.03	125.11
44	NH	501	GTP	N9-C8-N7	-2.80	108.21	113.40
44	RH	501	GTP	N9-C8-N7	-2.79	108.22	113.40
42	1B	2601	ADP	C4-N9-C8	2.79	108.67	105.74
44	VN	501	GTP	N9-C8-N7	-2.79	108.22	113.40
44	OH	501	GTP	C2-N1-C6	-2.79	120.05	125.11
44	TH	501	GTP	N9-C8-N7	-2.79	108.23	113.40
44	QH	501	GTP	N9-C8-N7	-2.78	108.24	113.40
44	RF	501	GTP	N9-C8-N7	-2.78	108.25	113.40
44	VB	501	GTP	C2-N1-C6	-2.78	120.07	125.11
44	ZF	501	GTP	C2-N1-C6	-2.77	120.09	125.11
44	VH	501	GTP	N9-C8-N7	-2.77	108.27	113.40
44	RD	501	GTP	N9-C8-N7	-2.76	108.29	113.40
44	SH	501	GTP	N9-C8-N7	-2.76	108.29	113.40
44	YJ	501	GTP	N9-C8-N7	-2.75	108.30	113.40
44	ZH	501	GTP	N9-C8-N7	-2.75	108.30	113.40
44	UL	501	GTP	N9-C8-N7	-2.75	108.30	113.40
44	PJ	501	GTP	N9-C8-N7	-2.75	108.30	113.40
44	VP	501	GTP	N9-C8-N7	-2.75	108.30	113.40
44	UJ	501	GTP	N9-C8-N7	-2.75	108.30	113.40
44	RJ	501	GTP	N9-C8-N7	-2.74	108.31	113.40
44	ZP	501	GTP	C2-N1-C6	-2.74	120.14	125.11
44	NJ	501	GTP	O3G-PG-O3B	2.74	113.83	104.64
44	RP	501	GTP	N9-C8-N7	-2.74	108.32	113.40
44	PN	501	GTP	N9-C8-N7	-2.74	108.33	113.40
44	ZB	501	GTP	C2-N1-C6	-2.74	120.15	125.11
44	WH	501	GTP	N9-C8-N7	-2.73	108.33	113.40
44	UB	501	GTP	N9-C8-N7	-2.73	108.34	113.40
44	ZD	501	GTP	C2-N1-C6	-2.73	120.16	125.11
44	XF	501	GTP	N9-C8-N7	-2.73	108.34	113.40
44	OF	501	GTP	N9-C8-N7	-2.72	108.35	113.40
42	1C	2601	ADP	C2-N1-C6	2.72	123.20	118.73
44	UD	501	GTP	N9-C8-N7	-2.72	108.35	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	OD	501	GTP	N9-C8-N7	-2.72	108.36	113.40
44	ZF	501	GTP	N9-C8-N7	-2.72	108.36	113.40
44	SL	501	GTP	N9-C8-N7	-2.72	108.36	113.40
44	TF	501	GTP	N9-C8-N7	-2.71	108.37	113.40
44	TB	501	GTP	N9-C8-N7	-2.71	108.37	113.40
44	QJ	501	GTP	N9-C8-N7	-2.71	108.38	113.40
44	OJ	501	GTP	N9-C8-N7	-2.71	108.38	113.40
44	XJ	501	GTP	N9-C8-N7	-2.70	108.39	113.40
44	YN	501	GTP	N9-C8-N7	-2.70	108.39	113.40
44	ZB	501	GTP	N9-C8-N7	-2.70	108.39	113.40
44	NN	501	GTP	N9-C8-N7	-2.70	108.39	113.40
44	TN	501	GTP	N9-C8-N7	-2.70	108.39	113.40
44	NL	501	GTP	N9-C8-N7	-2.70	108.39	113.40
44	OP	501	GTP	N9-C8-N7	-2.70	108.39	113.40
44	VF	501	GTP	N9-C8-N7	-2.70	108.39	113.40
44	SJ	501	GTP	N9-C8-N7	-2.70	108.40	113.40
44	ZN	501	GTP	N9-C8-N7	-2.70	108.40	113.40
44	YB	501	GTP	N9-C8-N7	-2.70	108.40	113.40
44	PF	501	GTP	N9-C8-N7	-2.69	108.40	113.40
44	WF	501	GTP	N9-C8-N7	-2.69	108.41	113.40
44	UN	501	GTP	N9-C8-N7	-2.69	108.41	113.40
44	TP	501	GTP	N9-C8-N7	-2.69	108.42	113.40
46	NC	501	GDP	C4-C5-N7	-2.69	106.41	110.67
44	XD	501	GTP	N9-C8-N7	-2.69	108.42	113.40
44	NF	501	GTP	N9-C8-N7	-2.69	108.42	113.40
44	QN	501	GTP	N9-C8-N7	-2.69	108.42	113.40
44	TJ	501	GTP	N9-C8-N7	-2.69	108.42	113.40
44	XN	501	GTP	N9-C8-N7	-2.68	108.42	113.40
44	UF	501	GTP	N9-C8-N7	-2.68	108.43	113.40
44	WD	501	GTP	N9-C8-N7	-2.68	108.43	113.40
44	WB	501	GTP	N9-C8-N7	-2.68	108.44	113.40
44	QL	501	GTP	N9-C8-N7	-2.68	108.44	113.40
44	SD	501	GTP	N9-C8-N7	-2.68	108.44	113.40
44	VB	501	GTP	N9-C8-N7	-2.68	108.44	113.40
44	ZP	501	GTP	N9-C8-N7	-2.68	108.44	113.40
44	YF	501	GTP	N9-C8-N7	-2.67	108.44	113.40
46	RM	501	GDP	C4-C5-N7	-2.67	106.44	110.67
44	VL	501	GTP	N9-C8-N7	-2.67	108.44	113.40
44	OL	501	GTP	N9-C8-N7	-2.67	108.45	113.40
44	ZD	501	GTP	N9-C8-N7	-2.67	108.45	113.40
46	QG	501	GDP	C4-C5-N7	-2.67	106.44	110.67
44	TD	501	GTP	N9-C8-N7	-2.67	108.46	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	YP	501	GTP	N9-C8-N7	-2.67	108.46	113.40
44	ZJ	501	GTP	N9-C8-N7	-2.66	108.46	113.40
44	QP	501	GTP	N9-C8-N7	-2.66	108.47	113.40
44	PD	501	GTP	N9-C8-N7	-2.66	108.47	113.40
44	YH	501	GTP	N9-C8-N7	-2.66	108.47	113.40
46	WE	501	GDP	C4-C5-N7	-2.66	106.45	110.67
44	NJ	501	GTP	N9-C8-N7	-2.66	108.47	113.40
44	ZL	501	GTP	N9-C8-N7	-2.66	108.47	113.40
44	RN	501	GTP	N9-C8-N7	-2.66	108.47	113.40
44	PH	501	GTP	N9-C8-N7	-2.66	108.48	113.40
44	XB	501	GTP	N9-C8-N7	-2.65	108.48	113.40
46	RE	501	GDP	C4-C5-N7	-2.65	106.47	110.67
44	NH	501	GTP	C8-N7-C5	2.65	108.98	104.26
44	SB	501	GTP	N9-C8-N7	-2.65	108.49	113.40
44	SP	501	GTP	N9-C8-N7	-2.64	108.50	113.40
44	XH	501	GTP	N9-C8-N7	-2.64	108.50	113.40
44	TL	501	GTP	N9-C8-N7	-2.64	108.50	113.40
44	XL	501	GTP	N9-C8-N7	-2.64	108.51	113.40
46	XK	501	GDP	C2'-C3'-C4'	2.64	107.70	102.61
44	ND	501	GTP	N9-C8-N7	-2.64	108.51	113.40
46	PM	501	GDP	C4-C5-N7	-2.64	106.49	110.67
44	VD	501	GTP	N9-C8-N7	-2.63	108.52	113.40
44	OH	501	GTP	N9-C8-N7	-2.63	108.52	113.40
44	UP	501	GTP	N9-C8-N7	-2.63	108.52	113.40
44	WN	501	GTP	N9-C8-N7	-2.63	108.52	113.40
44	QD	501	GTP	N9-C8-N7	-2.63	108.52	113.40
44	YD	501	GTP	N9-C8-N7	-2.63	108.52	113.40
46	QO	501	GDP	C4-C5-N7	-2.63	106.50	110.67
44	RF	501	GTP	C8-N7-C5	2.63	108.94	104.26
46	RG	501	GDP	C4-C5-N7	-2.63	106.51	110.67
46	TK	501	GDP	C4-C5-N7	-2.63	106.51	110.67
46	NI	501	GDP	C4-C5-N7	-2.62	106.51	110.67
46	TO	501	GDP	C4-C5-N7	-2.62	106.51	110.67
44	SN	501	GTP	N9-C8-N7	-2.62	108.53	113.40
46	VM	501	GDP	C4-C5-N7	-2.62	106.52	110.67
44	ON	501	GTP	N9-C8-N7	-2.62	108.54	113.40
44	YL	501	GTP	C8-N7-C5	2.62	108.93	104.26
46	RI	502	GDP	C4-C5-N7	-2.62	106.52	110.67
46	ZE	501	GDP	C4-C5-N7	-2.62	106.52	110.67
46	XI	501	GDP	C4-C5-N7	-2.62	106.52	110.67
46	RO	501	GDP	C4-C5-N7	-2.62	106.52	110.67
43	1B	2602	ANP	O1B-PB-N3B	-2.62	107.92	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	WK	501	GDP	C4-C5-N7	-2.62	106.53	110.67
44	SJ	501	GTP	C5-C6-N1	2.61	119.91	113.25
46	PG	501	GDP	C4-C5-N7	-2.61	106.53	110.67
46	TC	501	GDP	C4-C5-N7	-2.61	106.53	110.67
44	WJ	501	GTP	N9-C8-N7	-2.61	108.56	113.40
44	PJ	501	GTP	C5-C6-N1	2.61	119.90	113.25
44	UJ	501	GTP	C8-N7-C5	2.61	108.91	104.26
46	XA	501	GDP	C4-C5-N7	-2.61	106.53	110.67
44	SH	501	GTP	C8-N7-C5	2.61	108.91	104.26
46	WM	501	GDP	C4-C5-N7	-2.61	106.53	110.67
44	UD	501	GTP	C5-C6-N1	2.61	119.89	113.25
44	UH	501	GTP	N9-C8-N7	-2.61	108.56	113.40
46	ZM	501	GDP	C4-C5-N7	-2.61	106.54	110.67
46	UE	501	GDP	C4-C5-N7	-2.61	106.54	110.67
42	1B	2601	ADP	N6-C6-N1	-2.61	112.57	118.38
44	NB	501	GTP	N9-C8-N7	-2.61	108.57	113.40
46	YO	501	GDP	C4-C5-N7	-2.61	106.54	110.67
44	NN	501	GTP	C5-C6-N1	2.61	119.89	113.25
46	XE	501	GDP	C4-C5-N7	-2.60	106.54	110.67
44	UF	501	GTP	C5-C6-N1	2.60	119.88	113.25
46	NG	502	GDP	C4-C5-N7	-2.60	106.54	110.67
46	UI	501	GDP	C4-C5-N7	-2.60	106.54	110.67
46	SG	502	GDP	C4-C5-N7	-2.60	106.55	110.67
46	TI	501	GDP	C4-C5-N7	-2.60	106.55	110.67
44	RL	501	GTP	C5-C6-N1	2.60	119.88	113.25
46	YK	501	GDP	C4-C5-N7	-2.60	106.55	110.67
44	PP	501	GTP	N9-C8-N7	-2.60	108.58	113.40
46	PK	501	GDP	C4-C5-N7	-2.60	106.55	110.67
46	WO	501	GDP	C4-C5-N7	-2.60	106.55	110.67
44	VJ	501	GTP	N9-C8-N7	-2.59	108.59	113.40
46	WG	502	GDP	C4-C5-N7	-2.59	106.56	110.67
44	SF	501	GTP	N9-C8-N7	-2.59	108.59	113.40
46	OE	501	GDP	C4-C5-N7	-2.59	106.56	110.67
44	WF	501	GTP	C8-N7-C5	2.59	108.87	104.26
44	UH	501	GTP	C5-C6-N1	2.59	119.83	113.25
46	XC	501	GDP	C4-C5-N7	-2.59	106.57	110.67
44	NB	501	GTP	C5-C6-N1	2.58	119.83	113.25
44	TH	501	GTP	C8-N7-C5	2.58	108.86	104.26
46	QC	501	GDP	C4-C5-N7	-2.58	106.58	110.67
46	ZI	501	GDP	C4-C5-N7	-2.58	106.58	110.67
44	TH	501	GTP	C5-C6-N1	2.58	119.81	113.25
46	NK	501	GDP	C4-C5-N7	-2.58	106.58	110.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	QI	501	GDP	C4-C5-N7	-2.58	106.58	110.67
46	XO	501	GDP	C4-C5-N7	-2.58	106.58	110.67
46	QE	501	GDP	C4-C5-N7	-2.58	106.59	110.67
46	RC	501	GDP	C4-C5-N7	-2.58	106.59	110.67
46	VC	501	GDP	C4-C5-N7	-2.58	106.59	110.67
44	RP	501	GTP	C8-N7-C5	2.57	108.85	104.26
44	RF	501	GTP	C5-C6-N1	2.57	119.80	113.25
44	RH	501	GTP	C8-N7-C5	2.57	108.84	104.26
44	NN	501	GTP	C8-N7-C5	2.57	108.84	104.26
46	TE	501	GDP	C4-C5-N7	-2.57	106.60	110.67
44	QH	501	GTP	C8-N7-C5	2.57	108.84	104.26
44	NH	501	GTP	C5-C6-N1	2.57	119.79	113.25
44	UJ	501	GTP	C5-C6-N1	2.57	119.79	113.25
46	PI	502	GDP	C4-C5-N7	-2.57	106.60	110.67
44	QN	501	GTP	C5-C6-N1	2.57	119.79	113.25
46	PE	501	GDP	C4-C5-N7	-2.57	106.60	110.67
44	PL	501	GTP	C8-N7-C5	2.56	108.83	104.26
44	WL	501	GTP	C5-C6-N1	2.56	119.78	113.25
44	VP	501	GTP	C2-N1-C6	-2.56	120.46	125.11
46	SM	501	GDP	C4-C5-N7	-2.56	106.61	110.67
44	WH	501	GTP	C5-C6-N1	2.56	119.78	113.25
44	UN	501	GTP	C8-N7-C5	2.56	108.83	104.26
44	QF	501	GTP	N9-C8-N7	-2.56	108.65	113.40
46	YE	501	GDP	C4-C5-N7	-2.56	106.61	110.67
44	WF	501	GTP	C5-C6-N1	2.56	119.77	113.25
44	YB	501	GTP	C8-N7-C5	2.56	108.82	104.26
44	OP	501	GTP	C5-C6-N1	2.56	119.76	113.25
46	QK	501	GDP	C4-C5-N7	-2.56	106.62	110.67
46	TM	502	GDP	C4-C5-N7	-2.56	106.62	110.67
44	WL	501	GTP	N9-C8-N7	-2.56	108.66	113.40
46	YC	501	GDP	C4-C5-N7	-2.56	106.62	110.67
46	RK	501	GDP	C4-C5-N7	-2.56	106.62	110.67
44	YP	501	GTP	C5-C6-N1	2.55	119.76	113.25
44	QL	501	GTP	C5-C6-N1	2.55	119.75	113.25
44	VH	501	GTP	C8-N7-C5	2.55	108.81	104.26
44	TJ	501	GTP	C5-C6-N1	2.55	119.75	113.25
46	NO	501	GDP	C4-C5-N7	-2.55	106.62	110.67
46	YG	501	GDP	C4-C5-N7	-2.55	106.62	110.67
46	ZK	501	GDP	C4-C5-N7	-2.55	106.63	110.67
44	RL	501	GTP	C8-N7-C5	2.55	108.81	104.26
46	UM	501	GDP	C4-C5-N7	-2.55	106.63	110.67
44	TF	501	GTP	C8-N7-C5	2.55	108.80	104.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	SP	501	GTP	C5-C6-N1	2.55	119.74	113.25
44	VJ	501	GTP	C5-C6-N1	2.55	119.74	113.25
44	QH	501	GTP	C5-C6-N1	2.55	119.74	113.25
46	ZO	501	GDP	C4-C5-N7	-2.55	106.63	110.67
44	PJ	501	GTP	C8-N7-C5	2.55	108.80	104.26
44	PN	501	GTP	C5-C6-N1	2.54	119.73	113.25
44	PP	501	GTP	C5-C6-N1	2.54	119.73	113.25
44	RD	501	GTP	C5-C6-N1	2.54	119.73	113.25
44	ZJ	501	GTP	C5-C6-N1	2.54	119.73	113.25
46	PQ	501	GDP	C4-C5-N7	-2.54	106.64	110.67
44	RD	501	GTP	C8-N7-C5	2.54	108.79	104.26
44	VH	501	GTP	C5-C6-N1	2.54	119.72	113.25
46	VK	501	GDP	C4-C5-N7	-2.54	106.64	110.67
44	WD	501	GTP	C8-N7-C5	2.54	108.79	104.26
44	TL	501	GTP	C5-C6-N1	2.54	119.72	113.25
44	QF	501	GTP	C5-C6-N1	2.54	119.72	113.25
44	RH	501	GTP	C5-C6-N1	2.54	119.72	113.25
44	SP	501	GTP	C8-N7-C5	2.54	108.79	104.26
44	SD	501	GTP	C8-N7-C5	2.54	108.79	104.26
44	UN	501	GTP	C5-C6-N1	2.54	119.72	113.25
44	XF	501	GTP	C5-C6-N1	2.54	119.72	113.25
44	ZH	501	GTP	C8-N7-C5	2.54	108.78	104.26
44	SH	501	GTP	C5-C6-N1	2.54	119.72	113.25
44	YF	501	GTP	C5-C6-N1	2.54	119.72	113.25
44	NF	501	GTP	C8-N7-C5	2.54	108.78	104.26
46	SC	502	GDP	C4-C5-N7	-2.54	106.65	110.67
46	UK	501	GDP	C4-C5-N7	-2.54	106.65	110.67
44	TN	501	GTP	C5-C6-N1	2.54	119.71	113.25
46	XG	501	GDP	C4-C5-N7	-2.54	106.65	110.67
44	ON	501	GTP	C5-C6-N1	2.54	119.71	113.25
44	OF	501	GTP	C8-N7-C5	2.54	108.78	104.26
44	OL	501	GTP	C8-N7-C5	2.54	108.78	104.26
44	SJ	501	GTP	O6-C6-C5	-2.54	119.84	126.53
42	1B	2601	ADP	C5-C4-N9	2.54	108.58	105.81
44	UB	501	GTP	C8-N7-C5	2.54	108.78	104.26
44	WB	501	GTP	C5-C6-N1	2.54	119.71	113.25
44	ZH	501	GTP	C5-C6-N1	2.54	119.71	113.25
44	NL	501	GTP	C8-N7-C5	2.53	108.78	104.26
44	YJ	501	GTP	C8-N7-C5	2.53	108.78	104.26
44	QN	501	GTP	C8-N7-C5	2.53	108.78	104.26
44	XF	501	GTP	C8-N7-C5	2.53	108.78	104.26
44	RP	501	GTP	C5-C6-N1	2.53	119.70	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	SL	501	GTP	C5-C6-N1	2.53	119.70	113.25
44	VL	501	GTP	C8-N7-C5	2.53	108.77	104.26
44	UB	501	GTP	C5-C6-N1	2.53	119.70	113.25
44	TB	501	GTP	C8-N7-C5	2.53	108.77	104.26
46	XM	502	GDP	C4-C5-N7	-2.53	106.66	110.67
44	TP	501	GTP	C5-C6-N1	2.53	119.70	113.25
44	PD	501	GTP	C8-N7-C5	2.53	108.77	104.26
44	OJ	501	GTP	C8-N7-C5	2.53	108.77	104.26
46	TG	502	GDP	C4-C5-N7	-2.53	106.66	110.67
44	OF	501	GTP	C5-C6-N1	2.53	119.69	113.25
44	UL	501	GTP	C8-N7-C5	2.53	108.77	104.26
44	WJ	501	GTP	C5-C6-N1	2.53	119.69	113.25
44	NF	501	GTP	C5-C6-N1	2.53	119.69	113.25
44	QJ	501	GTP	C8-N7-C5	2.53	108.76	104.26
44	WH	501	GTP	C8-N7-C5	2.53	108.76	104.26
46	WI	501	GDP	C4-C5-N7	-2.53	106.67	110.67
44	SF	501	GTP	C5-C6-N1	2.53	119.68	113.25
44	RL	501	GTP	O6-C6-C5	-2.53	119.86	126.53
44	QJ	501	GTP	C5-C6-N1	2.53	119.68	113.25
44	VD	501	GTP	C5-C6-N1	2.53	119.68	113.25
44	OP	501	GTP	O6-C6-C5	-2.53	119.87	126.53
46	VE	501	GDP	C4-C5-N7	-2.52	106.67	110.67
44	XL	501	GTP	C5-C6-N1	2.52	119.68	113.25
44	XD	501	GTP	C8-N7-C5	2.52	108.76	104.26
46	ZG	501	GDP	C4-C5-N7	-2.52	106.67	110.67
44	QP	501	GTP	C8-N7-C5	2.52	108.76	104.26
44	SJ	501	GTP	C8-N7-C5	2.52	108.76	104.26
44	NJ	501	GTP	C5-C6-N1	2.52	119.68	113.25
44	OJ	501	GTP	C5-C6-N1	2.52	119.68	113.25
44	PF	501	GTP	C5-C6-N1	2.52	119.68	113.25
44	QD	501	GTP	C5-C6-N1	2.52	119.68	113.25
44	OD	501	GTP	C8-N7-C5	2.52	108.75	104.26
44	ZN	501	GTP	C8-N7-C5	2.52	108.75	104.26
46	SE	501	GDP	C4-C5-N7	-2.52	106.67	110.67
44	TJ	501	GTP	C8-N7-C5	2.52	108.75	104.26
44	WD	501	GTP	C5-C6-N1	2.52	119.67	113.25
44	PL	501	GTP	C5-C6-N1	2.52	119.67	113.25
44	ND	501	GTP	C8-N7-C5	2.52	108.75	104.26
44	SL	501	GTP	C8-N7-C5	2.52	108.75	104.26
44	PD	501	GTP	C5-C6-N1	2.52	119.66	113.25
44	VN	501	GTP	C5-C6-N1	2.52	119.66	113.25
44	WN	501	GTP	C5-C6-N1	2.52	119.66	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	UH	501	GTP	C8-N7-C5	2.52	108.74	104.26
46	OC	501	GDP	C4-C5-N7	-2.52	106.68	110.67
44	ND	501	GTP	C5-C6-N1	2.52	119.66	113.25
46	QQ	501	GDP	C4-C5-N7	-2.52	106.68	110.67
44	YH	501	GTP	C8-N7-C5	2.52	108.74	104.26
44	YN	501	GTP	C8-N7-C5	2.51	108.74	104.26
44	PN	501	GTP	C8-N7-C5	2.51	108.74	104.26
44	WJ	501	GTP	C8-N7-C5	2.51	108.74	104.26
44	XB	501	GTP	C5-C6-N1	2.51	119.65	113.25
44	YN	501	GTP	C5-C6-N1	2.51	119.65	113.25
44	YP	501	GTP	C8-N7-C5	2.51	108.74	104.26
44	OL	501	GTP	C5-C6-N1	2.51	119.65	113.25
44	TD	501	GTP	C5-C6-N1	2.51	119.65	113.25
44	XH	501	GTP	C5-C6-N1	2.51	119.65	113.25
46	NM	501	GDP	C4-C5-N7	-2.51	106.69	110.67
44	NJ	501	GTP	C8-N7-C5	2.51	108.73	104.26
44	PP	501	GTP	C8-N7-C5	2.51	108.73	104.26
44	RN	501	GTP	C8-N7-C5	2.51	108.73	104.26
46	WA	501	GDP	C4-C5-N7	-2.51	106.69	110.67
44	VL	501	GTP	C5-C6-N1	2.51	119.64	113.25
44	YJ	501	GTP	C5-C6-N1	2.51	119.64	113.25
44	RJ	501	GTP	C8-N7-C5	2.51	108.73	104.26
44	TN	501	GTP	C8-N7-C5	2.51	108.73	104.26
44	XJ	501	GTP	C5-C6-N1	2.51	119.64	113.25
44	ZL	501	GTP	C5-C6-N1	2.51	119.64	113.25
44	SB	501	GTP	C8-N7-C5	2.51	108.73	104.26
44	YB	501	GTP	C5-C6-N1	2.51	119.64	113.25
44	TD	501	GTP	C8-N7-C5	2.51	108.72	104.26
44	NL	501	GTP	C5-C6-N1	2.50	119.63	113.25
44	SD	501	GTP	C5-C6-N1	2.50	119.63	113.25
44	TP	501	GTP	C8-N7-C5	2.50	108.72	104.26
44	UL	501	GTP	C5-C6-N1	2.50	119.62	113.25
44	YH	501	GTP	C5-C6-N1	2.50	119.62	113.25
44	SB	501	GTP	C5-C6-N1	2.50	119.62	113.25
44	YF	501	GTP	C8-N7-C5	2.50	108.72	104.26
44	VN	501	GTP	C8-N7-C5	2.50	108.72	104.26
44	TB	501	GTP	C5-C6-N1	2.50	119.61	113.25
46	SK	501	GDP	C4-C5-N7	-2.50	106.71	110.67
44	XD	501	GTP	C5-C6-N1	2.50	119.61	113.25
44	UD	501	GTP	C8-N7-C5	2.50	108.71	104.26
44	ON	501	GTP	C8-N7-C5	2.50	108.71	104.26
44	ZJ	501	GTP	C8-N7-C5	2.50	108.71	104.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	RN	501	GTP	C5-C6-N1	2.50	119.61	113.25
44	RJ	501	GTP	C5-C6-N1	2.50	119.61	113.25
44	WB	501	GTP	C8-N7-C5	2.50	108.70	104.26
44	VJ	501	GTP	O6-C6-C5	-2.49	119.95	126.53
44	ZF	501	GTP	C8-N7-C5	2.49	108.70	104.26
44	TF	501	GTP	C5-C6-N1	2.49	119.60	113.25
46	OG	501	GDP	C4-C5-N7	-2.49	106.72	110.67
46	VO	501	GDP	C4-C5-N7	-2.49	106.72	110.67
44	QD	501	GTP	C8-N7-C5	2.49	108.70	104.26
44	QL	501	GTP	C8-N7-C5	2.49	108.70	104.26
44	PJ	501	GTP	O6-C6-C5	-2.49	119.96	126.53
44	ZN	501	GTP	C5-C6-N1	2.49	119.59	113.25
44	OP	501	GTP	C8-N7-C5	2.49	108.69	104.26
44	ZB	501	GTP	C8-N7-C5	2.49	108.69	104.26
46	OI	501	GDP	C4-C5-N7	-2.49	106.73	110.67
44	XN	501	GTP	C8-N7-C5	2.49	108.69	104.26
44	VD	501	GTP	O6-C6-C5	-2.49	119.97	126.53
44	XN	501	GTP	C5-C6-N1	2.49	119.58	113.25
44	ZL	501	GTP	C8-N7-C5	2.49	108.69	104.26
44	PH	501	GTP	C8-N7-C5	2.48	108.69	104.26
44	WL	501	GTP	C8-N7-C5	2.48	108.69	104.26
44	QP	501	GTP	C5-C6-N1	2.48	119.58	113.25
44	YL	501	GTP	C5-C6-N1	2.48	119.58	113.25
46	UO	501	GDP	C4-C5-N7	-2.48	106.73	110.67
44	XB	501	GTP	C8-N7-C5	2.48	108.68	104.26
44	UP	501	GTP	C8-N7-C5	2.48	108.68	104.26
44	YD	501	GTP	C5-C6-N1	2.48	119.56	113.25
44	UF	501	GTP	C8-N7-C5	2.48	108.67	104.26
44	UP	501	GTP	C5-C6-N1	2.48	119.56	113.25
46	UG	501	GDP	C4-C5-N7	-2.48	106.74	110.67
44	SN	501	GTP	C5-C6-N1	2.48	119.56	113.25
44	VF	501	GTP	C5-C6-N1	2.48	119.56	113.25
44	XF	501	GTP	O3G-PG-O3B	2.48	112.94	104.64
44	YP	501	GTP	O6-C6-C5	-2.47	120.00	126.53
44	VB	501	GTP	C8-N7-C5	2.47	108.67	104.26
44	PN	501	GTP	O6-C6-C5	-2.47	120.00	126.53
44	OD	501	GTP	C5-C6-N1	2.47	119.55	113.25
44	VF	501	GTP	C8-N7-C5	2.47	108.67	104.26
44	NB	501	GTP	C8-N7-C5	2.47	108.66	104.26
44	TH	501	GTP	O6-C6-C5	-2.47	120.01	126.53
44	TJ	501	GTP	O6-C6-C5	-2.47	120.01	126.53
44	ZL	501	GTP	O6-C6-C5	-2.47	120.01	126.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	PF	501	GTP	C8-N7-C5	2.47	108.66	104.26
44	XH	501	GTP	C8-N7-C5	2.47	108.66	104.26
44	XJ	501	GTP	C8-N7-C5	2.47	108.66	104.26
44	YD	501	GTP	C8-N7-C5	2.47	108.66	104.26
44	VD	501	GTP	C8-N7-C5	2.47	108.66	104.26
44	XL	501	GTP	C8-N7-C5	2.47	108.66	104.26
44	SF	501	GTP	C8-N7-C5	2.47	108.66	104.26
46	OQ	501	GDP	C4-C5-N7	-2.47	106.76	110.67
44	RD	501	GTP	O6-C6-C5	-2.47	120.02	126.53
44	WN	501	GTP	C8-N7-C5	2.47	108.65	104.26
44	UH	501	GTP	O6-C6-C5	-2.46	120.03	126.53
44	XL	501	GTP	O6-C6-C5	-2.46	120.03	126.53
44	ZD	501	GTP	C8-N7-C5	2.46	108.65	104.26
44	VH	501	GTP	O6-C6-C5	-2.46	120.04	126.53
44	TL	501	GTP	C8-N7-C5	2.46	108.64	104.26
44	ZP	501	GTP	C8-N7-C5	2.46	108.64	104.26
46	PO	501	GDP	C4-C5-N7	-2.46	106.77	110.67
44	WH	501	GTP	O6-C6-C5	-2.46	120.05	126.53
44	QN	501	GTP	O6-C6-C5	-2.46	120.05	126.53
44	TP	501	GTP	O6-C6-C5	-2.46	120.05	126.53
44	PH	501	GTP	O6-C6-C5	-2.45	120.06	126.53
44	QL	501	GTP	O6-C6-C5	-2.45	120.06	126.53
44	PH	501	GTP	C5-C6-N1	2.45	119.50	113.25
44	SN	501	GTP	C8-N7-C5	2.45	108.63	104.26
44	VP	501	GTP	C8-N7-C5	2.45	108.63	104.26
44	WB	501	GTP	O6-C6-C5	-2.45	120.06	126.53
44	YB	501	GTP	O6-C6-C5	-2.45	120.07	126.53
44	PD	501	GTP	O6-C6-C5	-2.45	120.07	126.53
46	SO	502	GDP	C4-C5-N7	-2.45	106.79	110.67
46	XK	501	GDP	C4-C5-N7	-2.44	106.80	110.67
46	YM	501	GDP	C4-C5-N7	-2.44	106.80	110.67
44	VB	501	GTP	C5-C6-N1	2.44	119.47	113.25
44	XF	501	GTP	O6-C6-C5	-2.44	120.09	126.53
44	YF	501	GTP	O6-C6-C5	-2.44	120.09	126.53
44	QF	501	GTP	C8-N7-C5	2.44	108.61	104.26
44	NJ	501	GTP	O6-C6-C5	-2.44	120.09	126.53
44	ZF	501	GTP	C5-C6-N1	2.44	119.47	113.25
44	UB	501	GTP	O6-C6-C5	-2.44	120.09	126.53
44	ZD	501	GTP	C5-C6-N1	2.44	119.46	113.25
44	RJ	501	GTP	O6-C6-C5	-2.44	120.10	126.53
44	TD	501	GTP	O6-C6-C5	-2.44	120.10	126.53
44	SP	501	GTP	O6-C6-C5	-2.44	120.10	126.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	XB	501	GTP	O6-C6-C5	-2.44	120.10	126.53
44	OJ	501	GTP	O6-C6-C5	-2.44	120.10	126.53
44	ZJ	501	GTP	O6-C6-C5	-2.44	120.10	126.53
44	RH	501	GTP	O6-C6-C5	-2.44	120.10	126.53
44	WJ	501	GTP	O6-C6-C5	-2.44	120.10	126.53
44	ZB	501	GTP	C5-C6-N1	2.44	119.45	113.25
42	1C	2601	ADP	N3-C4-N9	2.43	131.31	127.17
44	ON	501	GTP	O6-C6-C5	-2.43	120.11	126.53
44	SL	501	GTP	O6-C6-C5	-2.43	120.11	126.53
44	XH	501	GTP	O6-C6-C5	-2.43	120.11	126.53
44	OH	501	GTP	C5-C6-N1	2.43	119.45	113.25
44	TB	501	GTP	O6-C6-C5	-2.43	120.11	126.53
44	QF	501	GTP	O6-C6-C5	-2.43	120.11	126.53
44	TN	501	GTP	O6-C6-C5	-2.43	120.12	126.53
44	XD	501	GTP	O6-C6-C5	-2.43	120.12	126.53
44	OH	501	GTP	O6-C6-C5	-2.43	120.12	126.53
44	QJ	501	GTP	O6-C6-C5	-2.43	120.12	126.53
44	WN	501	GTP	O6-C6-C5	-2.43	120.12	126.53
44	VP	501	GTP	C5-C6-N1	2.43	119.43	113.25
44	NB	501	GTP	O6-C6-C5	-2.43	120.13	126.53
44	TL	501	GTP	O6-C6-C5	-2.43	120.13	126.53
46	VG	501	GDP	C4-C5-N7	-2.43	106.83	110.67
46	PQ	501	GDP	C3'-C2'-C1'	2.42	106.04	101.46
44	XJ	501	GTP	O6-C6-C5	-2.42	120.14	126.53
46	UC	501	GDP	O6-C6-C5	-2.42	120.14	126.53
44	VL	501	GTP	O6-C6-C5	-2.42	120.15	126.53
44	SB	501	GTP	O6-C6-C5	-2.42	120.15	126.53
44	QD	501	GTP	O6-C6-C5	-2.42	120.15	126.53
44	YH	501	GTP	O6-C6-C5	-2.42	120.15	126.53
44	PL	501	GTP	O6-C6-C5	-2.42	120.16	126.53
44	XN	501	GTP	O6-C6-C5	-2.42	120.16	126.53
44	WF	501	GTP	O6-C6-C5	-2.41	120.16	126.53
46	VI	501	GDP	C4-C5-N7	-2.41	106.84	110.67
44	VJ	501	GTP	C8-N7-C5	2.41	108.56	104.26
44	NH	501	GTP	O6-C6-C5	-2.41	120.16	126.53
44	YD	501	GTP	O6-C6-C5	-2.41	120.16	126.53
46	QM	501	GDP	C4-C5-N7	-2.41	106.85	110.67
44	ZP	501	GTP	C5-C6-N1	2.41	119.39	113.25
44	YN	501	GTP	O6-C6-C5	-2.41	120.17	126.53
46	QE	501	GDP	C3'-C2'-C1'	2.41	106.02	101.46
44	UF	501	GTP	O6-C6-C5	-2.41	120.17	126.53
44	SF	501	GTP	O6-C6-C5	-2.41	120.18	126.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	UJ	501	GTP	O6-C6-C5	-2.41	120.18	126.53
44	PF	501	GTP	O6-C6-C5	-2.41	120.18	126.53
44	VP	501	GTP	O6-C6-C5	-2.40	120.19	126.53
44	UL	501	GTP	O6-C6-C5	-2.40	120.19	126.53
44	ND	501	GTP	O6-C6-C5	-2.40	120.19	126.53
44	NF	501	GTP	O6-C6-C5	-2.40	120.19	126.53
44	VN	501	GTP	O6-C6-C5	-2.40	120.20	126.53
44	QH	501	GTP	O6-C6-C5	-2.40	120.20	126.53
44	NL	501	GTP	O6-C6-C5	-2.40	120.20	126.53
44	ZP	501	GTP	O6-C6-C5	-2.40	120.20	126.53
43	C3	2001	ANP	C5-C4-N9	-2.40	103.20	105.81
44	YJ	501	GTP	O6-C6-C5	-2.40	120.20	126.53
44	TF	501	GTP	O6-C6-C5	-2.40	120.20	126.53
44	YL	501	GTP	O6-C6-C5	-2.40	120.20	126.53
44	UN	501	GTP	O6-C6-C5	-2.40	120.21	126.53
44	RF	501	GTP	O6-C6-C5	-2.40	120.21	126.53
44	WD	501	GTP	O6-C6-C5	-2.40	120.21	126.53
44	SD	501	GTP	O6-C6-C5	-2.39	120.21	126.53
44	VB	501	GTP	O6-C6-C5	-2.39	120.21	126.53
46	QG	501	GDP	C3'-C2'-C1'	2.39	105.99	101.46
44	SN	501	GTP	O6-C6-C5	-2.39	120.22	126.53
44	VF	501	GTP	O6-C6-C5	-2.39	120.22	126.53
44	QP	501	GTP	O6-C6-C5	-2.39	120.23	126.53
42	1D	2601	ADP	N6-C6-N1	-2.39	113.06	118.38
44	ZD	501	GTP	O6-C6-C5	-2.39	120.24	126.53
44	OH	501	GTP	C8-N7-C5	2.38	108.51	104.26
44	OL	501	GTP	O6-C6-C5	-2.38	120.24	126.53
44	ZB	501	GTP	O6-C6-C5	-2.38	120.24	126.53
46	ZC	501	GDP	C4-C5-N7	-2.38	106.89	110.67
46	OM	501	GDP	C4-C5-N7	-2.38	106.90	110.67
44	OD	501	GTP	O6-C6-C5	-2.38	120.25	126.53
44	SH	501	GTP	O6-C6-C5	-2.38	120.25	126.53
44	OF	501	GTP	O6-C6-C5	-2.38	120.25	126.53
44	ZN	501	GTP	O6-C6-C5	-2.37	120.26	126.53
46	OK	501	GDP	C4-C5-N7	-2.37	106.91	110.67
44	PP	501	GTP	O6-C6-C5	-2.37	120.27	126.53
44	WL	501	GTP	O6-C6-C5	-2.37	120.28	126.53
46	NE	501	GDP	C2'-C3'-C4'	2.37	107.18	102.61
44	RP	501	GTP	O6-C6-C5	-2.36	120.29	126.53
46	NO	501	GDP	C3'-C2'-C1'	2.36	105.92	101.46
44	UD	501	GTP	O6-C6-C5	-2.36	120.31	126.53
44	UP	501	GTP	O6-C6-C5	-2.36	120.31	126.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	NB	501	GTP	C3'-C2'-C1'	2.36	105.92	101.46
42	1A	2601	ADP	N3-C4-N9	2.36	131.17	127.17
44	ZF	501	GTP	O6-C6-C5	-2.35	120.33	126.53
46	OO	501	GDP	O6-C6-C5	-2.35	120.33	126.53
44	YH	501	GTP	O2A-PA-O3A	2.35	113.62	107.27
46	PC	501	GDP	C4-C5-N7	-2.35	106.95	110.67
46	VI	501	GDP	O6-C6-C5	-2.34	120.36	126.53
46	SI	501	GDP	C4-C5-N7	-2.34	106.96	110.67
46	NE	501	GDP	C4-C5-N7	-2.33	106.98	110.67
46	OQ	501	GDP	C3'-C2'-C1'	2.33	105.87	101.46
46	PO	501	GDP	C3'-C2'-C1'	2.33	105.86	101.46
44	NN	501	GTP	O6-C6-C5	-2.33	120.39	126.53
46	VC	501	GDP	C3'-C2'-C1'	2.32	105.86	101.46
46	OO	501	GDP	C4-C5-N7	-2.32	106.99	110.67
46	YC	501	GDP	C3'-C2'-C1'	2.32	105.85	101.46
46	OC	501	GDP	C3'-C2'-C1'	2.32	105.84	101.46
44	ZH	501	GTP	O6-C6-C5	-2.31	120.44	126.53
44	XD	501	GTP	O2A-PA-O3A	2.30	113.49	107.27
44	OL	501	GTP	O3G-PG-O3B	2.30	112.34	104.64
46	VG	501	GDP	O6-C6-C5	-2.29	120.48	126.53
44	RH	501	GTP	O2A-PA-O3A	2.29	113.47	107.27
44	RN	501	GTP	O6-C6-C5	-2.29	120.49	126.53
46	SM	501	GDP	C3'-C2'-C1'	2.28	105.78	101.46
43	C3	2001	ANP	C4-C5-N7	2.28	113.19	110.58
46	PG	501	GDP	C3'-C2'-C1'	2.28	105.77	101.46
44	OJ	501	GTP	C3'-C2'-C1'	2.27	105.75	101.46
46	SO	502	GDP	O6-C6-C5	-2.27	120.55	126.53
46	ZM	501	GDP	C3'-C2'-C1'	2.26	105.75	101.46
46	ZC	501	GDP	C2'-C1'-N9	-2.26	106.97	113.25
42	1B	2601	ADP	C5-C6-N6	2.26	128.87	123.29
44	TH	501	GTP	O2B-PB-O3A	2.25	113.35	107.27
44	QN	501	GTP	C3'-C2'-C1'	2.24	105.70	101.46
46	OM	501	GDP	O6-C6-C5	-2.24	120.62	126.53
46	TC	501	GDP	C3'-C2'-C1'	2.24	105.69	101.46
44	SP	501	GTP	C3'-C2'-C1'	2.23	105.68	101.46
46	OG	501	GDP	O6-C6-C5	-2.23	120.64	126.53
46	YO	501	GDP	O6-C6-C5	-2.22	120.67	126.53
46	SK	501	GDP	C3'-C2'-C1'	2.21	105.65	101.46
44	QL	501	GTP	C3'-C2'-C1'	2.21	105.64	101.46
44	QD	501	GTP	O2A-PA-O3A	2.21	113.24	107.27
44	PJ	501	GTP	C3'-C2'-C1'	2.21	105.64	101.46
46	NG	502	GDP	C3'-C2'-C1'	2.21	105.64	101.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	1C	2602	ANP	O1B-PB-N3B	-2.20	108.53	111.77
44	RP	501	GTP	O2A-PA-O3A	2.20	113.22	107.27
46	UC	501	GDP	C4-C5-N7	-2.20	107.18	110.67
44	QD	501	GTP	O2B-PB-O3A	2.20	113.22	107.27
46	QQ	501	GDP	O6-C6-C5	-2.20	120.72	126.53
44	QD	501	GTP	C3'-C2'-C1'	2.20	105.62	101.46
46	NE	501	GDP	O6-C6-C5	-2.20	120.73	126.53
44	UN	501	GTP	O3G-PG-O3B	2.20	112.00	104.64
46	OK	501	GDP	O6-C6-C5	-2.19	120.75	126.53
44	PD	501	GTP	C3'-C2'-C1'	2.19	105.60	101.46
43	C2	2001	ANP	C4-N9-C1'	2.18	131.74	126.63
44	TP	501	GTP	O2A-PA-O3A	2.18	113.17	107.27
46	PI	502	GDP	C3'-C2'-C1'	2.18	105.59	101.46
43	1C	2602	ANP	O1G-PG-N3B	-2.18	108.56	111.77
46	TM	502	GDP	C3'-C2'-C1'	2.18	105.59	101.46
46	WO	501	GDP	C3'-C2'-C1'	2.18	105.58	101.46
46	RC	501	GDP	C3'-C2'-C1'	2.18	105.58	101.46
46	OQ	501	GDP	O6-C6-C5	-2.18	120.78	126.53
42	1D	2601	ADP	N3-C4-N9	2.17	130.87	127.17
46	WA	501	GDP	O6-C6-C5	-2.17	120.80	126.53
44	PF	501	GTP	C3'-C2'-C1'	2.17	105.57	101.46
44	PF	501	GTP	C2'-C1'-N9	-2.17	107.21	113.25
46	SE	501	GDP	C3'-C2'-C1'	2.17	105.57	101.46
44	TF	501	GTP	C3'-C2'-C1'	2.17	105.56	101.46
44	PJ	501	GTP	O3G-PG-O3B	2.16	111.89	104.64
46	UG	501	GDP	O6-C6-C5	-2.16	120.82	126.53
44	YP	501	GTP	C3'-C2'-C1'	2.16	105.55	101.46
46	UO	501	GDP	O6-C6-C5	-2.16	120.83	126.53
46	QM	501	GDP	O6-C6-C5	-2.16	120.83	126.53
46	SI	501	GDP	C2'-C3'-C4'	2.16	106.78	102.61
46	ZG	501	GDP	O6-C6-C5	-2.16	120.83	126.53
46	OM	501	GDP	C3'-C2'-C1'	2.16	105.54	101.46
44	QN	501	GTP	O2A-PA-O3A	2.16	113.10	107.27
44	RF	501	GTP	O3G-PG-O3B	2.16	111.86	104.64
46	WC	501	GDP	C8-N7-C5	2.15	108.09	104.26
46	SE	501	GDP	O6-C6-C5	-2.15	120.86	126.53
44	TL	501	GTP	C3'-C2'-C1'	2.15	105.53	101.46
46	VO	501	GDP	O6-C6-C5	-2.15	120.87	126.53
44	TD	501	GTP	C3'-C2'-C1'	2.15	105.52	101.46
46	WI	501	GDP	O6-C6-C5	-2.14	120.87	126.53
44	ZH	501	GTP	C3'-C2'-C1'	2.14	105.52	101.46
44	VL	501	GTP	C3'-C2'-C1'	2.14	105.52	101.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	RG	501	GDP	O6-C6-C5	-2.14	120.88	126.53
46	PO	501	GDP	O6-C6-C5	-2.14	120.88	126.53
46	XI	501	GDP	O6-C6-C5	-2.14	120.88	126.53
42	1B	2601	ADP	N3-C4-N9	2.14	130.81	127.17
46	VK	501	GDP	O6-C6-C5	-2.14	120.89	126.53
46	QC	501	GDP	O6-C6-C5	-2.14	120.89	126.53
46	TG	502	GDP	O6-C6-C5	-2.14	120.89	126.53
44	SF	501	GTP	C3'-C2'-C1'	2.13	105.50	101.46
44	WL	501	GTP	C3'-C2'-C1'	2.13	105.50	101.46
46	PC	501	GDP	C3'-C2'-C1'	2.13	105.49	101.46
44	RH	501	GTP	O2B-PB-O3A	2.13	113.03	107.27
46	PE	501	GDP	O6-C6-C5	-2.13	120.91	126.53
46	PQ	501	GDP	O6-C6-C5	-2.13	120.92	126.53
44	QF	501	GTP	C3'-C2'-C1'	2.13	105.49	101.46
44	UP	501	GTP	C3'-C2'-C1'	2.13	105.49	101.46
46	NM	501	GDP	O6-C6-C5	-2.13	120.92	126.53
46	QI	501	GDP	O6-C6-C5	-2.12	120.93	126.53
46	PC	501	GDP	O6-C6-C5	-2.12	120.93	126.53
42	1D	2601	ADP	C5-C4-N9	2.12	108.12	105.81
46	SK	501	GDP	O6-C6-C5	-2.12	120.93	126.53
46	TM	502	GDP	O6-C6-C5	-2.12	120.94	126.53
46	OE	501	GDP	O6-C6-C5	-2.12	120.94	126.53
44	ND	501	GTP	C3'-C2'-C1'	2.12	105.47	101.46
44	UN	501	GTP	C3'-C2'-C1'	2.12	105.47	101.46
46	YE	501	GDP	O6-C6-C5	-2.12	120.95	126.53
46	RK	501	GDP	O6-C6-C5	-2.11	120.95	126.53
46	XO	501	GDP	O6-C6-C5	-2.11	120.95	126.53
44	YB	501	GTP	C3'-C2'-C1'	2.11	105.46	101.46
46	UM	501	GDP	O6-C6-C5	-2.11	120.95	126.53
46	TC	501	GDP	O6-C6-C5	-2.11	120.96	126.53
46	VC	501	GDP	O6-C6-C5	-2.11	120.96	126.53
46	WM	501	GDP	O6-C6-C5	-2.11	120.96	126.53
46	OI	501	GDP	O6-C6-C5	-2.11	120.96	126.53
46	XC	501	GDP	O6-C6-C5	-2.11	120.96	126.53
46	RI	502	GDP	O6-C6-C5	-2.11	120.97	126.53
46	YK	501	GDP	O6-C6-C5	-2.11	120.97	126.53
46	VG	501	GDP	C3'-C2'-C1'	2.11	105.45	101.46
46	ZC	501	GDP	O6-C6-C5	-2.11	120.97	126.53
46	YM	501	GDP	O6-C6-C5	-2.11	120.97	126.53
46	XK	501	GDP	O6-C6-C5	-2.11	120.97	126.53
46	XM	502	GDP	O6-C6-C5	-2.11	120.97	126.53
44	UL	501	GTP	O3G-PG-O3B	2.11	111.70	104.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	XH	501	GTP	C3'-C2'-C1'	2.11	105.45	101.46
44	WJ	501	GTP	O2A-PA-O3A	2.11	112.97	107.27
44	VJ	501	GTP	O3G-PG-O3B	2.11	111.69	104.64
44	UF	501	GTP	C3'-C2'-C1'	2.11	105.44	101.46
44	UH	501	GTP	C3'-C2'-C1'	2.11	105.44	101.46
46	XA	501	GDP	O6-C6-C5	-2.10	120.98	126.53
44	SB	501	GTP	C3'-C2'-C1'	2.10	105.44	101.46
46	ZE	501	GDP	O6-C6-C5	-2.10	120.98	126.53
44	YF	501	GTP	C3'-C2'-C1'	2.10	105.44	101.46
46	XG	501	GDP	O6-C6-C5	-2.10	120.98	126.53
46	ZO	501	GDP	C3'-C2'-C1'	2.10	105.44	101.46
46	TI	501	GDP	O6-C6-C5	-2.10	120.98	126.53
46	ZK	501	GDP	O6-C6-C5	-2.10	120.98	126.53
46	ZO	501	GDP	O6-C6-C5	-2.10	120.99	126.53
46	SI	501	GDP	O6-C6-C5	-2.10	121.00	126.53
46	SC	502	GDP	O6-C6-C5	-2.10	121.00	126.53
46	NG	502	GDP	O6-C6-C5	-2.09	121.00	126.53
46	SM	501	GDP	O6-C6-C5	-2.09	121.01	126.53
44	NL	501	GTP	C3'-C2'-C1'	2.09	105.42	101.46
46	RC	501	GDP	O6-C6-C5	-2.09	121.01	126.53
44	WN	501	GTP	C3'-C2'-C1'	2.09	105.42	101.46
44	YP	501	GTP	O2A-PA-O3A	2.09	112.92	107.27
46	TE	501	GDP	O6-C6-C5	-2.09	121.02	126.53
46	ZI	501	GDP	O6-C6-C5	-2.09	121.02	126.53
46	SG	502	GDP	O6-C6-C5	-2.09	121.02	126.53
46	UK	501	GDP	O6-C6-C5	-2.09	121.02	126.53
44	NJ	501	GTP	C3'-C2'-C1'	2.09	105.41	101.46
44	PP	501	GTP	C3'-C2'-C1'	2.09	105.41	101.46
46	NO	501	GDP	O6-C6-C5	-2.08	121.03	126.53
46	PG	501	GDP	O6-C6-C5	-2.08	121.03	126.53
44	WD	501	GTP	C3'-C2'-C1'	2.08	105.40	101.46
42	1D	2601	ADP	C5-C6-N6	2.08	128.43	123.29
44	SN	501	GTP	C3'-C2'-C1'	2.08	105.39	101.46
46	QM	501	GDP	C3'-C2'-C1'	2.08	105.39	101.46
46	ZM	501	GDP	O6-C6-C5	-2.08	121.05	126.53
44	WJ	501	GTP	C3'-C2'-C1'	2.07	105.39	101.46
46	VM	501	GDP	O6-C6-C5	-2.07	121.06	126.53
46	PI	502	GDP	O6-C6-C5	-2.07	121.06	126.53
46	WO	501	GDP	O6-C6-C5	-2.07	121.06	126.53
46	XC	501	GDP	C3'-C2'-C1'	2.07	105.38	101.46
44	PH	501	GTP	C3'-C2'-C1'	2.07	105.38	101.46
46	PK	501	GDP	O6-C6-C5	-2.07	121.07	126.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	NI	501	GDP	O6-C6-C5	-2.07	121.07	126.53
46	WE	501	GDP	O6-C6-C5	-2.07	121.07	126.53
44	ON	501	GTP	C3'-C2'-C1'	2.07	105.38	101.46
46	QQ	501	GDP	C3'-C2'-C1'	2.07	105.38	101.46
44	SJ	501	GTP	C3'-C2'-C1'	2.07	105.37	101.46
44	RN	501	GTP	C3'-C2'-C1'	2.07	105.37	101.46
46	OC	501	GDP	O6-C6-C5	-2.07	121.08	126.53
46	WG	502	GDP	O6-C6-C5	-2.07	121.08	126.53
46	QE	501	GDP	O6-C6-C5	-2.06	121.09	126.53
46	TO	501	GDP	O6-C6-C5	-2.06	121.09	126.53
44	YN	501	GTP	O3G-PG-O3B	2.06	111.55	104.64
46	YG	501	GDP	O6-C6-C5	-2.06	121.09	126.53
44	QH	501	GTP	C3'-C2'-C1'	2.06	105.36	101.46
46	RO	501	GDP	O6-C6-C5	-2.06	121.10	126.53
44	ZF	501	GTP	C3'-C2'-C1'	2.06	105.35	101.46
44	YL	501	GTP	O3G-PG-O3B	2.06	111.53	104.64
44	NH	501	GTP	C3'-C2'-C1'	2.06	105.35	101.46
44	ZB	501	GTP	C3'-C2'-C1'	2.06	105.35	101.46
46	QC	501	GDP	C3'-C2'-C1'	2.06	105.35	101.46
46	ZK	501	GDP	C3'-C2'-C1'	2.06	105.35	101.46
46	RI	502	GDP	C3'-C2'-C1'	2.06	105.35	101.46
46	UG	501	GDP	C3'-C2'-C1'	2.06	105.35	101.46
44	ZL	501	GTP	C3'-C2'-C1'	2.05	105.35	101.46
46	XE	501	GDP	O6-C6-C5	-2.05	121.12	126.53
44	YD	501	GTP	O3G-PG-O3B	2.05	111.51	104.64
46	PE	501	GDP	C3'-C2'-C1'	2.05	105.34	101.46
46	NK	501	GDP	O6-C6-C5	-2.05	121.12	126.53
44	ZP	501	GTP	C3'-C2'-C1'	2.05	105.34	101.46
44	XD	501	GTP	O2B-PB-O3A	2.05	112.81	107.27
44	UJ	501	GTP	C3'-C2'-C1'	2.05	105.34	101.46
46	QK	501	GDP	O6-C6-C5	-2.05	121.13	126.53
44	SH	501	GTP	C3'-C2'-C1'	2.05	105.33	101.46
46	QO	501	GDP	O6-C6-C5	-2.04	121.14	126.53
44	NN	501	GTP	C3'-C2'-C1'	2.04	105.33	101.46
46	TK	501	GDP	O6-C6-C5	-2.04	121.14	126.53
44	YN	501	GTP	C3'-C2'-C1'	2.04	105.33	101.46
46	YC	501	GDP	O6-C6-C5	-2.04	121.14	126.53
44	WJ	501	GTP	O2B-PB-O3A	2.04	112.79	107.27
46	UC	501	GDP	C5-C6-N1	2.04	118.45	113.25
44	XD	501	GTP	C3'-C2'-C1'	2.04	105.32	101.46
46	VE	501	GDP	O6-C6-C5	-2.04	121.15	126.53
46	UE	501	GDP	O6-C6-C5	-2.04	121.15	126.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	1B	2601	ADP	C3'-C2'-C1'	2.04	105.32	101.46
46	RE	501	GDP	O6-C6-C5	-2.04	121.16	126.53
46	WC	501	GDP	O6-C6-C5	-2.03	121.16	126.53
44	YH	501	GTP	C3'-C2'-C1'	2.03	105.31	101.46
44	RP	501	GTP	O2B-PB-O3A	2.03	112.76	107.27
43	C2	2001	ANP	C1'-N9-C8	-2.03	122.59	127.09
46	OK	501	GDP	C5-C6-N1	2.03	118.42	113.25
46	QM	501	GDP	C2'-C3'-C4'	2.03	106.53	102.61
46	TE	501	GDP	C3'-C2'-C1'	2.03	105.30	101.46
44	ZJ	501	GTP	C3'-C2'-C1'	2.03	105.30	101.46
44	OL	501	GTP	C3'-C2'-C1'	2.03	105.30	101.46
46	OI	501	GDP	C3'-C2'-C1'	2.03	105.30	101.46
44	VL	501	GTP	O3G-PG-O3B	2.02	111.42	104.64
46	VO	501	GDP	C2'-C3'-C4'	2.02	106.52	102.61
44	QJ	501	GTP	C3'-C2'-C1'	2.02	105.29	101.46
44	YD	501	GTP	C3'-C2'-C1'	2.02	105.29	101.46
46	NC	501	GDP	O6-C6-C5	-2.02	121.20	126.53
46	RM	501	GDP	O6-C6-C5	-2.02	121.20	126.53
46	WK	501	GDP	O6-C6-C5	-2.02	121.20	126.53
44	TN	501	GTP	C3'-C2'-C1'	2.02	105.28	101.46
44	SH	501	GTP	O3G-PG-O3B	2.01	111.39	104.64
44	OH	501	GTP	C3'-C2'-C1'	2.01	105.27	101.46
44	TP	501	GTP	C3'-C2'-C1'	2.01	105.27	101.46
44	TB	501	GTP	C3'-C2'-C1'	2.01	105.26	101.46
44	ZD	501	GTP	C3'-C2'-C1'	2.01	105.26	101.46
46	UI	501	GDP	O6-C6-C5	-2.01	121.23	126.53
46	UI	501	GDP	C5-C6-N1	2.00	118.36	113.25
46	OG	501	GDP	C5-C6-N1	2.00	118.36	113.25
44	ZD	501	GTP	O3G-PG-O3B	2.00	111.36	104.64
46	QG	501	GDP	O6-C6-C5	-2.00	121.25	126.53
44	VD	501	GTP	C3'-C2'-C1'	2.00	105.25	101.46
44	XL	501	GTP	C3'-C2'-C1'	2.00	105.25	101.46
44	SL	501	GTP	C3'-C2'-C1'	2.00	105.25	101.46

There are no chirality outliers.

All (633) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
42	1D	2601	ADP	C5'-O5'-PA-O1A
43	1A	2602	ANP	PB-N3B-PG-O1G
43	1A	2602	ANP	PG-N3B-PB-O1B
43	1A	2602	ANP	PA-O3A-PB-O2B

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Mol	Chain	Res	Type	Atoms
43	1A	2602	ANP	C5'-O5'-PA-O1A
43	1A	2602	ANP	C5'-O5'-PA-O2A
43	1A	2602	ANP	C5'-O5'-PA-O3A
43	1B	2602	ANP	PB-N3B-PG-O1G
43	1B	2602	ANP	PG-N3B-PB-O1B
43	1B	2602	ANP	PB-O3A-PA-O5'
43	1B	2602	ANP	C5'-O5'-PA-O2A
43	1B	2602	ANP	C5'-O5'-PA-O3A
43	1B	2602	ANP	O4'-C4'-C5'-O5'
43	1B	2602	ANP	C3'-C4'-C5'-O5'
43	1C	2602	ANP	PB-N3B-PG-O1G
43	1C	2602	ANP	PG-N3B-PB-O1B
43	1C	2602	ANP	PA-O3A-PB-O2B
43	1C	2602	ANP	C5'-O5'-PA-O3A
43	1C	2602	ANP	O4'-C4'-C5'-O5'
43	1D	2602	ANP	PB-N3B-PG-O1G
43	1D	2602	ANP	PG-N3B-PB-O1B
43	1D	2602	ANP	PG-N3B-PB-O3A
43	1D	2602	ANP	PA-O3A-PB-O2B
43	1D	2602	ANP	C5'-O5'-PA-O1A
43	1D	2602	ANP	C5'-O5'-PA-O3A
43	1D	2602	ANP	O4'-C4'-C5'-O5'
43	C0	2001	ANP	PB-N3B-PG-O1G
43	C1	2001	ANP	PB-N3B-PG-O1G
43	C2	2001	ANP	PB-N3B-PG-O1G
43	C3	2001	ANP	PB-N3B-PG-O1G
44	NB	501	GTP	C5'-O5'-PA-O3A
44	NB	501	GTP	C5'-O5'-PA-O1A
44	NB	501	GTP	C5'-O5'-PA-O2A
44	NH	501	GTP	C5'-O5'-PA-O1A
44	NJ	501	GTP	PB-O3B-PG-O3G
44	NL	501	GTP	C5'-O5'-PA-O3A
44	NL	501	GTP	C5'-O5'-PA-O1A
44	OD	501	GTP	C5'-O5'-PA-O3A
44	OD	501	GTP	C5'-O5'-PA-O1A
44	OD	501	GTP	C5'-O5'-PA-O2A
44	OH	501	GTP	C5'-O5'-PA-O3A
44	OH	501	GTP	C5'-O5'-PA-O1A
44	OH	501	GTP	C5'-O5'-PA-O2A
44	OJ	501	GTP	C5'-O5'-PA-O3A
44	OJ	501	GTP	C4'-C5'-O5'-PA
44	OL	501	GTP	C5'-O5'-PA-O3A

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Mol	Chain	Res	Type	Atoms
44	OL	501	GTP	C5'-O5'-PA-O1A
44	ON	501	GTP	C5'-O5'-PA-O3A
44	ON	501	GTP	C5'-O5'-PA-O2A
44	PF	501	GTP	C5'-O5'-PA-O3A
44	PF	501	GTP	C5'-O5'-PA-O1A
44	PH	501	GTP	C5'-O5'-PA-O3A
44	PH	501	GTP	C5'-O5'-PA-O1A
44	PH	501	GTP	C5'-O5'-PA-O2A
44	PJ	501	GTP	C5'-O5'-PA-O3A
44	PJ	501	GTP	C5'-O5'-PA-O1A
44	PJ	501	GTP	C5'-O5'-PA-O2A
44	PP	501	GTP	C5'-O5'-PA-O3A
44	PP	501	GTP	C5'-O5'-PA-O1A
44	QD	501	GTP	C5'-O5'-PA-O3A
44	QD	501	GTP	C5'-O5'-PA-O1A
44	QD	501	GTP	C5'-O5'-PA-O2A
44	QF	501	GTP	C5'-O5'-PA-O3A
44	QF	501	GTP	C5'-O5'-PA-O2A
44	QL	501	GTP	C5'-O5'-PA-O3A
44	QL	501	GTP	C5'-O5'-PA-O2A
44	QN	501	GTP	C5'-O5'-PA-O3A
44	QN	501	GTP	C5'-O5'-PA-O1A
44	QN	501	GTP	C5'-O5'-PA-O2A
44	QP	501	GTP	C5'-O5'-PA-O1A
44	QP	501	GTP	C5'-O5'-PA-O2A
44	RH	501	GTP	C5'-O5'-PA-O3A
44	RH	501	GTP	C5'-O5'-PA-O1A
44	RH	501	GTP	C5'-O5'-PA-O2A
44	RJ	501	GTP	C5'-O5'-PA-O1A
44	RL	501	GTP	C5'-O5'-PA-O3A
44	RL	501	GTP	C5'-O5'-PA-O2A
44	RN	501	GTP	C5'-O5'-PA-O3A
44	RN	501	GTP	C5'-O5'-PA-O1A
44	RN	501	GTP	C5'-O5'-PA-O2A
44	RP	501	GTP	C5'-O5'-PA-O3A
44	RP	501	GTP	C5'-O5'-PA-O1A
44	RP	501	GTP	C5'-O5'-PA-O2A
44	SF	501	GTP	C5'-O5'-PA-O3A
44	SF	501	GTP	C5'-O5'-PA-O1A
44	SH	501	GTP	PB-O3B-PG-O3G
44	SH	501	GTP	C5'-O5'-PA-O3A
44	SH	501	GTP	C5'-O5'-PA-O1A

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Mol	Chain	Res	Type	Atoms
44	SH	501	GTP	C5'-O5'-PA-O2A
44	TH	501	GTP	C5'-O5'-PA-O3A
44	TH	501	GTP	C5'-O5'-PA-O1A
44	TJ	501	GTP	C5'-O5'-PA-O3A
44	TJ	501	GTP	C5'-O5'-PA-O1A
44	TJ	501	GTP	C5'-O5'-PA-O2A
44	TP	501	GTP	C5'-O5'-PA-O3A
44	TP	501	GTP	C5'-O5'-PA-O1A
44	TP	501	GTP	C5'-O5'-PA-O2A
44	UD	501	GTP	C5'-O5'-PA-O3A
44	UD	501	GTP	C5'-O5'-PA-O1A
44	UD	501	GTP	C5'-O5'-PA-O2A
44	UH	501	GTP	C5'-O5'-PA-O3A
44	UH	501	GTP	C5'-O5'-PA-O1A
44	UH	501	GTP	C5'-O5'-PA-O2A
44	UL	501	GTP	C5'-O5'-PA-O3A
44	UL	501	GTP	C5'-O5'-PA-O1A
44	UN	501	GTP	C5'-O5'-PA-O3A
44	UN	501	GTP	C5'-O5'-PA-O1A
44	VD	501	GTP	C5'-O5'-PA-O3A
44	VD	501	GTP	C5'-O5'-PA-O2A
44	VJ	501	GTP	C5'-O5'-PA-O3A
44	VJ	501	GTP	C5'-O5'-PA-O1A
44	VJ	501	GTP	C5'-O5'-PA-O2A
44	VL	501	GTP	C5'-O5'-PA-O1A
44	WH	501	GTP	C5'-O5'-PA-O3A
44	WH	501	GTP	C5'-O5'-PA-O1A
44	WH	501	GTP	C5'-O5'-PA-O2A
44	WJ	501	GTP	C5'-O5'-PA-O3A
44	WJ	501	GTP	C5'-O5'-PA-O1A
44	WL	501	GTP	C5'-O5'-PA-O3A
44	WL	501	GTP	C5'-O5'-PA-O1A
44	WL	501	GTP	C5'-O5'-PA-O2A
44	WN	501	GTP	C5'-O5'-PA-O1A
44	WN	501	GTP	C5'-O5'-PA-O2A
44	WN	501	GTP	O4'-C4'-C5'-O5'
44	XF	501	GTP	C5'-O5'-PA-O3A
44	XF	501	GTP	C5'-O5'-PA-O1A
44	XH	501	GTP	C5'-O5'-PA-O3A
44	XH	501	GTP	C5'-O5'-PA-O1A
44	XH	501	GTP	C5'-O5'-PA-O2A
44	XL	501	GTP	C5'-O5'-PA-O3A

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Mol	Chain	Res	Type	Atoms
44	XL	501	GTP	C5'-O5'-PA-O1A
44	XL	501	GTP	C5'-O5'-PA-O2A
44	YB	501	GTP	C5'-O5'-PA-O3A
44	YB	501	GTP	C5'-O5'-PA-O1A
44	YB	501	GTP	C5'-O5'-PA-O2A
44	YF	501	GTP	C5'-O5'-PA-O1A
44	YH	501	GTP	C5'-O5'-PA-O3A
44	YH	501	GTP	C5'-O5'-PA-O1A
44	YH	501	GTP	C5'-O5'-PA-O2A
44	YJ	501	GTP	C5'-O5'-PA-O1A
44	YL	501	GTP	C5'-O5'-PA-O3A
44	YL	501	GTP	C5'-O5'-PA-O1A
44	YL	501	GTP	C5'-O5'-PA-O2A
44	YP	501	GTP	C5'-O5'-PA-O3A
44	YP	501	GTP	C5'-O5'-PA-O1A
44	YP	501	GTP	C5'-O5'-PA-O2A
44	ZD	501	GTP	C5'-O5'-PA-O1A
44	ZH	501	GTP	C5'-O5'-PA-O3A
44	ZH	501	GTP	C5'-O5'-PA-O1A
44	ZH	501	GTP	C5'-O5'-PA-O2A
44	ZN	501	GTP	C5'-O5'-PA-O1A
46	OE	501	GDP	O4'-C4'-C5'-O5'
46	OM	501	GDP	O4'-C4'-C5'-O5'
46	PQ	501	GDP	C5'-O5'-PA-O1A
46	QG	501	GDP	C5'-O5'-PA-O1A
46	RE	501	GDP	O4'-C4'-C5'-O5'
46	UE	501	GDP	PA-O3A-PB-O2B
46	VI	501	GDP	C5'-O5'-PA-O3A
46	VI	501	GDP	C5'-O5'-PA-O2A
46	VI	501	GDP	O4'-C4'-C5'-O5'
46	VM	501	GDP	C5'-O5'-PA-O3A
46	VM	501	GDP	C5'-O5'-PA-O2A
46	WC	501	GDP	C5'-O5'-PA-O3A
46	WC	501	GDP	C5'-O5'-PA-O2A
46	WC	501	GDP	O4'-C4'-C5'-O5'
46	WC	501	GDP	C3'-C4'-C5'-O5'
46	YE	501	GDP	O4'-C4'-C5'-O5'
46	ZM	501	GDP	C5'-O5'-PA-O1A
43	1A	2602	ANP	C3'-C4'-C5'-O5'
43	1C	2602	ANP	C3'-C4'-C5'-O5'
43	1D	2602	ANP	C3'-C4'-C5'-O5'
44	OD	501	GTP	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
44	OL	501	GTP	O4'-C4'-C5'-O5'
44	OL	501	GTP	C3'-C4'-C5'-O5'
44	WF	501	GTP	O4'-C4'-C5'-O5'
44	WN	501	GTP	C3'-C4'-C5'-O5'
46	OE	501	GDP	C3'-C4'-C5'-O5'
46	OM	501	GDP	C3'-C4'-C5'-O5'
46	RE	501	GDP	C3'-C4'-C5'-O5'
46	TK	501	GDP	O4'-C4'-C5'-O5'
46	TK	501	GDP	C3'-C4'-C5'-O5'
46	UO	501	GDP	O4'-C4'-C5'-O5'
46	VI	501	GDP	C3'-C4'-C5'-O5'
46	WE	501	GDP	O4'-C4'-C5'-O5'
46	WE	501	GDP	C3'-C4'-C5'-O5'
46	YE	501	GDP	C3'-C4'-C5'-O5'
46	YI	501	GDP	O4'-C4'-C5'-O5'
46	YI	501	GDP	C3'-C4'-C5'-O5'
46	YM	501	GDP	O4'-C4'-C5'-O5'
46	YM	501	GDP	C3'-C4'-C5'-O5'
43	1B	2602	ANP	C4'-C5'-O5'-PA
42	1A	2601	ADP	C3'-C4'-C5'-O5'
42	1B	2601	ADP	O4'-C4'-C5'-O5'
42	1B	2601	ADP	C3'-C4'-C5'-O5'
42	1C	2601	ADP	O4'-C4'-C5'-O5'
42	1C	2601	ADP	C3'-C4'-C5'-O5'
43	1A	2602	ANP	O4'-C4'-C5'-O5'
43	C3	2001	ANP	O4'-C4'-C5'-O5'
44	OD	501	GTP	C3'-C4'-C5'-O5'
44	SF	501	GTP	O4'-C4'-C5'-O5'
44	WF	501	GTP	C3'-C4'-C5'-O5'
44	WL	501	GTP	O4'-C4'-C5'-O5'
44	WL	501	GTP	C3'-C4'-C5'-O5'
46	RG	501	GDP	O4'-C4'-C5'-O5'
46	RG	501	GDP	C3'-C4'-C5'-O5'
46	SG	502	GDP	O4'-C4'-C5'-O5'
46	SG	502	GDP	C3'-C4'-C5'-O5'
46	UO	501	GDP	C3'-C4'-C5'-O5'
46	XO	501	GDP	O4'-C4'-C5'-O5'
46	XO	501	GDP	C3'-C4'-C5'-O5'
46	YC	501	GDP	O4'-C4'-C5'-O5'
46	YC	501	GDP	C3'-C4'-C5'-O5'
46	ZG	501	GDP	O4'-C4'-C5'-O5'
46	ZG	501	GDP	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
44	QL	501	GTP	C4'-C5'-O5'-PA
42	1A	2601	ADP	O4'-C4'-C5'-O5'
43	C3	2001	ANP	C3'-C4'-C5'-O5'
44	SF	501	GTP	C3'-C4'-C5'-O5'
46	WA	501	GDP	C3'-C4'-C5'-O5'
46	XG	501	GDP	C3'-C4'-C5'-O5'
43	C0	2001	ANP	C4'-C5'-O5'-PA
44	PP	501	GTP	C3'-C4'-C5'-O5'
44	QP	501	GTP	C3'-C4'-C5'-O5'
44	RF	501	GTP	C3'-C4'-C5'-O5'
44	SD	501	GTP	C3'-C4'-C5'-O5'
44	VJ	501	GTP	C3'-C4'-C5'-O5'
46	PE	501	GDP	C3'-C4'-C5'-O5'
46	RM	501	GDP	C3'-C4'-C5'-O5'
46	RO	501	GDP	C3'-C4'-C5'-O5'
46	SO	502	GDP	C3'-C4'-C5'-O5'
46	XC	501	GDP	C3'-C4'-C5'-O5'
46	XM	502	GDP	C3'-C4'-C5'-O5'
46	YO	501	GDP	C3'-C4'-C5'-O5'
42	1D	2601	ADP	O4'-C4'-C5'-O5'
44	UL	501	GTP	C3'-C4'-C5'-O5'
44	XL	501	GTP	C3'-C4'-C5'-O5'
46	OC	501	GDP	C3'-C4'-C5'-O5'
46	OO	501	GDP	C3'-C4'-C5'-O5'
46	VO	501	GDP	C3'-C4'-C5'-O5'
46	WA	501	GDP	O4'-C4'-C5'-O5'
46	XC	501	GDP	O4'-C4'-C5'-O5'
46	XG	501	GDP	O4'-C4'-C5'-O5'
44	RF	501	GTP	O4'-C4'-C5'-O5'
44	WJ	501	GTP	C3'-C4'-C5'-O5'
46	PE	501	GDP	O4'-C4'-C5'-O5'
44	UD	501	GTP	C4'-C5'-O5'-PA
44	XL	501	GTP	C4'-C5'-O5'-PA
44	NL	501	GTP	PB-O3B-PG-O1G
44	OD	501	GTP	PB-O3B-PG-O1G
42	1D	2601	ADP	C3'-C4'-C5'-O5'
44	ND	501	GTP	C3'-C4'-C5'-O5'
44	QP	501	GTP	O4'-C4'-C5'-O5'
46	YO	501	GDP	O4'-C4'-C5'-O5'
44	ND	501	GTP	PA-O3A-PB-O1B
44	OD	501	GTP	PA-O3A-PB-O1B
44	QP	501	GTP	PA-O3A-PB-O1B

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Mol	Chain	Res	Type	Atoms
44	WN	501	GTP	PA-O3A-PB-O1B
44	YF	501	GTP	PA-O3A-PB-O1B
44	ZF	501	GTP	PA-O3A-PB-O1B
43	C1	2001	ANP	C4'-C5'-O5'-PA
43	C2	2001	ANP	C4'-C5'-O5'-PA
43	C3	2001	ANP	C4'-C5'-O5'-PA
44	NB	501	GTP	C4'-C5'-O5'-PA
44	SD	501	GTP	O4'-C4'-C5'-O5'
46	RO	501	GDP	O4'-C4'-C5'-O5'
44	ON	501	GTP	C4'-C5'-O5'-PA
44	QF	501	GTP	C4'-C5'-O5'-PA
44	RL	501	GTP	C4'-C5'-O5'-PA
44	SH	501	GTP	C4'-C5'-O5'-PA
44	VD	501	GTP	C4'-C5'-O5'-PA
44	ZH	501	GTP	C4'-C5'-O5'-PA
46	RM	501	GDP	O4'-C4'-C5'-O5'
44	QD	501	GTP	C4'-C5'-O5'-PA
44	RN	501	GTP	C4'-C5'-O5'-PA
44	XH	501	GTP	C4'-C5'-O5'-PA
44	NH	501	GTP	C3'-C4'-C5'-O5'
44	OJ	501	GTP	C3'-C4'-C5'-O5'
44	PP	501	GTP	O4'-C4'-C5'-O5'
44	VJ	501	GTP	O4'-C4'-C5'-O5'
46	OI	501	GDP	C3'-C4'-C5'-O5'
46	OK	501	GDP	C3'-C4'-C5'-O5'
46	TI	501	GDP	C3'-C4'-C5'-O5'
44	NJ	501	GTP	PB-O3B-PG-O1G
44	RF	501	GTP	PB-O3B-PG-O1G
44	WF	501	GTP	PB-O3B-PG-O1G
44	YJ	501	GTP	PB-O3B-PG-O1G
46	PC	501	GDP	PA-O3A-PB-O3B
46	YC	501	GDP	PA-O3A-PB-O2B
44	QL	501	GTP	C3'-C4'-C5'-O5'
44	YB	501	GTP	C3'-C4'-C5'-O5'
46	NC	501	GDP	C3'-C4'-C5'-O5'
46	NG	502	GDP	C3'-C4'-C5'-O5'
46	QM	501	GDP	C3'-C4'-C5'-O5'
46	SO	502	GDP	O4'-C4'-C5'-O5'
46	XM	502	GDP	O4'-C4'-C5'-O5'
44	YL	501	GTP	C4'-C5'-O5'-PA
43	1A	2602	ANP	C2'-C1'-N9-C8
43	1B	2602	ANP	C2'-C1'-N9-C8

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Mol	Chain	Res	Type	Atoms
43	1C	2602	ANP	C2'-C1'-N9-C8
43	1D	2602	ANP	C2'-C1'-N9-C8
42	1A	2601	ADP	PB-O3A-PA-O2A
42	1C	2601	ADP	PB-O3A-PA-O2A
44	NJ	501	GTP	PG-O3B-PB-O1B
44	NN	501	GTP	PG-O3B-PB-O1B
44	OF	501	GTP	PA-O3A-PB-O1B
44	OL	501	GTP	PG-O3B-PB-O1B
44	OL	501	GTP	PA-O3A-PB-O2B
44	PD	501	GTP	PA-O3A-PB-O2B
44	PH	501	GTP	PG-O3B-PB-O1B
44	PN	501	GTP	PG-O3B-PB-O1B
44	RD	501	GTP	PG-O3B-PB-O1B
44	RD	501	GTP	PA-O3A-PB-O2B
44	RP	501	GTP	PB-O3A-PA-O2A
44	SB	501	GTP	PG-O3B-PB-O1B
44	SL	501	GTP	PA-O3A-PB-O2B
44	SN	501	GTP	PG-O3B-PB-O1B
44	TB	501	GTP	PA-O3A-PB-O2B
44	TD	501	GTP	PG-O3B-PB-O1B
44	TD	501	GTP	PA-O3A-PB-O2B
44	TF	501	GTP	PG-O3B-PB-O1B
44	TF	501	GTP	PA-O3A-PB-O2B
44	TJ	501	GTP	PB-O3A-PA-O2A
44	TN	501	GTP	PA-O3A-PB-O2B
44	UB	501	GTP	PA-O3A-PB-O1B
44	UF	501	GTP	PG-O3B-PB-O1B
44	UL	501	GTP	PG-O3B-PB-O1B
44	UP	501	GTP	PA-O3A-PB-O2B
44	VB	501	GTP	PA-O3A-PB-O2B
44	VP	501	GTP	PA-O3A-PB-O2B
44	WJ	501	GTP	PB-O3A-PA-O2A
44	ZD	501	GTP	PA-O3A-PB-O2B
44	ZF	501	GTP	PG-O3B-PB-O1B
44	ZP	501	GTP	PA-O3A-PB-O2B
44	PH	501	GTP	C4'-C5'-O5'-PA
44	RH	501	GTP	C4'-C5'-O5'-PA
44	RP	501	GTP	C4'-C5'-O5'-PA
44	UH	501	GTP	C4'-C5'-O5'-PA
44	YP	501	GTP	C4'-C5'-O5'-PA
43	1D	2602	ANP	PB-O3A-PA-O1A
44	ND	501	GTP	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
44	WJ	501	GTP	O4'-C4'-C5'-O5'
46	OC	501	GDP	O4'-C4'-C5'-O5'
46	OO	501	GDP	O4'-C4'-C5'-O5'
46	SC	502	GDP	C3'-C4'-C5'-O5'
46	VO	501	GDP	O4'-C4'-C5'-O5'
46	YG	501	GDP	C3'-C4'-C5'-O5'
42	1A	2601	ADP	C5'-O5'-PA-O1A
42	1A	2601	ADP	C5'-O5'-PA-O2A
42	1A	2601	ADP	C5'-O5'-PA-O3A
42	1B	2601	ADP	C5'-O5'-PA-O1A
42	1B	2601	ADP	C5'-O5'-PA-O2A
42	1B	2601	ADP	C5'-O5'-PA-O3A
42	1C	2601	ADP	C5'-O5'-PA-O1A
42	1C	2601	ADP	C5'-O5'-PA-O2A
42	1C	2601	ADP	C5'-O5'-PA-O3A
42	1D	2601	ADP	C5'-O5'-PA-O2A
42	1D	2601	ADP	C5'-O5'-PA-O3A
43	1B	2602	ANP	C5'-O5'-PA-O1A
43	1C	2602	ANP	C5'-O5'-PA-O1A
44	ND	501	GTP	C5'-O5'-PA-O3A
44	ND	501	GTP	C5'-O5'-PA-O1A
44	ND	501	GTP	C5'-O5'-PA-O2A
44	NH	501	GTP	C5'-O5'-PA-O3A
44	NH	501	GTP	C5'-O5'-PA-O2A
44	NJ	501	GTP	C5'-O5'-PA-O1A
44	NN	501	GTP	C5'-O5'-PA-O1A
44	OJ	501	GTP	C5'-O5'-PA-O2A
44	OP	501	GTP	C5'-O5'-PA-O2A
44	PD	501	GTP	C5'-O5'-PA-O1A
44	PF	501	GTP	C5'-O5'-PA-O2A
44	PP	501	GTP	C5'-O5'-PA-O2A
44	QP	501	GTP	C5'-O5'-PA-O3A
44	RD	501	GTP	C5'-O5'-PA-O1A
44	RJ	501	GTP	C5'-O5'-PA-O3A
44	RJ	501	GTP	C5'-O5'-PA-O2A
44	SB	501	GTP	C5'-O5'-PA-O1A
44	SD	501	GTP	C5'-O5'-PA-O3A
44	SD	501	GTP	C5'-O5'-PA-O1A
44	SD	501	GTP	C5'-O5'-PA-O2A
44	TH	501	GTP	C5'-O5'-PA-O2A
44	TL	501	GTP	C5'-O5'-PA-O1A
44	UL	501	GTP	C5'-O5'-PA-O2A

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Mol	Chain	Res	Type	Atoms
44	UN	501	GTP	C5'-O5'-PA-O2A
44	VF	501	GTP	C5'-O5'-PA-O1A
44	VH	501	GTP	C5'-O5'-PA-O2A
44	VL	501	GTP	C5'-O5'-PA-O3A
44	VL	501	GTP	C5'-O5'-PA-O2A
44	WD	501	GTP	C5'-O5'-PA-O3A
44	WD	501	GTP	C5'-O5'-PA-O1A
44	WD	501	GTP	C5'-O5'-PA-O2A
44	WJ	501	GTP	C5'-O5'-PA-O2A
44	WN	501	GTP	C5'-O5'-PA-O3A
44	XB	501	GTP	C5'-O5'-PA-O1A
44	XF	501	GTP	C5'-O5'-PA-O2A
44	YJ	501	GTP	C5'-O5'-PA-O3A
44	YJ	501	GTP	C5'-O5'-PA-O2A
44	ZD	501	GTP	C5'-O5'-PA-O3A
44	ZF	501	GTP	C5'-O5'-PA-O1A
44	ZJ	501	GTP	C5'-O5'-PA-O3A
44	ZJ	501	GTP	C5'-O5'-PA-O1A
44	ZJ	501	GTP	C5'-O5'-PA-O2A
44	ZN	501	GTP	C5'-O5'-PA-O3A
44	ZN	501	GTP	C5'-O5'-PA-O2A
44	ZP	501	GTP	C5'-O5'-PA-O1A
46	NM	501	GDP	C5'-O5'-PA-O1A
46	NO	501	GDP	C5'-O5'-PA-O1A
46	PO	501	GDP	C5'-O5'-PA-O1A
46	RE	501	GDP	C5'-O5'-PA-O3A
46	RK	501	GDP	C5'-O5'-PA-O1A
46	TE	501	GDP	C5'-O5'-PA-O1A
46	XE	501	GDP	C5'-O5'-PA-O1A
46	ZE	501	GDP	C5'-O5'-PA-O1A
46	ZK	501	GDP	C5'-O5'-PA-O1A
44	OH	501	GTP	C4'-C5'-O5'-PA
44	PJ	501	GTP	C4'-C5'-O5'-PA
44	PP	501	GTP	C4'-C5'-O5'-PA
44	TH	501	GTP	C4'-C5'-O5'-PA
44	TJ	501	GTP	C4'-C5'-O5'-PA
44	TP	501	GTP	C4'-C5'-O5'-PA
44	UL	501	GTP	C4'-C5'-O5'-PA
44	UN	501	GTP	C4'-C5'-O5'-PA
44	VL	501	GTP	C4'-C5'-O5'-PA
44	WH	501	GTP	C4'-C5'-O5'-PA
44	WL	501	GTP	C4'-C5'-O5'-PA

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Mol	Chain	Res	Type	Atoms
44	YH	501	GTP	C4'-C5'-O5'-PA
44	ZN	501	GTP	C4'-C5'-O5'-PA
44	NH	501	GTP	O4'-C4'-C5'-O5'
44	YB	501	GTP	O4'-C4'-C5'-O5'
44	OP	501	GTP	C4'-C5'-O5'-PA
44	WJ	501	GTP	C4'-C5'-O5'-PA
42	1B	2601	ADP	PB-O3A-PA-O2A
42	1D	2601	ADP	PB-O3A-PA-O2A
44	NJ	501	GTP	PA-O3A-PB-O2B
44	NL	501	GTP	PA-O3A-PB-O2B
44	NN	501	GTP	PA-O3A-PB-O1B
44	OP	501	GTP	PA-O3A-PB-O2B
44	PL	501	GTP	PA-O3A-PB-O2B
44	QH	501	GTP	PA-O3A-PB-O2B
44	QJ	501	GTP	PA-O3A-PB-O2B
44	RH	501	GTP	PB-O3A-PA-O2A
44	SB	501	GTP	PA-O3A-PB-O2B
44	SD	501	GTP	PA-O3A-PB-O2B
44	SF	501	GTP	PA-O3A-PB-O2B
44	TH	501	GTP	PB-O3A-PA-O2A
44	TL	501	GTP	PA-O3A-PB-O2B
44	UF	501	GTP	PA-O3A-PB-O2B
44	UJ	501	GTP	PA-O3A-PB-O2B
44	VF	501	GTP	PA-O3A-PB-O2B
44	VH	501	GTP	PB-O3A-PA-O2A
44	VN	501	GTP	PA-O3A-PB-O2B
44	WD	501	GTP	PA-O3A-PB-O2B
44	XB	501	GTP	PA-O3A-PB-O2B
44	XJ	501	GTP	PA-O3A-PB-O2B
44	XN	501	GTP	PA-O3A-PB-O2B
44	YB	501	GTP	PA-O3A-PB-O1B
44	YD	501	GTP	PA-O3A-PB-O2B
44	YN	501	GTP	PA-O3A-PB-O2B
44	ZB	501	GTP	PA-O3A-PB-O2B
44	ZJ	501	GTP	PA-O3A-PB-O2B
44	ZN	501	GTP	PA-O3A-PB-O2B
46	QE	501	GDP	C3'-C4'-C5'-O5'
43	1C	2602	ANP	C4'-C5'-O5'-PA
44	QN	501	GTP	C4'-C5'-O5'-PA
44	YJ	501	GTP	C4'-C5'-O5'-PA
44	OF	501	GTP	C4'-C5'-O5'-PA
44	QH	501	GTP	C4'-C5'-O5'-PA

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Mol	Chain	Res	Type	Atoms
44	WB	501	GTP	C4'-C5'-O5'-PA
46	PK	501	GDP	PA-O3A-PB-O1B
44	XL	501	GTP	O4'-C4'-C5'-O5'
46	NE	501	GDP	C3'-C4'-C5'-O5'
43	1A	2602	ANP	C2'-C1'-N9-C4
44	PN	501	GTP	C4'-C5'-O5'-PA
44	RF	501	GTP	C4'-C5'-O5'-PA
44	TB	501	GTP	C4'-C5'-O5'-PA
44	UB	501	GTP	C4'-C5'-O5'-PA
44	UJ	501	GTP	C4'-C5'-O5'-PA
44	UP	501	GTP	C4'-C5'-O5'-PA
44	VH	501	GTP	C4'-C5'-O5'-PA
44	VJ	501	GTP	C4'-C5'-O5'-PA
46	VM	501	GDP	C4'-C5'-O5'-PA
43	1A	2602	ANP	PB-O3A-PA-O2A
46	OI	501	GDP	O4'-C4'-C5'-O5'
46	OK	501	GDP	O4'-C4'-C5'-O5'
46	ZO	501	GDP	C3'-C4'-C5'-O5'
44	NB	501	GTP	PA-O3A-PB-O2B
44	ND	501	GTP	PA-O3A-PB-O2B
44	PF	501	GTP	PG-O3B-PB-O1B
44	PH	501	GTP	PA-O3A-PB-O2B
44	PN	501	GTP	PA-O3A-PB-O2B
44	PP	501	GTP	PA-O3A-PB-O2B
44	QH	501	GTP	PG-O3B-PB-O1B
44	QP	501	GTP	PA-O3A-PB-O2B
44	RJ	501	GTP	PG-O3B-PB-O1B
44	RJ	501	GTP	PA-O3A-PB-O2B
44	SL	501	GTP	PG-O3B-PB-O1B
44	TB	501	GTP	PG-O3B-PB-O1B
44	VF	501	GTP	PA-O3A-PB-O1B
44	WB	501	GTP	PA-O3A-PB-O2B
44	WD	501	GTP	PA-O3A-PB-O1B
44	ZL	501	GTP	PA-O3A-PB-O2B
44	PF	501	GTP	C4'-C5'-O5'-PA
44	SP	501	GTP	C4'-C5'-O5'-PA
43	1D	2602	ANP	O4'-C1'-N9-C8
46	SE	501	GDP	C3'-C4'-C5'-O5'
46	SK	501	GDP	C3'-C4'-C5'-O5'
46	TI	501	GDP	O4'-C4'-C5'-O5'
46	UK	501	GDP	C3'-C4'-C5'-O5'
44	NF	501	GTP	C4'-C5'-O5'-PA

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Mol	Chain	Res	Type	Atoms
44	RJ	501	GTP	C4'-C5'-O5'-PA
44	VB	501	GTP	C4'-C5'-O5'-PA
44	YN	501	GTP	C4'-C5'-O5'-PA
46	NC	501	GDP	O4'-C4'-C5'-O5'
44	SH	501	GTP	PB-O3B-PG-O1G
44	SH	501	GTP	PB-O3B-PG-O2G
46	NI	501	GDP	PA-O3A-PB-O2B
46	PK	501	GDP	PA-O3A-PB-O2B
46	PK	501	GDP	PA-O3A-PB-O3B
46	VM	501	GDP	PA-O3A-PB-O3B
46	XI	501	GDP	PA-O3A-PB-O2B
44	RL	501	GTP	C3'-C4'-C5'-O5'
46	NG	502	GDP	O4'-C4'-C5'-O5'
46	QM	501	GDP	O4'-C4'-C5'-O5'
46	VG	501	GDP	C3'-C4'-C5'-O5'
43	1B	2602	ANP	O4'-C1'-N9-C8
43	1C	2602	ANP	O4'-C1'-N9-C8
44	PH	501	GTP	C3'-C4'-C5'-O5'
44	WH	501	GTP	C3'-C4'-C5'-O5'
46	TC	501	GDP	C3'-C4'-C5'-O5'
46	UC	501	GDP	C3'-C4'-C5'-O5'
44	VP	501	GTP	C4'-C5'-O5'-PA
43	1B	2602	ANP	PB-O3A-PA-O2A
42	1A	2601	ADP	PB-O3A-PA-O1A
42	1B	2601	ADP	PB-O3A-PA-O1A
42	1C	2601	ADP	PB-O3A-PA-O1A
44	NB	501	GTP	PA-O3A-PB-O1B
44	NJ	501	GTP	PA-O3A-PB-O1B
44	NN	501	GTP	PA-O3A-PB-O2B
44	OD	501	GTP	PA-O3A-PB-O2B
44	PD	501	GTP	PA-O3A-PB-O1B
44	PH	501	GTP	PA-O3A-PB-O1B
44	PN	501	GTP	PA-O3A-PB-O1B
44	PP	501	GTP	PG-O3B-PB-O2B
44	PP	501	GTP	PA-O3A-PB-O1B
44	QH	501	GTP	PG-O3B-PB-O2B
44	QH	501	GTP	PA-O3A-PB-O1B
44	QN	501	GTP	PG-O3B-PB-O2B
44	QN	501	GTP	PB-O3A-PA-O2A
44	RH	501	GTP	PB-O3A-PA-O1A
44	RJ	501	GTP	PA-O3A-PB-O1B
44	SD	501	GTP	PA-O3A-PB-O1B

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Mol	Chain	Res	Type	Atoms
44	SN	501	GTP	PA-O3A-PB-O1B
44	SN	501	GTP	PA-O3A-PB-O2B
44	TB	501	GTP	PA-O3A-PB-O1B
44	TD	501	GTP	PA-O3A-PB-O1B
44	TL	501	GTP	PG-O3B-PB-O2B
44	TN	501	GTP	PA-O3A-PB-O1B
44	UF	501	GTP	PA-O3A-PB-O1B
44	UJ	501	GTP	PA-O3A-PB-O1B
44	UP	501	GTP	PG-O3B-PB-O2B
44	UP	501	GTP	PA-O3A-PB-O1B
44	VB	501	GTP	PA-O3A-PB-O1B
44	VH	501	GTP	PB-O3A-PA-O1A
44	VP	501	GTP	PG-O3B-PB-O2B
44	WB	501	GTP	PA-O3A-PB-O1B
44	WH	501	GTP	PA-O3A-PB-O2B
44	WN	501	GTP	PA-O3A-PB-O2B
44	XH	501	GTP	PA-O3A-PB-O1B
44	XH	501	GTP	PA-O3A-PB-O2B
44	XN	501	GTP	PA-O3A-PB-O1B
44	YB	501	GTP	PA-O3A-PB-O2B
44	YF	501	GTP	PG-O3B-PB-O2B
44	YF	501	GTP	PA-O3A-PB-O2B
44	ZB	501	GTP	PG-O3B-PB-O1B
44	ZB	501	GTP	PA-O3A-PB-O1B
44	ZD	501	GTP	PA-O3A-PB-O1B
44	ZF	501	GTP	PA-O3A-PB-O2B
44	ZN	501	GTP	PG-O3B-PB-O2B
44	ZP	501	GTP	PG-O3B-PB-O1B
44	ZP	501	GTP	PA-O3A-PB-O1B
43	1A	2602	ANP	O4'-C1'-N9-C8
44	UL	501	GTP	O4'-C4'-C5'-O5'
46	OQ	501	GDP	C3'-C4'-C5'-O5'
46	QO	501	GDP	C3'-C4'-C5'-O5'
46	XA	501	GDP	C3'-C4'-C5'-O5'
46	XK	501	GDP	C3'-C4'-C5'-O5'
44	PL	501	GTP	C4'-C5'-O5'-PA
43	1A	2602	ANP	PA-O3A-PB-O1B
43	1D	2602	ANP	PA-O3A-PB-O1B
43	C0	2001	ANP	PA-O3A-PB-O1B
46	NK	501	GDP	C3'-C4'-C5'-O5'
46	QQ	501	GDP	C3'-C4'-C5'-O5'
43	1D	2602	ANP	C4'-C5'-O5'-PA

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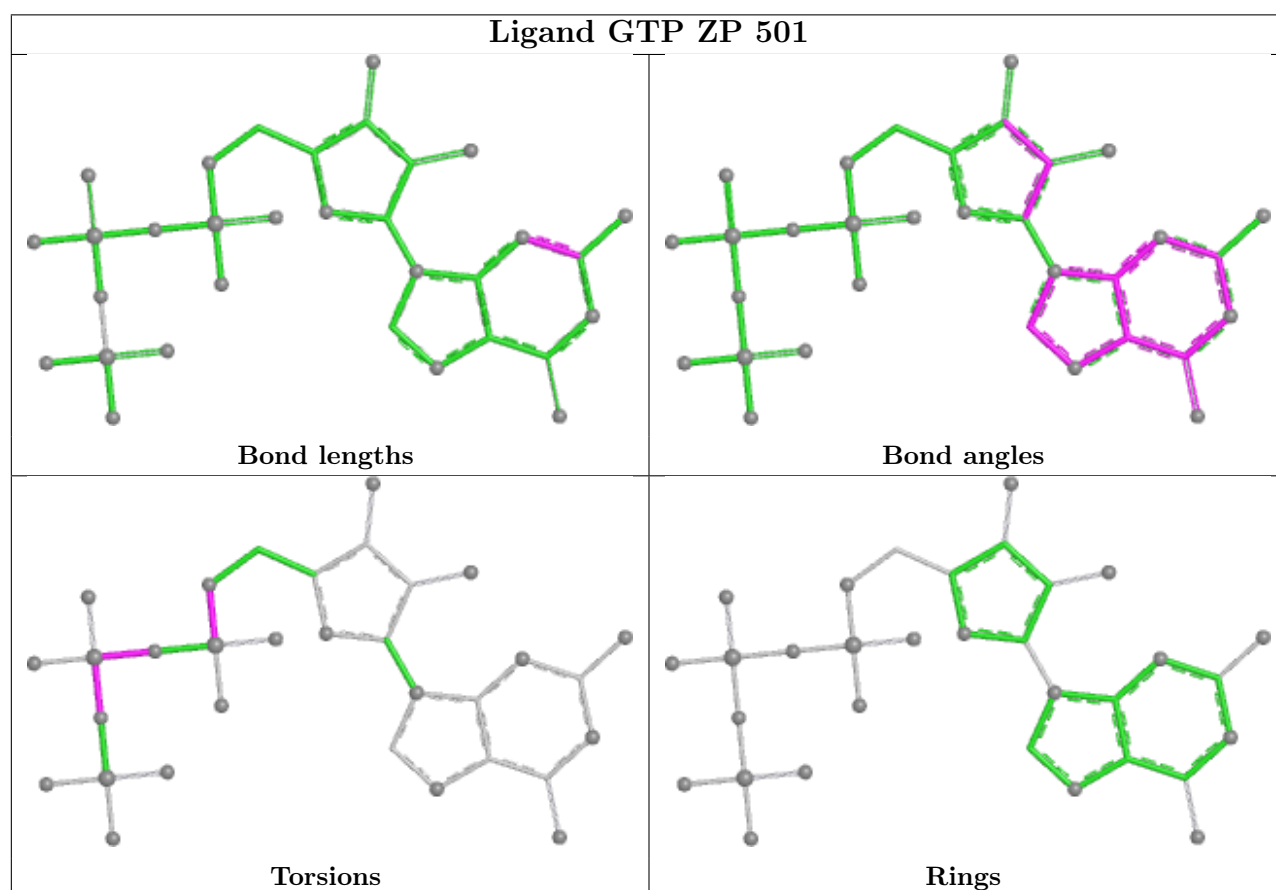
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Mol	Chain	Res	Type	Atoms
44	NH	501	GTP	C4'-C5'-O5'-PA
44	XF	501	GTP	C4'-C5'-O5'-PA
44	ZB	501	GTP	C4'-C5'-O5'-PA
43	C3	2001	ANP	PG-N3B-PB-O3A
43	1A	2602	ANP	PB-O3A-PA-O1A
44	NB	501	GTP	PG-O3B-PB-O2B
44	NJ	501	GTP	PG-O3B-PB-O2B
44	NL	501	GTP	PA-O3A-PB-O1B
44	NN	501	GTP	PG-O3B-PB-O2B
44	OF	501	GTP	PG-O3B-PB-O2B
44	OL	501	GTP	PG-O3B-PB-O2B
44	PH	501	GTP	PG-O3B-PB-O2B
44	PL	501	GTP	PA-O3A-PB-O1B
44	QJ	501	GTP	PA-O3A-PB-O1B
44	QN	501	GTP	PB-O3A-PA-O1A
44	RD	501	GTP	PG-O3B-PB-O2B
44	SB	501	GTP	PG-O3B-PB-O2B
44	TD	501	GTP	PG-O3B-PB-O2B
44	TF	501	GTP	PG-O3B-PB-O2B
44	TH	501	GTP	PB-O3A-PA-O1A
44	TL	501	GTP	PA-O3A-PB-O1B
44	UB	501	GTP	PA-O3A-PB-O2B
44	UF	501	GTP	PG-O3B-PB-O2B
44	UL	501	GTP	PG-O3B-PB-O2B
44	VB	501	GTP	PG-O3B-PB-O2B
44	VN	501	GTP	PA-O3A-PB-O1B
44	WH	501	GTP	PA-O3A-PB-O1B
44	XB	501	GTP	PA-O3A-PB-O1B
44	XD	501	GTP	PG-O3B-PB-O2B
44	XH	501	GTP	PG-O3B-PB-O1B
44	XH	501	GTP	PG-O3B-PB-O2B
44	XJ	501	GTP	PG-O3B-PB-O2B
44	XJ	501	GTP	PA-O3A-PB-O1B
44	YD	501	GTP	PA-O3A-PB-O1B
44	YN	501	GTP	PA-O3A-PB-O1B
44	ZB	501	GTP	PG-O3B-PB-O2B
44	ZF	501	GTP	PG-O3B-PB-O2B
44	ZJ	501	GTP	PA-O3A-PB-O1B
44	ZN	501	GTP	PA-O3A-PB-O1B
46	SC	502	GDP	O4'-C4'-C5'-O5'
46	ZE	501	GDP	C3'-C4'-C5'-O5'

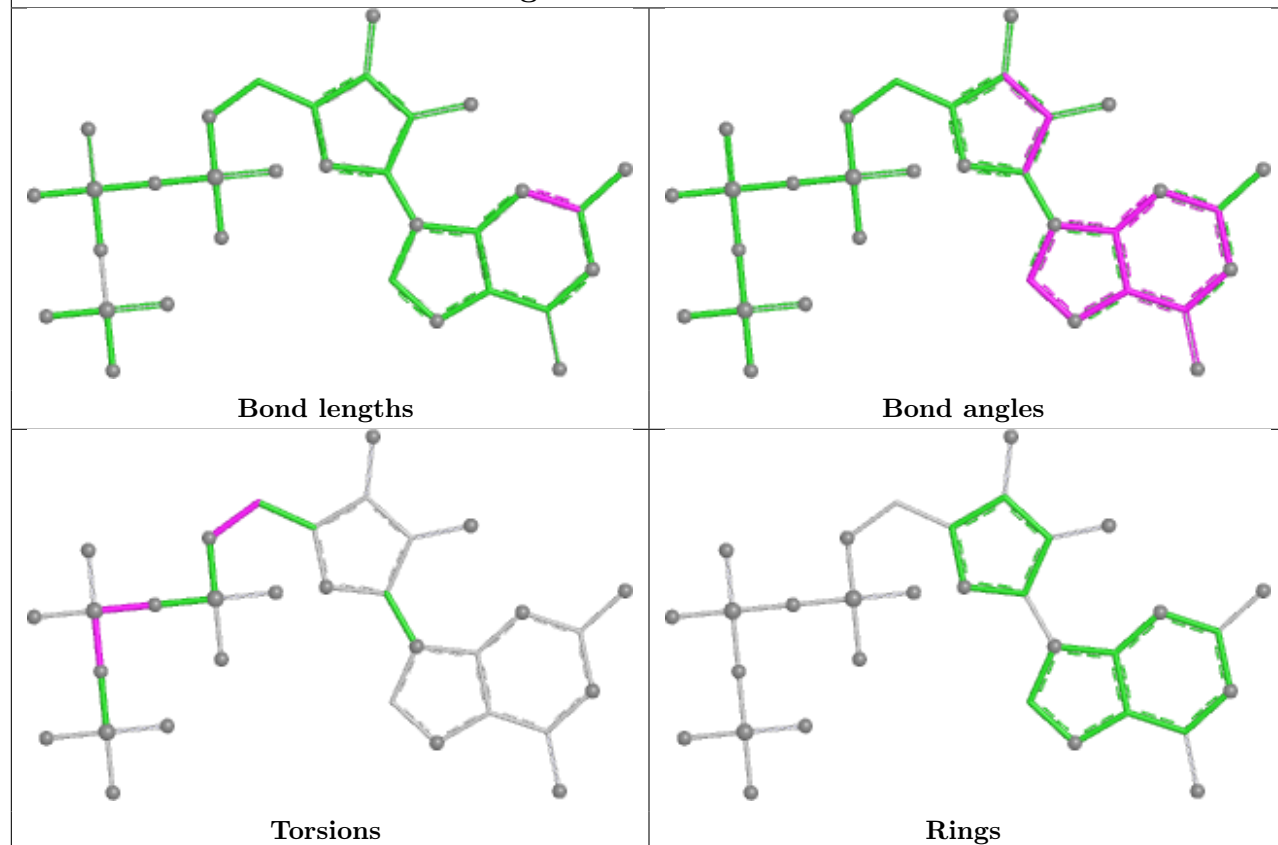
There are no ring outliers.

No monomer is involved in short contacts.

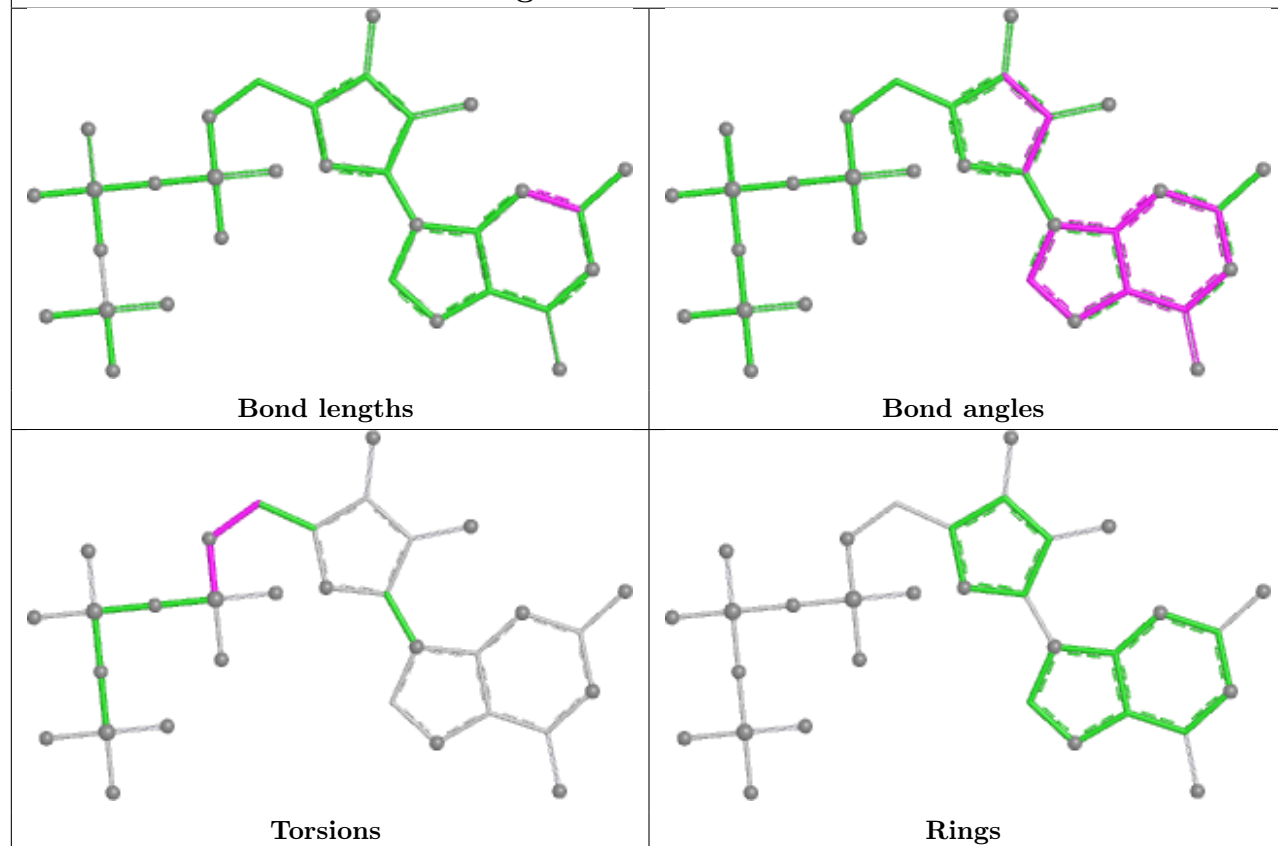
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

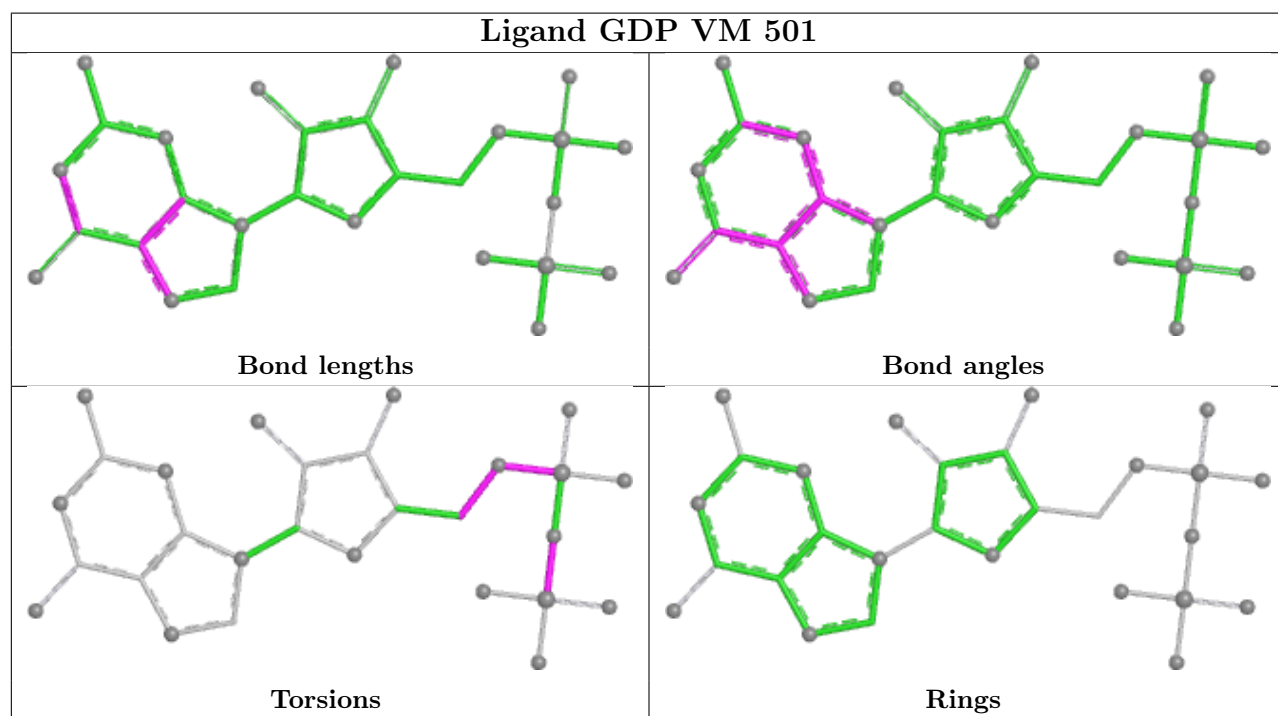
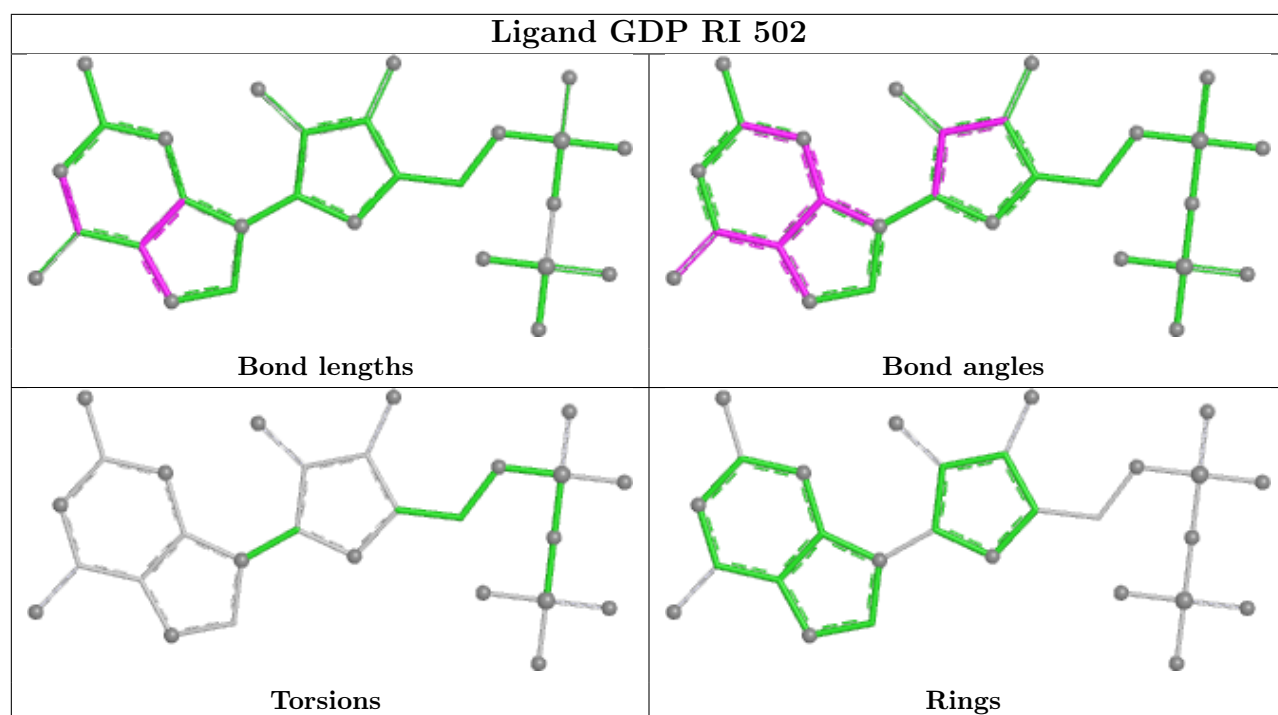


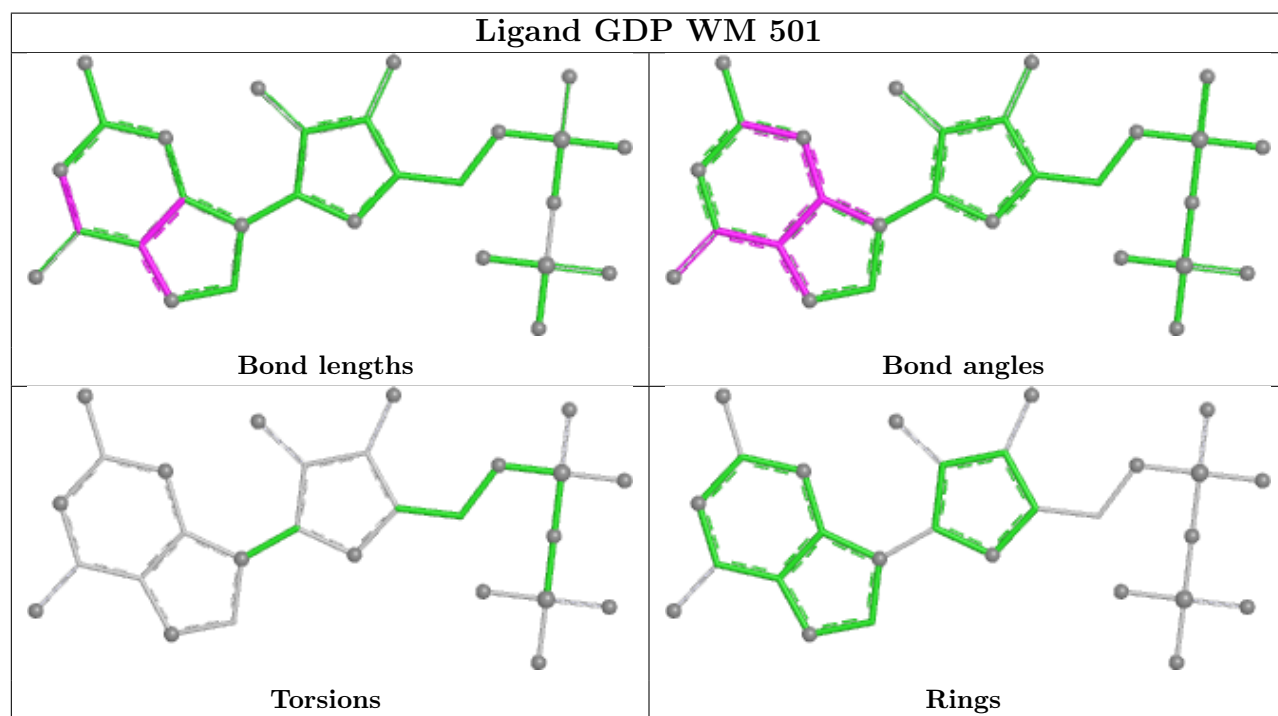
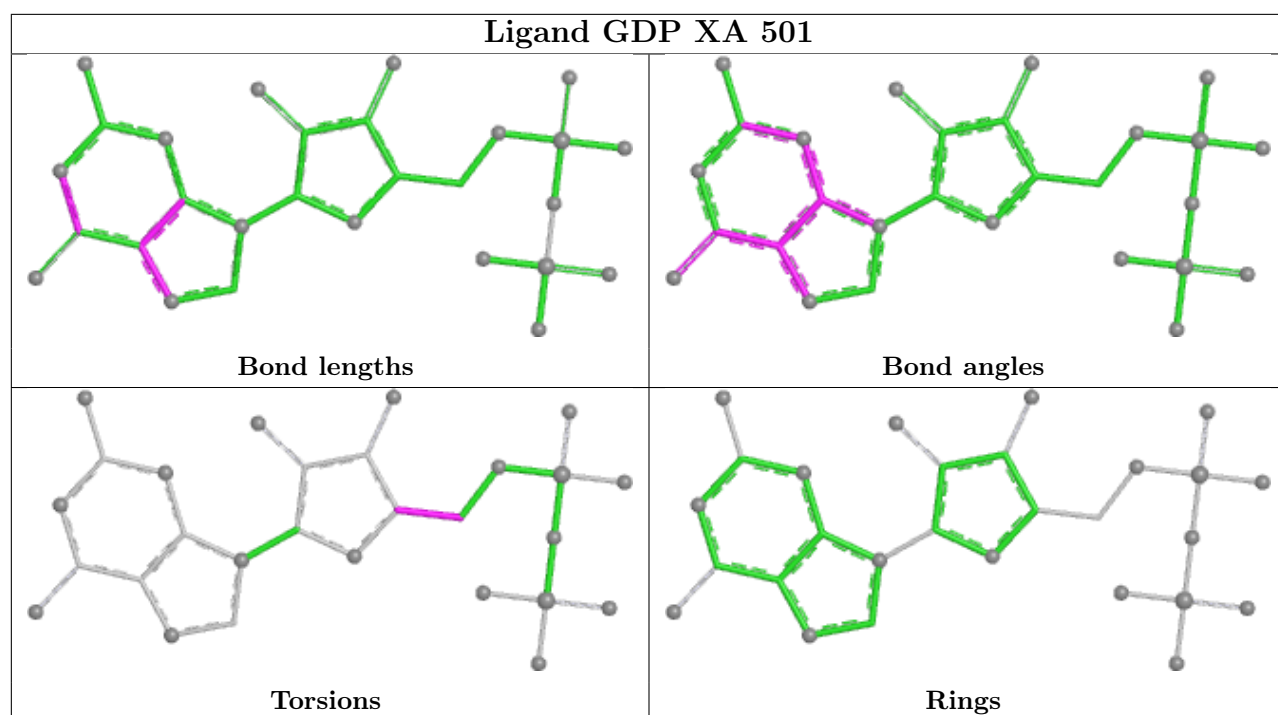
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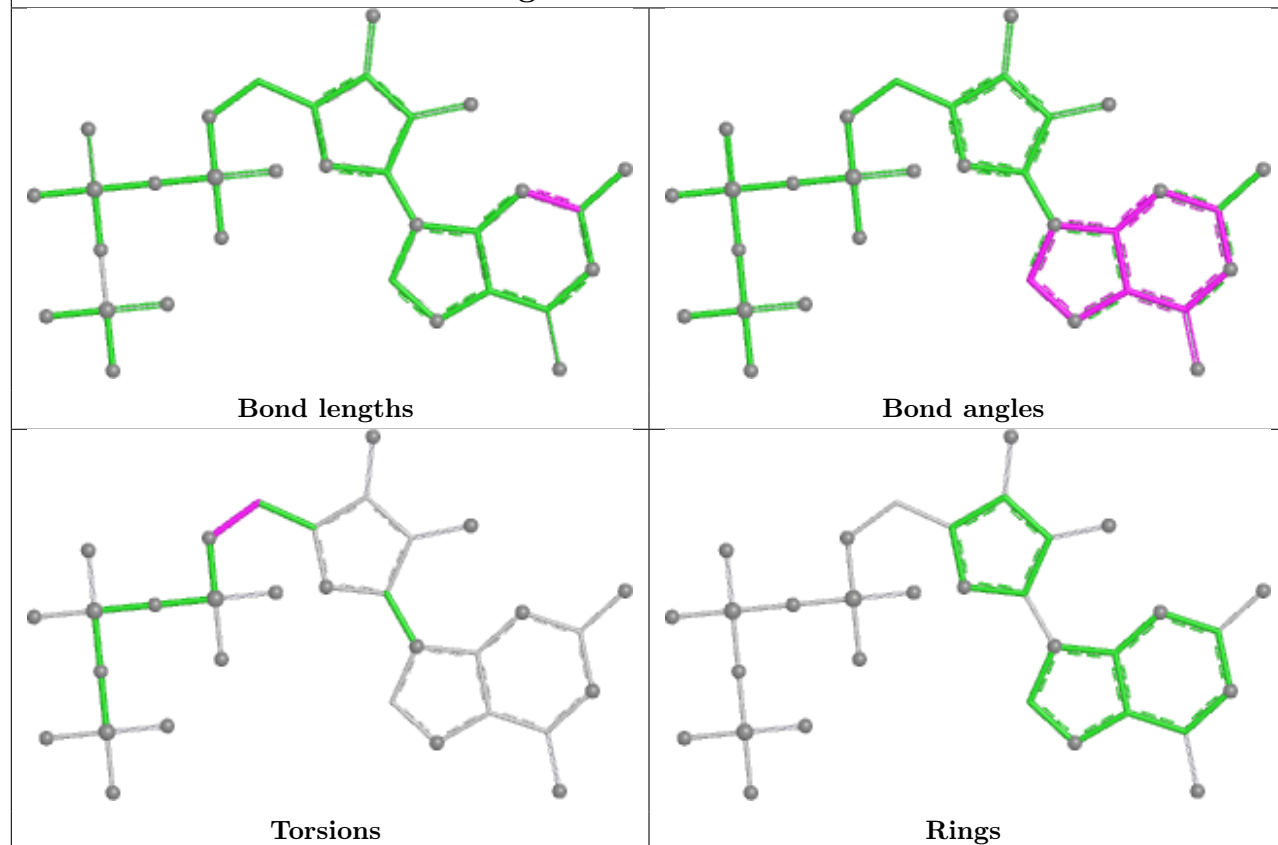
Ligand GTP OH 501



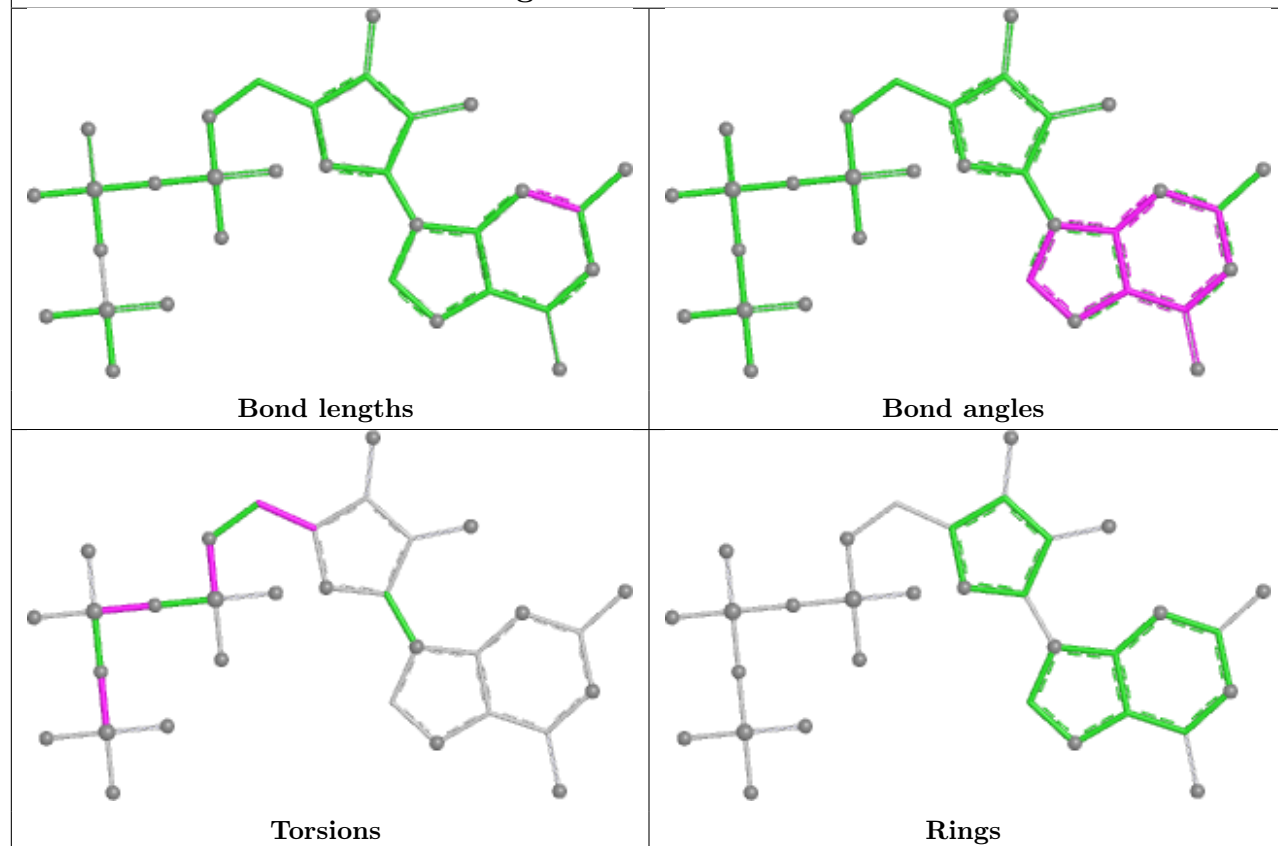




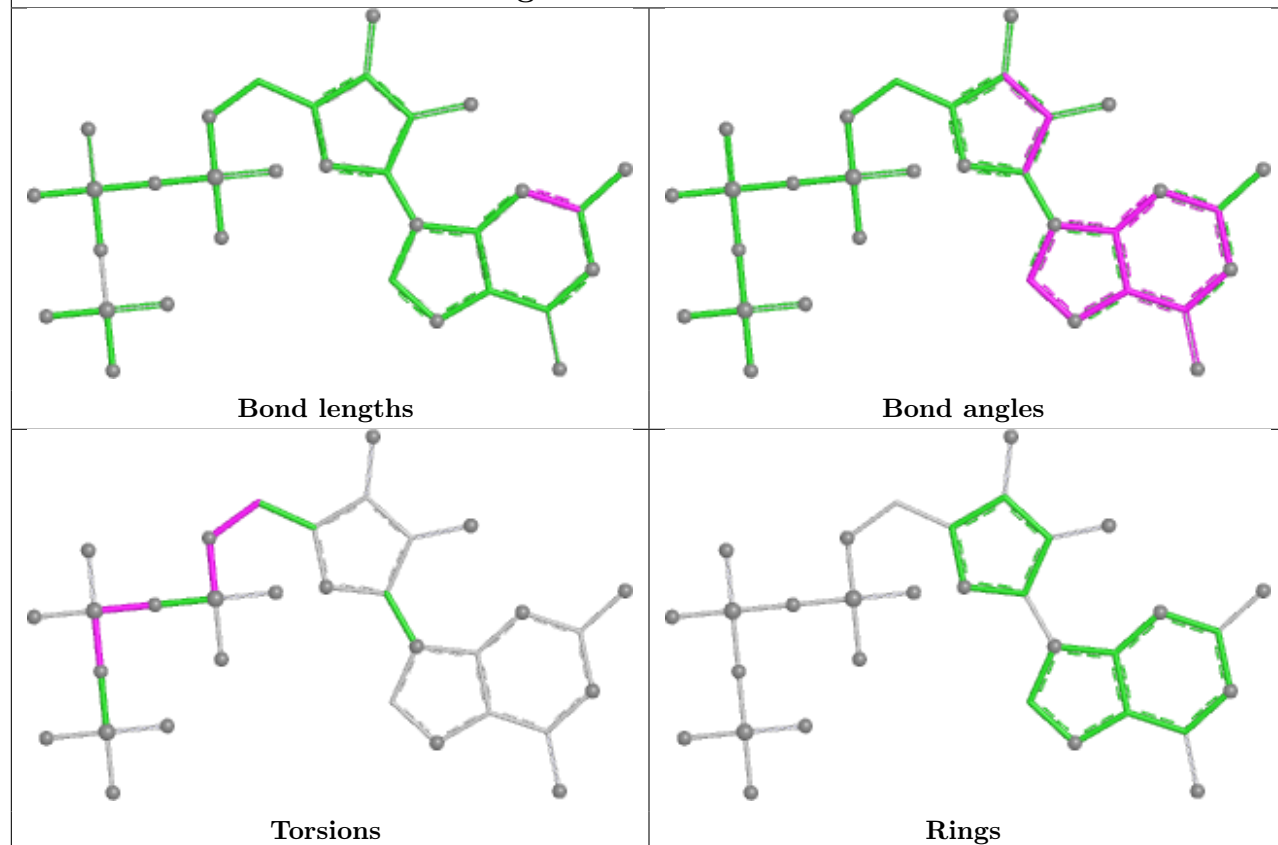
Ligand GTP NF 501



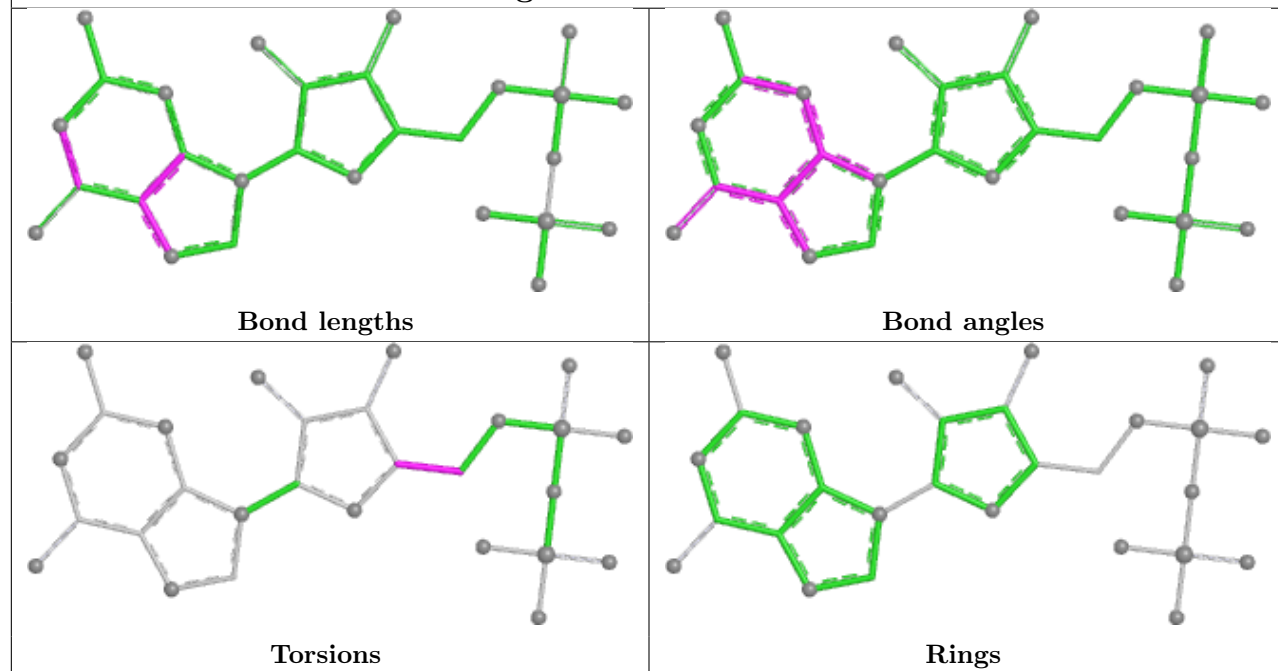
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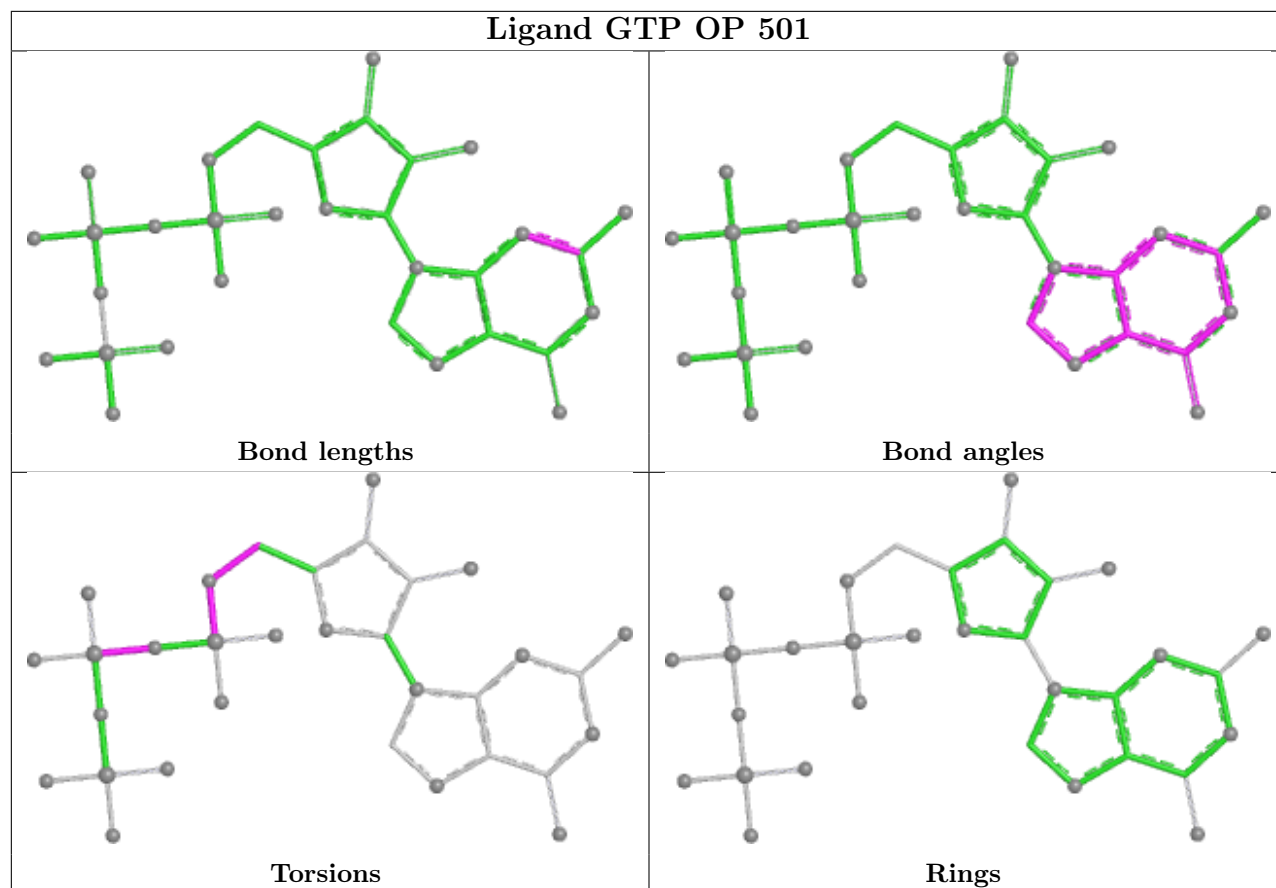
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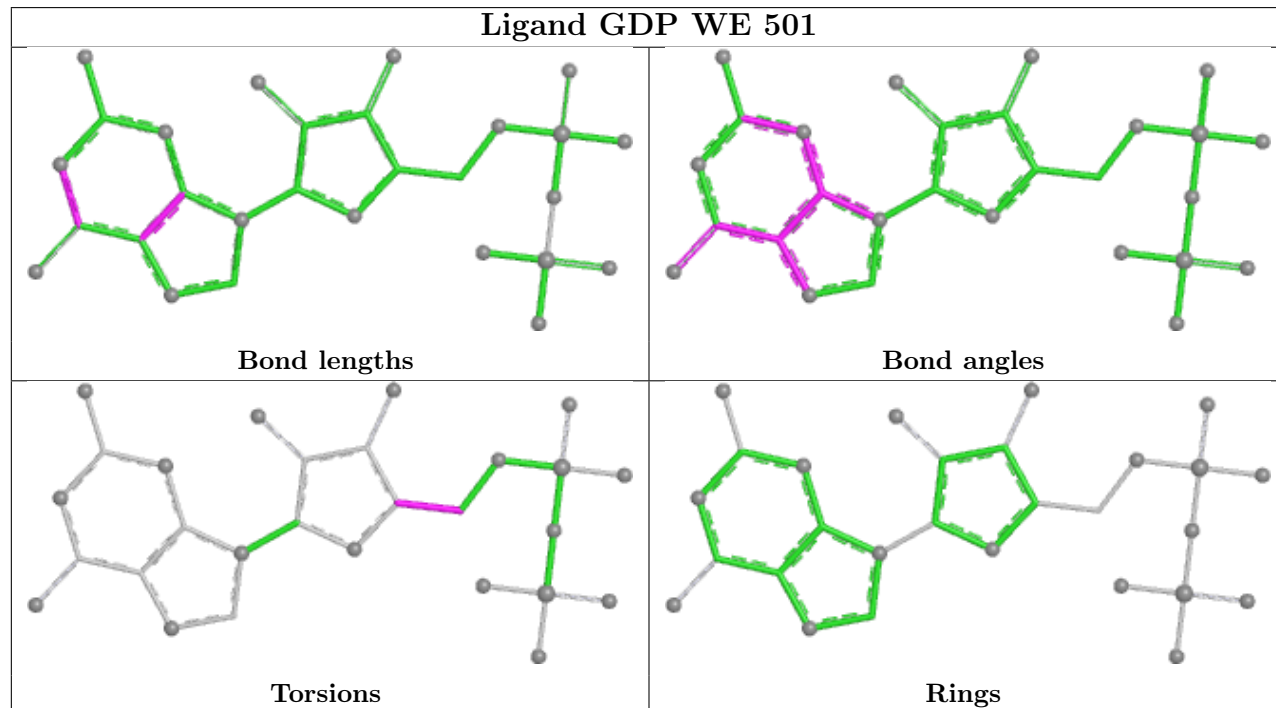
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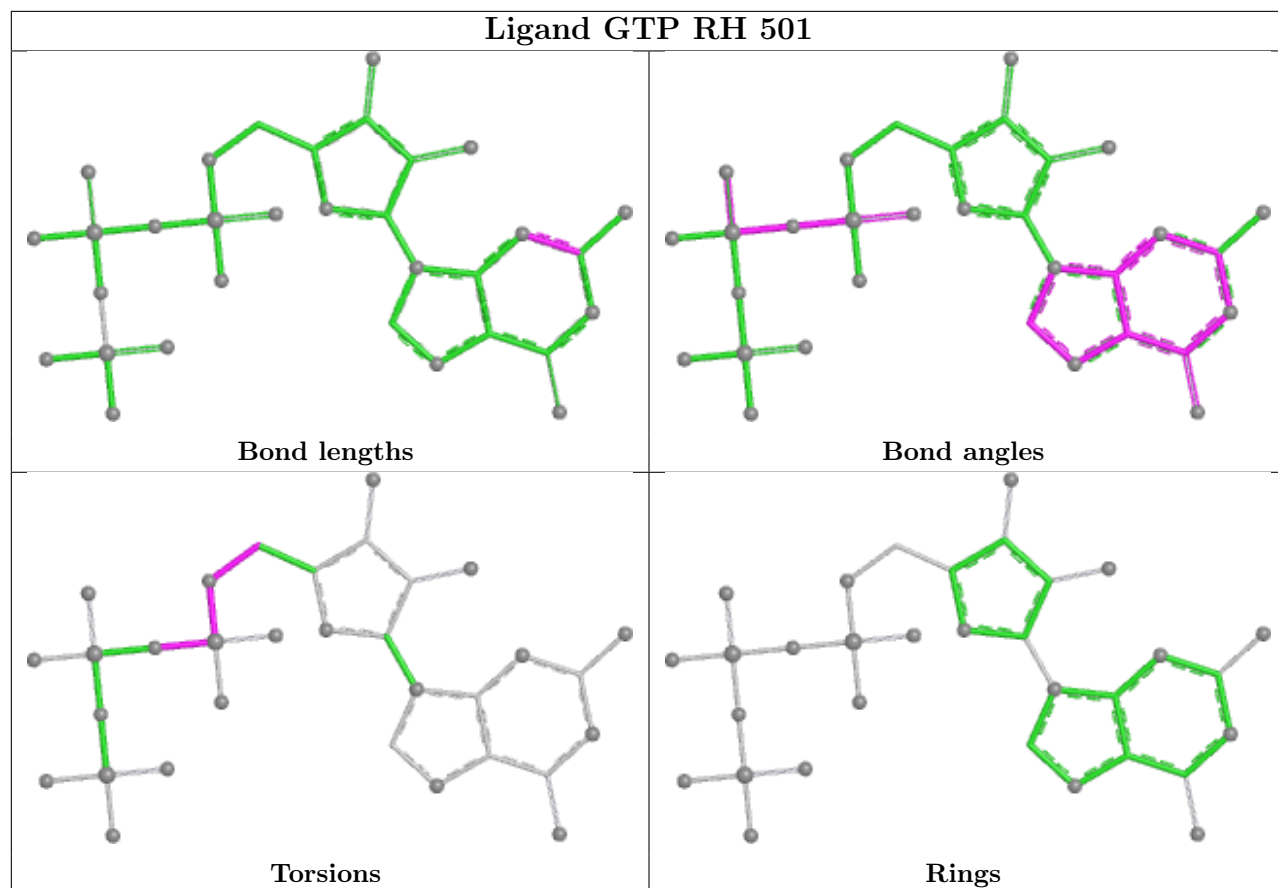
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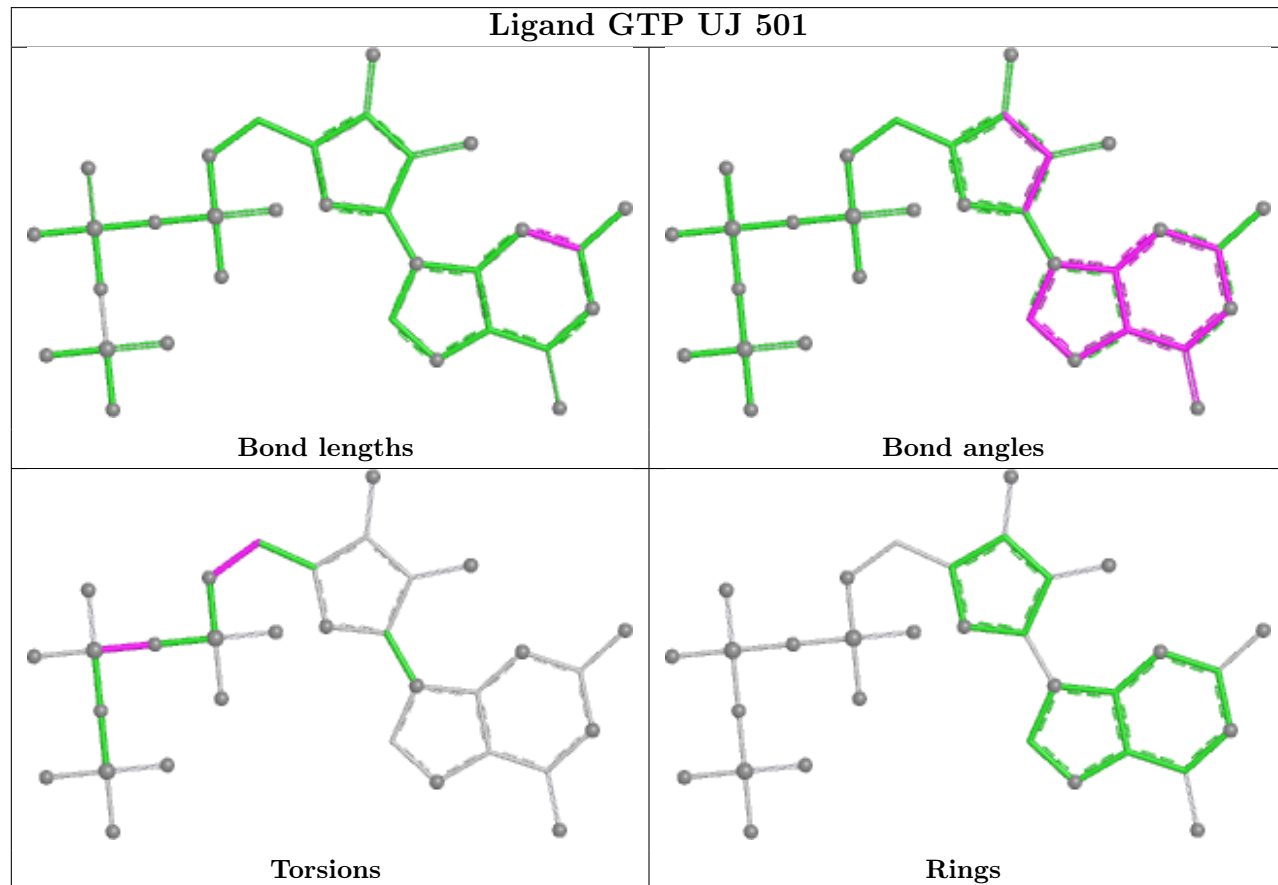
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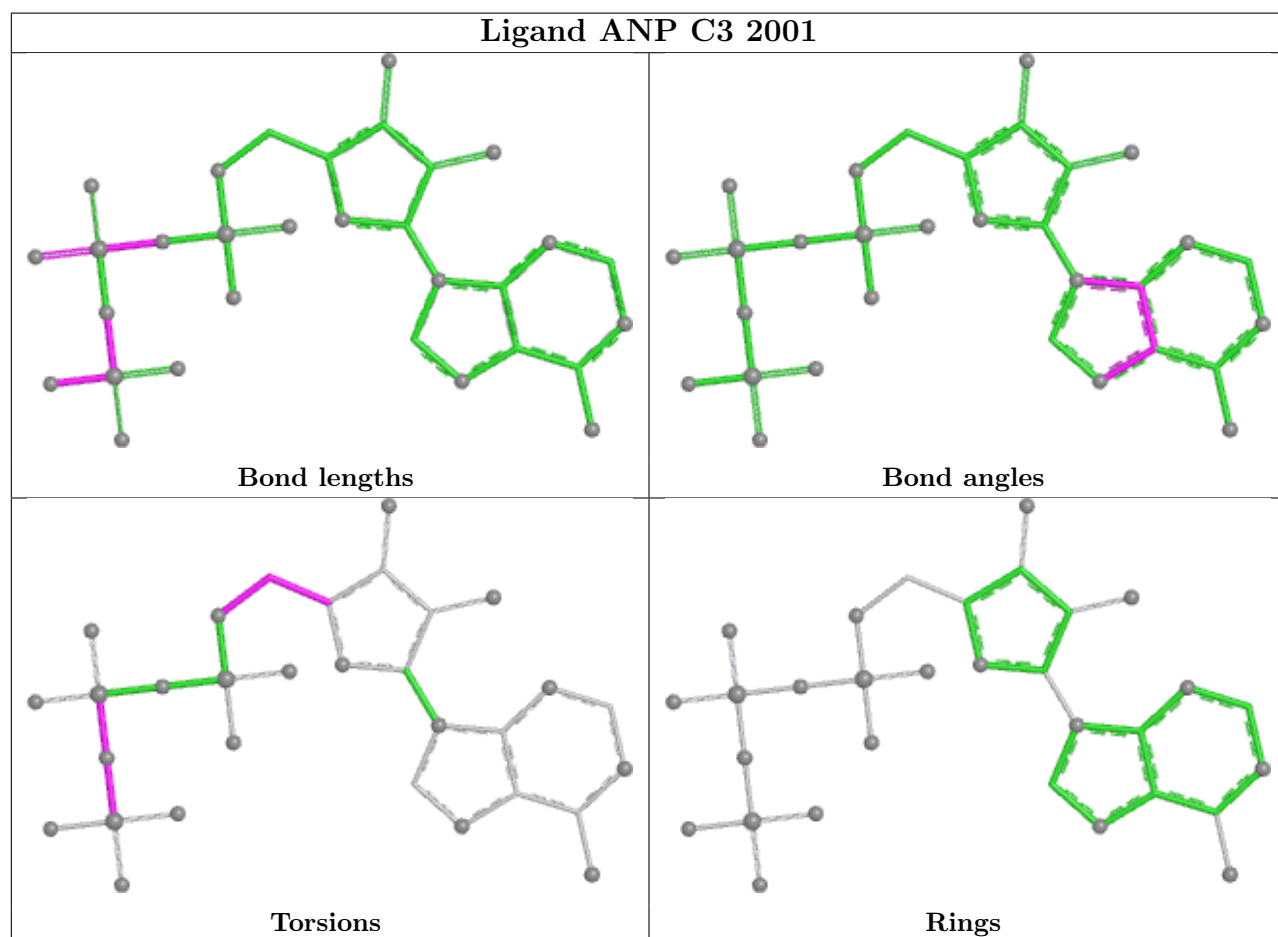
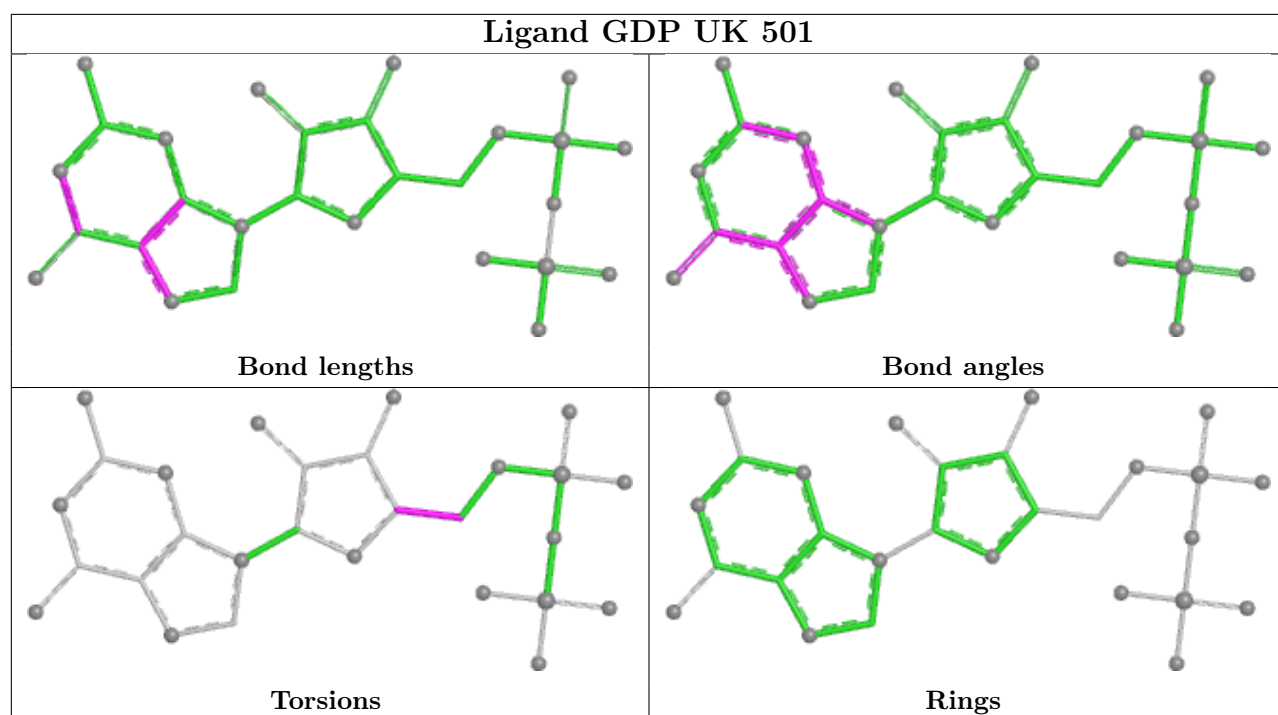


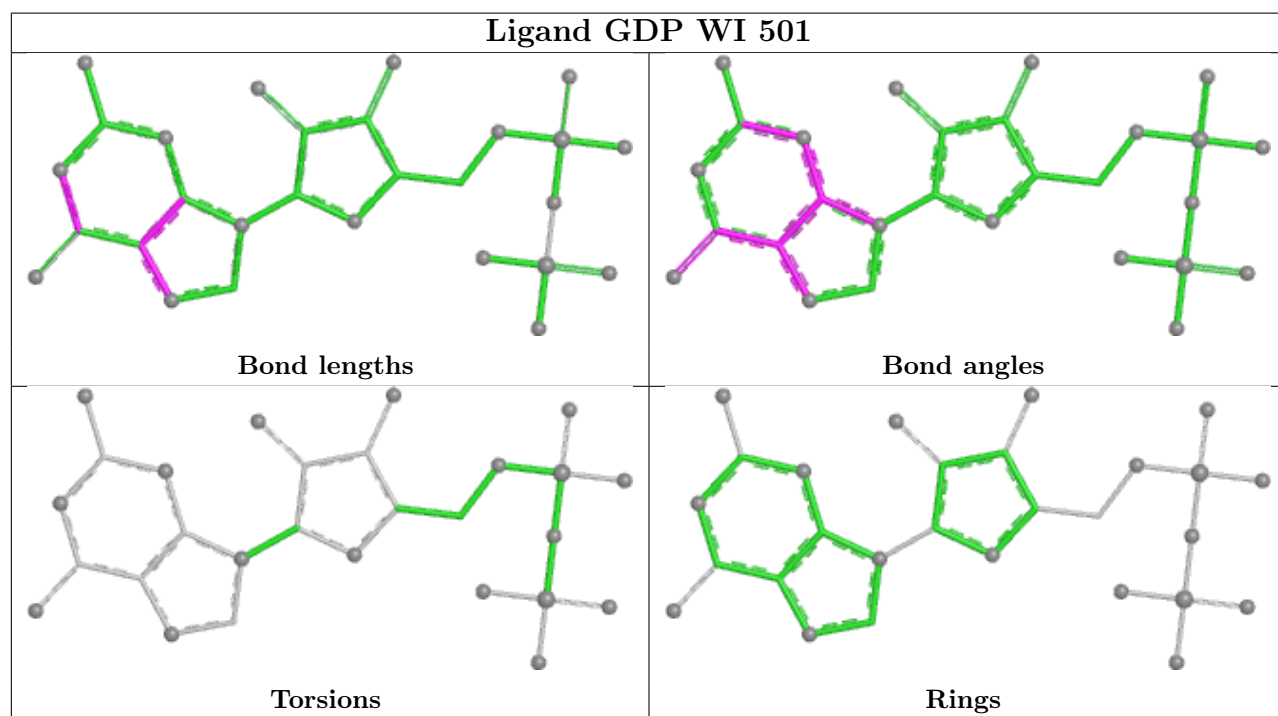
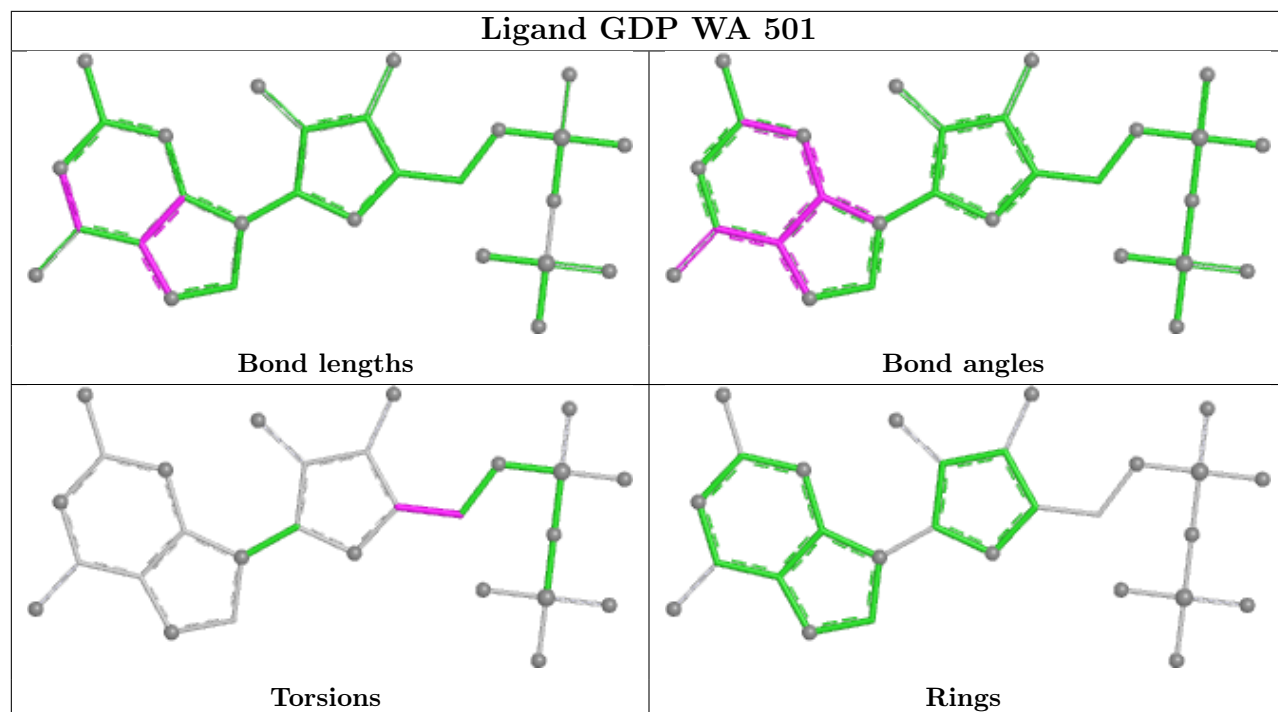
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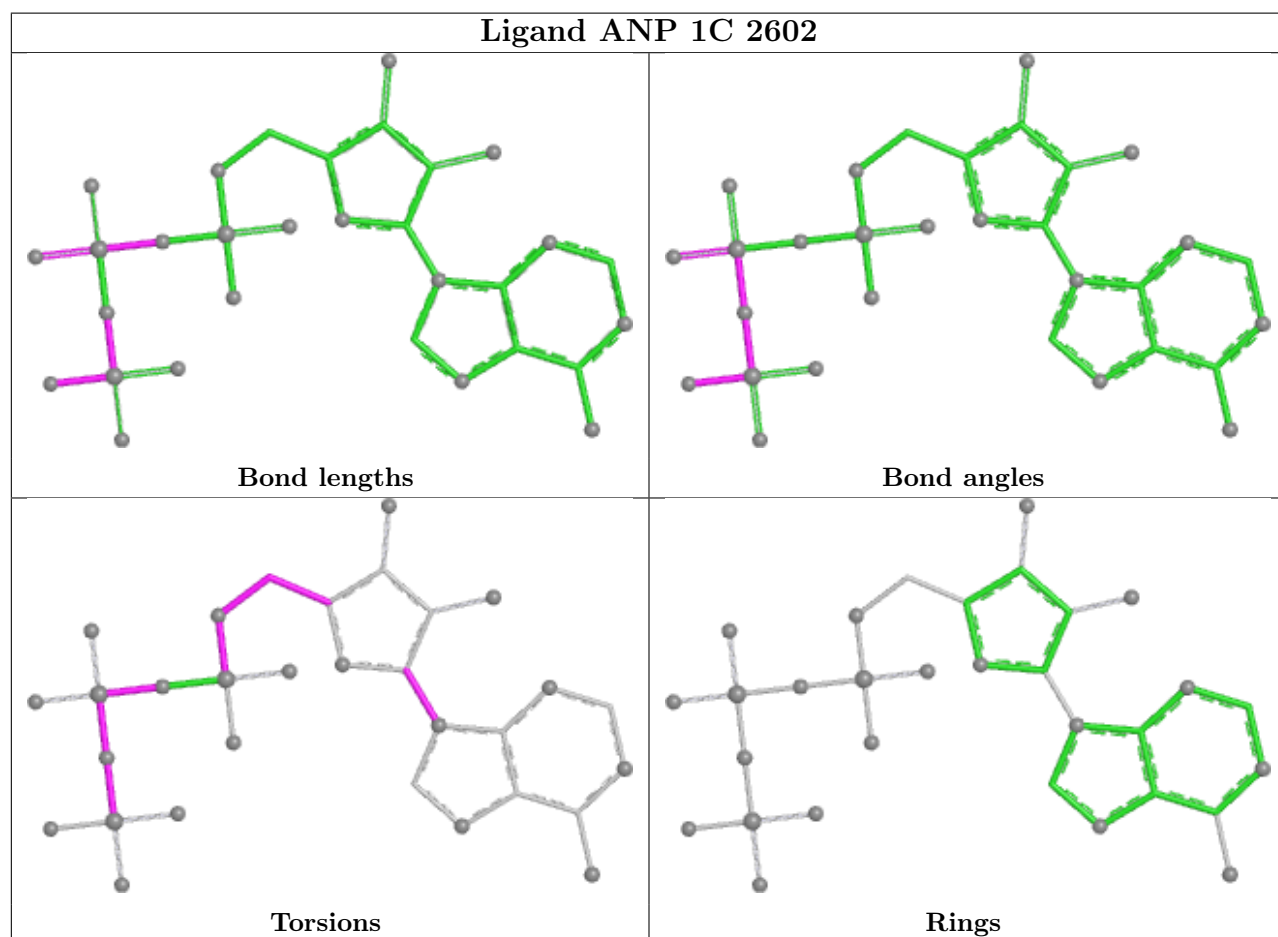
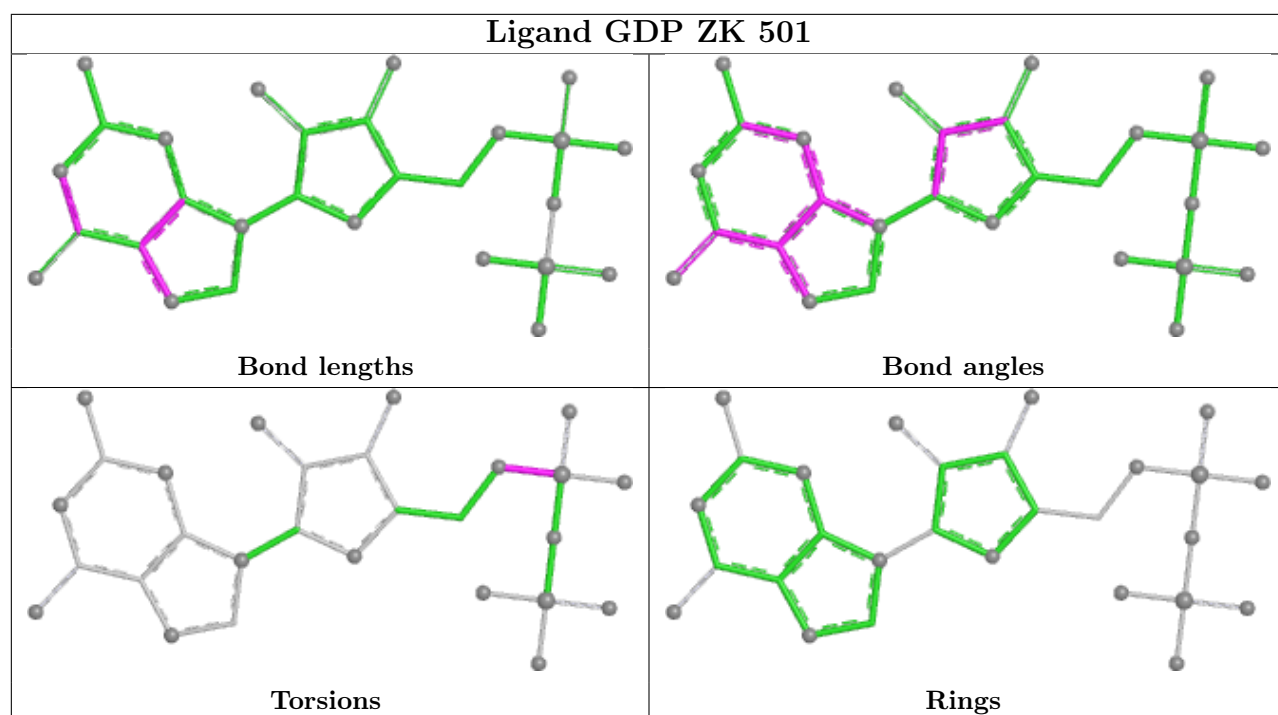


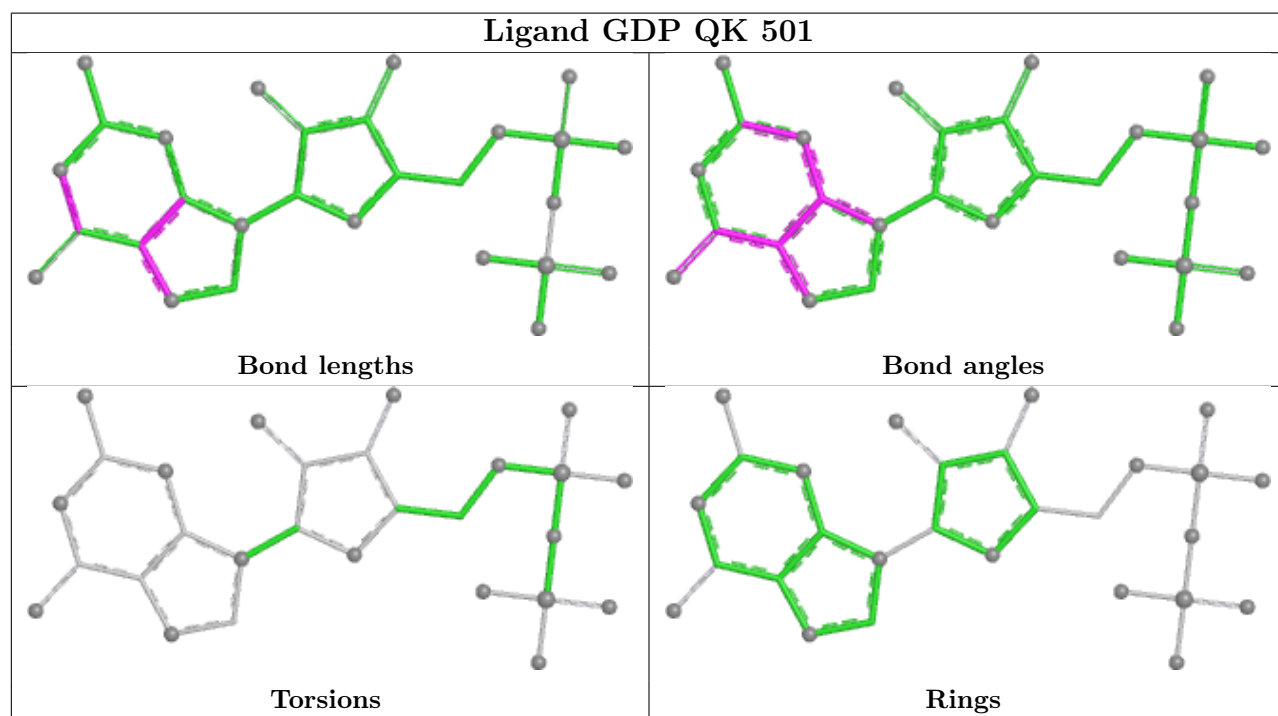
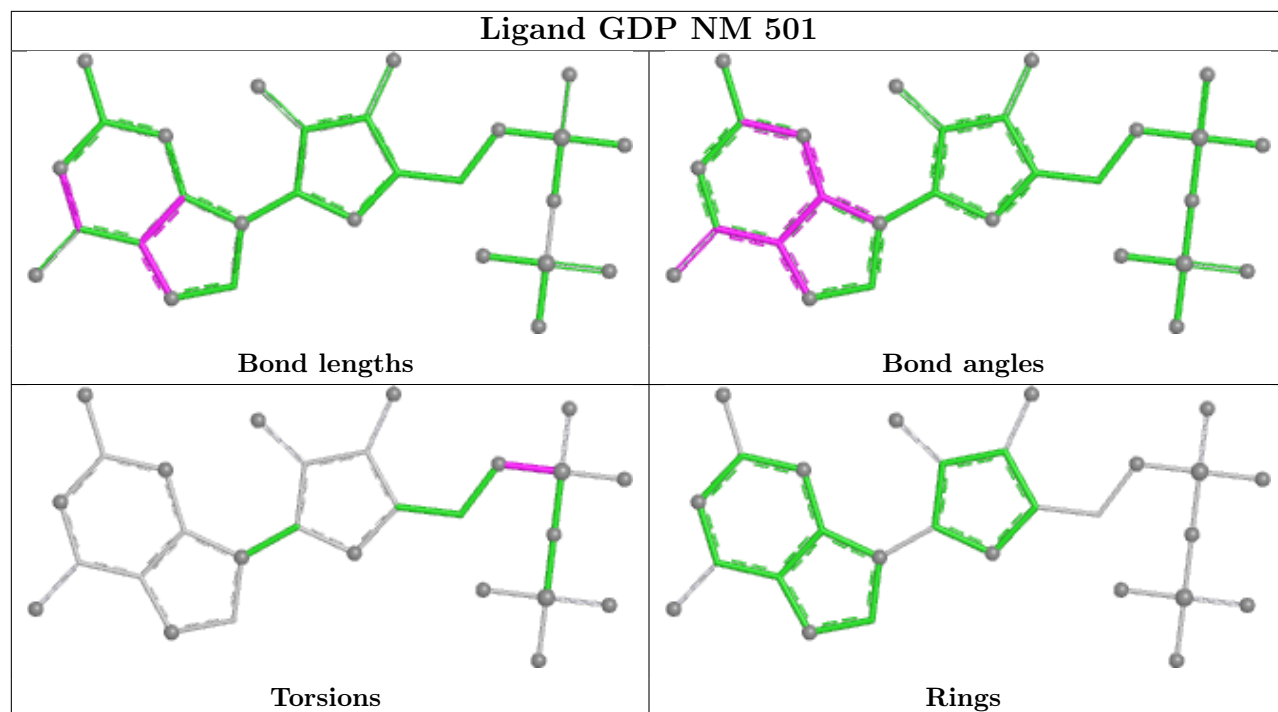
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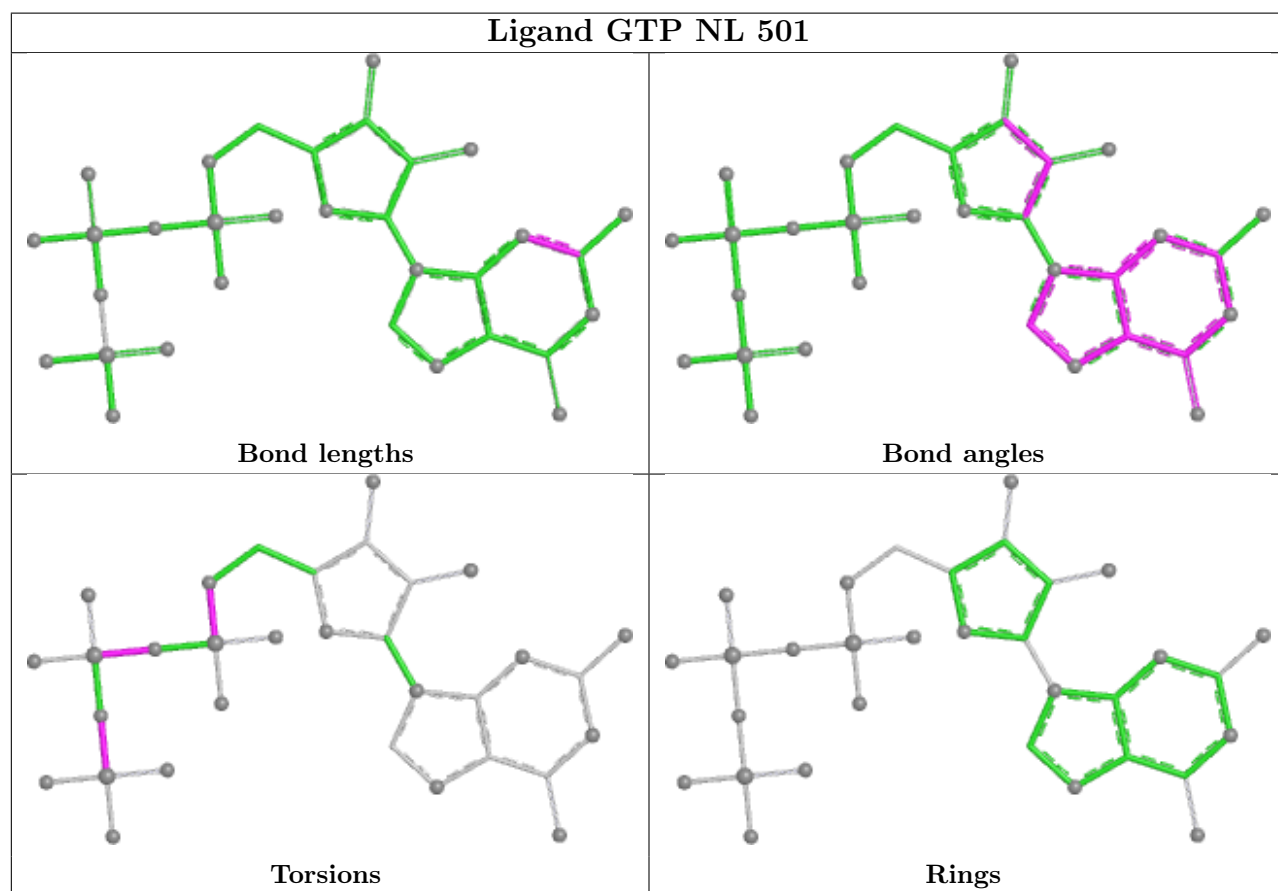
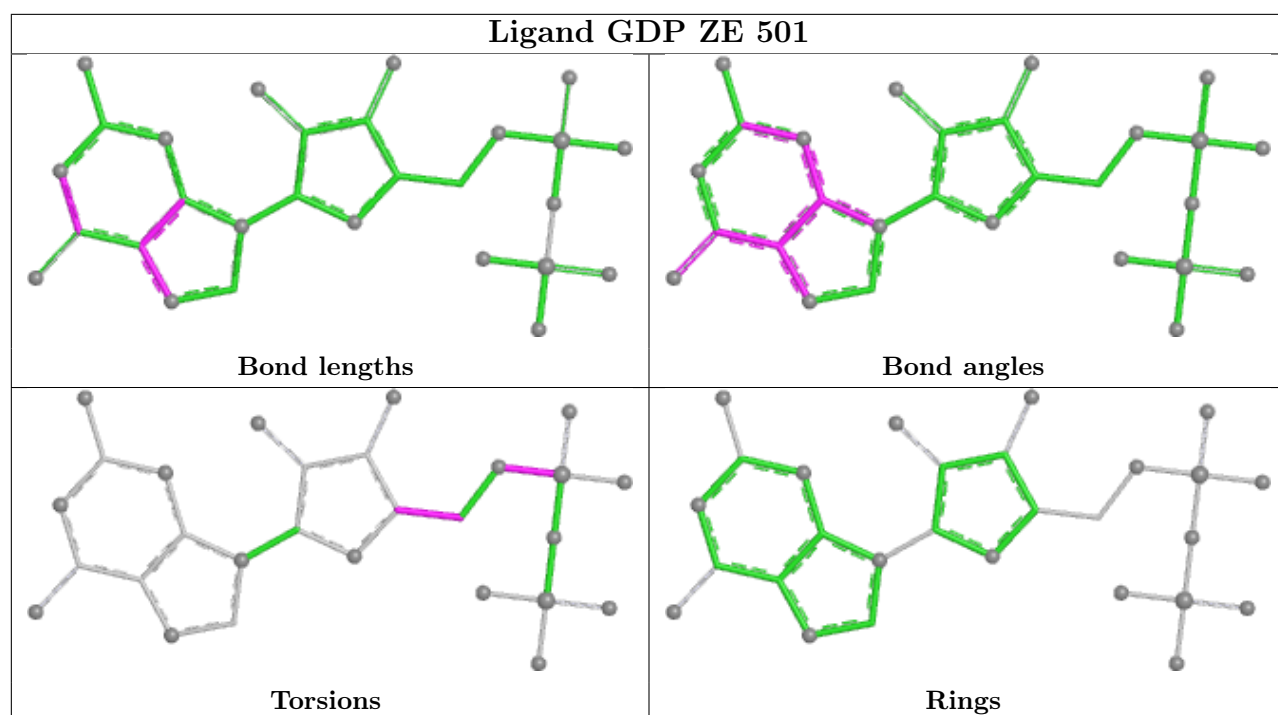


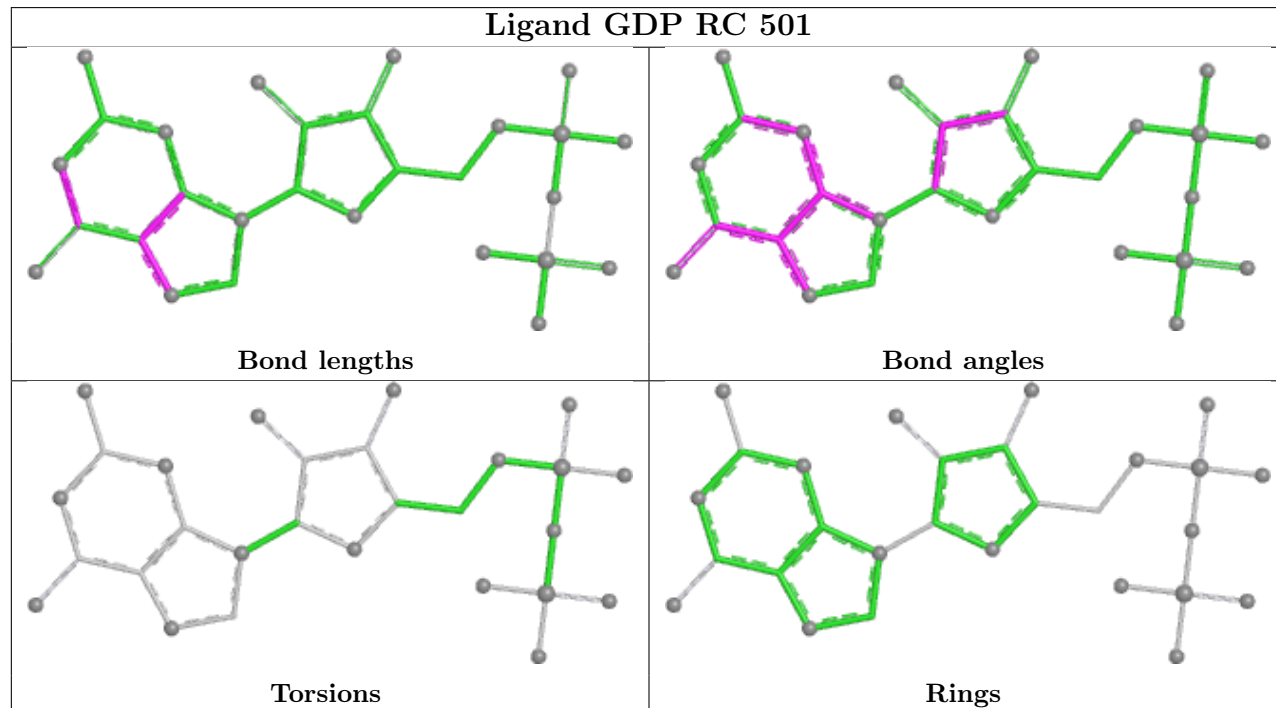
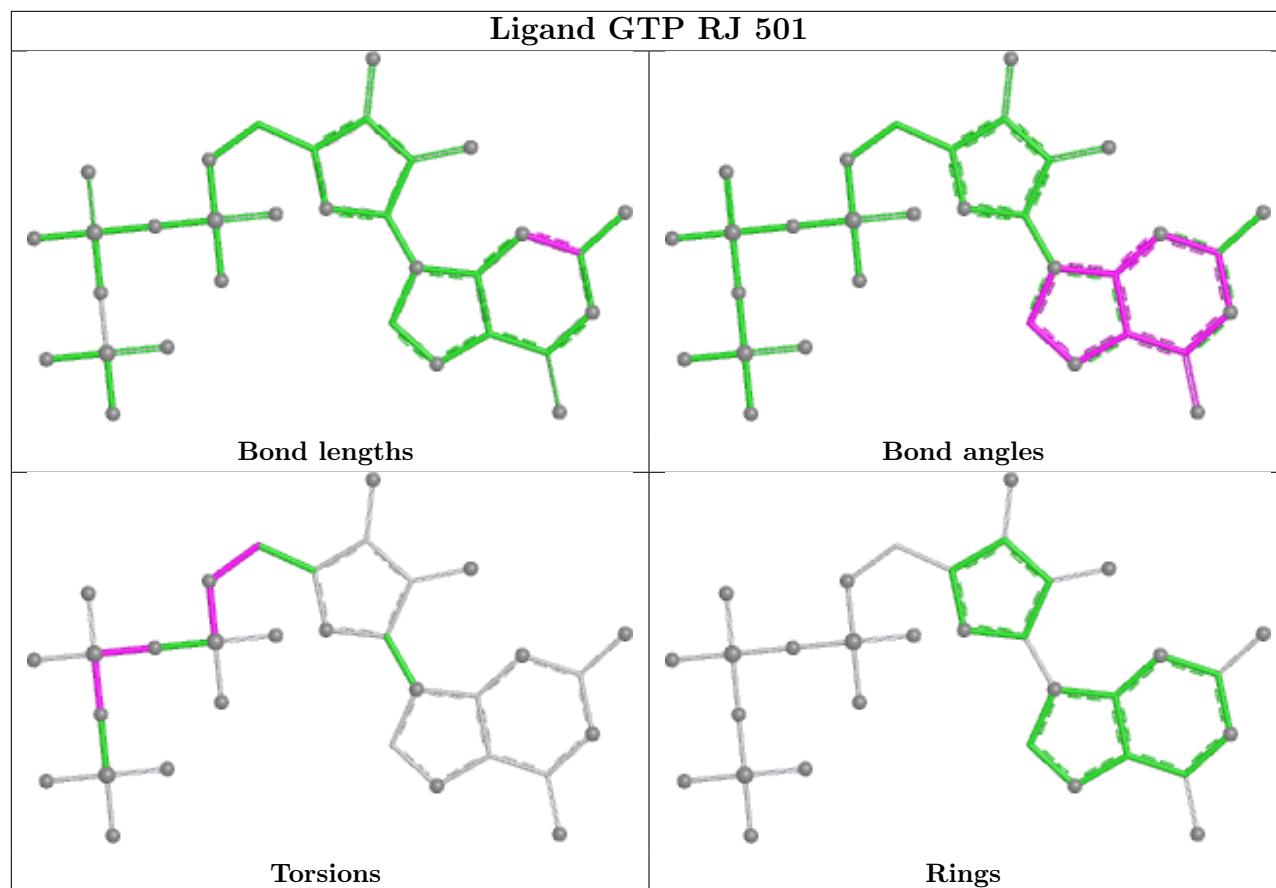


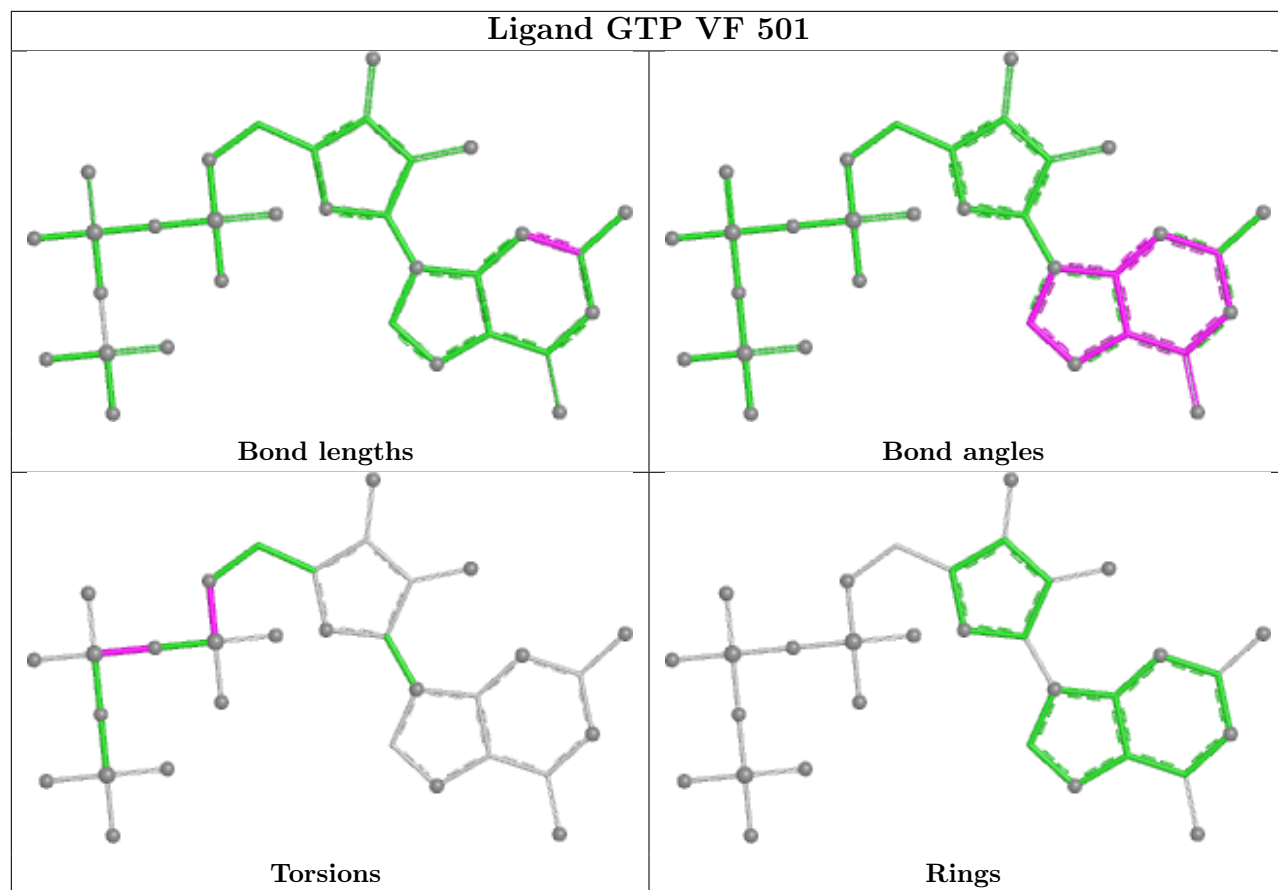




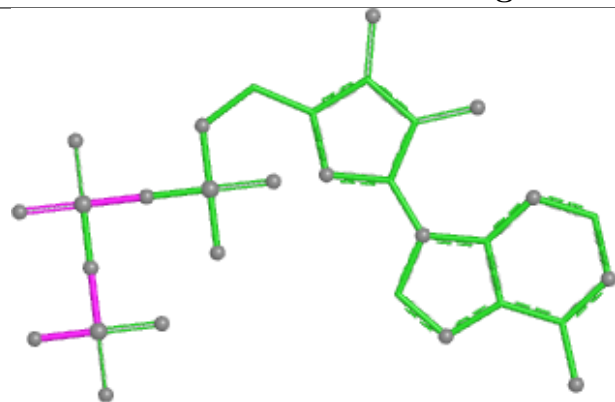




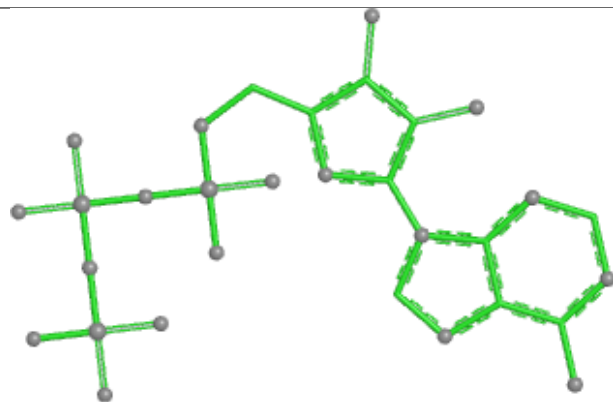




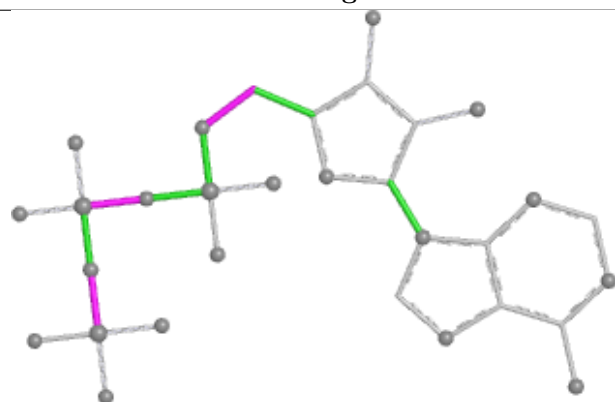
Ligand ANP C0 2001



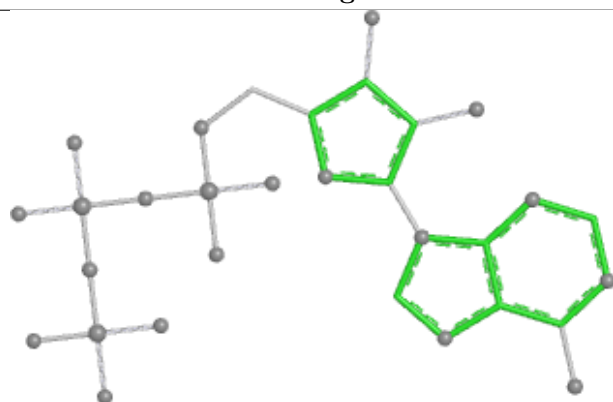
Bond lengths



Bond angles

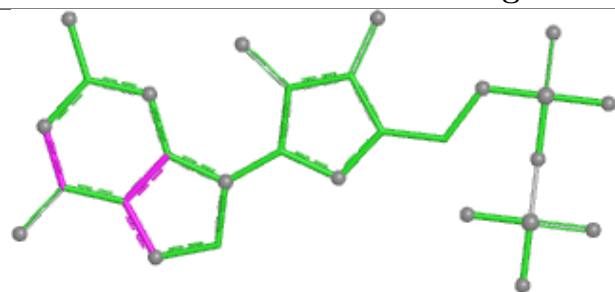


Torsions

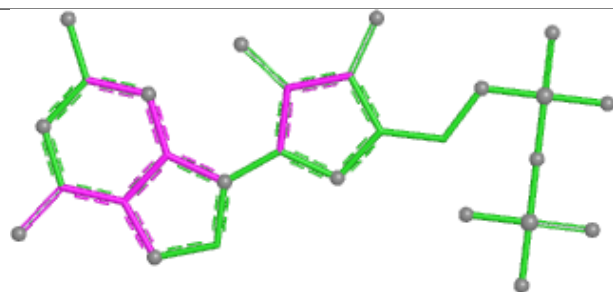


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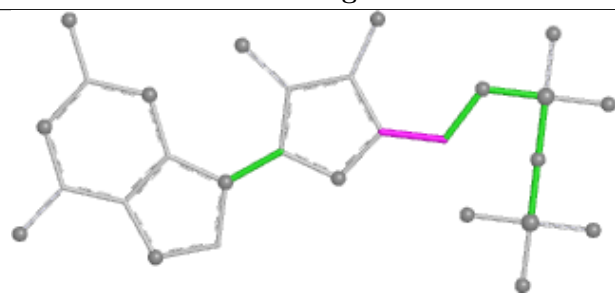
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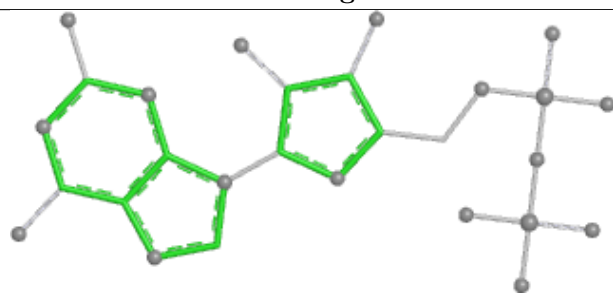
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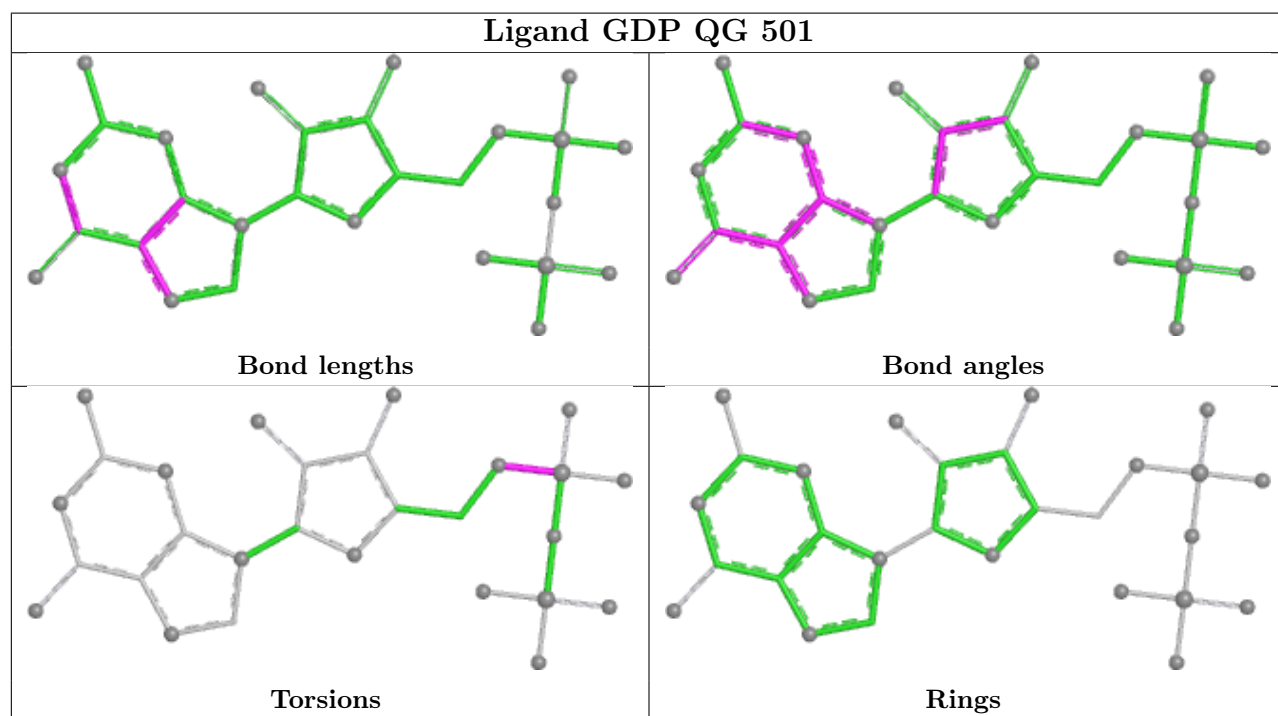
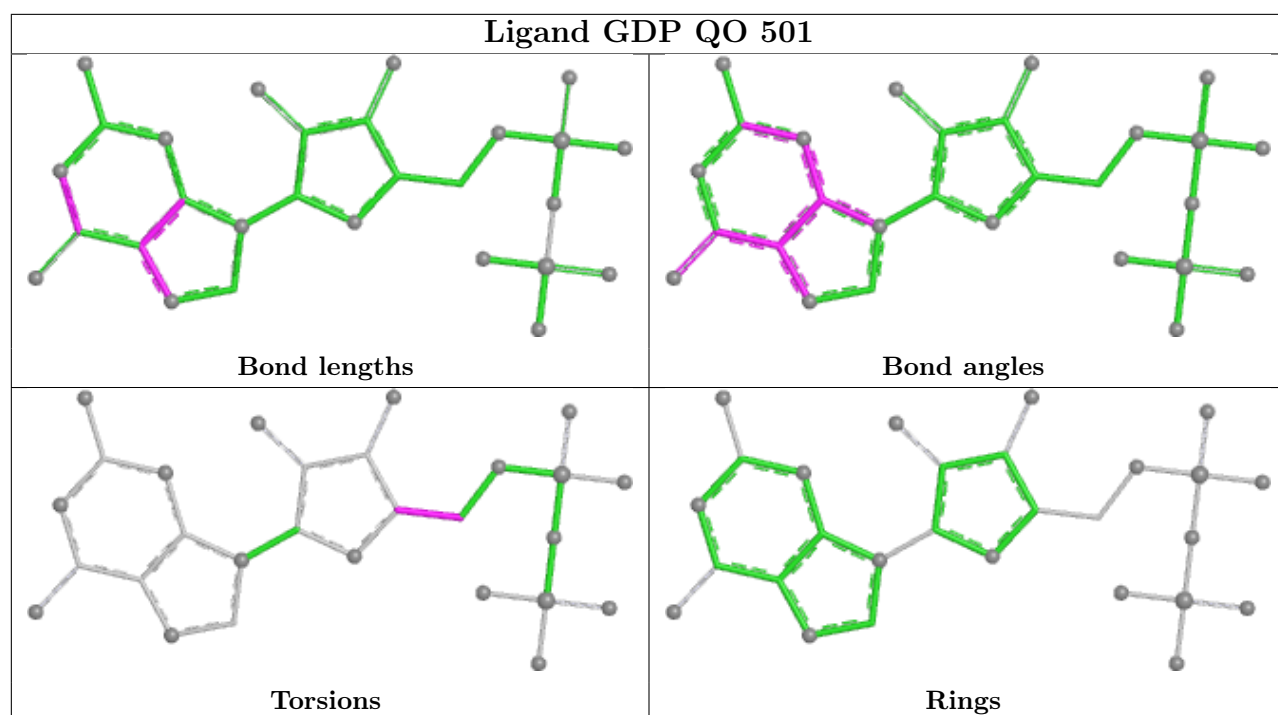
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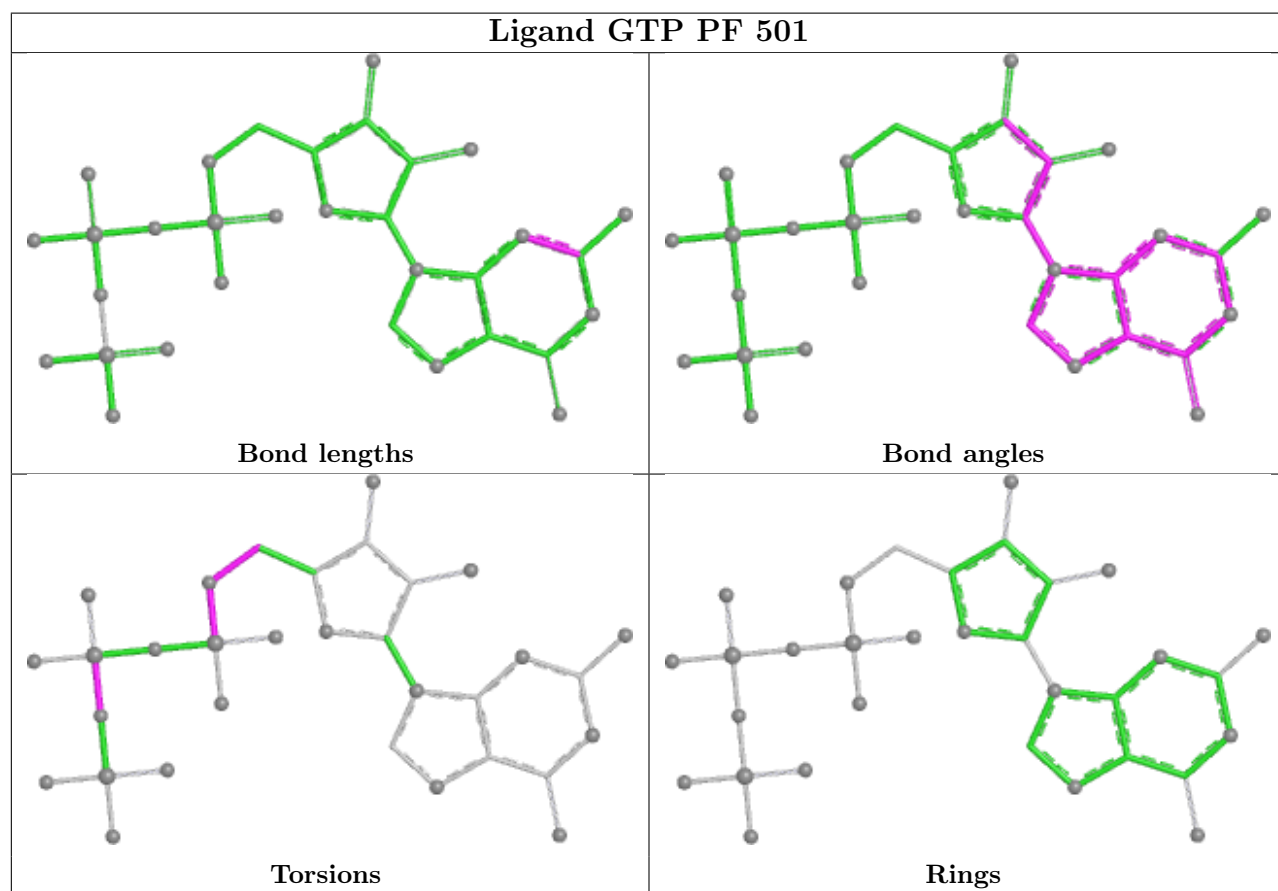
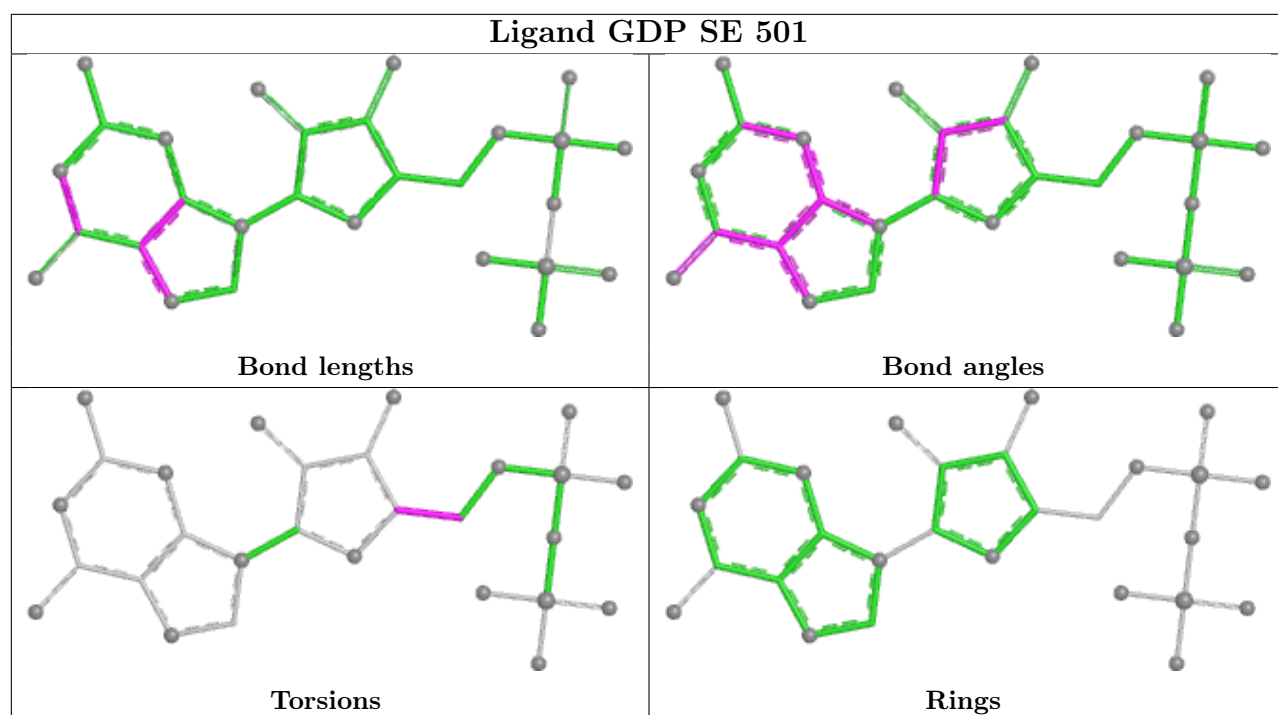


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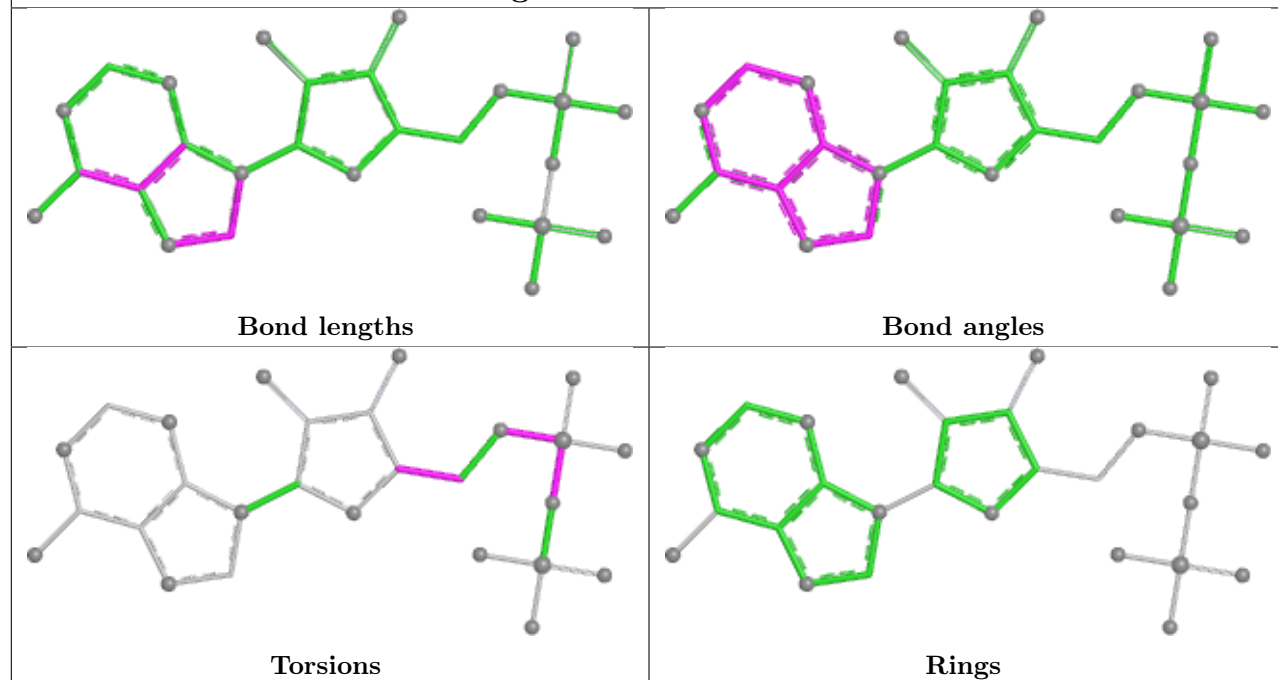


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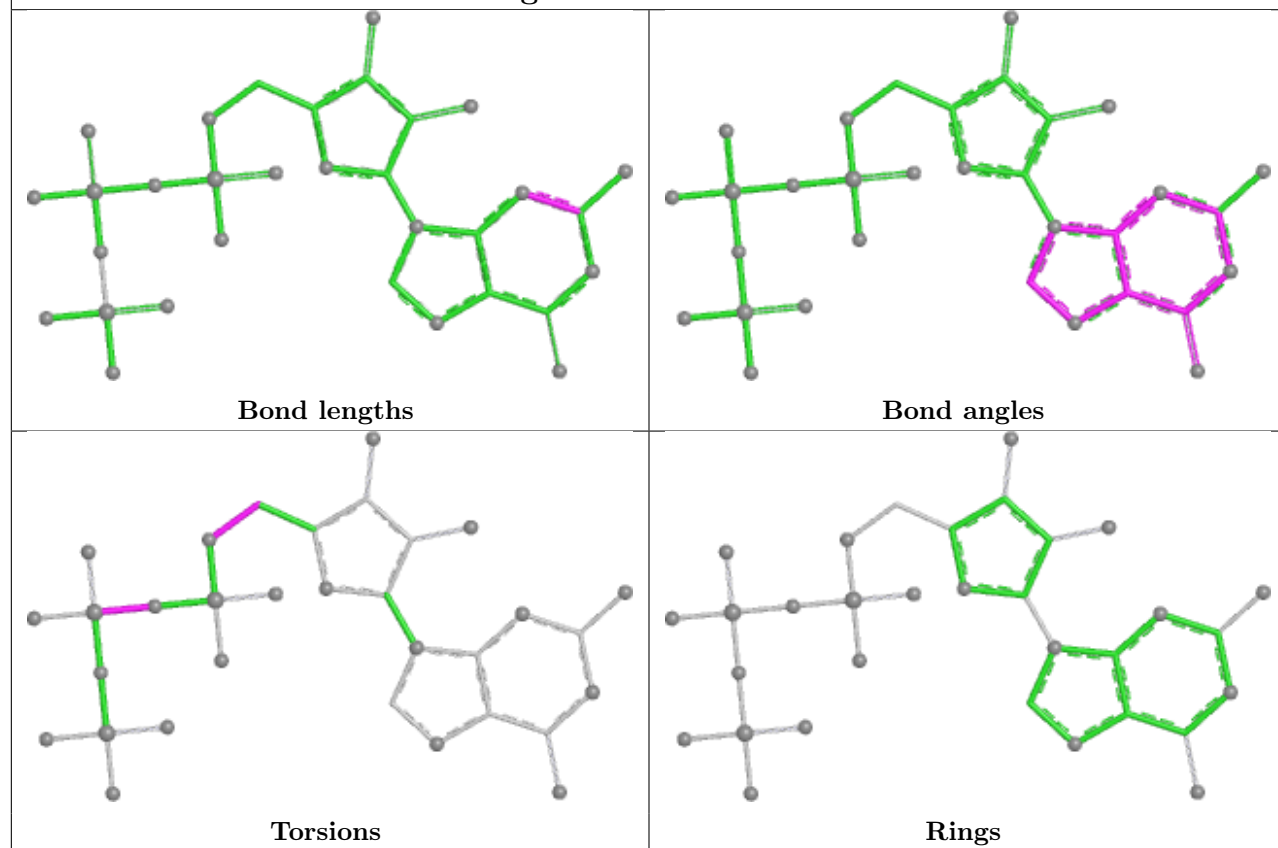


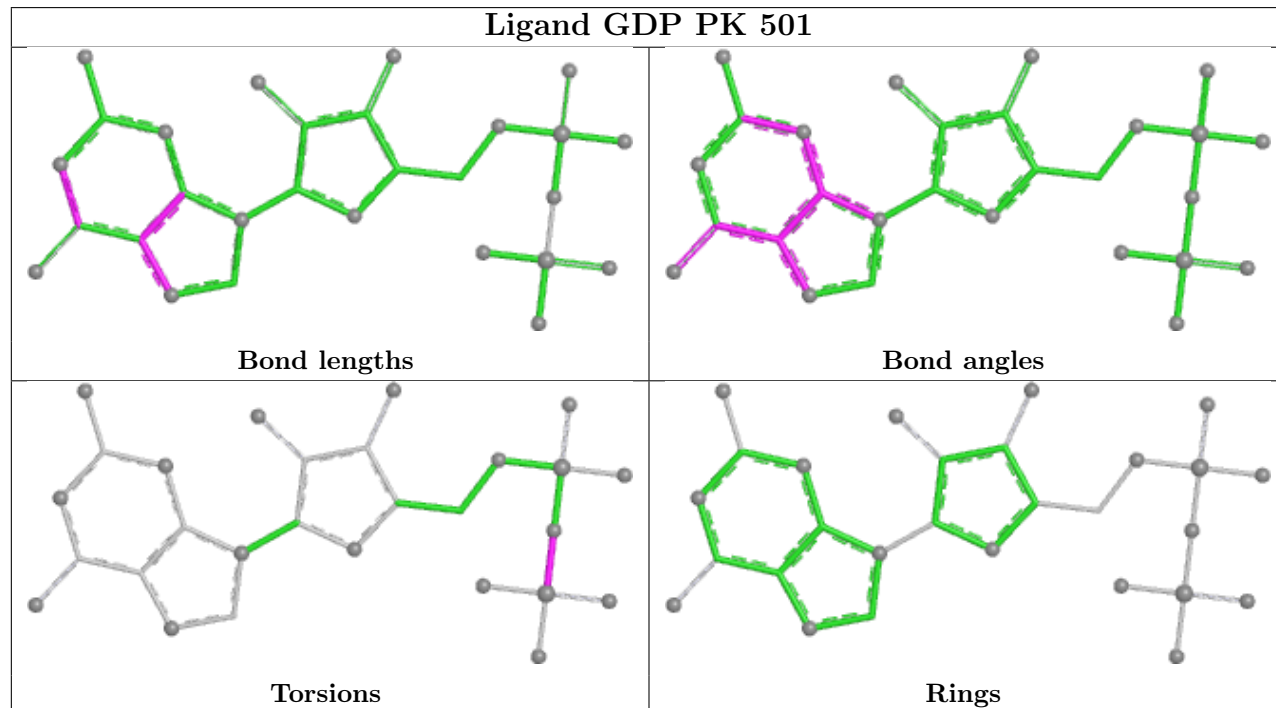
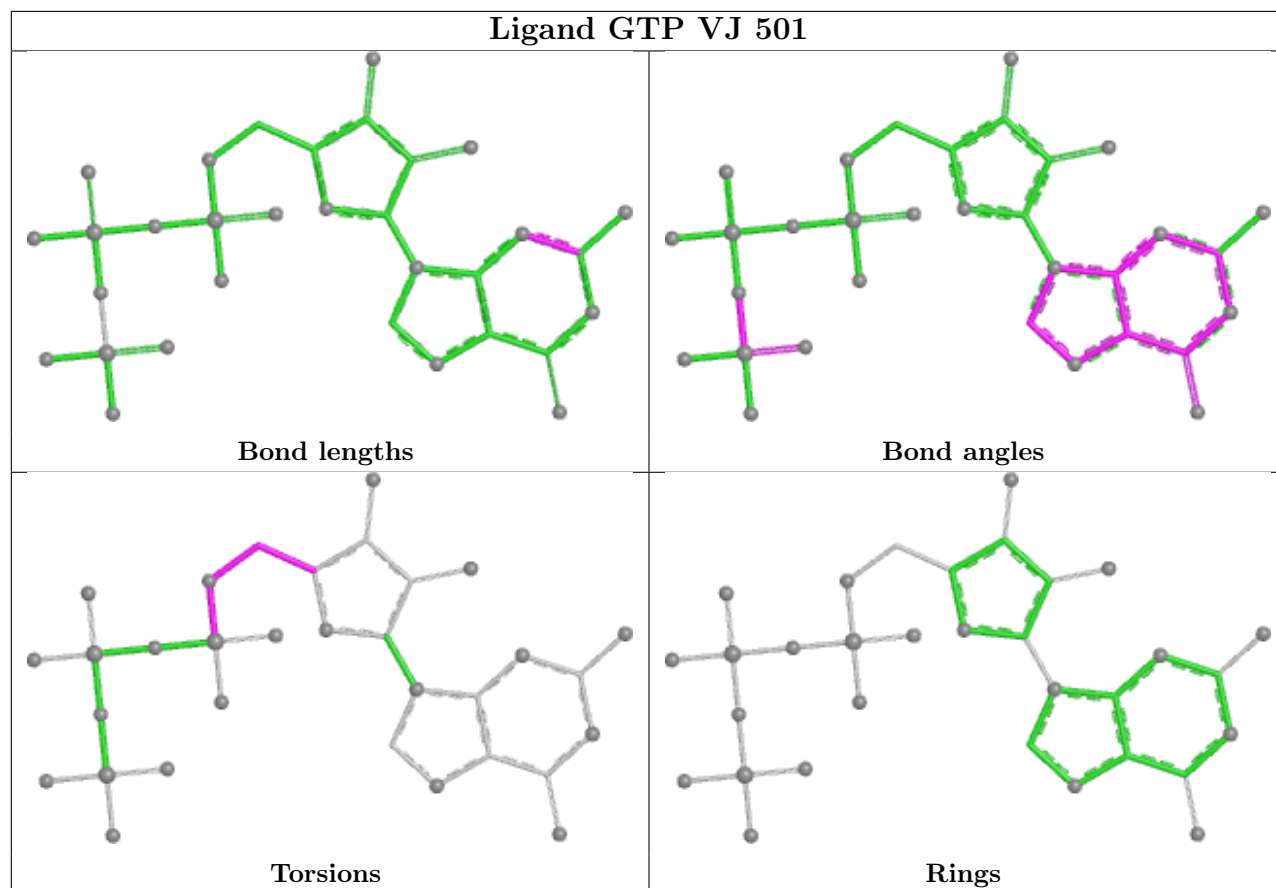


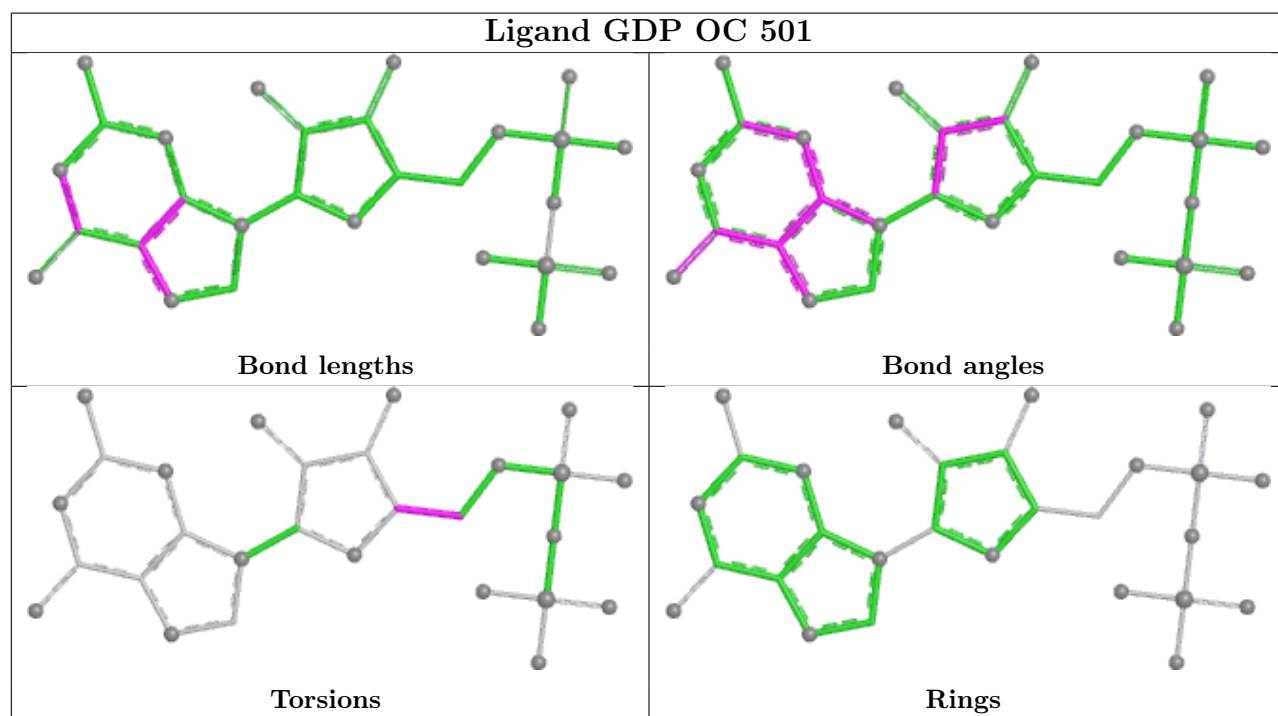
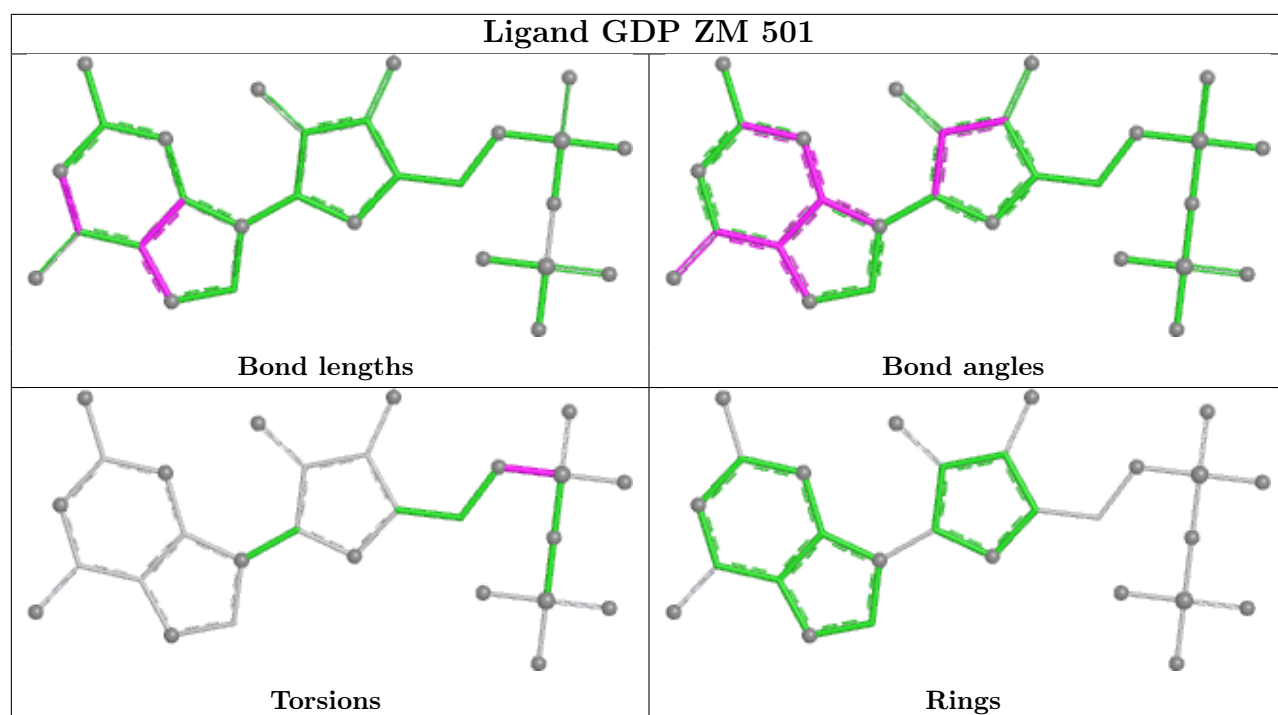
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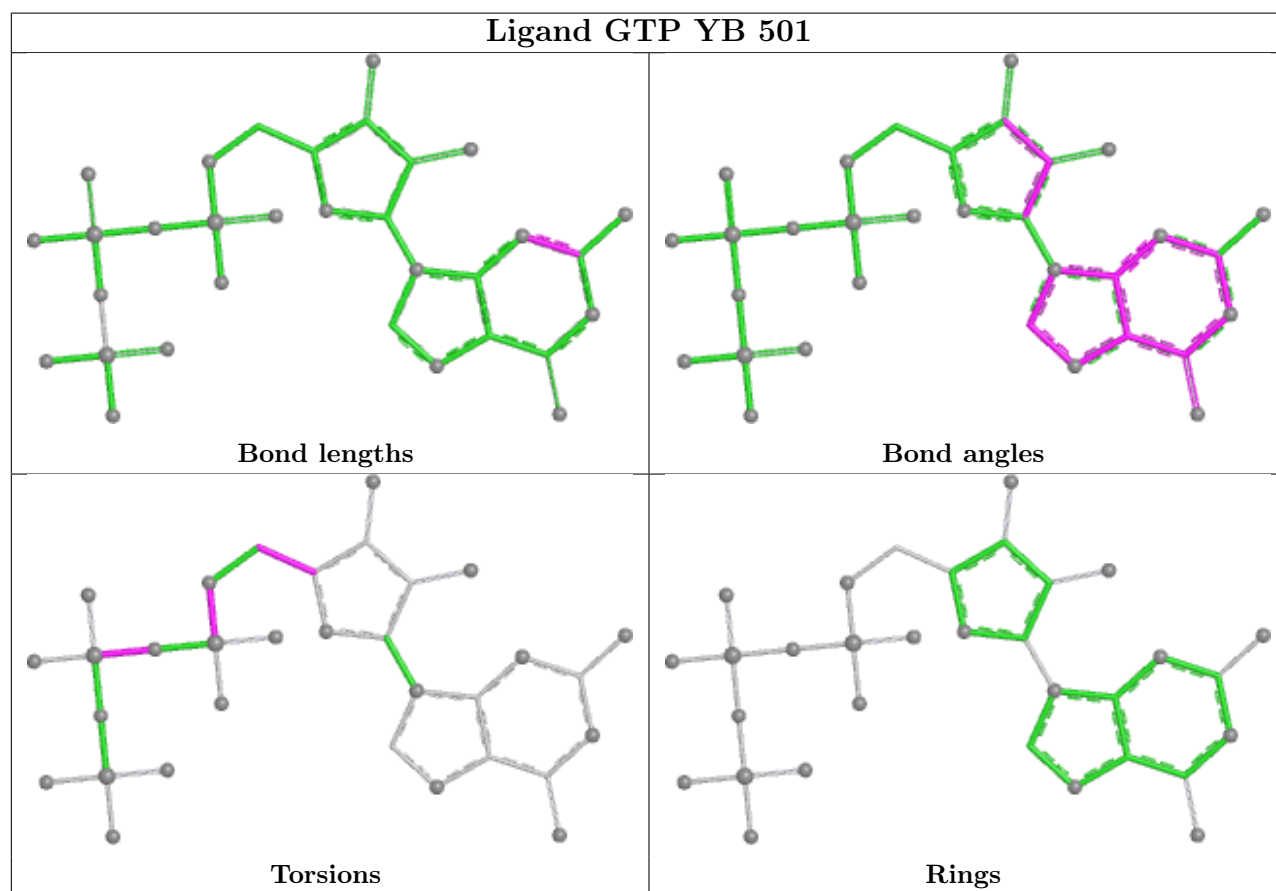
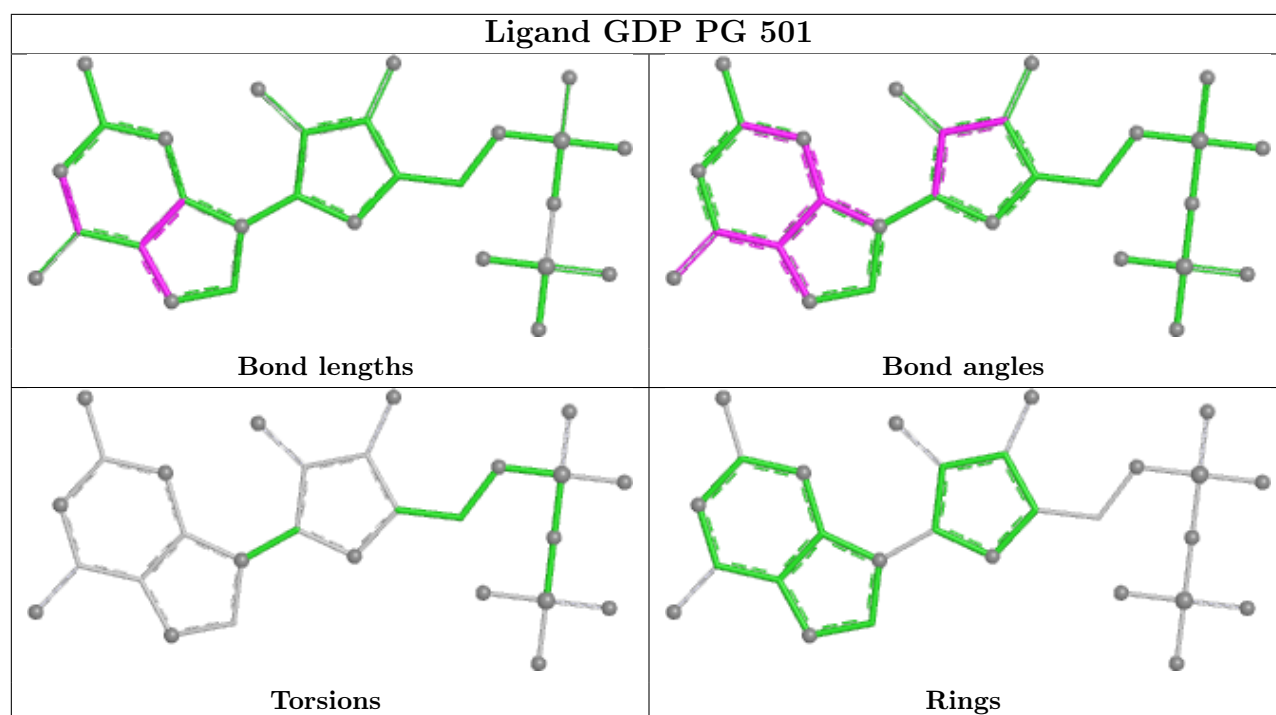


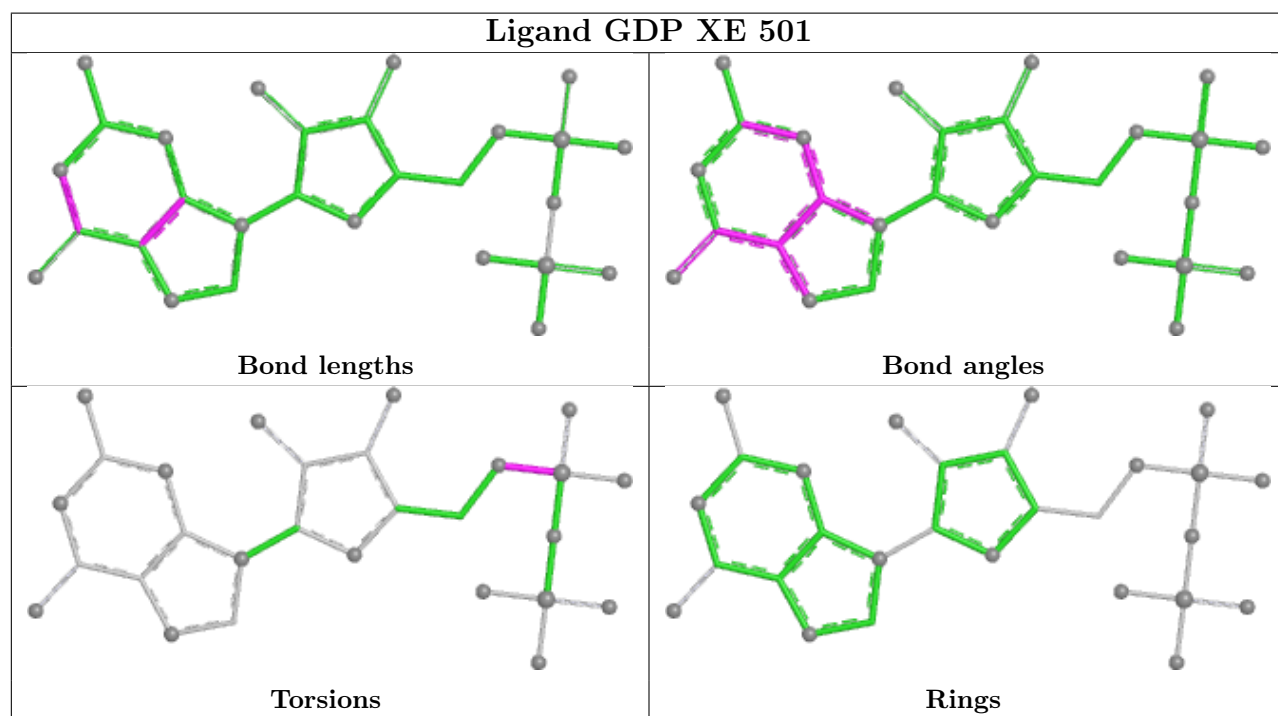
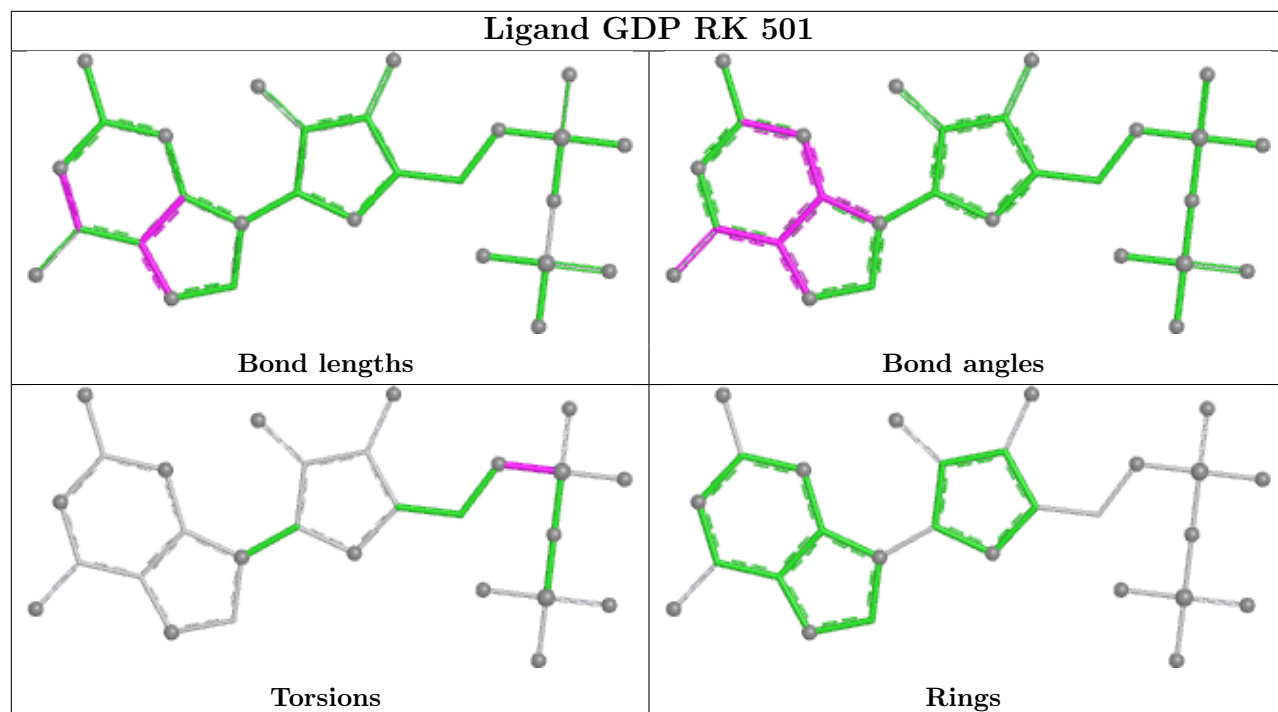
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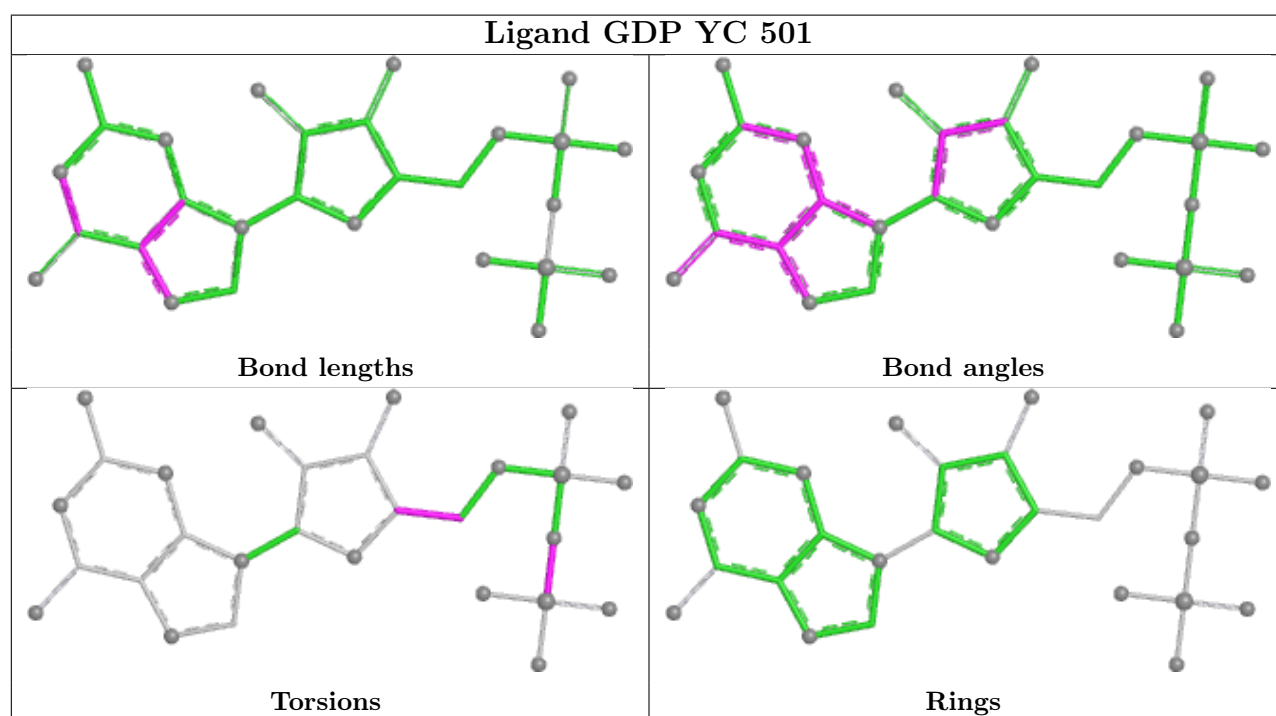
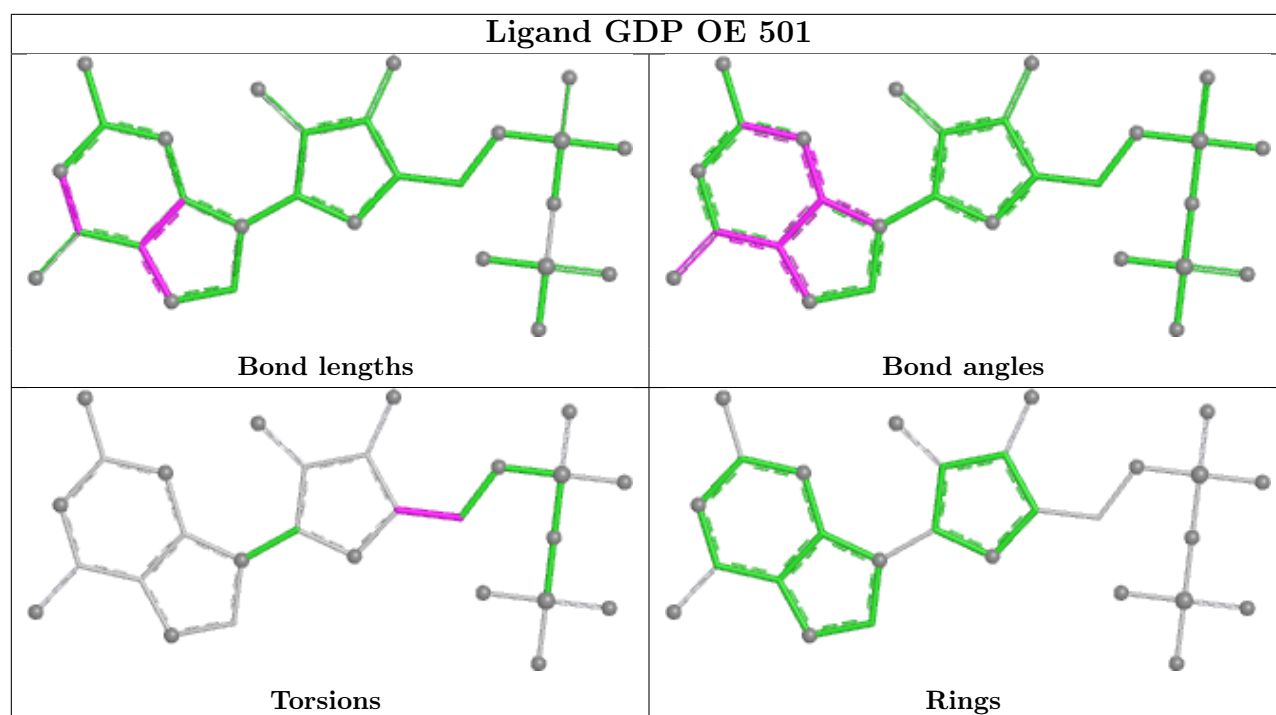


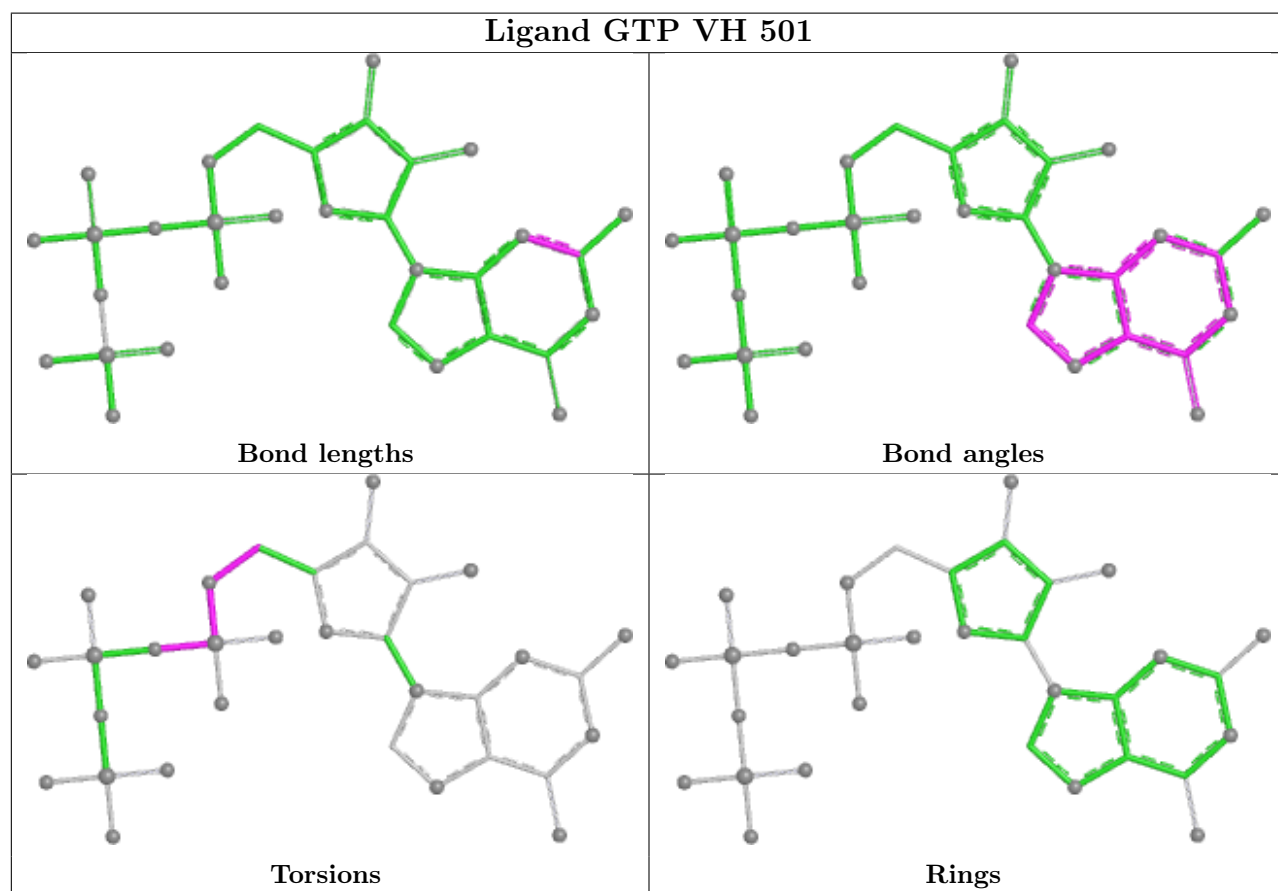
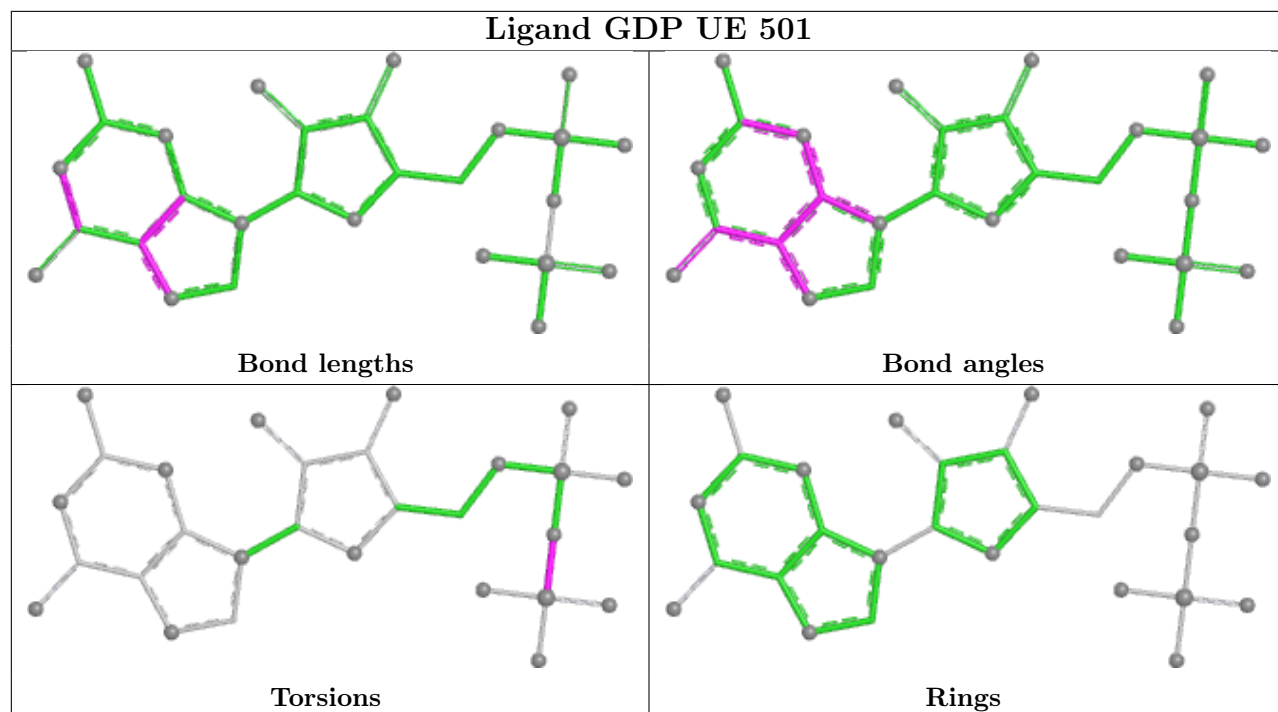


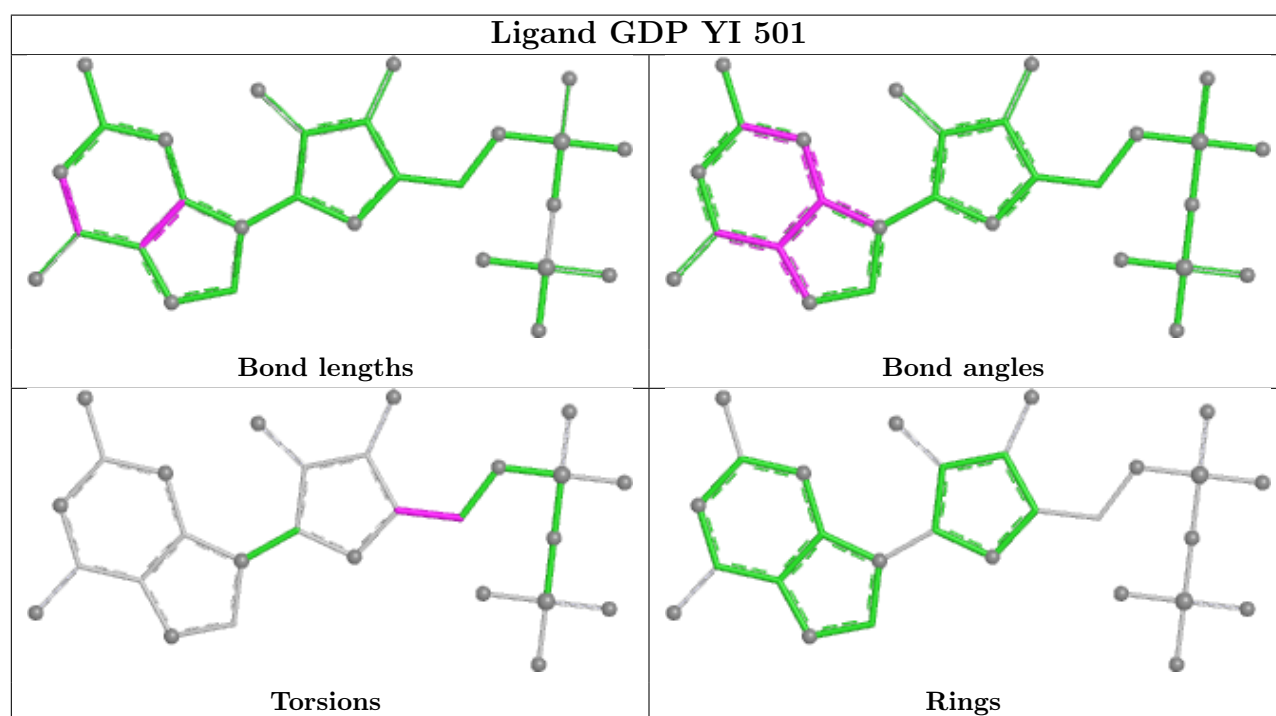
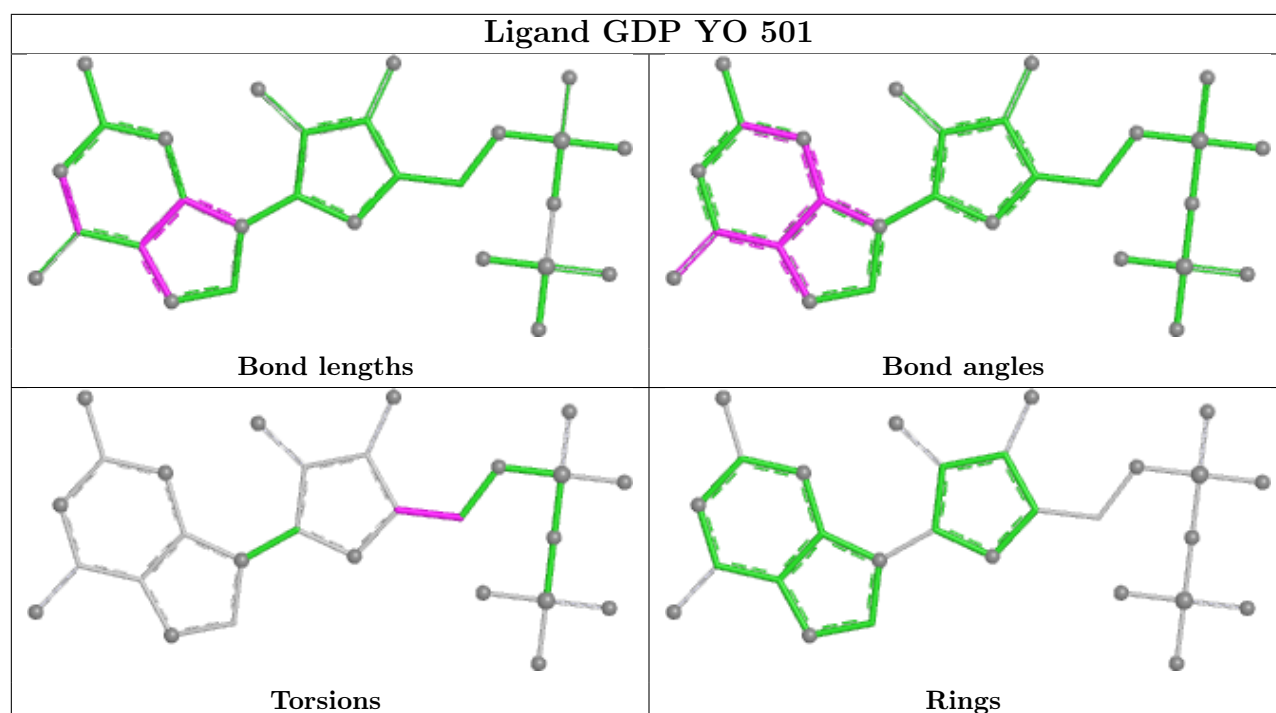




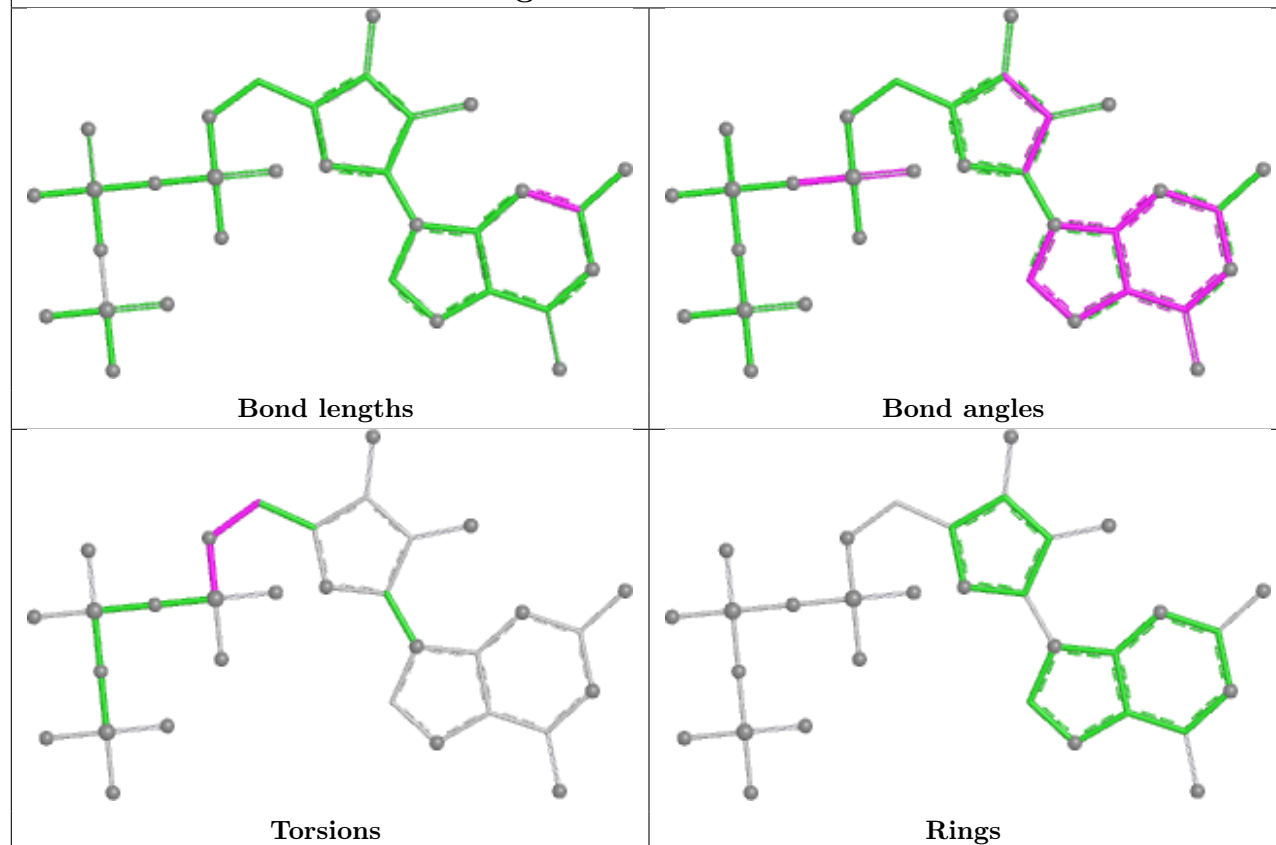




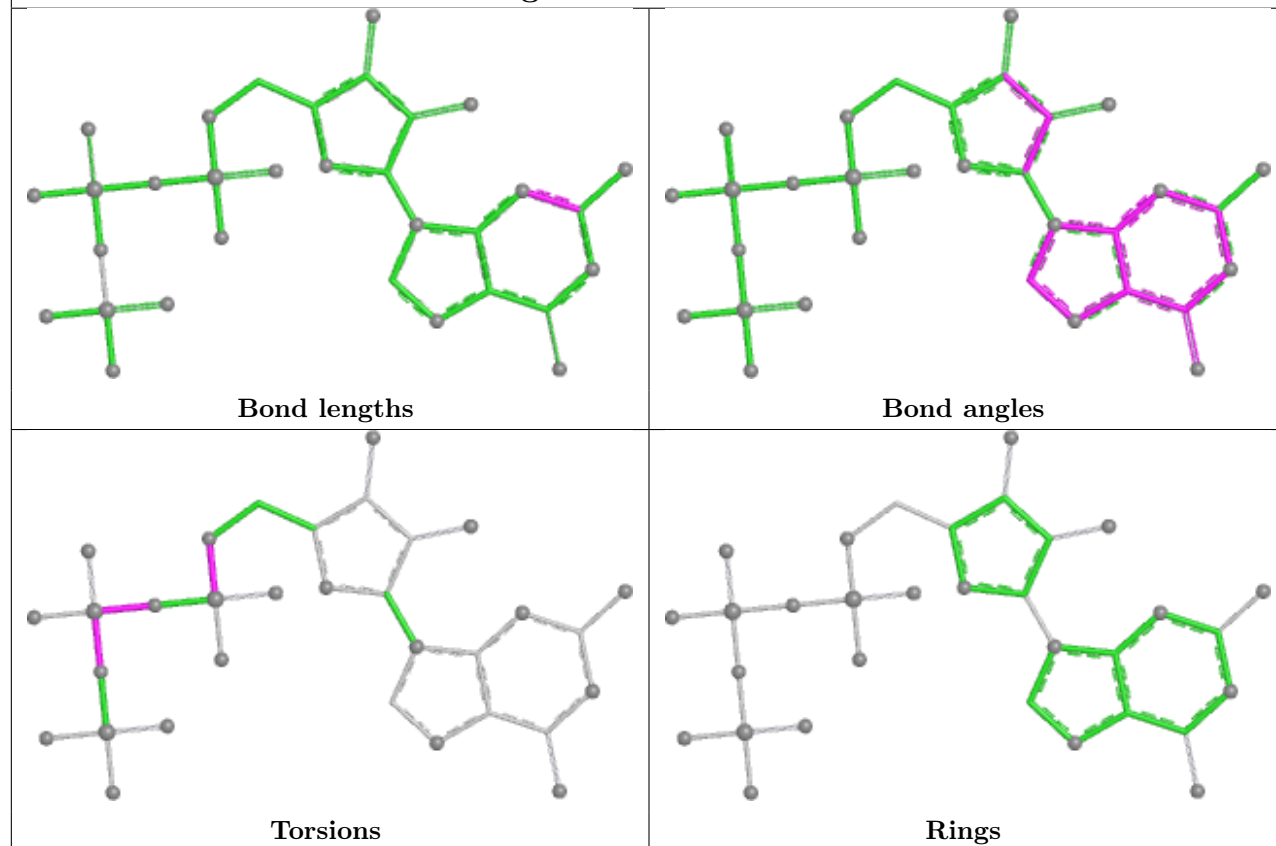




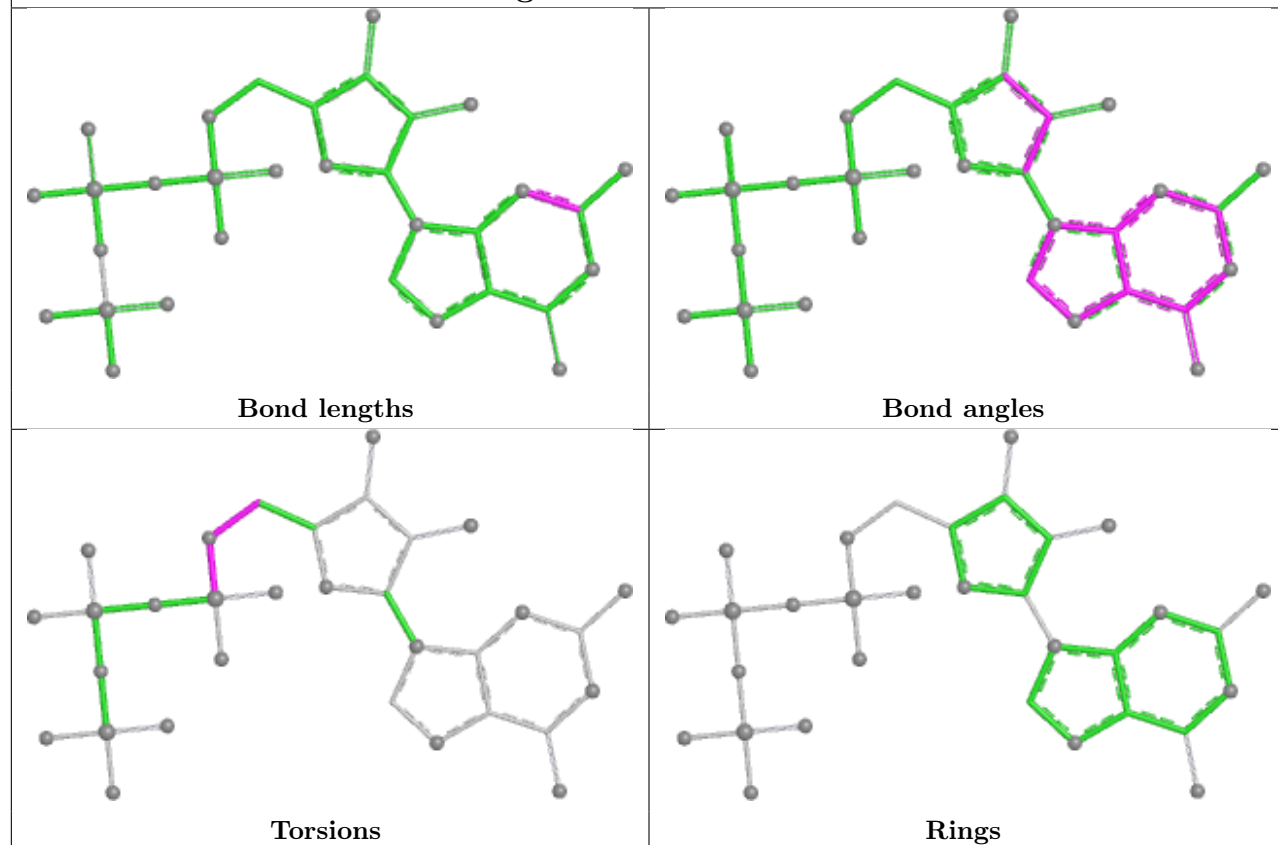
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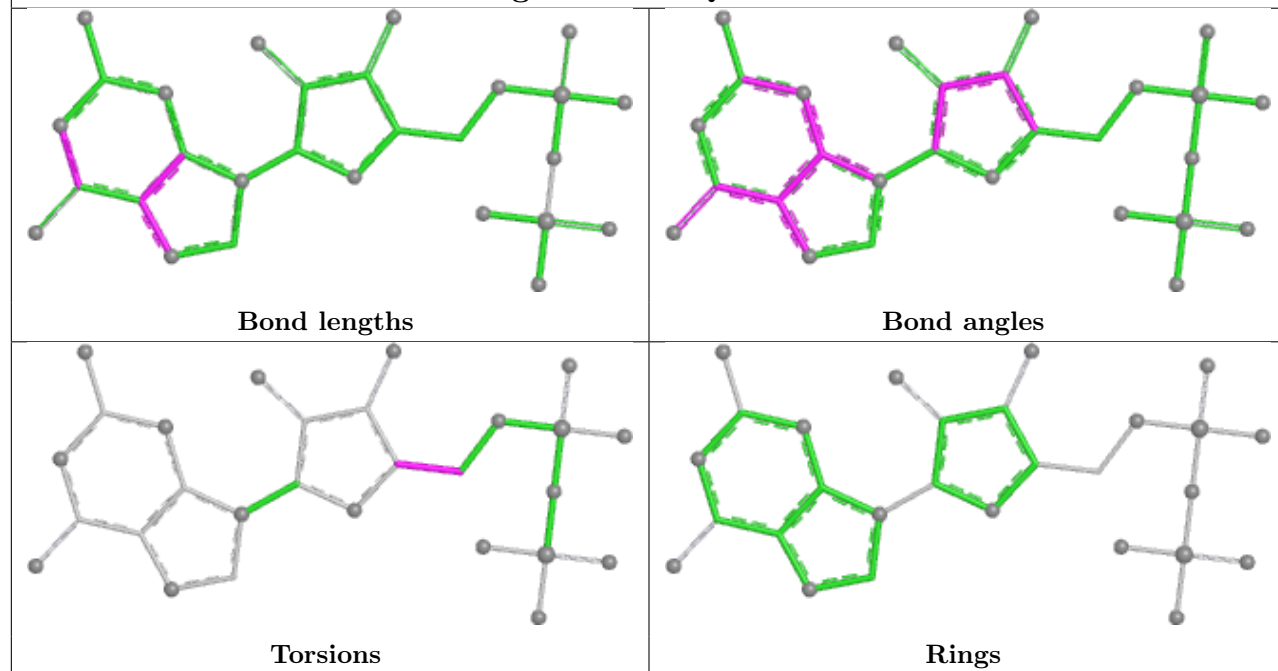
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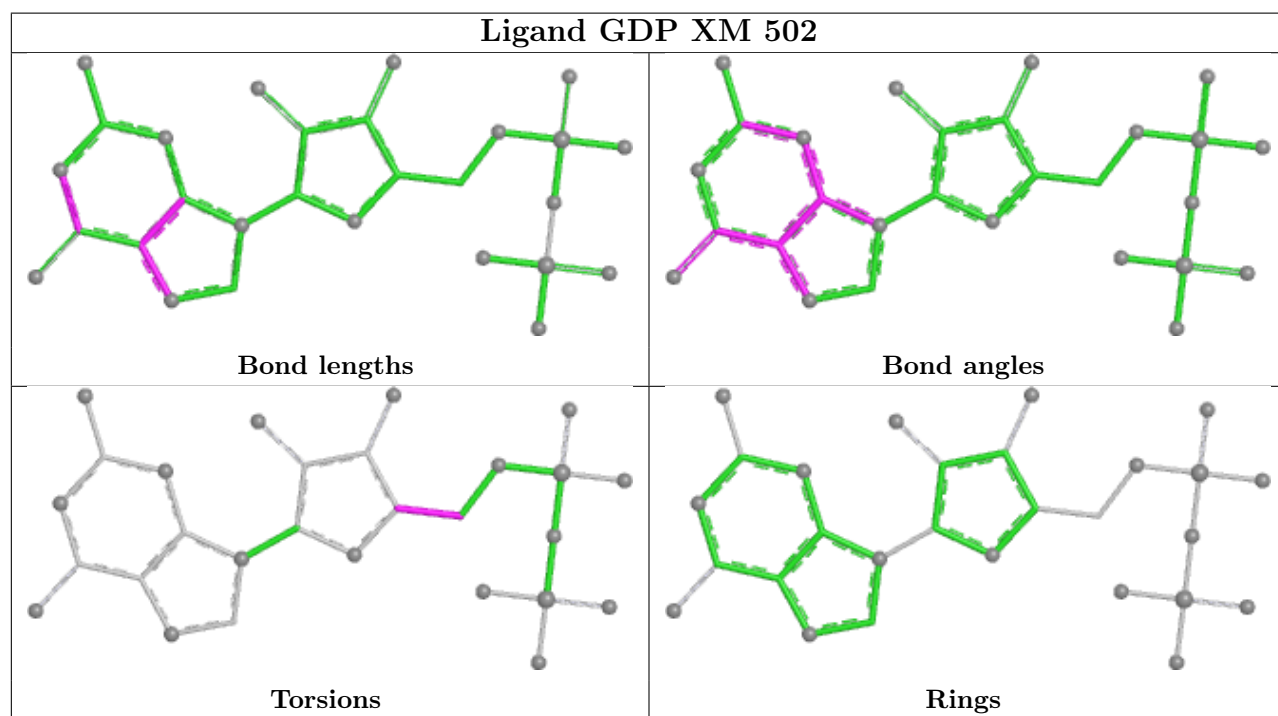
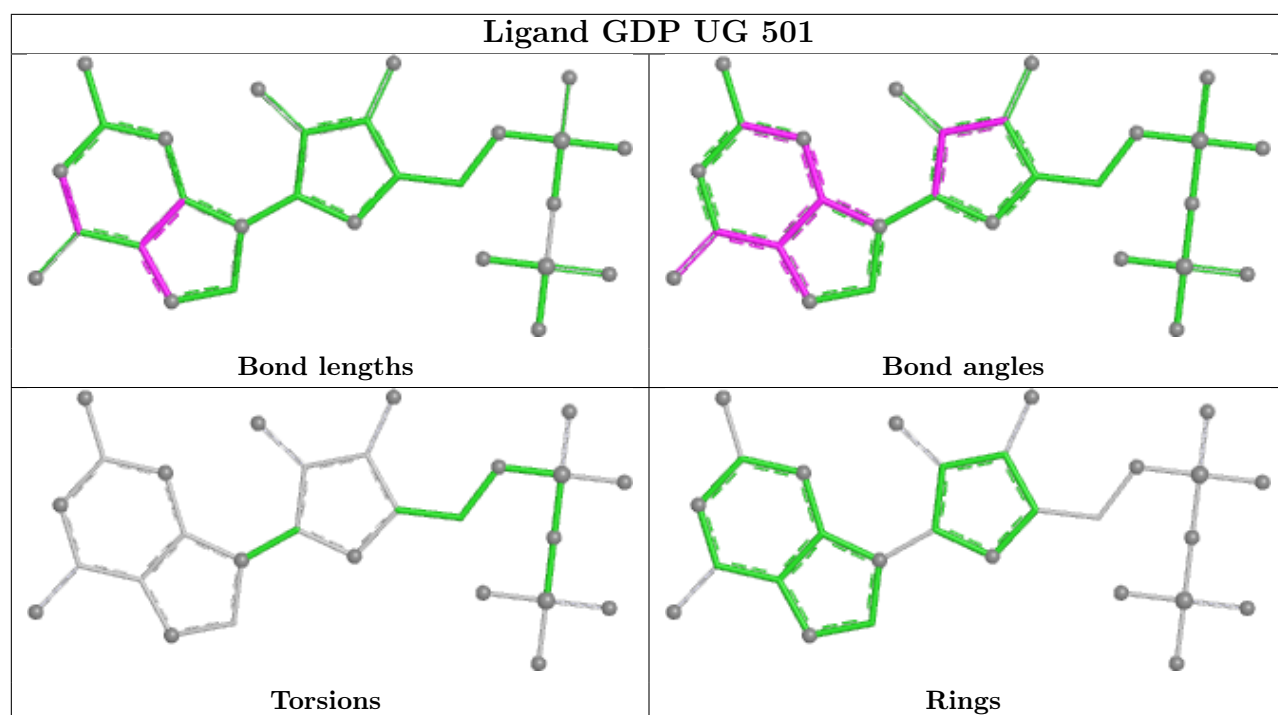


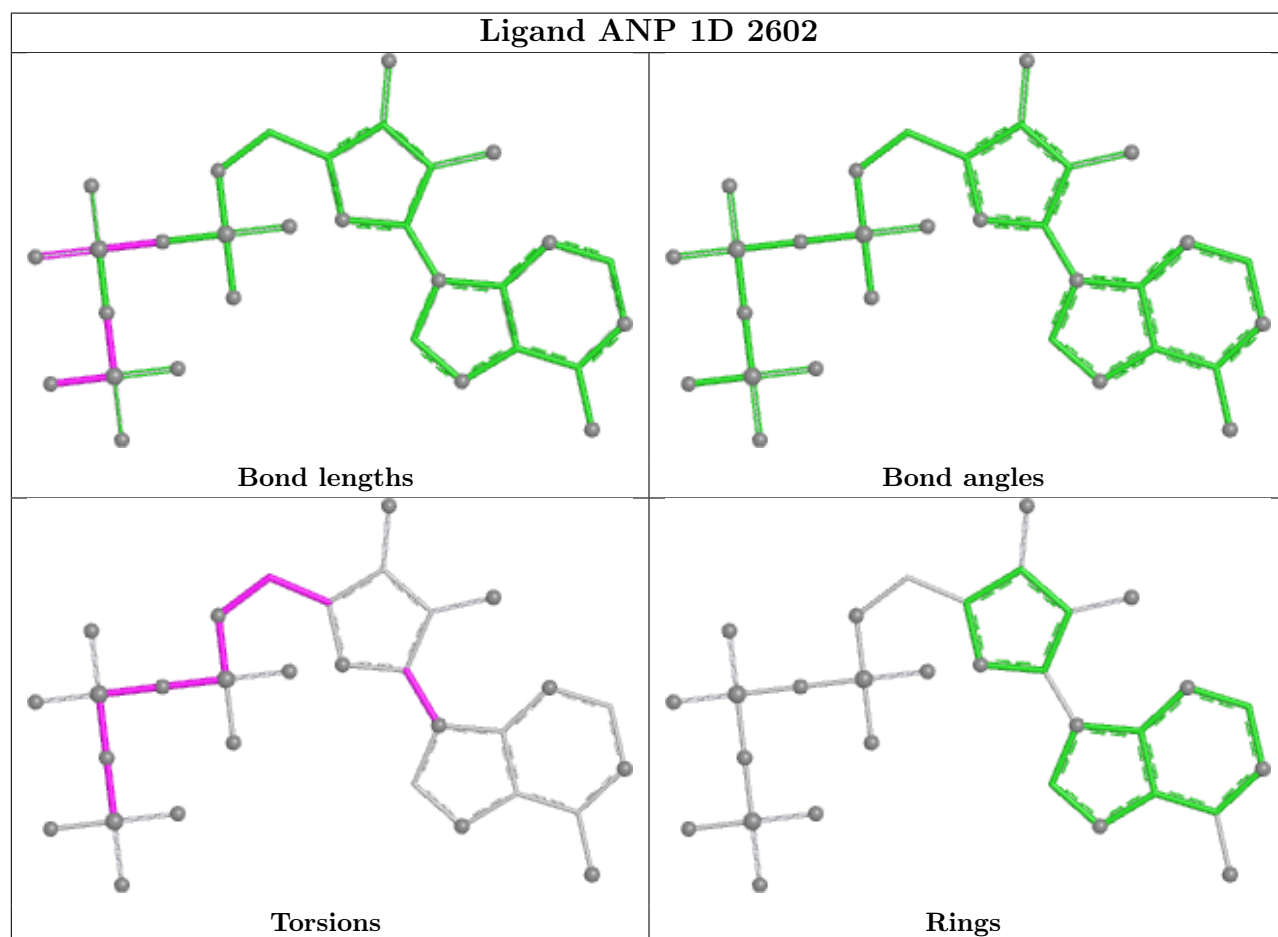
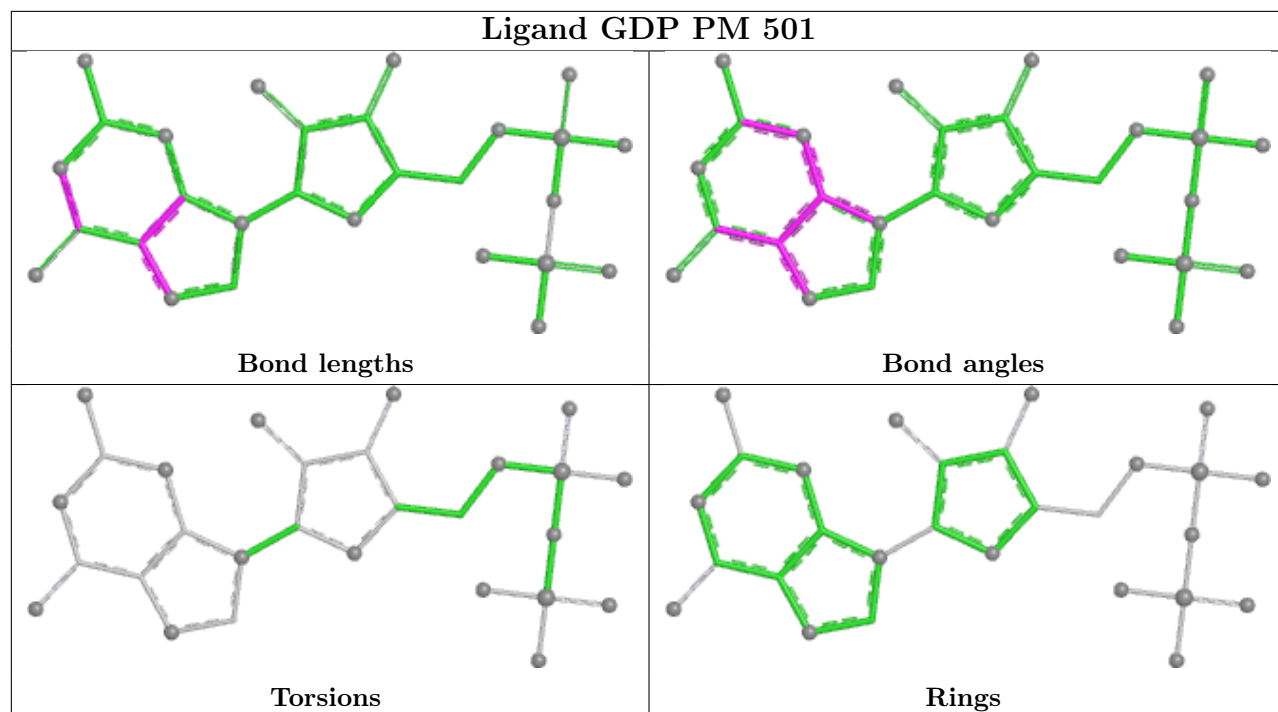
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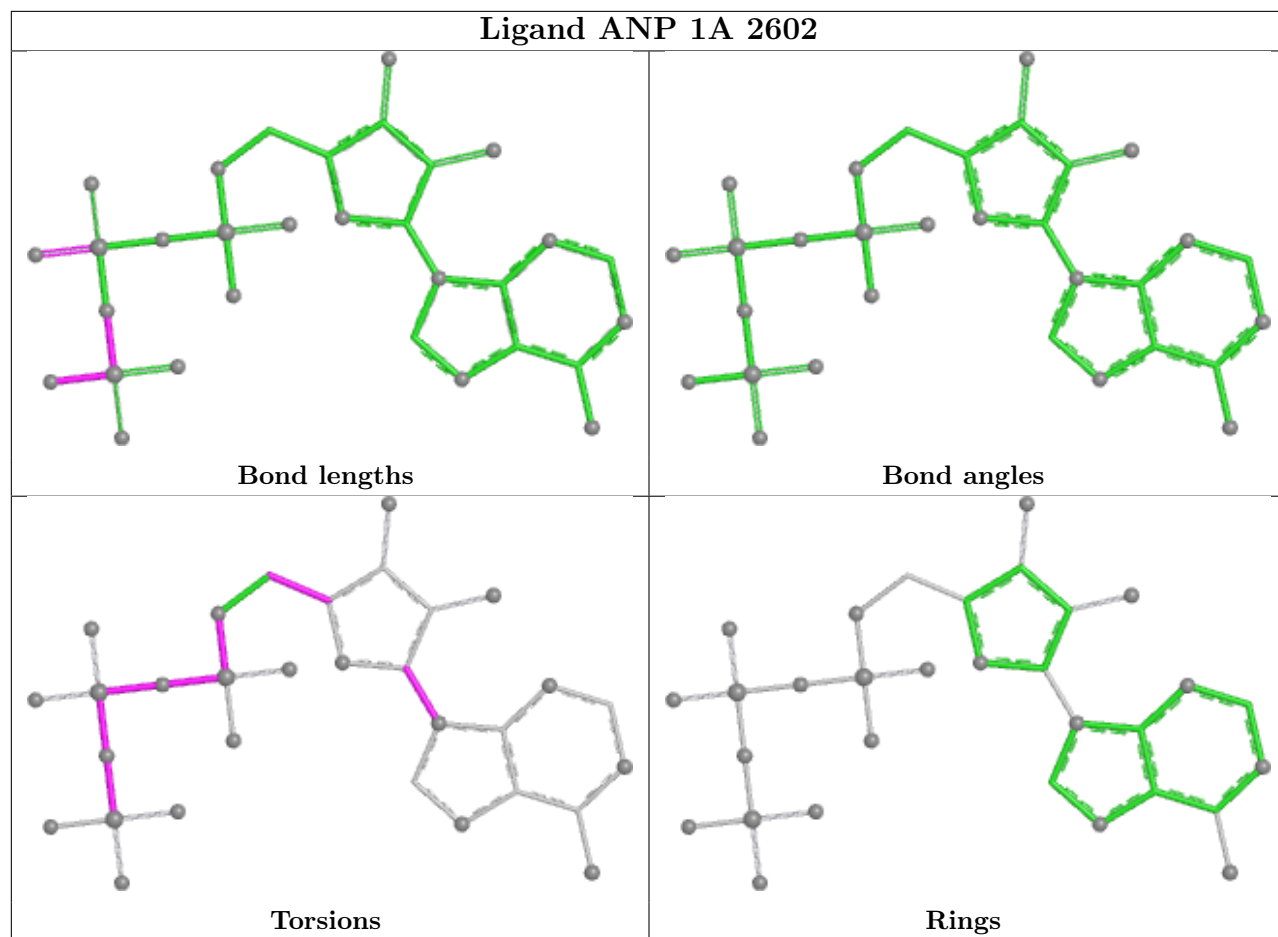
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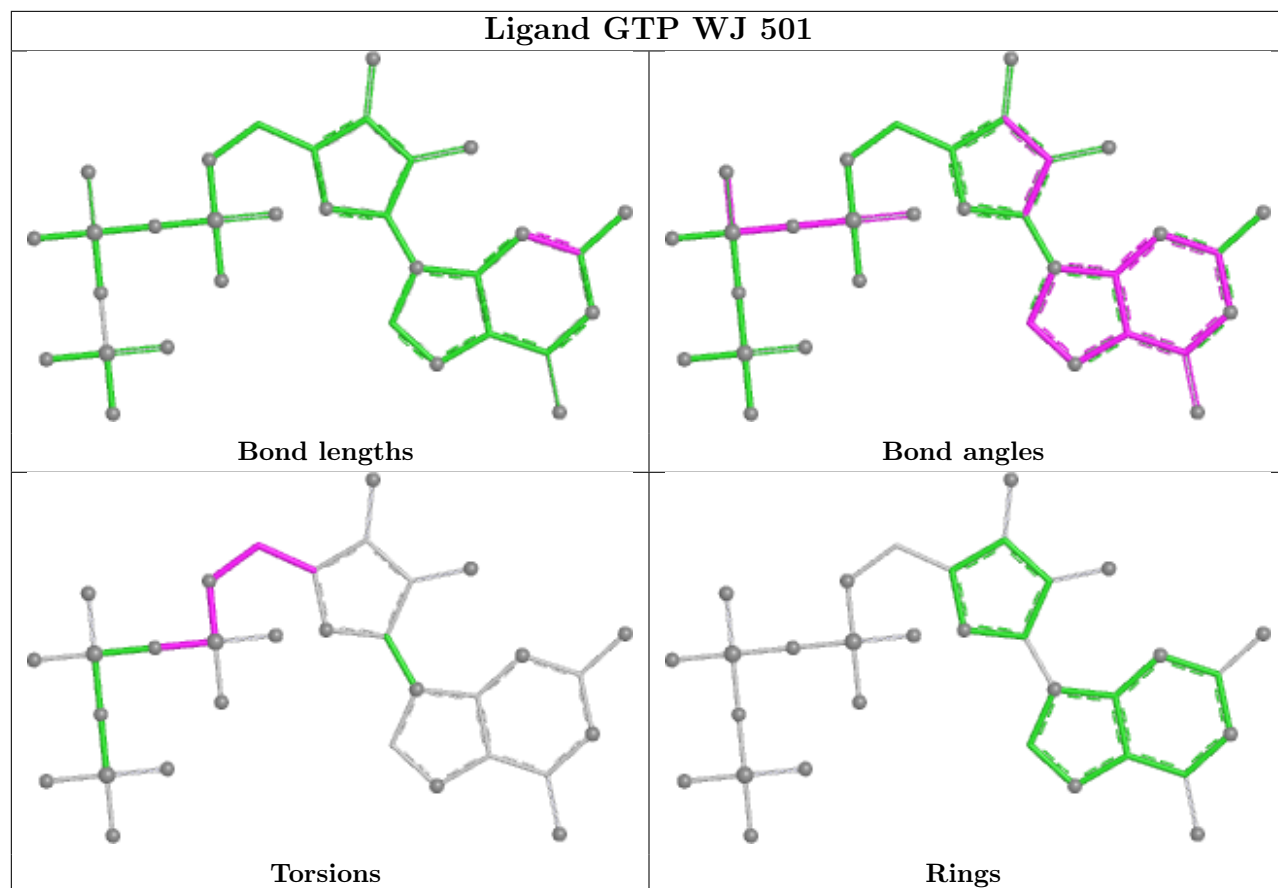




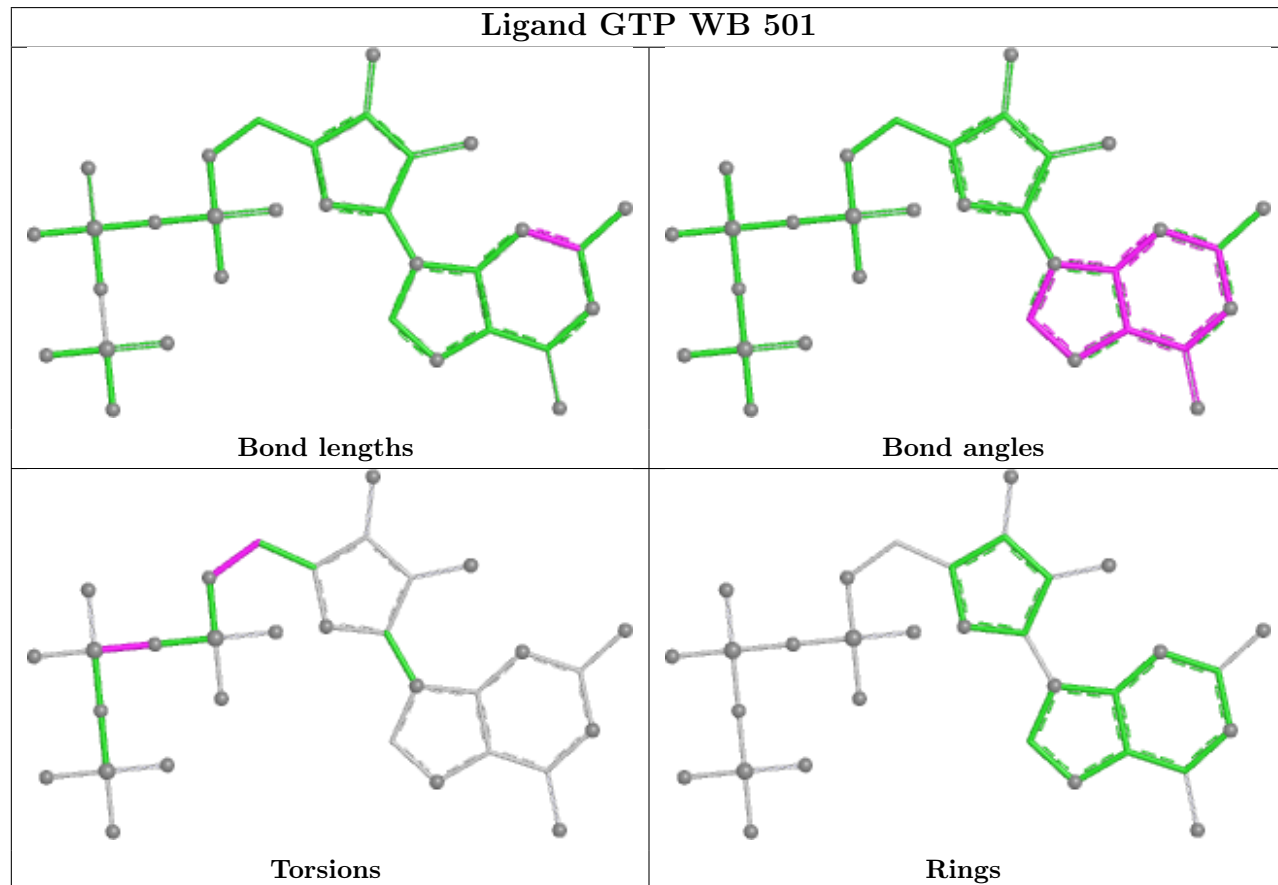
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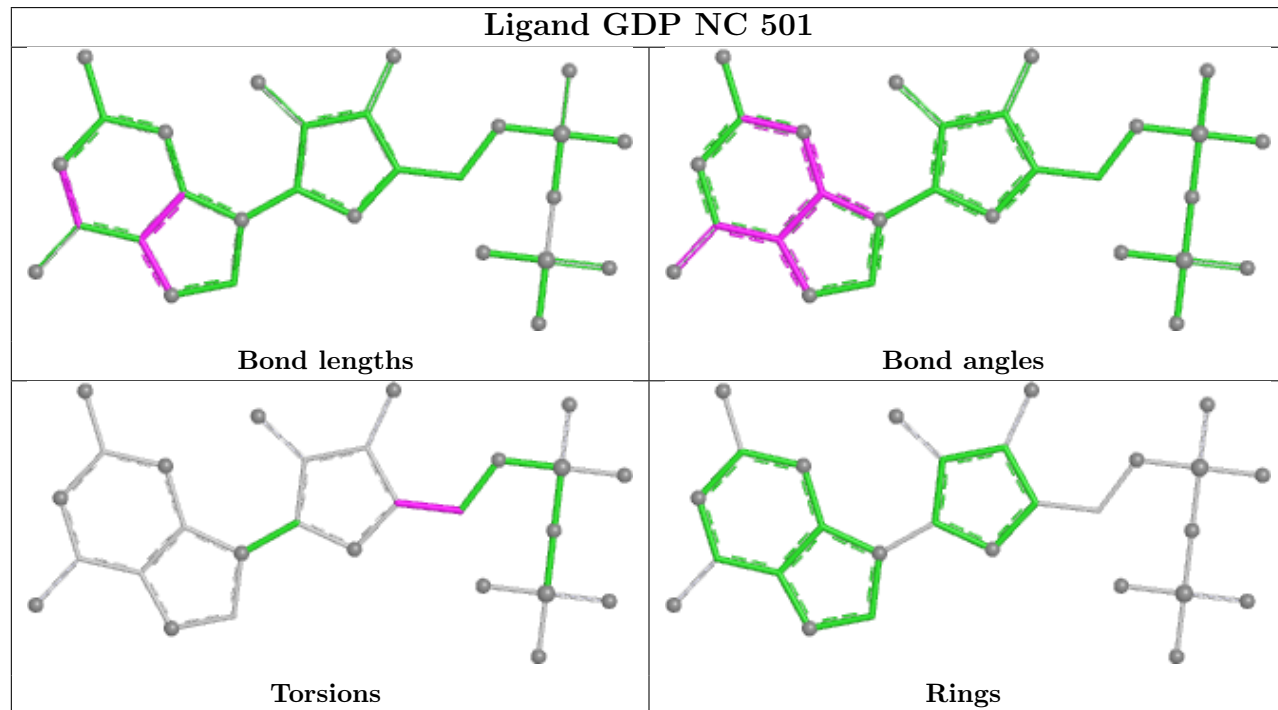
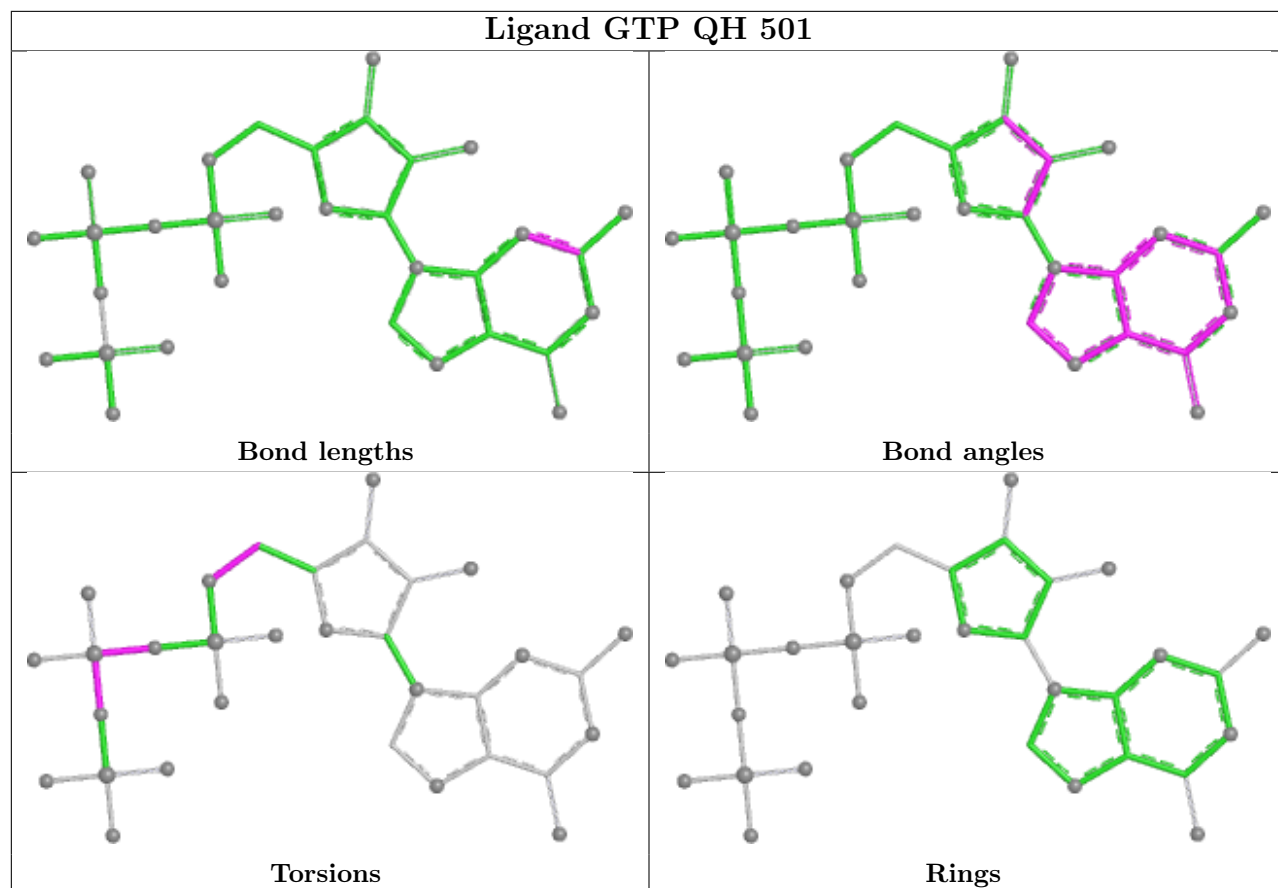


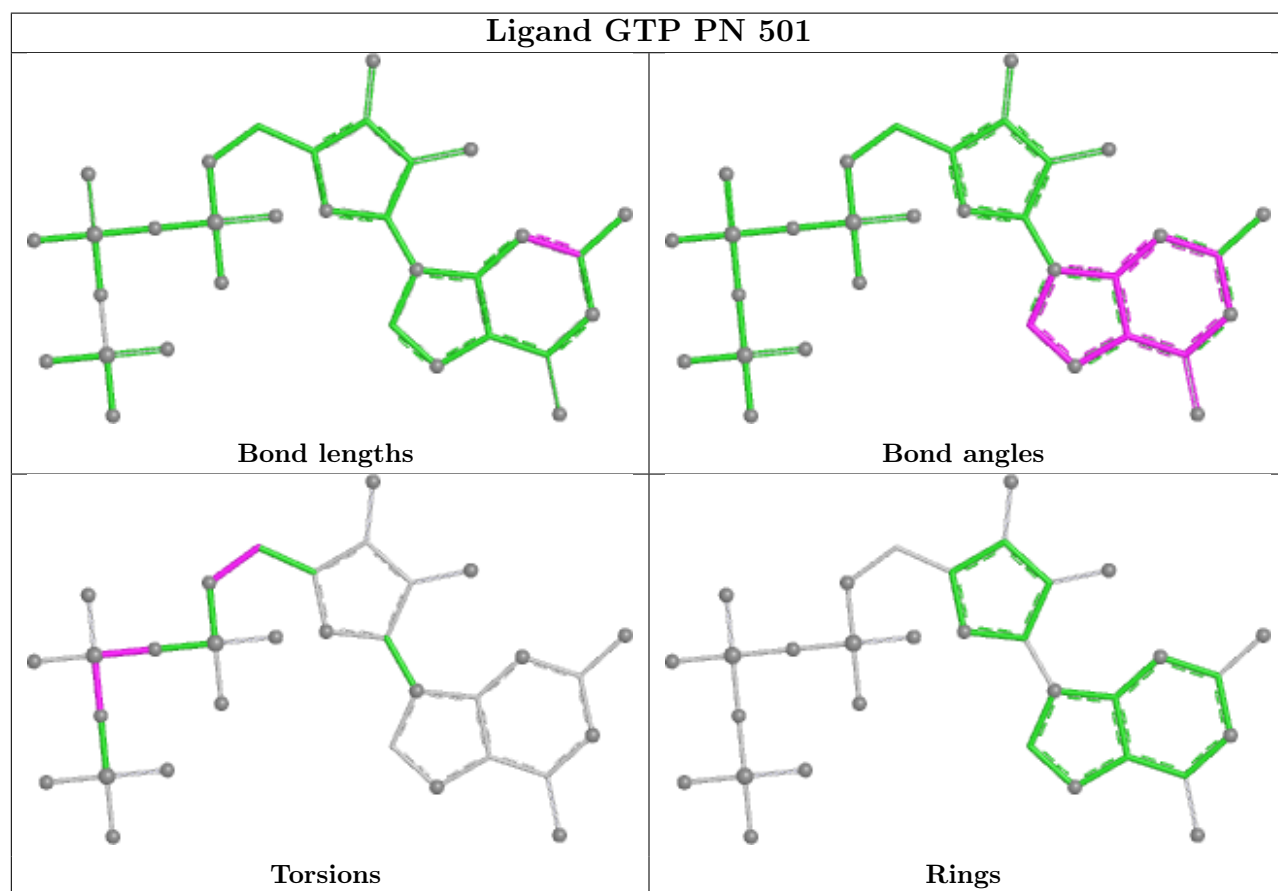
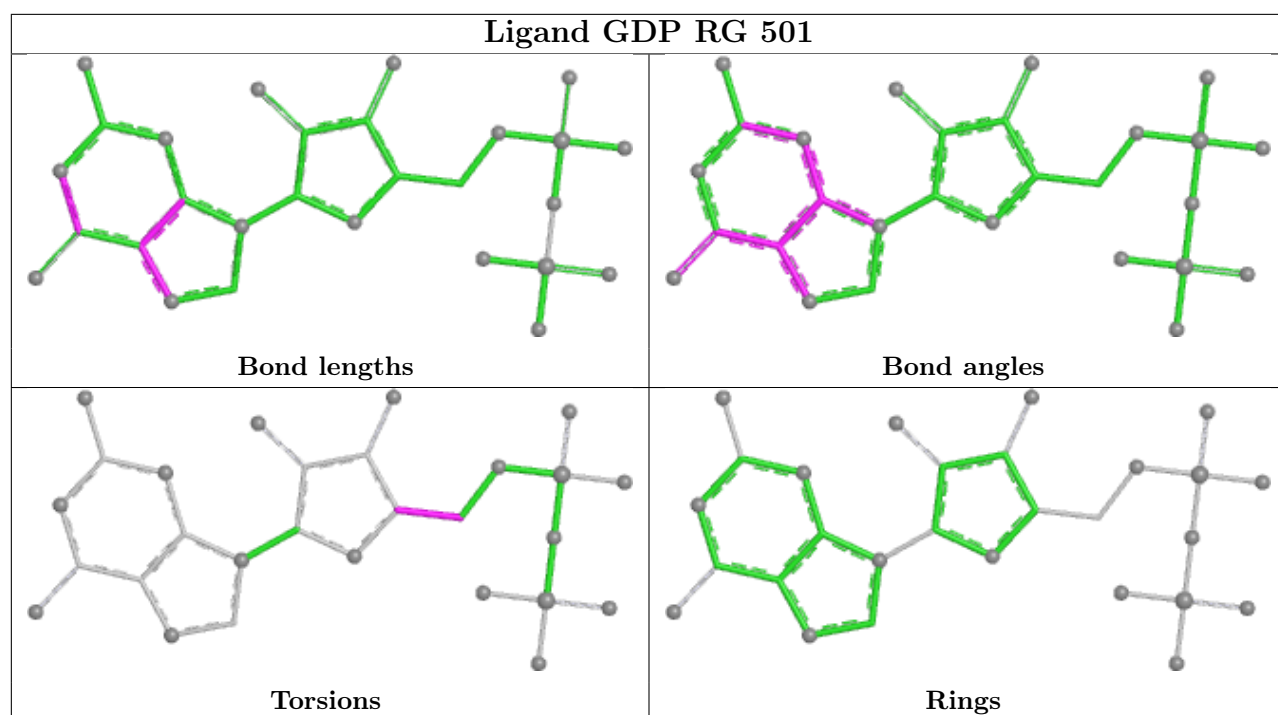
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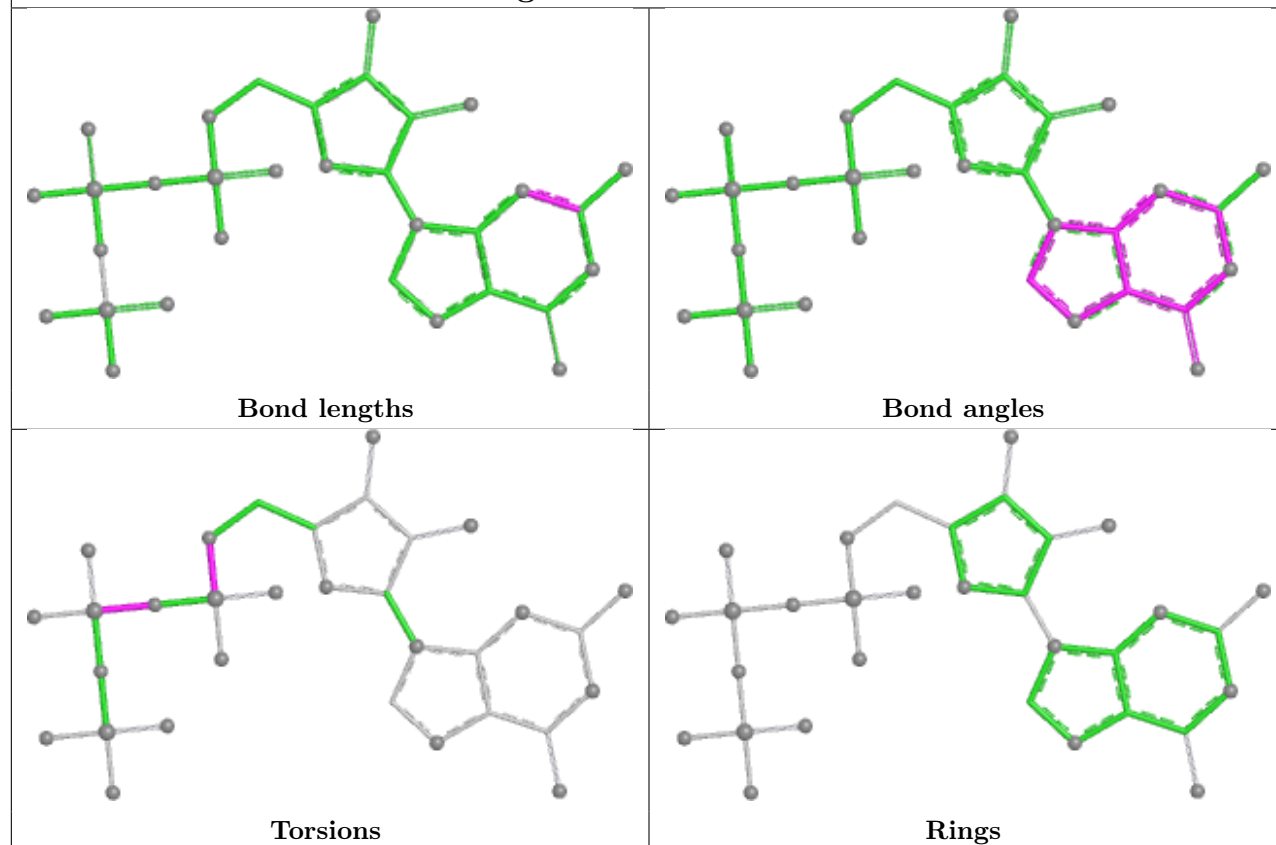
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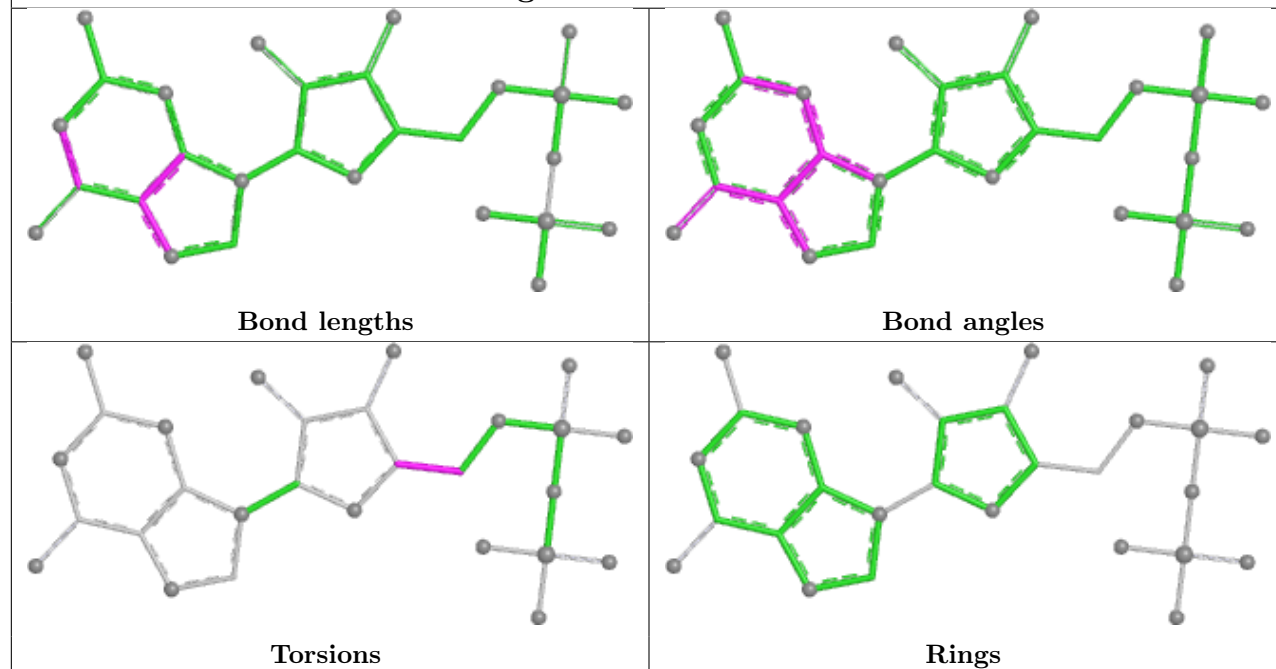


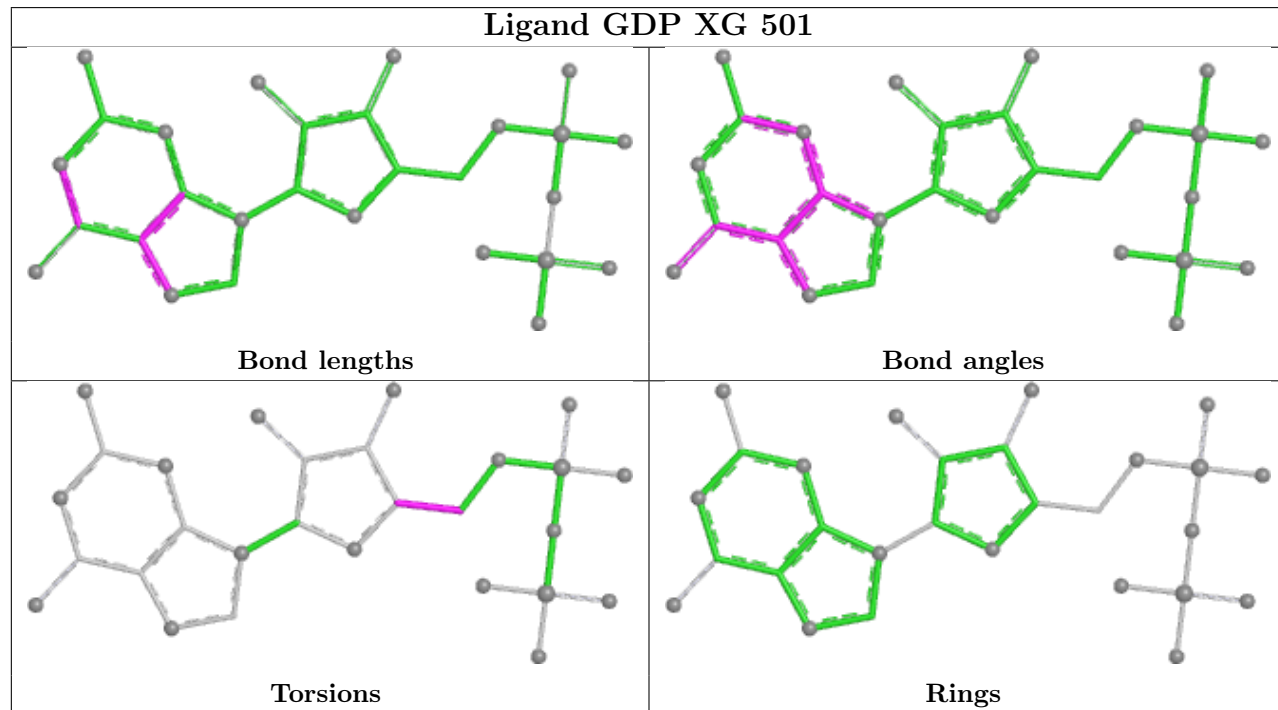
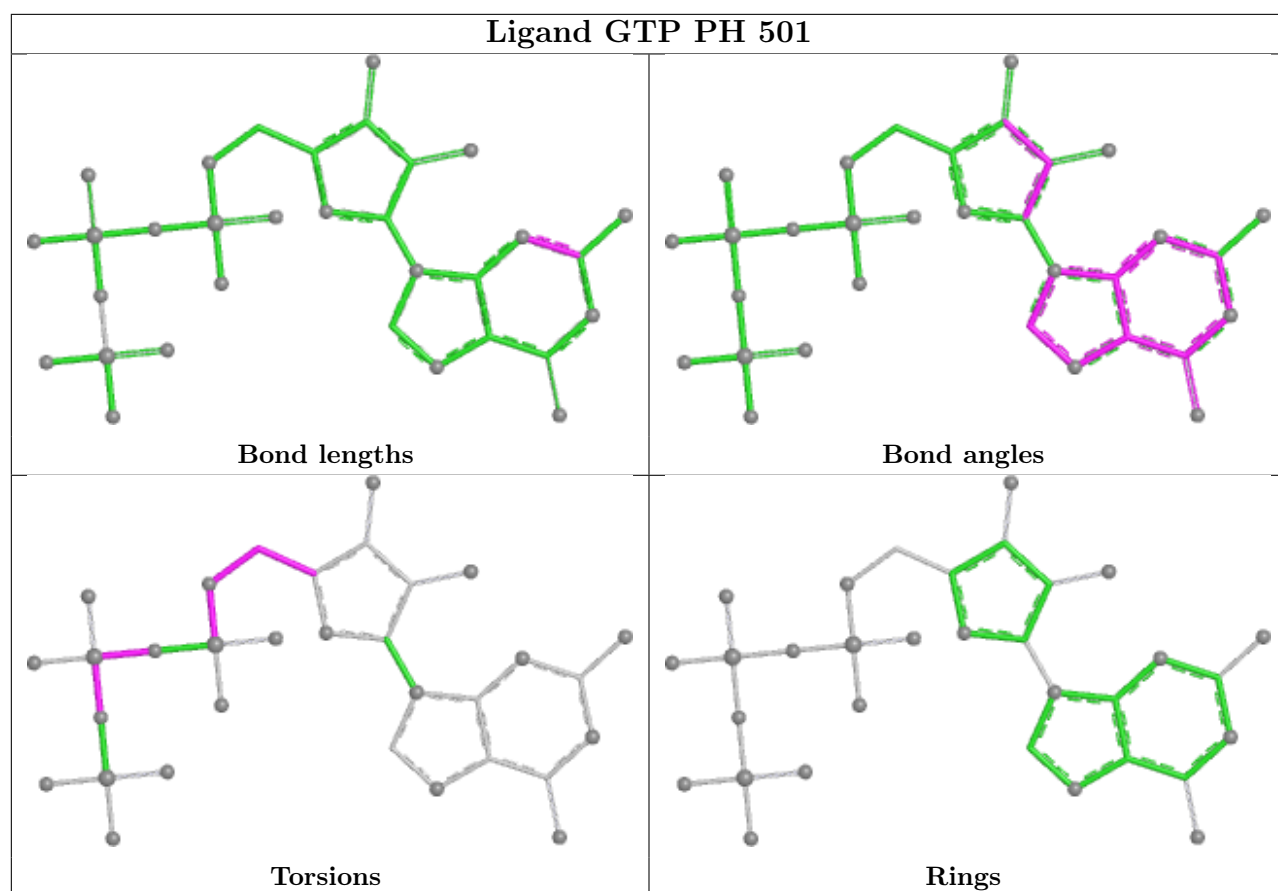


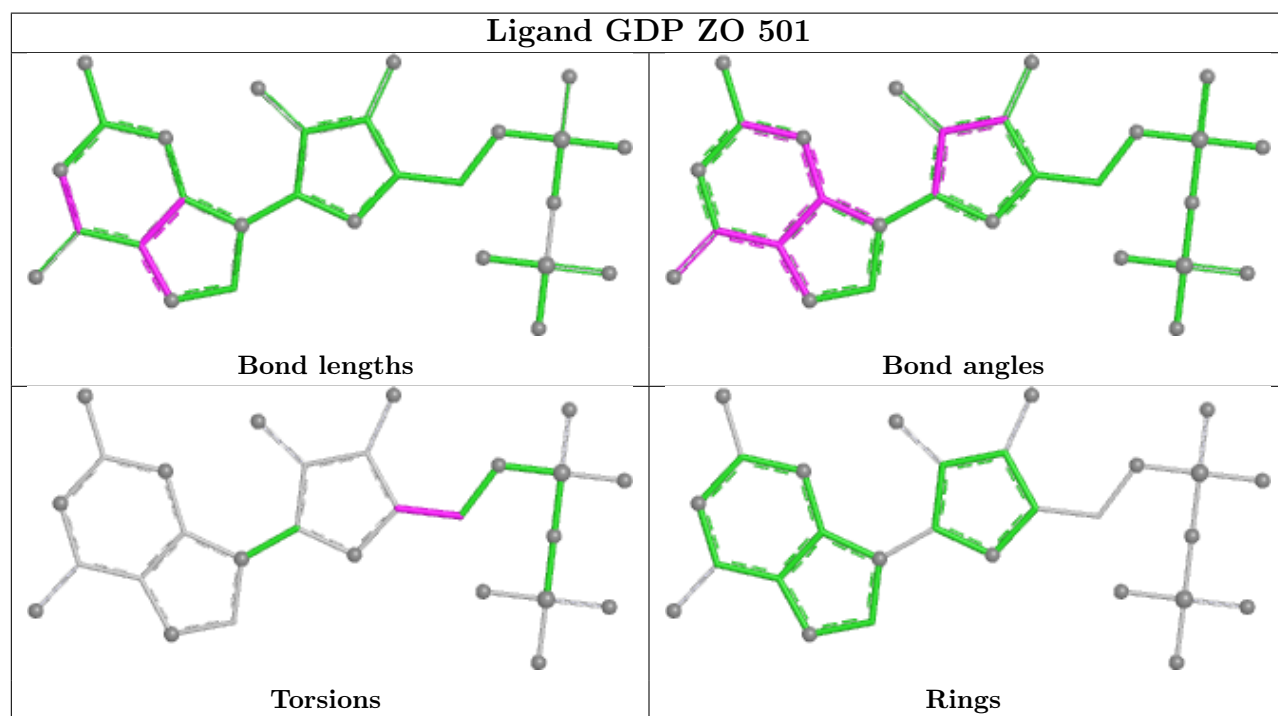
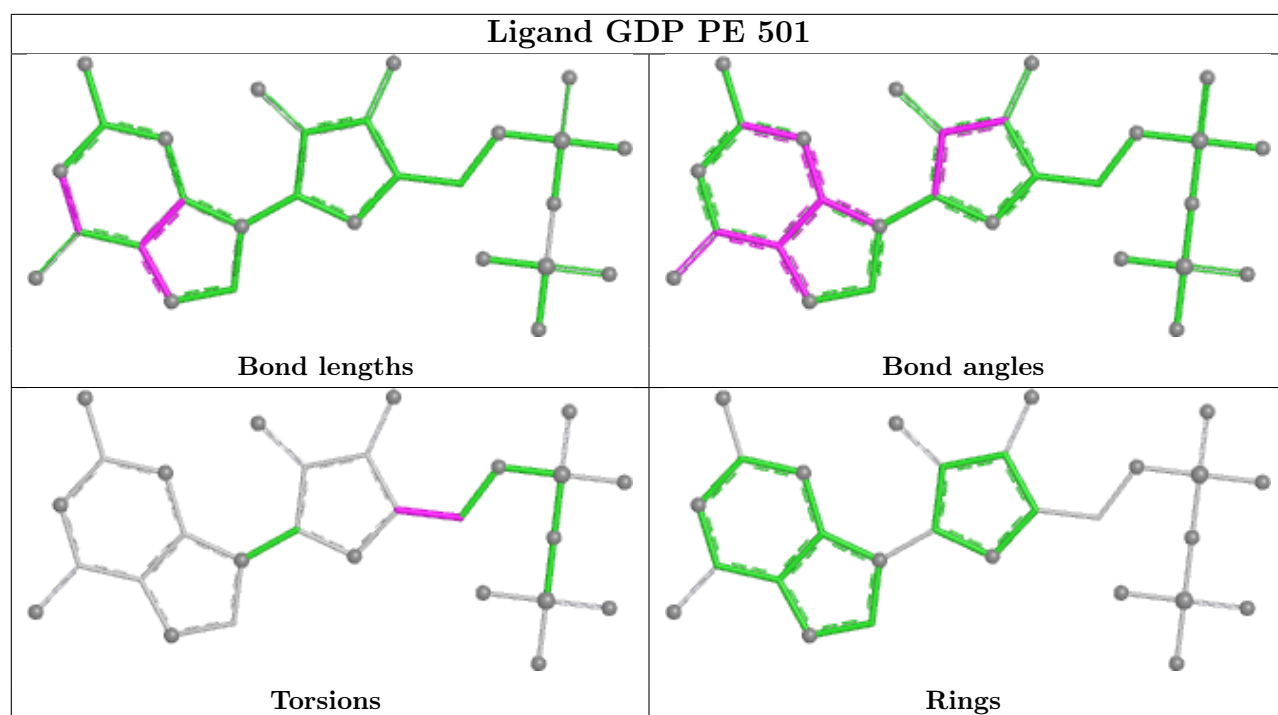
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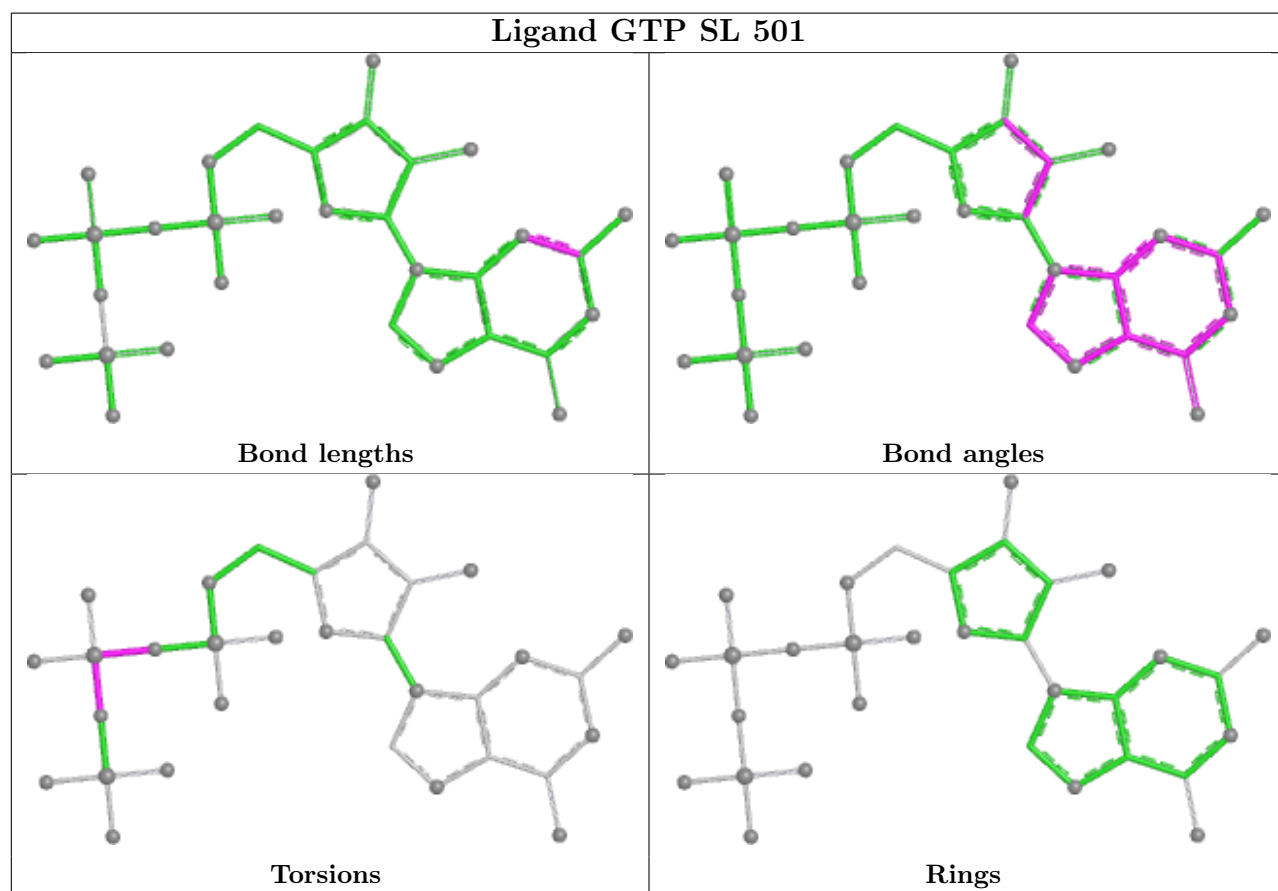
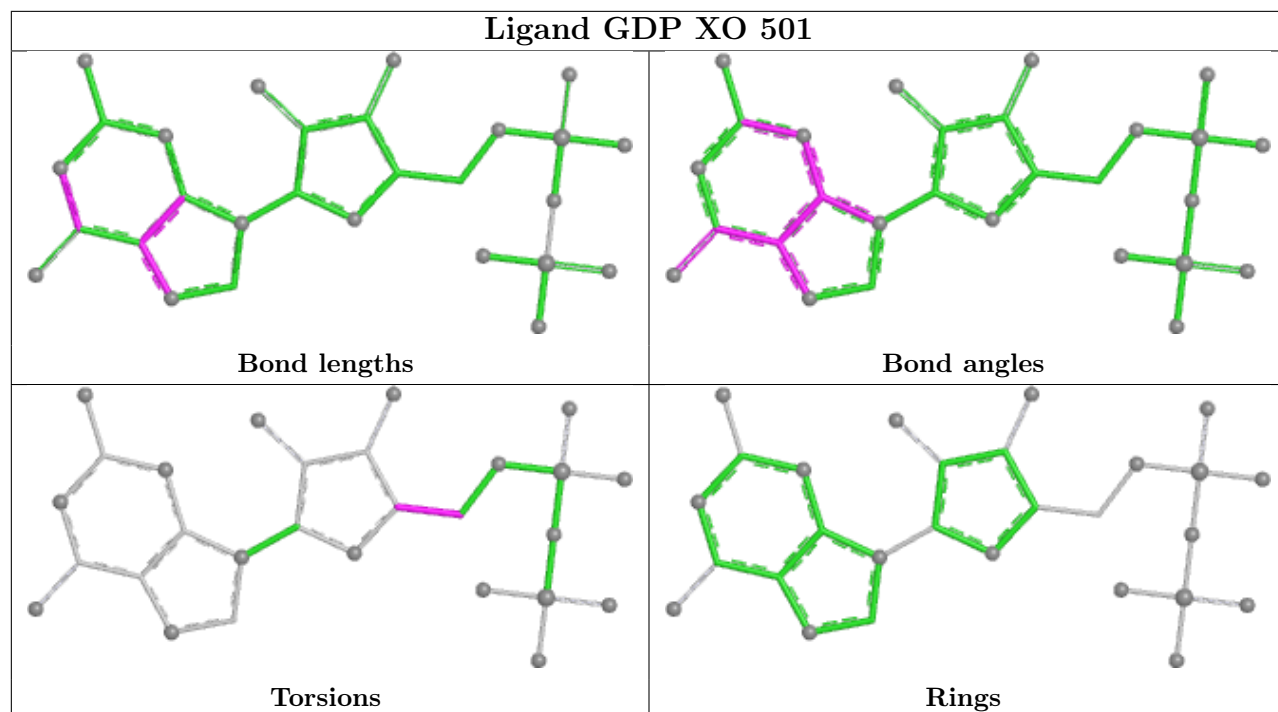


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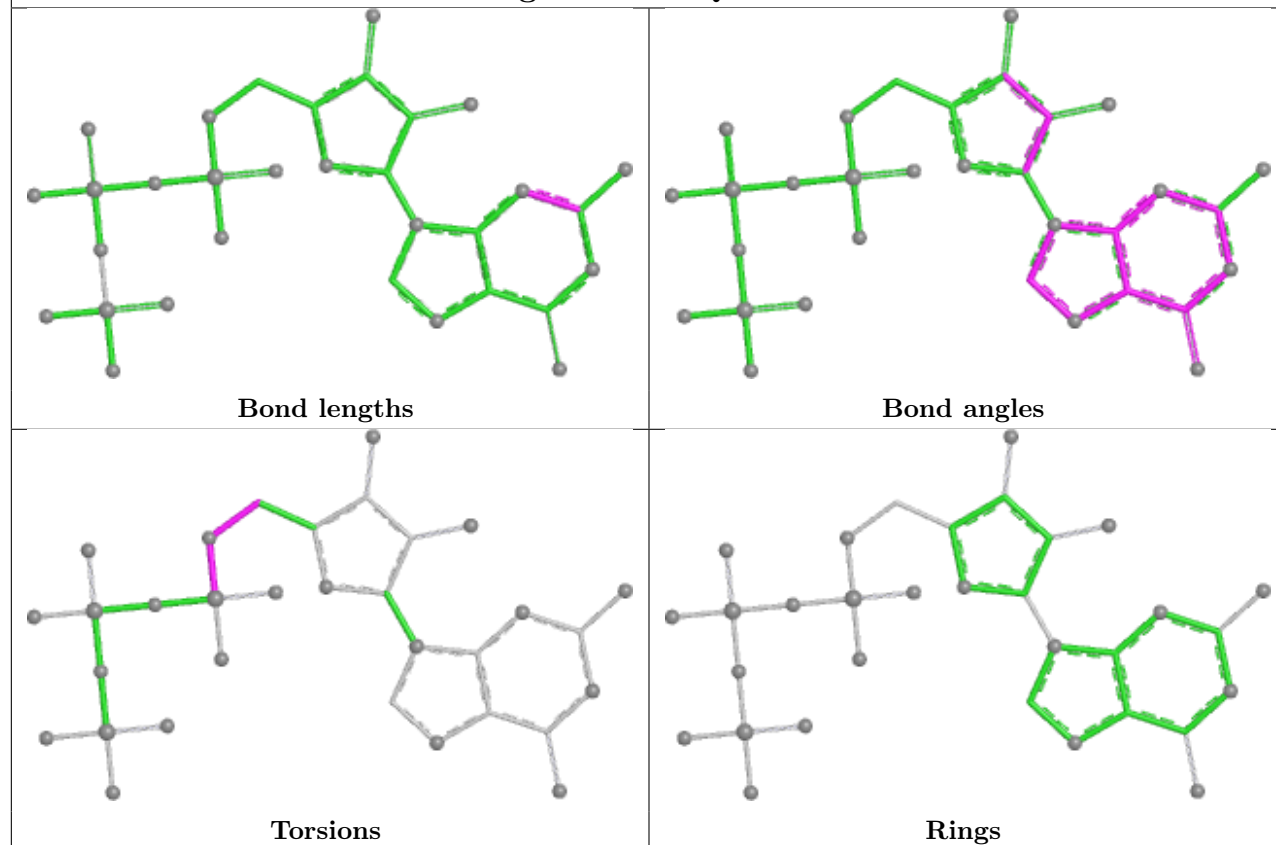




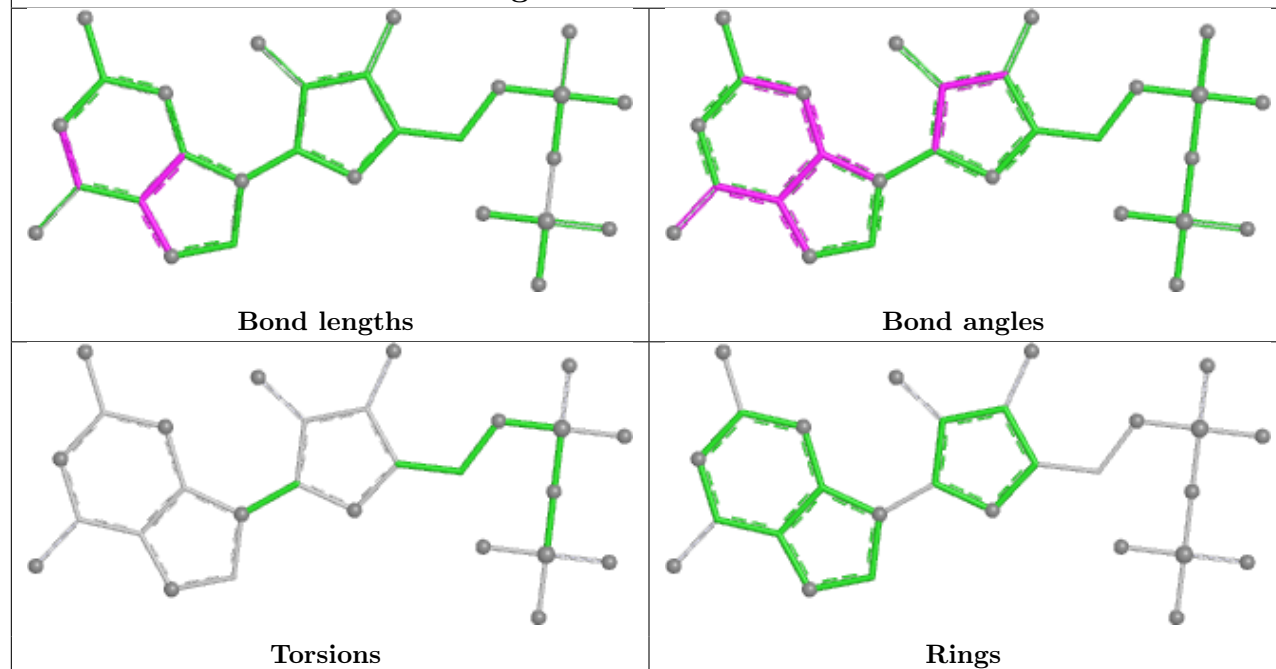




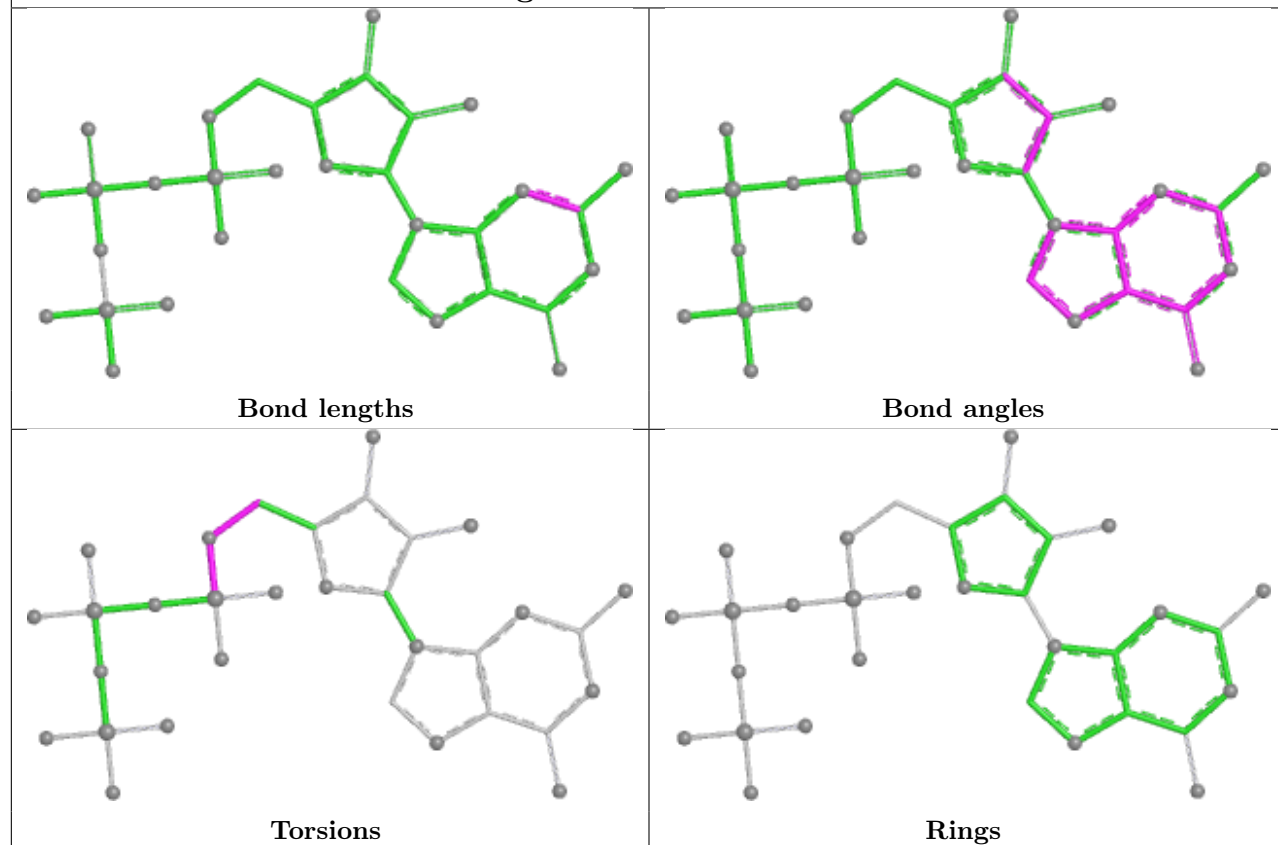
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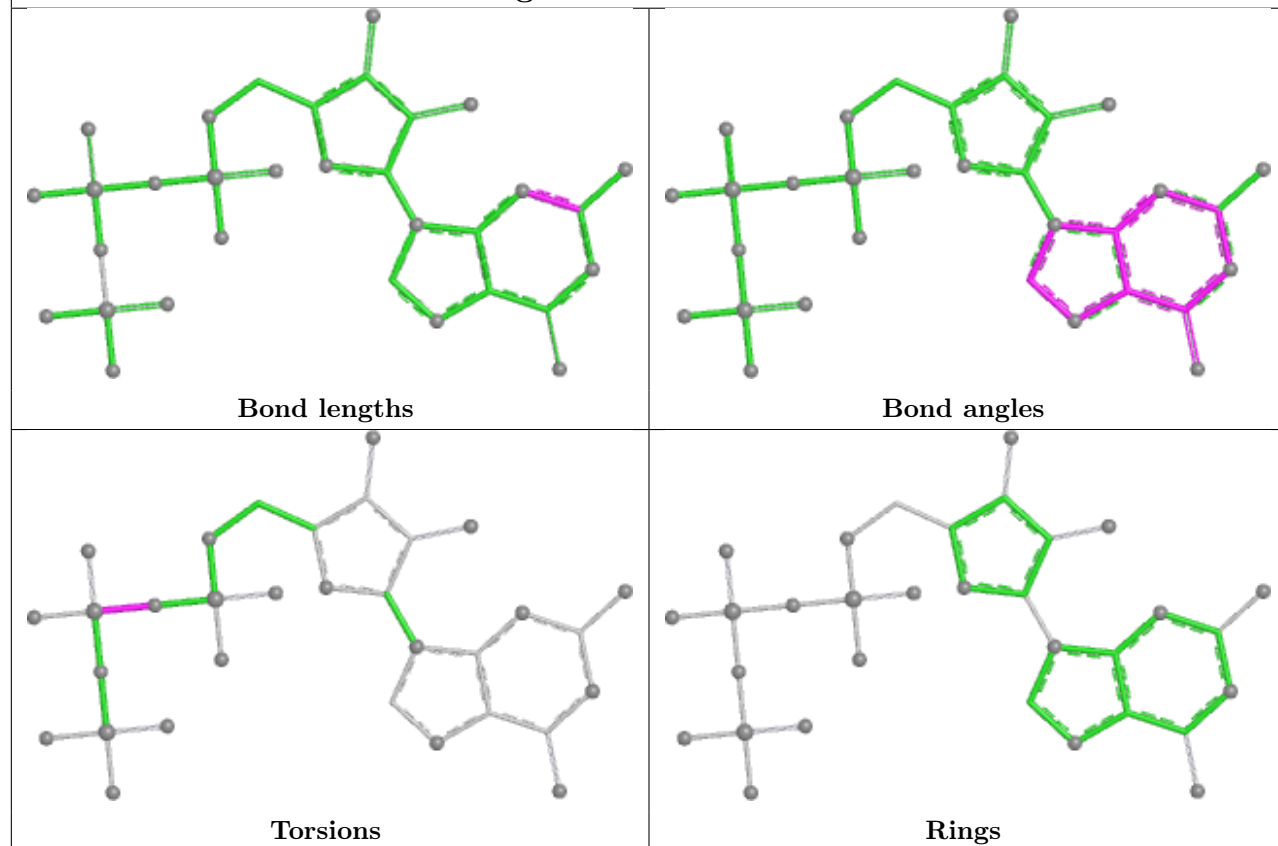
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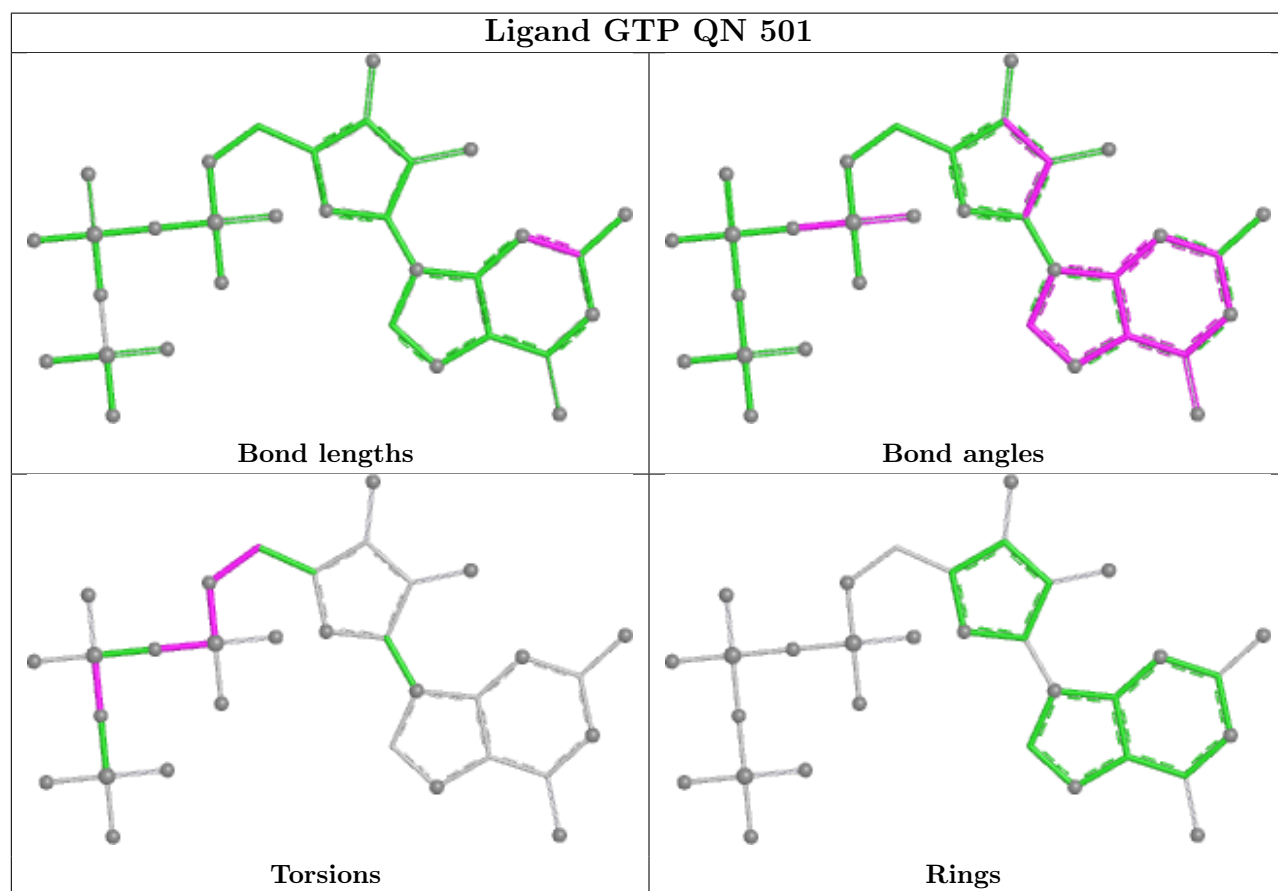
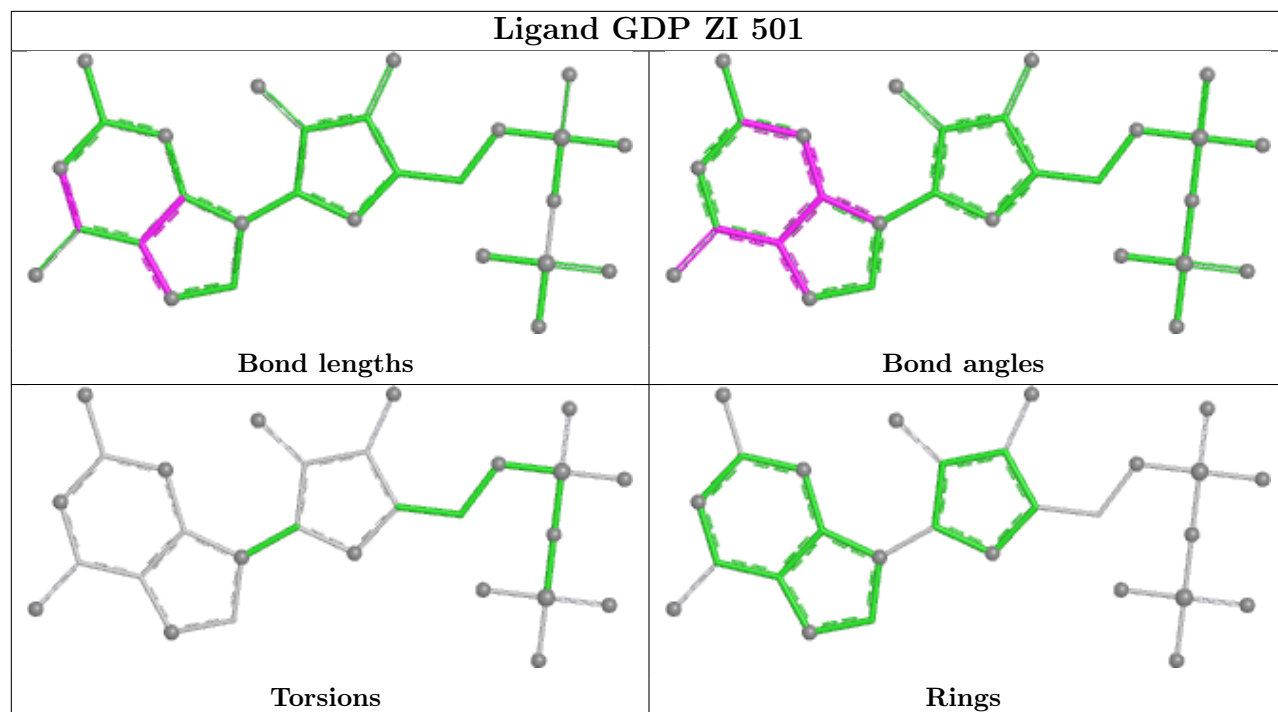


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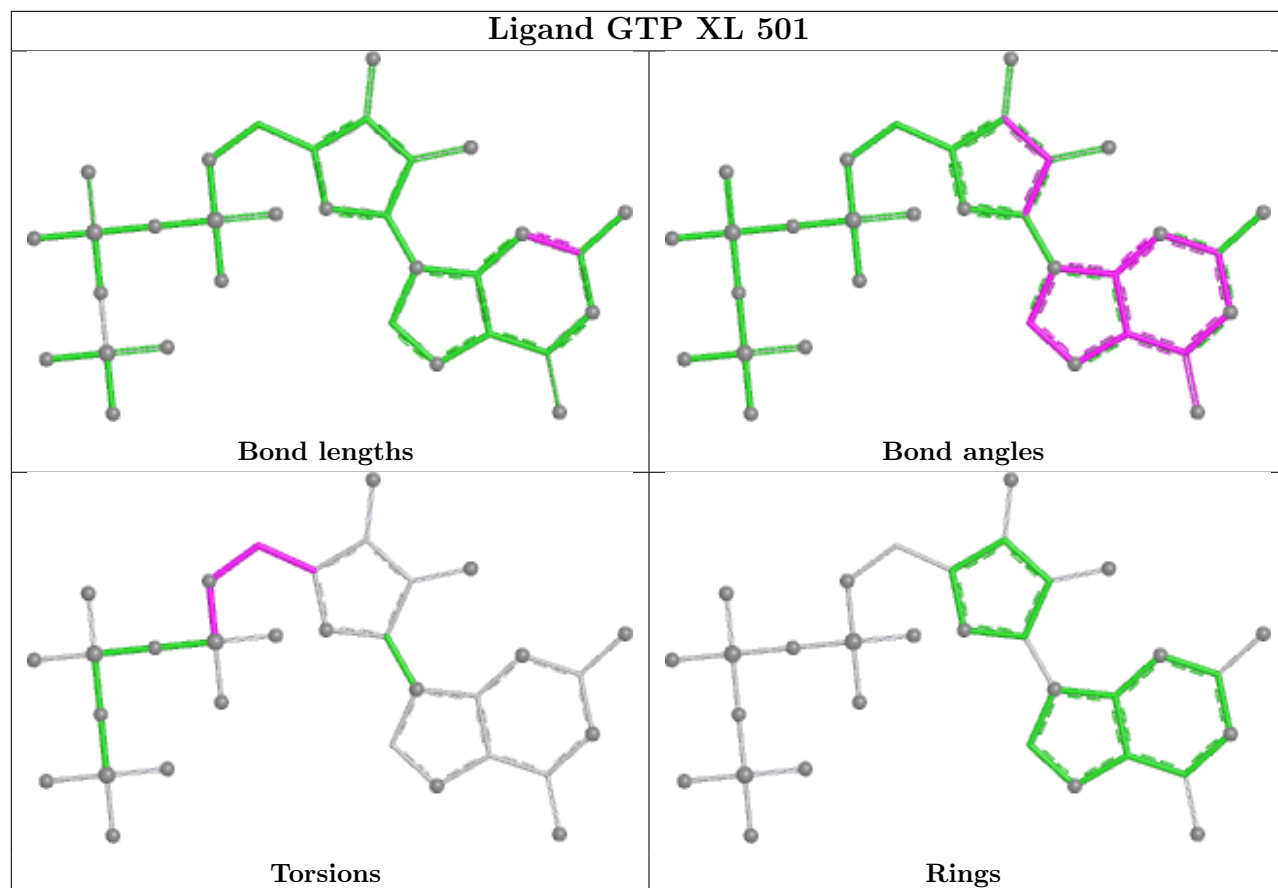


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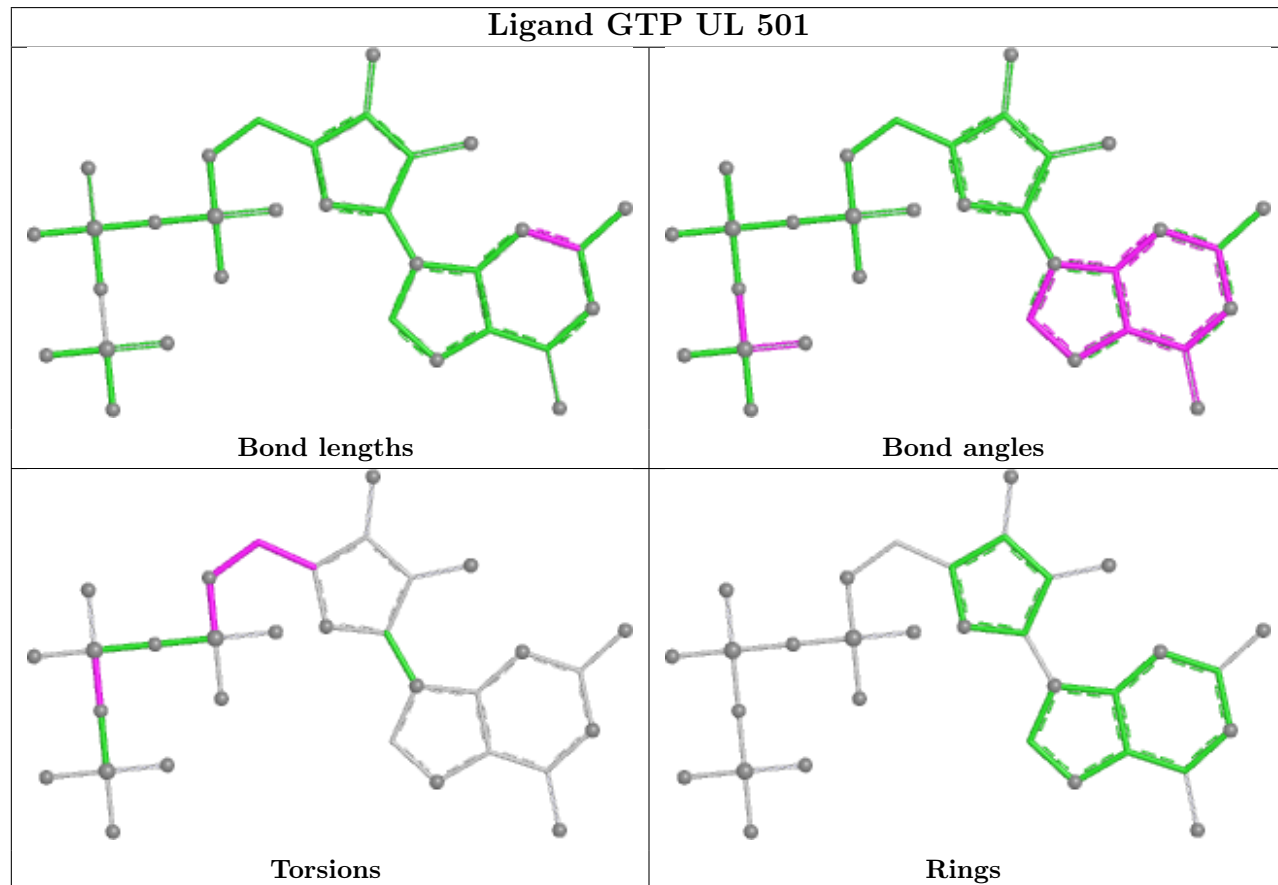




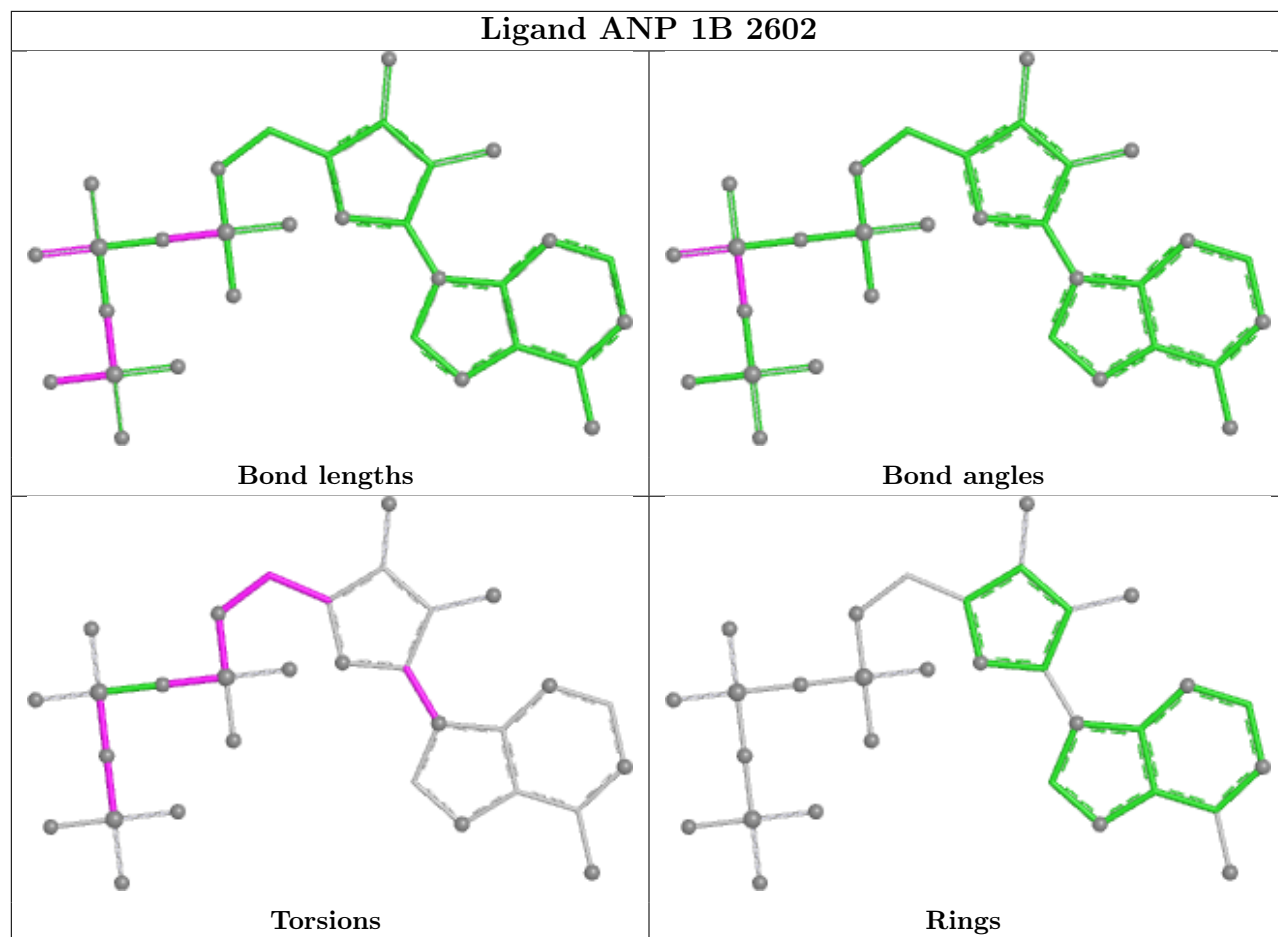
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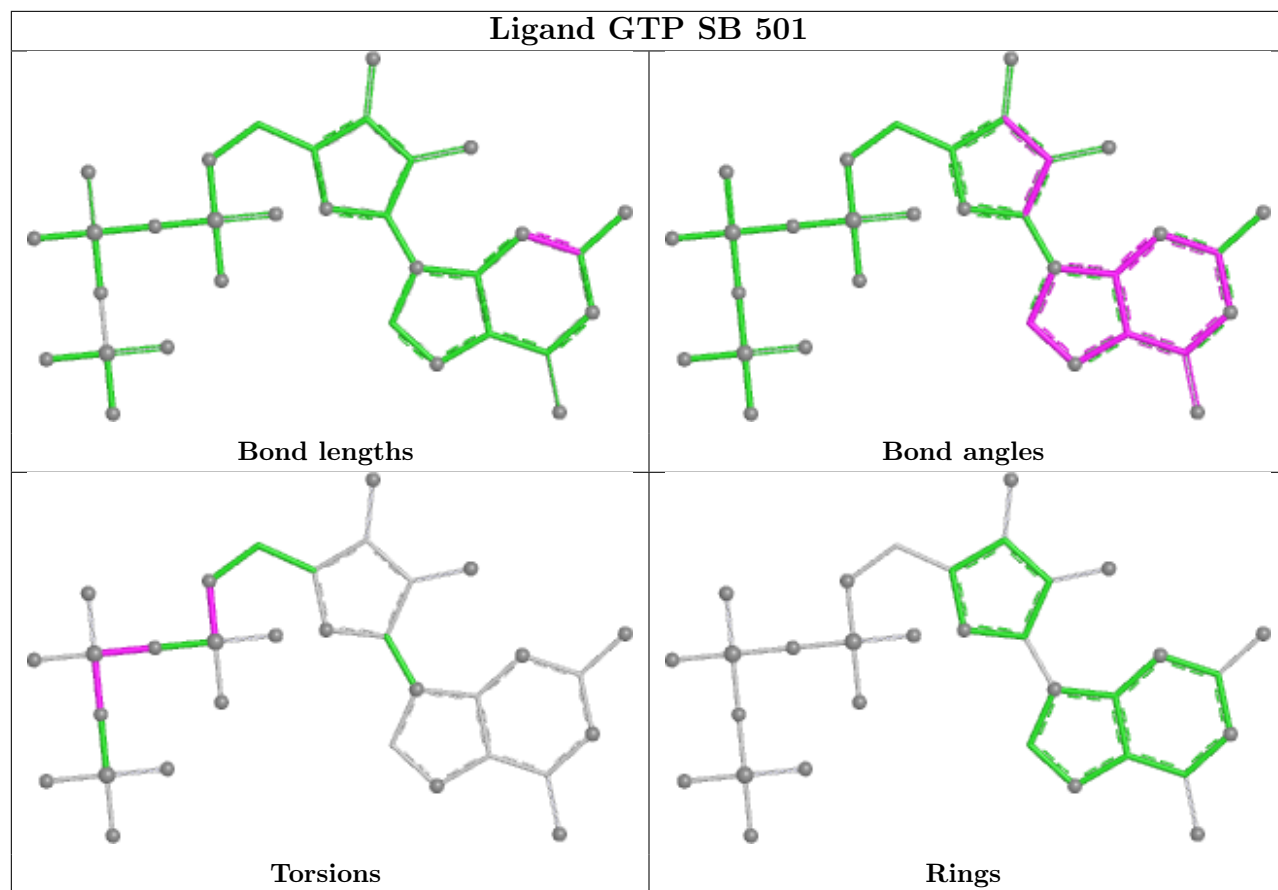


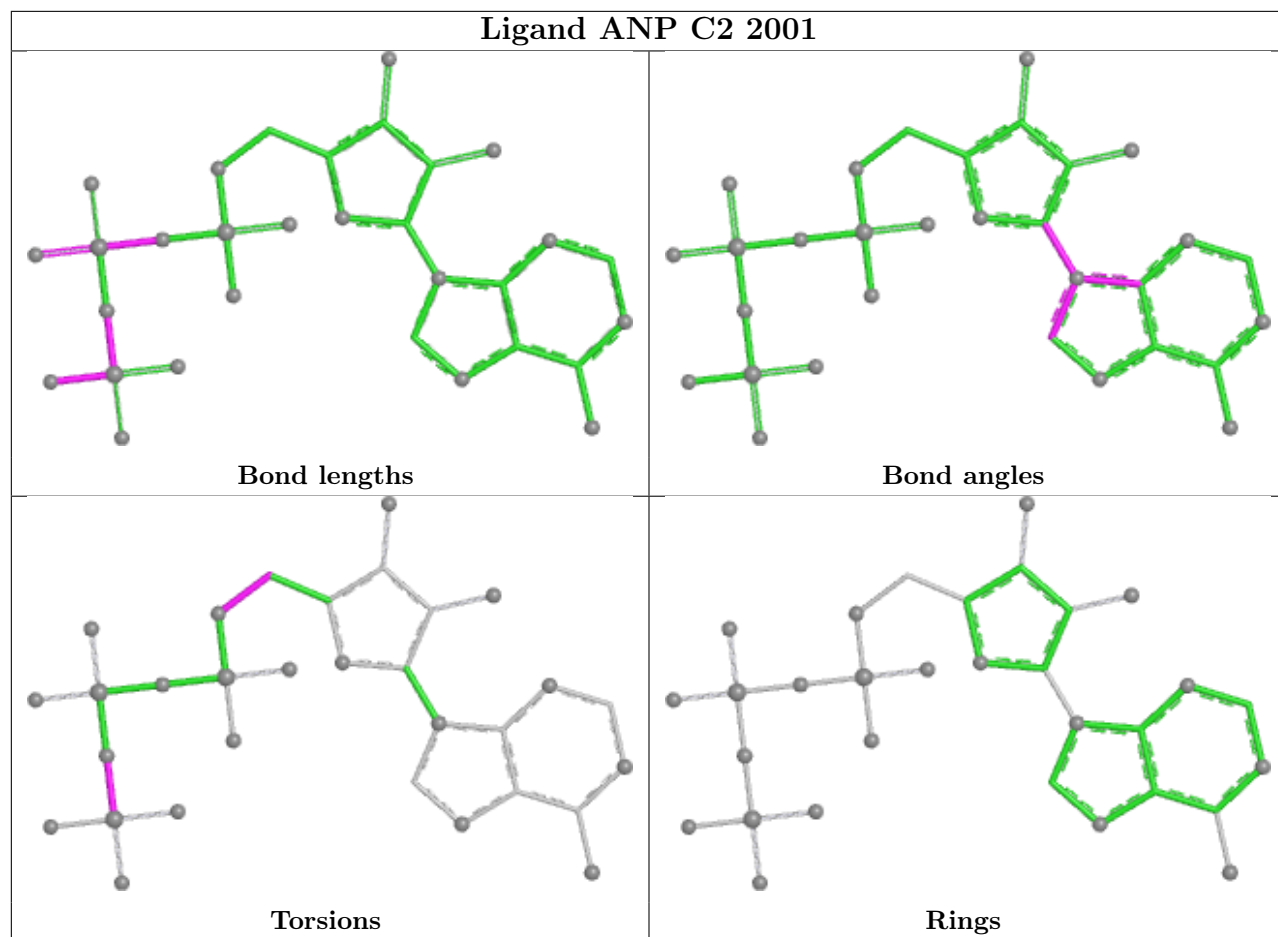
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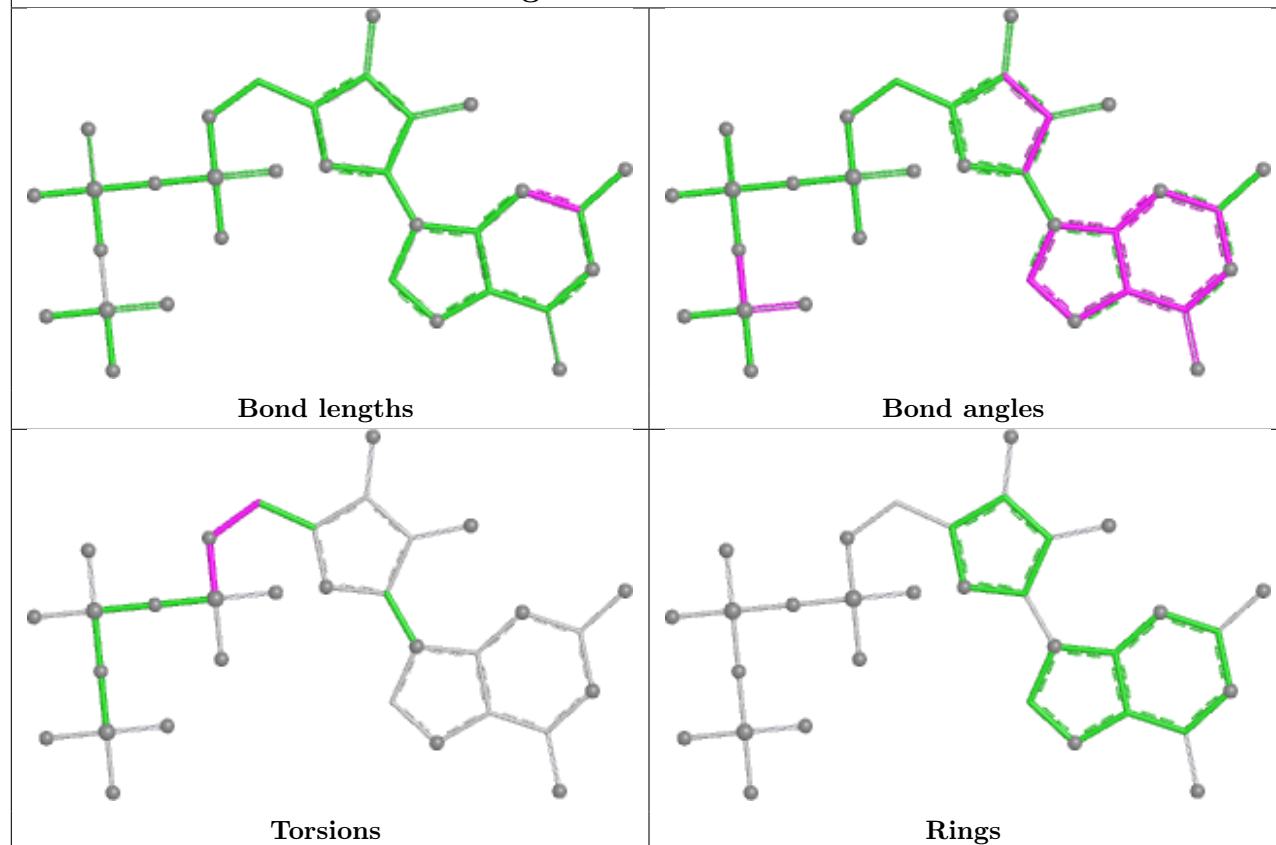
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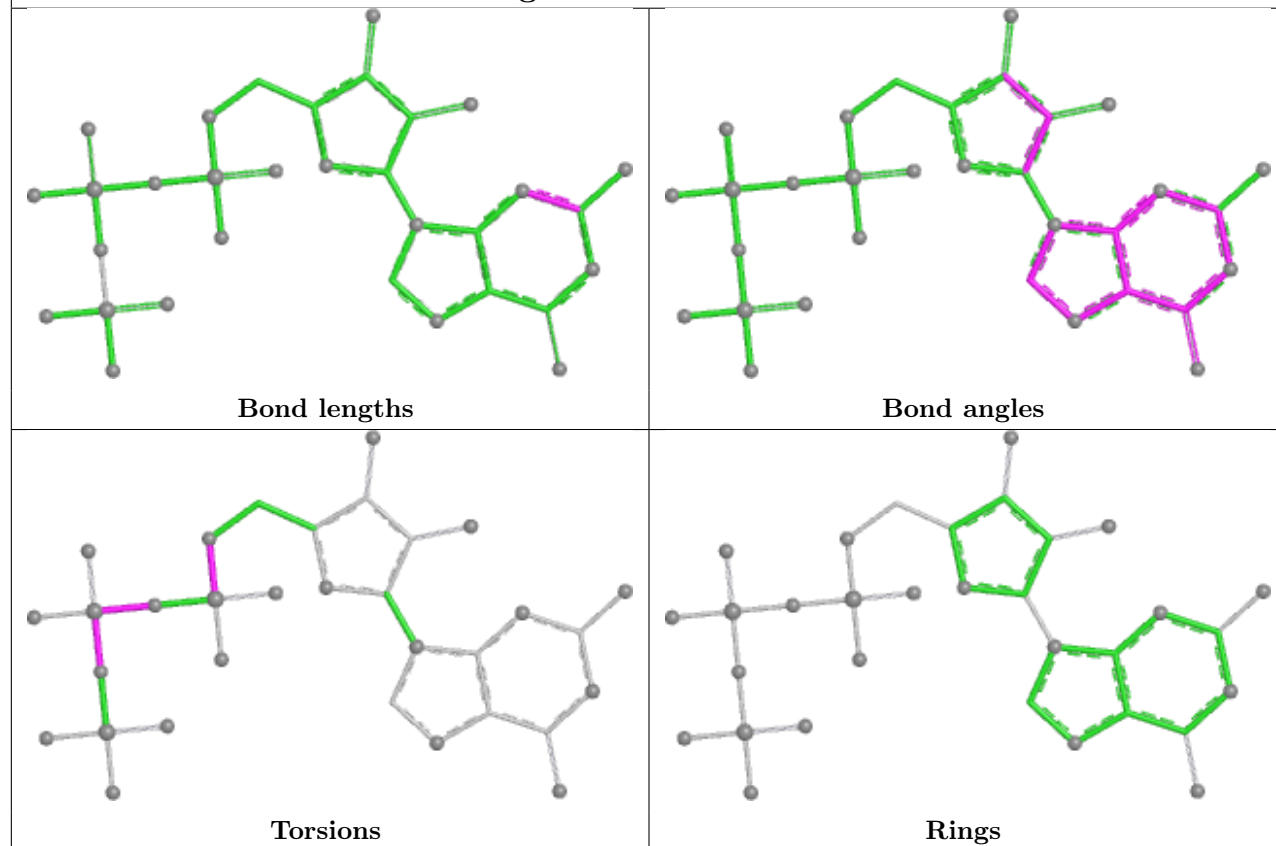


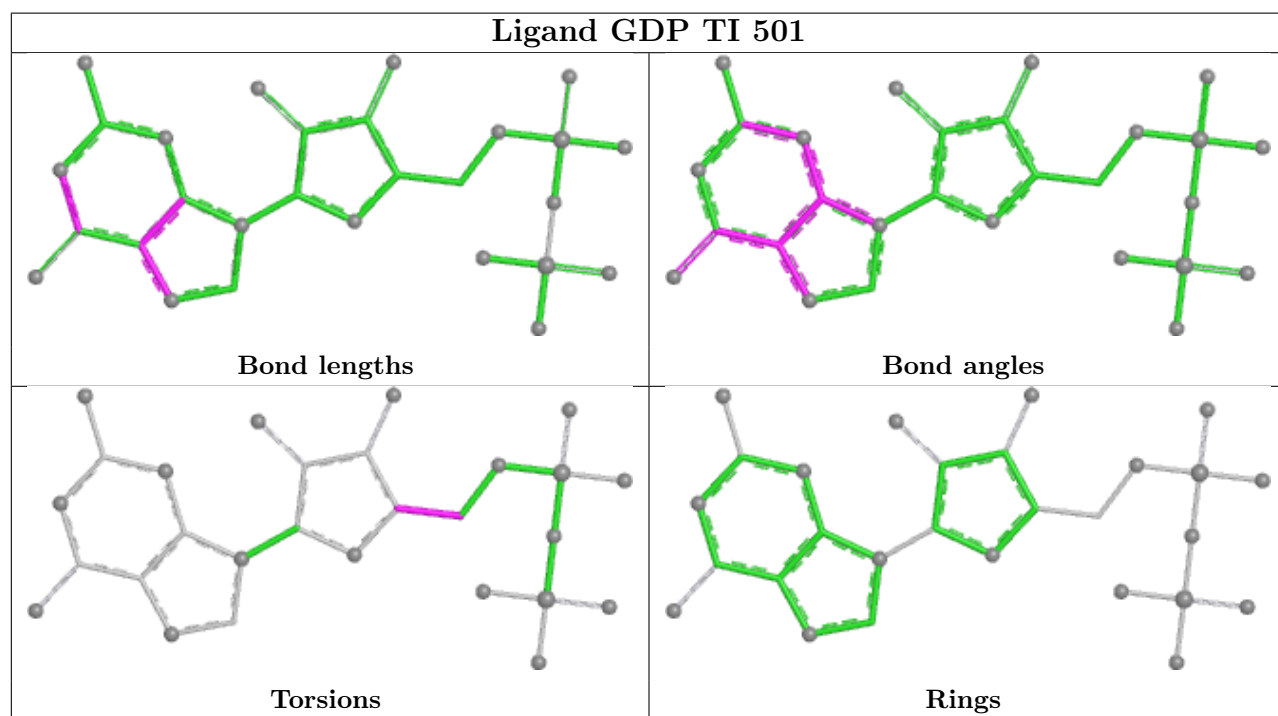
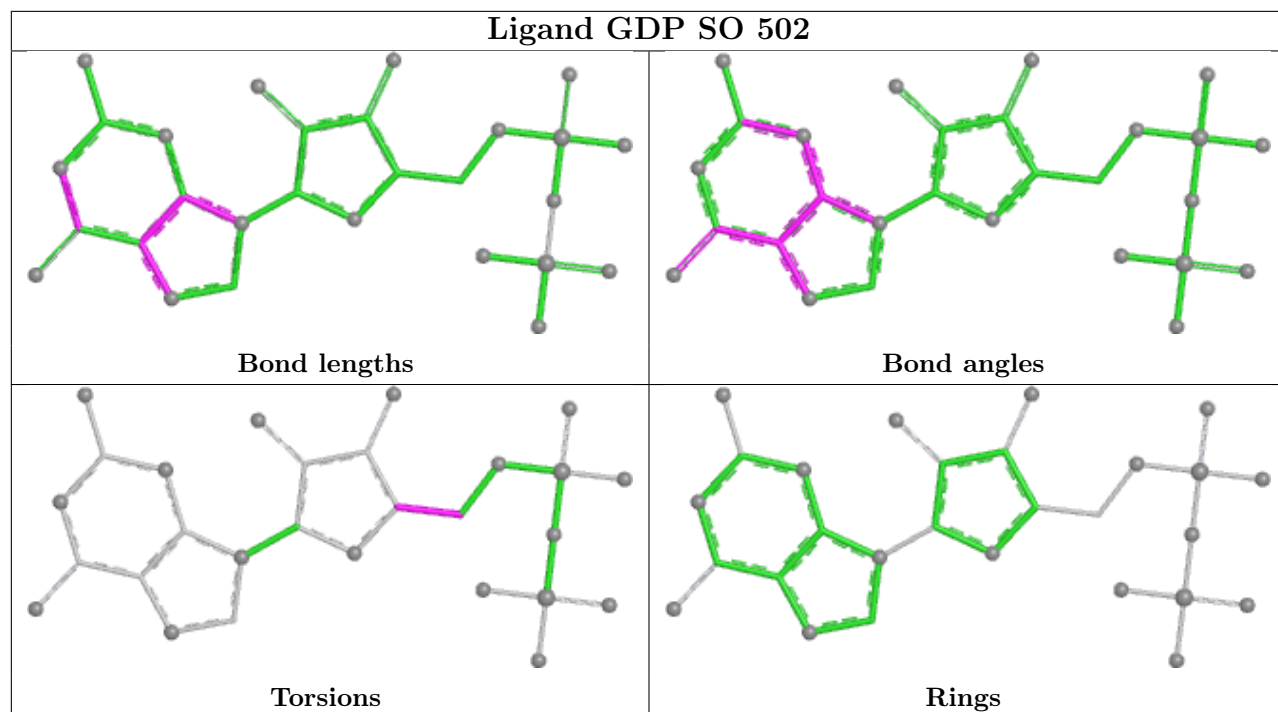


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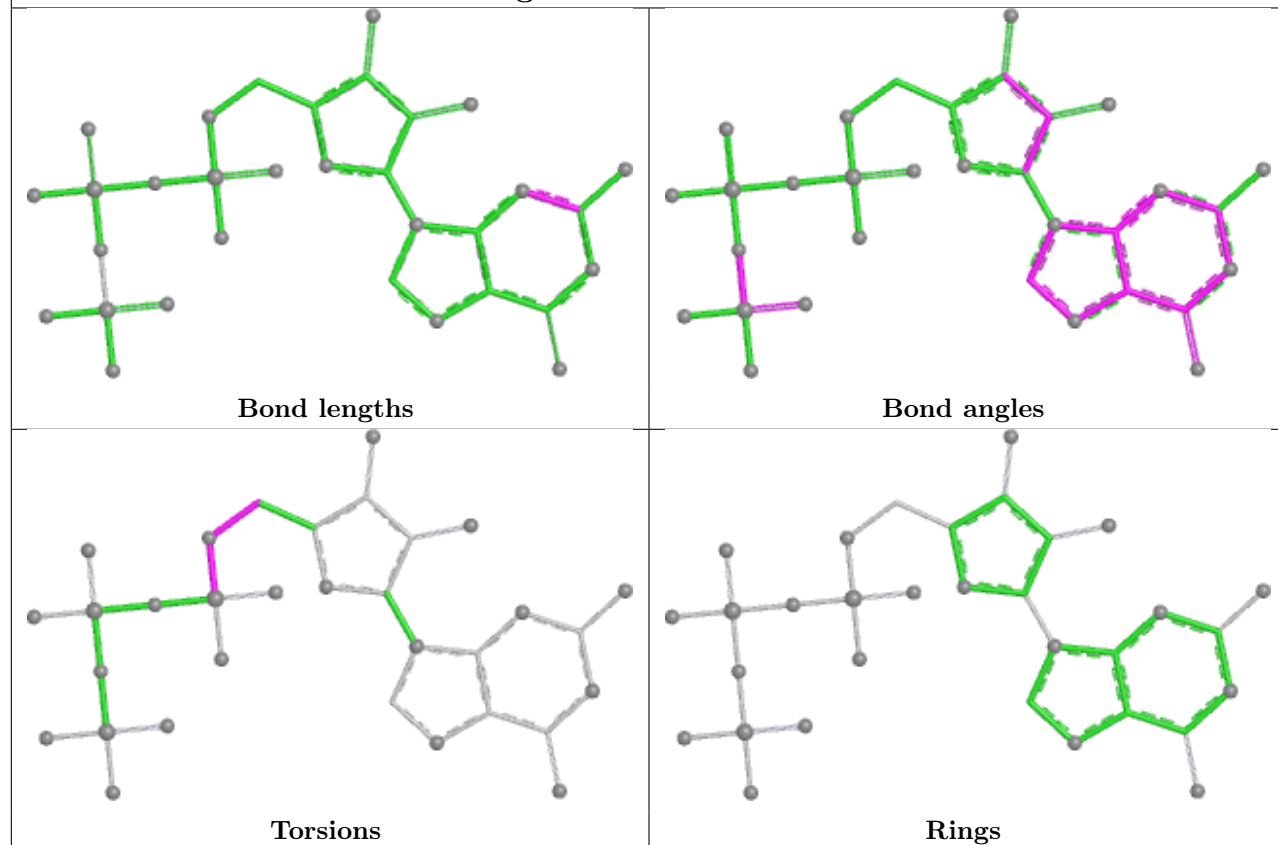


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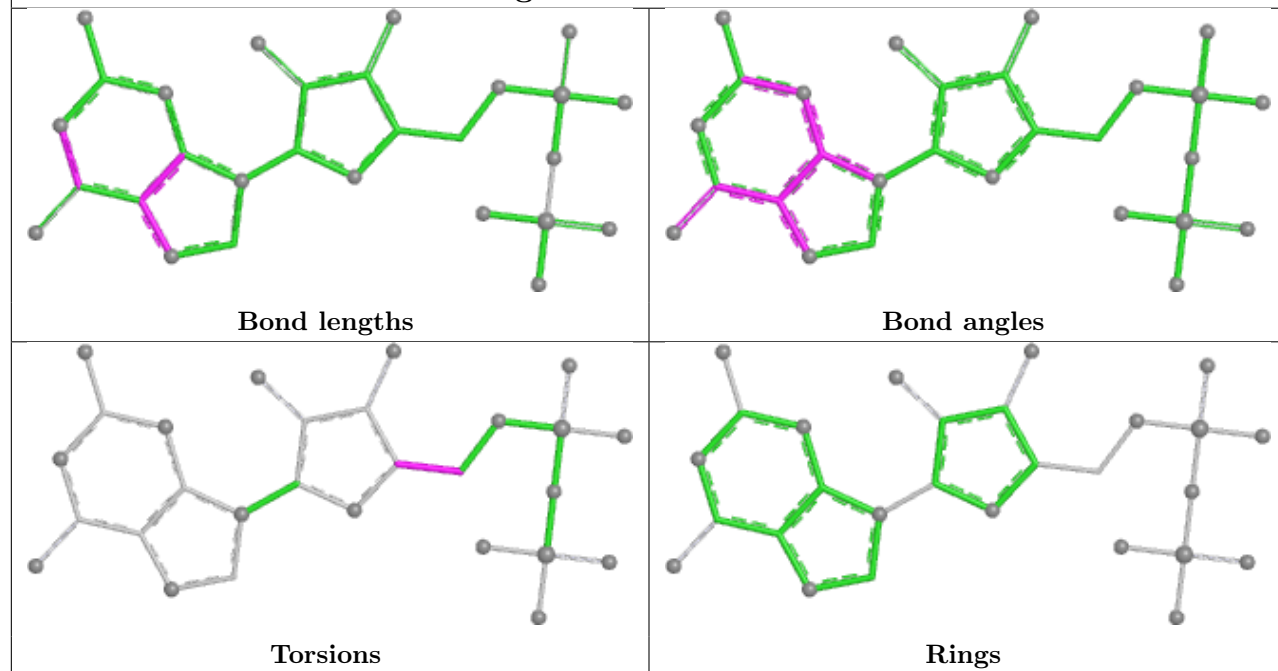




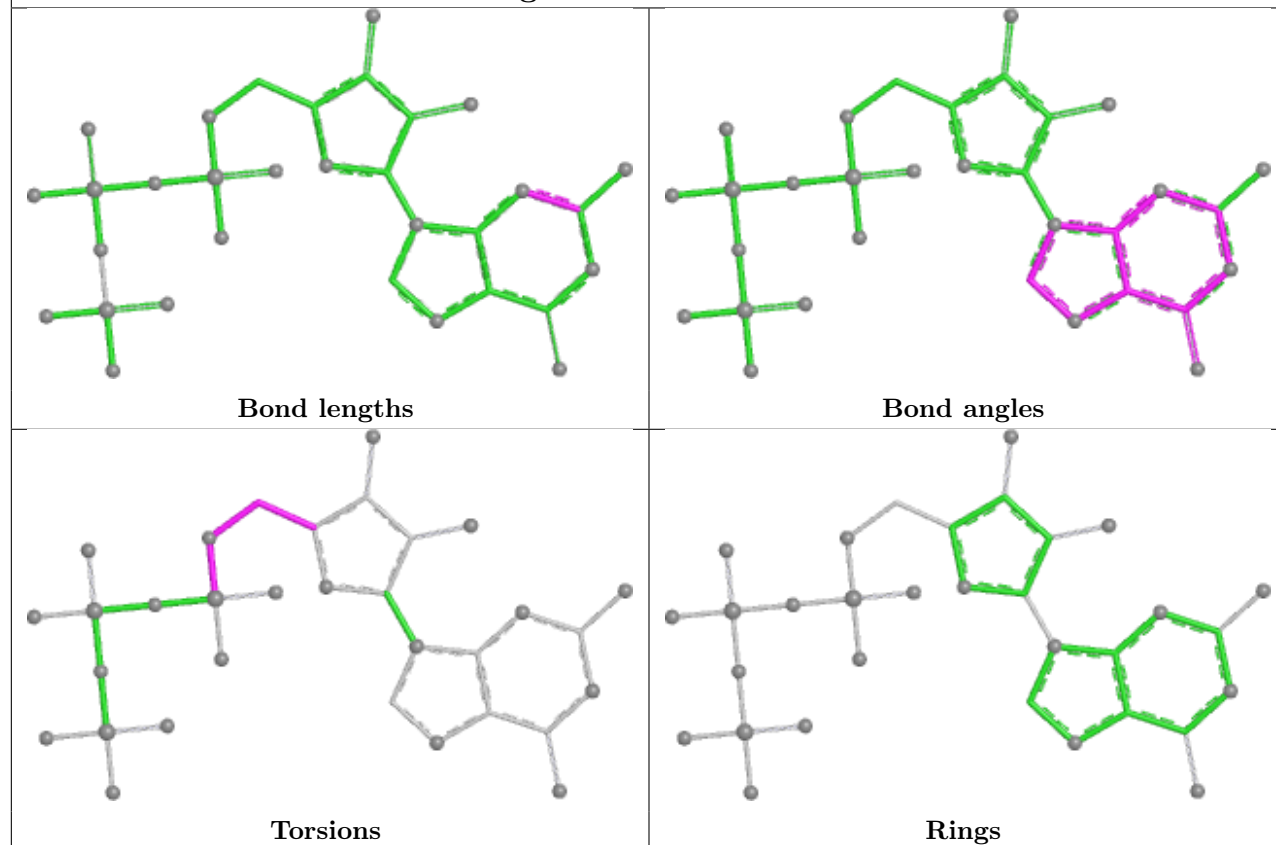
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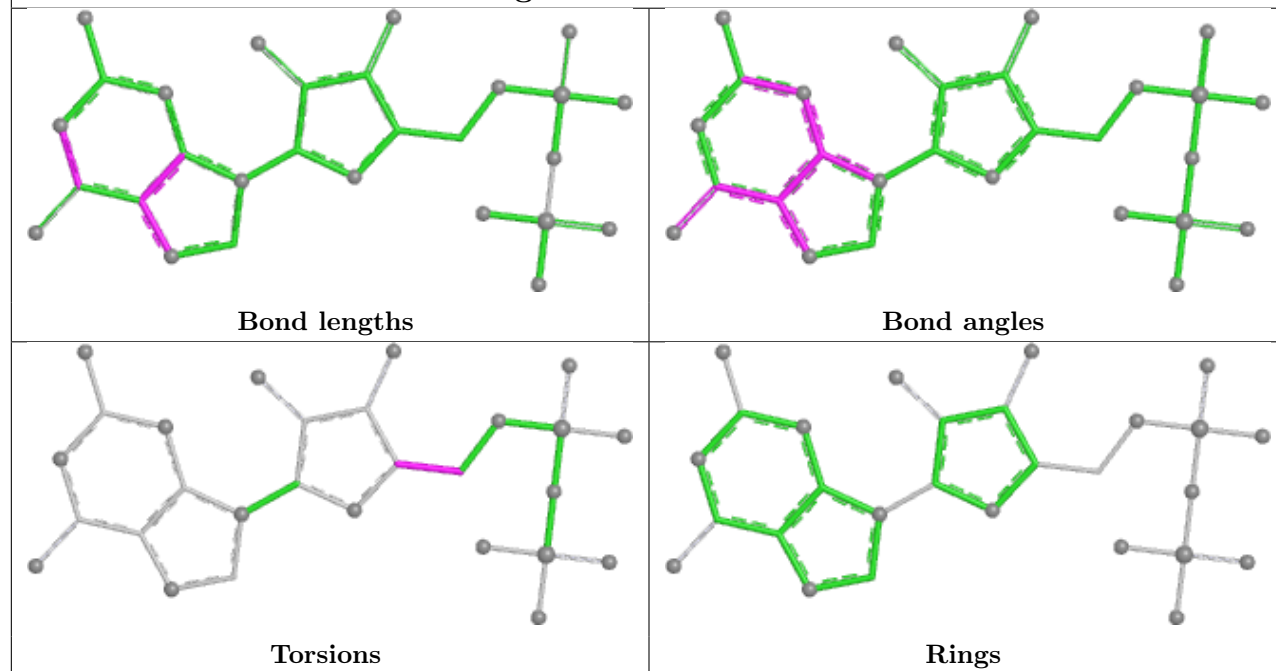
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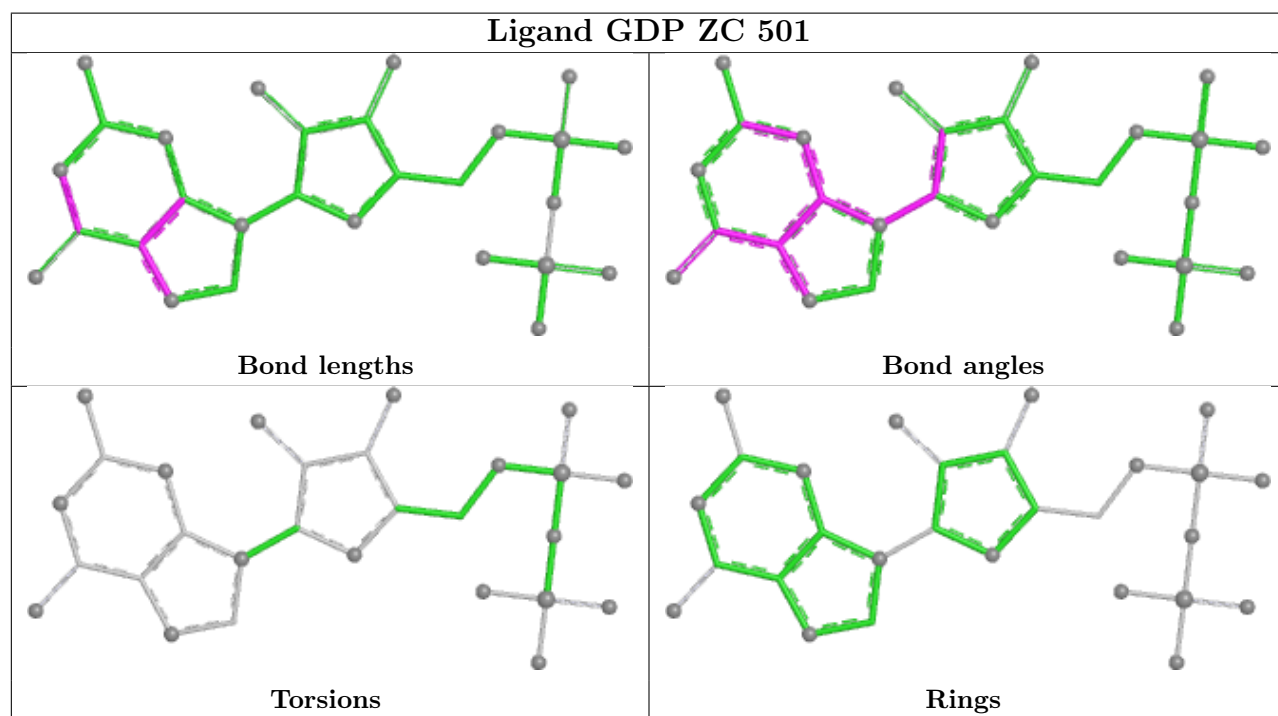
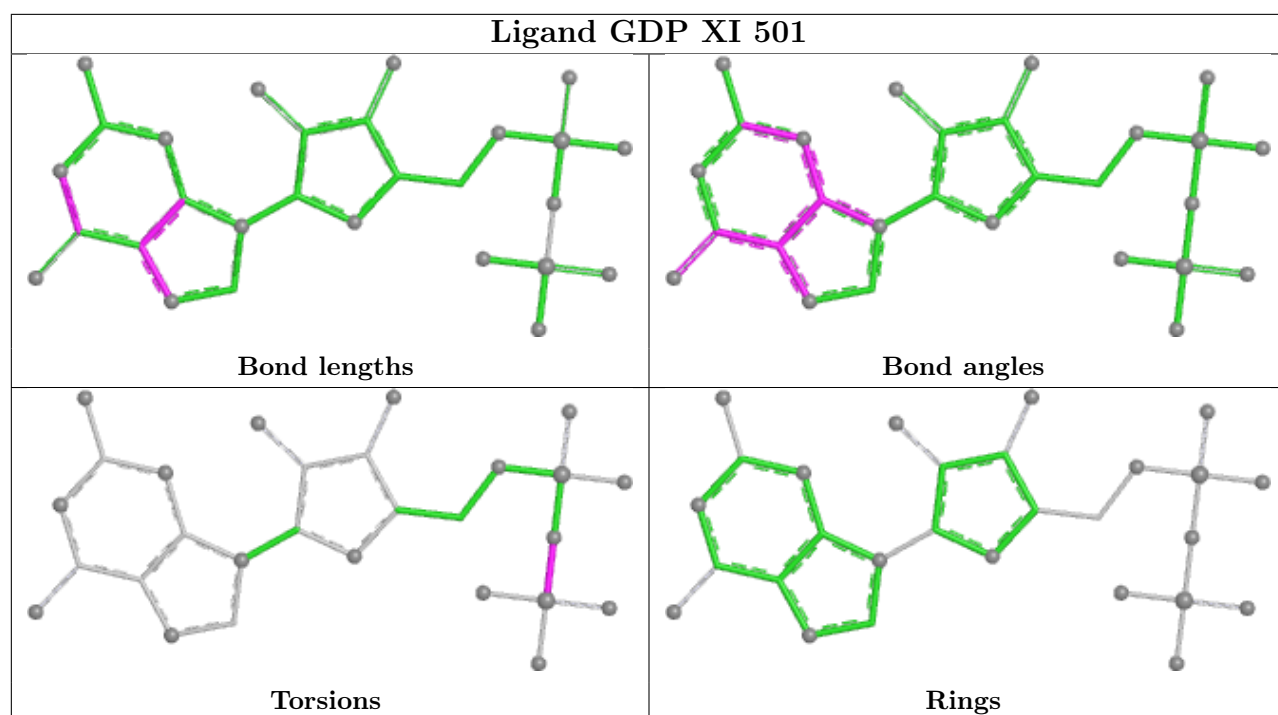


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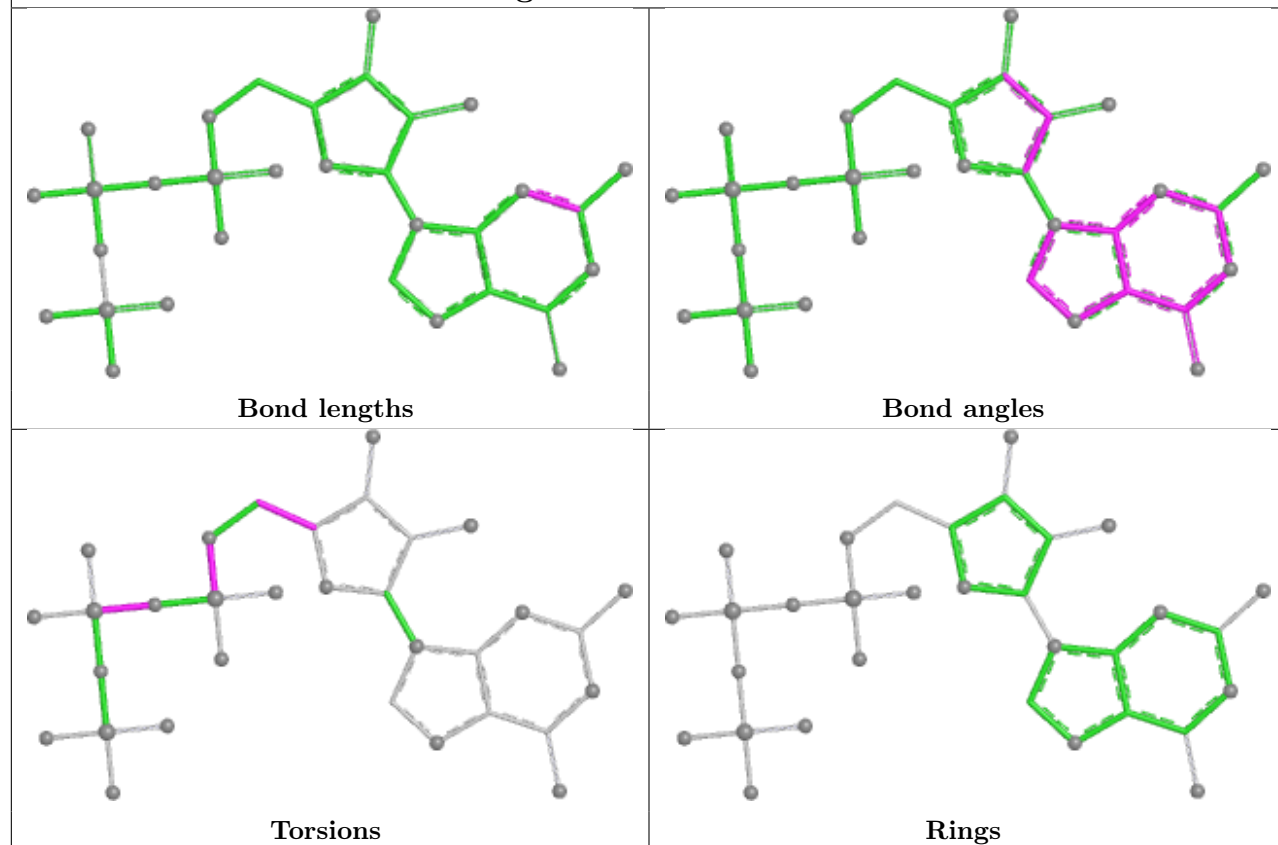


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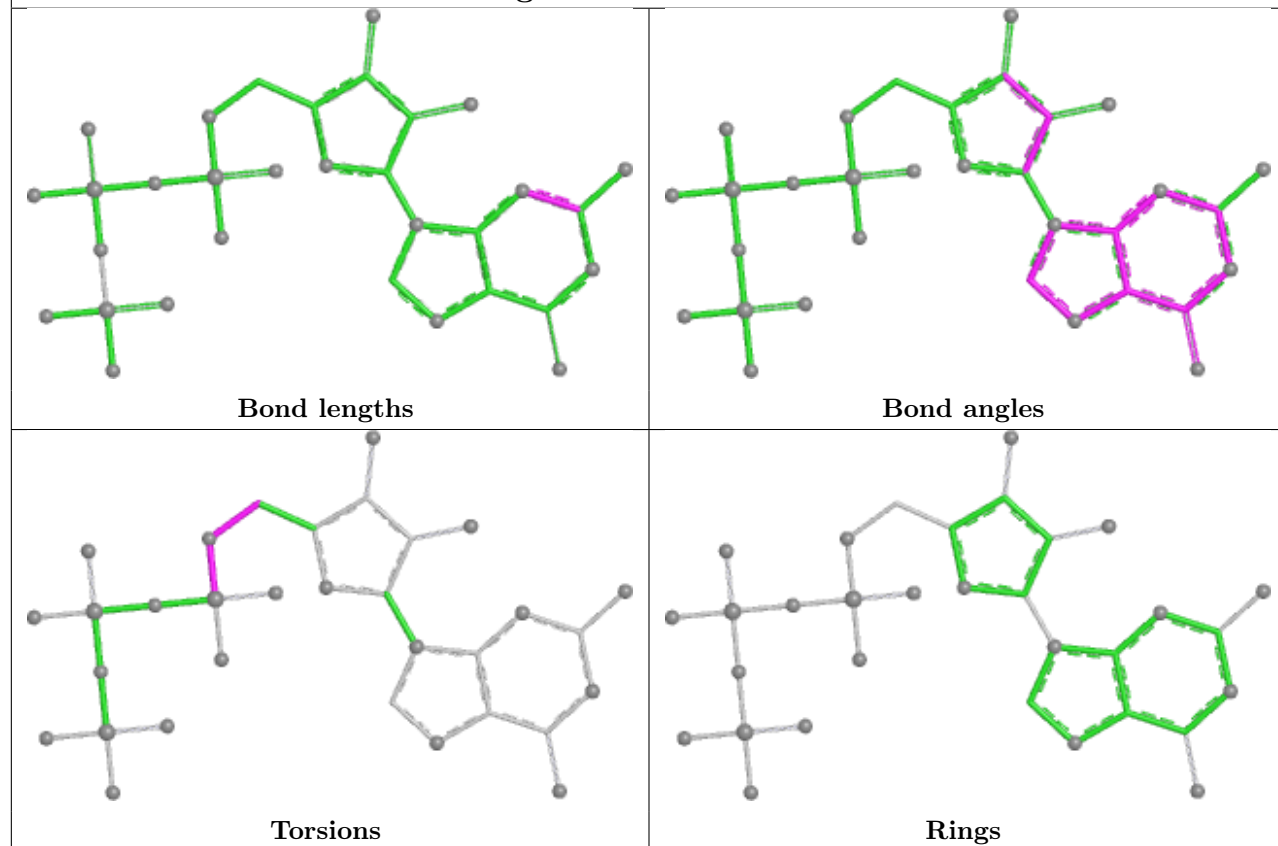


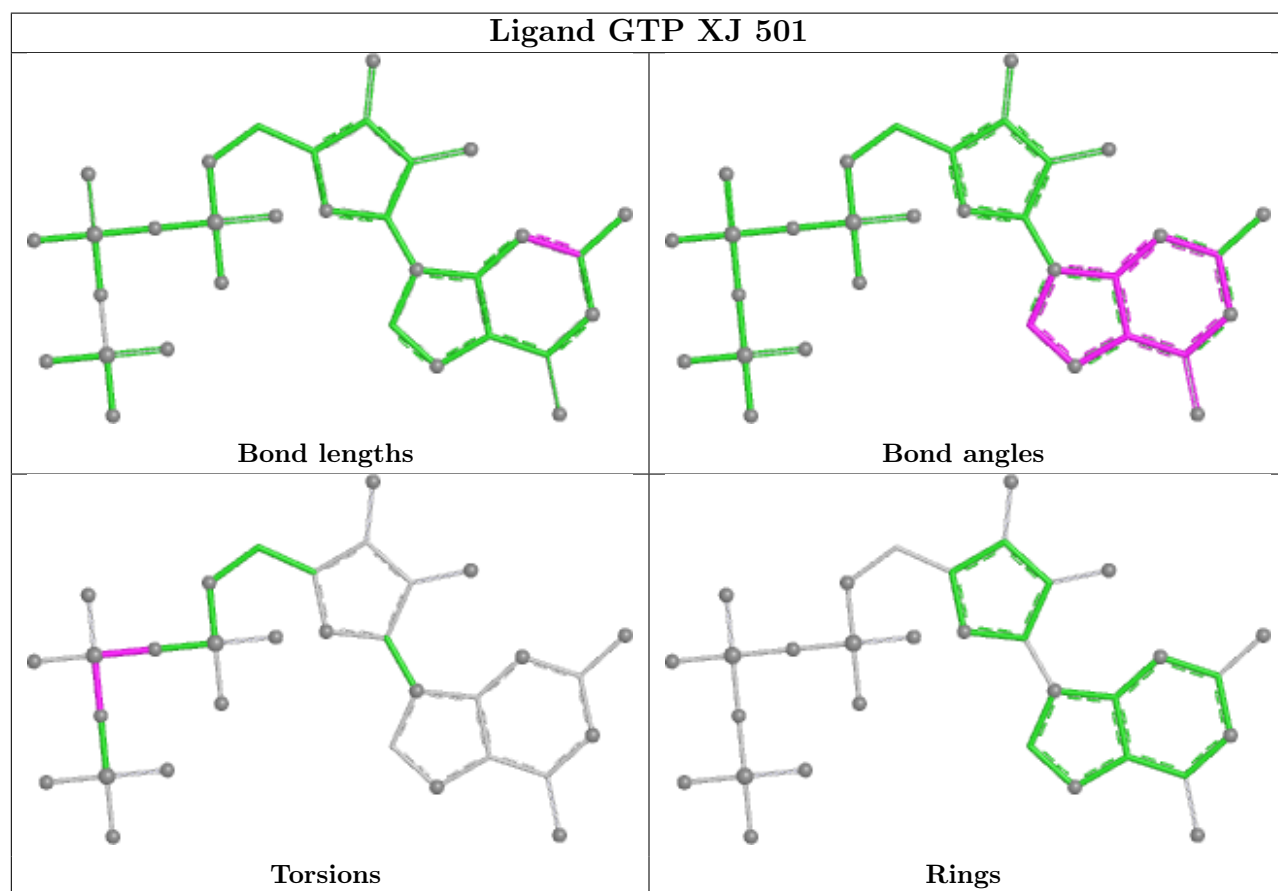
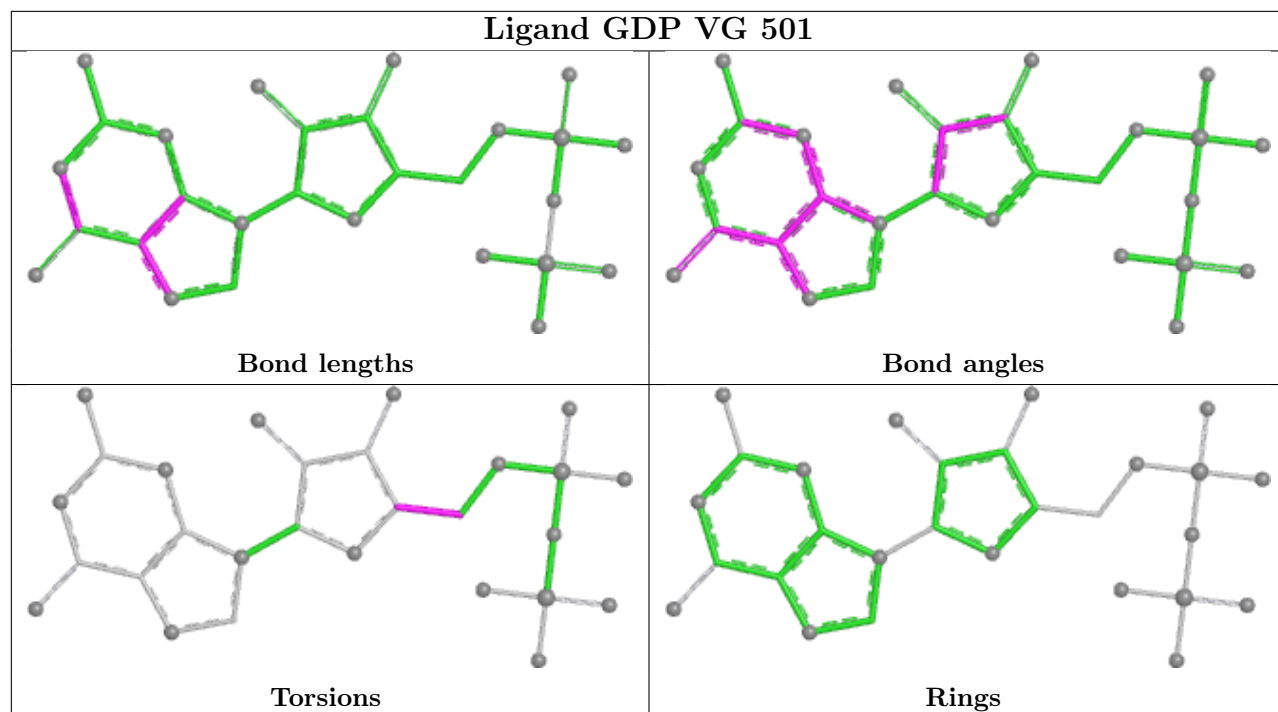


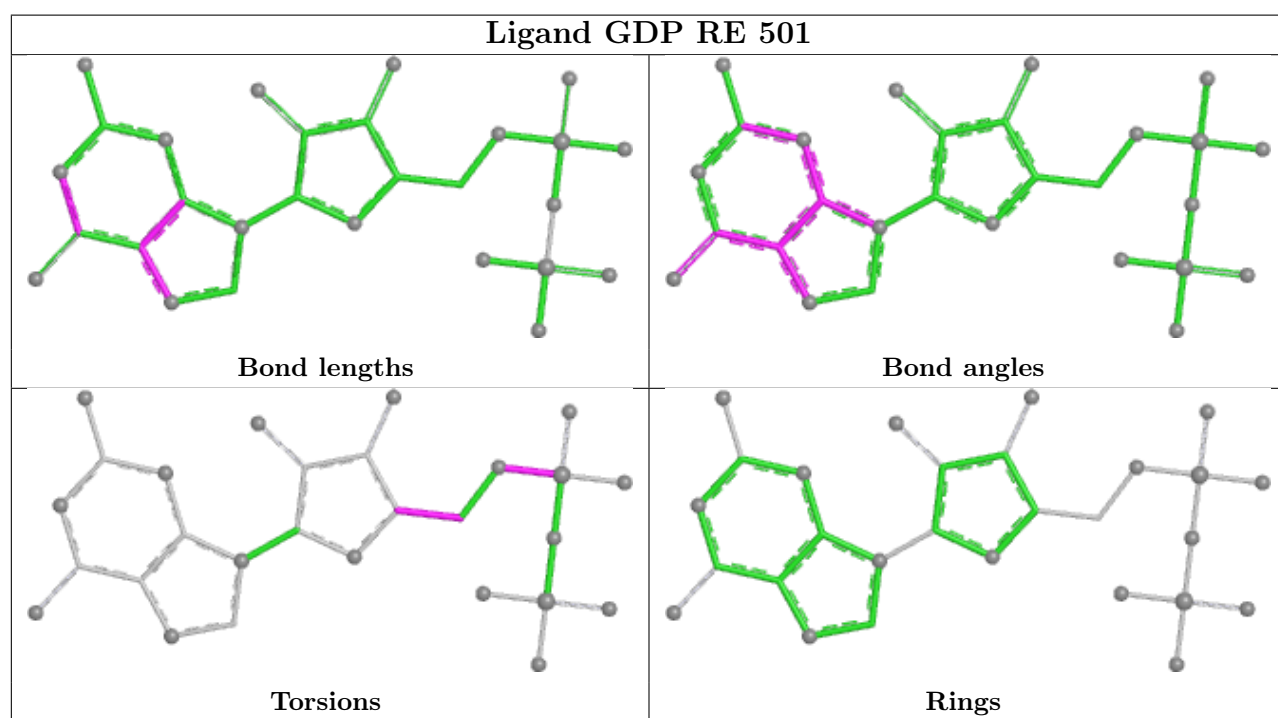
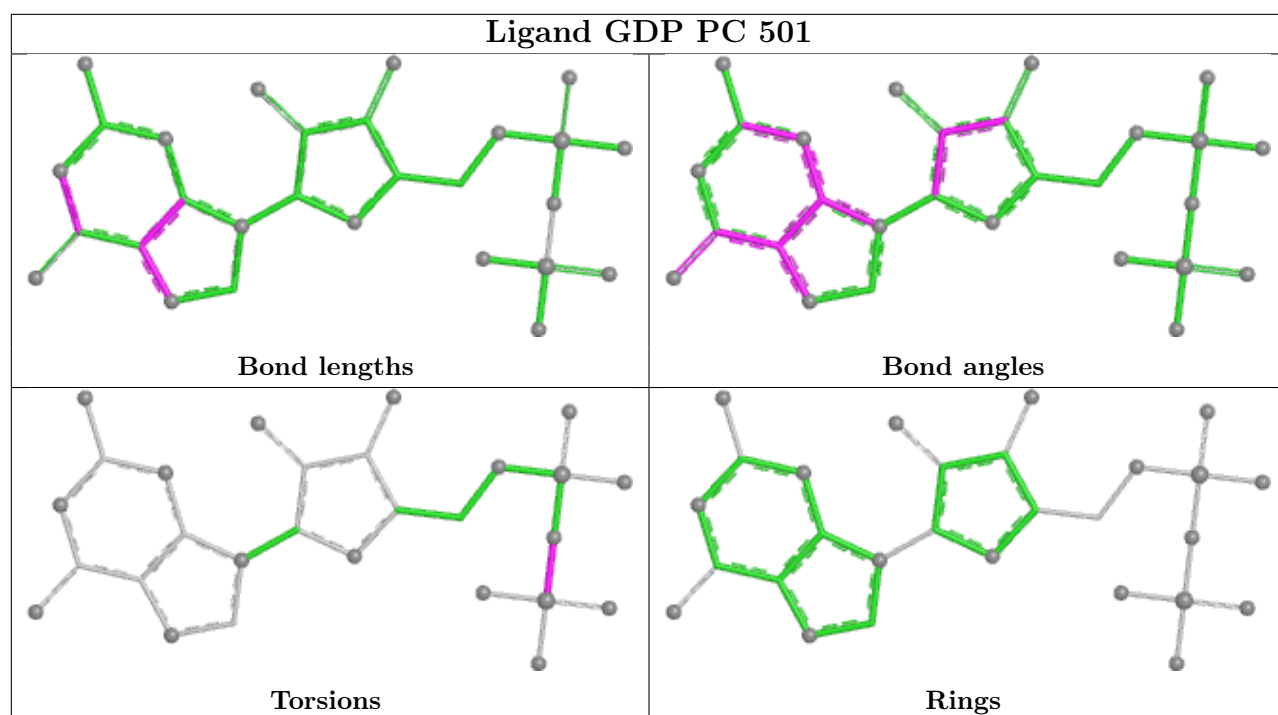
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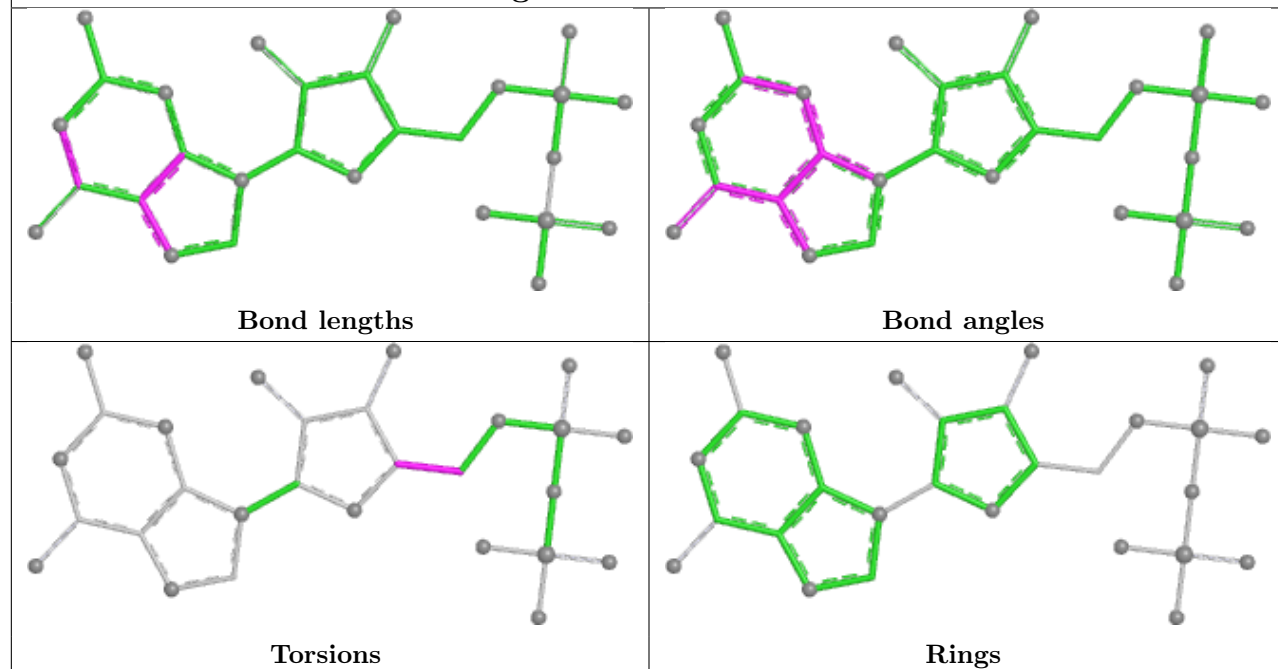
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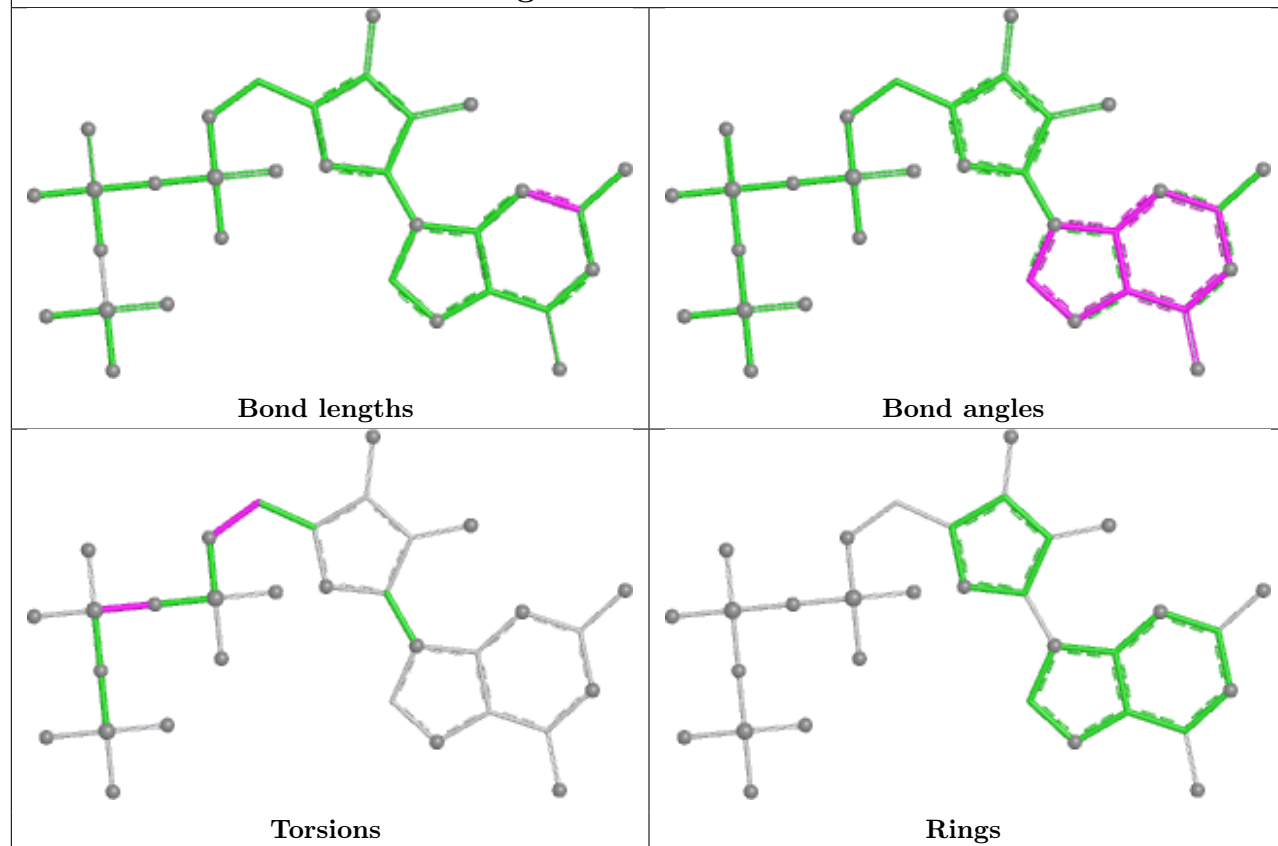


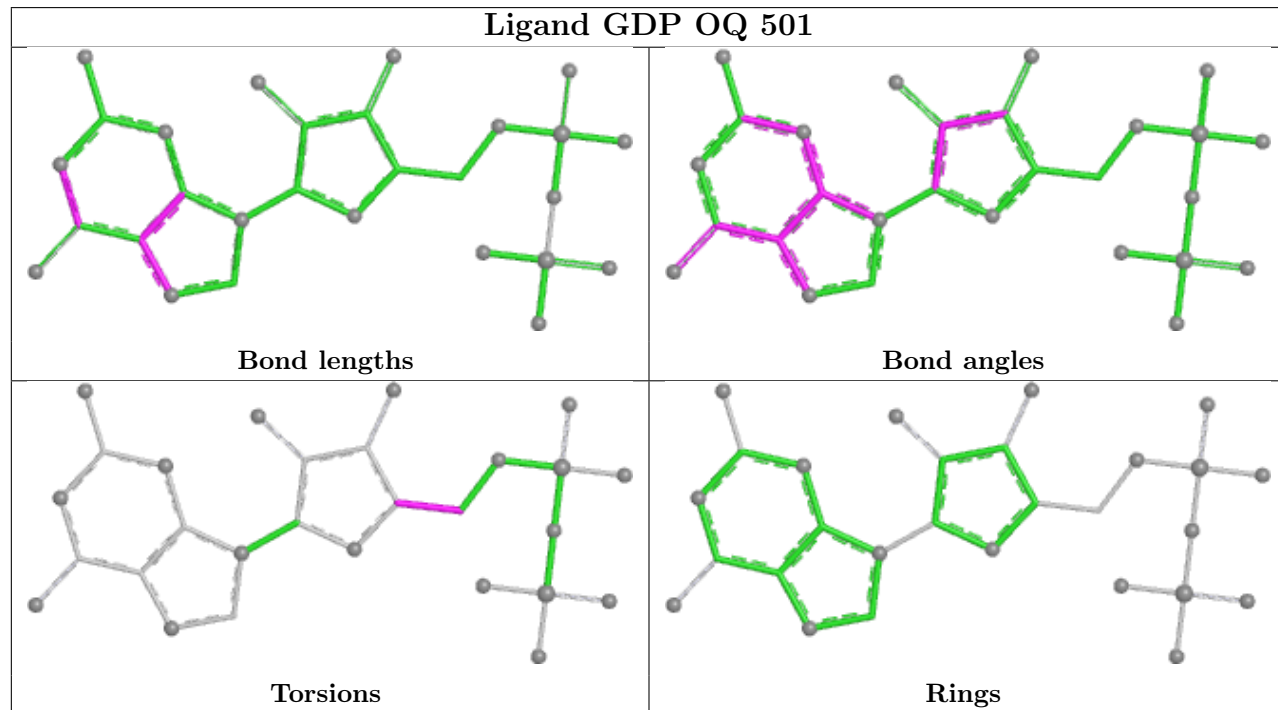
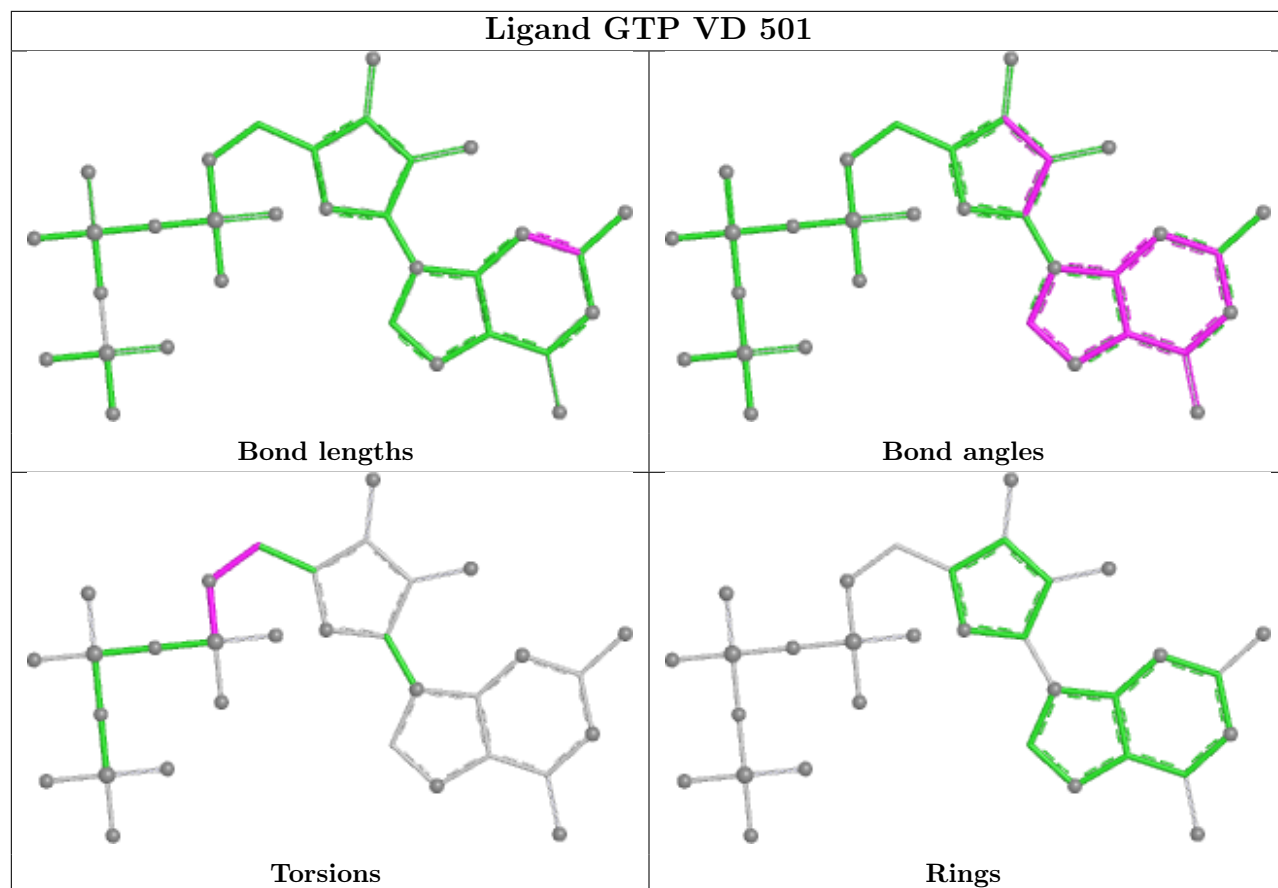


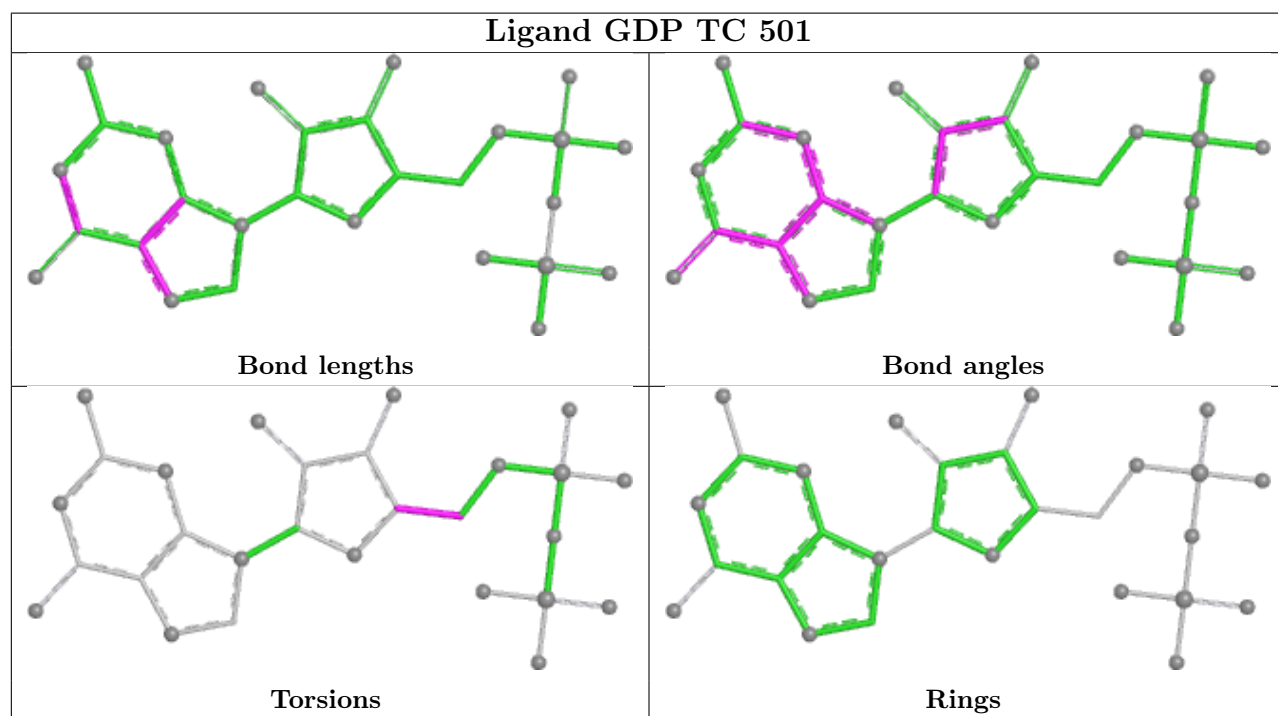
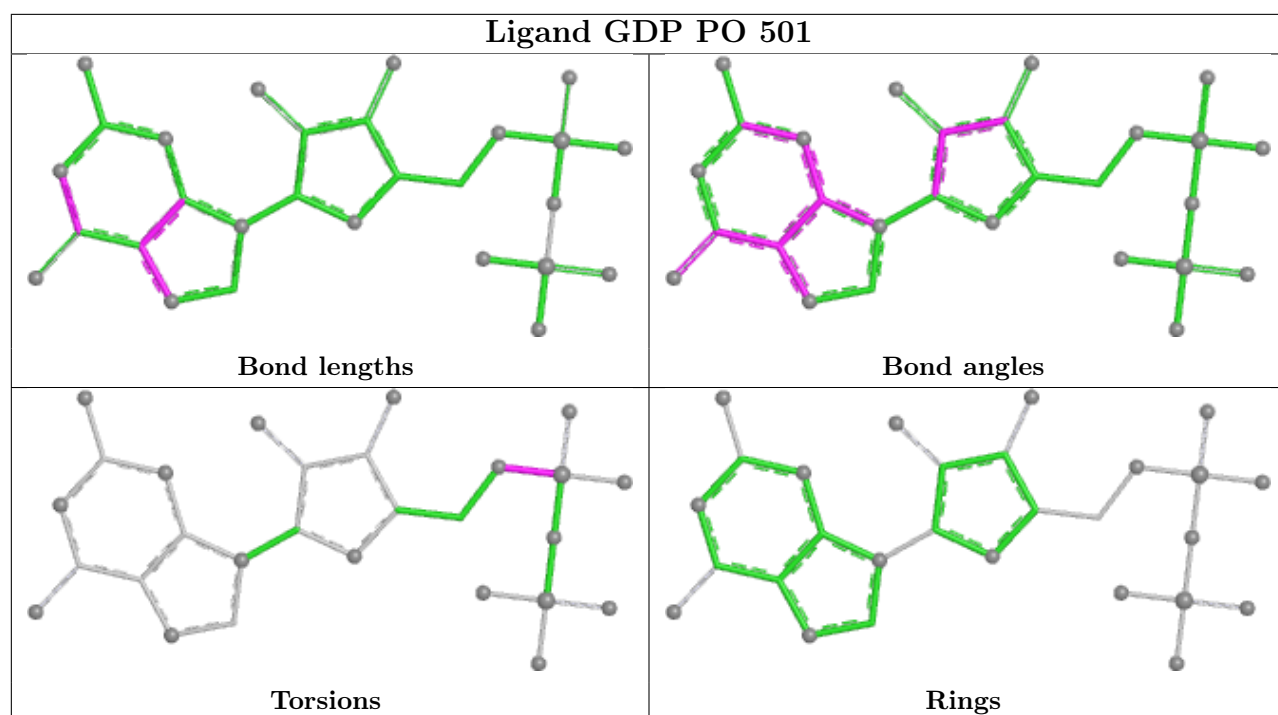
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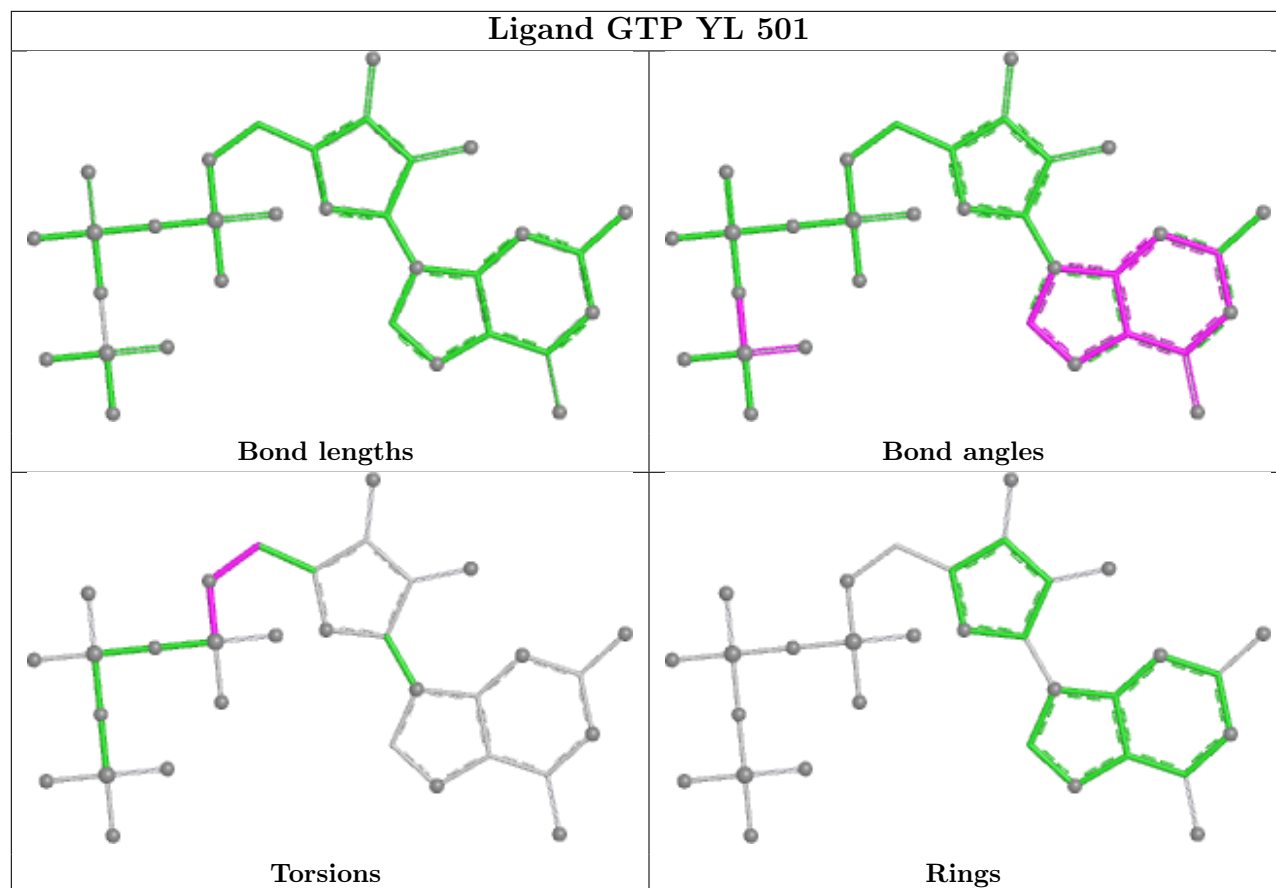
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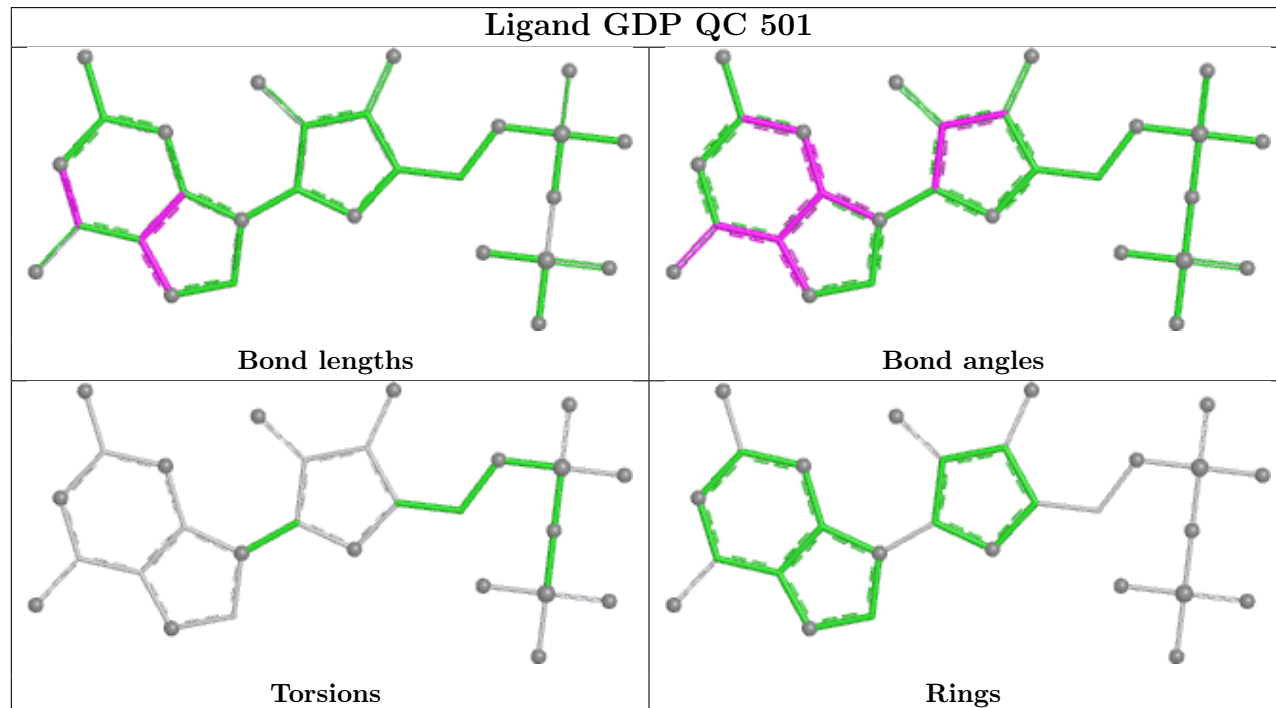


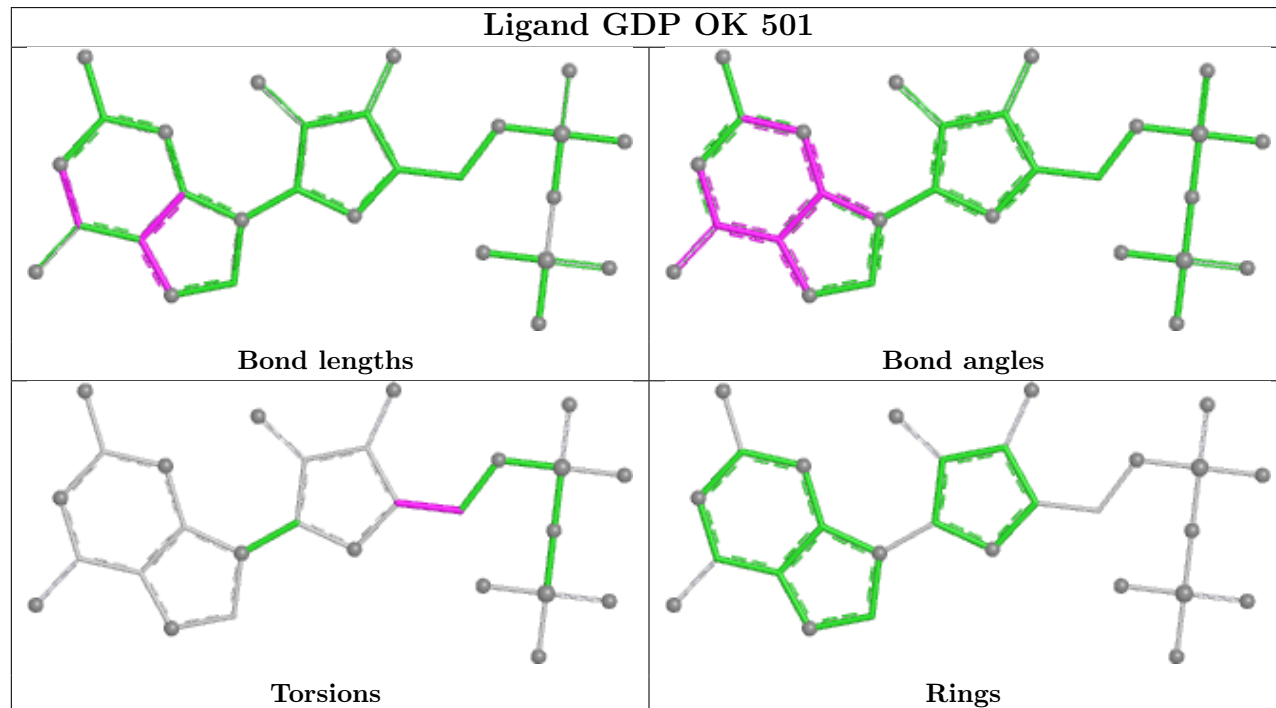
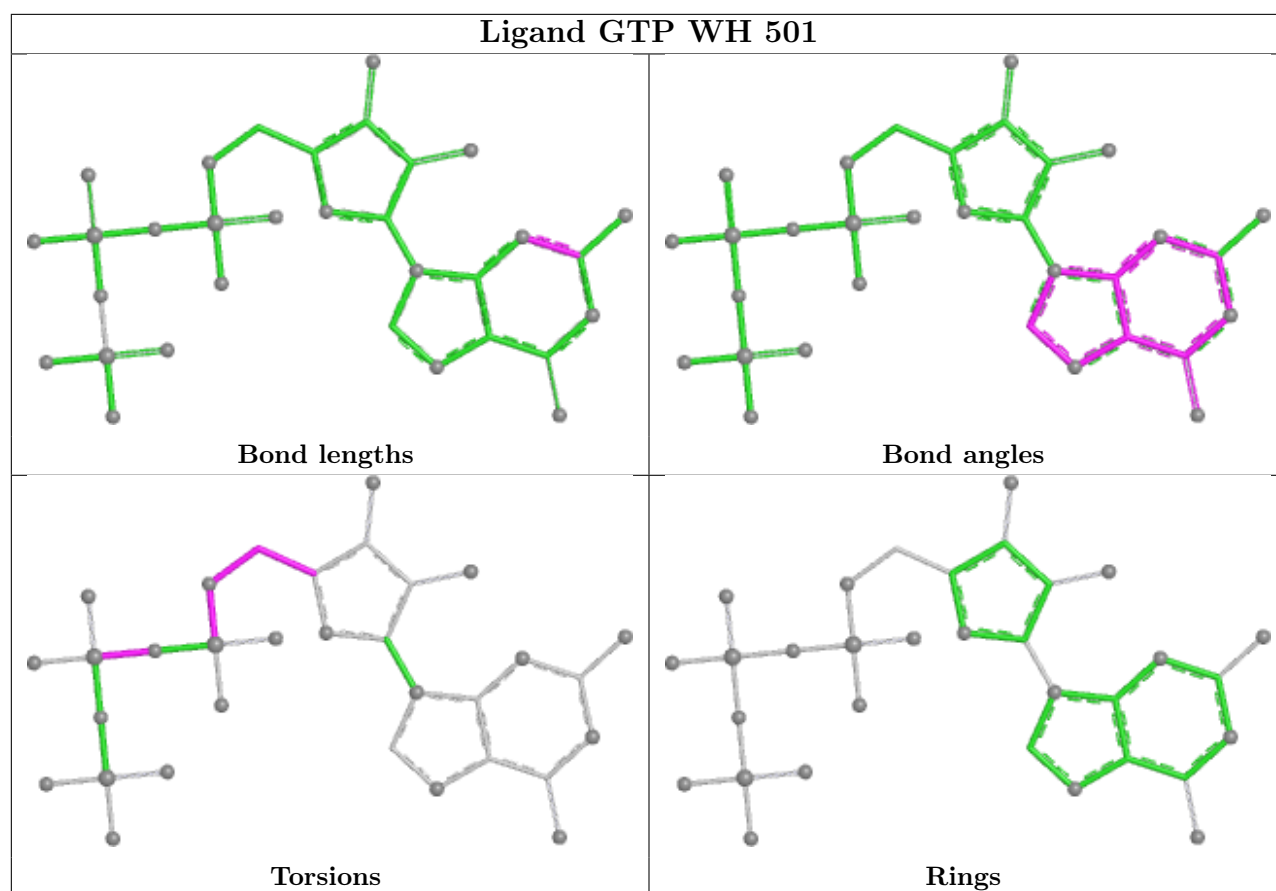


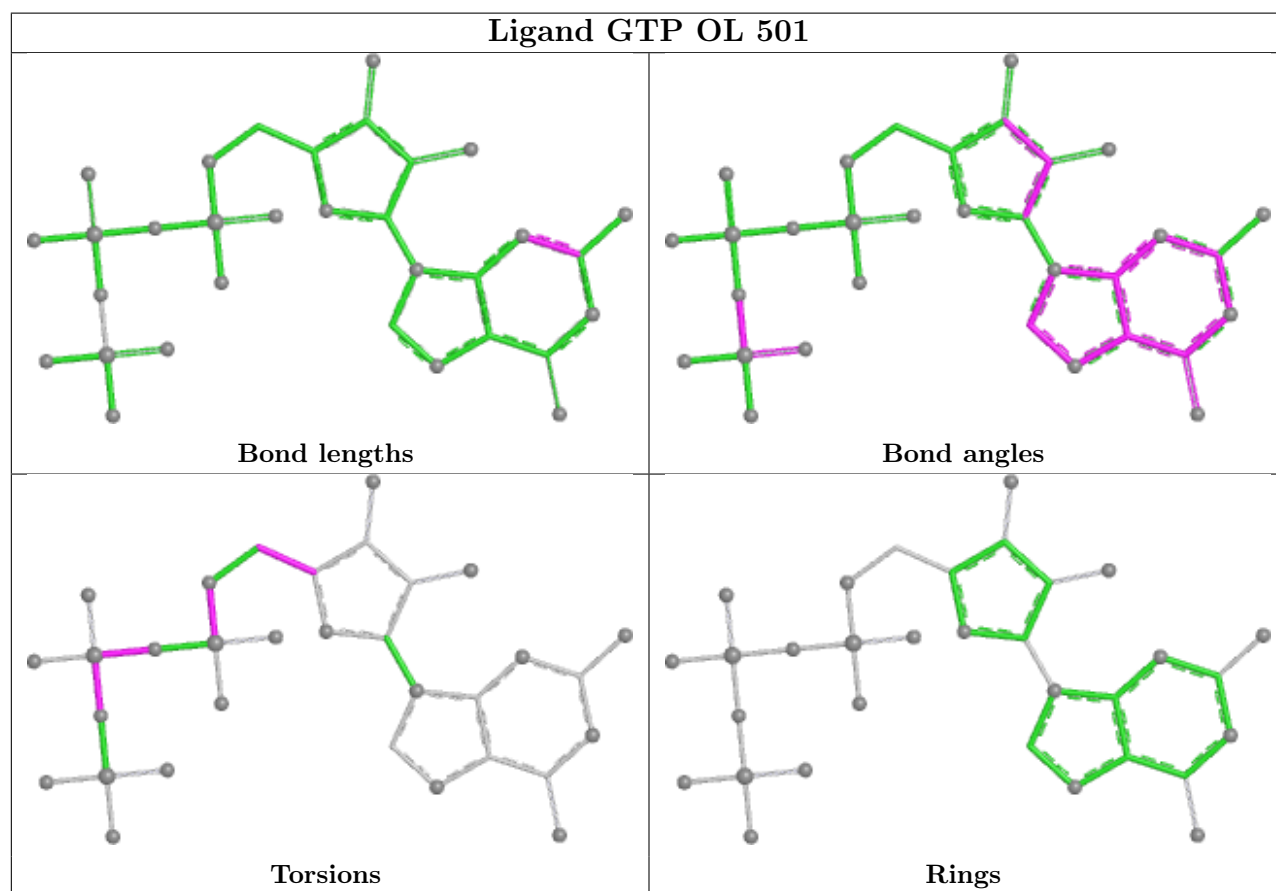
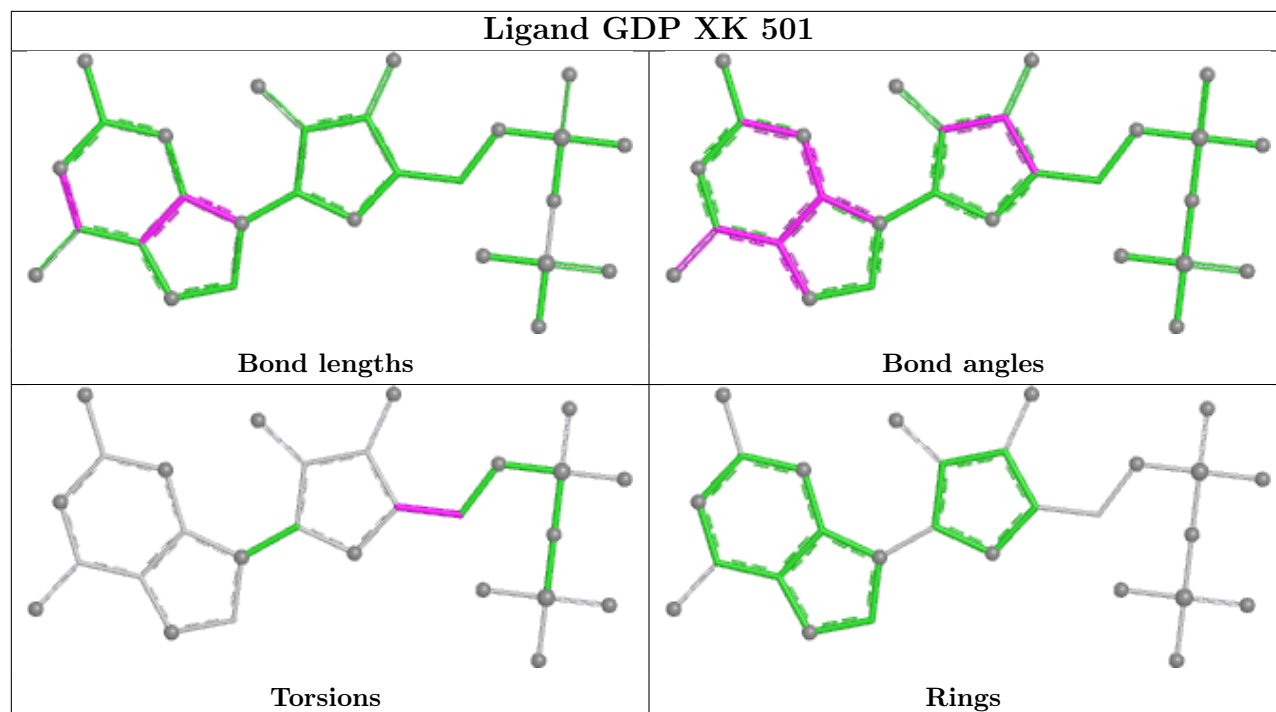
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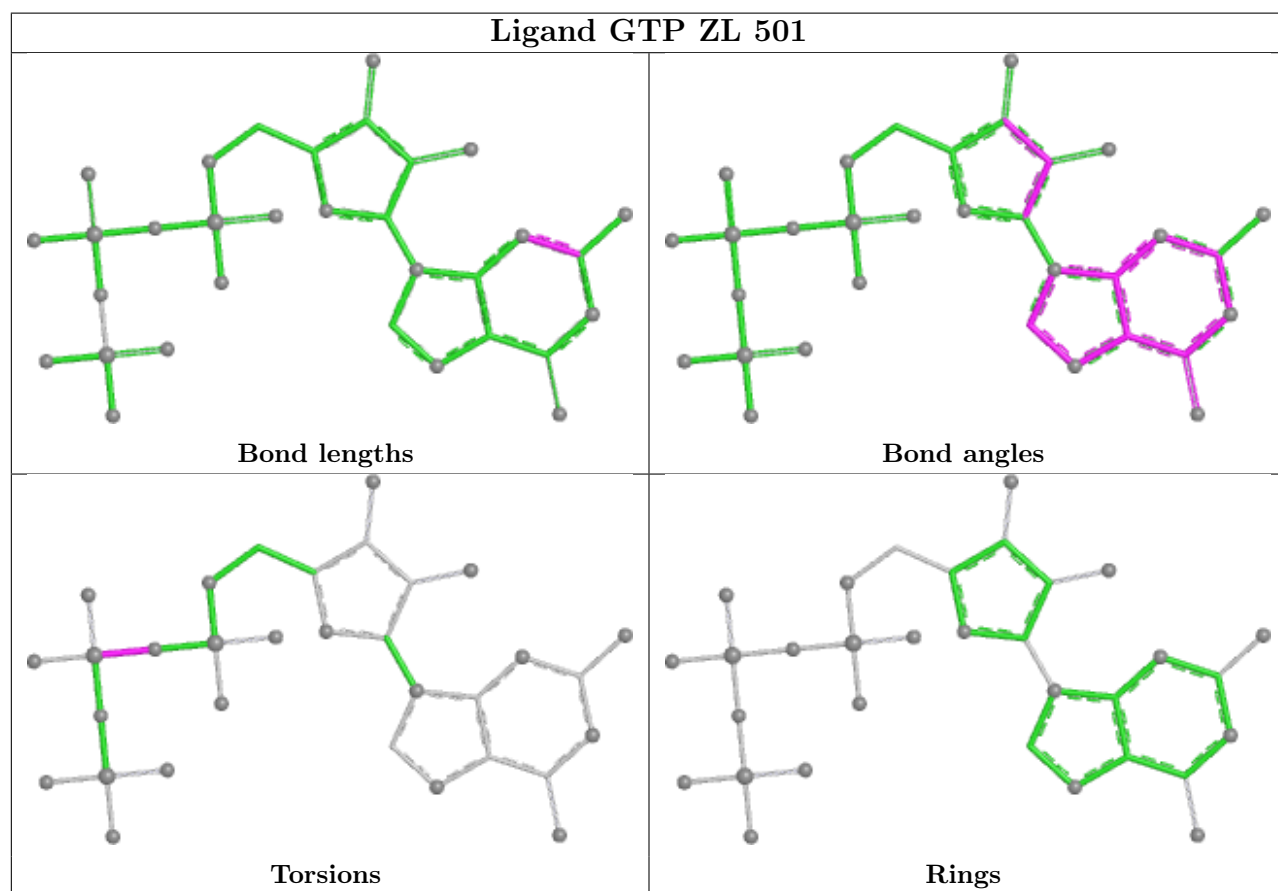
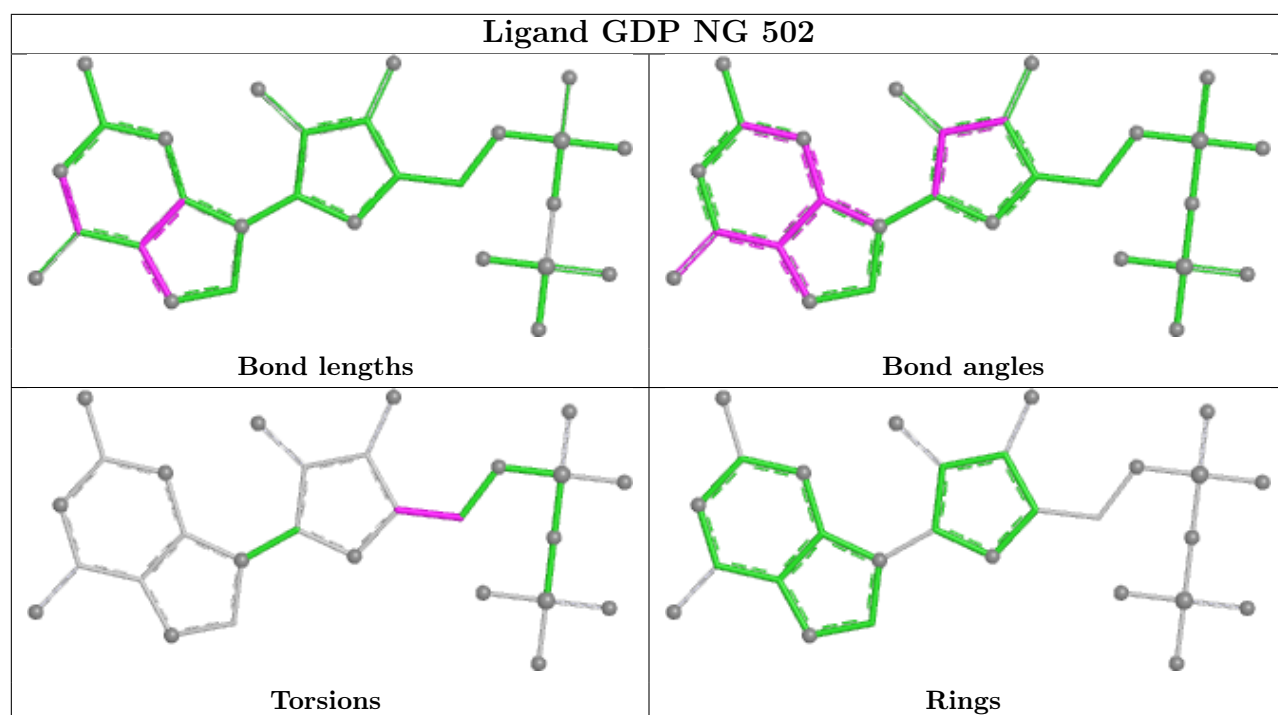


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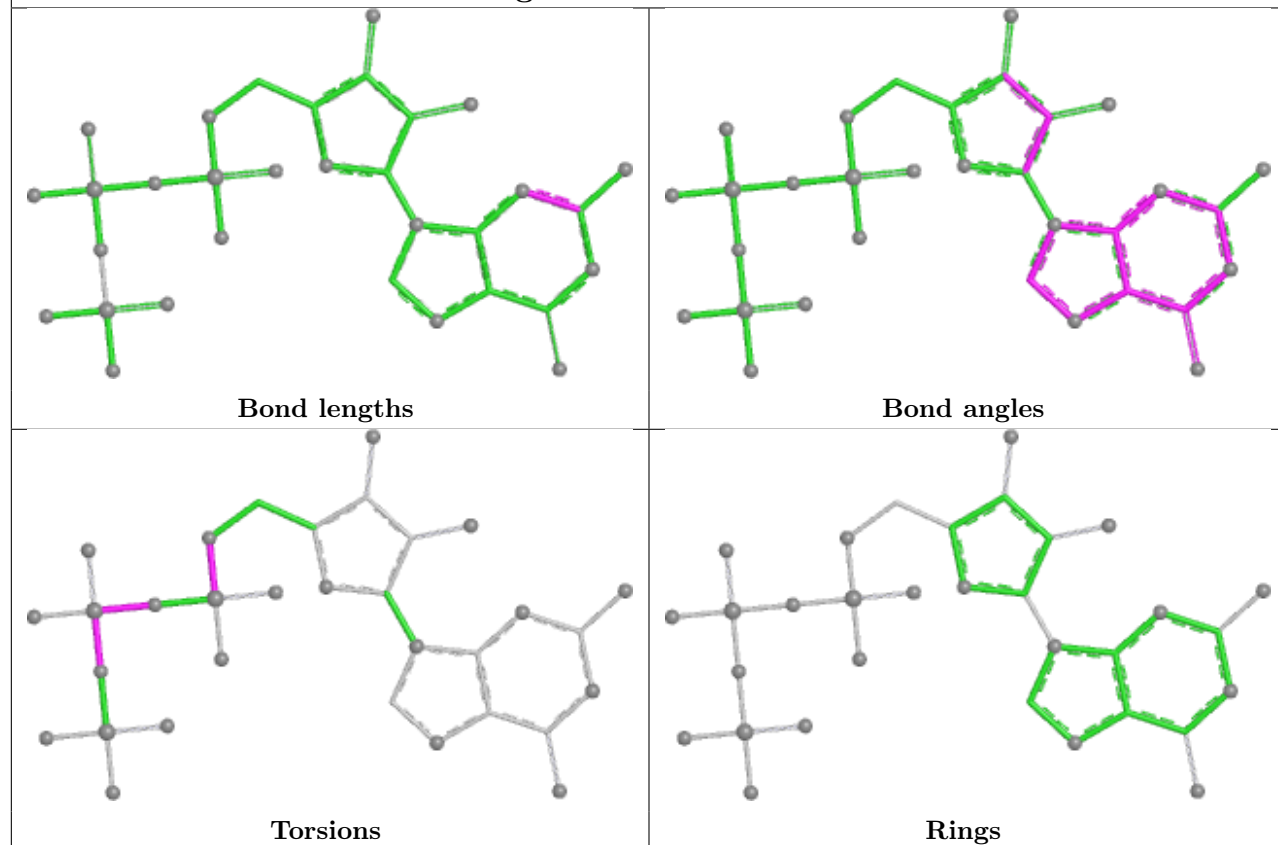




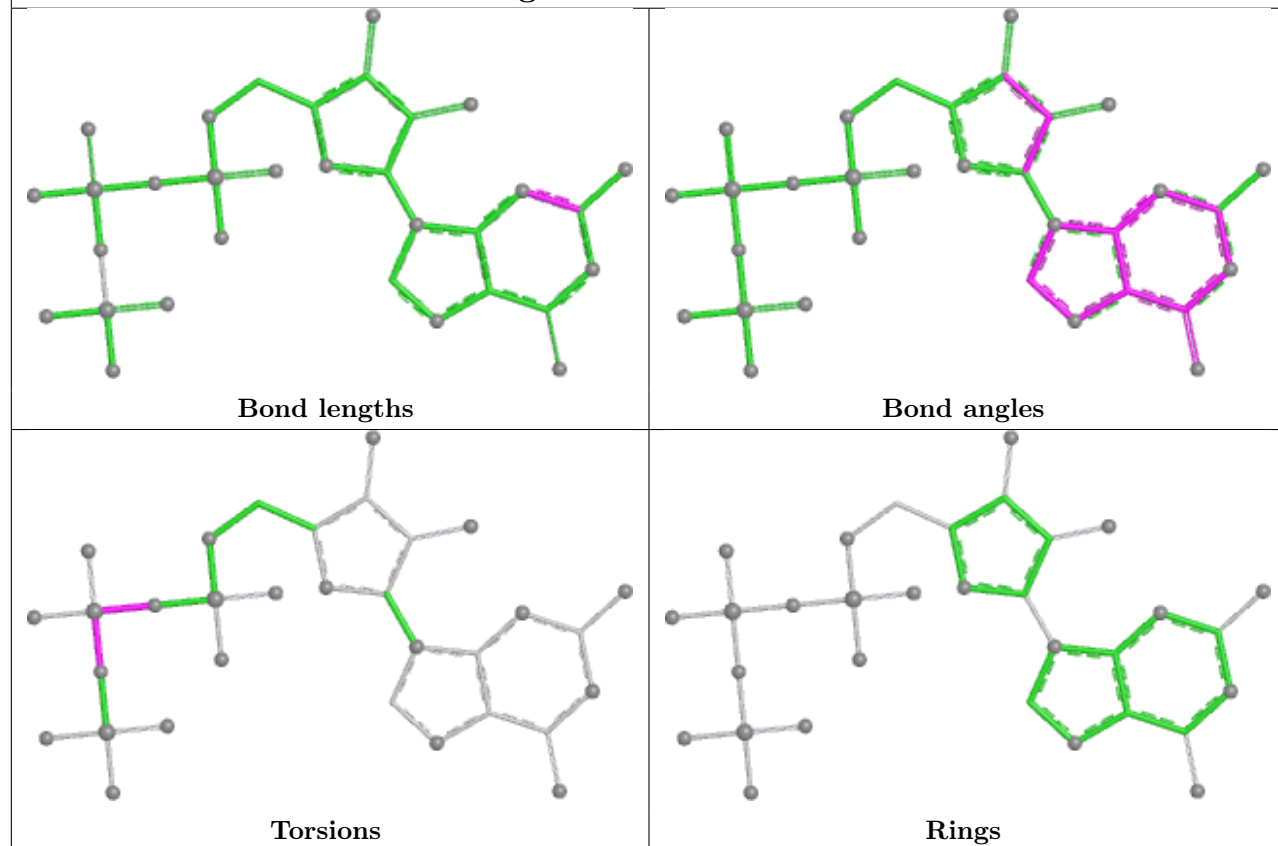


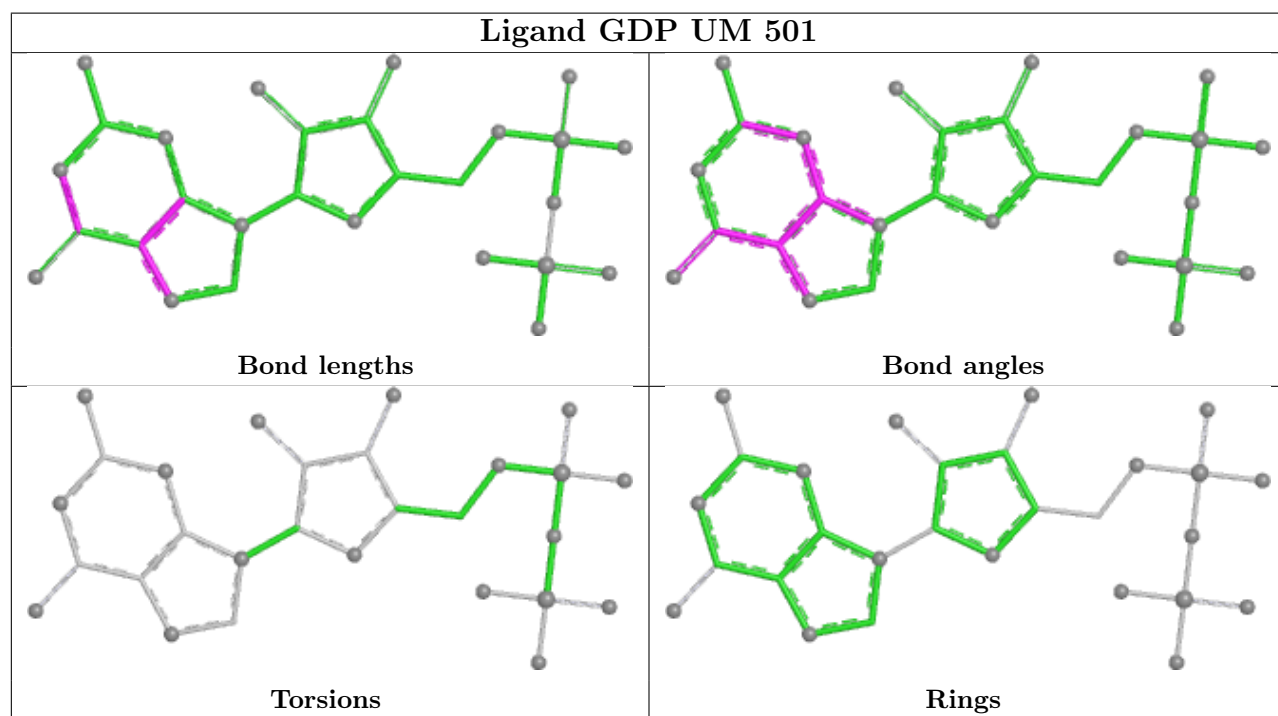
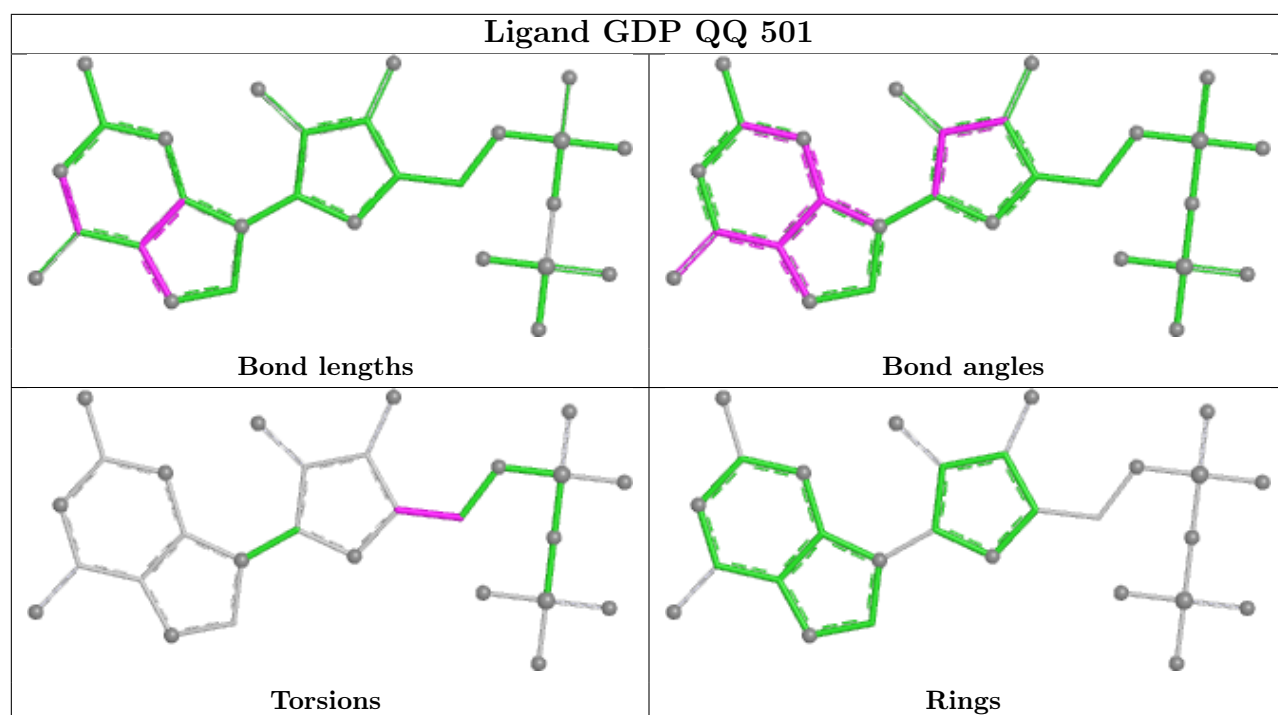


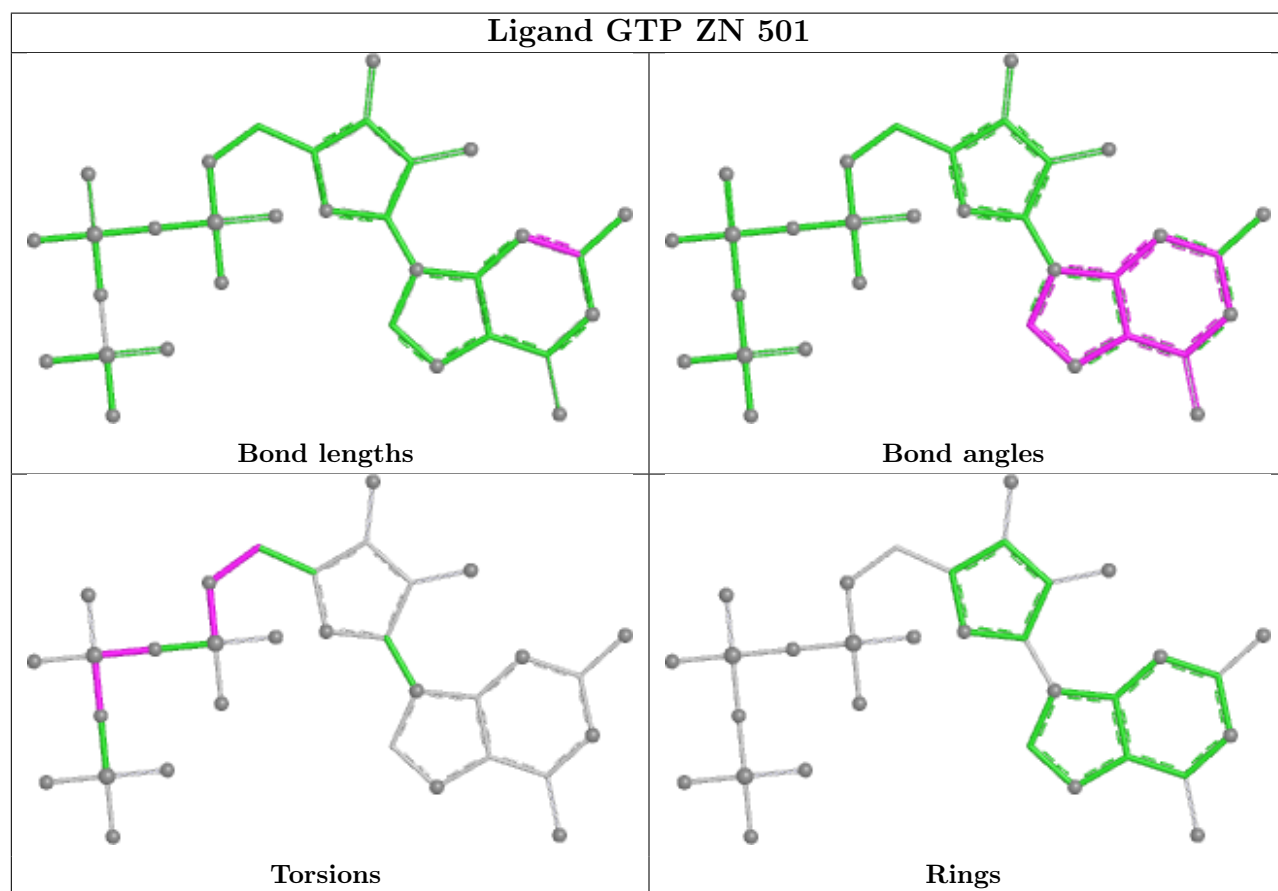
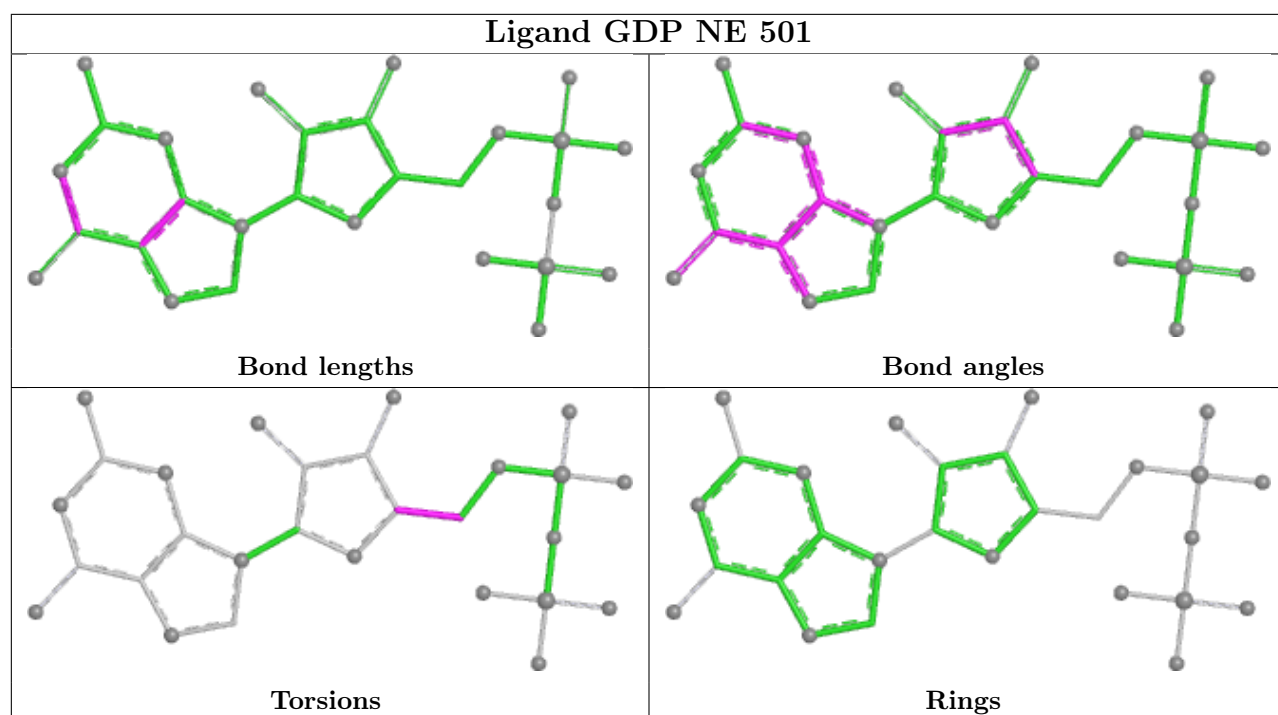
Ligand GTP NN 501



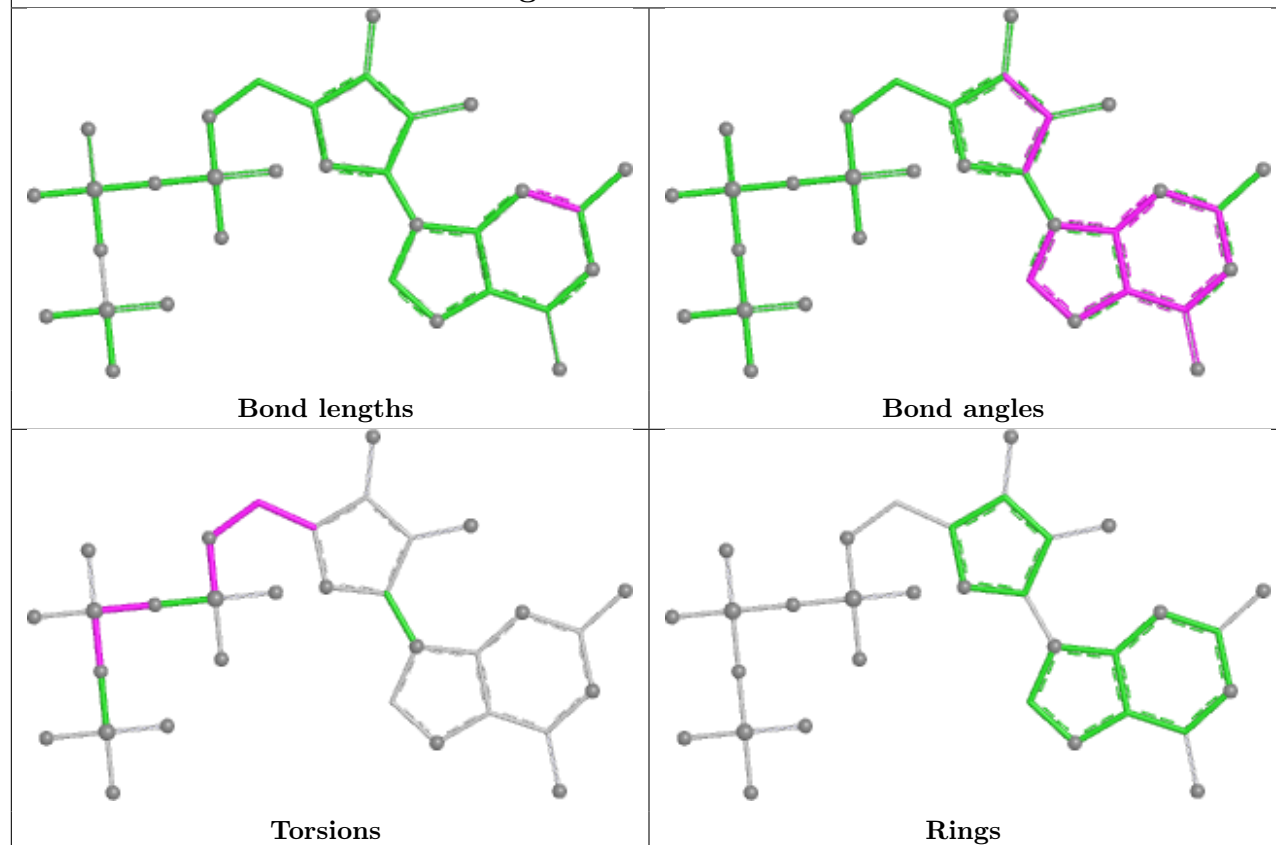
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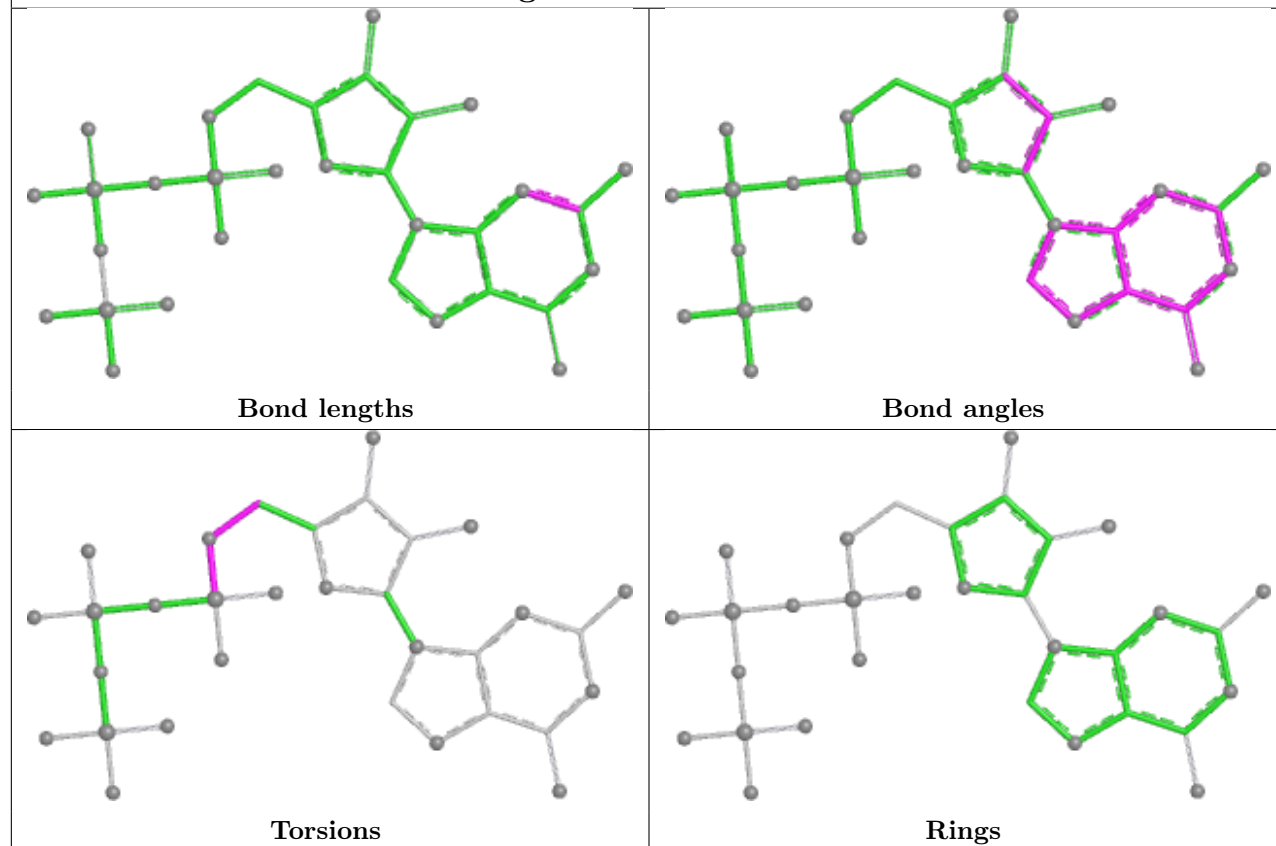


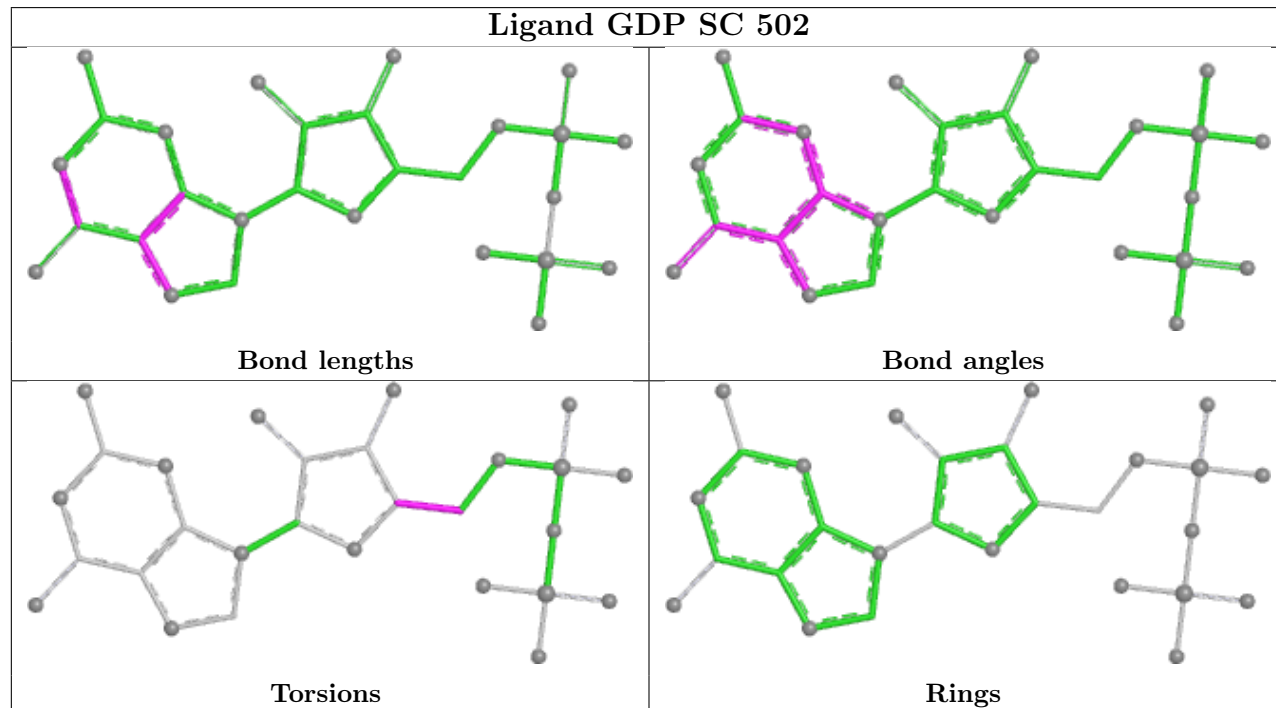
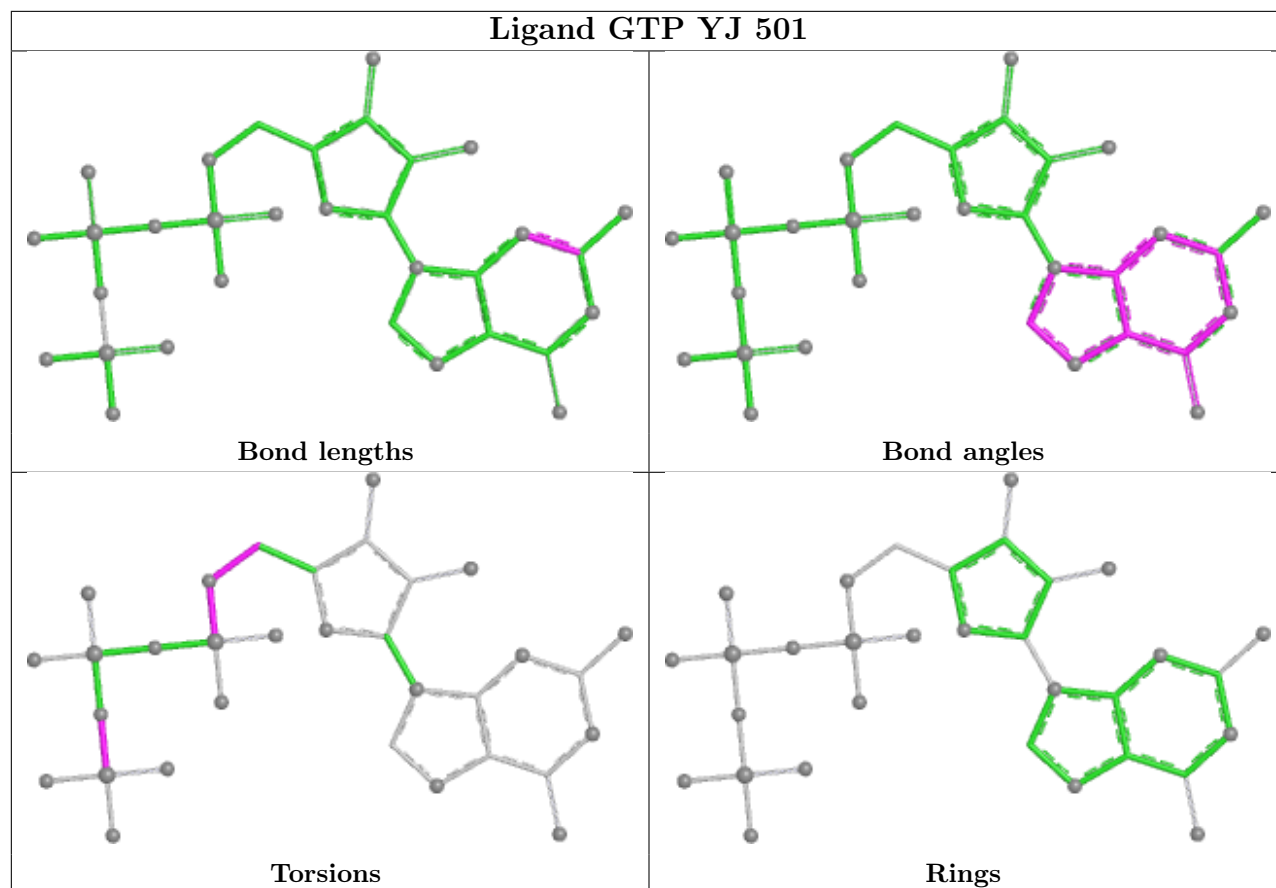


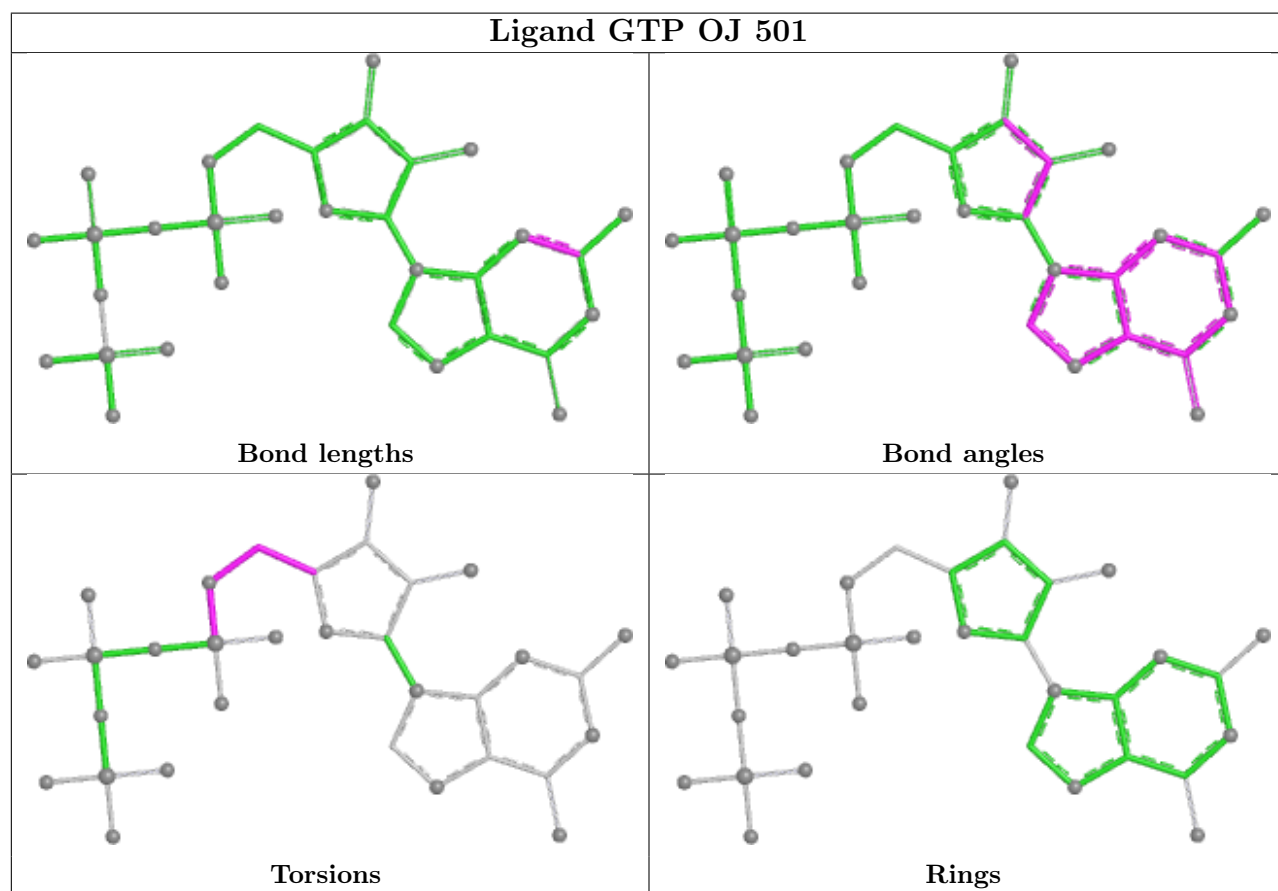
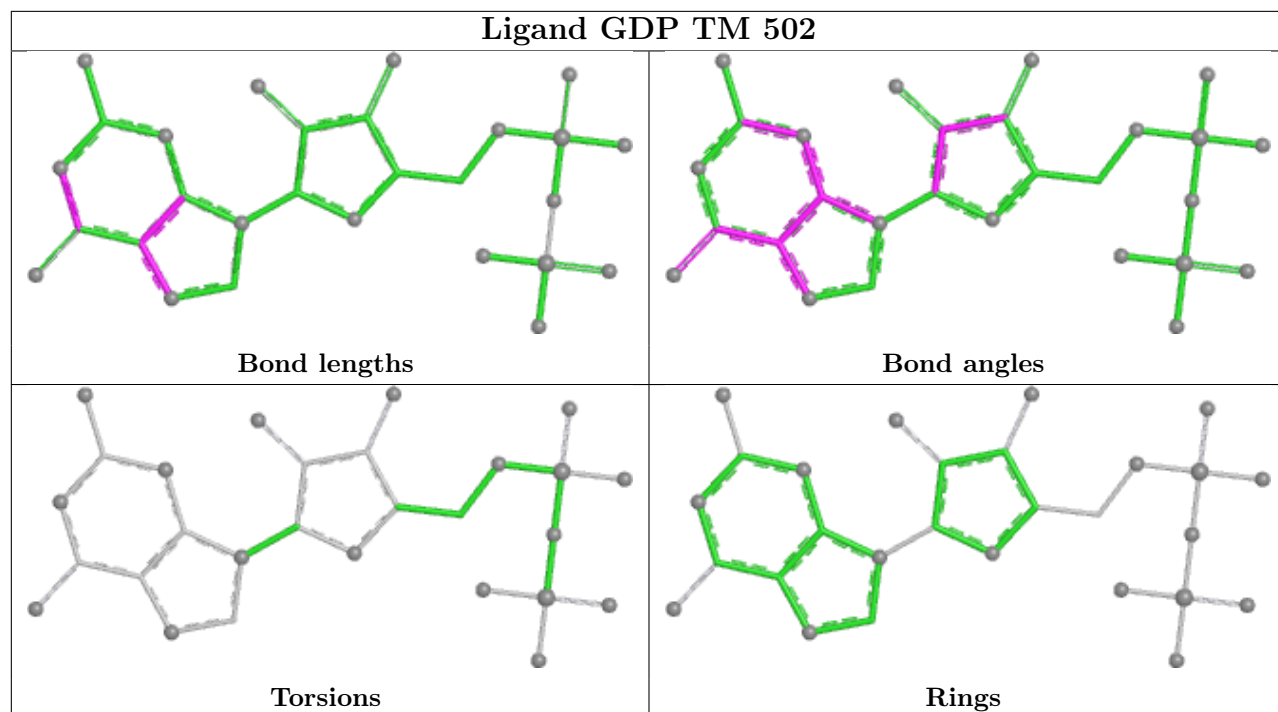
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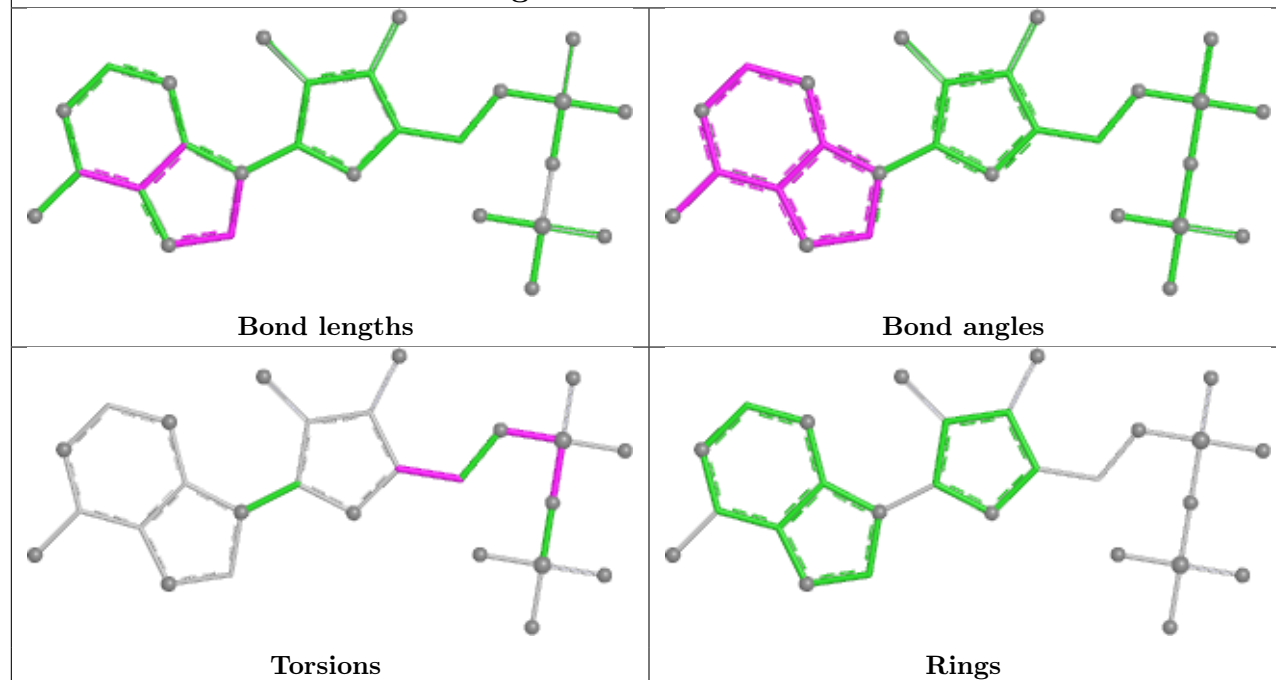
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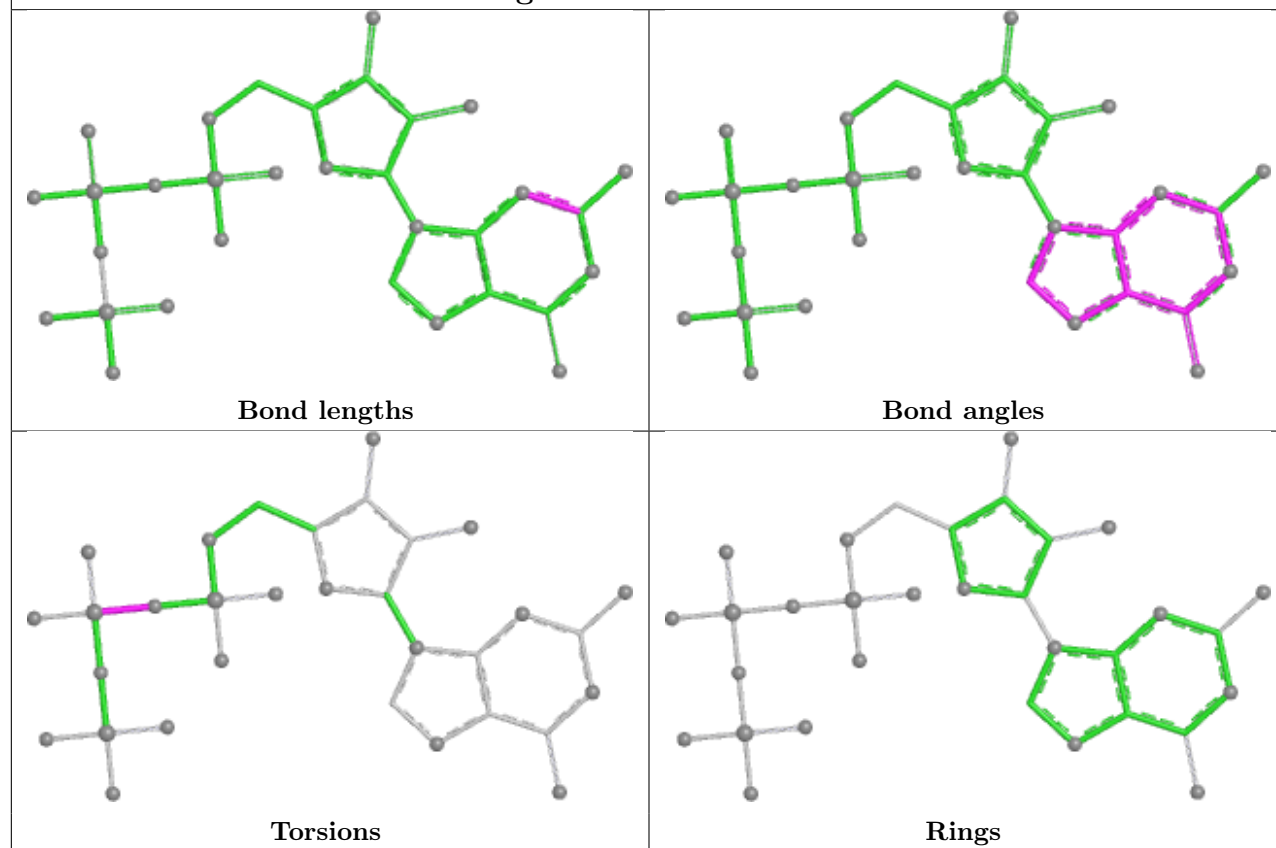


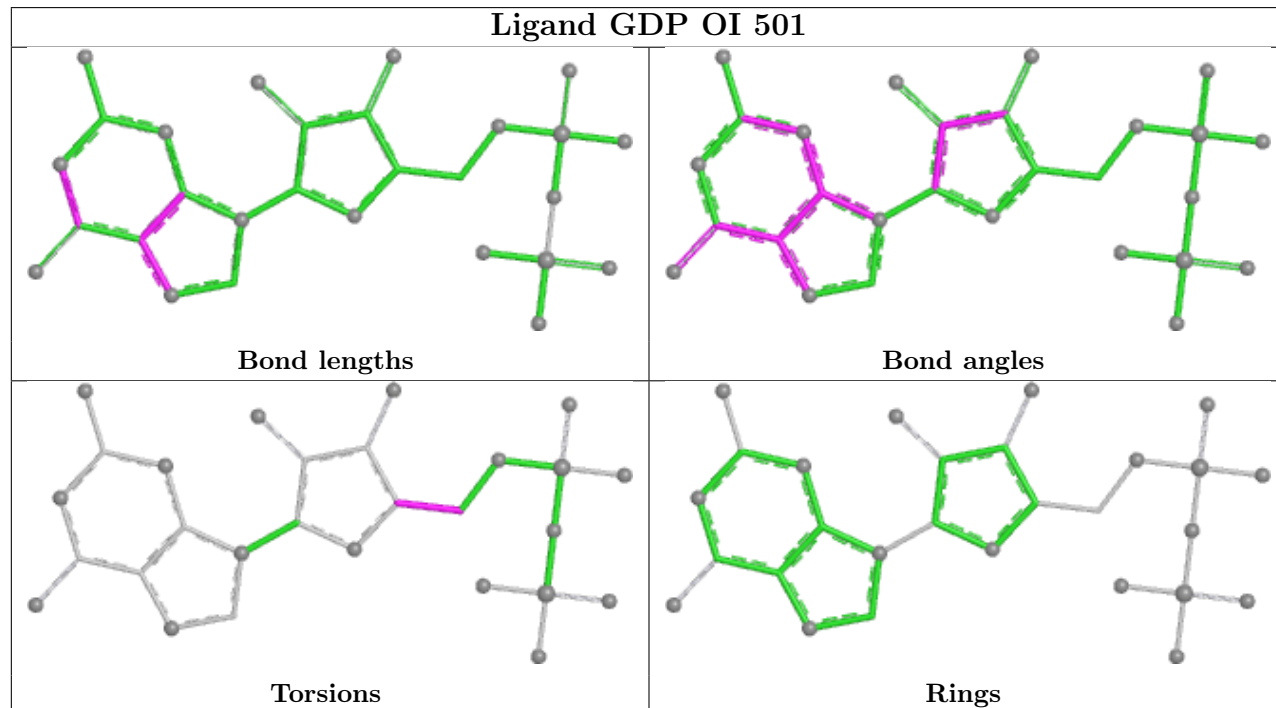
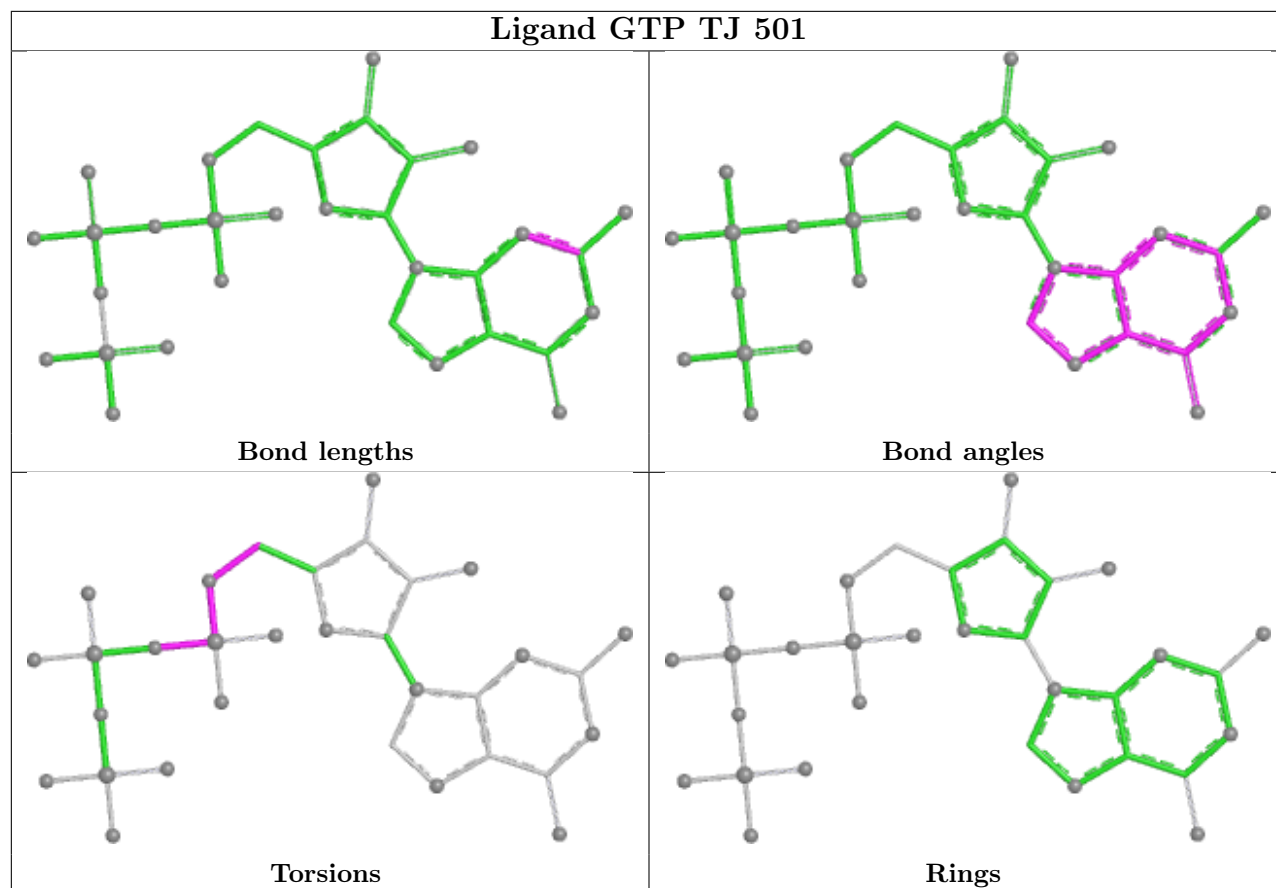


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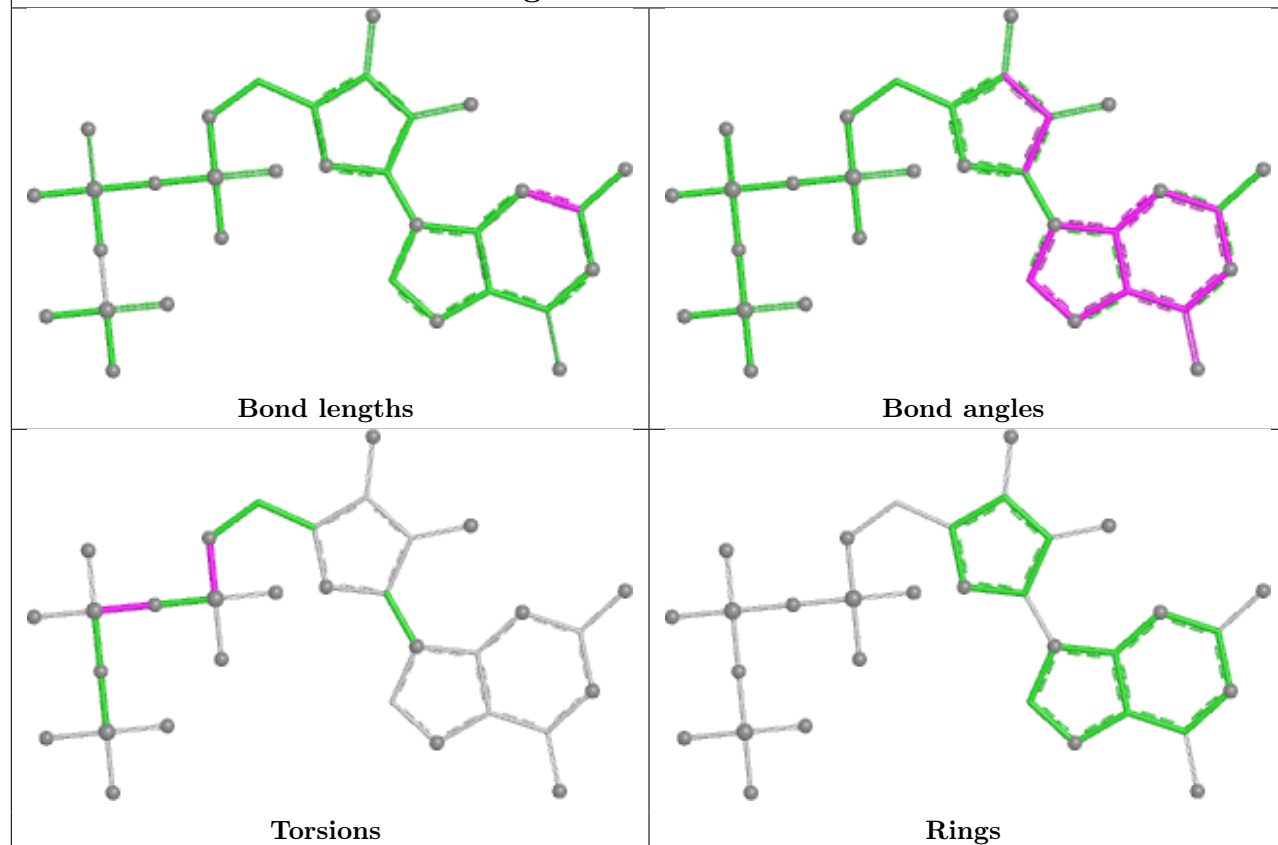


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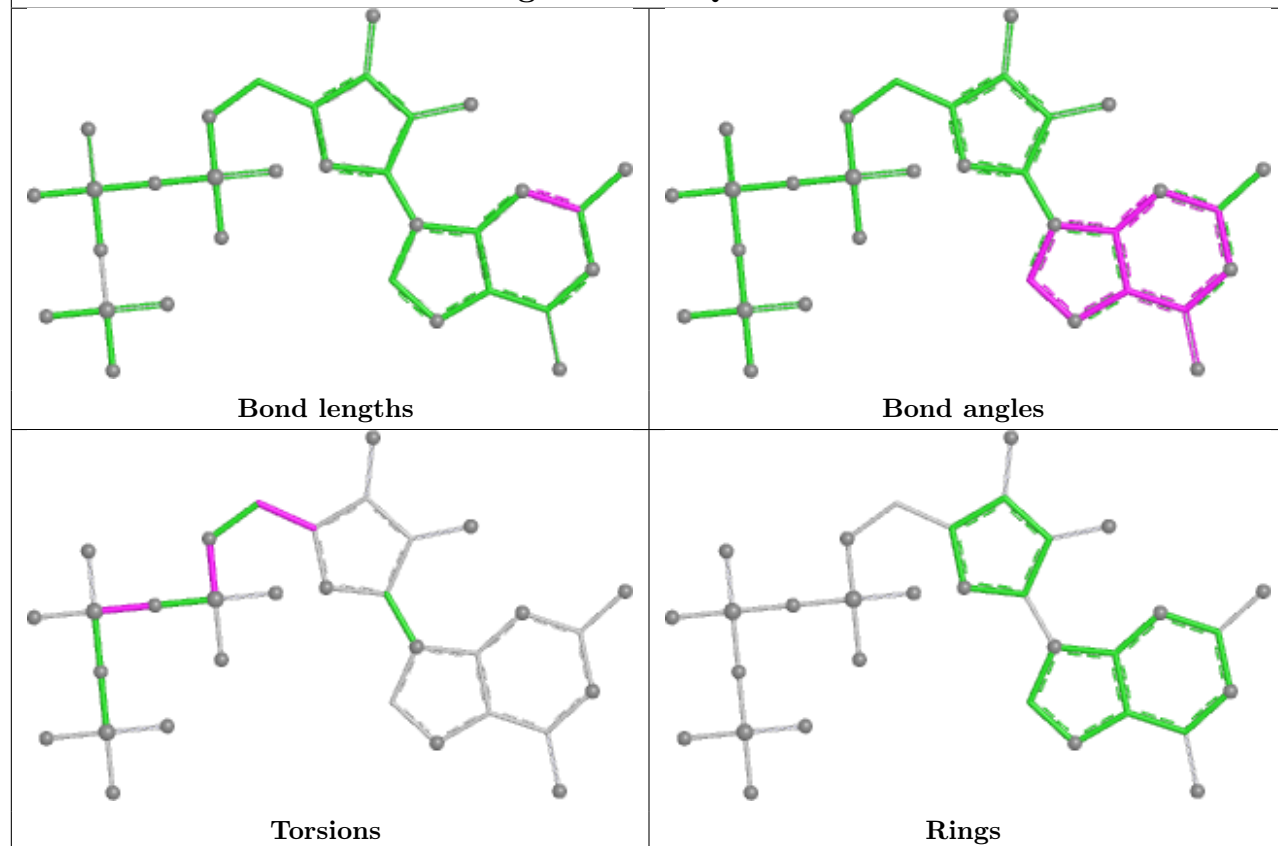


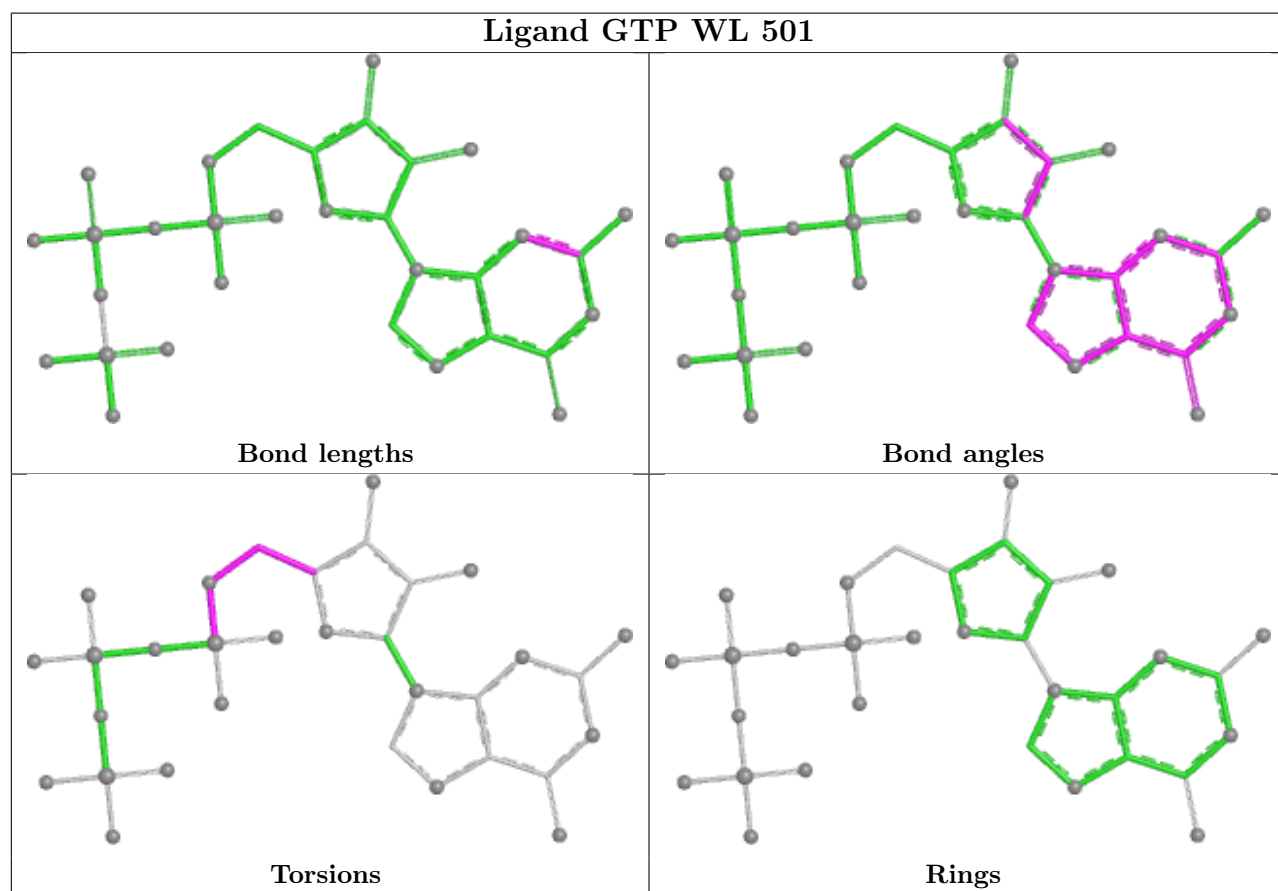
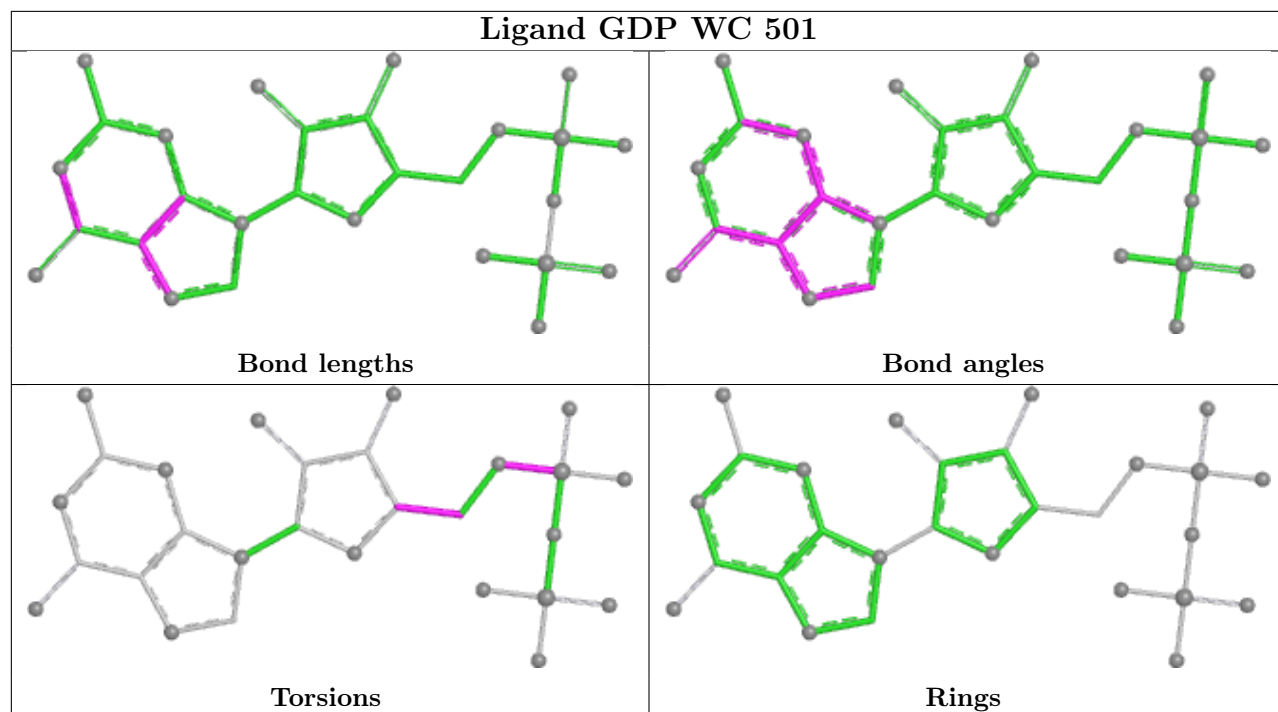


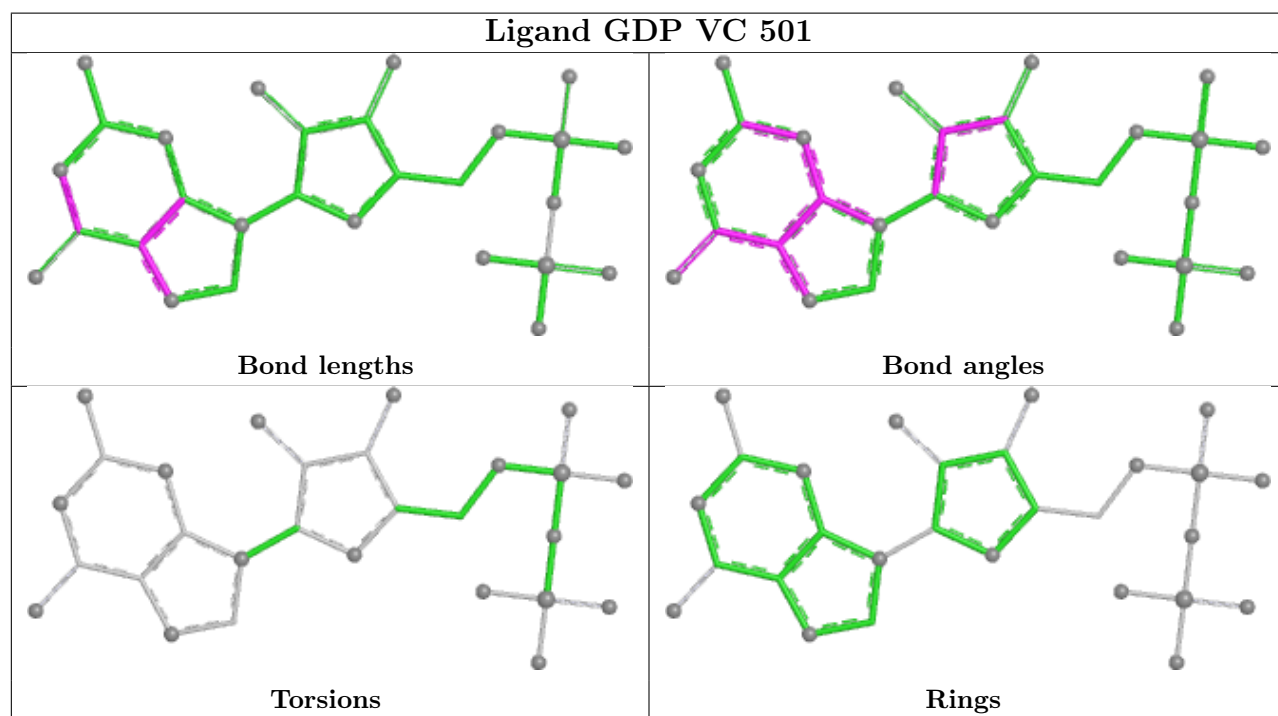
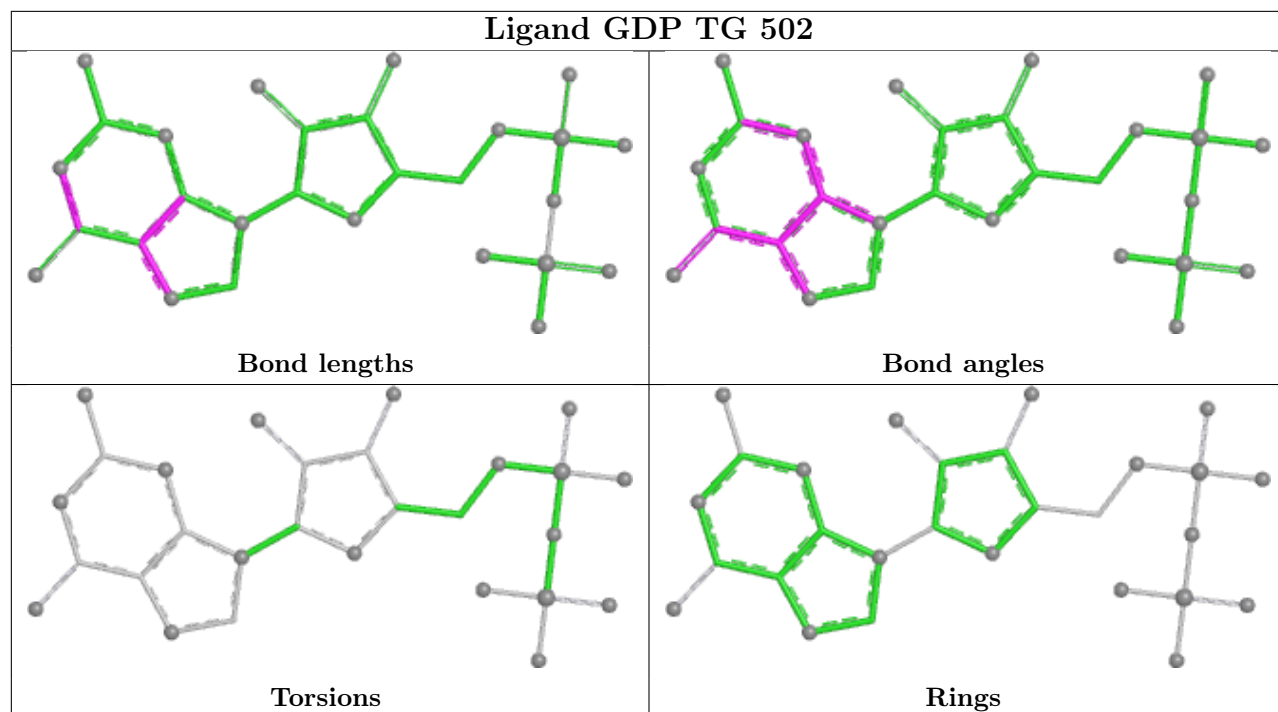
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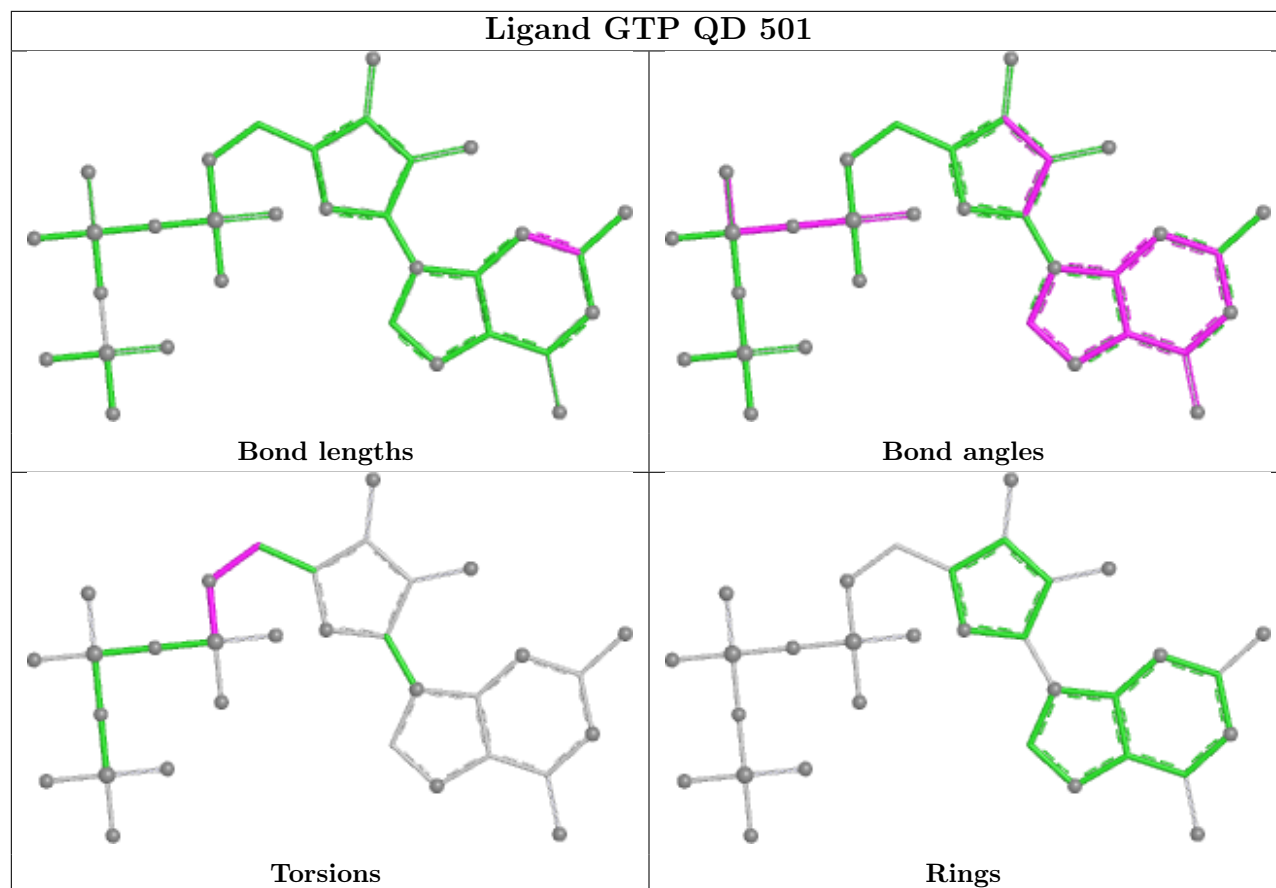
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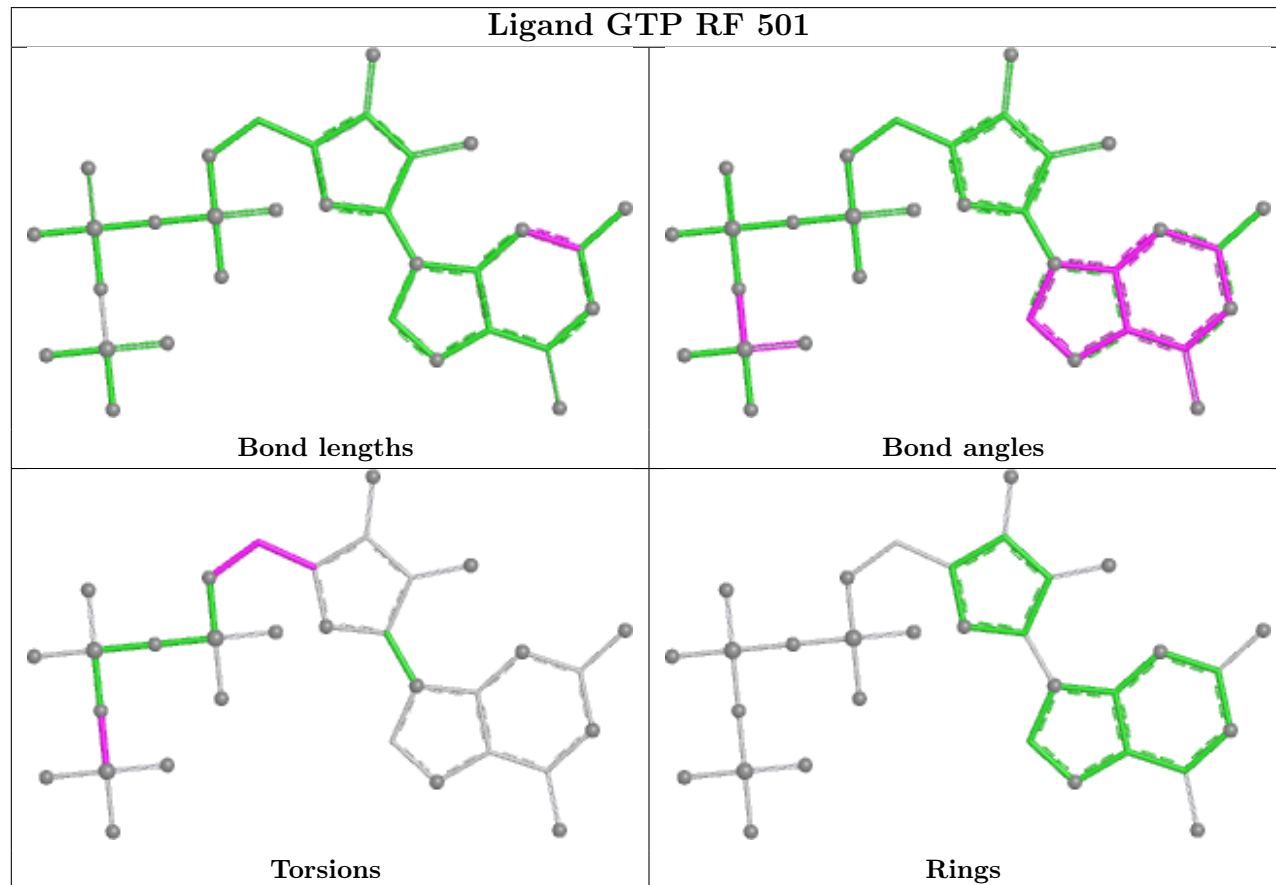


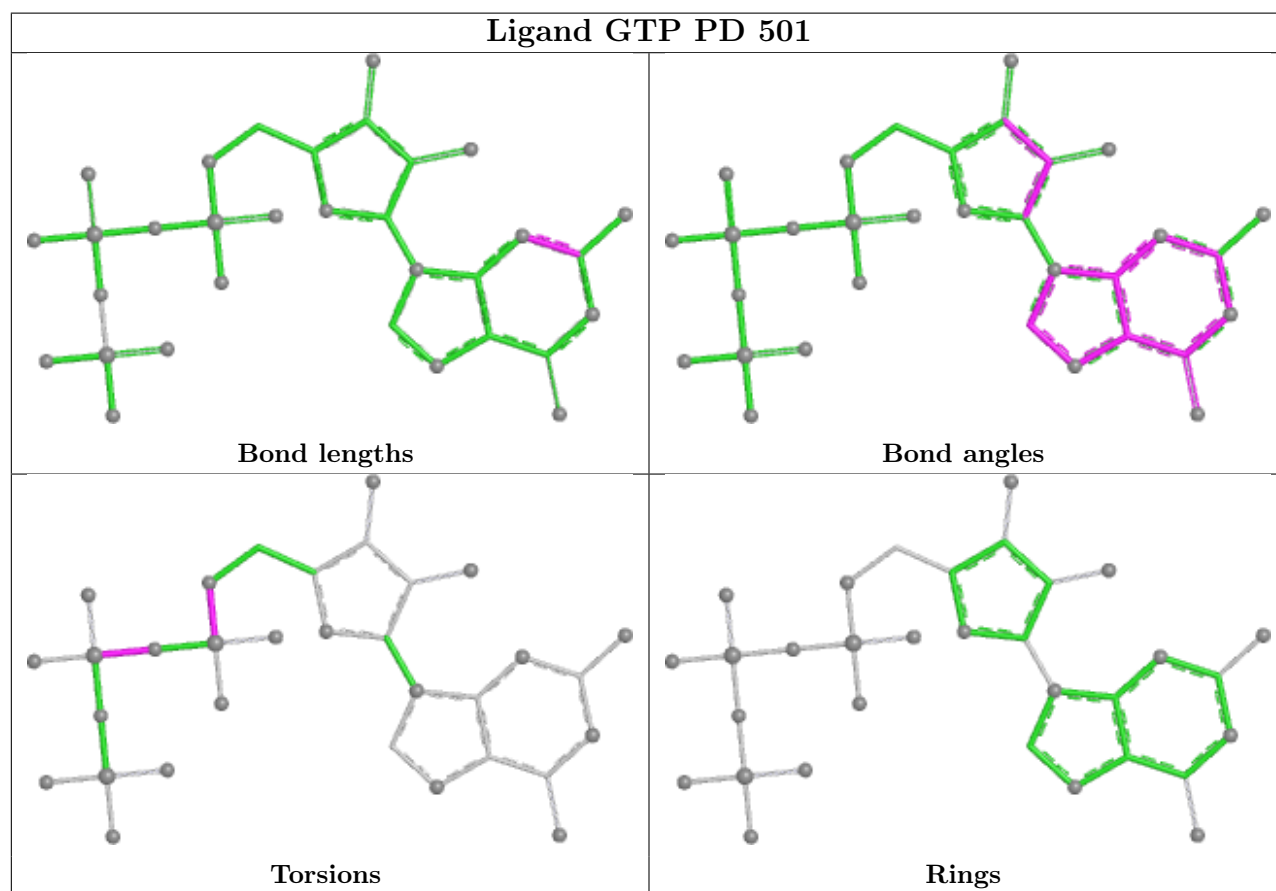
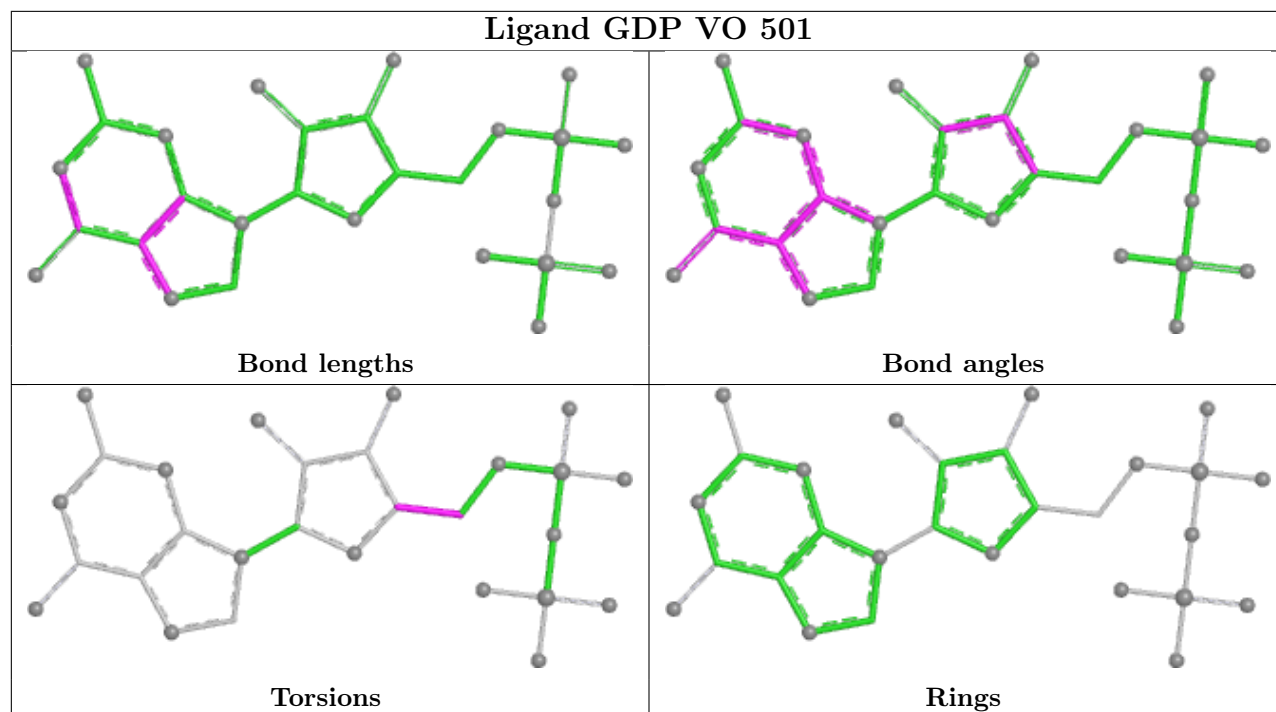


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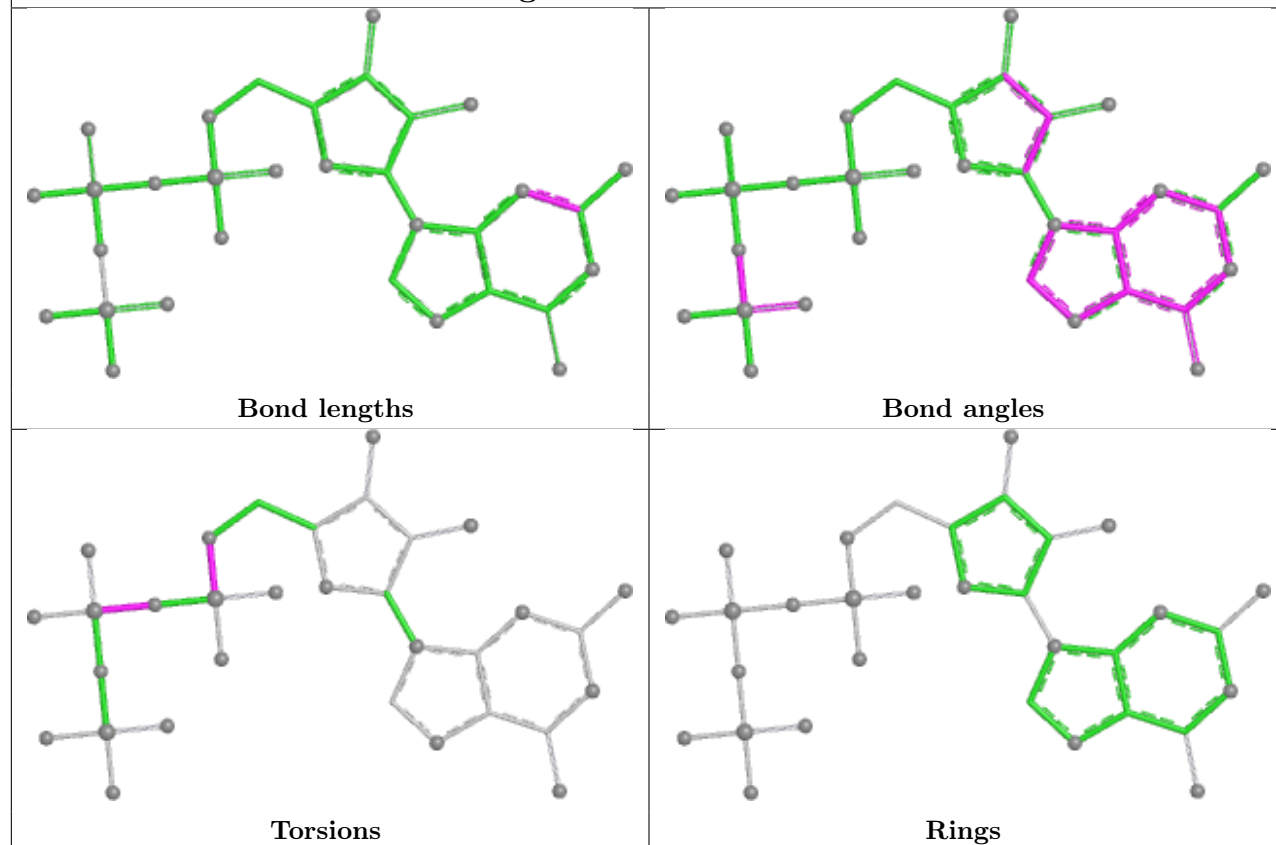


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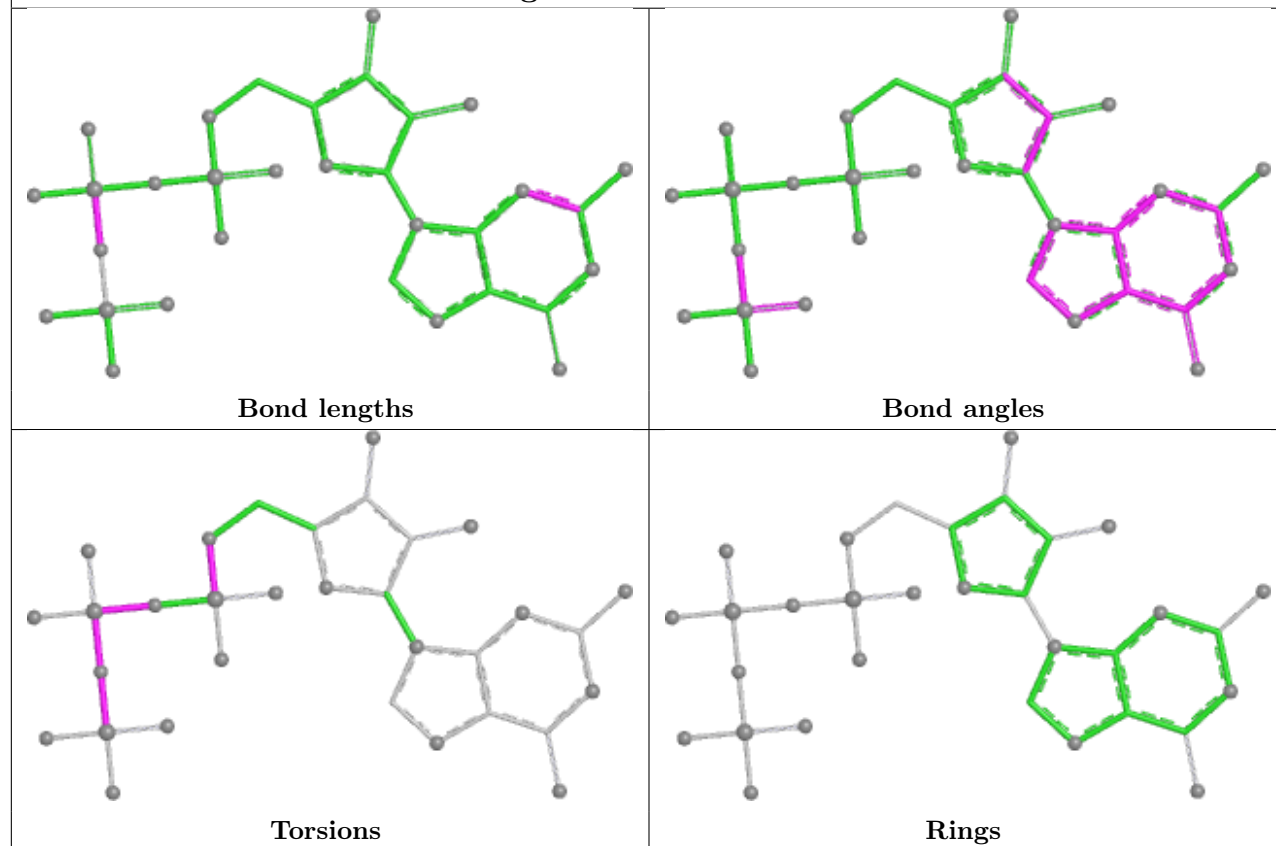


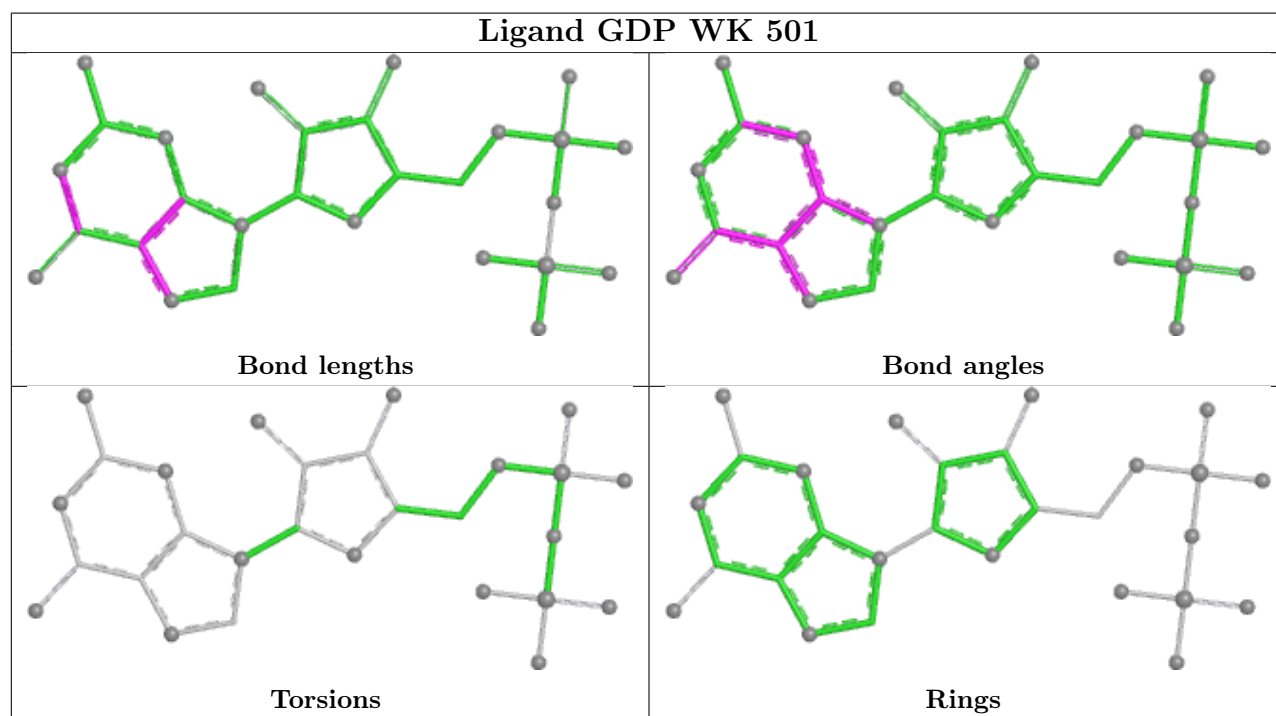
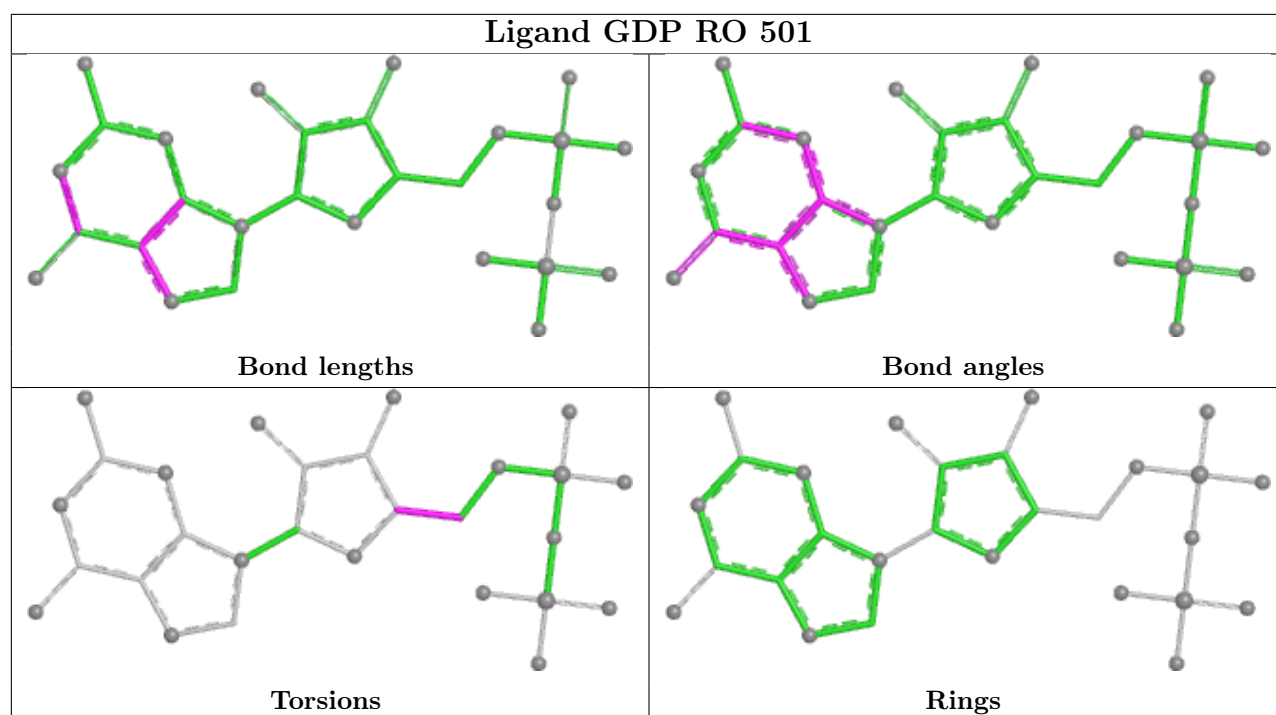


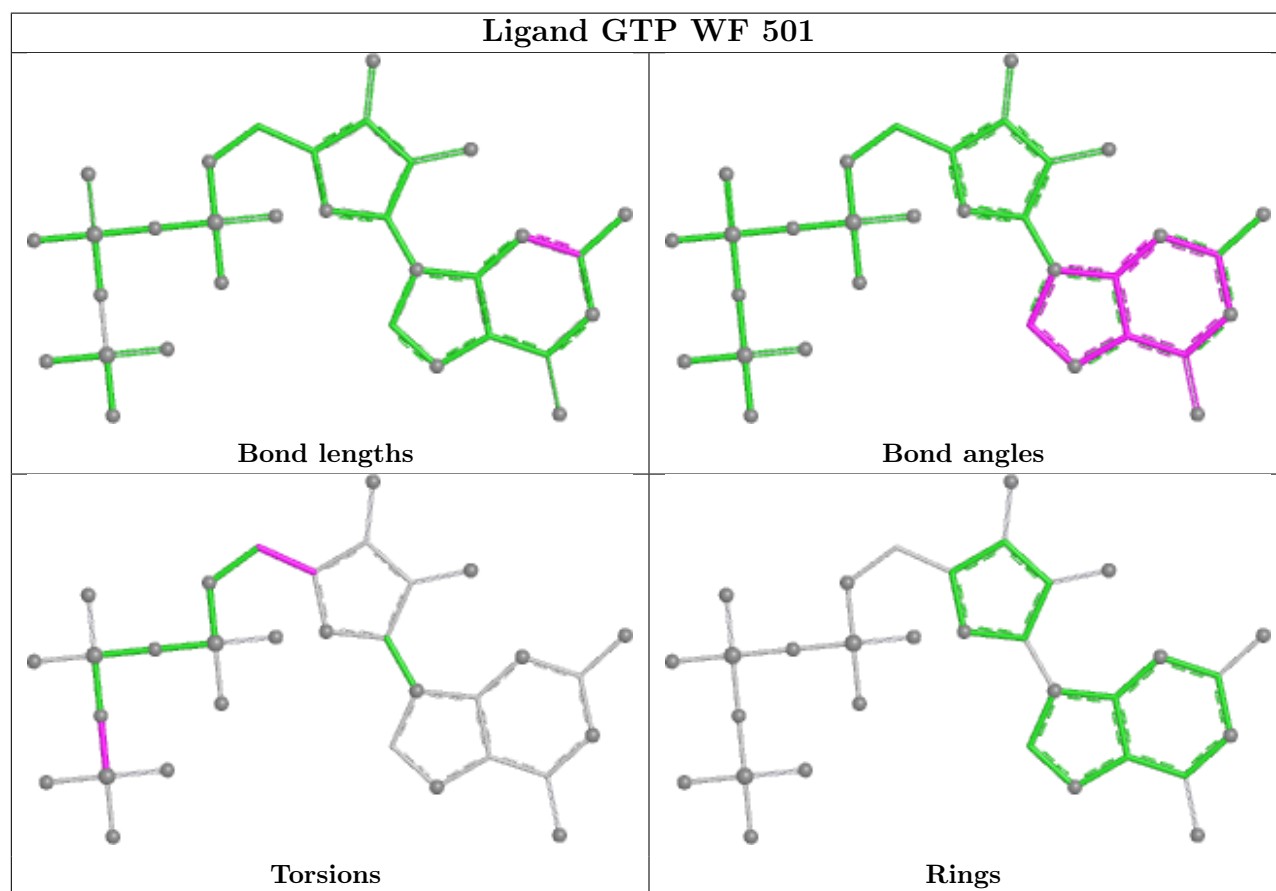
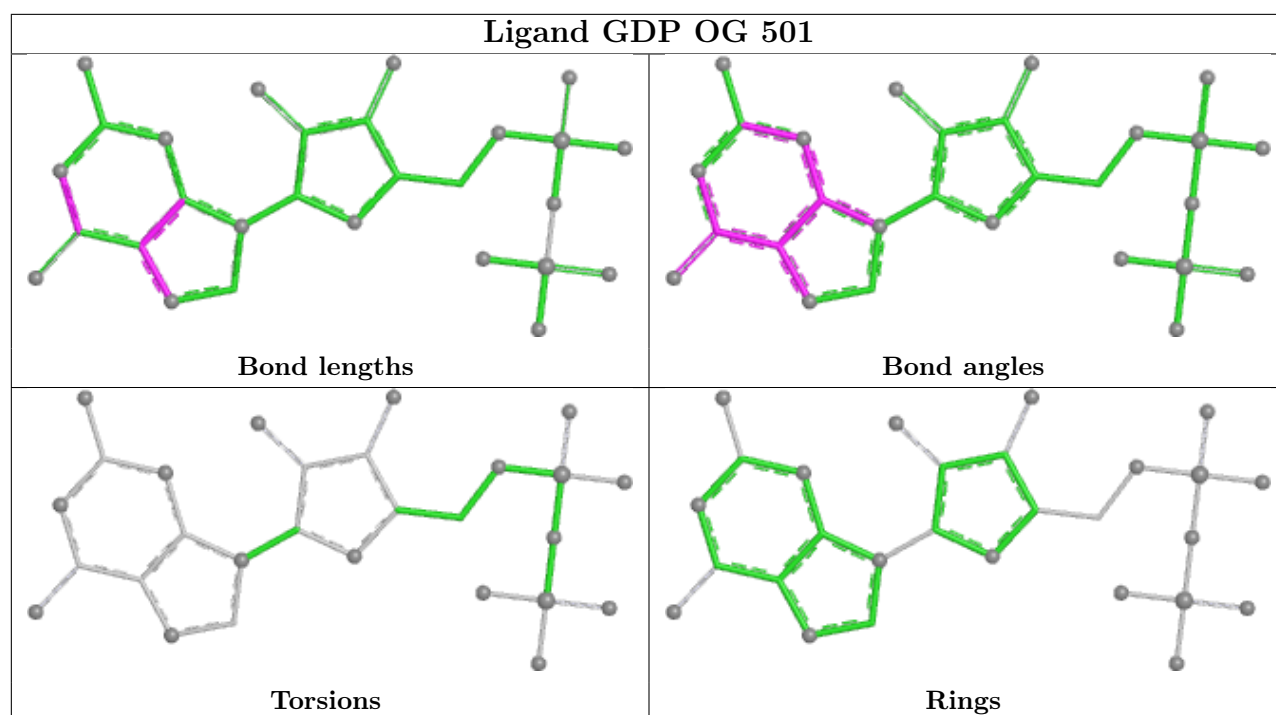
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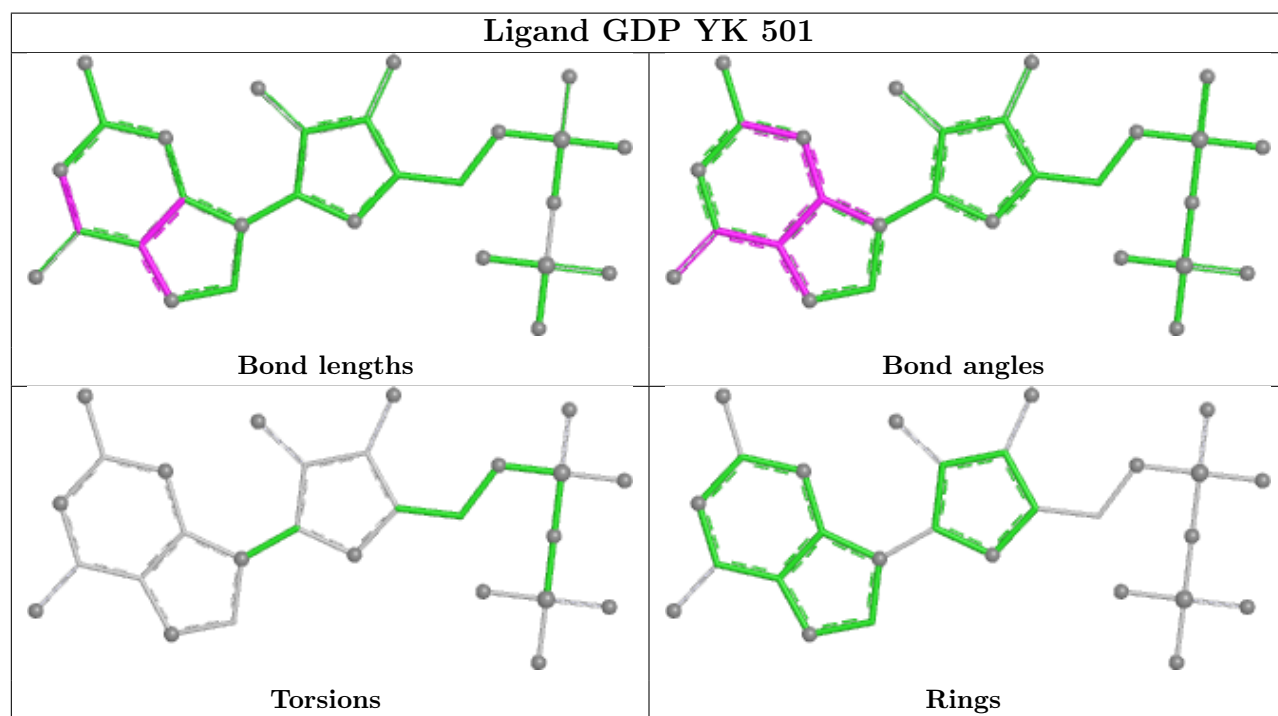
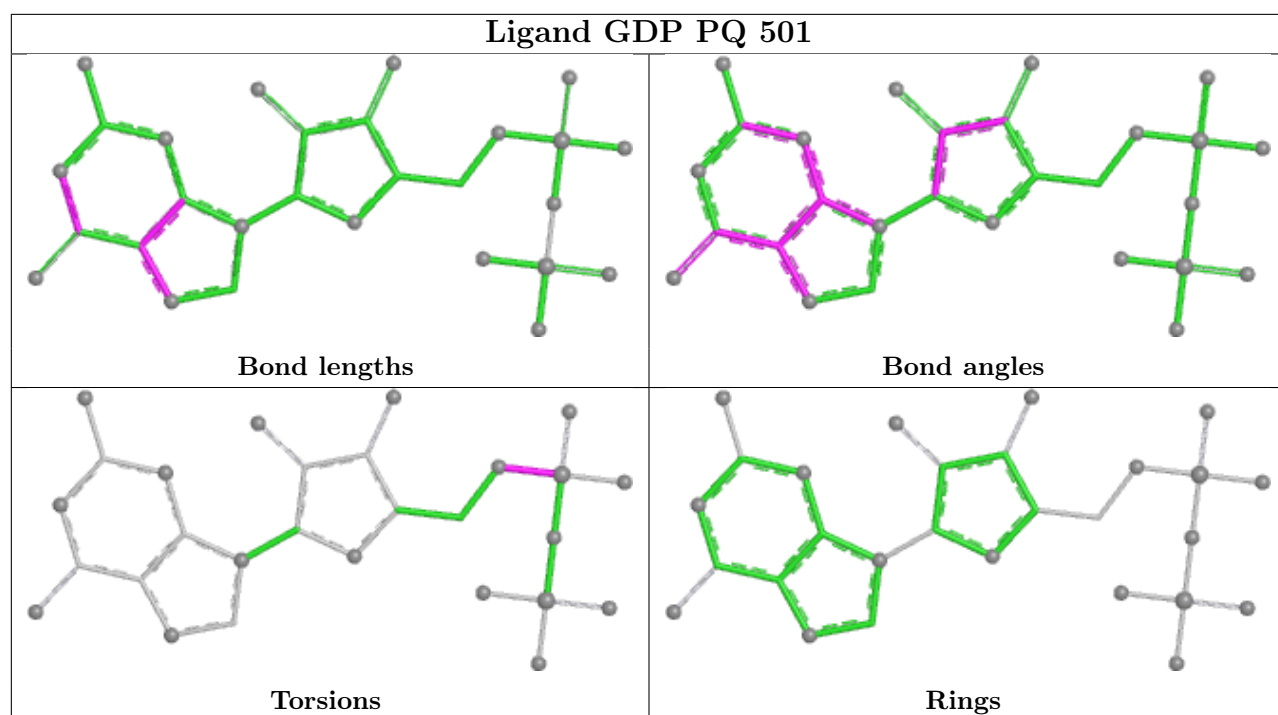


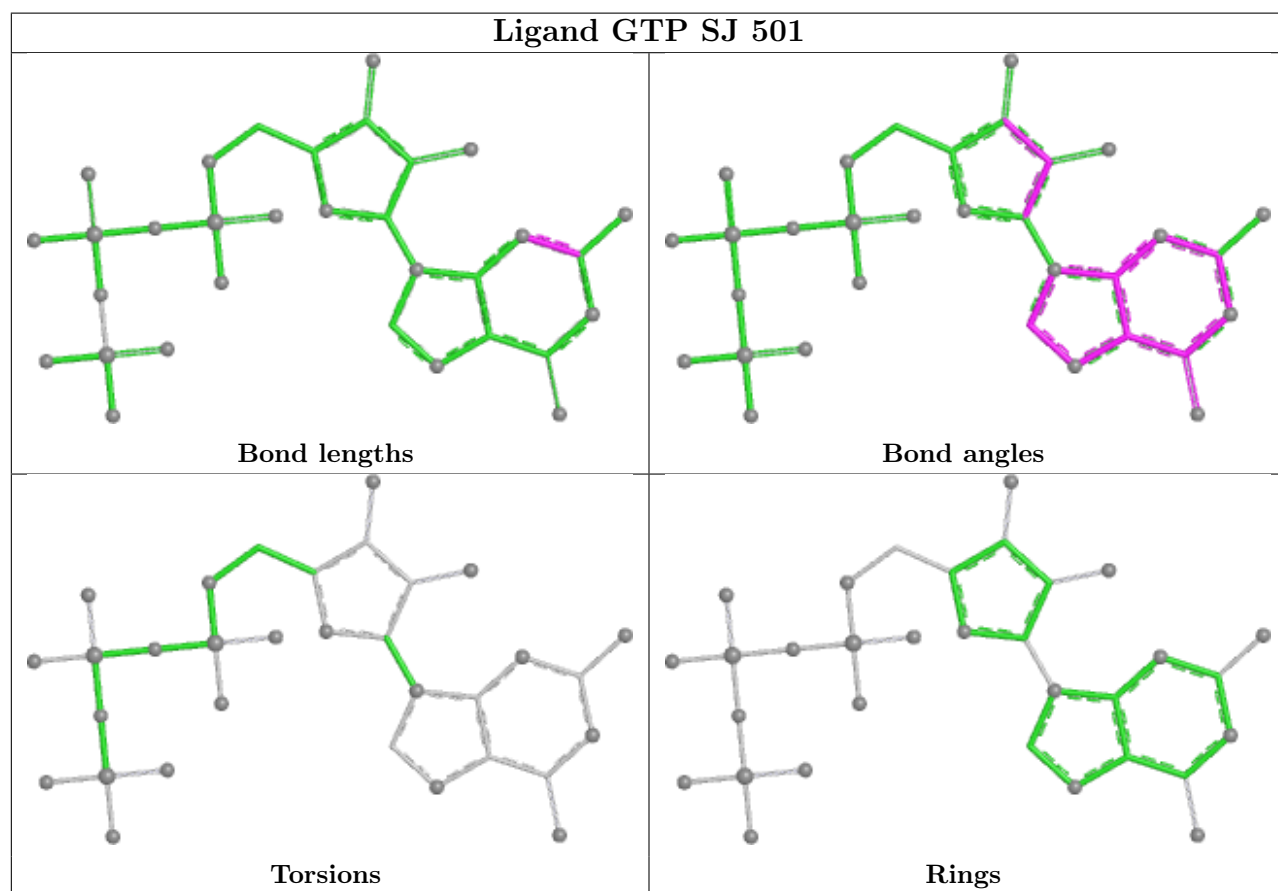
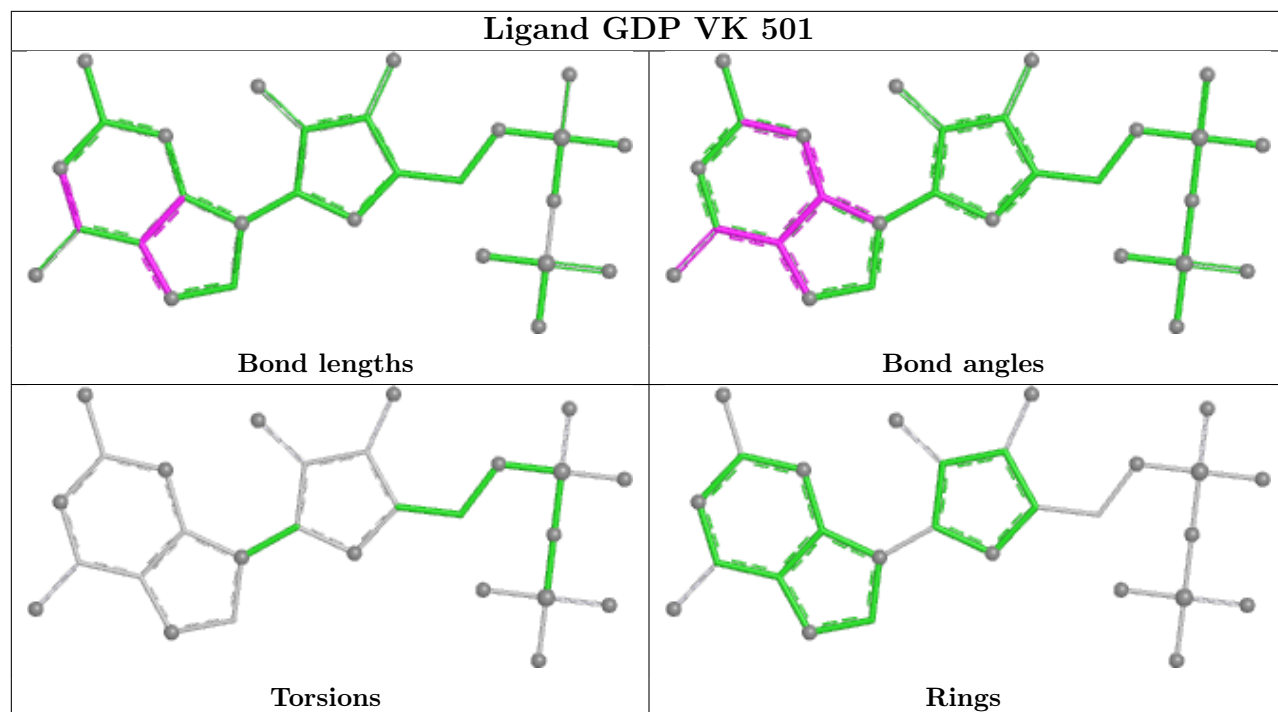
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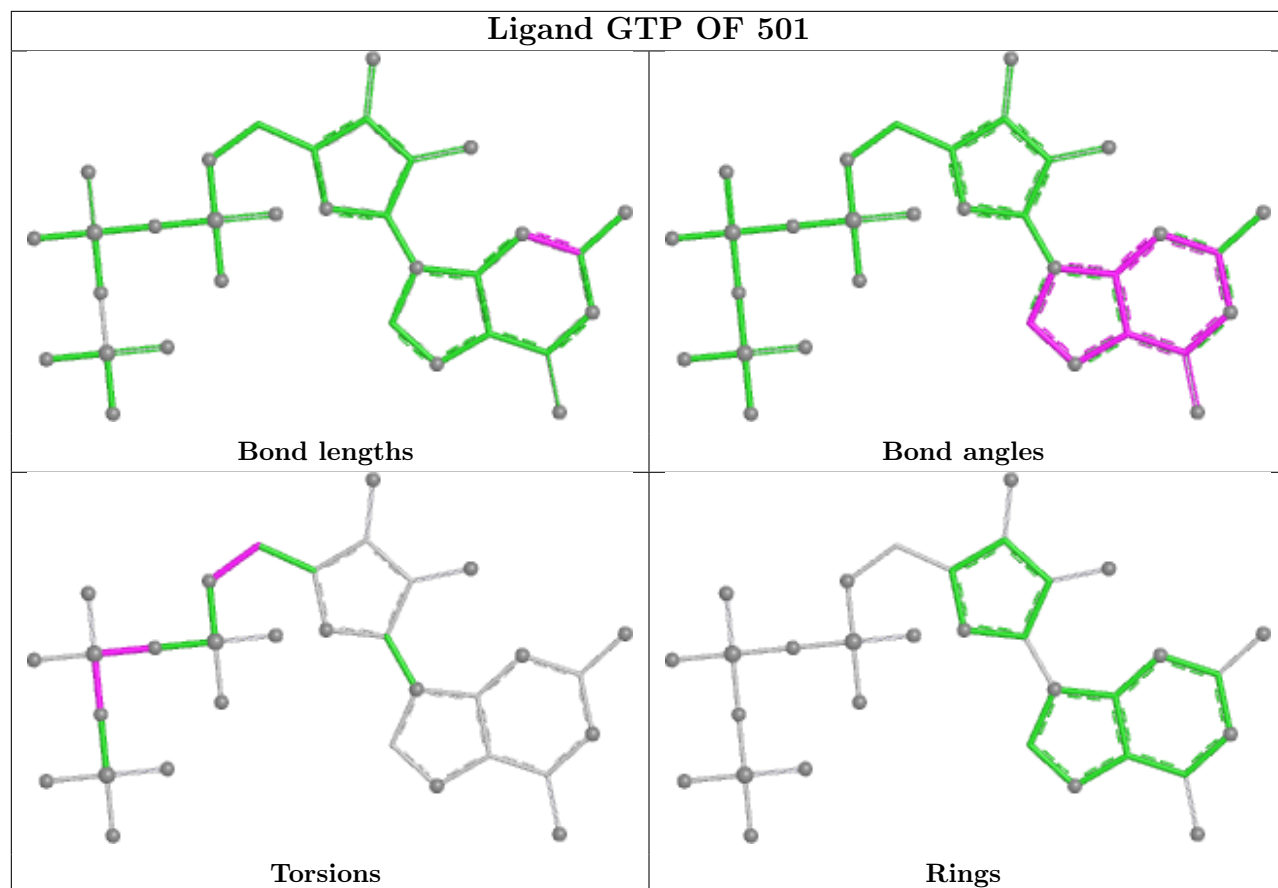




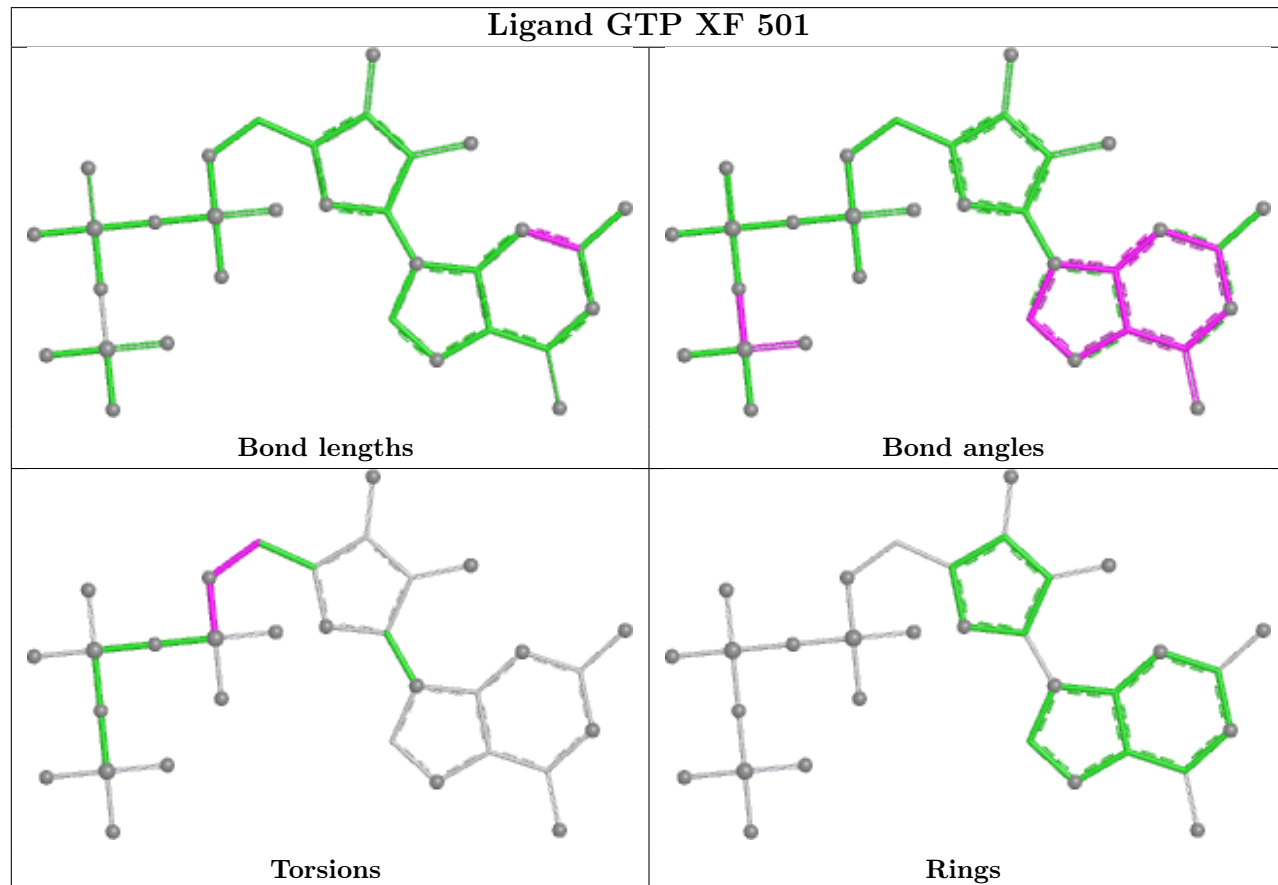




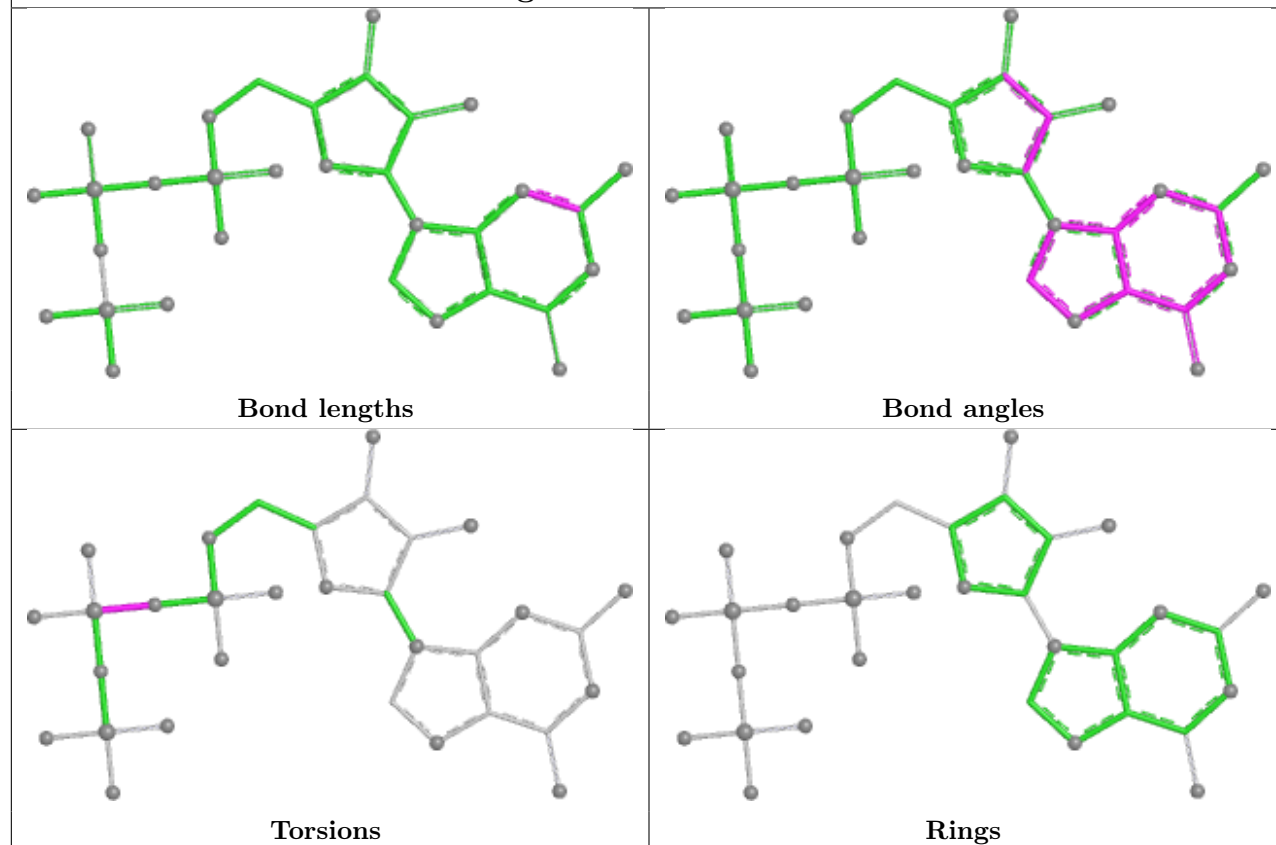
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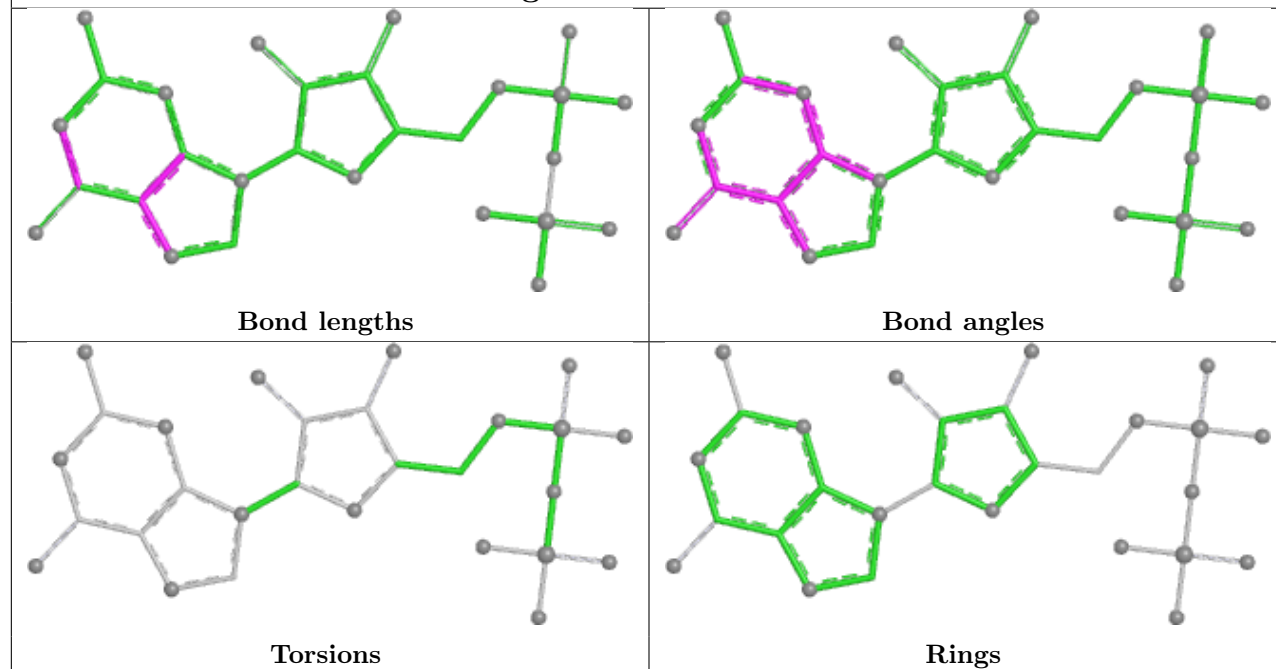
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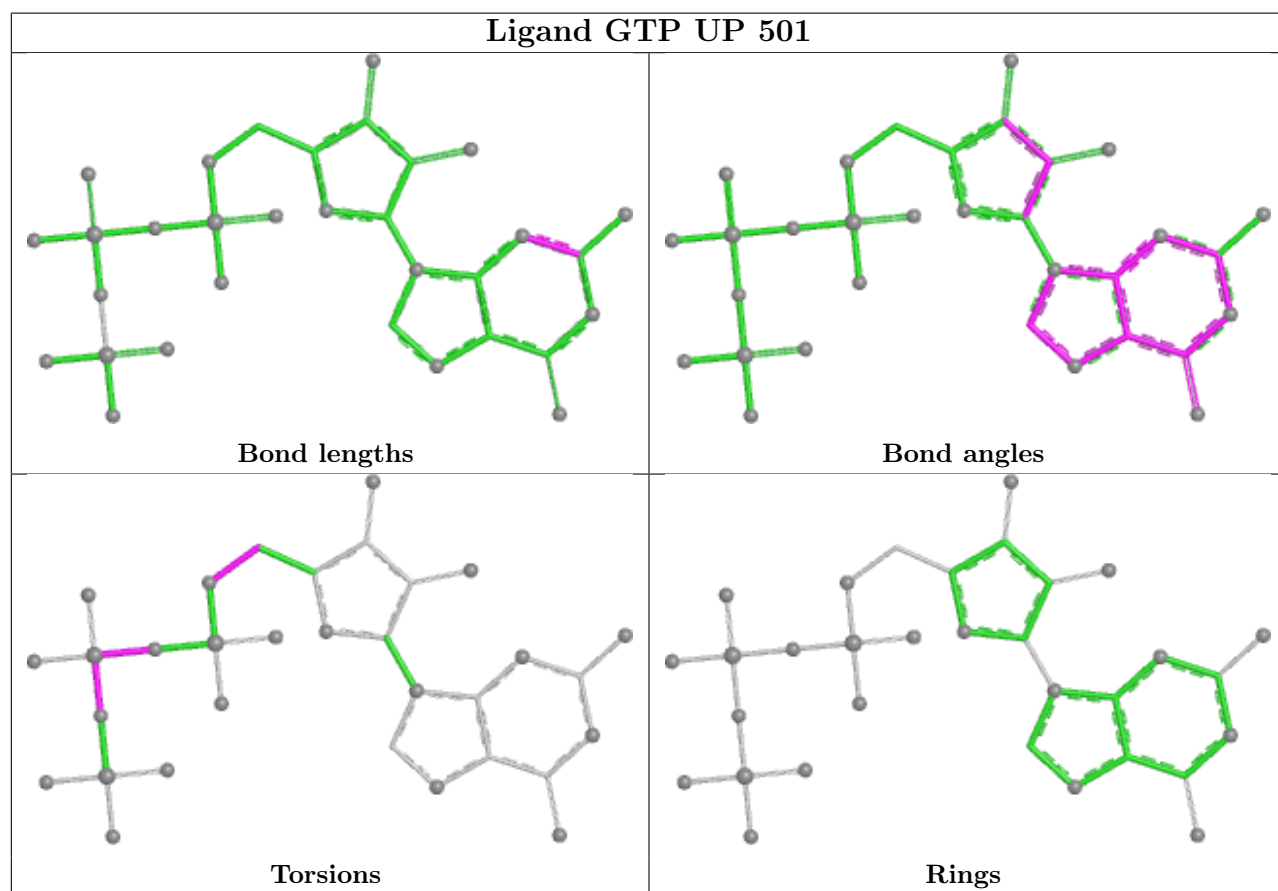
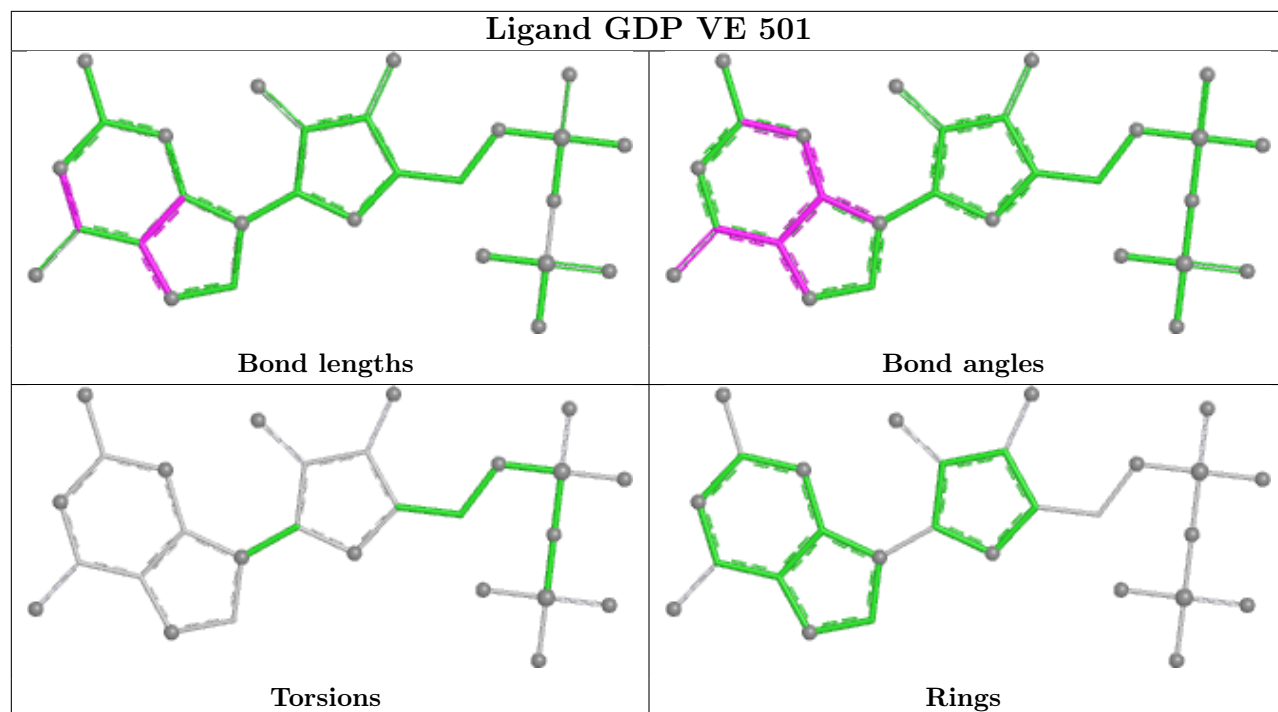


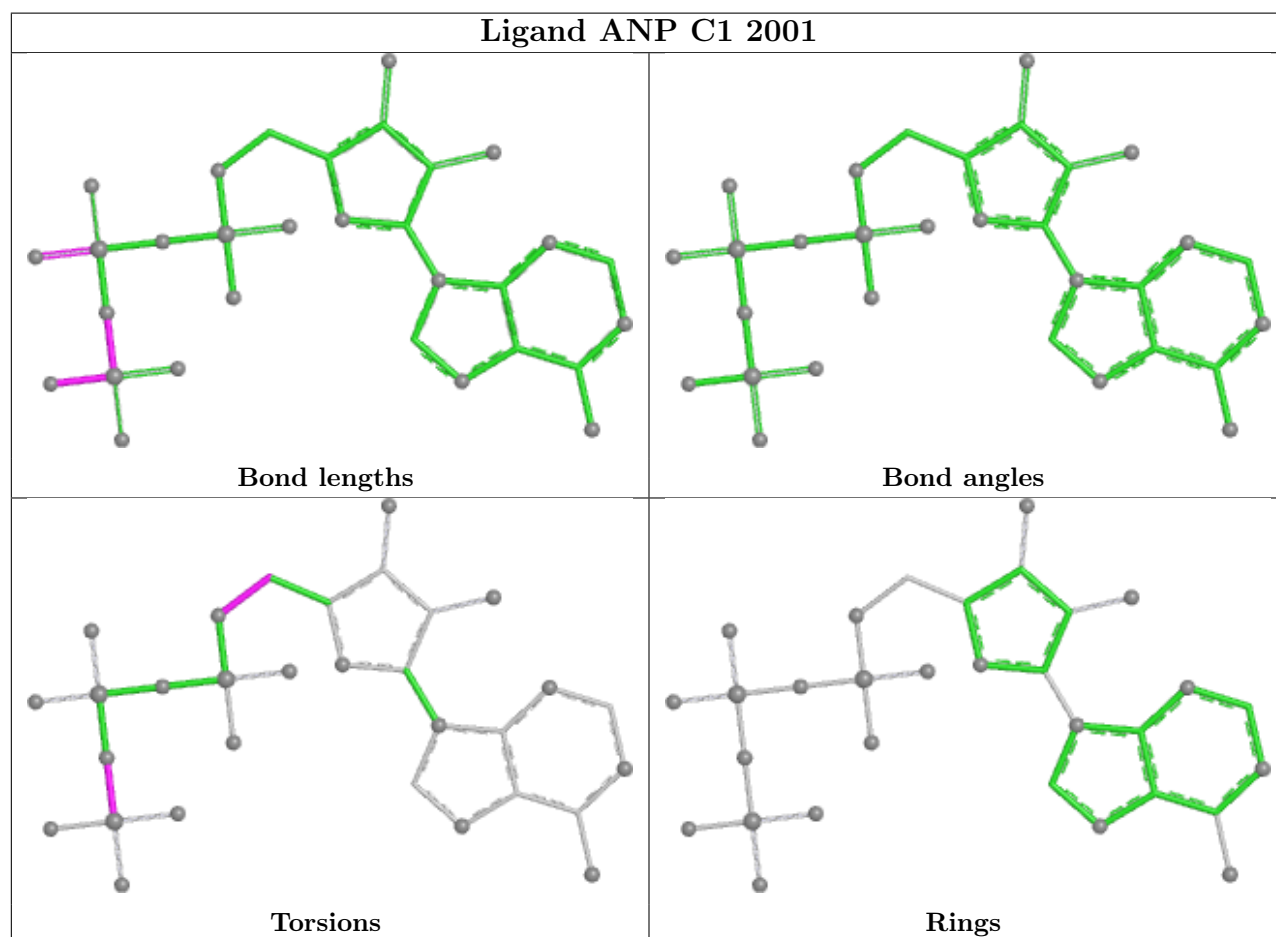
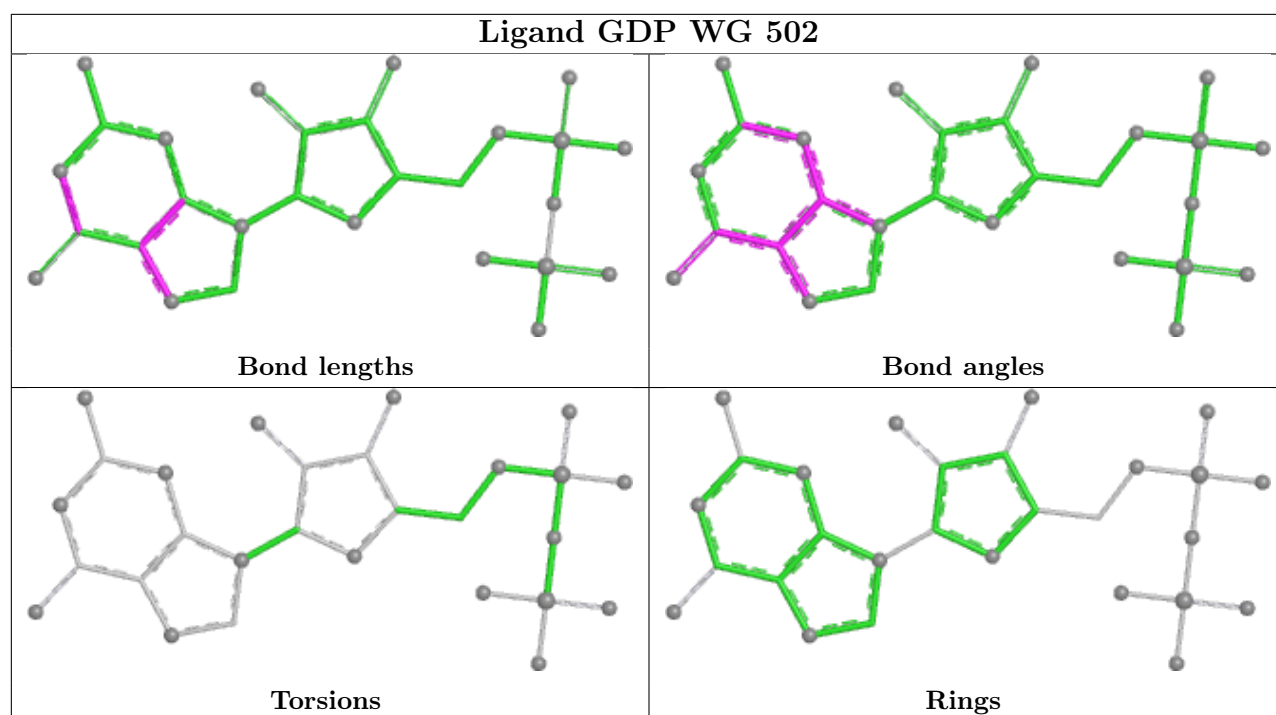
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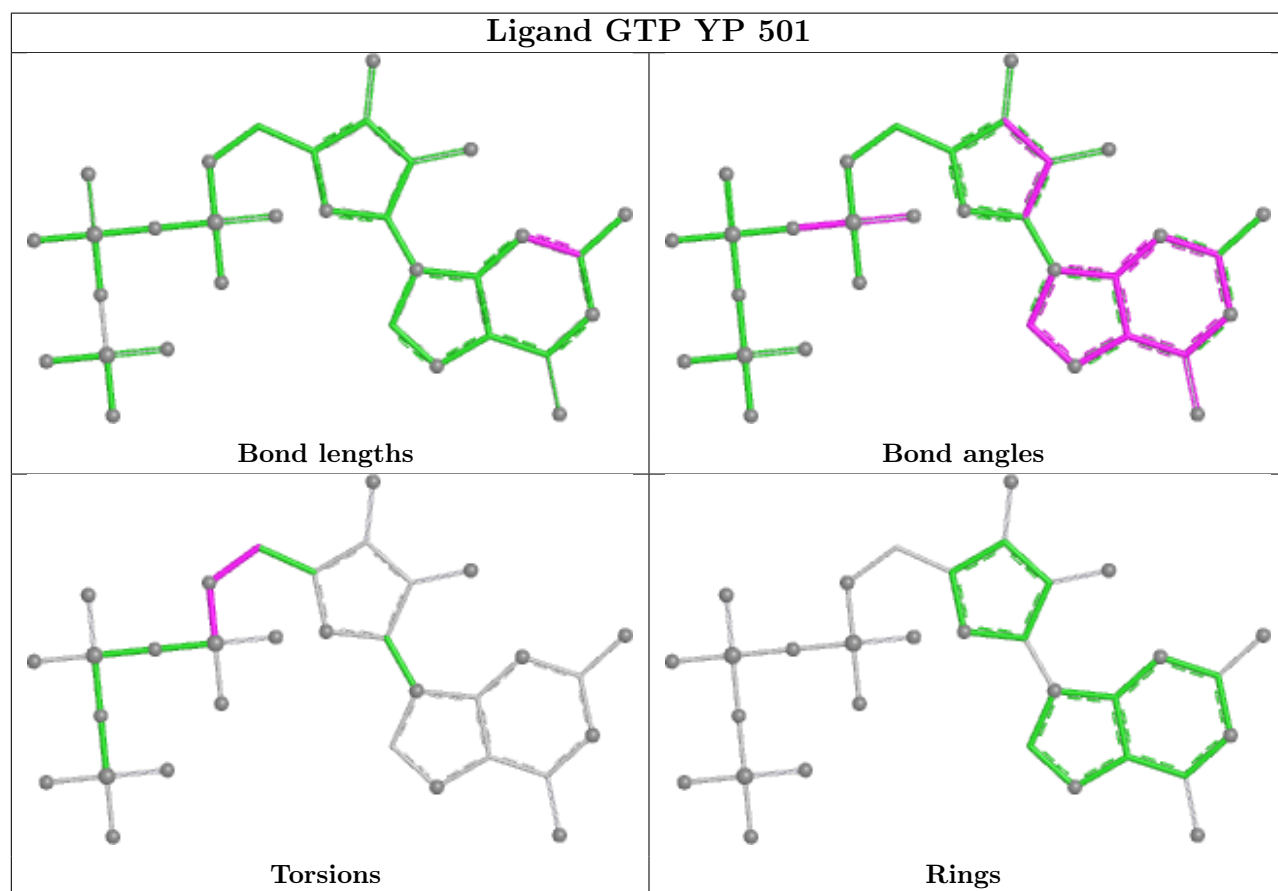
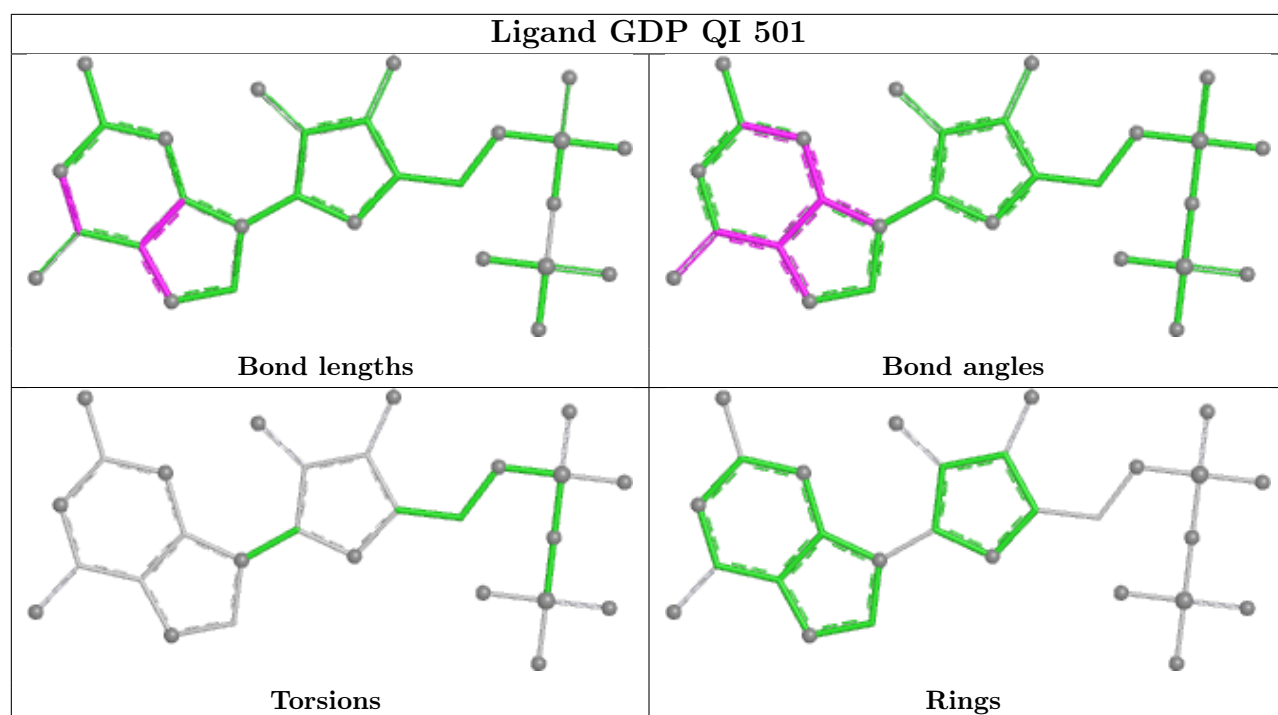


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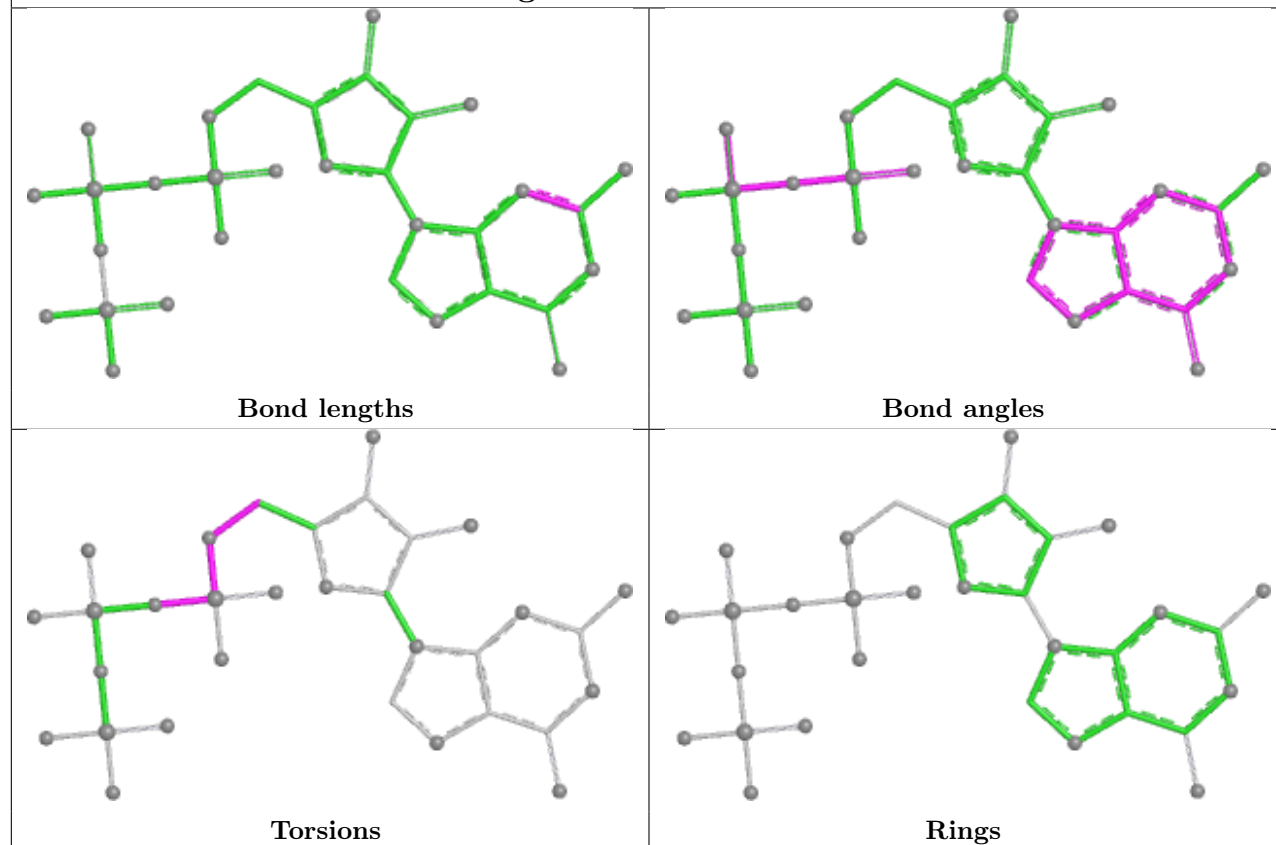




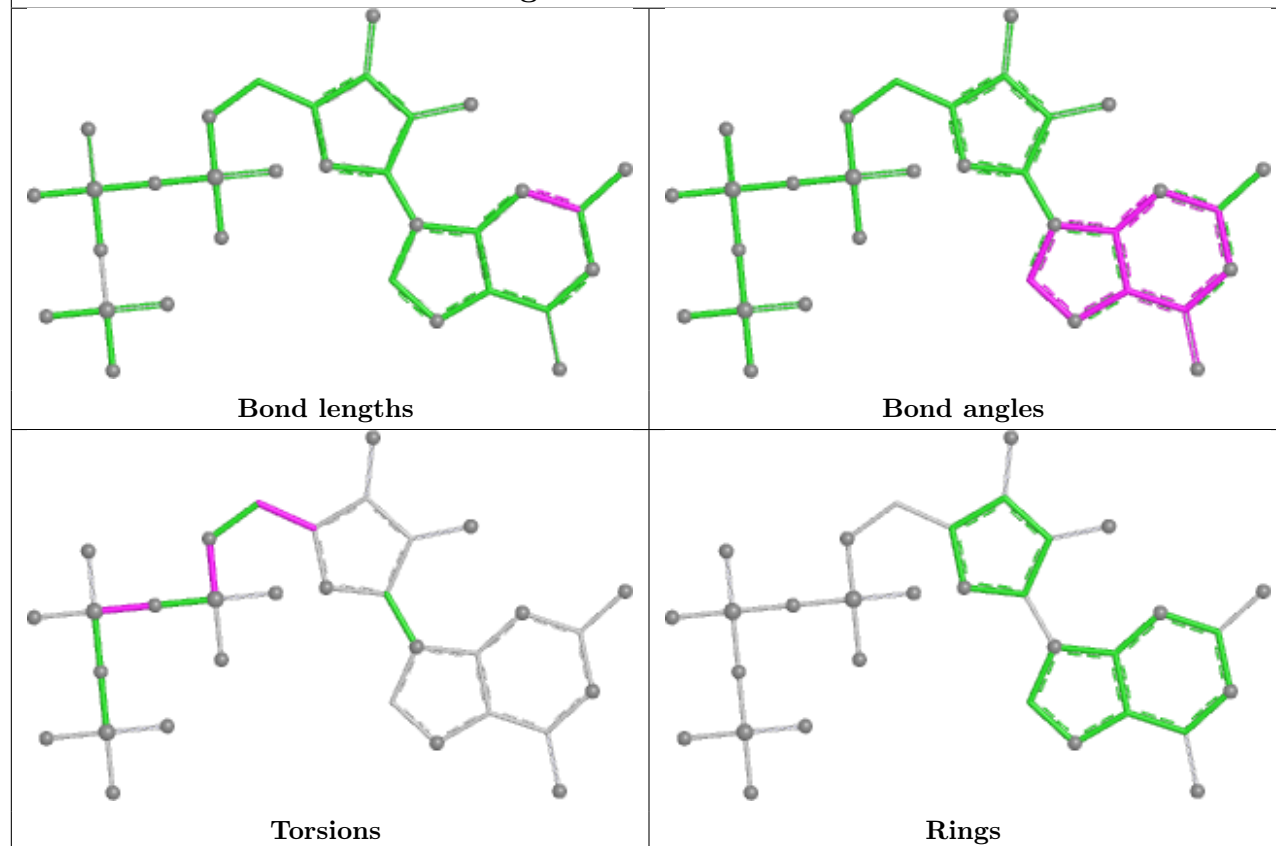


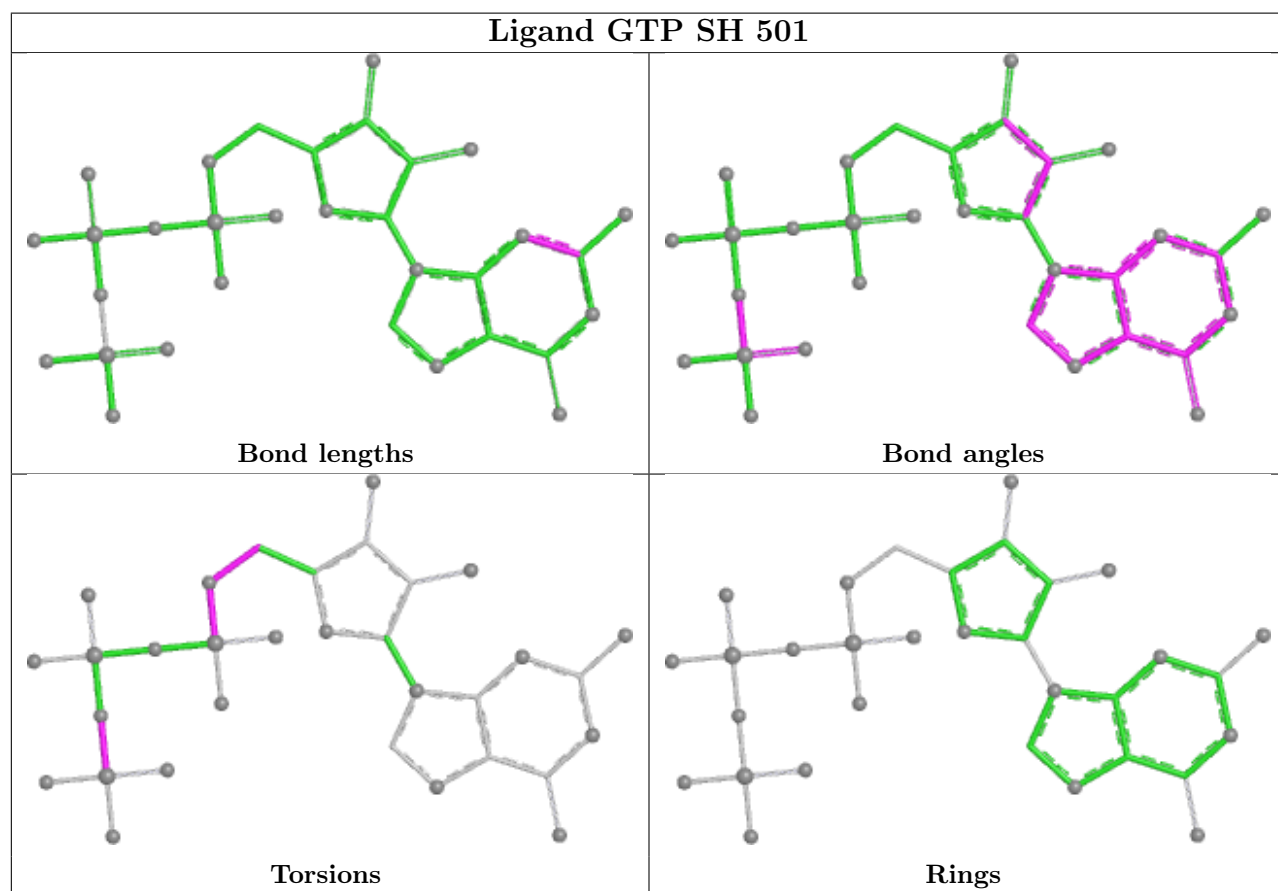
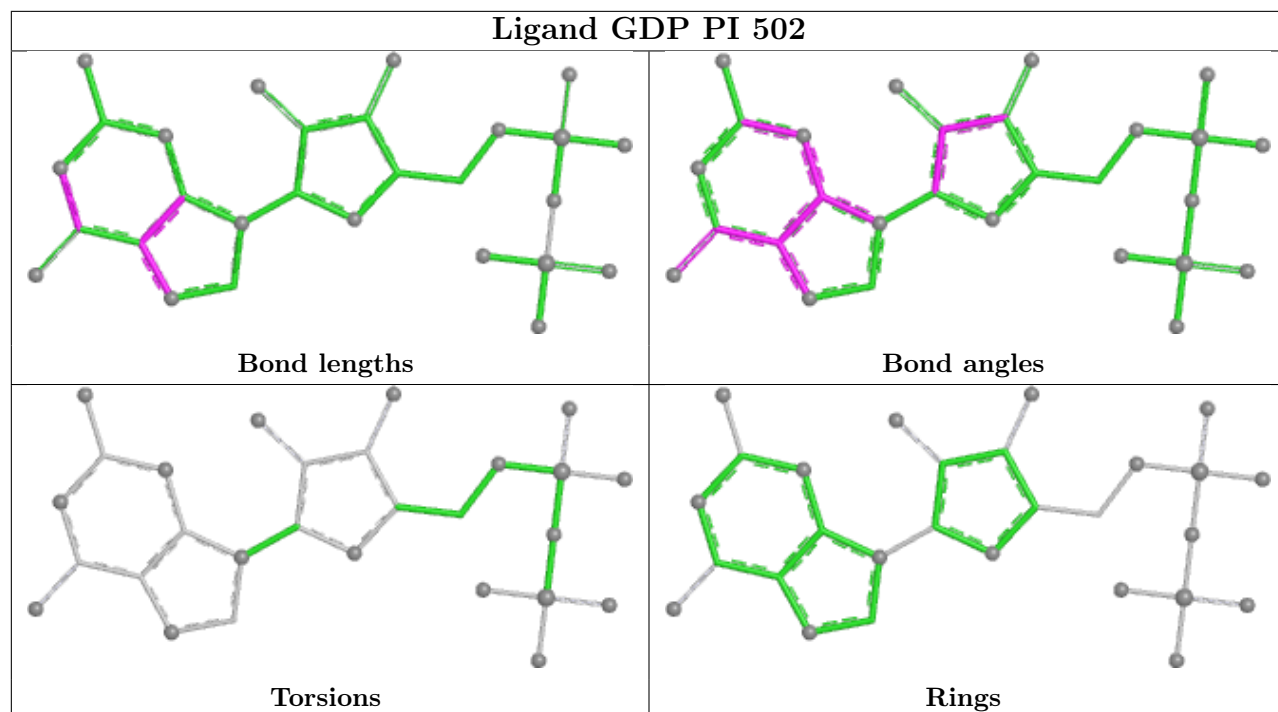


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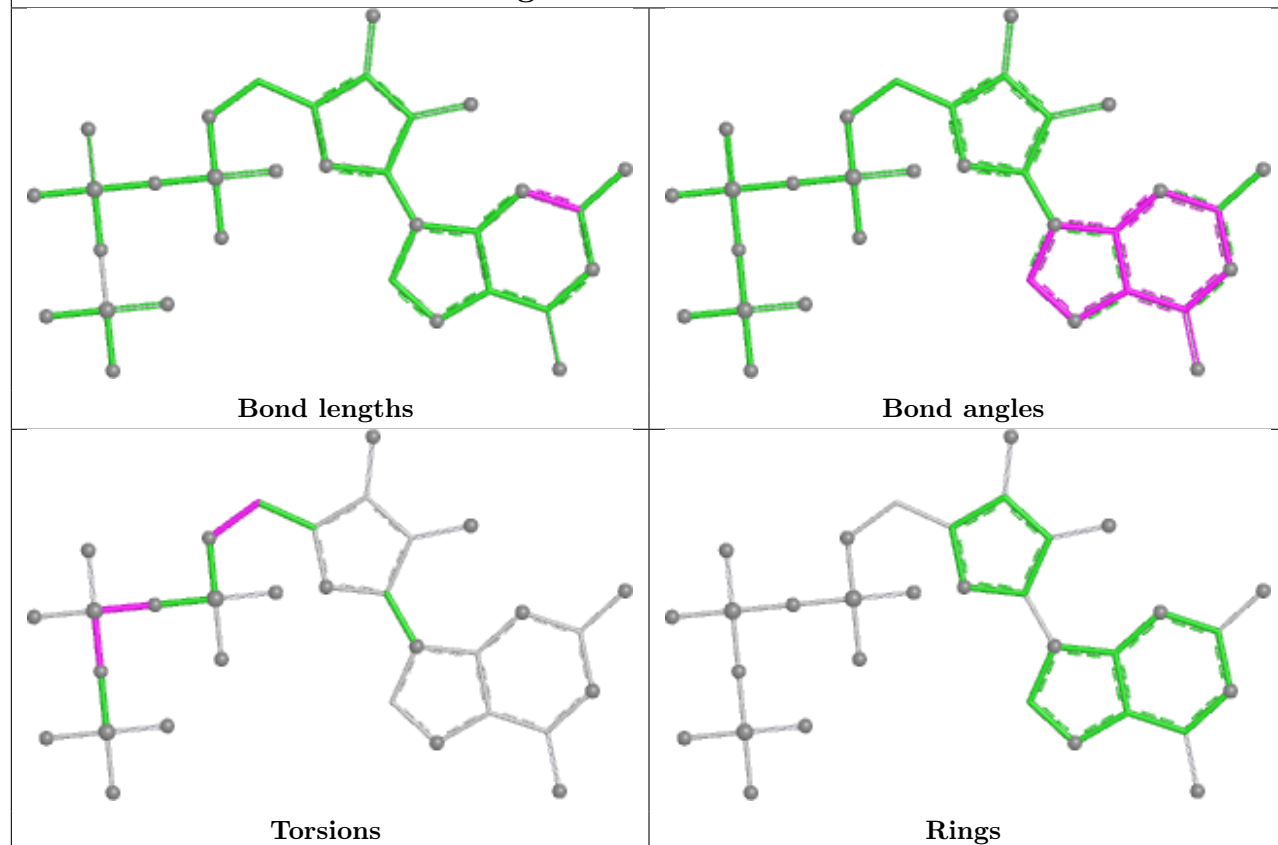


Ligand GTP SD 501

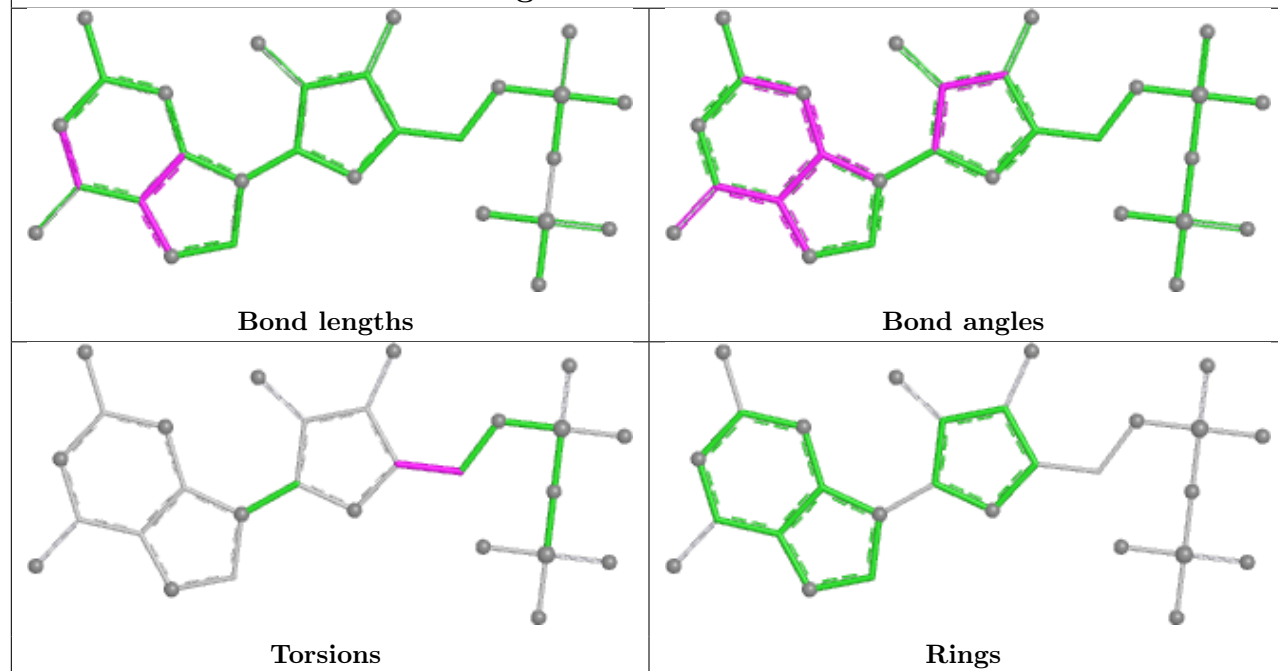


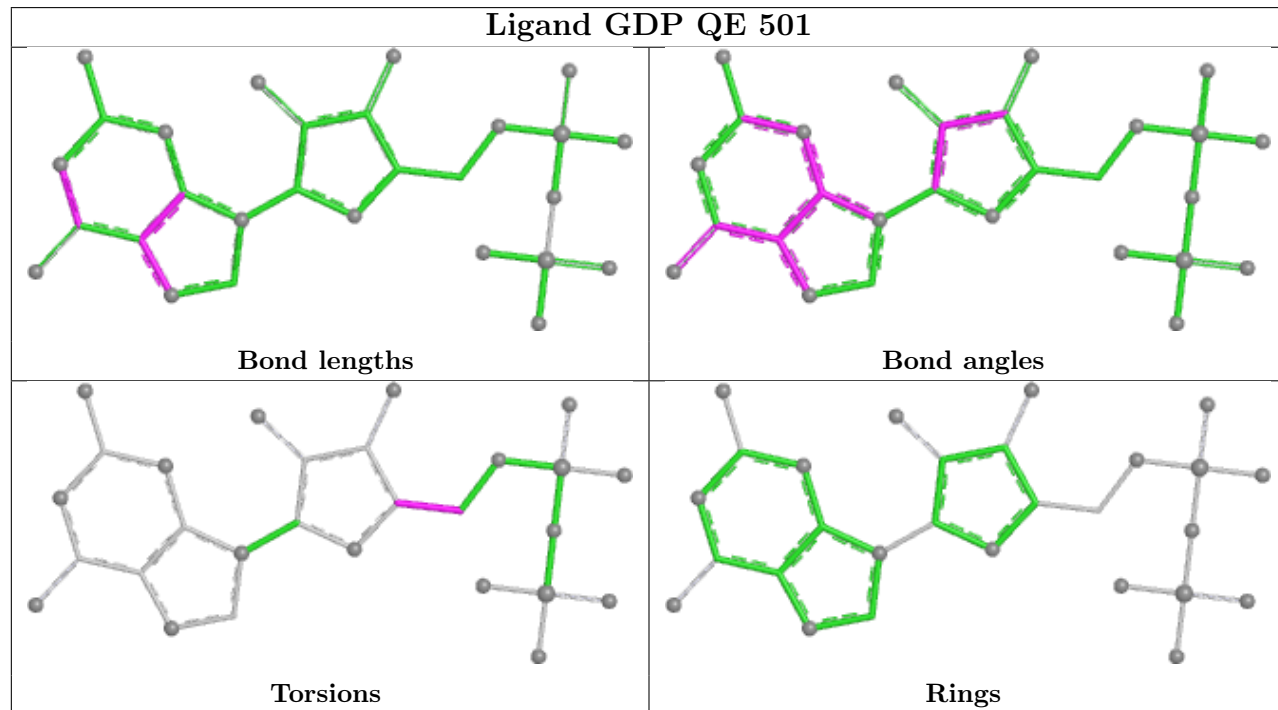
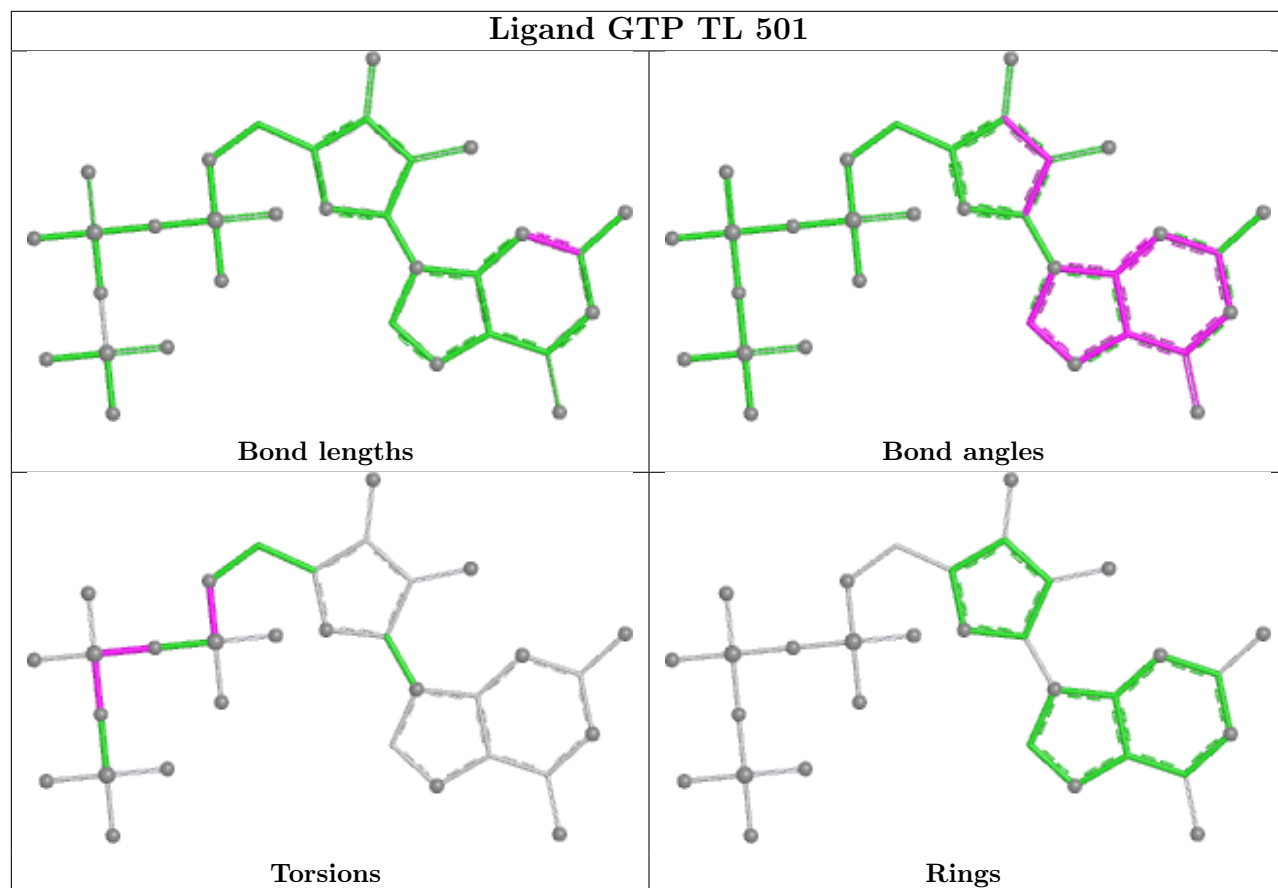


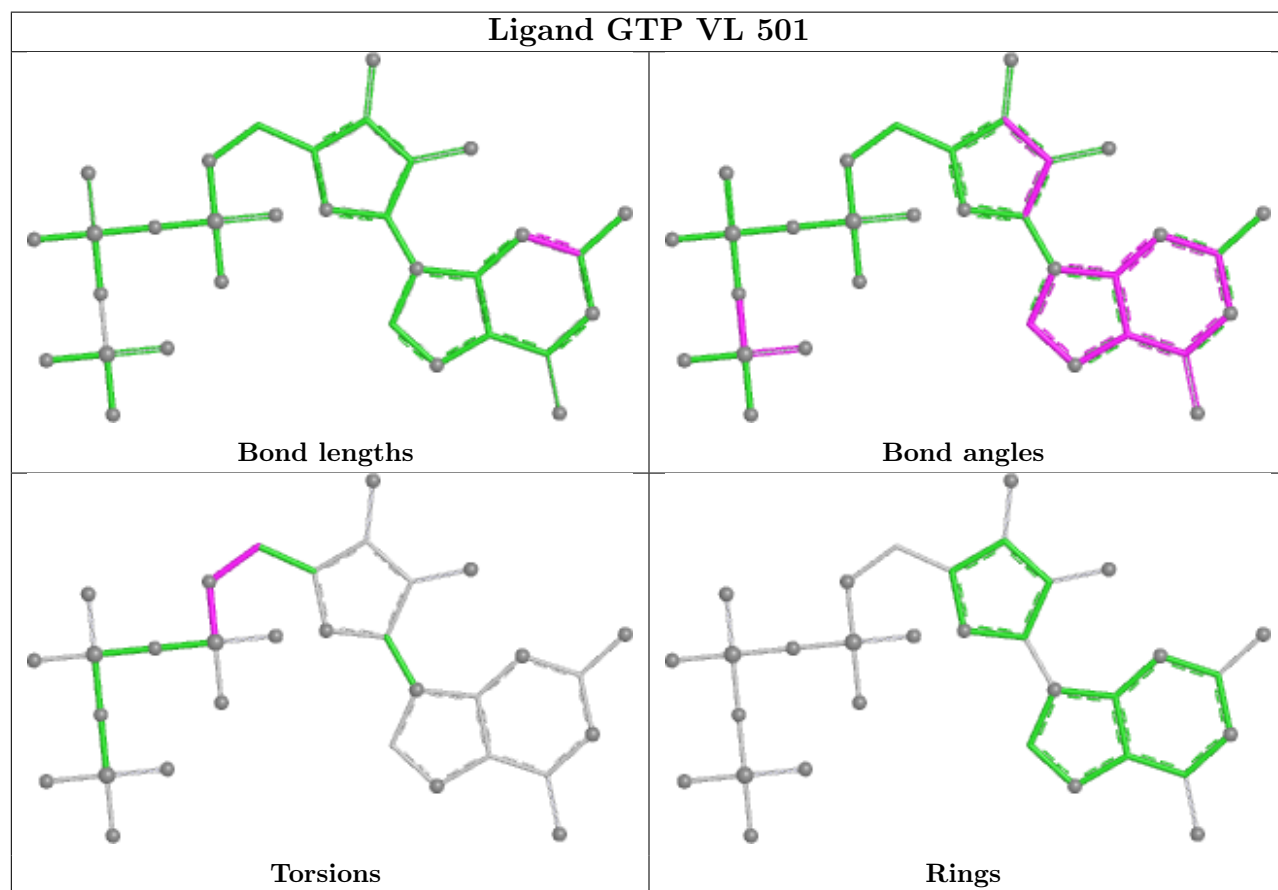
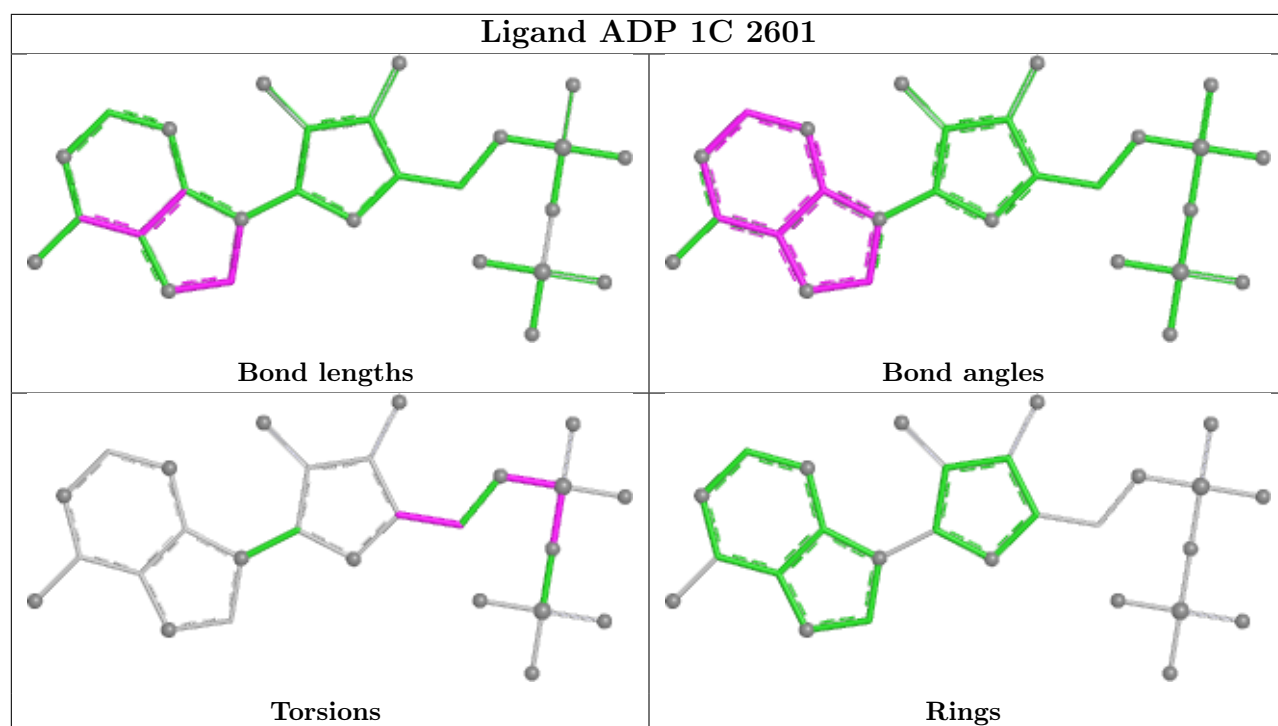
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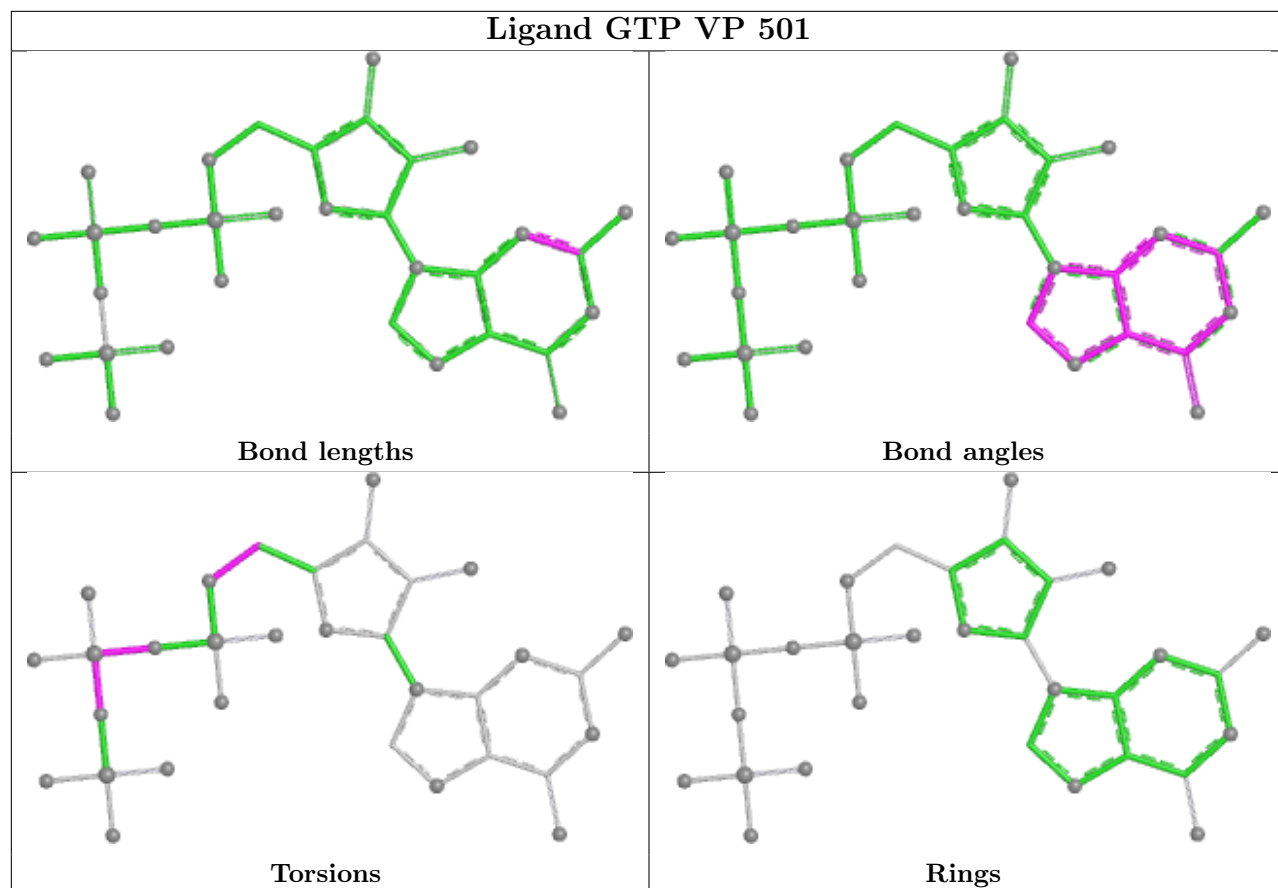
Ligand GDP XC 501



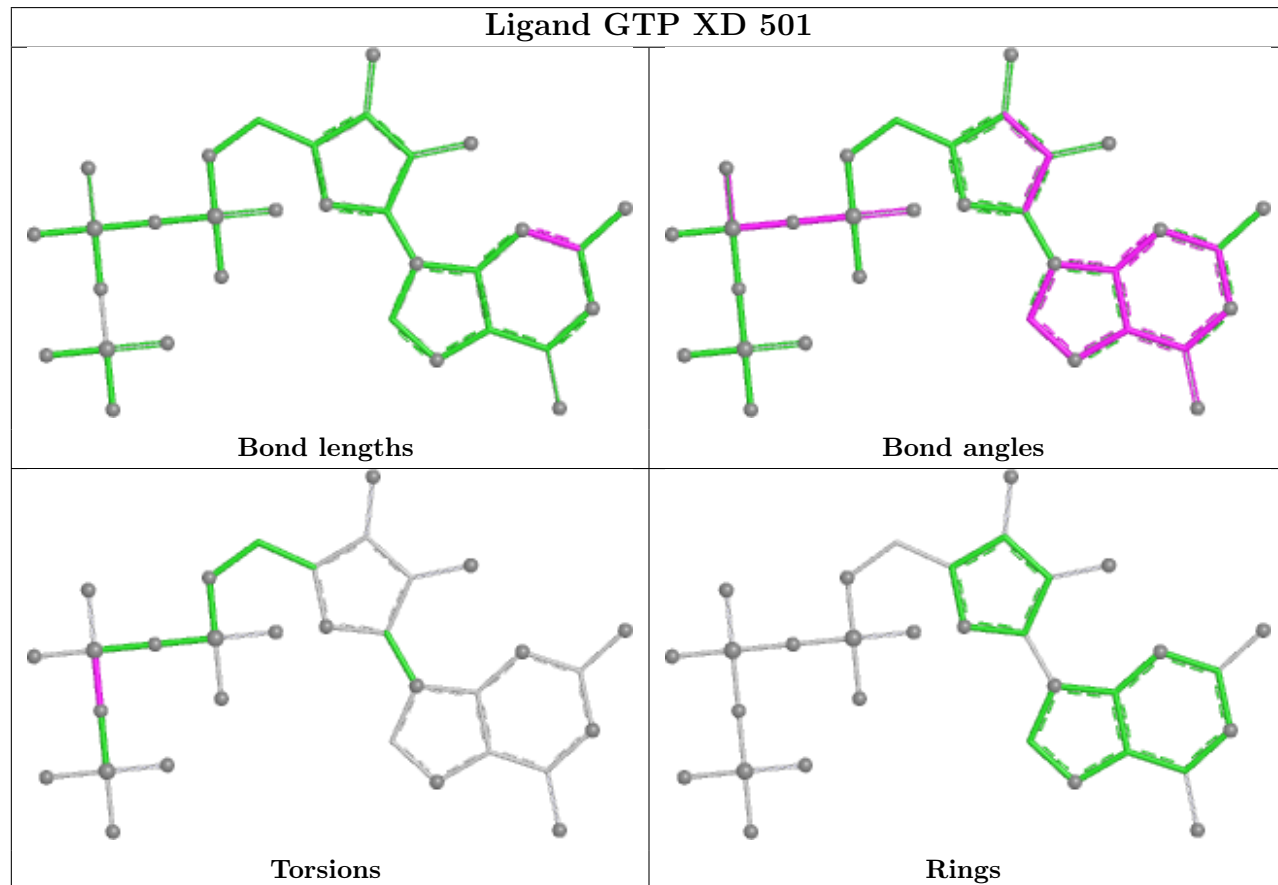


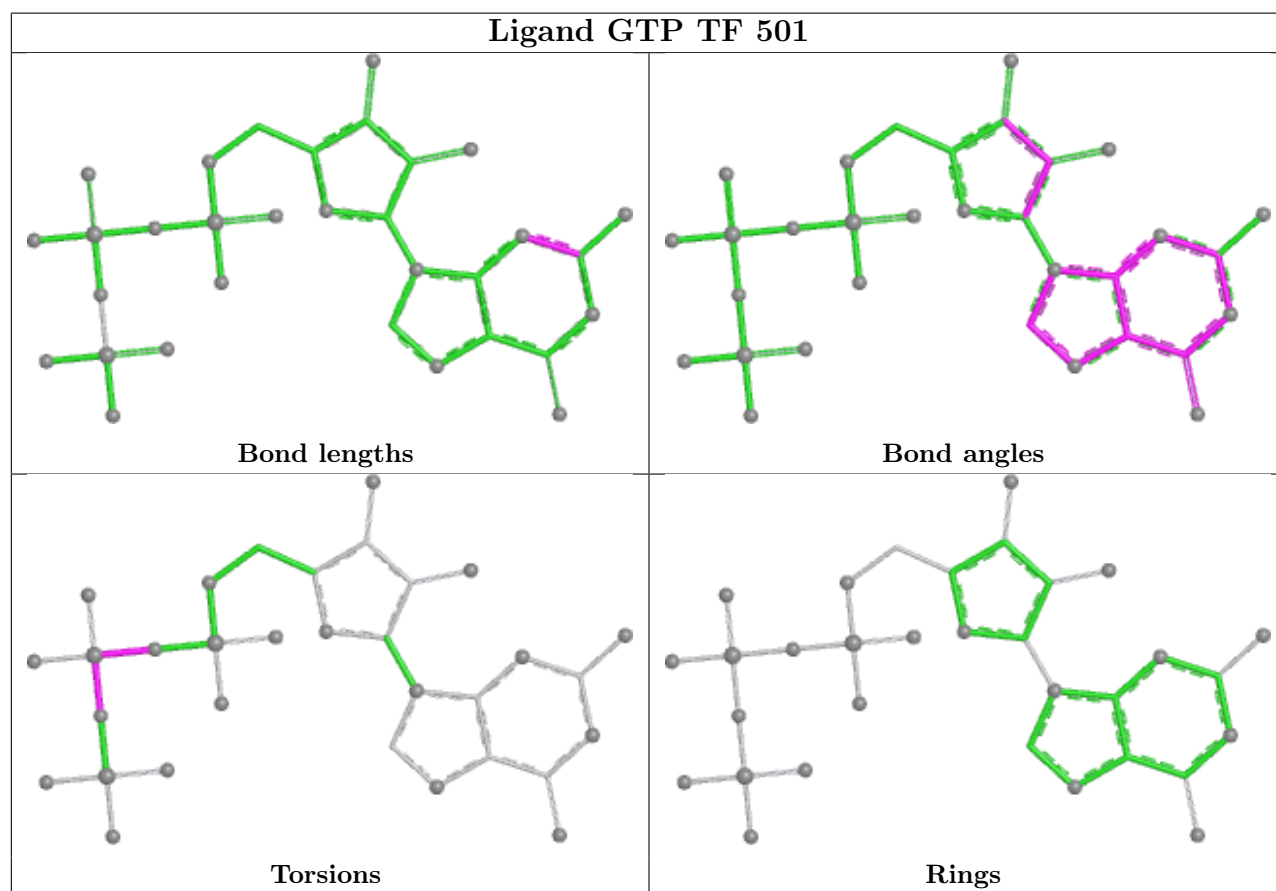
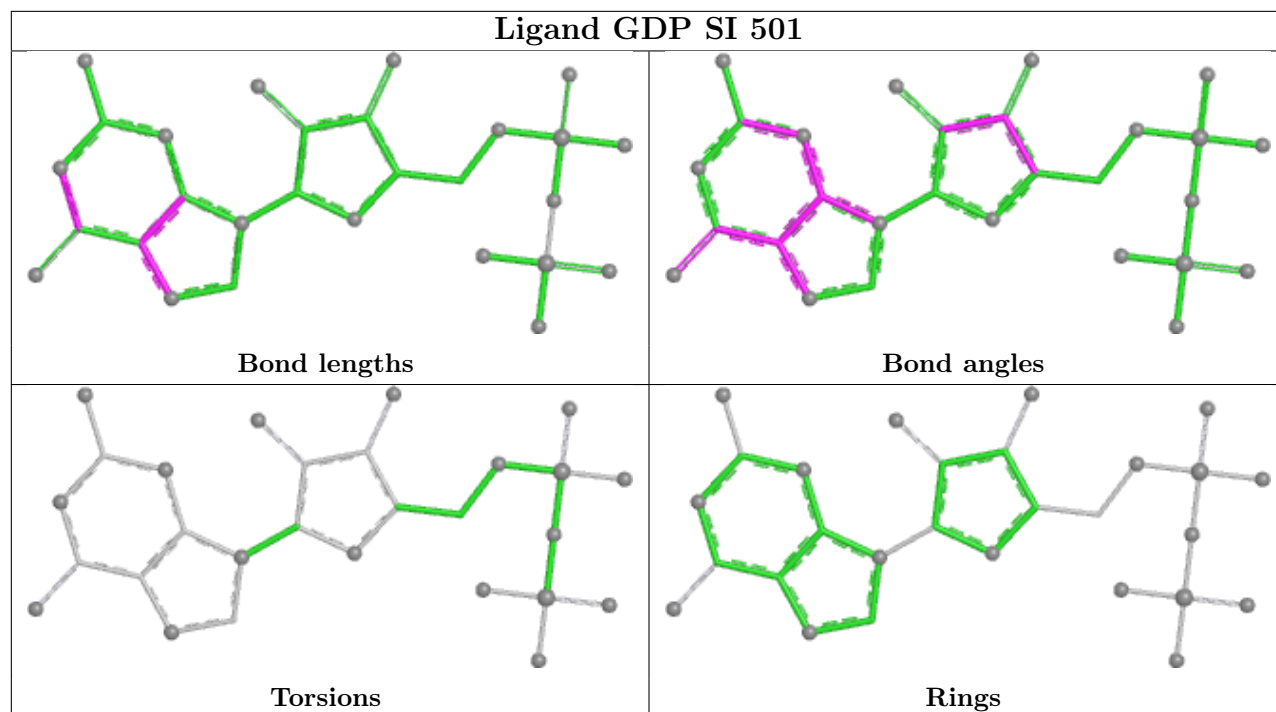


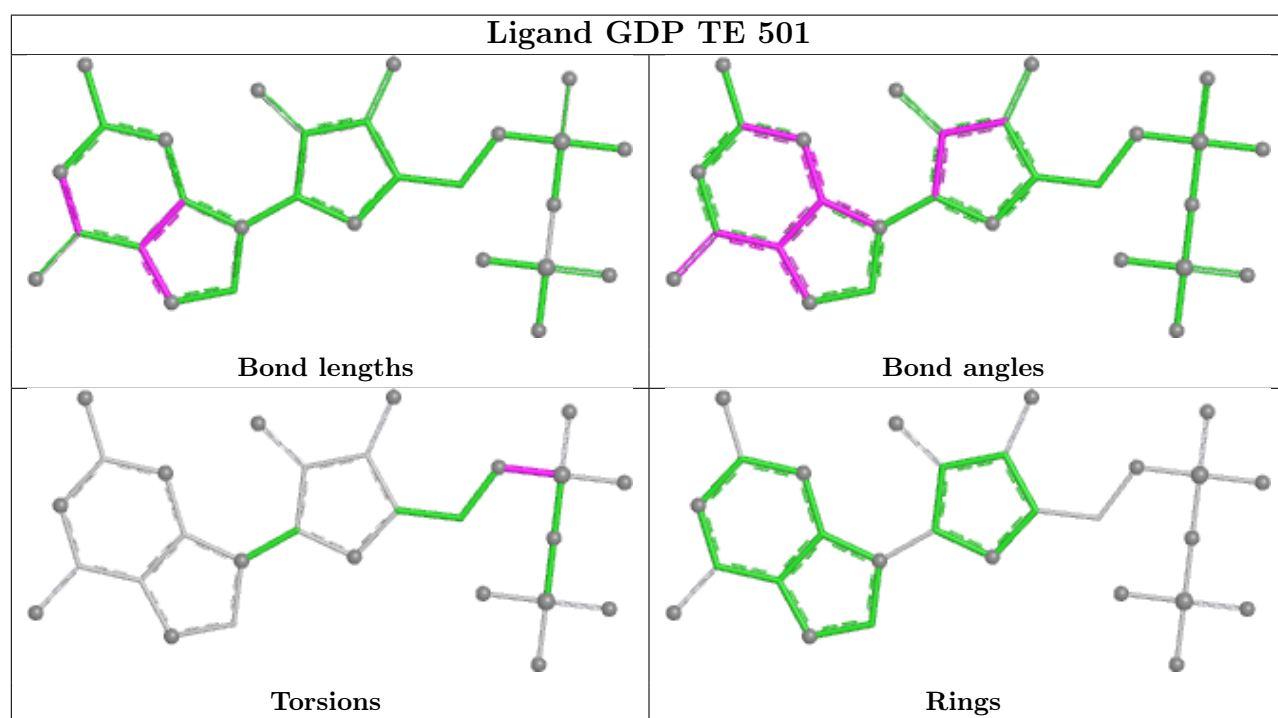
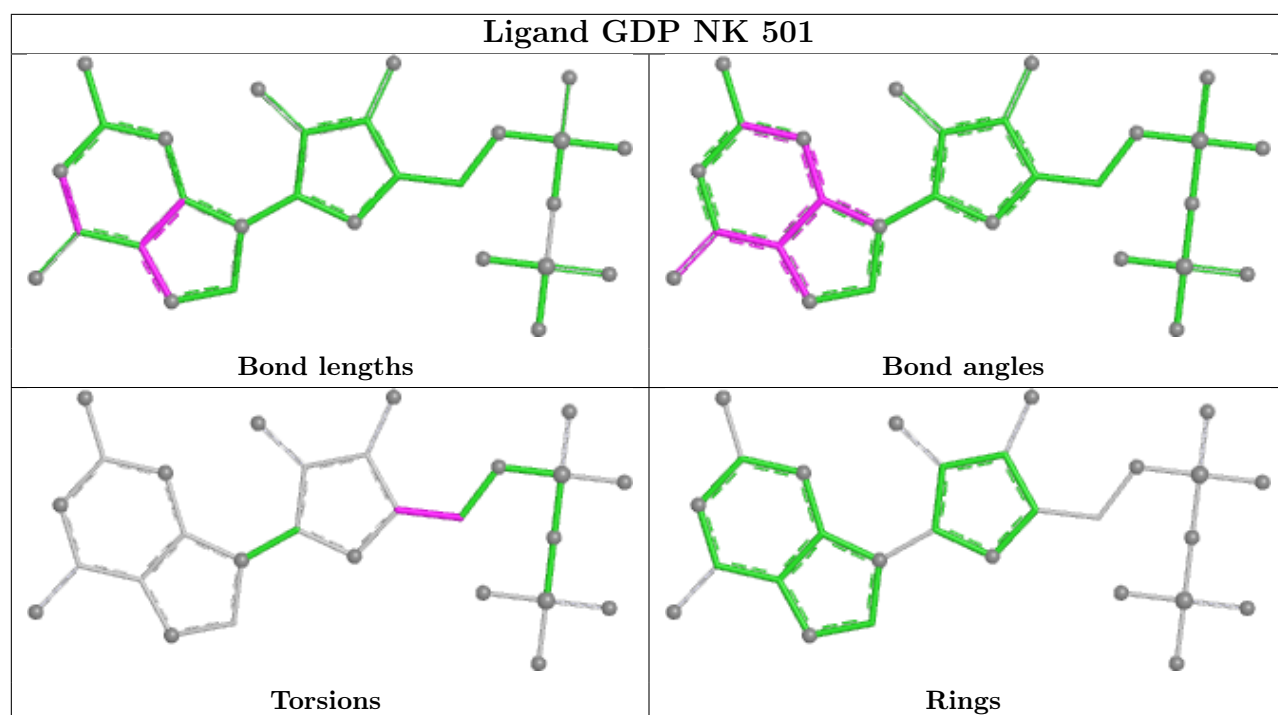
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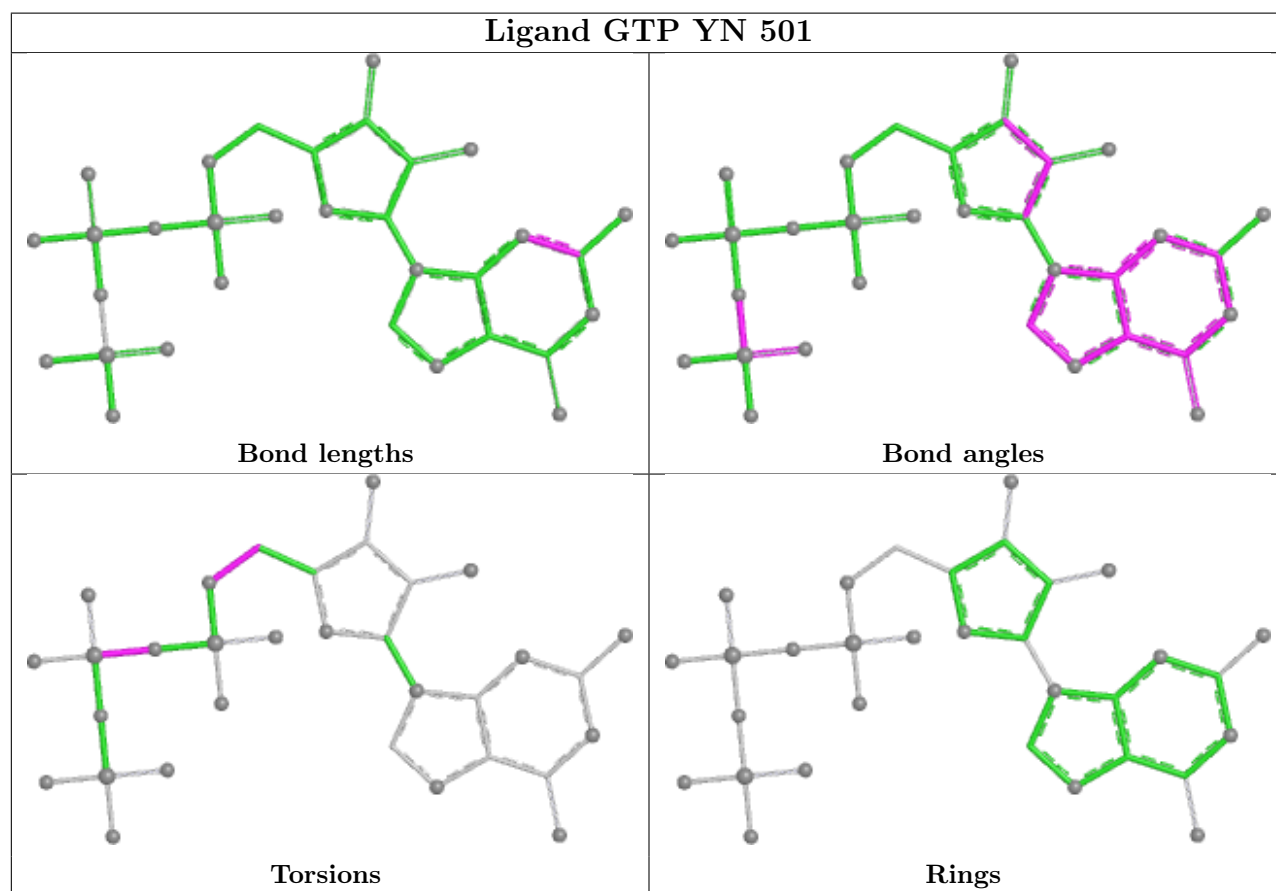
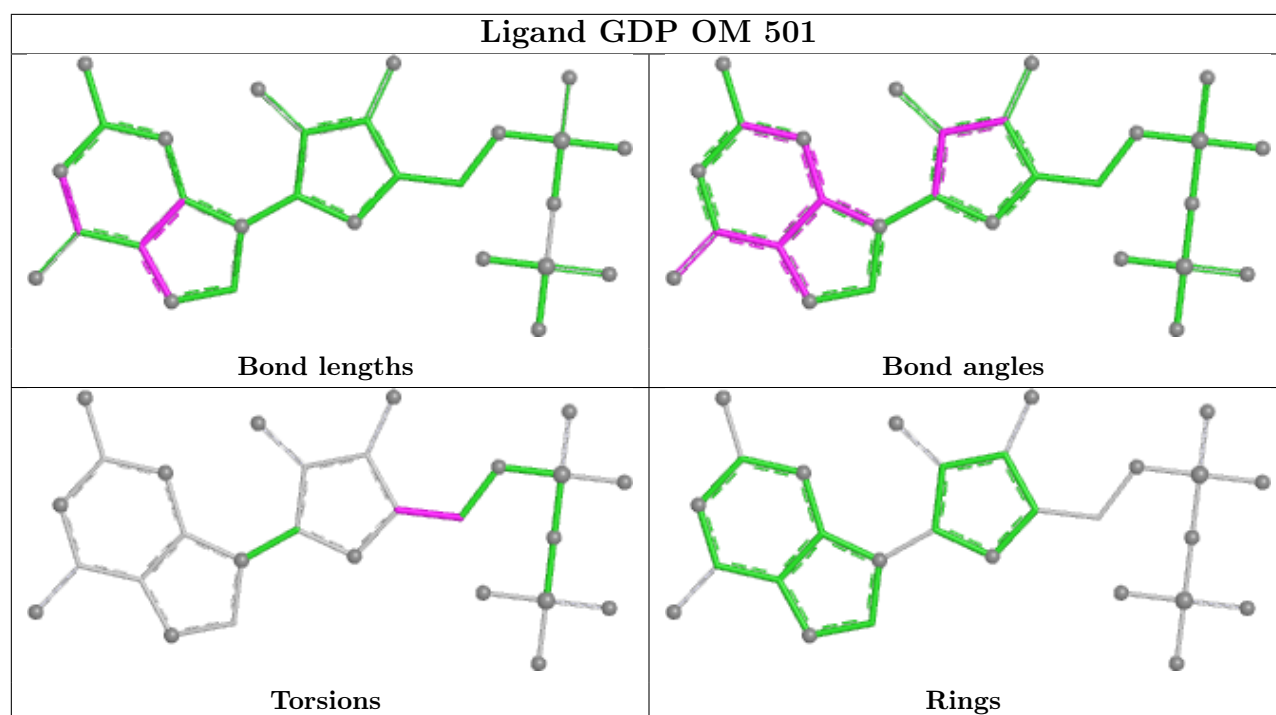


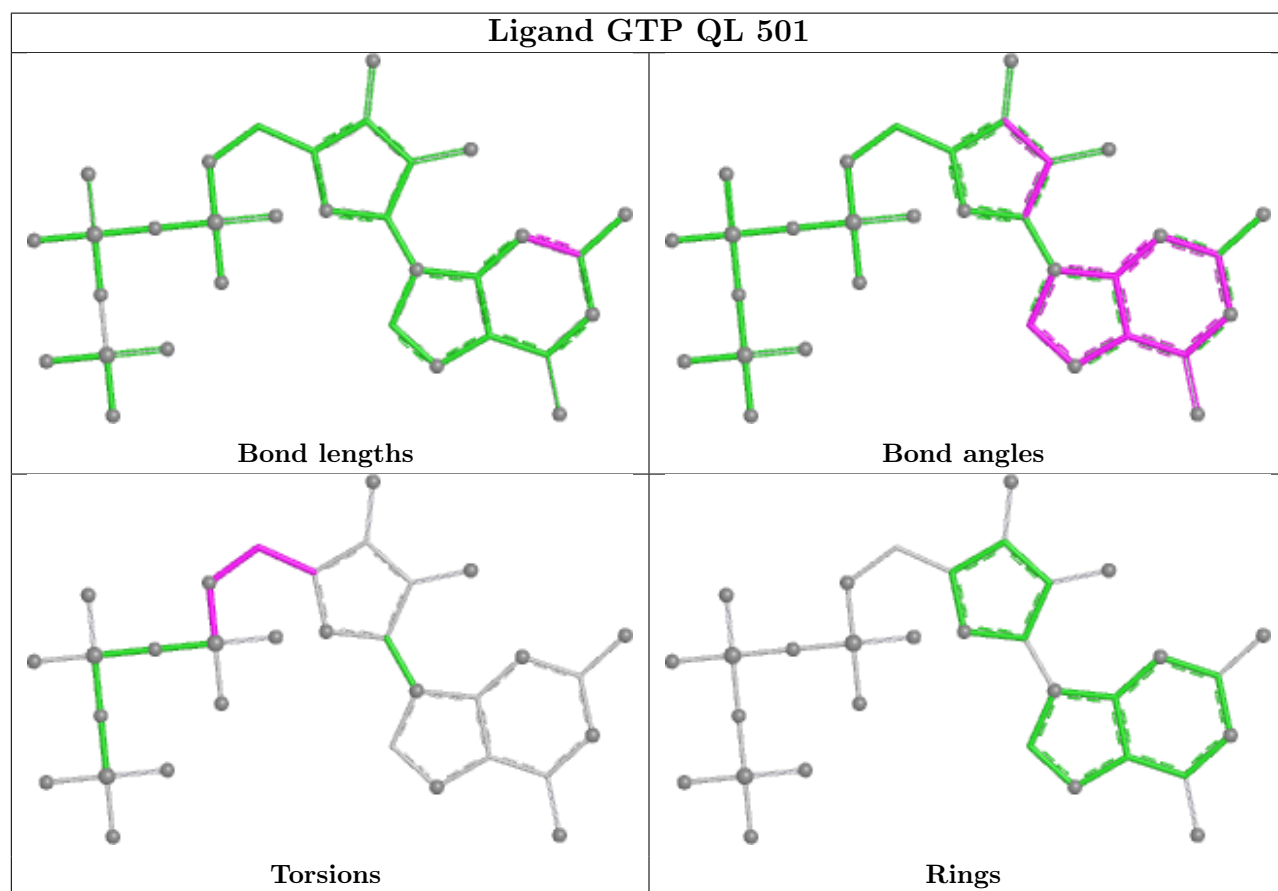
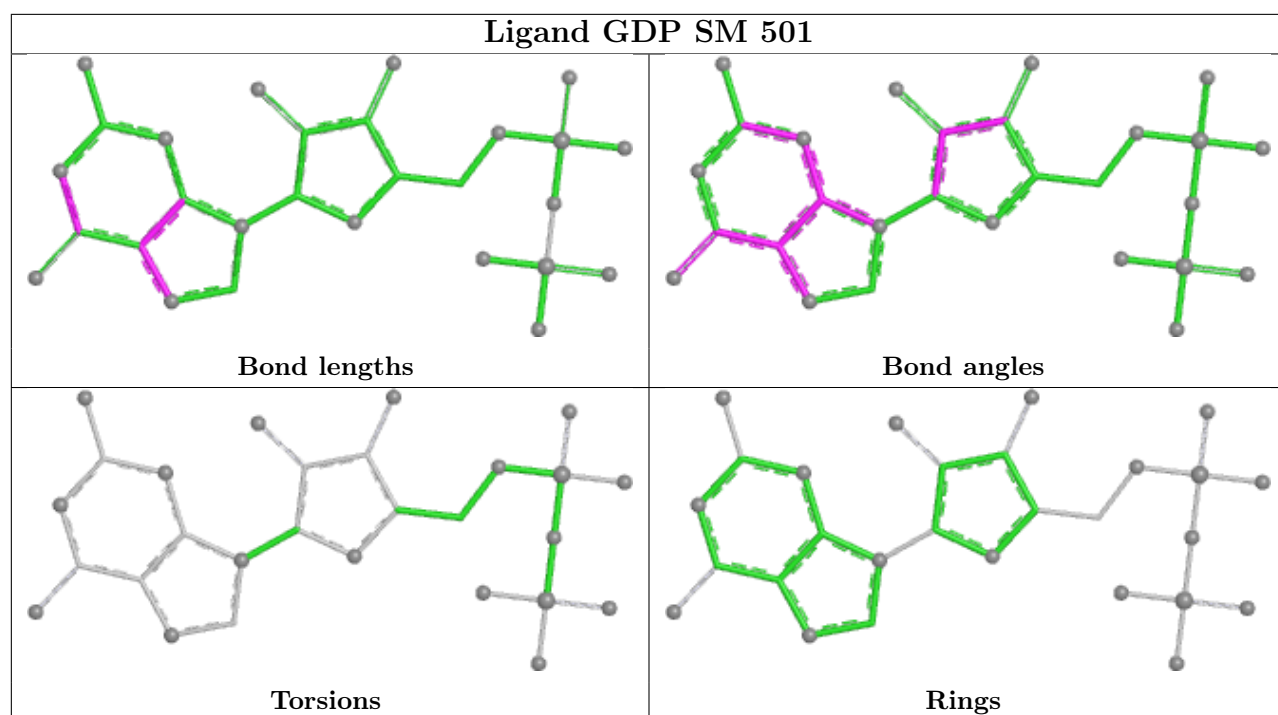
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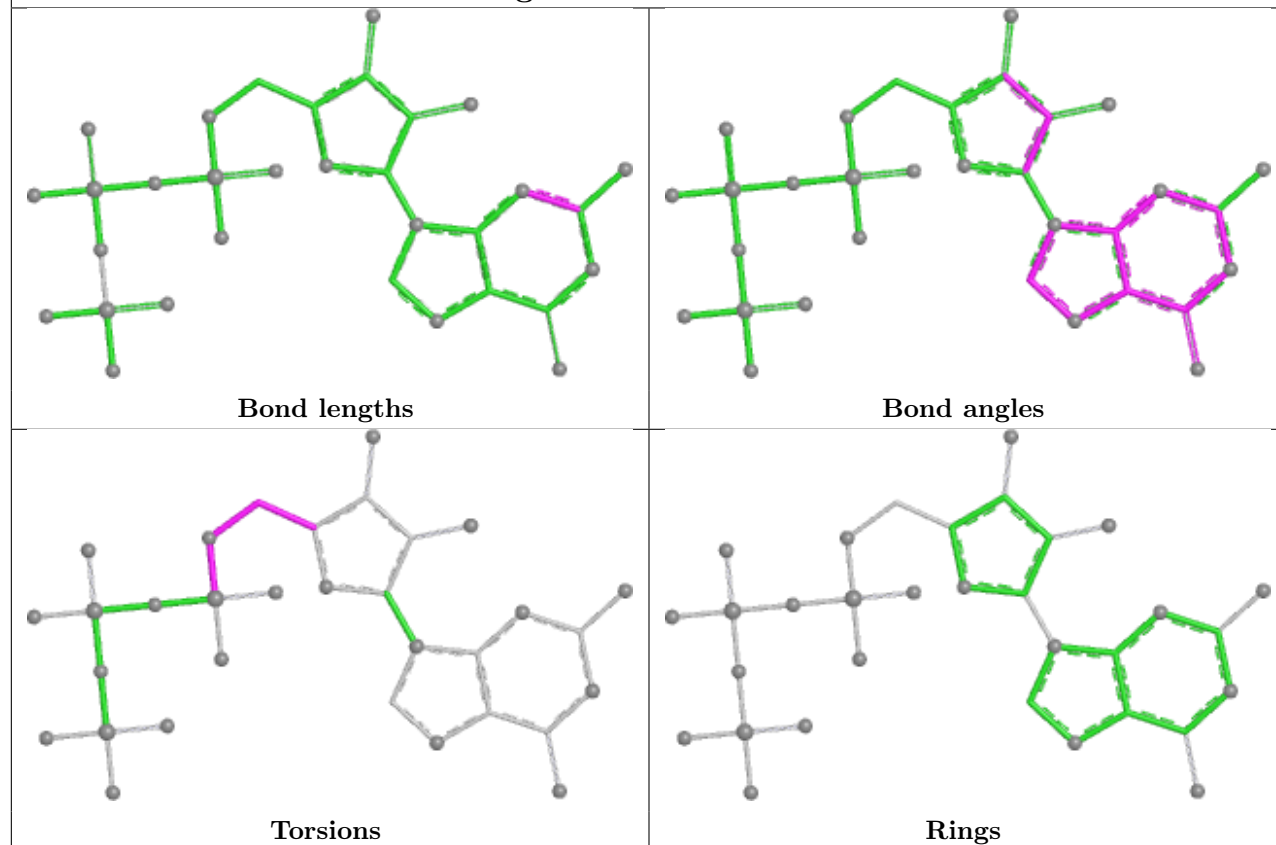




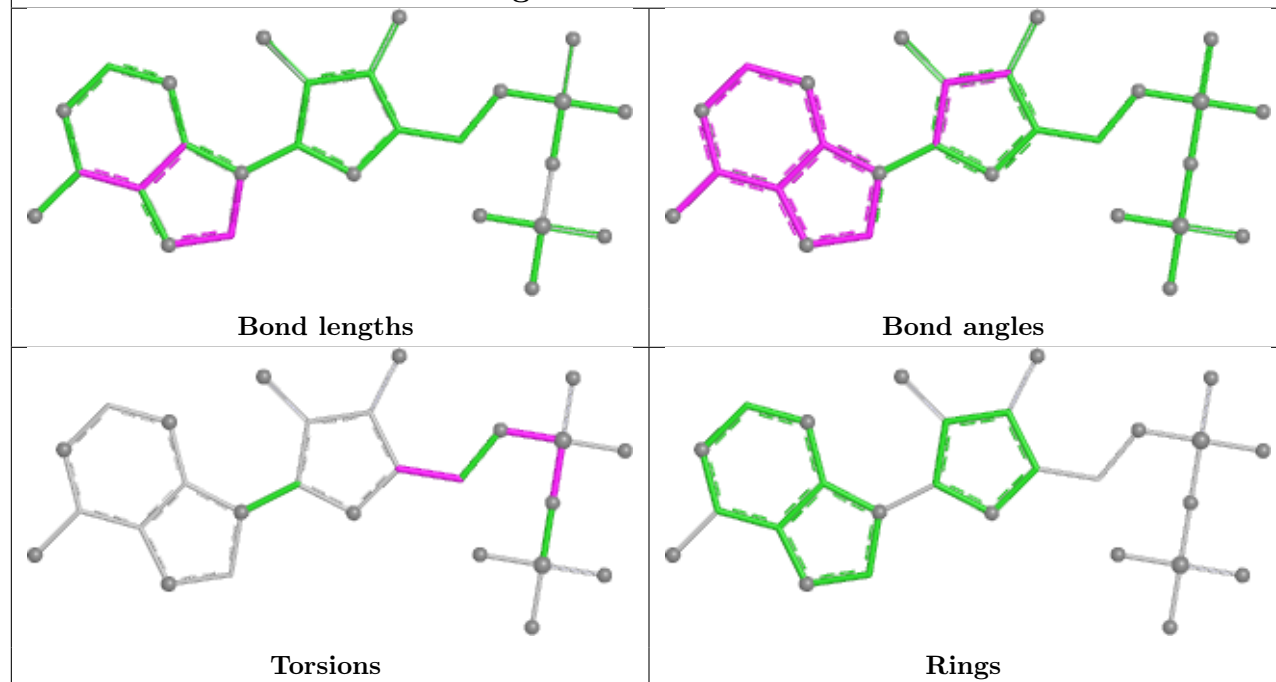


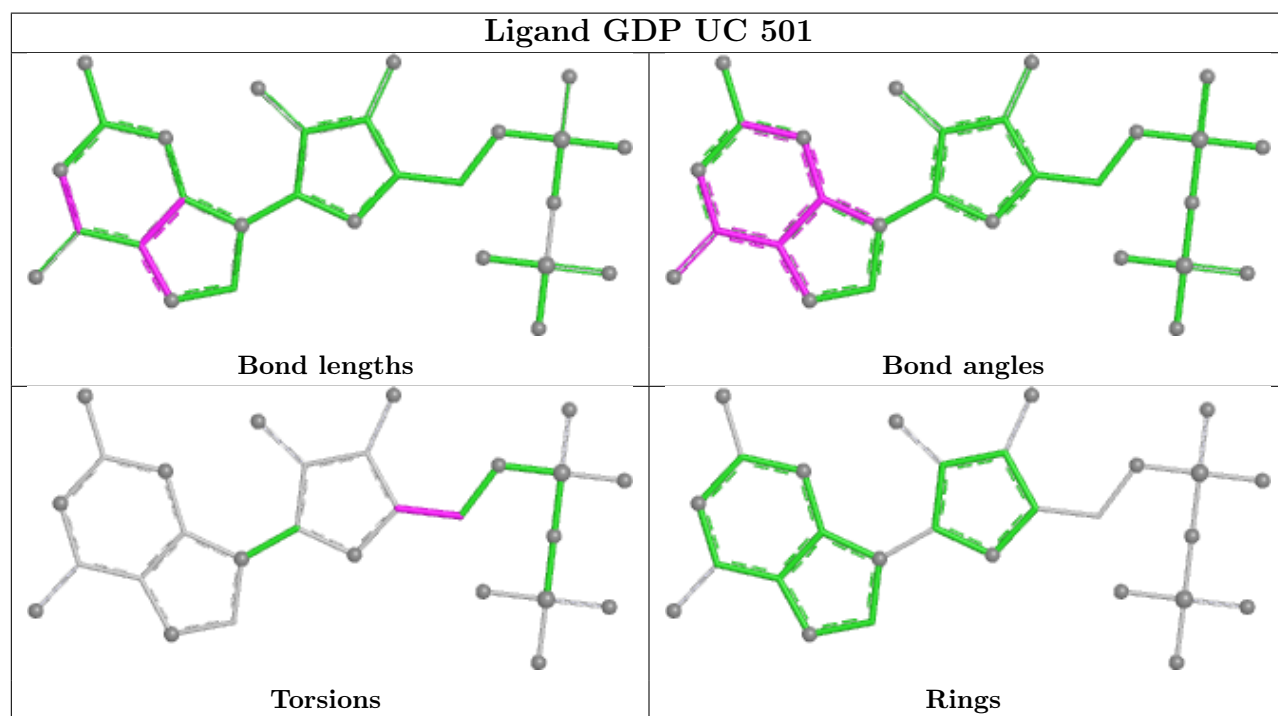
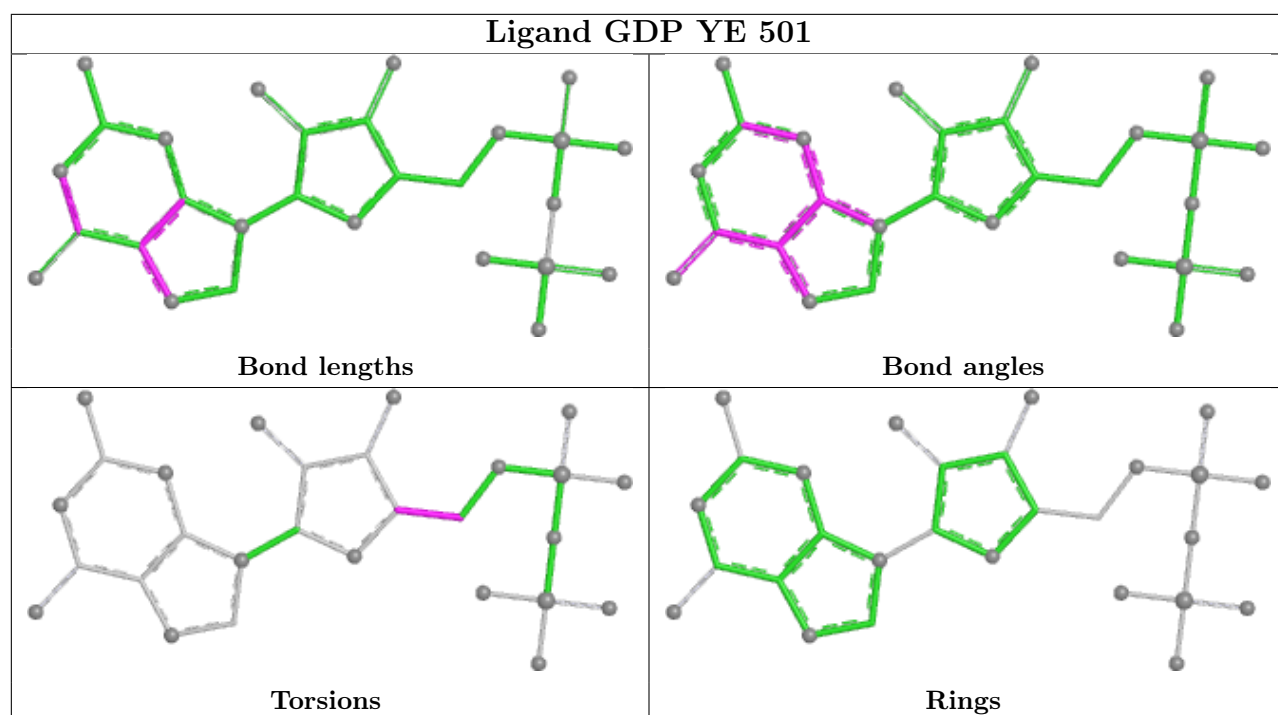


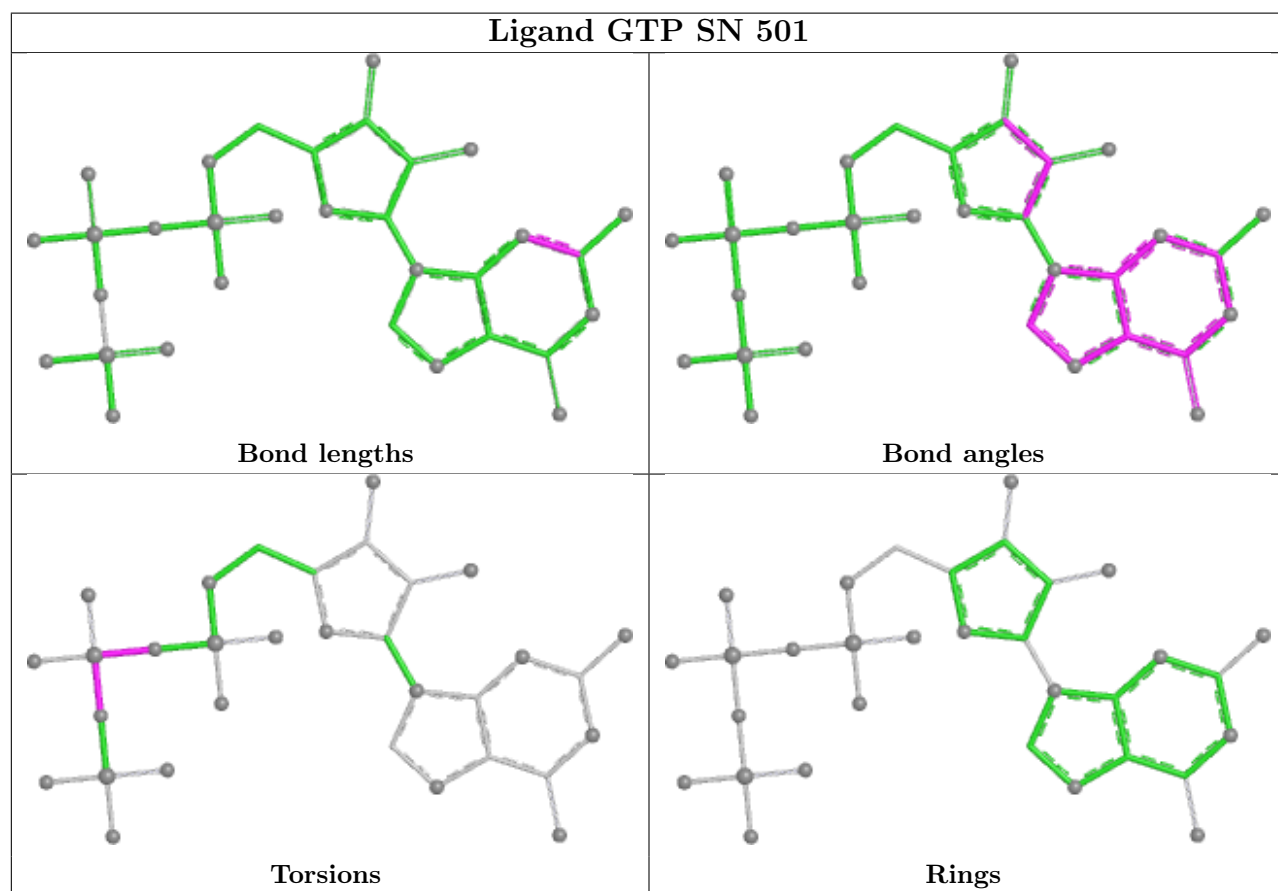
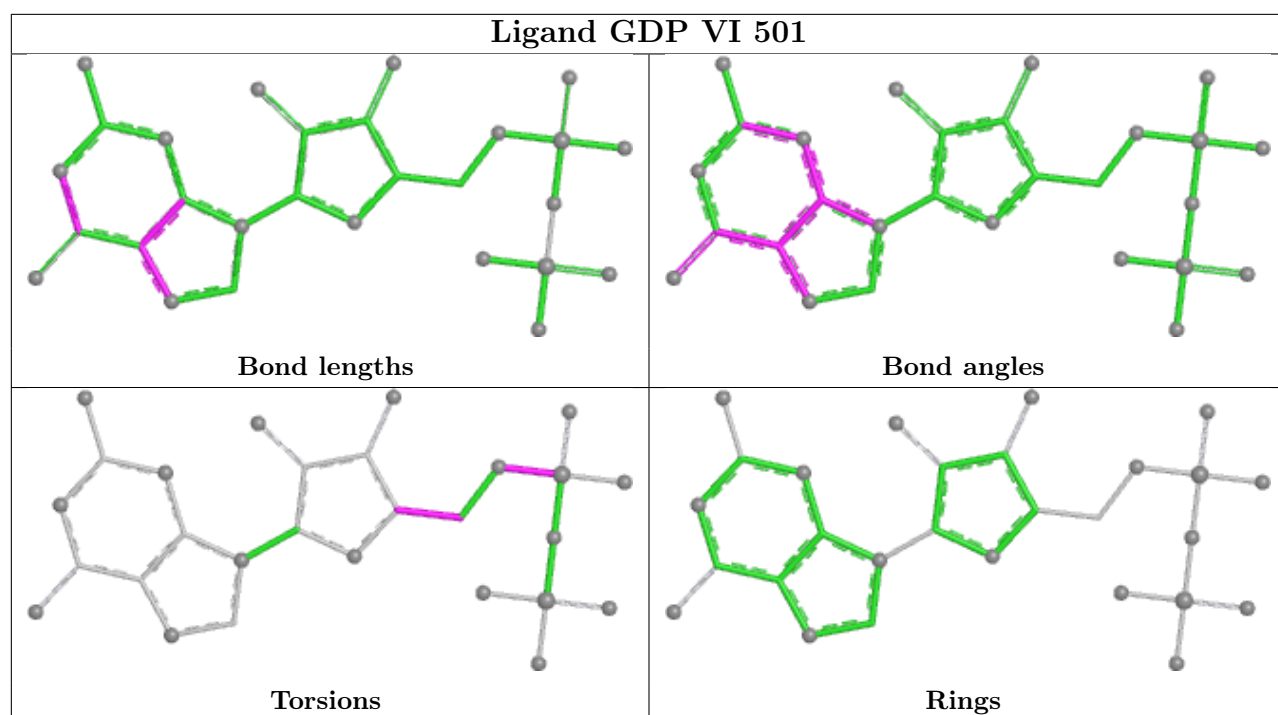
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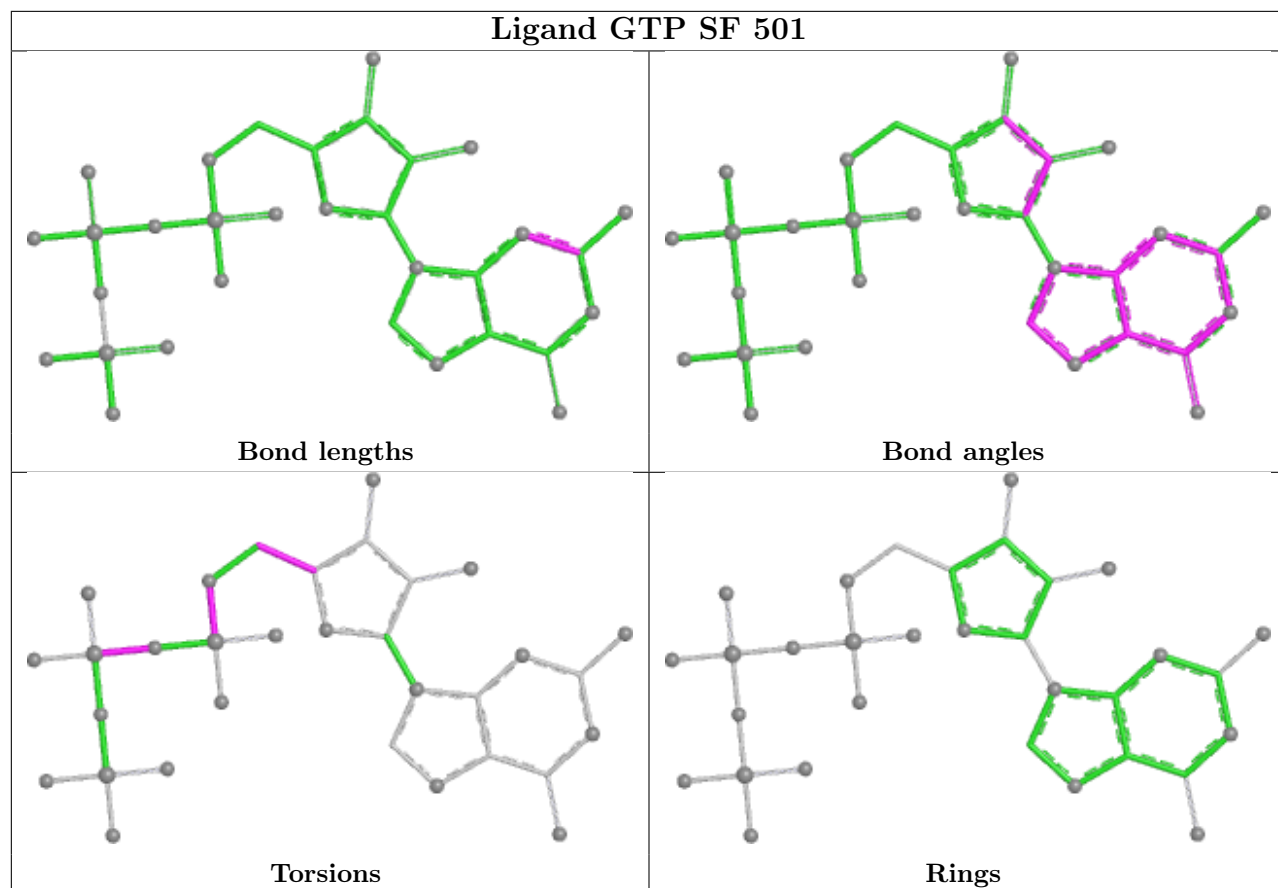
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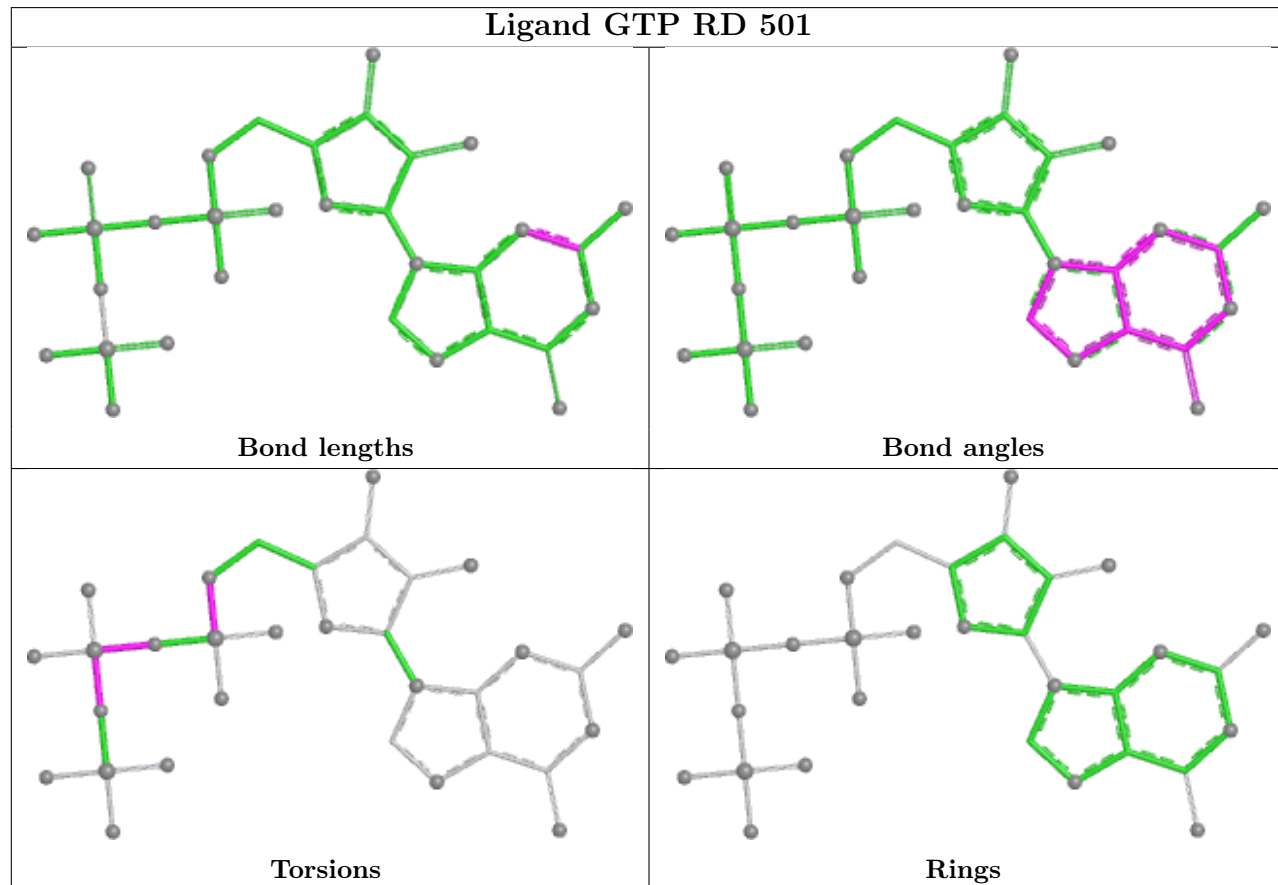


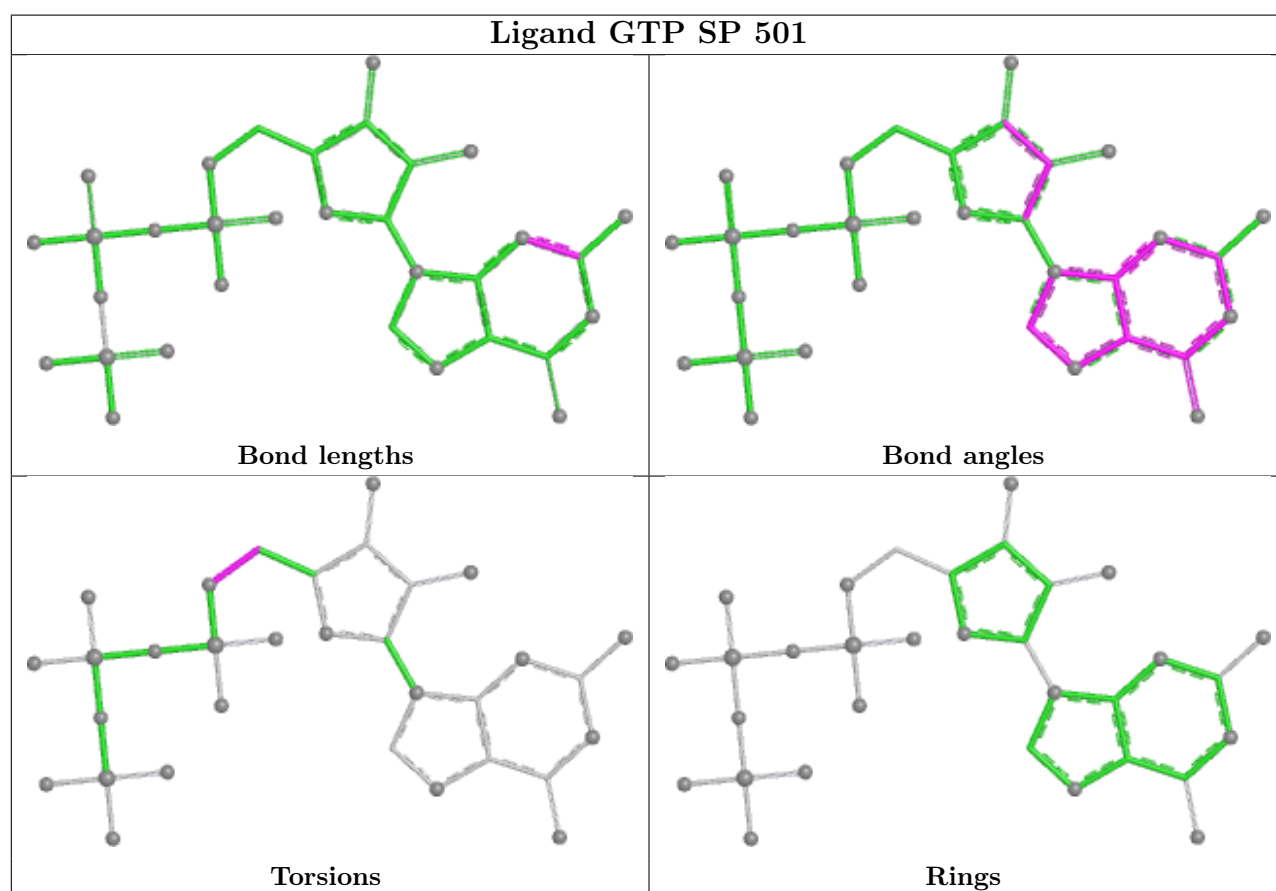
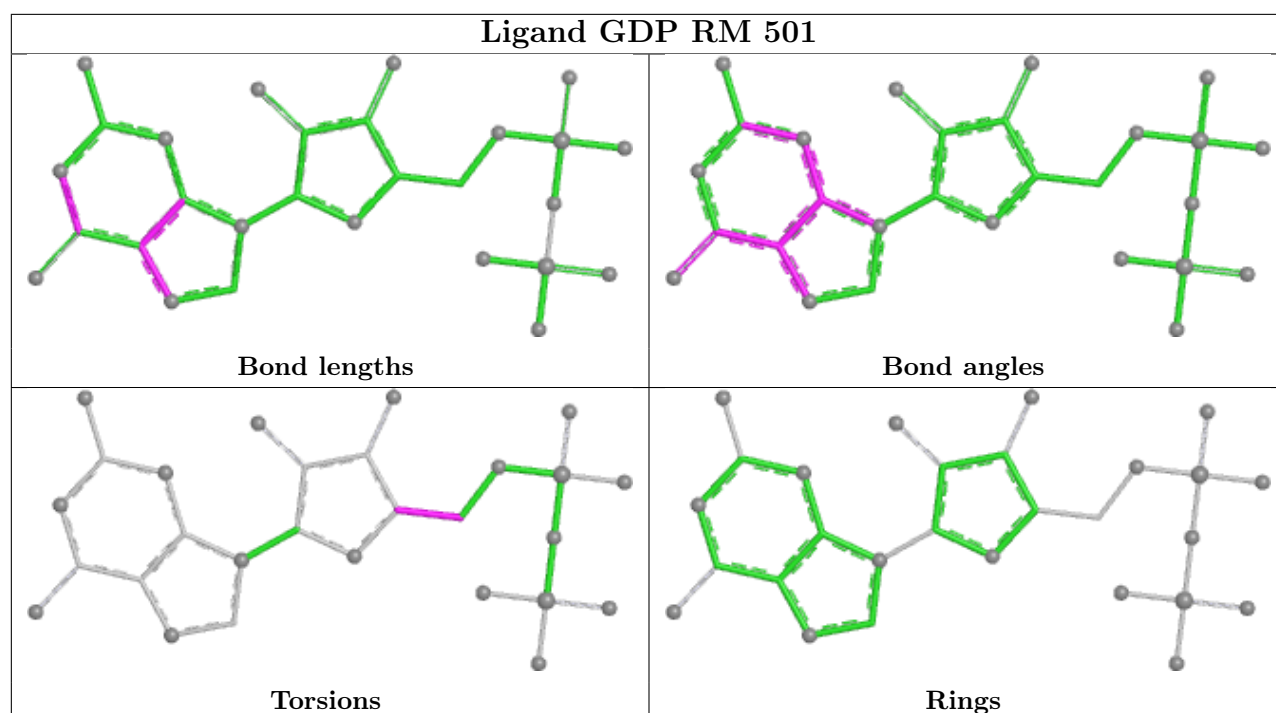


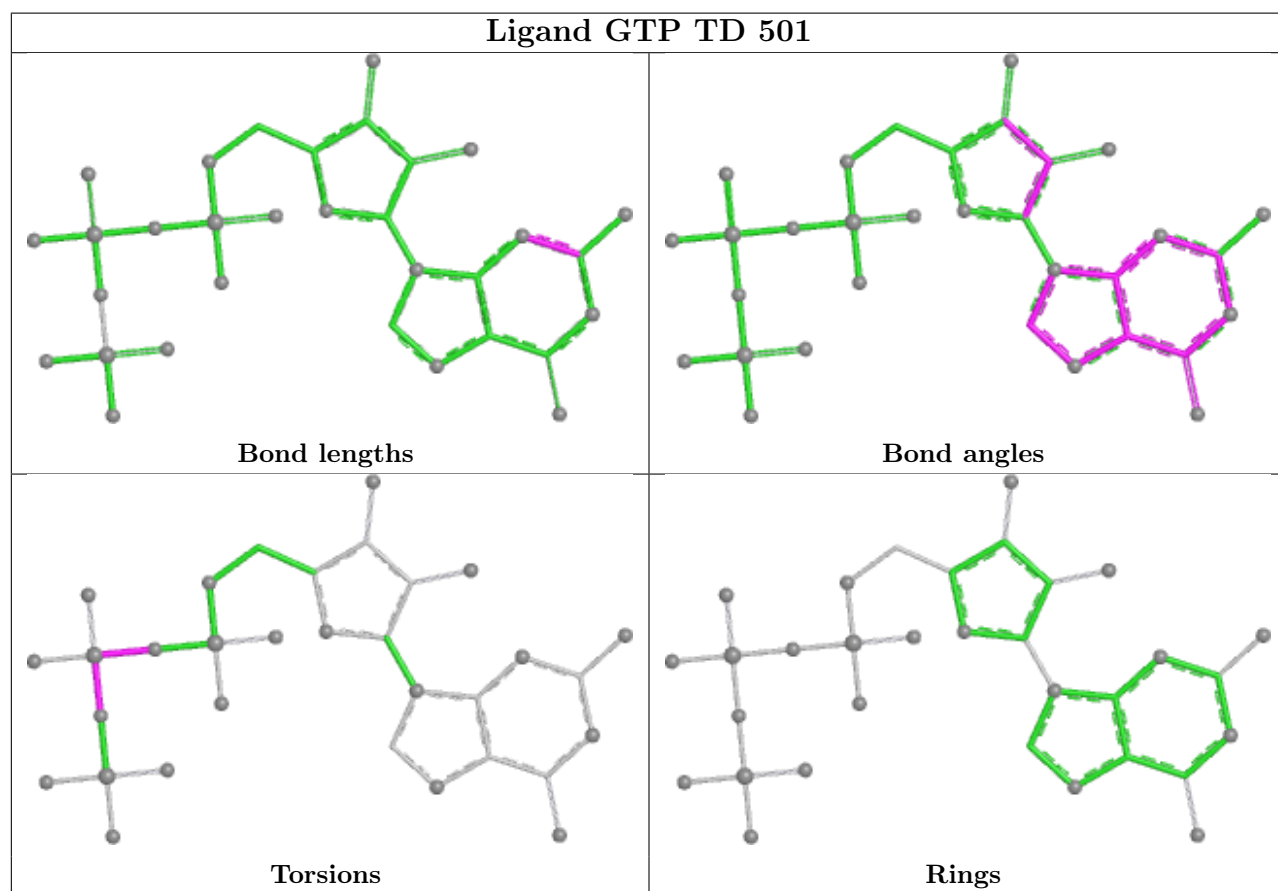
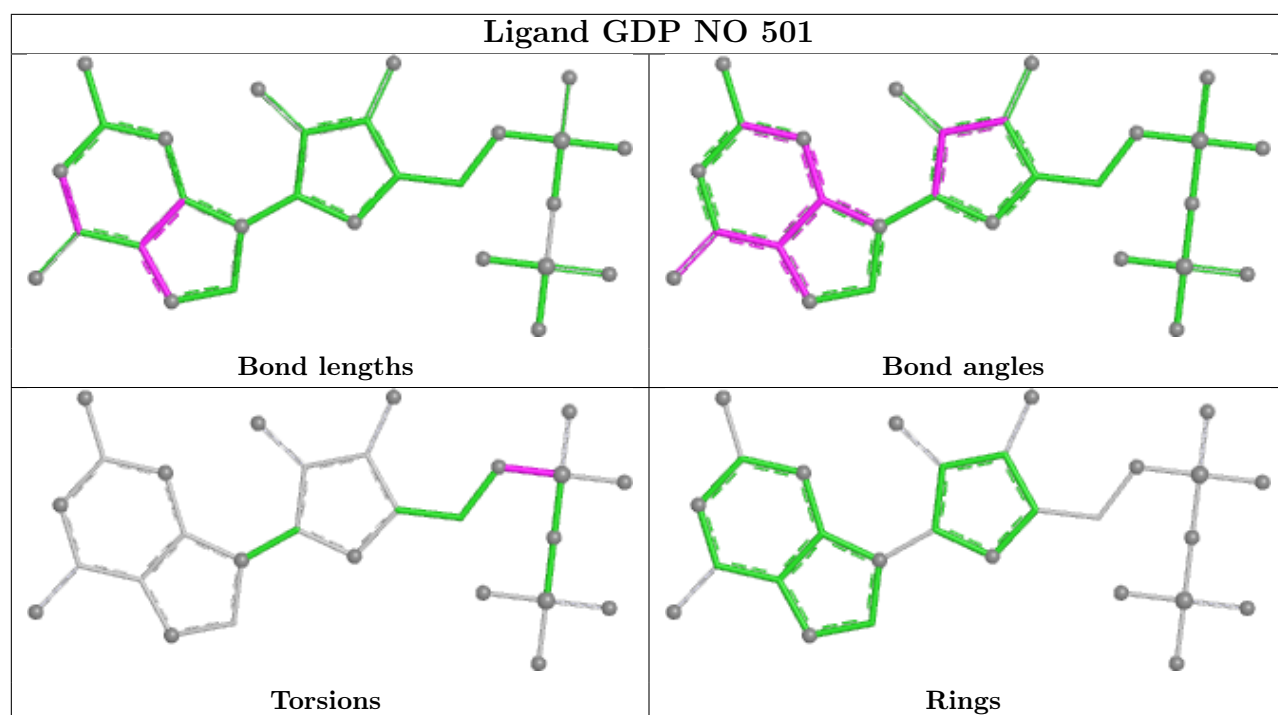
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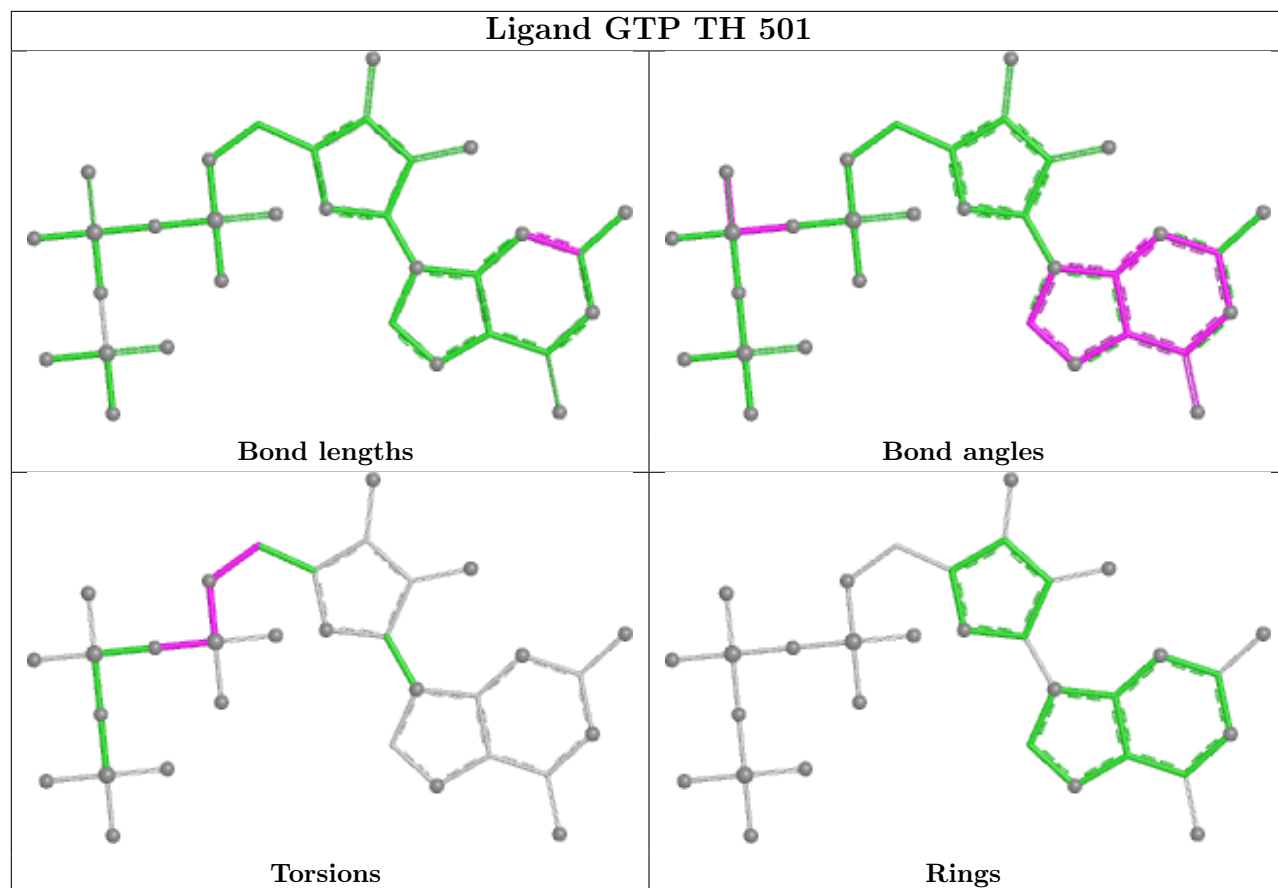
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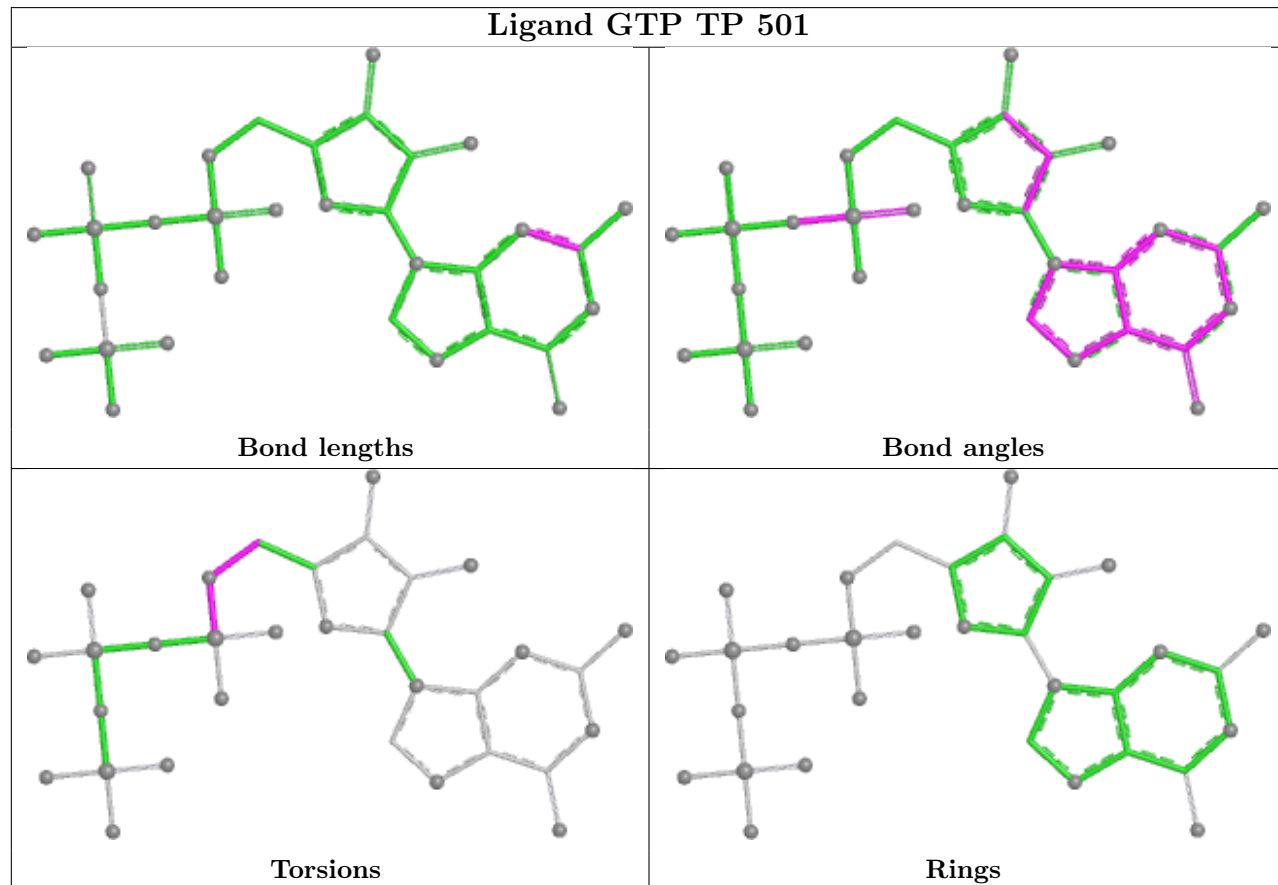




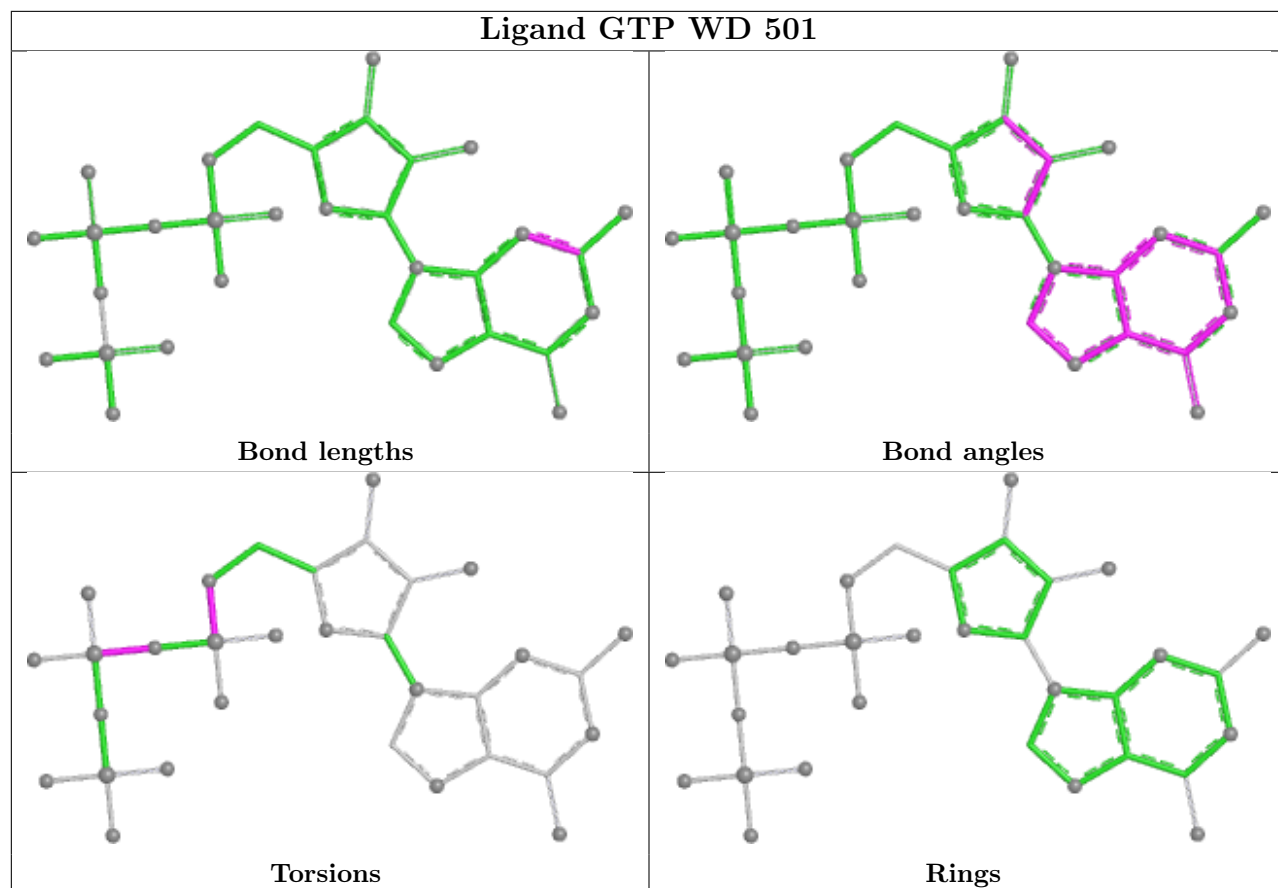
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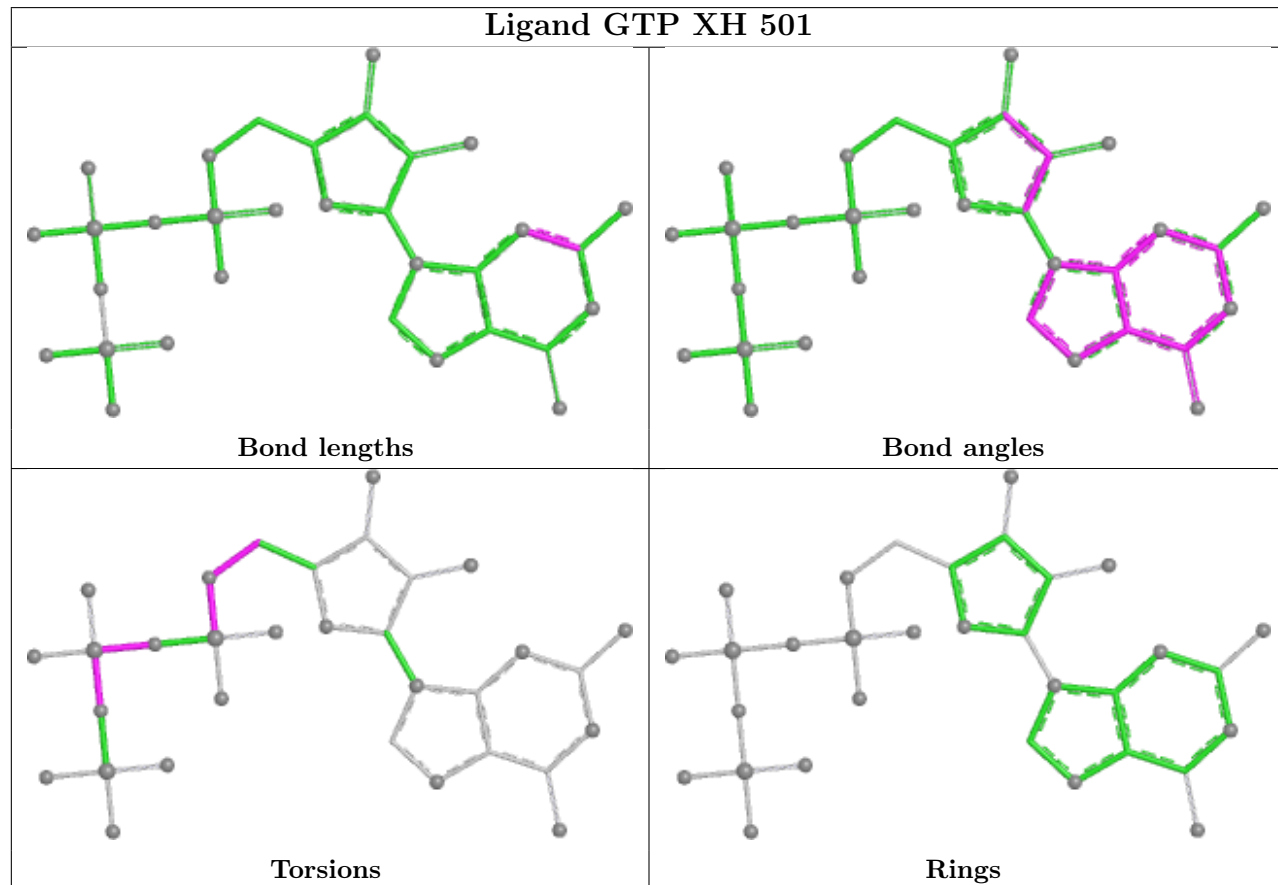
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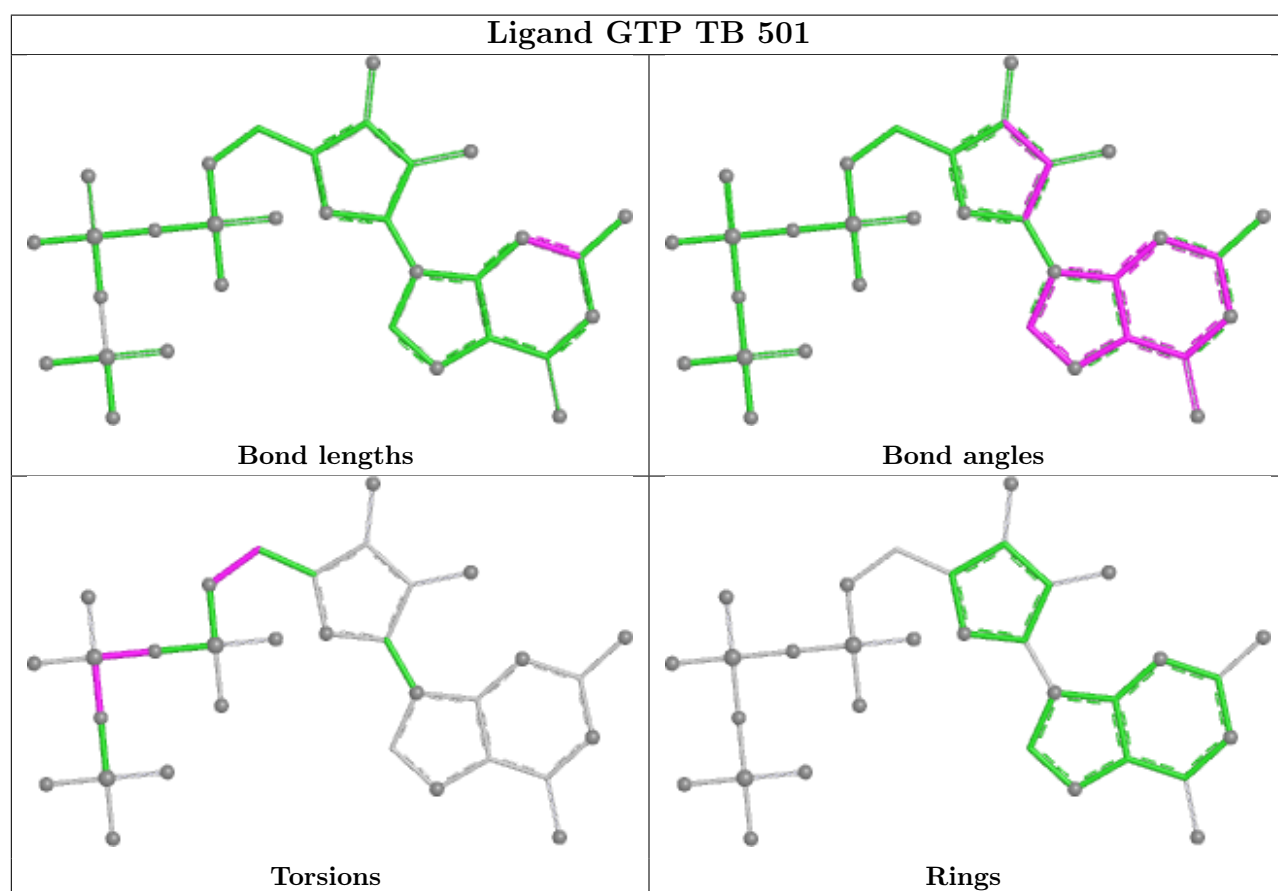
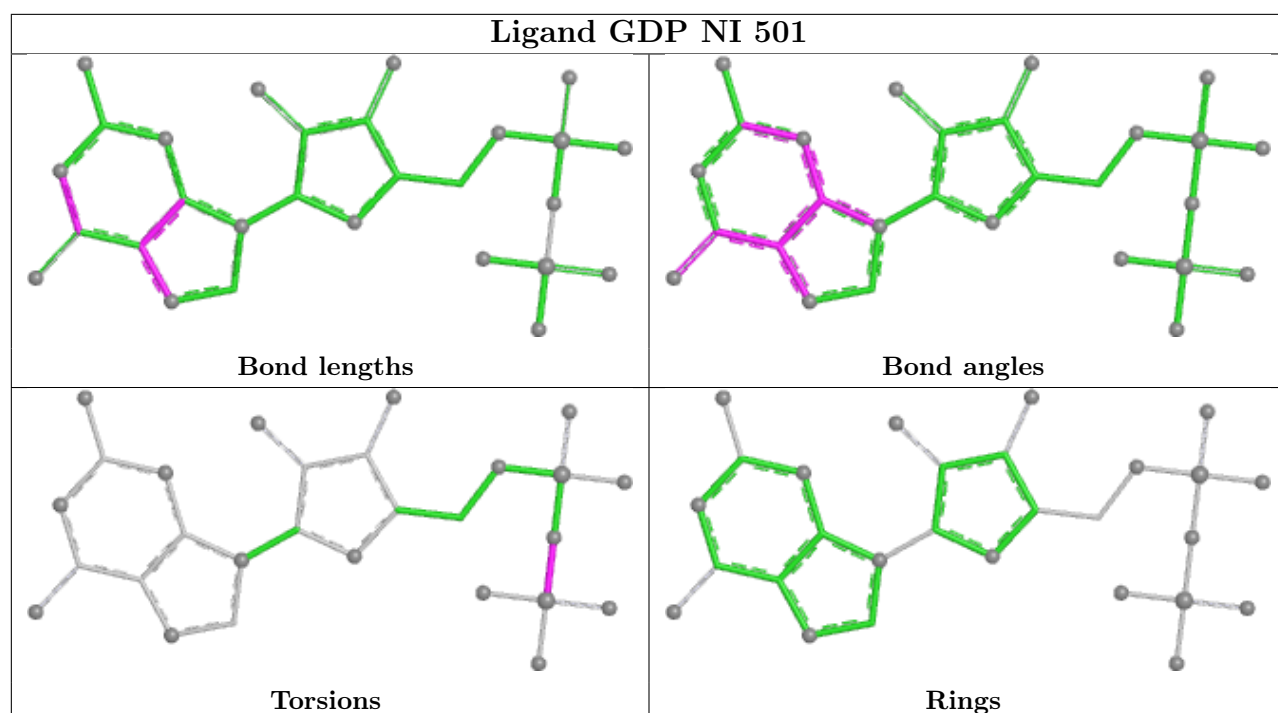


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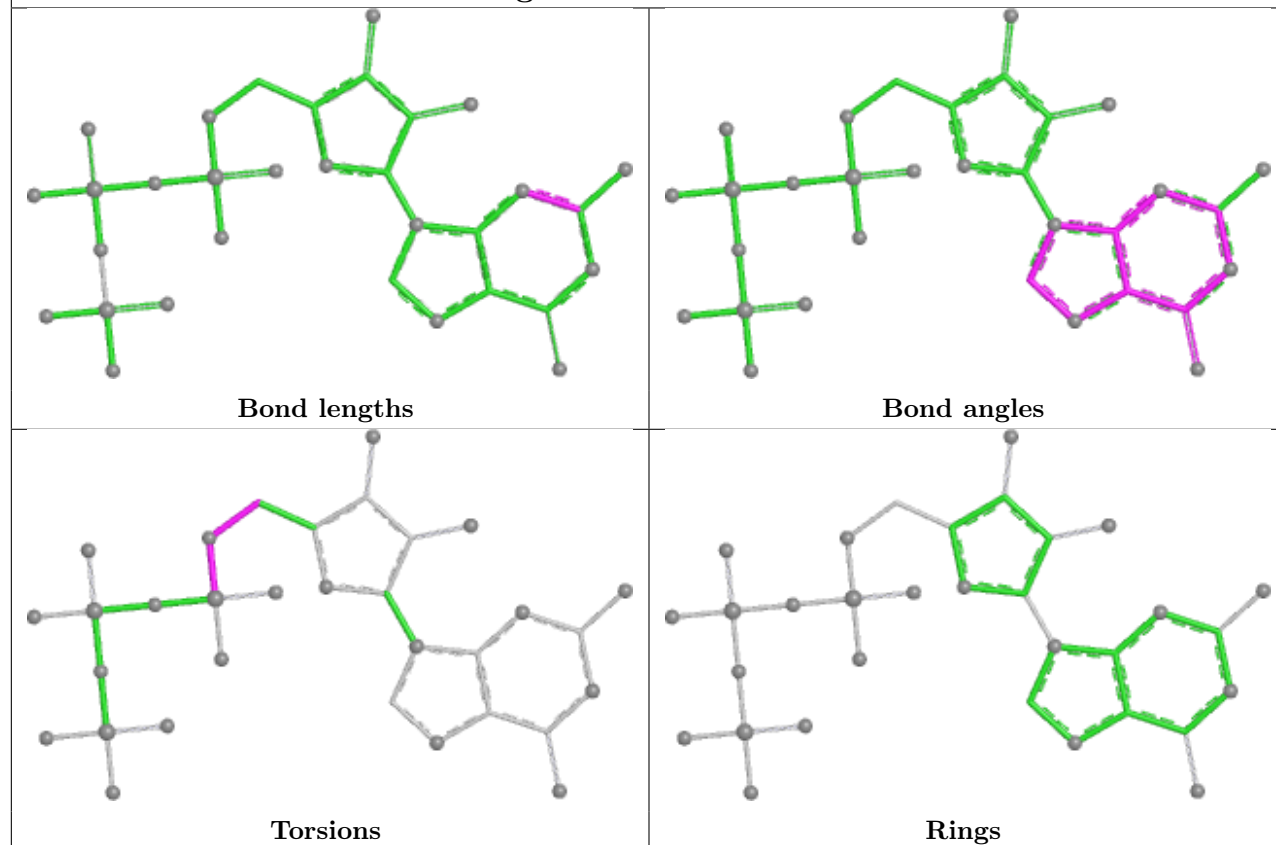


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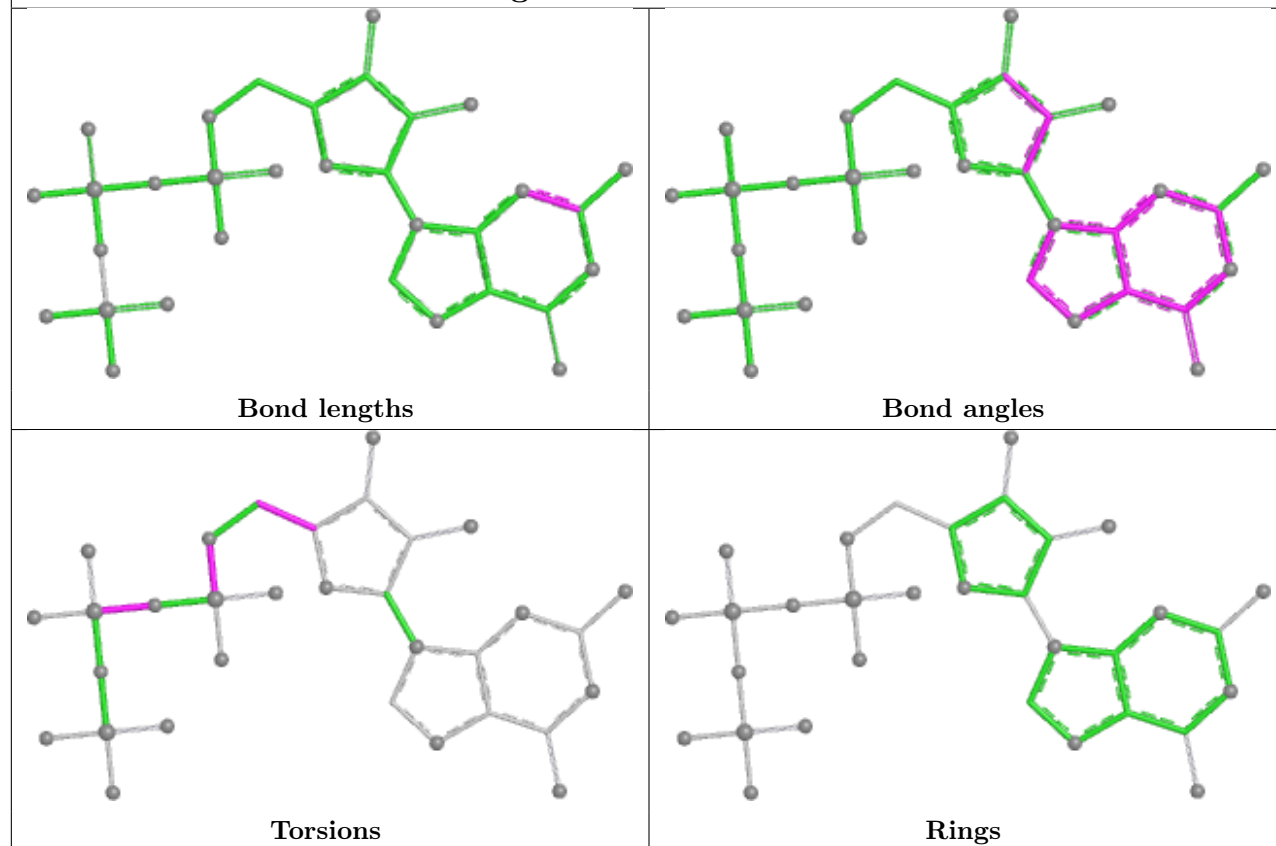


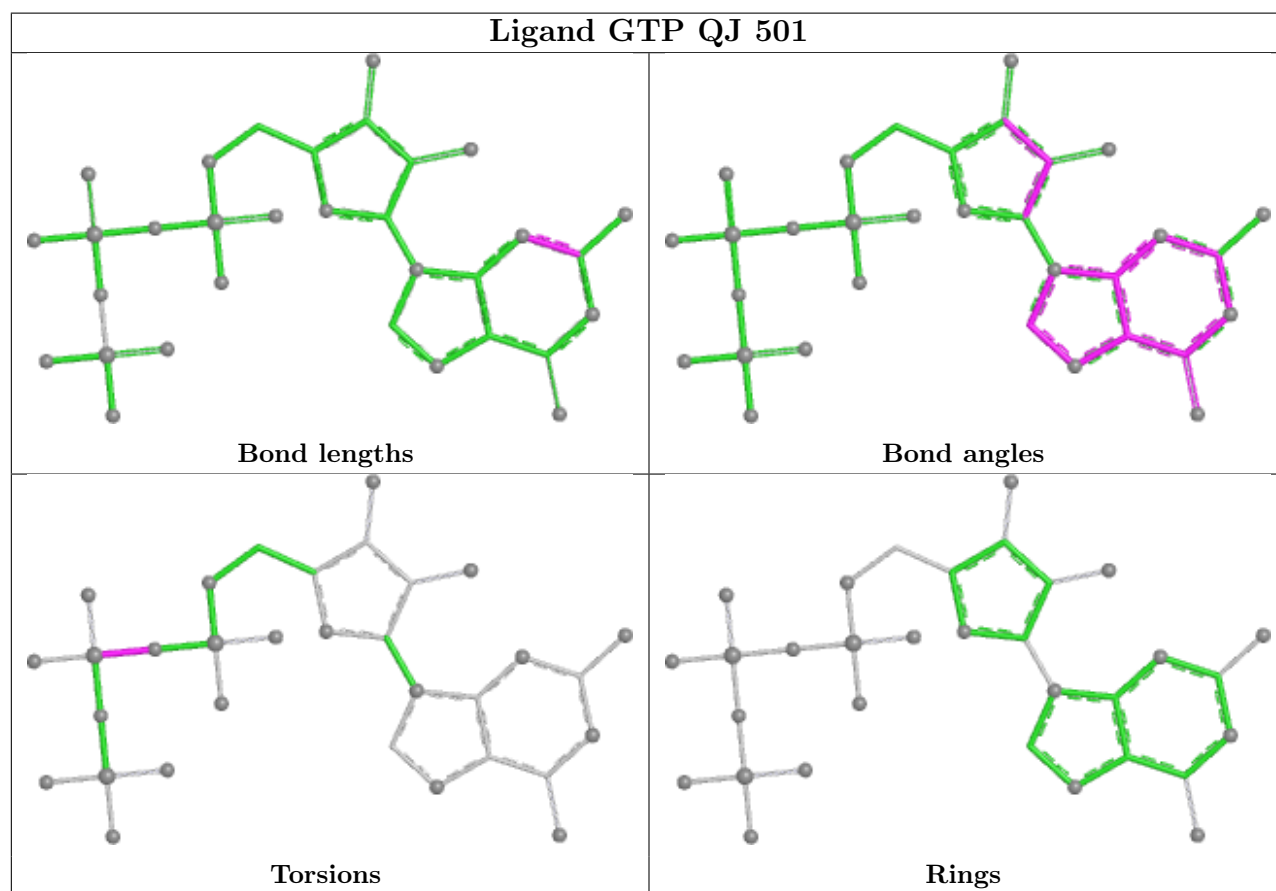
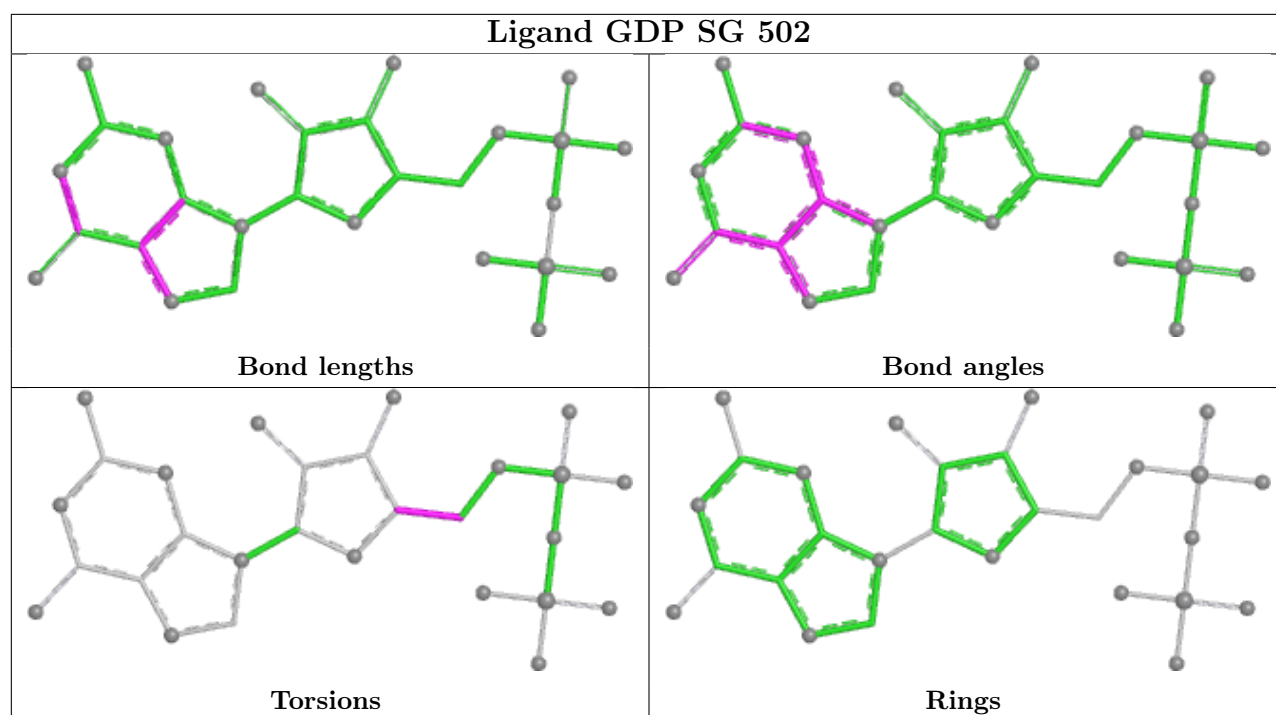


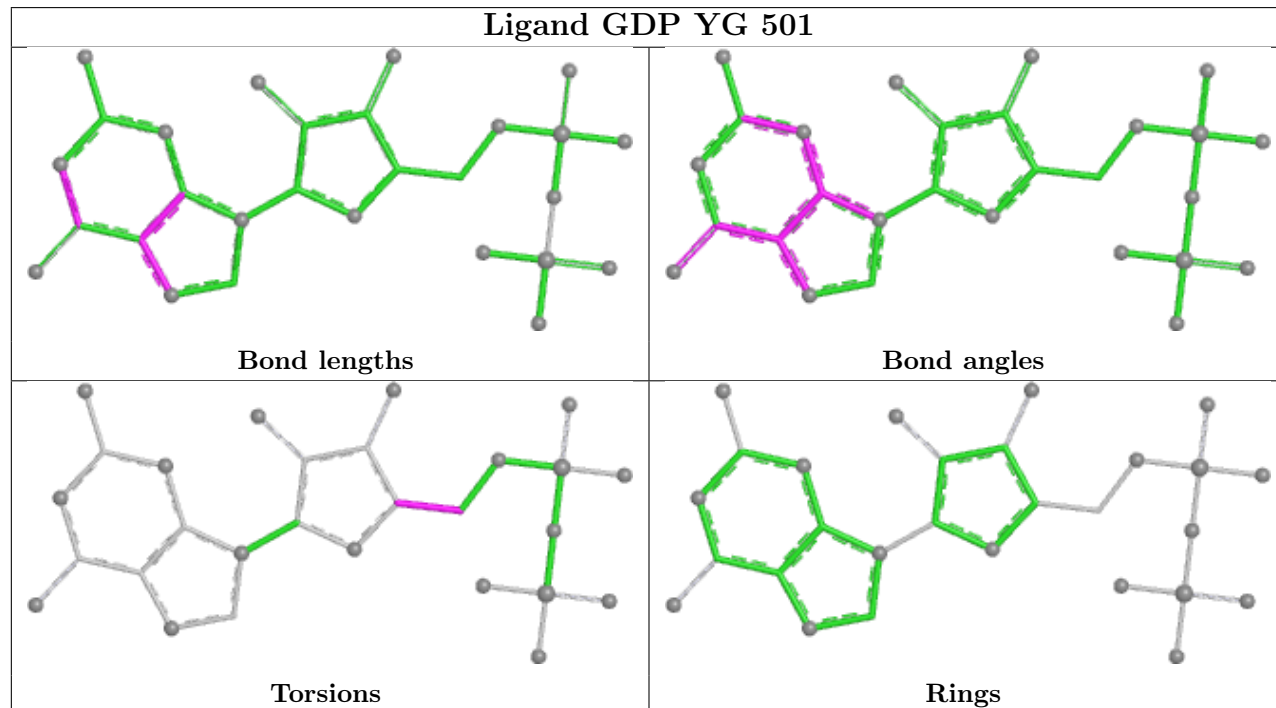
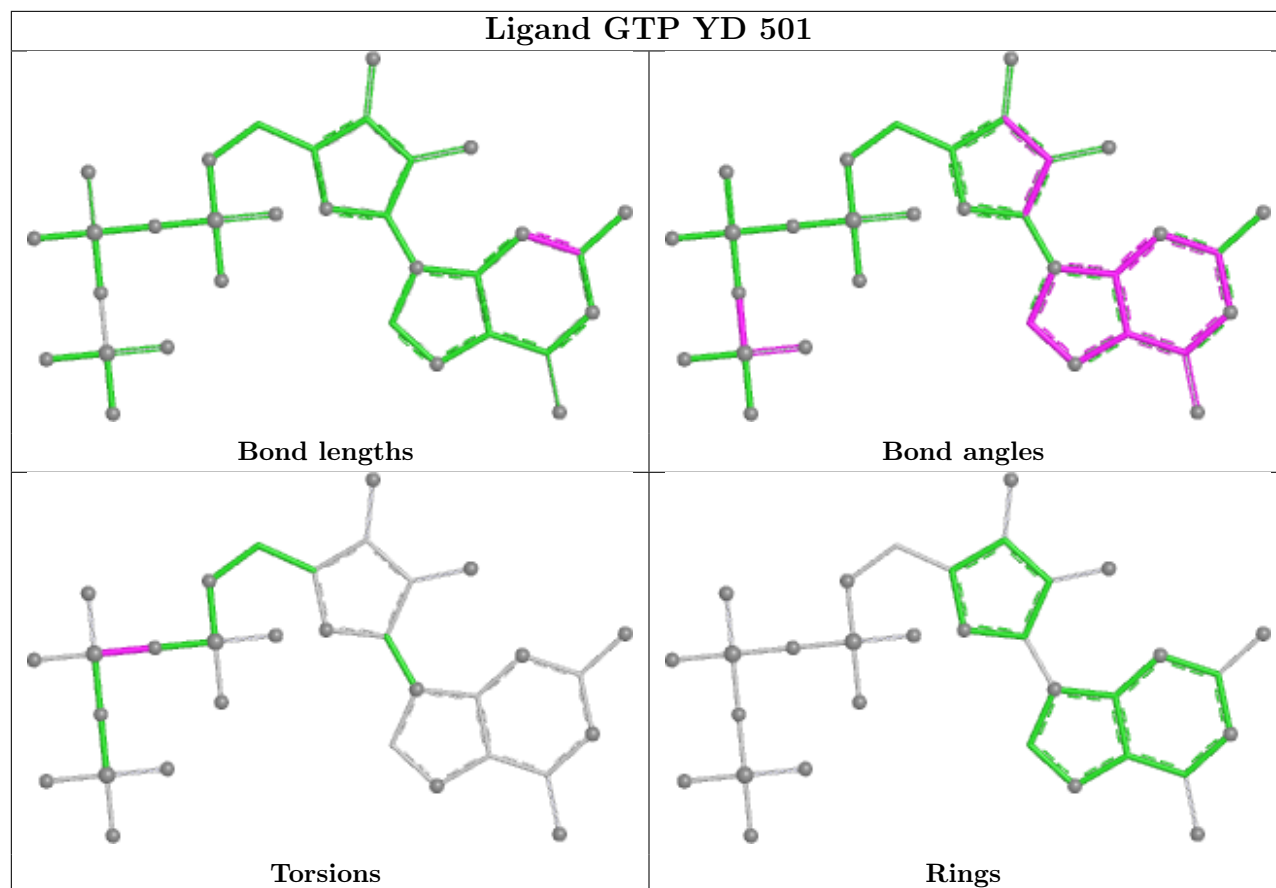
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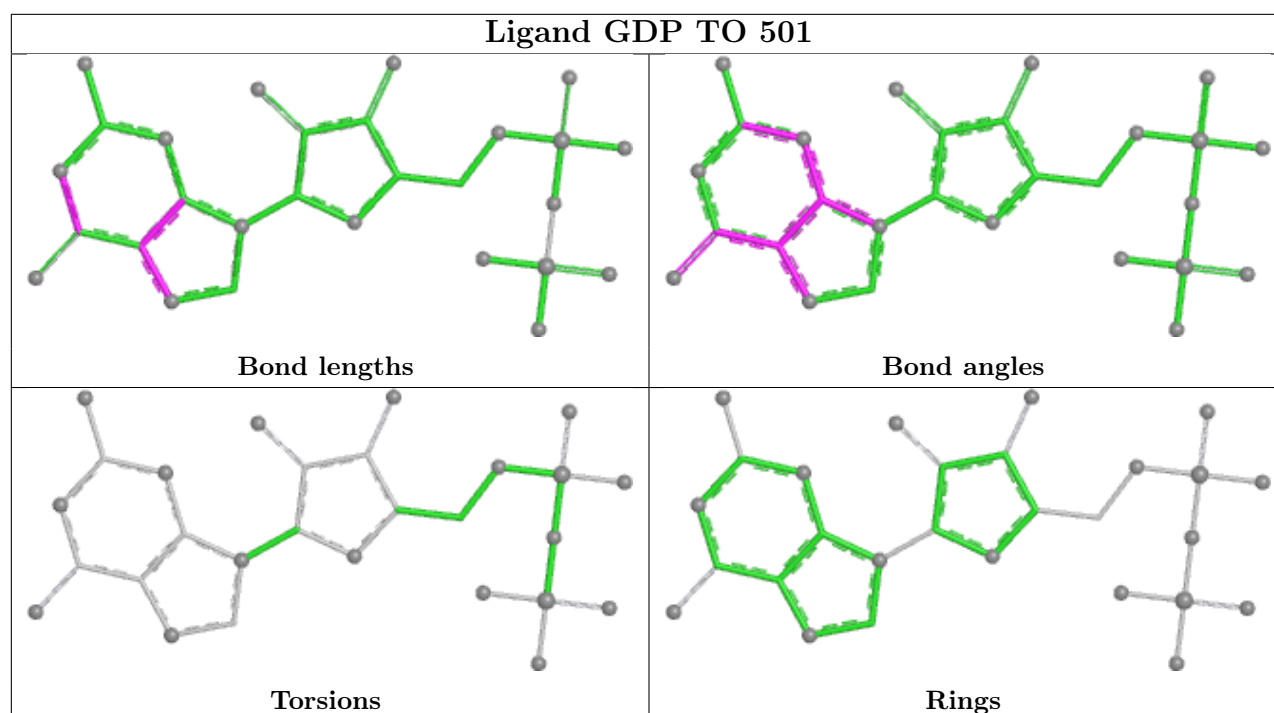


Ligand GTP WN 501









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
36	W6	1
36	W4	1
36	W5	1
36	W3	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	W6	43:UNK	C	53:UNK	N	8.65
1	W4	43:UNK	C	53:UNK	N	8.49
1	W5	43:UNK	C	53:UNK	N	8.22
1	W3	43:UNK	C	53:UNK	N	7.05

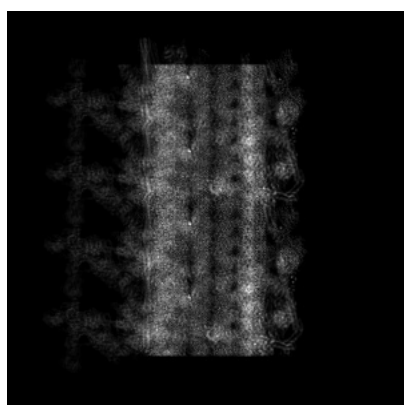
5 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-25381. These allow visual inspection of the internal detail of the map and identification of artifacts.

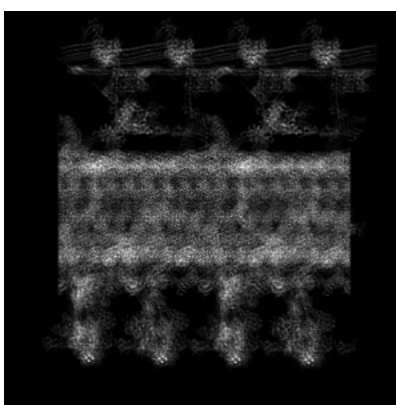
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

5.1 Orthogonal projections [i](#)

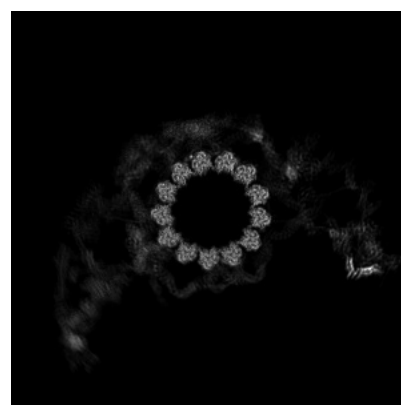
5.1.1 Primary map



X



Y



Z

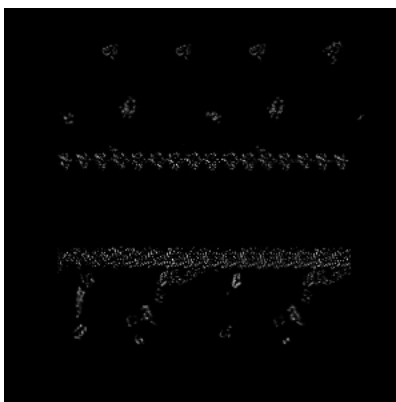
The images above show the map projected in three orthogonal directions.

5.2 Central slices [i](#)

5.2.1 Primary map



X Index: 320



Y Index: 320



Z Index: 320

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

5.3 Largest variance slices [i](#)

5.3.1 Primary map



X Index: 389



Y Index: 388

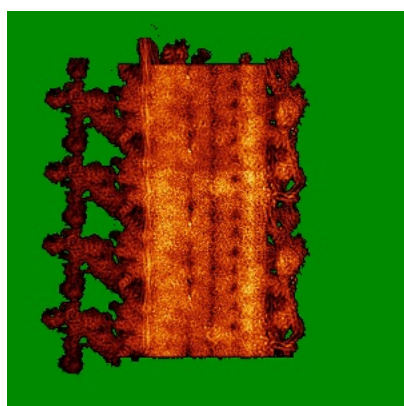


Z Index: 354

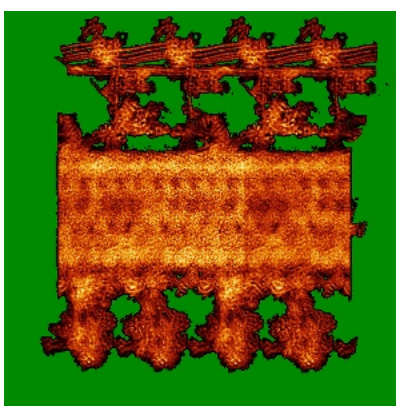
The images above show the largest variance slices of the map in three orthogonal directions.

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

5.4.1 Primary map



X



Y

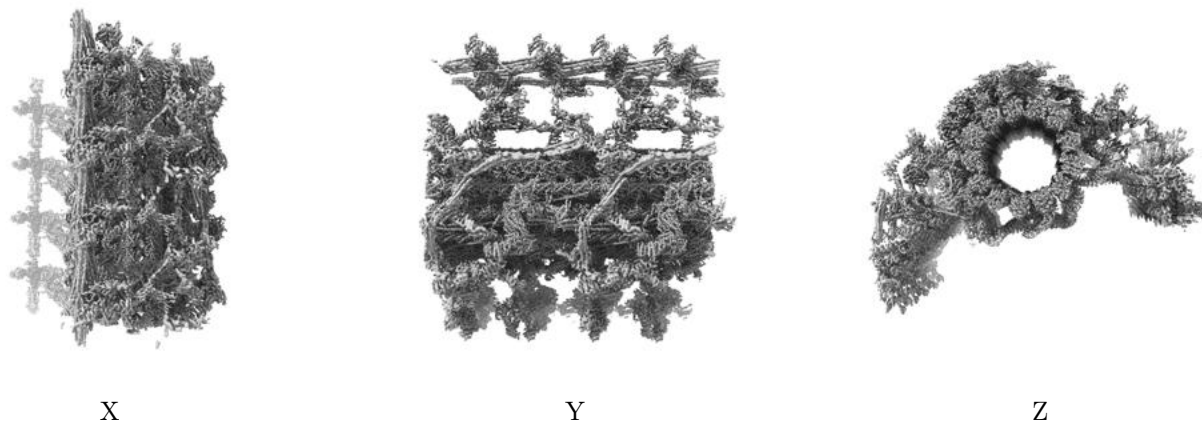


Z

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

5.5 Orthogonal surface views [i](#)

5.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

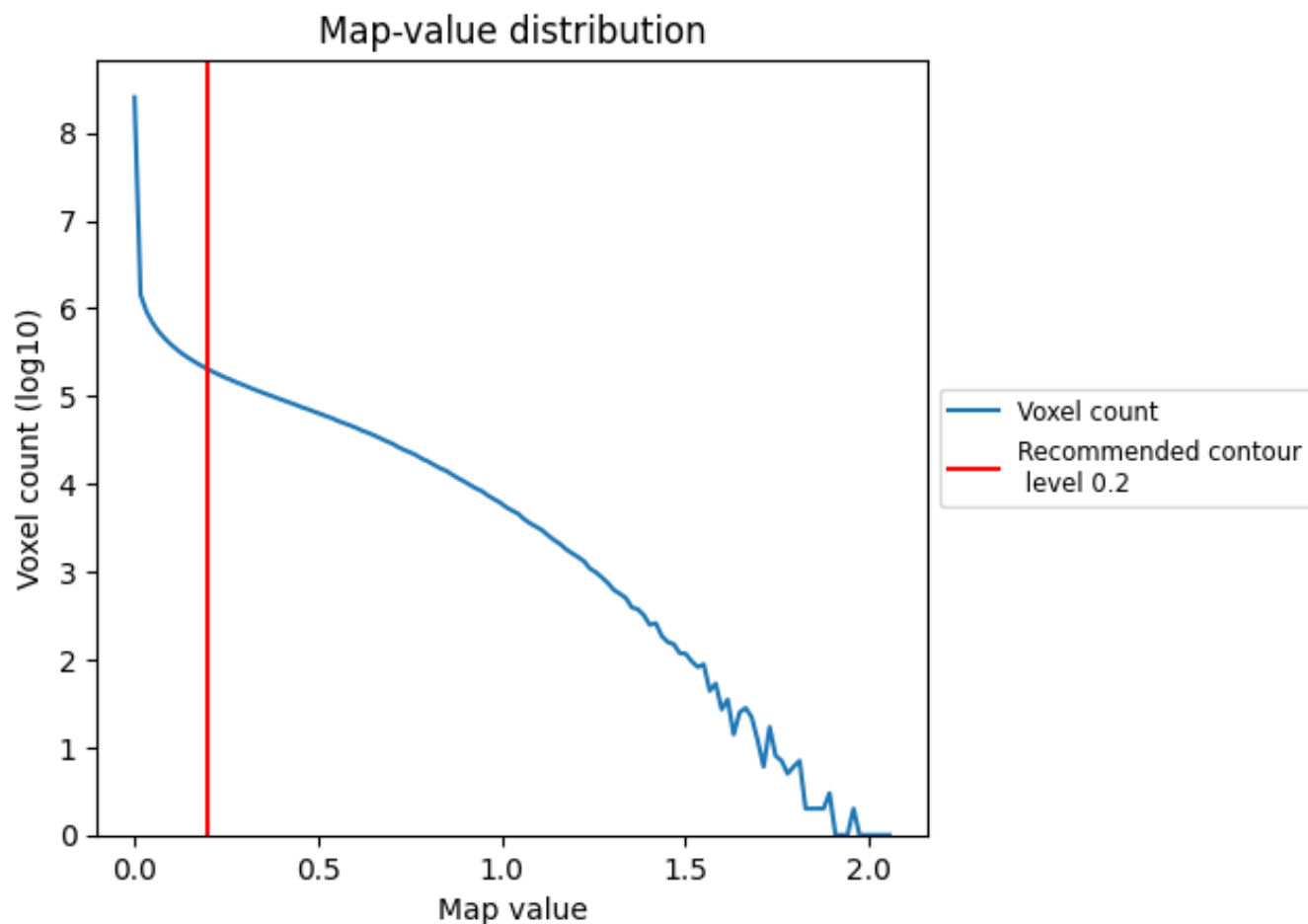
5.6 Mask visualisation [i](#)

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

6 Map analysis [i](#)

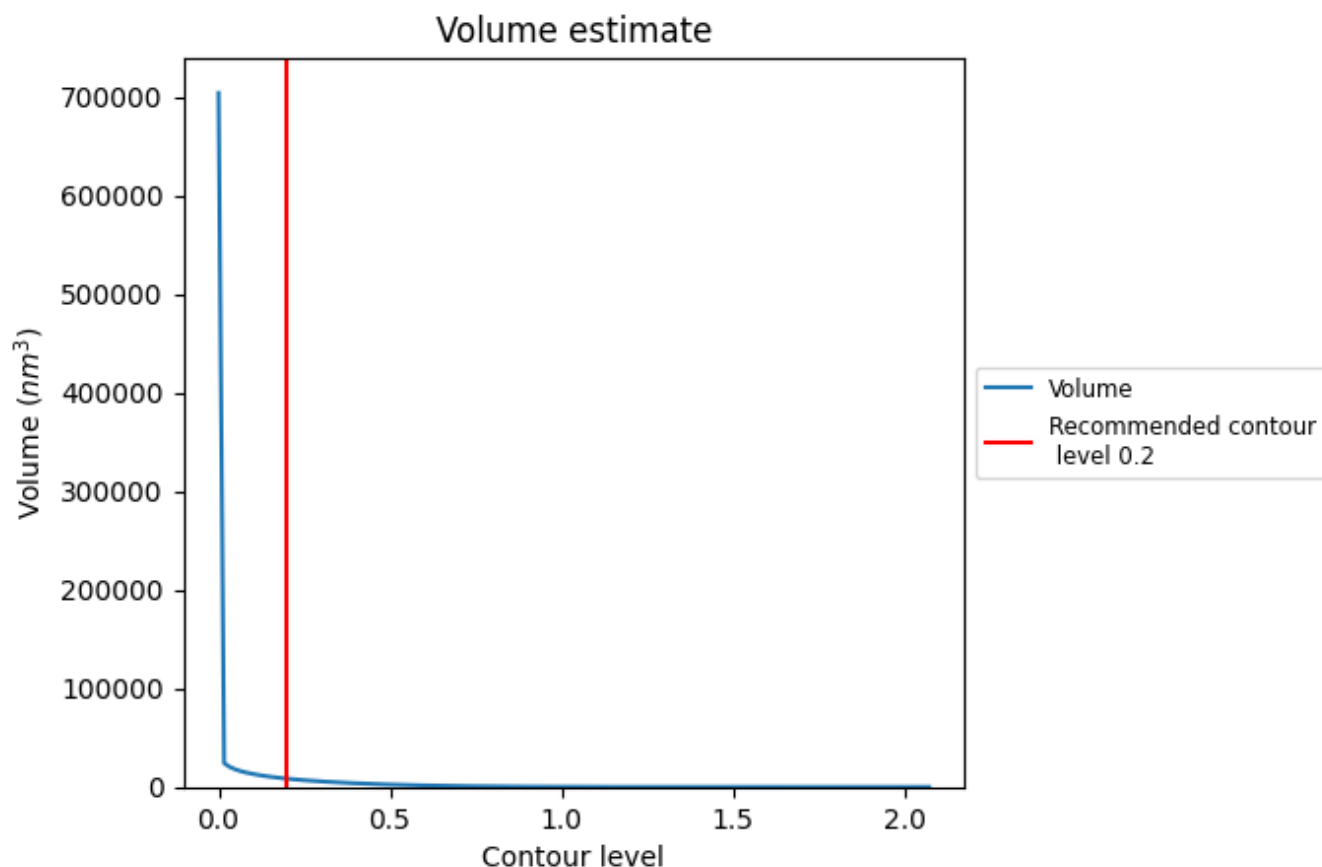
This section contains the results of statistical analysis of the map.

6.1 Map-value distribution [i](#)



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

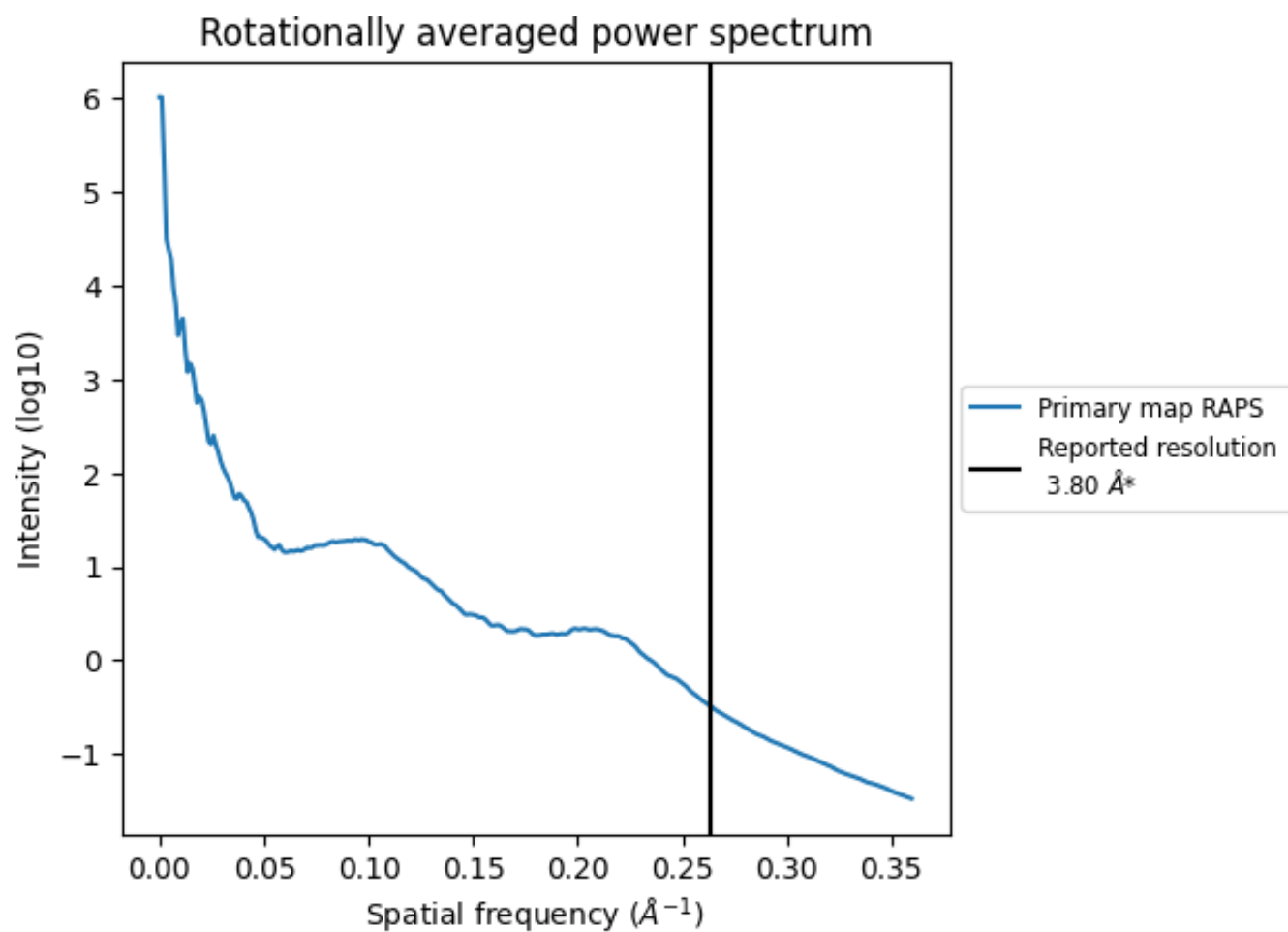
6.2 Volume estimate [i](#)



The volume at the recommended contour level is 8382 nm^3 ; this corresponds to an approximate mass of 7572 kDa.

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

6.3 Rotationally averaged power spectrum ⓘ

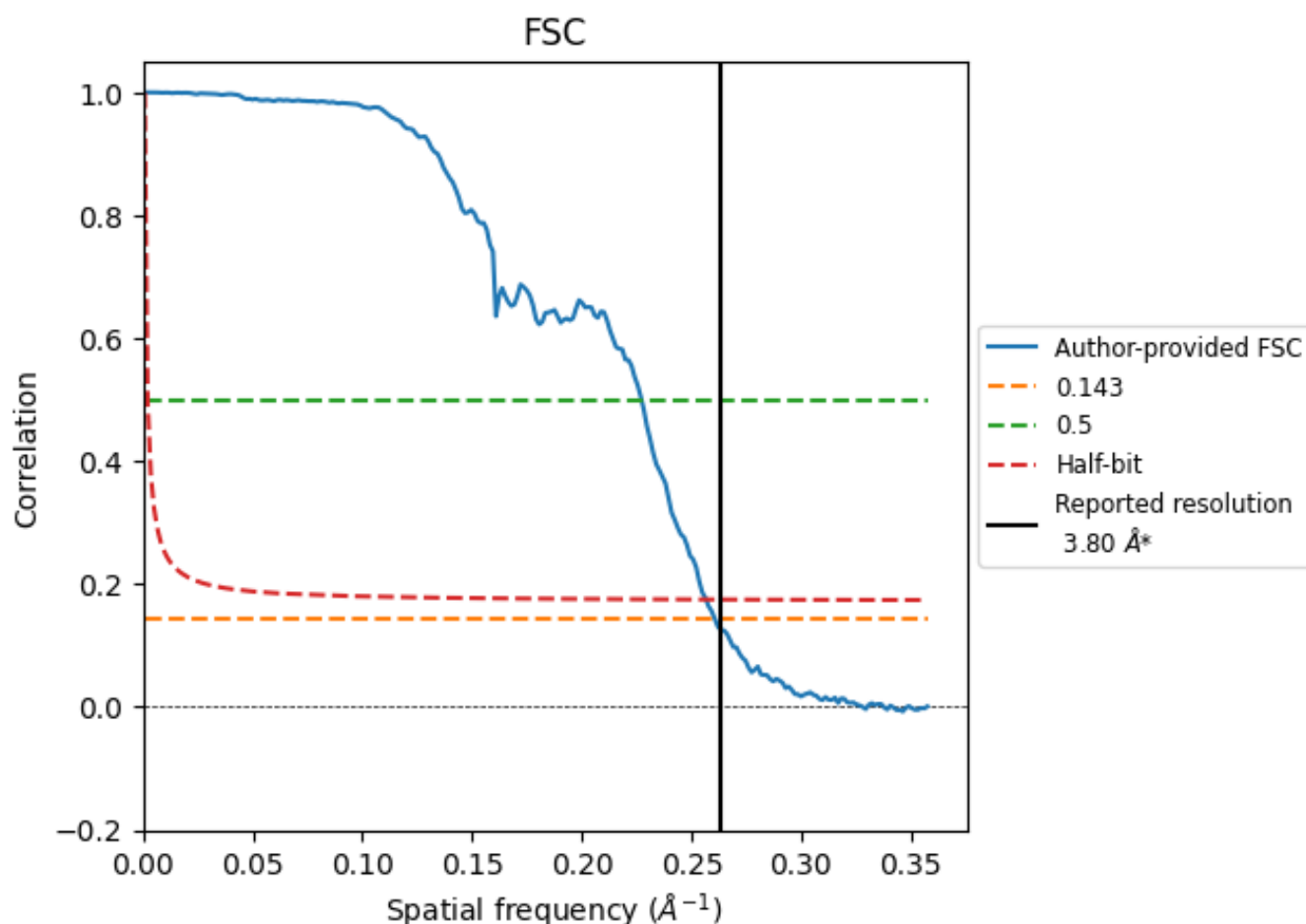


*Reported resolution corresponds to spatial frequency of 0.263 Å⁻¹

7 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

7.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.263 Å⁻¹

7.2 Resolution estimates [i](#)

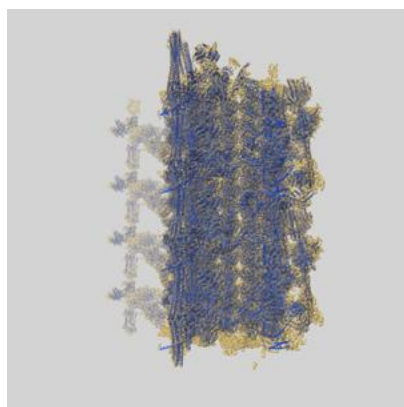
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.84	4.40	3.90
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

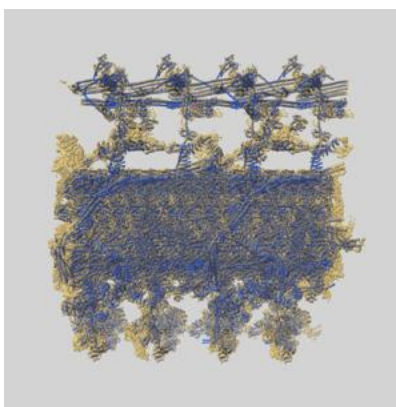
8 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-25381 and PDB model 7SQC. Per-residue inclusion information can be found in section ?? on page ??.

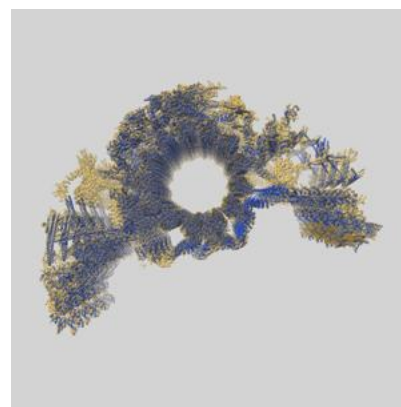
8.1 Map-model overlay [i](#)



X



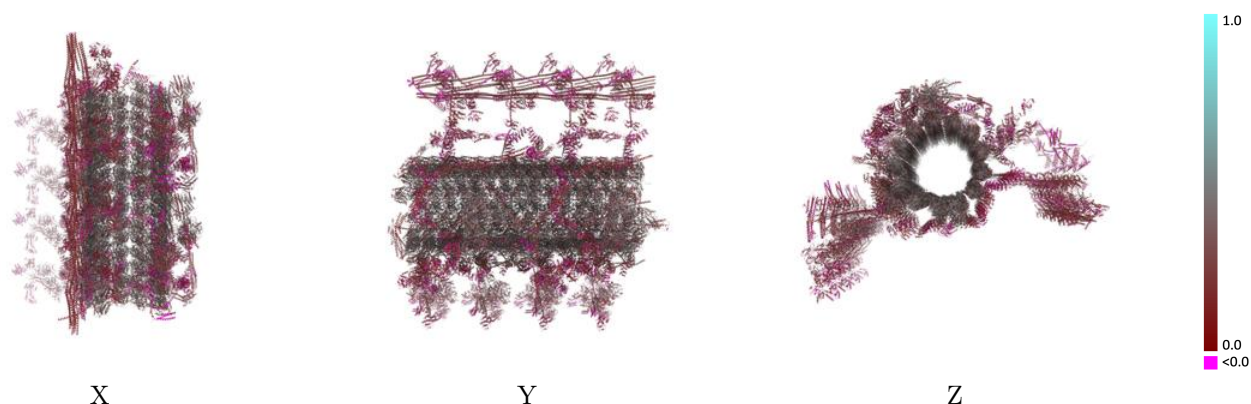
Y



Z

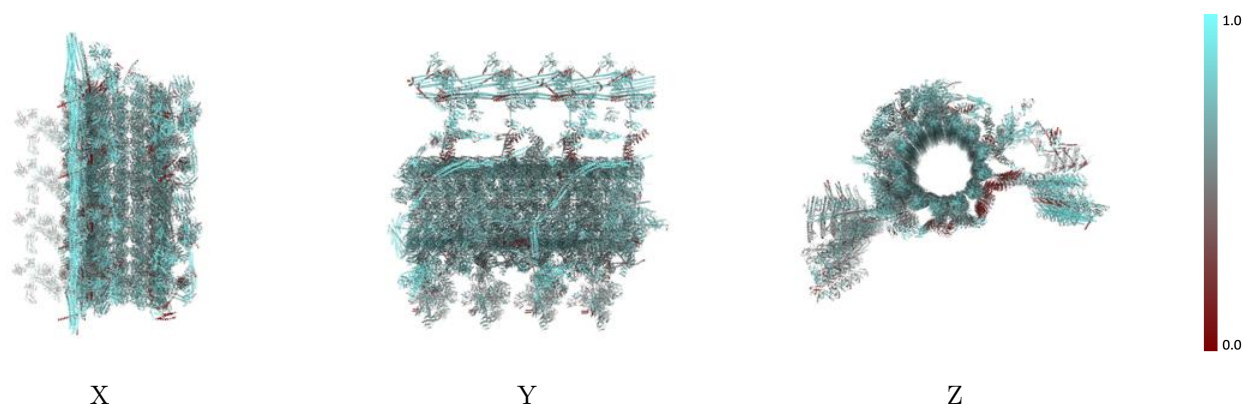
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



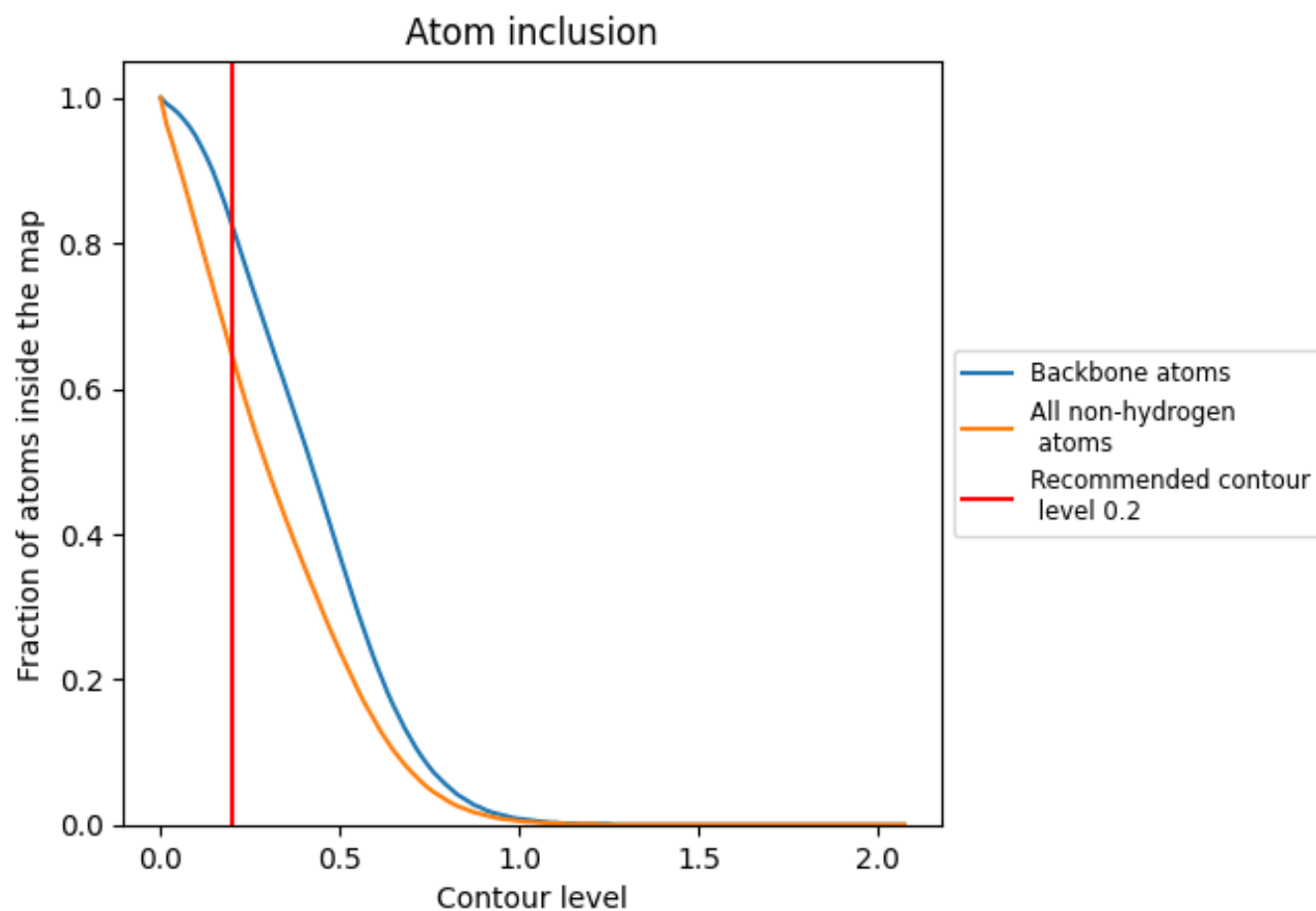
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.2).

8.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 64% of all non-hydrogen atoms, are inside the map.

8.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6440	 0.3260
0A	 0.5400	 0.2560
0B	 0.4840	 0.2440
0C	 0.5440	 0.2670
0D	 0.5000	 0.2480
0E	 0.5440	 0.2550
0F	 0.5130	 0.2510
0G	 0.5400	 0.2570
0H	 0.4780	 0.2400
0I	 0.7530	 0.2350
0J	 0.8020	 0.2280
0K	 0.7600	 0.2400
0L	 0.8620	 0.2450
1A	 0.5250	 0.1960
1B	 0.5370	 0.1990
1C	 0.5270	 0.1920
1D	 0.5300	 0.1940
1F	 0.8000	 0.2010
1G	 0.8680	 0.2140
1H	 0.7450	 0.1940
1I	 0.7530	 0.2010
1J	 0.8720	 0.2120
1K	 0.8630	 0.2140
1L	 0.7900	 0.2050
1M	 0.5180	 0.1590
1N	 0.8730	 0.2110
1O	 0.8670	 0.2140
1P	 0.8090	 0.2110
1Q	 0.5730	 0.1800
1R	 0.8830	 0.2170
1S	 0.8690	 0.2170
1T	 0.7910	 0.2100
1U	 0.5590	 0.1920
1V	 0.8880	 0.2210
1W	 0.8490	 0.2200



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Chain	Atom inclusion	Q-score
1X	 0.7850	 0.2090
1Y	 0.5080	 0.1750
2A	 0.6170	 0.2240
2B	 0.6370	 0.2410
2E	 0.3840	 0.1550
2F	 0.3670	 0.1730
2H	 0.5630	 0.1400
2I	 0.5770	 0.1450
2K	 0.6870	 0.2350
2L	 0.5820	 0.1640
2M	 0.5710	 0.1580
2N	 0.6150	 0.2020
2O	 0.6710	 0.2340
2P	 0.7100	 0.2490
2Q	 0.2700	 0.0310
3A	 0.7220	 0.2550
3B	 0.6570	 0.2240
3C	 0.7040	 0.2400
3D	 0.6550	 0.2270
3K	 0.6730	 0.1890
3L	 0.7010	 0.1910
3M	 0.6720	 0.1830
3N	 0.6950	 0.2070
3O	 0.6990	 0.1990
3P	 0.6790	 0.2040
4A	 0.7290	 0.2440
4B	 0.5910	 0.1980
4C	 0.6630	 0.2030
4D	 0.7240	 0.2420
4E	 0.5880	 0.1990
4F	 0.5070	 0.1370
4G	 0.7200	 0.2420
4H	 0.5840	 0.2070
4I	 0.6490	 0.1980
4J	 0.7090	 0.2410
4K	 0.5950	 0.2070
4L	 0.4990	 0.1540
5A	 0.6910	 0.2210
5B	 0.6910	 0.2220
5C	 0.6870	 0.2270
5D	 0.6900	 0.2280
6A	 0.6040	 0.1940

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Chain	Atom inclusion	Q-score
6B	 0.6180	 0.1960
6C	 0.3970	 0.1440
6D	 0.4230	 0.1440
7A	 0.5030	 0.1930
7B	 0.4930	 0.1190
7C	 0.6530	 0.1640
7D	 0.5050	 0.1170
7E	 0.6800	 0.1920
7F	 0.5140	 0.1170
7G	 0.5020	 0.1970
7H	 0.5130	 0.1170
7I	 0.4840	 0.1910
7J	 0.5050	 0.1170
7K	 0.4840	 0.1940
7L	 0.5760	 0.1690
8A	 0.5820	 0.3630
8B	 0.5400	 0.3770
8C	 0.5920	 0.3640
8D	 0.4830	 0.3420
9A	 0.6690	 0.2390
9B	 0.6670	 0.2370
9C	 0.6660	 0.2370
9D	 0.6630	 0.2380
9E	 0.6750	 0.1980
9F	 0.6980	 0.2070
A0	 0.6290	 0.4090
A1	 0.6200	 0.3950
A2	 0.6290	 0.3990
A3	 0.5850	 0.3760
A4	 0.5410	 0.3830
B0	 0.6160	 0.3210
B1	 0.5950	 0.3120
B2	 0.5600	 0.2890
C0	 0.5400	 0.1880
C1	 0.5560	 0.2100
C2	 0.5460	 0.2190
C3	 0.5400	 0.2090
C4	 0.5210	 0.3220
D0	 0.6260	 0.2920
D1	 0.5580	 0.1950
D2	 0.6520	 0.3340
D3	 0.5550	 0.1990

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Chain	Atom inclusion	Q-score
D4	 0.6080	 0.2770
D5	 0.5440	 0.1860
D6	 0.6460	 0.3050
D7	 0.5580	 0.2030
E0	 0.5850	 0.3760
E1	 0.5530	 0.3500
E2	 0.5490	 0.3600
E3	 0.5510	 0.3570
F0	 0.6840	 0.3190
F1	 0.6470	 0.3340
F2	 0.6580	 0.3630
F3	 0.6140	 0.3190
G0	 0.5670	 0.2200
G1	 0.5920	 0.2960
G2	 0.5710	 0.2330
G3	 0.6090	 0.3140
G4	 0.5500	 0.2130
G5	 0.5820	 0.2930
H0	 0.3990	 0.1930
H1	 0.2410	 0.1130
H2	 0.3150	 0.1530
H3	 0.3310	 0.1250
H4	 0.3410	 0.1870
H5	 0.2860	 0.0920
H6	 0.2860	 0.1560
H7	 0.2440	 0.1220
I0	 0.5560	 0.2240
I1	 0.5340	 0.1360
J0	 0.4800	 0.1310
J1	 0.5520	 0.1390
J2	 0.4750	 0.1310
J3	 0.5300	 0.1440
K0	 0.6420	 0.2500
K1	 0.5630	 0.1780
K2	 0.6340	 0.2250
K3	 0.5710	 0.1740
L0	 0.5490	 0.2310
L1	 0.5720	 0.2110
L2	 0.5420	 0.2260
L3	 0.5490	 0.1910
M0	 0.6470	 0.3680
M1	 0.6060	 0.3740

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Chain	Atom inclusion	Q-score
N0	 0.7290	 0.2560
N1	 0.7040	 0.2880
N2	 0.7390	 0.2560
N3	 0.6960	 0.2900
NB	 0.7130	 0.3830
NC	 0.6810	 0.3730
ND	 0.6820	 0.3780
NE	 0.6770	 0.3800
NF	 0.6940	 0.3680
NG	 0.6770	 0.3780
NH	 0.6870	 0.4050
NI	 0.6840	 0.4030
NJ	 0.7190	 0.3980
NK	 0.6960	 0.3900
NL	 0.6930	 0.3950
NM	 0.6950	 0.3970
NN	 0.6940	 0.3790
NO	 0.6710	 0.3630
O0	 0.5110	 0.2360
O1	 0.4970	 0.2990
O2	 0.4280	 0.2510
OC	 0.6800	 0.3840
OD	 0.6890	 0.3560
OE	 0.6290	 0.3320
OF	 0.6620	 0.3690
OG	 0.6650	 0.3670
OH	 0.7080	 0.3710
OI	 0.7020	 0.3890
OJ	 0.6900	 0.4030
OK	 0.6910	 0.3990
OL	 0.6980	 0.3770
OM	 0.6510	 0.3490
ON	 0.6850	 0.3910
OO	 0.6880	 0.3890
OP	 0.7000	 0.3720
OQ	 0.6950	 0.3810
P0	 0.8150	 0.3060
P1	 0.8540	 0.2960
P2	 0.8140	 0.3280
P3	 0.8410	 0.2890
PC	 0.6590	 0.3690
PD	 0.6800	 0.3460

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Chain	Atom inclusion	Q-score
PE	 0.6370	 0.3440
PF	 0.6610	 0.3700
PG	 0.6690	 0.3700
PH	 0.6910	 0.3580
PI	 0.6720	 0.3840
PJ	 0.6900	 0.3930
PK	 0.6690	 0.3890
PL	 0.6980	 0.3660
PM	 0.6570	 0.3650
PN	 0.6680	 0.3830
PO	 0.6740	 0.3830
PP	 0.6900	 0.3610
PQ	 0.6590	 0.3690
Q0	 0.6590	 0.3700
Q1	 0.6640	 0.3680
QC	 0.6790	 0.3750
QD	 0.7180	 0.3690
QE	 0.6890	 0.3820
QF	 0.6660	 0.3780
QG	 0.6840	 0.3710
QH	 0.7110	 0.3790
QI	 0.6870	 0.3900
QJ	 0.6890	 0.3950
QK	 0.6950	 0.3910
QL	 0.7240	 0.3950
QM	 0.6950	 0.3940
QN	 0.6860	 0.3960
QO	 0.6930	 0.3910
QP	 0.7060	 0.3690
QQ	 0.6720	 0.3740
R0	 0.6730	 0.2110
R1	 0.6580	 0.2020
RC	 0.6730	 0.3620
RD	 0.6700	 0.3440
RE	 0.6690	 0.3700
RF	 0.6720	 0.3660
RG	 0.6800	 0.3740
RH	 0.6920	 0.3830
RI	 0.6700	 0.3850
RJ	 0.6730	 0.3860
RK	 0.6800	 0.3760
RL	 0.6840	 0.3650

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Chain	Atom inclusion	Q-score
RM	 0.6770	 0.3850
RN	 0.6780	 0.3850
RO	 0.6910	 0.3880
RP	 0.6820	 0.3700
S0	 0.6110	 0.3880
S1	 0.6250	 0.4140
S2	 0.5690	 0.3540
S3	 0.5980	 0.3840
S5	 0.9370	 0.4940
SB	 0.6610	 0.3740
SC	 0.6870	 0.3600
SD	 0.6610	 0.3600
SE	 0.6720	 0.3700
SF	 0.6780	 0.3710
SG	 0.7110	 0.3870
SH	 0.6940	 0.4060
SI	 0.6900	 0.4070
SJ	 0.6770	 0.3970
SK	 0.7040	 0.3900
SL	 0.6850	 0.3870
SM	 0.6890	 0.3880
SN	 0.6940	 0.3900
SO	 0.7140	 0.3980
SP	 0.6840	 0.3860
T0	 0.5060	 0.3210
T1	 0.5040	 0.3220
T2	 0.4870	 0.3080
T3	 0.3470	 0.2280
TB	 0.6840	 0.4030
TC	 0.7030	 0.3900
TD	 0.6580	 0.3840
TE	 0.6640	 0.3800
TF	 0.6740	 0.3820
TG	 0.7110	 0.3950
TH	 0.7200	 0.4310
TI	 0.7040	 0.4200
TJ	 0.6860	 0.4200
TK	 0.7130	 0.4100
TL	 0.6910	 0.4110
TM	 0.6800	 0.3980
TN	 0.6890	 0.4030
TO	 0.7060	 0.3990

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Chain	Atom inclusion	Q-score
TP	 0.7110	 0.4130
U0	 0.5020	 0.2450
U1	 0.5330	 0.2630
UB	 0.7090	 0.4200
UC	 0.7220	 0.4020
UD	 0.6780	 0.3910
UE	 0.6710	 0.3950
UF	 0.6810	 0.3920
UG	 0.7160	 0.4120
UH	 0.7060	 0.4230
UI	 0.6860	 0.4270
UJ	 0.7150	 0.4370
UK	 0.7290	 0.4110
UL	 0.6930	 0.4050
UM	 0.6880	 0.4210
UN	 0.6920	 0.4200
UO	 0.7090	 0.4040
UP	 0.6990	 0.4120
V0	 0.8200	 0.2050
V1	 0.8230	 0.2010
VB	 0.7010	 0.4250
VC	 0.6970	 0.4080
VD	 0.6740	 0.4120
VE	 0.6800	 0.4110
VF	 0.7020	 0.4160
VG	 0.7260	 0.4410
VH	 0.7000	 0.4390
VI	 0.7070	 0.4430
VJ	 0.7120	 0.4410
VK	 0.7200	 0.4340
VL	 0.6980	 0.4330
VM	 0.7030	 0.4340
VN	 0.7150	 0.4340
VO	 0.7150	 0.4290
VP	 0.6920	 0.4250
W0	 0.7960	 0.2120
W1	 0.8040	 0.2130
W3	 0.6500	 0.4120
W4	 0.6620	 0.4420
W5	 0.6030	 0.4050
W6	 0.5740	 0.4070
W7	 0.8700	 0.4620

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Chain	Atom inclusion	Q-score
W8	 0.9020	 0.4900
W9	 0.8740	 0.4470
WA	 0.6790	 0.4160
WB	 0.6900	 0.4070
WC	 0.6760	 0.4010
WD	 0.6750	 0.3970
WE	 0.6530	 0.3830
WF	 0.6850	 0.4020
WG	 0.7030	 0.4340
WH	 0.6970	 0.4390
WI	 0.6920	 0.4370
WJ	 0.7050	 0.4310
WK	 0.7070	 0.4330
WL	 0.6920	 0.4250
WM	 0.6900	 0.4210
WN	 0.6920	 0.4110
WO	 0.6930	 0.4170
X0	 0.5450	 0.2590
X1	 0.5660	 0.2810
X2	 0.5630	 0.2810
X3	 0.5670	 0.2800
XA	 0.6910	 0.4230
XB	 0.7180	 0.4180
XC	 0.6900	 0.4040
XD	 0.6710	 0.4010
XE	 0.6680	 0.3910
XF	 0.7140	 0.4130
XG	 0.7160	 0.4390
XH	 0.7160	 0.4450
XI	 0.7040	 0.4400
XJ	 0.7250	 0.4420
XK	 0.7070	 0.4310
XL	 0.7010	 0.4240
XM	 0.6970	 0.4250
XN	 0.7050	 0.4180
XO	 0.7020	 0.4200
Y0	 0.5360	 0.2770
Y1	 0.5430	 0.2920
Y2	 0.5380	 0.2720
Y3	 0.5430	 0.2920
Y4	 0.5380	 0.2730
Y5	 0.5450	 0.2950

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Chain	Atom inclusion	Q-score
Y6	 0.5300	 0.2740
Y7	 0.5480	 0.2930
YB	 0.6920	 0.4190
YC	 0.7070	 0.4050
YD	 0.6710	 0.3890
YE	 0.6650	 0.3960
YF	 0.6630	 0.3950
YG	 0.7100	 0.4130
YH	 0.7150	 0.4390
YI	 0.7000	 0.4340
YJ	 0.6900	 0.4370
YK	 0.7200	 0.4310
YL	 0.6970	 0.4260
YM	 0.6860	 0.4230
YN	 0.6840	 0.4190
YO	 0.7050	 0.4080
YP	 0.7050	 0.4210
Z0	 0.5180	 0.2220
Z1	 0.5100	 0.2150
Z2	 0.5130	 0.2160
Z3	 0.5200	 0.2190
ZB	 0.6850	 0.3750
ZC	 0.6810	 0.3670
ZD	 0.6620	 0.3630
ZE	 0.6660	 0.3770
ZF	 0.6870	 0.3840
ZG	 0.6920	 0.3920
ZH	 0.6890	 0.4040
ZI	 0.6890	 0.4080
ZJ	 0.6960	 0.4020
ZK	 0.7010	 0.3900
ZL	 0.6870	 0.3940
ZM	 0.6840	 0.4000
ZN	 0.6960	 0.3970
ZO	 0.6830	 0.3730
ZP	 0.6780	 0.3770