



Full wwPDB EM Validation Report ⓘ

Nov 14, 2022 – 11:53 pm GMT

PDB ID : 7ZQD
EMDB ID : EMD-14871
Title : Dimeric PSI of Chlamydomonas reinhardtii at 2.97 Å resolution
Authors : Naschberger, A.; Amunts, A.
Deposited on : 2022-04-29
Resolution : 2.97 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:

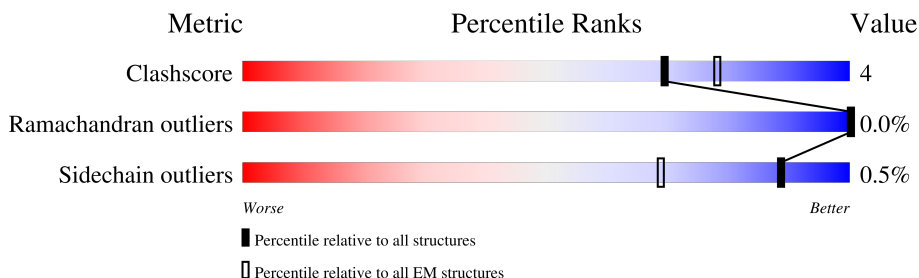
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

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 2.97 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	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	751	
1	A2	751	
2	B	735	
2	B2	735	
3	C	81	
3	C2	81	
4	D	196	
4	D2	196	




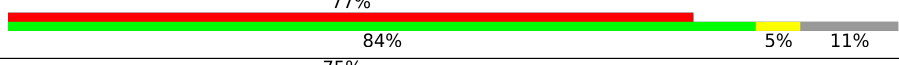
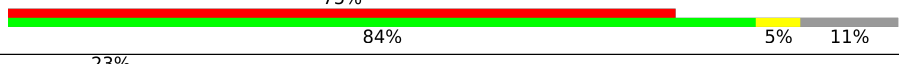
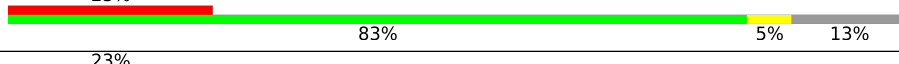
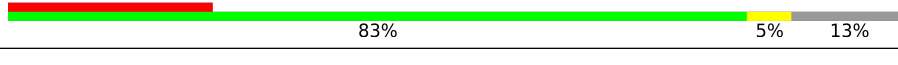
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Mol	Chain	Length	Quality of chain
5	E	97	15% 65% 34%
5	E2	97	16% 65% 34%
6	F	227	7% 67% 6% 27%
6	F2	227	9% 67% 6% 27%
7	G	126	24% 71% 5% 25%
7	G2	126	23% 71% 5% 25%
8	I	106	5% 31% 65%
8	I2	106	5% 31% 65%
9	J	40	8% 95% 5%
9	J2	40	5% 95% 5%
10	L	196	36% 59% 37%
10	L2	196	37% 59% 37%
11	K	113	46% 69% 7% 24%
11	K2	113	50% 69% 7% 24%
12	1	228	16% 80% 5% 15%
12	12	228	15% 81% 15%
12	Z	228	57% 79% 7% 15%
12	Z2	228	57% 79% 7% 15%
13	3	298	17% 68% 8% 24%
13	32	298	17% 68% 8% 24%
14	7	241	16% 85% 12%
14	72	241	17% 85% 12%
15	8	243	13% 86% 11%
15	82	243	12% 86% 11%
16	4	264	69% 77% 20%

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Mol	Chain	Length	Quality of chain
16	42	264	
17	5	257	
17	52	257	
18	6	257	
18	62	257	
19	9	213	
19	92	213	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CL0	A	801	X	-	-	-
20	CL0	A2	801	X	-	-	-
21	CLA	1	602	X	-	-	-
21	CLA	1	603	X	-	-	-
21	CLA	1	604	X	-	-	-
21	CLA	1	608	X	-	-	-
21	CLA	1	609	X	-	-	-
21	CLA	1	610	X	-	-	-
21	CLA	1	611	X	-	-	-
21	CLA	1	612	X	-	-	-
21	CLA	1	613	X	-	-	-
21	CLA	1	614	X	-	-	-
21	CLA	1	616	X	-	-	-
21	CLA	12	602	X	-	-	-
21	CLA	12	603	X	-	-	-
21	CLA	12	604	X	-	-	-
21	CLA	12	608	X	-	-	-
21	CLA	12	609	X	-	-	-
21	CLA	12	610	X	-	-	-
21	CLA	12	611	X	-	-	-
21	CLA	12	612	X	-	-	-
21	CLA	12	613	X	-	-	-
21	CLA	12	614	X	-	-	-
21	CLA	12	616	X	-	-	-
21	CLA	3	602	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	3	603	X	-	-	-
21	CLA	3	604	X	-	-	-
21	CLA	3	606	X	-	-	-
21	CLA	3	607	X	-	-	-
21	CLA	3	609	X	-	-	-
21	CLA	3	610	X	-	-	-
21	CLA	3	611	X	-	-	-
21	CLA	3	612	X	-	-	-
21	CLA	3	613	X	-	-	-
21	CLA	3	614	X	-	-	-
21	CLA	3	615	X	-	-	-
21	CLA	3	617	X	-	-	-
21	CLA	32	602	X	-	-	-
21	CLA	32	603	X	-	-	-
21	CLA	32	604	X	-	-	-
21	CLA	32	606	X	-	-	-
21	CLA	32	607	X	-	-	-
21	CLA	32	609	X	-	-	-
21	CLA	32	610	X	-	-	-
21	CLA	32	611	X	-	-	-
21	CLA	32	612	X	-	-	-
21	CLA	32	613	X	-	-	-
21	CLA	32	614	X	-	-	-
21	CLA	32	615	X	-	-	-
21	CLA	32	617	X	-	-	-
21	CLA	4	602	X	-	-	-
21	CLA	4	603	X	-	-	-
21	CLA	4	604	X	-	-	-
21	CLA	4	609	X	-	-	-
21	CLA	4	610	X	-	-	-
21	CLA	4	611	X	-	-	-
21	CLA	4	612	X	-	-	-
21	CLA	4	613	X	-	-	-
21	CLA	4	614	X	-	-	-
21	CLA	4	616	X	-	-	-
21	CLA	42	602	X	-	-	-
21	CLA	42	603	X	-	-	-
21	CLA	42	604	X	-	-	-
21	CLA	42	609	X	-	-	-
21	CLA	42	610	X	-	-	-
21	CLA	42	611	X	-	-	-
21	CLA	42	612	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	42	613	X	-	-	-
21	CLA	42	614	X	-	-	-
21	CLA	42	616	X	-	-	-
21	CLA	5	601	X	-	-	-
21	CLA	5	602	X	-	-	-
21	CLA	5	603	X	-	-	-
21	CLA	5	604	X	-	-	-
21	CLA	5	609	X	-	-	-
21	CLA	5	610	X	-	-	-
21	CLA	5	611	X	-	-	-
21	CLA	5	612	X	-	-	-
21	CLA	5	613	X	-	-	-
21	CLA	5	614	X	-	-	-
21	CLA	5	616	X	-	-	-
21	CLA	5	617	X	-	-	-
21	CLA	5	621	X	-	-	-
21	CLA	52	601	X	-	-	-
21	CLA	52	602	X	-	-	-
21	CLA	52	603	X	-	-	-
21	CLA	52	604	X	-	-	-
21	CLA	52	609	X	-	-	-
21	CLA	52	610	X	-	-	-
21	CLA	52	611	X	-	-	-
21	CLA	52	612	X	-	-	-
21	CLA	52	613	X	-	-	-
21	CLA	52	614	X	-	-	-
21	CLA	52	616	X	-	-	-
21	CLA	52	617	X	-	-	-
21	CLA	52	621	X	-	-	-
21	CLA	6	602	X	-	-	-
21	CLA	6	603	X	-	-	-
21	CLA	6	604	X	-	-	-
21	CLA	6	609	X	-	-	-
21	CLA	6	610	X	-	-	-
21	CLA	6	611	X	-	-	-
21	CLA	6	612	X	-	-	-
21	CLA	6	613	X	-	-	-
21	CLA	6	614	X	-	-	-
21	CLA	6	617	X	-	-	-
21	CLA	6	622	X	-	-	-
21	CLA	62	602	X	-	-	-
21	CLA	62	603	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	62	604	X	-	-	-
21	CLA	62	609	X	-	-	-
21	CLA	62	610	X	-	-	-
21	CLA	62	611	X	-	-	-
21	CLA	62	612	X	-	-	-
21	CLA	62	613	X	-	-	-
21	CLA	62	614	X	-	-	-
21	CLA	62	617	X	-	-	-
21	CLA	62	622	X	-	-	-
21	CLA	7	602	X	-	-	-
21	CLA	7	603	X	-	-	-
21	CLA	7	604	X	-	-	-
21	CLA	7	608	X	-	-	-
21	CLA	7	609	X	-	-	-
21	CLA	7	610	X	-	-	-
21	CLA	7	611	X	-	-	-
21	CLA	7	612	X	-	-	-
21	CLA	7	613	X	-	-	-
21	CLA	7	614	X	-	-	-
21	CLA	7	616	X	-	-	-
21	CLA	7	620	X	-	-	-
21	CLA	72	602	X	-	-	-
21	CLA	72	603	X	-	-	-
21	CLA	72	604	X	-	-	-
21	CLA	72	608	X	-	-	-
21	CLA	72	609	X	-	-	-
21	CLA	72	610	X	-	-	-
21	CLA	72	611	X	-	-	-
21	CLA	72	612	X	-	-	-
21	CLA	72	613	X	-	-	-
21	CLA	72	614	X	-	-	-
21	CLA	72	616	X	-	-	-
21	CLA	72	620	X	-	-	-
21	CLA	8	602	X	-	-	-
21	CLA	8	603	X	-	-	-
21	CLA	8	604	X	-	-	-
21	CLA	8	608	X	-	-	-
21	CLA	8	609	X	-	-	-
21	CLA	8	610	X	-	-	-
21	CLA	8	611	X	-	-	-
21	CLA	8	612	X	-	-	-
21	CLA	8	613	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	8	614	X	-	-	-
21	CLA	8	616	X	-	-	-
21	CLA	82	602	X	-	-	-
21	CLA	82	603	X	-	-	-
21	CLA	82	604	X	-	-	-
21	CLA	82	608	X	-	-	-
21	CLA	82	609	X	-	-	-
21	CLA	82	610	X	-	-	-
21	CLA	82	611	X	-	-	-
21	CLA	82	612	X	-	-	-
21	CLA	82	613	X	-	-	-
21	CLA	82	614	X	-	-	-
21	CLA	82	616	X	-	-	-
21	CLA	9	601	X	-	-	-
21	CLA	9	602	X	-	-	-
21	CLA	9	603	X	-	-	-
21	CLA	9	604	X	-	-	-
21	CLA	9	609	X	-	-	-
21	CLA	9	610	X	-	-	-
21	CLA	9	611	X	-	-	-
21	CLA	9	612	X	-	-	-
21	CLA	9	613	X	-	-	-
21	CLA	9	614	X	-	-	-
21	CLA	92	601	X	-	-	-
21	CLA	92	602	X	-	-	-
21	CLA	92	603	X	-	-	-
21	CLA	92	604	X	-	-	-
21	CLA	92	609	X	-	-	-
21	CLA	92	610	X	-	-	-
21	CLA	92	611	X	-	-	-
21	CLA	92	612	X	-	-	-
21	CLA	92	613	X	-	-	-
21	CLA	92	614	X	-	-	-
21	CLA	A	802	X	-	-	-
21	CLA	A	803	X	-	-	-
21	CLA	A	804	X	-	-	-
21	CLA	A	805	X	-	-	-
21	CLA	A	806	X	-	-	-
21	CLA	A	807	X	-	-	-
21	CLA	A	808	X	-	-	-
21	CLA	A	809	X	-	-	-
21	CLA	A	810	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	A	811	X	-	-	-
21	CLA	A	812	X	-	-	-
21	CLA	A	813	X	-	-	-
21	CLA	A	814	X	-	-	-
21	CLA	A	815	X	-	-	-
21	CLA	A	816	X	-	-	-
21	CLA	A	817	X	-	-	-
21	CLA	A	818	X	-	-	-
21	CLA	A	819	X	-	-	-
21	CLA	A	820	X	-	-	-
21	CLA	A	821	X	-	-	-
21	CLA	A	822	X	-	-	-
21	CLA	A	823	X	-	-	-
21	CLA	A	824	X	-	-	-
21	CLA	A	825	X	-	-	-
21	CLA	A	826	X	-	-	-
21	CLA	A	827	X	-	-	-
21	CLA	A	828	X	-	-	-
21	CLA	A	829	X	-	-	-
21	CLA	A	830	X	-	-	-
21	CLA	A	831	X	-	-	-
21	CLA	A	832	X	-	-	-
21	CLA	A	833	X	-	-	-
21	CLA	A	834	X	-	-	-
21	CLA	A	835	X	-	-	-
21	CLA	A	836	X	-	-	-
21	CLA	A	837	X	-	-	-
21	CLA	A	838	X	-	-	-
21	CLA	A	839	X	-	-	-
21	CLA	A	840	X	-	-	-
21	CLA	A	841	X	-	-	-
21	CLA	A	842	X	-	-	-
21	CLA	A	843	X	-	-	-
21	CLA	A	845	X	-	-	-
21	CLA	A	854	X	-	-	-
21	CLA	A2	802	X	-	-	-
21	CLA	A2	803	X	-	-	-
21	CLA	A2	804	X	-	-	-
21	CLA	A2	805	X	-	-	-
21	CLA	A2	806	X	-	-	-
21	CLA	A2	807	X	-	-	-
21	CLA	A2	808	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	A2	809	X	-	-	-
21	CLA	A2	810	X	-	-	-
21	CLA	A2	811	X	-	-	-
21	CLA	A2	812	X	-	-	-
21	CLA	A2	813	X	-	-	-
21	CLA	A2	814	X	-	-	-
21	CLA	A2	815	X	-	-	-
21	CLA	A2	816	X	-	-	-
21	CLA	A2	817	X	-	-	-
21	CLA	A2	818	X	-	-	-
21	CLA	A2	819	X	-	-	-
21	CLA	A2	820	X	-	-	-
21	CLA	A2	821	X	-	-	-
21	CLA	A2	822	X	-	-	-
21	CLA	A2	823	X	-	-	-
21	CLA	A2	824	X	-	-	-
21	CLA	A2	825	X	-	-	-
21	CLA	A2	826	X	-	-	-
21	CLA	A2	827	X	-	-	-
21	CLA	A2	828	X	-	-	-
21	CLA	A2	829	X	-	-	-
21	CLA	A2	830	X	-	-	-
21	CLA	A2	831	X	-	-	-
21	CLA	A2	832	X	-	-	-
21	CLA	A2	833	X	-	-	-
21	CLA	A2	834	X	-	-	-
21	CLA	A2	835	X	-	-	-
21	CLA	A2	836	X	-	-	-
21	CLA	A2	837	X	-	-	-
21	CLA	A2	838	X	-	-	-
21	CLA	A2	839	X	-	-	-
21	CLA	A2	840	X	-	-	-
21	CLA	A2	841	X	-	-	-
21	CLA	A2	842	X	-	-	-
21	CLA	A2	843	X	-	-	-
21	CLA	A2	845	X	-	-	-
21	CLA	A2	854	X	-	-	-
21	CLA	B	802	X	-	-	-
21	CLA	B	803	X	-	-	-
21	CLA	B	804	X	-	-	-
21	CLA	B	805	X	-	-	-
21	CLA	B	806	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	B	807	X	-	-	-
21	CLA	B	808	X	-	-	-
21	CLA	B	809	X	-	-	-
21	CLA	B	810	X	-	-	-
21	CLA	B	811	X	-	-	-
21	CLA	B	812	X	-	-	-
21	CLA	B	813	X	-	-	-
21	CLA	B	814	X	-	-	-
21	CLA	B	815	X	-	-	-
21	CLA	B	816	X	-	-	-
21	CLA	B	817	X	-	-	-
21	CLA	B	818	X	-	-	-
21	CLA	B	819	X	-	-	-
21	CLA	B	820	X	-	-	-
21	CLA	B	821	X	-	-	-
21	CLA	B	822	X	-	-	-
21	CLA	B	823	X	-	-	-
21	CLA	B	824	X	-	-	-
21	CLA	B	825	X	-	-	-
21	CLA	B	826	X	-	-	-
21	CLA	B	827	X	-	-	-
21	CLA	B	828	X	-	-	-
21	CLA	B	829	X	-	-	-
21	CLA	B	830	X	-	-	-
21	CLA	B	831	X	-	-	-
21	CLA	B	832	X	-	-	-
21	CLA	B	833	X	-	-	-
21	CLA	B	834	X	-	-	-
21	CLA	B	835	X	-	-	-
21	CLA	B	836	X	-	-	-
21	CLA	B	837	X	-	-	-
21	CLA	B	838	X	-	-	-
21	CLA	B	839	X	-	-	-
21	CLA	B	840	X	-	-	-
21	CLA	B	841	X	-	-	-
21	CLA	B2	802	X	-	-	-
21	CLA	B2	803	X	-	-	-
21	CLA	B2	804	X	-	-	-
21	CLA	B2	805	X	-	-	-
21	CLA	B2	806	X	-	-	-
21	CLA	B2	807	X	-	-	-
21	CLA	B2	808	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	B2	809	X	-	-	-
21	CLA	B2	810	X	-	-	-
21	CLA	B2	811	X	-	-	-
21	CLA	B2	812	X	-	-	-
21	CLA	B2	813	X	-	-	-
21	CLA	B2	814	X	-	-	-
21	CLA	B2	815	X	-	-	-
21	CLA	B2	816	X	-	-	-
21	CLA	B2	817	X	-	-	-
21	CLA	B2	818	X	-	-	-
21	CLA	B2	819	X	-	-	-
21	CLA	B2	820	X	-	-	-
21	CLA	B2	821	X	-	-	-
21	CLA	B2	822	X	-	-	-
21	CLA	B2	823	X	-	-	-
21	CLA	B2	824	X	-	-	-
21	CLA	B2	825	X	-	-	-
21	CLA	B2	826	X	-	-	-
21	CLA	B2	827	X	-	-	-
21	CLA	B2	828	X	-	-	-
21	CLA	B2	829	X	-	-	-
21	CLA	B2	830	X	-	-	-
21	CLA	B2	831	X	-	-	-
21	CLA	B2	832	X	-	-	-
21	CLA	B2	833	X	-	-	-
21	CLA	B2	834	X	-	-	-
21	CLA	B2	835	X	-	-	-
21	CLA	B2	836	X	-	-	-
21	CLA	B2	837	X	-	-	-
21	CLA	B2	838	X	-	-	-
21	CLA	B2	839	X	-	-	-
21	CLA	B2	840	X	-	-	-
21	CLA	B2	841	X	-	-	-
21	CLA	F	301	X	-	-	-
21	CLA	F	303	X	-	-	-
21	CLA	F	304	X	-	-	-
21	CLA	F2	301	X	-	-	-
21	CLA	F2	303	X	-	-	-
21	CLA	F2	304	X	-	-	-
21	CLA	G	203	X	-	-	-
21	CLA	G	204	X	-	-	-
21	CLA	G2	203	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	G2	204	X	-	-	-
21	CLA	J	101	X	-	-	-
21	CLA	J2	101	X	-	-	-
21	CLA	K	201	X	-	-	-
21	CLA	K	203	X	-	-	-
21	CLA	K	204	X	-	-	-
21	CLA	K	206	X	-	-	-
21	CLA	K2	201	X	-	-	-
21	CLA	K2	203	X	-	-	-
21	CLA	K2	204	X	-	-	-
21	CLA	K2	206	X	-	-	-
21	CLA	L	203	X	-	-	-
21	CLA	L	204	X	-	-	-
21	CLA	L2	203	X	-	-	-
21	CLA	L2	204	X	-	-	-
21	CLA	Z	602	X	-	-	-
21	CLA	Z	603	X	-	-	-
21	CLA	Z	604	X	-	-	-
21	CLA	Z	608	X	-	-	-
21	CLA	Z	609	X	-	-	-
21	CLA	Z	610	X	-	-	-
21	CLA	Z	611	X	-	-	-
21	CLA	Z	612	X	-	-	-
21	CLA	Z	613	X	-	-	-
21	CLA	Z	614	X	-	-	-
21	CLA	Z	616	X	-	-	-
21	CLA	Z2	602	X	-	-	-
21	CLA	Z2	603	X	-	-	-
21	CLA	Z2	604	X	-	-	-
21	CLA	Z2	608	X	-	-	-
21	CLA	Z2	609	X	-	-	-
21	CLA	Z2	610	X	-	-	-
21	CLA	Z2	611	X	-	-	-
21	CLA	Z2	612	X	-	-	-
21	CLA	Z2	613	X	-	-	-
21	CLA	Z2	614	X	-	-	-
21	CLA	Z2	616	X	-	-	-
30	CHL	1	601	X	-	-	-
30	CHL	1	606	X	-	-	-
30	CHL	1	607	X	-	-	-
30	CHL	12	601	X	-	-	-
30	CHL	12	606	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	CHL	12	607	X	-	-	-
30	CHL	3	608	X	-	-	-
30	CHL	32	608	X	-	-	-
30	CHL	4	601	X	-	-	-
30	CHL	4	606	X	-	-	-
30	CHL	4	607	X	-	-	-
30	CHL	4	608	X	-	-	-
30	CHL	4	618	X	-	-	-
30	CHL	42	601	X	-	-	-
30	CHL	42	606	X	-	-	-
30	CHL	42	607	X	-	-	-
30	CHL	42	608	X	-	-	-
30	CHL	42	618	X	-	-	-
30	CHL	5	606	X	-	-	-
30	CHL	5	607	X	-	-	-
30	CHL	5	608	X	-	-	-
30	CHL	5	618	X	-	-	-
30	CHL	52	606	X	-	-	-
30	CHL	52	607	X	-	-	-
30	CHL	52	608	X	-	-	-
30	CHL	52	618	X	-	-	-
30	CHL	6	601	X	-	-	-
30	CHL	6	606	X	-	-	-
30	CHL	6	607	X	-	-	-
30	CHL	6	608	X	-	-	-
30	CHL	6	616	X	-	-	-
30	CHL	6	618	X	-	-	-
30	CHL	62	601	X	-	-	-
30	CHL	62	606	X	-	-	-
30	CHL	62	607	X	-	-	-
30	CHL	62	608	X	-	-	-
30	CHL	62	616	X	-	-	-
30	CHL	62	618	X	-	-	-
30	CHL	7	601	X	-	-	-
30	CHL	7	606	X	-	-	-
30	CHL	7	607	X	-	-	-
30	CHL	72	601	X	-	-	-
30	CHL	72	606	X	-	-	-
30	CHL	72	607	X	-	-	-
30	CHL	8	601	X	-	-	-
30	CHL	8	606	X	-	-	-
30	CHL	8	607	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	CHL	82	601	X	-	-	-
30	CHL	82	606	X	-	-	-
30	CHL	82	607	X	-	-	-
30	CHL	9	606	X	-	-	-
30	CHL	9	607	X	-	-	-
30	CHL	92	606	X	-	-	-
30	CHL	92	607	X	-	-	-
30	CHL	Z	601	X	-	-	-
30	CHL	Z	606	X	-	-	-
30	CHL	Z	607	X	-	-	-
30	CHL	Z2	601	X	-	-	-
30	CHL	Z2	606	X	-	-	-
30	CHL	Z2	607	X	-	-	-
31	XAT	5	624	X	-	-	-
31	XAT	52	624	X	-	-	-

2 Entry composition [i](#)

There are 33 unique types of molecules in this entry. The entry contains 202818 atoms, of which 101988 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 Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
1	A	742	Total	C	H	N	O	S	0	0
			11500	3808	5675	994	1001	22		
1	A2	742	Total	C	H	N	O	S	0	0
			11500	3808	5675	994	1001	22		

- Molecule 2 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
2	B	733	Total	C	H	N	O	S	0	0
			11400	3824	5576	977	1005	18		
2	B2	733	Total	C	H	N	O	S	0	0
			11400	3824	5576	977	1005	18		

- Molecule 3 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
3	C	80	Total	C	H	N	O	S	0	0
			1183	369	582	103	117	12		
3	C2	80	Total	C	H	N	O	S	0	0
			1183	369	582	103	117	12		

- Molecule 4 is a protein called Photosystem I reaction center subunit II, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
4	D	144	Total	C	H	N	O	S	0	0
			2284	725	1151	200	201	7		
4	D2	144	Total	C	H	N	O	S	0	0
			2284	725	1151	200	201	7		

- Molecule 5 is a protein called Photosystem I reaction center subunit IV, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	64	Total	C	H	N	O	0	0
			1011	322	505	89	95		
5	E2	64	Total	C	H	N	O	0	0
			1011	322	505	89	95		

- Molecule 6 is a protein called Photosystem I reaction center subunit III, chloroplastic.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	F	165	Total	C	H	N	O	S	0	0
			2568	817	1302	213	233	3		
6	F2	165	Total	C	H	N	O	S	0	0
			2568	817	1302	213	233	3		

- Molecule 7 is a protein called Photosystem I reaction center subunit V, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	95	Total	C	H	N	O	0	0
			1393	452	687	119	135		
7	G2	95	Total	C	H	N	O	0	0
			1393	452	687	119	135		

- Molecule 8 is a protein called Photosystem I reaction center subunit VIII.

Mol	Chain	Residues	Atoms					AltConf	Trace	
8	I	37	Total	C	H	N	O	S	0	0
			573	195	292	39	46	1		
8	I2	37	Total	C	H	N	O	S	0	0
			573	195	292	39	46	1		

- Molecule 9 is a protein called Photosystem I reaction center subunit IX.

Mol	Chain	Residues	Atoms					AltConf	Trace	
9	J	40	Total	C	H	N	O	S	0	0
			657	224	328	46	58	1		
9	J2	40	Total	C	H	N	O	S	0	0
			657	224	328	46	58	1		

- Molecule 10 is a protein called PSI subunit V.

Mol	Chain	Residues	Atoms					AltConf	Trace	
10	L	124	Total	C	H	N	O	S	0	0
			1806	586	907	146	164	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
10	L2	124	1806	586	907	146	164	3	0	0

- Molecule 11 is a protein called Photosystem I reaction center subunit psak, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
11	K	86	1203	370	620	100	111	2	0	0
11	K2	86	1203	370	620	100	111	2	0	0

- Molecule 12 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
12	1	194	2842	941	1397	240	261	3	0	0
12	Z	194	2842	941	1397	240	261	3	0	0
12	12	194	2842	941	1397	240	261	3	0	0
12	Z2	194	2842	941	1397	240	261	3	0	0

- Molecule 13 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
13	3	227	3431	1128	1695	283	317	8	0	0
13	32	227	3431	1128	1695	283	317	8	0	0

- Molecule 14 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
14	7	213	3240	1072	1590	274	298	6	0	0
14	72	213	3240	1072	1590	274	298	6	0	0

- Molecule 15 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
15	8	217	3280	1073	1630	280	293	4	0	0
15	82	217	3280	1073	1630	280	293	4	0	0

- Molecule 16 is a protein called Chlorophyll a-b binding protein, chloroplastic (Lhca4).

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
16	4	212	3251	1080	1603	268	295	5	0	0
16	42	212	3251	1080	1603	268	295	5	0	0

- Molecule 17 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
17	5	227	3522	1154	1747	297	316	8	0	0
17	52	227	3522	1154	1747	297	316	8	0	0

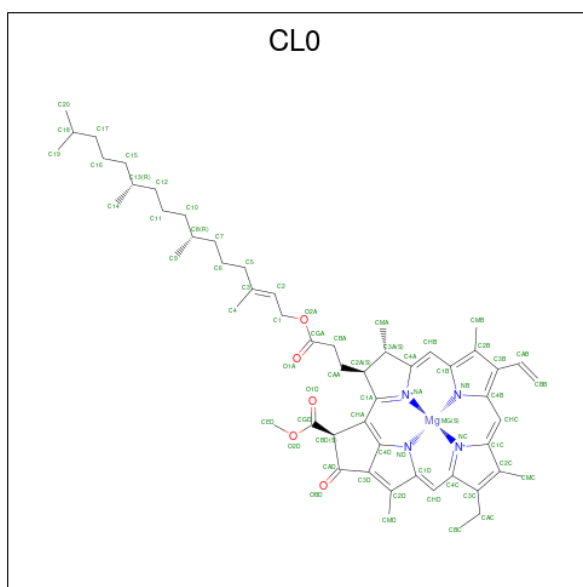
- Molecule 18 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
18	6	230	3542	1167	1770	293	306	6	0	0
18	62	230	3542	1167	1770	293	306	6	0	0

- Molecule 19 is a protein called Chlorophyll a-b binding protein, chloroplastic.

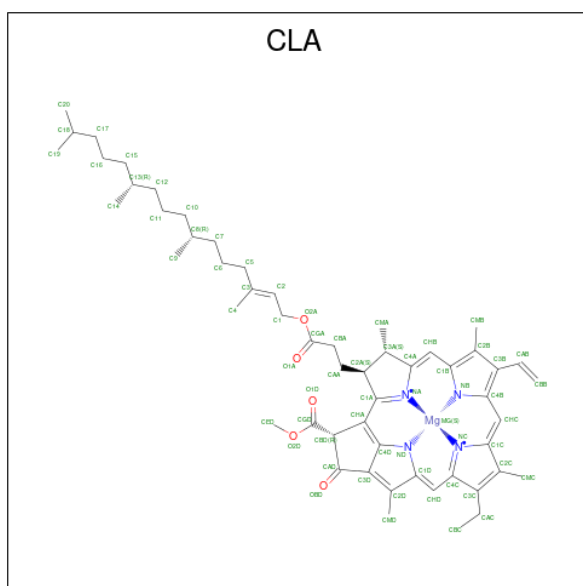
Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
19	9	186	2820	918	1400	238	257	7	0	0
19	92	186	2820	918	1400	238	257	7	0	0

- Molecule 20 is CHLOROPHYLL A ISOMER (three-letter code: CL0) (formula: C₅₅H₇₂MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf	
			Total	C	H	Mg	N		O
20	A	1	137	55	72	1	4	5	0
20	A2	1	137	55	72	1	4	5	0

- Molecule 21 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf	
			Total	C	H	Mg	N		O
21	A	1	5574	2278	2856	44	176	220	0

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Mol	Chain	Residues	Atoms						AltConf
21	B	1	Total	C	H	Mg	N	O	0
			5043	2063	2580	40	160	200	
21	B	1	Total	C	H	Mg	N	O	0
			5043	2063	2580	40	160	200	
21	B	1	Total	C	H	Mg	N	O	0
			5043	2063	2580	40	160	200	
21	B	1	Total	C	H	Mg	N	O	0
			5043	2063	2580	40	160	200	
21	B	1	Total	C	H	Mg	N	O	0
			5043	2063	2580	40	160	200	
21	B	1	Total	C	H	Mg	N	O	0
			5043	2063	2580	40	160	200	
21	B	1	Total	C	H	Mg	N	O	0
			5043	2063	2580	40	160	200	
21	B	1	Total	C	H	Mg	N	O	0
			5043	2063	2580	40	160	200	
21	B	1	Total	C	H	Mg	N	O	0
			5043	2063	2580	40	160	200	
21	B	1	Total	C	H	Mg	N	O	0
			5043	2063	2580	40	160	200	
21	B	1	Total	C	H	Mg	N	O	0
			5043	2063	2580	40	160	200	
21	B	1	Total	C	H	Mg	N	O	0
			5043	2063	2580	40	160	200	
21	B	1	Total	C	H	Mg	N	O	0
			5043	2063	2580	40	160	200	
21	B	1	Total	C	H	Mg	N	O	0
			5043	2063	2580	40	160	200	
21	B	1	Total	C	H	Mg	N	O	0
			5043	2063	2580	40	160	200	
21	F	1	Total	C	H	Mg	N	O	0
			352	145	177	3	12	15	

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Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	Mg	N	O	
21	F	1	Total 352	C 145	H 177	Mg 3	N 12	O 15	0
21	F	1	Total 352	C 145	H 177	Mg 3	N 12	O 15	0
21	G	1	Total 198	C 86	H 92	Mg 2	N 8	O 10	0
21	G	1	Total 198	C 86	H 92	Mg 2	N 8	O 10	0
21	J	1	Total 104	C 45	H 49	Mg 1	N 4	O 5	0
21	L	1	Total 215	C 90	H 105	Mg 2	N 8	O 10	0
21	L	1	Total 215	C 90	H 105	Mg 2	N 8	O 10	0
21	K	1	Total 354	C 156	H 158	Mg 4	N 16	O 20	0
21	K	1	Total 354	C 156	H 158	Mg 4	N 16	O 20	0
21	K	1	Total 354	C 156	H 158	Mg 4	N 16	O 20	0
21	K	1	Total 354	C 156	H 158	Mg 4	N 16	O 20	0
21	1	1	Total 1264	C 529	H 625	Mg 11	N 44	O 55	0
21	1	1	Total 1264	C 529	H 625	Mg 11	N 44	O 55	0
21	1	1	Total 1264	C 529	H 625	Mg 11	N 44	O 55	0
21	1	1	Total 1264	C 529	H 625	Mg 11	N 44	O 55	0
21	1	1	Total 1264	C 529	H 625	Mg 11	N 44	O 55	0
21	1	1	Total 1264	C 529	H 625	Mg 11	N 44	O 55	0
21	1	1	Total 1264	C 529	H 625	Mg 11	N 44	O 55	0
21	1	1	Total 1264	C 529	H 625	Mg 11	N 44	O 55	0
21	1	1	Total 1264	C 529	H 625	Mg 11	N 44	O 55	0
21	1	1	Total 1264	C 529	H 625	Mg 11	N 44	O 55	0

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Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	Mg	N	O	
21	1	1	Total 1264	C 529	H 625	Mg 11	N 44	O 55	0
21	3	1	Total 1458	C 612	H 718	Mg 13	N 52	O 63	0
21	3	1	Total 1458	C 612	H 718	Mg 13	N 52	O 63	0
21	3	1	Total 1458	C 612	H 718	Mg 13	N 52	O 63	0
21	3	1	Total 1458	C 612	H 718	Mg 13	N 52	O 63	0
21	3	1	Total 1458	C 612	H 718	Mg 13	N 52	O 63	0
21	3	1	Total 1458	C 612	H 718	Mg 13	N 52	O 63	0
21	3	1	Total 1458	C 612	H 718	Mg 13	N 52	O 63	0
21	3	1	Total 1458	C 612	H 718	Mg 13	N 52	O 63	0
21	3	1	Total 1458	C 612	H 718	Mg 13	N 52	O 63	0
21	3	1	Total 1458	C 612	H 718	Mg 13	N 52	O 63	0
21	3	1	Total 1458	C 612	H 718	Mg 13	N 52	O 63	0
21	3	1	Total 1458	C 612	H 718	Mg 13	N 52	O 63	0
21	3	1	Total 1458	C 612	H 718	Mg 13	N 52	O 63	0
21	3	1	Total 1458	C 612	H 718	Mg 13	N 52	O 63	0
21	7	1	Total 1250	C 534	H 598	Mg 12	N 48	O 58	0
21	7	1	Total 1250	C 534	H 598	Mg 12	N 48	O 58	0
21	7	1	Total 1250	C 534	H 598	Mg 12	N 48	O 58	0
21	7	1	Total 1250	C 534	H 598	Mg 12	N 48	O 58	0
21	7	1	Total 1250	C 534	H 598	Mg 12	N 48	O 58	0
21	7	1	Total 1250	C 534	H 598	Mg 12	N 48	O 58	0
21	7	1	Total 1250	C 534	H 598	Mg 12	N 48	O 58	0

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Mol	Chain	Residues	Atoms					AltConf	
			Total	C	H	Mg	N		O
21	7	1	Total	C	H	Mg	N	O	0
			1250	534	598	12	48	58	
21	7	1	Total	C	H	Mg	N	O	0
			1250	534	598	12	48	58	
21	7	1	Total	C	H	Mg	N	O	0
			1250	534	598	12	48	58	
21	7	1	Total	C	H	Mg	N	O	0
			1250	534	598	12	48	58	
21	8	1	Total	C	H	Mg	N	O	0
			1192	504	578	11	44	55	
21	8	1	Total	C	H	Mg	N	O	0
			1192	504	578	11	44	55	
21	8	1	Total	C	H	Mg	N	O	0
			1192	504	578	11	44	55	
21	8	1	Total	C	H	Mg	N	O	0
			1192	504	578	11	44	55	
21	8	1	Total	C	H	Mg	N	O	0
			1192	504	578	11	44	55	
21	8	1	Total	C	H	Mg	N	O	0
			1192	504	578	11	44	55	
21	8	1	Total	C	H	Mg	N	O	0
			1192	504	578	11	44	55	
21	8	1	Total	C	H	Mg	N	O	0
			1192	504	578	11	44	55	
21	8	1	Total	C	H	Mg	N	O	0
			1192	504	578	11	44	55	
21	Z	1	Total	C	H	Mg	N	O	0
			1220	517	593	11	44	55	
21	Z	1	Total	C	H	Mg	N	O	0
			1220	517	593	11	44	55	
21	Z	1	Total	C	H	Mg	N	O	0
			1220	517	593	11	44	55	
21	Z	1	Total	C	H	Mg	N	O	0
			1220	517	593	11	44	55	
21	Z	1	Total	C	H	Mg	N	O	0
			1220	517	593	11	44	55	

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Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	Mg	N	O	
21	Z	1	Total 1220	C 517	H 593	Mg 11	N 44	O 55	0
21	Z	1	Total 1220	C 517	H 593	Mg 11	N 44	O 55	0
21	Z	1	Total 1220	C 517	H 593	Mg 11	N 44	O 55	0
21	Z	1	Total 1220	C 517	H 593	Mg 11	N 44	O 55	0
21	Z	1	Total 1220	C 517	H 593	Mg 11	N 44	O 55	0
21	Z	1	Total 1220	C 517	H 593	Mg 11	N 44	O 55	0
21	4	1	Total 1099	C 465	H 534	Mg 10	N 40	O 50	0
21	4	1	Total 1099	C 465	H 534	Mg 10	N 40	O 50	0
21	4	1	Total 1099	C 465	H 534	Mg 10	N 40	O 50	0
21	4	1	Total 1099	C 465	H 534	Mg 10	N 40	O 50	0
21	4	1	Total 1099	C 465	H 534	Mg 10	N 40	O 50	0
21	4	1	Total 1099	C 465	H 534	Mg 10	N 40	O 50	0
21	4	1	Total 1099	C 465	H 534	Mg 10	N 40	O 50	0
21	4	1	Total 1099	C 465	H 534	Mg 10	N 40	O 50	0
21	4	1	Total 1099	C 465	H 534	Mg 10	N 40	O 50	0
21	4	1	Total 1099	C 465	H 534	Mg 10	N 40	O 50	0
21	5	1	Total 1452	C 610	H 712	Mg 13	N 52	O 65	0
21	5	1	Total 1452	C 610	H 712	Mg 13	N 52	O 65	0
21	5	1	Total 1452	C 610	H 712	Mg 13	N 52	O 65	0
21	5	1	Total 1452	C 610	H 712	Mg 13	N 52	O 65	0
21	5	1	Total 1452	C 610	H 712	Mg 13	N 52	O 65	0

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Mol	Chain	Residues	Atoms					AltConf	
			Total	C	H	Mg	N		O
21	5	1	Total 1452	C 610	H 712	Mg 13	N 52	O 65	0
21	5	1	Total 1452	C 610	H 712	Mg 13	N 52	O 65	0
21	5	1	Total 1452	C 610	H 712	Mg 13	N 52	O 65	0
21	5	1	Total 1452	C 610	H 712	Mg 13	N 52	O 65	0
21	5	1	Total 1452	C 610	H 712	Mg 13	N 52	O 65	0
21	5	1	Total 1452	C 610	H 712	Mg 13	N 52	O 65	0
21	5	1	Total 1452	C 610	H 712	Mg 13	N 52	O 65	0
21	5	1	Total 1452	C 610	H 712	Mg 13	N 52	O 65	0
21	5	1	Total 1452	C 610	H 712	Mg 13	N 52	O 65	0
21	6	1	Total 1233	C 518	H 605	Mg 11	N 44	O 55	0
21	6	1	Total 1233	C 518	H 605	Mg 11	N 44	O 55	0
21	6	1	Total 1233	C 518	H 605	Mg 11	N 44	O 55	0
21	6	1	Total 1233	C 518	H 605	Mg 11	N 44	O 55	0
21	6	1	Total 1233	C 518	H 605	Mg 11	N 44	O 55	0
21	6	1	Total 1233	C 518	H 605	Mg 11	N 44	O 55	0
21	6	1	Total 1233	C 518	H 605	Mg 11	N 44	O 55	0
21	6	1	Total 1233	C 518	H 605	Mg 11	N 44	O 55	0
21	6	1	Total 1233	C 518	H 605	Mg 11	N 44	O 55	0
21	6	1	Total 1233	C 518	H 605	Mg 11	N 44	O 55	0
21	6	1	Total 1233	C 518	H 605	Mg 11	N 44	O 55	0
21	6	1	Total 1233	C 518	H 605	Mg 11	N 44	O 55	0
21	9	1	Total 1100	C 465	H 535	Mg 10	N 40	O 50	0
21	9	1	Total 1100	C 465	H 535	Mg 10	N 40	O 50	0

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Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	Mg	N	O	
21	9	1	Total 1100	C 465	H 535	Mg 10	N 40	O 50	0
21	9	1	Total 1100	C 465	H 535	Mg 10	N 40	O 50	0
21	9	1	Total 1100	C 465	H 535	Mg 10	N 40	O 50	0
21	9	1	Total 1100	C 465	H 535	Mg 10	N 40	O 50	0
21	9	1	Total 1100	C 465	H 535	Mg 10	N 40	O 50	0
21	9	1	Total 1100	C 465	H 535	Mg 10	N 40	O 50	0
21	9	1	Total 1100	C 465	H 535	Mg 10	N 40	O 50	0
21	9	1	Total 1100	C 465	H 535	Mg 10	N 40	O 50	0
21	A2	1	Total 5574	C 2278	H 2856	Mg 44	N 176	O 220	0
21	A2	1	Total 5574	C 2278	H 2856	Mg 44	N 176	O 220	0
21	A2	1	Total 5574	C 2278	H 2856	Mg 44	N 176	O 220	0
21	A2	1	Total 5574	C 2278	H 2856	Mg 44	N 176	O 220	0
21	A2	1	Total 5574	C 2278	H 2856	Mg 44	N 176	O 220	0
21	A2	1	Total 5574	C 2278	H 2856	Mg 44	N 176	O 220	0
21	A2	1	Total 5574	C 2278	H 2856	Mg 44	N 176	O 220	0
21	A2	1	Total 5574	C 2278	H 2856	Mg 44	N 176	O 220	0
21	A2	1	Total 5574	C 2278	H 2856	Mg 44	N 176	O 220	0
21	A2	1	Total 5574	C 2278	H 2856	Mg 44	N 176	O 220	0
21	A2	1	Total 5574	C 2278	H 2856	Mg 44	N 176	O 220	0
21	A2	1	Total 5574	C 2278	H 2856	Mg 44	N 176	O 220	0

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Mol	Chain	Residues	Atoms						AltConf
21	A2	1	Total	C	H	Mg	N	O	0
			5574	2278	2856	44	176	220	
21	A2	1	Total	C	H	Mg	N	O	0
			5574	2278	2856	44	176	220	
21	A2	1	Total	C	H	Mg	N	O	0
			5574	2278	2856	44	176	220	
21	A2	1	Total	C	H	Mg	N	O	0
			5574	2278	2856	44	176	220	
21	A2	1	Total	C	H	Mg	N	O	0
			5574	2278	2856	44	176	220	
21	A2	1	Total	C	H	Mg	N	O	0
			5574	2278	2856	44	176	220	
21	A2	1	Total	C	H	Mg	N	O	0
			5574	2278	2856	44	176	220	
21	A2	1	Total	C	H	Mg	N	O	0
			5574	2278	2856	44	176	220	
21	A2	1	Total	C	H	Mg	N	O	0
			5574	2278	2856	44	176	220	
21	B2	1	Total	C	H	Mg	N	O	0
			5043	2063	2580	40	160	200	
21	B2	1	Total	C	H	Mg	N	O	0
			5043	2063	2580	40	160	200	
21	B2	1	Total	C	H	Mg	N	O	0
			5043	2063	2580	40	160	200	
21	B2	1	Total	C	H	Mg	N	O	0
			5043	2063	2580	40	160	200	
21	B2	1	Total	C	H	Mg	N	O	0
			5043	2063	2580	40	160	200	
21	B2	1	Total	C	H	Mg	N	O	0
			5043	2063	2580	40	160	200	
21	B2	1	Total	C	H	Mg	N	O	0
			5043	2063	2580	40	160	200	
21	B2	1	Total	C	H	Mg	N	O	0
			5043	2063	2580	40	160	200	
21	B2	1	Total	C	H	Mg	N	O	0
			5043	2063	2580	40	160	200	
21	B2	1	Total	C	H	Mg	N	O	0
			5043	2063	2580	40	160	200	

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Mol	Chain	Residues	Atoms						AltConf
21	B2	1	Total	C	H	Mg	N	O	0
			5043	2063	2580	40	160	200	
21	B2	1	Total	C	H	Mg	N	O	0
			5043	2063	2580	40	160	200	
21	B2	1	Total	C	H	Mg	N	O	0
			5043	2063	2580	40	160	200	
21	B2	1	Total	C	H	Mg	N	O	0
			5043	2063	2580	40	160	200	
21	B2	1	Total	C	H	Mg	N	O	0
			5043	2063	2580	40	160	200	
21	B2	1	Total	C	H	Mg	N	O	0
			5043	2063	2580	40	160	200	
21	B2	1	Total	C	H	Mg	N	O	0
			5043	2063	2580	40	160	200	
21	F2	1	Total	C	H	Mg	N	O	0
			352	145	177	3	12	15	
21	F2	1	Total	C	H	Mg	N	O	0
			352	145	177	3	12	15	
21	F2	1	Total	C	H	Mg	N	O	0
			352	145	177	3	12	15	
21	G2	1	Total	C	H	Mg	N	O	0
			198	86	92	2	8	10	
21	G2	1	Total	C	H	Mg	N	O	0
			198	86	92	2	8	10	
21	J2	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
21	L2	1	Total	C	H	Mg	N	O	0
			215	90	105	2	8	10	
21	L2	1	Total	C	H	Mg	N	O	0
			215	90	105	2	8	10	
21	K2	1	Total	C	H	Mg	N	O	0
			354	156	158	4	16	20	
21	K2	1	Total	C	H	Mg	N	O	0
			354	156	158	4	16	20	
21	K2	1	Total	C	H	Mg	N	O	0
			354	156	158	4	16	20	
21	K2	1	Total	C	H	Mg	N	O	0
			354	156	158	4	16	20	
21	12	1	Total	C	H	Mg	N	O	0
			1264	529	625	11	44	55	

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Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	Mg	N	O	
21	12	1	1264	529	625	11	44	55	0
21	12	1	1264	529	625	11	44	55	0
21	12	1	1264	529	625	11	44	55	0
21	12	1	1264	529	625	11	44	55	0
21	12	1	1264	529	625	11	44	55	0
21	12	1	1264	529	625	11	44	55	0
21	12	1	1264	529	625	11	44	55	0
21	12	1	1264	529	625	11	44	55	0
21	12	1	1264	529	625	11	44	55	0
21	12	1	1264	529	625	11	44	55	0
21	12	1	1264	529	625	11	44	55	0
21	32	1	1458	612	718	13	52	63	0
21	32	1	1458	612	718	13	52	63	0
21	32	1	1458	612	718	13	52	63	0
21	32	1	1458	612	718	13	52	63	0
21	32	1	1458	612	718	13	52	63	0
21	32	1	1458	612	718	13	52	63	0
21	32	1	1458	612	718	13	52	63	0
21	32	1	1458	612	718	13	52	63	0
21	32	1	1458	612	718	13	52	63	0
21	32	1	1458	612	718	13	52	63	0
21	32	1	1458	612	718	13	52	63	0
21	32	1	1458	612	718	13	52	63	0

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Mol	Chain	Residues	Atoms					AltConf	
			Total	C	H	Mg	N		O
21	32	1	Total 1458	C 612	H 718	Mg 13	N 52	O 63	0
21	32	1	Total 1458	C 612	H 718	Mg 13	N 52	O 63	0
21	72	1	Total 1250	C 534	H 598	Mg 12	N 48	O 58	0
21	72	1	Total 1250	C 534	H 598	Mg 12	N 48	O 58	0
21	72	1	Total 1250	C 534	H 598	Mg 12	N 48	O 58	0
21	72	1	Total 1250	C 534	H 598	Mg 12	N 48	O 58	0
21	72	1	Total 1250	C 534	H 598	Mg 12	N 48	O 58	0
21	72	1	Total 1250	C 534	H 598	Mg 12	N 48	O 58	0
21	72	1	Total 1250	C 534	H 598	Mg 12	N 48	O 58	0
21	72	1	Total 1250	C 534	H 598	Mg 12	N 48	O 58	0
21	72	1	Total 1250	C 534	H 598	Mg 12	N 48	O 58	0
21	72	1	Total 1250	C 534	H 598	Mg 12	N 48	O 58	0
21	72	1	Total 1250	C 534	H 598	Mg 12	N 48	O 58	0
21	72	1	Total 1250	C 534	H 598	Mg 12	N 48	O 58	0
21	72	1	Total 1250	C 534	H 598	Mg 12	N 48	O 58	0
21	72	1	Total 1250	C 534	H 598	Mg 12	N 48	O 58	0
21	72	1	Total 1250	C 534	H 598	Mg 12	N 48	O 58	0
21	72	1	Total 1250	C 534	H 598	Mg 12	N 48	O 58	0
21	82	1	Total 1192	C 504	H 578	Mg 11	N 44	O 55	0
21	82	1	Total 1192	C 504	H 578	Mg 11	N 44	O 55	0
21	82	1	Total 1192	C 504	H 578	Mg 11	N 44	O 55	0
21	82	1	Total 1192	C 504	H 578	Mg 11	N 44	O 55	0
21	82	1	Total 1192	C 504	H 578	Mg 11	N 44	O 55	0
21	82	1	Total 1192	C 504	H 578	Mg 11	N 44	O 55	0
21	82	1	Total 1192	C 504	H 578	Mg 11	N 44	O 55	0
21	82	1	Total 1192	C 504	H 578	Mg 11	N 44	O 55	0

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Mol	Chain	Residues	Atoms					AltConf	
			Total	C	H	Mg	N		O
21	82	1	Total 1192	C 504	H 578	Mg 11	N 44	O 55	0
21	82	1	Total 1192	C 504	H 578	Mg 11	N 44	O 55	0
21	82	1	Total 1192	C 504	H 578	Mg 11	N 44	O 55	0
21	82	1	Total 1192	C 504	H 578	Mg 11	N 44	O 55	0
21	Z2	1	Total 1220	C 517	H 593	Mg 11	N 44	O 55	0
21	Z2	1	Total 1220	C 517	H 593	Mg 11	N 44	O 55	0
21	Z2	1	Total 1220	C 517	H 593	Mg 11	N 44	O 55	0
21	Z2	1	Total 1220	C 517	H 593	Mg 11	N 44	O 55	0
21	Z2	1	Total 1220	C 517	H 593	Mg 11	N 44	O 55	0
21	Z2	1	Total 1220	C 517	H 593	Mg 11	N 44	O 55	0
21	Z2	1	Total 1220	C 517	H 593	Mg 11	N 44	O 55	0
21	Z2	1	Total 1220	C 517	H 593	Mg 11	N 44	O 55	0
21	Z2	1	Total 1220	C 517	H 593	Mg 11	N 44	O 55	0
21	Z2	1	Total 1220	C 517	H 593	Mg 11	N 44	O 55	0
21	Z2	1	Total 1220	C 517	H 593	Mg 11	N 44	O 55	0
21	42	1	Total 1099	C 465	H 534	Mg 10	N 40	O 50	0
21	42	1	Total 1099	C 465	H 534	Mg 10	N 40	O 50	0
21	42	1	Total 1099	C 465	H 534	Mg 10	N 40	O 50	0
21	42	1	Total 1099	C 465	H 534	Mg 10	N 40	O 50	0
21	42	1	Total 1099	C 465	H 534	Mg 10	N 40	O 50	0
21	42	1	Total 1099	C 465	H 534	Mg 10	N 40	O 50	0

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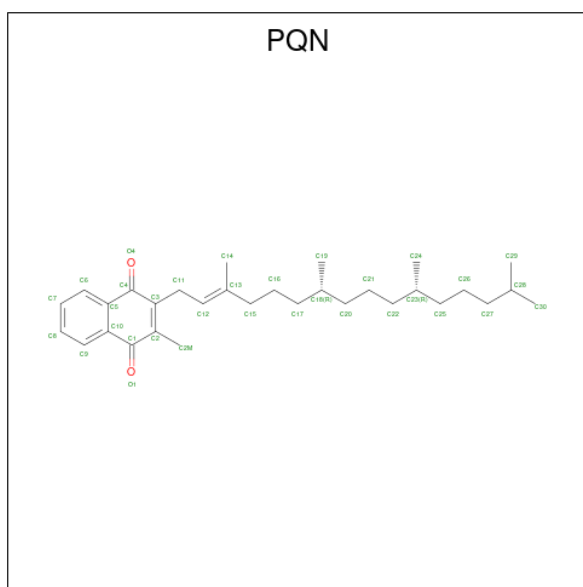
Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	Mg	N	O	
21	42	1	Total 1099	C 465	H 534	Mg 10	N 40	O 50	0
21	42	1	Total 1099	C 465	H 534	Mg 10	N 40	O 50	0
21	42	1	Total 1099	C 465	H 534	Mg 10	N 40	O 50	0
21	42	1	Total 1099	C 465	H 534	Mg 10	N 40	O 50	0
21	52	1	Total 1452	C 610	H 712	Mg 13	N 52	O 65	0
21	52	1	Total 1452	C 610	H 712	Mg 13	N 52	O 65	0
21	52	1	Total 1452	C 610	H 712	Mg 13	N 52	O 65	0
21	52	1	Total 1452	C 610	H 712	Mg 13	N 52	O 65	0
21	52	1	Total 1452	C 610	H 712	Mg 13	N 52	O 65	0
21	52	1	Total 1452	C 610	H 712	Mg 13	N 52	O 65	0
21	52	1	Total 1452	C 610	H 712	Mg 13	N 52	O 65	0
21	52	1	Total 1452	C 610	H 712	Mg 13	N 52	O 65	0
21	52	1	Total 1452	C 610	H 712	Mg 13	N 52	O 65	0
21	52	1	Total 1452	C 610	H 712	Mg 13	N 52	O 65	0
21	52	1	Total 1452	C 610	H 712	Mg 13	N 52	O 65	0
21	52	1	Total 1452	C 610	H 712	Mg 13	N 52	O 65	0
21	52	1	Total 1452	C 610	H 712	Mg 13	N 52	O 65	0
21	52	1	Total 1452	C 610	H 712	Mg 13	N 52	O 65	0
21	62	1	Total 1233	C 518	H 605	Mg 11	N 44	O 55	0
21	62	1	Total 1233	C 518	H 605	Mg 11	N 44	O 55	0
21	62	1	Total 1233	C 518	H 605	Mg 11	N 44	O 55	0
21	62	1	Total 1233	C 518	H 605	Mg 11	N 44	O 55	0

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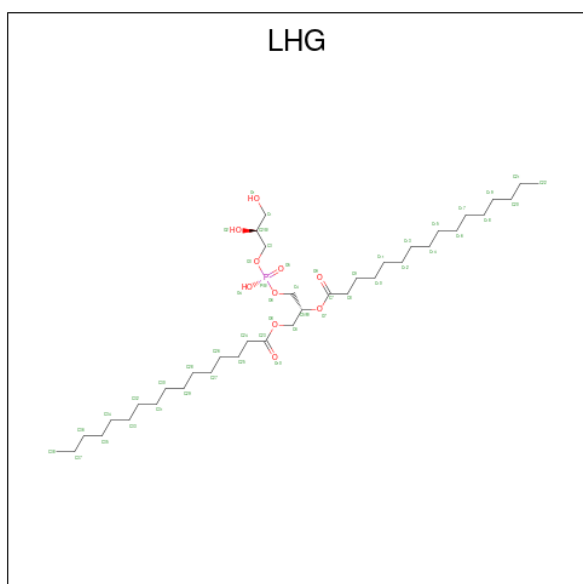
Mol	Chain	Residues	Atoms					AltConf	
			Total	C	H	Mg	N		O
21	62	1	Total 1233	C 518	H 605	Mg 11	N 44	O 55	0
21	62	1	Total 1233	C 518	H 605	Mg 11	N 44	O 55	0
21	62	1	Total 1233	C 518	H 605	Mg 11	N 44	O 55	0
21	62	1	Total 1233	C 518	H 605	Mg 11	N 44	O 55	0
21	62	1	Total 1233	C 518	H 605	Mg 11	N 44	O 55	0
21	62	1	Total 1233	C 518	H 605	Mg 11	N 44	O 55	0
21	62	1	Total 1233	C 518	H 605	Mg 11	N 44	O 55	0
21	92	1	Total 1100	C 465	H 535	Mg 10	N 40	O 50	0
21	92	1	Total 1100	C 465	H 535	Mg 10	N 40	O 50	0
21	92	1	Total 1100	C 465	H 535	Mg 10	N 40	O 50	0
21	92	1	Total 1100	C 465	H 535	Mg 10	N 40	O 50	0
21	92	1	Total 1100	C 465	H 535	Mg 10	N 40	O 50	0
21	92	1	Total 1100	C 465	H 535	Mg 10	N 40	O 50	0
21	92	1	Total 1100	C 465	H 535	Mg 10	N 40	O 50	0
21	92	1	Total 1100	C 465	H 535	Mg 10	N 40	O 50	0
21	92	1	Total 1100	C 465	H 535	Mg 10	N 40	O 50	0
21	92	1	Total 1100	C 465	H 535	Mg 10	N 40	O 50	0

- Molecule 22 is PHYLLOQUINONE (three-letter code: PQN) (formula: C₃₁H₄₆O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	H	O	
22	A	1	79	31	46	2	0
22	B	1	79	31	46	2	0
22	A2	1	79	31	46	2	0
22	B2	1	79	31	46	2	0

- Molecule 23 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$) (labeled as "Ligand of Interest" by depositor).



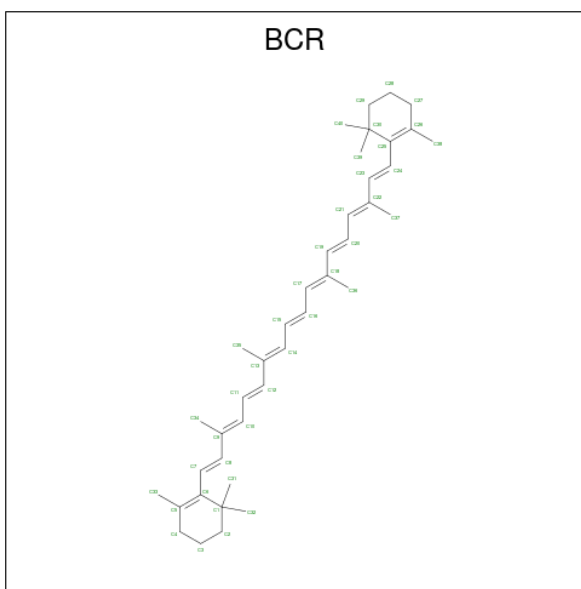
Mol	Chain	Residues	Atoms					AltConf
23	A	1	Total	C	H	O	P	0
			210	65	123	20	2	
23	A	1	Total	C	H	O	P	0
			210	65	123	20	2	
23	B	1	Total	C	H	O	P	0
			108	34	63	10	1	
23	1	1	Total	C	H	O	P	0
			87	28	48	10	1	
23	3	1	Total	C	H	O	P	0
			177	56	99	20	2	
23	3	1	Total	C	H	O	P	0
			177	56	99	20	2	
23	7	1	Total	C	H	O	P	0
			123	38	74	10	1	
23	8	1	Total	C	H	O	P	0
			105	33	61	10	1	
23	Z	1	Total	C	H	O	P	0
			87	28	48	10	1	
23	4	1	Total	C	H	O	P	0
			210	65	123	20	2	
23	4	1	Total	C	H	O	P	0
			210	65	123	20	2	
23	5	1	Total	C	H	O	P	0
			81	26	44	10	1	
23	6	1	Total	C	H	O	P	0
			201	63	116	20	2	
23	6	1	Total	C	H	O	P	0
			201	63	116	20	2	
23	9	1	Total	C	H	O	P	0
			96	30	55	10	1	
23	A2	1	Total	C	H	O	P	0
			210	65	123	20	2	
23	A2	1	Total	C	H	O	P	0
			210	65	123	20	2	
23	B2	1	Total	C	H	O	P	0
			108	34	63	10	1	
23	12	1	Total	C	H	O	P	0
			87	28	48	10	1	
23	32	1	Total	C	H	O	P	0
			177	56	99	20	2	
23	32	1	Total	C	H	O	P	0
			177	56	99	20	2	
23	72	1	Total	C	H	O	P	0
			123	38	74	10	1	

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	H	O	P	
23	82	1	Total	C	H	O	P	0
			105	33	61	10	1	
23	Z2	1	Total	C	H	O	P	0
			87	28	48	10	1	
23	42	1	Total	C	H	O	P	0
			210	65	123	20	2	
23	42	1	Total	C	H	O	P	0
			210	65	123	20	2	
23	52	1	Total	C	H	O	P	0
			81	26	44	10	1	
23	62	1	Total	C	H	O	P	0
			201	63	116	20	2	
23	62	1	Total	C	H	O	P	0
			201	63	116	20	2	
23	92	1	Total	C	H	O	P	0
			96	30	55	10	1	

- Molecule 24 is BETA-CAROTENE (three-letter code: BCR) (formula: C₄₀H₅₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	H	
24	A	1	Total	C	H	0
			480	200	280	
24	A	1	Total	C	H	0
			480	200	280	
24	A	1	Total	C	H	0
			480	200	280	

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Mol	Chain	Residues	Atoms			AltConf
			Total	C	H	
24	A	1	480	200	280	0
24	A	1	480	200	280	0
24	B	1	672	280	392	0
24	B	1	672	280	392	0
24	B	1	672	280	392	0
24	B	1	672	280	392	0
24	B	1	672	280	392	0
24	B	1	672	280	392	0
24	B	1	672	280	392	0
24	B	1	672	280	392	0
24	G	1	96	40	56	0
24	I	1	96	40	56	0
24	J	1	96	40	56	0
24	L	1	192	80	112	0
24	L	1	192	80	112	0
24	K	1	192	80	112	0
24	K	1	192	80	112	0
24	3	1	288	120	168	0
24	3	1	288	120	168	0
24	3	1	288	120	168	0
24	7	1	96	40	56	0
24	8	1	96	40	56	0

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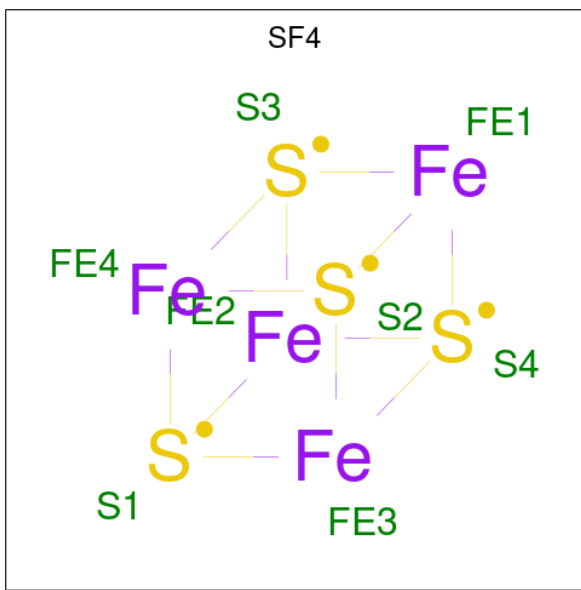
Mol	Chain	Residues	Atoms			AltConf
			Total	C	H	
24	4	1	96	40	56	0
24	5	1	96	40	56	0
24	6	1	96	40	56	0
24	9	1	96	40	56	0
24	A2	1	480	200	280	0
24	A2	1	480	200	280	0
24	A2	1	480	200	280	0
24	A2	1	480	200	280	0
24	A2	1	480	200	280	0
24	B2	1	672	280	392	0
24	B2	1	672	280	392	0
24	B2	1	672	280	392	0
24	B2	1	672	280	392	0
24	B2	1	672	280	392	0
24	B2	1	672	280	392	0
24	B2	1	672	280	392	0
24	B2	1	672	280	392	0
24	G2	1	96	40	56	0
24	I2	1	96	40	56	0
24	J2	1	96	40	56	0
24	L2	1	192	80	112	0
24	L2	1	192	80	112	0

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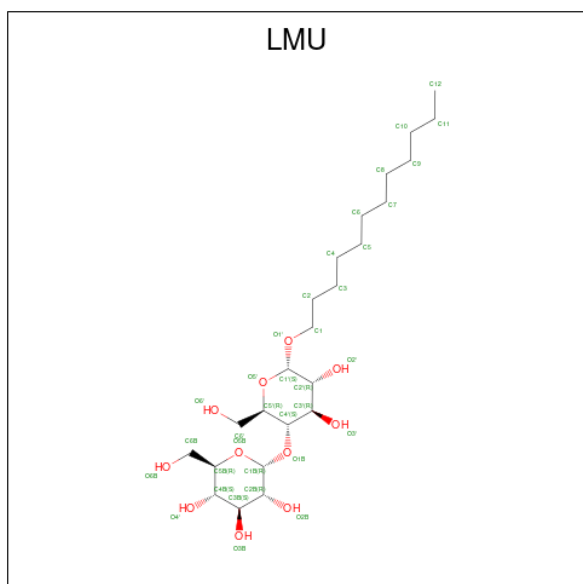
Mol	Chain	Residues	Atoms			AltConf
			Total	C	H	
24	K2	1	192	80	112	0
24	K2	1	192	80	112	0
24	32	1	288	120	168	0
24	32	1	288	120	168	0
24	32	1	288	120	168	0
24	72	1	96	40	56	0
24	82	1	96	40	56	0
24	42	1	96	40	56	0
24	52	1	96	40	56	0
24	62	1	96	40	56	0
24	92	1	96	40	56	0

- Molecule 25 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
25	A	1	Total	Fe	S	0
			8	4	4	
25	C	1	Total	Fe	S	0
			16	8	8	
25	C	1	Total	Fe	S	0
			16	8	8	
25	A2	1	Total	Fe	S	0
			8	4	4	
25	C2	1	Total	Fe	S	0
			16	8	8	
25	C2	1	Total	Fe	S	0
			16	8	8	

- Molecule 26 is DODECYL-ALPHA-D-MALTOSE (three-letter code: LMU) (formula: $C_{24}H_{46}O_{11}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
26	A	1	Total	C	H	O	0
			458	139	262	57	
26	A	1	Total	C	H	O	0
			458	139	262	57	
26	A	1	Total	C	H	O	0
			458	139	262	57	
26	A	1	Total	C	H	O	0
			458	139	262	57	
26	A	1	Total	C	H	O	0
			458	139	262	57	

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Mol	Chain	Residues	Atoms				AltConf
26	A	1	Total	C	H	O	0
			458	139	262	57	
26	A	1	Total	C	H	O	0
			458	139	262	57	
26	B	1	Total	C	H	O	0
			81	24	46	11	
26	G	1	Total	C	H	O	0
			59	18	35	6	
26	K	1	Total	C	H	O	0
			59	18	35	6	
26	1	1	Total	C	H	O	0
			349	107	201	41	
26	1	1	Total	C	H	O	0
			349	107	201	41	
26	1	1	Total	C	H	O	0
			349	107	201	41	
26	1	1	Total	C	H	O	0
			349	107	201	41	
26	1	1	Total	C	H	O	0
			349	107	201	41	
26	1	1	Total	C	H	O	0
			349	107	201	41	
26	7	1	Total	C	H	O	0
			173	53	92	28	
26	7	1	Total	C	H	O	0
			173	53	92	28	
26	7	1	Total	C	H	O	0
			173	53	92	28	
26	8	1	Total	C	H	O	0
			258	78	151	29	
26	8	1	Total	C	H	O	0
			258	78	151	29	
26	8	1	Total	C	H	O	0
			258	78	151	29	
26	8	1	Total	C	H	O	0
			258	78	151	29	
26	Z	1	Total	C	H	O	0
			116	36	63	17	
26	Z	1	Total	C	H	O	0
			116	36	63	17	
26	4	1	Total	C	H	O	0
			116	36	63	17	

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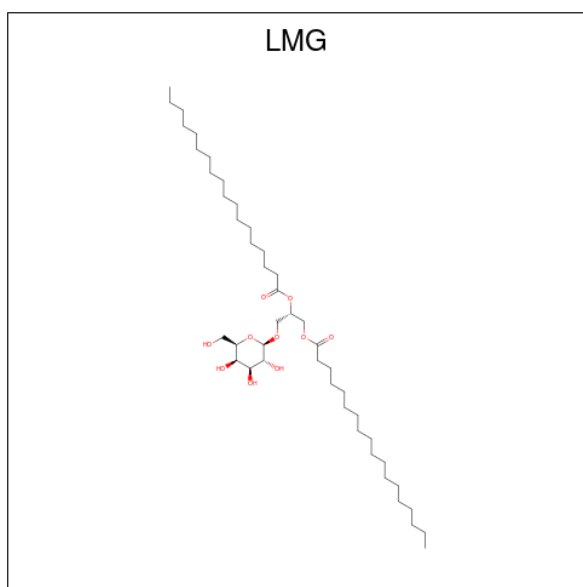
Mol	Chain	Residues	Atoms				AltConf
26	4	1	Total	C	H	O	0
			116	36	63	17	
26	5	1	Total	C	H	O	0
			59	18	35	6	
26	6	1	Total	C	H	O	0
			221	68	129	24	
26	6	1	Total	C	H	O	0
			221	68	129	24	
26	6	1	Total	C	H	O	0
			221	68	129	24	
26	6	1	Total	C	H	O	0
			221	68	129	24	
26	9	1	Total	C	H	O	0
			59	18	35	6	
26	A2	1	Total	C	H	O	0
			458	139	262	57	
26	A2	1	Total	C	H	O	0
			458	139	262	57	
26	A2	1	Total	C	H	O	0
			458	139	262	57	
26	A2	1	Total	C	H	O	0
			458	139	262	57	
26	A2	1	Total	C	H	O	0
			458	139	262	57	
26	A2	1	Total	C	H	O	0
			458	139	262	57	
26	A2	1	Total	C	H	O	0
			458	139	262	57	
26	B2	1	Total	C	H	O	0
			81	24	46	11	
26	G2	1	Total	C	H	O	0
			59	18	35	6	
26	K2	1	Total	C	H	O	0
			59	18	35	6	
26	12	1	Total	C	H	O	0
			349	107	201	41	
26	12	1	Total	C	H	O	0
			349	107	201	41	
26	12	1	Total	C	H	O	0
			349	107	201	41	
26	12	1	Total	C	H	O	0
			349	107	201	41	

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Mol	Chain	Residues	Atoms				AltConf
26	12	1	Total	C	H	O	0
			349	107	201	41	
26	12	1	Total	C	H	O	0
			349	107	201	41	
26	72	1	Total	C	H	O	0
			173	53	92	28	
26	72	1	Total	C	H	O	0
			173	53	92	28	
26	72	1	Total	C	H	O	0
			173	53	92	28	
26	82	1	Total	C	H	O	0
			258	78	151	29	
26	82	1	Total	C	H	O	0
			258	78	151	29	
26	82	1	Total	C	H	O	0
			258	78	151	29	
26	82	1	Total	C	H	O	0
			258	78	151	29	
26	Z2	1	Total	C	H	O	0
			116	36	63	17	
26	Z2	1	Total	C	H	O	0
			116	36	63	17	
26	42	1	Total	C	H	O	0
			116	36	63	17	
26	42	1	Total	C	H	O	0
			116	36	63	17	
26	52	1	Total	C	H	O	0
			59	18	35	6	
26	62	1	Total	C	H	O	0
			221	68	129	24	
26	62	1	Total	C	H	O	0
			221	68	129	24	
26	62	1	Total	C	H	O	0
			221	68	129	24	
26	62	1	Total	C	H	O	0
			221	68	129	24	
26	92	1	Total	C	H	O	0
			59	18	35	6	

- Molecule 27 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C₄₅H₈₆O₁₀) (labeled as "Ligand of Interest" by depositor).



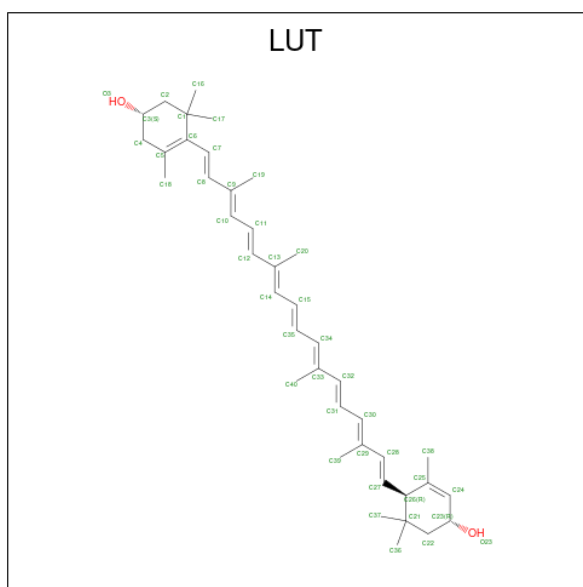
Mol	Chain	Residues	Atoms				AltConf
			Total	C	H	O	
27	A	1	195	64	111	20	0
27	A	1	195	64	111	20	0
27	B	1	177	59	98	20	0
27	B	1	177	59	98	20	0
27	J	1	174	57	97	20	0
27	J	1	174	57	97	20	0
27	1	1	174	58	96	20	0
27	1	1	174	58	96	20	0
27	3	1	120	40	75	5	0
27	7	1	81	27	44	10	0
27	8	1	165	54	91	20	0
27	8	1	165	54	91	20	0
27	4	1	96	31	55	10	0
27	6	1	55	18	35	2	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	H	O	
27	9	1	Total 105	C 34	H 61	O 10	0
27	A2	1	Total 195	C 64	H 111	O 20	0
27	A2	1	Total 195	C 64	H 111	O 20	0
27	B2	1	Total 177	C 59	H 98	O 20	0
27	B2	1	Total 177	C 59	H 98	O 20	0
27	J2	1	Total 174	C 57	H 97	O 20	0
27	J2	1	Total 174	C 57	H 97	O 20	0
27	12	1	Total 174	C 58	H 96	O 20	0
27	12	1	Total 174	C 58	H 96	O 20	0
27	32	1	Total 120	C 40	H 75	O 5	0
27	72	1	Total 81	C 27	H 44	O 10	0
27	82	1	Total 165	C 54	H 91	O 20	0
27	82	1	Total 165	C 54	H 91	O 20	0
27	42	1	Total 96	C 31	H 55	O 10	0
27	62	1	Total 55	C 18	H 35	O 2	0
27	92	1	Total 105	C 34	H 61	O 10	0

- Molecule 28 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (three-letter code: LUT) (formula: C₄₀H₅₆O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	H	O	
28	A	1	Total	C	H	O	0
			98	40	56	2	
28	F	1	Total	C	H	O	0
			98	40	56	2	
28	1	1	Total	C	H	O	0
			196	80	112	4	
28	1	1	Total	C	H	O	0
			196	80	112	4	
28	3	1	Total	C	H	O	0
			294	120	168	6	
28	3	1	Total	C	H	O	0
			294	120	168	6	
28	3	1	Total	C	H	O	0
			294	120	168	6	
28	7	1	Total	C	H	O	0
			196	80	112	4	
28	7	1	Total	C	H	O	0
			196	80	112	4	
28	8	1	Total	C	H	O	0
			98	40	56	2	
28	Z	1	Total	C	H	O	0
			157	65	89	3	
28	Z	1	Total	C	H	O	0
			157	65	89	3	
28	4	1	Total	C	H	O	0
			98	40	56	2	
28	5	1	Total	C	H	O	0
			196	80	112	4	

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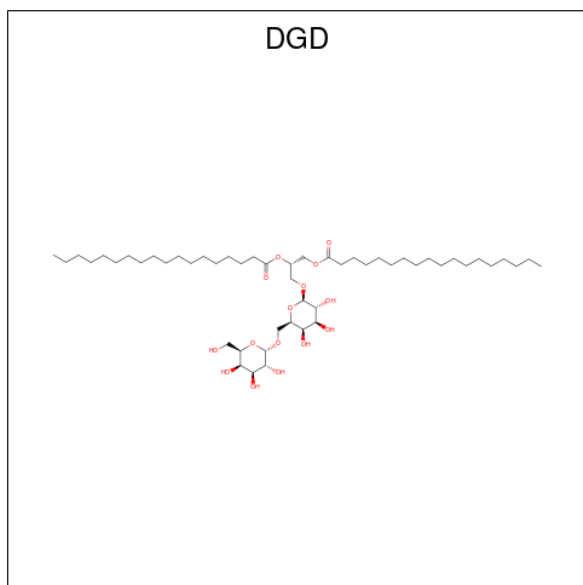
Mol	Chain	Residues	Atoms				AltConf
			Total	C	H	O	
28	5	1	Total 196	C 80	H 112	O 4	0
28	6	1	Total 98	C 40	H 56	O 2	0
28	9	1	Total 196	C 80	H 112	O 4	0
28	9	1	Total 196	C 80	H 112	O 4	0
28	A2	1	Total 98	C 40	H 56	O 2	0
28	F2	1	Total 98	C 40	H 56	O 2	0
28	12	1	Total 196	C 80	H 112	O 4	0
28	12	1	Total 196	C 80	H 112	O 4	0
28	32	1	Total 294	C 120	H 168	O 6	0
28	32	1	Total 294	C 120	H 168	O 6	0
28	32	1	Total 294	C 120	H 168	O 6	0
28	72	1	Total 196	C 80	H 112	O 4	0
28	72	1	Total 196	C 80	H 112	O 4	0
28	82	1	Total 98	C 40	H 56	O 2	0
28	Z2	1	Total 157	C 65	H 89	O 3	0
28	Z2	1	Total 157	C 65	H 89	O 3	0
28	42	1	Total 98	C 40	H 56	O 2	0
28	52	1	Total 196	C 80	H 112	O 4	0
28	52	1	Total 196	C 80	H 112	O 4	0
28	62	1	Total 98	C 40	H 56	O 2	0
28	92	1	Total 196	C 80	H 112	O 4	0

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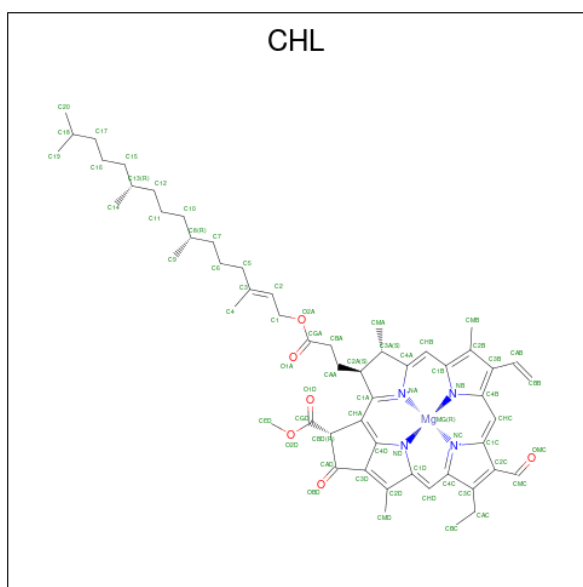
Mol	Chain	Residues	Atoms				AltConf
			Total	C	H	O	
28	92	1	196	80	112	4	0

- Molecule 29 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	H	O	
29	B	1	138	44	79	15	0
29	B2	1	138	44	79	15	0

- Molecule 30 is CHLOROPHYLL B (three-letter code: CHL) (formula: $C_{55}H_{70}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	Mg	N	O	
30	1	1	Total	C	H	Mg	N	O	0
			290	125	132	3	12	18	
30	1	1	Total	C	H	Mg	N	O	0
			290	125	132	3	12	18	
30	1	1	Total	C	H	Mg	N	O	0
			290	125	132	3	12	18	
30	3	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	
30	7	1	Total	C	H	Mg	N	O	0
			290	125	132	3	12	18	
30	7	1	Total	C	H	Mg	N	O	0
			290	125	132	3	12	18	
30	7	1	Total	C	H	Mg	N	O	0
			290	125	132	3	12	18	
30	8	1	Total	C	H	Mg	N	O	0
			408	165	210	3	12	18	
30	8	1	Total	C	H	Mg	N	O	0
			408	165	210	3	12	18	
30	8	1	Total	C	H	Mg	N	O	0
			408	165	210	3	12	18	
30	Z	1	Total	C	H	Mg	N	O	0
			349	145	171	3	12	18	
30	Z	1	Total	C	H	Mg	N	O	0
			349	145	171	3	12	18	
30	Z	1	Total	C	H	Mg	N	O	0
			349	145	171	3	12	18	
30	4	1	Total	C	H	Mg	N	O	0
			588	245	288	5	20	30	

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Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	Mg	N	O	
30	4	1	Total 588	C 245	H 288	Mg 5	N 20	O 30	0
30	4	1	Total 588	C 245	H 288	Mg 5	N 20	O 30	0
30	4	1	Total 588	C 245	H 288	Mg 5	N 20	O 30	0
30	4	1	Total 588	C 245	H 288	Mg 5	N 20	O 30	0
30	5	1	Total 373	C 164	H 167	Mg 4	N 16	O 22	0
30	5	1	Total 373	C 164	H 167	Mg 4	N 16	O 22	0
30	5	1	Total 373	C 164	H 167	Mg 4	N 16	O 22	0
30	5	1	Total 373	C 164	H 167	Mg 4	N 16	O 22	0
30	6	1	Total 677	C 286	H 327	Mg 6	N 24	O 34	0
30	6	1	Total 677	C 286	H 327	Mg 6	N 24	O 34	0
30	6	1	Total 677	C 286	H 327	Mg 6	N 24	O 34	0
30	6	1	Total 677	C 286	H 327	Mg 6	N 24	O 34	0
30	6	1	Total 677	C 286	H 327	Mg 6	N 24	O 34	0
30	6	1	Total 677	C 286	H 327	Mg 6	N 24	O 34	0
30	6	1	Total 677	C 286	H 327	Mg 6	N 24	O 34	0
30	9	1	Total 157	C 73	H 64	Mg 2	N 8	O 10	0
30	9	1	Total 157	C 73	H 64	Mg 2	N 8	O 10	0
30	12	1	Total 290	C 125	H 132	Mg 3	N 12	O 18	0
30	12	1	Total 290	C 125	H 132	Mg 3	N 12	O 18	0
30	12	1	Total 290	C 125	H 132	Mg 3	N 12	O 18	0
30	32	1	Total 136	C 55	H 70	Mg 1	N 4	O 6	0
30	72	1	Total 290	C 125	H 132	Mg 3	N 12	O 18	0

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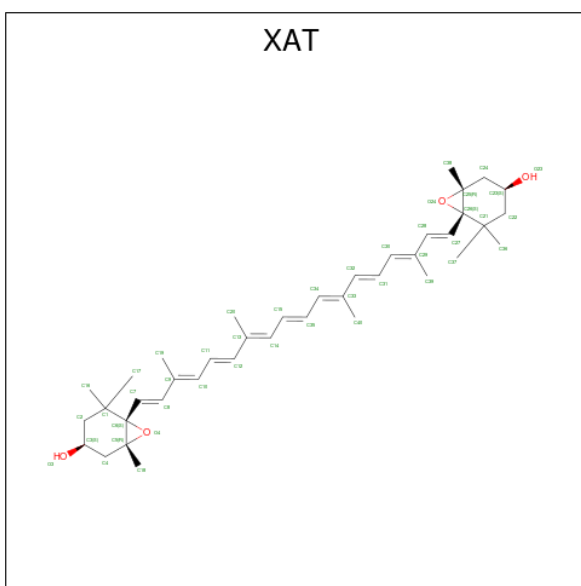
Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	Mg	N	O	
30	72	1	Total 290	C 125	H 132	Mg 3	N 12	O 18	0
30	72	1	Total 290	C 125	H 132	Mg 3	N 12	O 18	0
30	82	1	Total 408	C 165	H 210	Mg 3	N 12	O 18	0
30	82	1	Total 408	C 165	H 210	Mg 3	N 12	O 18	0
30	82	1	Total 408	C 165	H 210	Mg 3	N 12	O 18	0
30	Z2	1	Total 349	C 145	H 171	Mg 3	N 12	O 18	0
30	Z2	1	Total 349	C 145	H 171	Mg 3	N 12	O 18	0
30	Z2	1	Total 349	C 145	H 171	Mg 3	N 12	O 18	0
30	42	1	Total 588	C 245	H 288	Mg 5	N 20	O 30	0
30	42	1	Total 588	C 245	H 288	Mg 5	N 20	O 30	0
30	42	1	Total 588	C 245	H 288	Mg 5	N 20	O 30	0
30	42	1	Total 588	C 245	H 288	Mg 5	N 20	O 30	0
30	42	1	Total 588	C 245	H 288	Mg 5	N 20	O 30	0
30	42	1	Total 588	C 245	H 288	Mg 5	N 20	O 30	0
30	52	1	Total 373	C 164	H 167	Mg 4	N 16	O 22	0
30	52	1	Total 373	C 164	H 167	Mg 4	N 16	O 22	0
30	52	1	Total 373	C 164	H 167	Mg 4	N 16	O 22	0
30	52	1	Total 373	C 164	H 167	Mg 4	N 16	O 22	0
30	62	1	Total 677	C 286	H 327	Mg 6	N 24	O 34	0
30	62	1	Total 677	C 286	H 327	Mg 6	N 24	O 34	0
30	62	1	Total 677	C 286	H 327	Mg 6	N 24	O 34	0
30	62	1	Total 677	C 286	H 327	Mg 6	N 24	O 34	0

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Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	Mg	N	O	
30	62	1	Total	C	H	Mg	N	O	0
			677	286	327	6	24	34	
30	62	1	Total	C	H	Mg	N	O	0
			677	286	327	6	24	34	
30	92	1	Total	C	H	Mg	N	O	0
			157	73	64	2	8	10	
30	92	1	Total	C	H	Mg	N	O	0
			157	73	64	2	8	10	

- Molecule 31 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (three-letter code: XAT) (formula: C₄₀H₅₆O₄) (labeled as "Ligand of Interest" by depositor).



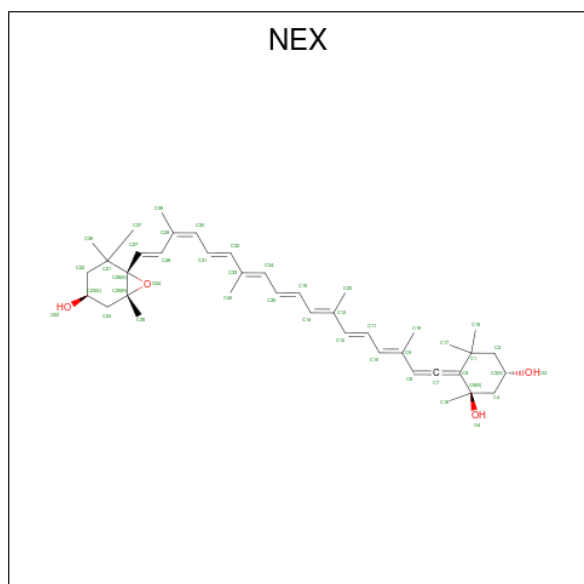
Mol	Chain	Residues	Atoms				AltConf
			Total	C	H	O	
31	1	1	Total	C	H	O	0
			100	40	56	4	
31	7	1	Total	C	H	O	0
			100	40	56	4	
31	8	1	Total	C	H	O	0
			100	40	56	4	
31	Z	1	Total	C	H	O	0
			100	40	56	4	
31	4	1	Total	C	H	O	0
			100	40	56	4	
31	5	1	Total	C	H	O	0
			100	40	56	4	

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	H	O	
31	6	1	Total 100	C 40	H 56	O 4	0
31	12	1	Total 100	C 40	H 56	O 4	0
31	72	1	Total 100	C 40	H 56	O 4	0
31	82	1	Total 100	C 40	H 56	O 4	0
31	Z2	1	Total 100	C 40	H 56	O 4	0
31	42	1	Total 100	C 40	H 56	O 4	0
31	52	1	Total 100	C 40	H 56	O 4	0
31	62	1	Total 100	C 40	H 56	O 4	0

- Molecule 32 is (1R,3R)-6-{(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-2,2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL]-3,7,12,16-TETRAMETHYLOCTADEC-1,3,5,7,9,11,13,15,17-NONAENYLIDENE}-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (three-letter code: NEX) (formula: C₄₀H₅₆O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	H	O	
32	5	1	Total 100	C 40	H 56	O 4	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	H	O	
32	6	1	100	40	56	4	0
32	52	1	100	40	56	4	0
32	62	1	100	40	56	4	0

- Molecule 33 is water.

Mol	Chain	Residues	Atoms		AltConf
33	H	10	Total	O	0
			160	160	
33	H	19	Total	O	0
			160	160	
33	H	1	Total	O	0
			160	160	
33	H	1	Total	O	0
			160	160	
33	H	4	Total	O	0
			160	160	
33	H	1	Total	O	0
			160	160	
33	H	1	Total	O	0
			160	160	
33	H	7	Total	O	0
			160	160	
33	H	6	Total	O	0
			160	160	
33	H	6	Total	O	0
			160	160	
33	H	6	Total	O	0
			160	160	
33	H	5	Total	O	0
			160	160	
33	H	3	Total	O	0
			160	160	
33	H	5	Total	O	0
			160	160	
33	H	5	Total	O	0
			160	160	
33	H	1	Total	O	0
			160	160	

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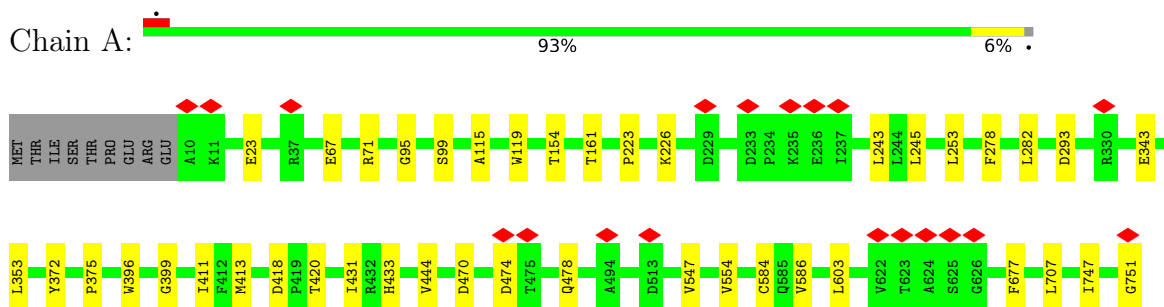
Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
33	H	11	Total 160	O 160	0
33	H	18	Total 160	O 160	0
33	H	1	Total 160	O 160	0
33	H	1	Total 160	O 160	0
33	H	4	Total 160	O 160	0
33	H	1	Total 160	O 160	0
33	H	1	Total 160	O 160	0
33	H	7	Total 160	O 160	0
33	H	5	Total 160	O 160	0
33	H	6	Total 160	O 160	0
33	H	5	Total 160	O 160	0
33	H	5	Total 160	O 160	0
33	H	3	Total 160	O 160	0
33	H	5	Total 160	O 160	0
33	H	5	Total 160	O 160	0
33	H	1	Total 160	O 160	0

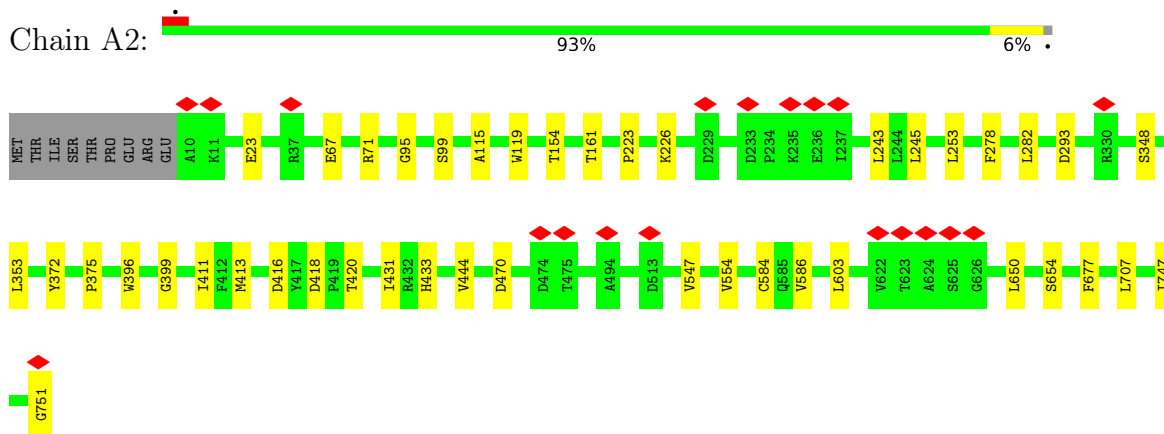
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

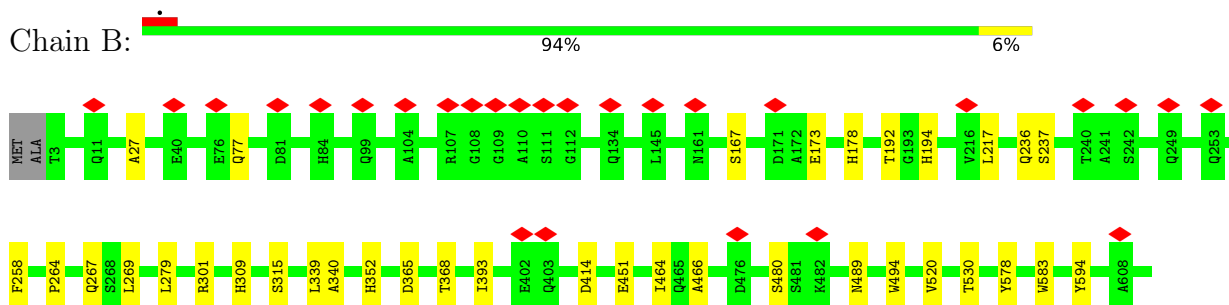
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

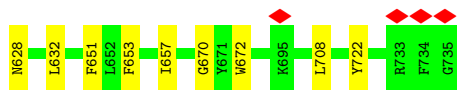


- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

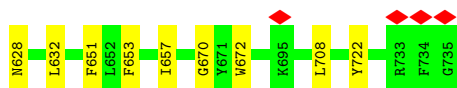
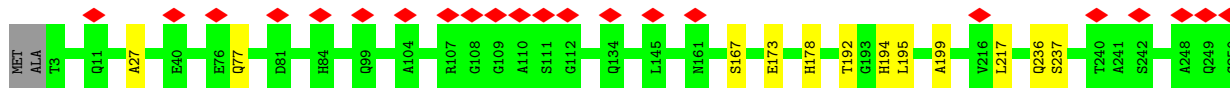


- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

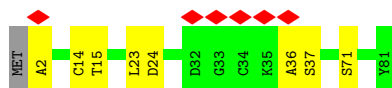
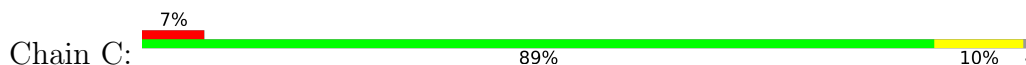




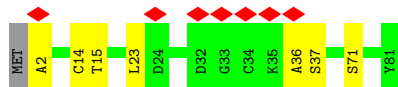
• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



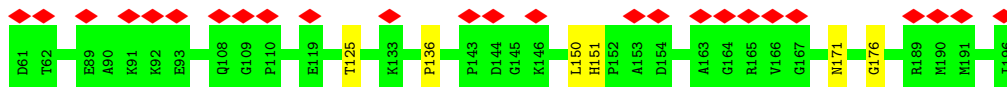
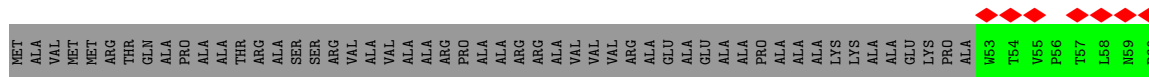
• Molecule 3: Photosystem I iron-sulfur center



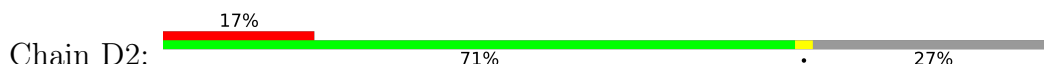
• Molecule 3: Photosystem I iron-sulfur center

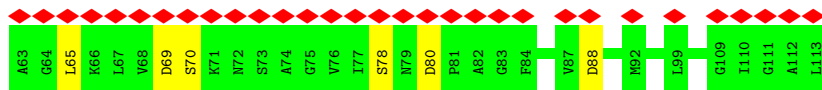


• Molecule 4: Photosystem I reaction center subunit II, chloroplastic

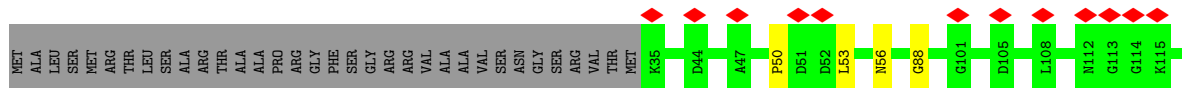
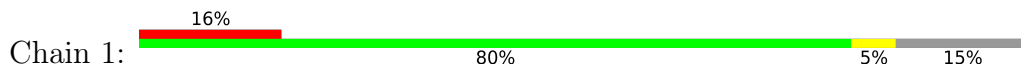


• Molecule 4: Photosystem I reaction center subunit II, chloroplastic

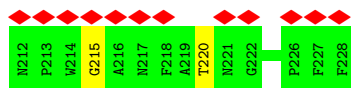
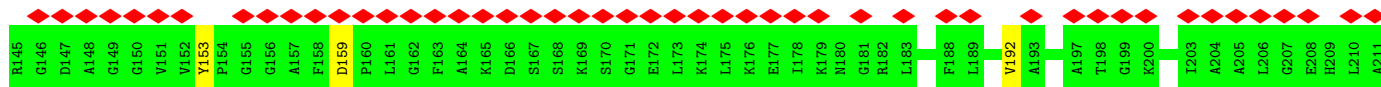
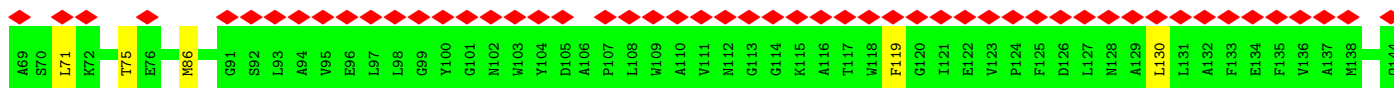
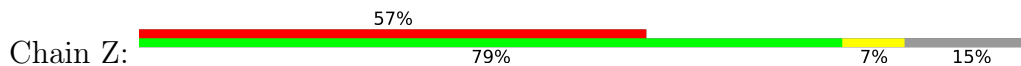




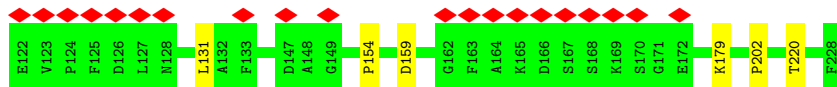
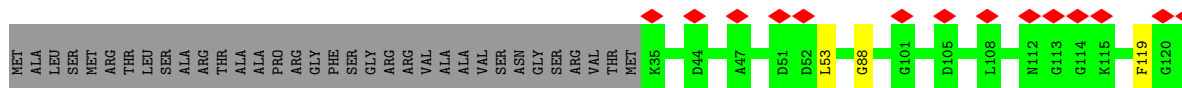
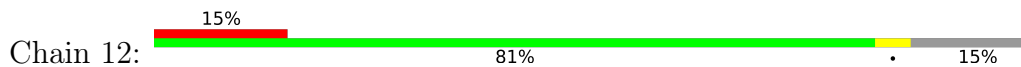
• Molecule 12: Chlorophyll a-b binding protein, chloroplastic



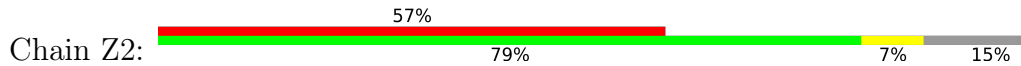
• Molecule 12: Chlorophyll a-b binding protein, chloroplastic

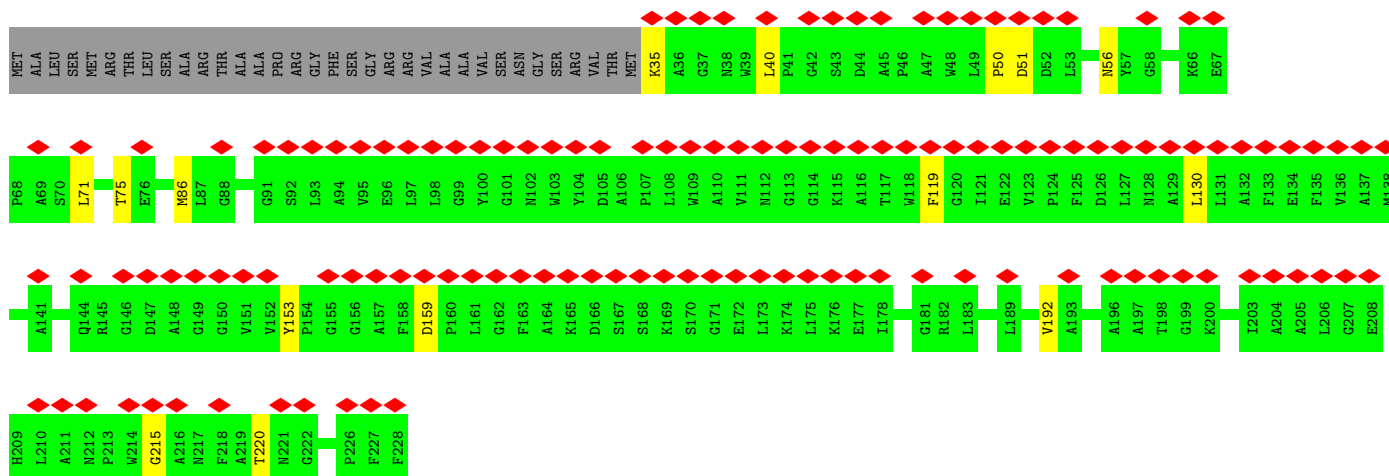


• Molecule 12: Chlorophyll a-b binding protein, chloroplastic

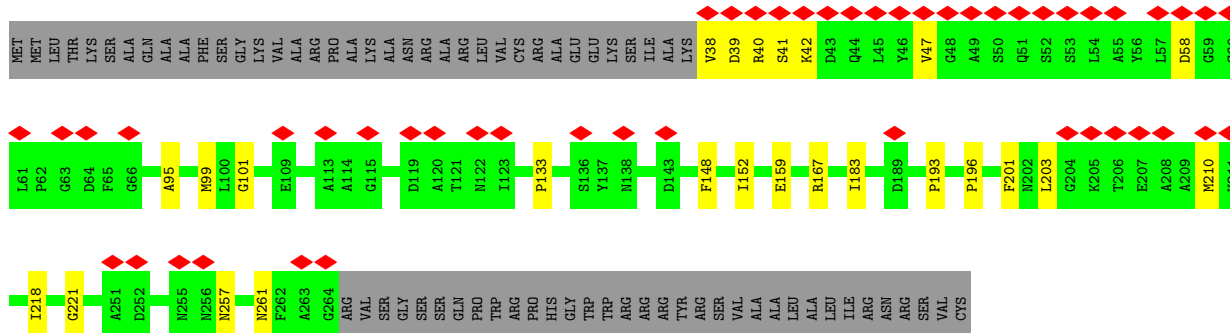


• Molecule 12: Chlorophyll a-b binding protein, chloroplastic

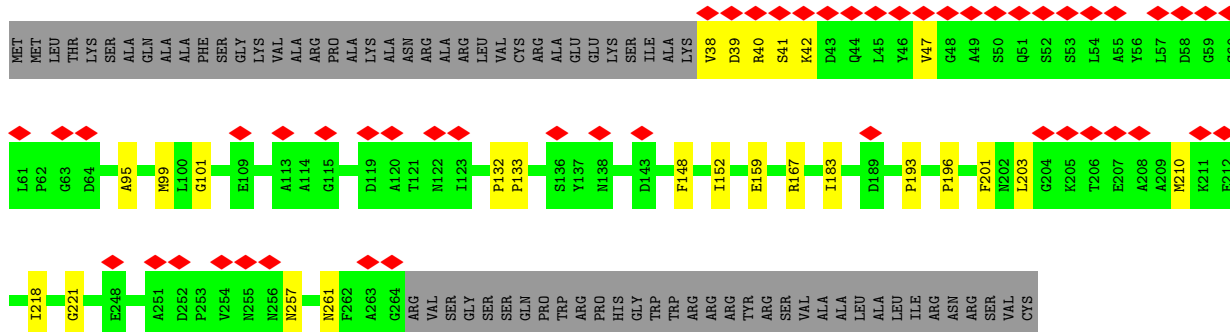




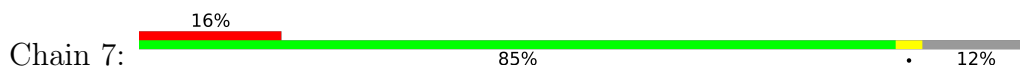
• Molecule 13: Chlorophyll a-b binding protein, chloroplastic

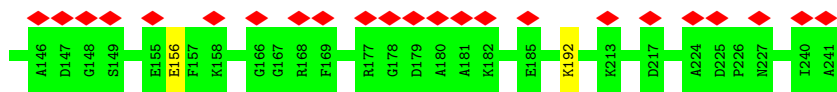


• Molecule 13: Chlorophyll a-b binding protein, chloroplastic

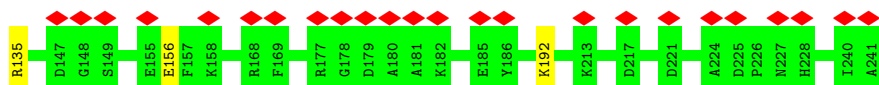
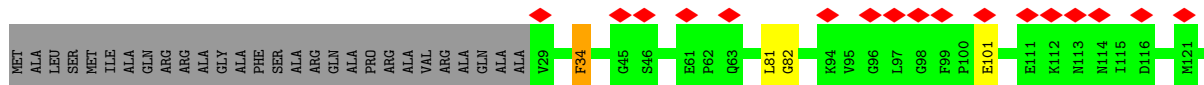
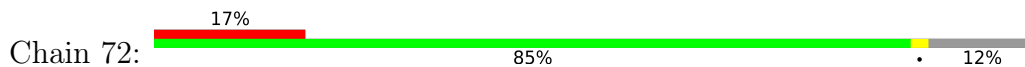


• Molecule 14: Chlorophyll a-b binding protein, chloroplastic

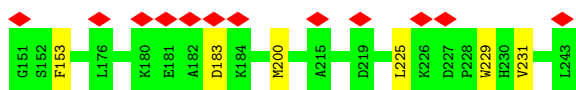
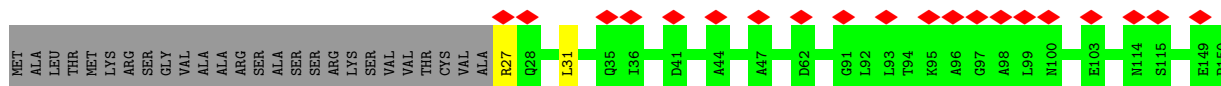
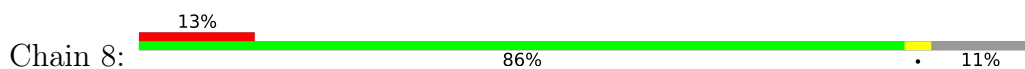




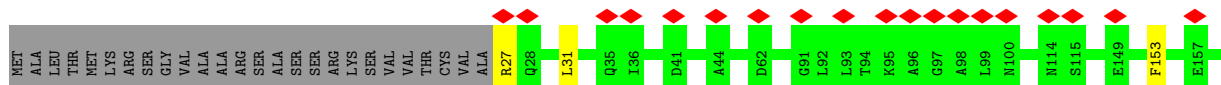
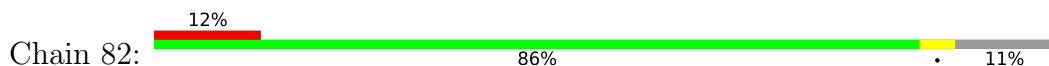
• Molecule 14: Chlorophyll a-b binding protein, chloroplastic



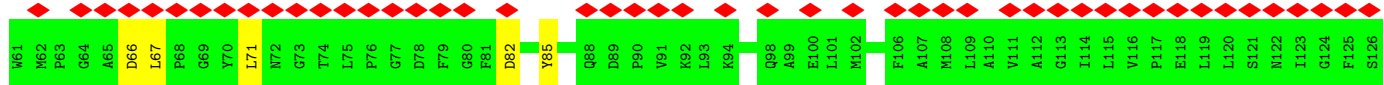
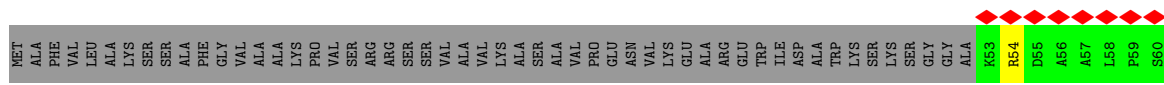
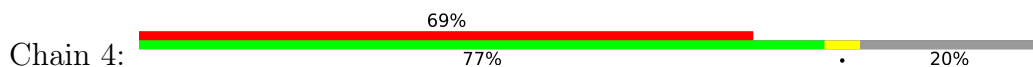
• Molecule 15: Chlorophyll a-b binding protein, chloroplastic

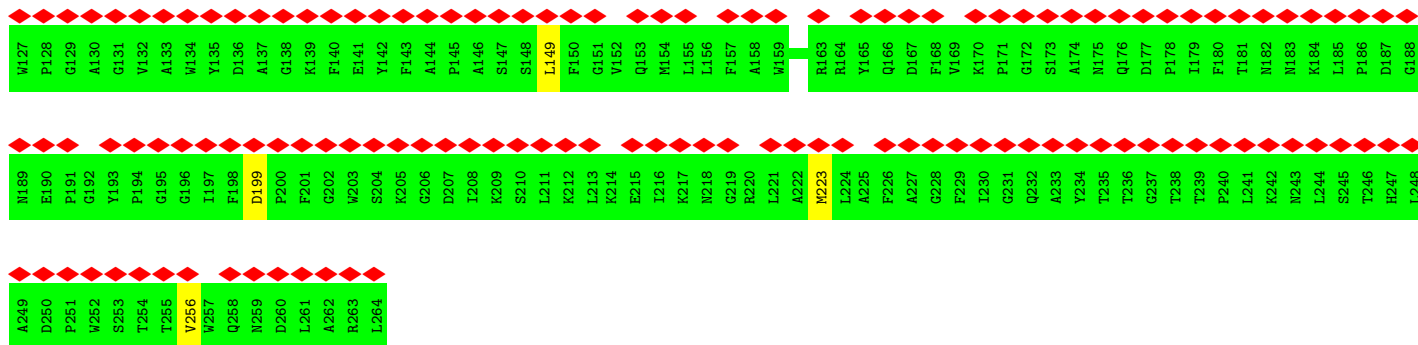


• Molecule 15: Chlorophyll a-b binding protein, chloroplastic

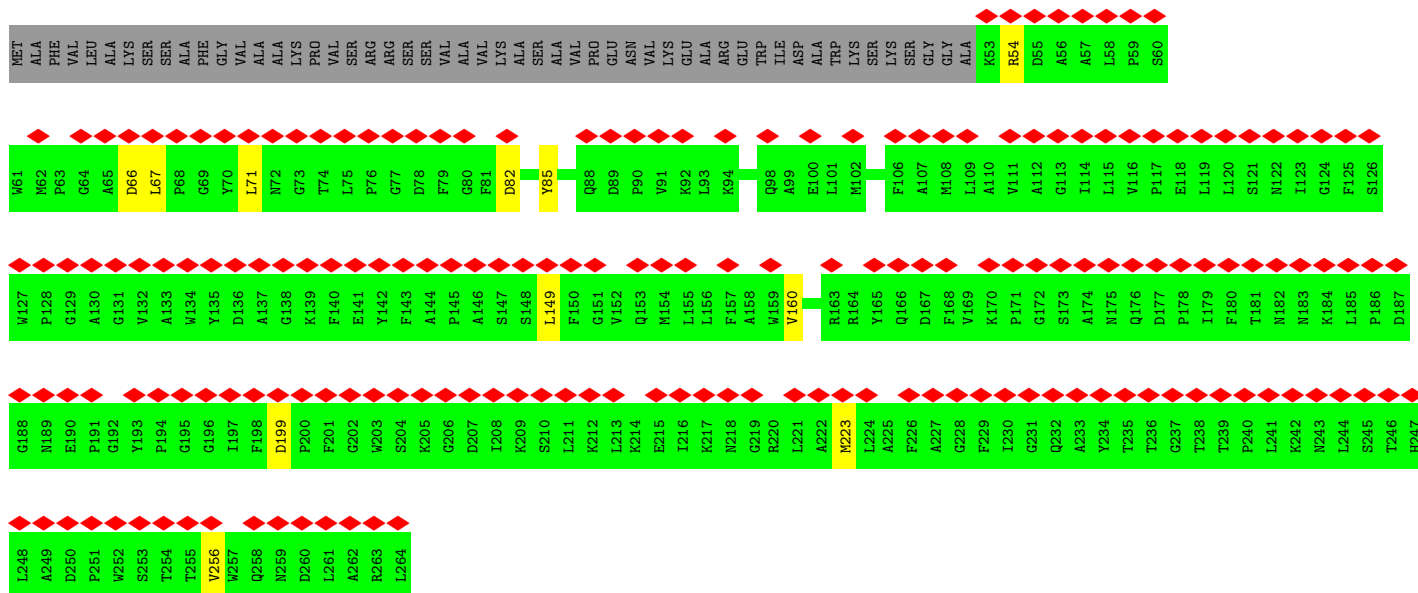
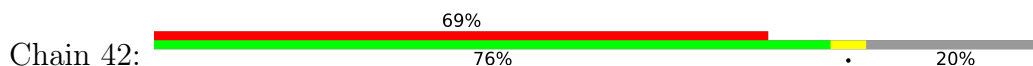


• Molecule 16: Chlorophyll a-b binding protein, chloroplastic (Lhca4)

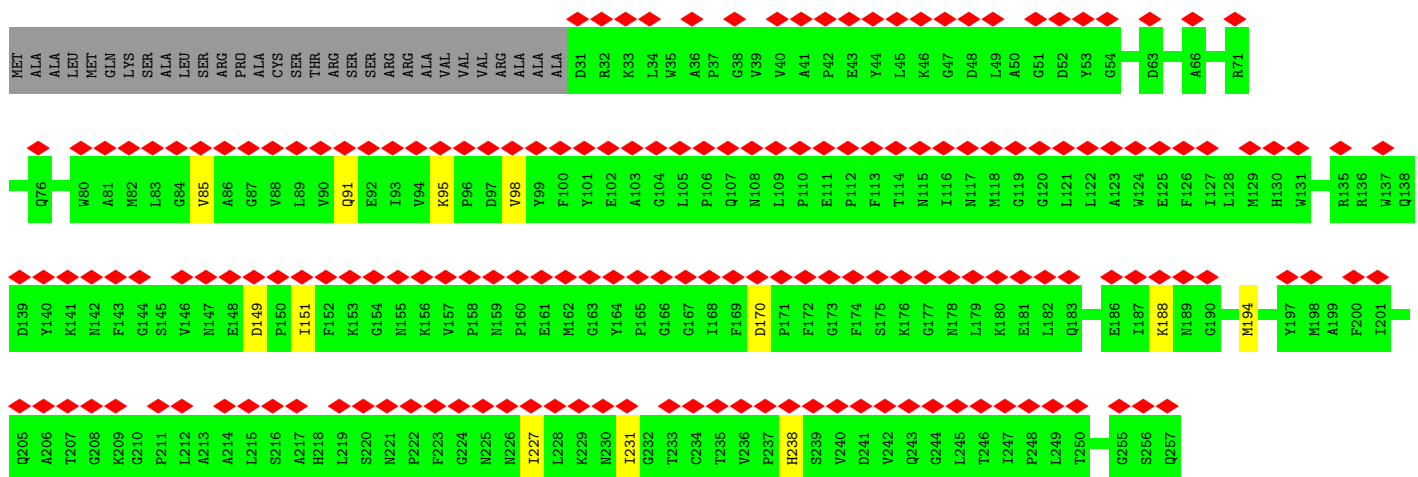
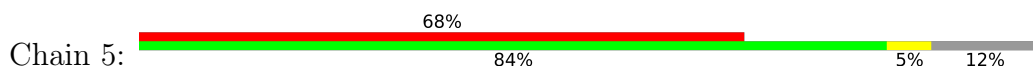




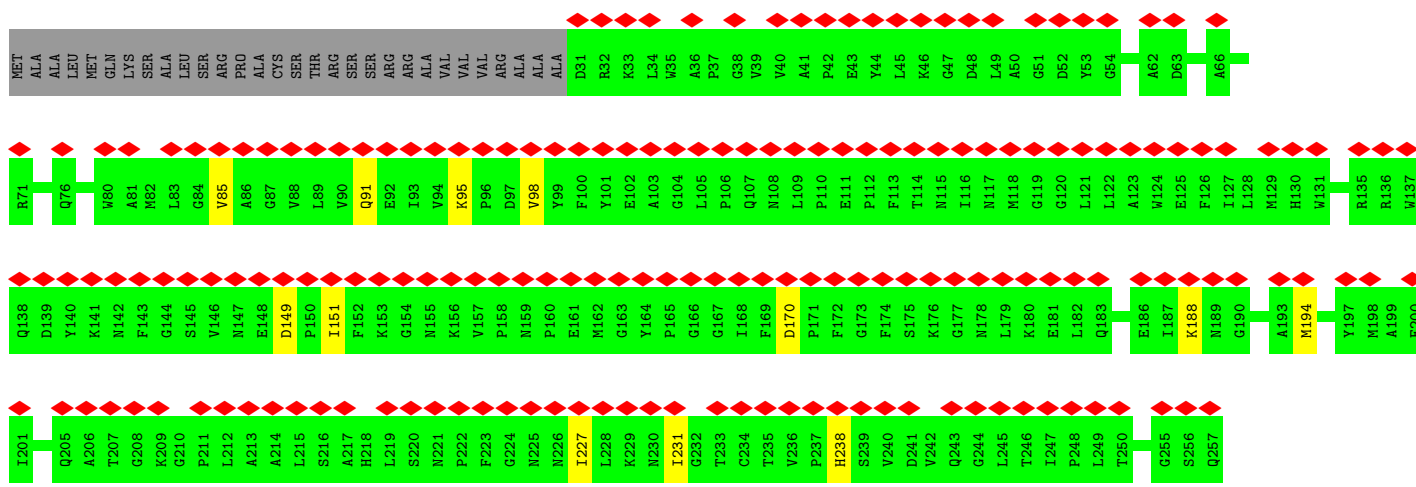
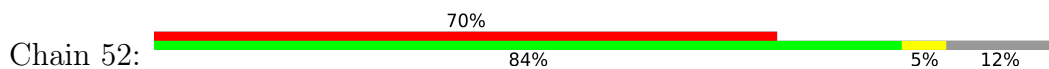
• Molecule 16: Chlorophyll a-b binding protein, chloroplastic (Lhca4)



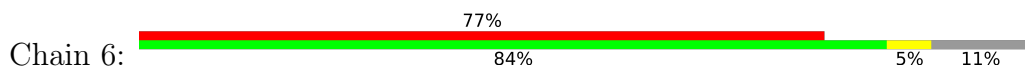
• Molecule 17: Chlorophyll a-b binding protein, chloroplastic



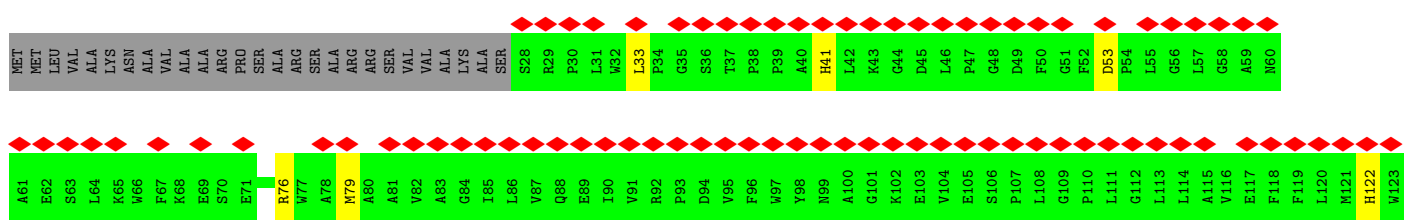
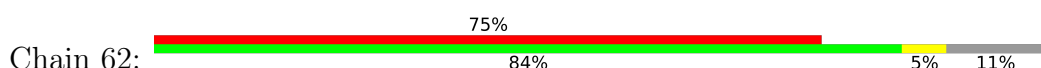
• Molecule 17: Chlorophyll a-b binding protein, chloroplastic

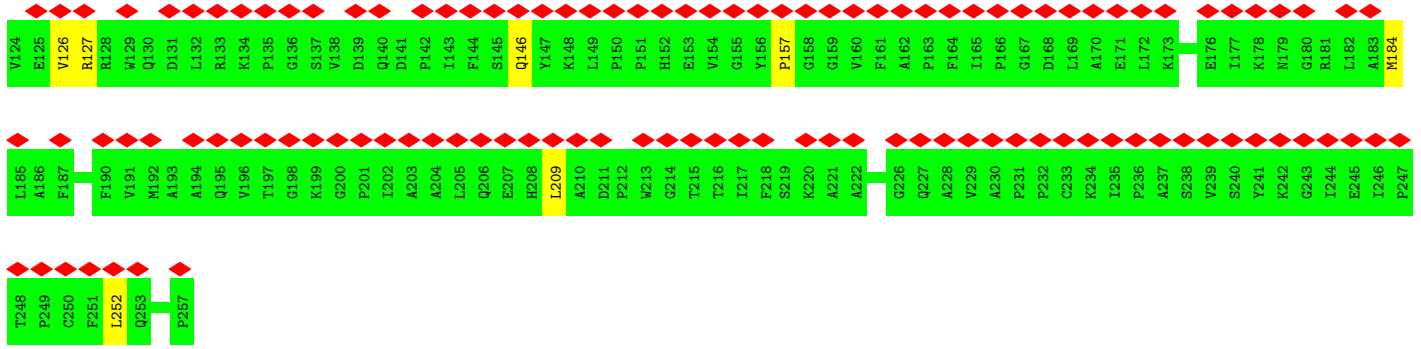


• Molecule 18: Chlorophyll a-b binding protein, chloroplastic

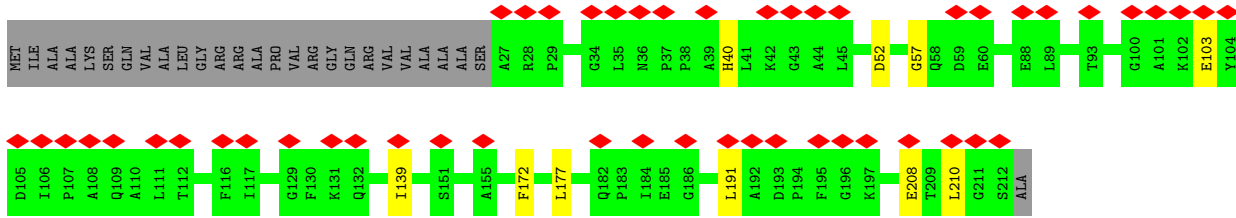
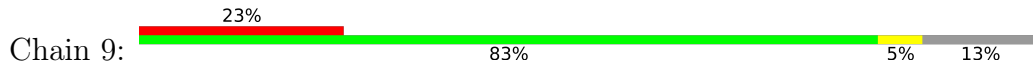


• Molecule 18: Chlorophyll a-b binding protein, chloroplastic

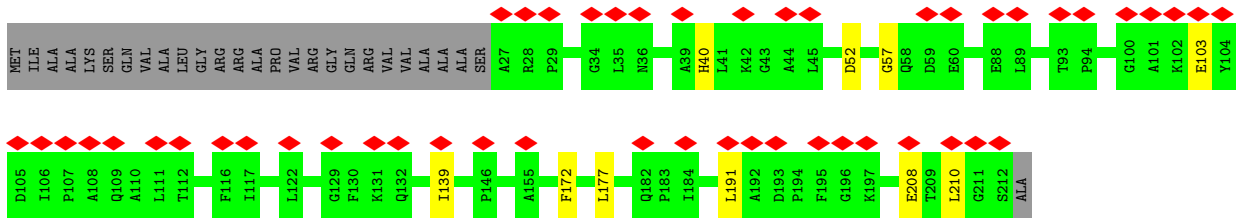
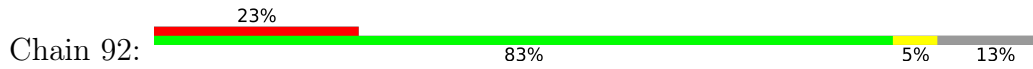




• Molecule 19: Chlorophyll a-b binding protein, chloroplastic



• Molecule 19: Chlorophyll a-b binding protein, chloroplastic



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	17439	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45.8	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.183	Depositor
Minimum map value	-0.090	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.036	Depositor
Map size (\AA)	588.0, 588.0, 588.0	wwPDB
Map dimensions	700, 700, 700	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.84, 0.84, 0.84	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: XAT, PQN, CL0, BCR, DGD, NEX, SF4, AME, CHL, CLA, LHG, LMG, LMU, LUT

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 $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.26	0/6021	0.43	0/8208
1	A2	0.26	0/6021	0.43	0/8208
2	B	0.27	0/6036	0.42	0/8240
2	B2	0.27	0/6036	0.42	0/8240
3	C	0.27	0/611	0.51	0/826
3	C2	0.27	0/611	0.51	0/826
4	D	0.27	0/1161	0.48	0/1567
4	D2	0.27	0/1161	0.48	0/1567
5	E	0.28	0/516	0.47	0/700
5	E2	0.28	0/516	0.47	0/700
6	F	0.26	0/1292	0.43	0/1747
6	F2	0.26	0/1292	0.43	0/1747
7	G	0.25	0/721	0.43	0/980
7	G2	0.26	0/721	0.43	0/980
8	I	0.27	0/293	0.38	0/406
8	I2	0.28	0/293	0.38	0/406
9	J	0.28	0/329	0.41	0/452
9	J2	0.28	0/329	0.41	0/452
10	L	0.26	0/920	0.42	0/1257
10	L2	0.26	0/920	0.42	0/1257
11	K	0.26	0/588	0.43	0/795
11	K2	0.26	0/588	0.43	0/795
12	1	0.26	0/1491	0.42	0/2028
12	12	0.26	0/1491	0.42	0/2028
12	Z	0.25	0/1491	0.40	0/2028
12	Z2	0.25	0/1491	0.40	0/2028
13	3	0.27	0/1784	0.43	0/2420
13	32	0.27	0/1784	0.43	0/2420
14	7	0.26	0/1702	0.41	0/2310
14	72	0.26	0/1702	0.41	0/2310
15	8	0.26	0/1701	0.42	0/2315
15	82	0.26	0/1701	0.42	0/2315

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	4	0.25	0/1703	0.40	0/2321
16	42	0.25	0/1703	0.40	0/2321
17	5	0.24	0/1830	0.41	0/2492
17	52	0.24	0/1830	0.41	0/2492
18	6	0.25	0/1834	0.41	0/2505
18	62	0.25	0/1834	0.41	0/2505
19	9	0.26	0/1461	0.42	0/1987
19	92	0.26	0/1461	0.42	0/1987
All	All	0.26	0/66970	0.42	0/91168

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5825	5675	5675	30	0
1	A2	5825	5675	5675	29	0
2	B	5824	5576	5577	39	0
2	B2	5824	5576	5577	40	0
3	C	601	582	581	4	0
3	C2	601	582	581	3	0
4	D	1133	1151	1150	4	0
4	D2	1133	1151	1150	2	0
5	E	506	505	504	1	0
5	E2	506	505	504	1	0
6	F	1266	1302	1301	11	0
6	F2	1266	1302	1301	10	0
7	G	706	687	686	4	0
7	G2	706	687	686	4	0
8	I	281	292	292	3	0
8	I2	281	292	292	3	0
9	J	329	328	328	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	J2	329	328	328	1	0
10	L	899	907	905	8	0
10	L2	899	907	905	9	0
11	K	583	620	620	5	0
11	K2	583	620	620	5	0
12	1	1445	1397	1396	11	0
12	12	1445	1397	1396	10	0
12	Z	1445	1397	1396	13	0
12	Z2	1445	1397	1396	13	0
13	3	1736	1695	1694	16	0
13	32	1736	1695	1694	15	0
14	7	1650	1590	1589	8	0
14	72	1650	1590	1589	8	0
15	8	1650	1630	1629	7	0
15	82	1650	1630	1629	8	0
16	4	1648	1603	1602	9	0
16	42	1648	1603	1602	10	0
17	5	1775	1747	1746	10	0
17	52	1775	1747	1746	10	0
18	6	1772	1770	1770	13	0
18	62	1772	1770	1770	13	0
19	9	1420	1400	1399	9	0
19	92	1420	1400	1399	9	0
20	A	65	72	72	1	0
20	A2	65	72	72	1	0
21	1	639	625	625	14	0
21	12	639	625	625	14	0
21	3	740	718	718	19	0
21	32	740	718	718	20	0
21	4	565	534	534	10	0
21	42	565	534	534	11	0
21	5	740	712	712	10	0
21	52	740	712	712	10	0
21	6	628	605	605	10	0
21	62	628	605	605	9	0
21	7	652	598	598	7	0
21	72	652	598	598	7	0
21	8	614	578	578	14	0
21	82	614	578	578	12	0
21	9	565	535	535	5	0
21	92	565	535	535	5	0
21	A	2718	2856	2856	41	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	A2	2718	2856	2856	41	0
21	B	2463	2580	2580	45	0
21	B2	2463	2580	2580	46	0
21	F	175	177	177	1	0
21	F2	175	177	177	1	0
21	G	106	92	92	0	0
21	G2	106	92	92	0	0
21	J	55	49	49	1	0
21	J2	55	49	49	1	0
21	K	196	158	158	1	0
21	K2	196	158	158	1	0
21	L	110	105	105	2	0
21	L2	110	105	105	1	0
21	Z	627	593	593	13	0
21	Z2	627	593	593	15	0
22	A	33	46	46	0	0
22	A2	33	46	46	0	0
22	B	33	46	46	1	0
22	B2	33	46	46	1	0
23	1	39	48	48	1	0
23	12	39	48	48	1	0
23	3	78	99	99	1	0
23	32	78	99	99	1	0
23	4	87	123	123	1	0
23	42	87	123	123	1	0
23	5	37	44	44	1	0
23	52	37	44	44	1	0
23	6	85	116	116	0	0
23	62	85	116	116	0	0
23	7	49	74	74	1	0
23	72	49	74	74	1	0
23	8	44	61	61	0	0
23	82	44	61	61	0	0
23	9	41	55	55	0	0
23	92	41	55	55	0	0
23	A	87	123	123	0	0
23	A2	87	123	123	0	0
23	B	45	63	63	0	0
23	B2	45	63	63	0	0
23	Z	39	48	48	0	0
23	Z2	39	48	48	1	0
24	3	120	168	168	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	32	120	168	168	4	0
24	4	40	56	56	0	0
24	42	40	56	56	1	0
24	5	40	56	56	0	0
24	52	40	56	56	0	0
24	6	40	56	56	3	0
24	62	40	56	56	2	0
24	7	40	56	56	0	0
24	72	40	56	56	0	0
24	8	40	56	56	2	0
24	82	40	56	56	2	0
24	9	40	56	56	1	0
24	92	40	56	56	2	0
24	A	200	280	280	12	0
24	A2	200	280	280	9	0
24	B	280	392	392	12	0
24	B2	280	392	392	12	0
24	G	40	56	56	0	0
24	G2	40	56	56	2	0
24	I	40	56	56	1	0
24	I2	40	56	56	1	0
24	J	40	56	56	1	0
24	J2	40	56	56	1	0
24	K	80	112	112	5	0
24	K2	80	112	112	6	0
24	L	80	112	112	5	0
24	L2	80	112	112	5	0
25	A	8	0	0	0	0
25	A2	8	0	0	0	0
25	C	16	0	0	0	0
25	C2	16	0	0	0	0
26	1	148	201	201	0	0
26	12	148	201	201	0	0
26	4	53	63	63	1	0
26	42	53	63	63	1	0
26	5	24	35	35	0	0
26	52	24	35	35	0	0
26	6	92	129	129	0	0
26	62	92	129	129	0	0
26	7	81	92	92	1	0
26	72	81	92	92	1	0
26	8	107	151	151	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	82	107	151	151	1	0
26	9	24	35	35	1	0
26	92	24	35	35	1	0
26	A	196	262	262	4	0
26	A2	196	262	262	2	0
26	B	35	46	46	3	0
26	B2	35	46	46	2	0
26	G	24	35	35	0	0
26	G2	24	35	35	0	0
26	K	24	35	35	0	0
26	K2	24	35	35	0	0
26	Z	53	63	63	1	0
26	Z2	53	63	63	1	0
27	1	78	96	96	0	0
27	12	78	96	96	0	0
27	3	45	75	75	1	0
27	32	45	75	75	1	0
27	4	41	55	55	0	0
27	42	41	55	55	0	0
27	6	20	35	35	0	0
27	62	20	35	35	0	0
27	7	37	44	44	0	0
27	72	37	44	44	0	0
27	8	74	91	91	1	0
27	82	74	91	91	0	0
27	9	44	61	61	2	0
27	92	44	61	61	2	0
27	A	84	111	111	1	0
27	A2	84	111	111	1	0
27	B	79	98	98	1	0
27	B2	79	98	98	1	0
27	J	77	97	97	2	0
27	J2	77	97	97	2	0
28	1	84	112	112	4	0
28	12	84	112	112	4	0
28	3	126	168	168	6	0
28	32	126	168	168	6	0
28	4	42	56	56	2	0
28	42	42	56	56	2	0
28	5	84	112	112	3	0
28	52	84	112	112	3	0
28	6	42	56	56	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	62	42	56	56	2	0
28	7	84	112	112	5	0
28	72	84	112	112	5	0
28	8	42	56	56	0	0
28	82	42	56	56	1	0
28	9	84	112	112	5	0
28	92	84	112	112	5	0
28	A	42	56	56	1	0
28	A2	42	56	56	2	0
28	F	42	56	56	4	0
28	F2	42	56	56	3	0
28	Z	68	89	89	2	0
28	Z2	68	89	89	2	0
29	B	59	79	79	1	0
29	B2	59	79	79	1	0
30	1	158	132	132	1	0
30	12	158	132	132	0	0
30	3	66	70	70	1	0
30	32	66	70	70	2	0
30	4	300	288	288	7	0
30	42	300	288	288	5	0
30	5	206	167	167	1	0
30	52	206	167	167	1	0
30	6	350	327	327	10	0
30	62	350	327	327	9	0
30	7	158	132	132	3	0
30	72	158	132	132	2	0
30	8	198	210	210	4	0
30	82	198	210	210	4	0
30	9	93	64	64	0	0
30	92	93	64	64	0	0
30	Z	178	171	171	4	0
30	Z2	178	171	171	4	0
31	1	44	56	56	2	0
31	12	44	56	56	2	0
31	4	44	56	56	1	0
31	42	44	56	56	1	0
31	5	44	56	56	1	0
31	52	44	56	56	1	0
31	6	44	56	56	1	0
31	62	44	56	56	1	0
31	7	44	56	56	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	72	44	56	56	2	0
31	8	44	56	56	1	0
31	82	44	56	56	1	0
31	Z	44	56	56	1	0
31	Z2	44	56	56	1	0
32	5	44	56	56	0	0
32	52	44	56	56	0	0
32	6	44	56	56	1	0
32	62	44	56	56	1	0
33	H	160	0	0	17	0
All	All	100830	101988	101960	751	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (751) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:7:624:LUT:H381	28:7:624:LUT:H28	1.51	0.93
28:72:624:LUT:H381	28:72:624:LUT:H28	1.51	0.91
26:B:853:LMU:H2O1	26:B:853:LMU:H6'	1.13	0.90
1:A2:95:GLY:O	1:A2:99:SER:OG	1.95	0.83
17:5:170:ASP:OD1	28:5:620:LUT:O23	1.96	0.82
1:A:95:GLY:O	1:A:99:SER:OG	1.96	0.82
17:52:170:ASP:OD1	28:52:620:LUT:O23	1.96	0.82
2:B2:301:ARG:NH1	7:G2:68:GLY:O	2.14	0.80
4:D:171:ASN:OD1	33:H:41:HOH:O	2.00	0.80
2:B:301:ARG:NH1	7:G:68:GLY:O	2.15	0.79
2:B:167:SER:OG	7:G:78:ASP:OD1	2.00	0.78
2:B2:167:SER:OG	7:G2:78:ASP:OD1	2.00	0.78
2:B:628:ASN:O	33:H:14:HOH:O	2.02	0.77
6:F2:184:GLU:OE1	33:H:176:HOH:O	2.03	0.76
2:B2:628:ASN:O	33:H:111:HOH:O	2.03	0.76
7:G2:58:ARG:NH2	7:G2:99:ASP:OD2	2.19	0.76
7:G:58:ARG:NH2	7:G:99:ASP:OD2	2.19	0.75
6:F:184:GLU:OE1	33:H:88:HOH:O	2.04	0.75
12:1:179:LYS:NZ	23:1:620:LHG:O5	2.20	0.73
2:B2:269:LEU:O	33:H:109:HOH:O	2.05	0.73
1:A:226:LYS:NZ	1:A:253:LEU:O	2.21	0.73
1:A2:226:LYS:NZ	1:A2:253:LEU:O	2.22	0.73
12:12:179:LYS:NZ	23:12:620:LHG:O5	2.21	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:42:601:CHL:OBD	18:62:127:ARG:NH1	2.23	0.72
28:72:624:LUT:H381	28:72:624:LUT:C28	2.19	0.72
2:B:269:LEU:O	33:H:12:HOH:O	2.05	0.72
13:32:40:ARG:O	13:32:41:SER:OG	2.07	0.72
30:4:601:CHL:OBD	18:6:127:ARG:NH1	2.22	0.72
12:Z:130:LEU:HD11	30:Z:606:CHL:HMD3	1.72	0.71
26:72:628:LMU:O6'	33:H:169:HOH:O	2.08	0.71
26:7:628:LMU:O6'	33:H:81:HOH:O	2.08	0.70
26:B2:853:LMU:O6'	26:B2:853:LMU:O2B	1.99	0.69
12:Z2:130:LEU:HD11	30:Z2:606:CHL:HMD3	1.72	0.69
13:3:40:ARG:O	13:3:41:SER:OG	2.06	0.69
19:92:191:LEU:HD21	21:92:614:CLA:HMC3	1.73	0.69
28:7:624:LUT:H381	28:7:624:LUT:C28	2.19	0.69
19:9:191:LEU:HD21	21:9:614:CLA:HMC3	1.73	0.69
21:72:608:CLA:O1A	21:72:610:CLA:HMD2	1.94	0.68
13:32:159:GLU:OE2	33:H:131:HOH:O	2.12	0.68
2:B:27:ALA:HA	21:B:829:CLA:H43	1.76	0.68
21:7:608:CLA:O1A	21:7:610:CLA:HMD2	1.94	0.68
1:A2:23:GLU:OE2	27:A2:860:LMG:O5	2.06	0.67
1:A:23:GLU:OE2	27:A:860:LMG:O5	2.07	0.66
2:B2:27:ALA:HA	21:B2:829:CLA:H43	1.77	0.66
13:3:159:GLU:OE2	33:H:37:HOH:O	2.13	0.66
21:5:621:CLA:HBC3	21:5:621:CLA:HMC1	1.78	0.66
21:A2:803:CLA:HBB1	21:A2:803:CLA:HMB1	1.78	0.66
21:A2:854:CLA:HMB3	21:B2:802:CLA:H193	1.78	0.65
21:52:621:CLA:HMC1	21:52:621:CLA:HBC3	1.78	0.65
30:62:606:CHL:OMC	33:H:162:HOH:O	2.15	0.65
13:32:148:PHE:CE2	13:32:152:ILE:HD11	2.32	0.65
30:8:606:CHL:OMC	33:H:55:HOH:O	2.15	0.65
30:6:606:CHL:OMC	33:H:73:HOH:O	2.15	0.65
21:A:803:CLA:HMB1	21:A:803:CLA:HBB1	1.78	0.64
21:62:602:CLA:HMC2	31:62:624:XAT:C11	2.27	0.64
21:A:854:CLA:HMB3	21:B:802:CLA:H193	1.79	0.64
6:F:63:ASP:N	6:F:67:LEU:O	2.30	0.64
21:6:602:CLA:HMC2	31:6:624:XAT:C11	2.27	0.64
2:B2:315:SER:OG	21:B2:841:CLA:O1A	2.08	0.64
6:F2:63:ASP:N	6:F2:67:LEU:O	2.30	0.64
2:B:315:SER:OG	21:B:841:CLA:O1A	2.08	0.64
21:Z2:603:CLA:HED2	21:Z2:603:CLA:H43	1.80	0.64
13:3:148:PHE:CE2	13:3:152:ILE:HD11	2.32	0.64
30:82:606:CHL:OMC	33:H:144:HOH:O	2.15	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:Z:616:CLA:H72	21:Z:616:CLA:H41	1.79	0.63
21:Z:603:CLA:HED2	21:Z:603:CLA:H43	1.80	0.63
2:B:217:LEU:CD1	19:9:210:LEU:HD23	2.29	0.63
21:A:811:CLA:H11	21:A:813:CLA:H42	1.80	0.63
19:9:208:GLU:N	19:9:208:GLU:OE1	2.31	0.63
2:B2:217:LEU:CD1	19:92:210:LEU:HD23	2.29	0.63
21:Z2:616:CLA:H41	21:Z2:616:CLA:C7	2.29	0.63
21:Z2:616:CLA:H41	21:Z2:616:CLA:H72	1.79	0.63
19:92:208:GLU:N	19:92:208:GLU:OE1	2.31	0.63
12:Z:50:PRO:O	12:Z:56:ASN:ND2	2.32	0.62
21:Z:616:CLA:H41	21:Z:616:CLA:C7	2.29	0.62
11:K:78:SER:OG	21:K:201:CLA:O1D	2.17	0.62
13:32:193:PRO:CG	30:32:608:CHL:HMD2	2.30	0.62
21:82:604:CLA:O1A	30:82:606:CHL:HMD2	2.00	0.61
13:3:193:PRO:CG	30:3:608:CHL:HMD2	2.30	0.61
21:A2:811:CLA:H11	21:A2:813:CLA:H42	1.81	0.61
21:8:604:CLA:O1A	30:8:606:CHL:HMD2	2.00	0.61
11:K2:78:SER:OG	21:K2:201:CLA:O1D	2.18	0.61
14:7:192:LYS:NZ	23:7:625:LHG:O5	2.34	0.60
21:3:607:CLA:H93	24:3:719:BCR:H392	1.83	0.60
21:32:607:CLA:H93	24:32:719:BCR:H392	1.83	0.60
18:6:146:GLN:OE1	18:6:146:GLN:N	2.33	0.60
18:62:146:GLN:OE1	18:62:146:GLN:N	2.33	0.60
12:Z:40:LEU:HD13	30:Z:601:CHL:HMA3	1.83	0.59
18:62:41:HIS:NE2	18:62:53:ASP:OD2	2.32	0.59
1:A2:396:TRP:HB3	21:A2:829:CLA:HMC3	1.84	0.59
14:72:192:LYS:NZ	23:72:625:LHG:O5	2.34	0.59
12:Z2:50:PRO:O	12:Z2:56:ASN:ND2	2.31	0.59
13:3:257:ASN:O	13:3:261:ASN:ND2	2.36	0.59
21:5:602:CLA:H41	21:5:603:CLA:O1A	2.02	0.59
13:32:167:ARG:NH1	27:32:722:LMG:O1	2.36	0.59
21:52:602:CLA:H41	21:52:603:CLA:O1A	2.02	0.59
21:A:810:CLA:HAB	21:B:833:CLA:HMD2	1.85	0.59
12:Z2:40:LEU:HD13	30:Z2:601:CHL:HMA3	1.83	0.59
13:3:167:ARG:NH1	27:3:722:LMG:O1	2.36	0.58
2:B2:708:LEU:HD23	29:B2:850:DGD:HA22	1.86	0.58
30:42:608:CHL:O1A	21:42:610:CLA:HMD2	2.03	0.58
16:4:54:ARG:NH1	16:4:71:LEU:O	2.36	0.58
2:B2:339:LEU:HD21	21:B2:829:CLA:HAB	1.86	0.58
13:32:257:ASN:O	13:32:261:ASN:ND2	2.36	0.58
21:B2:816:CLA:H142	21:B2:816:CLA:H101	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:42:54:ARG:NH1	16:42:71:LEU:O	2.36	0.58
21:12:603:CLA:HED2	21:12:603:CLA:H43	1.85	0.58
2:B:339:LEU:HD21	21:B:829:CLA:HAB	1.86	0.58
1:A:396:TRP:HB3	21:A:829:CLA:HMC3	1.85	0.57
27:9:620:LMG:HO2	27:9:620:LMG:C10	2.16	0.57
1:A:161:THR:HG21	21:A:817:CLA:HBA1	1.85	0.57
30:4:608:CHL:O1A	21:4:610:CLA:HMD2	2.03	0.57
18:6:41:HIS:NE2	18:6:53:ASP:OD2	2.32	0.57
21:A2:810:CLA:HAB	21:B2:833:CLA:HMD2	1.85	0.57
21:B:816:CLA:H101	21:B:816:CLA:H142	1.86	0.57
21:1:603:CLA:HED2	21:1:603:CLA:H43	1.84	0.57
21:7:620:CLA:O1A	18:6:252:LEU:N	2.38	0.57
21:A2:840:CLA:O1A	21:A2:840:CLA:H42	2.04	0.57
12:12:159:ASP:OD1	28:12:617:LUT:O23	2.23	0.57
14:72:156:GLU:N	14:72:156:GLU:OE1	2.38	0.57
21:42:602:CLA:HMC2	31:42:620:XAT:C11	2.35	0.57
12:1:220:THR:O	12:1:220:THR:HG22	2.05	0.57
21:4:602:CLA:HMC2	31:4:620:XAT:C11	2.35	0.57
21:5:621:CLA:HED2	21:5:621:CLA:O1A	2.05	0.57
21:A:840:CLA:H42	21:A:840:CLA:O1A	2.05	0.56
1:A2:161:THR:HG21	21:A2:817:CLA:HBA1	1.85	0.56
21:B2:838:CLA:HMB1	21:B2:838:CLA:HBB1	1.87	0.56
21:Z2:603:CLA:H43	21:Z2:603:CLA:CED	2.36	0.56
21:72:620:CLA:O1A	18:62:252:LEU:N	2.38	0.56
21:A:838:CLA:HBB1	21:A:838:CLA:HMB1	1.88	0.56
21:A2:829:CLA:HMB1	21:A2:829:CLA:HBB1	1.87	0.56
12:12:220:THR:HG22	12:12:220:THR:O	2.05	0.56
21:12:613:CLA:H143	21:12:613:CLA:H102	1.87	0.56
21:52:621:CLA:HED2	21:52:621:CLA:O1A	2.05	0.56
27:92:620:LMG:HO2	27:92:620:LMG:C10	2.19	0.56
24:A:851:BCR:H23C	24:A:851:BCR:H403	1.88	0.56
21:3:602:CLA:HMC2	28:3:622:LUT:C11	2.36	0.56
12:1:53:LEU:HD23	21:1:602:CLA:HED2	1.87	0.56
21:A2:822:CLA:HMB2	21:A2:826:CLA:HMA3	1.88	0.56
14:7:156:GLU:N	14:7:156:GLU:OE1	2.38	0.56
21:B:823:CLA:HAB	21:B:830:CLA:HMD2	1.88	0.56
24:A2:851:BCR:H403	24:A2:851:BCR:H23C	1.88	0.56
21:1:613:CLA:H102	21:1:613:CLA:H143	1.86	0.55
14:7:101:GLU:N	14:7:101:GLU:OE1	2.39	0.55
21:32:602:CLA:HMC2	28:32:622:LUT:C11	2.36	0.55
21:A:829:CLA:HBB1	21:A:829:CLA:HMB1	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:822:CLA:HMB2	21:A:826:CLA:HMA3	1.88	0.55
13:32:99:MET:HE3	21:32:610:CLA:HMC3	1.87	0.55
2:B:393:ILE:HD13	21:B:829:CLA:HED1	1.89	0.55
21:Z:603:CLA:H43	21:Z:603:CLA:CED	2.35	0.55
21:A2:838:CLA:HMB1	21:A2:838:CLA:HBB1	1.88	0.55
21:B2:836:CLA:HBB1	21:B2:836:CLA:HMB1	1.88	0.55
14:72:101:GLU:OE1	14:72:101:GLU:N	2.39	0.55
16:4:149:LEU:HD13	30:4:606:CHL:HMD3	1.89	0.55
26:9:624:LMU:O5'	8:I2:74:TRP:CZ2	2.60	0.55
12:12:53:LEU:HD23	21:12:602:CLA:HED2	1.87	0.55
16:4:256:VAL:N	21:4:613:CLA:O1A	2.39	0.55
21:A2:833:CLA:OBD	10:L2:57:THR:HG21	2.07	0.55
6:F2:204:LEU:HA	21:82:603:CLA:H42	1.89	0.55
4:D:125:THR:HG23	4:D:136:PRO:HG2	1.89	0.55
13:3:95:ALA:HB1	13:3:221:GLY:HA3	1.89	0.55
21:8:602:CLA:HMC2	31:8:618:XAT:C11	2.36	0.55
21:12:608:CLA:HMA1	28:12:619:LUT:H203	1.89	0.55
21:82:602:CLA:HMC2	31:82:618:XAT:C11	2.36	0.55
18:62:76:ARG:NH1	30:62:608:CHL:OBD	2.37	0.55
21:B:838:CLA:HBB1	21:B:838:CLA:HMB1	1.87	0.54
28:7:624:LUT:H383	15:8:229:TRP:CE2	2.42	0.54
2:B2:393:ILE:HD13	21:B2:829:CLA:HED1	1.89	0.54
16:42:149:LEU:HD13	30:42:606:CHL:HMD3	1.89	0.54
8:I:74:TRP:CZ2	26:92:624:LMU:O5'	2.60	0.54
21:1:603:CLA:H43	21:1:603:CLA:CED	2.38	0.54
28:72:624:LUT:H383	15:82:229:TRP:CE2	2.42	0.54
16:42:256:VAL:N	21:42:613:CLA:O1A	2.39	0.54
21:5:602:CLA:HMC2	31:5:624:XAT:C11	2.38	0.54
21:B2:823:CLA:HAB	21:B2:830:CLA:HMD2	1.88	0.54
12:1:119:PHE:CE1	21:1:604:CLA:HMD2	2.43	0.54
21:B:836:CLA:HBB1	21:B:836:CLA:HMB1	1.89	0.54
12:1:159:ASP:OD1	28:1:617:LUT:O23	2.23	0.54
13:3:99:MET:HE3	21:3:610:CLA:HMC3	1.89	0.54
21:3:615:CLA:H193	17:5:227:ILE:HG21	1.89	0.54
24:L2:205:BCR:C23	24:L2:205:BCR:H403	2.38	0.54
6:F:204:LEU:HA	21:8:603:CLA:H42	1.89	0.54
21:A:833:CLA:OBD	10:L:57:THR:HG21	2.07	0.54
21:1:608:CLA:HMA1	28:1:619:LUT:H203	1.89	0.54
2:B2:653:PHE:CZ	2:B2:657:ILE:HD11	2.43	0.54
13:32:95:ALA:HB1	13:32:221:GLY:HA3	1.89	0.54
18:6:184:MET:HE3	21:6:602:CLA:HMC3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:12:119:PHE:CE1	21:12:604:CLA:HMD2	2.43	0.54
24:L:205:BCR:C23	24:L:205:BCR:H403	2.38	0.53
6:F:208:GLN:OE1	6:F:212:ARG:NH2	2.42	0.53
4:D2:125:THR:HG23	4:D2:136:PRO:HG2	1.89	0.53
6:F2:165:TYR:HD1	28:F2:305:LUT:HO3	1.56	0.53
21:32:606:CLA:HMC2	28:32:622:LUT:H363	1.90	0.53
2:B:464:ILE:HD11	21:B:836:CLA:H12	1.90	0.53
21:32:615:CLA:H193	17:52:227:ILE:HG21	1.89	0.53
2:B2:464:ILE:HD11	21:B2:836:CLA:H12	1.90	0.53
26:A:858:LMU:H2O1	26:A:858:LMU:H3O2	1.57	0.53
7:G2:50:ARG:NH2	7:G2:91:ASP:OD1	2.42	0.53
21:Z2:608:CLA:H12	28:Z2:617:LUT:H383	1.90	0.53
26:A2:858:LMU:O3'	26:A2:858:LMU:O2B	2.26	0.53
21:12:603:CLA:H43	21:12:603:CLA:CED	2.38	0.53
21:52:602:CLA:HMC2	31:52:624:XAT:C11	2.38	0.53
21:B2:834:CLA:H141	27:B2:854:LMG:C34	2.38	0.53
26:B:853:LMU:O6'	26:B:853:LMU:O2B	1.99	0.53
21:Z:608:CLA:H12	28:Z:617:LUT:H383	1.90	0.53
6:F2:208:GLN:OE1	6:F2:212:ARG:NH2	2.42	0.53
2:B:217:LEU:HD13	19:9:210:LEU:HD23	1.91	0.52
21:F2:304:CLA:O1A	21:F2:304:CLA:C2	2.58	0.52
2:B:653:PHE:CZ	2:B:657:ILE:HD11	2.44	0.52
2:B:722:TYR:HB2	21:B:802:CLA:HED2	1.92	0.52
21:3:606:CLA:HMC2	28:3:622:LUT:H363	1.90	0.52
21:B:834:CLA:H141	27:B:854:LMG:C34	2.39	0.52
7:G:50:ARG:NH2	7:G:91:ASP:OD1	2.42	0.52
2:B2:393:ILE:HG21	21:B2:829:CLA:HED1	1.91	0.52
2:B2:722:TYR:HB2	21:B2:802:CLA:HED2	1.91	0.52
6:F:64:ILE:HD11	6:F:143:TYR:CD2	2.45	0.52
21:F:304:CLA:O1A	21:F:304:CLA:C2	2.58	0.52
16:4:149:LEU:CD1	30:4:606:CHL:HMD3	2.40	0.52
21:A2:843:CLA:H93	21:A2:843:CLA:H121	1.91	0.52
18:62:33:LEU:HD13	30:62:601:CHL:HMA3	1.92	0.52
21:92:610:CLA:HMB1	21:92:610:CLA:HBB1	1.92	0.52
13:3:210:MET:CE	21:3:610:CLA:HED3	2.40	0.52
13:32:210:MET:CE	21:32:610:CLA:HED3	2.40	0.52
16:42:149:LEU:CD1	30:42:606:CHL:HMD3	2.40	0.52
24:A:848:BCR:H362	24:A:849:BCR:H21C	1.92	0.52
30:6:608:CHL:H11	28:6:621:LUT:H383	1.92	0.52
24:B:801:BCR:H331	24:B:801:BCR:C8	2.40	0.52
6:F2:64:ILE:HD11	6:F2:143:TYR:CD2	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:12:610:CLA:HMC2	28:12:617:LUT:C31	2.40	0.52
23:32:623:LHG:HC62	21:52:616:CLA:HMD3	1.92	0.52
21:3:603:CLA:HMD3	24:3:719:BCR:H403	1.92	0.51
21:32:603:CLA:HMD3	24:32:719:BCR:H403	1.92	0.51
23:3:623:LHG:HC62	21:5:616:CLA:HMD3	1.92	0.51
24:A2:848:BCR:H362	24:A2:849:BCR:H21C	1.92	0.51
8:I2:72:PRO:HG3	8:I2:74:TRP:CZ2	2.46	0.51
21:42:610:CLA:HBB1	21:42:610:CLA:HMB1	1.92	0.51
21:A:802:CLA:H141	21:A:804:CLA:H191	1.92	0.51
21:1:610:CLA:HMC2	28:1:617:LUT:C31	2.41	0.51
3:C2:14:CYS:O	3:C2:15:THR:OG1	2.26	0.51
24:B:843:BCR:H331	24:B:843:BCR:C8	2.40	0.51
21:A2:854:CLA:HMD3	21:B2:802:CLA:O1A	2.10	0.51
2:B2:217:LEU:HD13	19:92:210:LEU:HD23	1.91	0.51
21:42:613:CLA:H43	21:42:614:CLA:OBD	2.11	0.51
30:62:608:CHL:H11	28:62:621:LUT:H383	1.92	0.51
21:A:843:CLA:H93	21:A:843:CLA:H121	1.91	0.51
21:A:854:CLA:HMD3	21:B:802:CLA:O1A	2.10	0.51
24:J:102:BCR:H331	24:J:102:BCR:C8	2.40	0.51
12:Z2:71:LEU:O	12:Z2:75:THR:HG23	2.11	0.51
21:62:613:CLA:CHB	21:62:614:CLA:HMD3	2.40	0.51
8:I:72:PRO:HG3	8:I:74:TRP:CZ2	2.46	0.51
21:32:615:CLA:H42	17:52:231:ILE:CG1	2.41	0.51
30:8:601:CHL:CBB	21:8:602:CLA:HMD2	2.41	0.51
30:4:606:CHL:C4A	33:H:64:HOH:O	2.28	0.51
18:6:76:ARG:NH1	30:6:608:CHL:OBD	2.37	0.51
18:62:184:MET:HE3	21:62:602:CLA:HMC3	1.93	0.51
2:B:708:LEU:HD23	29:B:850:DGD:HA22	1.93	0.51
21:6:613:CLA:CHB	21:6:614:CLA:HMD3	2.40	0.51
21:9:610:CLA:HBB1	21:9:610:CLA:HMB1	1.92	0.51
21:B:841:CLA:HMC3	21:1:603:CLA:H12	1.93	0.51
21:4:610:CLA:HBB1	21:4:610:CLA:HMB1	1.92	0.51
21:4:613:CLA:H43	21:4:614:CLA:OBD	2.11	0.51
21:92:602:CLA:HMC2	28:92:617:LUT:C31	2.41	0.51
2:B:393:ILE:HG21	21:B:829:CLA:HED1	1.92	0.50
21:3:615:CLA:H42	17:5:231:ILE:CG1	2.41	0.50
24:B2:843:BCR:H331	24:B2:843:BCR:C8	2.40	0.50
24:J2:102:BCR:H331	24:J2:102:BCR:C8	2.40	0.50
12:Z:71:LEU:O	12:Z:75:THR:HG23	2.11	0.50
21:9:602:CLA:HMC2	28:9:617:LUT:C31	2.42	0.50
21:A2:802:CLA:H141	21:A2:804:CLA:H191	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:82:601:CHL:CBB	21:82:602:CLA:HMD2	2.41	0.50
24:A2:852:BCR:H331	24:A2:852:BCR:C8	2.42	0.50
12:Z:86:MET:HE3	21:Z:610:CLA:HMC3	1.94	0.50
24:B2:801:BCR:H331	24:B2:801:BCR:C8	2.40	0.50
12:Z2:86:MET:HE3	21:Z2:610:CLA:HMC3	1.93	0.50
21:A:818:CLA:H91	24:K:207:BCR:HC21	1.94	0.50
21:B2:841:CLA:HMC3	21:12:603:CLA:H12	1.93	0.50
18:62:157:PRO:HD3	30:62:608:CHL:HMD2	1.93	0.50
1:A:67:GLU:OE2	1:A:71:ARG:NH2	2.45	0.50
24:A:852:BCR:H331	24:A:852:BCR:C8	2.41	0.50
1:A:444:VAL:HG21	21:A:840:CLA:HMC3	1.94	0.49
18:6:33:LEU:HD13	30:6:601:CHL:HMA3	1.92	0.49
18:6:157:PRO:HD3	30:6:608:CHL:HMD2	1.94	0.49
20:A2:801:CL0:H13	21:A2:854:CLA:OBD	2.12	0.49
21:32:611:CLA:H41	21:32:611:CLA:H71	1.94	0.49
1:A2:444:VAL:HG21	21:A2:840:CLA:HMC3	1.94	0.49
21:32:602:CLA:HBA1	28:32:622:LUT:H182	1.94	0.49
15:82:31:LEU:HD13	30:82:601:CHL:HMA3	1.93	0.49
1:A2:67:GLU:OE2	1:A2:71:ARG:NH2	2.45	0.49
15:8:31:LEU:HD13	30:8:601:CHL:HMA3	1.94	0.49
21:32:610:CLA:HMC2	28:32:621:LUT:C31	2.43	0.49
1:A:413:MET:HE3	1:A:431:ILE:HD11	1.95	0.49
21:A2:818:CLA:H91	24:K2:207:BCR:HC21	1.94	0.49
24:B2:844:BCR:H382	24:B2:844:BCR:H23C	1.94	0.49
17:52:194:MET:HE3	21:52:602:CLA:HMC3	1.94	0.49
20:A:801:CL0:H13	21:A:854:CLA:OBD	2.13	0.49
2:B:520:VAL:HG11	2:B:594:TYR:CG	2.47	0.49
2:B2:340:ALA:HB2	24:B2:847:BCR:H372	1.95	0.49
19:9:40:HIS:ND1	19:9:57:GLY:O	2.46	0.49
24:L2:205:BCR:C8	24:L2:205:BCR:H331	2.43	0.49
12:Z2:130:LEU:CD1	30:Z2:606:CHL:HMD3	2.43	0.49
21:B2:834:CLA:H2	21:B2:835:CLA:HMB2	1.95	0.49
19:92:40:HIS:ND1	19:92:57:GLY:O	2.46	0.49
21:3:610:CLA:HMC2	28:3:621:LUT:C31	2.43	0.49
2:B2:77:GLN:OE1	2:B2:77:GLN:N	2.46	0.49
13:32:39:ASP:HB2	13:32:47:VAL:HG23	1.95	0.49
21:82:604:CLA:H43	24:82:619:BCR:H272	1.95	0.49
21:B:834:CLA:H2	21:B:835:CLA:HMB2	1.95	0.49
13:3:39:ASP:HB2	13:3:47:VAL:HG23	1.95	0.49
14:7:135:ARG:NH1	21:7:609:CLA:O1D	2.44	0.48
2:B2:520:VAL:HG11	2:B2:594:TYR:CG	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:82:183:ASP:OD1	15:82:183:ASP:N	2.46	0.48
17:52:85:VAL:HG11	28:52:620:LUT:H12	1.95	0.48
21:3:602:CLA:HBA1	28:3:622:LUT:H182	1.94	0.48
21:A2:803:CLA:OBD	21:B2:802:CLA:HMB3	2.13	0.48
21:A:803:CLA:OBD	21:B:802:CLA:HMB3	2.12	0.48
2:B:340:ALA:HB2	24:B:847:BCR:H372	1.95	0.48
21:3:611:CLA:H41	21:3:611:CLA:H71	1.94	0.48
12:Z:130:LEU:CD1	30:Z:606:CHL:HMD3	2.43	0.48
30:4:606:CHL:C1A	33:H:64:HOH:O	2.36	0.48
19:9:103:GLU:N	19:9:103:GLU:OE1	2.46	0.48
1:A2:399:GLY:HA3	1:A2:603:LEU:HD11	1.95	0.48
21:A2:854:CLA:HBB1	21:A2:854:CLA:HMB1	1.95	0.48
21:A:854:CLA:HBB1	21:A:854:CLA:HMB1	1.95	0.48
1:A2:353:LEU:HB2	21:A2:806:CLA:HMD3	1.96	0.48
2:B:309:HIS:HA	21:B:841:CLA:HMD1	1.95	0.48
24:B:844:BCR:H382	24:B:844:BCR:H23C	1.95	0.48
2:B2:309:HIS:HA	21:B2:841:CLA:HMD1	1.95	0.48
19:9:52:ASP:OD1	28:9:617:LUT:O23	2.31	0.48
1:A:547:VAL:HG11	21:A:840:CLA:HMB3	1.95	0.48
28:F:305:LUT:C28	28:F:305:LUT:H381	2.40	0.48
1:A2:547:VAL:HG11	21:A2:840:CLA:HMB3	1.96	0.48
21:A2:802:CLA:HMC2	21:A2:854:CLA:CAC	2.44	0.48
21:B:839:CLA:H93	24:I:172:BCR:H333	1.96	0.48
17:5:85:VAL:HG11	28:5:620:LUT:H12	1.95	0.48
10:L2:58:PRO:O	10:L2:62:ALA:HB2	2.14	0.48
11:K2:57:VAL:HG23	11:K2:88:ASP:OD1	2.14	0.48
18:62:79:MET:HE3	21:62:610:CLA:HMC3	1.96	0.48
21:62:609:CLA:HMB2	21:62:617:CLA:C2C	2.44	0.48
24:L:205:BCR:H331	24:L:205:BCR:C8	2.43	0.47
21:8:604:CLA:H43	24:8:619:BCR:H272	1.95	0.47
21:B2:829:CLA:HMB1	21:B2:829:CLA:HBB1	1.96	0.47
19:92:103:GLU:N	19:92:103:GLU:OE1	2.47	0.47
2:B:466:ALA:O	2:B:480:SER:OG	2.28	0.47
3:C:14:CYS:O	3:C:15:THR:OG1	2.26	0.47
18:6:79:MET:HE3	21:6:610:CLA:HMC3	1.94	0.47
2:B2:489:ASN:ND2	21:B2:835:CLA:HMD1	2.29	0.47
15:82:200:MET:HE3	21:82:602:CLA:HMC3	1.97	0.47
10:L:128:LEU:HD22	24:L:205:BCR:H401	1.96	0.47
17:5:194:MET:HE3	21:5:602:CLA:HMC3	1.96	0.47
21:6:609:CLA:HMB2	21:6:617:CLA:C2C	2.44	0.47
2:B:192:THR:HG21	2:B:279:LEU:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:489:ASN:ND2	21:B:835:CLA:HMD1	2.29	0.47
21:B2:839:CLA:H93	24:I2:172:BCR:H333	1.96	0.47
16:4:199:ASP:OD1	28:4:619:LUT:O23	2.29	0.47
21:6:610:CLA:HMC2	28:6:621:LUT:C31	2.45	0.47
21:Z2:602:CLA:HMC2	31:Z2:618:XAT:C11	2.43	0.47
21:Z:602:CLA:HMC2	31:Z:618:XAT:C11	2.43	0.47
1:A:223:PRO:HB2	1:A:243:LEU:HD13	1.96	0.47
1:A:353:LEU:HB2	21:A:806:CLA:HMD3	1.96	0.47
1:A:399:GLY:HA3	1:A:603:LEU:HD11	1.95	0.47
21:A:817:CLA:HMD2	13:3:133:PRO:HG3	1.97	0.47
13:3:201:PHE:O	13:3:203:LEU:N	2.47	0.47
15:8:183:ASP:N	15:8:183:ASP:OD1	2.46	0.47
21:8:611:CLA:HMB2	26:8:625:LMU:H41	1.97	0.47
1:A2:433:HIS:HB3	10:L2:55:LEU:HD22	1.96	0.47
10:L2:128:LEU:HD22	24:L2:205:BCR:H401	1.96	0.47
21:62:610:CLA:HMC2	28:62:621:LUT:C31	2.45	0.47
10:L:58:PRO:O	10:L:62:ALA:HB2	2.14	0.47
11:K:57:VAL:HG23	11:K:88:ASP:OD1	2.14	0.47
21:4:612:CLA:HMC2	28:4:619:LUT:C11	2.45	0.47
1:A:433:HIS:HB3	10:L:55:LEU:HD22	1.96	0.47
21:A:802:CLA:HMC2	21:A:854:CLA:CAC	2.45	0.47
1:A2:413:MET:CE	1:A2:431:ILE:HD11	2.45	0.47
21:B2:841:CLA:HBC1	26:B2:853:LMU:H2'	1.96	0.47
21:8:604:CLA:H142	21:Z:616:CLA:HMB2	1.96	0.47
6:F:165:TYR:HD1	28:F:305:LUT:HO3	1.63	0.46
21:A:820:CLA:HMB1	21:A:820:CLA:HBB1	1.97	0.46
1:A2:223:PRO:HB2	1:A2:243:LEU:HD13	1.96	0.46
2:B2:192:THR:HG21	2:B2:279:LEU:HB2	1.96	0.46
24:B2:845:BCR:H342	19:92:177:LEU:HD21	1.98	0.46
8:I2:80:VAL:HB	8:I2:81:PRO:HD3	1.97	0.46
21:B:821:CLA:H191	12:1:131:LEU:HD22	1.98	0.46
4:D2:176:GLY:N	5:E2:49:GLU:OE1	2.49	0.46
13:32:201:PHE:O	13:32:203:LEU:N	2.47	0.46
21:72:610:CLA:HMC2	28:72:621:LUT:C31	2.45	0.46
16:4:82:ASP:OD1	16:4:85:TYR:N	2.49	0.46
21:82:604:CLA:H142	21:Z2:616:CLA:HMB2	1.96	0.46
21:B:841:CLA:HBC1	26:B:853:LMU:H2'	1.97	0.46
12:1:88:GLY:HA2	31:1:618:XAT:H181	1.98	0.46
12:1:202:PRO:O	28:1:617:LUT:O3	2.32	0.46
21:7:610:CLA:HMC2	28:7:621:LUT:C31	2.45	0.46
28:F2:305:LUT:C28	28:F2:305:LUT:H381	2.40	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:80:VAL:HB	8:I:81:PRO:HD3	1.97	0.46
21:A2:820:CLA:HBB1	21:A2:820:CLA:HMB1	1.97	0.46
12:12:88:GLY:HA2	31:12:618:XAT:H181	1.98	0.46
21:82:611:CLA:HMB2	26:82:625:LMU:H41	1.97	0.46
30:42:607:CHL:O1A	26:42:625:LMU:O6'	2.32	0.46
21:42:612:CLA:HMC2	28:42:619:LUT:C11	2.45	0.46
17:52:188:LYS:NZ	23:52:623:LHG:O5	2.49	0.46
24:B:845:BCR:H342	19:9:177:LEU:HD21	1.98	0.46
21:32:615:CLA:H42	17:52:231:ILE:HG13	1.98	0.46
16:42:199:ASP:OD1	28:42:619:LUT:O23	2.29	0.46
30:62:607:CHL:H42	32:62:625:NEX:H403	1.97	0.46
21:B:829:CLA:HBB1	21:B:829:CLA:HMB1	1.96	0.46
4:D:176:GLY:N	5:E:49:GLU:OE1	2.49	0.46
30:6:607:CHL:H42	32:6:625:NEX:H403	1.97	0.46
21:A:833:CLA:H42	10:L:65:VAL:HG13	1.97	0.46
1:A2:677:PHE:CG	24:A2:852:BCR:H363	2.51	0.46
21:A2:802:CLA:HBB1	21:A2:802:CLA:HMB1	1.98	0.46
21:A2:817:CLA:HMD2	13:32:133:PRO:HG3	1.96	0.46
10:L2:74:ALA:HB2	21:L2:203:CLA:HMD1	1.98	0.46
1:A:677:PHE:CG	24:A:852:BCR:H363	2.51	0.46
10:L:57:THR:HG22	10:L:58:PRO:HD2	1.98	0.46
21:A2:826:CLA:C14	21:A2:826:CLA:HMD2	2.46	0.46
21:B2:832:CLA:CAB	21:B2:833:CLA:HMB2	2.46	0.46
2:B:269:LEU:HD13	21:B:817:CLA:HMA2	1.98	0.45
2:B:365:ASP:OD2	2:B:368:THR:OG1	2.29	0.45
17:5:188:LYS:NZ	23:5:623:LHG:O5	2.49	0.45
21:Z2:603:CLA:HMD2	21:Z2:609:CLA:C1D	2.46	0.45
18:62:122:HIS:O	18:62:126:VAL:HG23	2.16	0.45
15:8:200:MET:HE3	21:8:602:CLA:HMC3	1.97	0.45
17:5:149:ASP:OD1	17:5:151:ILE:N	2.49	0.45
21:B2:821:CLA:H191	12:12:131:LEU:HD22	1.98	0.45
16:42:82:ASP:OD1	16:42:85:TYR:N	2.49	0.45
12:1:154:PRO:CG	21:1:608:CLA:HMD2	2.47	0.45
12:12:119:PHE:CZ	21:12:604:CLA:HMD2	2.51	0.45
21:A:809:CLA:H91	21:A:812:CLA:H201	1.98	0.45
2:B:77:GLN:OE1	2:B:77:GLN:N	2.46	0.45
24:9:623:BCR:H20C	24:9:623:BCR:H361	1.83	0.45
21:42:603:CLA:HMD2	21:42:609:CLA:C1D	2.47	0.45
1:A:411:ILE:HD13	21:A:831:CLA:CED	2.47	0.45
2:B:236:GLN:O	2:B:237:SER:OG	2.33	0.45
21:1:603:CLA:H61	21:1:603:CLA:H41	1.87	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:Z:601:CHL:CBB	21:Z:602:CLA:HMD2	2.46	0.45
21:Z:603:CLA:HMD2	21:Z:609:CLA:C1D	2.46	0.45
2:B2:269:LEU:HD13	21:B2:817:CLA:HMA2	1.98	0.45
10:L2:57:THR:HG22	10:L2:58:PRO:HD2	1.98	0.45
30:Z2:601:CHL:CBB	21:Z2:602:CLA:HMD2	2.47	0.45
1:A:413:MET:CE	1:A:431:ILE:HD11	2.46	0.45
21:A:826:CLA:C14	21:A:826:CLA:HMD2	2.46	0.45
2:B:451:GLU:OE2	6:F:114:ARG:NH1	2.49	0.45
24:B:845:BCR:H331	24:B:845:BCR:C8	2.47	0.45
12:1:119:PHE:CZ	21:1:604:CLA:HMD2	2.51	0.45
1:A2:413:MET:HE1	1:A2:431:ILE:HD11	1.98	0.45
21:A:802:CLA:HBB1	21:A:802:CLA:HMB1	1.98	0.45
21:4:611:CLA:C1D	21:4:612:CLA:HMD2	2.47	0.45
12:12:202:PRO:O	28:12:617:LUT:O3	2.33	0.45
21:B:832:CLA:CAB	21:B:833:CLA:HMB2	2.46	0.45
24:K2:202:BCR:C23	24:K2:202:BCR:H392	2.47	0.45
21:42:611:CLA:C1D	21:42:612:CLA:HMD2	2.46	0.45
17:52:149:ASP:OD1	17:52:151:ILE:N	2.49	0.45
24:K:202:BCR:H392	24:K:202:BCR:C23	2.47	0.45
12:Z:35:LYS:N	12:Z:51:ASP:OD1	2.50	0.45
18:6:33:LEU:HD13	30:6:601:CHL:CMA	2.47	0.45
21:32:612:CLA:HMC2	28:32:621:LUT:C11	2.47	0.45
17:52:95:LYS:HB3	17:52:98:VAL:HG13	1.99	0.45
24:62:623:BCR:H331	24:62:623:BCR:C8	2.46	0.45
19:92:172:PHE:CE1	28:92:616:LUT:H182	2.52	0.45
21:3:615:CLA:H42	17:5:231:ILE:HG13	1.98	0.44
18:6:122:HIS:O	18:6:126:VAL:HG23	2.16	0.44
19:9:172:PHE:CE1	28:9:616:LUT:H182	2.52	0.44
1:A2:411:ILE:HD13	21:A2:831:CLA:CED	2.47	0.44
2:B2:264:PRO:O	2:B2:267:GLN:NE2	2.50	0.44
21:72:602:CLA:HMC2	31:72:622:XAT:C11	2.47	0.44
21:A:826:CLA:HBB1	21:A:826:CLA:HMB1	2.00	0.44
26:A:862:LMU:O2'	26:A:863:LMU:O6B	2.03	0.44
2:B:414:ASP:O	6:F:227:ARG:NH1	2.50	0.44
1:A2:245:LEU:O	26:A2:857:LMU:O2B	2.34	0.44
1:A2:650:LEU:O	1:A2:654:SER:OG	2.28	0.44
24:A2:850:BCR:H24C	24:A2:850:BCR:H371	1.86	0.44
12:12:154:PRO:CG	21:12:608:CLA:HMD2	2.46	0.44
18:62:33:LEU:HD12	30:62:601:CHL:HED2	1.99	0.44
1:A:119:TRP:CD2	21:A:810:CLA:HED3	2.52	0.44
21:B:819:CLA:HMB2	21:B:824:CLA:HMA3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:3:612:CLA:HMC2	28:3:621:LUT:C11	2.47	0.44
21:A2:833:CLA:H42	10:L2:65:VAL:HG13	1.97	0.44
21:12:609:CLA:HBB1	21:12:609:CLA:HMB1	2.00	0.44
21:7:602:CLA:HMC2	31:7:622:XAT:C11	2.47	0.44
24:6:623:BCR:H331	24:6:623:BCR:C8	2.46	0.44
21:B2:811:CLA:C9	21:B2:813:CLA:HMB3	2.48	0.44
12:Z2:35:LYS:N	12:Z2:51:ASP:OD1	2.50	0.44
14:7:81:LEU:HD22	21:7:610:CLA:H201	1.99	0.44
12:Z:119:PHE:CZ	21:Z:604:CLA:HMD2	2.52	0.44
21:A2:809:CLA:H91	21:A2:812:CLA:H201	1.98	0.44
13:32:101:GLY:HA2	28:32:622:LUT:H381	2.00	0.44
14:72:34:PHE:CE1	30:72:601:CHL:HED2	2.53	0.44
21:B:811:CLA:C9	21:B:813:CLA:HMB3	2.48	0.44
21:Z:613:CLA:CGA	21:Z:613:CLA:C1A	2.96	0.44
21:4:603:CLA:HMD2	21:4:609:CLA:C1D	2.47	0.44
2:B2:414:ASP:O	6:F2:227:ARG:NH1	2.51	0.44
2:B2:451:GLU:OE2	6:F2:114:ARG:NH1	2.50	0.44
24:32:719:BCR:C8	24:32:719:BCR:H331	2.48	0.44
27:92:620:LMG:O9	27:92:620:LMG:O2	2.33	0.44
24:B:844:BCR:C8	24:B:844:BCR:H331	2.47	0.44
14:7:34:PHE:HE1	30:7:601:CHL:HED2	1.83	0.44
24:B2:845:BCR:H331	24:B2:845:BCR:C8	2.47	0.44
21:92:610:CLA:HMC2	28:92:616:LUT:C31	2.48	0.44
10:L:74:ALA:HB2	21:L:203:CLA:HMD1	1.98	0.44
21:1:609:CLA:HMB1	21:1:609:CLA:HBB1	2.00	0.44
1:A2:470:ASP:HB3	21:A2:835:CLA:HED3	1.99	0.44
21:A2:826:CLA:HBB1	21:A2:826:CLA:HMB1	2.00	0.44
21:Z2:603:CLA:H61	21:Z2:603:CLA:H41	1.83	0.44
21:Z2:611:CLA:C1B	23:Z2:620:LHG:O4	2.59	0.44
16:42:54:ARG:HD3	16:42:67:LEU:HD12	1.99	0.44
21:52:617:CLA:H61	21:52:617:CLA:H41	1.90	0.44
17:5:95:LYS:HB3	17:5:98:VAL:HG13	1.99	0.44
14:72:135:ARG:NH1	21:72:609:CLA:O1D	2.44	0.44
12:Z2:119:PHE:CZ	21:Z2:604:CLA:HMD2	2.52	0.44
21:42:613:CLA:H62	21:42:613:CLA:H41	1.93	0.44
16:4:54:ARG:HD3	16:4:67:LEU:HD12	1.99	0.43
18:6:33:LEU:HD12	30:6:601:CHL:HED2	1.99	0.43
1:A2:586:VAL:HG13	2:B2:670:GLY:HA3	1.99	0.43
14:72:34:PHE:HE1	30:72:601:CHL:HED2	1.83	0.43
1:A:282:LEU:HD21	1:A:375:PRO:HD2	1.99	0.43
24:K:202:BCR:H331	24:K:202:BCR:C8	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:7:624:LUT:H383	15:8:229:TRP:CZ2	2.53	0.43
24:K2:202:BCR:H403	24:K2:202:BCR:H23C	1.99	0.43
1:A:418:ASP:OD2	1:A:420:THR:OG1	2.31	0.43
21:B:816:CLA:H142	21:B:816:CLA:C10	2.49	0.43
21:3:603:CLA:HBB1	21:3:603:CLA:HMB1	2.01	0.43
24:B2:844:BCR:C8	24:B2:844:BCR:H331	2.47	0.43
21:12:603:CLA:H61	21:12:603:CLA:H41	1.87	0.43
21:32:603:CLA:HBC1	21:32:609:CLA:CBC	2.48	0.43
21:72:610:CLA:H13	21:62:603:CLA:H142	2.00	0.43
21:42:610:CLA:H62	21:42:610:CLA:H41	1.94	0.43
21:52:621:CLA:HAA2	21:52:621:CLA:CB D	2.49	0.43
21:B:806:CLA:H2	21:B:806:CLA:HED3	2.00	0.43
21:3:603:CLA:HBC1	21:3:609:CLA:CBC	2.48	0.43
15:8:225:LEU:HD21	21:8:614:CLA:HMC3	2.01	0.43
1:A:586:VAL:HG13	2:B:670:GLY:HA3	1.99	0.43
2:B:264:PRO:O	2:B:267:GLN:NE2	2.51	0.43
2:B:632:LEU:HD21	2:B:651:PHE:CD1	2.54	0.43
14:7:34:PHE:CE1	30:7:601:CHL:HED2	2.53	0.43
28:72:624:LUT:H383	15:82:229:TRP:CZ2	2.53	0.43
21:Z2:613:CLA:C1A	21:Z2:613:CLA:CGA	2.96	0.43
24:K:202:BCR:H23C	24:K:202:BCR:H403	1.99	0.43
24:K:207:BCR:H24C	24:K:207:BCR:H371	1.88	0.43
21:5:621:CLA:CB D	21:5:621:CLA:HAA2	2.49	0.43
1:A2:119:TRP:CD2	21:A2:810:CLA:HED3	2.53	0.43
6:F2:193:THR:HG21	27:J2:104:LMG:H142	2.00	0.43
26:A:858:LMU:O3'	26:A:858:LMU:O2B	2.26	0.43
24:L:201:BCR:H24C	24:L:201:BCR:H371	1.91	0.43
11:K:50:ARG:NH1	11:K:80:ASP:OD2	2.51	0.43
21:9:610:CLA:HMC2	28:9:616:LUT:C31	2.48	0.43
1:A2:282:LEU:HD21	1:A2:375:PRO:HD2	1.99	0.43
24:A2:849:BCR:C8	24:A2:849:BCR:H331	2.49	0.43
21:B2:819:CLA:HMB2	21:B2:824:CLA:HMA3	2.00	0.43
18:62:33:LEU:HD13	30:62:601:CHL:CMA	2.47	0.43
2:B:173:GLU:OE1	2:B:173:GLU:N	2.50	0.43
2:B:178:HIS:CG	21:B:813:CLA:HMC2	2.53	0.43
21:B:808:CLA:CGA	21:B:808:CLA:C1A	2.97	0.43
13:3:210:MET:HE2	21:3:610:CLA:HED3	2.01	0.43
21:32:607:CLA:HMC1	21:32:607:CLA:HBC2	2.01	0.43
14:72:81:LEU:HD22	21:72:610:CLA:H201	1.99	0.43
30:1:601:CHL:H62	30:1:601:CHL:H41	1.77	0.43
1:A2:418:ASP:OD2	1:A2:420:THR:OG1	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:B:848:BCR:H24C	24:B:848:BCR:H371	1.91	0.43
24:L:205:BCR:H403	24:L:205:BCR:H23C	2.01	0.43
24:3:719:BCR:C8	24:3:719:BCR:H331	2.47	0.43
28:92:617:LUT:C28	28:92:617:LUT:H381	2.47	0.43
1:A:470:ASP:HB3	21:A:835:CLA:HED3	1.99	0.42
1:A:584:CYS:O	2:B:670:GLY:N	2.51	0.42
24:A:849:BCR:C8	24:A:849:BCR:H331	2.49	0.42
13:3:101:GLY:HA2	28:3:622:LUT:H381	2.00	0.42
21:8:604:CLA:HMB1	21:8:604:CLA:HBB1	2.01	0.42
21:A2:854:CLA:HMB3	21:B2:802:CLA:C19	2.48	0.42
2:B2:178:HIS:CG	21:B2:813:CLA:HMC2	2.53	0.42
2:B2:365:ASP:OD2	2:B2:368:THR:OG1	2.29	0.42
2:B2:530:THR:HG21	2:B2:583:TRP:CE2	2.54	0.42
21:B2:806:CLA:H2	21:B2:806:CLA:HED3	2.00	0.42
21:B2:808:CLA:H142	21:B2:808:CLA:HMB2	2.01	0.42
24:B2:848:BCR:H20C	24:B2:848:BCR:H361	1.91	0.42
3:C2:36:ALA:O	3:C2:37:SER:OG	2.30	0.42
21:32:615:CLA:C19	17:52:227:ILE:HG21	2.49	0.42
21:82:604:CLA:HMB1	21:82:604:CLA:HBB1	2.01	0.42
21:62:613:CLA:C1B	21:62:614:CLA:HMD3	2.49	0.42
19:92:52:ASP:OD1	28:92:617:LUT:O23	2.31	0.42
6:F:193:THR:HG21	27:J:104:LMG:H142	2.00	0.42
21:3:607:CLA:HMC1	21:3:607:CLA:HBC2	2.01	0.42
28:9:617:LUT:C28	28:9:617:LUT:H381	2.48	0.42
27:9:620:LMG:O9	27:9:620:LMG:O2	2.33	0.42
11:K2:50:ARG:NH1	11:K2:80:ASP:OD2	2.51	0.42
24:K2:202:BCR:H331	24:K2:202:BCR:C8	2.48	0.42
1:A:554:VAL:HG11	21:A:822:CLA:H203	2.01	0.42
24:A:850:BCR:C8	24:A:850:BCR:H331	2.49	0.42
21:3:615:CLA:C19	17:5:227:ILE:HG21	2.49	0.42
21:7:610:CLA:H13	21:6:603:CLA:H142	2.00	0.42
21:A2:829:CLA:H72	21:A2:829:CLA:C12	2.50	0.42
21:B2:808:CLA:CGA	21:B2:808:CLA:C1A	2.97	0.42
24:G2:205:BCR:H20C	24:G2:205:BCR:H361	1.89	0.42
27:J2:103:LMG:O1	27:J2:103:LMG:HC61	2.20	0.42
24:92:623:BCR:H361	24:92:623:BCR:H20C	1.83	0.42
21:6:613:CLA:C1B	21:6:614:CLA:HMD3	2.49	0.42
1:A2:348:SER:OG	1:A2:416:ASP:OD2	2.30	0.42
24:K2:207:BCR:H20C	24:K2:207:BCR:H361	1.90	0.42
21:32:603:CLA:HBB1	21:32:603:CLA:HMB1	2.01	0.42
21:B:808:CLA:HMB2	21:B:808:CLA:H142	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:2:ALA:N	3:C:71:SER:O	2.53	0.42
21:5:616:CLA:H62	21:5:616:CLA:H41	1.93	0.42
2:B2:494:TRP:CH2	21:B2:835:CLA:HED3	2.55	0.42
1:A:115:ALA:HB3	21:A:809:CLA:HED3	2.01	0.42
21:A:802:CLA:CGA	21:A:802:CLA:H3A	2.50	0.42
2:B:194:HIS:CE1	21:B:814:CLA:NA	2.87	0.42
21:B:837:CLA:H41	28:F:305:LUT:C37	2.49	0.42
24:B:843:BCR:H24C	24:B:843:BCR:H371	1.91	0.42
27:J:103:LMG:O1	27:J:103:LMG:HC61	2.20	0.42
24:3:719:BCR:H24C	24:3:719:BCR:H371	1.85	0.42
1:A2:584:CYS:O	2:B2:670:GLY:N	2.51	0.42
24:A2:850:BCR:C8	24:A2:850:BCR:H331	2.49	0.42
21:B2:837:CLA:H41	28:F2:305:LUT:C37	2.50	0.42
24:3:718:BCR:H24C	24:3:718:BCR:H371	1.90	0.42
12:Z:220:THR:HG22	12:Z:220:THR:O	2.20	0.42
1:A2:115:ALA:HB3	21:A2:809:CLA:HED3	2.01	0.42
2:B2:236:GLN:O	2:B2:237:SER:OG	2.33	0.42
24:B2:843:BCR:H24C	24:B2:843:BCR:H371	1.91	0.42
15:82:225:LEU:HD21	21:82:614:CLA:HMC3	2.01	0.42
2:B:494:TRP:CH2	21:B:835:CLA:HED3	2.55	0.42
21:B:806:CLA:HMC2	24:B:844:BCR:H401	2.01	0.42
21:B:840:CLA:H122	21:B:840:CLA:H91	2.02	0.42
21:8:610:CLA:HBB1	21:8:610:CLA:HMB1	2.02	0.42
30:4:607:CHL:O1A	26:4:625:LMU:O6'	2.33	0.42
1:A2:747:ILE:O	1:A2:751:GLY:N	2.51	0.42
2:B:672:TRP:CZ2	22:B:842:PQN:H2M3	2.55	0.42
12:1:50:PRO:O	12:1:56:ASN:ND2	2.52	0.42
21:3:615:CLA:HAA2	21:5:616:CLA:HED2	2.02	0.42
2:B2:632:LEU:HD21	2:B2:651:PHE:CD1	2.54	0.42
21:A:829:CLA:H62	21:A:829:CLA:H41	1.83	0.42
24:A:848:BCR:H24C	24:A:848:BCR:H371	1.87	0.42
13:3:183:ILE:HG22	13:3:196:PRO:HG2	2.02	0.42
21:B2:816:CLA:H142	21:B2:816:CLA:C10	2.48	0.42
21:52:610:CLA:H62	21:52:610:CLA:H41	1.83	0.42
1:A:707:LEU:HD23	6:F:216:LEU:HD23	2.02	0.41
13:3:58:ASP:OD1	13:3:58:ASP:N	2.53	0.41
1:A2:554:VAL:HG11	21:A2:822:CLA:H203	2.01	0.41
2:B2:194:HIS:CE1	21:B2:814:CLA:NA	2.87	0.41
24:L2:205:BCR:H403	24:L2:205:BCR:H23C	2.01	0.41
24:K2:202:BCR:H24C	24:K2:202:BCR:H371	1.92	0.41
21:32:615:CLA:HAA2	21:52:616:CLA:HED2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z2:220:THR:HG22	12:Z2:220:THR:O	2.20	0.41
24:A:851:BCR:H371	24:A:851:BCR:H24C	1.89	0.41
11:K:69:ASP:OD1	11:K:70:SER:N	2.54	0.41
24:3:719:BCR:H20C	24:3:719:BCR:H361	1.91	0.41
16:4:66:ASP:O	23:4:623:LHG:O4	2.39	0.41
21:9:612:CLA:HBB1	21:9:612:CLA:HMB1	2.03	0.41
21:12:602:CLA:HMC2	31:12:618:XAT:C31	2.49	0.41
13:32:183:ILE:HG22	13:32:196:PRO:HG2	2.02	0.41
12:Z2:192:VAL:HG13	26:Z2:622:LMU:O2'	2.20	0.41
1:A:747:ILE:O	1:A:751:GLY:N	2.51	0.41
2:B:632:LEU:HD21	2:B:651:PHE:CG	2.55	0.41
21:B:837:CLA:HBB1	21:B:837:CLA:HMB1	2.02	0.41
12:Z:215:GLY:O	12:Z:220:THR:HG21	2.20	0.41
24:A2:848:BCR:H361	24:A2:848:BCR:H20C	1.85	0.41
3:C2:2:ALA:N	3:C2:71:SER:O	2.53	0.41
1:A:343:GLU:OE1	1:A:343:GLU:N	2.48	0.41
21:A:829:CLA:H72	21:A:829:CLA:C12	2.50	0.41
18:6:209:LEU:HD21	21:6:614:CLA:HMC3	2.03	0.41
21:A2:802:CLA:CGA	21:A2:802:CLA:H3A	2.50	0.41
2:B2:195:LEU:HA	2:B2:199:ALA:HB3	2.02	0.41
21:B2:827:CLA:H141	21:B2:829:CLA:H143	2.03	0.41
21:B2:837:CLA:HBB1	21:B2:837:CLA:HMB1	2.02	0.41
30:52:608:CHL:H12	28:52:620:LUT:H383	2.02	0.41
9:J:32:TYR:OH	21:J:101:CLA:HED3	2.21	0.41
21:L:203:CLA:H62	21:L:203:CLA:H41	1.90	0.41
21:1:602:CLA:HMC2	31:1:618:XAT:C31	2.49	0.41
21:8:603:CLA:HMD2	21:8:609:CLA:CHD	2.51	0.41
2:B2:352:HIS:CE1	21:B2:826:CLA:NB	2.89	0.41
12:Z2:159:ASP:OD1	28:Z2:617:LUT:O23	2.38	0.41
15:8:231:VAL:HG12	21:8:613:CLA:HED1	2.02	0.41
24:6:623:BCR:H20C	24:6:623:BCR:H361	1.96	0.41
1:A2:707:LEU:HD23	6:F2:216:LEU:HD23	2.02	0.41
21:A2:840:CLA:HBB1	21:A2:840:CLA:HMB1	2.03	0.41
24:A2:850:BCR:H20C	24:A2:850:BCR:H361	1.89	0.41
2:B2:632:LEU:HD21	2:B2:651:PHE:CG	2.56	0.41
21:B2:806:CLA:HMC2	24:B2:844:BCR:H401	2.02	0.41
24:B2:801:BCR:H24C	24:B2:801:BCR:H371	1.92	0.41
24:G2:205:BCR:H24C	24:G2:205:BCR:H371	1.87	0.41
15:82:231:VAL:HG12	21:82:613:CLA:HED1	2.03	0.41
21:B:827:CLA:H141	21:B:829:CLA:H143	2.02	0.41
6:F:212:ARG:NH2	27:8:626:LMG:O3	2.47	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:5:608:CHL:H12	28:5:620:LUT:H383	2.02	0.41
24:32:719:BCR:H24C	24:32:719:BCR:H371	1.85	0.41
24:3:620:BCR:H24C	24:3:620:BCR:H371	1.92	0.41
12:Z:192:VAL:HG13	26:Z:622:LMU:O2'	2.20	0.41
21:A2:820:CLA:CAD	21:A2:830:CLA:H41	2.51	0.41
21:A2:833:CLA:C4	10:L2:65:VAL:HG13	2.51	0.41
21:B2:817:CLA:HMC1	21:B2:817:CLA:HBC3	2.02	0.41
12:Z2:153:TYR:HB3	21:Z2:610:CLA:HED2	2.03	0.41
16:42:66:ASP:O	23:42:623:LHG:O4	2.39	0.41
24:92:623:BCR:H24C	24:92:623:BCR:H371	1.89	0.41
1:A:245:LEU:O	26:A:857:LMU:O2B	2.34	0.41
1:A:474:ASP:O	1:A:478:GLN:NE2	2.54	0.41
21:A:833:CLA:C4	10:L:65:VAL:HG13	2.51	0.41
21:A:840:CLA:HMB1	21:A:840:CLA:HBB1	2.03	0.41
24:A:848:BCR:H20C	24:A:848:BCR:H361	1.86	0.41
24:A:851:BCR:H20C	24:A:851:BCR:H361	1.94	0.41
28:A:856:LUT:H8	28:A:856:LUT:H171	2.03	0.41
2:B:352:HIS:CE1	21:B:826:CLA:NB	2.88	0.41
21:B:837:CLA:H41	28:F:305:LUT:H371	2.03	0.41
21:B:840:CLA:H91	21:B:840:CLA:C12	2.51	0.41
3:C:36:ALA:O	3:C:37:SER:OG	2.31	0.41
21:1:613:CLA:H2	21:1:614:CLA:HMD1	2.02	0.41
30:7:601:CHL:H61	30:7:601:CHL:H41	1.84	0.41
21:B2:840:CLA:C12	21:B2:840:CLA:H91	2.51	0.41
30:32:608:CHL:H191	21:32:610:CLA:H142	2.03	0.41
12:Z2:215:GLY:O	12:Z2:220:THR:HG21	2.20	0.41
21:A:811:CLA:C1	21:A:813:CLA:H42	2.50	0.41
24:A:852:BCR:H24C	24:A:852:BCR:H371	1.91	0.41
3:C:24:ASP:OD2	4:D:151:HIS:ND1	2.50	0.41
12:Z:159:ASP:OD1	28:Z:617:LUT:O23	2.38	0.41
2:B2:293:ARG:N	2:B2:300:HIS:O	2.53	0.41
2:B2:672:TRP:CZ2	22:B2:842:PQN:H2M3	2.56	0.41
11:K2:69:ASP:OD1	11:K2:70:SER:N	2.54	0.41
21:12:613:CLA:H2	21:12:614:CLA:HMD1	2.03	0.41
21:32:615:CLA:H61	21:32:615:CLA:H41	1.94	0.41
15:82:217:PRO:O	28:82:617:LUT:O3	2.39	0.41
24:82:619:BCR:HC8	24:82:619:BCR:H311	2.02	0.41
2:B:530:THR:HG21	2:B:583:TRP:CE2	2.55	0.40
24:B:845:BCR:H24C	24:B:845:BCR:H371	1.84	0.40
26:8:627:LMU:H2'	26:8:627:LMU:H6D	2.03	0.40
21:5:621:CLA:HAA2	21:5:621:CLA:HBD	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:B2:832:CLA:HBB1	24:B2:801:BCR:H323	2.03	0.40
11:K2:65:LEU:HD12	11:K2:65:LEU:N	2.37	0.40
21:92:612:CLA:HMB1	21:92:612:CLA:HBB1	2.03	0.40
21:B:834:CLA:HMD2	21:B:835:CLA:CHC	2.51	0.40
11:K:65:LEU:N	11:K:65:LEU:HD12	2.37	0.40
30:6:606:CHL:HMB2	24:6:623:BCR:H373	2.03	0.40
30:6:608:CHL:O2A	21:6:610:CLA:HMD2	2.21	0.40
21:A2:832:CLA:HED2	10:L2:55:LEU:HD21	2.02	0.40
21:B2:840:CLA:H62	21:B2:840:CLA:H41	1.85	0.40
13:32:132:PRO:N	13:32:133:PRO:CD	2.84	0.40
21:82:610:CLA:HMB1	21:82:610:CLA:HBB1	2.03	0.40
16:42:160:VAL:HG11	24:42:621:BCR:H362	2.03	0.40
16:4:223:MET:HE3	21:4:602:CLA:HMC3	2.04	0.40
28:A2:856:LUT:C28	28:A2:856:LUT:H381	2.51	0.40
21:B2:840:CLA:H91	21:B2:840:CLA:H122	2.02	0.40
24:L2:201:BCR:H24C	24:L2:201:BCR:H371	1.91	0.40
1:A:411:ILE:HD13	21:A:831:CLA:HED1	2.04	0.40
24:A:852:BCR:H20C	24:A:852:BCR:H361	1.88	0.40
24:B:844:BCR:H24C	24:B:844:BCR:H371	1.97	0.40
24:8:619:BCR:HC8	24:8:619:BCR:H311	2.02	0.40
12:Z:153:TYR:HB3	21:Z:610:CLA:HED2	2.03	0.40
28:A2:856:LUT:H171	28:A2:856:LUT:H8	2.03	0.40
2:B2:173:GLU:OE1	2:B2:173:GLU:N	2.50	0.40
9:J2:32:TYR:OH	21:J2:101:CLA:HED3	2.21	0.40
21:B:817:CLA:HBC3	21:B:817:CLA:HMC1	2.02	0.40
14:7:110:VAL:HG13	14:7:115:ILE:O	2.22	0.40
21:8:612:CLA:H43	21:4:609:CLA:H11	2.04	0.40
14:72:82:GLY:HA2	31:72:622:XAT:H381	2.03	0.40
16:42:223:MET:HE3	21:42:602:CLA:HMC3	2.04	0.40
18:62:209:LEU:HD21	21:62:614:CLA:HMC3	2.03	0.40
30:62:606:CHL:HMB2	24:62:623:BCR:H373	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	740/751 (98%)	727 (98%)	13 (2%)	0	100	100
1	A2	740/751 (98%)	727 (98%)	13 (2%)	0	100	100
2	B	731/735 (100%)	718 (98%)	13 (2%)	0	100	100
2	B2	731/735 (100%)	718 (98%)	13 (2%)	0	100	100
3	C	78/81 (96%)	76 (97%)	2 (3%)	0	100	100
3	C2	78/81 (96%)	76 (97%)	2 (3%)	0	100	100
4	D	142/196 (72%)	139 (98%)	3 (2%)	0	100	100
4	D2	142/196 (72%)	139 (98%)	3 (2%)	0	100	100
5	E	62/97 (64%)	62 (100%)	0	0	100	100
5	E2	62/97 (64%)	62 (100%)	0	0	100	100
6	F	163/227 (72%)	163 (100%)	0	0	100	100
6	F2	163/227 (72%)	162 (99%)	1 (1%)	0	100	100
7	G	93/126 (74%)	92 (99%)	1 (1%)	0	100	100
7	G2	93/126 (74%)	92 (99%)	1 (1%)	0	100	100
8	I	35/106 (33%)	35 (100%)	0	0	100	100
8	I2	35/106 (33%)	35 (100%)	0	0	100	100
9	J	38/40 (95%)	37 (97%)	1 (3%)	0	100	100
9	J2	38/40 (95%)	37 (97%)	1 (3%)	0	100	100
10	L	120/196 (61%)	118 (98%)	2 (2%)	0	100	100
10	L2	120/196 (61%)	118 (98%)	2 (2%)	0	100	100
11	K	84/113 (74%)	82 (98%)	2 (2%)	0	100	100
11	K2	84/113 (74%)	82 (98%)	2 (2%)	0	100	100
12	1	192/228 (84%)	192 (100%)	0	0	100	100
12	12	192/228 (84%)	192 (100%)	0	0	100	100
12	Z	192/228 (84%)	190 (99%)	2 (1%)	0	100	100
12	Z2	192/228 (84%)	190 (99%)	2 (1%)	0	100	100
13	3	225/298 (76%)	218 (97%)	7 (3%)	0	100	100
13	32	225/298 (76%)	218 (97%)	7 (3%)	0	100	100
14	7	211/241 (88%)	210 (100%)	1 (0%)	0	100	100
14	72	211/241 (88%)	210 (100%)	1 (0%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	8	215/243 (88%)	212 (99%)	3 (1%)	0	100	100
15	82	215/243 (88%)	212 (99%)	3 (1%)	0	100	100
16	4	210/264 (80%)	207 (99%)	3 (1%)	0	100	100
16	42	210/264 (80%)	207 (99%)	3 (1%)	0	100	100
17	5	225/257 (88%)	220 (98%)	5 (2%)	0	100	100
17	52	225/257 (88%)	220 (98%)	5 (2%)	0	100	100
18	6	228/257 (89%)	225 (99%)	3 (1%)	0	100	100
18	62	228/257 (89%)	225 (99%)	3 (1%)	0	100	100
19	9	184/213 (86%)	179 (97%)	4 (2%)	1 (0%)	29	66
19	92	184/213 (86%)	179 (97%)	4 (2%)	1 (0%)	29	66
All	All	8336/9794 (85%)	8203 (98%)	131 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
19	9	139	ILE
19	92	139	ILE

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	601/610 (98%)	597 (99%)	4 (1%)	84	93
1	A2	601/610 (98%)	597 (99%)	4 (1%)	84	93
2	B	596/597 (100%)	594 (100%)	2 (0%)	92	97
2	B2	596/597 (100%)	595 (100%)	1 (0%)	93	98
3	C	69/70 (99%)	68 (99%)	1 (1%)	67	86
3	C2	69/70 (99%)	68 (99%)	1 (1%)	67	86
4	D	121/152 (80%)	120 (99%)	1 (1%)	81	92
4	D2	121/152 (80%)	120 (99%)	1 (1%)	81	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	55/81 (68%)	55 (100%)	0	100	100
5	E2	55/81 (68%)	55 (100%)	0	100	100
6	F	127/169 (75%)	126 (99%)	1 (1%)	81	92
6	F2	127/169 (75%)	126 (99%)	1 (1%)	81	92
7	G	71/94 (76%)	71 (100%)	0	100	100
7	G2	71/94 (76%)	71 (100%)	0	100	100
8	I	31/76 (41%)	31 (100%)	0	100	100
8	I2	31/76 (41%)	31 (100%)	0	100	100
9	J	35/35 (100%)	35 (100%)	0	100	100
9	J2	35/35 (100%)	35 (100%)	0	100	100
10	L	90/148 (61%)	89 (99%)	1 (1%)	73	90
10	L2	90/148 (61%)	89 (99%)	1 (1%)	73	90
11	K	59/80 (74%)	59 (100%)	0	100	100
11	K2	59/80 (74%)	59 (100%)	0	100	100
12	1	137/162 (85%)	137 (100%)	0	100	100
12	12	137/162 (85%)	137 (100%)	0	100	100
12	Z	137/162 (85%)	137 (100%)	0	100	100
12	Z2	137/162 (85%)	137 (100%)	0	100	100
13	3	174/230 (76%)	171 (98%)	3 (2%)	60	84
13	32	174/230 (76%)	171 (98%)	3 (2%)	60	84
14	7	164/181 (91%)	163 (99%)	1 (1%)	86	94
14	72	164/181 (91%)	163 (99%)	1 (1%)	86	94
15	8	163/183 (89%)	161 (99%)	2 (1%)	71	89
15	82	163/183 (89%)	161 (99%)	2 (1%)	71	89
16	4	166/205 (81%)	166 (100%)	0	100	100
16	42	166/205 (81%)	166 (100%)	0	100	100
17	5	184/206 (89%)	182 (99%)	2 (1%)	73	90
17	52	184/206 (89%)	182 (99%)	2 (1%)	73	90
18	6	184/203 (91%)	184 (100%)	0	100	100
18	62	184/203 (91%)	184 (100%)	0	100	100
19	9	142/159 (89%)	142 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	92	142/159 (89%)	142 (100%)	0	100	100
All	All	6612/7606 (87%)	6577 (100%)	35 (0%)	89	95

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	154	THR
1	A	278	PHE
1	A	293	ASP
1	A	372	TYR
2	B	258	PHE
2	B	578	TYR
3	C	23	LEU
4	D	150	LEU
6	F	162	TYR
10	L	64	ILE
13	3	38	VAL
13	3	42	LYS
13	3	218	ILE
14	7	34	PHE
15	8	27	ARG
15	8	153	PHE
17	5	91	GLN
17	5	238	HIS
1	A2	154	THR
1	A2	278	PHE
1	A2	293	ASP
1	A2	372	TYR
2	B2	258	PHE
3	C2	23	LEU
4	D2	150	LEU
6	F2	162	TYR
10	L2	64	ILE
13	32	38	VAL
13	32	42	LYS
13	32	218	ILE
14	72	34	PHE
15	82	27	ARG
15	82	153	PHE
17	52	91	GLN
17	52	238	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
12	1	195	HIS
13	3	256	ASN
19	9	109	GLN
7	G2	121	GLN
12	12	195	HIS
13	32	256	ASN
19	92	109	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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
9	AME	J2	1	9	9,10,11	0.51	0	9,11,13	0.89	1 (11%)
9	AME	J	1	9	9,10,11	0.50	0	9,11,13	0.89	1 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	AME	J2	1	9	-	2/9/10/12	-
9	AME	J	1	9	-	2/9/10/12	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	J2	1	AME	O-C-CA	-2.52	118.17	124.78
9	J	1	AME	O-C-CA	-2.51	118.20	124.78

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	J	1	AME	C-CA-CB-CG
9	J	1	AME	N-CA-CB-CG
9	J2	1	AME	C-CA-CB-CG
9	J2	1	AME	N-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

706 ligands are modelled in this entry.

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	$\# Z > 2$
21	CLA	72	604	33	51,59,73	1.17	3 (5%)	59,96,113	0.97	2 (3%)
21	CLA	32	613	13	60,68,73	1.07	3 (5%)	70,107,113	0.89	2 (2%)
21	CLA	32	604	33	65,73,73	1.04	3 (4%)	76,113,113	0.86	2 (2%)
30	CHL	5	618	17	43,51,74	2.50	9 (20%)	45,86,114	1.44	7 (15%)
21	CLA	12	610	12	65,73,73	1.01	4 (6%)	76,113,113	0.85	2 (2%)
21	CLA	B	818	-	65,73,73	1.02	3 (4%)	76,113,113	0.85	2 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	32	602	13	60,68,73	1.06	3 (5%)	70,107,113	0.89	2 (2%)
26	LMU	12	623	-	24,24,36	0.14	0	29,29,47	0.27	0
21	CLA	G2	204	7	46,54,73	1.23	3 (6%)	53,90,113	1.01	2 (3%)
21	CLA	82	610	15	65,73,73	1.02	3 (4%)	76,113,113	0.84	2 (2%)
21	CLA	42	604	33	50,58,73	1.18	3 (6%)	58,95,113	1.00	3 (5%)
21	CLA	7	602	14	65,73,73	1.02	3 (4%)	76,113,113	0.85	2 (2%)
30	CHL	42	606	33	56,64,74	2.17	9 (16%)	61,102,114	1.32	8 (13%)
30	CHL	42	608	-	66,74,74	2.03	10 (15%)	73,114,114	1.13	7 (9%)
30	CHL	9	606	-	42,50,74	2.58	11 (26%)	44,85,114	1.43	7 (15%)
21	CLA	42	616	16	45,53,73	1.26	3 (6%)	52,89,113	1.03	2 (3%)
21	CLA	42	613	16	65,73,73	1.04	3 (4%)	76,113,113	0.86	2 (2%)
28	LUT	92	616	-	42,43,43	0.26	0	51,60,60	0.37	0
30	CHL	8	606	33	66,74,74	1.99	10 (15%)	73,114,114	1.13	8 (10%)
21	CLA	5	617	-	65,73,73	1.03	3 (4%)	76,113,113	0.85	2 (2%)
21	CLA	42	602	16	60,68,73	1.07	3 (5%)	70,107,113	0.88	2 (2%)
24	BCR	62	623	-	41,41,41	0.16	0	56,56,56	0.35	0
30	CHL	3	608	33	66,74,74	2.00	10 (15%)	73,114,114	1.15	7 (9%)
21	CLA	7	608	33	50,58,73	1.18	3 (6%)	58,95,113	0.97	2 (3%)
21	CLA	B	826	-	65,73,73	1.02	3 (4%)	76,113,113	0.83	2 (2%)
31	XAT	52	624	-	39,47,47	0.10	0	54,74,74	0.58	0
21	CLA	1	614	-	60,68,73	1.09	3 (5%)	70,107,113	0.93	2 (2%)
30	CHL	52	607	33	66,74,74	2.04	9 (13%)	73,114,114	1.18	8 (10%)
21	CLA	8	612	15	55,63,73	1.12	3 (5%)	64,101,113	0.91	2 (3%)
26	LMU	6	632	-	20,20,36	0.15	0	25,25,47	0.26	0
21	CLA	4	611	23	60,68,73	1.08	3 (5%)	70,107,113	0.90	3 (4%)
21	CLA	A	824	-	45,53,73	1.22	3 (6%)	52,89,113	1.05	2 (3%)
30	CHL	12	606	33	46,54,74	2.40	10 (21%)	49,90,114	1.38	7 (14%)
26	LMU	1	623	-	24,24,36	0.13	0	29,29,47	0.27	0
28	LUT	7	621	-	42,43,43	0.25	0	51,60,60	0.38	0
27	LMG	4	624	-	41,41,55	0.19	0	49,49,63	0.26	0
21	CLA	A2	823	-	65,73,73	1.04	4 (6%)	76,113,113	0.86	2 (2%)
24	BCR	3	620	-	41,41,41	0.19	0	56,56,56	0.36	0
30	CHL	82	606	33	66,74,74	1.99	9 (13%)	73,114,114	1.13	8 (10%)
23	LHG	4	622	21	48,48,48	0.24	0	51,54,54	0.27	0
21	CLA	A	817	33	55,63,73	1.14	3 (5%)	64,101,113	0.92	2 (3%)
21	CLA	3	613	13	60,68,73	1.07	3 (5%)	70,107,113	0.89	2 (2%)
30	CHL	4	618	16	46,54,74	2.43	9 (19%)	49,90,114	1.38	7 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	B	829	-	65,73,73	1.00	4 (6%)	76,113,113	0.87	2 (2%)
21	CLA	A	836	-	65,73,73	1.04	4 (6%)	76,113,113	0.86	2 (2%)
21	CLA	B2	831	-	55,63,73	1.09	4 (7%)	64,101,113	0.93	3 (4%)
21	CLA	52	611	23	55,63,73	1.12	3 (5%)	64,101,113	0.93	2 (3%)
25	SF4	A2	853	1,2	0,12,12	-	-	-	-	-
21	CLA	9	609	19	51,59,73	1.16	3 (5%)	59,96,113	0.97	2 (3%)
21	CLA	6	603	-	65,73,73	1.04	3 (4%)	76,113,113	0.83	2 (2%)
24	BCR	32	620	-	41,41,41	0.19	0	56,56,56	0.36	0
21	CLA	32	610	13	65,73,73	1.03	4 (6%)	76,113,113	0.87	2 (2%)
23	LHG	Z2	620	21	38,38,48	0.26	0	41,44,54	0.28	0
29	DGD	B	850	-	60,60,67	0.18	0	74,74,81	0.52	0
21	CLA	92	611	23	65,73,73	1.03	3 (4%)	76,113,113	0.86	2 (2%)
30	CHL	52	618	17	43,51,74	2.50	9 (20%)	45,86,114	1.44	7 (15%)
21	CLA	62	603	-	65,73,73	1.04	3 (4%)	76,113,113	0.83	2 (2%)
21	CLA	92	604	19	53,61,73	1.13	4 (7%)	61,98,113	0.96	3 (4%)
21	CLA	A2	843	33	65,73,73	1.02	4 (6%)	76,113,113	0.88	2 (2%)
26	LMU	92	624	-	24,24,36	0.15	0	29,29,47	0.37	0
26	LMU	82	627	-	36,36,36	0.10	0	47,47,47	0.37	0
27	LMG	72	626	-	37,37,55	0.19	0	45,45,63	0.27	0
21	CLA	6	610	18	60,68,73	1.08	3 (5%)	70,107,113	0.89	2 (2%)
21	CLA	12	602	12	60,68,73	1.06	4 (6%)	70,107,113	0.90	2 (2%)
31	XAT	Z	618	-	39,47,47	0.13	0	54,74,74	0.56	0
28	LUT	32	622	-	42,43,43	0.32	0	51,60,60	0.35	0
24	BCR	B2	845	-	41,41,41	0.13	0	56,56,56	0.37	0
21	CLA	92	602	19	60,68,73	1.07	3 (5%)	70,107,113	0.89	2 (2%)
26	LMU	4	625	-	34,34,36	0.11	0	45,45,47	0.20	0
30	CHL	5	607	33	66,74,74	2.05	9 (13%)	73,114,114	1.19	9 (12%)
23	LHG	32	623	-	46,46,48	0.23	0	49,52,54	0.26	0
21	CLA	8	611	23	45,53,73	1.24	3 (6%)	52,89,113	1.07	3 (5%)
26	LMU	7	627	-	33,33,36	0.11	0	44,44,47	0.16	0
21	CLA	62	610	18	60,68,73	1.07	3 (5%)	70,107,113	0.89	2 (2%)
21	CLA	A	840	-	65,73,73	1.03	3 (4%)	76,113,113	0.86	2 (2%)
21	CLA	B	821	-	65,73,73	1.02	4 (6%)	76,113,113	0.85	2 (2%)
26	LMU	A2	858	-	36,36,36	0.08	0	47,47,47	0.19	0
21	CLA	A	842	-	65,73,73	0.99	4 (6%)	76,113,113	0.85	2 (2%)
21	CLA	B	813	-	65,73,73	1.03	3 (4%)	76,113,113	0.86	2 (2%)
21	CLA	A	822	33	65,73,73	1.03	4 (6%)	76,113,113	0.85	2 (2%)
31	XAT	4	620	-	39,47,47	0.10	0	54,74,74	0.65	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	BCR	B	845	-	41,41,41	0.14	0	56,56,56	0.37	0
25	SF4	C2	101	3	0,12,12	-	-	-		
21	CLA	Z2	608	33	50,58,73	1.19	3 (6%)	58,95,113	1.00	2 (3%)
21	CLA	6	602	18	65,73,73	1.03	3 (4%)	76,113,113	0.87	2 (2%)
21	CLA	B	820	-	56,64,73	1.12	3 (5%)	65,102,113	0.90	2 (3%)
21	CLA	A2	821	-	55,63,73	1.12	3 (5%)	64,101,113	0.90	2 (3%)
21	CLA	A	838	-	51,59,73	1.17	3 (5%)	59,96,113	0.98	2 (3%)
21	CLA	F	303	33	45,53,73	1.25	3 (6%)	52,89,113	1.02	2 (3%)
21	CLA	82	604	33	60,68,73	1.09	4 (6%)	70,107,113	0.92	2 (2%)
23	LHG	12	620	21	38,38,48	0.26	0	41,44,54	0.29	0
21	CLA	32	615	33	65,73,73	1.05	3 (4%)	76,113,113	0.86	2 (2%)
21	CLA	F	304	6	65,73,73	1.05	3 (4%)	76,113,113	0.95	3 (3%)
21	CLA	B2	819	33	60,68,73	1.07	4 (6%)	70,107,113	0.89	2 (2%)
21	CLA	B2	809	2	65,73,73	1.03	3 (4%)	76,113,113	0.83	2 (2%)
21	CLA	32	612	13	46,54,73	1.23	3 (6%)	53,90,113	0.99	2 (3%)
21	CLA	82	616	15	45,53,73	1.24	3 (6%)	52,89,113	1.06	3 (5%)
21	CLA	A2	802	-	65,73,73	1.01	4 (6%)	76,113,113	0.81	2 (2%)
21	CLA	A2	803	33	65,73,73	1.03	4 (6%)	76,113,113	0.85	2 (2%)
21	CLA	7	614	-	43,51,73	1.28	3 (6%)	49,86,113	1.07	2 (4%)
21	CLA	32	607	13	55,63,73	1.12	3 (5%)	64,101,113	0.95	3 (4%)
21	CLA	8	614	-	57,65,73	1.11	3 (5%)	66,103,113	0.90	2 (3%)
23	LHG	5	623	21	36,36,48	0.26	0	39,42,54	0.27	0
21	CLA	A2	806	-	65,73,73	1.02	4 (6%)	76,113,113	0.89	3 (3%)
21	CLA	G	203	-	60,68,73	1.08	3 (5%)	70,107,113	0.84	2 (2%)
24	BCR	B2	846	-	41,41,41	0.13	0	56,56,56	0.34	0
26	LMU	A2	861	-	24,24,36	0.13	0	29,29,47	0.30	0
24	BCR	K2	202	-	41,41,41	0.15	0	56,56,56	0.36	0
21	CLA	42	612	16	45,53,73	1.27	3 (6%)	52,89,113	1.00	2 (3%)
21	CLA	Z2	610	12	60,68,73	1.07	3 (5%)	70,107,113	0.88	2 (2%)
30	CHL	1	607	33	46,54,74	2.38	10 (21%)	49,90,114	1.42	10 (20%)
30	CHL	6	608	33	51,59,74	2.31	10 (19%)	55,96,114	1.32	8 (14%)
27	LMG	32	722	-	44,44,55	0.21	0	46,46,63	0.26	0
21	CLA	A	837	1	57,65,73	1.11	4 (7%)	66,103,113	0.93	2 (3%)
24	BCR	5	622	-	41,41,41	0.17	0	56,56,56	0.32	0
26	LMU	6	631	-	24,24,36	0.15	0	29,29,47	0.28	0
21	CLA	B	825	33	65,73,73	1.01	4 (6%)	76,113,113	0.83	2 (2%)
21	CLA	B2	820	-	56,64,73	1.12	3 (5%)	65,102,113	0.91	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	A2	810	1	65,73,73	1.03	3 (4%)	76,113,113	0.87	2 (2%)
21	CLA	52	601	17	65,73,73	1.05	3 (4%)	76,113,113	0.87	2 (2%)
21	CLA	82	609	15	45,53,73	1.24	3 (6%)	52,89,113	1.01	2 (3%)
24	BCR	92	623	-	41,41,41	0.15	0	56,56,56	0.34	0
21	CLA	5	614	-	45,53,73	1.27	3 (6%)	52,89,113	1.03	2 (3%)
21	CLA	3	615	33	65,73,73	1.05	3 (4%)	76,113,113	0.87	2 (2%)
21	CLA	A	833	-	65,73,73	1.03	4 (6%)	76,113,113	0.86	2 (2%)
23	LHG	A	846	-	48,48,48	0.24	0	51,54,54	0.29	0
29	DGD	B2	850	-	60,60,67	0.17	0	74,74,81	0.34	0
21	CLA	42	609	16	60,68,73	1.10	3 (5%)	70,107,113	0.92	2 (2%)
21	CLA	J2	101	9	55,63,73	1.13	3 (5%)	64,101,113	0.92	2 (3%)
21	CLA	9	612	19	65,73,73	1.03	3 (4%)	76,113,113	0.84	2 (2%)
21	CLA	82	608	33	50,58,73	1.19	3 (6%)	58,95,113	0.98	2 (3%)
27	LMG	1	624	-	36,36,55	0.20	0	44,44,63	0.19	0
21	CLA	A	845	23	45,53,73	1.24	3 (6%)	52,89,113	0.99	2 (3%)
30	CHL	72	601	14	66,74,74	2.01	10 (15%)	73,114,114	1.15	7 (9%)
30	CHL	6	607	33	66,74,74	2.06	9 (13%)	73,114,114	1.18	8 (10%)
21	CLA	A2	831	-	65,73,73	1.04	4 (6%)	76,113,113	0.86	2 (2%)
24	BCR	B	844	-	41,41,41	0.13	0	56,56,56	0.45	0
30	CHL	Z2	606	33	46,54,74	2.40	10 (21%)	49,90,114	1.37	7 (14%)
21	CLA	1	602	12	60,68,73	1.06	4 (6%)	70,107,113	0.91	2 (2%)
24	BCR	A2	849	-	41,41,41	0.17	0	56,56,56	0.31	0
26	LMU	1	626	-	24,24,36	0.12	0	29,29,47	0.27	0
21	CLA	A2	845	23	45,53,73	1.25	3 (6%)	52,89,113	1.00	2 (3%)
21	CLA	5	610	17	60,68,73	1.06	3 (5%)	70,107,113	0.89	2 (2%)
21	CLA	52	610	17	60,68,73	1.07	3 (5%)	70,107,113	0.88	2 (2%)
26	LMU	12	626	-	24,24,36	0.12	0	29,29,47	0.27	0
21	CLA	B2	826	-	65,73,73	1.02	3 (4%)	76,113,113	0.82	2 (2%)
23	LHG	3	623	-	46,46,48	0.23	0	49,52,54	0.26	0
31	XAT	8	618	-	39,47,47	0.16	0	54,74,74	0.57	0
30	CHL	12	607	33	46,54,74	2.37	10 (21%)	49,90,114	1.42	10 (20%)
21	CLA	Z2	612	12	45,53,73	1.26	3 (6%)	52,89,113	1.01	2 (3%)
21	CLA	42	610	16	60,68,73	1.08	3 (5%)	70,107,113	0.88	2 (2%)
21	CLA	Z	603	-	55,63,73	1.15	3 (5%)	64,101,113	0.91	2 (3%)
21	CLA	92	614	-	45,53,73	1.26	3 (6%)	52,89,113	1.03	3 (5%)
21	CLA	B2	807	-	55,63,73	1.13	3 (5%)	64,101,113	0.94	2 (3%)
24	BCR	A2	851	-	41,41,41	0.13	0	56,56,56	0.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	LHG	42	622	21	48,48,48	0.24	0	51,54,54	0.27	0
27	LMG	B	852	-	43,43,55	0.18	0	51,51,63	0.24	0
21	CLA	62	613	33	65,73,73	1.04	3 (4%)	76,113,113	0.87	2 (2%)
21	CLA	B	808	-	65,73,73	1.03	3 (4%)	76,113,113	0.85	2 (2%)
25	SF4	A	853	1,2	0,12,12	-	-	-	-	-
24	BCR	A	848	-	41,41,41	0.14	0	56,56,56	0.30	0
21	CLA	8	616	15	45,53,73	1.24	3 (6%)	52,89,113	1.05	3 (5%)
21	CLA	A	828	-	65,73,73	1.05	3 (4%)	76,113,113	0.81	2 (2%)
21	CLA	5	601	17	65,73,73	1.05	3 (4%)	76,113,113	0.87	2 (2%)
21	CLA	32	609	13	61,69,73	1.05	3 (4%)	71,108,113	0.87	2 (2%)
31	XAT	6	624	-	39,47,47	0.12	0	54,74,74	0.60	0
21	CLA	B	807	-	55,63,73	1.13	3 (5%)	64,101,113	0.94	2 (3%)
21	CLA	12	611	23	61,69,73	1.06	3 (4%)	71,108,113	0.87	2 (2%)
21	CLA	Z	613	33	65,73,73	1.03	3 (4%)	76,113,113	0.89	3 (3%)
24	BCR	A	849	-	41,41,41	0.17	0	56,56,56	0.31	0
21	CLA	3	612	13	46,54,73	1.23	3 (6%)	53,90,113	1.00	2 (3%)
21	CLA	A	811	-	65,73,73	1.02	4 (6%)	76,113,113	0.87	2 (2%)
21	CLA	8	609	15	45,53,73	1.23	3 (6%)	52,89,113	1.01	2 (3%)
21	CLA	A	854	33	65,73,73	1.05	4 (6%)	76,113,113	0.80	2 (2%)
21	CLA	3	607	13	55,63,73	1.12	3 (5%)	64,101,113	0.95	3 (4%)
21	CLA	5	611	23	55,63,73	1.13	3 (5%)	64,101,113	0.93	2 (3%)
21	CLA	92	601	19	46,54,73	1.24	3 (6%)	53,90,113	1.03	2 (3%)
21	CLA	7	620	33	53,61,73	1.14	3 (5%)	61,98,113	0.93	2 (3%)
27	LMG	1	628	-	42,42,55	0.19	0	50,50,63	0.28	0
26	LMU	82	625	-	24,24,36	0.12	0	29,29,47	0.28	0
21	CLA	A	841	-	65,73,73	1.02	4 (6%)	76,113,113	0.87	2 (2%)
21	CLA	F2	301	33	65,73,73	1.01	3 (4%)	76,113,113	0.83	2 (2%)
26	LMU	B	853	-	36,36,36	0.13	0	47,47,47	0.67	2 (4%)
21	CLA	Z2	614	-	50,58,73	1.19	3 (6%)	58,95,113	0.99	3 (5%)
21	CLA	82	612	15	55,63,73	1.13	3 (5%)	64,101,113	0.91	2 (3%)
22	PQN	A	844	-	34,34,34	0.31	0	42,45,45	0.36	0
21	CLA	7	612	14	52,60,73	1.16	3 (5%)	60,97,113	0.94	2 (3%)
21	CLA	72	612	14	52,60,73	1.16	3 (5%)	60,97,113	0.93	2 (3%)
26	LMU	Z2	622	-	32,32,36	0.10	0	43,43,47	0.17	0
21	CLA	A2	826	33	65,73,73	1.05	3 (4%)	76,113,113	0.84	2 (2%)
24	BCR	82	619	-	41,41,41	0.14	0	56,56,56	0.32	0
23	LHG	6	619	21	48,48,48	0.23	0	51,54,54	0.24	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	B2	815	-	65,73,73	1.02	3 (4%)	76,113,113	0.85	2 (2%)
27	LMG	3	722	-	44,44,55	0.21	0	46,46,63	0.25	0
26	LMU	12	621	-	36,36,36	0.10	0	47,47,47	0.28	0
21	CLA	L	204	-	45,53,73	1.26	3 (6%)	52,89,113	1.05	3 (5%)
21	CLA	72	610	14	65,73,73	1.02	3 (4%)	76,113,113	0.92	2 (2%)
23	LHG	62	619	21	48,48,48	0.23	0	51,54,54	0.24	0
30	CHL	52	608	33	51,59,74	2.29	10 (19%)	55,96,114	1.33	8 (14%)
21	CLA	5	609	17	65,73,73	1.03	3 (4%)	76,113,113	0.85	3 (3%)
21	CLA	A2	820	-	65,73,73	1.02	4 (6%)	76,113,113	0.88	2 (2%)
31	XAT	7	622	-	39,47,47	0.13	0	54,74,74	0.57	0
21	CLA	B	835	33	45,53,73	1.26	3 (6%)	52,89,113	1.03	2 (3%)
21	CLA	A	827	33	65,73,73	1.04	4 (6%)	76,113,113	0.87	2 (2%)
21	CLA	72	603	-	52,60,73	1.14	3 (5%)	60,97,113	0.98	2 (3%)
21	CLA	52	621	33	46,54,73	1.27	3 (6%)	53,90,113	1.12	5 (9%)
21	CLA	52	602	17	65,73,73	1.04	3 (4%)	76,113,113	0.84	2 (2%)
26	LMU	K	208	-	24,24,36	0.12	0	29,29,47	0.30	0
28	LUT	A	856	-	42,43,43	0.28	0	51,60,60	0.35	0
21	CLA	A	803	33	65,73,73	1.02	4 (6%)	76,113,113	0.86	2 (2%)
21	CLA	B2	811	-	65,73,73	1.02	3 (4%)	76,113,113	0.87	2 (2%)
28	LUT	32	720	-	42,43,43	0.22	0	51,60,60	0.33	0
21	CLA	B	809	2	65,73,73	1.03	3 (4%)	76,113,113	0.83	2 (2%)
26	LMU	1	622	-	19,19,36	0.14	0	24,24,47	0.31	0
21	CLA	B	812	-	65,73,73	1.03	4 (6%)	76,113,113	0.88	2 (2%)
21	CLA	3	611	-	65,73,73	1.04	3 (4%)	76,113,113	0.86	2 (2%)
21	CLA	B	817	-	65,73,73	1.03	3 (4%)	76,113,113	0.86	2 (2%)
26	LMU	12	622	-	19,19,36	0.14	0	24,24,47	0.31	0
21	CLA	A2	835	-	65,73,73	1.04	3 (4%)	76,113,113	0.86	2 (2%)
28	LUT	1	617	-	42,43,43	0.26	0	51,60,60	0.40	0
21	CLA	A	806	-	65,73,73	1.01	4 (6%)	76,113,113	0.88	3 (3%)
30	CHL	4	606	33	56,64,74	2.17	10 (17%)	61,102,114	1.31	8 (13%)
21	CLA	A2	836	-	65,73,73	1.05	4 (6%)	76,113,113	0.86	2 (2%)
21	CLA	12	614	-	60,68,73	1.08	3 (5%)	70,107,113	0.93	2 (2%)
26	LMU	Z	621	-	22,22,36	0.15	0	27,27,47	0.26	0
21	CLA	A2	838	-	51,59,73	1.17	3 (5%)	59,96,113	0.98	2 (3%)
30	CHL	8	601	15	66,74,74	1.99	10 (15%)	73,114,114	1.10	7 (9%)
30	CHL	72	607	33	46,54,74	2.37	8 (17%)	49,90,114	1.38	7 (14%)
30	CHL	Z	606	33	46,54,74	2.41	10 (21%)	49,90,114	1.37	7 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	5	604	33	55,63,73	1.13	3 (5%)	64,101,113	0.94	2 (3%)
21	CLA	52	604	33	55,63,73	1.13	3 (5%)	64,101,113	0.94	2 (3%)
21	CLA	1	610	12	65,73,73	1.01	3 (4%)	76,113,113	0.86	2 (2%)
21	CLA	B2	805	-	65,73,73	1.01	3 (4%)	76,113,113	0.88	2 (2%)
23	LHG	52	623	21	36,36,48	0.26	0	39,42,54	0.27	0
21	CLA	Z	612	12	45,53,73	1.26	3 (6%)	52,89,113	1.01	2 (3%)
30	CHL	4	608	-	66,74,74	2.02	10 (15%)	73,114,114	1.13	7 (9%)
21	CLA	A	815	-	55,63,73	1.13	3 (5%)	64,101,113	0.90	2 (3%)
21	CLA	B	840	-	65,73,73	1.01	4 (6%)	76,113,113	0.87	2 (2%)
30	CHL	92	606	-	42,50,74	2.57	11 (26%)	44,85,114	1.43	7 (15%)
27	LMG	J	104	-	35,35,55	0.20	0	43,43,63	0.20	0
21	CLA	A	818	-	65,73,73	1.03	3 (4%)	76,113,113	0.85	2 (2%)
24	BCR	G2	205	-	41,41,41	0.14	0	56,56,56	0.32	0
21	CLA	B2	836	-	60,68,73	1.07	3 (5%)	70,107,113	0.90	2 (2%)
21	CLA	4	602	16	60,68,73	1.07	3 (5%)	70,107,113	0.88	2 (2%)
21	CLA	A	807	1	65,73,73	1.03	4 (6%)	76,113,113	0.81	2 (2%)
23	LHG	3	721	-	30,30,48	0.27	0	33,36,54	0.35	0
21	CLA	A2	840	-	65,73,73	1.03	3 (4%)	76,113,113	0.86	2 (2%)
21	CLA	Z2	616	12	60,68,73	1.08	3 (5%)	70,107,113	0.89	2 (2%)
26	LMU	8	627	-	36,36,36	0.10	0	47,47,47	0.37	0
23	LHG	A	847	21	37,37,48	0.26	0	40,43,54	0.30	0
21	CLA	1	611	23	61,69,73	1.06	3 (4%)	71,108,113	0.87	2 (2%)
21	CLA	A2	822	33	65,73,73	1.03	4 (6%)	76,113,113	0.85	2 (2%)
21	CLA	42	614	-	55,63,73	1.15	3 (5%)	64,101,113	0.93	2 (3%)
26	LMU	52	627	-	24,24,36	0.13	0	29,29,47	0.26	0
28	LUT	82	617	-	42,43,43	0.29	0	51,60,60	0.42	0
21	CLA	9	611	23	65,73,73	1.03	3 (4%)	76,113,113	0.86	2 (2%)
30	CHL	Z	607	33	66,74,74	1.99	9 (13%)	73,114,114	1.16	8 (10%)
21	CLA	A2	808	-	50,58,73	1.17	3 (6%)	58,95,113	0.95	2 (3%)
27	LMG	7	626	-	37,37,55	0.20	0	45,45,63	0.27	0
21	CLA	B	814	-	60,68,73	1.07	3 (5%)	70,107,113	0.89	3 (4%)
21	CLA	F2	303	33	45,53,73	1.25	3 (6%)	52,89,113	1.02	2 (3%)
25	SF4	C	101	3	0,12,12	-	-	-	-	-
21	CLA	92	613	19	65,73,73	1.01	3 (4%)	76,113,113	0.89	2 (2%)
26	LMU	B2	853	-	36,36,36	0.13	0	47,47,47	0.67	2 (4%)
21	CLA	B	832	-	65,73,73	1.00	4 (6%)	76,113,113	0.86	2 (2%)
21	CLA	B	804	-	45,53,73	1.25	3 (6%)	52,89,113	1.00	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	52	609	17	65,73,73	1.03	3 (4%)	76,113,113	0.85	3 (3%)
21	CLA	1	603	-	57,65,73	1.10	3 (5%)	66,103,113	0.92	2 (3%)
30	CHL	62	608	33	51,59,74	2.32	10 (19%)	55,96,114	1.33	8 (14%)
26	LMU	A	865	-	24,24,36	0.13	0	29,29,47	0.47	0
21	CLA	62	622	33	55,63,73	1.12	3 (5%)	64,101,113	0.91	2 (3%)
21	CLA	A2	814	-	65,73,73	1.03	3 (4%)	76,113,113	0.83	2 (2%)
27	LMG	J2	104	-	35,35,55	0.20	0	43,43,63	0.20	0
21	CLA	92	609	19	51,59,73	1.17	3 (5%)	59,96,113	0.97	3 (5%)
31	XAT	12	618	-	39,47,47	0.13	0	54,74,74	0.69	2 (3%)
21	CLA	B2	818	-	65,73,73	1.02	4 (6%)	76,113,113	0.86	2 (2%)
24	BCR	9	623	-	41,41,41	0.14	0	56,56,56	0.34	0
24	BCR	52	622	-	41,41,41	0.17	0	56,56,56	0.32	0
21	CLA	72	620	33	53,61,73	1.15	3 (5%)	61,98,113	0.94	2 (3%)
21	CLA	A2	832	-	55,63,73	1.12	3 (5%)	64,101,113	0.95	2 (3%)
21	CLA	A2	824	-	45,53,73	1.22	4 (8%)	52,89,113	1.05	2 (3%)
21	CLA	3	609	13	61,69,73	1.05	3 (4%)	71,108,113	0.88	2 (2%)
31	XAT	42	620	-	39,47,47	0.11	0	54,74,74	0.65	0
32	NEX	52	625	-	38,46,46	0.46	1 (2%)	50,70,70	0.80	2 (4%)
21	CLA	12	604	33	50,58,73	1.17	3 (6%)	58,95,113	0.99	2 (3%)
24	BCR	L	201	-	41,41,41	0.17	0	56,56,56	0.36	0
26	LMU	8	624	-	24,24,36	0.14	0	29,29,47	0.26	0
21	CLA	B	830	-	45,53,73	1.20	4 (8%)	52,89,113	1.03	2 (3%)
30	CHL	6	616	18	66,74,74	2.01	10 (15%)	73,114,114	1.17	9 (12%)
21	CLA	B	819	33	60,68,73	1.07	3 (5%)	70,107,113	0.89	2 (2%)
21	CLA	G2	203	-	60,68,73	1.07	3 (5%)	70,107,113	0.84	2 (2%)
24	BCR	8	619	-	41,41,41	0.14	0	56,56,56	0.31	0
21	CLA	7	616	14	46,54,73	1.22	4 (8%)	53,90,113	1.01	2 (3%)
21	CLA	Z	602	12	60,68,73	1.07	3 (5%)	70,107,113	0.92	2 (2%)
21	CLA	8	603	-	65,73,73	1.05	3 (4%)	76,113,113	0.84	2 (2%)
21	CLA	12	616	12	46,54,73	1.21	3 (6%)	53,90,113	1.02	2 (3%)
21	CLA	72	616	14	46,54,73	1.22	3 (6%)	53,90,113	1.02	2 (3%)
26	LMU	A2	862	-	20,20,36	0.13	0	25,25,47	0.28	0
30	CHL	62	616	18	66,74,74	2.01	10 (15%)	73,114,114	1.17	9 (12%)
30	CHL	9	607	33	51,59,74	2.36	9 (17%)	55,96,114	1.32	8 (14%)
21	CLA	B2	813	-	65,73,73	1.03	3 (4%)	76,113,113	0.85	2 (2%)
30	CHL	42	618	16	46,54,74	2.42	9 (19%)	49,90,114	1.38	7 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	3	617	13	46,54,73	1.22	3 (6%)	53,90,113	1.02	2 (3%)
21	CLA	A	805	-	55,63,73	1.11	4 (7%)	64,101,113	0.90	2 (3%)
24	BCR	L2	205	-	41,41,41	0.15	0	56,56,56	0.37	0
23	LHG	6	629	-	35,35,48	0.26	0	38,41,54	0.28	0
24	BCR	42	621	-	41,41,41	0.14	0	56,56,56	0.35	0
21	CLA	6	611	23	58,66,73	1.10	3 (5%)	67,104,113	0.91	2 (2%)
26	LMU	Z2	621	-	22,22,36	0.15	0	27,27,47	0.27	0
24	BCR	A2	852	-	41,41,41	0.14	0	56,56,56	0.38	0
21	CLA	A	826	33	65,73,73	1.05	3 (4%)	76,113,113	0.84	2 (2%)
21	CLA	A	831	-	65,73,73	1.03	3 (4%)	76,113,113	0.86	2 (2%)
27	LMG	42	624	-	41,41,55	0.19	0	49,49,63	0.26	0
21	CLA	1	604	33	50,58,73	1.16	3 (6%)	58,95,113	0.99	2 (3%)
24	BCR	K	207	-	41,41,41	0.14	0	56,56,56	0.27	0
23	LHG	B	851	21	44,44,48	0.25	0	47,50,54	0.31	0
26	LMU	A	858	-	36,36,36	0.08	0	47,47,47	0.19	0
21	CLA	3	614	-	45,53,73	1.25	3 (6%)	52,89,113	1.04	2 (3%)
28	LUT	12	619	-	42,43,43	0.21	0	51,60,60	0.40	0
28	LUT	3	720	-	42,43,43	0.23	0	51,60,60	0.34	0
21	CLA	A	832	-	55,63,73	1.12	4 (7%)	64,101,113	0.94	2 (3%)
21	CLA	A2	834	-	65,73,73	1.03	3 (4%)	76,113,113	0.87	2 (2%)
28	LUT	3	622	-	42,43,43	0.31	0	51,60,60	0.34	0
21	CLA	B2	817	-	65,73,73	1.04	4 (6%)	76,113,113	0.86	2 (2%)
26	LMU	K2	208	-	24,24,36	0.11	0	29,29,47	0.31	0
23	LHG	1	620	21	38,38,48	0.26	0	41,44,54	0.29	0
27	LMG	J2	103	-	42,42,55	0.18	0	50,50,63	0.39	0
21	CLA	32	611	-	65,73,73	1.04	3 (4%)	76,113,113	0.86	2 (2%)
28	LUT	5	626	-	42,43,43	0.24	0	51,60,60	0.36	0
28	LUT	32	621	-	42,43,43	0.29	0	51,60,60	0.37	0
21	CLA	B	802	-	65,73,73	1.01	3 (4%)	76,113,113	0.85	3 (3%)
21	CLA	4	612	16	45,53,73	1.28	3 (6%)	52,89,113	1.01	2 (3%)
24	BCR	32	719	-	41,41,41	0.11	0	56,56,56	0.40	0
26	LMU	1	627	-	22,22,36	0.13	0	27,27,47	0.29	0
30	CHL	52	606	33	46,54,74	2.40	9 (19%)	49,90,114	1.37	7 (14%)
21	CLA	B	810	-	65,73,73	1.03	3 (4%)	76,113,113	0.87	2 (2%)
24	BCR	L	205	-	41,41,41	0.15	0	56,56,56	0.37	0
21	CLA	12	613	33	65,73,73	1.02	4 (6%)	76,113,113	0.88	2 (2%)
21	CLA	B2	821	-	65,73,73	1.03	4 (6%)	76,113,113	0.86	2 (2%)
21	CLA	B2	833	-	58,66,73	1.05	4 (6%)	67,104,113	0.95	3 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	A2	827	33	65,73,73	1.03	4 (6%)	76,113,113	0.87	2 (2%)
31	XAT	Z2	618	-	39,47,47	0.14	0	54,74,74	0.56	0
23	LHG	7	625	21	48,48,48	0.24	0	51,54,54	0.23	0
26	LMU	7	628	-	22,22,36	0.15	0	27,27,47	0.33	0
26	LMU	6	630	-	24,24,36	0.15	0	29,29,47	0.29	0
26	LMU	5	627	-	24,24,36	0.13	0	29,29,47	0.26	0
21	CLA	B	841	23	65,73,73	1.03	3 (4%)	76,113,113	0.88	2 (2%)
21	CLA	52	612	17	45,53,73	1.25	3 (6%)	52,89,113	1.01	2 (3%)
21	CLA	12	609	12	65,73,73	1.04	3 (4%)	76,113,113	0.86	2 (2%)
21	CLA	72	608	33	50,58,73	1.18	3 (6%)	58,95,113	0.96	2 (3%)
21	CLA	A2	816	-	65,73,73	1.03	3 (4%)	76,113,113	0.87	2 (2%)
21	CLA	5	602	17	65,73,73	1.03	3 (4%)	76,113,113	0.84	2 (2%)
21	CLA	6	604	-	65,73,73	1.04	3 (4%)	76,113,113	0.85	2 (2%)
21	CLA	B2	828	-	65,73,73	1.02	3 (4%)	76,113,113	0.84	2 (2%)
21	CLA	92	612	19	65,73,73	1.03	3 (4%)	76,113,113	0.84	2 (2%)
23	LHG	62	629	-	35,35,48	0.27	0	38,41,54	0.28	0
30	CHL	42	601	16	66,74,74	2.00	10 (15%)	73,114,114	1.14	7 (9%)
21	CLA	62	604	-	65,73,73	1.03	3 (4%)	76,113,113	0.85	2 (2%)
26	LMU	A	857	-	35,35,36	0.10	0	46,46,47	0.18	0
21	CLA	1	608	33	65,73,73	1.04	3 (4%)	76,113,113	0.86	2 (2%)
28	LUT	3	621	-	42,43,43	0.29	0	51,60,60	0.37	0
21	CLA	62	611	23	58,66,73	1.10	3 (5%)	67,104,113	0.91	2 (2%)
21	CLA	12	608	33	65,73,73	1.05	3 (4%)	76,113,113	0.87	2 (2%)
21	CLA	A2	841	-	65,73,73	1.02	4 (6%)	76,113,113	0.87	2 (2%)
21	CLA	6	613	33	65,73,73	1.04	3 (4%)	76,113,113	0.88	2 (2%)
21	CLA	B	834	-	60,68,73	1.06	3 (5%)	70,107,113	0.90	2 (2%)
28	LUT	Z2	617	-	42,43,43	0.27	0	51,60,60	0.40	0
21	CLA	7	611	23	65,73,73	1.03	3 (4%)	76,113,113	0.84	2 (2%)
21	CLA	4	614	-	55,63,73	1.14	3 (5%)	64,101,113	0.94	2 (3%)
24	BCR	A2	850	-	41,41,41	0.15	0	56,56,56	0.24	0
27	LMG	82	626	-	32,32,55	0.20	0	40,40,63	0.19	0
21	CLA	B	823	-	65,73,73	1.02	4 (6%)	76,113,113	0.89	2 (2%)
28	LUT	4	619	-	42,43,43	0.25	0	51,60,60	0.43	0
21	CLA	1	616	12	46,54,73	1.22	3 (6%)	53,90,113	1.03	2 (3%)
26	LMU	A2	857	-	35,35,36	0.10	0	46,46,47	0.17	0
21	CLA	1	613	33	65,73,73	1.02	4 (6%)	76,113,113	0.88	2 (2%)
21	CLA	B	803	-	65,73,73	1.03	3 (4%)	76,113,113	0.83	2 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	Z	610	12	60,68,73	1.06	3 (5%)	70,107,113	0.88	2 (2%)
21	CLA	52	617	-	65,73,73	1.04	3 (4%)	76,113,113	0.85	2 (2%)
32	NEX	5	625	-	38,46,46	0.54	1 (2%)	50,70,70	0.80	2 (4%)
21	CLA	32	617	13	46,54,73	1.22	3 (6%)	53,90,113	1.02	2 (3%)
24	BCR	I2	172	-	41,41,41	0.19	0	56,56,56	0.37	0
21	CLA	B2	810	-	65,73,73	1.02	3 (4%)	76,113,113	0.87	2 (2%)
21	CLA	7	603	-	52,60,73	1.14	3 (5%)	60,97,113	0.98	2 (3%)
28	LUT	72	621	-	42,43,43	0.25	0	51,60,60	0.38	0
21	CLA	52	614	-	45,53,73	1.26	3 (6%)	52,89,113	1.03	2 (3%)
28	LUT	52	626	-	42,43,43	0.23	0	51,60,60	0.36	0
27	LMG	62	633	-	19,19,55	0.31	0	19,19,63	0.30	0
24	BCR	I	172	-	41,41,41	0.20	0	56,56,56	0.37	0
28	LUT	7	624	-	42,43,43	0.21	0	51,60,60	0.41	0
21	CLA	A	809	1	65,73,73	1.03	4 (6%)	76,113,113	0.94	4 (5%)
28	LUT	52	620	-	42,43,43	0.24	0	51,60,60	0.44	0
21	CLA	B	824	33	65,73,73	1.04	3 (4%)	76,113,113	0.85	2 (2%)
21	CLA	B2	812	-	65,73,73	1.03	4 (6%)	76,113,113	0.87	2 (2%)
27	LMG	9	620	21	44,44,55	0.18	0	52,52,63	0.35	0
21	CLA	3	603	-	65,73,73	1.02	3 (4%)	76,113,113	0.84	2 (2%)
21	CLA	9	603	27,19	55,63,73	1.13	4 (7%)	64,101,113	0.93	2 (3%)
23	LHG	B2	851	21	44,44,48	0.25	0	47,50,54	0.31	0
24	BCR	72	623	-	41,41,41	0.15	0	56,56,56	0.38	0
21	CLA	B2	830	-	45,53,73	1.22	4 (8%)	52,89,113	1.05	2 (3%)
21	CLA	7	610	14	65,73,73	1.02	3 (4%)	76,113,113	0.91	2 (2%)
21	CLA	Z	608	33	50,58,73	1.19	3 (6%)	58,95,113	1.00	2 (3%)
21	CLA	32	614	-	45,53,73	1.25	3 (6%)	52,89,113	1.03	2 (3%)
21	CLA	K	201	11	45,53,73	1.27	3 (6%)	52,89,113	1.01	2 (3%)
21	CLA	62	614	-	50,58,73	1.19	3 (6%)	58,95,113	0.99	2 (3%)
21	CLA	Z2	604	33	57,65,73	1.10	3 (5%)	66,103,113	0.93	2 (3%)
26	LMU	12	627	-	22,22,36	0.14	0	27,27,47	0.30	0
21	CLA	92	610	19	60,68,73	1.07	4 (6%)	70,107,113	0.94	3 (4%)
21	CLA	A	820	-	65,73,73	1.02	4 (6%)	76,113,113	0.87	3 (3%)
26	LMU	82	624	-	24,24,36	0.15	0	29,29,47	0.26	0
26	LMU	A2	865	-	24,24,36	0.13	0	29,29,47	0.46	0
21	CLA	A	821	-	55,63,73	1.11	3 (5%)	64,101,113	0.90	2 (3%)
21	CLA	9	610	19	60,68,73	1.08	4 (6%)	70,107,113	0.94	3 (4%)
21	CLA	Z	611	23	60,68,73	1.07	3 (5%)	70,107,113	0.91	2 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	A2	828	-	65,73,73	1.05	3 (4%)	76,113,113	0.80	2 (2%)
21	CLA	A2	805	-	55,63,73	1.10	4 (7%)	64,101,113	0.90	2 (3%)
27	LMG	B2	852	-	43,43,55	0.18	0	51,51,63	0.24	0
21	CLA	A2	815	-	55,63,73	1.13	3 (5%)	64,101,113	0.90	2 (3%)
21	CLA	A	829	-	65,73,73	1.04	3 (4%)	76,113,113	0.84	2 (2%)
21	CLA	B2	832	-	65,73,73	1.01	4 (6%)	76,113,113	0.86	2 (2%)
28	LUT	9	617	-	42,43,43	0.21	0	51,60,60	0.38	0
24	BCR	3	719	-	41,41,41	0.12	0	56,56,56	0.40	0
21	CLA	B	839	33	65,73,73	1.06	3 (4%)	76,113,113	0.89	2 (2%)
21	CLA	B2	814	-	60,68,73	1.07	3 (5%)	70,107,113	0.90	3 (4%)
21	CLA	Z2	609	12	65,73,73	1.06	3 (4%)	76,113,113	0.86	2 (2%)
26	LMU	8	628	-	24,24,36	0.16	0	29,29,47	0.32	0
21	CLA	A2	813	-	65,73,73	1.04	3 (4%)	76,113,113	0.90	2 (2%)
27	LMG	A	860	-	36,36,55	0.20	0	44,44,63	0.26	0
28	LUT	Z	617	-	42,43,43	0.26	0	51,60,60	0.40	0
21	CLA	A2	833	-	65,73,73	1.03	4 (6%)	76,113,113	0.86	2 (2%)
21	CLA	8	604	33	60,68,73	1.09	3 (5%)	70,107,113	0.92	2 (2%)
26	LMU	62	631	-	24,24,36	0.15	0	29,29,47	0.28	0
21	CLA	B2	825	33	65,73,73	1.02	4 (6%)	76,113,113	0.82	2 (2%)
30	CHL	1	601	12	66,74,74	1.97	9 (13%)	73,114,114	1.13	7 (9%)
21	CLA	A2	839	-	65,73,73	1.04	4 (6%)	76,113,113	0.87	2 (2%)
24	BCR	B	848	-	41,41,41	0.13	0	56,56,56	0.46	0
21	CLA	12	612	12	45,53,73	1.26	3 (6%)	52,89,113	1.01	2 (3%)
21	CLA	92	603	27,19	55,63,73	1.13	3 (5%)	64,101,113	0.94	2 (3%)
21	CLA	A	839	-	65,73,73	1.03	4 (6%)	76,113,113	0.86	2 (2%)
23	LHG	82	620	21	43,43,48	0.25	0	46,49,54	0.26	0
28	LUT	9	616	-	42,43,43	0.26	0	51,60,60	0.37	0
26	LMU	8	625	-	24,24,36	0.12	0	29,29,47	0.28	0
21	CLA	5	612	17	45,53,73	1.26	3 (6%)	52,89,113	1.02	2 (3%)
24	BCR	G	205	-	41,41,41	0.14	0	56,56,56	0.32	0
21	CLA	A2	842	-	65,73,73	1.00	4 (6%)	76,113,113	0.86	2 (2%)
27	LMG	12	628	-	42,42,55	0.19	0	50,50,63	0.28	0
26	LMU	G	206	-	24,24,36	0.14	0	29,29,47	0.25	0
30	CHL	6	601	18	66,74,74	2.02	10 (15%)	73,114,114	1.19	8 (10%)
21	CLA	7	613	14	65,73,73	1.03	3 (4%)	76,113,113	0.87	2 (2%)
21	CLA	72	609	14	45,53,73	1.25	3 (6%)	52,89,113	1.01	2 (3%)
21	CLA	Z	614	-	50,58,73	1.18	3 (6%)	58,95,113	0.99	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	CHL	62	601	18	66,74,74	2.01	9 (13%)	73,114,114	1.19	8 (10%)
30	CHL	62	607	33	66,74,74	2.05	9 (13%)	73,114,114	1.18	8 (10%)
28	LUT	6	621	-	42,43,43	0.24	0	51,60,60	0.39	0
26	LMU	Z	622	-	32,32,36	0.11	0	43,43,47	0.17	0
27	LMG	J	103	-	42,42,55	0.18	0	50,50,63	0.39	0
30	CHL	7	607	33	46,54,74	2.37	9 (19%)	49,90,114	1.39	7 (14%)
23	LHG	72	625	21	48,48,48	0.23	0	51,54,54	0.23	0
21	CLA	B2	841	23	65,73,73	1.02	3 (4%)	76,113,113	0.88	2 (2%)
21	CLA	12	603	-	57,65,73	1.10	3 (5%)	66,103,113	0.91	2 (3%)
26	LMU	6	628	-	24,24,36	0.13	0	29,29,47	0.29	0
21	CLA	B2	829	-	65,73,73	0.99	4 (6%)	76,113,113	0.87	2 (2%)
26	LMU	A	861	-	24,24,36	0.13	0	29,29,47	0.30	0
21	CLA	4	616	16	45,53,73	1.26	3 (6%)	52,89,113	1.04	2 (3%)
24	BCR	J	102	-	41,41,41	0.14	0	56,56,56	0.31	0
21	CLA	B2	834	-	60,68,73	1.06	3 (5%)	70,107,113	0.91	2 (2%)
21	CLA	B	822	-	59,67,73	1.08	3 (5%)	68,105,113	0.91	2 (2%)
21	CLA	A2	812	-	65,73,73	1.00	4 (6%)	76,113,113	0.84	2 (2%)
27	LMG	B2	854	-	36,36,55	0.20	0	44,44,63	0.17	0
24	BCR	B2	843	-	41,41,41	0.16	0	56,56,56	0.30	0
26	LMU	A2	863	-	36,36,36	0.10	0	47,47,47	0.27	0
25	SF4	C	102	3	0,12,12	-	-	-	-	-
21	CLA	6	617	-	45,53,73	1.26	3 (6%)	52,89,113	1.03	3 (5%)
26	LMU	A	863	-	36,36,36	0.10	0	47,47,47	0.27	0
21	CLA	A	808	-	50,58,73	1.18	4 (8%)	58,95,113	0.96	2 (3%)
21	CLA	A2	837	1	57,65,73	1.12	3 (5%)	66,103,113	0.94	2 (3%)
21	CLA	B2	803	-	65,73,73	1.03	3 (4%)	76,113,113	0.83	2 (2%)
21	CLA	52	616	17	53,61,73	1.16	3 (5%)	61,98,113	0.97	2 (3%)
26	LMU	4	626	-	20,20,36	0.15	0	25,25,47	0.28	0
27	LMG	8	626	-	32,32,55	0.20	0	40,40,63	0.19	0
20	CL0	A2	801	-	65,73,73	1.96	9 (13%)	76,113,113	1.11	7 (9%)
21	CLA	A	843	33	65,73,73	1.03	4 (6%)	76,113,113	0.88	2 (2%)
21	CLA	9	604	19	53,61,73	1.14	4 (7%)	61,98,113	0.97	3 (4%)
21	CLA	Z	609	12	65,73,73	1.06	3 (4%)	76,113,113	0.86	2 (2%)
28	LUT	A2	856	-	42,43,43	0.27	0	51,60,60	0.35	0
30	CHL	4	607	33	66,74,74	2.00	10 (15%)	73,114,114	1.14	8 (10%)
27	LMG	8	629	-	42,42,55	0.19	0	50,50,63	0.16	0
21	CLA	6	612	18	45,53,73	1.25	3 (6%)	52,89,113	1.02	2 (3%)
21	CLA	B	838	-	50,58,73	1.19	3 (6%)	58,95,113	0.97	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	LHG	A2	846	-	48,48,48	0.24	0	51,54,54	0.29	0
27	LMG	A2	859	-	48,48,55	0.18	0	56,56,63	0.17	0
25	SF4	C2	102	3	0,12,12	-	-	-	-	-
32	NEX	6	625	-	38,46,46	0.19	0	50,70,70	0.83	2 (4%)
26	LMU	7	629	-	28,28,36	0.10	0	39,39,47	0.27	0
24	BCR	B	846	-	41,41,41	0.13	0	56,56,56	0.33	0
21	CLA	B2	840	-	65,73,73	1.01	4 (6%)	76,113,113	0.86	2 (2%)
21	CLA	72	602	14	65,73,73	1.03	3 (4%)	76,113,113	0.86	2 (2%)
21	CLA	32	603	-	65,73,73	1.03	3 (4%)	76,113,113	0.84	2 (2%)
30	CHL	92	607	33	51,59,74	2.37	9 (17%)	55,96,114	1.34	9 (16%)
21	CLA	Z	616	12	60,68,73	1.08	3 (5%)	70,107,113	0.89	2 (2%)
23	LHG	9	622	21	40,40,48	0.25	0	43,46,54	0.28	0
21	CLA	6	609	18	55,63,73	1.12	3 (5%)	64,101,113	0.97	3 (4%)
21	CLA	B2	808	-	65,73,73	1.03	3 (4%)	76,113,113	0.84	2 (2%)
21	CLA	A2	807	1	65,73,73	1.02	4 (6%)	76,113,113	0.81	2 (2%)
21	CLA	B2	838	-	50,58,73	1.18	3 (6%)	58,95,113	0.96	2 (3%)
26	LMU	62	632	-	20,20,36	0.16	0	25,25,47	0.26	0
26	LMU	G2	206	-	24,24,36	0.14	0	29,29,47	0.25	0
28	LUT	5	620	-	42,43,43	0.25	0	51,60,60	0.44	0
21	CLA	B	837	-	65,73,73	1.03	4 (6%)	76,113,113	0.86	2 (2%)
30	CHL	5	606	33	46,54,74	2.41	9 (19%)	49,90,114	1.36	7 (14%)
22	PQN	B2	842	-	34,34,34	0.30	0	42,45,45	0.37	0
21	CLA	J	101	9	55,63,73	1.13	3 (5%)	64,101,113	0.92	2 (3%)
28	LUT	F	305	-	42,43,43	0.39	0	51,60,60	0.78	1 (1%)
21	CLA	B2	839	33	65,73,73	1.05	3 (4%)	76,113,113	0.88	2 (2%)
31	XAT	62	624	-	39,47,47	0.12	0	54,74,74	0.59	0
21	CLA	72	613	14	65,73,73	1.03	3 (4%)	76,113,113	0.87	2 (2%)
21	CLA	B	811	-	65,73,73	1.03	4 (6%)	76,113,113	0.87	2 (2%)
21	CLA	4	609	16	60,68,73	1.09	3 (5%)	70,107,113	0.91	2 (2%)
21	CLA	42	603	16	65,73,73	1.05	4 (6%)	76,113,113	0.85	2 (2%)
26	LMU	42	625	-	34,34,36	0.11	0	45,45,47	0.20	0
21	CLA	B2	802	-	65,73,73	1.01	3 (4%)	76,113,113	0.85	3 (3%)
21	CLA	B	833	-	58,66,73	1.05	4 (6%)	67,104,113	0.95	2 (2%)
27	LMG	A2	860	-	36,36,55	0.20	0	44,44,63	0.26	0
30	CHL	42	607	33	66,74,74	2.00	10 (15%)	73,114,114	1.14	8 (10%)
30	CHL	82	601	15	66,74,74	1.98	10 (15%)	73,114,114	1.10	7 (9%)
30	CHL	Z2	601	12	66,74,74	1.98	9 (13%)	73,114,114	1.14	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	CHL	7	601	14	66,74,74	2.01	10 (15%)	73,114,114	1.14	7 (9%)
21	CLA	A2	811	-	65,73,73	1.01	4 (6%)	76,113,113	0.86	2 (2%)
21	CLA	F2	304	6	65,73,73	1.05	3 (4%)	76,113,113	0.94	3 (3%)
21	CLA	82	602	15	62,70,73	1.07	4 (6%)	72,109,113	0.88	2 (2%)
24	BCR	B	847	-	41,41,41	0.19	0	56,56,56	0.41	0
28	LUT	Z2	619	-	26,26,43	0.36	0	34,35,60	0.37	0
31	XAT	5	624	-	39,47,47	0.11	0	54,74,74	0.59	0
21	CLA	B2	837	-	65,73,73	1.02	4 (6%)	76,113,113	0.86	2 (2%)
21	CLA	5	621	33	46,54,73	1.28	3 (6%)	53,90,113	1.13	5 (9%)
21	CLA	62	612	18	45,53,73	1.25	3 (6%)	52,89,113	1.02	2 (3%)
31	XAT	1	618	-	39,47,47	0.13	0	54,74,74	0.68	2 (3%)
21	CLA	A2	829	-	65,73,73	1.04	3 (4%)	76,113,113	0.84	2 (2%)
21	CLA	K	203	33	60,68,73	1.09	3 (5%)	70,107,113	0.89	2 (2%)
21	CLA	32	606	33	42,50,73	1.28	3 (7%)	48,85,113	1.07	2 (4%)
24	BCR	B	843	-	41,41,41	0.16	0	56,56,56	0.31	0
32	NEX	62	625	-	38,46,46	0.28	0	50,70,70	0.85	2 (4%)
28	LUT	8	617	-	42,43,43	0.29	0	51,60,60	0.42	0
21	CLA	1	612	12	45,53,73	1.25	3 (6%)	52,89,113	1.01	2 (3%)
24	BCR	3	718	-	41,41,41	0.15	0	56,56,56	0.34	0
21	CLA	8	610	15	65,73,73	1.02	3 (4%)	76,113,113	0.86	2 (2%)
24	BCR	B2	844	-	41,41,41	0.14	0	56,56,56	0.45	0
27	LMG	A	859	-	48,48,55	0.18	0	56,56,63	0.17	0
24	BCR	4	621	-	41,41,41	0.13	0	56,56,56	0.36	0
23	LHG	32	721	-	30,30,48	0.27	0	33,36,54	0.35	0
26	LMU	9	624	-	24,24,36	0.15	0	29,29,47	0.38	0
30	CHL	1	606	33	46,54,74	2.40	10 (21%)	49,90,114	1.38	7 (14%)
21	CLA	A	819	-	60,68,73	1.09	3 (5%)	70,107,113	0.92	2 (2%)
24	BCR	32	718	-	41,41,41	0.16	0	56,56,56	0.34	0
21	CLA	B	816	-	65,73,73	1.02	3 (4%)	76,113,113	0.88	2 (2%)
21	CLA	Z2	603	-	55,63,73	1.14	3 (5%)	64,101,113	0.92	2 (3%)
27	LMG	92	620	21	44,44,55	0.18	0	52,52,63	0.36	0
24	BCR	7	623	-	41,41,41	0.15	0	56,56,56	0.38	0
21	CLA	A	835	-	65,73,73	1.03	3 (4%)	76,113,113	0.86	2 (2%)
21	CLA	5	616	17	53,61,73	1.15	3 (5%)	61,98,113	0.96	2 (3%)
21	CLA	1	609	12	65,73,73	1.04	3 (4%)	76,113,113	0.87	2 (2%)
30	CHL	4	601	16	66,74,74	2.00	9 (13%)	73,114,114	1.15	7 (9%)
21	CLA	82	611	23	45,53,73	1.24	3 (6%)	52,89,113	1.07	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	3	606	33	42,50,73	1.28	3 (7%)	48,85,113	1.07	2 (4%)
21	CLA	Z2	611	23	60,68,73	1.06	3 (5%)	70,107,113	0.91	2 (2%)
24	BCR	B2	801	-	41,41,41	0.17	0	56,56,56	0.38	0
21	CLA	K2	204	-	46,54,73	1.21	3 (6%)	53,90,113	1.04	2 (3%)
23	LHG	42	623	-	37,37,48	0.25	0	40,43,54	0.29	0
21	CLA	A	812	-	65,73,73	1.00	4 (6%)	76,113,113	0.85	2 (2%)
30	CHL	8	607	33	66,74,74	2.01	8 (12%)	73,114,114	1.16	8 (10%)
23	LHG	A2	847	21	37,37,48	0.26	0	40,43,54	0.29	0
21	CLA	K	204	-	46,54,73	1.23	3 (6%)	53,90,113	1.05	3 (5%)
26	LMU	72	627	-	33,33,36	0.11	0	44,44,47	0.16	0
21	CLA	B2	816	-	65,73,73	1.01	3 (4%)	76,113,113	0.88	2 (2%)
30	CHL	6	606	33	58,66,74	2.16	9 (15%)	63,104,114	1.23	7 (11%)
24	BCR	B2	848	-	41,41,41	0.13	0	56,56,56	0.46	0
21	CLA	L2	204	-	45,53,73	1.26	3 (6%)	52,89,113	1.05	3 (5%)
26	LMU	72	629	-	28,28,36	0.10	0	39,39,47	0.27	0
21	CLA	A	830	-	65,73,73	1.03	3 (4%)	76,113,113	0.85	2 (2%)
26	LMU	42	626	-	20,20,36	0.15	0	25,25,47	0.28	0
21	CLA	A2	825	-	55,63,73	1.12	3 (5%)	64,101,113	0.94	2 (3%)
23	LHG	Z	620	21	38,38,48	0.25	0	41,44,54	0.28	0
27	LMG	82	629	-	42,42,55	0.19	0	50,50,63	0.16	0
21	CLA	62	602	18	65,73,73	1.03	3 (4%)	76,113,113	0.86	2 (2%)
21	CLA	B	827	-	65,73,73	1.04	3 (4%)	76,113,113	0.87	2 (2%)
24	BCR	A2	848	-	41,41,41	0.13	0	56,56,56	0.30	0
21	CLA	A2	817	33	55,63,73	1.14	3 (5%)	64,101,113	0.92	2 (3%)
26	LMU	12	625	-	24,24,36	0.12	0	29,29,47	0.31	0
30	CHL	82	607	33	66,74,74	2.01	8 (12%)	73,114,114	1.16	8 (10%)
24	BCR	L2	201	-	41,41,41	0.17	0	56,56,56	0.35	0
24	BCR	J2	102	-	41,41,41	0.16	0	56,56,56	0.30	0
21	CLA	8	602	15	62,70,73	1.06	4 (6%)	72,109,113	0.88	2 (2%)
21	CLA	72	611	23	65,73,73	1.03	3 (4%)	76,113,113	0.85	2 (2%)
21	CLA	A2	818	-	65,73,73	1.01	3 (4%)	76,113,113	0.84	2 (2%)
27	LMG	12	624	-	36,36,55	0.20	0	44,44,63	0.18	0
21	CLA	K2	201	11	45,53,73	1.27	3 (6%)	52,89,113	1.00	2 (3%)
22	PQN	A2	844	-	34,34,34	0.31	0	42,45,45	0.36	0
27	LMG	6	633	-	19,19,55	0.31	0	19,19,63	0.29	0
21	CLA	4	613	16	65,73,73	1.04	3 (4%)	76,113,113	0.88	2 (2%)
21	CLA	42	611	23	60,68,73	1.08	3 (5%)	70,107,113	0.90	3 (4%)
30	CHL	12	601	12	66,74,74	1.97	9 (13%)	73,114,114	1.12	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	A2	830	-	65,73,73	1.01	3 (4%)	76,113,113	0.85	2 (2%)
21	CLA	A	813	-	65,73,73	1.04	3 (4%)	76,113,113	0.90	2 (2%)
21	CLA	B	828	-	65,73,73	1.03	3 (4%)	76,113,113	0.84	2 (2%)
28	LUT	62	621	-	42,43,43	0.23	0	51,60,60	0.39	0
21	CLA	A	814	-	65,73,73	1.03	3 (4%)	76,113,113	0.84	2 (2%)
21	CLA	K2	203	33	60,68,73	1.10	3 (5%)	70,107,113	0.89	2 (2%)
21	CLA	A2	819	-	60,68,73	1.08	3 (5%)	70,107,113	0.91	2 (2%)
21	CLA	9	601	19	46,54,73	1.23	3 (6%)	53,90,113	1.03	2 (3%)
26	LMU	82	628	-	24,24,36	0.16	0	29,29,47	0.31	0
28	LUT	92	617	-	42,43,43	0.21	0	51,60,60	0.38	0
21	CLA	6	614	-	50,58,73	1.19	3 (6%)	58,95,113	0.99	2 (3%)
21	CLA	B2	827	-	65,73,73	1.04	3 (4%)	76,113,113	0.87	2 (2%)
21	CLA	A	804	-	65,73,73	1.02	4 (6%)	76,113,113	0.85	2 (2%)
21	CLA	Z2	613	33	65,73,73	1.03	3 (4%)	76,113,113	0.88	3 (3%)
26	LMU	72	628	-	22,22,36	0.15	0	27,27,47	0.33	0
21	CLA	52	613	17	56,64,73	1.11	3 (5%)	65,102,113	0.93	2 (3%)
26	LMU	62	628	-	24,24,36	0.13	0	29,29,47	0.30	0
21	CLA	4	603	16	65,73,73	1.06	4 (6%)	76,113,113	0.85	2 (2%)
21	CLA	A	816	-	65,73,73	1.03	3 (4%)	76,113,113	0.87	2 (2%)
21	CLA	B2	822	-	59,67,73	1.07	3 (5%)	68,105,113	0.91	2 (2%)
21	CLA	62	617	-	45,53,73	1.25	3 (6%)	52,89,113	1.03	2 (3%)
21	CLA	9	614	-	45,53,73	1.26	3 (6%)	52,89,113	1.03	2 (3%)
21	CLA	B2	806	2	65,73,73	1.04	3 (4%)	76,113,113	0.79	2 (2%)
20	CL0	A	801	-	65,73,73	1.96	9 (13%)	76,113,113	1.10	7 (9%)
24	BCR	A	852	-	41,41,41	0.14	0	56,56,56	0.39	0
21	CLA	B	805	-	65,73,73	1.00	4 (6%)	76,113,113	0.88	2 (2%)
21	CLA	4	604	33	50,58,73	1.18	3 (6%)	58,95,113	0.99	3 (5%)
30	CHL	62	606	33	58,66,74	2.16	9 (15%)	63,104,114	1.23	7 (11%)
21	CLA	K	206	11	45,53,73	1.24	3 (6%)	52,89,113	1.02	2 (3%)
21	CLA	B	815	-	65,73,73	1.02	3 (4%)	76,113,113	0.85	2 (2%)
26	LMU	62	630	-	24,24,36	0.15	0	29,29,47	0.28	0
21	CLA	5	603	-	65,73,73	1.03	3 (4%)	76,113,113	0.87	2 (2%)
21	CLA	72	614	-	43,51,73	1.27	3 (6%)	49,86,113	1.07	2 (4%)
21	CLA	9	613	19	65,73,73	1.01	3 (4%)	76,113,113	0.89	2 (2%)
21	CLA	52	603	-	65,73,73	1.04	3 (4%)	76,113,113	0.86	3 (3%)
28	LUT	F2	305	-	42,43,43	0.38	0	51,60,60	0.78	1 (1%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	XAT	82	618	-	39,47,47	0.15	0	54,74,74	0.57	0
28	LUT	72	624	-	42,43,43	0.21	0	51,60,60	0.41	0
21	CLA	4	610	16	60,68,73	1.08	3 (5%)	70,107,113	0.88	2 (2%)
30	CHL	Z	601	12	66,74,74	1.99	11 (16%)	73,114,114	1.15	7 (9%)
21	CLA	A2	804	-	65,73,73	1.01	4 (6%)	76,113,113	0.84	2 (2%)
21	CLA	B	806	2	65,73,73	1.03	3 (4%)	76,113,113	0.78	2 (2%)
21	CLA	B	831	-	55,63,73	1.10	4 (7%)	64,101,113	0.93	3 (4%)
21	CLA	8	613	15	65,73,73	1.02	3 (4%)	76,113,113	0.86	2 (2%)
24	BCR	B	801	-	41,41,41	0.17	0	56,56,56	0.38	0
27	LMG	B	854	-	36,36,55	0.19	0	44,44,63	0.17	0
21	CLA	L	203	-	65,73,73	1.03	3 (4%)	76,113,113	0.84	2 (2%)
21	CLA	B2	835	33	45,53,73	1.24	3 (6%)	52,89,113	1.02	2 (3%)
21	CLA	62	609	18	55,63,73	1.12	3 (5%)	64,101,113	0.97	3 (4%)
21	CLA	A	810	1	65,73,73	1.03	3 (4%)	76,113,113	0.87	2 (2%)
21	CLA	A	825	-	55,63,73	1.12	4 (7%)	64,101,113	0.93	2 (3%)
24	BCR	K2	207	-	41,41,41	0.14	0	56,56,56	0.28	0
30	CHL	7	606	33	46,54,74	2.38	10 (21%)	49,90,114	1.36	8 (16%)
30	CHL	72	606	33	46,54,74	2.38	10 (21%)	49,90,114	1.38	8 (16%)
21	CLA	7	604	33	51,59,73	1.16	3 (5%)	59,96,113	0.96	2 (3%)
21	CLA	A	834	-	65,73,73	1.04	4 (6%)	76,113,113	0.87	2 (2%)
26	LMU	A	862	-	20,20,36	0.14	0	25,25,47	0.28	0
21	CLA	B2	823	-	65,73,73	1.03	4 (6%)	76,113,113	0.90	2 (2%)
21	CLA	82	614	-	57,65,73	1.12	3 (5%)	66,103,113	0.90	2 (3%)
21	CLA	8	608	33	50,58,73	1.19	3 (6%)	58,95,113	0.97	2 (3%)
24	BCR	A	850	-	41,41,41	0.15	0	56,56,56	0.24	0
21	CLA	L2	203	-	65,73,73	1.03	3 (4%)	76,113,113	0.84	2 (2%)
21	CLA	B	836	-	60,68,73	1.07	3 (5%)	70,107,113	0.91	2 (2%)
26	LMU	A2	864	-	24,24,36	0.12	0	29,29,47	0.29	0
21	CLA	6	622	33	55,63,73	1.13	3 (5%)	64,101,113	0.92	2 (3%)
28	LUT	1	619	-	42,43,43	0.21	0	51,60,60	0.40	0
21	CLA	B2	804	-	45,53,73	1.24	3 (6%)	52,89,113	0.99	2 (3%)
23	LHG	8	620	21	43,43,48	0.25	0	46,49,54	0.26	0
24	BCR	6	623	-	41,41,41	0.16	0	56,56,56	0.35	0
28	LUT	Z	619	-	26,26,43	0.36	0	34,35,60	0.37	0
23	LHG	4	623	-	37,37,48	0.25	0	40,43,54	0.28	0
23	LHG	92	622	21	40,40,48	0.25	0	43,46,54	0.28	0
26	LMU	A	864	-	24,24,36	0.12	0	29,29,47	0.28	0
26	LMU	1	625	-	24,24,36	0.11	0	29,29,47	0.30	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	CHL	6	618	18	43,51,74	2.49	10 (23%)	45,86,114	1.47	9 (20%)
21	CLA	82	613	15	65,73,73	1.02	3 (4%)	76,113,113	0.87	2 (2%)
21	CLA	3	610	13	65,73,73	1.02	3 (4%)	76,113,113	0.87	2 (2%)
21	CLA	A	823	-	65,73,73	1.03	3 (4%)	76,113,113	0.86	3 (3%)
30	CHL	62	618	18	43,51,74	2.50	10 (23%)	45,86,114	1.46	9 (20%)
21	CLA	7	609	14	45,53,73	1.25	3 (6%)	52,89,113	1.00	2 (3%)
21	CLA	Z2	602	12	60,68,73	1.07	3 (5%)	70,107,113	0.91	2 (2%)
21	CLA	A2	854	33	65,73,73	1.06	3 (4%)	76,113,113	0.81	2 (2%)
21	CLA	A	802	-	65,73,73	1.01	4 (6%)	76,113,113	0.82	2 (2%)
21	CLA	G	204	7	46,54,73	1.23	3 (6%)	53,90,113	1.01	2 (3%)
24	BCR	B2	847	-	41,41,41	0.19	0	56,56,56	0.41	0
21	CLA	3	604	33	65,73,73	1.03	3 (4%)	76,113,113	0.86	2 (2%)
24	BCR	A	851	-	41,41,41	0.14	0	56,56,56	0.33	0
21	CLA	Z	604	33	57,65,73	1.10	3 (5%)	66,103,113	0.92	2 (3%)
28	LUT	12	617	-	42,43,43	0.26	0	51,60,60	0.40	0
21	CLA	82	603	-	65,73,73	1.06	4 (6%)	76,113,113	0.84	2 (2%)
22	PQN	B	842	-	34,34,34	0.31	0	42,45,45	0.37	0
21	CLA	B2	824	33	65,73,73	1.04	3 (4%)	76,113,113	0.86	2 (2%)
24	BCR	K	202	-	41,41,41	0.15	0	56,56,56	0.36	0
21	CLA	K2	206	11	45,53,73	1.25	3 (6%)	52,89,113	1.04	2 (3%)
21	CLA	3	602	13	60,68,73	1.07	4 (6%)	70,107,113	0.88	2 (2%)
21	CLA	9	602	19	60,68,73	1.07	4 (6%)	70,107,113	0.89	2 (2%)
21	CLA	5	613	17	56,64,73	1.11	3 (5%)	65,102,113	0.94	2 (3%)
21	CLA	F	301	33	65,73,73	1.00	3 (4%)	76,113,113	0.83	2 (2%)
28	LUT	42	619	-	42,43,43	0.25	0	51,60,60	0.43	0
30	CHL	5	608	33	51,59,74	2.29	10 (19%)	55,96,114	1.33	8 (14%)
21	CLA	A2	809	1	65,73,73	1.04	4 (6%)	76,113,113	0.93	3 (3%)
30	CHL	32	608	33	66,74,74	2.00	10 (15%)	73,114,114	1.15	7 (9%)
30	CHL	Z2	607	33	66,74,74	2.00	9 (13%)	73,114,114	1.16	7 (9%)
31	XAT	72	622	-	39,47,47	0.12	0	54,74,74	0.57	0
26	LMU	1	621	-	36,36,36	0.10	0	47,47,47	0.28	0

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
21	CLA	72	604	33	1/1/17/20	1/21/99/115	-
21	CLA	32	613	13	1/1/19/20	3/31/109/115	-
21	CLA	32	604	33	1/1/20/20	1/37/115/115	-
30	CHL	5	618	17	3/3/20/26	2/12/110/137	-
21	CLA	12	610	12	1/1/20/20	0/37/115/115	-
21	CLA	B	818	-	1/1/20/20	2/37/115/115	-
21	CLA	32	602	13	1/1/19/20	1/31/109/115	-
26	LMU	12	623	-	-	1/15/35/61	0/1/1/2
21	CLA	G2	204	7	1/1/15/20	4/15/93/115	-
21	CLA	82	610	15	1/1/20/20	2/37/115/115	-
21	CLA	42	604	33	1/1/17/20	1/19/97/115	-
21	CLA	7	602	14	1/1/20/20	2/37/115/115	-
30	CHL	42	606	33	3/3/24/26	1/27/125/137	-
30	CHL	42	608	-	3/3/26/26	3/39/137/137	-
30	CHL	9	606	-	3/3/20/26	0/10/108/137	-
21	CLA	42	616	16	1/1/15/20	0/13/91/115	-
21	CLA	42	613	16	1/1/20/20	5/37/115/115	-
28	LUT	92	616	-	-	2/29/67/67	0/2/2/2
30	CHL	8	606	33	3/3/26/26	3/39/137/137	-
21	CLA	5	617	-	1/1/20/20	6/37/115/115	-
21	CLA	42	602	16	1/1/19/20	2/31/109/115	-
24	BCR	62	623	-	-	2/29/63/63	0/2/2/2
30	CHL	3	608	33	3/3/26/26	3/39/137/137	-
21	CLA	7	608	33	1/1/17/20	0/19/97/115	-
21	CLA	B	826	-	1/1/20/20	3/37/115/115	-
31	XAT	52	624	-	1/1/26/26	0/31/93/93	0/4/4/4
21	CLA	1	614	-	1/1/19/20	4/31/109/115	-
30	CHL	52	607	33	3/3/26/26	8/39/137/137	-
21	CLA	8	612	15	1/1/18/20	6/25/103/115	-
26	LMU	6	632	-	-	3/11/31/61	0/1/1/2
21	CLA	4	611	23	1/1/19/20	4/31/109/115	-
21	CLA	A	824	-	1/1/15/20	2/13/91/115	-
30	CHL	12	606	33	3/3/21/26	0/15/113/137	-
26	LMU	1	623	-	-	1/15/35/61	0/1/1/2
28	LUT	7	621	-	-	2/29/67/67	0/2/2/2
27	LMG	4	624	-	-	5/36/56/70	0/1/1/1
21	CLA	A2	823	-	1/1/20/20	6/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CHL	82	606	33	3/3/26/26	3/39/137/137	-
24	BCR	3	620	-	-	4/29/63/63	0/2/2/2
23	LHG	4	622	21	-	13/53/53/53	-
21	CLA	A	817	33	1/1/18/20	4/25/103/115	-
21	CLA	3	613	13	1/1/19/20	3/31/109/115	-
30	CHL	4	618	16	3/3/21/26	2/15/113/137	-
21	CLA	B	829	-	1/1/20/20	3/37/115/115	-
21	CLA	A	836	-	1/1/20/20	4/37/115/115	-
21	CLA	B2	831	-	1/1/18/20	1/25/103/115	-
21	CLA	52	611	23	1/1/18/20	2/25/103/115	-
25	SF4	A2	853	1,2	-	-	0/6/5/5
21	CLA	9	609	19	1/1/17/20	2/21/99/115	-
21	CLA	6	603	-	1/1/20/20	7/37/115/115	-
24	BCR	32	620	-	-	4/29/63/63	0/2/2/2
21	CLA	32	610	13	1/1/20/20	0/37/115/115	-
23	LHG	Z2	620	21	-	6/43/43/53	-
29	DGD	B	850	-	-	15/48/88/95	0/2/2/2
21	CLA	92	611	23	1/1/20/20	4/37/115/115	-
30	CHL	52	618	17	3/3/20/26	2/12/110/137	-
21	CLA	62	603	-	1/1/20/20	7/37/115/115	-
21	CLA	92	604	19	1/1/17/20	1/23/101/115	-
21	CLA	A2	843	33	1/1/20/20	5/37/115/115	-
26	LMU	92	624	-	-	4/15/35/61	0/1/1/2
26	LMU	82	627	-	-	9/21/61/61	0/2/2/2
27	LMG	72	626	-	-	7/32/52/70	0/1/1/1
21	CLA	6	610	18	1/1/19/20	3/31/109/115	-
21	CLA	12	602	12	1/1/19/20	2/31/109/115	-
31	XAT	Z	618	-	-	0/31/93/93	0/4/4/4
28	LUT	32	622	-	-	2/29/67/67	0/2/2/2
24	BCR	B2	845	-	-	4/29/63/63	0/2/2/2
21	CLA	92	602	19	1/1/19/20	2/31/109/115	-
30	CHL	5	607	33	3/3/26/26	8/39/137/137	-
26	LMU	4	625	-	-	3/19/59/61	0/2/2/2
23	LHG	32	623	-	-	13/51/51/53	-
21	CLA	8	611	23	1/1/15/20	2/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	LMU	7	627	-	-	2/18/58/61	0/2/2/2
21	CLA	62	610	18	1/1/19/20	2/31/109/115	-
21	CLA	A	840	-	1/1/20/20	9/37/115/115	-
21	CLA	B	821	-	1/1/20/20	3/37/115/115	-
26	LMU	A2	858	-	-	6/21/61/61	0/2/2/2
21	CLA	A	842	-	1/1/20/20	1/37/115/115	-
21	CLA	B	813	-	1/1/20/20	4/37/115/115	-
21	CLA	A	822	33	1/1/20/20	0/37/115/115	-
31	XAT	4	620	-	-	0/31/93/93	0/4/4/4
24	BCR	B	845	-	-	4/29/63/63	0/2/2/2
25	SF4	C2	101	3	-	-	0/6/5/5
21	CLA	Z2	608	33	1/1/17/20	0/19/97/115	-
21	CLA	6	602	18	1/1/20/20	2/37/115/115	-
21	CLA	B	820	-	1/1/18/20	5/27/105/115	-
21	CLA	A2	821	-	1/1/18/20	2/25/103/115	-
21	CLA	A	838	-	1/1/17/20	1/21/99/115	-
21	CLA	F	303	33	1/1/15/20	2/13/91/115	-
21	CLA	82	604	33	1/1/19/20	2/31/109/115	-
23	LHG	12	620	21	-	9/43/43/53	-
21	CLA	32	615	33	1/1/20/20	6/37/115/115	-
21	CLA	F	304	6	1/1/20/20	7/37/115/115	-
21	CLA	B2	819	33	1/1/19/20	3/31/109/115	-
21	CLA	B2	809	2	1/1/20/20	6/37/115/115	-
21	CLA	32	612	13	1/1/15/20	1/15/93/115	-
21	CLA	82	616	15	1/1/15/20	0/13/91/115	-
21	CLA	A2	802	-	1/1/20/20	0/37/115/115	-
21	CLA	A2	803	33	1/1/20/20	2/37/115/115	-
21	CLA	7	614	-	1/1/14/20	4/11/89/115	-
21	CLA	32	607	13	1/1/18/20	4/25/103/115	-
21	CLA	8	614	-	1/1/18/20	7/28/106/115	-
23	LHG	5	623	21	-	12/41/41/53	-
21	CLA	A2	806	-	1/1/20/20	12/37/115/115	-
21	CLA	G	203	-	1/1/19/20	3/31/109/115	-
24	BCR	B2	846	-	-	2/29/63/63	0/2/2/2
26	LMU	A2	861	-	-	3/15/35/61	0/1/1/2
24	BCR	K2	202	-	-	2/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	42	612	16	1/1/15/20	4/13/91/115	-
21	CLA	Z2	610	12	1/1/19/20	0/31/109/115	-
30	CHL	1	607	33	3/3/21/26	3/15/113/137	-
30	CHL	6	608	33	3/3/23/26	0/21/119/137	-
27	LMG	32	722	-	-	5/46/46/70	-
21	CLA	A	837	1	1/1/18/20	3/28/106/115	-
24	BCR	5	622	-	-	3/29/63/63	0/2/2/2
26	LMU	6	631	-	-	4/15/35/61	0/1/1/2
21	CLA	B	825	33	1/1/20/20	2/37/115/115	-
21	CLA	B2	820	-	1/1/18/20	4/27/105/115	-
21	CLA	A2	810	1	1/1/20/20	8/37/115/115	-
21	CLA	52	601	17	1/1/20/20	5/37/115/115	-
21	CLA	82	609	15	1/1/15/20	0/13/91/115	-
24	BCR	92	623	-	-	2/29/63/63	0/2/2/2
21	CLA	5	614	-	1/1/15/20	2/13/91/115	-
21	CLA	3	615	33	1/1/20/20	6/37/115/115	-
21	CLA	A	833	-	1/1/20/20	1/37/115/115	-
23	LHG	A	846	-	-	10/53/53/53	-
29	DGD	B2	850	-	-	10/48/88/95	0/2/2/2
21	CLA	42	609	16	1/1/19/20	5/31/109/115	-
21	CLA	J2	101	9	1/1/18/20	5/25/103/115	-
21	CLA	9	612	19	1/1/20/20	5/37/115/115	-
21	CLA	82	608	33	1/1/17/20	0/19/97/115	-
27	LMG	1	624	-	-	4/31/51/70	0/1/1/1
21	CLA	A	845	23	1/1/15/20	4/13/91/115	-
30	CHL	72	601	14	3/3/26/26	5/39/137/137	-
30	CHL	6	607	33	3/3/26/26	7/39/137/137	-
21	CLA	A2	831	-	1/1/20/20	2/37/115/115	-
24	BCR	B	844	-	-	0/29/63/63	0/2/2/2
30	CHL	Z2	606	33	3/3/21/26	5/15/113/137	-
21	CLA	1	602	12	1/1/19/20	2/31/109/115	-
24	BCR	A2	849	-	-	0/29/63/63	0/2/2/2
26	LMU	1	626	-	-	0/15/35/61	0/1/1/2
21	CLA	A2	845	23	1/1/15/20	4/13/91/115	-
21	CLA	5	610	17	1/1/19/20	2/31/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	52	610	17	1/1/19/20	2/31/109/115	-
26	LMU	12	626	-	-	0/15/35/61	0/1/1/2
21	CLA	B2	826	-	1/1/20/20	3/37/115/115	-
23	LHG	3	623	-	-	13/51/51/53	-
31	XAT	8	618	-	-	0/31/93/93	0/4/4/4
30	CHL	12	607	33	3/3/21/26	3/15/113/137	-
21	CLA	Z2	612	12	1/1/15/20	3/13/91/115	-
21	CLA	42	610	16	1/1/19/20	3/31/109/115	-
21	CLA	Z	603	-	1/1/18/20	6/25/103/115	-
21	CLA	92	614	-	1/1/15/20	3/13/91/115	-
21	CLA	B2	807	-	1/1/18/20	2/25/103/115	-
24	BCR	A2	851	-	-	2/29/63/63	0/2/2/2
23	LHG	42	622	21	-	13/53/53/53	-
27	LMG	B	852	-	-	7/38/58/70	0/1/1/1
21	CLA	62	613	33	1/1/20/20	4/37/115/115	-
21	CLA	B	808	-	1/1/20/20	7/37/115/115	-
25	SF4	A	853	1,2	-	-	0/6/5/5
24	BCR	A	848	-	-	2/29/63/63	0/2/2/2
21	CLA	8	616	15	1/1/15/20	0/13/91/115	-
21	CLA	A	828	-	1/1/20/20	6/37/115/115	-
21	CLA	5	601	17	1/1/20/20	5/37/115/115	-
21	CLA	32	609	13	1/1/19/20	3/33/111/115	-
31	XAT	6	624	-	-	0/31/93/93	0/4/4/4
21	CLA	B	807	-	1/1/18/20	2/25/103/115	-
21	CLA	12	611	23	1/1/19/20	3/33/111/115	-
21	CLA	Z	613	33	1/1/20/20	2/37/115/115	-
24	BCR	A	849	-	-	0/29/63/63	0/2/2/2
21	CLA	3	612	13	1/1/15/20	1/15/93/115	-
21	CLA	A	811	-	1/1/20/20	5/37/115/115	-
21	CLA	8	609	15	1/1/15/20	0/13/91/115	-
21	CLA	A	854	33	1/1/20/20	1/37/115/115	-
21	CLA	3	607	13	1/1/18/20	4/25/103/115	-
21	CLA	5	611	23	1/1/18/20	2/25/103/115	-
21	CLA	92	601	19	1/1/15/20	0/15/93/115	-
21	CLA	7	620	33	1/1/17/20	5/23/101/115	-
27	LMG	1	628	-	-	6/37/57/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	LMU	82	625	-	-	2/15/35/61	0/1/1/2
21	CLA	A	841	-	1/1/20/20	7/37/115/115	-
21	CLA	F2	301	33	1/1/20/20	3/37/115/115	-
26	LMU	B	853	-	-	7/21/61/61	0/2/2/2
21	CLA	Z2	614	-	1/1/17/20	0/19/97/115	-
21	CLA	82	612	15	1/1/18/20	6/25/103/115	-
22	PQN	A	844	-	-	3/23/43/43	0/2/2/2
21	CLA	7	612	14	1/1/17/20	3/22/100/115	-
21	CLA	72	612	14	1/1/17/20	3/22/100/115	-
26	LMU	Z2	622	-	-	3/17/57/61	0/2/2/2
21	CLA	A2	826	33	1/1/20/20	9/37/115/115	-
24	BCR	82	619	-	-	4/29/63/63	0/2/2/2
23	LHG	6	619	21	-	5/53/53/53	-
21	CLA	B2	815	-	1/1/20/20	4/37/115/115	-
27	LMG	3	722	-	-	6/46/46/70	-
26	LMU	12	621	-	-	6/21/61/61	0/2/2/2
21	CLA	L	204	-	1/1/15/20	2/13/91/115	-
21	CLA	72	610	14	1/1/20/20	4/37/115/115	-
23	LHG	62	619	21	-	5/53/53/53	-
30	CHL	52	608	33	3/3/23/26	0/21/119/137	-
21	CLA	5	609	17	1/1/20/20	2/37/115/115	-
21	CLA	A2	820	-	1/1/20/20	8/37/115/115	-
31	XAT	7	622	-	-	0/31/93/93	0/4/4/4
21	CLA	B	835	33	1/1/15/20	0/13/91/115	-
21	CLA	A	827	33	1/1/20/20	3/37/115/115	-
21	CLA	72	603	-	1/1/17/20	5/22/100/115	-
21	CLA	52	621	33	1/1/15/20	8/15/93/115	-
21	CLA	52	602	17	1/1/20/20	0/37/115/115	-
26	LMU	K	208	-	-	3/15/35/61	0/1/1/2
28	LUT	A	856	-	-	4/29/67/67	0/2/2/2
21	CLA	A	803	33	1/1/20/20	2/37/115/115	-
21	CLA	B2	811	-	1/1/20/20	8/37/115/115	-
28	LUT	32	720	-	-	0/29/67/67	0/2/2/2
21	CLA	B	809	2	1/1/20/20	6/37/115/115	-
26	LMU	1	622	-	-	4/10/30/61	0/1/1/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	B	812	-	1/1/20/20	2/37/115/115	-
21	CLA	3	611	-	1/1/20/20	3/37/115/115	-
21	CLA	B	817	-	1/1/20/20	6/37/115/115	-
26	LMU	12	622	-	-	4/10/30/61	0/1/1/2
21	CLA	A2	835	-	1/1/20/20	4/37/115/115	-
28	LUT	1	617	-	-	2/29/67/67	0/2/2/2
21	CLA	A	806	-	1/1/20/20	12/37/115/115	-
30	CHL	4	606	33	3/3/24/26	1/27/125/137	-
21	CLA	A2	836	-	1/1/20/20	4/37/115/115	-
21	CLA	12	614	-	1/1/19/20	5/31/109/115	-
26	LMU	Z	621	-	-	2/13/33/61	0/1/1/2
21	CLA	A2	838	-	1/1/17/20	1/21/99/115	-
30	CHL	8	601	15	3/3/26/26	10/39/137/137	-
30	CHL	72	607	33	3/3/21/26	1/15/113/137	-
30	CHL	Z	606	33	3/3/21/26	5/15/113/137	-
21	CLA	5	604	33	1/1/18/20	4/25/103/115	-
21	CLA	52	604	33	1/1/18/20	4/25/103/115	-
21	CLA	1	610	12	1/1/20/20	0/37/115/115	-
21	CLA	B2	805	-	1/1/20/20	9/37/115/115	-
23	LHG	52	623	21	-	12/41/41/53	-
21	CLA	Z	612	12	1/1/15/20	3/13/91/115	-
30	CHL	4	608	-	3/3/26/26	3/39/137/137	-
21	CLA	A	815	-	1/1/18/20	3/25/103/115	-
21	CLA	B	840	-	1/1/20/20	5/37/115/115	-
30	CHL	92	606	-	3/3/20/26	0/10/108/137	-
27	LMG	J	104	-	-	8/30/50/70	0/1/1/1
21	CLA	A	818	-	1/1/20/20	2/37/115/115	-
24	BCR	G2	205	-	-	2/29/63/63	0/2/2/2
21	CLA	B2	836	-	1/1/19/20	5/31/109/115	-
21	CLA	4	602	16	1/1/19/20	2/31/109/115	-
21	CLA	A	807	1	1/1/20/20	3/37/115/115	-
23	LHG	3	721	-	-	12/35/35/53	-
21	CLA	A2	840	-	1/1/20/20	9/37/115/115	-
21	CLA	Z2	616	12	1/1/19/20	2/31/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	LMU	8	627	-	-	9/21/61/61	0/2/2/2
23	LHG	A	847	21	-	6/42/42/53	-
21	CLA	1	611	23	1/1/19/20	3/33/111/115	-
21	CLA	A2	822	33	1/1/20/20	0/37/115/115	-
21	CLA	42	614	-	1/1/18/20	4/25/103/115	-
26	LMU	52	627	-	-	1/15/35/61	0/1/1/2
28	LUT	82	617	-	-	2/29/67/67	0/2/2/2
21	CLA	9	611	23	1/1/20/20	4/37/115/115	-
30	CHL	Z	607	33	3/3/26/26	4/39/137/137	-
21	CLA	A2	808	-	1/1/17/20	1/19/97/115	-
27	LMG	7	626	-	-	7/32/52/70	0/1/1/1
21	CLA	B	814	-	1/1/19/20	3/31/109/115	-
21	CLA	F2	303	33	1/1/15/20	2/13/91/115	-
25	SF4	C	101	3	-	-	0/6/5/5
21	CLA	92	613	19	1/1/20/20	4/37/115/115	-
26	LMU	B2	853	-	-	7/21/61/61	0/2/2/2
21	CLA	B	832	-	1/1/20/20	3/37/115/115	-
21	CLA	B	804	-	1/1/15/20	5/13/91/115	-
21	CLA	52	609	17	1/1/20/20	2/37/115/115	-
21	CLA	1	603	-	1/1/18/20	4/28/106/115	-
30	CHL	62	608	33	3/3/23/26	0/21/119/137	-
26	LMU	A	865	-	-	3/15/35/61	0/1/1/2
21	CLA	62	622	33	1/1/18/20	3/25/103/115	-
21	CLA	A2	814	-	1/1/20/20	6/37/115/115	-
27	LMG	J2	104	-	-	8/30/50/70	0/1/1/1
21	CLA	92	609	19	1/1/17/20	2/21/99/115	-
31	XAT	12	618	-	-	0/31/93/93	0/4/4/4
21	CLA	B2	818	-	1/1/20/20	2/37/115/115	-
24	BCR	9	623	-	-	2/29/63/63	0/2/2/2
24	BCR	52	622	-	-	3/29/63/63	0/2/2/2
21	CLA	72	620	33	1/1/17/20	5/23/101/115	-
21	CLA	A2	832	-	1/1/18/20	1/25/103/115	-
21	CLA	A2	824	-	1/1/15/20	2/13/91/115	-
21	CLA	3	609	13	1/1/19/20	3/33/111/115	-
31	XAT	42	620	-	-	0/31/93/93	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	NEX	52	625	-	-	2/27/83/83	1/3/3/3
21	CLA	12	604	33	1/1/17/20	1/19/97/115	-
24	BCR	L	201	-	-	4/29/63/63	0/2/2/2
26	LMU	8	624	-	-	1/15/35/61	0/1/1/2
21	CLA	B	830	-	1/1/15/20	0/13/91/115	-
30	CHL	6	616	18	3/3/26/26	5/39/137/137	-
21	CLA	B	819	33	1/1/19/20	3/31/109/115	-
21	CLA	G2	203	-	1/1/19/20	3/31/109/115	-
24	BCR	8	619	-	-	4/29/63/63	0/2/2/2
21	CLA	7	616	14	1/1/15/20	3/15/93/115	-
21	CLA	Z	602	12	1/1/19/20	1/31/109/115	-
21	CLA	8	603	-	1/1/20/20	5/37/115/115	-
21	CLA	12	616	12	1/1/15/20	2/15/93/115	-
21	CLA	72	616	14	1/1/15/20	3/15/93/115	-
30	CHL	62	616	18	3/3/26/26	5/39/137/137	-
26	LMU	A2	862	-	-	2/11/31/61	0/1/1/2
30	CHL	9	607	33	3/3/23/26	8/21/119/137	-
21	CLA	B2	813	-	1/1/20/20	4/37/115/115	-
30	CHL	42	618	16	3/3/21/26	2/15/113/137	-
21	CLA	3	617	13	1/1/15/20	2/15/93/115	-
21	CLA	A	805	-	1/1/18/20	1/25/103/115	-
24	BCR	L2	205	-	-	2/29/63/63	0/2/2/2
23	LHG	6	629	-	-	10/40/40/53	-
24	BCR	42	621	-	-	2/29/63/63	0/2/2/2
21	CLA	6	611	23	1/1/18/20	2/29/107/115	-
26	LMU	Z2	621	-	-	2/13/33/61	0/1/1/2
24	BCR	A2	852	-	-	4/29/63/63	0/2/2/2
21	CLA	A	826	33	1/1/20/20	9/37/115/115	-
21	CLA	A	831	-	1/1/20/20	2/37/115/115	-
27	LMG	42	624	-	-	5/36/56/70	0/1/1/1
21	CLA	1	604	33	1/1/17/20	1/19/97/115	-
24	BCR	K	207	-	-	4/29/63/63	0/2/2/2
23	LHG	B	851	21	-	13/49/49/53	-
26	LMU	A	858	-	-	6/21/61/61	0/2/2/2
21	CLA	3	614	-	1/1/15/20	0/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	LUT	12	619	-	-	2/29/67/67	0/2/2/2
28	LUT	3	720	-	-	0/29/67/67	0/2/2/2
21	CLA	A	832	-	1/1/18/20	1/25/103/115	-
21	CLA	A2	834	-	1/1/20/20	5/37/115/115	-
28	LUT	3	622	-	-	2/29/67/67	0/2/2/2
21	CLA	B2	817	-	1/1/20/20	6/37/115/115	-
26	LMU	K2	208	-	-	3/15/35/61	0/1/1/2
23	LHG	1	620	21	-	9/43/43/53	-
27	LMG	J2	103	-	-	2/37/57/70	0/1/1/1
21	CLA	32	611	-	1/1/20/20	3/37/115/115	-
28	LUT	5	626	-	-	4/29/67/67	0/2/2/2
28	LUT	32	621	-	-	2/29/67/67	0/2/2/2
21	CLA	B	802	-	1/1/20/20	4/37/115/115	-
21	CLA	4	612	16	1/1/15/20	4/13/91/115	-
24	BCR	32	719	-	-	2/29/63/63	0/2/2/2
26	LMU	1	627	-	-	3/13/33/61	0/1/1/2
30	CHL	52	606	33	3/3/21/26	0/15/113/137	-
21	CLA	B	810	-	1/1/20/20	3/37/115/115	-
24	BCR	L	205	-	-	2/29/63/63	0/2/2/2
21	CLA	12	613	33	1/1/20/20	4/37/115/115	-
21	CLA	B2	821	-	1/1/20/20	2/37/115/115	-
21	CLA	B2	833	-	1/1/18/20	4/29/107/115	-
21	CLA	A2	827	33	1/1/20/20	3/37/115/115	-
31	XAT	Z2	618	-	-	0/31/93/93	0/4/4/4
23	LHG	7	625	21	-	16/53/53/53	-
26	LMU	7	628	-	-	3/13/33/61	0/1/1/2
26	LMU	6	630	-	-	1/15/35/61	0/1/1/2
26	LMU	5	627	-	-	1/15/35/61	0/1/1/2
21	CLA	B	841	23	1/1/20/20	5/37/115/115	-
21	CLA	52	612	17	1/1/15/20	3/13/91/115	-
21	CLA	12	609	12	1/1/20/20	5/37/115/115	-
21	CLA	72	608	33	1/1/17/20	0/19/97/115	-
21	CLA	A2	816	-	1/1/20/20	6/37/115/115	-
21	CLA	5	602	17	1/1/20/20	0/37/115/115	-
21	CLA	6	604	-	1/1/20/20	4/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	B2	828	-	1/1/20/20	4/37/115/115	-
21	CLA	92	612	19	1/1/20/20	6/37/115/115	-
23	LHG	62	629	-	-	10/40/40/53	-
30	CHL	42	601	16	3/3/26/26	6/39/137/137	-
21	CLA	62	604	-	1/1/20/20	4/37/115/115	-
26	LMU	A	857	-	-	3/20/60/61	0/2/2/2
21	CLA	1	608	33	1/1/20/20	2/37/115/115	-
28	LUT	3	621	-	-	2/29/67/67	0/2/2/2
21	CLA	62	611	23	1/1/18/20	2/29/107/115	-
21	CLA	12	608	33	1/1/20/20	2/37/115/115	-
21	CLA	A2	841	-	1/1/20/20	7/37/115/115	-
21	CLA	6	613	33	1/1/20/20	3/37/115/115	-
21	CLA	B	834	-	1/1/19/20	6/31/109/115	-
28	LUT	Z2	617	-	-	2/29/67/67	0/2/2/2
21	CLA	7	611	23	1/1/20/20	5/37/115/115	-
21	CLA	4	614	-	1/1/18/20	4/25/103/115	-
24	BCR	A2	850	-	-	1/29/63/63	0/2/2/2
27	LMG	82	626	-	-	6/27/47/70	0/1/1/1
21	CLA	B	823	-	1/1/20/20	7/37/115/115	-
28	LUT	4	619	-	-	2/29/67/67	0/2/2/2
21	CLA	1	616	12	1/1/15/20	2/15/93/115	-
26	LMU	A2	857	-	-	3/20/60/61	0/2/2/2
21	CLA	1	613	33	1/1/20/20	4/37/115/115	-
21	CLA	B	803	-	1/1/20/20	2/37/115/115	-
21	CLA	Z	610	12	1/1/19/20	0/31/109/115	-
21	CLA	52	617	-	1/1/20/20	6/37/115/115	-
32	NEX	5	625	-	-	2/27/83/83	1/3/3/3
21	CLA	32	617	13	1/1/15/20	2/15/93/115	-
24	BCR	I2	172	-	-	0/29/63/63	0/2/2/2
21	CLA	B2	810	-	1/1/20/20	3/37/115/115	-
21	CLA	7	603	-	1/1/17/20	4/22/100/115	-
28	LUT	72	621	-	-	2/29/67/67	0/2/2/2
21	CLA	52	614	-	1/1/15/20	2/13/91/115	-
28	LUT	52	626	-	-	4/29/67/67	0/2/2/2
27	LMG	62	633	-	-	1/17/17/70	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	BCR	I	172	-	-	0/29/63/63	0/2/2/2
28	LUT	7	624	-	-	4/29/67/67	0/2/2/2
21	CLA	A	809	1	1/1/20/20	5/37/115/115	-
28	LUT	52	620	-	-	2/29/67/67	0/2/2/2
21	CLA	B	824	33	1/1/20/20	3/37/115/115	-
21	CLA	B2	812	-	1/1/20/20	3/37/115/115	-
27	LMG	9	620	21	-	6/39/59/70	0/1/1/1
21	CLA	3	603	-	1/1/20/20	5/37/115/115	-
21	CLA	9	603	27,19	1/1/18/20	4/25/103/115	-
23	LHG	B2	851	21	-	13/49/49/53	-
24	BCR	72	623	-	-	2/29/63/63	0/2/2/2
21	CLA	B2	830	-	1/1/15/20	0/13/91/115	-
21	CLA	7	610	14	1/1/20/20	4/37/115/115	-
21	CLA	Z	608	33	1/1/17/20	0/19/97/115	-
21	CLA	32	614	-	1/1/15/20	0/13/91/115	-
21	CLA	K	201	11	1/1/15/20	1/13/91/115	-
21	CLA	62	614	-	1/1/17/20	0/19/97/115	-
21	CLA	Z2	604	33	1/1/18/20	3/28/106/115	-
26	LMU	12	627	-	-	3/13/33/61	0/1/1/2
21	CLA	92	610	19	1/1/19/20	0/31/109/115	-
21	CLA	A	820	-	1/1/20/20	8/37/115/115	-
26	LMU	82	624	-	-	1/15/35/61	0/1/1/2
26	LMU	A2	865	-	-	3/15/35/61	0/1/1/2
21	CLA	A	821	-	1/1/18/20	2/25/103/115	-
21	CLA	9	610	19	1/1/19/20	0/31/109/115	-
21	CLA	Z	611	23	1/1/19/20	4/31/109/115	-
21	CLA	A2	828	-	1/1/20/20	6/37/115/115	-
21	CLA	A2	805	-	1/1/18/20	1/25/103/115	-
27	LMG	B2	852	-	-	7/38/58/70	0/1/1/1
21	CLA	A2	815	-	1/1/18/20	3/25/103/115	-
21	CLA	A	829	-	1/1/20/20	7/37/115/115	-
21	CLA	B2	832	-	1/1/20/20	3/37/115/115	-
28	LUT	9	617	-	-	0/29/67/67	0/2/2/2
24	BCR	3	719	-	-	2/29/63/63	0/2/2/2
21	CLA	B	839	33	1/1/20/20	4/37/115/115	-
21	CLA	B2	814	-	1/1/19/20	3/31/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	Z2	609	12	1/1/20/20	7/37/115/115	-
26	LMU	8	628	-	-	4/15/35/61	0/1/1/2
21	CLA	A2	813	-	1/1/20/20	5/37/115/115	-
27	LMG	A	860	-	-	6/31/51/70	0/1/1/1
28	LUT	Z	617	-	-	2/29/67/67	0/2/2/2
21	CLA	A2	833	-	1/1/20/20	1/37/115/115	-
21	CLA	8	604	33	1/1/19/20	2/31/109/115	-
26	LMU	62	631	-	-	4/15/35/61	0/1/1/2
21	CLA	B2	825	33	1/1/20/20	3/37/115/115	-
30	CHL	1	601	12	3/3/26/26	10/39/137/137	-
21	CLA	A2	839	-	1/1/20/20	2/37/115/115	-
24	BCR	B	848	-	-	2/29/63/63	0/2/2/2
21	CLA	12	612	12	1/1/15/20	3/13/91/115	-
21	CLA	92	603	27,19	1/1/18/20	4/25/103/115	-
21	CLA	A	839	-	1/1/20/20	2/37/115/115	-
23	LHG	82	620	21	-	16/48/48/53	-
28	LUT	9	616	-	-	2/29/67/67	0/2/2/2
26	LMU	8	625	-	-	2/15/35/61	0/1/1/2
21	CLA	5	612	17	1/1/15/20	3/13/91/115	-
24	BCR	G	205	-	-	2/29/63/63	0/2/2/2
21	CLA	A2	842	-	1/1/20/20	1/37/115/115	-
30	CHL	6	601	18	3/3/26/26	8/39/137/137	-
26	LMU	G	206	-	-	4/15/35/61	0/1/1/2
27	LMG	12	628	-	-	6/37/57/70	0/1/1/1
21	CLA	7	613	14	1/1/20/20	1/37/115/115	-
21	CLA	72	609	14	1/1/15/20	0/13/91/115	-
21	CLA	Z	614	-	1/1/17/20	0/19/97/115	-
30	CHL	62	601	18	3/3/26/26	8/39/137/137	-
30	CHL	62	607	33	3/3/26/26	7/39/137/137	-
28	LUT	6	621	-	-	2/29/67/67	0/2/2/2
26	LMU	Z	622	-	-	3/17/57/61	0/2/2/2
27	LMG	J	103	-	-	2/37/57/70	0/1/1/1
30	CHL	7	607	33	3/3/21/26	1/15/113/137	-
23	LHG	72	625	21	-	15/53/53/53	-
21	CLA	B2	841	23	1/1/20/20	5/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	12	603	-	1/1/18/20	4/28/106/115	-
26	LMU	6	628	-	-	2/15/35/61	0/1/1/2
21	CLA	B2	829	-	1/1/20/20	4/37/115/115	-
26	LMU	A	861	-	-	3/15/35/61	0/1/1/2
21	CLA	4	616	16	1/1/15/20	0/13/91/115	-
24	BCR	J	102	-	-	2/29/63/63	0/2/2/2
21	CLA	B2	834	-	1/1/19/20	6/31/109/115	-
21	CLA	B	822	-	1/1/18/20	5/30/108/115	-
21	CLA	A2	812	-	1/1/20/20	8/37/115/115	-
27	LMG	B2	854	-	-	2/31/51/70	0/1/1/1
24	BCR	B2	843	-	-	0/29/63/63	0/2/2/2
26	LMU	A2	863	-	-	7/21/61/61	0/2/2/2
25	SF4	C	102	3	-	-	0/6/5/5
21	CLA	6	617	-	1/1/15/20	1/13/91/115	-
26	LMU	A	863	-	-	7/21/61/61	0/2/2/2
21	CLA	A	808	-	1/1/17/20	1/19/97/115	-
21	CLA	A2	837	1	1/1/18/20	3/28/106/115	-
21	CLA	B2	803	-	1/1/20/20	2/37/115/115	-
21	CLA	52	616	17	1/1/17/20	4/23/101/115	-
26	LMU	4	626	-	-	0/11/31/61	0/1/1/2
27	LMG	8	626	-	-	6/27/47/70	0/1/1/1
20	CL0	A2	801	-	3/3/25/25	1/37/135/135	-
21	CLA	A	843	33	1/1/20/20	5/37/115/115	-
21	CLA	9	604	19	1/1/17/20	1/23/101/115	-
21	CLA	Z	609	12	1/1/20/20	7/37/115/115	-
28	LUT	A2	856	-	-	4/29/67/67	0/2/2/2
30	CHL	4	607	33	3/3/26/26	0/39/137/137	-
27	LMG	8	629	-	-	8/37/57/70	0/1/1/1
21	CLA	6	612	18	1/1/15/20	2/13/91/115	-
21	CLA	B	838	-	1/1/17/20	1/19/97/115	-
23	LHG	A2	846	-	-	10/53/53/53	-
27	LMG	A2	859	-	-	8/43/63/70	0/1/1/1
32	NEX	6	625	-	-	4/27/83/83	0/3/3/3
25	SF4	C2	102	3	-	-	0/6/5/5
26	LMU	7	629	-	-	4/13/53/61	0/2/2/2
24	BCR	B	846	-	-	2/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	B2	840	-	1/1/20/20	5/37/115/115	-
21	CLA	72	602	14	1/1/20/20	2/37/115/115	-
21	CLA	32	603	-	1/1/20/20	5/37/115/115	-
30	CHL	92	607	33	3/3/23/26	7/21/119/137	-
21	CLA	Z	616	12	1/1/19/20	2/31/109/115	-
23	LHG	9	622	21	-	13/45/45/53	-
21	CLA	6	609	18	1/1/18/20	2/25/103/115	-
21	CLA	B2	808	-	1/1/20/20	7/37/115/115	-
21	CLA	A2	807	1	1/1/20/20	3/37/115/115	-
21	CLA	B2	838	-	1/1/17/20	1/19/97/115	-
26	LMU	62	632	-	-	3/11/31/61	0/1/1/2
26	LMU	G2	206	-	-	4/15/35/61	0/1/1/2
28	LUT	5	620	-	-	2/29/67/67	0/2/2/2
21	CLA	B	837	-	1/1/20/20	2/37/115/115	-
30	CHL	5	606	33	3/3/21/26	0/15/113/137	-
22	PQN	B2	842	-	-	1/23/43/43	0/2/2/2
21	CLA	J	101	9	1/1/18/20	5/25/103/115	-
28	LUT	F	305	-	-	5/29/67/67	0/2/2/2
21	CLA	B2	839	33	1/1/20/20	4/37/115/115	-
31	XAT	62	624	-	-	0/31/93/93	0/4/4/4
21	CLA	72	613	14	1/1/20/20	1/37/115/115	-
21	CLA	B	811	-	1/1/20/20	8/37/115/115	-
21	CLA	4	609	16	1/1/19/20	5/31/109/115	-
21	CLA	42	603	16	1/1/20/20	6/37/115/115	-
26	LMU	42	625	-	-	3/19/59/61	0/2/2/2
21	CLA	B2	802	-	1/1/20/20	4/37/115/115	-
21	CLA	B	833	-	1/1/18/20	4/29/107/115	-
30	CHL	42	607	33	3/3/26/26	0/39/137/137	-
27	LMG	A2	860	-	-	7/31/51/70	0/1/1/1
30	CHL	82	601	15	3/3/26/26	10/39/137/137	-
30	CHL	Z2	601	12	3/3/26/26	7/39/137/137	-
30	CHL	7	601	14	3/3/26/26	5/39/137/137	-
21	CLA	A2	811	-	1/1/20/20	5/37/115/115	-
21	CLA	F2	304	6	1/1/20/20	7/37/115/115	-
21	CLA	82	602	15	1/1/19/20	2/34/112/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	BCR	B	847	-	-	2/29/63/63	0/2/2/2
31	XAT	5	624	-	1/1/26/26	0/31/93/93	0/4/4/4
28	LUT	Z2	619	-	-	2/18/37/67	0/1/1/2
21	CLA	B2	837	-	1/1/20/20	2/37/115/115	-
21	CLA	5	621	33	1/1/15/20	8/15/93/115	-
21	CLA	62	612	18	1/1/15/20	2/13/91/115	-
31	XAT	1	618	-	-	0/31/93/93	0/4/4/4
21	CLA	A2	829	-	1/1/20/20	7/37/115/115	-
21	CLA	K	203	33	1/1/19/20	4/31/109/115	-
21	CLA	32	606	33	1/1/14/20	0/10/88/115	-
24	BCR	B	843	-	-	0/29/63/63	0/2/2/2
32	NEX	62	625	-	-	5/27/83/83	0/3/3/3
28	LUT	8	617	-	-	2/29/67/67	0/2/2/2
21	CLA	1	612	12	1/1/15/20	3/13/91/115	-
24	BCR	3	718	-	-	2/29/63/63	0/2/2/2
21	CLA	8	610	15	1/1/20/20	2/37/115/115	-
24	BCR	B2	844	-	-	0/29/63/63	0/2/2/2
27	LMG	A	859	-	-	8/43/63/70	0/1/1/1
24	BCR	4	621	-	-	2/29/63/63	0/2/2/2
23	LHG	32	721	-	-	12/35/35/53	-
26	LMU	9	624	-	-	4/15/35/61	0/1/1/2
30	CHL	1	606	33	3/3/21/26	0/15/113/137	-
21	CLA	A	819	-	1/1/19/20	1/31/109/115	-
24	BCR	32	718	-	-	2/29/63/63	0/2/2/2
21	CLA	B	816	-	1/1/20/20	1/37/115/115	-
21	CLA	Z2	603	-	1/1/18/20	6/25/103/115	-
27	LMG	92	620	21	-	6/39/59/70	0/1/1/1
24	BCR	7	623	-	-	2/29/63/63	0/2/2/2
21	CLA	A	835	-	1/1/20/20	4/37/115/115	-
21	CLA	5	616	17	1/1/17/20	4/23/101/115	-
21	CLA	1	609	12	1/1/20/20	5/37/115/115	-
30	CHL	4	601	16	3/3/26/26	6/39/137/137	-
21	CLA	82	611	23	1/1/15/20	2/13/91/115	-
21	CLA	3	606	33	1/1/14/20	0/10/88/115	-
21	CLA	Z2	611	23	1/1/19/20	4/31/109/115	-
24	BCR	B2	801	-	-	0/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	K2	204	-	1/1/15/20	1/15/93/115	-
30	CHL	8	607	33	3/3/26/26	8/39/137/137	-
21	CLA	A	812	-	1/1/20/20	8/37/115/115	-
23	LHG	42	623	-	-	15/42/42/53	-
23	LHG	A2	847	21	-	6/42/42/53	-
21	CLA	K	204	-	1/1/15/20	1/15/93/115	-
26	LMU	72	627	-	-	2/18/58/61	0/2/2/2
21	CLA	B2	816	-	1/1/20/20	1/37/115/115	-
30	CHL	6	606	33	3/3/24/26	0/30/128/137	-
24	BCR	B2	848	-	-	2/29/63/63	0/2/2/2
21	CLA	L2	204	-	1/1/15/20	2/13/91/115	-
26	LMU	72	629	-	-	4/13/53/61	0/2/2/2
21	CLA	A	830	-	1/1/20/20	4/37/115/115	-
26	LMU	42	626	-	-	0/11/31/61	0/1/1/2
21	CLA	A2	825	-	1/1/18/20	6/25/103/115	-
23	LHG	Z	620	21	-	7/43/43/53	-
27	LMG	82	629	-	-	8/37/57/70	0/1/1/1
21	CLA	62	602	18	1/1/20/20	2/37/115/115	-
21	CLA	B	827	-	1/1/20/20	5/37/115/115	-
24	BCR	A2	848	-	-	2/29/63/63	0/2/2/2
21	CLA	A2	817	33	1/1/18/20	4/25/103/115	-
26	LMU	12	625	-	-	5/15/35/61	0/1/1/2
30	CHL	82	607	33	3/3/26/26	8/39/137/137	-
24	BCR	L2	201	-	-	4/29/63/63	0/2/2/2
24	BCR	J2	102	-	-	2/29/63/63	0/2/2/2
21	CLA	8	602	15	1/1/19/20	1/34/112/115	-
21	CLA	72	611	23	1/1/20/20	5/37/115/115	-
21	CLA	A2	818	-	1/1/20/20	2/37/115/115	-
27	LMG	12	624	-	-	4/31/51/70	0/1/1/1
21	CLA	K2	201	11	1/1/15/20	1/13/91/115	-
22	PQN	A2	844	-	-	3/23/43/43	0/2/2/2
27	LMG	6	633	-	-	1/17/17/70	-
21	CLA	4	613	16	1/1/20/20	5/37/115/115	-
21	CLA	42	611	23	1/1/19/20	4/31/109/115	-
30	CHL	12	601	12	3/3/26/26	10/39/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	A2	830	-	1/1/20/20	4/37/115/115	-
21	CLA	A	813	-	1/1/20/20	5/37/115/115	-
21	CLA	B	828	-	1/1/20/20	4/37/115/115	-
28	LUT	62	621	-	-	2/29/67/67	0/2/2/2
21	CLA	A	814	-	1/1/20/20	5/37/115/115	-
21	CLA	K2	203	33	1/1/19/20	4/31/109/115	-
21	CLA	A2	819	-	1/1/19/20	1/31/109/115	-
21	CLA	9	601	19	1/1/15/20	0/15/93/115	-
26	LMU	82	628	-	-	4/15/35/61	0/1/1/2
28	LUT	92	617	-	-	0/29/67/67	0/2/2/2
21	CLA	6	614	-	1/1/17/20	0/19/97/115	-
21	CLA	B2	827	-	1/1/20/20	5/37/115/115	-
21	CLA	A	804	-	1/1/20/20	5/37/115/115	-
21	CLA	Z2	613	33	1/1/20/20	2/37/115/115	-
26	LMU	72	628	-	-	3/13/33/61	0/1/1/2
21	CLA	52	613	17	1/1/18/20	4/27/105/115	-
26	LMU	62	628	-	-	2/15/35/61	0/1/1/2
21	CLA	4	603	16	1/1/20/20	6/37/115/115	-
21	CLA	A	816	-	1/1/20/20	6/37/115/115	-
21	CLA	B2	822	-	1/1/18/20	5/30/108/115	-
21	CLA	62	617	-	1/1/15/20	2/13/91/115	-
21	CLA	9	614	-	1/1/15/20	3/13/91/115	-
21	CLA	B2	806	2	1/1/20/20	3/37/115/115	-
20	CL0	A	801	-	3/3/25/25	1/37/135/135	-
24	BCR	A	852	-	-	4/29/63/63	0/2/2/2
21	CLA	B	805	-	1/1/20/20	9/37/115/115	-
21	CLA	4	604	33	1/1/17/20	1/19/97/115	-
30	CHL	62	606	33	3/3/24/26	0/30/128/137	-
21	CLA	K	206	11	1/1/15/20	2/13/91/115	-
21	CLA	B	815	-	1/1/20/20	4/37/115/115	-
26	LMU	62	630	-	-	1/15/35/61	0/1/1/2
21	CLA	5	603	-	1/1/20/20	16/37/115/115	-
21	CLA	72	614	-	1/1/14/20	4/11/89/115	-
21	CLA	9	613	19	1/1/20/20	4/37/115/115	-
21	CLA	52	603	-	1/1/20/20	16/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	LUT	F2	305	-	-	5/29/67/67	0/2/2/2
31	XAT	82	618	-	-	0/31/93/93	0/4/4/4
28	LUT	72	624	-	-	4/29/67/67	0/2/2/2
21	CLA	4	610	16	1/1/19/20	3/31/109/115	-
30	CHL	Z	601	12	3/3/26/26	7/39/137/137	-
21	CLA	A2	804	-	1/1/20/20	5/37/115/115	-
21	CLA	B	806	2	1/1/20/20	3/37/115/115	-
21	CLA	B	831	-	1/1/18/20	1/25/103/115	-
21	CLA	8	613	15	1/1/20/20	5/37/115/115	-
24	BCR	B	801	-	-	0/29/63/63	0/2/2/2
27	LMG	B	854	-	-	2/31/51/70	0/1/1/1
21	CLA	L	203	-	1/1/20/20	6/37/115/115	-
21	CLA	B2	835	33	1/1/15/20	1/13/91/115	-
21	CLA	62	609	18	1/1/18/20	2/25/103/115	-
21	CLA	A	810	1	1/1/20/20	8/37/115/115	-
21	CLA	A	825	-	1/1/18/20	6/25/103/115	-
24	BCR	K2	207	-	-	4/29/63/63	0/2/2/2
30	CHL	7	606	33	3/3/21/26	3/15/113/137	-
30	CHL	72	606	33	3/3/21/26	3/15/113/137	-
21	CLA	7	604	33	1/1/17/20	1/21/99/115	-
21	CLA	A	834	-	1/1/20/20	5/37/115/115	-
26	LMU	A	862	-	-	2/11/31/61	0/1/1/2
21	CLA	B2	823	-	1/1/20/20	7/37/115/115	-
21	CLA	82	614	-	1/1/18/20	7/28/106/115	-
21	CLA	8	608	33	1/1/17/20	0/19/97/115	-
24	BCR	A	850	-	-	1/29/63/63	0/2/2/2
21	CLA	L2	203	-	1/1/20/20	6/37/115/115	-
21	CLA	B	836	-	1/1/19/20	5/31/109/115	-
26	LMU	A2	864	-	-	2/15/35/61	0/1/1/2
21	CLA	6	622	33	1/1/18/20	3/25/103/115	-
28	LUT	1	619	-	-	2/29/67/67	0/2/2/2
21	CLA	B2	804	-	1/1/15/20	5/13/91/115	-
23	LHG	8	620	21	-	16/48/48/53	-
24	BCR	6	623	-	-	2/29/63/63	0/2/2/2
28	LUT	Z	619	-	-	2/18/37/67	0/1/1/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	LHG	4	623	-	-	15/42/42/53	-
30	CHL	6	618	18	3/3/20/26	2/12/110/137	-
23	LHG	92	622	21	-	13/45/45/53	-
26	LMU	A	864	-	-	2/15/35/61	0/1/1/2
26	LMU	1	625	-	-	5/15/35/61	0/1/1/2
21	CLA	82	613	15	1/1/20/20	5/37/115/115	-
21	CLA	3	610	13	1/1/20/20	0/37/115/115	-
21	CLA	A	823	-	1/1/20/20	6/37/115/115	-
30	CHL	62	618	18	3/3/20/26	2/12/110/137	-
21	CLA	7	609	14	1/1/15/20	0/13/91/115	-
21	CLA	Z2	602	12	1/1/19/20	1/31/109/115	-
21	CLA	A2	854	33	1/1/20/20	1/37/115/115	-
21	CLA	A	802	-	1/1/20/20	0/37/115/115	-
21	CLA	G	204	7	1/1/15/20	4/15/93/115	-
24	BCR	B2	847	-	-	2/29/63/63	0/2/2/2
21	CLA	3	604	33	1/1/20/20	1/37/115/115	-
24	BCR	A	851	-	-	2/29/63/63	0/2/2/2
21	CLA	Z	604	33	1/1/18/20	3/28/106/115	-
28	LUT	12	617	-	-	2/29/67/67	0/2/2/2
21	CLA	82	603	-	1/1/20/20	5/37/115/115	-
22	PQN	B	842	-	-	1/23/43/43	0/2/2/2
21	CLA	B2	824	33	1/1/20/20	3/37/115/115	-
24	BCR	K	202	-	-	2/29/63/63	0/2/2/2
21	CLA	K2	206	11	1/1/15/20	2/13/91/115	-
21	CLA	3	602	13	1/1/19/20	1/31/109/115	-
21	CLA	9	602	19	1/1/19/20	2/31/109/115	-
21	CLA	5	613	17	1/1/18/20	4/27/105/115	-
21	CLA	F	301	33	1/1/20/20	3/37/115/115	-
30	CHL	5	608	33	3/3/23/26	0/21/119/137	-
30	CHL	Z2	607	33	3/3/26/26	4/39/137/137	-
21	CLA	A2	809	1	1/1/20/20	5/37/115/115	-
30	CHL	32	608	33	3/3/26/26	3/39/137/137	-
28	LUT	42	619	-	-	2/29/67/67	0/2/2/2
31	XAT	72	622	-	-	0/31/93/93	0/4/4/4
26	LMU	1	621	-	-	6/21/61/61	0/2/2/2

All (1873) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	92	607	CHL	C4B-NB	12.30	1.46	1.35
30	6	607	CHL	C4B-NB	12.27	1.46	1.35
30	62	607	CHL	C4B-NB	12.20	1.46	1.35
30	9	607	CHL	C4B-NB	12.08	1.46	1.35
30	62	608	CHL	C4B-NB	12.05	1.46	1.35
30	6	608	CHL	C4B-NB	12.01	1.45	1.35
30	9	606	CHL	C4B-NB	11.99	1.45	1.35
30	62	618	CHL	C4B-NB	11.96	1.45	1.35
30	4	618	CHL	C4B-NB	11.96	1.45	1.35
30	42	608	CHL	C4B-NB	11.93	1.45	1.35
30	6	606	CHL	C4B-NB	11.91	1.45	1.35
30	5	618	CHL	C4B-NB	11.91	1.45	1.35
30	6	618	CHL	C4B-NB	11.90	1.45	1.35
30	52	618	CHL	C4B-NB	11.89	1.45	1.35
30	8	607	CHL	C4B-NB	11.88	1.45	1.35
30	42	618	CHL	C4B-NB	11.86	1.45	1.35
30	62	606	CHL	C4B-NB	11.85	1.45	1.35
30	4	608	CHL	C4B-NB	11.84	1.45	1.35
30	92	606	CHL	C4B-NB	11.84	1.45	1.35
30	5	608	CHL	C4B-NB	11.83	1.45	1.35
30	82	607	CHL	C4B-NB	11.83	1.45	1.35
30	5	607	CHL	C4B-NB	11.81	1.45	1.35
30	52	608	CHL	C4B-NB	11.79	1.45	1.35
30	7	601	CHL	C4B-NB	11.77	1.45	1.35
30	72	601	CHL	C4B-NB	11.77	1.45	1.35
30	52	607	CHL	C4B-NB	11.77	1.45	1.35
30	62	616	CHL	C4B-NB	11.77	1.45	1.35
30	Z2	606	CHL	C4B-NB	11.76	1.45	1.35
30	Z	606	CHL	C4B-NB	11.76	1.45	1.35
30	6	616	CHL	C4B-NB	11.75	1.45	1.35
30	5	606	CHL	C4B-NB	11.73	1.45	1.35
30	42	606	CHL	C4B-NB	11.72	1.45	1.35
30	1	606	CHL	C4B-NB	11.72	1.45	1.35
30	12	606	CHL	C4B-NB	11.72	1.45	1.35
30	42	601	CHL	C4B-NB	11.68	1.45	1.35
30	4	606	CHL	C4B-NB	11.67	1.45	1.35
30	Z2	607	CHL	C4B-NB	11.64	1.45	1.35
30	52	606	CHL	C4B-NB	11.63	1.45	1.35
30	4	601	CHL	C4B-NB	11.63	1.45	1.35
30	82	606	CHL	C4B-NB	11.62	1.45	1.35
30	6	601	CHL	C4B-NB	11.60	1.45	1.35
30	Z	607	CHL	C4B-NB	11.58	1.45	1.35
30	42	607	CHL	C4B-NB	11.57	1.45	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	4	607	CHL	C4B-NB	11.56	1.45	1.35
30	7	606	CHL	C4B-NB	11.55	1.45	1.35
30	7	607	CHL	C4B-NB	11.54	1.45	1.35
30	72	607	CHL	C4B-NB	11.53	1.45	1.35
30	8	606	CHL	C4B-NB	11.51	1.45	1.35
30	72	606	CHL	C4B-NB	11.50	1.45	1.35
30	62	601	CHL	C4B-NB	11.49	1.45	1.35
30	82	601	CHL	C4B-NB	11.49	1.45	1.35
30	8	601	CHL	C4B-NB	11.48	1.45	1.35
30	32	608	CHL	C4B-NB	11.42	1.45	1.35
30	3	608	CHL	C4B-NB	11.40	1.45	1.35
30	12	601	CHL	C4B-NB	11.36	1.45	1.35
30	Z	601	CHL	C4B-NB	11.36	1.45	1.35
30	1	601	CHL	C4B-NB	11.32	1.45	1.35
30	Z2	601	CHL	C4B-NB	11.30	1.45	1.35
30	1	607	CHL	C4B-NB	11.19	1.45	1.35
30	12	607	CHL	C4B-NB	11.11	1.45	1.35
20	A	801	CL0	C4B-NB	9.84	1.44	1.35
20	A2	801	CL0	C4B-NB	9.82	1.44	1.35
20	A	801	CL0	C1B-NB	6.54	1.41	1.35
20	A2	801	CL0	C1B-NB	6.54	1.41	1.35
30	9	607	CHL	MG-ND	-6.26	1.93	2.05
30	32	608	CHL	MG-ND	-6.10	1.93	2.05
30	3	608	CHL	MG-ND	-6.10	1.93	2.05
30	92	607	CHL	MG-ND	-6.07	1.93	2.05
30	Z2	601	CHL	MG-ND	-6.05	1.93	2.05
30	1	607	CHL	MG-ND	-6.05	1.93	2.05
30	Z	601	CHL	MG-ND	-6.05	1.93	2.05
30	6	601	CHL	MG-ND	-6.05	1.93	2.05
30	62	601	CHL	MG-ND	-6.03	1.93	2.05
30	Z	607	CHL	MG-ND	-6.01	1.93	2.05
30	Z2	607	CHL	MG-ND	-6.01	1.93	2.05
30	12	607	CHL	MG-ND	-6.01	1.93	2.05
30	7	607	CHL	MG-ND	-5.96	1.94	2.05
30	72	607	CHL	MG-ND	-5.96	1.94	2.05
30	5	606	CHL	MG-ND	-5.96	1.94	2.05
30	82	607	CHL	MG-ND	-5.95	1.94	2.05
30	82	601	CHL	MG-ND	-5.95	1.94	2.05
30	4	607	CHL	MG-ND	-5.94	1.94	2.05
30	4	608	CHL	MG-ND	-5.94	1.94	2.05
30	52	606	CHL	MG-ND	-5.93	1.94	2.05
30	42	601	CHL	MG-ND	-5.93	1.94	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	8	607	CHL	MG-ND	-5.93	1.94	2.05
30	12	606	CHL	MG-ND	-5.93	1.94	2.05
30	42	608	CHL	MG-ND	-5.91	1.94	2.05
30	8	601	CHL	MG-ND	-5.91	1.94	2.05
30	6	616	CHL	MG-ND	-5.91	1.94	2.05
30	62	616	CHL	MG-ND	-5.91	1.94	2.05
30	42	607	CHL	MG-ND	-5.90	1.94	2.05
30	4	606	CHL	MG-ND	-5.90	1.94	2.05
30	6	606	CHL	MG-ND	-5.90	1.94	2.05
30	62	606	CHL	MG-ND	-5.90	1.94	2.05
30	42	606	CHL	MG-ND	-5.89	1.94	2.05
30	4	601	CHL	MG-ND	-5.89	1.94	2.05
30	1	601	CHL	MG-ND	-5.88	1.94	2.05
30	1	606	CHL	MG-ND	-5.87	1.94	2.05
30	12	601	CHL	MG-ND	-5.87	1.94	2.05
30	9	606	CHL	MG-ND	-5.87	1.94	2.05
30	92	606	CHL	MG-ND	-5.87	1.94	2.05
30	62	608	CHL	MG-ND	-5.87	1.94	2.05
30	52	608	CHL	MG-ND	-5.86	1.94	2.05
30	5	607	CHL	MG-ND	-5.84	1.94	2.05
30	8	606	CHL	MG-ND	-5.84	1.94	2.05
30	5	608	CHL	MG-ND	-5.83	1.94	2.05
30	6	608	CHL	MG-ND	-5.83	1.94	2.05
30	82	606	CHL	MG-ND	-5.82	1.94	2.05
30	72	606	CHL	MG-ND	-5.81	1.94	2.05
30	6	607	CHL	MG-ND	-5.81	1.94	2.05
30	62	607	CHL	MG-ND	-5.81	1.94	2.05
30	52	607	CHL	MG-ND	-5.80	1.94	2.05
21	4	612	CLA	C1D-ND	5.79	1.44	1.37
30	7	601	CHL	MG-ND	-5.79	1.94	2.05
30	7	606	CHL	MG-ND	-5.78	1.94	2.05
30	72	601	CHL	MG-ND	-5.77	1.94	2.05
30	52	618	CHL	MG-ND	-5.77	1.94	2.05
21	5	621	CLA	C1D-ND	5.75	1.44	1.37
30	6	618	CHL	MG-ND	-5.73	1.94	2.05
30	Z2	606	CHL	MG-ND	-5.72	1.94	2.05
21	52	621	CLA	C1D-ND	5.71	1.44	1.37
30	62	618	CHL	MG-ND	-5.70	1.94	2.05
30	5	618	CHL	MG-ND	-5.70	1.94	2.05
21	42	612	CLA	C1D-ND	5.69	1.44	1.37
30	42	618	CHL	MG-ND	-5.69	1.94	2.05
21	Z	612	CLA	C1D-ND	5.68	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	Z2	612	CLA	C1D-ND	5.68	1.44	1.37
30	4	618	CHL	MG-ND	-5.67	1.94	2.05
30	Z	606	CHL	MG-ND	-5.67	1.94	2.05
21	6	614	CLA	C1D-ND	5.65	1.44	1.37
21	62	614	CLA	C1D-ND	5.65	1.44	1.37
21	4	603	CLA	C1D-ND	5.64	1.44	1.37
21	L2	204	CLA	C1D-ND	5.64	1.44	1.37
21	6	612	CLA	C1D-ND	5.62	1.44	1.37
21	62	612	CLA	C1D-ND	5.62	1.44	1.37
21	5	612	CLA	C1D-ND	5.60	1.44	1.37
21	42	603	CLA	C1D-ND	5.59	1.44	1.37
21	F	304	CLA	C1D-ND	5.59	1.44	1.37
21	F2	304	CLA	C1D-ND	5.59	1.44	1.37
21	82	612	CLA	C1D-ND	5.58	1.44	1.37
21	Z	603	CLA	C1D-ND	5.57	1.44	1.37
21	B	824	CLA	C1D-ND	5.57	1.44	1.37
21	5	601	CLA	C1D-ND	5.57	1.44	1.37
21	52	601	CLA	C1D-ND	5.57	1.44	1.37
21	L	204	CLA	C1D-ND	5.56	1.44	1.37
21	5	614	CLA	C1D-ND	5.56	1.44	1.37
21	52	612	CLA	C1D-ND	5.54	1.44	1.37
21	K2	206	CLA	C1D-ND	5.54	1.44	1.37
21	82	608	CLA	C1D-ND	5.54	1.44	1.37
21	8	612	CLA	C1D-ND	5.54	1.44	1.37
21	5	616	CLA	C1D-ND	5.54	1.44	1.37
21	52	616	CLA	C1D-ND	5.54	1.44	1.37
21	B2	824	CLA	C1D-ND	5.53	1.44	1.37
21	B	827	CLA	C1D-ND	5.53	1.44	1.37
21	72	620	CLA	C1D-ND	5.53	1.44	1.37
21	92	603	CLA	C1D-ND	5.53	1.44	1.37
21	B2	827	CLA	C1D-ND	5.53	1.44	1.37
21	92	601	CLA	C1D-ND	5.52	1.44	1.37
21	K2	203	CLA	C1D-ND	5.52	1.44	1.37
21	Z2	603	CLA	C1D-ND	5.52	1.44	1.37
30	12	607	CHL	MG-NA	-5.52	1.93	2.06
21	6	613	CLA	C1D-ND	5.52	1.44	1.37
21	52	614	CLA	C1D-ND	5.52	1.44	1.37
21	A	826	CLA	C1D-ND	5.51	1.44	1.37
21	G2	204	CLA	C1D-ND	5.51	1.44	1.37
21	12	612	CLA	C1D-ND	5.51	1.44	1.37
21	A2	817	CLA	C1D-ND	5.51	1.44	1.37
21	6	604	CLA	C1D-ND	5.51	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	1	612	CLA	C1D-ND	5.51	1.44	1.37
21	6	611	CLA	C1D-ND	5.51	1.44	1.37
21	52	603	CLA	C1D-ND	5.51	1.44	1.37
30	1	607	CHL	MG-NA	-5.50	1.93	2.06
21	8	608	CLA	C1D-ND	5.50	1.44	1.37
21	J	101	CLA	C1D-ND	5.50	1.44	1.37
21	Z	616	CLA	C1D-ND	5.49	1.44	1.37
21	Z2	616	CLA	C1D-ND	5.49	1.44	1.37
21	62	613	CLA	C1D-ND	5.49	1.44	1.37
21	9	603	CLA	C1D-ND	5.49	1.44	1.37
21	K	203	CLA	C1D-ND	5.49	1.44	1.37
21	3	615	CLA	C1D-ND	5.49	1.44	1.37
21	7	614	CLA	C1D-ND	5.49	1.44	1.37
21	5	603	CLA	C1D-ND	5.48	1.44	1.37
30	5	607	CHL	MG-NA	-5.47	1.93	2.06
30	52	607	CHL	MG-NA	-5.47	1.93	2.06
21	B	839	CLA	C1D-ND	5.47	1.44	1.37
21	J2	101	CLA	C1D-ND	5.47	1.44	1.37
21	9	601	CLA	C1D-ND	5.47	1.44	1.37
21	62	611	CLA	C1D-ND	5.47	1.44	1.37
21	4	616	CLA	C1D-ND	5.47	1.44	1.37
21	42	616	CLA	C1D-ND	5.47	1.44	1.37
21	82	603	CLA	C1D-ND	5.46	1.44	1.37
21	92	614	CLA	C1D-ND	5.46	1.44	1.37
21	7	620	CLA	C1D-ND	5.46	1.44	1.37
21	82	614	CLA	C1D-ND	5.45	1.44	1.37
21	A2	826	CLA	C1D-ND	5.45	1.44	1.37
21	42	614	CLA	C1D-ND	5.45	1.44	1.37
21	A	816	CLA	C1D-ND	5.45	1.44	1.37
21	G	204	CLA	C1D-ND	5.45	1.44	1.37
21	62	604	CLA	C1D-ND	5.44	1.44	1.37
21	A2	816	CLA	C1D-ND	5.44	1.44	1.37
21	Z2	614	CLA	C1D-ND	5.44	1.44	1.37
21	6	603	CLA	C1D-ND	5.44	1.44	1.37
21	9	614	CLA	C1D-ND	5.44	1.44	1.37
21	12	608	CLA	C1D-ND	5.43	1.44	1.37
21	32	615	CLA	C1D-ND	5.43	1.44	1.37
21	6	622	CLA	C1D-ND	5.43	1.44	1.37
21	A2	845	CLA	C1D-ND	5.43	1.44	1.37
21	K2	201	CLA	C1D-ND	5.42	1.44	1.37
21	A	817	CLA	C1D-ND	5.42	1.44	1.37
21	B2	839	CLA	C1D-ND	5.42	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	3	612	CLA	C1D-ND	5.42	1.44	1.37
21	F2	303	CLA	C1D-ND	5.42	1.44	1.37
21	K	206	CLA	C1D-ND	5.42	1.44	1.37
21	3	604	CLA	C1D-ND	5.42	1.44	1.37
21	6	602	CLA	C1D-ND	5.42	1.44	1.37
21	A	838	CLA	C1D-ND	5.42	1.44	1.37
21	A2	838	CLA	C1D-ND	5.42	1.44	1.37
21	3	614	CLA	C1D-ND	5.42	1.44	1.37
21	A2	835	CLA	C1D-ND	5.41	1.44	1.37
21	1	614	CLA	C1D-ND	5.41	1.44	1.37
30	62	601	CHL	MG-NA	-5.40	1.93	2.06
21	7	612	CLA	C1D-ND	5.40	1.44	1.37
21	92	612	CLA	C1D-ND	5.40	1.44	1.37
21	72	612	CLA	C1D-ND	5.40	1.44	1.37
21	32	604	CLA	C1D-ND	5.40	1.44	1.37
21	Z	609	CLA	C1D-ND	5.40	1.44	1.37
21	B	835	CLA	C1D-ND	5.40	1.44	1.37
21	5	611	CLA	C1D-ND	5.39	1.44	1.37
21	62	602	CLA	C1D-ND	5.39	1.44	1.37
21	62	603	CLA	C1D-ND	5.39	1.44	1.37
21	4	610	CLA	C1D-ND	5.39	1.44	1.37
21	4	614	CLA	C1D-ND	5.39	1.44	1.37
21	42	610	CLA	C1D-ND	5.39	1.44	1.37
21	Z2	609	CLA	C1D-ND	5.39	1.44	1.37
21	62	622	CLA	C1D-ND	5.39	1.44	1.37
21	Z	614	CLA	C1D-ND	5.39	1.44	1.37
21	72	614	CLA	C1D-ND	5.39	1.44	1.37
21	Z2	604	CLA	C1D-ND	5.38	1.44	1.37
21	5	613	CLA	C1D-ND	5.38	1.44	1.37
21	4	604	CLA	C1D-ND	5.37	1.44	1.37
21	32	614	CLA	C1D-ND	5.37	1.44	1.37
21	3	606	CLA	C1D-ND	5.37	1.44	1.37
21	52	602	CLA	C1D-ND	5.37	1.44	1.37
21	F	303	CLA	C1D-ND	5.37	1.44	1.37
21	42	604	CLA	C1D-ND	5.37	1.44	1.37
30	6	601	CHL	MG-NA	-5.37	1.93	2.06
21	B2	807	CLA	C1D-ND	5.36	1.44	1.37
21	32	612	CLA	C1D-ND	5.36	1.44	1.37
21	B	814	CLA	C1D-ND	5.36	1.44	1.37
21	6	617	CLA	C1D-ND	5.36	1.44	1.37
21	12	614	CLA	C1D-ND	5.36	1.44	1.37
21	A	815	CLA	C1D-ND	5.36	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	K	201	CLA	C1D-ND	5.36	1.44	1.37
21	A2	815	CLA	C1D-ND	5.36	1.44	1.37
21	Z	611	CLA	C1D-ND	5.35	1.44	1.37
21	A	840	CLA	C1D-ND	5.35	1.44	1.37
21	B	810	CLA	C1D-ND	5.35	1.44	1.37
21	A	819	CLA	C1D-ND	5.35	1.44	1.37
21	8	603	CLA	C1D-ND	5.35	1.44	1.37
21	A	845	CLA	C1D-ND	5.35	1.44	1.37
21	4	611	CLA	C1D-ND	5.35	1.44	1.37
21	42	611	CLA	C1D-ND	5.35	1.44	1.37
21	8	614	CLA	C1D-ND	5.35	1.44	1.37
21	9	612	CLA	C1D-ND	5.34	1.44	1.37
21	B	804	CLA	C1D-ND	5.34	1.44	1.37
21	B	808	CLA	C1D-ND	5.34	1.44	1.37
21	52	611	CLA	C1D-ND	5.34	1.44	1.37
21	B2	835	CLA	C1D-ND	5.34	1.44	1.37
21	3	611	CLA	C1D-ND	5.34	1.44	1.37
21	A	834	CLA	C1D-ND	5.34	1.44	1.37
21	A2	834	CLA	C1D-ND	5.34	1.44	1.37
21	K	204	CLA	C1D-ND	5.34	1.44	1.37
21	Z	602	CLA	C1D-ND	5.34	1.44	1.37
21	Z2	602	CLA	C1D-ND	5.34	1.44	1.37
21	1	608	CLA	C1D-ND	5.34	1.44	1.37
21	32	606	CLA	C1D-ND	5.34	1.44	1.37
21	A2	831	CLA	C1D-ND	5.34	1.44	1.37
21	52	617	CLA	C1D-ND	5.34	1.44	1.37
21	A	835	CLA	C1D-ND	5.34	1.44	1.37
21	62	610	CLA	C1D-ND	5.33	1.44	1.37
21	A	839	CLA	C1D-ND	5.33	1.44	1.37
21	Z	604	CLA	C1D-ND	5.33	1.44	1.37
21	Z2	611	CLA	C1D-ND	5.33	1.44	1.37
21	B	811	CLA	C1D-ND	5.33	1.44	1.37
21	1	609	CLA	C1D-ND	5.33	1.44	1.37
21	12	609	CLA	C1D-ND	5.33	1.44	1.37
21	B	807	CLA	C1D-ND	5.33	1.44	1.37
21	A2	839	CLA	C1D-ND	5.33	1.44	1.37
21	6	610	CLA	C1D-ND	5.32	1.44	1.37
21	A2	832	CLA	C1D-ND	5.32	1.44	1.37
21	A	832	CLA	C1D-ND	5.32	1.44	1.37
21	B2	814	CLA	C1D-ND	5.32	1.44	1.37
21	A2	840	CLA	C1D-ND	5.32	1.44	1.37
21	52	613	CLA	C1D-ND	5.32	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	822	CLA	C1D-ND	5.32	1.44	1.37
21	B2	822	CLA	C1D-ND	5.32	1.44	1.37
21	7	613	CLA	C1D-ND	5.32	1.44	1.37
21	A	828	CLA	C1D-ND	5.32	1.44	1.37
21	72	613	CLA	C1D-ND	5.31	1.44	1.37
21	5	604	CLA	C1D-ND	5.31	1.44	1.37
21	52	604	CLA	C1D-ND	5.31	1.44	1.37
21	B2	836	CLA	C1D-ND	5.31	1.44	1.37
21	52	609	CLA	C1D-ND	5.31	1.44	1.37
21	82	602	CLA	C1D-ND	5.30	1.44	1.37
21	A	831	CLA	C1D-ND	5.30	1.44	1.37
21	8	611	CLA	C1D-ND	5.30	1.44	1.37
21	7	603	CLA	C1D-ND	5.30	1.44	1.37
21	A	830	CLA	C1D-ND	5.30	1.44	1.37
21	B2	808	CLA	C1D-ND	5.30	1.44	1.37
21	A	818	CLA	C1D-ND	5.29	1.44	1.37
21	4	613	CLA	C1D-ND	5.29	1.44	1.37
21	5	602	CLA	C1D-ND	5.29	1.44	1.37
21	B2	804	CLA	C1D-ND	5.29	1.44	1.37
21	72	611	CLA	C1D-ND	5.29	1.44	1.37
21	72	602	CLA	C1D-ND	5.29	1.44	1.37
21	32	611	CLA	C1D-ND	5.29	1.44	1.37
21	B	836	CLA	C1D-ND	5.29	1.44	1.37
30	Z	601	CHL	MG-NA	-5.29	1.93	2.06
21	B	812	CLA	C1D-ND	5.28	1.44	1.37
21	1	603	CLA	C1D-ND	5.28	1.44	1.37
21	B2	812	CLA	C1D-ND	5.28	1.44	1.37
21	8	616	CLA	C1D-ND	5.28	1.44	1.37
21	82	616	CLA	C1D-ND	5.28	1.44	1.37
21	92	609	CLA	C1D-ND	5.28	1.44	1.37
21	8	613	CLA	C1D-ND	5.28	1.44	1.37
21	82	613	CLA	C1D-ND	5.28	1.44	1.37
21	8	602	CLA	C1D-ND	5.27	1.44	1.37
21	Z2	613	CLA	C1D-ND	5.27	1.44	1.37
21	72	604	CLA	C1D-ND	5.27	1.44	1.37
21	B	815	CLA	C1D-ND	5.27	1.44	1.37
21	Z	613	CLA	C1D-ND	5.27	1.44	1.37
21	B2	815	CLA	C1D-ND	5.27	1.44	1.37
21	12	603	CLA	C1D-ND	5.27	1.44	1.37
30	Z2	601	CHL	MG-NA	-5.26	1.93	2.06
21	7	604	CLA	C1D-ND	5.26	1.44	1.37
21	7	611	CLA	C1D-ND	5.26	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A2	819	CLA	C1D-ND	5.26	1.44	1.37
21	B2	810	CLA	C1D-ND	5.26	1.44	1.37
21	A2	828	CLA	C1D-ND	5.26	1.44	1.37
30	32	608	CHL	MG-NA	-5.26	1.93	2.06
21	72	603	CLA	C1D-ND	5.26	1.44	1.37
21	42	613	CLA	C1D-ND	5.26	1.44	1.37
21	62	617	CLA	C1D-ND	5.26	1.44	1.37
21	9	604	CLA	C1D-ND	5.25	1.44	1.37
21	A	813	CLA	C1D-ND	5.25	1.44	1.37
21	A2	813	CLA	C1D-ND	5.25	1.44	1.37
21	B	816	CLA	C1D-ND	5.25	1.44	1.37
21	5	617	CLA	C1D-ND	5.25	1.44	1.37
21	A2	820	CLA	C1D-ND	5.25	1.44	1.37
21	B	809	CLA	C1D-ND	5.25	1.44	1.37
21	A2	854	CLA	C1D-ND	5.24	1.44	1.37
21	B	820	CLA	C1D-ND	5.24	1.44	1.37
21	B2	811	CLA	C1D-ND	5.24	1.44	1.37
21	82	611	CLA	C1D-ND	5.24	1.44	1.37
21	B2	820	CLA	C1D-ND	5.24	1.44	1.37
21	1	613	CLA	C1D-ND	5.24	1.44	1.37
21	12	613	CLA	C1D-ND	5.24	1.44	1.37
21	K2	204	CLA	C1D-ND	5.23	1.44	1.37
30	3	608	CHL	MG-NA	-5.23	1.93	2.06
21	72	608	CLA	C1D-ND	5.23	1.44	1.37
21	3	613	CLA	C1D-ND	5.23	1.44	1.37
21	82	609	CLA	C1D-ND	5.23	1.44	1.37
21	A2	830	CLA	C1D-ND	5.23	1.44	1.37
21	32	613	CLA	C1D-ND	5.23	1.44	1.37
21	A2	814	CLA	C1D-ND	5.22	1.44	1.37
21	A	827	CLA	C1D-ND	5.22	1.44	1.37
21	7	602	CLA	C1D-ND	5.22	1.44	1.37
21	B2	809	CLA	C1D-ND	5.22	1.44	1.37
21	52	610	CLA	C1D-ND	5.22	1.44	1.37
21	B	837	CLA	C1D-ND	5.21	1.44	1.37
21	A	814	CLA	C1D-ND	5.21	1.44	1.37
21	G2	203	CLA	C1D-ND	5.21	1.44	1.37
21	A	854	CLA	C1D-ND	5.21	1.44	1.37
21	9	609	CLA	C1D-ND	5.21	1.44	1.37
21	B	813	CLA	C1D-ND	5.20	1.44	1.37
21	B2	813	CLA	C1D-ND	5.20	1.44	1.37
21	1	604	CLA	C1D-ND	5.20	1.44	1.37
21	3	607	CLA	C1D-ND	5.20	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	12	604	CLA	C1D-ND	5.20	1.44	1.37
21	B2	841	CLA	C1D-ND	5.20	1.44	1.37
21	5	609	CLA	C1D-ND	5.20	1.44	1.37
21	B2	816	CLA	C1D-ND	5.20	1.44	1.37
21	92	604	CLA	C1D-ND	5.20	1.44	1.37
21	G	203	CLA	C1D-ND	5.20	1.44	1.37
21	32	617	CLA	C1D-ND	5.20	1.44	1.37
21	3	602	CLA	C1D-ND	5.19	1.44	1.37
21	8	609	CLA	C1D-ND	5.19	1.44	1.37
21	1	611	CLA	C1D-ND	5.19	1.44	1.37
21	72	616	CLA	C1D-ND	5.19	1.44	1.37
21	B	828	CLA	C1D-ND	5.18	1.44	1.37
21	A	822	CLA	C1D-ND	5.18	1.44	1.37
21	A2	822	CLA	C1D-ND	5.18	1.44	1.37
21	42	609	CLA	C1D-ND	5.18	1.44	1.37
21	32	607	CLA	C1D-ND	5.18	1.44	1.37
21	A2	821	CLA	C1D-ND	5.17	1.44	1.37
21	3	617	CLA	C1D-ND	5.17	1.44	1.37
21	62	609	CLA	C1D-ND	5.17	1.44	1.37
21	5	610	CLA	C1D-ND	5.17	1.44	1.37
21	A	808	CLA	C1D-ND	5.17	1.44	1.37
21	4	602	CLA	C1D-ND	5.17	1.44	1.37
21	42	602	CLA	C1D-ND	5.17	1.44	1.37
30	1	601	CHL	MG-NA	-5.16	1.94	2.06
21	B	841	CLA	C1D-ND	5.16	1.44	1.37
21	A	829	CLA	C1D-ND	5.16	1.44	1.37
21	B2	806	CLA	C1D-ND	5.16	1.44	1.37
30	12	601	CHL	MG-NA	-5.16	1.94	2.06
21	12	611	CLA	C1D-ND	5.16	1.44	1.37
21	7	608	CLA	C1D-ND	5.15	1.44	1.37
21	4	609	CLA	C1D-ND	5.15	1.44	1.37
21	A2	829	CLA	C1D-ND	5.15	1.44	1.37
21	92	602	CLA	C1D-ND	5.15	1.44	1.37
21	7	609	CLA	C1D-ND	5.14	1.44	1.37
21	B2	837	CLA	C1D-ND	5.14	1.44	1.37
21	Z2	608	CLA	C1D-ND	5.14	1.44	1.37
21	7	616	CLA	C1D-ND	5.14	1.44	1.37
21	Z	608	CLA	C1D-ND	5.14	1.44	1.37
21	6	609	CLA	C1D-ND	5.14	1.44	1.37
21	Z2	610	CLA	C1D-ND	5.14	1.44	1.37
21	B2	802	CLA	C1D-ND	5.13	1.44	1.37
21	A	820	CLA	C1D-ND	5.13	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A2	827	CLA	C1D-ND	5.13	1.44	1.37
21	L2	203	CLA	C1D-ND	5.13	1.44	1.37
21	A2	841	CLA	C1D-ND	5.13	1.44	1.37
21	9	610	CLA	C1D-ND	5.12	1.44	1.37
21	B2	828	CLA	C1D-ND	5.12	1.44	1.37
21	A2	808	CLA	C1D-ND	5.12	1.44	1.37
30	4	601	CHL	MG-NA	-5.12	1.94	2.06
21	B	826	CLA	C1D-ND	5.12	1.44	1.37
30	7	601	CHL	MG-NA	-5.12	1.94	2.06
21	A2	836	CLA	C1D-ND	5.11	1.44	1.37
21	A	841	CLA	C1D-ND	5.11	1.44	1.37
21	L	203	CLA	C1D-ND	5.11	1.44	1.37
21	A2	818	CLA	C1D-ND	5.11	1.44	1.37
30	42	601	CHL	MG-NA	-5.11	1.94	2.06
21	8	604	CLA	C1D-ND	5.11	1.44	1.37
21	A	811	CLA	C1D-ND	5.11	1.44	1.37
21	A	807	CLA	C1D-ND	5.10	1.44	1.37
21	A2	811	CLA	C1D-ND	5.10	1.44	1.37
21	B2	805	CLA	C1D-ND	5.10	1.44	1.37
30	42	607	CHL	MG-NA	-5.10	1.94	2.06
21	A	821	CLA	C1D-ND	5.09	1.44	1.37
21	B2	826	CLA	C1D-ND	5.09	1.44	1.37
21	82	604	CLA	C1D-ND	5.09	1.44	1.37
30	72	601	CHL	MG-NA	-5.09	1.94	2.06
21	A	804	CLA	C1D-ND	5.09	1.44	1.37
21	A	824	CLA	C1D-ND	5.09	1.44	1.37
21	32	602	CLA	C1D-ND	5.09	1.44	1.37
21	B2	834	CLA	C1D-ND	5.08	1.44	1.37
21	92	610	CLA	C1D-ND	5.08	1.44	1.37
21	32	603	CLA	C1D-ND	5.08	1.44	1.37
21	A	805	CLA	C1D-ND	5.08	1.44	1.37
21	A2	824	CLA	C1D-ND	5.08	1.44	1.37
21	B	806	CLA	C1D-ND	5.08	1.44	1.37
30	4	607	CHL	MG-NA	-5.08	1.94	2.06
21	A	833	CLA	C1D-ND	5.07	1.44	1.37
21	9	613	CLA	C1D-ND	5.07	1.44	1.37
21	92	613	CLA	C1D-ND	5.07	1.44	1.37
21	72	609	CLA	C1D-ND	5.07	1.44	1.37
21	3	610	CLA	C1D-ND	5.07	1.44	1.37
21	B2	817	CLA	C1D-ND	5.07	1.44	1.37
21	32	610	CLA	C1D-ND	5.07	1.44	1.37
30	Z2	606	CHL	MG-NA	-5.07	1.94	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A2	833	CLA	C1D-ND	5.06	1.44	1.37
21	9	602	CLA	C1D-ND	5.06	1.44	1.37
21	A	836	CLA	C1D-ND	5.06	1.44	1.37
21	A2	807	CLA	C1D-ND	5.06	1.44	1.37
21	A	843	CLA	C1D-ND	5.05	1.44	1.37
21	A2	843	CLA	C1D-ND	5.05	1.44	1.37
21	3	609	CLA	C1D-ND	5.05	1.44	1.37
21	B2	819	CLA	C1D-ND	5.05	1.44	1.37
21	32	609	CLA	C1D-ND	5.05	1.44	1.37
30	4	618	CHL	MG-NA	-5.05	1.94	2.06
30	42	618	CHL	MG-NA	-5.04	1.94	2.06
21	A2	804	CLA	C1D-ND	5.04	1.44	1.37
21	B2	832	CLA	C1D-ND	5.04	1.44	1.37
21	A2	837	CLA	C1D-ND	5.04	1.44	1.37
21	B	802	CLA	C1D-ND	5.04	1.44	1.37
21	B	838	CLA	C1D-ND	5.04	1.44	1.37
21	B2	838	CLA	C1D-ND	5.04	1.44	1.37
21	A2	803	CLA	C1D-ND	5.04	1.44	1.37
21	F2	301	CLA	C1D-ND	5.04	1.44	1.37
30	52	618	CHL	MG-NA	-5.03	1.94	2.06
30	62	616	CHL	MG-NA	-5.03	1.94	2.06
21	B	819	CLA	C1D-ND	5.03	1.44	1.37
21	B	831	CLA	C1D-ND	5.03	1.44	1.37
21	B	834	CLA	C1D-ND	5.03	1.44	1.37
30	Z	606	CHL	MG-NA	-5.03	1.94	2.06
30	8	601	CHL	MG-NA	-5.03	1.94	2.06
21	9	611	CLA	C1D-ND	5.03	1.44	1.37
30	4	606	CHL	MG-NA	-5.03	1.94	2.06
21	A	837	CLA	C1D-ND	5.02	1.44	1.37
21	8	610	CLA	C1D-ND	5.02	1.44	1.37
30	8	606	CHL	MG-NA	-5.02	1.94	2.06
30	82	606	CHL	MG-NA	-5.02	1.94	2.06
21	A	825	CLA	C1D-ND	5.02	1.44	1.37
30	82	601	CHL	MG-NA	-5.02	1.94	2.06
21	B	840	CLA	C1D-ND	5.01	1.43	1.37
21	B2	840	CLA	C1D-ND	5.01	1.43	1.37
30	7	606	CHL	MG-NA	-5.01	1.94	2.06
30	72	606	CHL	MG-NA	-5.01	1.94	2.06
21	Z	610	CLA	C1D-ND	5.01	1.43	1.37
30	5	618	CHL	MG-NA	-5.01	1.94	2.06
21	A	809	CLA	C1D-ND	5.01	1.43	1.37
21	A2	809	CLA	C1D-ND	5.01	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	818	CLA	C1D-ND	5.01	1.43	1.37
30	92	606	CHL	MG-NA	-5.01	1.94	2.06
21	A2	805	CLA	C1D-ND	5.00	1.43	1.37
21	12	602	CLA	C1D-ND	5.00	1.43	1.37
21	82	610	CLA	C1D-ND	5.00	1.43	1.37
21	A2	825	CLA	C1D-ND	5.00	1.43	1.37
30	6	608	CHL	MG-NA	-5.00	1.94	2.06
30	62	608	CHL	MG-NA	-5.00	1.94	2.06
21	B2	818	CLA	C1D-ND	5.00	1.43	1.37
30	6	616	CHL	MG-NA	-5.00	1.94	2.06
21	A	803	CLA	C1D-ND	4.99	1.43	1.37
21	B	817	CLA	C1D-ND	4.99	1.43	1.37
21	B2	821	CLA	C1D-ND	4.99	1.43	1.37
21	3	603	CLA	C1D-ND	4.99	1.43	1.37
30	6	607	CHL	MG-NA	-4.99	1.94	2.06
21	A2	823	CLA	C1D-ND	4.99	1.43	1.37
21	1	616	CLA	C1D-ND	4.98	1.43	1.37
21	A2	806	CLA	C1D-ND	4.98	1.43	1.37
30	92	607	CHL	MG-NA	-4.98	1.94	2.06
30	42	606	CHL	MG-NA	-4.98	1.94	2.06
21	92	611	CLA	C1D-ND	4.97	1.43	1.37
21	B2	831	CLA	C1D-ND	4.97	1.43	1.37
21	A	810	CLA	C1D-ND	4.97	1.43	1.37
21	A	823	CLA	C1D-ND	4.97	1.43	1.37
30	9	606	CHL	MG-NA	-4.96	1.94	2.06
21	A2	842	CLA	C1D-ND	4.96	1.43	1.37
30	Z	607	CHL	MG-NA	-4.96	1.94	2.06
30	Z2	607	CHL	MG-NA	-4.96	1.94	2.06
20	A	801	CL0	MG-NA	-4.96	1.94	2.06
30	72	607	CHL	MG-NA	-4.96	1.94	2.06
21	12	610	CLA	C1D-ND	4.95	1.43	1.37
21	1	602	CLA	C1D-ND	4.95	1.43	1.37
30	52	608	CHL	MG-NA	-4.95	1.94	2.06
21	B	805	CLA	C1D-ND	4.95	1.43	1.37
30	42	608	CHL	MG-NA	-4.95	1.94	2.06
21	A2	810	CLA	C1D-ND	4.95	1.43	1.37
21	F	301	CLA	C1D-ND	4.94	1.43	1.37
30	52	606	CHL	MG-NA	-4.94	1.94	2.06
21	1	610	CLA	C1D-ND	4.94	1.43	1.37
30	62	607	CHL	MG-NA	-4.94	1.94	2.06
21	12	616	CLA	C1D-ND	4.94	1.43	1.37
30	5	608	CHL	MG-NA	-4.94	1.94	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	832	CLA	C1D-ND	4.93	1.43	1.37
21	B2	803	CLA	C1D-ND	4.93	1.43	1.37
30	5	606	CHL	MG-NA	-4.93	1.94	2.06
21	A	812	CLA	C1D-ND	4.93	1.43	1.37
21	A2	812	CLA	C1D-ND	4.93	1.43	1.37
21	B2	830	CLA	C1D-ND	4.93	1.43	1.37
30	4	608	CHL	MG-NA	-4.92	1.94	2.06
20	A2	801	CL0	MG-NA	-4.92	1.94	2.06
30	62	618	CHL	MG-NA	-4.92	1.94	2.06
21	A	806	CLA	C1D-ND	4.91	1.43	1.37
30	6	618	CHL	MG-NA	-4.91	1.94	2.06
30	7	607	CHL	MG-NA	-4.91	1.94	2.06
21	7	610	CLA	C1D-ND	4.90	1.43	1.37
21	72	610	CLA	C1D-ND	4.90	1.43	1.37
21	B	803	CLA	C1D-ND	4.89	1.43	1.37
30	1	606	CHL	MG-NA	-4.89	1.94	2.06
21	B	821	CLA	C1D-ND	4.88	1.43	1.37
30	12	606	CHL	MG-NA	-4.88	1.94	2.06
30	6	606	CHL	MG-NA	-4.86	1.94	2.06
21	A	842	CLA	C1D-ND	4.85	1.43	1.37
30	62	606	CHL	MG-NA	-4.85	1.94	2.06
21	B	830	CLA	C1D-ND	4.84	1.43	1.37
21	B2	825	CLA	C1D-ND	4.77	1.43	1.37
30	8	607	CHL	MG-NA	-4.77	1.94	2.06
30	9	607	CHL	MG-NA	-4.75	1.95	2.06
21	B2	823	CLA	C1D-ND	4.72	1.43	1.37
30	82	607	CHL	MG-NA	-4.72	1.95	2.06
21	B	825	CLA	C1D-ND	4.71	1.43	1.37
21	B	829	CLA	C1D-ND	4.70	1.43	1.37
21	A	802	CLA	C1D-ND	4.69	1.43	1.37
30	9	607	CHL	C1B-NB	4.68	1.39	1.35
21	B	833	CLA	C1D-ND	4.68	1.43	1.37
21	B2	833	CLA	C1D-ND	4.68	1.43	1.37
21	B	823	CLA	C1D-ND	4.68	1.43	1.37
21	B2	829	CLA	C1D-ND	4.67	1.43	1.37
21	A	810	CLA	MG-ND	-4.67	1.96	2.05
21	A2	802	CLA	C1D-ND	4.65	1.43	1.37
21	A2	810	CLA	MG-ND	-4.65	1.96	2.05
20	A2	801	CL0	MG-ND	-4.63	1.96	2.05
20	A	801	CL0	MG-ND	-4.62	1.96	2.05
21	A2	837	CLA	MG-ND	-4.61	1.96	2.05
21	A2	854	CLA	MG-ND	-4.59	1.96	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	837	CLA	MG-ND	-4.55	1.96	2.05
21	B	838	CLA	MG-ND	-4.55	1.96	2.05
21	B	821	CLA	MG-ND	-4.55	1.96	2.05
21	B2	821	CLA	MG-ND	-4.55	1.96	2.05
21	A	854	CLA	MG-ND	-4.55	1.96	2.05
21	A	829	CLA	MG-ND	-4.53	1.96	2.05
21	K	201	CLA	MG-ND	-4.53	1.96	2.05
21	B2	838	CLA	MG-ND	-4.53	1.96	2.05
21	B	803	CLA	MG-ND	-4.52	1.96	2.05
21	B2	803	CLA	MG-ND	-4.51	1.96	2.05
21	1	616	CLA	MG-ND	-4.49	1.96	2.05
21	A2	823	CLA	MG-ND	-4.48	1.96	2.05
21	72	610	CLA	MG-ND	-4.48	1.96	2.05
21	A	803	CLA	MG-ND	-4.48	1.96	2.05
21	A2	803	CLA	MG-ND	-4.48	1.96	2.05
21	K2	201	CLA	MG-ND	-4.48	1.96	2.05
21	72	609	CLA	MG-ND	-4.48	1.96	2.05
21	A2	829	CLA	MG-ND	-4.47	1.96	2.05
21	B	806	CLA	MG-ND	-4.47	1.96	2.05
21	7	610	CLA	MG-ND	-4.46	1.96	2.05
21	A	823	CLA	MG-ND	-4.46	1.97	2.05
21	B2	806	CLA	MG-ND	-4.44	1.97	2.05
21	A	819	CLA	MG-ND	-4.43	1.97	2.05
21	A	825	CLA	MG-ND	-4.42	1.97	2.05
21	A2	833	CLA	MG-ND	-4.42	1.97	2.05
21	32	617	CLA	MG-ND	-4.41	1.97	2.05
21	A	833	CLA	MG-ND	-4.41	1.97	2.05
21	B	829	CLA	MG-ND	-4.41	1.97	2.05
21	A2	802	CLA	MG-ND	-4.41	1.97	2.05
21	7	609	CLA	MG-ND	-4.41	1.97	2.05
21	32	603	CLA	MG-ND	-4.41	1.97	2.05
21	92	602	CLA	MG-ND	-4.40	1.97	2.05
21	A	817	CLA	MG-ND	-4.40	1.97	2.05
21	B2	820	CLA	MG-ND	-4.40	1.97	2.05
21	A2	825	CLA	MG-ND	-4.40	1.97	2.05
21	3	603	CLA	MG-ND	-4.40	1.97	2.05
21	12	616	CLA	MG-ND	-4.40	1.97	2.05
21	9	602	CLA	MG-ND	-4.40	1.97	2.05
21	5	621	CLA	MG-ND	-4.40	1.97	2.05
21	52	621	CLA	MG-ND	-4.39	1.97	2.05
21	A	802	CLA	MG-ND	-4.39	1.97	2.05
21	B	839	CLA	MG-ND	-4.38	1.97	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A2	817	CLA	MG-ND	-4.38	1.97	2.05
21	A2	819	CLA	MG-ND	-4.38	1.97	2.05
21	3	617	CLA	MG-ND	-4.37	1.97	2.05
21	B2	839	CLA	MG-ND	-4.37	1.97	2.05
21	B	820	CLA	MG-ND	-4.37	1.97	2.05
20	A2	801	CL0	C1D-ND	4.37	1.43	1.37
21	B2	817	CLA	MG-ND	-4.37	1.97	2.05
21	72	608	CLA	MG-ND	-4.37	1.97	2.05
21	7	608	CLA	MG-ND	-4.36	1.97	2.05
21	B2	829	CLA	MG-ND	-4.35	1.97	2.05
21	Z	608	CLA	MG-ND	-4.35	1.97	2.05
21	4	609	CLA	MG-ND	-4.34	1.97	2.05
21	82	602	CLA	MG-ND	-4.34	1.97	2.05
21	B	818	CLA	MG-ND	-4.34	1.97	2.05
21	Z2	609	CLA	MG-ND	-4.34	1.97	2.05
21	A2	808	CLA	MG-ND	-4.33	1.97	2.05
21	A2	828	CLA	MG-ND	-4.33	1.97	2.05
21	82	610	CLA	MG-ND	-4.33	1.97	2.05
21	32	611	CLA	MG-ND	-4.33	1.97	2.05
21	A2	843	CLA	MG-ND	-4.33	1.97	2.05
20	A	801	CL0	C1D-ND	4.33	1.43	1.37
21	Z2	608	CLA	MG-ND	-4.33	1.97	2.05
21	A	828	CLA	MG-ND	-4.33	1.97	2.05
21	8	602	CLA	MG-ND	-4.32	1.97	2.05
21	A	843	CLA	MG-ND	-4.32	1.97	2.05
21	B2	819	CLA	MG-ND	-4.32	1.97	2.05
21	1	602	CLA	MG-ND	-4.32	1.97	2.05
21	12	602	CLA	MG-ND	-4.32	1.97	2.05
21	B	819	CLA	MG-ND	-4.32	1.97	2.05
21	A2	813	CLA	MG-ND	-4.32	1.97	2.05
21	A	836	CLA	MG-ND	-4.31	1.97	2.05
21	B2	818	CLA	MG-ND	-4.31	1.97	2.05
21	A2	836	CLA	MG-ND	-4.31	1.97	2.05
21	72	613	CLA	MG-ND	-4.31	1.97	2.05
21	1	608	CLA	MG-ND	-4.31	1.97	2.05
21	1	611	CLA	MG-ND	-4.31	1.97	2.05
21	42	609	CLA	MG-ND	-4.31	1.97	2.05
21	B2	823	CLA	MG-ND	-4.31	1.97	2.05
21	A	808	CLA	MG-ND	-4.30	1.97	2.05
21	B2	809	CLA	MG-ND	-4.30	1.97	2.05
21	3	611	CLA	MG-ND	-4.30	1.97	2.05
21	B2	812	CLA	MG-ND	-4.30	1.97	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	813	CLA	MG-ND	-4.30	1.97	2.05
21	3	609	CLA	MG-ND	-4.30	1.97	2.05
21	32	609	CLA	MG-ND	-4.30	1.97	2.05
21	G2	203	CLA	MG-ND	-4.30	1.97	2.05
21	82	604	CLA	MG-ND	-4.30	1.97	2.05
21	12	611	CLA	MG-ND	-4.30	1.97	2.05
21	7	613	CLA	MG-ND	-4.29	1.97	2.05
21	32	607	CLA	MG-ND	-4.29	1.97	2.05
21	B	823	CLA	MG-ND	-4.29	1.97	2.05
21	32	610	CLA	MG-ND	-4.29	1.97	2.05
21	A	815	CLA	MG-ND	-4.29	1.97	2.05
21	Z	609	CLA	MG-ND	-4.29	1.97	2.05
21	4	602	CLA	MG-ND	-4.29	1.97	2.05
21	B	807	CLA	MG-ND	-4.28	1.97	2.05
21	12	608	CLA	MG-ND	-4.28	1.97	2.05
21	B	812	CLA	MG-ND	-4.28	1.97	2.05
21	B	817	CLA	MG-ND	-4.28	1.97	2.05
21	52	602	CLA	MG-ND	-4.28	1.97	2.05
21	G	203	CLA	MG-ND	-4.28	1.97	2.05
21	K2	203	CLA	MG-ND	-4.27	1.97	2.05
21	B2	826	CLA	MG-ND	-4.27	1.97	2.05
21	A	807	CLA	MG-ND	-4.27	1.97	2.05
21	A2	807	CLA	MG-ND	-4.27	1.97	2.05
21	8	610	CLA	MG-ND	-4.27	1.97	2.05
21	42	602	CLA	MG-ND	-4.27	1.97	2.05
21	B	813	CLA	MG-ND	-4.27	1.97	2.05
21	3	607	CLA	MG-ND	-4.27	1.97	2.05
21	B2	813	CLA	MG-ND	-4.26	1.97	2.05
21	A	814	CLA	MG-ND	-4.26	1.97	2.05
21	B	809	CLA	MG-ND	-4.26	1.97	2.05
21	32	613	CLA	MG-ND	-4.26	1.97	2.05
21	92	611	CLA	MG-ND	-4.26	1.97	2.05
21	A	824	CLA	MG-ND	-4.26	1.97	2.05
21	A2	815	CLA	MG-ND	-4.26	1.97	2.05
21	5	602	CLA	MG-ND	-4.26	1.97	2.05
21	8	604	CLA	MG-ND	-4.25	1.97	2.05
21	L2	203	CLA	MG-ND	-4.25	1.97	2.05
21	9	613	CLA	MG-ND	-4.25	1.97	2.05
21	A2	821	CLA	MG-ND	-4.25	1.97	2.05
21	3	613	CLA	MG-ND	-4.25	1.97	2.05
21	A2	814	CLA	MG-ND	-4.25	1.97	2.05
21	3	610	CLA	MG-ND	-4.24	1.97	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	4	613	CLA	MG-ND	-4.24	1.97	2.05
21	92	601	CLA	MG-ND	-4.24	1.97	2.05
21	A	826	CLA	MG-ND	-4.24	1.97	2.05
21	8	603	CLA	MG-ND	-4.24	1.97	2.05
21	82	603	CLA	MG-ND	-4.24	1.97	2.05
21	1	610	CLA	MG-ND	-4.23	1.97	2.05
21	B	826	CLA	MG-ND	-4.23	1.97	2.05
21	A2	826	CLA	MG-ND	-4.23	1.97	2.05
21	72	604	CLA	MG-ND	-4.23	1.97	2.05
21	92	613	CLA	MG-ND	-4.23	1.97	2.05
21	32	606	CLA	MG-ND	-4.23	1.97	2.05
21	6	617	CLA	MG-ND	-4.23	1.97	2.05
21	Z2	602	CLA	MG-ND	-4.23	1.97	2.05
21	62	617	CLA	MG-ND	-4.23	1.97	2.05
21	9	610	CLA	MG-ND	-4.23	1.97	2.05
21	A	821	CLA	MG-ND	-4.23	1.97	2.05
21	9	601	CLA	MG-ND	-4.22	1.97	2.05
21	3	615	CLA	MG-ND	-4.22	1.97	2.05
21	B2	807	CLA	MG-ND	-4.22	1.97	2.05
21	32	615	CLA	MG-ND	-4.22	1.97	2.05
21	J2	101	CLA	MG-ND	-4.22	1.97	2.05
21	3	606	CLA	MG-ND	-4.22	1.97	2.05
21	B2	837	CLA	MG-ND	-4.22	1.97	2.05
21	B	835	CLA	MG-ND	-4.22	1.97	2.05
21	K	203	CLA	MG-ND	-4.22	1.97	2.05
21	5	604	CLA	MG-ND	-4.22	1.97	2.05
21	9	611	CLA	MG-ND	-4.22	1.97	2.05
21	52	604	CLA	MG-ND	-4.22	1.97	2.05
21	B	833	CLA	MG-ND	-4.22	1.97	2.05
21	B	837	CLA	MG-ND	-4.22	1.97	2.05
21	A2	839	CLA	MG-ND	-4.22	1.97	2.05
21	32	602	CLA	MG-ND	-4.21	1.97	2.05
21	A	805	CLA	MG-ND	-4.21	1.97	2.05
21	1	603	CLA	MG-ND	-4.21	1.97	2.05
21	Z	603	CLA	MG-ND	-4.21	1.97	2.05
21	5	611	CLA	MG-ND	-4.21	1.97	2.05
21	72	602	CLA	MG-ND	-4.21	1.97	2.05
21	3	602	CLA	MG-ND	-4.21	1.97	2.05
21	12	604	CLA	MG-ND	-4.21	1.97	2.05
21	1	614	CLA	MG-ND	-4.21	1.97	2.05
21	A2	824	CLA	MG-ND	-4.21	1.97	2.05
21	B	815	CLA	MG-ND	-4.21	1.97	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	12	614	CLA	MG-ND	-4.21	1.97	2.05
21	L	203	CLA	MG-ND	-4.21	1.97	2.05
21	1	609	CLA	MG-ND	-4.21	1.97	2.05
21	82	608	CLA	MG-ND	-4.21	1.97	2.05
21	B	834	CLA	MG-ND	-4.21	1.97	2.05
21	A	839	CLA	MG-ND	-4.20	1.97	2.05
21	8	611	CLA	MG-ND	-4.20	1.97	2.05
21	82	611	CLA	MG-ND	-4.20	1.97	2.05
21	B2	811	CLA	MG-ND	-4.20	1.97	2.05
21	A2	834	CLA	MG-ND	-4.19	1.97	2.05
21	B2	833	CLA	MG-ND	-4.19	1.97	2.05
21	B	841	CLA	MG-ND	-4.19	1.97	2.05
21	72	614	CLA	MG-ND	-4.19	1.97	2.05
21	A2	822	CLA	MG-ND	-4.19	1.97	2.05
21	8	608	CLA	MG-ND	-4.19	1.97	2.05
21	B2	834	CLA	MG-ND	-4.19	1.97	2.05
21	52	611	CLA	MG-ND	-4.19	1.97	2.05
21	A	834	CLA	MG-ND	-4.19	1.97	2.05
21	6	622	CLA	MG-ND	-4.19	1.97	2.05
21	82	609	CLA	MG-ND	-4.19	1.97	2.05
21	42	616	CLA	MG-ND	-4.19	1.97	2.05
21	A	831	CLA	MG-ND	-4.19	1.97	2.05
21	52	601	CLA	MG-ND	-4.19	1.97	2.05
21	42	613	CLA	MG-ND	-4.18	1.97	2.05
21	62	613	CLA	MG-ND	-4.18	1.97	2.05
21	92	610	CLA	MG-ND	-4.18	1.97	2.05
21	9	604	CLA	MG-ND	-4.18	1.97	2.05
21	B	811	CLA	MG-ND	-4.18	1.97	2.05
21	3	612	CLA	MG-ND	-4.18	1.97	2.05
21	A2	805	CLA	MG-ND	-4.18	1.97	2.05
21	Z2	603	CLA	MG-ND	-4.18	1.97	2.05
21	Z	602	CLA	MG-ND	-4.18	1.97	2.05
21	7	604	CLA	MG-ND	-4.18	1.97	2.05
21	92	609	CLA	MG-ND	-4.18	1.97	2.05
21	K	204	CLA	MG-ND	-4.18	1.97	2.05
21	7	611	CLA	MG-ND	-4.18	1.97	2.05
21	B2	830	CLA	MG-ND	-4.18	1.97	2.05
21	32	604	CLA	MG-ND	-4.18	1.97	2.05
21	12	610	CLA	MG-ND	-4.18	1.97	2.05
21	B2	815	CLA	MG-ND	-4.17	1.97	2.05
21	B	825	CLA	MG-ND	-4.17	1.97	2.05
21	4	616	CLA	MG-ND	-4.17	1.97	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	6	613	CLA	MG-ND	-4.17	1.97	2.05
21	Z2	616	CLA	MG-ND	-4.17	1.97	2.05
21	92	604	CLA	MG-ND	-4.17	1.97	2.05
21	7	614	CLA	MG-ND	-4.17	1.97	2.05
21	7	612	CLA	MG-ND	-4.17	1.97	2.05
21	72	616	CLA	MG-ND	-4.17	1.97	2.05
21	9	609	CLA	MG-ND	-4.16	1.97	2.05
21	B2	841	CLA	MG-ND	-4.16	1.97	2.05
21	32	612	CLA	MG-ND	-4.16	1.97	2.05
21	12	603	CLA	MG-ND	-4.16	1.97	2.05
21	B2	825	CLA	MG-ND	-4.16	1.97	2.05
21	A	822	CLA	MG-ND	-4.16	1.97	2.05
21	F	303	CLA	MG-ND	-4.16	1.97	2.05
21	92	612	CLA	MG-ND	-4.16	1.97	2.05
21	F2	301	CLA	MG-ND	-4.16	1.97	2.05
21	12	609	CLA	MG-ND	-4.16	1.97	2.05
21	F2	303	CLA	MG-ND	-4.16	1.97	2.05
21	F	301	CLA	MG-ND	-4.16	1.97	2.05
21	J	101	CLA	MG-ND	-4.16	1.97	2.05
21	A2	831	CLA	MG-ND	-4.16	1.97	2.05
21	42	603	CLA	MG-ND	-4.16	1.97	2.05
21	Z	610	CLA	MG-ND	-4.16	1.97	2.05
21	4	603	CLA	MG-ND	-4.16	1.97	2.05
21	Z2	610	CLA	MG-ND	-4.16	1.97	2.05
21	92	614	CLA	MG-ND	-4.16	1.97	2.05
21	72	611	CLA	MG-ND	-4.16	1.97	2.05
21	42	604	CLA	MG-ND	-4.16	1.97	2.05
21	B2	835	CLA	MG-ND	-4.16	1.97	2.05
21	9	612	CLA	MG-ND	-4.16	1.97	2.05
21	3	614	CLA	MG-ND	-4.15	1.97	2.05
21	1	604	CLA	MG-ND	-4.15	1.97	2.05
21	7	602	CLA	MG-ND	-4.15	1.97	2.05
21	8	609	CLA	MG-ND	-4.15	1.97	2.05
21	4	614	CLA	MG-ND	-4.15	1.97	2.05
21	42	614	CLA	MG-ND	-4.15	1.97	2.05
21	K2	206	CLA	MG-ND	-4.15	1.97	2.05
21	9	614	CLA	MG-ND	-4.15	1.97	2.05
21	A	804	CLA	MG-ND	-4.15	1.97	2.05
21	B	810	CLA	MG-ND	-4.15	1.97	2.05
21	6	610	CLA	MG-ND	-4.14	1.97	2.05
21	32	614	CLA	MG-ND	-4.14	1.97	2.05
21	3	604	CLA	MG-ND	-4.14	1.97	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B2	804	CLA	MG-ND	-4.14	1.97	2.05
21	6	604	CLA	MG-ND	-4.14	1.97	2.05
21	4	611	CLA	MG-ND	-4.14	1.97	2.05
21	8	614	CLA	MG-ND	-4.14	1.97	2.05
21	82	614	CLA	MG-ND	-4.14	1.97	2.05
21	62	622	CLA	MG-ND	-4.14	1.97	2.05
21	5	614	CLA	MG-ND	-4.14	1.97	2.05
21	4	604	CLA	MG-ND	-4.14	1.97	2.05
21	A2	845	CLA	MG-ND	-4.14	1.97	2.05
21	12	612	CLA	MG-ND	-4.13	1.97	2.05
21	Z	604	CLA	MG-ND	-4.13	1.97	2.05
21	Z	613	CLA	MG-ND	-4.13	1.97	2.05
21	A2	809	CLA	MG-ND	-4.13	1.97	2.05
21	A	841	CLA	MG-ND	-4.13	1.97	2.05
21	42	611	CLA	MG-ND	-4.13	1.97	2.05
21	62	611	CLA	MG-ND	-4.13	1.97	2.05
21	B	804	CLA	MG-ND	-4.13	1.97	2.05
21	6	603	CLA	MG-ND	-4.13	1.97	2.05
21	Z2	614	CLA	MG-ND	-4.13	1.97	2.05
21	Z2	613	CLA	MG-ND	-4.13	1.97	2.05
21	62	610	CLA	MG-ND	-4.13	1.97	2.05
21	7	616	CLA	MG-ND	-4.12	1.97	2.05
21	A	832	CLA	MG-ND	-4.12	1.97	2.05
21	6	611	CLA	MG-ND	-4.12	1.97	2.05
21	B2	824	CLA	MG-ND	-4.12	1.97	2.05
21	1	612	CLA	MG-ND	-4.12	1.97	2.05
21	6	609	CLA	MG-ND	-4.12	1.97	2.05
21	A	818	CLA	MG-ND	-4.12	1.97	2.05
21	Z	616	CLA	MG-ND	-4.12	1.97	2.05
21	72	612	CLA	MG-ND	-4.12	1.97	2.05
21	Z2	604	CLA	MG-ND	-4.12	1.97	2.05
21	62	604	CLA	MG-ND	-4.12	1.97	2.05
21	5	601	CLA	MG-ND	-4.11	1.97	2.05
21	K2	204	CLA	MG-ND	-4.11	1.97	2.05
21	B	830	CLA	MG-ND	-4.11	1.97	2.05
21	B	831	CLA	MG-ND	-4.11	1.97	2.05
21	52	614	CLA	MG-ND	-4.11	1.97	2.05
21	62	609	CLA	MG-ND	-4.11	1.97	2.05
21	A2	835	CLA	MG-ND	-4.11	1.97	2.05
21	A	811	CLA	MG-ND	-4.11	1.97	2.05
21	A2	804	CLA	MG-ND	-4.11	1.97	2.05
21	B2	828	CLA	MG-ND	-4.11	1.97	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	4	612	CLA	MG-ND	-4.11	1.97	2.05
21	12	613	CLA	MG-ND	-4.11	1.97	2.05
21	1	613	CLA	MG-ND	-4.11	1.97	2.05
21	A2	841	CLA	MG-ND	-4.11	1.97	2.05
21	52	610	CLA	MG-ND	-4.11	1.97	2.05
21	A	845	CLA	MG-ND	-4.10	1.97	2.05
21	B2	822	CLA	MG-ND	-4.10	1.97	2.05
21	72	620	CLA	MG-ND	-4.10	1.97	2.05
21	A2	840	CLA	MG-ND	-4.10	1.97	2.05
21	B	822	CLA	MG-ND	-4.10	1.97	2.05
21	K	206	CLA	MG-ND	-4.10	1.97	2.05
21	8	613	CLA	MG-ND	-4.10	1.97	2.05
21	82	613	CLA	MG-ND	-4.10	1.97	2.05
21	A2	832	CLA	MG-ND	-4.10	1.97	2.05
21	A	809	CLA	MG-ND	-4.10	1.97	2.05
21	Z	614	CLA	MG-ND	-4.10	1.97	2.05
21	B2	810	CLA	MG-ND	-4.10	1.97	2.05
21	A2	811	CLA	MG-ND	-4.10	1.97	2.05
21	52	616	CLA	MG-ND	-4.10	1.97	2.05
21	B	824	CLA	MG-ND	-4.10	1.97	2.05
21	5	610	CLA	MG-ND	-4.09	1.97	2.05
21	7	620	CLA	MG-ND	-4.09	1.97	2.05
21	7	603	CLA	MG-ND	-4.09	1.97	2.05
21	62	603	CLA	MG-ND	-4.09	1.97	2.05
21	52	612	CLA	MG-ND	-4.09	1.97	2.05
21	B2	832	CLA	MG-ND	-4.08	1.97	2.05
21	B	816	CLA	MG-ND	-4.08	1.97	2.05
21	Z	611	CLA	MG-ND	-4.08	1.97	2.05
21	A	835	CLA	MG-ND	-4.08	1.97	2.05
21	B2	816	CLA	MG-ND	-4.08	1.97	2.05
21	A2	818	CLA	MG-ND	-4.08	1.97	2.05
21	G	204	CLA	MG-ND	-4.08	1.97	2.05
21	A	827	CLA	MG-ND	-4.08	1.97	2.05
21	Z2	611	CLA	MG-ND	-4.08	1.97	2.05
21	4	610	CLA	MG-ND	-4.07	1.97	2.05
21	6	602	CLA	MG-ND	-4.07	1.97	2.05
21	A2	827	CLA	MG-ND	-4.07	1.97	2.05
21	62	602	CLA	MG-ND	-4.07	1.97	2.05
21	A2	816	CLA	MG-ND	-4.07	1.97	2.05
21	A	816	CLA	MG-ND	-4.07	1.97	2.05
21	A	840	CLA	MG-ND	-4.07	1.97	2.05
21	52	609	CLA	MG-ND	-4.07	1.97	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	82	616	CLA	MG-ND	-4.07	1.97	2.05
21	B	827	CLA	MG-ND	-4.06	1.97	2.05
21	B2	827	CLA	MG-ND	-4.06	1.97	2.05
21	B	832	CLA	MG-ND	-4.06	1.97	2.05
21	B	802	CLA	MG-ND	-4.06	1.97	2.05
21	B2	836	CLA	MG-ND	-4.06	1.97	2.05
21	B2	805	CLA	MG-ND	-4.06	1.97	2.05
21	A	838	CLA	MG-ND	-4.06	1.97	2.05
21	B	828	CLA	MG-ND	-4.06	1.97	2.05
21	52	617	CLA	MG-ND	-4.06	1.97	2.05
21	92	603	CLA	MG-ND	-4.06	1.97	2.05
21	5	609	CLA	MG-ND	-4.05	1.97	2.05
21	A	830	CLA	MG-ND	-4.05	1.97	2.05
21	B2	802	CLA	MG-ND	-4.05	1.97	2.05
21	A	820	CLA	MG-ND	-4.05	1.97	2.05
21	B	836	CLA	MG-ND	-4.05	1.97	2.05
21	G2	204	CLA	MG-ND	-4.05	1.97	2.05
21	5	612	CLA	MG-ND	-4.05	1.97	2.05
21	5	616	CLA	MG-ND	-4.05	1.97	2.05
21	A2	820	CLA	MG-ND	-4.05	1.97	2.05
21	5	613	CLA	MG-ND	-4.05	1.97	2.05
21	52	613	CLA	MG-ND	-4.05	1.97	2.05
21	42	612	CLA	MG-ND	-4.05	1.97	2.05
21	42	610	CLA	MG-ND	-4.05	1.97	2.05
21	6	612	CLA	MG-ND	-4.05	1.97	2.05
21	72	603	CLA	MG-ND	-4.04	1.97	2.05
21	F	304	CLA	MG-ND	-4.04	1.97	2.05
21	8	616	CLA	MG-ND	-4.04	1.97	2.05
21	F2	304	CLA	MG-ND	-4.04	1.97	2.05
21	9	603	CLA	MG-ND	-4.03	1.97	2.05
21	A2	830	CLA	MG-ND	-4.03	1.97	2.05
21	B2	831	CLA	MG-ND	-4.03	1.97	2.05
21	B2	840	CLA	MG-ND	-4.03	1.97	2.05
21	5	617	CLA	MG-ND	-4.03	1.97	2.05
21	L	204	CLA	MG-ND	-4.02	1.97	2.05
21	B	805	CLA	MG-ND	-4.01	1.97	2.05
21	A2	842	CLA	MG-ND	-4.01	1.97	2.05
21	A	812	CLA	MG-ND	-4.01	1.97	2.05
21	B	840	CLA	MG-ND	-4.01	1.97	2.05
21	A2	812	CLA	MG-ND	-4.01	1.97	2.05
21	A	842	CLA	MG-ND	-4.01	1.97	2.05
21	A2	806	CLA	MG-ND	-4.00	1.97	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A2	838	CLA	MG-ND	-3.99	1.97	2.05
21	B	808	CLA	MG-ND	-3.99	1.97	2.05
21	B2	814	CLA	MG-ND	-3.99	1.97	2.05
21	62	612	CLA	MG-ND	-3.99	1.97	2.05
21	B	814	CLA	MG-ND	-3.98	1.97	2.05
21	B2	808	CLA	MG-ND	-3.98	1.97	2.05
20	A2	801	CL0	MG-NC	-3.98	1.96	2.06
20	A	801	CL0	MG-NC	-3.97	1.96	2.06
21	L2	204	CLA	MG-ND	-3.97	1.97	2.05
21	A	806	CLA	MG-ND	-3.95	1.98	2.05
21	6	614	CLA	MG-ND	-3.94	1.98	2.05
21	62	614	CLA	MG-ND	-3.94	1.98	2.05
21	Z2	612	CLA	MG-ND	-3.93	1.98	2.05
21	5	603	CLA	MG-ND	-3.93	1.98	2.05
21	52	603	CLA	MG-ND	-3.93	1.98	2.05
21	8	612	CLA	MG-ND	-3.91	1.98	2.05
21	82	612	CLA	MG-ND	-3.91	1.98	2.05
21	Z	612	CLA	MG-ND	-3.86	1.98	2.05
30	92	607	CHL	C1B-NB	3.75	1.38	1.35
30	4	618	CHL	C1D-ND	3.67	1.42	1.37
30	6	606	CHL	C1D-ND	3.65	1.42	1.37
30	6	607	CHL	C1D-ND	3.65	1.42	1.37
30	82	607	CHL	C1D-ND	3.64	1.42	1.37
30	62	606	CHL	C1D-ND	3.63	1.42	1.37
30	52	618	CHL	C1D-ND	3.63	1.42	1.37
30	42	618	CHL	C1D-ND	3.61	1.42	1.37
30	Z	606	CHL	C1D-ND	3.60	1.42	1.37
30	62	608	CHL	C1D-ND	3.59	1.42	1.37
30	5	618	CHL	C1D-ND	3.58	1.42	1.37
30	62	607	CHL	C1D-ND	3.57	1.42	1.37
30	8	607	CHL	C1D-ND	3.57	1.42	1.37
30	6	618	CHL	C1D-ND	3.55	1.42	1.37
30	62	618	CHL	C1D-ND	3.55	1.42	1.37
30	5	606	CHL	C1D-ND	3.54	1.42	1.37
30	42	601	CHL	C1D-ND	3.54	1.42	1.37
30	6	608	CHL	C1D-ND	3.52	1.42	1.37
30	4	606	CHL	C1D-ND	3.50	1.42	1.37
30	4	601	CHL	C1D-ND	3.50	1.42	1.37
30	8	606	CHL	C1D-ND	3.50	1.42	1.37
30	42	606	CHL	C1D-ND	3.50	1.42	1.37
30	52	606	CHL	C1D-ND	3.50	1.42	1.37
30	4	608	CHL	C1D-ND	3.48	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	42	608	CHL	C1D-ND	3.48	1.42	1.37
30	52	608	CHL	C1D-ND	3.44	1.42	1.37
30	82	606	CHL	C1D-ND	3.43	1.42	1.37
30	8	601	CHL	C1D-ND	3.43	1.42	1.37
30	Z2	606	CHL	C1D-ND	3.43	1.42	1.37
30	92	607	CHL	C1D-ND	3.41	1.42	1.37
30	5	608	CHL	C1D-ND	3.40	1.42	1.37
30	62	601	CHL	C1D-ND	3.40	1.42	1.37
30	1	606	CHL	C1D-ND	3.40	1.42	1.37
30	62	616	CHL	C1D-ND	3.39	1.42	1.37
30	92	606	CHL	C1D-ND	3.39	1.41	1.37
30	12	606	CHL	C1D-ND	3.38	1.41	1.37
30	82	601	CHL	C1D-ND	3.38	1.41	1.37
30	9	606	CHL	C3A-C2A	-3.35	1.51	1.54
30	92	606	CHL	C3A-C2A	-3.34	1.51	1.54
30	5	607	CHL	C1D-ND	3.34	1.41	1.37
30	6	601	CHL	C1D-ND	3.33	1.41	1.37
30	72	606	CHL	C1D-ND	3.32	1.41	1.37
30	6	616	CHL	C1D-ND	3.32	1.41	1.37
30	9	606	CHL	C1D-ND	3.31	1.41	1.37
30	7	606	CHL	C1D-ND	3.31	1.41	1.37
30	1	601	CHL	C1D-ND	3.28	1.41	1.37
30	4	607	CHL	C1D-ND	3.27	1.41	1.37
30	Z	601	CHL	C1D-ND	3.26	1.41	1.37
30	72	601	CHL	C1D-ND	3.26	1.41	1.37
30	12	601	CHL	C1D-ND	3.25	1.41	1.37
30	Z2	607	CHL	C1D-ND	3.25	1.41	1.37
30	7	607	CHL	C1D-ND	3.24	1.41	1.37
30	52	607	CHL	C1D-ND	3.24	1.41	1.37
30	7	601	CHL	C1D-ND	3.23	1.41	1.37
30	Z	607	CHL	C1D-ND	3.22	1.41	1.37
30	72	607	CHL	C1D-ND	3.21	1.41	1.37
32	5	625	NEX	C1-C6	-3.20	1.49	1.54
30	42	607	CHL	C1D-ND	3.20	1.41	1.37
30	Z2	601	CHL	C1D-ND	3.19	1.41	1.37
30	52	607	CHL	C1B-NB	3.17	1.38	1.35
30	1	607	CHL	MG-NC	-3.16	1.98	2.06
30	52	607	CHL	MG-NC	-3.16	1.98	2.06
30	3	608	CHL	C1D-ND	3.16	1.41	1.37
30	12	607	CHL	MG-NC	-3.14	1.98	2.06
30	5	607	CHL	MG-NC	-3.14	1.98	2.06
30	7	607	CHL	C3B-C2B	-3.12	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	62	607	CHL	MG-NC	-3.12	1.98	2.06
30	1	601	CHL	C3B-C2B	-3.12	1.36	1.40
30	82	607	CHL	C3B-C2B	-3.11	1.36	1.40
30	8	607	CHL	C3B-C2B	-3.09	1.36	1.40
30	6	601	CHL	MG-NC	-3.09	1.98	2.06
30	6	607	CHL	MG-NC	-3.09	1.98	2.06
30	32	608	CHL	C1D-ND	3.09	1.41	1.37
30	5	607	CHL	C1B-NB	3.08	1.38	1.35
30	12	601	CHL	C3B-C2B	-3.08	1.36	1.40
30	62	601	CHL	MG-NC	-3.07	1.99	2.06
30	72	607	CHL	C3B-C2B	-3.04	1.36	1.40
30	32	608	CHL	C3B-C2B	-3.04	1.36	1.40
30	3	608	CHL	C3B-C2B	-3.04	1.36	1.40
30	1	607	CHL	C3B-C2B	-3.04	1.36	1.40
30	52	606	CHL	C3B-C2B	-3.03	1.36	1.40
30	Z2	607	CHL	C3B-C2B	-3.02	1.36	1.40
30	92	606	CHL	C3B-C2B	-3.02	1.36	1.40
30	5	607	CHL	C3B-C2B	-3.01	1.36	1.40
30	1	606	CHL	C3B-C2B	-3.00	1.36	1.40
30	12	607	CHL	C3B-C2B	-2.99	1.36	1.40
30	42	607	CHL	C3B-C2B	-2.99	1.36	1.40
30	Z	607	CHL	C3B-C2B	-2.99	1.36	1.40
30	62	606	CHL	C3B-C2B	-2.99	1.36	1.40
30	Z	606	CHL	C3B-C2B	-2.98	1.36	1.40
30	9	606	CHL	C3B-C2B	-2.98	1.36	1.40
30	6	608	CHL	MG-NC	-2.98	1.99	2.06
30	62	608	CHL	MG-NC	-2.98	1.99	2.06
30	72	601	CHL	MG-NC	-2.97	1.99	2.06
30	12	606	CHL	C3B-C2B	-2.96	1.36	1.40
30	52	607	CHL	C3B-C2B	-2.96	1.36	1.40
30	7	601	CHL	MG-NC	-2.96	1.99	2.06
30	42	618	CHL	MG-NC	-2.96	1.99	2.06
30	4	618	CHL	MG-NC	-2.96	1.99	2.06
30	4	607	CHL	C3B-C2B	-2.96	1.36	1.40
30	5	618	CHL	MG-NC	-2.96	1.99	2.06
30	5	606	CHL	C3B-C2B	-2.96	1.36	1.40
30	52	608	CHL	C3B-C2B	-2.95	1.36	1.40
30	52	608	CHL	MG-NC	-2.95	1.99	2.06
30	7	606	CHL	MG-NC	-2.95	1.99	2.06
30	72	606	CHL	MG-NC	-2.95	1.99	2.06
30	6	606	CHL	C3B-C2B	-2.95	1.36	1.40
30	5	608	CHL	C3B-C2B	-2.94	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	Z2	606	CHL	C3B-C2B	-2.94	1.36	1.40
30	8	606	CHL	MG-NC	-2.94	1.99	2.06
30	82	606	CHL	MG-NC	-2.94	1.99	2.06
30	52	618	CHL	MG-NC	-2.94	1.99	2.06
30	8	601	CHL	MG-NC	-2.93	1.99	2.06
30	82	601	CHL	MG-NC	-2.93	1.99	2.06
30	6	616	CHL	C3B-C2B	-2.93	1.36	1.40
30	5	608	CHL	MG-NC	-2.92	1.99	2.06
30	52	618	CHL	C3B-C2B	-2.92	1.36	1.40
30	6	607	CHL	C3B-C2B	-2.92	1.36	1.40
30	62	607	CHL	C3B-C2B	-2.92	1.36	1.40
30	1	607	CHL	C1D-ND	2.91	1.41	1.37
30	12	607	CHL	C1D-ND	2.91	1.41	1.37
30	5	618	CHL	C3B-C2B	-2.90	1.36	1.40
30	4	608	CHL	C3B-C2B	-2.90	1.36	1.40
30	7	606	CHL	C3B-C2B	-2.90	1.36	1.40
30	72	606	CHL	C3B-C2B	-2.90	1.36	1.40
30	62	616	CHL	C3B-C2B	-2.90	1.36	1.40
30	Z	606	CHL	MG-NC	-2.90	1.99	2.06
30	42	618	CHL	C3B-C2B	-2.90	1.36	1.40
30	6	608	CHL	C3B-C2B	-2.89	1.36	1.40
30	62	608	CHL	C3B-C2B	-2.89	1.36	1.40
30	1	601	CHL	MG-NC	-2.89	1.99	2.06
30	62	606	CHL	MG-NC	-2.88	1.99	2.06
30	62	601	CHL	C1B-NB	2.88	1.37	1.35
30	Z2	606	CHL	MG-NC	-2.88	1.99	2.06
30	42	608	CHL	C3B-C2B	-2.87	1.36	1.40
30	4	618	CHL	C3B-C2B	-2.87	1.36	1.40
30	7	601	CHL	C3B-C2B	-2.87	1.36	1.40
30	62	618	CHL	C3B-C2B	-2.87	1.36	1.40
30	42	606	CHL	C3B-C2B	-2.87	1.36	1.40
30	4	606	CHL	C3B-C2B	-2.87	1.36	1.40
30	9	607	CHL	C1D-ND	2.87	1.41	1.37
30	9	606	CHL	MG-NC	-2.87	1.99	2.06
30	1	606	CHL	MG-NC	-2.87	1.99	2.06
30	42	607	CHL	C1B-NB	2.86	1.37	1.35
30	8	601	CHL	C3B-C2B	-2.86	1.36	1.40
30	82	601	CHL	C3B-C2B	-2.86	1.36	1.40
30	6	616	CHL	MG-NC	-2.86	1.99	2.06
30	52	606	CHL	MG-NC	-2.86	1.99	2.06
30	12	601	CHL	MG-NC	-2.85	1.99	2.06
30	Z	601	CHL	C3B-C2B	-2.85	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	Z2	601	CHL	C3B-C2B	-2.85	1.36	1.40
30	4	601	CHL	C3B-C2B	-2.85	1.36	1.40
30	42	601	CHL	C3B-C2B	-2.85	1.36	1.40
30	4	607	CHL	MG-NC	-2.85	1.99	2.06
30	Z	601	CHL	MG-NC	-2.85	1.99	2.06
30	6	606	CHL	MG-NC	-2.85	1.99	2.06
30	Z2	601	CHL	MG-NC	-2.85	1.99	2.06
30	92	606	CHL	MG-NC	-2.85	1.99	2.06
30	4	607	CHL	C1B-NB	2.85	1.37	1.35
30	12	606	CHL	MG-NC	-2.85	1.99	2.06
30	4	608	CHL	MG-NC	-2.85	1.99	2.06
30	42	608	CHL	MG-NC	-2.85	1.99	2.06
30	6	618	CHL	C3B-C2B	-2.84	1.36	1.40
30	42	606	CHL	MG-NC	-2.84	1.99	2.06
30	7	607	CHL	MG-NC	-2.84	1.99	2.06
30	72	601	CHL	C3B-C2B	-2.84	1.36	1.40
30	92	607	CHL	C3B-C2B	-2.84	1.36	1.40
30	82	607	CHL	MG-NC	-2.84	1.99	2.06
30	8	606	CHL	C3B-C2B	-2.84	1.36	1.40
30	82	606	CHL	C3B-C2B	-2.84	1.36	1.40
30	42	607	CHL	MG-NC	-2.84	1.99	2.06
30	6	618	CHL	MG-NC	-2.84	1.99	2.06
30	62	618	CHL	MG-NC	-2.84	1.99	2.06
30	4	608	CHL	C1B-NB	2.83	1.37	1.35
30	62	616	CHL	MG-NC	-2.83	1.99	2.06
30	4	606	CHL	MG-NC	-2.82	1.99	2.06
30	Z	607	CHL	MG-NC	-2.81	1.99	2.06
30	Z2	607	CHL	MG-NC	-2.81	1.99	2.06
30	42	618	CHL	C1B-NB	2.81	1.37	1.35
30	6	601	CHL	C1B-NB	2.81	1.37	1.35
30	72	607	CHL	MG-NC	-2.81	1.99	2.06
30	Z	601	CHL	C1B-NB	2.80	1.37	1.35
30	Z2	601	CHL	C1B-NB	2.80	1.37	1.35
30	92	607	CHL	MG-NC	-2.79	1.99	2.06
30	8	607	CHL	MG-NC	-2.78	1.99	2.06
30	6	601	CHL	C3B-C2B	-2.78	1.36	1.40
30	62	601	CHL	C3B-C2B	-2.78	1.36	1.40
30	5	606	CHL	MG-NC	-2.77	1.99	2.06
30	6	606	CHL	C1B-NB	2.77	1.37	1.35
30	62	606	CHL	C1B-NB	2.77	1.37	1.35
30	32	608	CHL	MG-NC	-2.76	1.99	2.06
30	Z	607	CHL	C1B-NB	2.76	1.37	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	6	616	CHL	C1B-NB	2.76	1.37	1.35
30	62	616	CHL	C1B-NB	2.76	1.37	1.35
30	5	608	CHL	C1B-NB	2.76	1.37	1.35
30	62	608	CHL	C1B-NB	2.75	1.37	1.35
30	3	608	CHL	MG-NC	-2.75	1.99	2.06
30	9	606	CHL	C1B-NB	2.74	1.37	1.35
30	92	606	CHL	C1B-NB	2.74	1.37	1.35
30	9	607	CHL	MG-NC	-2.73	1.99	2.06
30	42	608	CHL	C1B-NB	2.73	1.37	1.35
30	4	618	CHL	C1B-NB	2.73	1.37	1.35
30	5	606	CHL	C1B-NB	2.73	1.37	1.35
30	4	601	CHL	MG-NC	-2.72	1.99	2.06
30	42	601	CHL	MG-NC	-2.72	1.99	2.06
30	Z	606	CHL	C1B-NB	2.72	1.37	1.35
30	6	618	CHL	C1B-NB	2.71	1.37	1.35
30	62	618	CHL	C1B-NB	2.71	1.37	1.35
32	52	625	NEX	C1-C6	-2.71	1.50	1.54
30	Z2	606	CHL	C1B-NB	2.71	1.37	1.35
30	12	607	CHL	C1B-NB	2.70	1.37	1.35
30	52	606	CHL	C1B-NB	2.70	1.37	1.35
30	3	608	CHL	C1B-NB	2.69	1.37	1.35
30	6	608	CHL	C1B-NB	2.68	1.37	1.35
30	32	608	CHL	C1B-NB	2.68	1.37	1.35
30	1	607	CHL	C1B-NB	2.68	1.37	1.35
30	4	601	CHL	C1B-NB	2.67	1.37	1.35
30	Z2	607	CHL	C1B-NB	2.67	1.37	1.35
30	9	607	CHL	C3B-C2B	-2.64	1.36	1.40
30	52	618	CHL	C1B-NB	2.64	1.37	1.35
30	52	608	CHL	C1B-NB	2.60	1.37	1.35
30	42	601	CHL	C1B-NB	2.60	1.37	1.35
30	5	618	CHL	C1B-NB	2.60	1.37	1.35
30	72	606	CHL	C1B-NB	2.57	1.37	1.35
21	A2	829	CLA	C1D-C2D	-2.56	1.40	1.45
21	A	829	CLA	C1D-C2D	-2.56	1.40	1.45
30	7	606	CHL	C1B-NB	2.56	1.37	1.35
21	B	806	CLA	C1D-C2D	-2.56	1.40	1.45
21	A	802	CLA	C1D-C2D	-2.56	1.40	1.45
30	8	606	CHL	C1B-NB	2.55	1.37	1.35
30	82	606	CHL	C1B-NB	2.55	1.37	1.35
30	62	607	CHL	C1B-NB	2.55	1.37	1.35
30	1	601	CHL	C1B-NB	2.54	1.37	1.35
21	B2	802	CLA	C1D-C2D	-2.54	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	9	607	CHL	C1D-C2D	-2.53	1.40	1.45
21	B2	806	CLA	C1D-C2D	-2.53	1.40	1.45
21	B	802	CLA	C1D-C2D	-2.53	1.40	1.45
21	A2	802	CLA	C1D-C2D	-2.52	1.40	1.45
21	A	828	CLA	C1D-C2D	-2.51	1.40	1.45
21	K2	201	CLA	C1D-C2D	-2.51	1.40	1.45
30	8	601	CHL	C1B-NB	2.51	1.37	1.35
21	A2	828	CLA	C1D-C2D	-2.51	1.40	1.45
30	7	601	CHL	C1B-NB	2.50	1.37	1.35
30	72	601	CHL	C1B-NB	2.50	1.37	1.35
21	A	819	CLA	C1D-C2D	-2.50	1.40	1.45
21	B2	803	CLA	C1D-C2D	-2.50	1.40	1.45
21	B	803	CLA	C1D-C2D	-2.50	1.40	1.45
21	A2	854	CLA	C1D-C2D	-2.50	1.40	1.45
21	K	201	CLA	C1D-C2D	-2.50	1.40	1.45
21	A2	810	CLA	C1D-C2D	-2.50	1.40	1.45
21	7	612	CLA	C1D-C2D	-2.49	1.40	1.45
21	A	807	CLA	C1D-C2D	-2.49	1.40	1.45
30	6	607	CHL	C1B-NB	2.49	1.37	1.35
21	A2	842	CLA	C1D-C2D	-2.49	1.40	1.45
21	B	838	CLA	C1D-C2D	-2.48	1.40	1.45
21	32	603	CLA	C1D-C2D	-2.48	1.40	1.45
21	A	854	CLA	C1D-C2D	-2.48	1.40	1.45
21	A2	826	CLA	C1D-C2D	-2.47	1.40	1.45
21	F	301	CLA	C1D-C2D	-2.47	1.40	1.45
21	F2	301	CLA	C1D-C2D	-2.47	1.40	1.45
21	A2	807	CLA	C1D-C2D	-2.47	1.40	1.45
21	A	826	CLA	C1D-C2D	-2.47	1.40	1.45
21	5	621	CLA	C1D-C2D	-2.47	1.40	1.45
30	4	606	CHL	C1B-NB	2.47	1.37	1.35
21	8	610	CLA	C1D-C2D	-2.46	1.40	1.45
21	B2	824	CLA	C1D-C2D	-2.46	1.40	1.45
21	A	814	CLA	C1D-C2D	-2.46	1.40	1.45
21	3	603	CLA	C1D-C2D	-2.46	1.40	1.45
21	A2	814	CLA	C1D-C2D	-2.46	1.40	1.45
21	B	824	CLA	C1D-C2D	-2.46	1.40	1.45
21	B	809	CLA	C1D-C2D	-2.46	1.40	1.45
21	8	608	CLA	C1D-C2D	-2.45	1.40	1.45
21	B2	838	CLA	C1D-C2D	-2.45	1.40	1.45
21	A2	838	CLA	C1D-C2D	-2.45	1.40	1.45
21	72	612	CLA	C1D-C2D	-2.45	1.40	1.45
21	A	813	CLA	C1D-C2D	-2.45	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	810	CLA	C1D-C2D	-2.45	1.40	1.45
21	A	830	CLA	C1D-C2D	-2.45	1.40	1.45
21	A	821	CLA	C1D-C2D	-2.45	1.40	1.45
21	B2	825	CLA	C1D-C2D	-2.44	1.40	1.45
21	A2	808	CLA	C1D-C2D	-2.44	1.40	1.45
21	A	808	CLA	C1D-C2D	-2.44	1.40	1.45
21	B2	809	CLA	C1D-C2D	-2.44	1.40	1.45
20	A2	801	CL0	C1D-C2D	-2.44	1.40	1.45
21	A	842	CLA	C1D-C2D	-2.44	1.40	1.45
21	A2	805	CLA	C1D-C2D	-2.44	1.40	1.45
21	A	812	CLA	C1D-C2D	-2.44	1.40	1.45
21	A2	819	CLA	C1D-C2D	-2.43	1.40	1.45
21	A	805	CLA	C1D-C2D	-2.43	1.40	1.45
30	82	601	CHL	C1B-NB	2.43	1.37	1.35
21	B	825	CLA	C1D-C2D	-2.43	1.40	1.45
21	A	818	CLA	C1D-C2D	-2.43	1.40	1.45
21	B	835	CLA	C1D-C2D	-2.43	1.40	1.45
21	52	621	CLA	C1D-C2D	-2.43	1.40	1.45
21	A	843	CLA	C1D-C2D	-2.43	1.40	1.45
21	A2	845	CLA	C1D-C2D	-2.42	1.40	1.45
30	92	607	CHL	C1D-C2D	-2.42	1.40	1.45
21	B	813	CLA	C1D-C2D	-2.42	1.40	1.45
21	B	829	CLA	C1D-C2D	-2.42	1.40	1.45
21	B2	829	CLA	C1D-C2D	-2.42	1.40	1.45
21	82	608	CLA	C1D-C2D	-2.42	1.40	1.45
21	B2	820	CLA	C1D-C2D	-2.42	1.40	1.45
21	1	612	CLA	C1D-C2D	-2.42	1.40	1.45
21	A2	818	CLA	C1D-C2D	-2.42	1.40	1.45
21	A2	830	CLA	C1D-C2D	-2.42	1.40	1.45
30	42	606	CHL	C1B-NB	2.42	1.37	1.35
21	A2	815	CLA	C1D-C2D	-2.42	1.40	1.45
21	A	845	CLA	C1D-C2D	-2.42	1.40	1.45
21	B2	827	CLA	C1D-C2D	-2.42	1.40	1.45
21	A	815	CLA	C1D-C2D	-2.42	1.40	1.45
21	B	808	CLA	C1D-C2D	-2.42	1.40	1.45
21	A	827	CLA	C1D-C2D	-2.42	1.40	1.45
21	B2	808	CLA	C1D-C2D	-2.42	1.40	1.45
21	9	602	CLA	C1D-C2D	-2.41	1.40	1.45
21	82	612	CLA	C1D-C2D	-2.41	1.40	1.45
21	B	827	CLA	C1D-C2D	-2.41	1.40	1.45
21	B2	813	CLA	C1D-C2D	-2.41	1.40	1.45
21	A2	813	CLA	C1D-C2D	-2.41	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A2	821	CLA	C1D-C2D	-2.41	1.40	1.45
21	B	816	CLA	C1D-C2D	-2.41	1.40	1.45
21	A	834	CLA	C1D-C2D	-2.41	1.40	1.45
21	B	805	CLA	C1D-C2D	-2.41	1.40	1.45
21	7	608	CLA	C1D-C2D	-2.41	1.40	1.45
21	8	602	CLA	C1D-C2D	-2.40	1.40	1.45
21	A2	806	CLA	C1D-C2D	-2.40	1.40	1.45
21	32	615	CLA	C1D-C2D	-2.40	1.40	1.45
21	K2	203	CLA	C1D-C2D	-2.40	1.40	1.45
21	Z2	609	CLA	C1D-C2D	-2.40	1.40	1.45
21	K	203	CLA	C1D-C2D	-2.40	1.40	1.45
21	A2	834	CLA	C1D-C2D	-2.40	1.40	1.45
21	J	101	CLA	C1D-C2D	-2.40	1.40	1.45
21	J2	101	CLA	C1D-C2D	-2.40	1.40	1.45
21	1	616	CLA	C1D-C2D	-2.40	1.40	1.45
21	12	616	CLA	C1D-C2D	-2.40	1.40	1.45
21	B	840	CLA	C1D-C2D	-2.40	1.40	1.45
21	F	303	CLA	C1D-C2D	-2.40	1.40	1.45
21	F2	303	CLA	C1D-C2D	-2.40	1.40	1.45
21	A	804	CLA	C1D-C2D	-2.40	1.40	1.45
21	5	602	CLA	C1D-C2D	-2.40	1.40	1.45
21	3	615	CLA	C1D-C2D	-2.40	1.40	1.45
21	A2	839	CLA	C1D-C2D	-2.40	1.40	1.45
21	12	612	CLA	C1D-C2D	-2.40	1.40	1.45
21	B	819	CLA	C1D-C2D	-2.40	1.40	1.45
21	8	612	CLA	C1D-C2D	-2.40	1.40	1.45
21	B2	837	CLA	C1D-C2D	-2.40	1.40	1.45
21	B2	834	CLA	C1D-C2D	-2.39	1.40	1.45
21	A	833	CLA	C1D-C2D	-2.39	1.40	1.45
20	A	801	CL0	C1D-C2D	-2.39	1.40	1.45
21	A	822	CLA	C1D-C2D	-2.39	1.40	1.45
21	3	606	CLA	C1D-C2D	-2.39	1.40	1.45
21	12	614	CLA	C1D-C2D	-2.39	1.40	1.45
21	52	602	CLA	C1D-C2D	-2.39	1.40	1.45
30	12	601	CHL	C1B-NB	2.39	1.37	1.35
21	1	611	CLA	C1D-C2D	-2.39	1.40	1.45
21	42	603	CLA	C1D-C2D	-2.39	1.40	1.45
30	82	607	CHL	C1D-C2D	-2.39	1.40	1.45
30	8	607	CHL	C1D-C2D	-2.39	1.40	1.45
21	A	820	CLA	C1D-C2D	-2.39	1.40	1.45
21	A2	843	CLA	C1D-C2D	-2.39	1.40	1.45
21	92	603	CLA	C1D-C2D	-2.39	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	832	CLA	C1D-C2D	-2.39	1.40	1.45
21	G	203	CLA	C1D-C2D	-2.39	1.40	1.45
21	A2	817	CLA	C1D-C2D	-2.39	1.40	1.45
21	A	838	CLA	C1D-C2D	-2.39	1.40	1.45
21	B	841	CLA	C1D-C2D	-2.39	1.40	1.45
21	A2	812	CLA	C1D-C2D	-2.39	1.40	1.45
21	B2	835	CLA	C1D-C2D	-2.38	1.40	1.45
21	12	611	CLA	C1D-C2D	-2.38	1.40	1.45
21	A	817	CLA	C1D-C2D	-2.38	1.40	1.45
21	A2	827	CLA	C1D-C2D	-2.38	1.40	1.45
21	3	613	CLA	C1D-C2D	-2.38	1.40	1.45
21	A	841	CLA	C1D-C2D	-2.38	1.40	1.45
21	42	609	CLA	C1D-C2D	-2.38	1.40	1.45
21	72	613	CLA	C1D-C2D	-2.38	1.40	1.45
30	72	607	CHL	C1B-NB	2.38	1.37	1.35
21	A2	809	CLA	C1D-C2D	-2.38	1.40	1.45
21	A	840	CLA	C1D-C2D	-2.38	1.40	1.45
21	Z	612	CLA	C1D-C2D	-2.38	1.40	1.45
21	A	806	CLA	C1D-C2D	-2.38	1.40	1.45
21	B	820	CLA	C1D-C2D	-2.38	1.40	1.45
21	B	818	CLA	C1D-C2D	-2.38	1.40	1.45
21	7	614	CLA	C1D-C2D	-2.38	1.40	1.45
21	Z	609	CLA	C1D-C2D	-2.38	1.40	1.45
21	4	602	CLA	C1D-C2D	-2.38	1.40	1.45
21	B2	818	CLA	C1D-C2D	-2.38	1.40	1.45
21	B2	816	CLA	C1D-C2D	-2.38	1.40	1.45
21	82	610	CLA	C1D-C2D	-2.37	1.40	1.45
21	A2	841	CLA	C1D-C2D	-2.37	1.40	1.45
21	B	836	CLA	C1D-C2D	-2.37	1.40	1.45
21	72	609	CLA	C1D-C2D	-2.37	1.40	1.45
21	3	617	CLA	C1D-C2D	-2.37	1.40	1.45
21	B2	819	CLA	C1D-C2D	-2.37	1.40	1.45
21	32	612	CLA	C1D-C2D	-2.37	1.40	1.45
21	1	609	CLA	C1D-C2D	-2.37	1.40	1.45
21	1	613	CLA	C1D-C2D	-2.37	1.40	1.45
21	6	622	CLA	C1D-C2D	-2.37	1.40	1.45
21	A2	837	CLA	C1D-C2D	-2.37	1.40	1.45
21	12	609	CLA	C1D-C2D	-2.37	1.40	1.45
21	12	613	CLA	C1D-C2D	-2.37	1.40	1.45
21	62	622	CLA	C1D-C2D	-2.37	1.40	1.45
21	B2	805	CLA	C1D-C2D	-2.37	1.40	1.45
21	A	832	CLA	C1D-C2D	-2.37	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A2	820	CLA	C1D-C2D	-2.37	1.40	1.45
30	8	601	CHL	C1D-C2D	-2.37	1.40	1.45
21	A2	831	CLA	C1D-C2D	-2.37	1.40	1.45
21	92	602	CLA	C1D-C2D	-2.37	1.40	1.45
21	B	811	CLA	C1D-C2D	-2.37	1.40	1.45
21	B	821	CLA	C1D-C2D	-2.37	1.40	1.45
21	Z	603	CLA	C1D-C2D	-2.37	1.40	1.45
21	B2	811	CLA	C1D-C2D	-2.37	1.40	1.45
21	B2	821	CLA	C1D-C2D	-2.37	1.40	1.45
21	Z2	603	CLA	C1D-C2D	-2.37	1.40	1.45
21	52	617	CLA	C1D-C2D	-2.37	1.40	1.45
21	7	602	CLA	C1D-C2D	-2.37	1.40	1.45
21	B2	828	CLA	C1D-C2D	-2.37	1.40	1.45
21	A	831	CLA	C1D-C2D	-2.37	1.40	1.45
21	7	620	CLA	C1D-C2D	-2.37	1.40	1.45
21	72	620	CLA	C1D-C2D	-2.37	1.40	1.45
21	B2	815	CLA	C1D-C2D	-2.37	1.40	1.45
30	82	601	CHL	C1D-C2D	-2.37	1.40	1.45
21	82	609	CLA	C1D-C2D	-2.37	1.40	1.45
21	B2	831	CLA	C1D-C2D	-2.37	1.40	1.45
21	B2	832	CLA	C1D-C2D	-2.37	1.40	1.45
21	32	604	CLA	C1D-C2D	-2.37	1.40	1.45
21	82	602	CLA	C1D-C2D	-2.37	1.40	1.45
21	82	613	CLA	C1D-C2D	-2.37	1.40	1.45
21	B	828	CLA	C1D-C2D	-2.36	1.40	1.45
21	B	837	CLA	C1D-C2D	-2.36	1.40	1.45
21	7	611	CLA	C1D-C2D	-2.36	1.40	1.45
21	72	611	CLA	C1D-C2D	-2.36	1.40	1.45
21	1	603	CLA	C1D-C2D	-2.36	1.40	1.45
21	8	603	CLA	C1D-C2D	-2.36	1.40	1.45
21	82	603	CLA	C1D-C2D	-2.36	1.40	1.45
21	F	304	CLA	C1D-C2D	-2.36	1.40	1.45
21	F2	304	CLA	C1D-C2D	-2.36	1.40	1.45
21	52	616	CLA	C1D-C2D	-2.36	1.40	1.45
21	3	610	CLA	C1D-C2D	-2.36	1.40	1.45
21	A2	822	CLA	C1D-C2D	-2.36	1.40	1.45
21	B2	833	CLA	C1D-C2D	-2.36	1.40	1.45
21	7	616	CLA	C1D-C2D	-2.36	1.40	1.45
21	4	603	CLA	C1D-C2D	-2.36	1.40	1.45
21	6	603	CLA	C1D-C2D	-2.36	1.40	1.45
21	A	825	CLA	C1D-C2D	-2.36	1.40	1.45
21	B	804	CLA	C1D-C2D	-2.36	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A2	803	CLA	C1D-C2D	-2.36	1.40	1.45
21	A2	823	CLA	C1D-C2D	-2.36	1.40	1.45
21	A2	840	CLA	C1D-C2D	-2.36	1.40	1.45
21	A2	825	CLA	C1D-C2D	-2.36	1.40	1.45
21	A2	804	CLA	C1D-C2D	-2.36	1.40	1.45
21	G2	203	CLA	C1D-C2D	-2.36	1.40	1.45
21	5	614	CLA	C1D-C2D	-2.36	1.40	1.45
21	B2	830	CLA	C1D-C2D	-2.36	1.40	1.45
21	52	614	CLA	C1D-C2D	-2.36	1.40	1.45
21	52	613	CLA	C1D-C2D	-2.36	1.40	1.45
21	7	613	CLA	C1D-C2D	-2.36	1.40	1.45
21	5	601	CLA	C1D-C2D	-2.36	1.40	1.45
21	K	204	CLA	C1D-C2D	-2.36	1.40	1.45
21	32	606	CLA	C1D-C2D	-2.36	1.40	1.45
21	72	608	CLA	C1D-C2D	-2.36	1.40	1.45
21	9	612	CLA	C1D-C2D	-2.36	1.40	1.45
21	A2	836	CLA	C1D-C2D	-2.36	1.40	1.45
21	92	612	CLA	C1D-C2D	-2.36	1.40	1.45
21	5	617	CLA	C1D-C2D	-2.36	1.40	1.45
21	52	610	CLA	C1D-C2D	-2.36	1.40	1.45
21	4	612	CLA	C1D-C2D	-2.35	1.40	1.45
21	42	612	CLA	C1D-C2D	-2.35	1.40	1.45
21	A	811	CLA	C1D-C2D	-2.35	1.40	1.45
21	42	602	CLA	C1D-C2D	-2.35	1.40	1.45
21	B	815	CLA	C1D-C2D	-2.35	1.40	1.45
21	8	614	CLA	C1D-C2D	-2.35	1.40	1.45
21	82	614	CLA	C1D-C2D	-2.35	1.40	1.45
21	52	601	CLA	C1D-C2D	-2.35	1.40	1.45
21	32	613	CLA	C1D-C2D	-2.35	1.40	1.45
21	3	609	CLA	C1D-C2D	-2.35	1.40	1.45
21	8	609	CLA	C1D-C2D	-2.35	1.40	1.45
21	B	826	CLA	C1D-C2D	-2.35	1.40	1.45
21	32	602	CLA	C1D-C2D	-2.35	1.40	1.45
21	7	604	CLA	C1D-C2D	-2.35	1.40	1.45
21	3	612	CLA	C1D-C2D	-2.35	1.40	1.45
21	72	602	CLA	C1D-C2D	-2.35	1.40	1.45
21	3	604	CLA	C1D-C2D	-2.35	1.40	1.45
21	Z2	612	CLA	C1D-C2D	-2.35	1.40	1.45
21	A	839	CLA	C1D-C2D	-2.35	1.40	1.45
21	B	839	CLA	C1D-C2D	-2.35	1.40	1.45
21	1	614	CLA	C1D-C2D	-2.35	1.40	1.45
21	6	609	CLA	C1D-C2D	-2.35	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	62	612	CLA	C1D-C2D	-2.35	1.40	1.45
21	B	834	CLA	C1D-C2D	-2.35	1.40	1.45
21	1	602	CLA	C1D-C2D	-2.35	1.40	1.45
21	A2	832	CLA	C1D-C2D	-2.35	1.40	1.45
21	12	602	CLA	C1D-C2D	-2.35	1.40	1.45
21	B2	836	CLA	C1D-C2D	-2.35	1.40	1.45
21	B2	841	CLA	C1D-C2D	-2.35	1.40	1.45
21	7	609	CLA	C1D-C2D	-2.35	1.40	1.45
21	K2	206	CLA	C1D-C2D	-2.35	1.40	1.45
21	62	609	CLA	C1D-C2D	-2.35	1.40	1.45
21	9	603	CLA	C1D-C2D	-2.34	1.40	1.45
21	52	612	CLA	C1D-C2D	-2.34	1.40	1.45
21	B2	812	CLA	C1D-C2D	-2.34	1.40	1.45
21	6	602	CLA	C1D-C2D	-2.34	1.40	1.45
21	B2	840	CLA	C1D-C2D	-2.34	1.40	1.45
21	B	831	CLA	C1D-C2D	-2.34	1.40	1.45
21	B2	817	CLA	C1D-C2D	-2.34	1.40	1.45
21	A	836	CLA	C1D-C2D	-2.34	1.40	1.45
21	3	614	CLA	C1D-C2D	-2.34	1.40	1.45
21	8	604	CLA	C1D-C2D	-2.34	1.40	1.45
21	5	610	CLA	C1D-C2D	-2.34	1.40	1.45
21	62	603	CLA	C1D-C2D	-2.34	1.40	1.45
21	8	613	CLA	C1D-C2D	-2.34	1.40	1.45
21	12	610	CLA	C1D-C2D	-2.34	1.40	1.45
21	Z2	616	CLA	C1D-C2D	-2.34	1.40	1.45
30	7	607	CHL	C1D-C2D	-2.34	1.40	1.45
21	5	613	CLA	C1D-C2D	-2.34	1.40	1.45
21	A	824	CLA	C1D-C2D	-2.34	1.40	1.45
21	Z	616	CLA	C1D-C2D	-2.34	1.40	1.45
21	B2	804	CLA	C1D-C2D	-2.34	1.40	1.45
21	K	206	CLA	C1D-C2D	-2.34	1.40	1.45
21	B2	807	CLA	C1D-C2D	-2.34	1.40	1.45
21	B2	814	CLA	C1D-C2D	-2.34	1.40	1.45
21	B	812	CLA	C1D-C2D	-2.34	1.40	1.45
21	B	817	CLA	C1D-C2D	-2.34	1.40	1.45
21	A2	833	CLA	C1D-C2D	-2.34	1.40	1.45
21	6	612	CLA	C1D-C2D	-2.33	1.40	1.45
21	32	610	CLA	C1D-C2D	-2.33	1.40	1.45
21	92	609	CLA	C1D-C2D	-2.33	1.40	1.45
21	A2	824	CLA	C1D-C2D	-2.33	1.40	1.45
21	7	610	CLA	C1D-C2D	-2.33	1.40	1.45
21	5	611	CLA	C1D-C2D	-2.33	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	72	610	CLA	C1D-C2D	-2.33	1.40	1.45
21	52	611	CLA	C1D-C2D	-2.33	1.40	1.45
21	4	613	CLA	C1D-C2D	-2.33	1.40	1.45
21	A	809	CLA	C1D-C2D	-2.33	1.40	1.45
21	B	823	CLA	C1D-C2D	-2.33	1.40	1.45
21	32	617	CLA	C1D-C2D	-2.33	1.40	1.45
30	1	606	CHL	C1B-NB	2.33	1.37	1.35
21	9	611	CLA	C1D-C2D	-2.33	1.40	1.45
21	A	837	CLA	C1D-C2D	-2.33	1.40	1.45
21	12	608	CLA	C1D-C2D	-2.33	1.40	1.45
21	42	616	CLA	C1D-C2D	-2.33	1.40	1.45
21	72	604	CLA	C1D-C2D	-2.33	1.40	1.45
21	B	833	CLA	C1D-C2D	-2.33	1.40	1.45
21	5	609	CLA	C1D-C2D	-2.33	1.40	1.45
21	6	604	CLA	C1D-C2D	-2.33	1.40	1.45
21	B2	826	CLA	C1D-C2D	-2.33	1.40	1.45
21	52	609	CLA	C1D-C2D	-2.33	1.40	1.45
21	62	604	CLA	C1D-C2D	-2.33	1.40	1.45
21	A	803	CLA	C1D-C2D	-2.33	1.40	1.45
21	3	602	CLA	C1D-C2D	-2.33	1.40	1.45
21	B2	823	CLA	C1D-C2D	-2.33	1.40	1.45
21	32	609	CLA	C1D-C2D	-2.33	1.40	1.45
21	92	613	CLA	C1D-C2D	-2.33	1.40	1.45
21	5	616	CLA	C1D-C2D	-2.33	1.40	1.45
21	Z2	608	CLA	C1D-C2D	-2.33	1.40	1.45
21	1	610	CLA	C1D-C2D	-2.33	1.40	1.45
21	5	604	CLA	C1D-C2D	-2.33	1.40	1.45
21	72	614	CLA	C1D-C2D	-2.33	1.40	1.45
21	Z2	614	CLA	C1D-C2D	-2.33	1.40	1.45
21	5	612	CLA	C1D-C2D	-2.33	1.40	1.45
21	G	204	CLA	C1D-C2D	-2.32	1.40	1.45
21	6	611	CLA	C1D-C2D	-2.32	1.40	1.45
21	Z	602	CLA	C1D-C2D	-2.32	1.40	1.45
21	12	603	CLA	C1D-C2D	-2.32	1.40	1.45
21	72	616	CLA	C1D-C2D	-2.32	1.40	1.45
21	L2	203	CLA	C1D-C2D	-2.32	1.40	1.45
30	Z	601	CHL	C1D-C2D	-2.32	1.40	1.45
21	92	604	CLA	C1D-C2D	-2.32	1.40	1.45
30	7	607	CHL	C1B-NB	2.32	1.37	1.35
21	A2	816	CLA	C1D-C2D	-2.32	1.40	1.45
21	4	616	CLA	C1D-C2D	-2.32	1.40	1.45
30	12	606	CHL	C1B-NB	2.32	1.37	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	823	CLA	C1D-C2D	-2.32	1.40	1.45
21	Z	613	CLA	C1D-C2D	-2.31	1.40	1.45
21	6	613	CLA	C1D-C2D	-2.31	1.40	1.45
21	9	613	CLA	C1D-C2D	-2.31	1.40	1.45
21	B	807	CLA	C1D-C2D	-2.31	1.40	1.45
30	7	601	CHL	C2C-C1C	2.31	1.49	1.44
21	A	816	CLA	C1D-C2D	-2.31	1.40	1.45
21	B2	822	CLA	C1D-C2D	-2.31	1.40	1.45
21	62	614	CLA	C1D-C2D	-2.31	1.40	1.45
21	A	835	CLA	C1D-C2D	-2.31	1.40	1.45
21	4	614	CLA	C1D-C2D	-2.31	1.40	1.45
21	42	614	CLA	C1D-C2D	-2.31	1.40	1.45
21	42	613	CLA	C1D-C2D	-2.31	1.40	1.45
21	B2	810	CLA	C1D-C2D	-2.31	1.40	1.45
30	4	601	CHL	C1D-C2D	-2.31	1.40	1.45
21	G2	204	CLA	C1D-C2D	-2.31	1.40	1.45
21	K2	204	CLA	C1D-C2D	-2.31	1.40	1.45
21	7	603	CLA	C1D-C2D	-2.30	1.40	1.45
30	1	606	CHL	C2C-C1C	2.30	1.49	1.44
21	B	830	CLA	C1D-C2D	-2.30	1.40	1.45
21	3	611	CLA	C1D-C2D	-2.30	1.40	1.45
21	A2	811	CLA	C1D-C2D	-2.30	1.40	1.45
21	62	610	CLA	C1D-C2D	-2.30	1.40	1.45
30	52	606	CHL	C1D-C2D	-2.30	1.40	1.45
21	Z	611	CLA	C1D-C2D	-2.30	1.40	1.45
21	L	203	CLA	C1D-C2D	-2.30	1.40	1.45
21	62	602	CLA	C1D-C2D	-2.30	1.40	1.45
21	42	610	CLA	C1D-C2D	-2.30	1.40	1.45
21	42	604	CLA	C1D-C2D	-2.30	1.40	1.45
21	52	604	CLA	C1D-C2D	-2.30	1.40	1.45
21	6	617	CLA	C1D-C2D	-2.30	1.40	1.45
21	62	617	CLA	C1D-C2D	-2.30	1.40	1.45
21	B2	839	CLA	C1D-C2D	-2.30	1.40	1.45
30	12	606	CHL	C1D-C2D	-2.30	1.40	1.45
21	B	822	CLA	C1D-C2D	-2.30	1.40	1.45
21	8	611	CLA	C1D-C2D	-2.30	1.40	1.45
21	82	611	CLA	C1D-C2D	-2.30	1.40	1.45
30	6	616	CHL	C2C-C1C	2.30	1.49	1.44
21	4	611	CLA	C1D-C2D	-2.30	1.40	1.45
21	42	611	CLA	C1D-C2D	-2.30	1.40	1.45
30	52	608	CHL	C1D-C2D	-2.30	1.40	1.45
30	72	601	CHL	C2C-C1C	2.29	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	52	607	CHL	C1D-C2D	-2.29	1.40	1.45
21	1	608	CLA	C1D-C2D	-2.29	1.40	1.45
30	6	606	CHL	C1D-C2D	-2.29	1.40	1.45
30	62	606	CHL	C1D-C2D	-2.29	1.40	1.45
21	9	604	CLA	C1D-C2D	-2.29	1.40	1.45
21	9	609	CLA	C1D-C2D	-2.29	1.40	1.45
30	62	607	CHL	C1D-C2D	-2.29	1.40	1.45
21	B	810	CLA	C1D-C2D	-2.29	1.40	1.45
30	Z	607	CHL	C1D-C2D	-2.29	1.40	1.45
21	92	614	CLA	C1D-C2D	-2.29	1.40	1.45
21	Z	610	CLA	C1D-C2D	-2.29	1.40	1.45
21	Z2	610	CLA	C1D-C2D	-2.29	1.40	1.45
21	Z2	613	CLA	C1D-C2D	-2.29	1.40	1.45
21	92	610	CLA	C1D-C2D	-2.29	1.40	1.45
30	12	601	CHL	C1D-C2D	-2.29	1.40	1.45
21	92	601	CLA	C1D-C2D	-2.29	1.40	1.45
30	72	607	CHL	C1D-C2D	-2.29	1.40	1.45
30	1	601	CHL	C1D-C2D	-2.29	1.40	1.45
21	A2	835	CLA	C1D-C2D	-2.29	1.40	1.45
30	7	601	CHL	C1D-C2D	-2.29	1.40	1.45
30	5	606	CHL	C1D-C2D	-2.29	1.40	1.45
30	72	601	CHL	C1D-C2D	-2.29	1.40	1.45
21	Z2	602	CLA	C1D-C2D	-2.29	1.40	1.45
30	3	608	CHL	C1D-C2D	-2.28	1.40	1.45
21	32	614	CLA	C1D-C2D	-2.28	1.40	1.45
21	5	603	CLA	C1D-C2D	-2.28	1.40	1.45
21	52	603	CLA	C1D-C2D	-2.28	1.40	1.45
30	5	607	CHL	C1D-C2D	-2.28	1.40	1.45
21	4	604	CLA	C1D-C2D	-2.28	1.40	1.45
21	6	610	CLA	C1D-C2D	-2.28	1.40	1.45
21	8	616	CLA	C1D-C2D	-2.28	1.40	1.45
21	82	616	CLA	C1D-C2D	-2.28	1.40	1.45
30	12	606	CHL	C2C-C1C	2.28	1.49	1.44
30	72	606	CHL	C1D-C2D	-2.28	1.40	1.45
21	62	611	CLA	C1D-C2D	-2.28	1.40	1.45
21	1	604	CLA	C1D-C2D	-2.28	1.40	1.45
21	Z	608	CLA	C1D-C2D	-2.28	1.40	1.45
30	42	601	CHL	C1D-C2D	-2.28	1.40	1.45
21	72	603	CLA	C1D-C2D	-2.28	1.40	1.45
21	Z2	611	CLA	C1D-C2D	-2.28	1.40	1.45
30	9	606	CHL	C1D-C2D	-2.28	1.40	1.45
21	4	610	CLA	C1D-C2D	-2.28	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	1	606	CHL	C1D-C2D	-2.28	1.40	1.45
21	32	607	CLA	C1D-C2D	-2.28	1.40	1.45
21	4	609	CLA	C1D-C2D	-2.27	1.40	1.45
30	42	607	CHL	C1D-C2D	-2.27	1.40	1.45
30	62	618	CHL	C1D-C2D	-2.27	1.40	1.45
30	62	601	CHL	C1D-C2D	-2.27	1.40	1.45
30	Z2	601	CHL	C1D-C2D	-2.27	1.40	1.45
21	82	604	CLA	C1D-C2D	-2.27	1.40	1.45
30	Z2	607	CHL	C1D-C2D	-2.27	1.40	1.45
30	92	606	CHL	C1D-C2D	-2.27	1.40	1.45
21	32	611	CLA	C1D-C2D	-2.27	1.40	1.45
21	Z	614	CLA	C1D-C2D	-2.27	1.40	1.45
21	9	614	CLA	C1D-C2D	-2.27	1.40	1.45
21	3	607	CLA	C1D-C2D	-2.27	1.40	1.45
21	6	614	CLA	C1D-C2D	-2.26	1.40	1.45
21	9	601	CLA	C1D-C2D	-2.26	1.40	1.45
30	4	607	CHL	C1D-C2D	-2.26	1.40	1.45
30	7	606	CHL	C1D-C2D	-2.26	1.40	1.45
30	6	618	CHL	C1D-C2D	-2.26	1.40	1.45
21	B	814	CLA	C1D-C2D	-2.26	1.40	1.45
30	42	608	CHL	C1D-C2D	-2.26	1.40	1.45
30	4	608	CHL	C1D-C2D	-2.26	1.40	1.45
21	92	611	CLA	C1D-C2D	-2.26	1.40	1.45
30	12	607	CHL	C1D-C2D	-2.26	1.40	1.45
30	62	606	CHL	C2C-C1C	2.26	1.49	1.44
21	62	613	CLA	C1D-C2D	-2.26	1.40	1.45
30	5	608	CHL	C1D-C2D	-2.25	1.40	1.45
21	Z	604	CLA	C1D-C2D	-2.25	1.40	1.45
21	Z2	604	CLA	C1D-C2D	-2.25	1.40	1.45
30	6	608	CHL	C1D-C2D	-2.25	1.40	1.45
30	62	608	CHL	C1D-C2D	-2.25	1.40	1.45
30	Z	606	CHL	C2C-C1C	2.25	1.49	1.44
30	6	607	CHL	C1D-C2D	-2.25	1.40	1.45
21	9	610	CLA	C1D-C2D	-2.25	1.40	1.45
30	4	606	CHL	C1D-C2D	-2.25	1.40	1.45
21	L	204	CLA	C1D-C2D	-2.24	1.40	1.45
30	32	608	CHL	C1D-C2D	-2.24	1.40	1.45
30	42	606	CHL	C1D-C2D	-2.24	1.40	1.45
30	42	618	CHL	C1D-C2D	-2.24	1.40	1.45
30	62	616	CHL	C2C-C1C	2.24	1.49	1.44
21	L2	204	CLA	C1D-C2D	-2.24	1.40	1.45
30	1	607	CHL	C1D-C2D	-2.24	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	4	618	CHL	C1D-C2D	-2.24	1.40	1.45
30	4	618	CHL	C2C-C1C	2.24	1.49	1.44
30	42	618	CHL	C2C-C1C	2.24	1.49	1.44
21	12	604	CLA	C1D-C2D	-2.23	1.40	1.45
30	5	618	CHL	C2C-C1C	2.23	1.49	1.44
30	6	601	CHL	C1D-C2D	-2.23	1.40	1.45
30	5	606	CHL	C2C-C1C	2.23	1.49	1.44
30	5	618	CHL	C1D-C2D	-2.23	1.40	1.45
30	6	606	CHL	C2C-C1C	2.22	1.49	1.44
30	8	606	CHL	C1D-C2D	-2.22	1.40	1.45
30	52	618	CHL	C1D-C2D	-2.21	1.41	1.45
30	6	618	CHL	C2C-C1C	2.21	1.49	1.44
30	52	606	CHL	C2C-C1C	2.21	1.49	1.44
30	6	616	CHL	C1D-C2D	-2.21	1.41	1.45
30	82	606	CHL	C1D-C2D	-2.21	1.41	1.45
20	A2	801	CL0	C1C-C2C	2.21	1.48	1.44
30	62	618	CHL	C2C-C1C	2.20	1.49	1.44
20	A	801	CL0	C1C-C2C	2.20	1.48	1.44
30	Z2	606	CHL	C1D-C2D	-2.20	1.41	1.45
30	Z2	606	CHL	C2C-C1C	2.20	1.49	1.44
30	7	606	CHL	C2C-C1C	2.20	1.49	1.44
30	72	606	CHL	C2C-C1C	2.20	1.49	1.44
30	6	601	CHL	C2C-C1C	2.20	1.49	1.44
30	62	601	CHL	C2C-C1C	2.19	1.49	1.44
30	Z	606	CHL	C1D-C2D	-2.19	1.41	1.45
30	62	616	CHL	C1D-C2D	-2.18	1.41	1.45
30	4	601	CHL	C2C-C1C	2.17	1.49	1.44
30	42	601	CHL	C2C-C1C	2.17	1.49	1.44
30	52	618	CHL	C2C-C1C	2.17	1.49	1.44
30	5	608	CHL	C2C-C1C	2.17	1.49	1.44
30	6	607	CHL	C2C-C1C	2.15	1.49	1.44
30	62	607	CHL	C2C-C1C	2.14	1.49	1.44
30	52	608	CHL	C2C-C1C	2.14	1.49	1.44
30	3	608	CHL	C3D-C4D	-2.12	1.39	1.44
30	9	606	CHL	C2C-C1C	2.12	1.49	1.44
30	8	607	CHL	C2C-C1C	2.11	1.49	1.44
30	92	606	CHL	C2C-C1C	2.11	1.49	1.44
30	32	608	CHL	C2C-C1C	2.10	1.49	1.44
30	42	608	CHL	C2C-C1C	2.10	1.49	1.44
30	6	608	CHL	C2C-C1C	2.10	1.49	1.44
30	1	607	CHL	C3D-C4D	-2.10	1.39	1.44
30	12	607	CHL	C3D-C4D	-2.10	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	32	608	CHL	C3D-C4D	-2.10	1.39	1.44
21	B2	840	CLA	C3D-C4D	-2.10	1.39	1.44
30	82	606	CHL	C2C-C1C	2.09	1.49	1.44
30	82	607	CHL	C2C-C1C	2.09	1.49	1.44
21	B	840	CLA	C3D-C4D	-2.09	1.39	1.44
30	8	601	CHL	C2C-C1C	2.09	1.49	1.44
30	62	608	CHL	C2C-C1C	2.09	1.49	1.44
30	4	608	CHL	C2C-C1C	2.09	1.49	1.44
21	A	806	CLA	C3D-C4D	-2.08	1.39	1.44
21	A2	806	CLA	C3D-C4D	-2.08	1.39	1.44
21	A2	827	CLA	C3D-C4D	-2.08	1.39	1.44
30	8	606	CHL	C2C-C1C	2.08	1.49	1.44
21	A	833	CLA	C3D-C4D	-2.07	1.39	1.44
30	9	606	CHL	C3D-C4D	-2.07	1.39	1.44
30	3	608	CHL	C2C-C1C	2.07	1.49	1.44
21	B2	830	CLA	C3D-C4D	-2.07	1.39	1.44
21	92	610	CLA	C3D-C4D	-2.07	1.39	1.44
30	82	601	CHL	C2C-C1C	2.07	1.49	1.44
30	Z	601	CHL	C2C-C1C	2.07	1.49	1.44
30	Z2	601	CHL	C2C-C1C	2.07	1.49	1.44
30	7	601	CHL	C3D-C4D	-2.07	1.39	1.44
21	B2	829	CLA	C3D-C4D	-2.07	1.39	1.44
20	A2	801	CL0	C3D-C4D	-2.07	1.39	1.44
21	9	610	CLA	C3D-C4D	-2.07	1.39	1.44
21	A	809	CLA	C3D-C4D	-2.06	1.39	1.44
21	B2	825	CLA	C3D-C4D	-2.06	1.39	1.44
30	5	607	CHL	C3D-C4D	-2.06	1.39	1.44
30	52	607	CHL	C3D-C4D	-2.06	1.39	1.44
21	B2	831	CLA	C3D-C4D	-2.06	1.39	1.44
21	A2	842	CLA	C3D-C4D	-2.06	1.39	1.44
21	A	842	CLA	C3D-C4D	-2.06	1.39	1.44
21	B	833	CLA	C3D-C4D	-2.06	1.39	1.44
30	1	601	CHL	C3D-C4D	-2.06	1.39	1.44
30	12	601	CHL	C3D-C4D	-2.06	1.39	1.44
21	12	602	CLA	C3D-C4D	-2.06	1.39	1.44
21	A	803	CLA	C3D-C4D	-2.05	1.39	1.44
30	8	606	CHL	C3D-C4D	-2.05	1.39	1.44
21	1	602	CLA	C3D-C4D	-2.05	1.39	1.44
21	A	802	CLA	C3D-C4D	-2.05	1.39	1.44
21	A	805	CLA	C3D-C4D	-2.05	1.39	1.44
21	A	822	CLA	C3D-C4D	-2.05	1.39	1.44
21	A2	822	CLA	C3D-C4D	-2.05	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	72	606	CHL	C3D-C4D	-2.05	1.39	1.44
21	A	827	CLA	C3D-C4D	-2.05	1.39	1.44
30	42	606	CHL	C2C-C1C	2.05	1.49	1.44
21	B	837	CLA	C3D-C4D	-2.05	1.39	1.44
30	82	601	CHL	C3D-C4D	-2.04	1.39	1.44
21	B	823	CLA	C3D-C4D	-2.04	1.39	1.44
21	A	843	CLA	C3D-C4D	-2.04	1.39	1.44
21	B2	833	CLA	C3D-C4D	-2.04	1.39	1.44
30	42	607	CHL	C3D-C4D	-2.04	1.39	1.44
30	62	608	CHL	C3D-C4D	-2.04	1.39	1.44
21	A	834	CLA	C3D-C4D	-2.04	1.39	1.44
21	B	825	CLA	C3D-C4D	-2.04	1.39	1.44
30	62	616	CHL	C3D-C4D	-2.04	1.39	1.44
21	B2	823	CLA	C3D-C4D	-2.04	1.39	1.44
30	4	606	CHL	C2C-C1C	2.04	1.48	1.44
21	B	830	CLA	C3D-C4D	-2.04	1.39	1.44
21	A2	803	CLA	C3D-C4D	-2.04	1.39	1.44
21	12	610	CLA	C3D-C4D	-2.04	1.39	1.44
21	A	808	CLA	C3D-C4D	-2.04	1.39	1.44
21	A	812	CLA	C3D-C4D	-2.04	1.39	1.44
21	A	841	CLA	C3D-C4D	-2.04	1.39	1.44
21	A2	841	CLA	C3D-C4D	-2.04	1.39	1.44
30	Z2	606	CHL	C3D-C4D	-2.04	1.39	1.44
30	92	606	CHL	C3D-C4D	-2.04	1.39	1.44
21	B	829	CLA	C3D-C4D	-2.04	1.39	1.44
21	B	831	CLA	C3D-C4D	-2.04	1.39	1.44
30	4	608	CHL	C3D-C4D	-2.03	1.39	1.44
30	42	608	CHL	C3D-C4D	-2.03	1.39	1.44
30	9	607	CHL	C3D-C4D	-2.03	1.39	1.44
21	B2	818	CLA	C3D-C4D	-2.03	1.39	1.44
30	8	601	CHL	C3D-C4D	-2.03	1.39	1.44
30	Z2	607	CHL	C3D-C4D	-2.03	1.39	1.44
30	92	607	CHL	C3D-C4D	-2.03	1.39	1.44
21	A2	809	CLA	C3D-C4D	-2.03	1.39	1.44
21	A2	839	CLA	C3D-C4D	-2.03	1.39	1.44
30	7	606	CHL	C3D-C4D	-2.03	1.39	1.44
30	72	601	CHL	C3D-C4D	-2.03	1.39	1.44
21	B2	837	CLA	C3D-C4D	-2.03	1.39	1.44
21	32	610	CLA	C3D-C4D	-2.03	1.39	1.44
30	6	608	CHL	C3D-C4D	-2.03	1.39	1.44
30	Z	601	CHL	C3D-C4D	-2.03	1.39	1.44
21	4	603	CLA	C3D-C4D	-2.03	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	821	CLA	C3D-C4D	-2.03	1.39	1.44
21	9	604	CLA	C3D-C4D	-2.03	1.39	1.44
21	B2	821	CLA	C3D-C4D	-2.03	1.39	1.44
21	82	602	CLA	C3D-C4D	-2.03	1.39	1.44
21	92	604	CLA	C3D-C4D	-2.03	1.39	1.44
30	1	606	CHL	C3D-C4D	-2.03	1.39	1.44
20	A	801	CL0	C3D-C4D	-2.03	1.39	1.44
21	A	825	CLA	C3D-C4D	-2.03	1.39	1.44
30	6	616	CHL	C3D-C4D	-2.03	1.39	1.44
21	A2	833	CLA	C3D-C4D	-2.02	1.39	1.44
30	4	607	CHL	C2C-C1C	2.02	1.48	1.44
30	42	607	CHL	C2C-C1C	2.02	1.48	1.44
21	A	839	CLA	C3D-C4D	-2.02	1.39	1.44
21	A2	805	CLA	C3D-C4D	-2.02	1.39	1.44
30	1	607	CHL	C4B-CHC	-2.02	1.35	1.41
30	12	607	CHL	C4B-CHC	-2.02	1.35	1.41
21	B2	832	CLA	C3D-C4D	-2.02	1.39	1.44
21	B	812	CLA	C3D-C4D	-2.02	1.39	1.44
21	B2	812	CLA	C3D-C4D	-2.02	1.39	1.44
21	B2	819	CLA	C3D-C4D	-2.02	1.39	1.44
21	A	820	CLA	C3D-C4D	-2.02	1.39	1.44
21	A2	802	CLA	C3D-C4D	-2.02	1.39	1.44
21	A2	843	CLA	C3D-C4D	-2.02	1.39	1.44
21	A2	812	CLA	C3D-C4D	-2.02	1.39	1.44
21	A2	820	CLA	C3D-C4D	-2.02	1.39	1.44
21	B	832	CLA	C3D-C4D	-2.02	1.39	1.44
21	82	603	CLA	C3D-C4D	-2.02	1.39	1.44
30	Z	606	CHL	C3D-C4D	-2.02	1.39	1.44
30	42	601	CHL	C3D-C4D	-2.01	1.39	1.44
21	A	836	CLA	C3D-C4D	-2.01	1.39	1.44
21	A	807	CLA	C3D-C4D	-2.01	1.39	1.44
21	A2	807	CLA	C3D-C4D	-2.01	1.39	1.44
21	A2	824	CLA	C3D-C4D	-2.01	1.39	1.44
21	1	613	CLA	C3D-C4D	-2.01	1.39	1.44
21	A2	831	CLA	C3D-C4D	-2.01	1.39	1.44
21	12	613	CLA	C3D-C4D	-2.01	1.39	1.44
21	9	603	CLA	C3D-C4D	-2.01	1.39	1.44
21	9	602	CLA	C3D-C4D	-2.01	1.39	1.44
21	A2	823	CLA	C3D-C4D	-2.01	1.39	1.44
21	A	837	CLA	C3D-C4D	-2.01	1.39	1.44
21	A2	836	CLA	C3D-C4D	-2.01	1.39	1.44
30	Z	607	CHL	C3D-C4D	-2.01	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	811	CLA	C3D-C4D	-2.01	1.39	1.44
21	B	805	CLA	C3D-C4D	-2.01	1.39	1.44
21	A2	811	CLA	C3D-C4D	-2.01	1.39	1.44
30	7	607	CHL	C3D-C4D	-2.01	1.39	1.44
21	A	832	CLA	C3D-C4D	-2.01	1.39	1.44
21	B	811	CLA	C3D-C4D	-2.01	1.39	1.44
21	3	602	CLA	C3D-C4D	-2.01	1.39	1.44
21	8	602	CLA	C3D-C4D	-2.01	1.39	1.44
21	82	604	CLA	C3D-C4D	-2.01	1.39	1.44
30	12	606	CHL	C3D-C4D	-2.01	1.39	1.44
30	5	608	CHL	C3D-C4D	-2.01	1.39	1.44
30	6	601	CHL	C3D-C4D	-2.01	1.39	1.44
21	A	804	CLA	C3D-C4D	-2.00	1.39	1.44
21	42	603	CLA	C3D-C4D	-2.00	1.39	1.44
30	4	606	CHL	C3D-C4D	-2.00	1.39	1.44
30	Z	601	CHL	C4B-CHC	-2.00	1.35	1.41
30	6	618	CHL	C3D-C4D	-2.00	1.39	1.44
30	62	618	CHL	C3D-C4D	-2.00	1.39	1.44
21	A	854	CLA	C3D-C4D	-2.00	1.39	1.44
21	7	616	CLA	C3D-C4D	-2.00	1.39	1.44
21	B2	817	CLA	C3D-C4D	-2.00	1.39	1.44
30	4	607	CHL	C3D-C4D	-2.00	1.39	1.44
21	A2	804	CLA	C3D-C4D	-2.00	1.39	1.44
30	52	608	CHL	C3D-C4D	-2.00	1.39	1.44

All (1334) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	92	610	CLA	C1D-ND-C4D	-4.52	103.12	106.33
21	9	610	CLA	C1D-ND-C4D	-4.50	103.14	106.33
21	Z	613	CLA	C1D-ND-C4D	-4.41	103.20	106.33
21	9	604	CLA	C1D-ND-C4D	-4.38	103.22	106.33
30	3	608	CHL	CHD-C1D-ND	-4.36	120.44	124.45
21	92	604	CLA	C1D-ND-C4D	-4.36	103.24	106.33
21	5	603	CLA	C1D-ND-C4D	-4.34	103.25	106.33
21	8	616	CLA	C1D-ND-C4D	-4.34	103.25	106.33
21	82	616	CLA	C1D-ND-C4D	-4.34	103.25	106.33
30	32	608	CHL	CHD-C1D-ND	-4.34	120.47	124.45
21	B2	814	CLA	C1D-ND-C4D	-4.33	103.26	106.33
30	12	607	CHL	CHD-C1D-ND	-4.33	120.47	124.45
21	Z2	613	CLA	C1D-ND-C4D	-4.33	103.26	106.33
21	K	204	CLA	C1D-ND-C4D	-4.33	103.26	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	92	603	CLA	C1D-ND-C4D	-4.33	103.26	106.33
30	1	607	CHL	CHD-C1D-ND	-4.33	120.48	124.45
21	1	613	CLA	C1D-ND-C4D	-4.33	103.26	106.33
21	12	613	CLA	C1D-ND-C4D	-4.33	103.26	106.33
21	5	609	CLA	C1D-ND-C4D	-4.32	103.27	106.33
21	A	816	CLA	C1D-ND-C4D	-4.32	103.27	106.33
21	6	614	CLA	C1D-ND-C4D	-4.32	103.27	106.33
21	52	609	CLA	C1D-ND-C4D	-4.32	103.27	106.33
21	62	614	CLA	C1D-ND-C4D	-4.32	103.27	106.33
21	42	604	CLA	C1D-ND-C4D	-4.31	103.27	106.33
21	52	603	CLA	C1D-ND-C4D	-4.31	103.27	106.33
21	B	840	CLA	C1D-ND-C4D	-4.30	103.28	106.33
21	B	808	CLA	C1D-ND-C4D	-4.30	103.28	106.33
21	5	617	CLA	C1D-ND-C4D	-4.30	103.28	106.33
21	52	617	CLA	C1D-ND-C4D	-4.30	103.28	106.33
21	8	611	CLA	C1D-ND-C4D	-4.29	103.29	106.33
21	5	614	CLA	C1D-ND-C4D	-4.29	103.29	106.33
21	Z	611	CLA	C1D-ND-C4D	-4.28	103.29	106.33
21	B2	840	CLA	C1D-ND-C4D	-4.28	103.29	106.33
21	Z2	611	CLA	C1D-ND-C4D	-4.28	103.29	106.33
21	5	613	CLA	C1D-ND-C4D	-4.28	103.30	106.33
21	92	609	CLA	C1D-ND-C4D	-4.28	103.30	106.33
21	B	814	CLA	C1D-ND-C4D	-4.27	103.30	106.33
21	9	603	CLA	C1D-ND-C4D	-4.27	103.30	106.33
21	Z	614	CLA	C1D-ND-C4D	-4.27	103.30	106.33
21	3	614	CLA	C1D-ND-C4D	-4.27	103.30	106.33
21	82	611	CLA	C1D-ND-C4D	-4.27	103.30	106.33
21	F	303	CLA	C1D-ND-C4D	-4.27	103.31	106.33
21	A	809	CLA	C1D-ND-C4D	-4.26	103.31	106.33
21	B	822	CLA	C1D-ND-C4D	-4.26	103.31	106.33
21	32	607	CLA	C1D-ND-C4D	-4.26	103.31	106.33
21	4	616	CLA	C1D-ND-C4D	-4.26	103.31	106.33
21	6	609	CLA	C1D-ND-C4D	-4.26	103.31	106.33
21	52	613	CLA	C1D-ND-C4D	-4.26	103.31	106.33
21	A2	816	CLA	C1D-ND-C4D	-4.25	103.31	106.33
21	82	613	CLA	C1D-ND-C4D	-4.25	103.31	106.33
21	B2	822	CLA	C1D-ND-C4D	-4.25	103.31	106.33
21	4	604	CLA	C1D-ND-C4D	-4.25	103.31	106.33
21	A2	806	CLA	C1D-ND-C4D	-4.25	103.32	106.33
21	52	614	CLA	C1D-ND-C4D	-4.25	103.32	106.33
21	7	603	CLA	C1D-ND-C4D	-4.25	103.32	106.33
21	62	609	CLA	C1D-ND-C4D	-4.25	103.32	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	62	612	CLA	C1D-ND-C4D	-4.24	103.32	106.33
30	42	606	CHL	CHD-C1D-ND	-4.24	120.55	124.45
21	B2	808	CLA	C1D-ND-C4D	-4.24	103.32	106.33
21	L	204	CLA	C1D-ND-C4D	-4.24	103.32	106.33
21	A	820	CLA	C1D-ND-C4D	-4.24	103.32	106.33
21	K2	204	CLA	C1D-ND-C4D	-4.24	103.33	106.33
30	Z	606	CHL	CHD-C1D-ND	-4.23	120.56	124.45
21	6	602	CLA	C1D-ND-C4D	-4.23	103.33	106.33
21	Z2	614	CLA	C1D-ND-C4D	-4.23	103.33	106.33
21	4	612	CLA	C1D-ND-C4D	-4.23	103.33	106.33
30	6	608	CHL	CHD-C1D-ND	-4.23	120.57	124.45
21	A2	809	CLA	C1D-ND-C4D	-4.22	103.33	106.33
21	6	613	CLA	C1D-ND-C4D	-4.22	103.33	106.33
30	Z2	606	CHL	CHD-C1D-ND	-4.22	120.58	124.45
21	5	611	CLA	C1D-ND-C4D	-4.22	103.34	106.33
21	A2	839	CLA	C1D-ND-C4D	-4.22	103.34	106.33
30	62	608	CHL	CHD-C1D-ND	-4.22	120.58	124.45
21	L2	204	CLA	C1D-ND-C4D	-4.22	103.34	106.33
21	72	614	CLA	C1D-ND-C4D	-4.22	103.34	106.33
21	4	611	CLA	C1D-ND-C4D	-4.22	103.34	106.33
21	42	611	CLA	C1D-ND-C4D	-4.22	103.34	106.33
21	32	614	CLA	C1D-ND-C4D	-4.21	103.34	106.33
21	42	616	CLA	C1D-ND-C4D	-4.21	103.34	106.33
21	32	610	CLA	C1D-ND-C4D	-4.21	103.34	106.33
21	F	304	CLA	C1D-ND-C4D	-4.21	103.34	106.33
21	Z	612	CLA	C1D-ND-C4D	-4.21	103.34	106.33
21	6	617	CLA	C1D-ND-C4D	-4.21	103.34	106.33
21	72	604	CLA	C1D-ND-C4D	-4.21	103.34	106.33
21	Z2	612	CLA	C1D-ND-C4D	-4.21	103.34	106.33
30	4	606	CHL	CHD-C1D-ND	-4.21	120.59	124.45
21	B	836	CLA	C1D-ND-C4D	-4.21	103.34	106.33
21	6	610	CLA	C1D-ND-C4D	-4.21	103.34	106.33
21	3	612	CLA	C1D-ND-C4D	-4.21	103.35	106.33
21	9	614	CLA	C1D-ND-C4D	-4.21	103.35	106.33
21	72	603	CLA	C1D-ND-C4D	-4.20	103.35	106.33
21	9	609	CLA	C1D-ND-C4D	-4.20	103.35	106.33
21	A2	822	CLA	C1D-ND-C4D	-4.20	103.35	106.33
21	F2	303	CLA	C1D-ND-C4D	-4.20	103.35	106.33
21	B	816	CLA	C1D-ND-C4D	-4.20	103.35	106.33
21	3	604	CLA	C1D-ND-C4D	-4.20	103.35	106.33
21	A2	820	CLA	C1D-ND-C4D	-4.20	103.35	106.33
21	62	610	CLA	C1D-ND-C4D	-4.19	103.36	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	1	602	CLA	C1D-ND-C4D	-4.19	103.36	106.33
21	32	602	CLA	C1D-ND-C4D	-4.19	103.36	106.33
21	A	804	CLA	C1D-ND-C4D	-4.19	103.36	106.33
21	52	611	CLA	C1D-ND-C4D	-4.19	103.36	106.33
21	3	607	CLA	C1D-ND-C4D	-4.19	103.36	106.33
21	7	614	CLA	C1D-ND-C4D	-4.19	103.36	106.33
21	A	822	CLA	C1D-ND-C4D	-4.19	103.36	106.33
21	6	612	CLA	C1D-ND-C4D	-4.19	103.36	106.33
21	A	818	CLA	C1D-ND-C4D	-4.19	103.36	106.33
21	3	602	CLA	C1D-ND-C4D	-4.19	103.36	106.33
21	F2	304	CLA	C1D-ND-C4D	-4.19	103.36	106.33
21	Z2	604	CLA	C1D-ND-C4D	-4.19	103.36	106.33
21	1	616	CLA	C1D-ND-C4D	-4.18	103.36	106.33
21	62	602	CLA	C1D-ND-C4D	-4.18	103.36	106.33
30	8	606	CHL	CHD-C1D-ND	-4.18	120.61	124.45
21	A	835	CLA	C1D-ND-C4D	-4.18	103.36	106.33
21	62	617	CLA	C1D-ND-C4D	-4.18	103.36	106.33
21	B	810	CLA	C1D-ND-C4D	-4.18	103.36	106.33
21	62	613	CLA	C1D-ND-C4D	-4.18	103.36	106.33
21	A2	831	CLA	C1D-ND-C4D	-4.18	103.37	106.33
21	62	611	CLA	C1D-ND-C4D	-4.18	103.37	106.33
21	8	613	CLA	C1D-ND-C4D	-4.18	103.37	106.33
21	32	612	CLA	C1D-ND-C4D	-4.18	103.37	106.33
21	B	807	CLA	C1D-ND-C4D	-4.18	103.37	106.33
21	1	614	CLA	C1D-ND-C4D	-4.18	103.37	106.33
21	92	614	CLA	C1D-ND-C4D	-4.17	103.37	106.33
21	72	616	CLA	C1D-ND-C4D	-4.17	103.37	106.33
21	A	834	CLA	C1D-ND-C4D	-4.17	103.37	106.33
21	8	612	CLA	C1D-ND-C4D	-4.17	103.37	106.33
21	4	614	CLA	C1D-ND-C4D	-4.17	103.37	106.33
21	52	616	CLA	C1D-ND-C4D	-4.17	103.37	106.33
21	12	614	CLA	C1D-ND-C4D	-4.17	103.37	106.33
21	72	602	CLA	C1D-ND-C4D	-4.17	103.37	106.33
21	Z	604	CLA	C1D-ND-C4D	-4.17	103.38	106.33
21	42	603	CLA	C1D-ND-C4D	-4.17	103.38	106.33
21	1	610	CLA	C1D-ND-C4D	-4.16	103.38	106.33
21	B2	810	CLA	C1D-ND-C4D	-4.16	103.38	106.33
21	A	831	CLA	C1D-ND-C4D	-4.16	103.38	106.33
21	1	609	CLA	C1D-ND-C4D	-4.16	103.38	106.33
21	82	603	CLA	C1D-ND-C4D	-4.16	103.38	106.33
21	5	612	CLA	C1D-ND-C4D	-4.16	103.38	106.33
21	B2	816	CLA	C1D-ND-C4D	-4.16	103.38	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	K2	206	CLA	C1D-ND-C4D	-4.16	103.38	106.33
21	B	813	CLA	C1D-ND-C4D	-4.16	103.38	106.33
21	9	601	CLA	C1D-ND-C4D	-4.16	103.38	106.33
21	3	610	CLA	C1D-ND-C4D	-4.16	103.38	106.33
21	B	831	CLA	C1D-ND-C4D	-4.16	103.38	106.33
21	B	833	CLA	C1D-ND-C4D	-4.16	103.38	106.33
21	6	604	CLA	C1D-ND-C4D	-4.16	103.38	106.33
21	B2	836	CLA	C1D-ND-C4D	-4.16	103.38	106.33
21	32	604	CLA	C1D-ND-C4D	-4.16	103.38	106.33
21	A	832	CLA	C1D-ND-C4D	-4.15	103.38	106.33
21	B2	834	CLA	C1D-ND-C4D	-4.15	103.38	106.33
21	A	830	CLA	C1D-ND-C4D	-4.15	103.39	106.33
21	B	834	CLA	C1D-ND-C4D	-4.15	103.39	106.33
21	6	611	CLA	C1D-ND-C4D	-4.15	103.39	106.33
21	B2	833	CLA	C1D-ND-C4D	-4.15	103.39	106.33
21	42	612	CLA	C1D-ND-C4D	-4.15	103.39	106.33
21	B	839	CLA	C1D-ND-C4D	-4.15	103.39	106.33
30	42	618	CHL	CHD-C1D-ND	-4.15	120.64	124.45
30	7	601	CHL	CHD-C1D-ND	-4.15	120.64	124.45
21	Z	610	CLA	C1D-ND-C4D	-4.15	103.39	106.33
21	B2	831	CLA	C1D-ND-C4D	-4.15	103.39	106.33
21	A2	841	CLA	C1D-ND-C4D	-4.15	103.39	106.33
30	72	601	CHL	CHD-C1D-ND	-4.15	120.64	124.45
21	A	811	CLA	C1D-ND-C4D	-4.14	103.39	106.33
21	A2	834	CLA	C1D-ND-C4D	-4.14	103.39	106.33
21	A	806	CLA	C1D-ND-C4D	-4.14	103.39	106.33
21	A	841	CLA	C1D-ND-C4D	-4.14	103.39	106.33
21	3	611	CLA	C1D-ND-C4D	-4.14	103.39	106.33
21	4	603	CLA	C1D-ND-C4D	-4.14	103.39	106.33
21	92	601	CLA	C1D-ND-C4D	-4.14	103.39	106.33
21	G2	204	CLA	C1D-ND-C4D	-4.14	103.39	106.33
21	12	609	CLA	C1D-ND-C4D	-4.14	103.39	106.33
21	7	612	CLA	C1D-ND-C4D	-4.14	103.39	106.33
30	62	601	CHL	CHD-C1D-ND	-4.14	120.65	124.45
21	A2	832	CLA	C1D-ND-C4D	-4.14	103.40	106.33
21	A	813	CLA	C1D-ND-C4D	-4.14	103.40	106.33
21	A	838	CLA	C1D-ND-C4D	-4.14	103.40	106.33
21	A2	813	CLA	C1D-ND-C4D	-4.14	103.40	106.33
21	12	610	CLA	C1D-ND-C4D	-4.14	103.40	106.33
21	A2	804	CLA	C1D-ND-C4D	-4.13	103.40	106.33
21	B2	835	CLA	C1D-ND-C4D	-4.13	103.40	106.33
21	Z2	616	CLA	C1D-ND-C4D	-4.13	103.40	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	4	618	CHL	CHD-C1D-ND	-4.13	120.66	124.45
21	32	611	CLA	C1D-ND-C4D	-4.13	103.40	106.33
21	5	616	CLA	C1D-ND-C4D	-4.13	103.40	106.33
21	A2	830	CLA	C1D-ND-C4D	-4.13	103.40	106.33
21	12	604	CLA	C1D-ND-C4D	-4.13	103.40	106.33
21	A	823	CLA	C1D-ND-C4D	-4.13	103.40	106.33
21	A2	827	CLA	C1D-ND-C4D	-4.13	103.40	106.33
30	1	601	CHL	CHD-C1D-ND	-4.13	120.66	124.45
21	12	602	CLA	C1D-ND-C4D	-4.13	103.40	106.33
30	72	606	CHL	CHD-C1D-ND	-4.13	120.66	124.45
21	B	811	CLA	C1D-ND-C4D	-4.13	103.40	106.33
21	A	839	CLA	C1D-ND-C4D	-4.12	103.41	106.33
21	B	835	CLA	C1D-ND-C4D	-4.12	103.41	106.33
21	A2	818	CLA	C1D-ND-C4D	-4.12	103.41	106.33
21	7	616	CLA	C1D-ND-C4D	-4.12	103.41	106.33
21	82	608	CLA	C1D-ND-C4D	-4.12	103.41	106.33
21	1	611	CLA	C1D-ND-C4D	-4.12	103.41	106.33
30	62	616	CHL	CHD-C1D-ND	-4.12	120.67	124.45
21	B	837	CLA	C1D-ND-C4D	-4.12	103.41	106.33
21	7	604	CLA	C1D-ND-C4D	-4.12	103.41	106.33
21	Z	616	CLA	C1D-ND-C4D	-4.12	103.41	106.33
21	A2	824	CLA	C1D-ND-C4D	-4.12	103.41	106.33
21	A2	835	CLA	C1D-ND-C4D	-4.12	103.41	106.33
21	B2	830	CLA	C1D-ND-C4D	-4.12	103.41	106.33
30	62	618	CHL	CHD-C1D-ND	-4.12	120.67	124.45
21	4	602	CLA	C1D-ND-C4D	-4.12	103.41	106.33
21	B2	805	CLA	C1D-ND-C4D	-4.12	103.41	106.33
21	12	612	CLA	C1D-ND-C4D	-4.12	103.41	106.33
30	Z	601	CHL	CHD-C1D-ND	-4.12	120.67	124.45
21	A	827	CLA	C1D-ND-C4D	-4.12	103.41	106.33
21	B	828	CLA	C1D-ND-C4D	-4.12	103.41	106.33
21	A2	842	CLA	C1D-ND-C4D	-4.12	103.41	106.33
30	6	601	CHL	CHD-C1D-ND	-4.12	120.67	124.45
30	12	601	CHL	CHD-C1D-ND	-4.12	120.67	124.45
21	72	611	CLA	C1D-ND-C4D	-4.11	103.41	106.33
30	82	606	CHL	CHD-C1D-ND	-4.11	120.67	124.45
21	1	612	CLA	C1D-ND-C4D	-4.11	103.41	106.33
21	B2	813	CLA	C1D-ND-C4D	-4.11	103.41	106.33
21	72	613	CLA	C1D-ND-C4D	-4.11	103.41	106.33
21	72	620	CLA	C1D-ND-C4D	-4.11	103.41	106.33
21	Z	602	CLA	C1D-ND-C4D	-4.11	103.42	106.33
21	Z	608	CLA	C1D-ND-C4D	-4.11	103.42	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B2	827	CLA	C1D-ND-C4D	-4.11	103.42	106.33
21	5	610	CLA	C1D-ND-C4D	-4.11	103.42	106.33
21	82	612	CLA	C1D-ND-C4D	-4.11	103.42	106.33
21	52	612	CLA	C1D-ND-C4D	-4.11	103.42	106.33
21	B2	837	CLA	C1D-ND-C4D	-4.11	103.42	106.33
21	52	604	CLA	C1D-ND-C4D	-4.11	103.42	106.33
21	A	812	CLA	C1D-ND-C4D	-4.11	103.42	106.33
21	Z2	610	CLA	C1D-ND-C4D	-4.11	103.42	106.33
21	62	603	CLA	C1D-ND-C4D	-4.11	103.42	106.33
21	12	611	CLA	C1D-ND-C4D	-4.10	103.42	106.33
21	82	614	CLA	C1D-ND-C4D	-4.10	103.42	106.33
21	Z2	602	CLA	C1D-ND-C4D	-4.10	103.42	106.33
21	A	808	CLA	C1D-ND-C4D	-4.10	103.42	106.33
21	B	812	CLA	C1D-ND-C4D	-4.10	103.42	106.33
21	B2	812	CLA	C1D-ND-C4D	-4.10	103.42	106.33
21	9	613	CLA	C1D-ND-C4D	-4.10	103.42	106.33
21	92	602	CLA	C1D-ND-C4D	-4.10	103.42	106.33
21	4	610	CLA	C1D-ND-C4D	-4.10	103.42	106.33
21	A2	823	CLA	C1D-ND-C4D	-4.10	103.42	106.33
21	42	610	CLA	C1D-ND-C4D	-4.10	103.42	106.33
21	G	204	CLA	C1D-ND-C4D	-4.10	103.42	106.33
21	3	606	CLA	C1D-ND-C4D	-4.10	103.42	106.33
21	B2	828	CLA	C1D-ND-C4D	-4.10	103.42	106.33
21	12	608	CLA	C1D-ND-C4D	-4.10	103.42	106.33
21	B	805	CLA	C1D-ND-C4D	-4.09	103.43	106.33
21	B2	807	CLA	C1D-ND-C4D	-4.09	103.43	106.33
30	6	616	CHL	CHD-C1D-ND	-4.09	120.69	124.45
21	8	603	CLA	C1D-ND-C4D	-4.09	103.43	106.33
21	Z2	603	CLA	C1D-ND-C4D	-4.09	103.43	106.33
21	42	614	CLA	C1D-ND-C4D	-4.09	103.43	106.33
21	7	608	CLA	C1D-ND-C4D	-4.09	103.43	106.33
21	7	611	CLA	C1D-ND-C4D	-4.09	103.43	106.33
21	7	602	CLA	C1D-ND-C4D	-4.09	103.43	106.33
30	6	607	CHL	CHD-C1D-ND	-4.09	120.69	124.45
21	7	620	CLA	C1D-ND-C4D	-4.09	103.43	106.33
30	52	608	CHL	CHD-C1D-ND	-4.09	120.70	124.45
21	L2	203	CLA	C1D-ND-C4D	-4.09	103.43	106.33
21	72	612	CLA	C1D-ND-C4D	-4.09	103.43	106.33
21	92	613	CLA	C1D-ND-C4D	-4.09	103.43	106.33
21	1	604	CLA	C1D-ND-C4D	-4.09	103.43	106.33
30	62	607	CHL	CHD-C1D-ND	-4.08	120.70	124.45
21	A	843	CLA	C1D-ND-C4D	-4.08	103.43	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B2	819	CLA	C1D-ND-C4D	-4.08	103.43	106.33
21	B2	839	CLA	C1D-ND-C4D	-4.08	103.43	106.33
21	7	613	CLA	C1D-ND-C4D	-4.08	103.44	106.33
21	Z	603	CLA	C1D-ND-C4D	-4.08	103.44	106.33
21	K2	203	CLA	C1D-ND-C4D	-4.08	103.44	106.33
30	5	618	CHL	CHD-C1D-ND	-4.08	120.70	124.45
21	A	833	CLA	C1D-ND-C4D	-4.08	103.44	106.33
21	8	614	CLA	C1D-ND-C4D	-4.08	103.44	106.33
21	42	602	CLA	C1D-ND-C4D	-4.08	103.44	106.33
30	6	618	CHL	CHD-C1D-ND	-4.08	120.70	124.45
21	92	612	CLA	C1D-ND-C4D	-4.08	103.44	106.33
30	52	618	CHL	CHD-C1D-ND	-4.08	120.71	124.45
21	32	606	CLA	C1D-ND-C4D	-4.08	103.44	106.33
30	5	608	CHL	CHD-C1D-ND	-4.08	120.71	124.45
21	B2	818	CLA	C1D-ND-C4D	-4.08	103.44	106.33
30	4	607	CHL	CHD-C1D-ND	-4.08	120.71	124.45
30	Z2	601	CHL	CHD-C1D-ND	-4.08	120.71	124.45
30	42	608	CHL	CHD-C1D-ND	-4.07	120.71	124.45
21	A	824	CLA	C1D-ND-C4D	-4.07	103.44	106.33
21	9	602	CLA	C1D-ND-C4D	-4.07	103.44	106.33
21	A2	843	CLA	C1D-ND-C4D	-4.07	103.44	106.33
21	62	604	CLA	C1D-ND-C4D	-4.07	103.44	106.33
21	1	608	CLA	C1D-ND-C4D	-4.07	103.44	106.33
21	A2	811	CLA	C1D-ND-C4D	-4.07	103.44	106.33
21	52	601	CLA	C1D-ND-C4D	-4.07	103.44	106.33
21	B	841	CLA	C1D-ND-C4D	-4.07	103.44	106.33
21	B2	832	CLA	C1D-ND-C4D	-4.07	103.44	106.33
21	5	604	CLA	C1D-ND-C4D	-4.07	103.45	106.33
21	52	610	CLA	C1D-ND-C4D	-4.07	103.45	106.33
21	B2	811	CLA	C1D-ND-C4D	-4.06	103.45	106.33
21	Z2	608	CLA	C1D-ND-C4D	-4.06	103.45	106.33
21	B	827	CLA	C1D-ND-C4D	-4.06	103.45	106.33
21	9	612	CLA	C1D-ND-C4D	-4.06	103.45	106.33
21	A2	833	CLA	C1D-ND-C4D	-4.06	103.45	106.33
21	12	616	CLA	C1D-ND-C4D	-4.06	103.45	106.33
30	42	607	CHL	CHD-C1D-ND	-4.06	120.72	124.45
21	B	819	CLA	C1D-ND-C4D	-4.06	103.45	106.33
21	K	203	CLA	C1D-ND-C4D	-4.06	103.45	106.33
21	A2	838	CLA	C1D-ND-C4D	-4.06	103.45	106.33
21	52	602	CLA	C1D-ND-C4D	-4.06	103.45	106.33
30	4	601	CHL	CHD-C1D-ND	-4.06	120.72	124.45
21	B	832	CLA	C1D-ND-C4D	-4.05	103.45	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	8	601	CHL	CHD-C1D-ND	-4.05	120.73	124.45
30	4	608	CHL	CHD-C1D-ND	-4.05	120.73	124.45
21	A2	821	CLA	C1D-ND-C4D	-4.05	103.46	106.33
21	8	604	CLA	C1D-ND-C4D	-4.05	103.46	106.33
21	6	603	CLA	C1D-ND-C4D	-4.05	103.46	106.33
21	3	613	CLA	C1D-ND-C4D	-4.05	103.46	106.33
21	8	609	CLA	C1D-ND-C4D	-4.05	103.46	106.33
21	A	842	CLA	C1D-ND-C4D	-4.05	103.46	106.33
21	82	604	CLA	C1D-ND-C4D	-4.05	103.46	106.33
30	5	607	CHL	CHD-C1D-ND	-4.05	120.74	124.45
21	6	622	CLA	C1D-ND-C4D	-4.04	103.46	106.33
30	42	601	CHL	CHD-C1D-ND	-4.04	120.74	124.45
21	32	613	CLA	C1D-ND-C4D	-4.04	103.46	106.33
30	7	606	CHL	CHD-C1D-ND	-4.04	120.74	124.45
21	B	818	CLA	C1D-ND-C4D	-4.04	103.47	106.33
21	B	804	CLA	C1D-ND-C4D	-4.04	103.47	106.33
21	A2	845	CLA	C1D-ND-C4D	-4.04	103.47	106.33
21	9	611	CLA	C1D-ND-C4D	-4.04	103.47	106.33
21	82	602	CLA	C1D-ND-C4D	-4.04	103.47	106.33
21	A	814	CLA	C1D-ND-C4D	-4.03	103.47	106.33
21	K	206	CLA	C1D-ND-C4D	-4.03	103.47	106.33
21	A2	812	CLA	C1D-ND-C4D	-4.03	103.47	106.33
21	B2	804	CLA	C1D-ND-C4D	-4.03	103.47	106.33
21	A	821	CLA	C1D-ND-C4D	-4.03	103.47	106.33
21	A	845	CLA	C1D-ND-C4D	-4.03	103.47	106.33
21	B2	823	CLA	C1D-ND-C4D	-4.03	103.47	106.33
30	52	606	CHL	CHD-C1D-ND	-4.03	120.75	124.45
21	B2	841	CLA	C1D-ND-C4D	-4.02	103.48	106.33
21	5	602	CLA	C1D-ND-C4D	-4.02	103.48	106.33
30	7	607	CHL	CHD-C1D-ND	-4.02	120.76	124.45
30	82	601	CHL	CHD-C1D-ND	-4.02	120.76	124.45
21	1	603	CLA	C1D-ND-C4D	-4.02	103.48	106.33
21	J2	101	CLA	C1D-ND-C4D	-4.02	103.48	106.33
21	3	609	CLA	C1D-ND-C4D	-4.02	103.48	106.33
21	5	601	CLA	C1D-ND-C4D	-4.02	103.48	106.33
21	L	203	CLA	C1D-ND-C4D	-4.01	103.48	106.33
21	A2	840	CLA	C1D-ND-C4D	-4.01	103.48	106.33
30	9	606	CHL	CHD-C1D-ND	-4.01	120.77	124.45
21	B	825	CLA	C1D-ND-C4D	-4.01	103.49	106.33
21	32	609	CLA	C1D-ND-C4D	-4.01	103.49	106.33
21	B2	820	CLA	C1D-ND-C4D	-4.01	103.49	106.33
21	92	611	CLA	C1D-ND-C4D	-4.01	103.49	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	52	607	CHL	CHD-C1D-ND	-4.01	120.77	124.45
21	72	608	CLA	C1D-ND-C4D	-4.00	103.49	106.33
21	4	613	CLA	C1D-ND-C4D	-4.00	103.49	106.33
21	A	840	CLA	C1D-ND-C4D	-4.00	103.49	106.33
21	A2	808	CLA	C1D-ND-C4D	-4.00	103.49	106.33
21	82	609	CLA	C1D-ND-C4D	-4.00	103.50	106.33
21	8	602	CLA	C1D-ND-C4D	-4.00	103.50	106.33
21	8	608	CLA	C1D-ND-C4D	-4.00	103.50	106.33
30	Z	607	CHL	CHD-C1D-ND	-4.00	120.78	124.45
30	92	606	CHL	CHD-C1D-ND	-3.99	120.78	124.45
30	5	606	CHL	CHD-C1D-ND	-3.99	120.78	124.45
21	12	603	CLA	C1D-ND-C4D	-3.99	103.50	106.33
21	8	610	CLA	C1D-ND-C4D	-3.99	103.50	106.33
21	72	609	CLA	C1D-ND-C4D	-3.99	103.50	106.33
21	B	823	CLA	C1D-ND-C4D	-3.99	103.50	106.33
30	Z2	607	CHL	CHD-C1D-ND	-3.98	120.79	124.45
21	A2	814	CLA	C1D-ND-C4D	-3.98	103.51	106.33
21	62	622	CLA	C1D-ND-C4D	-3.98	103.51	106.33
21	A	817	CLA	C1D-ND-C4D	-3.97	103.51	106.33
21	B2	815	CLA	C1D-ND-C4D	-3.97	103.51	106.33
30	62	606	CHL	CHD-C1D-ND	-3.97	120.81	124.45
21	B	829	CLA	C1D-ND-C4D	-3.97	103.52	106.33
21	A2	825	CLA	C1D-ND-C4D	-3.97	103.52	106.33
21	A	836	CLA	C1D-ND-C4D	-3.97	103.52	106.33
21	3	615	CLA	C1D-ND-C4D	-3.97	103.52	106.33
21	F	301	CLA	C1D-ND-C4D	-3.97	103.52	106.33
21	B	815	CLA	C1D-ND-C4D	-3.96	103.52	106.33
21	B2	825	CLA	C1D-ND-C4D	-3.96	103.52	106.33
30	1	606	CHL	CHD-C1D-ND	-3.96	120.82	124.45
21	B2	821	CLA	C1D-ND-C4D	-3.95	103.53	106.33
21	A	825	CLA	C1D-ND-C4D	-3.95	103.53	106.33
21	B	820	CLA	C1D-ND-C4D	-3.95	103.53	106.33
21	J	101	CLA	C1D-ND-C4D	-3.95	103.53	106.33
21	B	830	CLA	C1D-ND-C4D	-3.94	103.53	106.33
30	12	606	CHL	CHD-C1D-ND	-3.94	120.83	124.45
21	A	815	CLA	C1D-ND-C4D	-3.94	103.53	106.33
21	A2	836	CLA	C1D-ND-C4D	-3.94	103.53	106.33
21	B2	829	CLA	C1D-ND-C4D	-3.94	103.54	106.33
21	B	826	CLA	C1D-ND-C4D	-3.93	103.54	106.33
21	B2	817	CLA	C1D-ND-C4D	-3.93	103.54	106.33
21	A	803	CLA	C1D-ND-C4D	-3.93	103.54	106.33
21	A	819	CLA	C1D-ND-C4D	-3.93	103.54	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	828	CLA	C1D-ND-C4D	-3.93	103.55	106.33
30	6	606	CHL	CHD-C1D-ND	-3.93	120.84	124.45
30	72	607	CHL	CHD-C1D-ND	-3.93	120.85	124.45
21	A2	805	CLA	C1D-ND-C4D	-3.92	103.55	106.33
21	A2	815	CLA	C1D-ND-C4D	-3.92	103.55	106.33
21	F2	301	CLA	C1D-ND-C4D	-3.92	103.55	106.33
21	42	609	CLA	C1D-ND-C4D	-3.92	103.55	106.33
21	32	617	CLA	C1D-ND-C4D	-3.92	103.55	106.33
21	A	805	CLA	C1D-ND-C4D	-3.92	103.55	106.33
21	82	610	CLA	C1D-ND-C4D	-3.91	103.55	106.33
20	A2	801	CL0	CHD-C1D-ND	-3.91	120.86	124.45
32	62	625	NEX	C5-C6-C1	3.91	123.58	119.70
21	4	609	CLA	C1D-ND-C4D	-3.90	103.56	106.33
21	B	821	CLA	C1D-ND-C4D	-3.90	103.56	106.33
21	B2	824	CLA	C1D-ND-C4D	-3.90	103.57	106.33
21	7	609	CLA	C1D-ND-C4D	-3.89	103.57	106.33
21	32	615	CLA	C1D-ND-C4D	-3.89	103.57	106.33
21	A2	817	CLA	C1D-ND-C4D	-3.89	103.57	106.33
21	B2	809	CLA	C1D-ND-C4D	-3.89	103.57	106.33
21	42	613	CLA	C1D-ND-C4D	-3.89	103.57	106.33
21	B2	826	CLA	C1D-ND-C4D	-3.89	103.58	106.33
21	B	809	CLA	C1D-ND-C4D	-3.88	103.58	106.33
21	B	817	CLA	C1D-ND-C4D	-3.88	103.58	106.33
21	A2	803	CLA	C1D-ND-C4D	-3.87	103.58	106.33
30	92	607	CHL	CHD-C1D-ND	-3.87	120.90	124.45
21	B	824	CLA	C1D-ND-C4D	-3.87	103.58	106.33
21	3	617	CLA	C1D-ND-C4D	-3.87	103.59	106.33
20	A	801	CL0	CHD-C1D-ND	-3.86	120.91	124.45
21	Z2	609	CLA	C1D-ND-C4D	-3.86	103.60	106.33
21	A2	828	CLA	C1D-ND-C4D	-3.85	103.60	106.33
21	A2	819	CLA	C1D-ND-C4D	-3.84	103.60	106.33
21	G2	203	CLA	C1D-ND-C4D	-3.83	103.61	106.33
21	A2	837	CLA	C1D-ND-C4D	-3.83	103.61	106.33
21	G	203	CLA	C1D-ND-C4D	-3.82	103.62	106.33
32	52	625	NEX	O24-C25-C24	-3.82	110.51	113.38
21	A2	807	CLA	C1D-ND-C4D	-3.81	103.63	106.33
21	A	826	CLA	C1D-ND-C4D	-3.81	103.63	106.33
21	A2	826	CLA	C1D-ND-C4D	-3.81	103.63	106.33
30	8	607	CHL	CHD-C1D-ND	-3.81	120.95	124.45
21	A2	854	CLA	C1D-ND-C4D	-3.80	103.63	106.33
21	72	610	CLA	CHD-C1D-ND	-3.80	120.97	124.45
21	A	807	CLA	C1D-ND-C4D	-3.80	103.64	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	7	610	CLA	CHD-C1D-ND	-3.79	120.97	124.45
21	32	603	CLA	C1D-ND-C4D	-3.78	103.65	106.33
30	82	607	CHL	CHD-C1D-ND	-3.78	120.98	124.45
21	Z	609	CLA	C1D-ND-C4D	-3.78	103.65	106.33
32	6	625	NEX	C5-C6-C1	3.76	123.43	119.70
32	5	625	NEX	O24-C25-C24	-3.76	110.56	113.38
21	A	854	CLA	C1D-ND-C4D	-3.76	103.67	106.33
21	B2	802	CLA	C1D-ND-C4D	-3.75	103.67	106.33
21	3	603	CLA	C1D-ND-C4D	-3.75	103.67	106.33
21	A	837	CLA	C1D-ND-C4D	-3.74	103.68	106.33
21	B	838	CLA	C1D-ND-C4D	-3.73	103.69	106.33
30	9	607	CHL	CHD-C1D-ND	-3.72	121.03	124.45
21	A	802	CLA	C1D-ND-C4D	-3.72	103.69	106.33
21	A2	829	CLA	C1D-ND-C4D	-3.72	103.69	106.33
21	B	802	CLA	C1D-ND-C4D	-3.72	103.69	106.33
21	B	833	CLA	CHD-C1D-ND	-3.71	121.05	124.45
21	B2	833	CLA	CHD-C1D-ND	-3.71	121.05	124.45
20	A2	801	CL0	C1D-ND-C4D	-3.69	103.71	106.33
21	A2	802	CLA	C1D-ND-C4D	-3.69	103.72	106.33
21	K	201	CLA	C1D-ND-C4D	-3.68	103.72	106.33
21	72	610	CLA	C1D-ND-C4D	-3.67	103.73	106.33
21	A2	810	CLA	C1D-ND-C4D	-3.66	103.73	106.33
21	B2	806	CLA	C1D-ND-C4D	-3.66	103.74	106.33
30	9	607	CHL	C1B-CHB-C4A	-3.66	122.87	130.12
21	B2	838	CLA	C1D-ND-C4D	-3.66	103.74	106.33
30	5	607	CHL	C1D-ND-C4D	-3.66	103.74	106.33
30	62	608	CHL	C1D-ND-C4D	-3.66	103.74	106.33
21	5	621	CLA	C1D-ND-C4D	-3.65	103.75	106.33
30	8	606	CHL	C1D-ND-C4D	-3.64	103.75	106.33
21	B	806	CLA	C1D-ND-C4D	-3.63	103.76	106.33
20	A	801	CL0	C1D-ND-C4D	-3.62	103.76	106.33
21	A2	823	CLA	CHD-C1D-ND	-3.62	121.12	124.45
21	A	829	CLA	C1D-ND-C4D	-3.61	103.77	106.33
21	A	810	CLA	C1D-ND-C4D	-3.61	103.77	106.33
21	7	610	CLA	C1D-ND-C4D	-3.61	103.77	106.33
30	72	606	CHL	C1D-ND-C4D	-3.61	103.77	106.33
21	A2	806	CLA	CHD-C1D-ND	-3.61	121.14	124.45
30	6	608	CHL	C1D-ND-C4D	-3.60	103.78	106.33
21	A	823	CLA	CHD-C1D-ND	-3.60	121.15	124.45
21	1	604	CLA	CHD-C1D-ND	-3.60	121.15	124.45
21	52	621	CLA	C1D-ND-C4D	-3.59	103.78	106.33
21	92	610	CLA	CHD-C1D-ND	-3.59	121.16	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	4	608	CHL	C1D-ND-C4D	-3.59	103.79	106.33
30	6	618	CHL	C1D-ND-C4D	-3.59	103.79	106.33
30	52	608	CHL	C1D-ND-C4D	-3.59	103.79	106.33
30	52	607	CHL	C1D-ND-C4D	-3.58	103.79	106.33
20	A2	801	CL0	CHC-C1C-NC	3.58	129.64	124.20
30	82	606	CHL	C1D-ND-C4D	-3.58	103.79	106.33
21	12	604	CLA	CHD-C1D-ND	-3.57	121.17	124.45
21	A2	809	CLA	CHD-C1D-ND	-3.57	121.17	124.45
21	K2	201	CLA	C1D-ND-C4D	-3.57	103.80	106.33
21	A	809	CLA	CHD-C1D-ND	-3.56	121.18	124.45
30	92	607	CHL	C1D-ND-C4D	-3.56	103.80	106.33
30	62	607	CHL	C1D-ND-C4D	-3.56	103.81	106.33
30	1	601	CHL	C1D-ND-C4D	-3.56	103.81	106.33
21	5	616	CLA	CHD-C1D-ND	-3.55	121.19	124.45
30	42	607	CHL	C1D-ND-C4D	-3.55	103.81	106.33
30	62	616	CHL	C1D-ND-C4D	-3.55	103.81	106.33
21	B2	834	CLA	CHD-C1D-ND	-3.55	121.19	124.45
30	42	601	CHL	C1D-ND-C4D	-3.55	103.82	106.33
20	A	801	CL0	CHC-C1C-NC	3.54	129.58	124.20
21	A	806	CLA	CHD-C1D-ND	-3.54	121.20	124.45
30	9	606	CHL	C1D-ND-C4D	-3.54	103.82	106.33
30	12	601	CHL	C1D-ND-C4D	-3.54	103.82	106.33
30	62	618	CHL	C1D-ND-C4D	-3.54	103.82	106.33
21	B2	830	CLA	CHD-C1D-ND	-3.54	121.20	124.45
30	4	607	CHL	C1D-ND-C4D	-3.53	103.82	106.33
21	52	616	CLA	CHD-C1D-ND	-3.53	121.21	124.45
21	B	803	CLA	CHD-C1D-ND	-3.53	121.21	124.45
30	5	608	CHL	C1D-ND-C4D	-3.53	103.83	106.33
30	6	607	CHL	C1D-ND-C4D	-3.53	103.83	106.33
21	9	610	CLA	CHD-C1D-ND	-3.53	121.21	124.45
21	62	614	CLA	CHD-C1D-ND	-3.52	121.22	124.45
30	5	618	CHL	C1D-ND-C4D	-3.52	103.83	106.33
21	B2	803	CLA	CHD-C1D-ND	-3.52	121.22	124.45
30	92	606	CHL	C1D-ND-C4D	-3.52	103.83	106.33
30	Z	606	CHL	C1D-ND-C4D	-3.52	103.84	106.33
30	6	616	CHL	C1D-ND-C4D	-3.51	103.84	106.33
21	12	608	CLA	CHD-C1D-ND	-3.51	121.22	124.45
21	82	616	CLA	CHD-C1D-ND	-3.51	121.22	124.45
30	4	618	CHL	C1D-ND-C4D	-3.51	103.84	106.33
30	42	606	CHL	C1D-ND-C4D	-3.51	103.84	106.33
30	42	608	CHL	C1D-ND-C4D	-3.51	103.84	106.33
21	42	610	CLA	CHD-C1D-ND	-3.51	121.23	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	6	614	CLA	CHD-C1D-ND	-3.50	121.23	124.45
21	1	610	CLA	CHD-C1D-ND	-3.50	121.23	124.45
30	52	618	CHL	C1D-ND-C4D	-3.50	103.85	106.33
21	5	610	CLA	CHD-C1D-ND	-3.49	121.24	124.45
21	6	610	CLA	CHD-C1D-ND	-3.49	121.24	124.45
30	42	618	CHL	C1D-ND-C4D	-3.49	103.85	106.33
21	B	829	CLA	CHD-C1D-ND	-3.49	121.25	124.45
21	B2	829	CLA	CHD-C1D-ND	-3.48	121.25	124.45
21	8	616	CLA	CHD-C1D-ND	-3.48	121.25	124.45
21	4	610	CLA	CHD-C1D-ND	-3.48	121.26	124.45
30	7	606	CHL	C1D-ND-C4D	-3.48	103.86	106.33
30	4	601	CHL	C1D-ND-C4D	-3.47	103.87	106.33
30	5	607	CHL	C1B-CHB-C4A	-3.47	123.24	130.12
30	12	606	CHL	C1D-ND-C4D	-3.47	103.87	106.33
21	B	841	CLA	CHD-C1D-ND	-3.47	121.27	124.45
21	9	604	CLA	CHD-C1D-ND	-3.47	121.27	124.45
21	A	812	CLA	CHD-C1D-ND	-3.47	121.27	124.45
21	A2	812	CLA	CHD-C1D-ND	-3.47	121.27	124.45
21	B	834	CLA	CHD-C1D-ND	-3.47	121.27	124.45
21	L2	203	CLA	CHD-C1D-ND	-3.46	121.27	124.45
21	12	610	CLA	CHD-C1D-ND	-3.46	121.27	124.45
21	62	610	CLA	CHD-C1D-ND	-3.46	121.27	124.45
30	7	601	CHL	C1D-ND-C4D	-3.46	103.88	106.33
21	5	613	CLA	CHD-C1D-ND	-3.46	121.27	124.45
21	A2	841	CLA	CHD-C1D-ND	-3.46	121.27	124.45
21	A	827	CLA	CHD-C1D-ND	-3.46	121.28	124.45
30	62	606	CHL	C1D-ND-C4D	-3.45	103.88	106.33
21	B	830	CLA	CHD-C1D-ND	-3.45	121.28	124.45
21	A	836	CLA	CHD-C1D-ND	-3.45	121.28	124.45
32	62	625	NEX	O24-C25-C24	-3.45	110.79	113.38
21	42	604	CLA	CHD-C1D-ND	-3.45	121.28	124.45
30	52	607	CHL	C1B-CHB-C4A	-3.45	123.29	130.12
30	Z2	606	CHL	C1D-ND-C4D	-3.45	103.89	106.33
21	52	610	CLA	CHD-C1D-ND	-3.45	121.28	124.45
30	32	608	CHL	C1D-ND-C4D	-3.45	103.89	106.33
21	A	841	CLA	CHD-C1D-ND	-3.45	121.29	124.45
21	92	609	CLA	CHD-C1D-ND	-3.45	121.29	124.45
21	9	611	CLA	CHD-C1D-ND	-3.45	121.29	124.45
30	1	606	CHL	C1D-ND-C4D	-3.44	103.89	106.33
30	Z	607	CHL	C1D-ND-C4D	-3.44	103.89	106.33
21	A	811	CLA	CHD-C1D-ND	-3.44	121.29	124.45
21	Z	604	CLA	CHD-C1D-ND	-3.44	121.29	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	62	609	CLA	CHD-C1D-ND	-3.44	121.29	124.45
21	92	604	CLA	CHD-C1D-ND	-3.44	121.29	124.45
21	Z	613	CLA	CHD-C1D-ND	-3.44	121.30	124.45
21	B2	805	CLA	CHD-C1D-ND	-3.44	121.30	124.45
21	A	804	CLA	CHD-C1D-ND	-3.44	121.30	124.45
21	B2	841	CLA	CHD-C1D-ND	-3.44	121.30	124.45
21	B	805	CLA	CHD-C1D-ND	-3.43	121.30	124.45
30	3	608	CHL	C1D-ND-C4D	-3.43	103.90	106.33
21	5	603	CLA	CHD-C1D-ND	-3.43	121.30	124.45
21	Z2	614	CLA	CHD-C1D-ND	-3.43	121.30	124.45
21	B	822	CLA	CHD-C1D-ND	-3.43	121.30	124.45
21	A2	836	CLA	CHD-C1D-ND	-3.43	121.30	124.45
21	B2	822	CLA	CHD-C1D-ND	-3.43	121.30	124.45
21	3	614	CLA	CHD-C1D-ND	-3.43	121.30	124.45
21	Z2	604	CLA	CHD-C1D-ND	-3.43	121.30	124.45
30	4	606	CHL	C1D-ND-C4D	-3.43	103.90	106.33
21	L	203	CLA	CHD-C1D-ND	-3.43	121.30	124.45
21	B2	823	CLA	CHD-C1D-ND	-3.43	121.30	124.45
21	B2	840	CLA	CHD-C1D-ND	-3.43	121.31	124.45
30	Z2	607	CHL	C1D-ND-C4D	-3.43	103.90	106.33
21	7	603	CLA	CHD-C1D-ND	-3.43	121.31	124.45
21	52	613	CLA	CHD-C1D-ND	-3.42	121.31	124.45
32	6	625	NEX	O24-C25-C24	-3.42	110.81	113.38
30	92	607	CHL	C1B-CHB-C4A	-3.42	123.34	130.12
21	B	840	CLA	CHD-C1D-ND	-3.42	121.31	124.45
21	A2	827	CLA	CHD-C1D-ND	-3.42	121.31	124.45
21	6	617	CLA	CHD-C1D-ND	-3.42	121.31	124.45
21	Z	610	CLA	CHD-C1D-ND	-3.42	121.31	124.45
21	A2	820	CLA	CHD-C1D-ND	-3.42	121.31	124.45
30	72	601	CHL	C1D-ND-C4D	-3.42	103.91	106.33
21	1	608	CLA	CHD-C1D-ND	-3.42	121.31	124.45
21	A2	837	CLA	CHD-C1D-ND	-3.42	121.31	124.45
21	B2	814	CLA	CHD-C1D-ND	-3.42	121.31	124.45
21	6	609	CLA	CHD-C1D-ND	-3.41	121.32	124.45
21	B2	828	CLA	CHD-C1D-ND	-3.41	121.32	124.45
21	72	616	CLA	CHD-C1D-ND	-3.41	121.32	124.45
30	6	606	CHL	C1D-ND-C4D	-3.41	103.91	106.33
21	92	611	CLA	CHD-C1D-ND	-3.41	121.32	124.45
21	B2	837	CLA	CHD-C1D-ND	-3.41	121.32	124.45
21	B	839	CLA	CHD-C1D-ND	-3.41	121.32	124.45
21	B	828	CLA	CHD-C1D-ND	-3.41	121.32	124.45
21	A2	831	CLA	CHD-C1D-ND	-3.40	121.33	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	72	603	CLA	CHD-C1D-ND	-3.40	121.33	124.45
21	9	613	CLA	CHD-C1D-ND	-3.40	121.33	124.45
21	62	617	CLA	CHD-C1D-ND	-3.40	121.33	124.45
21	Z	614	CLA	CHD-C1D-ND	-3.40	121.33	124.45
21	B2	819	CLA	CHD-C1D-ND	-3.40	121.33	124.45
21	B	831	CLA	CHD-C1D-ND	-3.40	121.33	124.45
21	32	602	CLA	CHD-C1D-ND	-3.40	121.33	124.45
21	8	604	CLA	CHD-C1D-ND	-3.40	121.33	124.45
21	9	609	CLA	CHD-C1D-ND	-3.40	121.33	124.45
21	Z2	610	CLA	CHD-C1D-ND	-3.40	121.33	124.45
21	B2	803	CLA	C1D-ND-C4D	-3.40	103.92	106.33
21	A	802	CLA	CHD-C1D-ND	-3.40	121.33	124.45
21	9	614	CLA	CHD-C1D-ND	-3.39	121.33	124.45
21	32	614	CLA	CHD-C1D-ND	-3.39	121.33	124.45
21	A	831	CLA	CHD-C1D-ND	-3.39	121.34	124.45
21	A2	811	CLA	CHD-C1D-ND	-3.39	121.34	124.45
21	6	602	CLA	CHD-C1D-ND	-3.39	121.34	124.45
21	52	603	CLA	CHD-C1D-ND	-3.39	121.34	124.45
21	L	204	CLA	CHD-C1D-ND	-3.39	121.34	124.45
21	4	604	CLA	CHD-C1D-ND	-3.39	121.34	124.45
21	Z2	608	CLA	CHD-C1D-ND	-3.39	121.34	124.45
30	7	607	CHL	C1D-ND-C4D	-3.39	103.93	106.33
21	A	830	CLA	CHD-C1D-ND	-3.39	121.34	124.45
21	B	807	CLA	CHD-C1D-ND	-3.39	121.34	124.45
21	Z	608	CLA	CHD-C1D-ND	-3.39	121.34	124.45
21	5	617	CLA	CHD-C1D-ND	-3.39	121.34	124.45
21	A	803	CLA	CHD-C1D-ND	-3.39	121.34	124.45
21	7	616	CLA	CHD-C1D-ND	-3.39	121.34	124.45
21	B	812	CLA	CHD-C1D-ND	-3.38	121.34	124.45
21	B	819	CLA	CHD-C1D-ND	-3.38	121.34	124.45
21	Z	602	CLA	CHD-C1D-ND	-3.38	121.35	124.45
21	4	616	CLA	CHD-C1D-ND	-3.38	121.35	124.45
21	A2	832	CLA	CHD-C1D-ND	-3.38	121.35	124.45
30	52	606	CHL	C1D-ND-C4D	-3.38	103.93	106.33
30	6	601	CHL	C1B-CHB-C4A	-3.38	123.42	130.12
21	82	602	CLA	CHD-C1D-ND	-3.38	121.35	124.45
21	52	617	CLA	CHD-C1D-ND	-3.38	121.35	124.45
21	A	820	CLA	CHD-C1D-ND	-3.38	121.35	124.45
21	4	613	CLA	CHD-C1D-ND	-3.38	121.35	124.45
21	B2	807	CLA	CHD-C1D-ND	-3.38	121.35	124.45
21	1	603	CLA	CHD-C1D-ND	-3.38	121.35	124.45
21	8	602	CLA	CHD-C1D-ND	-3.38	121.35	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	5	606	CHL	C1D-ND-C4D	-3.37	103.94	106.33
21	72	611	CLA	CHD-C1D-ND	-3.37	121.35	124.45
30	12	607	CHL	C1D-ND-C4D	-3.37	103.94	106.33
21	B2	821	CLA	CHD-C1D-ND	-3.37	121.36	124.45
21	L2	204	CLA	CHD-C1D-ND	-3.37	121.36	124.45
21	Z2	613	CLA	CHD-C1D-ND	-3.37	121.36	124.45
21	42	616	CLA	CHD-C1D-ND	-3.37	121.36	124.45
21	A	837	CLA	CHD-C1D-ND	-3.37	121.36	124.45
21	B2	831	CLA	CHD-C1D-ND	-3.37	121.36	124.45
21	92	613	CLA	CHD-C1D-ND	-3.37	121.36	124.45
30	1	607	CHL	C1D-ND-C4D	-3.37	103.94	106.33
21	A2	803	CLA	CHD-C1D-ND	-3.37	121.36	124.45
21	B	803	CLA	C1D-ND-C4D	-3.37	103.94	106.33
21	A	833	CLA	CHD-C1D-ND	-3.37	121.36	124.45
21	7	608	CLA	CHD-C1D-ND	-3.36	121.36	124.45
21	92	614	CLA	CHD-C1D-ND	-3.36	121.36	124.45
21	B	823	CLA	CHD-C1D-ND	-3.36	121.37	124.45
21	A2	816	CLA	CHD-C1D-ND	-3.36	121.37	124.45
21	B2	832	CLA	CHD-C1D-ND	-3.36	121.37	124.45
21	A2	830	CLA	CHD-C1D-ND	-3.36	121.37	124.45
21	3	610	CLA	CHD-C1D-ND	-3.36	121.37	124.45
21	1	609	CLA	CHD-C1D-ND	-3.36	121.37	124.45
21	A2	833	CLA	CHD-C1D-ND	-3.36	121.37	124.45
21	82	604	CLA	CHD-C1D-ND	-3.36	121.37	124.45
21	A2	804	CLA	CHD-C1D-ND	-3.36	121.37	124.45
21	12	609	CLA	CHD-C1D-ND	-3.36	121.37	124.45
21	82	614	CLA	CHD-C1D-ND	-3.36	121.37	124.45
21	6	613	CLA	CHD-C1D-ND	-3.35	121.37	124.45
21	42	614	CLA	CHD-C1D-ND	-3.35	121.38	124.45
21	7	611	CLA	CHD-C1D-ND	-3.35	121.38	124.45
21	4	614	CLA	CHD-C1D-ND	-3.35	121.38	124.45
21	6	622	CLA	CHD-C1D-ND	-3.35	121.38	124.45
21	B	814	CLA	CHD-C1D-ND	-3.35	121.38	124.45
21	B	837	CLA	CHD-C1D-ND	-3.35	121.38	124.45
21	32	604	CLA	CHD-C1D-ND	-3.34	121.38	124.45
21	B2	839	CLA	CHD-C1D-ND	-3.34	121.38	124.45
21	A2	802	CLA	CHD-C1D-ND	-3.34	121.38	124.45
30	62	601	CHL	C1B-CHB-C4A	-3.34	123.50	130.12
21	8	614	CLA	CHD-C1D-ND	-3.34	121.38	124.45
21	82	613	CLA	CHD-C1D-ND	-3.34	121.39	124.45
21	5	609	CLA	CHD-C1D-ND	-3.34	121.39	124.45
21	3	604	CLA	CHD-C1D-ND	-3.34	121.39	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A2	835	CLA	CHD-C1D-ND	-3.34	121.39	124.45
21	A	816	CLA	CHD-C1D-ND	-3.34	121.39	124.45
21	62	622	CLA	CHD-C1D-ND	-3.34	121.39	124.45
21	3	602	CLA	CHD-C1D-ND	-3.33	121.39	124.45
21	Z2	602	CLA	CHD-C1D-ND	-3.33	121.39	124.45
21	B	821	CLA	CHD-C1D-ND	-3.33	121.39	124.45
21	52	614	CLA	CHD-C1D-ND	-3.33	121.39	124.45
21	Z	603	CLA	CHD-C1D-ND	-3.33	121.40	124.45
21	B	835	CLA	CHD-C1D-ND	-3.33	121.40	124.45
21	52	604	CLA	CHD-C1D-ND	-3.33	121.40	124.45
21	A	835	CLA	CHD-C1D-ND	-3.33	121.40	124.45
21	A	821	CLA	CHD-C1D-ND	-3.32	121.40	124.45
21	B	810	CLA	CHD-C1D-ND	-3.32	121.40	124.45
21	8	613	CLA	CHD-C1D-ND	-3.32	121.40	124.45
21	5	614	CLA	CHD-C1D-ND	-3.32	121.40	124.45
21	42	611	CLA	CHD-C1D-ND	-3.32	121.40	124.45
21	52	609	CLA	CHD-C1D-ND	-3.32	121.40	124.45
30	72	607	CHL	C1D-ND-C4D	-3.32	103.97	106.33
21	5	604	CLA	CHD-C1D-ND	-3.32	121.40	124.45
21	Z2	603	CLA	CHD-C1D-ND	-3.32	121.40	124.45
21	1	613	CLA	CHD-C1D-ND	-3.32	121.40	124.45
21	72	608	CLA	CHD-C1D-ND	-3.32	121.40	124.45
30	Z	601	CHL	C1D-ND-C4D	-3.32	103.98	106.33
21	42	609	CLA	CHD-C1D-ND	-3.32	121.41	124.45
21	A	832	CLA	CHD-C1D-ND	-3.31	121.41	124.45
21	32	610	CLA	CHD-C1D-ND	-3.31	121.41	124.45
21	A	840	CLA	CHD-C1D-ND	-3.31	121.41	124.45
21	12	613	CLA	CHD-C1D-ND	-3.31	121.41	124.45
21	B2	812	CLA	CHD-C1D-ND	-3.31	121.41	124.45
21	K	204	CLA	CHD-C1D-ND	-3.31	121.42	124.45
30	82	607	CHL	C1D-ND-C4D	-3.31	103.99	106.33
21	A2	821	CLA	CHD-C1D-ND	-3.31	121.42	124.45
21	A2	840	CLA	CHD-C1D-ND	-3.31	121.42	124.45
21	B	804	CLA	CHD-C1D-ND	-3.30	121.42	124.45
21	72	609	CLA	CHD-C1D-ND	-3.30	121.42	124.45
21	42	613	CLA	CHD-C1D-ND	-3.30	121.42	124.45
21	62	602	CLA	CHD-C1D-ND	-3.30	121.42	124.45
21	8	610	CLA	CHD-C1D-ND	-3.30	121.42	124.45
21	32	611	CLA	CHD-C1D-ND	-3.30	121.42	124.45
21	B	832	CLA	CHD-C1D-ND	-3.30	121.42	124.45
21	B	838	CLA	CHD-C1D-ND	-3.29	121.43	124.45
21	B2	838	CLA	CHD-C1D-ND	-3.29	121.43	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	82	603	CLA	CHD-C1D-ND	-3.29	121.43	124.45
21	3	611	CLA	CHD-C1D-ND	-3.29	121.43	124.45
21	82	609	CLA	CHD-C1D-ND	-3.29	121.43	124.45
21	4	611	CLA	CHD-C1D-ND	-3.29	121.43	124.45
21	12	603	CLA	CHD-C1D-ND	-3.29	121.43	124.45
21	A	843	CLA	CHD-C1D-ND	-3.28	121.44	124.45
21	B	818	CLA	CHD-C1D-ND	-3.28	121.44	124.45
21	A2	824	CLA	CHD-C1D-ND	-3.28	121.44	124.45
21	8	611	CLA	CHD-C1D-ND	-3.28	121.44	124.45
21	A	822	CLA	CHD-C1D-ND	-3.28	121.44	124.45
21	A	824	CLA	CHD-C1D-ND	-3.28	121.44	124.45
21	3	609	CLA	CHD-C1D-ND	-3.28	121.44	124.45
30	8	607	CHL	C1D-ND-C4D	-3.28	104.01	106.33
21	B2	810	CLA	CHD-C1D-ND	-3.28	121.44	124.45
21	8	603	CLA	CHD-C1D-ND	-3.27	121.44	124.45
21	62	613	CLA	CHD-C1D-ND	-3.27	121.44	124.45
21	6	611	CLA	CHD-C1D-ND	-3.27	121.45	124.45
21	B2	835	CLA	CHD-C1D-ND	-3.27	121.45	124.45
30	12	607	CHL	C1B-CHB-C4A	-3.27	123.64	130.12
21	B	825	CLA	CHD-C1D-ND	-3.27	121.45	124.45
21	12	614	CLA	CHD-C1D-ND	-3.27	121.45	124.45
21	8	609	CLA	CHD-C1D-ND	-3.27	121.45	124.45
21	B	816	CLA	CHD-C1D-ND	-3.27	121.45	124.45
21	82	611	CLA	CHD-C1D-ND	-3.27	121.45	124.45
21	K2	204	CLA	CHD-C1D-ND	-3.27	121.45	124.45
21	A2	825	CLA	CHD-C1D-ND	-3.26	121.45	124.45
21	A2	842	CLA	CHD-C1D-ND	-3.26	121.46	124.45
21	3	612	CLA	CHD-C1D-ND	-3.26	121.46	124.45
21	B2	818	CLA	CHD-C1D-ND	-3.26	121.46	124.45
21	4	609	CLA	CHD-C1D-ND	-3.26	121.46	124.45
21	F	303	CLA	CHD-C1D-ND	-3.25	121.47	124.45
21	A2	839	CLA	CHD-C1D-ND	-3.25	121.47	124.45
21	92	603	CLA	CHD-C1D-ND	-3.25	121.47	124.45
30	62	601	CHL	C1D-ND-C4D	-3.25	104.03	106.33
21	4	602	CLA	CHD-C1D-ND	-3.25	121.47	124.45
21	32	607	CLA	CHD-C1D-ND	-3.25	121.47	124.45
30	8	601	CHL	C1D-ND-C4D	-3.25	104.03	106.33
21	K	203	CLA	CHD-C1D-ND	-3.25	121.47	124.45
21	7	609	CLA	CHD-C1D-ND	-3.25	121.47	124.45
21	32	609	CLA	CHD-C1D-ND	-3.25	121.47	124.45
21	B	811	CLA	CHD-C1D-ND	-3.25	121.47	124.45
21	3	607	CLA	CHD-C1D-ND	-3.25	121.47	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	836	CLA	CHD-C1D-ND	-3.24	121.47	124.45
30	4	607	CHL	C1B-CHB-C4A	-3.24	123.69	130.12
21	B2	811	CLA	CHD-C1D-ND	-3.24	121.47	124.45
21	Z2	616	CLA	CHD-C1D-ND	-3.24	121.47	124.45
21	1	602	CLA	CHD-C1D-ND	-3.24	121.47	124.45
21	F2	303	CLA	CHD-C1D-ND	-3.24	121.47	124.45
30	1	607	CHL	C1B-CHB-C4A	-3.24	123.70	130.12
21	3	615	CLA	CHD-C1D-ND	-3.24	121.48	124.45
21	A2	843	CLA	CHD-C1D-ND	-3.24	121.48	124.45
21	B2	804	CLA	CHD-C1D-ND	-3.24	121.48	124.45
21	1	614	CLA	CHD-C1D-ND	-3.24	121.48	124.45
21	92	601	CLA	CHD-C1D-ND	-3.24	121.48	124.45
21	42	602	CLA	CHD-C1D-ND	-3.24	121.48	124.45
21	A	818	CLA	CHD-C1D-ND	-3.24	121.48	124.45
21	3	606	CLA	CHD-C1D-ND	-3.24	121.48	124.45
21	K2	206	CLA	CHD-C1D-ND	-3.24	121.48	124.45
21	B2	816	CLA	CHD-C1D-ND	-3.23	121.48	124.45
21	B2	825	CLA	CHD-C1D-ND	-3.23	121.48	124.45
21	B	815	CLA	CHD-C1D-ND	-3.23	121.48	124.45
21	B2	815	CLA	CHD-C1D-ND	-3.23	121.48	124.45
21	72	602	CLA	CHD-C1D-ND	-3.23	121.48	124.45
21	A2	807	CLA	CHD-C1D-ND	-3.23	121.48	124.45
21	A2	822	CLA	CHD-C1D-ND	-3.23	121.48	124.45
21	82	610	CLA	CHD-C1D-ND	-3.23	121.48	124.45
30	Z2	601	CHL	C1D-ND-C4D	-3.23	104.04	106.33
21	6	604	CLA	CHD-C1D-ND	-3.23	121.49	124.45
21	32	612	CLA	CHD-C1D-ND	-3.23	121.49	124.45
21	B	826	CLA	CHD-C1D-ND	-3.23	121.49	124.45
21	A	808	CLA	CHD-C1D-ND	-3.22	121.49	124.45
21	12	602	CLA	CHD-C1D-ND	-3.22	121.49	124.45
21	Z	609	CLA	CHD-C1D-ND	-3.22	121.49	124.45
21	92	602	CLA	CHD-C1D-ND	-3.22	121.49	124.45
30	42	607	CHL	C1B-CHB-C4A	-3.22	123.74	130.12
21	A	815	CLA	CHD-C1D-ND	-3.22	121.50	124.45
21	7	614	CLA	CHD-C1D-ND	-3.22	121.50	124.45
21	Z2	611	CLA	CHD-C1D-ND	-3.22	121.50	124.45
21	K2	203	CLA	CHD-C1D-ND	-3.22	121.50	124.45
21	52	611	CLA	CHD-C1D-ND	-3.22	121.50	124.45
21	62	603	CLA	CHD-C1D-ND	-3.22	121.50	124.45
30	82	601	CHL	C1D-ND-C4D	-3.22	104.05	106.33
21	72	614	CLA	CHD-C1D-ND	-3.22	121.50	124.45
21	B2	826	CLA	CHD-C1D-ND	-3.21	121.50	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	825	CLA	CHD-C1D-ND	-3.21	121.50	124.45
21	9	601	CLA	CHD-C1D-ND	-3.21	121.50	124.45
30	6	601	CHL	C1D-ND-C4D	-3.21	104.05	106.33
21	8	612	CLA	CHD-C1D-ND	-3.21	121.50	124.45
21	G2	203	CLA	CHD-C1D-ND	-3.21	121.50	124.45
21	7	602	CLA	CHD-C1D-ND	-3.21	121.51	124.45
21	B2	827	CLA	CHD-C1D-ND	-3.21	121.51	124.45
21	Z	616	CLA	CHD-C1D-ND	-3.21	121.51	124.45
21	A	834	CLA	CHD-C1D-ND	-3.20	121.51	124.45
21	B	827	CLA	CHD-C1D-ND	-3.20	121.51	124.45
21	A2	834	CLA	CHD-C1D-ND	-3.20	121.51	124.45
21	5	611	CLA	CHD-C1D-ND	-3.20	121.51	124.45
21	62	611	CLA	CHD-C1D-ND	-3.20	121.51	124.45
21	A2	838	CLA	CHD-C1D-ND	-3.20	121.52	124.45
21	A2	815	CLA	CHD-C1D-ND	-3.20	121.52	124.45
21	6	603	CLA	CHD-C1D-ND	-3.20	121.52	124.45
21	9	602	CLA	CHD-C1D-ND	-3.20	121.52	124.45
21	Z	612	CLA	CHD-C1D-ND	-3.19	121.52	124.45
21	B2	836	CLA	CHD-C1D-ND	-3.19	121.52	124.45
21	32	606	CLA	CHD-C1D-ND	-3.19	121.52	124.45
21	A	839	CLA	CHD-C1D-ND	-3.19	121.52	124.45
21	G	203	CLA	CHD-C1D-ND	-3.19	121.52	124.45
21	Z	611	CLA	CHD-C1D-ND	-3.19	121.52	124.45
21	A2	808	CLA	CHD-C1D-ND	-3.19	121.52	124.45
21	B2	802	CLA	CHD-C1D-ND	-3.19	121.52	124.45
21	Z2	609	CLA	CHD-C1D-ND	-3.19	121.52	124.45
21	A2	818	CLA	CHD-C1D-ND	-3.19	121.52	124.45
21	92	612	CLA	CHD-C1D-ND	-3.19	121.53	124.45
21	A	845	CLA	CHD-C1D-ND	-3.19	121.53	124.45
21	32	615	CLA	CHD-C1D-ND	-3.19	121.53	124.45
30	72	601	CHL	C1B-CHB-C4A	-3.18	123.81	130.12
21	7	620	CLA	CHD-C1D-ND	-3.18	121.53	124.45
21	82	612	CLA	CHD-C1D-ND	-3.18	121.53	124.45
21	A	807	CLA	CHD-C1D-ND	-3.18	121.53	124.45
21	7	604	CLA	CHD-C1D-ND	-3.18	121.53	124.45
21	82	608	CLA	CHD-C1D-ND	-3.18	121.53	124.45
21	A	805	CLA	CHD-C1D-ND	-3.18	121.53	124.45
21	A	817	CLA	CHD-C1D-ND	-3.18	121.53	124.45
21	1	611	CLA	CHD-C1D-ND	-3.18	121.53	124.45
21	12	611	CLA	CHD-C1D-ND	-3.18	121.53	124.45
21	A2	805	CLA	CHD-C1D-ND	-3.18	121.53	124.45
21	1	612	CLA	CHD-C1D-ND	-3.18	121.53	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	6	607	CHL	C1B-CHB-C4A	-3.18	123.83	130.12
21	F	301	CLA	CHD-C1D-ND	-3.18	121.54	124.45
21	B	809	CLA	CHD-C1D-ND	-3.17	121.54	124.45
21	4	612	CLA	CHD-C1D-ND	-3.17	121.54	124.45
21	5	612	CLA	CHD-C1D-ND	-3.17	121.54	124.45
21	72	604	CLA	CHD-C1D-ND	-3.17	121.54	124.45
21	62	604	CLA	CHD-C1D-ND	-3.17	121.54	124.45
21	9	603	CLA	CHD-C1D-ND	-3.17	121.54	124.45
30	Z	607	CHL	C1B-CHB-C4A	-3.16	123.85	130.12
21	B	802	CLA	CHD-C1D-ND	-3.16	121.55	124.45
21	3	613	CLA	CHD-C1D-ND	-3.16	121.55	124.45
21	B	808	CLA	CHD-C1D-ND	-3.16	121.55	124.45
21	A	842	CLA	CHD-C1D-ND	-3.16	121.55	124.45
30	62	607	CHL	C1B-CHB-C4A	-3.15	123.87	130.12
21	B	817	CLA	CHD-C1D-ND	-3.15	121.56	124.45
21	B2	809	CLA	CHD-C1D-ND	-3.15	121.56	124.45
21	1	616	CLA	CHD-C1D-ND	-3.15	121.56	124.45
21	72	620	CLA	CHD-C1D-ND	-3.15	121.56	124.45
21	Z2	612	CLA	CHD-C1D-ND	-3.15	121.56	124.45
30	Z2	607	CHL	C1B-CHB-C4A	-3.15	123.88	130.12
21	8	608	CLA	CHD-C1D-ND	-3.15	121.56	124.45
21	42	603	CLA	CHD-C1D-ND	-3.15	121.56	124.45
30	7	601	CHL	C1B-CHB-C4A	-3.15	123.89	130.12
21	A	838	CLA	CHD-C1D-ND	-3.14	121.56	124.45
30	62	608	CHL	C1B-CHB-C4A	-3.14	123.89	130.12
21	7	613	CLA	CHD-C1D-ND	-3.14	121.56	124.45
21	52	602	CLA	CHD-C1D-ND	-3.14	121.56	124.45
21	K	206	CLA	CHD-C1D-ND	-3.14	121.57	124.45
21	72	613	CLA	CHD-C1D-ND	-3.14	121.57	124.45
30	9	607	CHL	C1D-ND-C4D	-3.14	104.11	106.33
21	B2	817	CLA	CHD-C1D-ND	-3.14	121.57	124.45
21	42	612	CLA	CHD-C1D-ND	-3.13	121.57	124.45
21	9	612	CLA	CHD-C1D-ND	-3.13	121.58	124.45
21	A2	845	CLA	CHD-C1D-ND	-3.13	121.58	124.45
21	32	613	CLA	CHD-C1D-ND	-3.13	121.58	124.45
30	4	608	CHL	C1B-CHB-C4A	-3.13	123.92	130.12
21	A2	854	CLA	CHD-C1D-ND	-3.13	121.58	124.45
30	42	608	CHL	C1B-CHB-C4A	-3.13	123.92	130.12
30	6	608	CHL	C1B-CHB-C4A	-3.13	123.92	130.12
21	A2	826	CLA	CHD-C1D-ND	-3.13	121.58	124.45
21	A	828	CLA	CHD-C1D-ND	-3.13	121.58	124.45
21	B2	820	CLA	CHD-C1D-ND	-3.12	121.58	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	F2	301	CLA	CHD-C1D-ND	-3.12	121.58	124.45
21	A	813	CLA	CHD-C1D-ND	-3.12	121.59	124.45
21	A2	813	CLA	CHD-C1D-ND	-3.12	121.59	124.45
21	52	612	CLA	CHD-C1D-ND	-3.12	121.59	124.45
21	G2	204	CLA	CHD-C1D-ND	-3.12	121.59	124.45
30	6	616	CHL	C1B-CHB-C4A	-3.11	123.95	130.12
21	5	602	CLA	CHD-C1D-ND	-3.11	121.59	124.45
21	A2	828	CLA	CHD-C1D-ND	-3.11	121.59	124.45
21	12	612	CLA	CHD-C1D-ND	-3.11	121.60	124.45
21	G	204	CLA	CHD-C1D-ND	-3.11	121.60	124.45
21	A2	817	CLA	CHD-C1D-ND	-3.11	121.60	124.45
21	7	612	CLA	CHD-C1D-ND	-3.10	121.60	124.45
30	62	616	CHL	C1B-CHB-C4A	-3.10	123.97	130.12
21	J2	101	CLA	CHD-C1D-ND	-3.10	121.60	124.45
21	32	617	CLA	CHD-C1D-ND	-3.10	121.60	124.45
21	A	826	CLA	CHD-C1D-ND	-3.10	121.61	124.45
21	5	601	CLA	CHD-C1D-ND	-3.10	121.61	124.45
21	52	601	CLA	CHD-C1D-ND	-3.10	121.61	124.45
21	B2	808	CLA	CHD-C1D-ND	-3.10	121.61	124.45
30	92	606	CHL	C1B-CHB-C4A	-3.09	123.99	130.12
21	4	603	CLA	CHD-C1D-ND	-3.09	121.61	124.45
30	1	601	CHL	C1B-CHB-C4A	-3.09	124.00	130.12
21	3	617	CLA	CHD-C1D-ND	-3.09	121.62	124.45
30	42	618	CHL	C1B-CHB-C4A	-3.08	124.01	130.12
30	12	601	CHL	C1B-CHB-C4A	-3.08	124.01	130.12
30	6	606	CHL	C1B-CHB-C4A	-3.08	124.01	130.12
30	4	618	CHL	C1B-CHB-C4A	-3.08	124.01	130.12
21	J	101	CLA	CHD-C1D-ND	-3.08	121.62	124.45
21	B	820	CLA	CHD-C1D-ND	-3.08	121.62	124.45
21	A	814	CLA	CHD-C1D-ND	-3.08	121.63	124.45
30	52	618	CHL	C1B-CHB-C4A	-3.07	124.03	130.12
30	62	606	CHL	C1B-CHB-C4A	-3.07	124.03	130.12
21	A2	814	CLA	CHD-C1D-ND	-3.07	121.63	124.45
30	9	606	CHL	C1B-CHB-C4A	-3.07	124.04	130.12
30	5	618	CHL	C1B-CHB-C4A	-3.06	124.05	130.12
21	A2	810	CLA	CHD-C1D-ND	-3.06	121.64	124.45
30	5	608	CHL	C1B-CHB-C4A	-3.06	124.05	130.12
30	52	608	CHL	C1B-CHB-C4A	-3.06	124.05	130.12
21	A	854	CLA	CHD-C1D-ND	-3.06	121.64	124.45
21	B	813	CLA	CHD-C1D-ND	-3.06	121.64	124.45
21	12	616	CLA	CHD-C1D-ND	-3.06	121.64	124.45
21	A	810	CLA	CHD-C1D-ND	-3.06	121.65	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	F	304	CLA	CHD-C1D-ND	-3.06	121.65	124.45
21	B2	824	CLA	CHD-C1D-ND	-3.06	121.65	124.45
21	F2	304	CLA	CHD-C1D-ND	-3.06	121.65	124.45
30	6	618	CHL	C1B-CHB-C4A	-3.05	124.07	130.12
21	62	612	CLA	CHD-C1D-ND	-3.05	121.65	124.45
21	A2	829	CLA	CHD-C1D-ND	-3.05	121.65	124.45
21	6	612	CLA	CHD-C1D-ND	-3.05	121.65	124.45
30	1	606	CHL	C1B-CHB-C4A	-3.05	124.09	130.12
21	72	612	CLA	CHD-C1D-ND	-3.04	121.66	124.45
30	62	618	CHL	C1B-CHB-C4A	-3.04	124.10	130.12
30	12	606	CHL	C1B-CHB-C4A	-3.04	124.10	130.12
30	42	606	CHL	C1B-CHB-C4A	-3.04	124.11	130.12
21	B2	813	CLA	CHD-C1D-ND	-3.03	121.67	124.45
20	A2	801	CL0	CHC-C1C-C2C	-3.03	118.35	126.72
30	4	606	CHL	C1B-CHB-C4A	-3.02	124.14	130.12
20	A	801	CL0	CHC-C1C-C2C	-3.01	118.40	126.72
30	7	607	CHL	C1B-CHB-C4A	-3.01	124.16	130.12
30	72	606	CHL	C1B-CHB-C4A	-3.00	124.18	130.12
21	A	829	CLA	CHD-C1D-ND	-2.99	121.70	124.45
21	B	824	CLA	CHD-C1D-ND	-2.99	121.70	124.45
21	32	603	CLA	CHD-C1D-ND	-2.99	121.71	124.45
30	7	601	CHL	CMB-C2B-C1B	-2.98	123.88	128.46
30	Z2	601	CHL	C1B-CHB-C4A	-2.98	124.21	130.12
21	3	603	CLA	CHD-C1D-ND	-2.98	121.72	124.45
30	Z	606	CHL	C1B-CHB-C4A	-2.98	124.22	130.12
30	72	607	CHL	C1B-CHB-C4A	-2.98	124.22	130.12
21	B2	806	CLA	CHD-C1D-ND	-2.98	121.72	124.45
30	4	606	CHL	CMB-C2B-C1B	-2.97	123.89	128.46
30	5	606	CHL	C1B-CHB-C4A	-2.97	124.23	130.12
30	52	606	CHL	C1B-CHB-C4A	-2.97	124.23	130.12
30	Z2	606	CHL	C1B-CHB-C4A	-2.97	124.24	130.12
30	Z	601	CHL	C1B-CHB-C4A	-2.96	124.25	130.12
30	72	601	CHL	CMB-C2B-C1B	-2.95	123.92	128.46
30	7	606	CHL	C1B-CHB-C4A	-2.95	124.27	130.12
30	82	606	CHL	C1B-CHB-C4A	-2.95	124.28	130.12
30	42	606	CHL	CMB-C2B-C1B	-2.95	123.94	128.46
30	8	606	CHL	C1B-CHB-C4A	-2.94	124.30	130.12
21	A	819	CLA	CHD-C1D-ND	-2.93	121.76	124.45
30	6	616	CHL	CMB-C2B-C1B	-2.92	123.98	128.46
30	4	601	CHL	C1B-CHB-C4A	-2.91	124.35	130.12
30	3	608	CHL	C1B-CHB-C4A	-2.91	124.36	130.12
30	62	616	CHL	CMB-C2B-C1B	-2.91	124.00	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	32	608	CHL	C1B-CHB-C4A	-2.90	124.37	130.12
30	8	607	CHL	C1B-CHB-C4A	-2.90	124.37	130.12
21	B	806	CLA	CHD-C1D-ND	-2.90	121.79	124.45
30	62	601	CHL	CMB-C2B-C1B	-2.89	124.02	128.46
30	42	601	CHL	C1B-CHB-C4A	-2.89	124.39	130.12
30	82	607	CHL	C1B-CHB-C4A	-2.88	124.41	130.12
30	6	601	CHL	CMB-C2B-C1B	-2.87	124.05	128.46
21	A2	819	CLA	CHD-C1D-ND	-2.86	121.82	124.45
30	62	608	CHL	CMB-C2B-C1B	-2.84	124.10	128.46
30	82	601	CHL	C1B-CHB-C4A	-2.84	124.49	130.12
30	8	601	CHL	C1B-CHB-C4A	-2.83	124.51	130.12
30	6	608	CHL	CMB-C2B-C1B	-2.82	124.13	128.46
21	5	621	CLA	CHD-C1D-ND	-2.81	121.87	124.45
30	5	608	CHL	CMB-C2B-C1B	-2.80	124.16	128.46
30	Z	601	CHL	CMB-C2B-C1B	-2.80	124.17	128.46
30	52	608	CHL	CMB-C2B-C1B	-2.79	124.17	128.46
30	12	606	CHL	CMB-C2B-C1B	-2.79	124.18	128.46
21	52	621	CLA	CHD-C1D-ND	-2.79	121.89	124.45
30	1	606	CHL	CMB-C2B-C1B	-2.79	124.18	128.46
30	6	618	CHL	CMB-C2B-C1B	-2.78	124.20	128.46
30	62	618	CHL	CMB-C2B-C1B	-2.77	124.20	128.46
30	42	607	CHL	CMB-C2B-C1B	-2.77	124.21	128.46
30	4	608	CHL	CMB-C2B-C1B	-2.76	124.22	128.46
30	Z2	601	CHL	CMB-C2B-C1B	-2.75	124.23	128.46
30	42	618	CHL	CMB-C2B-C1B	-2.75	124.24	128.46
30	1	607	CHL	CMB-C2B-C1B	-2.74	124.26	128.46
30	42	608	CHL	CMB-C2B-C1B	-2.73	124.26	128.46
30	7	607	CHL	CMB-C2B-C1B	-2.73	124.27	128.46
30	62	607	CHL	CMB-C2B-C1B	-2.73	124.27	128.46
21	K	201	CLA	CHD-C1D-ND	-2.72	121.95	124.45
30	72	607	CHL	CMB-C2B-C1B	-2.72	124.28	128.46
30	12	607	CHL	CMB-C2B-C1B	-2.72	124.29	128.46
30	6	607	CHL	CMB-C2B-C1B	-2.71	124.29	128.46
30	52	607	CHL	CMB-C2B-C1B	-2.71	124.29	128.46
30	4	618	CHL	CMB-C2B-C1B	-2.71	124.30	128.46
30	4	607	CHL	CMB-C2B-C1B	-2.71	124.30	128.46
30	82	607	CHL	CMB-C2B-C1B	-2.70	124.31	128.46
30	5	607	CHL	CMB-C2B-C1B	-2.69	124.33	128.46
30	8	607	CHL	CMB-C2B-C1B	-2.69	124.33	128.46
30	7	606	CHL	CMB-C2B-C1B	-2.69	124.33	128.46
30	72	606	CHL	CMB-C2B-C1B	-2.69	124.33	128.46
30	52	618	CHL	CMB-C2B-C1B	-2.68	124.34	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	62	606	CHL	CHB-C4A-NA	2.67	128.21	124.51
30	6	606	CHL	CHB-C4A-NA	2.67	128.21	124.51
21	K2	201	CLA	CHD-C1D-ND	-2.66	122.01	124.45
21	F2	304	CLA	O2A-C1-C2	2.66	115.61	108.64
30	5	618	CHL	CMB-C2B-C1B	-2.65	124.39	128.46
30	1	607	CHL	CHC-C1C-NC	2.65	128.22	124.20
30	Z2	607	CHL	CMB-C2B-C1B	-2.64	124.40	128.46
21	F	304	CLA	O2A-C1-C2	2.64	115.57	108.64
30	Z	607	CHL	CMB-C2B-C1B	-2.64	124.41	128.46
30	8	607	CHL	CHB-C4A-NA	2.63	128.15	124.51
30	62	601	CHL	CHA-C1A-NA	-2.63	120.38	126.40
30	12	601	CHL	CHB-C4A-NA	2.62	128.14	124.51
30	Z2	606	CHL	CMB-C2B-C1B	-2.61	124.45	128.46
30	12	607	CHL	CHC-C1C-NC	2.61	128.16	124.20
30	6	601	CHL	CHA-C1A-NA	-2.61	120.43	126.40
30	Z	606	CHL	CMB-C2B-C1B	-2.60	124.47	128.46
30	82	607	CHL	CHB-C4A-NA	2.59	128.10	124.51
30	8	607	CHL	CAA-C2A-C1A	2.58	120.44	111.97
30	82	607	CHL	CAA-C2A-C1A	2.58	120.43	111.97
30	7	607	CHL	CHB-C4A-NA	2.58	128.08	124.51
30	1	601	CHL	CHB-C4A-NA	2.57	128.07	124.51
30	92	607	CHL	CHC-C1C-NC	2.57	128.10	124.20
30	5	607	CHL	CHC-C1C-NC	2.57	128.10	124.20
30	1	601	CHL	CMB-C2B-C1B	-2.56	124.52	128.46
30	52	607	CHL	CHC-C1C-NC	2.56	128.09	124.20
30	32	608	CHL	CMB-C2B-C1B	-2.56	124.53	128.46
30	82	606	CHL	CMB-C2B-C1B	-2.56	124.53	128.46
30	6	606	CHL	CMB-C2B-C1B	-2.56	124.54	128.46
30	62	606	CHL	CMB-C2B-C1B	-2.56	124.54	128.46
30	42	601	CHL	CMB-C2B-C1B	-2.55	124.54	128.46
30	82	601	CHL	CHB-C4A-NA	2.55	128.04	124.51
30	52	606	CHL	CHB-C4A-NA	2.55	128.04	124.51
30	8	601	CHL	CHB-C4A-NA	2.55	128.04	124.51
30	5	606	CHL	CHB-C4A-NA	2.55	128.04	124.51
30	8	606	CHL	CMB-C2B-C1B	-2.55	124.54	128.46
30	8	607	CHL	CHA-C1A-NA	-2.55	120.56	126.40
30	3	608	CHL	CMB-C2B-C1B	-2.55	124.55	128.46
30	92	607	CHL	CMB-C2B-C1B	-2.55	124.55	128.46
30	62	618	CHL	CHB-C4A-NA	2.54	128.03	124.51
30	12	601	CHL	CMB-C2B-C1B	-2.54	124.55	128.46
30	72	607	CHL	CHB-C4A-NA	2.54	128.03	124.51
30	6	607	CHL	CHB-C4A-NA	2.54	128.02	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	6	618	CHL	CHB-C4A-NA	2.54	128.02	124.51
30	4	601	CHL	CMB-C2B-C1B	-2.54	124.57	128.46
30	9	607	CHL	CHA-C1A-NA	-2.53	120.59	126.40
30	62	607	CHL	CHB-C4A-NA	2.53	128.01	124.51
30	82	607	CHL	CHA-C1A-NA	-2.53	120.61	126.40
30	9	607	CHL	CHB-C4A-NA	2.52	127.99	124.51
30	3	608	CHL	CHB-C4A-NA	2.51	127.98	124.51
30	Z	601	CHL	CHC-C1C-NC	2.50	128.00	124.20
30	4	601	CHL	CHB-C4A-NA	2.50	127.97	124.51
30	Z2	601	CHL	CHC-C1C-NC	2.50	128.00	124.20
30	Z2	601	CHL	CHB-C4A-NA	2.50	127.97	124.51
30	42	606	CHL	CHB-C4A-NA	2.50	127.97	124.51
30	52	606	CHL	CMB-C2B-C1B	-2.50	124.63	128.46
30	42	606	CHL	CHC-C1C-NC	2.49	127.99	124.20
30	5	618	CHL	CHB-C4A-NA	2.49	127.96	124.51
30	32	608	CHL	CHB-C4A-NA	2.49	127.96	124.51
30	92	607	CHL	CHA-C1A-NA	-2.49	120.70	126.40
30	52	618	CHL	CHB-C4A-NA	2.49	127.95	124.51
30	52	606	CHL	CHA-C1A-NA	-2.48	120.71	126.40
30	7	607	CHL	CHC-C1C-NC	2.48	127.97	124.20
30	5	608	CHL	CHB-C4A-NA	2.48	127.94	124.51
30	52	608	CHL	CHB-C4A-NA	2.48	127.94	124.51
30	72	607	CHL	CHC-C1C-NC	2.48	127.96	124.20
30	4	601	CHL	CHA-C1A-NA	-2.48	120.72	126.40
26	B2	853	LMU	C1B-O5B-C5B	2.47	118.54	113.69
30	4	606	CHL	CHB-C4A-NA	2.47	127.93	124.51
30	42	601	CHL	CHA-C1A-NA	-2.47	120.74	126.40
30	42	601	CHL	CHB-C4A-NA	2.47	127.92	124.51
30	5	606	CHL	CMB-C2B-C1B	-2.46	124.68	128.46
30	42	618	CHL	CHB-C4A-NA	2.46	127.92	124.51
30	1	606	CHL	CHA-C1A-NA	-2.46	120.76	126.40
30	12	606	CHL	CHA-C1A-NA	-2.46	120.76	126.40
30	Z2	607	CHL	CHC-C1C-NC	2.46	127.93	124.20
30	12	607	CHL	CHA-C1A-NA	-2.46	120.77	126.40
21	52	621	CLA	C2A-C1A-CHA	2.46	128.16	123.86
30	Z	607	CHL	CHC-C1C-NC	2.45	127.92	124.20
30	4	618	CHL	CHB-C4A-NA	2.45	127.90	124.51
26	B	853	LMU	C1B-O5B-C5B	2.45	118.49	113.69
30	6	607	CHL	CHA-C1A-NA	-2.45	120.79	126.40
30	Z	601	CHL	CHB-C4A-NA	2.45	127.90	124.51
30	5	606	CHL	CHA-C1A-NA	-2.45	120.80	126.40
30	9	607	CHL	CHC-C1C-NC	2.45	127.91	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	1	607	CHL	CHA-C1A-NA	-2.44	120.80	126.40
21	5	621	CLA	C2A-C1A-CHA	2.44	128.13	123.86
30	92	607	CHL	CHB-C4A-NA	2.44	127.89	124.51
30	4	606	CHL	CHC-C1C-NC	2.44	127.91	124.20
30	6	606	CHL	CHA-C1A-NA	-2.43	120.82	126.40
30	62	608	CHL	CHA-C1A-NA	-2.43	120.83	126.40
30	6	607	CHL	CHC-C1C-NC	2.43	127.89	124.20
30	72	601	CHL	CHB-C4A-NA	2.43	127.87	124.51
30	62	607	CHL	CHA-C1A-NA	-2.43	120.83	126.40
30	62	601	CHL	C2A-C1A-CHA	2.43	128.10	123.86
30	1	606	CHL	CHB-C4A-NA	2.43	127.87	124.51
30	82	601	CHL	CHA-C1A-NA	-2.43	120.84	126.40
30	72	606	CHL	CHB-C4A-NA	2.43	127.87	124.51
30	5	618	CHL	CHA-C1A-NA	-2.42	120.84	126.40
30	62	606	CHL	CHA-C1A-NA	-2.42	120.86	126.40
30	6	608	CHL	CHA-C1A-NA	-2.42	120.86	126.40
30	72	607	CHL	CHA-C1A-NA	-2.42	120.86	126.40
30	12	606	CHL	CHB-C4A-NA	2.42	127.86	124.51
30	62	608	CHL	CHB-C4A-NA	2.42	127.86	124.51
30	52	618	CHL	CHA-C1A-NA	-2.42	120.86	126.40
30	92	606	CHL	CHB-C4A-NA	2.41	127.85	124.51
30	8	601	CHL	CHA-C1A-NA	-2.41	120.88	126.40
30	3	608	CHL	CHA-C1A-NA	-2.41	120.88	126.40
30	42	607	CHL	CHC-C1C-NC	2.40	127.85	124.20
30	82	606	CHL	CHB-C4A-NA	2.40	127.84	124.51
30	6	601	CHL	CHC-C1C-NC	2.40	127.85	124.20
30	62	618	CHL	CHA-C1A-NA	-2.40	120.89	126.40
30	6	608	CHL	CHC-C1C-NC	2.40	127.85	124.20
30	62	607	CHL	CHC-C1C-NC	2.40	127.84	124.20
30	4	601	CHL	CHC-C1C-NC	2.40	127.84	124.20
30	42	601	CHL	CHC-C1C-NC	2.40	127.84	124.20
30	32	608	CHL	CHA-C1A-NA	-2.40	120.91	126.40
30	6	618	CHL	CHA-C1A-NA	-2.40	120.91	126.40
30	7	607	CHL	CHA-C1A-NA	-2.40	120.91	126.40
30	12	607	CHL	CHB-C4A-NA	2.40	127.83	124.51
30	Z	607	CHL	CHA-C1A-NA	-2.39	120.91	126.40
30	6	601	CHL	C2A-C1A-CHA	2.39	128.05	123.86
32	5	625	NEX	C2-C1-C6	-2.39	106.89	109.21
30	8	601	CHL	CMB-C2B-C1B	-2.39	124.79	128.46
30	9	606	CHL	CHB-C4A-NA	2.39	127.82	124.51
30	1	601	CHL	CHC-C1C-NC	2.39	127.83	124.20
30	4	607	CHL	CHC-C1C-NC	2.39	127.83	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	42	608	CHL	CHA-C1A-NA	-2.38	120.94	126.40
30	62	616	CHL	CHC-C1C-NC	2.38	127.82	124.20
30	7	606	CHL	CHB-C4A-NA	2.38	127.81	124.51
30	6	618	CHL	CHC-C1C-NC	2.38	127.82	124.20
30	8	606	CHL	CHB-C4A-NA	2.38	127.81	124.51
30	82	601	CHL	CMB-C2B-C1B	-2.38	124.80	128.46
31	12	618	XAT	C7-C8-C9	2.38	129.22	125.53
30	Z2	601	CHL	CHA-C1A-NA	-2.38	120.95	126.40
30	82	606	CHL	CHC-C1C-NC	2.38	127.81	124.20
31	12	618	XAT	O4-C5-C4	-2.38	111.59	113.38
30	6	616	CHL	CHA-C1A-NA	-2.38	120.95	126.40
30	4	618	CHL	CHA-C1A-NA	-2.38	120.95	126.40
30	Z2	607	CHL	CHA-C1A-NA	-2.38	120.95	126.40
30	52	608	CHL	CHA-C1A-NA	-2.37	120.96	126.40
30	5	618	CHL	CHC-C1C-NC	2.37	127.80	124.20
21	5	621	CLA	CAA-C2A-C1A	2.37	119.75	111.97
30	8	606	CHL	CHC-C1C-NC	2.37	127.80	124.20
30	62	616	CHL	CHA-C1A-NA	-2.37	120.97	126.40
30	62	608	CHL	CHC-C1C-NC	2.37	127.80	124.20
30	1	607	CHL	CHB-C4A-NA	2.37	127.79	124.51
30	4	618	CHL	CHC-C1C-NC	2.37	127.80	124.20
30	4	607	CHL	CHA-C1A-NA	-2.37	120.97	126.40
30	4	608	CHL	CHA-C1A-NA	-2.37	120.97	126.40
30	62	601	CHL	CHC-C1C-NC	2.37	127.80	124.20
30	52	618	CHL	CHC-C1C-NC	2.37	127.80	124.20
21	52	621	CLA	CAA-C2A-C1A	2.37	119.73	111.97
30	5	608	CHL	CHA-C1A-NA	-2.36	120.98	126.40
30	42	607	CHL	CHA-C1A-NA	-2.36	120.98	126.40
30	6	616	CHL	CHC-C1C-NC	2.36	127.79	124.20
30	82	601	CHL	CHC-C1C-NC	2.36	127.79	124.20
30	5	608	CHL	CHC-C1C-NC	2.36	127.79	124.20
30	6	608	CHL	CHB-C4A-NA	2.36	127.77	124.51
30	12	601	CHL	CHC-C1C-NC	2.36	127.78	124.20
30	52	608	CHL	CHC-C1C-NC	2.36	127.78	124.20
30	7	601	CHL	CHB-C4A-NA	2.36	127.77	124.51
30	3	608	CHL	CHC-C1C-NC	2.36	127.78	124.20
30	32	608	CHL	CHC-C1C-NC	2.35	127.78	124.20
30	42	606	CHL	CHA-C1A-NA	-2.35	121.01	126.40
30	Z	601	CHL	CHA-C1A-NA	-2.35	121.01	126.40
30	6	601	CHL	CHB-C4A-NA	2.35	127.77	124.51
30	82	607	CHL	CHC-C1C-NC	2.35	127.77	124.20
30	42	618	CHL	CHA-C1A-NA	-2.35	121.01	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	52	606	CHL	CHC-C1C-NC	2.35	127.77	124.20
30	Z2	606	CHL	CHC-C1C-NC	2.35	127.77	124.20
30	4	608	CHL	CHC-C1C-NC	2.35	127.77	124.20
30	92	606	CHL	CHC-C1C-NC	2.35	127.76	124.20
30	42	618	CHL	CHC-C1C-NC	2.35	127.76	124.20
30	82	606	CHL	CHA-C1A-NA	-2.34	121.03	126.40
30	6	616	CHL	CHB-C4A-NA	2.34	127.75	124.51
30	42	608	CHL	CHC-C1C-NC	2.34	127.76	124.20
30	62	618	CHL	CHC-C1C-NC	2.34	127.76	124.20
30	5	606	CHL	CHC-C1C-NC	2.34	127.76	124.20
30	8	606	CHL	CHA-C1A-NA	-2.34	121.04	126.40
30	62	606	CHL	CHC-C1C-NC	2.33	127.75	124.20
30	1	601	CHL	CHA-C1A-NA	-2.33	121.06	126.40
30	62	616	CHL	CHB-C4A-NA	2.33	127.74	124.51
30	4	606	CHL	CHA-C1A-NA	-2.33	121.06	126.40
30	8	601	CHL	CHC-C1C-NC	2.33	127.74	124.20
30	8	607	CHL	CHC-C1C-NC	2.33	127.74	124.20
30	92	606	CHL	CMB-C2B-C1B	-2.33	124.88	128.46
30	6	606	CHL	CHC-C1C-NC	2.33	127.73	124.20
30	9	606	CHL	CHA-C1A-NA	-2.32	121.08	126.40
30	Z	607	CHL	CHB-C4A-NA	2.32	127.72	124.51
30	92	606	CHL	CHA-C1A-NA	-2.32	121.08	126.40
30	9	606	CHL	CHC-C1C-NC	2.32	127.73	124.20
30	Z	606	CHL	CHC-C1C-NC	2.32	127.73	124.20
30	Z2	607	CHL	CHB-C4A-NA	2.32	127.72	124.51
30	Z2	606	CHL	CHB-C4A-NA	2.32	127.72	124.51
30	72	606	CHL	CHA-C1A-NA	-2.32	121.09	126.40
30	1	606	CHL	CHC-C1C-NC	2.32	127.72	124.20
30	Z	606	CHL	CHB-C4A-NA	2.30	127.70	124.51
30	9	606	CHL	CMB-C2B-C1B	-2.30	124.92	128.46
30	72	606	CHL	CHC-C1C-NC	2.30	127.70	124.20
31	1	618	XAT	C7-C8-C9	2.30	129.10	125.53
31	1	618	XAT	O4-C5-C4	-2.30	111.65	113.38
30	12	606	CHL	CHC-C1C-NC	2.30	127.69	124.20
30	12	601	CHL	CHA-C1A-NA	-2.30	121.13	126.40
30	7	601	CHL	CHA-C1A-NA	-2.30	121.13	126.40
30	62	601	CHL	CHB-C4A-NA	2.29	127.68	124.51
30	72	601	CHL	CHA-C1A-NA	-2.29	121.16	126.40
30	7	606	CHL	CHC-C1C-NC	2.28	127.67	124.20
32	52	625	NEX	C2-C1-C6	-2.28	106.99	109.21
30	7	606	CHL	CHA-C1A-NA	-2.28	121.18	126.40
30	Z	606	CHL	CHA-C1A-NA	-2.26	121.22	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	Z2	606	CHL	CHA-C1A-NA	-2.26	121.23	126.40
21	A	809	CLA	C1-C2-C3	-2.26	122.14	126.04
30	9	607	CHL	CMB-C2B-C1B	-2.26	125.00	128.46
21	A2	809	CLA	C1-C2-C3	-2.25	122.15	126.04
30	4	608	CHL	CHB-C4A-NA	2.24	127.61	124.51
30	42	608	CHL	CHB-C4A-NA	2.24	127.61	124.51
30	7	601	CHL	CHC-C1C-NC	2.22	127.57	124.20
30	72	601	CHL	CHC-C1C-NC	2.22	127.57	124.20
30	5	607	CHL	CHB-C4A-NA	2.21	127.56	124.51
30	52	607	CHL	CHB-C4A-NA	2.21	127.56	124.51
30	1	607	CHL	C2A-C1A-CHA	2.20	127.70	123.86
30	12	607	CHL	C2A-C1A-CHA	2.19	127.69	123.86
30	6	616	CHL	C1-C2-C3	-2.18	122.27	126.04
21	92	610	CLA	C3D-C4D-ND	2.18	113.77	110.24
28	F	305	LUT	C8-C7-C6	2.18	133.32	127.20
30	4	607	CHL	CHB-C4A-NA	2.17	127.52	124.51
20	A	801	CL0	C2C-C1C-NC	2.17	112.01	109.97
21	9	610	CLA	C3D-C4D-ND	2.16	113.74	110.24
20	A2	801	CL0	C2C-C1C-NC	2.16	112.00	109.97
30	62	616	CHL	C1-C2-C3	-2.15	122.32	126.04
30	92	607	CHL	C1-C2-C3	-2.15	123.27	126.75
28	F2	305	LUT	C8-C7-C6	2.15	133.25	127.20
20	A2	801	CL0	CHA-C1A-NA	-2.15	121.48	126.40
30	9	607	CHL	C1-C2-C3	-2.15	123.28	126.75
20	A	801	CL0	CHA-C1A-NA	-2.14	121.49	126.40
21	B2	802	CLA	O2A-C1-C2	-2.14	103.01	108.64
21	52	621	CLA	CHA-C1A-NA	-2.12	121.54	126.40
30	42	607	CHL	CHB-C4A-NA	2.12	127.44	124.51
21	B	802	CLA	O2A-C1-C2	-2.12	103.06	108.64
30	4	606	CHL	C1-C2-C3	-2.11	122.39	126.04
30	42	606	CHL	C1-C2-C3	-2.11	122.40	126.04
20	A	801	CL0	C4A-NA-C1A	-2.11	105.76	106.71
21	5	621	CLA	CHA-C1A-NA	-2.10	121.58	126.40
30	52	607	CHL	CHA-C1A-NA	-2.10	121.59	126.40
30	5	607	CHL	CHA-C1A-NA	-2.10	121.60	126.40
30	6	607	CHL	C1-C2-C3	-2.09	122.44	126.04
21	Z	613	CLA	C3D-C4D-ND	2.08	113.60	110.24
20	A2	801	CL0	C4A-NA-C1A	-2.08	105.77	106.71
21	32	607	CLA	C3D-C4D-ND	2.07	113.59	110.24
21	62	609	CLA	CAA-C2A-C1A	-2.07	105.18	111.97
30	42	607	CHL	C3D-C4D-ND	2.07	113.59	110.24
30	62	608	CHL	C3D-C4D-ND	2.07	113.58	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	6	609	CLA	CAA-C2A-C1A	-2.06	105.21	111.97
21	Z2	613	CLA	C3D-C4D-ND	2.06	113.57	110.24
21	A2	806	CLA	C3D-C4D-ND	2.06	113.56	110.24
30	62	607	CHL	C1-C2-C3	-2.05	122.49	126.04
30	5	607	CHL	C3D-C4D-ND	2.05	113.56	110.24
30	62	616	CHL	C3D-C4D-ND	2.05	113.56	110.24
30	4	607	CHL	C3D-C4D-ND	2.05	113.55	110.24
21	4	604	CLA	C3D-C4D-ND	2.05	113.55	110.24
30	1	607	CHL	CHC-C1C-C2C	-2.04	118.70	126.11
21	B	814	CLA	C3D-C4D-ND	2.04	113.54	110.24
30	12	607	CHL	CHC-C1C-C2C	-2.04	118.71	126.11
21	6	617	CLA	C3D-C4D-ND	2.04	113.54	110.24
21	82	611	CLA	C3D-C4D-ND	2.04	113.54	110.24
30	6	616	CHL	C3D-C4D-ND	2.04	113.54	110.24
21	8	616	CLA	C3D-C4D-ND	2.04	113.53	110.24
21	B2	814	CLA	C3D-C4D-ND	2.04	113.53	110.24
21	B2	831	CLA	C3D-C4D-ND	2.04	113.53	110.24
21	82	616	CLA	C3D-C4D-ND	2.04	113.53	110.24
30	52	607	CHL	C3D-C4D-ND	2.04	113.53	110.24
26	B2	853	LMU	C1B-O1B-C4'	2.03	123.00	117.96
21	3	607	CLA	C3D-C4D-ND	2.03	113.53	110.24
21	8	611	CLA	C3D-C4D-ND	2.03	113.53	110.24
26	B	853	LMU	C1B-O1B-C4'	2.03	122.99	117.96
21	Z	614	CLA	C3D-C4D-ND	2.03	113.52	110.24
21	9	604	CLA	C3D-C4D-ND	2.03	113.52	110.24
21	42	604	CLA	C3D-C4D-ND	2.03	113.52	110.24
21	A	823	CLA	C3D-C4D-ND	2.03	113.52	110.24
21	K	204	CLA	C3D-C4D-ND	2.03	113.52	110.24
30	6	608	CHL	C3D-C4D-ND	2.03	113.52	110.24
21	A	820	CLA	C3D-C4D-ND	2.03	113.52	110.24
21	B	831	CLA	C3D-C4D-ND	2.03	113.52	110.24
21	A	806	CLA	C3D-C4D-ND	2.02	113.51	110.24
30	6	618	CHL	C3D-C4D-ND	2.02	113.51	110.24
21	5	609	CLA	C3D-C4D-ND	2.02	113.51	110.24
21	4	611	CLA	C3D-C4D-ND	2.02	113.51	110.24
21	42	611	CLA	C3D-C4D-ND	2.02	113.51	110.24
21	A	809	CLA	C3D-C4D-ND	2.02	113.51	110.24
21	52	609	CLA	C3D-C4D-ND	2.02	113.51	110.24
21	92	604	CLA	C3D-C4D-ND	2.02	113.51	110.24
30	82	606	CHL	C3D-C4D-ND	2.02	113.50	110.24
30	92	607	CHL	CHC-C1C-C2C	-2.02	118.79	126.11
21	52	603	CLA	C3D-C4D-ND	2.02	113.50	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	62	618	CHL	CAA-C2A-C1A	2.02	116.60	112.14
30	8	606	CHL	C3D-C4D-ND	2.01	113.50	110.24
30	12	607	CHL	C3D-C4D-ND	2.01	113.50	110.24
21	B2	833	CLA	C3D-C4D-ND	2.01	113.50	110.24
30	6	618	CHL	CAA-C2A-C1A	2.01	116.60	112.14
30	1	607	CHL	C3D-C4D-ND	2.01	113.49	110.24
30	72	606	CHL	C3D-C4D-ND	2.01	113.49	110.24
21	Z2	614	CLA	C3D-C4D-ND	2.01	113.48	110.24
30	7	606	CHL	C3D-C4D-ND	2.01	113.48	110.24
30	Z	607	CHL	CHC-C1C-C2C	-2.01	118.83	126.11
21	L	204	CLA	C3D-C4D-ND	2.01	113.48	110.24
21	L2	204	CLA	C3D-C4D-ND	2.01	113.48	110.24
30	5	608	CHL	C3D-C4D-ND	2.00	113.48	110.24
30	62	618	CHL	C3D-C4D-ND	2.00	113.48	110.24
21	92	609	CLA	C3D-C4D-ND	2.00	113.48	110.24
21	92	614	CLA	C3D-C4D-ND	2.00	113.47	110.24
30	5	607	CHL	C2A-C1A-CHA	2.00	127.36	123.86
30	52	608	CHL	C3D-C4D-ND	2.00	113.47	110.24

All (584) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
20	A	801	CL0	NA
20	A	801	CL0	NC
20	A	801	CL0	ND
20	A2	801	CL0	NA
20	A2	801	CL0	NC
20	A2	801	CL0	ND
21	A	802	CLA	ND
21	A	803	CLA	ND
21	A	804	CLA	ND
21	A	805	CLA	ND
21	A	806	CLA	ND
21	A	807	CLA	ND
21	A	808	CLA	ND
21	A	809	CLA	ND
21	A	810	CLA	ND
21	A	811	CLA	ND
21	A	812	CLA	ND
21	A	813	CLA	ND
21	A	814	CLA	ND
21	A	815	CLA	ND

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Mol	Chain	Res	Type	Atom
21	A	816	CLA	ND
21	A	817	CLA	ND
21	A	818	CLA	ND
21	A	819	CLA	ND
21	A	820	CLA	ND
21	A	821	CLA	ND
21	A	822	CLA	ND
21	A	823	CLA	ND
21	A	824	CLA	ND
21	A	825	CLA	ND
21	A	826	CLA	ND
21	A	827	CLA	ND
21	A	828	CLA	ND
21	A	829	CLA	ND
21	A	830	CLA	ND
21	A	831	CLA	ND
21	A	832	CLA	ND
21	A	833	CLA	ND
21	A	834	CLA	ND
21	A	835	CLA	ND
21	A	836	CLA	ND
21	A	837	CLA	ND
21	A	838	CLA	ND
21	A	839	CLA	ND
21	A	840	CLA	ND
21	A	841	CLA	ND
21	A	842	CLA	ND
21	A	843	CLA	ND
21	A	845	CLA	ND
21	A	854	CLA	ND
21	B	802	CLA	ND
21	B	803	CLA	ND
21	B	804	CLA	ND
21	B	805	CLA	ND
21	B	806	CLA	ND
21	B	807	CLA	ND
21	B	808	CLA	ND
21	B	809	CLA	ND
21	B	810	CLA	ND
21	B	811	CLA	ND
21	B	812	CLA	ND
21	B	813	CLA	ND

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Mol	Chain	Res	Type	Atom
21	B	814	CLA	ND
21	B	815	CLA	ND
21	B	816	CLA	ND
21	B	817	CLA	ND
21	B	818	CLA	ND
21	B	819	CLA	ND
21	B	820	CLA	ND
21	B	821	CLA	ND
21	B	822	CLA	ND
21	B	823	CLA	ND
21	B	824	CLA	ND
21	B	825	CLA	ND
21	B	826	CLA	ND
21	B	827	CLA	ND
21	B	828	CLA	ND
21	B	829	CLA	ND
21	B	830	CLA	ND
21	B	831	CLA	ND
21	B	832	CLA	ND
21	B	833	CLA	ND
21	B	834	CLA	ND
21	B	835	CLA	ND
21	B	836	CLA	ND
21	B	837	CLA	ND
21	B	838	CLA	ND
21	B	839	CLA	ND
21	B	840	CLA	ND
21	B	841	CLA	ND
21	F	301	CLA	ND
21	F	303	CLA	ND
21	F	304	CLA	ND
21	G	203	CLA	ND
21	G	204	CLA	ND
21	J	101	CLA	ND
21	L	203	CLA	ND
21	L	204	CLA	ND
21	K	201	CLA	ND
21	K	203	CLA	ND
21	K	204	CLA	ND
21	K	206	CLA	ND
21	1	602	CLA	ND
21	1	603	CLA	ND

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Mol	Chain	Res	Type	Atom
21	1	604	CLA	ND
21	1	608	CLA	ND
21	1	609	CLA	ND
21	1	610	CLA	ND
21	1	611	CLA	ND
21	1	612	CLA	ND
21	1	613	CLA	ND
21	1	614	CLA	ND
21	1	616	CLA	ND
21	3	602	CLA	ND
21	3	603	CLA	ND
21	3	604	CLA	ND
21	3	606	CLA	ND
21	3	607	CLA	ND
21	3	609	CLA	ND
21	3	610	CLA	ND
21	3	611	CLA	ND
21	3	612	CLA	ND
21	3	613	CLA	ND
21	3	614	CLA	ND
21	3	617	CLA	ND
21	3	615	CLA	ND
21	7	602	CLA	ND
21	7	603	CLA	ND
21	7	604	CLA	ND
21	7	608	CLA	ND
21	7	609	CLA	ND
21	7	610	CLA	ND
21	7	611	CLA	ND
21	7	612	CLA	ND
21	7	613	CLA	ND
21	7	614	CLA	ND
21	7	616	CLA	ND
21	7	620	CLA	ND
21	8	602	CLA	ND
21	8	603	CLA	ND
21	8	604	CLA	ND
21	8	608	CLA	ND
21	8	609	CLA	ND
21	8	610	CLA	ND
21	8	611	CLA	ND
21	8	612	CLA	ND

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Mol	Chain	Res	Type	Atom
21	8	613	CLA	ND
21	8	614	CLA	ND
21	8	616	CLA	ND
21	Z	602	CLA	ND
21	Z	603	CLA	ND
21	Z	604	CLA	ND
21	Z	608	CLA	ND
21	Z	609	CLA	ND
21	Z	610	CLA	ND
21	Z	611	CLA	ND
21	Z	612	CLA	ND
21	Z	613	CLA	ND
21	Z	614	CLA	ND
21	Z	616	CLA	ND
21	4	602	CLA	ND
21	4	603	CLA	ND
21	4	604	CLA	ND
21	4	609	CLA	ND
21	4	610	CLA	ND
21	4	611	CLA	ND
21	4	612	CLA	ND
21	4	613	CLA	ND
21	4	614	CLA	ND
21	4	616	CLA	ND
21	5	601	CLA	ND
21	5	602	CLA	ND
21	5	603	CLA	ND
21	5	604	CLA	ND
21	5	609	CLA	ND
21	5	610	CLA	ND
21	5	611	CLA	ND
21	5	612	CLA	ND
21	5	613	CLA	ND
21	5	614	CLA	ND
21	5	616	CLA	ND
21	5	617	CLA	ND
21	5	621	CLA	ND
21	6	602	CLA	ND
21	6	603	CLA	ND
21	6	604	CLA	ND
21	6	609	CLA	ND
21	6	610	CLA	ND

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Mol	Chain	Res	Type	Atom
21	6	611	CLA	ND
21	6	612	CLA	ND
21	6	613	CLA	ND
21	6	614	CLA	ND
21	6	617	CLA	ND
21	6	622	CLA	ND
21	9	601	CLA	ND
21	9	602	CLA	ND
21	9	603	CLA	ND
21	9	604	CLA	ND
21	9	609	CLA	ND
21	9	610	CLA	ND
21	9	611	CLA	ND
21	9	612	CLA	ND
21	9	613	CLA	ND
21	9	614	CLA	ND
21	A2	802	CLA	ND
21	A2	803	CLA	ND
21	A2	804	CLA	ND
21	A2	805	CLA	ND
21	A2	806	CLA	ND
21	A2	807	CLA	ND
21	A2	808	CLA	ND
21	A2	809	CLA	ND
21	A2	810	CLA	ND
21	A2	811	CLA	ND
21	A2	812	CLA	ND
21	A2	813	CLA	ND
21	A2	814	CLA	ND
21	A2	815	CLA	ND
21	A2	816	CLA	ND
21	A2	817	CLA	ND
21	A2	818	CLA	ND
21	A2	819	CLA	ND
21	A2	820	CLA	ND
21	A2	821	CLA	ND
21	A2	822	CLA	ND
21	A2	823	CLA	ND
21	A2	824	CLA	ND
21	A2	825	CLA	ND
21	A2	826	CLA	ND
21	A2	827	CLA	ND

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Mol	Chain	Res	Type	Atom
21	A2	828	CLA	ND
21	A2	829	CLA	ND
21	A2	830	CLA	ND
21	A2	831	CLA	ND
21	A2	832	CLA	ND
21	A2	833	CLA	ND
21	A2	834	CLA	ND
21	A2	835	CLA	ND
21	A2	836	CLA	ND
21	A2	837	CLA	ND
21	A2	838	CLA	ND
21	A2	839	CLA	ND
21	A2	840	CLA	ND
21	A2	841	CLA	ND
21	A2	842	CLA	ND
21	A2	843	CLA	ND
21	A2	845	CLA	ND
21	A2	854	CLA	ND
21	B2	802	CLA	ND
21	B2	803	CLA	ND
21	B2	804	CLA	ND
21	B2	805	CLA	ND
21	B2	806	CLA	ND
21	B2	807	CLA	ND
21	B2	808	CLA	ND
21	B2	809	CLA	ND
21	B2	810	CLA	ND
21	B2	811	CLA	ND
21	B2	812	CLA	ND
21	B2	813	CLA	ND
21	B2	814	CLA	ND
21	B2	815	CLA	ND
21	B2	816	CLA	ND
21	B2	817	CLA	ND
21	B2	818	CLA	ND
21	B2	819	CLA	ND
21	B2	820	CLA	ND
21	B2	821	CLA	ND
21	B2	822	CLA	ND
21	B2	823	CLA	ND
21	B2	824	CLA	ND
21	B2	825	CLA	ND

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Mol	Chain	Res	Type	Atom
21	B2	826	CLA	ND
21	B2	827	CLA	ND
21	B2	828	CLA	ND
21	B2	829	CLA	ND
21	B2	830	CLA	ND
21	B2	831	CLA	ND
21	B2	832	CLA	ND
21	B2	833	CLA	ND
21	B2	834	CLA	ND
21	B2	835	CLA	ND
21	B2	836	CLA	ND
21	B2	837	CLA	ND
21	B2	838	CLA	ND
21	B2	839	CLA	ND
21	B2	840	CLA	ND
21	B2	841	CLA	ND
21	F2	301	CLA	ND
21	F2	303	CLA	ND
21	F2	304	CLA	ND
21	G2	203	CLA	ND
21	G2	204	CLA	ND
21	J2	101	CLA	ND
21	L2	203	CLA	ND
21	L2	204	CLA	ND
21	K2	201	CLA	ND
21	K2	203	CLA	ND
21	K2	204	CLA	ND
21	K2	206	CLA	ND
21	12	602	CLA	ND
21	12	603	CLA	ND
21	12	604	CLA	ND
21	12	608	CLA	ND
21	12	609	CLA	ND
21	12	610	CLA	ND
21	12	611	CLA	ND
21	12	612	CLA	ND
21	12	613	CLA	ND
21	12	614	CLA	ND
21	12	616	CLA	ND
21	32	602	CLA	ND
21	32	603	CLA	ND
21	32	604	CLA	ND

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Mol	Chain	Res	Type	Atom
21	32	606	CLA	ND
21	32	607	CLA	ND
21	32	609	CLA	ND
21	32	610	CLA	ND
21	32	611	CLA	ND
21	32	612	CLA	ND
21	32	613	CLA	ND
21	32	614	CLA	ND
21	32	617	CLA	ND
21	32	615	CLA	ND
21	72	602	CLA	ND
21	72	603	CLA	ND
21	72	604	CLA	ND
21	72	608	CLA	ND
21	72	609	CLA	ND
21	72	610	CLA	ND
21	72	611	CLA	ND
21	72	612	CLA	ND
21	72	613	CLA	ND
21	72	614	CLA	ND
21	72	616	CLA	ND
21	72	620	CLA	ND
21	82	602	CLA	ND
21	82	603	CLA	ND
21	82	604	CLA	ND
21	82	608	CLA	ND
21	82	609	CLA	ND
21	82	610	CLA	ND
21	82	611	CLA	ND
21	82	612	CLA	ND
21	82	613	CLA	ND
21	82	614	CLA	ND
21	82	616	CLA	ND
21	Z2	602	CLA	ND
21	Z2	603	CLA	ND
21	Z2	604	CLA	ND
21	Z2	608	CLA	ND
21	Z2	609	CLA	ND
21	Z2	610	CLA	ND
21	Z2	611	CLA	ND
21	Z2	612	CLA	ND
21	Z2	613	CLA	ND

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Mol	Chain	Res	Type	Atom
21	Z2	614	CLA	ND
21	Z2	616	CLA	ND
21	42	602	CLA	ND
21	42	603	CLA	ND
21	42	604	CLA	ND
21	42	609	CLA	ND
21	42	610	CLA	ND
21	42	611	CLA	ND
21	42	612	CLA	ND
21	42	613	CLA	ND
21	42	614	CLA	ND
21	42	616	CLA	ND
21	52	601	CLA	ND
21	52	602	CLA	ND
21	52	603	CLA	ND
21	52	604	CLA	ND
21	52	609	CLA	ND
21	52	610	CLA	ND
21	52	611	CLA	ND
21	52	612	CLA	ND
21	52	613	CLA	ND
21	52	614	CLA	ND
21	52	616	CLA	ND
21	52	617	CLA	ND
21	52	621	CLA	ND
21	62	602	CLA	ND
21	62	603	CLA	ND
21	62	604	CLA	ND
21	62	609	CLA	ND
21	62	610	CLA	ND
21	62	611	CLA	ND
21	62	612	CLA	ND
21	62	613	CLA	ND
21	62	614	CLA	ND
21	62	617	CLA	ND
21	62	622	CLA	ND
21	92	601	CLA	ND
21	92	602	CLA	ND
21	92	603	CLA	ND
21	92	604	CLA	ND
21	92	609	CLA	ND
21	92	610	CLA	ND

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Mol	Chain	Res	Type	Atom
21	92	611	CLA	ND
21	92	612	CLA	ND
21	92	613	CLA	ND
21	92	614	CLA	ND
30	1	601	CHL	NA
30	1	601	CHL	NC
30	1	601	CHL	ND
30	1	606	CHL	NA
30	1	606	CHL	NC
30	1	606	CHL	ND
30	1	607	CHL	NA
30	1	607	CHL	NC
30	1	607	CHL	ND
30	3	608	CHL	NA
30	3	608	CHL	NC
30	3	608	CHL	ND
30	7	601	CHL	NA
30	7	601	CHL	NC
30	7	601	CHL	ND
30	7	606	CHL	NA
30	7	606	CHL	NC
30	7	606	CHL	ND
30	7	607	CHL	NA
30	7	607	CHL	NC
30	7	607	CHL	ND
30	8	601	CHL	NA
30	8	601	CHL	NC
30	8	601	CHL	ND
30	8	606	CHL	NA
30	8	606	CHL	NC
30	8	606	CHL	ND
30	8	607	CHL	NA
30	8	607	CHL	NC
30	8	607	CHL	ND
30	Z	601	CHL	NA
30	Z	601	CHL	NC
30	Z	601	CHL	ND
30	Z	606	CHL	NA
30	Z	606	CHL	NC
30	Z	606	CHL	ND
30	Z	607	CHL	NA
30	Z	607	CHL	NC

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Mol	Chain	Res	Type	Atom
30	Z	607	CHL	ND
30	4	601	CHL	NA
30	4	601	CHL	NC
30	4	601	CHL	ND
30	4	606	CHL	NA
30	4	606	CHL	NC
30	4	606	CHL	ND
30	4	607	CHL	NA
30	4	607	CHL	NC
30	4	607	CHL	ND
30	4	608	CHL	NA
30	4	608	CHL	NC
30	4	608	CHL	ND
30	4	618	CHL	NA
30	4	618	CHL	NC
30	4	618	CHL	ND
30	5	606	CHL	NA
30	5	606	CHL	NC
30	5	606	CHL	ND
30	5	607	CHL	NA
30	5	607	CHL	NC
30	5	607	CHL	ND
30	5	608	CHL	NA
30	5	608	CHL	NC
30	5	608	CHL	ND
30	5	618	CHL	NA
30	5	618	CHL	NC
30	5	618	CHL	ND
30	6	601	CHL	NA
30	6	601	CHL	NC
30	6	601	CHL	ND
30	6	606	CHL	NA
30	6	606	CHL	NC
30	6	606	CHL	ND
30	6	607	CHL	NA
30	6	607	CHL	NC
30	6	607	CHL	ND
30	6	608	CHL	NA
30	6	608	CHL	NC
30	6	608	CHL	ND
30	6	616	CHL	NA
30	6	616	CHL	NC

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Mol	Chain	Res	Type	Atom
30	6	616	CHL	ND
30	6	618	CHL	NA
30	6	618	CHL	NC
30	6	618	CHL	ND
30	9	606	CHL	NA
30	9	606	CHL	NC
30	9	606	CHL	ND
30	9	607	CHL	NA
30	9	607	CHL	NC
30	9	607	CHL	ND
30	12	601	CHL	NA
30	12	601	CHL	NC
30	12	601	CHL	ND
30	12	606	CHL	NA
30	12	606	CHL	NC
30	12	606	CHL	ND
30	12	607	CHL	NA
30	12	607	CHL	NC
30	12	607	CHL	ND
30	32	608	CHL	NA
30	32	608	CHL	NC
30	32	608	CHL	ND
30	72	601	CHL	NA
30	72	601	CHL	NC
30	72	601	CHL	ND
30	72	606	CHL	NA
30	72	606	CHL	NC
30	72	606	CHL	ND
30	72	607	CHL	NA
30	72	607	CHL	NC
30	72	607	CHL	ND
30	82	601	CHL	NA
30	82	601	CHL	NC
30	82	601	CHL	ND
30	82	606	CHL	NA
30	82	606	CHL	NC
30	82	606	CHL	ND
30	82	607	CHL	NA
30	82	607	CHL	NC
30	82	607	CHL	ND
30	Z2	601	CHL	NA
30	Z2	601	CHL	NC

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Mol	Chain	Res	Type	Atom
30	Z2	601	CHL	ND
30	Z2	606	CHL	NA
30	Z2	606	CHL	NC
30	Z2	606	CHL	ND
30	Z2	607	CHL	NA
30	Z2	607	CHL	NC
30	Z2	607	CHL	ND
30	42	601	CHL	NA
30	42	601	CHL	NC
30	42	601	CHL	ND
30	42	606	CHL	NA
30	42	606	CHL	NC
30	42	606	CHL	ND
30	42	607	CHL	NA
30	42	607	CHL	NC
30	42	607	CHL	ND
30	42	608	CHL	NA
30	42	608	CHL	NC
30	42	608	CHL	ND
30	42	618	CHL	NA
30	42	618	CHL	NC
30	42	618	CHL	ND
30	52	606	CHL	NA
30	52	606	CHL	NC
30	52	606	CHL	ND
30	52	607	CHL	NA
30	52	607	CHL	NC
30	52	607	CHL	ND
30	52	608	CHL	NA
30	52	608	CHL	NC
30	52	608	CHL	ND
30	52	618	CHL	NA
30	52	618	CHL	NC
30	52	618	CHL	ND
30	62	601	CHL	NA
30	62	601	CHL	NC
30	62	601	CHL	ND
30	62	606	CHL	NA
30	62	606	CHL	NC
30	62	606	CHL	ND
30	62	607	CHL	NA
30	62	607	CHL	NC

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Mol	Chain	Res	Type	Atom
30	62	607	CHL	ND
30	62	608	CHL	NA
30	62	608	CHL	NC
30	62	608	CHL	ND
30	62	616	CHL	NA
30	62	616	CHL	NC
30	62	616	CHL	ND
30	62	618	CHL	NA
30	62	618	CHL	NC
30	62	618	CHL	ND
30	92	606	CHL	NA
30	92	606	CHL	NC
30	92	606	CHL	ND
30	92	607	CHL	NA
30	92	607	CHL	NC
30	92	607	CHL	ND
31	5	624	XAT	C26
31	52	624	XAT	C26

All (2525) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
21	A	806	CLA	CHA-CBD-CGD-O1D
21	A	806	CLA	CHA-CBD-CGD-O2D
21	A	806	CLA	CAD-CBD-CGD-O1D
21	A	806	CLA	CAD-CBD-CGD-O2D
21	A	806	CLA	C4-C3-C5-C6
21	A	809	CLA	CHA-CBD-CGD-O1D
21	A	809	CLA	CHA-CBD-CGD-O2D
21	A	816	CLA	O2A-C1-C2-C3
21	A	825	CLA	CHA-CBD-CGD-O1D
21	A	825	CLA	CHA-CBD-CGD-O2D
21	A	835	CLA	CHA-CBD-CGD-O1D
21	A	835	CLA	CHA-CBD-CGD-O2D
21	A	837	CLA	CHA-CBD-CGD-O1D
21	A	837	CLA	CHA-CBD-CGD-O2D
21	A	840	CLA	CHA-CBD-CGD-O1D
21	A	840	CLA	CHA-CBD-CGD-O2D
21	A	841	CLA	CHA-CBD-CGD-O1D
21	A	841	CLA	CHA-CBD-CGD-O2D
21	A	843	CLA	O2A-C1-C2-C3
21	A	845	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
21	A	845	CLA	CHA-CBD-CGD-O2D
21	A	845	CLA	CAD-CBD-CGD-O1D
21	A	845	CLA	CAD-CBD-CGD-O2D
21	B	804	CLA	CHA-CBD-CGD-O2D
21	B	808	CLA	CHA-CBD-CGD-O1D
21	B	808	CLA	CHA-CBD-CGD-O2D
21	B	822	CLA	C2-C3-C5-C6
21	B	822	CLA	C4-C3-C5-C6
21	B	825	CLA	CHA-CBD-CGD-O1D
21	B	825	CLA	CHA-CBD-CGD-O2D
21	B	833	CLA	CHA-CBD-CGD-O1D
21	B	833	CLA	CHA-CBD-CGD-O2D
21	B	840	CLA	C4-C3-C5-C6
21	F	304	CLA	C1A-C2A-CAA-CBA
21	F	304	CLA	C2-C1-O2A-CGA
21	F	304	CLA	CHA-CBD-CGD-O1D
21	F	304	CLA	CHA-CBD-CGD-O2D
21	G	204	CLA	CHA-CBD-CGD-O1D
21	G	204	CLA	CHA-CBD-CGD-O2D
21	J	101	CLA	CHA-CBD-CGD-O1D
21	J	101	CLA	CHA-CBD-CGD-O2D
21	J	101	CLA	C2-C3-C5-C6
21	J	101	CLA	C4-C3-C5-C6
21	L	203	CLA	CHA-CBD-CGD-O1D
21	K	203	CLA	CHA-CBD-CGD-O1D
21	K	203	CLA	CHA-CBD-CGD-O2D
21	1	603	CLA	C2-C3-C5-C6
21	1	603	CLA	C4-C3-C5-C6
21	7	610	CLA	C1A-C2A-CAA-CBA
21	7	610	CLA	C3A-C2A-CAA-CBA
21	4	610	CLA	C4-C3-C5-C6
21	4	613	CLA	C2-C3-C5-C6
21	4	613	CLA	C4-C3-C5-C6
21	5	603	CLA	CHA-CBD-CGD-O2D
21	5	611	CLA	C2-C3-C5-C6
21	5	611	CLA	C4-C3-C5-C6
21	5	617	CLA	CHA-CBD-CGD-O1D
21	5	617	CLA	CHA-CBD-CGD-O2D
21	5	617	CLA	C2-C3-C5-C6
21	5	617	CLA	C4-C3-C5-C6
21	9	609	CLA	C4-C3-C5-C6
21	A2	806	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
21	A2	806	CLA	CHA-CBD-CGD-O2D
21	A2	806	CLA	CAD-CBD-CGD-O1D
21	A2	806	CLA	CAD-CBD-CGD-O2D
21	A2	806	CLA	C4-C3-C5-C6
21	A2	809	CLA	CHA-CBD-CGD-O1D
21	A2	809	CLA	CHA-CBD-CGD-O2D
21	A2	816	CLA	O2A-C1-C2-C3
21	A2	825	CLA	CHA-CBD-CGD-O1D
21	A2	825	CLA	CHA-CBD-CGD-O2D
21	A2	835	CLA	CHA-CBD-CGD-O1D
21	A2	835	CLA	CHA-CBD-CGD-O2D
21	A2	837	CLA	CHA-CBD-CGD-O1D
21	A2	837	CLA	CHA-CBD-CGD-O2D
21	A2	840	CLA	CHA-CBD-CGD-O1D
21	A2	840	CLA	CHA-CBD-CGD-O2D
21	A2	841	CLA	CHA-CBD-CGD-O1D
21	A2	841	CLA	CHA-CBD-CGD-O2D
21	A2	843	CLA	O2A-C1-C2-C3
21	A2	845	CLA	CHA-CBD-CGD-O1D
21	A2	845	CLA	CHA-CBD-CGD-O2D
21	A2	845	CLA	CAD-CBD-CGD-O1D
21	A2	845	CLA	CAD-CBD-CGD-O2D
21	B2	804	CLA	CHA-CBD-CGD-O2D
21	B2	808	CLA	CHA-CBD-CGD-O1D
21	B2	808	CLA	CHA-CBD-CGD-O2D
21	B2	822	CLA	C2-C3-C5-C6
21	B2	822	CLA	C4-C3-C5-C6
21	B2	823	CLA	CHA-CBD-CGD-O1D
21	B2	825	CLA	CHA-CBD-CGD-O1D
21	B2	825	CLA	CHA-CBD-CGD-O2D
21	B2	833	CLA	CHA-CBD-CGD-O1D
21	B2	833	CLA	CHA-CBD-CGD-O2D
21	B2	840	CLA	C4-C3-C5-C6
21	F2	304	CLA	C1A-C2A-CAA-CBA
21	F2	304	CLA	C2-C1-O2A-CGA
21	F2	304	CLA	CHA-CBD-CGD-O1D
21	F2	304	CLA	CHA-CBD-CGD-O2D
21	G2	204	CLA	CHA-CBD-CGD-O1D
21	G2	204	CLA	CHA-CBD-CGD-O2D
21	J2	101	CLA	CHA-CBD-CGD-O1D
21	J2	101	CLA	CHA-CBD-CGD-O2D
21	J2	101	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
21	J2	101	CLA	C4-C3-C5-C6
21	L2	203	CLA	CHA-CBD-CGD-O1D
21	K2	203	CLA	CHA-CBD-CGD-O1D
21	K2	203	CLA	CHA-CBD-CGD-O2D
21	12	603	CLA	C2-C3-C5-C6
21	12	603	CLA	C4-C3-C5-C6
21	72	610	CLA	C1A-C2A-CAA-CBA
21	72	610	CLA	C3A-C2A-CAA-CBA
21	42	610	CLA	C4-C3-C5-C6
21	42	613	CLA	C2-C3-C5-C6
21	42	613	CLA	C4-C3-C5-C6
21	52	603	CLA	CHA-CBD-CGD-O2D
21	52	611	CLA	C2-C3-C5-C6
21	52	611	CLA	C4-C3-C5-C6
21	52	617	CLA	CHA-CBD-CGD-O1D
21	52	617	CLA	CHA-CBD-CGD-O2D
21	52	617	CLA	C2-C3-C5-C6
21	52	617	CLA	C4-C3-C5-C6
21	92	609	CLA	C4-C3-C5-C6
23	A	846	LHG	C3-O3-P-O5
23	A	846	LHG	C4-O6-P-O5
23	3	721	LHG	C2-C3-O3-P
23	3	721	LHG	C3-O3-P-O4
23	3	721	LHG	C4-O6-P-O5
23	3	623	LHG	O2-C2-C3-O3
23	3	623	LHG	C3-O3-P-O5
23	3	623	LHG	O6-C4-C5-O7
23	7	625	LHG	C1-C2-C3-O3
23	7	625	LHG	C3-O3-P-O4
23	7	625	LHG	C3-O3-P-O5
23	7	625	LHG	C3-O3-P-O6
23	8	620	LHG	C3-O3-P-O5
23	8	620	LHG	C4-O6-P-O3
23	8	620	LHG	C4-O6-P-O4
23	4	622	LHG	C2-C3-O3-P
23	4	622	LHG	C3-O3-P-O4
23	4	623	LHG	C3-O3-P-O4
23	4	623	LHG	C3-O3-P-O5
23	4	623	LHG	C4-O6-P-O3
23	4	623	LHG	C4-O6-P-O4
23	4	623	LHG	C4-O6-P-O5
23	5	623	LHG	C3-O3-P-O5

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Mol	Chain	Res	Type	Atoms
23	5	623	LHG	C3-O3-P-O6
23	5	623	LHG	C4-O6-P-O3
23	5	623	LHG	C4-O6-P-O4
23	5	623	LHG	C4-O6-P-O5
23	6	629	LHG	C1-C2-C3-O3
23	6	629	LHG	C4-O6-P-O4
23	6	629	LHG	C4-O6-P-O5
23	9	622	LHG	C1-C2-C3-O3
23	9	622	LHG	C4-O6-P-O4
23	A2	846	LHG	C3-O3-P-O5
23	A2	846	LHG	C4-O6-P-O5
23	32	721	LHG	C2-C3-O3-P
23	32	721	LHG	C3-O3-P-O4
23	32	721	LHG	C4-O6-P-O5
23	32	623	LHG	O2-C2-C3-O3
23	32	623	LHG	C3-O3-P-O5
23	32	623	LHG	O6-C4-C5-O7
23	72	625	LHG	C1-C2-C3-O3
23	72	625	LHG	C3-O3-P-O4
23	72	625	LHG	C3-O3-P-O5
23	72	625	LHG	C3-O3-P-O6
23	82	620	LHG	C3-O3-P-O5
23	82	620	LHG	C4-O6-P-O3
23	82	620	LHG	C4-O6-P-O4
23	42	622	LHG	C2-C3-O3-P
23	42	622	LHG	C3-O3-P-O4
23	42	623	LHG	C3-O3-P-O4
23	42	623	LHG	C3-O3-P-O5
23	42	623	LHG	C4-O6-P-O3
23	42	623	LHG	C4-O6-P-O4
23	42	623	LHG	C4-O6-P-O5
23	52	623	LHG	C3-O3-P-O5
23	52	623	LHG	C3-O3-P-O6
23	52	623	LHG	C4-O6-P-O3
23	52	623	LHG	C4-O6-P-O4
23	52	623	LHG	C4-O6-P-O5
23	62	629	LHG	C1-C2-C3-O3
23	62	629	LHG	C4-O6-P-O4
23	62	629	LHG	C4-O6-P-O5
23	92	622	LHG	C1-C2-C3-O3
23	92	622	LHG	C4-O6-P-O4
24	A	848	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
24	A	851	BCR	C23-C24-C25-C26
24	A	851	BCR	C23-C24-C25-C30
24	B	847	BCR	C23-C24-C25-C30
24	J	102	BCR	C23-C24-C25-C26
24	L	201	BCR	C1-C6-C7-C8
24	3	620	BCR	C1-C6-C7-C8
24	3	620	BCR	C5-C6-C7-C8
24	3	718	BCR	C23-C24-C25-C30
24	8	619	BCR	C1-C6-C7-C8
24	8	619	BCR	C5-C6-C7-C8
24	9	623	BCR	C23-C24-C25-C26
24	A2	848	BCR	C1-C6-C7-C8
24	A2	851	BCR	C23-C24-C25-C26
24	A2	851	BCR	C23-C24-C25-C30
24	B2	847	BCR	C23-C24-C25-C30
24	J2	102	BCR	C23-C24-C25-C26
24	L2	201	BCR	C1-C6-C7-C8
24	32	620	BCR	C1-C6-C7-C8
24	32	620	BCR	C5-C6-C7-C8
24	32	718	BCR	C23-C24-C25-C30
24	82	619	BCR	C1-C6-C7-C8
24	82	619	BCR	C5-C6-C7-C8
24	92	623	BCR	C23-C24-C25-C26
26	A	858	LMU	O5'-C1'-O1'-C1
26	A	865	LMU	C2'-C1'-O1'-C1
26	A	865	LMU	O5'-C1'-O1'-C1
26	A	864	LMU	O5'-C1'-O1'-C1
26	B	853	LMU	O5'-C1'-O1'-C1
26	G	206	LMU	C2'-C1'-O1'-C1
26	G	206	LMU	O5'-C1'-O1'-C1
26	1	622	LMU	C2'-C1'-O1'-C1
26	1	622	LMU	O5'-C1'-O1'-C1
26	1	622	LMU	C2-C1-O1'-C1'
26	1	627	LMU	C2'-C1'-O1'-C1
26	1	627	LMU	O5'-C1'-O1'-C1
26	1	627	LMU	C2-C1-O1'-C1'
26	7	627	LMU	C2'-C1'-O1'-C1
26	7	627	LMU	O5'-C1'-O1'-C1
26	7	628	LMU	C2'-C1'-O1'-C1
26	7	628	LMU	O5'-C1'-O1'-C1
26	7	628	LMU	C2-C1-O1'-C1'
26	7	629	LMU	C2'-C1'-O1'-C1

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Mol	Chain	Res	Type	Atoms
26	7	629	LMU	O5'-C1'-O1'-C1
26	8	628	LMU	C2'-C1'-O1'-C1
26	8	628	LMU	O5'-C1'-O1'-C1
26	Z	622	LMU	C2-C1-O1'-C1'
26	Z	621	LMU	C2'-C1'-O1'-C1
26	Z	621	LMU	O5'-C1'-O1'-C1
26	4	625	LMU	C2'-C1'-O1'-C1
26	4	625	LMU	O5'-C1'-O1'-C1
26	5	627	LMU	C2-C1-O1'-C1'
26	6	632	LMU	C2'-C1'-O1'-C1
26	6	632	LMU	O5'-C1'-O1'-C1
26	6	632	LMU	C2-C1-O1'-C1'
26	6	628	LMU	C2'-C1'-O1'-C1
26	6	628	LMU	O5'-C1'-O1'-C1
26	6	631	LMU	C2'-C1'-O1'-C1
26	6	631	LMU	O5'-C1'-O1'-C1
26	A2	858	LMU	O5'-C1'-O1'-C1
26	A2	865	LMU	C2'-C1'-O1'-C1
26	A2	865	LMU	O5'-C1'-O1'-C1
26	A2	864	LMU	O5'-C1'-O1'-C1
26	B2	853	LMU	O5'-C1'-O1'-C1
26	G2	206	LMU	C2'-C1'-O1'-C1
26	G2	206	LMU	O5'-C1'-O1'-C1
26	12	622	LMU	C2'-C1'-O1'-C1
26	12	622	LMU	O5'-C1'-O1'-C1
26	12	622	LMU	C2-C1-O1'-C1'
26	12	627	LMU	C2'-C1'-O1'-C1
26	12	627	LMU	O5'-C1'-O1'-C1
26	12	627	LMU	C2-C1-O1'-C1'
26	72	627	LMU	C2'-C1'-O1'-C1
26	72	627	LMU	O5'-C1'-O1'-C1
26	72	628	LMU	C2'-C1'-O1'-C1
26	72	628	LMU	O5'-C1'-O1'-C1
26	72	628	LMU	C2-C1-O1'-C1'
26	72	629	LMU	C2'-C1'-O1'-C1
26	72	629	LMU	O5'-C1'-O1'-C1
26	82	628	LMU	C2'-C1'-O1'-C1
26	82	628	LMU	O5'-C1'-O1'-C1
26	Z2	622	LMU	C2-C1-O1'-C1'
26	Z2	621	LMU	C2'-C1'-O1'-C1
26	Z2	621	LMU	O5'-C1'-O1'-C1
26	42	625	LMU	C2'-C1'-O1'-C1

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Mol	Chain	Res	Type	Atoms
26	42	625	LMU	O5'-C1'-O1'-C1
26	52	627	LMU	C2-C1-O1'-C1'
26	62	632	LMU	C2'-C1'-O1'-C1
26	62	632	LMU	O5'-C1'-O1'-C1
26	62	632	LMU	C2-C1-O1'-C1'
26	62	628	LMU	C2'-C1'-O1'-C1
26	62	628	LMU	O5'-C1'-O1'-C1
26	62	631	LMU	C2'-C1'-O1'-C1
26	62	631	LMU	O5'-C1'-O1'-C1
27	A	859	LMG	C2-C1-O1-C7
27	A	859	LMG	O6-C1-O1-C7
27	A	860	LMG	C2-C1-O1-C7
27	A	860	LMG	O6-C1-O1-C7
27	B	854	LMG	C2-C1-O1-C7
27	B	854	LMG	O6-C1-O1-C7
27	7	626	LMG	C2-C1-O1-C7
27	7	626	LMG	O6-C1-O1-C7
27	8	626	LMG	C2-C1-O1-C7
27	8	626	LMG	O6-C1-O1-C7
27	8	629	LMG	C2-C1-O1-C7
27	8	629	LMG	O6-C1-O1-C7
27	4	624	LMG	O6-C1-O1-C7
27	9	620	LMG	C2-C1-O1-C7
27	9	620	LMG	O6-C1-O1-C7
27	A2	859	LMG	C2-C1-O1-C7
27	A2	859	LMG	O6-C1-O1-C7
27	A2	860	LMG	C2-C1-O1-C7
27	A2	860	LMG	O6-C1-O1-C7
27	B2	854	LMG	C2-C1-O1-C7
27	B2	854	LMG	O6-C1-O1-C7
27	72	626	LMG	C2-C1-O1-C7
27	72	626	LMG	O6-C1-O1-C7
27	82	626	LMG	C2-C1-O1-C7
27	82	626	LMG	O6-C1-O1-C7
27	82	629	LMG	C2-C1-O1-C7
27	82	629	LMG	O6-C1-O1-C7
27	42	624	LMG	O6-C1-O1-C7
27	92	620	LMG	C2-C1-O1-C7
27	92	620	LMG	O6-C1-O1-C7
28	A	856	LUT	C5-C6-C7-C8
28	A	856	LUT	C21-C26-C27-C28
28	A	856	LUT	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
28	F	305	LUT	C1-C6-C7-C8
28	F	305	LUT	C5-C6-C7-C8
28	F	305	LUT	C25-C26-C27-C28
28	3	621	LUT	C1-C6-C7-C8
28	3	622	LUT	C1-C6-C7-C8
28	7	624	LUT	C21-C26-C27-C28
28	7	624	LUT	C25-C26-C27-C28
28	7	624	LUT	C27-C28-C29-C30
28	7	624	LUT	C27-C28-C29-C39
28	5	620	LUT	C1-C6-C7-C8
28	6	621	LUT	C1-C6-C7-C8
28	A2	856	LUT	C1-C6-C7-C8
28	A2	856	LUT	C5-C6-C7-C8
28	A2	856	LUT	C21-C26-C27-C28
28	A2	856	LUT	C25-C26-C27-C28
28	F2	305	LUT	C1-C6-C7-C8
28	F2	305	LUT	C5-C6-C7-C8
28	F2	305	LUT	C25-C26-C27-C28
28	32	621	LUT	C1-C6-C7-C8
28	32	622	LUT	C1-C6-C7-C8
28	72	624	LUT	C21-C26-C27-C28
28	72	624	LUT	C25-C26-C27-C28
28	72	624	LUT	C27-C28-C29-C30
28	72	624	LUT	C27-C28-C29-C39
28	52	620	LUT	C1-C6-C7-C8
28	62	621	LUT	C1-C6-C7-C8
29	B	850	DGD	C2D-C1D-O3G-C3G
29	B	850	DGD	O6D-C1D-O3G-C3G
29	B2	850	DGD	C2D-C1D-O3G-C3G
29	B2	850	DGD	O6D-C1D-O3G-C3G
30	1	601	CHL	C2-C3-C5-C6
30	1	601	CHL	C4-C3-C5-C6
30	8	601	CHL	CHA-CBD-CGD-O1D
30	8	601	CHL	CHA-CBD-CGD-O2D
30	8	601	CHL	CAD-CBD-CGD-O1D
30	8	607	CHL	C2-C3-C5-C6
30	8	607	CHL	C4-C3-C5-C6
30	Z	606	CHL	C1A-C2A-CAA-CBA
30	6	616	CHL	CHA-CBD-CGD-O1D
30	6	616	CHL	CHA-CBD-CGD-O2D
30	12	601	CHL	C2-C3-C5-C6
30	12	601	CHL	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
30	82	601	CHL	CHA-CBD-CGD-O1D
30	82	601	CHL	CHA-CBD-CGD-O2D
30	82	601	CHL	CAD-CBD-CGD-O1D
30	82	607	CHL	C2-C3-C5-C6
30	82	607	CHL	C4-C3-C5-C6
30	Z2	606	CHL	C1A-C2A-CAA-CBA
30	62	616	CHL	CHA-CBD-CGD-O1D
30	62	616	CHL	CHA-CBD-CGD-O2D
26	A	858	LMU	O5B-C1B-O1B-C4'
26	A2	858	LMU	O5B-C1B-O1B-C4'
26	A	858	LMU	C2B-C1B-O1B-C4'
26	A2	858	LMU	C2B-C1B-O1B-C4'
30	9	607	CHL	CBD-CGD-O2D-CED
26	8	627	LMU	O5B-C1B-O1B-C4'
26	82	627	LMU	O5B-C1B-O1B-C4'
21	B	806	CLA	C3-C5-C6-C7
21	B2	806	CLA	C3-C5-C6-C7
26	A	863	LMU	O5B-C1B-O1B-C4'
26	A2	863	LMU	O5B-C1B-O1B-C4'
26	A	863	LMU	C2B-C1B-O1B-C4'
26	A2	863	LMU	C2B-C1B-O1B-C4'
21	L	203	CLA	C4-C3-C5-C6
21	L2	203	CLA	C4-C3-C5-C6
21	A	806	CLA	C2-C3-C5-C6
21	B	840	CLA	C2-C3-C5-C6
21	4	610	CLA	C2-C3-C5-C6
21	A2	806	CLA	C2-C3-C5-C6
21	B2	840	CLA	C2-C3-C5-C6
21	42	610	CLA	C2-C3-C5-C6
21	B	839	CLA	C2A-CAA-CBA-CGA
21	5	603	CLA	C2A-CAA-CBA-CGA
21	B2	839	CLA	C2A-CAA-CBA-CGA
21	52	603	CLA	C2A-CAA-CBA-CGA
26	8	627	LMU	C2B-C1B-O1B-C4'
26	82	627	LMU	C2B-C1B-O1B-C4'
26	B	853	LMU	C2B-C1B-O1B-C4'
26	B2	853	LMU	C2B-C1B-O1B-C4'
21	5	621	CLA	C2C-C3C-CAC-CBC
21	52	621	CLA	C2C-C3C-CAC-CBC
23	3	721	LHG	O2-C2-C3-O3
23	7	625	LHG	O2-C2-C3-O3
23	4	623	LHG	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
23	6	629	LHG	O2-C2-C3-O3
23	9	622	LHG	O2-C2-C3-O3
23	32	721	LHG	O2-C2-C3-O3
23	72	625	LHG	O2-C2-C3-O3
23	42	623	LHG	O2-C2-C3-O3
23	62	629	LHG	O2-C2-C3-O3
23	92	622	LHG	O2-C2-C3-O3
21	B	808	CLA	C3-C5-C6-C7
21	B2	808	CLA	C3-C5-C6-C7
21	A	825	CLA	C3-C5-C6-C7
21	A2	825	CLA	C3-C5-C6-C7
26	8	627	LMU	C5'-C4'-O1B-C1B
26	82	627	LMU	C5'-C4'-O1B-C1B
23	6	629	LHG	C2-C3-O3-P
23	62	629	LHG	C2-C3-O3-P
21	A	829	CLA	C4-C3-C5-C6
21	B	833	CLA	C4-C3-C5-C6
21	7	612	CLA	C4-C3-C5-C6
21	8	612	CLA	C4-C3-C5-C6
21	Z	603	CLA	C4-C3-C5-C6
21	A2	829	CLA	C4-C3-C5-C6
21	B2	833	CLA	C4-C3-C5-C6
21	72	612	CLA	C4-C3-C5-C6
21	82	612	CLA	C4-C3-C5-C6
21	Z2	603	CLA	C4-C3-C5-C6
21	A	829	CLA	C2-C3-C5-C6
21	B	833	CLA	C2-C3-C5-C6
21	L	203	CLA	C2-C3-C5-C6
21	7	612	CLA	C2-C3-C5-C6
21	8	612	CLA	C2-C3-C5-C6
21	Z	603	CLA	C2-C3-C5-C6
21	A2	829	CLA	C2-C3-C5-C6
21	B2	833	CLA	C2-C3-C5-C6
21	L2	203	CLA	C2-C3-C5-C6
21	72	612	CLA	C2-C3-C5-C6
21	82	612	CLA	C2-C3-C5-C6
21	Z2	603	CLA	C2-C3-C5-C6
21	A	830	CLA	C2A-CAA-CBA-CGA
21	A2	830	CLA	C2A-CAA-CBA-CGA
26	A	861	LMU	O5'-C1'-O1'-C1
26	A2	861	LMU	O5'-C1'-O1'-C1
23	1	620	LHG	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
23	3	623	LHG	C1-C2-C3-O3
23	12	620	LHG	C1-C2-C3-O3
23	32	623	LHG	C1-C2-C3-O3
23	1	620	LHG	O2-C2-C3-O3
23	12	620	LHG	O2-C2-C3-O3
26	A	858	LMU	C2'-C1'-O1'-C1
26	B	853	LMU	C2'-C1'-O1'-C1
26	A2	858	LMU	C2'-C1'-O1'-C1
26	B2	853	LMU	C2'-C1'-O1'-C1
21	A	806	CLA	C11-C10-C8-C9
21	B	808	CLA	C14-C13-C15-C16
21	B	809	CLA	C6-C7-C8-C9
21	G	203	CLA	C6-C7-C8-C9
21	1	609	CLA	C11-C10-C8-C9
21	4	609	CLA	C11-C10-C8-C9
21	5	603	CLA	C11-C10-C8-C9
21	5	603	CLA	C14-C13-C15-C16
21	A2	806	CLA	C11-C10-C8-C9
21	B2	808	CLA	C14-C13-C15-C16
21	B2	809	CLA	C6-C7-C8-C9
21	G2	203	CLA	C6-C7-C8-C9
21	12	609	CLA	C11-C10-C8-C9
21	42	609	CLA	C11-C10-C8-C9
21	52	603	CLA	C11-C10-C8-C9
21	52	603	CLA	C14-C13-C15-C16
30	1	601	CHL	C6-C7-C8-C9
30	12	601	CHL	C6-C7-C8-C9
30	6	616	CHL	C8-C10-C11-C12
30	62	616	CHL	C8-C10-C11-C12
27	4	624	LMG	C10-C11-C12-C13
27	42	624	LMG	C10-C11-C12-C13
21	B	803	CLA	C10-C11-C12-C13
21	B	818	CLA	C13-C15-C16-C17
21	B2	803	CLA	C10-C11-C12-C13
21	B2	818	CLA	C13-C15-C16-C17
21	5	617	CLA	C8-C10-C11-C12
21	12	611	CLA	C5-C6-C7-C8
21	52	617	CLA	C8-C10-C11-C12
26	B	853	LMU	O5B-C1B-O1B-C4'
26	B2	853	LMU	O5B-C1B-O1B-C4'
21	1	611	CLA	C5-C6-C7-C8
21	5	609	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
21	52	609	CLA	C10-C11-C12-C13
30	9	607	CHL	O1D-CGD-O2D-CED
21	A	840	CLA	C12-C13-C15-C16
21	B	817	CLA	C11-C10-C8-C7
21	7	611	CLA	C6-C7-C8-C10
21	5	601	CLA	C6-C7-C8-C10
21	A2	840	CLA	C12-C13-C15-C16
21	B2	817	CLA	C11-C10-C8-C7
21	72	611	CLA	C6-C7-C8-C10
21	52	601	CLA	C6-C7-C8-C10
21	B	823	CLA	C2A-CAA-CBA-CGA
21	B2	823	CLA	C2A-CAA-CBA-CGA
26	A	862	LMU	O5'-C1'-O1'-C1
26	A2	862	LMU	O5'-C1'-O1'-C1
21	5	621	CLA	C4C-C3C-CAC-CBC
23	8	620	LHG	O2-C2-C3-O3
23	82	620	LHG	O2-C2-C3-O3
21	Z	604	CLA	C3-C5-C6-C7
21	Z2	604	CLA	C3-C5-C6-C7
21	A	840	CLA	C15-C16-C17-C18
21	A2	840	CLA	C15-C16-C17-C18
26	8	627	LMU	C3'-C4'-O1B-C1B
26	82	627	LMU	C3'-C4'-O1B-C1B
21	52	621	CLA	C4C-C3C-CAC-CBC
21	A	813	CLA	C15-C16-C17-C18
21	A2	813	CLA	C15-C16-C17-C18
23	A	846	LHG	C4-O6-P-O3
23	A	847	LHG	C4-O6-P-O3
23	1	620	LHG	C3-O3-P-O6
23	3	721	LHG	C4-O6-P-O3
23	3	623	LHG	C3-O3-P-O6
23	3	623	LHG	C4-O6-P-O3
23	Z	620	LHG	C4-O6-P-O3
23	4	622	LHG	C3-O3-P-O6
23	6	629	LHG	C4-O6-P-O3
23	A2	846	LHG	C4-O6-P-O3
23	A2	847	LHG	C4-O6-P-O3
23	12	620	LHG	C3-O3-P-O6
23	32	721	LHG	C4-O6-P-O3
23	32	623	LHG	C3-O3-P-O6
23	32	623	LHG	C4-O6-P-O3
23	Z2	620	LHG	C4-O6-P-O3

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Mol	Chain	Res	Type	Atoms
23	42	622	LHG	C3-O3-P-O6
23	62	629	LHG	C4-O6-P-O3
21	A	818	CLA	C3-C5-C6-C7
21	4	603	CLA	C3-C5-C6-C7
21	A2	818	CLA	C3-C5-C6-C7
21	42	603	CLA	C3-C5-C6-C7
23	8	620	LHG	C1-C2-C3-O3
23	4	623	LHG	C1-C2-C3-O3
23	82	620	LHG	C1-C2-C3-O3
23	42	623	LHG	C1-C2-C3-O3
21	7	616	CLA	C2A-CAA-CBA-CGA
21	72	616	CLA	C2A-CAA-CBA-CGA
29	B	850	DGD	O6E-C5E-C6E-O5E
23	4	622	LHG	C9-C10-C11-C12
23	42	622	LHG	C9-C10-C11-C12
27	6	633	LMG	C17-C18-C19-C20
27	62	633	LMG	C17-C18-C19-C20
30	92	607	CHL	CBD-CGD-O2D-CED
29	B	850	DGD	C3A-C4A-C5A-C6A
23	B	851	LHG	O2-C2-C3-O3
23	B2	851	LHG	O2-C2-C3-O3
26	A	862	LMU	C2'-C1'-O1'-C1
26	A	863	LMU	C2'-C1'-O1'-C1
26	K	208	LMU	C2'-C1'-O1'-C1
26	A2	862	LMU	C2'-C1'-O1'-C1
26	A2	863	LMU	C2'-C1'-O1'-C1
26	K2	208	LMU	C2'-C1'-O1'-C1
21	3	603	CLA	C8-C10-C11-C12
21	32	603	CLA	C8-C10-C11-C12
21	A	813	CLA	C6-C7-C8-C9
21	A	820	CLA	C11-C12-C13-C14
21	A	826	CLA	C11-C10-C8-C9
21	A	839	CLA	C11-C12-C13-C14
21	A	843	CLA	C11-C12-C13-C14
21	L	203	CLA	C14-C13-C15-C16
21	7	611	CLA	C11-C12-C13-C14
21	6	613	CLA	C11-C10-C8-C9
21	A2	813	CLA	C6-C7-C8-C9
21	A2	820	CLA	C11-C12-C13-C14
21	A2	826	CLA	C11-C10-C8-C9
21	A2	839	CLA	C11-C12-C13-C14
21	A2	843	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
21	L2	203	CLA	C14-C13-C15-C16
21	72	611	CLA	C11-C12-C13-C14
21	62	613	CLA	C11-C10-C8-C9
21	1	614	CLA	C2A-CAA-CBA-CGA
21	12	614	CLA	C2A-CAA-CBA-CGA
21	B	820	CLA	C5-C6-C7-C8
30	Z	607	CHL	C10-C11-C12-C13
30	Z2	607	CHL	C10-C11-C12-C13
26	7	629	LMU	O5'-C5'-C6'-O6'
26	72	629	LMU	O5'-C5'-C6'-O6'
21	B2	820	CLA	C5-C6-C7-C8
23	6	619	LHG	C26-C27-C28-C29
23	62	619	LHG	C26-C27-C28-C29
29	B	850	DGD	CBB-CCB-CDB-CEB
30	9	607	CHL	CBA-CGA-O2A-C1
21	A	834	CLA	C3A-C2A-CAA-CBA
21	B	823	CLA	C3A-C2A-CAA-CBA
21	3	611	CLA	C3A-C2A-CAA-CBA
21	7	616	CLA	C3A-C2A-CAA-CBA
21	9	603	CLA	C3A-C2A-CAA-CBA
21	A2	834	CLA	C3A-C2A-CAA-CBA
21	B2	823	CLA	C3A-C2A-CAA-CBA
21	32	611	CLA	C3A-C2A-CAA-CBA
21	72	616	CLA	C3A-C2A-CAA-CBA
21	92	603	CLA	C3A-C2A-CAA-CBA
30	Z	606	CHL	C3A-C2A-CAA-CBA
30	9	607	CHL	C3A-C2A-CAA-CBA
30	Z2	606	CHL	C3A-C2A-CAA-CBA
30	92	607	CHL	C3A-C2A-CAA-CBA
26	B	853	LMU	C2-C1-O1'-C1'
26	1	621	LMU	C2-C1-O1'-C1'
26	1	625	LMU	C2-C1-O1'-C1'
26	8	624	LMU	C2-C1-O1'-C1'
26	B2	853	LMU	C2-C1-O1'-C1'
26	G2	206	LMU	C2-C1-O1'-C1'
26	12	621	LMU	C2-C1-O1'-C1'
26	12	625	LMU	C2-C1-O1'-C1'
26	82	624	LMU	C2-C1-O1'-C1'
21	A	826	CLA	O2A-C1-C2-C3
21	9	609	CLA	O2A-C1-C2-C3
21	9	613	CLA	O2A-C1-C2-C3
21	A2	826	CLA	O2A-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
21	92	609	CLA	O2A-C1-C2-C3
21	92	613	CLA	O2A-C1-C2-C3
30	4	606	CHL	O2A-C1-C2-C3
30	42	606	CHL	O2A-C1-C2-C3
23	8	620	LHG	C23-C24-C25-C26
23	82	620	LHG	C23-C24-C25-C26
21	B	820	CLA	C4-C3-C5-C6
21	B	828	CLA	C4-C3-C5-C6
21	B2	820	CLA	C4-C3-C5-C6
21	B2	828	CLA	C4-C3-C5-C6
21	62	613	CLA	C4-C3-C5-C6
30	6	607	CHL	C4-C3-C5-C6
30	62	607	CHL	C4-C3-C5-C6
21	B	820	CLA	C2-C3-C5-C6
21	B	828	CLA	C2-C3-C5-C6
21	Z	609	CLA	C2-C3-C5-C6
21	A2	835	CLA	C2-C3-C5-C6
21	B2	820	CLA	C2-C3-C5-C6
21	B2	828	CLA	C2-C3-C5-C6
21	Z2	609	CLA	C2-C3-C5-C6
30	6	607	CHL	C2-C3-C5-C6
30	62	607	CHL	C2-C3-C5-C6
21	A	806	CLA	C5-C6-C7-C8
21	9	612	CLA	C13-C15-C16-C17
21	A2	806	CLA	C5-C6-C7-C8
21	92	612	CLA	C13-C15-C16-C17
21	B	829	CLA	C5-C6-C7-C8
23	B	851	LHG	C1-C2-C3-O3
23	4	622	LHG	C1-C2-C3-O3
23	B2	851	LHG	C1-C2-C3-O3
23	42	622	LHG	C1-C2-C3-O3
21	9	611	CLA	C10-C11-C12-C13
21	B2	829	CLA	C5-C6-C7-C8
21	92	611	CLA	C10-C11-C12-C13
23	A	846	LHG	C23-C24-C25-C26
23	A2	846	LHG	C23-C24-C25-C26
24	A	848	BCR	C5-C6-C7-C8
24	B	846	BCR	C23-C24-C25-C26
24	B	846	BCR	C23-C24-C25-C30
24	B	847	BCR	C23-C24-C25-C26
24	B	848	BCR	C1-C6-C7-C8
24	B	848	BCR	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
24	J	102	BCR	C23-C24-C25-C30
24	K	202	BCR	C23-C24-C25-C26
24	K	202	BCR	C23-C24-C25-C30
24	K	207	BCR	C23-C24-C25-C26
24	K	207	BCR	C23-C24-C25-C30
24	3	620	BCR	C23-C24-C25-C26
24	3	620	BCR	C23-C24-C25-C30
24	3	719	BCR	C23-C24-C25-C26
24	3	719	BCR	C23-C24-C25-C30
24	7	623	BCR	C23-C24-C25-C26
24	7	623	BCR	C23-C24-C25-C30
24	8	619	BCR	C23-C24-C25-C26
24	8	619	BCR	C23-C24-C25-C30
24	4	621	BCR	C23-C24-C25-C26
24	4	621	BCR	C23-C24-C25-C30
24	5	622	BCR	C23-C24-C25-C26
24	5	622	BCR	C23-C24-C25-C30
24	6	623	BCR	C23-C24-C25-C26
24	6	623	BCR	C23-C24-C25-C30
24	9	623	BCR	C23-C24-C25-C30
24	A2	848	BCR	C5-C6-C7-C8
24	B2	846	BCR	C23-C24-C25-C26
24	B2	846	BCR	C23-C24-C25-C30
24	B2	847	BCR	C23-C24-C25-C26
24	B2	848	BCR	C1-C6-C7-C8
24	B2	848	BCR	C5-C6-C7-C8
24	J2	102	BCR	C23-C24-C25-C30
24	K2	202	BCR	C23-C24-C25-C26
24	K2	202	BCR	C23-C24-C25-C30
24	K2	207	BCR	C23-C24-C25-C26
24	K2	207	BCR	C23-C24-C25-C30
24	32	620	BCR	C23-C24-C25-C26
24	32	620	BCR	C23-C24-C25-C30
24	32	719	BCR	C23-C24-C25-C26
24	32	719	BCR	C23-C24-C25-C30
24	72	623	BCR	C23-C24-C25-C26
24	72	623	BCR	C23-C24-C25-C30
24	82	619	BCR	C23-C24-C25-C26
24	82	619	BCR	C23-C24-C25-C30
24	42	621	BCR	C23-C24-C25-C26
24	42	621	BCR	C23-C24-C25-C30
24	52	622	BCR	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
24	52	622	BCR	C23-C24-C25-C30
24	62	623	BCR	C23-C24-C25-C26
24	62	623	BCR	C23-C24-C25-C30
24	92	623	BCR	C23-C24-C25-C30
28	A	856	LUT	C1-C6-C7-C8
28	1	617	LUT	C1-C6-C7-C8
28	1	617	LUT	C5-C6-C7-C8
28	1	619	LUT	C1-C6-C7-C8
28	1	619	LUT	C5-C6-C7-C8
28	3	621	LUT	C5-C6-C7-C8
28	3	622	LUT	C5-C6-C7-C8
28	8	617	LUT	C1-C6-C7-C8
28	8	617	LUT	C5-C6-C7-C8
28	Z	617	LUT	C1-C6-C7-C8
28	Z	617	LUT	C5-C6-C7-C8
28	Z	619	LUT	C1-C6-C7-C8
28	Z	619	LUT	C5-C6-C7-C8
28	5	620	LUT	C5-C6-C7-C8
28	5	626	LUT	C1-C6-C7-C8
28	5	626	LUT	C5-C6-C7-C8
28	6	621	LUT	C5-C6-C7-C8
28	9	616	LUT	C1-C6-C7-C8
28	9	616	LUT	C5-C6-C7-C8
28	12	617	LUT	C1-C6-C7-C8
28	12	617	LUT	C5-C6-C7-C8
28	12	619	LUT	C1-C6-C7-C8
28	12	619	LUT	C5-C6-C7-C8
28	32	621	LUT	C5-C6-C7-C8
28	32	622	LUT	C5-C6-C7-C8
28	82	617	LUT	C1-C6-C7-C8
28	82	617	LUT	C5-C6-C7-C8
28	Z2	617	LUT	C1-C6-C7-C8
28	Z2	617	LUT	C5-C6-C7-C8
28	Z2	619	LUT	C1-C6-C7-C8
28	Z2	619	LUT	C5-C6-C7-C8
28	52	620	LUT	C5-C6-C7-C8
28	52	626	LUT	C1-C6-C7-C8
28	52	626	LUT	C5-C6-C7-C8
28	62	621	LUT	C5-C6-C7-C8
28	92	616	LUT	C1-C6-C7-C8
28	92	616	LUT	C5-C6-C7-C8
23	8	620	LHG	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
23	82	620	LHG	C17-C18-C19-C20
27	B	852	LMG	C11-C12-C13-C14
27	B2	852	LMG	C11-C12-C13-C14
21	4	609	CLA	C5-C6-C7-C8
21	3	607	CLA	C2C-C3C-CAC-CBC
21	A	826	CLA	C4-C3-C5-C6
21	A	835	CLA	C4-C3-C5-C6
21	Z	609	CLA	C4-C3-C5-C6
21	6	613	CLA	C4-C3-C5-C6
21	9	611	CLA	C4-C3-C5-C6
21	A2	826	CLA	C4-C3-C5-C6
21	A2	835	CLA	C4-C3-C5-C6
21	92	611	CLA	C4-C3-C5-C6
30	7	601	CHL	C4-C3-C5-C6
30	72	601	CHL	C4-C3-C5-C6
21	A	810	CLA	C11-C10-C8-C7
21	A	820	CLA	C11-C12-C13-C15
21	A	823	CLA	C11-C12-C13-C15
21	A	826	CLA	C2-C3-C5-C6
21	A	828	CLA	C12-C13-C15-C16
21	A	835	CLA	C2-C3-C5-C6
21	A	839	CLA	C11-C12-C13-C15
21	B	808	CLA	C12-C13-C15-C16
21	G	203	CLA	C6-C7-C8-C10
21	L	203	CLA	C12-C13-C15-C16
21	3	615	CLA	C11-C10-C8-C7
21	7	611	CLA	C11-C12-C13-C15
21	8	610	CLA	C11-C12-C13-C15
21	6	613	CLA	C2-C3-C5-C6
21	A2	810	CLA	C11-C10-C8-C7
21	A2	820	CLA	C11-C12-C13-C15
21	A2	823	CLA	C11-C12-C13-C15
21	A2	826	CLA	C2-C3-C5-C6
21	A2	839	CLA	C11-C12-C13-C15
21	B2	808	CLA	C12-C13-C15-C16
21	G2	203	CLA	C6-C7-C8-C10
21	L2	203	CLA	C12-C13-C15-C16
21	32	615	CLA	C11-C10-C8-C7
21	72	611	CLA	C11-C12-C13-C15
21	82	610	CLA	C11-C12-C13-C15
21	62	613	CLA	C2-C3-C5-C6
21	92	611	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
30	5	607	CHL	C6-C7-C8-C10
30	5	607	CHL	C11-C10-C8-C7
30	52	607	CHL	C6-C7-C8-C10
30	52	607	CHL	C11-C10-C8-C7
30	9	607	CHL	O1A-CGA-O2A-C1
21	32	607	CLA	C2C-C3C-CAC-CBC
29	B	850	DGD	C8B-C9B-CAB-CBB
21	42	609	CLA	C5-C6-C7-C8
30	92	607	CHL	CBA-CGA-O2A-C1
21	A	854	CLA	C2A-CAA-CBA-CGA
21	A2	854	CLA	C2A-CAA-CBA-CGA
26	92	624	LMU	C4-C5-C6-C7
26	9	624	LMU	C4-C5-C6-C7
26	A	863	LMU	O5'-C1'-O1'-C1
26	K	208	LMU	O5'-C1'-O1'-C1
26	A2	863	LMU	O5'-C1'-O1'-C1
26	K2	208	LMU	O5'-C1'-O1'-C1
21	B	817	CLA	C2C-C3C-CAC-CBC
21	B2	817	CLA	C2C-C3C-CAC-CBC
23	B	851	LHG	C17-C18-C19-C20
23	B2	851	LHG	C17-C18-C19-C20
21	Z2	609	CLA	C13-C15-C16-C17
21	5	603	CLA	C3-C5-C6-C7
21	52	603	CLA	C3-C5-C6-C7
21	Z	609	CLA	C13-C15-C16-C17
30	62	607	CHL	C15-C16-C17-C18
23	5	623	LHG	O7-C5-C6-O8
23	52	623	LHG	O7-C5-C6-O8
29	B	850	DGD	C5A-C6A-C7A-C8A
26	A	864	LMU	O5'-C5'-C6'-O6'
26	B	853	LMU	O5'-C5'-C6'-O6'
26	6	630	LMU	O5'-C5'-C6'-O6'
26	A2	864	LMU	O5'-C5'-C6'-O6'
26	B2	853	LMU	O5'-C5'-C6'-O6'
26	62	630	LMU	O5'-C5'-C6'-O6'
27	1	628	LMG	O6-C5-C6-O5
27	7	626	LMG	O6-C5-C6-O5
27	12	628	LMG	O6-C5-C6-O5
27	72	626	LMG	O6-C5-C6-O5
21	A	826	CLA	C10-C11-C12-C13
21	1	608	CLA	C10-C11-C12-C13
21	A2	826	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
21	12	608	CLA	C10-C11-C12-C13
30	6	607	CHL	C15-C16-C17-C18
21	Z2	609	CLA	C4-C3-C5-C6
21	B	839	CLA	C2-C3-C5-C6
21	9	611	CLA	C2-C3-C5-C6
21	B2	839	CLA	C2-C3-C5-C6
30	7	601	CHL	C2-C3-C5-C6
30	72	601	CHL	C2-C3-C5-C6
21	A	810	CLA	C11-C10-C8-C9
21	A	823	CLA	C11-C12-C13-C14
21	A	828	CLA	C14-C13-C15-C16
21	A	840	CLA	C14-C13-C15-C16
21	B	802	CLA	C11-C10-C8-C9
21	B	805	CLA	C14-C13-C15-C16
21	B	817	CLA	C11-C10-C8-C9
21	3	615	CLA	C11-C10-C8-C9
21	7	611	CLA	C6-C7-C8-C9
21	8	610	CLA	C11-C12-C13-C14
21	5	601	CLA	C6-C7-C8-C9
21	A2	810	CLA	C11-C10-C8-C9
21	A2	823	CLA	C11-C12-C13-C14
21	A2	828	CLA	C14-C13-C15-C16
21	A2	840	CLA	C14-C13-C15-C16
21	B2	802	CLA	C11-C10-C8-C9
21	B2	805	CLA	C14-C13-C15-C16
21	B2	817	CLA	C11-C10-C8-C9
21	32	615	CLA	C11-C10-C8-C9
21	72	611	CLA	C6-C7-C8-C9
21	82	610	CLA	C11-C12-C13-C14
21	52	601	CLA	C6-C7-C8-C9
30	5	607	CHL	C6-C7-C8-C9
30	5	607	CHL	C11-C10-C8-C9
30	52	607	CHL	C6-C7-C8-C9
30	52	607	CHL	C11-C10-C8-C9
26	1	622	LMU	O5'-C5'-C6'-O6'
26	12	622	LMU	O5'-C5'-C6'-O6'
27	A	860	LMG	O6-C5-C6-O5
27	8	626	LMG	O6-C5-C6-O5
27	A2	860	LMG	O6-C5-C6-O5
27	82	626	LMG	O6-C5-C6-O5
21	B	836	CLA	C10-C11-C12-C13
30	92	607	CHL	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
21	A	812	CLA	C1A-C2A-CAA-CBA
21	A	834	CLA	C1A-C2A-CAA-CBA
21	B	823	CLA	C1A-C2A-CAA-CBA
21	B	838	CLA	C1A-C2A-CAA-CBA
21	J	101	CLA	C1A-C2A-CAA-CBA
21	1	611	CLA	C1A-C2A-CAA-CBA
21	3	611	CLA	C1A-C2A-CAA-CBA
21	Z	609	CLA	C1A-C2A-CAA-CBA
21	9	603	CLA	C1A-C2A-CAA-CBA
21	A2	812	CLA	C1A-C2A-CAA-CBA
21	A2	834	CLA	C1A-C2A-CAA-CBA
21	B2	823	CLA	C1A-C2A-CAA-CBA
21	B2	838	CLA	C1A-C2A-CAA-CBA
21	J2	101	CLA	C1A-C2A-CAA-CBA
21	12	611	CLA	C1A-C2A-CAA-CBA
21	32	611	CLA	C1A-C2A-CAA-CBA
21	Z2	609	CLA	C1A-C2A-CAA-CBA
21	92	603	CLA	C1A-C2A-CAA-CBA
27	J	104	LMG	O6-C5-C6-O5
27	8	629	LMG	O6-C5-C6-O5
27	J2	104	LMG	O6-C5-C6-O5
27	82	629	LMG	O6-C5-C6-O5
30	9	607	CHL	C1A-C2A-CAA-CBA
30	92	607	CHL	C1A-C2A-CAA-CBA
21	B	824	CLA	C8-C10-C11-C12
21	B	840	CLA	C15-C16-C17-C18
21	K	203	CLA	C5-C6-C7-C8
21	B2	824	CLA	C8-C10-C11-C12
21	B2	836	CLA	C10-C11-C12-C13
21	B2	840	CLA	C15-C16-C17-C18
21	K2	203	CLA	C5-C6-C7-C8
23	4	623	LHG	C3-O3-P-O6
23	42	623	LHG	C3-O3-P-O6
26	1	625	LMU	O5'-C5'-C6'-O6'
26	12	625	LMU	O5'-C5'-C6'-O6'
27	9	620	LMG	O6-C5-C6-O5
26	12	621	LMU	O5B-C1B-O1B-C4'
21	A2	836	CLA	C8-C10-C11-C12
30	4	608	CHL	C15-C16-C17-C18
30	42	608	CHL	C15-C16-C17-C18
26	A	861	LMU	O5'-C5'-C6'-O6'
26	A2	861	LMU	O5'-C5'-C6'-O6'

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Mol	Chain	Res	Type	Atoms
27	92	620	LMG	O6-C5-C6-O5
23	A	847	LHG	O6-C4-C5-C6
23	3	721	LHG	O6-C4-C5-C6
23	5	623	LHG	O6-C4-C5-C6
23	A2	847	LHG	O6-C4-C5-C6
23	32	721	LHG	O6-C4-C5-C6
23	52	623	LHG	O6-C4-C5-C6
26	1	621	LMU	O5B-C1B-O1B-C4'
21	A	836	CLA	C8-C10-C11-C12
21	A	833	CLA	C3-C5-C6-C7
26	8	627	LMU	O5B-C5B-C6B-O6B
26	82	627	LMU	O5B-C5B-C6B-O6B
27	J	103	LMG	C16-C17-C18-C19
27	J2	103	LMG	C16-C17-C18-C19
27	1	628	LMG	C12-C13-C14-C15
27	12	628	LMG	C12-C13-C14-C15
30	82	607	CHL	C15-C16-C17-C18
26	A	857	LMU	O5B-C5B-C6B-O6B
26	8	625	LMU	O5'-C5'-C6'-O6'
26	A2	857	LMU	O5B-C5B-C6B-O6B
26	82	625	LMU	O5'-C5'-C6'-O6'
21	B	827	CLA	C3-C5-C6-C7
21	A2	833	CLA	C3-C5-C6-C7
21	B2	827	CLA	C3-C5-C6-C7
23	7	625	LHG	C4-C5-C6-O8
23	72	625	LHG	C4-C5-C6-O8
27	J	104	LMG	O1-C7-C8-C9
27	3	722	LMG	C33-C34-C35-C36
27	J2	104	LMG	O1-C7-C8-C9
27	32	722	LMG	C33-C34-C35-C36
21	A	834	CLA	C13-C15-C16-C17
30	8	607	CHL	C15-C16-C17-C18
27	A	860	LMG	C8-C7-O1-C1
27	J	104	LMG	C8-C7-O1-C1
27	A2	860	LMG	C8-C7-O1-C1
27	J2	104	LMG	C8-C7-O1-C1
21	A2	834	CLA	C13-C15-C16-C17
29	B	850	DGD	O2G-C1B-C2B-C3B
30	5	607	CHL	CAA-CBA-CGA-O2A
30	52	607	CHL	CAA-CBA-CGA-O2A
26	A2	858	LMU	O5B-C5B-C6B-O6B
26	A	858	LMU	O5B-C5B-C6B-O6B

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Mol	Chain	Res	Type	Atoms
21	Z	611	CLA	C10-C11-C12-C13
21	Z2	611	CLA	C10-C11-C12-C13
21	5	601	CLA	C10-C11-C12-C13
26	G	206	LMU	O5'-C5'-C6'-O6'
26	8	628	LMU	O5'-C5'-C6'-O6'
26	9	624	LMU	O5'-C5'-C6'-O6'
26	G2	206	LMU	O5'-C5'-C6'-O6'
26	82	628	LMU	O5'-C5'-C6'-O6'
27	4	624	LMG	O6-C5-C6-O5
27	42	624	LMG	O6-C5-C6-O5
21	A	817	CLA	C4-C3-C5-C6
21	A	828	CLA	C4-C3-C5-C6
21	A	830	CLA	C4-C3-C5-C6
21	A	841	CLA	C4-C3-C5-C6
21	B	839	CLA	C4-C3-C5-C6
21	1	609	CLA	C4-C3-C5-C6
21	9	612	CLA	C4-C3-C5-C6
21	A2	817	CLA	C4-C3-C5-C6
21	A2	828	CLA	C4-C3-C5-C6
21	A2	830	CLA	C4-C3-C5-C6
21	A2	841	CLA	C4-C3-C5-C6
21	B2	839	CLA	C4-C3-C5-C6
21	12	609	CLA	C4-C3-C5-C6
21	92	612	CLA	C4-C3-C5-C6
30	6	601	CHL	C4-C3-C5-C6
30	62	601	CHL	C4-C3-C5-C6
21	A	817	CLA	C2-C3-C5-C6
21	A	830	CLA	C2-C3-C5-C6
21	A	841	CLA	C2-C3-C5-C6
21	A2	817	CLA	C2-C3-C5-C6
21	A2	830	CLA	C2-C3-C5-C6
26	92	624	LMU	O5'-C5'-C6'-O6'
21	6	603	CLA	C5-C6-C7-C8
21	52	601	CLA	C10-C11-C12-C13
21	62	603	CLA	C5-C6-C7-C8
26	6	631	LMU	O5'-C5'-C6'-O6'
26	62	631	LMU	O5'-C5'-C6'-O6'
21	A	810	CLA	C2A-CAA-CBA-CGA
21	A2	810	CLA	C2A-CAA-CBA-CGA
21	A	806	CLA	C2-C1-O2A-CGA
21	5	603	CLA	C2-C1-O2A-CGA
21	A2	806	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
21	52	603	CLA	C2-C1-O2A-CGA
26	12	623	LMU	C11-C10-C9-C8
26	1	623	LMU	C11-C10-C9-C8
21	82	602	CLA	C8-C10-C11-C12
23	B	851	LHG	O7-C7-C8-C9
23	B2	851	LHG	O7-C7-C8-C9
23	B	851	LHG	O7-C5-C6-O8
23	B2	851	LHG	O7-C5-C6-O8
21	8	602	CLA	C8-C10-C11-C12
21	8	603	CLA	C15-C16-C17-C18
21	82	603	CLA	C15-C16-C17-C18
21	A	840	CLA	C4-C3-C5-C6
21	1	614	CLA	C4-C3-C5-C6
21	3	603	CLA	C4-C3-C5-C6
21	A2	840	CLA	C4-C3-C5-C6
21	12	614	CLA	C4-C3-C5-C6
21	32	603	CLA	C4-C3-C5-C6
23	9	622	LHG	C25-C26-C27-C28
23	92	622	LHG	C25-C26-C27-C28
29	B2	850	DGD	C2A-C3A-C4A-C5A
21	A	828	CLA	C2-C3-C5-C6
21	A	834	CLA	C11-C10-C8-C7
21	B	802	CLA	C11-C10-C8-C7
21	F	301	CLA	C11-C10-C8-C7
21	1	609	CLA	C2-C3-C5-C6
21	1	614	CLA	C2-C3-C5-C6
21	1	614	CLA	C6-C7-C8-C10
21	5	603	CLA	C11-C10-C8-C7
21	A2	828	CLA	C2-C3-C5-C6
21	A2	828	CLA	C12-C13-C15-C16
21	A2	834	CLA	C11-C10-C8-C7
21	A2	841	CLA	C2-C3-C5-C6
21	B2	802	CLA	C11-C10-C8-C7
21	F2	301	CLA	C11-C10-C8-C7
21	12	609	CLA	C2-C3-C5-C6
21	12	614	CLA	C2-C3-C5-C6
21	12	614	CLA	C6-C7-C8-C10
21	52	603	CLA	C11-C10-C8-C7
22	A	844	PQN	C17-C18-C20-C21
22	A2	844	PQN	C17-C18-C20-C21
30	1	601	CHL	C11-C12-C13-C15
30	12	601	CHL	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
21	B	827	CLA	C11-C10-C8-C9
21	B	834	CLA	C11-C10-C8-C9
21	Z	609	CLA	C11-C12-C13-C14
21	B2	827	CLA	C11-C10-C8-C9
21	B2	834	CLA	C11-C10-C8-C9
21	Z2	609	CLA	C11-C12-C13-C14
22	A	844	PQN	C19-C18-C20-C21
22	A2	844	PQN	C19-C18-C20-C21
30	Z	601	CHL	C6-C7-C8-C9
30	Z2	601	CHL	C6-C7-C8-C9
21	A	806	CLA	C2A-CAA-CBA-CGA
21	A2	806	CLA	C2A-CAA-CBA-CGA
21	B	811	CLA	C15-C16-C17-C18
21	5	603	CLA	C5-C6-C7-C8
21	B2	811	CLA	C15-C16-C17-C18
21	52	603	CLA	C5-C6-C7-C8
21	B	817	CLA	C13-C15-C16-C17
21	B	821	CLA	C10-C11-C12-C13
21	B2	817	CLA	C13-C15-C16-C17
21	B2	821	CLA	C10-C11-C12-C13
23	B	851	LHG	O6-C4-C5-C6
23	Z	620	LHG	O6-C4-C5-C6
23	B2	851	LHG	O6-C4-C5-C6
23	Z2	620	LHG	O6-C4-C5-C6
27	A	859	LMG	C40-C41-C42-C43
27	A2	859	LMG	C40-C41-C42-C43
21	B	826	CLA	C8-C10-C11-C12
21	B2	826	CLA	C8-C10-C11-C12
21	A	820	CLA	C4-C3-C5-C6
21	B	808	CLA	C4-C3-C5-C6
21	B	812	CLA	C4-C3-C5-C6
21	B	829	CLA	C4-C3-C5-C6
21	A2	820	CLA	C4-C3-C5-C6
21	B2	808	CLA	C4-C3-C5-C6
21	B2	812	CLA	C4-C3-C5-C6
21	B2	829	CLA	C4-C3-C5-C6
21	B	808	CLA	C2-C3-C5-C6
21	9	612	CLA	C2-C3-C5-C6
21	B2	808	CLA	C2-C3-C5-C6
21	92	612	CLA	C2-C3-C5-C6
30	6	601	CHL	C2-C3-C5-C6
30	62	601	CHL	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
21	A2	828	CLA	C8-C10-C11-C12
23	5	623	LHG	O2-C2-C3-O3
23	52	623	LHG	O2-C2-C3-O3
23	4	623	LHG	C13-C14-C15-C16
21	A	816	CLA	C13-C15-C16-C17
21	A	828	CLA	C8-C10-C11-C12
21	7	611	CLA	C8-C10-C11-C12
21	A2	816	CLA	C13-C15-C16-C17
21	72	611	CLA	C8-C10-C11-C12
23	42	623	LHG	C13-C14-C15-C16
21	B	805	CLA	C3A-C2A-CAA-CBA
21	B2	805	CLA	C3A-C2A-CAA-CBA
23	8	620	LHG	C26-C27-C28-C29
23	82	620	LHG	C26-C27-C28-C29
26	A	857	LMU	C2-C1-O1'-C1'
26	A	858	LMU	C2-C1-O1'-C1'
26	G	206	LMU	C2-C1-O1'-C1'
26	7	629	LMU	C2-C1-O1'-C1'
26	8	628	LMU	C2-C1-O1'-C1'
26	8	627	LMU	C2-C1-O1'-C1'
26	8	625	LMU	C2-C1-O1'-C1'
26	A2	857	LMU	C2-C1-O1'-C1'
26	A2	858	LMU	C2-C1-O1'-C1'
26	72	629	LMU	C2-C1-O1'-C1'
26	82	628	LMU	C2-C1-O1'-C1'
26	82	627	LMU	C2-C1-O1'-C1'
26	82	625	LMU	C2-C1-O1'-C1'
27	1	628	LMG	C14-C15-C16-C17
27	12	628	LMG	C14-C15-C16-C17
27	4	624	LMG	O1-C7-C8-C9
27	42	624	LMG	O1-C7-C8-C9
21	A	823	CLA	O2A-C1-C2-C3
21	A	827	CLA	O2A-C1-C2-C3
21	A2	823	CLA	O2A-C1-C2-C3
21	A2	827	CLA	O2A-C1-C2-C3
30	8	607	CHL	O2A-C1-C2-C3
30	Z	601	CHL	O2A-C1-C2-C3
30	82	607	CHL	O2A-C1-C2-C3
30	Z2	601	CHL	O2A-C1-C2-C3
30	92	607	CHL	O1D-CGD-O2D-CED
21	A	810	CLA	C4-C3-C5-C6
21	B	807	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
21	A2	810	CLA	C4-C3-C5-C6
21	B2	807	CLA	C4-C3-C5-C6
21	A	840	CLA	C2-C3-C5-C6
21	B	812	CLA	C2-C3-C5-C6
21	A2	840	CLA	C2-C3-C5-C6
21	B2	829	CLA	C2-C3-C5-C6
21	32	603	CLA	C2C-C3C-CAC-CBC
21	3	603	CLA	C2C-C3C-CAC-CBC
23	8	620	LHG	C3-O3-P-O6
23	82	620	LHG	C3-O3-P-O6
23	A	846	LHG	C27-C28-C29-C30
23	A2	846	LHG	C27-C28-C29-C30
23	A	847	LHG	O6-C4-C5-O7
23	B	851	LHG	O6-C4-C5-O7
23	A2	847	LHG	O6-C4-C5-O7
23	B2	851	LHG	O6-C4-C5-O7
23	4	622	LHG	O2-C2-C3-O3
23	8	620	LHG	C15-C16-C17-C18
23	82	620	LHG	C15-C16-C17-C18
27	8	626	LMG	O7-C8-C9-O8
27	82	626	LMG	O7-C8-C9-O8
21	A	812	CLA	C15-C16-C17-C18
21	12	609	CLA	C15-C16-C17-C18
21	A	815	CLA	C4-C3-C5-C6
21	A	812	CLA	C2-C1-O2A-CGA
21	A2	812	CLA	C2-C1-O2A-CGA
21	B	807	CLA	C2-C3-C5-C6
21	B	829	CLA	C2-C3-C5-C6
21	3	603	CLA	C2-C3-C5-C6
21	B2	807	CLA	C2-C3-C5-C6
21	B2	812	CLA	C2-C3-C5-C6
21	32	603	CLA	C2-C3-C5-C6
29	B2	850	DGD	C3A-C4A-C5A-C6A
21	A2	812	CLA	C15-C16-C17-C18
27	7	626	LMG	O8-C28-C29-C30
27	72	626	LMG	O8-C28-C29-C30
21	A	812	CLA	C6-C7-C8-C9
21	A2	812	CLA	C6-C7-C8-C9
21	1	609	CLA	C15-C16-C17-C18
29	B	850	DGD	C2A-C3A-C4A-C5A
21	A	803	CLA	C2A-CAA-CBA-CGA
21	A	809	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
21	A2	803	CLA	C2A-CAA-CBA-CGA
21	A2	809	CLA	C2A-CAA-CBA-CGA
24	L	201	BCR	C5-C6-C7-C8
24	K	207	BCR	C5-C6-C7-C8
24	3	718	BCR	C23-C24-C25-C26
24	L2	201	BCR	C5-C6-C7-C8
24	K2	207	BCR	C5-C6-C7-C8
24	32	718	BCR	C23-C24-C25-C26
28	7	621	LUT	C1-C6-C7-C8
28	7	621	LUT	C5-C6-C7-C8
28	4	619	LUT	C1-C6-C7-C8
28	72	621	LUT	C1-C6-C7-C8
28	72	621	LUT	C5-C6-C7-C8
28	42	619	LUT	C1-C6-C7-C8
23	62	619	LHG	C9-C10-C11-C12
23	6	619	LHG	C9-C10-C11-C12
23	3	623	LHG	O6-C4-C5-C6
23	6	629	LHG	O6-C4-C5-C6
23	32	623	LHG	O6-C4-C5-C6
23	62	629	LHG	O6-C4-C5-C6
21	A2	815	CLA	C4-C3-C5-C6
23	42	622	LHG	O2-C2-C3-O3
21	A	804	CLA	C11-C12-C13-C15
21	A	811	CLA	C6-C7-C8-C10
21	A	815	CLA	C2-C3-C5-C6
21	A	820	CLA	C2-C3-C5-C6
21	A	829	CLA	C6-C7-C8-C10
21	A	843	CLA	C11-C12-C13-C15
21	B	819	CLA	C11-C10-C8-C7
21	B	827	CLA	C11-C10-C8-C7
21	B	834	CLA	C11-C10-C8-C7
21	7	603	CLA	C2-C3-C5-C6
21	Z	609	CLA	C11-C12-C13-C15
21	A2	804	CLA	C11-C12-C13-C15
21	A2	811	CLA	C6-C7-C8-C10
21	A2	815	CLA	C2-C3-C5-C6
21	A2	820	CLA	C2-C3-C5-C6
21	A2	829	CLA	C6-C7-C8-C10
21	A2	843	CLA	C11-C12-C13-C15
21	B2	819	CLA	C11-C10-C8-C7
21	B2	827	CLA	C11-C10-C8-C7
21	B2	834	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
21	72	603	CLA	C2-C3-C5-C6
21	Z2	609	CLA	C11-C12-C13-C15
30	Z	601	CHL	C6-C7-C8-C10
30	6	616	CHL	C12-C13-C15-C16
30	Z2	601	CHL	C6-C7-C8-C10
30	62	616	CHL	C12-C13-C15-C16
27	3	722	LMG	O8-C28-C29-C30
21	9	613	CLA	C2A-CAA-CBA-CGA
21	92	613	CLA	C2A-CAA-CBA-CGA
26	B	853	LMU	C2-C3-C4-C5
26	B2	853	LMU	C2-C3-C4-C5
27	32	722	LMG	O8-C28-C29-C30
21	A	829	CLA	C10-C11-C12-C13
21	A2	829	CLA	C10-C11-C12-C13
26	4	625	LMU	C3-C4-C5-C6
21	A	805	CLA	CAD-CBD-CGD-O2D
21	A	808	CLA	CAD-CBD-CGD-O2D
21	A	823	CLA	CAD-CBD-CGD-O2D
21	A	826	CLA	CAD-CBD-CGD-O2D
21	A	827	CLA	CAD-CBD-CGD-O2D
21	A	838	CLA	CAD-CBD-CGD-O2D
21	A	842	CLA	CAD-CBD-CGD-O2D
21	B	810	CLA	CAD-CBD-CGD-O2D
21	B	811	CLA	CAD-CBD-CGD-O2D
21	B	814	CLA	CAD-CBD-CGD-O2D
21	B	820	CLA	CAD-CBD-CGD-O2D
21	B	824	CLA	CAD-CBD-CGD-O2D
21	B	826	CLA	CAD-CBD-CGD-O2D
21	B	839	CLA	CAD-CBD-CGD-O2D
21	K	201	CLA	CAD-CBD-CGD-O2D
21	1	604	CLA	CAD-CBD-CGD-O2D
21	1	608	CLA	CAD-CBD-CGD-O2D
21	1	612	CLA	CAD-CBD-CGD-O2D
21	3	612	CLA	CAD-CBD-CGD-O2D
21	4	604	CLA	CAD-CBD-CGD-O2D
21	4	614	CLA	CAD-CBD-CGD-O2D
21	5	621	CLA	CAD-CBD-CGD-O2D
21	9	613	CLA	CAD-CBD-CGD-O2D
21	A2	805	CLA	CAD-CBD-CGD-O2D
21	A2	808	CLA	CAD-CBD-CGD-O2D
21	A2	810	CLA	CAD-CBD-CGD-O2D
21	A2	823	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
21	A2	826	CLA	CAD-CBD-CGD-O2D
21	A2	827	CLA	CAD-CBD-CGD-O2D
21	A2	838	CLA	CAD-CBD-CGD-O2D
21	A2	842	CLA	CAD-CBD-CGD-O2D
21	B2	810	CLA	CAD-CBD-CGD-O2D
21	B2	811	CLA	CAD-CBD-CGD-O2D
21	B2	814	CLA	CAD-CBD-CGD-O2D
21	B2	820	CLA	CAD-CBD-CGD-O2D
21	B2	824	CLA	CAD-CBD-CGD-O2D
21	B2	826	CLA	CAD-CBD-CGD-O2D
21	B2	839	CLA	CAD-CBD-CGD-O2D
21	K2	201	CLA	CAD-CBD-CGD-O2D
21	12	604	CLA	CAD-CBD-CGD-O2D
21	12	608	CLA	CAD-CBD-CGD-O2D
21	12	612	CLA	CAD-CBD-CGD-O2D
21	32	612	CLA	CAD-CBD-CGD-O2D
21	42	604	CLA	CAD-CBD-CGD-O2D
21	42	614	CLA	CAD-CBD-CGD-O2D
21	52	621	CLA	CAD-CBD-CGD-O2D
21	92	613	CLA	CAD-CBD-CGD-O2D
21	A2	836	CLA	CAA-CBA-CGA-O2A
21	3	607	CLA	C4C-C3C-CAC-CBC
26	42	625	LMU	C3-C4-C5-C6
21	B2	815	CLA	C4-C3-C5-C6
23	72	625	LHG	C34-C35-C36-C37
26	1	621	LMU	O5'-C1'-O1'-C1
26	12	621	LMU	O5'-C1'-O1'-C1
27	B	852	LMG	O6-C1-O1-C7
27	B2	852	LMG	O6-C1-O1-C7
21	A	810	CLA	C2-C3-C5-C6
21	A2	810	CLA	C2-C3-C5-C6
23	7	625	LHG	C34-C35-C36-C37
27	8	626	LMG	C7-C8-C9-O8
27	82	626	LMG	C7-C8-C9-O8
27	A	859	LMG	C32-C33-C34-C35
23	Z	620	LHG	O6-C4-C5-O7
23	4	623	LHG	O6-C4-C5-O7
23	6	629	LHG	O6-C4-C5-O7
23	Z2	620	LHG	O6-C4-C5-O7
23	42	623	LHG	O6-C4-C5-O7
23	62	629	LHG	O6-C4-C5-O7
21	5	617	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
21	52	617	CLA	C10-C11-C12-C13
21	A	836	CLA	CAA-CBA-CGA-O2A
21	7	610	CLA	CBA-CGA-O2A-C1
21	72	610	CLA	CBA-CGA-O2A-C1
21	B	831	CLA	C2A-CAA-CBA-CGA
21	B2	831	CLA	C2A-CAA-CBA-CGA
27	A2	859	LMG	C32-C33-C34-C35
21	32	607	CLA	C4C-C3C-CAC-CBC
21	A	804	CLA	CHA-CBD-CGD-O1D
21	A	807	CLA	CHA-CBD-CGD-O1D
21	A	817	CLA	CHA-CBD-CGD-O1D
21	A	817	CLA	CHA-CBD-CGD-O2D
21	A	831	CLA	CHA-CBD-CGD-O1D
21	A	831	CLA	CHA-CBD-CGD-O2D
21	B	804	CLA	CHA-CBD-CGD-O1D
21	B	805	CLA	CHA-CBD-CGD-O1D
21	B	815	CLA	CHA-CBD-CGD-O1D
21	B	815	CLA	CHA-CBD-CGD-O2D
21	B	820	CLA	CHA-CBD-CGD-O1D
21	B	823	CLA	CHA-CBD-CGD-O1D
21	B	823	CLA	CHA-CBD-CGD-O2D
21	B	841	CLA	CHA-CBD-CGD-O1D
21	L	203	CLA	CHA-CBD-CGD-O2D
21	7	602	CLA	CHA-CBD-CGD-O1D
21	7	602	CLA	CHA-CBD-CGD-O2D
21	7	614	CLA	CHA-CBD-CGD-O1D
21	7	614	CLA	CHA-CBD-CGD-O2D
21	7	620	CLA	CHA-CBD-CGD-O1D
21	8	612	CLA	CHA-CBD-CGD-O1D
21	4	602	CLA	CHA-CBD-CGD-O1D
21	4	602	CLA	CHA-CBD-CGD-O2D
21	5	603	CLA	CHA-CBD-CGD-O1D
21	6	622	CLA	CHA-CBD-CGD-O1D
21	A2	804	CLA	CHA-CBD-CGD-O1D
21	A2	817	CLA	CHA-CBD-CGD-O1D
21	A2	817	CLA	CHA-CBD-CGD-O2D
21	A2	831	CLA	CHA-CBD-CGD-O1D
21	A2	831	CLA	CHA-CBD-CGD-O2D
21	B2	804	CLA	CHA-CBD-CGD-O1D
21	B2	805	CLA	CHA-CBD-CGD-O1D
21	B2	815	CLA	CHA-CBD-CGD-O1D
21	B2	823	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
21	B2	841	CLA	CHA-CBD-CGD-O1D
21	L2	203	CLA	CHA-CBD-CGD-O2D
21	72	602	CLA	CHA-CBD-CGD-O1D
21	72	602	CLA	CHA-CBD-CGD-O2D
21	72	614	CLA	CHA-CBD-CGD-O1D
21	72	614	CLA	CHA-CBD-CGD-O2D
21	72	620	CLA	CHA-CBD-CGD-O1D
21	42	602	CLA	CHA-CBD-CGD-O1D
21	42	602	CLA	CHA-CBD-CGD-O2D
21	52	603	CLA	CHA-CBD-CGD-O1D
21	62	622	CLA	CHA-CBD-CGD-O1D
30	1	601	CHL	CHA-CBD-CGD-O1D
30	1	601	CHL	CHA-CBD-CGD-O2D
30	1	607	CHL	CHA-CBD-CGD-O1D
30	5	618	CHL	CHA-CBD-CGD-O1D
30	5	618	CHL	CHA-CBD-CGD-O2D
30	6	601	CHL	CHA-CBD-CGD-O1D
30	12	601	CHL	CHA-CBD-CGD-O1D
30	12	601	CHL	CHA-CBD-CGD-O2D
30	12	607	CHL	CHA-CBD-CGD-O1D
30	52	618	CHL	CHA-CBD-CGD-O1D
30	52	618	CHL	CHA-CBD-CGD-O2D
30	62	601	CHL	CHA-CBD-CGD-O1D
23	42	622	LHG	C19-C20-C21-C22
27	3	722	LMG	C8-C7-O1-C1
27	32	722	LMG	C8-C7-O1-C1
23	4	622	LHG	C19-C20-C21-C22
23	7	625	LHG	O7-C5-C6-O8
23	72	625	LHG	O7-C5-C6-O8
27	4	624	LMG	O1-C7-C8-O7
27	42	624	LMG	O1-C7-C8-O7
23	4	623	LHG	C9-C10-C11-C12
26	8	627	LMU	C7-C8-C9-C10
30	32	608	CHL	C15-C16-C17-C18
23	42	623	LHG	C9-C10-C11-C12
30	3	608	CHL	C15-C16-C17-C18
21	A	811	CLA	C4-C3-C5-C6
21	B	813	CLA	C4-C3-C5-C6
21	B	815	CLA	C4-C3-C5-C6
21	7	603	CLA	C4-C3-C5-C6
21	A2	811	CLA	C4-C3-C5-C6
21	B2	813	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
21	72	603	CLA	C4-C3-C5-C6
26	82	627	LMU	C7-C8-C9-C10
21	B	813	CLA	C2-C3-C5-C6
21	B	815	CLA	C2-C3-C5-C6
21	B2	813	CLA	C2-C3-C5-C6
21	B2	815	CLA	C2-C3-C5-C6
21	A	811	CLA	C6-C7-C8-C9
21	A	829	CLA	C6-C7-C8-C9
21	A2	811	CLA	C6-C7-C8-C9
21	A2	829	CLA	C6-C7-C8-C9
21	A	812	CLA	C13-C15-C16-C17
21	Z	611	CLA	C5-C6-C7-C8
21	Z2	611	CLA	C5-C6-C7-C8
21	A	829	CLA	C8-C10-C11-C12
21	A2	812	CLA	C13-C15-C16-C17
21	A2	829	CLA	C8-C10-C11-C12
21	B	805	CLA	C1A-C2A-CAA-CBA
21	B	827	CLA	C1A-C2A-CAA-CBA
21	7	616	CLA	C1A-C2A-CAA-CBA
21	B2	805	CLA	C1A-C2A-CAA-CBA
21	B2	827	CLA	C1A-C2A-CAA-CBA
21	72	616	CLA	C1A-C2A-CAA-CBA
21	Z2	616	CLA	C5-C6-C7-C8
21	B	817	CLA	C4C-C3C-CAC-CBC
21	A	825	CLA	C2-C1-O2A-CGA
21	A	843	CLA	C2-C1-O2A-CGA
21	A2	825	CLA	C2-C1-O2A-CGA
30	9	607	CHL	C2-C1-O2A-CGA
23	A	846	LHG	C3-O3-P-O6
23	A	847	LHG	C3-O3-P-O6
23	A2	846	LHG	C3-O3-P-O6
23	A2	847	LHG	C3-O3-P-O6
23	7	625	LHG	C31-C32-C33-C34
21	B2	817	CLA	C4C-C3C-CAC-CBC
23	72	625	LHG	C31-C32-C33-C34
21	A	821	CLA	C4-C3-C5-C6
21	1	613	CLA	C4-C3-C5-C6
21	5	610	CLA	C4-C3-C5-C6
21	A2	821	CLA	C4-C3-C5-C6
21	12	613	CLA	C4-C3-C5-C6
21	52	610	CLA	C4-C3-C5-C6
23	A	846	LHG	C4-O6-P-O4

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Mol	Chain	Res	Type	Atoms
23	3	721	LHG	C3-O3-P-O5
23	3	721	LHG	C4-O6-P-O4
23	3	623	LHG	C3-O3-P-O4
23	3	623	LHG	C4-O6-P-O4
23	3	623	LHG	C4-O6-P-O5
23	7	625	LHG	C4-O6-P-O5
23	8	620	LHG	C3-O3-P-O4
23	8	620	LHG	C4-O6-P-O5
23	Z	620	LHG	C4-O6-P-O4
23	Z	620	LHG	C4-O6-P-O5
23	9	622	LHG	C4-O6-P-O5
23	A2	846	LHG	C4-O6-P-O4
23	32	721	LHG	C3-O3-P-O5
23	32	721	LHG	C4-O6-P-O4
23	32	623	LHG	C3-O3-P-O4
23	32	623	LHG	C4-O6-P-O4
23	32	623	LHG	C4-O6-P-O5
23	72	625	LHG	C4-O6-P-O5
23	82	620	LHG	C3-O3-P-O4
23	82	620	LHG	C4-O6-P-O5
23	Z2	620	LHG	C4-O6-P-O4
23	Z2	620	LHG	C4-O6-P-O5
23	92	622	LHG	C3-O3-P-O5
23	92	622	LHG	C4-O6-P-O5
21	Z	616	CLA	C5-C6-C7-C8
23	1	620	LHG	O6-C4-C5-C6
23	4	623	LHG	O6-C4-C5-C6
23	9	622	LHG	O6-C4-C5-C6
23	12	620	LHG	O6-C4-C5-C6
23	42	623	LHG	O6-C4-C5-C6
21	A	804	CLA	CAD-CBD-CGD-O1D
21	A	814	CLA	CAD-CBD-CGD-O1D
21	B	805	CLA	CAD-CBD-CGD-O1D
21	B	841	CLA	CAD-CBD-CGD-O1D
21	7	614	CLA	CAD-CBD-CGD-O1D
21	7	620	CLA	CAD-CBD-CGD-O1D
21	6	603	CLA	CAD-CBD-CGD-O1D
21	6	622	CLA	CAD-CBD-CGD-O1D
21	A2	804	CLA	CAD-CBD-CGD-O1D
21	A2	814	CLA	CAD-CBD-CGD-O1D
21	B2	805	CLA	CAD-CBD-CGD-O1D
21	B2	841	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
21	72	614	CLA	CAD-CBD-CGD-O1D
21	72	620	CLA	CAD-CBD-CGD-O1D
21	62	603	CLA	CAD-CBD-CGD-O1D
21	62	622	CLA	CAD-CBD-CGD-O1D
30	1	601	CHL	CAD-CBD-CGD-O1D
30	1	607	CHL	CAD-CBD-CGD-O1D
30	7	601	CHL	CAD-CBD-CGD-O1D
30	Z	601	CHL	CAD-CBD-CGD-O1D
30	4	601	CHL	CAD-CBD-CGD-O1D
30	6	601	CHL	CAD-CBD-CGD-O1D
30	12	601	CHL	CAD-CBD-CGD-O1D
30	12	607	CHL	CAD-CBD-CGD-O1D
30	72	601	CHL	CAD-CBD-CGD-O1D
30	Z2	601	CHL	CAD-CBD-CGD-O1D
30	42	601	CHL	CAD-CBD-CGD-O1D
30	62	601	CHL	CAD-CBD-CGD-O1D
29	B	850	DGD	C4E-C5E-C6E-O5E
23	3	721	LHG	C1-C2-C3-O3
23	32	721	LHG	C1-C2-C3-O3
21	A	841	CLA	C16-C17-C18-C20
21	A2	841	CLA	C16-C17-C18-C20
21	A	809	CLA	C12-C13-C15-C16
21	A	816	CLA	C12-C13-C15-C16
21	A	820	CLA	C6-C7-C8-C10
21	8	613	CLA	C12-C13-C15-C16
21	4	609	CLA	C11-C10-C8-C7
21	A2	809	CLA	C12-C13-C15-C16
21	A2	816	CLA	C12-C13-C15-C16
21	A2	820	CLA	C6-C7-C8-C10
21	82	613	CLA	C12-C13-C15-C16
21	42	609	CLA	C11-C10-C8-C7
23	1	620	LHG	O6-C4-C5-O7
23	5	623	LHG	O6-C4-C5-O7
23	12	620	LHG	O6-C4-C5-O7
23	52	623	LHG	O6-C4-C5-O7
28	5	626	LUT	C25-C26-C27-C28
28	52	626	LUT	C25-C26-C27-C28
30	8	607	CHL	C6-C7-C8-C10
30	4	601	CHL	C11-C10-C8-C7
30	6	607	CHL	C12-C13-C15-C16
30	82	607	CHL	C6-C7-C8-C10
30	42	601	CHL	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
30	62	607	CHL	C12-C13-C15-C16
27	A	859	LMG	C12-C13-C14-C15
27	A2	859	LMG	C12-C13-C14-C15
21	3	611	CLA	C3-C5-C6-C7
21	32	611	CLA	C3-C5-C6-C7
26	A	863	LMU	C2-C1-O1'-C1'
26	A2	863	LMU	C2-C1-O1'-C1'
30	Z	607	CHL	CAA-CBA-CGA-O2A
30	Z2	607	CHL	CAA-CBA-CGA-O2A
21	6	609	CLA	C2A-CAA-CBA-CGA
21	62	609	CLA	C2A-CAA-CBA-CGA
30	4	608	CHL	C2A-CAA-CBA-CGA
30	42	608	CHL	C2A-CAA-CBA-CGA
21	A	806	CLA	C3-C5-C6-C7
21	A2	806	CLA	C3-C5-C6-C7
21	3	615	CLA	CAA-CBA-CGA-O2A
29	B2	850	DGD	O2G-C1B-C2B-C3B
23	32	623	LHG	C32-C33-C34-C35
23	3	623	LHG	C32-C33-C34-C35
27	B	852	LMG	C8-C7-O1-C1
27	B2	852	LMG	C8-C7-O1-C1
21	32	615	CLA	CAA-CBA-CGA-O2A
21	A	812	CLA	C3-C5-C6-C7
21	A2	812	CLA	C3-C5-C6-C7
21	3	613	CLA	C4-C3-C5-C6
21	7	620	CLA	C4-C3-C5-C6
21	B2	805	CLA	C4-C3-C5-C6
21	32	613	CLA	C4-C3-C5-C6
21	72	620	CLA	C4-C3-C5-C6
26	A2	863	LMU	C5'-C4'-O1B-C1B
21	A	830	CLA	C13-C15-C16-C17
21	A2	830	CLA	C13-C15-C16-C17
21	A	804	CLA	C11-C12-C13-C14
21	B	819	CLA	C11-C10-C8-C9
21	B	841	CLA	C14-C13-C15-C16
21	8	613	CLA	C11-C12-C13-C14
21	A2	804	CLA	C11-C12-C13-C14
21	B2	819	CLA	C11-C10-C8-C9
21	B2	841	CLA	C14-C13-C15-C16
21	82	613	CLA	C11-C12-C13-C14
21	82	613	CLA	C14-C13-C15-C16
30	8	601	CHL	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
30	8	607	CHL	C6-C7-C8-C9
30	6	607	CHL	C6-C7-C8-C9
30	82	601	CHL	C14-C13-C15-C16
30	82	607	CHL	C6-C7-C8-C9
30	62	607	CHL	C6-C7-C8-C9
26	A	863	LMU	C5'-C4'-O1B-C1B
21	B	826	CLA	C13-C15-C16-C17
21	B2	826	CLA	C13-C15-C16-C17
23	B2	851	LHG	C23-C24-C25-C26
21	B	805	CLA	C4-C3-C5-C6
29	B	850	DGD	C7B-C8B-C9B-CAB
21	A	811	CLA	C2-C3-C5-C6
21	A2	811	CLA	C2-C3-C5-C6
23	6	629	LHG	C13-C14-C15-C16
23	4	623	LHG	C6-C5-O7-C7
23	42	623	LHG	C6-C5-O7-C7
29	B	850	DGD	C3G-C2G-O2G-C1B
23	92	622	LHG	O6-C4-C5-C6
21	B	836	CLA	C2-C1-O2A-CGA
21	A2	843	CLA	C2-C1-O2A-CGA
30	92	607	CHL	C2-C1-O2A-CGA
23	62	629	LHG	C13-C14-C15-C16
21	1	609	CLA	CAA-CBA-CGA-O2A
21	12	609	CLA	CAA-CBA-CGA-O2A
30	8	601	CHL	CAA-CBA-CGA-O2A
30	82	601	CHL	CAA-CBA-CGA-O2A
21	B	819	CLA	C3-C5-C6-C7
21	B2	819	CLA	C3-C5-C6-C7
27	8	629	LMG	C14-C15-C16-C17
23	4	622	LHG	C5-C4-O6-P
23	42	622	LHG	C5-C4-O6-P
27	82	629	LMG	C14-C15-C16-C17
23	3	721	LHG	O6-C4-C5-O7
23	9	622	LHG	O6-C4-C5-O7
23	32	721	LHG	O6-C4-C5-O7
23	92	622	LHG	O6-C4-C5-O7
26	A	863	LMU	C3'-C4'-O1B-C1B
26	A2	863	LMU	C3'-C4'-O1B-C1B
21	B	805	CLA	CAA-CBA-CGA-O2A
21	B2	805	CLA	CAA-CBA-CGA-O2A
21	6	604	CLA	C4-C3-C5-C6
21	62	604	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
24	G	205	BCR	C1-C6-C7-C8
24	K	207	BCR	C1-C6-C7-C8
24	G2	205	BCR	C1-C6-C7-C8
24	K2	207	BCR	C1-C6-C7-C8
21	A	829	CLA	C5-C6-C7-C8
21	A2	829	CLA	C5-C6-C7-C8
23	B	851	LHG	C23-C24-C25-C26
21	B2	818	CLA	C10-C11-C12-C13
21	B	818	CLA	C10-C11-C12-C13
21	A	823	CLA	C2A-CAA-CBA-CGA
21	A2	823	CLA	C2A-CAA-CBA-CGA
26	9	624	LMU	C2'-C1'-O1'-C1
26	92	624	LMU	C2'-C1'-O1'-C1
27	J	104	LMG	O1-C7-C8-O7
27	J2	104	LMG	O1-C7-C8-O7
23	1	620	LHG	C4-O6-P-O3
23	Z	620	LHG	C3-O3-P-O6
23	6	619	LHG	C4-O6-P-O3
23	12	620	LHG	C4-O6-P-O3
23	Z2	620	LHG	C3-O3-P-O6
23	62	619	LHG	C4-O6-P-O3
23	5	623	LHG	C4-C5-C6-O8
23	52	623	LHG	C4-C5-C6-O8
21	B	834	CLA	C4-C3-C5-C6
21	5	613	CLA	C4-C3-C5-C6
21	B2	834	CLA	C4-C3-C5-C6
21	52	613	CLA	C4-C3-C5-C6
21	A	813	CLA	C6-C7-C8-C10
21	A	826	CLA	C11-C10-C8-C7
21	A2	813	CLA	C6-C7-C8-C10
21	A2	826	CLA	C11-C10-C8-C7
21	A	809	CLA	C14-C13-C15-C16
21	F	301	CLA	C11-C10-C8-C9
21	8	613	CLA	C14-C13-C15-C16
21	A2	809	CLA	C14-C13-C15-C16
21	F2	301	CLA	C11-C10-C8-C9
30	1	601	CHL	C11-C12-C13-C14
30	6	616	CHL	C14-C13-C15-C16
30	12	601	CHL	C11-C12-C13-C14
30	62	616	CHL	C14-C13-C15-C16
21	5	601	CLA	C16-C17-C18-C20
21	52	601	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
26	A2	857	LMU	O1'-C1-C2-C3
26	82	627	LMU	C2-C3-C4-C5
26	8	627	LMU	C2-C3-C4-C5
29	B	850	DGD	CDB-CEB-CFB-CGB
23	9	622	LHG	C5-C4-O6-P
23	92	622	LHG	C5-C4-O6-P
23	5	623	LHG	C1-C2-C3-O3
23	52	623	LHG	C1-C2-C3-O3
26	A	857	LMU	O1'-C1-C2-C3
30	4	601	CHL	C4-C3-C5-C6
30	42	601	CHL	C4-C3-C5-C6
21	B2	805	CLA	C2-C3-C5-C6
21	72	620	CLA	C2-C3-C5-C6
21	5	601	CLA	C16-C17-C18-C19
21	52	601	CLA	C16-C17-C18-C19
21	3	603	CLA	C4C-C3C-CAC-CBC
21	32	603	CLA	C4C-C3C-CAC-CBC
23	B	851	LHG	O9-C7-C8-C9
23	B2	851	LHG	O9-C7-C8-C9
21	32	607	CLA	C4-C3-C5-C6
21	1	612	CLA	CAA-CBA-CGA-O2A
21	82	611	CLA	CAA-CBA-CGA-O1A
21	B	840	CLA	C10-C11-C12-C13
21	B2	840	CLA	C10-C11-C12-C13
21	B	805	CLA	C2-C3-C5-C6
21	7	620	CLA	C2-C3-C5-C6
21	B	832	CLA	C15-C16-C17-C18
27	8	629	LMG	C13-C14-C15-C16
21	8	611	CLA	CAA-CBA-CGA-O1A
21	12	612	CLA	CAA-CBA-CGA-O2A
21	5	616	CLA	C2-C1-O2A-CGA
21	B2	836	CLA	C2-C1-O2A-CGA
21	52	616	CLA	C2-C1-O2A-CGA
30	4	608	CHL	C2-C1-O2A-CGA
30	42	608	CHL	C2-C1-O2A-CGA
21	A2	841	CLA	C10-C11-C12-C13
21	B2	832	CLA	C15-C16-C17-C18
27	A	860	LMG	O1-C7-C8-O7
27	A2	860	LMG	O1-C7-C8-O7
23	42	622	LHG	C27-C28-C29-C30
21	A	841	CLA	C10-C11-C12-C13
27	82	629	LMG	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
21	4	609	CLA	C3A-C2A-CAA-CBA
21	5	621	CLA	C3A-C2A-CAA-CBA
21	42	609	CLA	C3A-C2A-CAA-CBA
21	52	621	CLA	C3A-C2A-CAA-CBA
21	B	804	CLA	CAA-CBA-CGA-O1A
21	B2	804	CLA	CAA-CBA-CGA-O1A
23	4	622	LHG	C27-C28-C29-C30
30	7	606	CHL	CAA-CBA-CGA-O2A
30	72	606	CHL	CAA-CBA-CGA-O2A
21	3	607	CLA	C4-C3-C5-C6
21	6	603	CLA	C4-C3-C5-C6
21	62	603	CLA	C4-C3-C5-C6
30	8	601	CHL	C4-C3-C5-C6
30	82	601	CHL	C4-C3-C5-C6
27	12	628	LMG	C11-C12-C13-C14
21	A	812	CLA	C14-C13-C15-C16
21	A	820	CLA	C6-C7-C8-C9
21	A	840	CLA	C11-C10-C8-C9
21	B	802	CLA	C14-C13-C15-C16
21	B	811	CLA	C11-C10-C8-C9
21	B	840	CLA	C11-C12-C13-C14
21	A2	812	CLA	C14-C13-C15-C16
21	A2	820	CLA	C6-C7-C8-C9
21	A2	840	CLA	C11-C10-C8-C9
21	B2	802	CLA	C14-C13-C15-C16
21	B2	811	CLA	C11-C10-C8-C9
21	B2	840	CLA	C11-C12-C13-C14
30	4	601	CHL	C11-C10-C8-C9
30	42	601	CHL	C11-C10-C8-C9
21	6	612	CLA	CAA-CBA-CGA-O1A
21	62	612	CLA	CAA-CBA-CGA-O1A
27	1	628	LMG	C11-C12-C13-C14
23	B	851	LHG	C4-C5-C6-O8
23	B2	851	LHG	C4-C5-C6-O8
24	A	852	BCR	C11-C10-C9-C34
24	A	852	BCR	C16-C17-C18-C36
24	B	845	BCR	C11-C10-C9-C34
24	B	845	BCR	C20-C21-C22-C37
24	L	201	BCR	C11-C10-C9-C34
24	A2	852	BCR	C11-C10-C9-C34
24	A2	852	BCR	C16-C17-C18-C36
24	B2	845	BCR	C11-C10-C9-C34

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Mol	Chain	Res	Type	Atoms
24	B2	845	BCR	C20-C21-C22-C37
24	L2	201	BCR	C11-C10-C9-C34
27	B	852	LMG	O1-C7-C8-C9
27	B2	852	LMG	O1-C7-C8-C9
28	F	305	LUT	C20-C13-C14-C15
28	5	626	LUT	C21-C26-C27-C28
28	F2	305	LUT	C20-C13-C14-C15
28	52	626	LUT	C21-C26-C27-C28
32	5	625	NEX	C39-C29-C30-C31
32	6	625	NEX	C39-C29-C30-C31
32	52	625	NEX	C39-C29-C30-C31
32	62	625	NEX	C39-C29-C30-C31
21	4	612	CLA	CAA-CBA-CGA-O1A
21	42	612	CLA	CAA-CBA-CGA-O1A
26	Z2	622	LMU	C5'-C4'-O1B-C1B
27	8	629	LMG	C15-C16-C17-C18
27	82	629	LMG	C15-C16-C17-C18
21	B	824	CLA	O2A-C1-C2-C3
21	B2	824	CLA	O2A-C1-C2-C3
30	Z	607	CHL	O2A-C1-C2-C3
30	6	607	CHL	O2A-C1-C2-C3
30	Z2	607	CHL	O2A-C1-C2-C3
30	62	607	CHL	O2A-C1-C2-C3
26	1	625	LMU	O5'-C1'-O1'-C1
26	9	624	LMU	O5'-C1'-O1'-C1
26	12	625	LMU	O5'-C1'-O1'-C1
26	92	624	LMU	O5'-C1'-O1'-C1
26	Z	622	LMU	C5'-C4'-O1B-C1B
21	82	611	CLA	CAA-CBA-CGA-O2A
21	K	206	CLA	CAA-CBA-CGA-O1A
21	8	611	CLA	CAA-CBA-CGA-O2A
21	K2	206	CLA	CAA-CBA-CGA-O1A
23	4	623	LHG	C4-C5-O7-C7
23	6	629	LHG	C4-C5-O7-C7
23	42	623	LHG	C4-C5-O7-C7
23	62	629	LHG	C4-C5-O7-C7
29	B2	850	DGD	C1G-C2G-O2G-C1B
30	3	608	CHL	C13-C15-C16-C17
30	32	608	CHL	C13-C15-C16-C17
21	A	819	CLA	C1A-C2A-CAA-CBA
21	7	614	CLA	C1A-C2A-CAA-CBA
21	5	621	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
21	A2	819	CLA	C1A-C2A-CAA-CBA
21	72	614	CLA	C1A-C2A-CAA-CBA
21	52	621	CLA	C1A-C2A-CAA-CBA
30	7	606	CHL	C1A-C2A-CAA-CBA
30	72	606	CHL	C1A-C2A-CAA-CBA
21	B	809	CLA	C6-C7-C8-C10
21	B	832	CLA	C11-C12-C13-C15
21	1	613	CLA	C2-C3-C5-C6
21	4	611	CLA	C6-C7-C8-C10
21	B2	809	CLA	C6-C7-C8-C10
21	B2	832	CLA	C11-C12-C13-C15
21	12	613	CLA	C2-C3-C5-C6
21	42	611	CLA	C6-C7-C8-C10
30	8	601	CHL	C11-C12-C13-C15
30	82	601	CHL	C11-C12-C13-C15
21	4	603	CLA	C10-C11-C12-C13
21	A2	827	CLA	C13-C15-C16-C17
21	42	603	CLA	C10-C11-C12-C13
21	7	610	CLA	O1A-CGA-O2A-C1
21	72	610	CLA	O1A-CGA-O2A-C1
21	Z	612	CLA	CAA-CBA-CGA-O1A
21	32	609	CLA	C4C-C3C-CAC-CBC
21	12	612	CLA	CAA-CBA-CGA-O1A
21	3	609	CLA	C4C-C3C-CAC-CBC
21	A	827	CLA	C13-C15-C16-C17
21	B	803	CLA	C8-C10-C11-C12
21	A2	810	CLA	C5-C6-C7-C8
21	B2	803	CLA	C8-C10-C11-C12
21	1	612	CLA	CAA-CBA-CGA-O1A
21	A	810	CLA	C5-C6-C7-C8
23	4	622	LHG	O6-C4-C5-C6
23	42	622	LHG	O6-C4-C5-C6
21	A	824	CLA	CAA-CBA-CGA-O2A
21	B	804	CLA	CAA-CBA-CGA-O2A
21	B2	804	CLA	CAA-CBA-CGA-O2A
21	B	810	CLA	C4-C3-C5-C6
21	4	603	CLA	C4-C3-C5-C6
21	4	611	CLA	C4-C3-C5-C6
21	5	603	CLA	C4-C3-C5-C6
21	B2	810	CLA	C4-C3-C5-C6
21	42	603	CLA	C4-C3-C5-C6
21	42	611	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
21	52	603	CLA	C4-C3-C5-C6
23	3	623	LHG	C28-C29-C30-C31
21	A2	824	CLA	CAA-CBA-CGA-O2A
21	Z2	612	CLA	CAA-CBA-CGA-O1A
26	Z2	622	LMU	C3'-C4'-O1B-C1B
21	A	825	CLA	C2C-C3C-CAC-CBC
24	A	852	BCR	C11-C10-C9-C8
24	A	852	BCR	C16-C17-C18-C19
24	B	845	BCR	C11-C10-C9-C8
24	B	845	BCR	C20-C21-C22-C23
24	L	201	BCR	C11-C10-C9-C8
24	A2	852	BCR	C11-C10-C9-C8
24	A2	852	BCR	C16-C17-C18-C19
24	B2	845	BCR	C11-C10-C9-C8
24	B2	845	BCR	C20-C21-C22-C23
24	L2	201	BCR	C11-C10-C9-C8
28	F	305	LUT	C12-C13-C14-C15
28	F2	305	LUT	C12-C13-C14-C15
32	5	625	NEX	C28-C29-C30-C31
32	6	625	NEX	C28-C29-C30-C31
32	52	625	NEX	C28-C29-C30-C31
32	62	625	NEX	C28-C29-C30-C31
26	Z	622	LMU	C3'-C4'-O1B-C1B
23	9	622	LHG	O7-C5-C6-O8
23	92	622	LHG	O7-C5-C6-O8
27	B	852	LMG	O1-C7-C8-O7
27	B2	852	LMG	O1-C7-C8-O7
29	B2	850	DGD	O1G-C1G-C2G-O2G
23	A2	846	LHG	C11-C12-C13-C14
23	32	623	LHG	C28-C29-C30-C31
30	5	607	CHL	CAA-CBA-CGA-O1A
23	A	846	LHG	C11-C12-C13-C14
32	62	625	NEX	C33-C34-C35-C15
21	5	612	CLA	CAA-CBA-CGA-O1A
21	52	612	CLA	CAA-CBA-CGA-O1A
26	62	631	LMU	C3-C4-C5-C6
21	A	824	CLA	CAA-CBA-CGA-O1A
21	A2	824	CLA	CAA-CBA-CGA-O1A
30	7	606	CHL	CAA-CBA-CGA-O1A
30	Z	606	CHL	CAA-CBA-CGA-O2A
30	72	606	CHL	CAA-CBA-CGA-O1A
30	Z2	606	CHL	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
26	6	631	LMU	C3-C4-C5-C6
27	82	629	LMG	C21-C22-C23-C24
21	5	604	CLA	C4-C3-C5-C6
21	52	604	CLA	C4-C3-C5-C6
30	8	606	CHL	C4-C3-C5-C6
30	5	607	CHL	C4-C3-C5-C6
30	82	606	CHL	C4-C3-C5-C6
30	52	607	CHL	C4-C3-C5-C6
26	K2	208	LMU	C5-C6-C7-C8
27	8	629	LMG	C21-C22-C23-C24
21	B	811	CLA	C2-C1-O2A-CGA
21	Z	609	CLA	C2-C1-O2A-CGA
21	B2	811	CLA	C2-C1-O2A-CGA
21	Z2	609	CLA	C2-C1-O2A-CGA
30	8	607	CHL	C2-C1-O2A-CGA
30	82	607	CHL	C2-C1-O2A-CGA
21	A	821	CLA	C2-C3-C5-C6
21	B	810	CLA	C2-C3-C5-C6
21	B	834	CLA	C2-C3-C5-C6
21	3	607	CLA	C2-C3-C5-C6
21	5	613	CLA	C2-C3-C5-C6
21	6	603	CLA	C2-C3-C5-C6
21	6	604	CLA	C2-C3-C5-C6
21	B2	810	CLA	C2-C3-C5-C6
21	B2	834	CLA	C2-C3-C5-C6
21	32	607	CLA	C2-C3-C5-C6
21	52	613	CLA	C2-C3-C5-C6
21	62	603	CLA	C2-C3-C5-C6
21	A2	825	CLA	C2C-C3C-CAC-CBC
26	K	208	LMU	C5-C6-C7-C8
21	B	841	CLA	C11-C10-C8-C9
21	B2	837	CLA	C11-C12-C13-C14
21	B2	841	CLA	C11-C10-C8-C9
21	K	206	CLA	CAA-CBA-CGA-O2A
21	4	612	CLA	CAA-CBA-CGA-O2A
21	9	614	CLA	CAA-CBA-CGA-O2A
21	K2	206	CLA	CAA-CBA-CGA-O2A
21	42	612	CLA	CAA-CBA-CGA-O2A
30	Z	606	CHL	CAA-CBA-CGA-O1A
30	Z2	606	CHL	CAA-CBA-CGA-O1A
21	7	604	CLA	C4-C3-C5-C6
21	72	604	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
30	52	607	CHL	CAA-CBA-CGA-O1A
21	5	621	CLA	C2A-CAA-CBA-CGA
21	52	621	CLA	C2A-CAA-CBA-CGA
21	6	612	CLA	CAA-CBA-CGA-O2A
21	62	612	CLA	CAA-CBA-CGA-O2A
21	92	614	CLA	CAA-CBA-CGA-O2A
24	L	205	BCR	C23-C24-C25-C26
24	5	622	BCR	C1-C6-C7-C8
24	L2	205	BCR	C23-C24-C25-C26
24	52	622	BCR	C1-C6-C7-C8
28	4	619	LUT	C5-C6-C7-C8
28	42	619	LUT	C5-C6-C7-C8
29	B2	850	DGD	C9B-CAB-CBB-CCB
21	4	613	CLA	CAA-CBA-CGA-O2A
21	42	613	CLA	CAA-CBA-CGA-O2A
21	B	834	CLA	C8-C10-C11-C12
21	B2	834	CLA	C8-C10-C11-C12
29	B	850	DGD	O1B-C1B-C2B-C3B
32	6	625	NEX	C33-C34-C35-C15
21	B	823	CLA	C4-C3-C5-C6
21	F	301	CLA	C4-C3-C5-C6
21	8	613	CLA	C4-C3-C5-C6
21	B2	823	CLA	C4-C3-C5-C6
21	F2	301	CLA	C4-C3-C5-C6
21	3	613	CLA	C2-C3-C5-C6
21	A2	821	CLA	C2-C3-C5-C6
21	32	613	CLA	C2-C3-C5-C6
21	62	604	CLA	C2-C3-C5-C6
30	42	601	CHL	C2-C3-C5-C6
21	52	612	CLA	CAA-CBA-CGA-O2A
27	7	626	LMG	C14-C15-C16-C17
21	92	614	CLA	CAA-CBA-CGA-O1A
27	72	626	LMG	C14-C15-C16-C17
21	5	612	CLA	CAA-CBA-CGA-O2A
21	9	614	CLA	CAA-CBA-CGA-O1A
26	1	621	LMU	C3'-C4'-O1B-C1B
21	B	841	CLA	C4-C3-C5-C6
21	8	614	CLA	C4-C3-C5-C6
21	B2	836	CLA	C4-C3-C5-C6
21	B2	841	CLA	C4-C3-C5-C6
21	82	613	CLA	C4-C3-C5-C6
21	82	614	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
21	52	609	CLA	C4-C3-C5-C6
26	12	621	LMU	C3'-C4'-O1B-C1B
21	A	812	CLA	C6-C7-C8-C10
21	1	613	CLA	C11-C12-C13-C15
21	A2	812	CLA	C6-C7-C8-C10
21	12	613	CLA	C11-C12-C13-C15
30	8	601	CHL	C2-C3-C5-C6
30	4	601	CHL	C2-C3-C5-C6
30	5	607	CHL	C2-C3-C5-C6
30	82	601	CHL	C2-C3-C5-C6
30	52	607	CHL	C2-C3-C5-C6
21	A2	807	CLA	CAA-CBA-CGA-O2A
26	1	625	LMU	C2'-C1'-O1'-C1
26	12	625	LMU	C2'-C1'-O1'-C1
23	4	623	LHG	O7-C5-C6-O8
23	42	623	LHG	O7-C5-C6-O8
27	7	626	LMG	O7-C8-C9-O8
27	9	620	LMG	O1-C7-C8-O7
27	72	626	LMG	O7-C8-C9-O8
27	92	620	LMG	O1-C7-C8-O7
21	A	807	CLA	CAA-CBA-CGA-O2A
21	B	811	CLA	CAA-CBA-CGA-O2A
21	5	616	CLA	CAA-CBA-CGA-O2A
21	B2	811	CLA	CAA-CBA-CGA-O2A
21	52	604	CLA	CAA-CBA-CGA-O2A
21	52	616	CLA	CAA-CBA-CGA-O2A
23	A	846	LHG	O8-C23-C24-C25
30	9	607	CHL	C2A-CAA-CBA-CGA
21	1	603	CLA	CAA-CBA-CGA-O2A
21	12	603	CLA	CAA-CBA-CGA-O2A
23	A2	846	LHG	O8-C23-C24-C25
21	A	814	CLA	C4-C3-C5-C6
21	B	836	CLA	C4-C3-C5-C6
21	3	615	CLA	C4-C3-C5-C6
21	5	609	CLA	C4-C3-C5-C6
21	A2	814	CLA	C4-C3-C5-C6
21	32	615	CLA	C4-C3-C5-C6
21	8	613	CLA	C2-C3-C5-C6
21	4	603	CLA	C2-C3-C5-C6
21	5	610	CLA	C2-C3-C5-C6
21	82	613	CLA	C2-C3-C5-C6
21	42	603	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
21	52	610	CLA	C2-C3-C5-C6
27	J	103	LMG	C22-C23-C24-C25
27	J2	103	LMG	C22-C23-C24-C25
21	5	604	CLA	CAA-CBA-CGA-O2A
21	A	806	CLA	C14-C13-C15-C16
21	B	837	CLA	C11-C12-C13-C14
21	A2	806	CLA	C14-C13-C15-C16
30	6	607	CHL	C14-C13-C15-C16
30	72	601	CHL	C11-C10-C8-C9
30	62	607	CHL	C14-C13-C15-C16
23	82	620	LHG	C12-C13-C14-C15
23	8	620	LHG	C12-C13-C14-C15
27	1	624	LMG	C31-C32-C33-C34
21	A	810	CLA	CAD-CBD-CGD-O2D
21	A	815	CLA	CAD-CBD-CGD-O2D
21	A	816	CLA	CAD-CBD-CGD-O2D
21	A	834	CLA	CAD-CBD-CGD-O2D
21	B	836	CLA	CAD-CBD-CGD-O2D
21	G	203	CLA	CAD-CBD-CGD-O2D
21	3	609	CLA	CAD-CBD-CGD-O2D
21	5	612	CLA	CAD-CBD-CGD-O2D
21	9	604	CLA	CAD-CBD-CGD-O2D
21	A2	807	CLA	CAD-CBD-CGD-O2D
21	A2	815	CLA	CAD-CBD-CGD-O2D
21	A2	816	CLA	CAD-CBD-CGD-O2D
21	A2	834	CLA	CAD-CBD-CGD-O2D
21	B2	836	CLA	CAD-CBD-CGD-O2D
21	G2	203	CLA	CAD-CBD-CGD-O2D
21	32	609	CLA	CAD-CBD-CGD-O2D
21	52	612	CLA	CAD-CBD-CGD-O2D
21	92	604	CLA	CAD-CBD-CGD-O2D
30	8	601	CHL	CAD-CBD-CGD-O2D
30	82	601	CHL	CAD-CBD-CGD-O2D
27	12	624	LMG	C31-C32-C33-C34
32	6	625	NEX	C9-C10-C11-C12
26	A	865	LMU	C5-C6-C7-C8
26	A2	865	LMU	C5-C6-C7-C8
21	B	814	CLA	CAA-CBA-CGA-O2A
21	4	614	CLA	CAA-CBA-CGA-O2A
21	B2	814	CLA	CAA-CBA-CGA-O2A
27	1	624	LMG	O7-C10-C11-C12
27	9	620	LMG	O7-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
27	12	624	LMG	O7-C10-C11-C12
27	92	620	LMG	O7-C10-C11-C12
21	B	811	CLA	C4-C3-C5-C6
21	Z	604	CLA	C4-C3-C5-C6
21	5	616	CLA	C4-C3-C5-C6
21	6	611	CLA	C4-C3-C5-C6
21	B2	811	CLA	C4-C3-C5-C6
21	Z2	604	CLA	C4-C3-C5-C6
21	52	616	CLA	C4-C3-C5-C6
21	62	611	CLA	C4-C3-C5-C6
30	Z	601	CHL	C4-C3-C5-C6
30	Z2	601	CHL	C4-C3-C5-C6
21	32	604	CLA	C3-C5-C6-C7
21	B	811	CLA	C2-C3-C5-C6
21	Z	604	CLA	C2-C3-C5-C6
21	4	611	CLA	C2-C3-C5-C6
21	5	603	CLA	C2-C3-C5-C6
21	B2	811	CLA	C2-C3-C5-C6
21	Z2	604	CLA	C2-C3-C5-C6
21	42	611	CLA	C2-C3-C5-C6
21	52	603	CLA	C2-C3-C5-C6
21	B	817	CLA	CAA-CBA-CGA-O2A
21	B2	817	CLA	CAA-CBA-CGA-O2A
27	J	104	LMG	O7-C10-C11-C12
27	8	626	LMG	O8-C28-C29-C30
27	J2	104	LMG	O7-C10-C11-C12
27	82	626	LMG	O8-C28-C29-C30
23	72	625	LHG	C10-C11-C12-C13
23	4	622	LHG	O6-C4-C5-O7
23	42	622	LHG	O6-C4-C5-O7
21	3	604	CLA	C3-C5-C6-C7
23	42	622	LHG	O8-C23-C24-C25
21	Z	612	CLA	CAA-CBA-CGA-O2A
23	7	625	LHG	C10-C11-C12-C13
21	B	821	CLA	O2A-C1-C2-C3
21	1	611	CLA	O2A-C1-C2-C3
21	B2	821	CLA	O2A-C1-C2-C3
21	12	611	CLA	O2A-C1-C2-C3
26	1	621	LMU	C2B-C1B-O1B-C4'
26	12	621	LMU	C2B-C1B-O1B-C4'
27	A2	859	LMG	C13-C14-C15-C16
21	8	604	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
21	82	604	CLA	CAA-CBA-CGA-O2A
23	4	622	LHG	O8-C23-C24-C25
27	A	859	LMG	C13-C14-C15-C16
21	A	804	CLA	CHA-CBD-CGD-O2D
21	A	811	CLA	CHA-CBD-CGD-O2D
21	A	814	CLA	CHA-CBD-CGD-O1D
21	A	820	CLA	CHA-CBD-CGD-O1D
21	A	820	CLA	CHA-CBD-CGD-O2D
21	A	832	CLA	CHA-CBD-CGD-O2D
21	B	805	CLA	CHA-CBD-CGD-O2D
21	B	821	CLA	CHA-CBD-CGD-O2D
21	B	822	CLA	CHA-CBD-CGD-O1D
21	B	822	CLA	CHA-CBD-CGD-O2D
21	B	828	CLA	CHA-CBD-CGD-O1D
21	B	828	CLA	CHA-CBD-CGD-O2D
21	K	204	CLA	CHA-CBD-CGD-O1D
21	1	602	CLA	CHA-CBD-CGD-O2D
21	1	616	CLA	CHA-CBD-CGD-O1D
21	1	616	CLA	CHA-CBD-CGD-O2D
21	3	602	CLA	CHA-CBD-CGD-O2D
21	7	620	CLA	CHA-CBD-CGD-O2D
21	8	603	CLA	CHA-CBD-CGD-O1D
21	8	603	CLA	CHA-CBD-CGD-O2D
21	8	612	CLA	CHA-CBD-CGD-O2D
21	8	614	CLA	CHA-CBD-CGD-O1D
21	8	614	CLA	CHA-CBD-CGD-O2D
21	Z	602	CLA	CHA-CBD-CGD-O2D
21	Z	603	CLA	CHA-CBD-CGD-O1D
21	Z	603	CLA	CHA-CBD-CGD-O2D
21	Z	612	CLA	CHA-CBD-CGD-O1D
21	Z	613	CLA	CHA-CBD-CGD-O1D
21	Z	613	CLA	CHA-CBD-CGD-O2D
21	4	612	CLA	CHA-CBD-CGD-O1D
21	4	612	CLA	CHA-CBD-CGD-O2D
21	5	613	CLA	CHA-CBD-CGD-O2D
21	6	602	CLA	CHA-CBD-CGD-O1D
21	6	602	CLA	CHA-CBD-CGD-O2D
21	6	604	CLA	CHA-CBD-CGD-O1D
21	6	604	CLA	CHA-CBD-CGD-O2D
21	6	610	CLA	CHA-CBD-CGD-O1D
21	6	610	CLA	CHA-CBD-CGD-O2D
21	6	617	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
21	6	622	CLA	CHA-CBD-CGD-O2D
21	9	602	CLA	CHA-CBD-CGD-O1D
21	9	602	CLA	CHA-CBD-CGD-O2D
21	9	603	CLA	CHA-CBD-CGD-O1D
21	9	603	CLA	CHA-CBD-CGD-O2D
21	9	612	CLA	CHA-CBD-CGD-O1D
21	9	612	CLA	CHA-CBD-CGD-O2D
21	A2	804	CLA	CHA-CBD-CGD-O2D
21	A2	811	CLA	CHA-CBD-CGD-O2D
21	A2	814	CLA	CHA-CBD-CGD-O1D
21	A2	820	CLA	CHA-CBD-CGD-O1D
21	A2	820	CLA	CHA-CBD-CGD-O2D
21	A2	832	CLA	CHA-CBD-CGD-O2D
21	B2	805	CLA	CHA-CBD-CGD-O2D
21	B2	815	CLA	CHA-CBD-CGD-O2D
21	B2	822	CLA	CHA-CBD-CGD-O1D
21	B2	822	CLA	CHA-CBD-CGD-O2D
21	B2	828	CLA	CHA-CBD-CGD-O1D
21	B2	828	CLA	CHA-CBD-CGD-O2D
21	B2	829	CLA	CHA-CBD-CGD-O2D
21	K2	204	CLA	CHA-CBD-CGD-O1D
21	12	602	CLA	CHA-CBD-CGD-O2D
21	12	616	CLA	CHA-CBD-CGD-O1D
21	12	616	CLA	CHA-CBD-CGD-O2D
21	32	602	CLA	CHA-CBD-CGD-O2D
21	72	603	CLA	CHA-CBD-CGD-O1D
21	72	620	CLA	CHA-CBD-CGD-O2D
21	82	602	CLA	CHA-CBD-CGD-O2D
21	82	603	CLA	CHA-CBD-CGD-O1D
21	82	603	CLA	CHA-CBD-CGD-O2D
21	82	612	CLA	CHA-CBD-CGD-O1D
21	82	612	CLA	CHA-CBD-CGD-O2D
21	82	614	CLA	CHA-CBD-CGD-O1D
21	82	614	CLA	CHA-CBD-CGD-O2D
21	Z2	602	CLA	CHA-CBD-CGD-O2D
21	Z2	603	CLA	CHA-CBD-CGD-O1D
21	Z2	603	CLA	CHA-CBD-CGD-O2D
21	Z2	612	CLA	CHA-CBD-CGD-O1D
21	Z2	613	CLA	CHA-CBD-CGD-O1D
21	Z2	613	CLA	CHA-CBD-CGD-O2D
21	42	612	CLA	CHA-CBD-CGD-O1D
21	42	612	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
21	52	613	CLA	CHA-CBD-CGD-O2D
21	62	602	CLA	CHA-CBD-CGD-O1D
21	62	602	CLA	CHA-CBD-CGD-O2D
21	62	604	CLA	CHA-CBD-CGD-O1D
21	62	604	CLA	CHA-CBD-CGD-O2D
21	62	610	CLA	CHA-CBD-CGD-O1D
21	62	610	CLA	CHA-CBD-CGD-O2D
21	62	617	CLA	CHA-CBD-CGD-O2D
21	62	622	CLA	CHA-CBD-CGD-O2D
21	92	602	CLA	CHA-CBD-CGD-O1D
21	92	602	CLA	CHA-CBD-CGD-O2D
21	92	603	CLA	CHA-CBD-CGD-O1D
21	92	603	CLA	CHA-CBD-CGD-O2D
21	92	612	CLA	CHA-CBD-CGD-O1D
21	92	612	CLA	CHA-CBD-CGD-O2D
30	1	607	CHL	CHA-CBD-CGD-O2D
30	7	601	CHL	CHA-CBD-CGD-O1D
30	Z	601	CHL	CHA-CBD-CGD-O1D
30	Z	607	CHL	CHA-CBD-CGD-O2D
30	4	601	CHL	CHA-CBD-CGD-O1D
30	4	618	CHL	CHA-CBD-CGD-O1D
30	4	618	CHL	CHA-CBD-CGD-O2D
30	6	601	CHL	CHA-CBD-CGD-O2D
30	6	618	CHL	CHA-CBD-CGD-O1D
30	6	618	CHL	CHA-CBD-CGD-O2D
30	12	607	CHL	CHA-CBD-CGD-O2D
30	72	601	CHL	CHA-CBD-CGD-O1D
30	Z2	601	CHL	CHA-CBD-CGD-O1D
30	Z2	607	CHL	CHA-CBD-CGD-O2D
30	42	601	CHL	CHA-CBD-CGD-O1D
30	42	618	CHL	CHA-CBD-CGD-O1D
30	42	618	CHL	CHA-CBD-CGD-O2D
30	62	601	CHL	CHA-CBD-CGD-O2D
30	62	618	CHL	CHA-CBD-CGD-O1D
30	62	618	CHL	CHA-CBD-CGD-O2D
32	62	625	NEX	C9-C10-C11-C12
21	6	609	CLA	C4-C3-C5-C6
21	62	609	CLA	C4-C3-C5-C6
21	G2	204	CLA	CAA-CBA-CGA-O2A
21	42	614	CLA	CAA-CBA-CGA-O2A
21	G	204	CLA	CAA-CBA-CGA-O2A
21	Z	603	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
21	72	603	CLA	CAA-CBA-CGA-O2A
23	1	620	LHG	O7-C5-C6-O8
23	12	620	LHG	O7-C5-C6-O8
27	1	624	LMG	O1-C7-C8-O7
27	12	624	LMG	O1-C7-C8-O7
21	Z2	612	CLA	CAA-CBA-CGA-O2A
21	7	603	CLA	CAA-CBA-CGA-O2A
21	8	614	CLA	CAA-CBA-CGA-O2A
21	A2	826	CLA	CAA-CBA-CGA-O2A
21	82	614	CLA	CAA-CBA-CGA-O2A
21	52	621	CLA	CAA-CBA-CGA-O2A
23	3	721	LHG	O7-C7-C8-C9
23	32	721	LHG	O7-C7-C8-C9
27	1	628	LMG	O8-C28-C29-C30
27	12	628	LMG	O8-C28-C29-C30
27	7	626	LMG	O10-C28-C29-C30
21	52	614	CLA	CAA-CBA-CGA-O2A
26	1	621	LMU	C5'-C4'-O1B-C1B
26	12	621	LMU	C5'-C4'-O1B-C1B
27	72	626	LMG	O10-C28-C29-C30
21	B	834	CLA	CAA-CBA-CGA-O2A
21	5	603	CLA	CAA-CBA-CGA-O2A
21	Z2	603	CLA	CAA-CBA-CGA-O2A
21	52	603	CLA	CAA-CBA-CGA-O2A
21	5	603	CLA	C12-C13-C15-C16
21	6	611	CLA	C2-C3-C5-C6
21	B2	836	CLA	C2-C3-C5-C6
21	52	603	CLA	C12-C13-C15-C16
21	62	611	CLA	C2-C3-C5-C6
22	B	842	PQN	C16-C17-C18-C20
26	1	625	LMU	C2-C3-C4-C5
21	5	621	CLA	CAA-CBA-CGA-O2A
21	42	603	CLA	CAA-CBA-CGA-O2A
21	5	614	CLA	CAA-CBA-CGA-O2A
21	A	816	CLA	C14-C13-C15-C16
21	A2	816	CLA	C14-C13-C15-C16
30	8	601	CHL	C11-C10-C8-C9
30	82	601	CHL	C11-C10-C8-C9
21	5	604	CLA	CAA-CBA-CGA-O1A
21	52	604	CLA	CAA-CBA-CGA-O1A
26	12	625	LMU	C2-C3-C4-C5
21	A	826	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
21	F	304	CLA	CAA-CBA-CGA-O2A
21	F2	304	CLA	CAA-CBA-CGA-O2A
27	J	104	LMG	O8-C28-C29-C30
21	B	809	CLA	C3-C5-C6-C7
21	B2	809	CLA	C3-C5-C6-C7
21	B	814	CLA	CAA-CBA-CGA-O1A
21	B2	814	CLA	CAA-CBA-CGA-O1A
23	42	622	LHG	O10-C23-C24-C25
27	J2	104	LMG	O9-C10-C11-C12
21	A2	825	CLA	C4C-C3C-CAC-CBC
21	B2	834	CLA	CAA-CBA-CGA-O2A
27	J2	104	LMG	O8-C28-C29-C30
20	A2	801	CL0	C5-C6-C7-C8
21	12	603	CLA	CAA-CBA-CGA-O1A
23	A	846	LHG	O10-C23-C24-C25
23	4	622	LHG	O10-C23-C24-C25
30	Z2	601	CHL	C5-C6-C7-C8
30	32	608	CHL	C4-C3-C5-C6
21	A	814	CLA	C2-C3-C5-C6
21	A2	814	CLA	C2-C3-C5-C6
21	4	603	CLA	CAA-CBA-CGA-O2A
20	A	801	CL0	C5-C6-C7-C8
30	Z	601	CHL	C5-C6-C7-C8
21	A	825	CLA	C4C-C3C-CAC-CBC
23	A2	846	LHG	O10-C23-C24-C25
27	J	104	LMG	O9-C10-C11-C12
21	9	613	CLA	CBA-CGA-O2A-C1
21	92	613	CLA	CBA-CGA-O2A-C1
26	82	627	LMU	C4-C5-C6-C7
21	A	836	CLA	C1A-C2A-CAA-CBA
21	3	615	CLA	C1A-C2A-CAA-CBA
21	8	614	CLA	C1A-C2A-CAA-CBA
21	Z	611	CLA	C1A-C2A-CAA-CBA
21	4	613	CLA	C1A-C2A-CAA-CBA
21	5	603	CLA	C1A-C2A-CAA-CBA
21	A2	836	CLA	C1A-C2A-CAA-CBA
21	32	615	CLA	C1A-C2A-CAA-CBA
21	82	614	CLA	C1A-C2A-CAA-CBA
21	Z2	611	CLA	C1A-C2A-CAA-CBA
21	42	613	CLA	C1A-C2A-CAA-CBA
21	52	603	CLA	C1A-C2A-CAA-CBA
30	8	607	CHL	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
30	6	601	CHL	C1A-C2A-CAA-CBA
30	82	607	CHL	C1A-C2A-CAA-CBA
30	62	601	CHL	C1A-C2A-CAA-CBA
21	B	811	CLA	CAA-CBA-CGA-O1A
21	1	603	CLA	CAA-CBA-CGA-O1A
21	B2	811	CLA	CAA-CBA-CGA-O1A
27	J2	104	LMG	O10-C28-C29-C30
26	8	627	LMU	C4-C5-C6-C7
27	B	852	LMG	C12-C13-C14-C15
21	4	609	CLA	C2-C1-O2A-CGA
21	42	609	CLA	C2-C1-O2A-CGA
21	B	827	CLA	C8-C10-C11-C12
21	A	826	CLA	CAA-CBA-CGA-O1A
23	8	620	LHG	C4-C5-C6-O8
23	9	622	LHG	C4-C5-C6-O8
23	82	620	LHG	C4-C5-C6-O8
23	92	622	LHG	C4-C5-C6-O8
27	A2	860	LMG	O8-C28-C29-C30
29	B2	850	DGD	C7B-C8B-C9B-CAB
21	B2	827	CLA	C8-C10-C11-C12
21	A	818	CLA	C2A-CAA-CBA-CGA
21	A2	818	CLA	C2A-CAA-CBA-CGA
21	A	807	CLA	CAA-CBA-CGA-O1A
23	3	721	LHG	O9-C7-C8-C9
27	J	104	LMG	O10-C28-C29-C30
27	9	620	LMG	O9-C10-C11-C12
27	92	620	LMG	O9-C10-C11-C12
27	A	859	LMG	C29-C30-C31-C32
27	B2	852	LMG	C12-C13-C14-C15
23	1	620	LHG	C11-C10-C9-C8
27	A2	859	LMG	C29-C30-C31-C32
30	3	608	CHL	C4-C3-C5-C6
21	A	813	CLA	CAA-CBA-CGA-O2A
21	B	806	CLA	CAA-CBA-CGA-O2A
21	B	809	CLA	CAA-CBA-CGA-O2A
21	A2	813	CLA	CAA-CBA-CGA-O2A
21	B2	806	CLA	CAA-CBA-CGA-O2A
27	A	860	LMG	O8-C28-C29-C30
21	4	614	CLA	CAA-CBA-CGA-O1A
21	5	621	CLA	CAA-CBA-CGA-O1A
21	A2	807	CLA	CAA-CBA-CGA-O1A
21	A2	826	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
27	1	624	LMG	O9-C10-C11-C12
27	12	624	LMG	O9-C10-C11-C12
21	B	836	CLA	C2-C3-C5-C6
21	6	603	CLA	C13-C15-C16-C17
21	62	603	CLA	C13-C15-C16-C17
23	12	620	LHG	C11-C10-C9-C8
23	A	847	LHG	C3-O3-P-O5
23	A	847	LHG	C4-O6-P-O5
23	1	620	LHG	C3-O3-P-O5
23	7	625	LHG	C4-O6-P-O4
23	9	622	LHG	C3-O3-P-O5
23	A2	847	LHG	C3-O3-P-O5
23	A2	847	LHG	C4-O6-P-O5
23	12	620	LHG	C3-O3-P-O5
23	72	625	LHG	C4-O6-P-O4
21	F	304	CLA	CAA-CBA-CGA-O1A
21	8	604	CLA	CAA-CBA-CGA-O1A
21	5	616	CLA	CAA-CBA-CGA-O1A
21	F2	304	CLA	CAA-CBA-CGA-O1A
21	82	604	CLA	CAA-CBA-CGA-O1A
21	42	614	CLA	CAA-CBA-CGA-O1A
21	52	616	CLA	CAA-CBA-CGA-O1A
21	52	621	CLA	CAA-CBA-CGA-O1A
23	32	721	LHG	O9-C7-C8-C9
29	B	850	DGD	O6E-C1E-O5D-C6D
23	7	625	LHG	O6-C4-C5-C6
24	A	850	BCR	C23-C24-C25-C30
24	G	205	BCR	C5-C6-C7-C8
24	L	205	BCR	C23-C24-C25-C30
24	A2	850	BCR	C23-C24-C25-C30
24	G2	205	BCR	C5-C6-C7-C8
24	L2	205	BCR	C23-C24-C25-C30
21	8	614	CLA	CAA-CBA-CGA-O1A
21	82	614	CLA	CAA-CBA-CGA-O1A
23	9	622	LHG	C26-C27-C28-C29
21	7	613	CLA	CAA-CBA-CGA-O2A
21	8	603	CLA	CAA-CBA-CGA-O2A
21	82	603	CLA	CAA-CBA-CGA-O2A
21	L	204	CLA	CAA-CBA-CGA-O2A
21	3	617	CLA	C2C-C3C-CAC-CBC
21	3	617	CLA	C4C-C3C-CAC-CBC
23	92	622	LHG	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
21	G	204	CLA	CAA-CBA-CGA-O1A
21	G2	204	CLA	CAA-CBA-CGA-O1A
21	A	810	CLA	C8-C10-C11-C12
21	3	613	CLA	C10-C11-C12-C13
21	32	617	CLA	C4C-C3C-CAC-CBC
21	5	614	CLA	CAA-CBA-CGA-O1A
21	L2	204	CLA	CAA-CBA-CGA-O2A
21	8	612	CLA	CAA-CBA-CGA-O2A
21	B2	809	CLA	CAA-CBA-CGA-O2A
27	82	629	LMG	O8-C28-C29-C30
21	A2	810	CLA	C8-C10-C11-C12
21	32	613	CLA	C10-C11-C12-C13
21	7	603	CLA	CAA-CBA-CGA-O1A
21	A2	813	CLA	CAA-CBA-CGA-O1A
23	9	622	LHG	C29-C30-C31-C32
21	3	609	CLA	C2C-C3C-CAC-CBC
23	92	622	LHG	C29-C30-C31-C32
21	52	614	CLA	CAA-CBA-CGA-O1A
21	A	828	CLA	CAD-CBD-CGD-O1D
21	B	804	CLA	CAD-CBD-CGD-O1D
21	B	813	CLA	CAD-CBD-CGD-O1D
21	5	613	CLA	CAD-CBD-CGD-O1D
21	6	610	CLA	CAD-CBD-CGD-O1D
21	9	614	CLA	CAD-CBD-CGD-O1D
21	A2	828	CLA	CAD-CBD-CGD-O1D
21	B2	804	CLA	CAD-CBD-CGD-O1D
21	B2	813	CLA	CAD-CBD-CGD-O1D
21	52	613	CLA	CAD-CBD-CGD-O1D
21	62	613	CLA	CAD-CBD-CGD-O1D
21	62	617	CLA	CAD-CBD-CGD-O1D
21	92	614	CLA	CAD-CBD-CGD-O1D
29	B2	850	DGD	C3G-C2G-O2G-C1B
30	Z	606	CHL	CAD-CBD-CGD-O1D
30	Z2	606	CHL	CAD-CBD-CGD-O1D
21	72	603	CLA	CAA-CBA-CGA-O1A
27	A	859	LMG	C30-C31-C32-C33
21	82	612	CLA	CAA-CBA-CGA-O2A
27	8	629	LMG	O8-C28-C29-C30
21	A	823	CLA	C6-C7-C8-C9
21	B	832	CLA	C11-C12-C13-C14
21	4	611	CLA	C6-C7-C8-C9
21	A2	823	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
21	B2	825	CLA	C6-C7-C8-C9
21	B2	832	CLA	C11-C12-C13-C14
21	42	611	CLA	C6-C7-C8-C9
21	92	612	CLA	C11-C12-C13-C14
30	7	601	CHL	C11-C10-C8-C9
30	8	606	CHL	C11-C10-C8-C9
30	8	606	CHL	C14-C13-C15-C16
30	82	606	CHL	C11-C10-C8-C9
30	82	606	CHL	C14-C13-C15-C16
21	32	617	CLA	C2C-C3C-CAC-CBC
21	A	813	CLA	CAA-CBA-CGA-O1A
21	B	823	CLA	CAA-CBA-CGA-O2A
21	K	203	CLA	CAA-CBA-CGA-O2A
21	1	613	CLA	CAA-CBA-CGA-O2A
21	A2	814	CLA	CAA-CBA-CGA-O2A
21	A2	816	CLA	CAA-CBA-CGA-O2A
21	62	603	CLA	CAA-CBA-CGA-O2A
23	6	619	LHG	O7-C7-C8-C9
23	62	619	LHG	O7-C7-C8-C9
27	B2	852	LMG	O7-C10-C11-C12
27	32	722	LMG	O7-C10-C11-C12
27	A2	859	LMG	C30-C31-C32-C33
21	F	303	CLA	CAA-CBA-CGA-O2A
21	L	204	CLA	CAA-CBA-CGA-O1A
21	Z2	611	CLA	C4C-C3C-CAC-CBC
21	32	609	CLA	C2C-C3C-CAC-CBC
21	B2	823	CLA	CAA-CBA-CGA-O2A
21	72	612	CLA	CAA-CBA-CGA-O2A
23	B	851	LHG	O8-C23-C24-C25
23	72	625	LHG	O8-C23-C24-C25
27	B	852	LMG	O7-C10-C11-C12
21	L2	204	CLA	CAA-CBA-CGA-O1A
21	Z	603	CLA	CAA-CBA-CGA-O1A
21	Z2	603	CLA	CAA-CBA-CGA-O1A
27	3	722	LMG	O9-C10-C11-C12
27	12	628	LMG	O10-C28-C29-C30
21	A	803	CLA	C4-C3-C5-C6
21	A2	803	CLA	C4-C3-C5-C6
23	3	623	LHG	C24-C25-C26-C27
23	32	623	LHG	C24-C25-C26-C27
21	A	836	CLA	C3A-C2A-CAA-CBA
21	A	840	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
21	A	841	CLA	C11-C10-C8-C7
21	A	843	CLA	C11-C10-C8-C7
21	B	822	CLA	C6-C7-C8-C10
21	B	837	CLA	C11-C12-C13-C15
21	F	304	CLA	C3A-C2A-CAA-CBA
21	3	615	CLA	C3A-C2A-CAA-CBA
21	8	614	CLA	C3A-C2A-CAA-CBA
21	4	613	CLA	C3A-C2A-CAA-CBA
21	4	614	CLA	C3A-C2A-CAA-CBA
21	5	603	CLA	C3A-C2A-CAA-CBA
21	5	604	CLA	C3A-C2A-CAA-CBA
21	9	611	CLA	C3A-C2A-CAA-CBA
21	A2	836	CLA	C3A-C2A-CAA-CBA
21	A2	840	CLA	C6-C7-C8-C10
21	A2	841	CLA	C11-C10-C8-C7
21	A2	843	CLA	C11-C10-C8-C7
21	B2	822	CLA	C6-C7-C8-C10
21	B2	837	CLA	C11-C12-C13-C15
21	F2	304	CLA	C3A-C2A-CAA-CBA
21	32	615	CLA	C3A-C2A-CAA-CBA
21	82	614	CLA	C3A-C2A-CAA-CBA
21	42	613	CLA	C3A-C2A-CAA-CBA
21	42	614	CLA	C3A-C2A-CAA-CBA
21	52	603	CLA	C3A-C2A-CAA-CBA
21	52	604	CLA	C3A-C2A-CAA-CBA
21	92	611	CLA	C3A-C2A-CAA-CBA
22	A	844	PQN	C21-C22-C23-C25
22	A2	844	PQN	C21-C22-C23-C25
22	B2	842	PQN	C16-C17-C18-C20
30	1	601	CHL	C6-C7-C8-C10
30	1	601	CHL	C11-C10-C8-C7
30	12	601	CHL	C6-C7-C8-C10
30	12	601	CHL	C11-C10-C8-C7
21	5	603	CLA	CAA-CBA-CGA-O1A
21	6	603	CLA	CAA-CBA-CGA-O1A
23	6	619	LHG	O9-C7-C8-C9
27	1	628	LMG	O10-C28-C29-C30
27	A2	860	LMG	O10-C28-C29-C30
27	32	722	LMG	O9-C10-C11-C12
21	A	814	CLA	CAA-CBA-CGA-O2A
21	6	603	CLA	CAA-CBA-CGA-O2A
21	K2	203	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
21	12	613	CLA	CAA-CBA-CGA-O2A
21	72	613	CLA	CAA-CBA-CGA-O2A
23	7	625	LHG	O7-C7-C8-C9
23	8	620	LHG	O7-C7-C8-C9
23	72	625	LHG	O7-C7-C8-C9
23	82	620	LHG	O7-C7-C8-C9
27	3	722	LMG	O7-C10-C11-C12
30	6	601	CHL	CAA-CBA-CGA-O2A
30	62	601	CHL	CAA-CBA-CGA-O2A
21	Z	611	CLA	C4C-C3C-CAC-CBC
21	B	806	CLA	CAA-CBA-CGA-O1A
21	B	809	CLA	CAA-CBA-CGA-O1A
21	B2	806	CLA	CAA-CBA-CGA-O1A
21	62	603	CLA	CAA-CBA-CGA-O1A
23	B	851	LHG	O10-C23-C24-C25
23	8	620	LHG	O9-C7-C8-C9
23	72	625	LHG	O9-C7-C8-C9
23	82	620	LHG	O9-C7-C8-C9
23	62	619	LHG	O9-C7-C8-C9
30	6	601	CHL	CAA-CBA-CGA-O1A
21	F	303	CLA	CAA-CBA-CGA-O1A
32	62	625	NEX	C13-C14-C15-C35
26	A	861	LMU	C2-C1-O1'-C1'
26	A2	861	LMU	C2-C1-O1'-C1'
21	A	837	CLA	CAA-CBA-CGA-O2A
21	A2	837	CLA	CAA-CBA-CGA-O2A
23	B2	851	LHG	O8-C23-C24-C25
23	52	623	LHG	O8-C23-C24-C25
21	B	813	CLA	C8-C10-C11-C12
21	B2	813	CLA	C8-C10-C11-C12
21	8	612	CLA	CAA-CBA-CGA-O1A
21	4	603	CLA	CAA-CBA-CGA-O1A
21	82	603	CLA	CAA-CBA-CGA-O1A
21	82	612	CLA	CAA-CBA-CGA-O1A
21	42	603	CLA	CAA-CBA-CGA-O1A
21	52	603	CLA	CAA-CBA-CGA-O1A
23	7	625	LHG	O9-C7-C8-C9
30	62	601	CHL	CAA-CBA-CGA-O1A
21	B2	835	CLA	CAA-CBA-CGA-O2A
21	F2	303	CLA	CAA-CBA-CGA-O1A
21	F2	303	CLA	CAA-CBA-CGA-O2A
21	B	802	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
21	B2	802	CLA	C8-C10-C11-C12
23	Z	620	LHG	C5-C6-O8-C23
21	A	816	CLA	CAA-CBA-CGA-O2A
21	1	602	CLA	CAA-CBA-CGA-O2A
21	B2	812	CLA	CAA-CBA-CGA-O2A
21	12	602	CLA	CAA-CBA-CGA-O2A
23	7	625	LHG	O8-C23-C24-C25
23	5	623	LHG	O8-C23-C24-C25
21	8	603	CLA	CAA-CBA-CGA-O1A
27	3	722	LMG	O10-C28-C29-C30
30	7	607	CHL	CAA-CBA-CGA-O2A
30	72	607	CHL	CAA-CBA-CGA-O2A
21	B	809	CLA	C8-C10-C11-C12
21	4	610	CLA	C5-C6-C7-C8
21	B2	809	CLA	C8-C10-C11-C12
21	42	610	CLA	C5-C6-C7-C8
23	B	851	LHG	C25-C26-C27-C28
21	Z	616	CLA	C3-C5-C6-C7
21	Z2	616	CLA	C3-C5-C6-C7
21	A2	814	CLA	CAA-CBA-CGA-O1A
21	B2	809	CLA	CAA-CBA-CGA-O1A
23	B2	851	LHG	O10-C23-C24-C25
23	B2	851	LHG	C25-C26-C27-C28
21	B	816	CLA	CAA-CBA-CGA-O2A
21	7	612	CLA	CAA-CBA-CGA-O2A
21	B2	816	CLA	CAA-CBA-CGA-O2A
21	12	614	CLA	CAA-CBA-CGA-O2A

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	52	625	NEX	C1-C2-C3-C4-C5-C6
32	5	625	NEX	C1-C2-C3-C4-C5-C6

402 monomers are involved in 578 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	12	610	CLA	1	0
21	32	602	CLA	2	0
21	82	610	CLA	1	0
21	7	602	CLA	1	0
30	42	606	CHL	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	42	608	CHL	1	0
21	42	613	CLA	3	0
28	92	616	LUT	2	0
30	8	606	CHL	2	0
21	42	602	CLA	2	0
24	62	623	BCR	2	0
30	3	608	CHL	1	0
21	7	608	CLA	1	0
21	B	826	CLA	1	0
31	52	624	XAT	1	0
21	1	614	CLA	1	0
21	8	612	CLA	1	0
21	4	611	CLA	1	0
28	7	621	LUT	1	0
24	3	620	BCR	1	0
30	82	606	CHL	2	0
21	A	817	CLA	2	0
21	B	829	CLA	6	0
21	6	603	CLA	1	0
21	32	610	CLA	4	0
23	Z2	620	LHG	1	0
29	B	850	DGD	1	0
21	62	603	CLA	1	0
21	A2	843	CLA	1	0
26	92	624	LMU	1	0
21	6	610	CLA	3	0
21	12	602	CLA	2	0
31	Z	618	XAT	1	0
28	32	622	LUT	4	0
24	B2	845	BCR	2	0
21	92	602	CLA	1	0
26	4	625	LMU	1	0
23	32	623	LHG	1	0
21	8	611	CLA	1	0
21	62	610	CLA	2	0
21	A	840	CLA	4	0
21	B	821	CLA	1	0
26	A2	858	LMU	1	0
21	B	813	CLA	2	0
21	A	822	CLA	2	0
31	4	620	XAT	1	0
24	B	845	BCR	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	Z2	608	CLA	1	0
21	6	602	CLA	2	0
21	A	838	CLA	1	0
21	82	604	CLA	4	0
23	12	620	LHG	1	0
21	32	615	CLA	6	0
21	F	304	CLA	1	0
21	B2	819	CLA	1	0
21	32	612	CLA	1	0
21	A2	802	CLA	4	0
21	A2	803	CLA	2	0
21	32	607	CLA	2	0
21	8	614	CLA	1	0
23	5	623	LHG	1	0
21	A2	806	CLA	1	0
24	K2	202	BCR	4	0
21	42	612	CLA	2	0
21	Z2	610	CLA	2	0
30	6	608	CHL	4	0
27	32	722	LMG	1	0
21	A2	810	CLA	2	0
24	92	623	BCR	2	0
21	3	615	CLA	5	0
21	A	833	CLA	3	0
29	B2	850	DGD	1	0
21	42	609	CLA	1	0
21	J2	101	CLA	1	0
21	9	612	CLA	1	0
30	72	601	CHL	2	0
30	6	607	CHL	1	0
21	A2	831	CLA	1	0
24	B	844	BCR	4	0
30	Z2	606	CHL	2	0
21	1	602	CLA	2	0
24	A2	849	BCR	2	0
21	52	610	CLA	1	0
21	B2	826	CLA	1	0
23	3	623	LHG	1	0
31	8	618	XAT	1	0
21	42	610	CLA	3	0
21	Z	603	CLA	3	0
21	92	614	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	A2	851	BCR	1	0
21	62	613	CLA	2	0
21	B	808	CLA	2	0
24	A	848	BCR	3	0
21	32	609	CLA	1	0
31	6	624	XAT	1	0
21	Z	613	CLA	1	0
24	A	849	BCR	2	0
21	3	612	CLA	1	0
21	A	811	CLA	2	0
21	8	609	CLA	1	0
21	A	854	CLA	5	0
21	3	607	CLA	2	0
21	7	620	CLA	1	0
26	82	625	LMU	1	0
26	B	853	LMU	3	0
26	Z2	622	LMU	1	0
21	A2	826	CLA	3	0
24	82	619	BCR	2	0
27	3	722	LMG	1	0
21	72	610	CLA	4	0
30	52	608	CHL	1	0
21	A2	820	CLA	2	0
31	7	622	XAT	1	0
21	B	835	CLA	4	0
21	52	621	CLA	3	0
21	52	602	CLA	3	0
28	A	856	LUT	1	0
21	A	803	CLA	2	0
21	B2	811	CLA	1	0
21	3	611	CLA	1	0
21	B	817	CLA	2	0
21	A2	835	CLA	1	0
28	1	617	LUT	3	0
21	A	806	CLA	1	0
30	4	606	CHL	4	0
21	12	614	CLA	1	0
21	A2	838	CLA	1	0
30	8	601	CHL	2	0
30	Z	606	CHL	2	0
21	1	610	CLA	1	0
23	52	623	LHG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	4	608	CHL	1	0
21	B	840	CLA	2	0
27	J	104	LMG	1	0
21	A	818	CLA	1	0
24	G2	205	BCR	2	0
21	B2	836	CLA	2	0
21	4	602	CLA	2	0
21	A2	840	CLA	4	0
21	Z2	616	CLA	3	0
26	8	627	LMU	1	0
21	A2	822	CLA	2	0
21	42	614	CLA	1	0
28	82	617	LUT	1	0
21	B	814	CLA	1	0
26	B2	853	LMU	2	0
21	B	832	CLA	1	0
21	1	603	CLA	4	0
30	62	608	CHL	3	0
27	J2	104	LMG	1	0
31	12	618	XAT	2	0
24	9	623	BCR	1	0
21	72	620	CLA	1	0
21	A2	832	CLA	1	0
21	3	609	CLA	1	0
31	42	620	XAT	1	0
21	12	604	CLA	2	0
24	L	201	BCR	1	0
21	B	830	CLA	1	0
21	B	819	CLA	1	0
24	8	619	BCR	2	0
21	Z	602	CLA	2	0
21	8	603	CLA	2	0
21	B2	813	CLA	2	0
24	L2	205	BCR	4	0
24	42	621	BCR	1	0
24	A2	852	BCR	2	0
21	A	826	CLA	3	0
21	A	831	CLA	2	0
21	1	604	CLA	2	0
24	K	207	BCR	2	0
26	A	858	LMU	2	0
28	12	619	LUT	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	3	622	LUT	4	0
21	B2	817	CLA	2	0
23	1	620	LHG	1	0
27	J2	103	LMG	1	0
21	32	611	CLA	1	0
28	32	621	LUT	2	0
21	B	802	CLA	4	0
21	4	612	CLA	2	0
24	32	719	BCR	4	0
24	L	205	BCR	4	0
21	12	613	CLA	2	0
21	B2	821	CLA	1	0
21	B2	833	CLA	2	0
31	Z2	618	XAT	1	0
23	7	625	LHG	1	0
26	7	628	LMU	1	0
21	B	841	CLA	4	0
21	12	609	CLA	1	0
21	72	608	CLA	1	0
21	5	602	CLA	3	0
21	92	612	CLA	1	0
30	42	601	CHL	1	0
26	A	857	LMU	1	0
21	1	608	CLA	2	0
28	3	621	LUT	2	0
21	12	608	CLA	2	0
21	6	613	CLA	2	0
21	B	834	CLA	3	0
28	Z2	617	LUT	2	0
21	4	614	CLA	1	0
24	A2	850	BCR	3	0
21	B	823	CLA	1	0
28	4	619	LUT	2	0
26	A2	857	LMU	1	0
21	1	613	CLA	2	0
21	Z	610	CLA	2	0
21	52	617	CLA	1	0
24	I2	172	BCR	1	0
28	72	621	LUT	1	0
24	I	172	BCR	1	0
28	7	624	LUT	4	0
21	A	809	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	52	620	LUT	3	0
21	B	824	CLA	1	0
27	9	620	LMG	2	0
21	3	603	CLA	3	0
21	B2	830	CLA	1	0
21	7	610	CLA	4	0
21	Z	608	CLA	1	0
21	K	201	CLA	1	0
21	62	614	CLA	3	0
21	Z2	604	CLA	1	0
21	92	610	CLA	2	0
21	A	820	CLA	1	0
21	9	610	CLA	2	0
21	A	829	CLA	4	0
21	B2	832	CLA	2	0
28	9	617	LUT	3	0
24	3	719	BCR	5	0
21	B	839	CLA	1	0
21	B2	814	CLA	1	0
21	Z2	609	CLA	1	0
21	A2	813	CLA	1	0
27	A	860	LMG	1	0
28	Z	617	LUT	2	0
21	A2	833	CLA	3	0
21	8	604	CLA	4	0
30	1	601	CHL	1	0
24	B	848	BCR	1	0
28	9	616	LUT	2	0
26	8	625	LMU	1	0
30	6	601	CHL	3	0
21	72	609	CLA	1	0
30	62	601	CHL	3	0
30	62	607	CHL	1	0
28	6	621	LUT	2	0
26	Z	622	LMU	1	0
27	J	103	LMG	1	0
23	72	625	LHG	1	0
21	B2	841	CLA	4	0
21	12	603	CLA	4	0
21	B2	829	CLA	6	0
24	J	102	BCR	1	0
21	B2	834	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	A2	812	CLA	1	0
27	B2	854	LMG	1	0
24	B2	843	BCR	2	0
21	6	617	CLA	1	0
26	A	863	LMU	1	0
21	52	616	CLA	2	0
27	8	626	LMG	1	0
20	A2	801	CL0	1	0
21	A	843	CLA	1	0
21	Z	609	CLA	1	0
28	A2	856	LUT	2	0
30	4	607	CHL	1	0
21	B	838	CLA	1	0
32	6	625	NEX	1	0
21	B2	840	CLA	3	0
21	72	602	CLA	1	0
21	32	603	CLA	3	0
21	Z	616	CLA	3	0
21	6	609	CLA	1	0
21	B2	808	CLA	2	0
21	B2	838	CLA	1	0
28	5	620	LUT	3	0
21	B	837	CLA	3	0
22	B2	842	PQN	1	0
21	J	101	CLA	1	0
28	F	305	LUT	4	0
21	B2	839	CLA	1	0
31	62	624	XAT	1	0
21	B	811	CLA	1	0
21	4	609	CLA	2	0
21	42	603	CLA	1	0
26	42	625	LMU	1	0
21	B2	802	CLA	5	0
21	B	833	CLA	2	0
27	A2	860	LMG	1	0
30	42	607	CHL	1	0
30	82	601	CHL	2	0
30	Z2	601	CHL	2	0
30	7	601	CHL	3	0
21	A2	811	CLA	1	0
21	F2	304	CLA	1	0
21	82	602	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	B	847	BCR	1	0
31	5	624	XAT	1	0
21	B2	837	CLA	2	0
21	5	621	CLA	4	0
31	1	618	XAT	2	0
21	A2	829	CLA	3	0
21	32	606	CLA	1	0
24	B	843	BCR	2	0
32	62	625	NEX	1	0
24	3	718	BCR	1	0
21	8	610	CLA	1	0
24	B2	844	BCR	3	0
26	9	624	LMU	1	0
21	B	816	CLA	2	0
21	Z2	603	CLA	4	0
27	92	620	LMG	2	0
21	A	835	CLA	1	0
21	5	616	CLA	3	0
21	1	609	CLA	1	0
30	4	601	CHL	1	0
21	82	611	CLA	1	0
21	3	606	CLA	1	0
21	Z2	611	CLA	1	0
24	B2	801	BCR	3	0
23	42	623	LHG	1	0
21	A	812	CLA	1	0
21	B2	816	CLA	2	0
30	6	606	CHL	2	0
24	B2	848	BCR	1	0
21	62	602	CLA	2	0
21	B	827	CLA	1	0
24	A2	848	BCR	2	0
21	A2	817	CLA	2	0
24	L2	201	BCR	1	0
24	J2	102	BCR	1	0
21	8	602	CLA	3	0
21	A2	818	CLA	1	0
21	K2	201	CLA	1	0
21	4	613	CLA	2	0
21	42	611	CLA	1	0
21	A2	830	CLA	1	0
21	A	813	CLA	2	0

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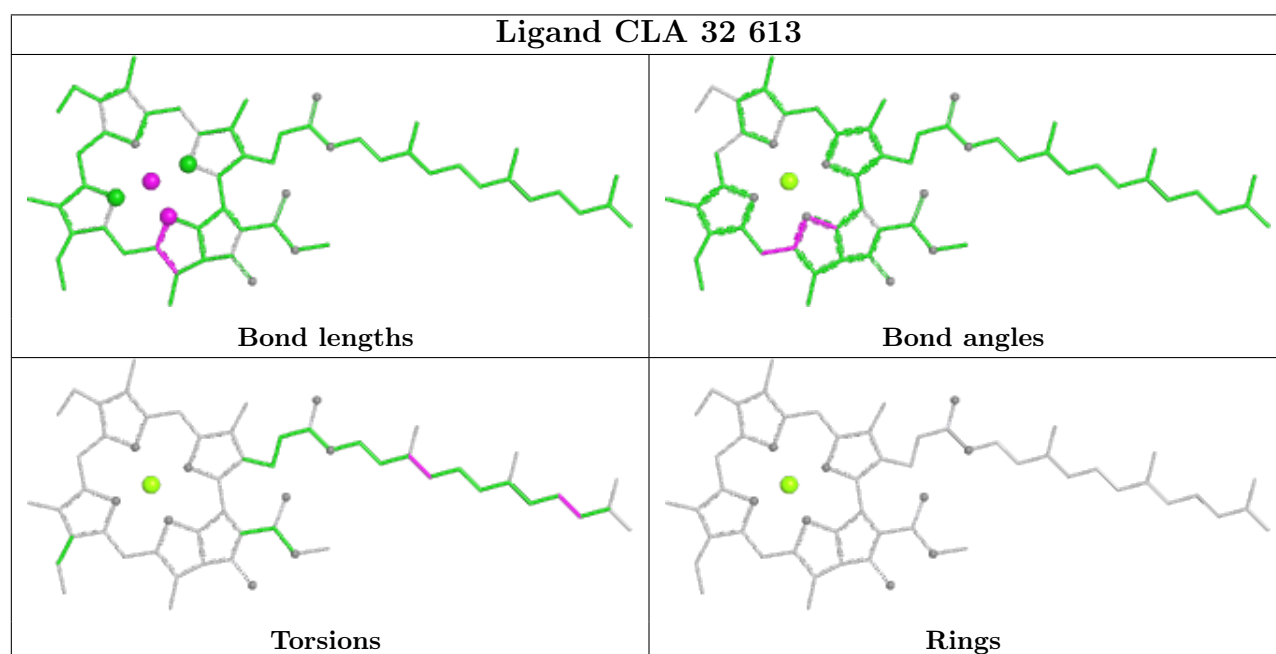
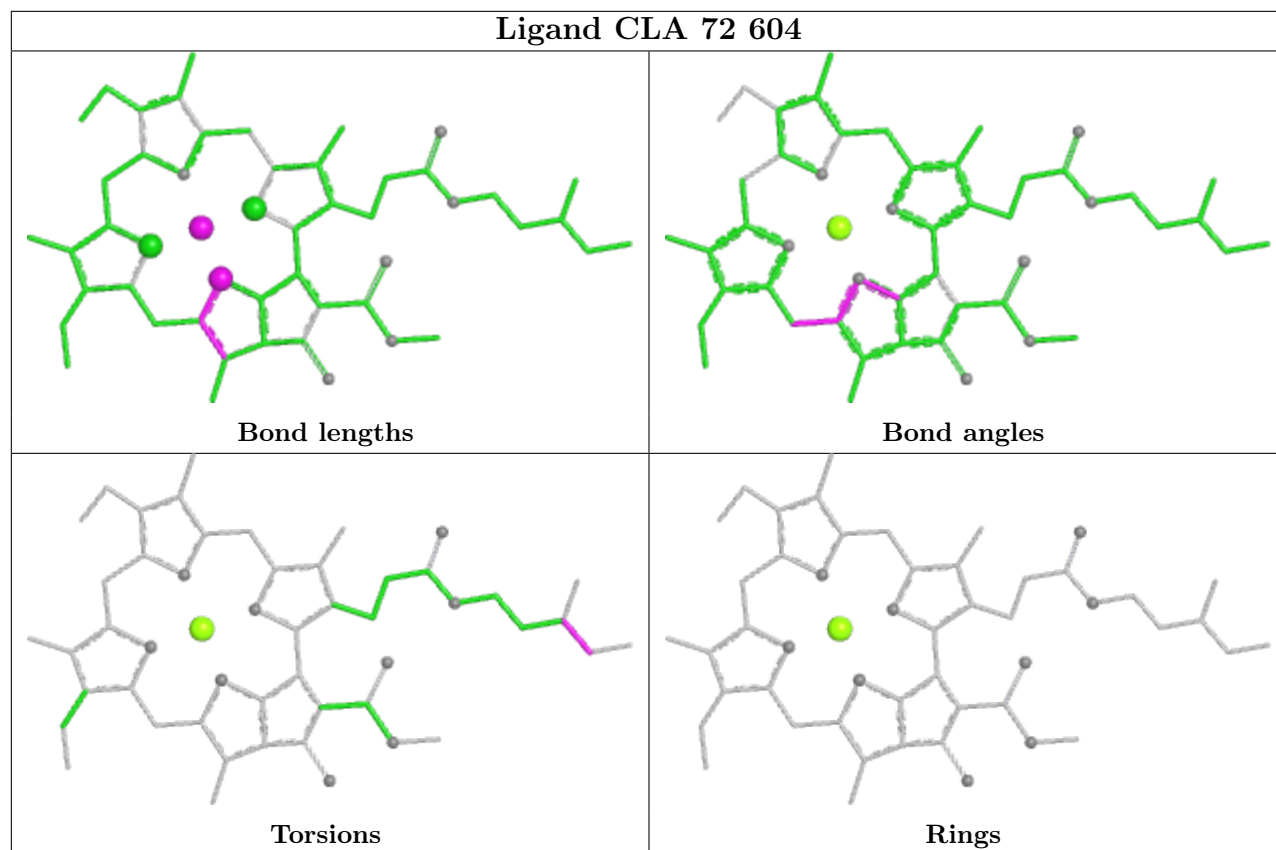
Mol	Chain	Res	Type	Clashes	Symm-Clashes
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28	92	617	LUT	3	0
21	6	614	CLA	3	0
21	B2	827	CLA	1	0
21	A	804	CLA	1	0
21	Z2	613	CLA	1	0
26	72	628	LMU	1	0
21	4	603	CLA	1	0
21	62	617	CLA	1	0
21	9	614	CLA	1	0
21	B2	806	CLA	2	0
20	A	801	CL0	1	0
24	A	852	BCR	4	0
30	62	606	CHL	2	0
21	5	603	CLA	1	0
21	52	603	CLA	1	0
28	F2	305	LUT	3	0
31	82	618	XAT	1	0
28	72	624	LUT	4	0
21	4	610	CLA	2	0
30	Z	601	CHL	2	0
21	A2	804	CLA	1	0
21	B	806	CLA	2	0
21	8	613	CLA	1	0
24	B	801	BCR	1	0
27	B	854	LMG	1	0
21	L	203	CLA	2	0
21	B2	835	CLA	3	0
21	62	609	CLA	1	0
21	A	810	CLA	2	0
24	K2	207	BCR	2	0
26	A	862	LMU	1	0
21	B2	823	CLA	1	0
21	82	614	CLA	1	0
24	A	850	BCR	1	0
21	L2	203	CLA	1	0
21	B	836	CLA	2	0
28	1	619	LUT	1	0
24	6	623	BCR	3	0
23	4	623	LHG	1	0
21	82	613	CLA	1	0
21	3	610	CLA	4	0

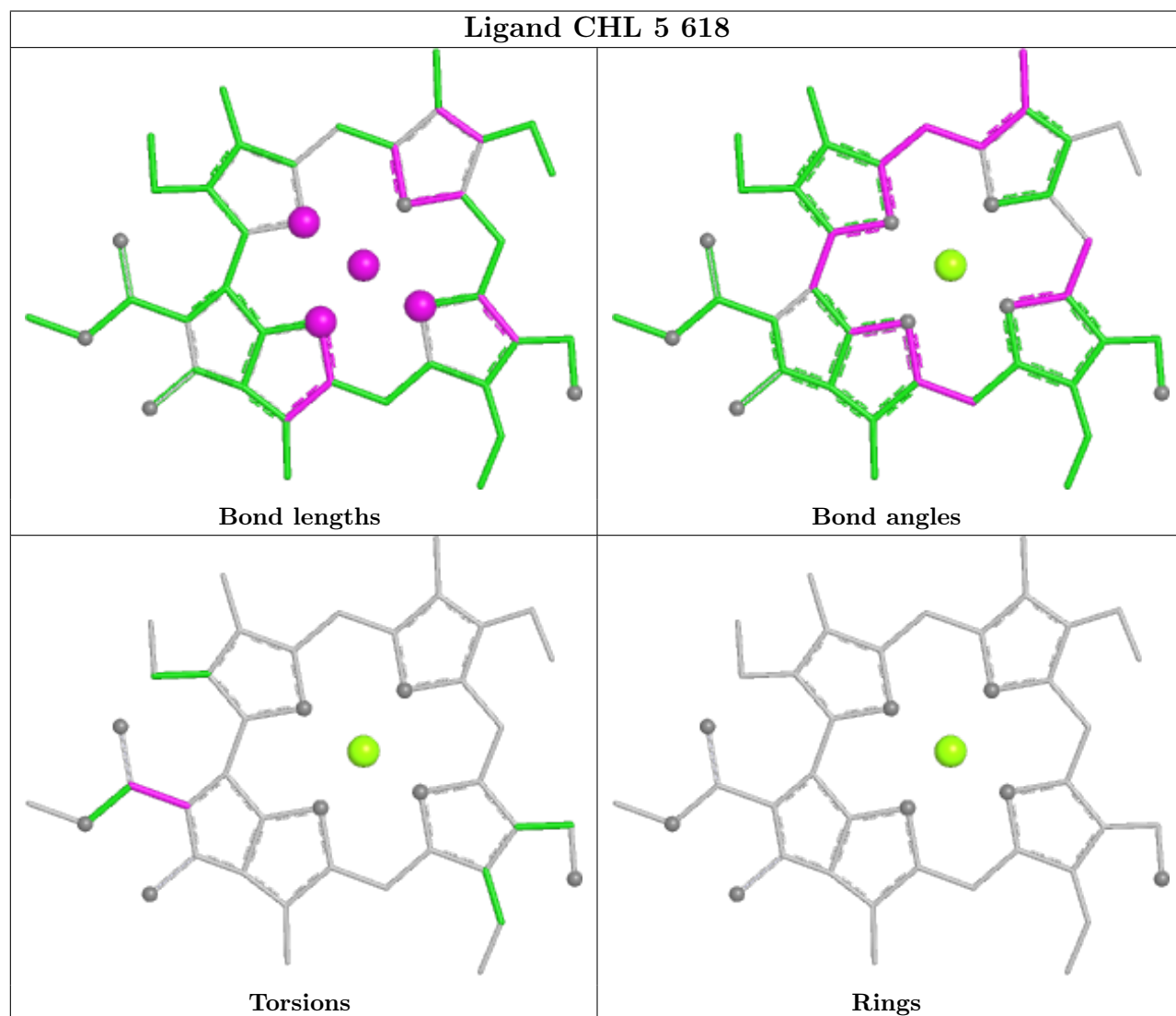
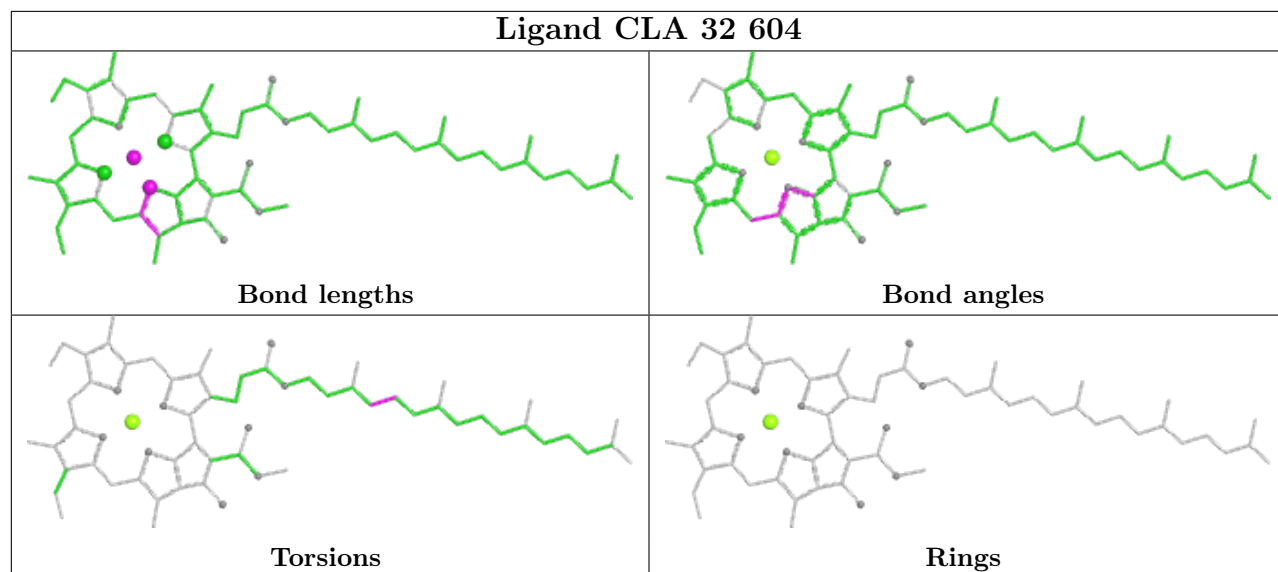
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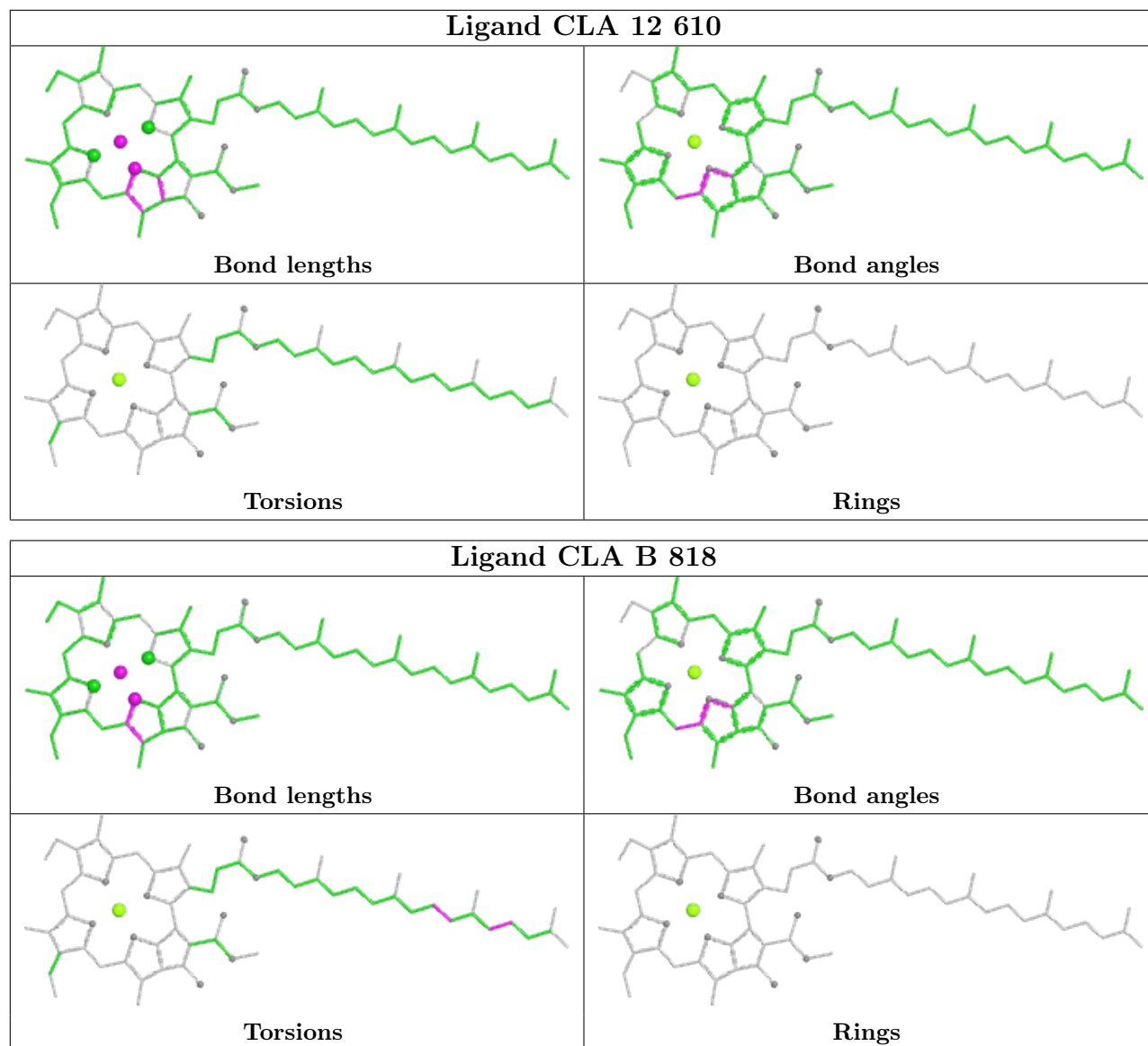
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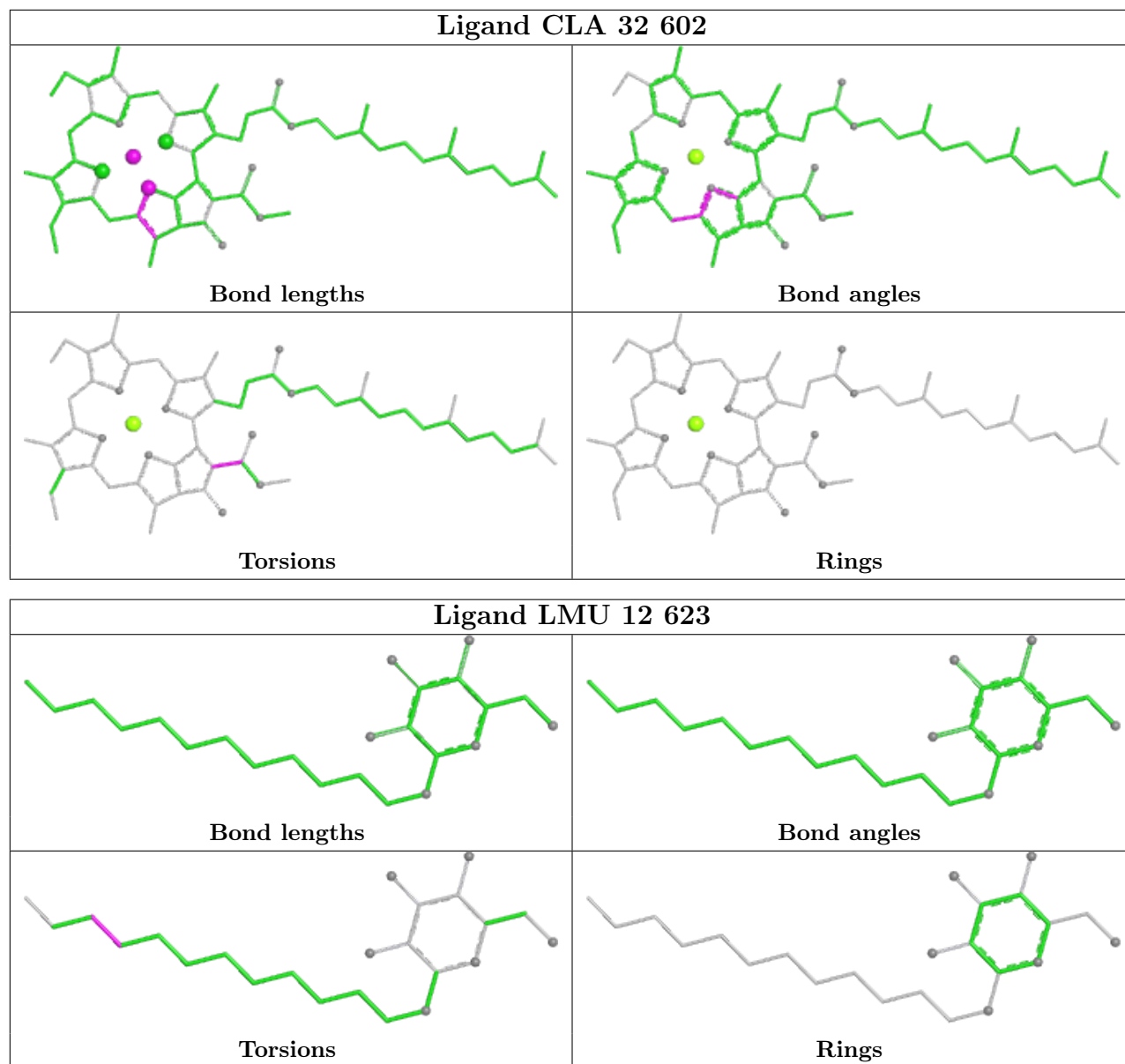
Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	7	609	CLA	1	0
21	Z2	602	CLA	2	0
21	A2	854	CLA	6	0
21	A	802	CLA	4	0
24	B2	847	BCR	1	0
24	A	851	BCR	3	0
21	Z	604	CLA	1	0
28	12	617	LUT	3	0
21	82	603	CLA	1	0
22	B	842	PQN	1	0
21	B2	824	CLA	1	0
24	K	202	BCR	3	0
21	3	602	CLA	2	0
21	9	602	CLA	1	0
28	42	619	LUT	2	0
30	5	608	CHL	1	0
21	A2	809	CLA	2	0
30	32	608	CHL	2	0
31	72	622	XAT	2	0

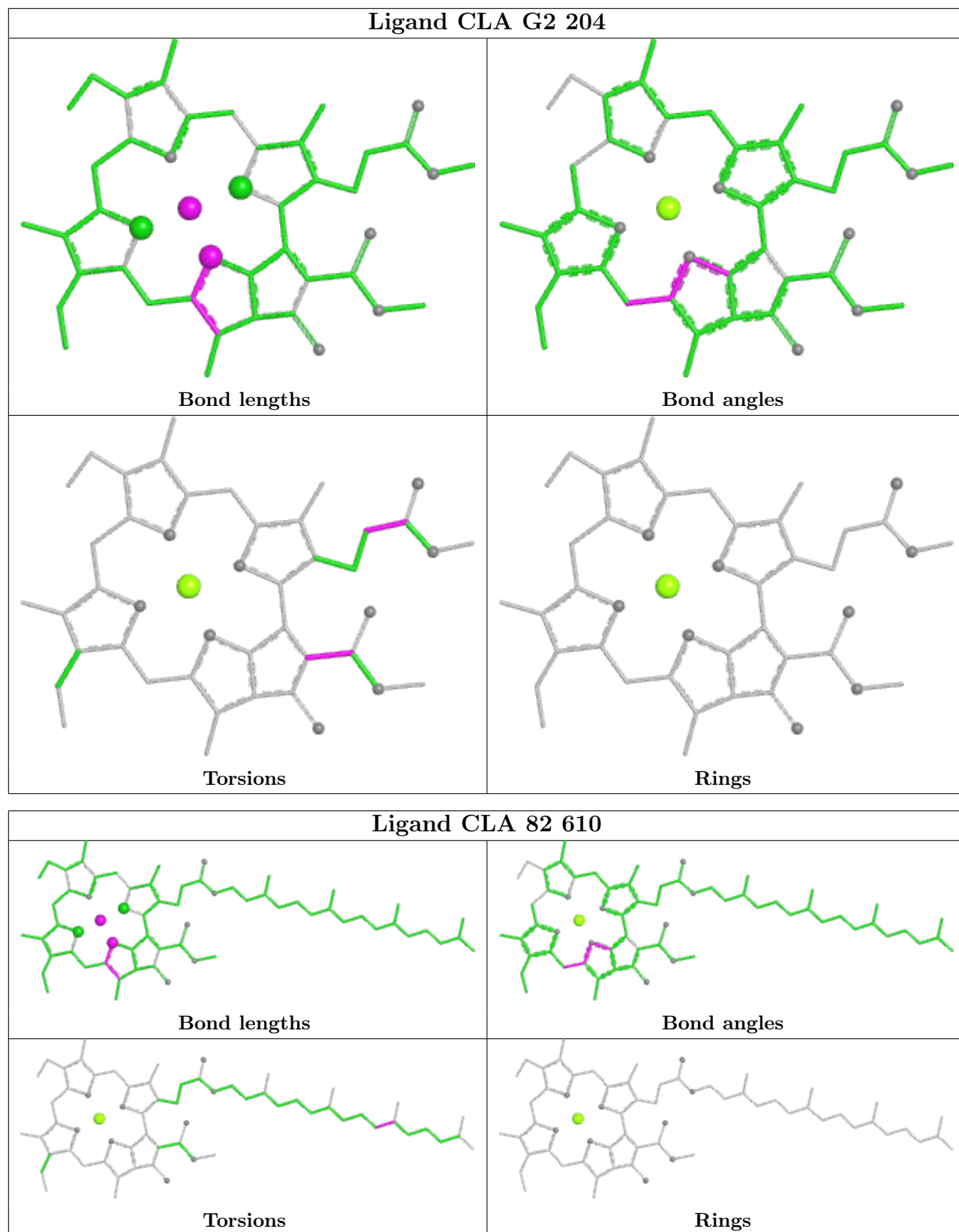
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

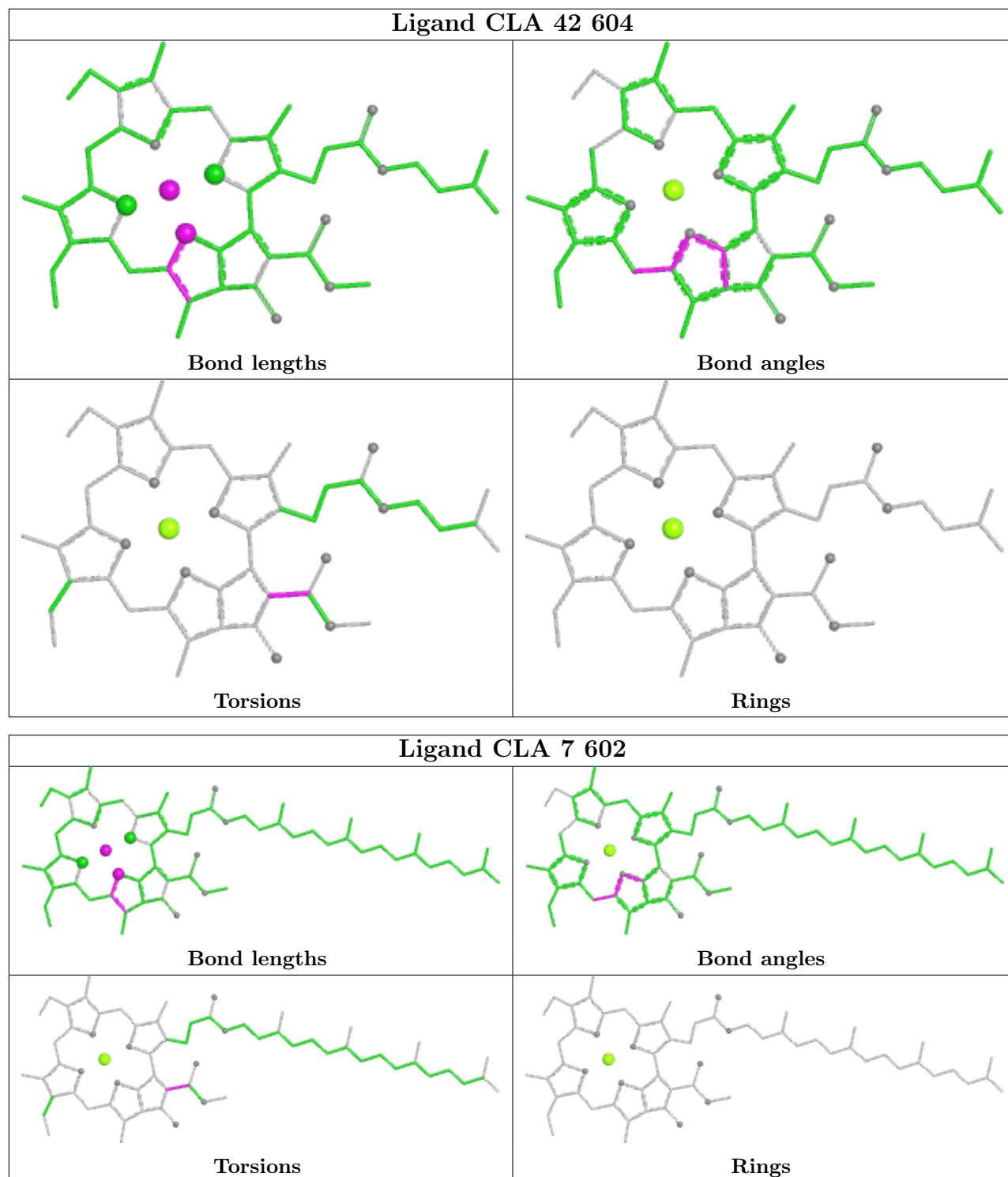


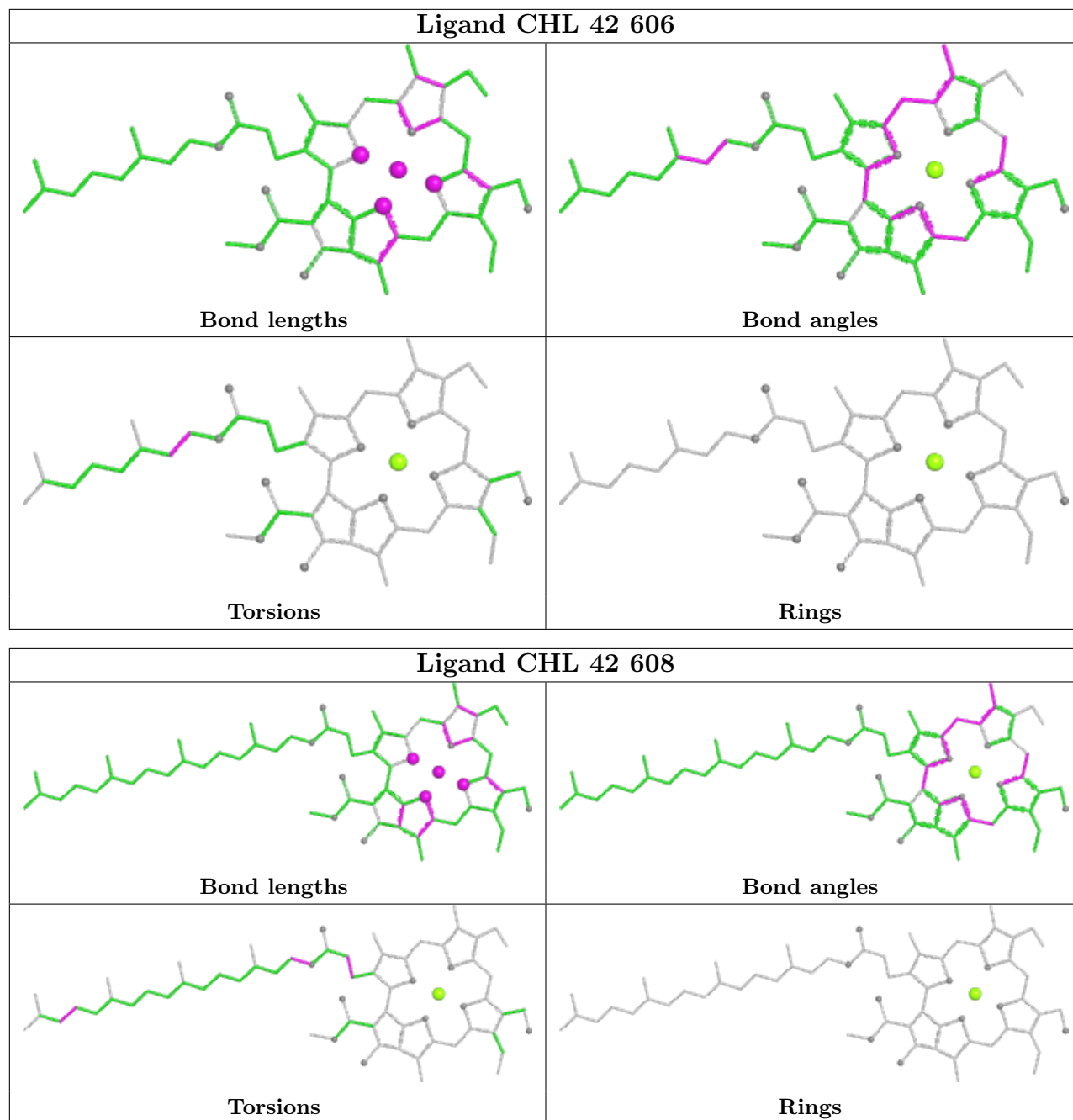


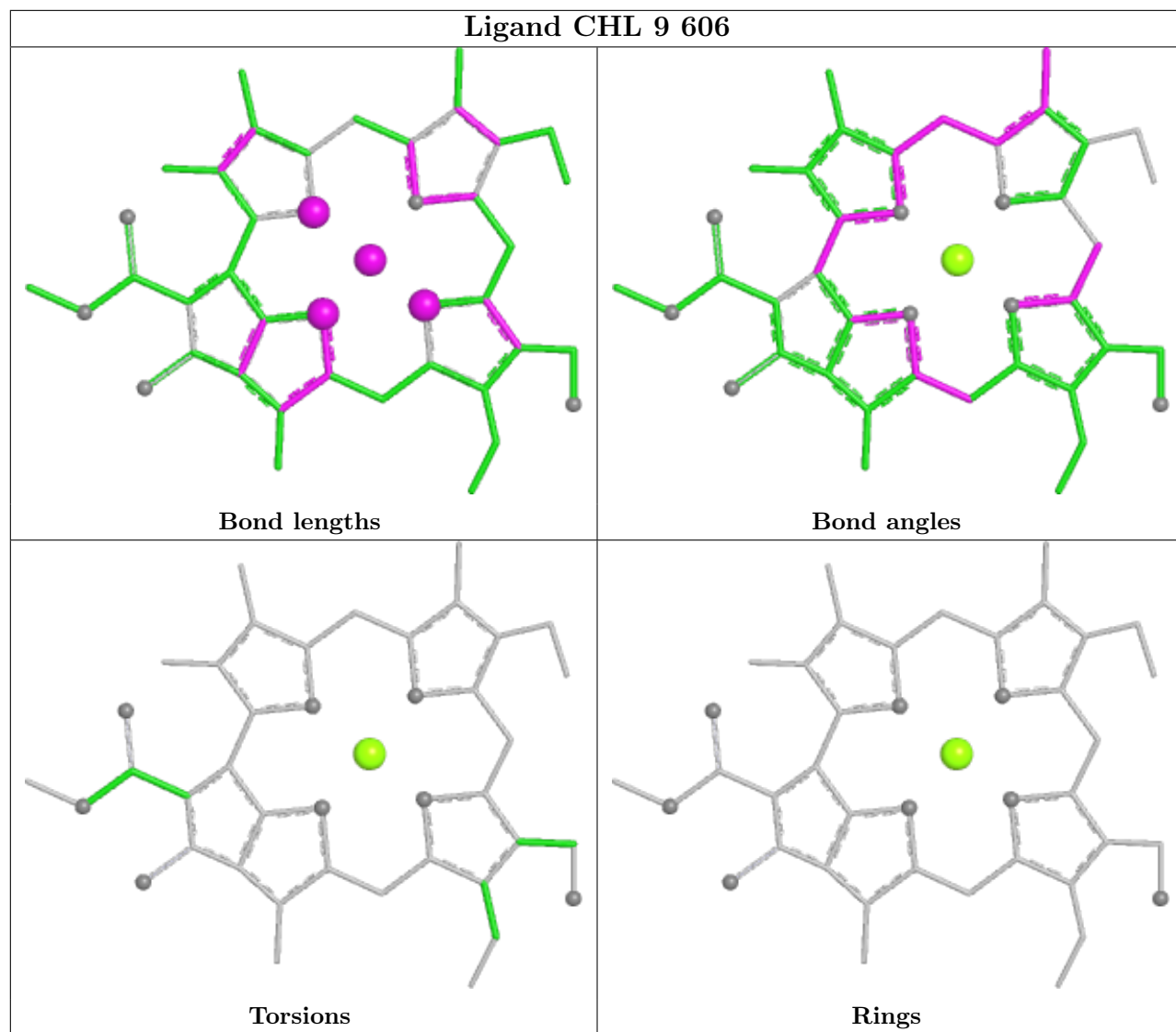


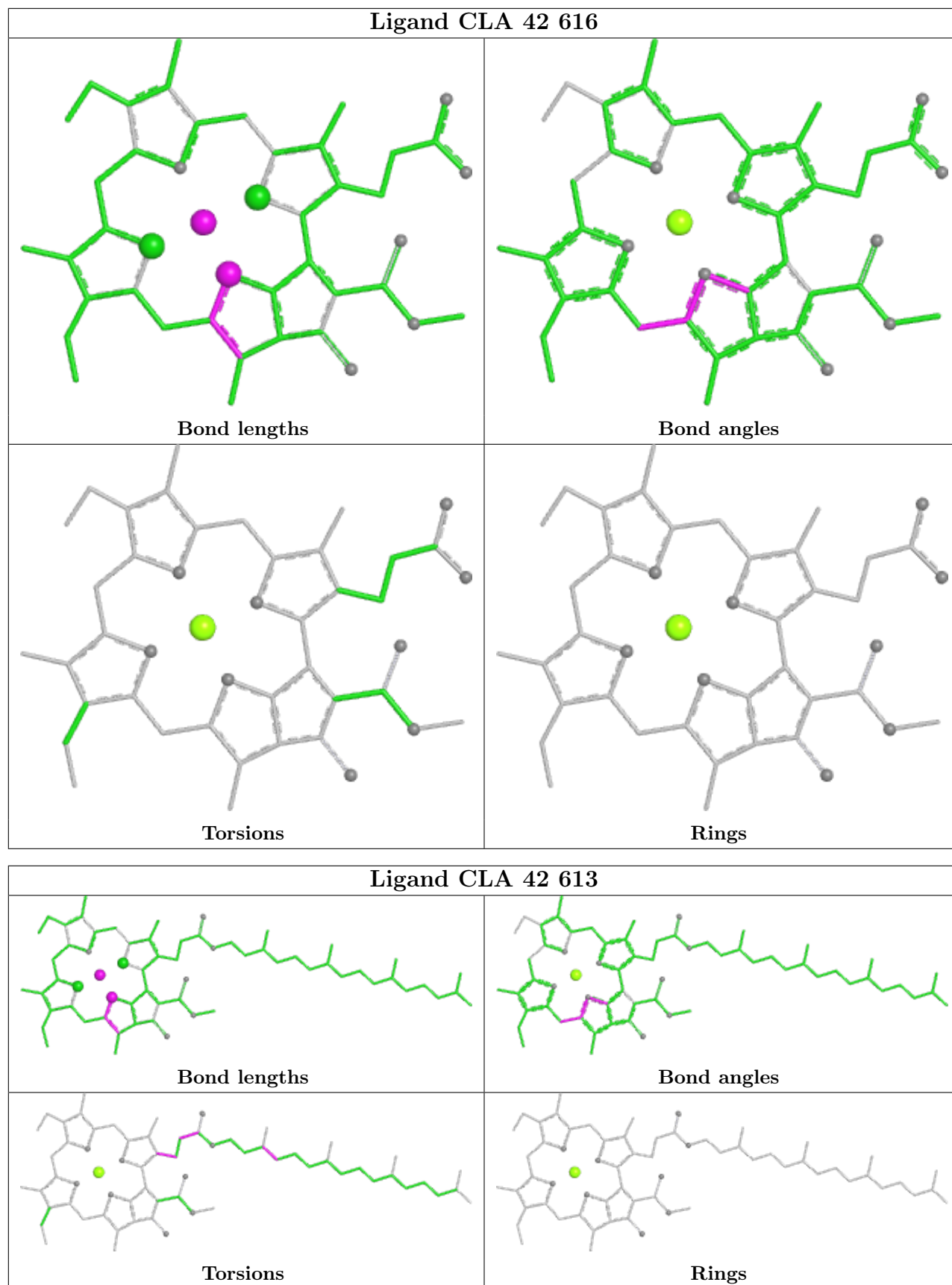


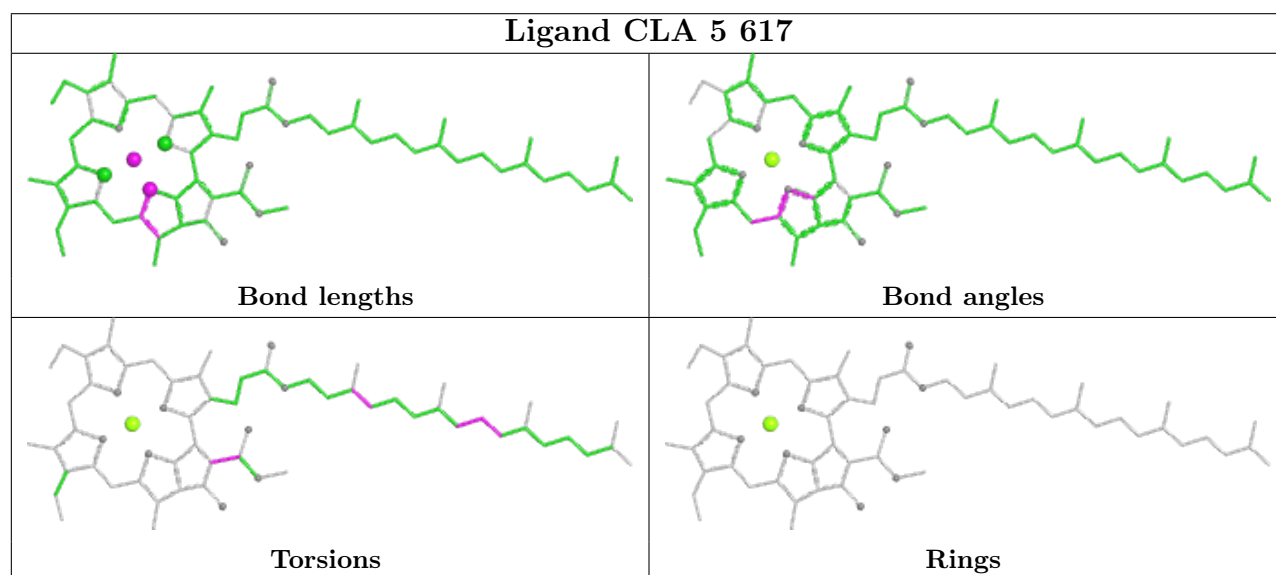
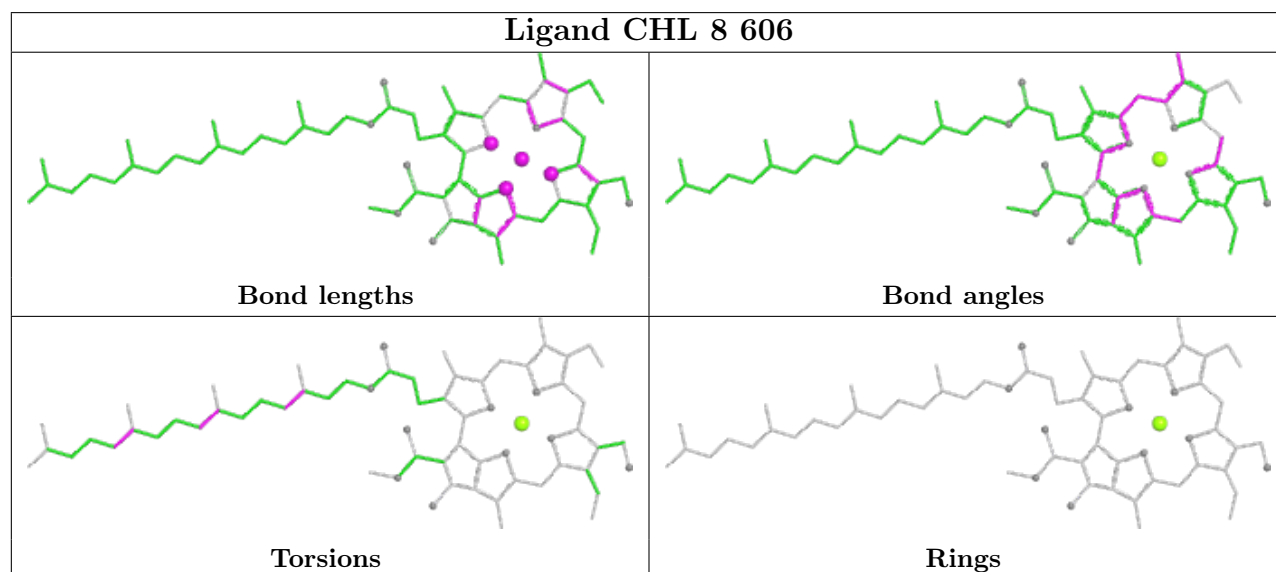
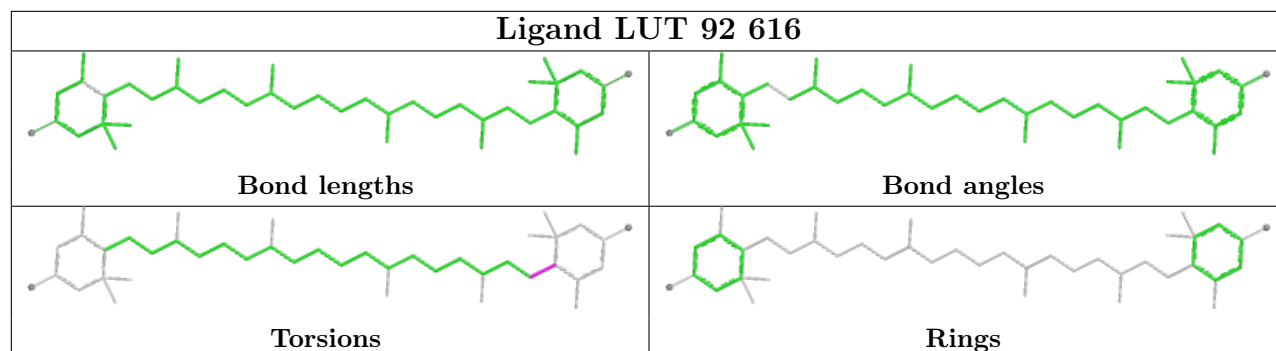


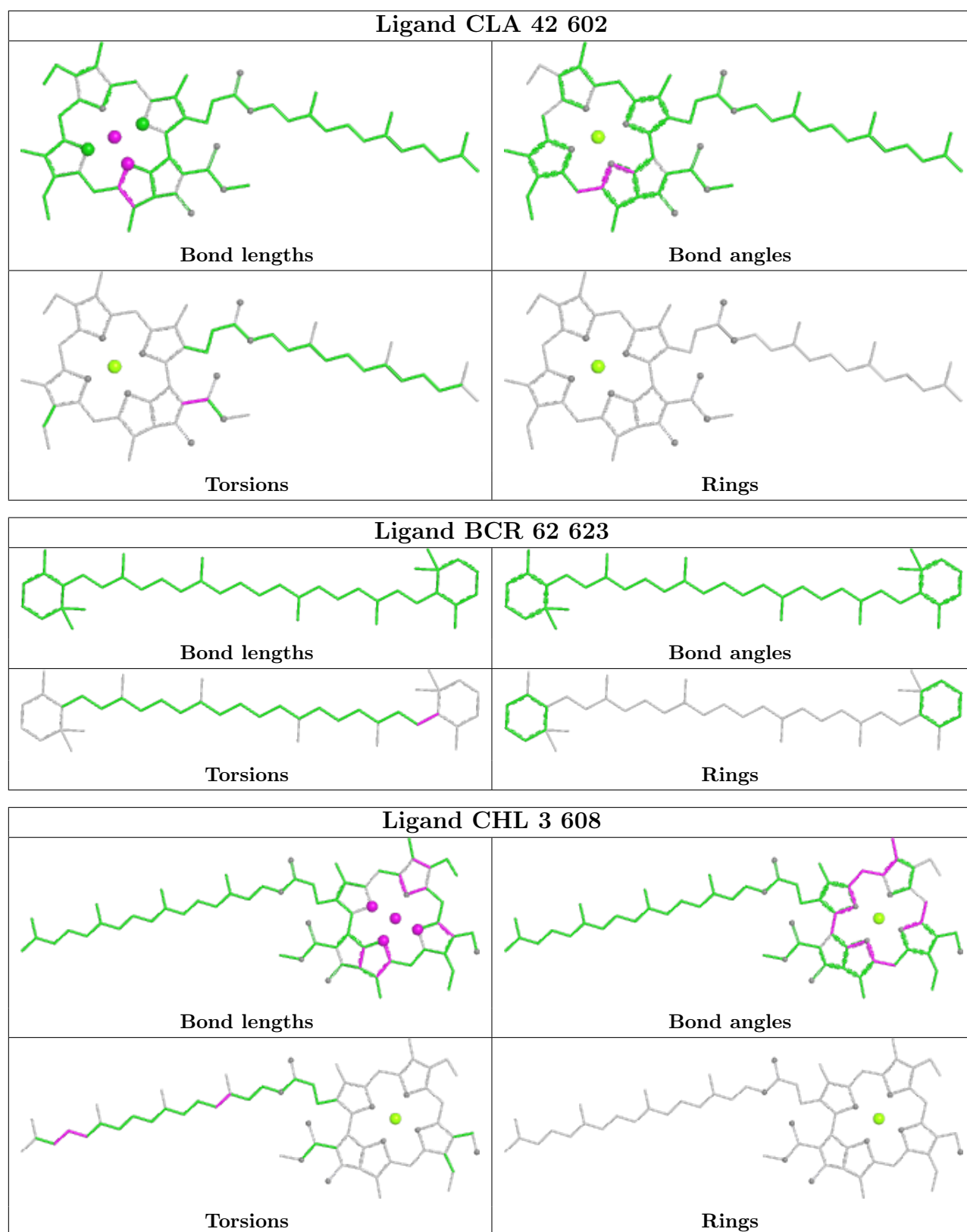


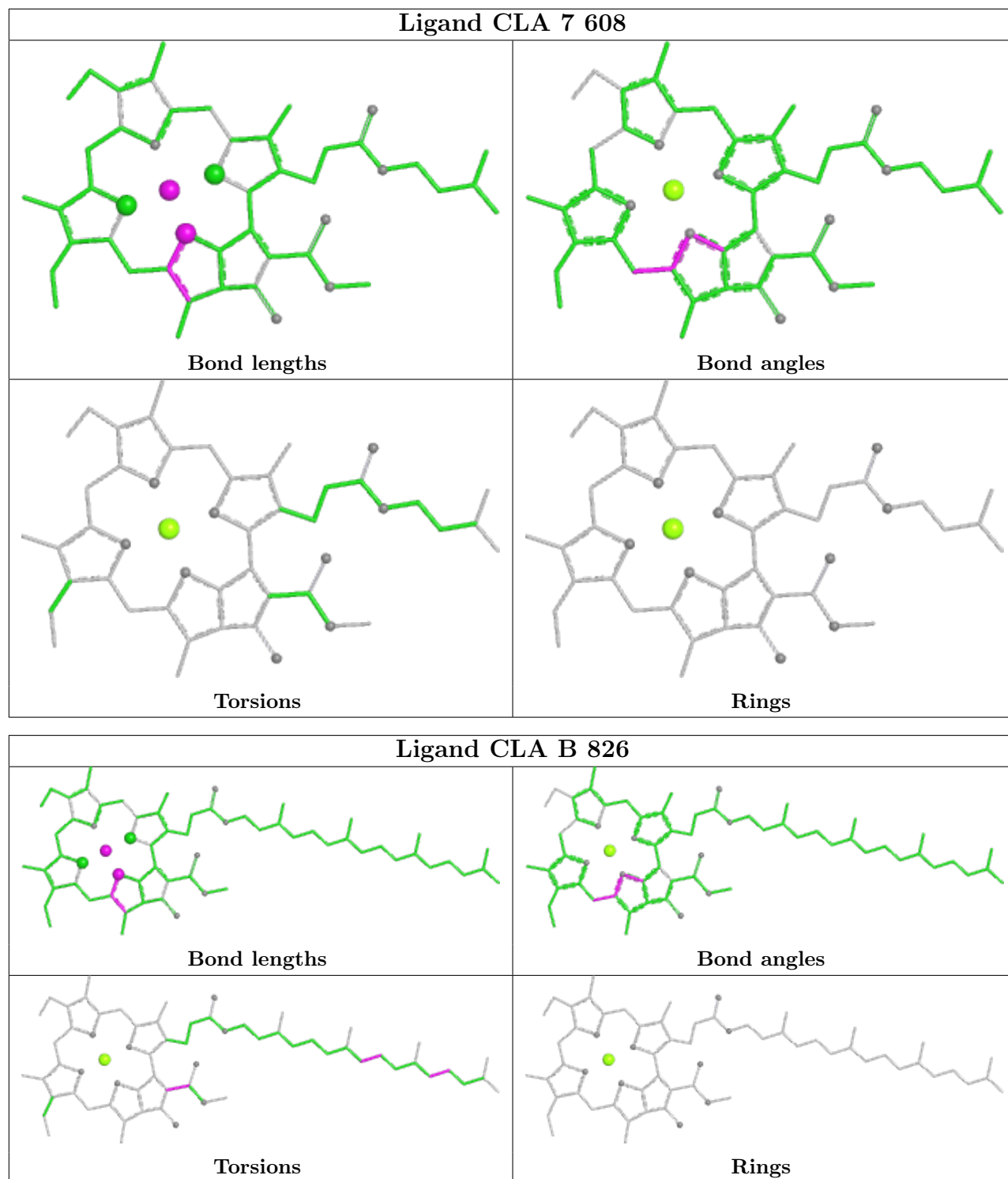


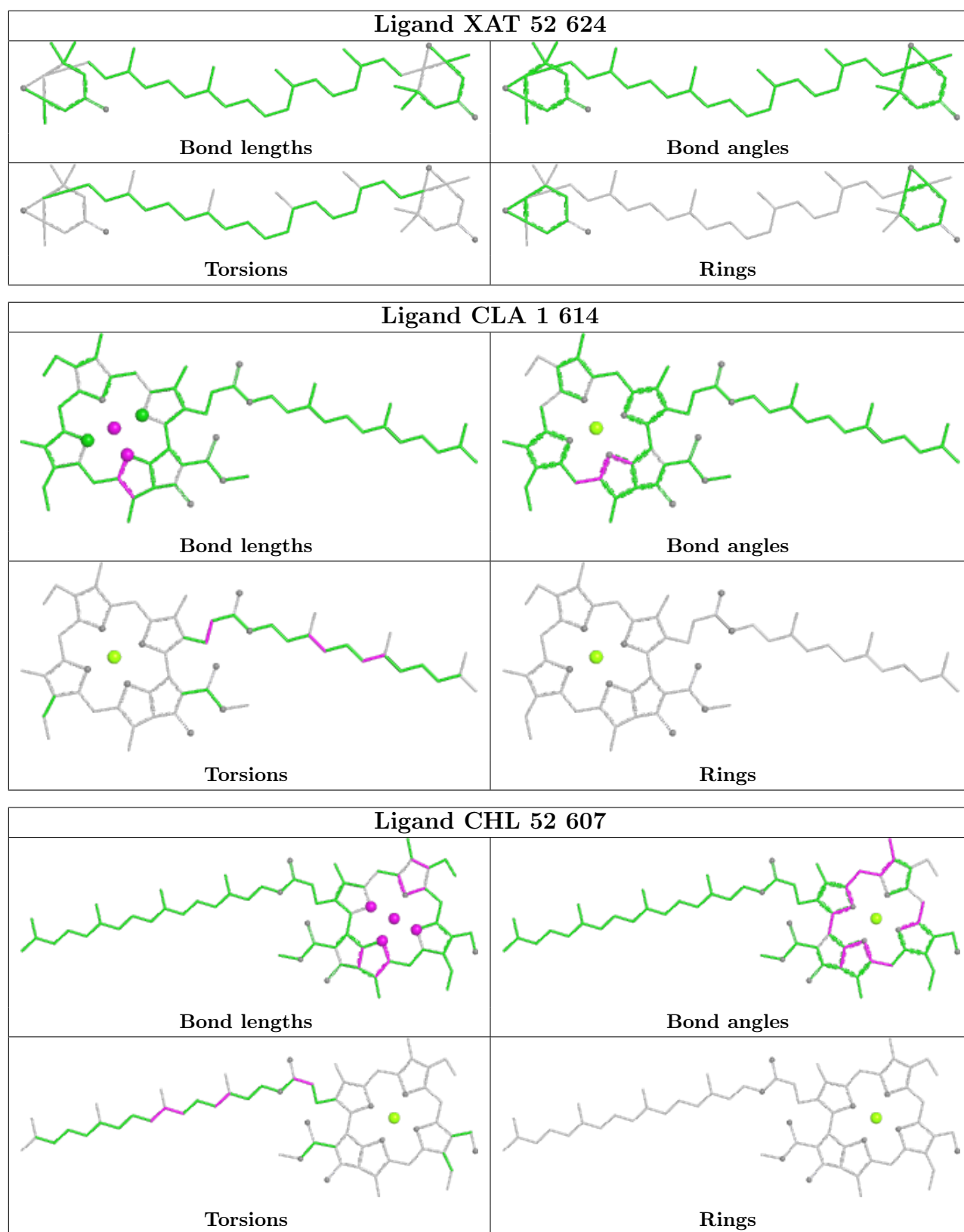


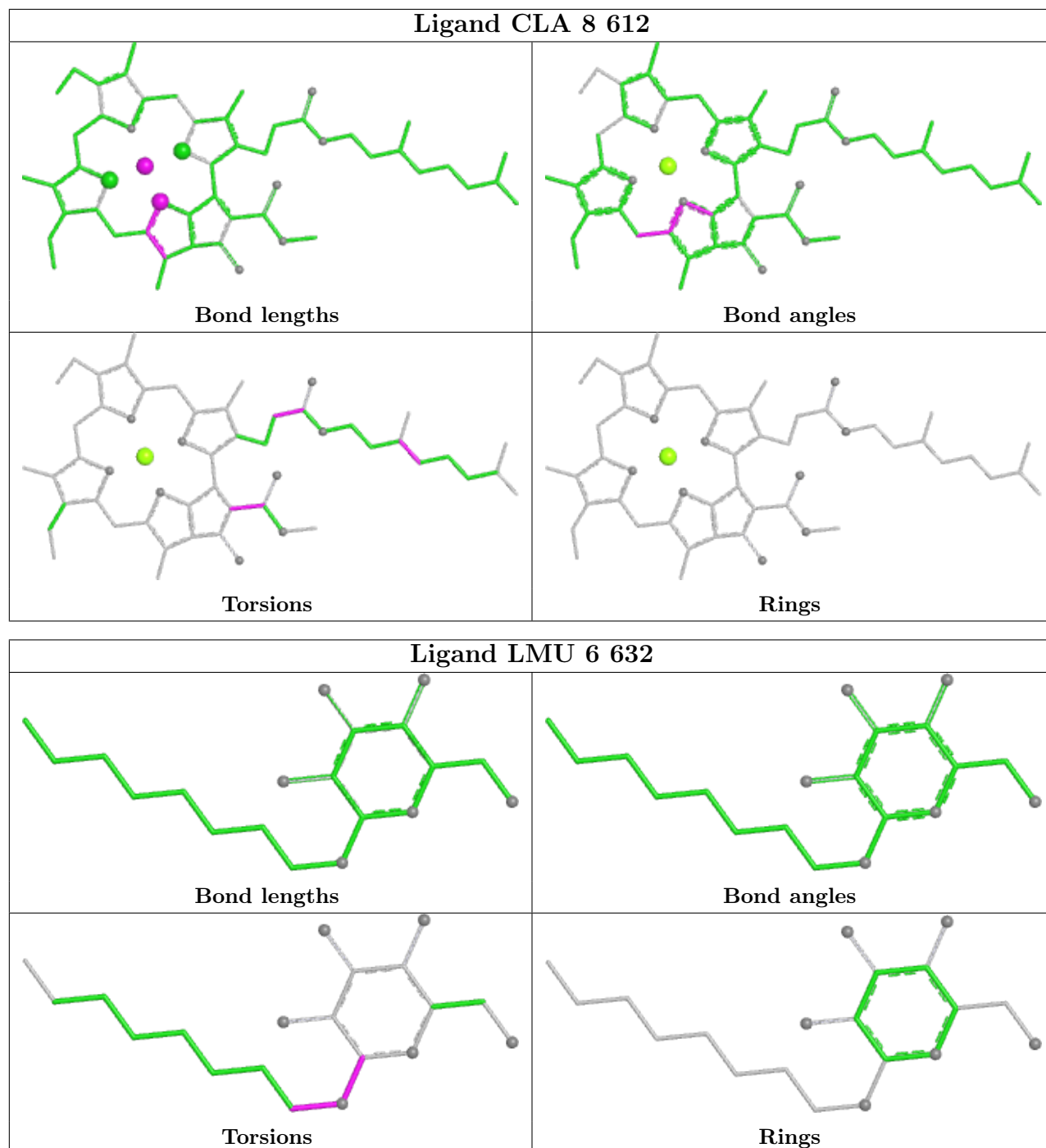


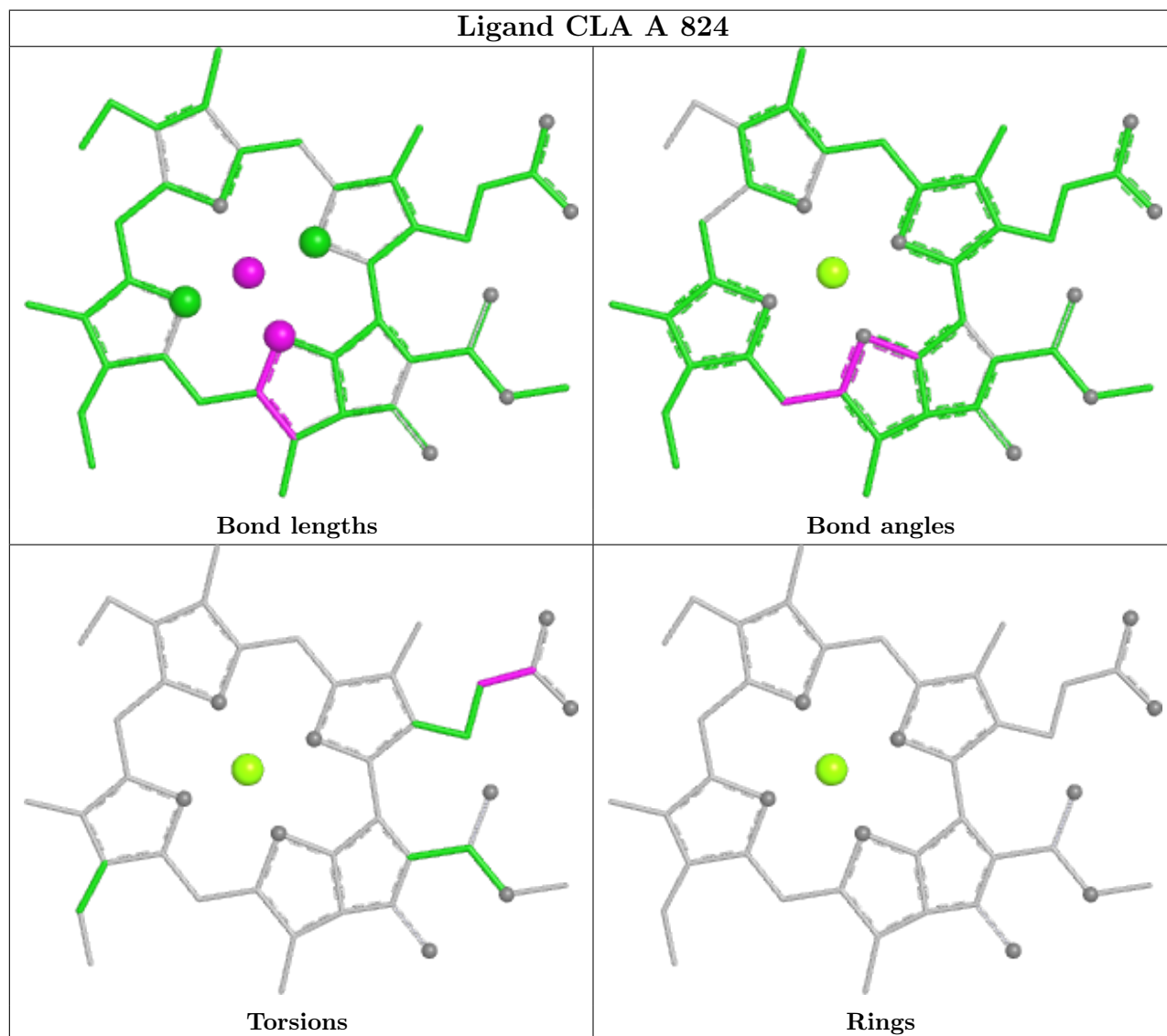
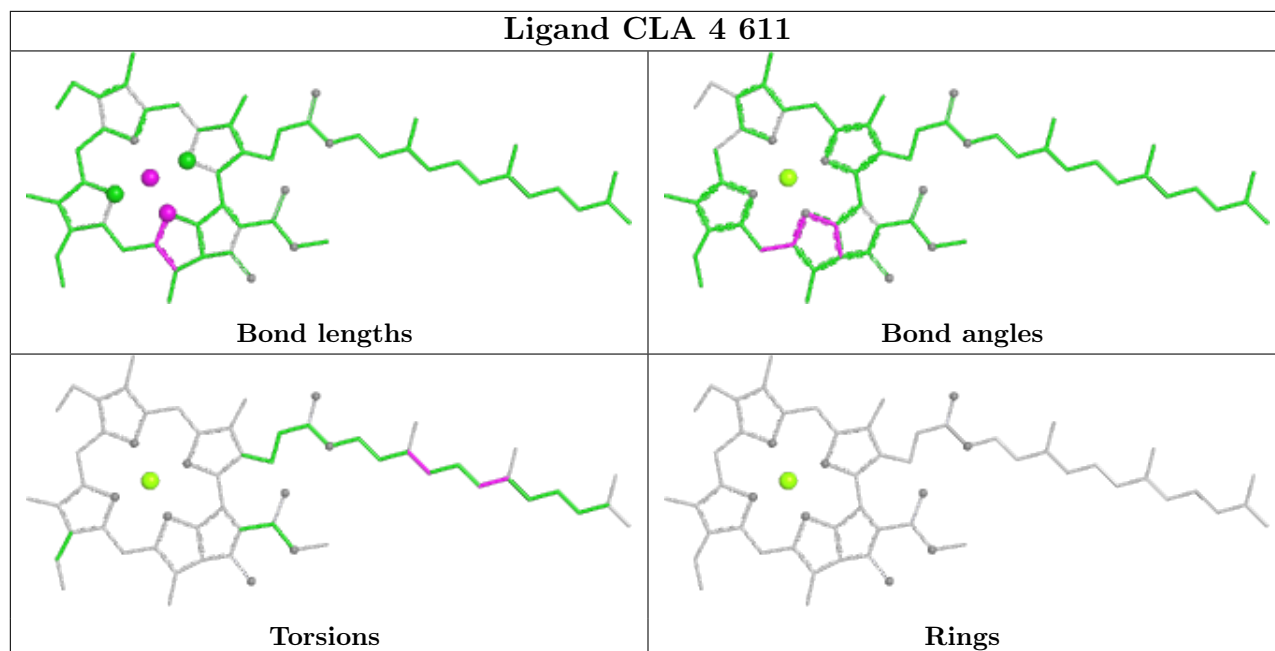


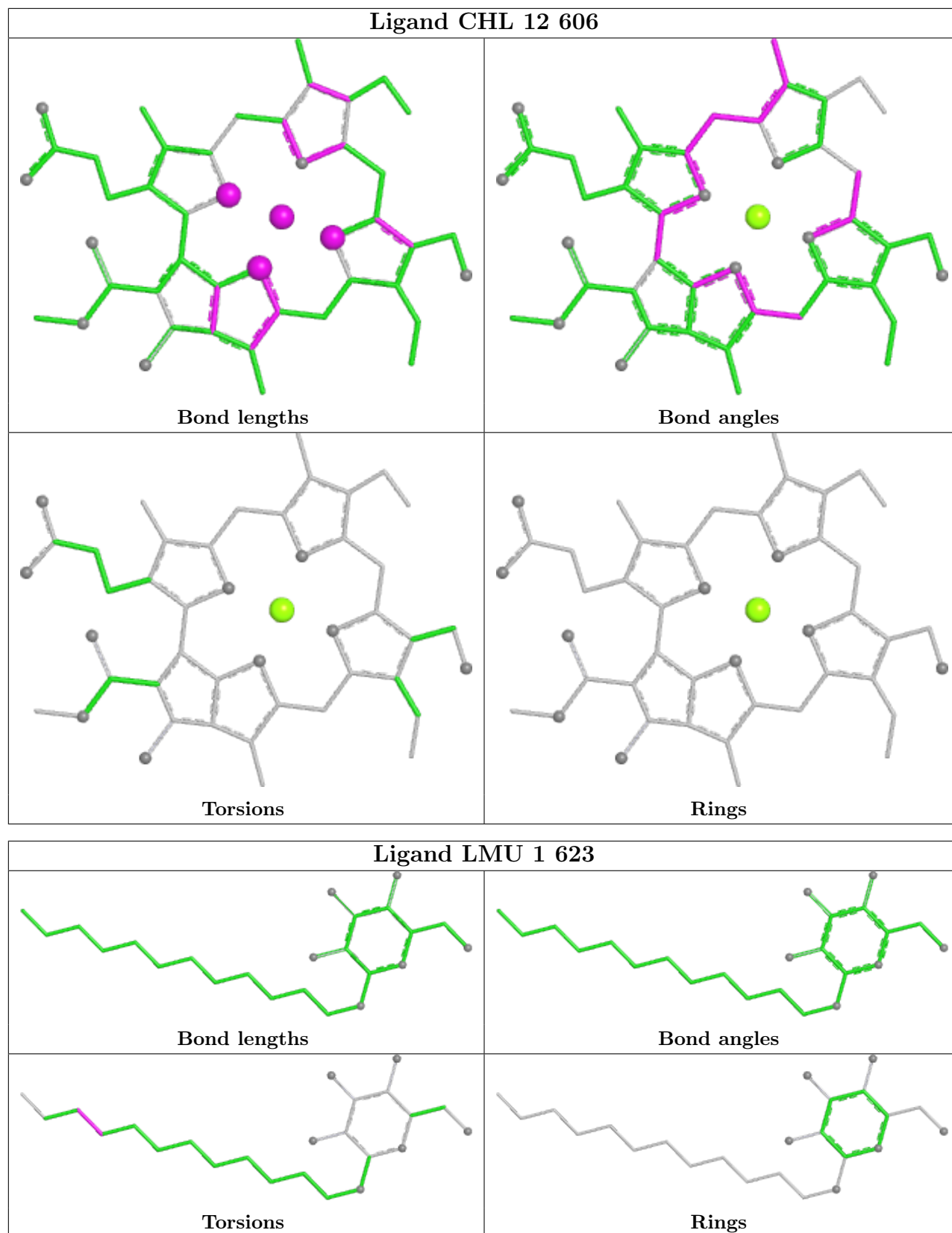


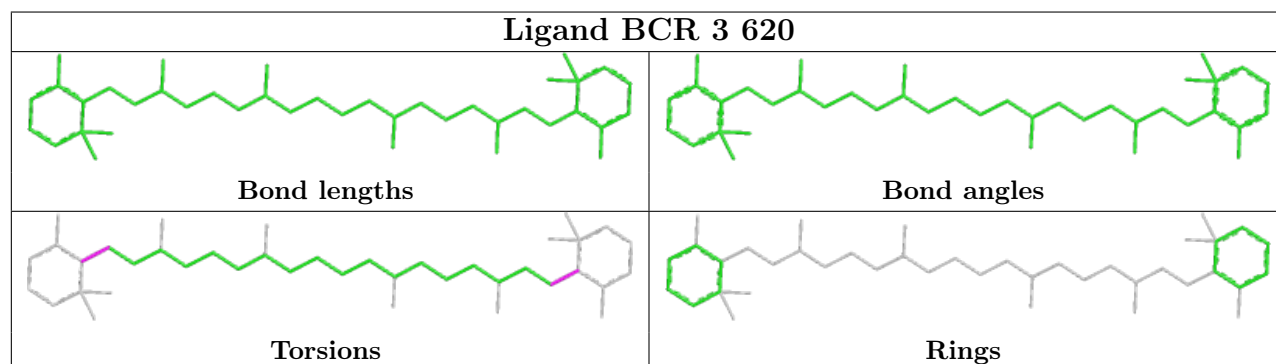
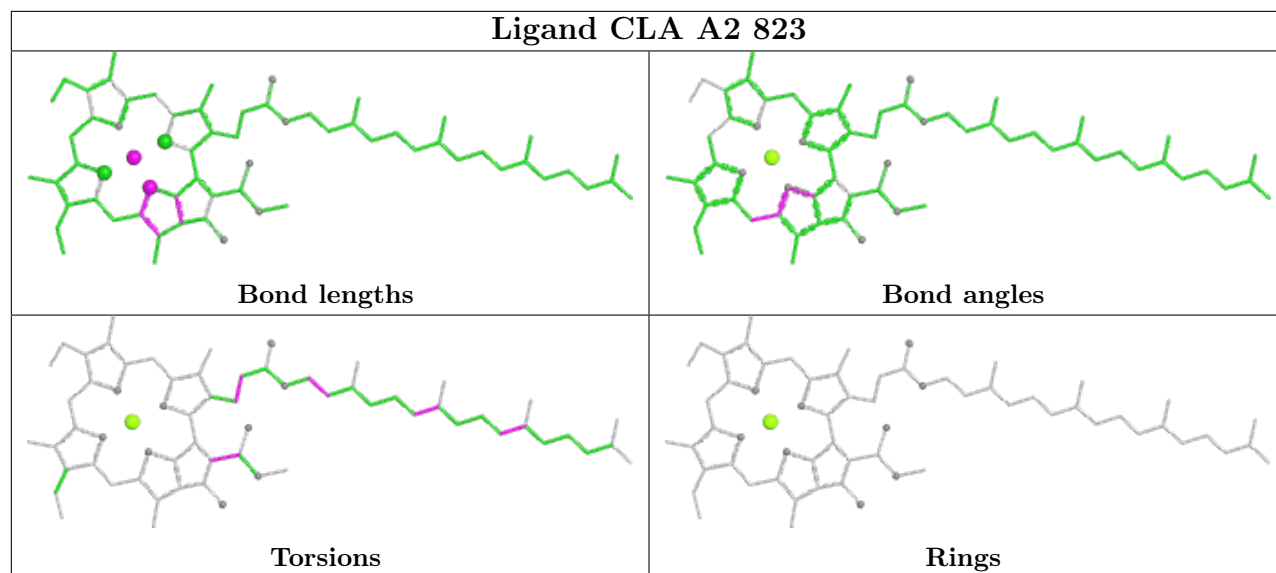
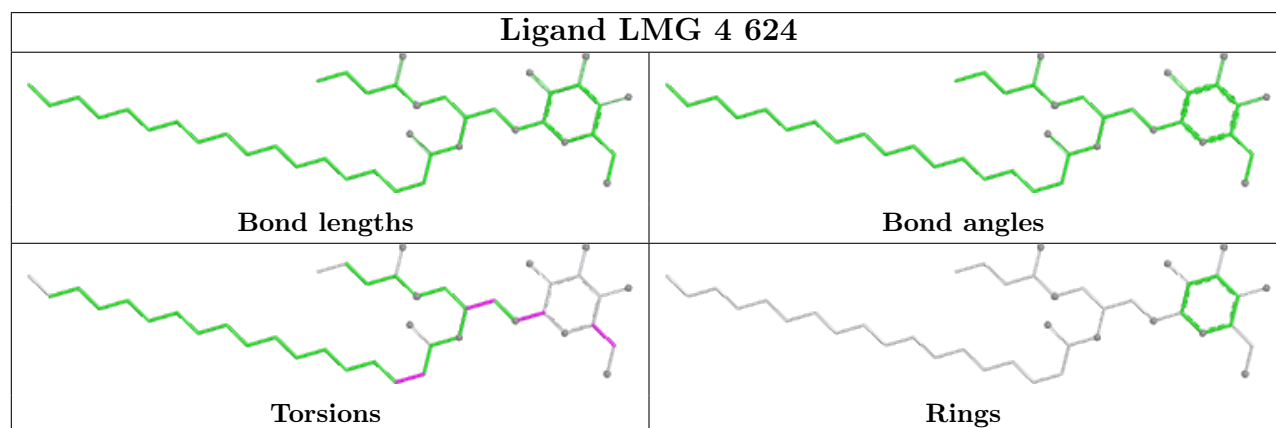
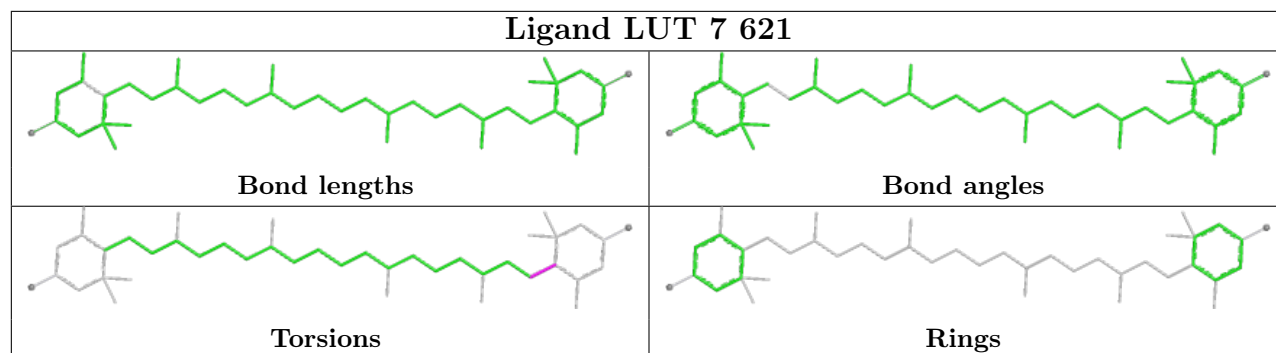


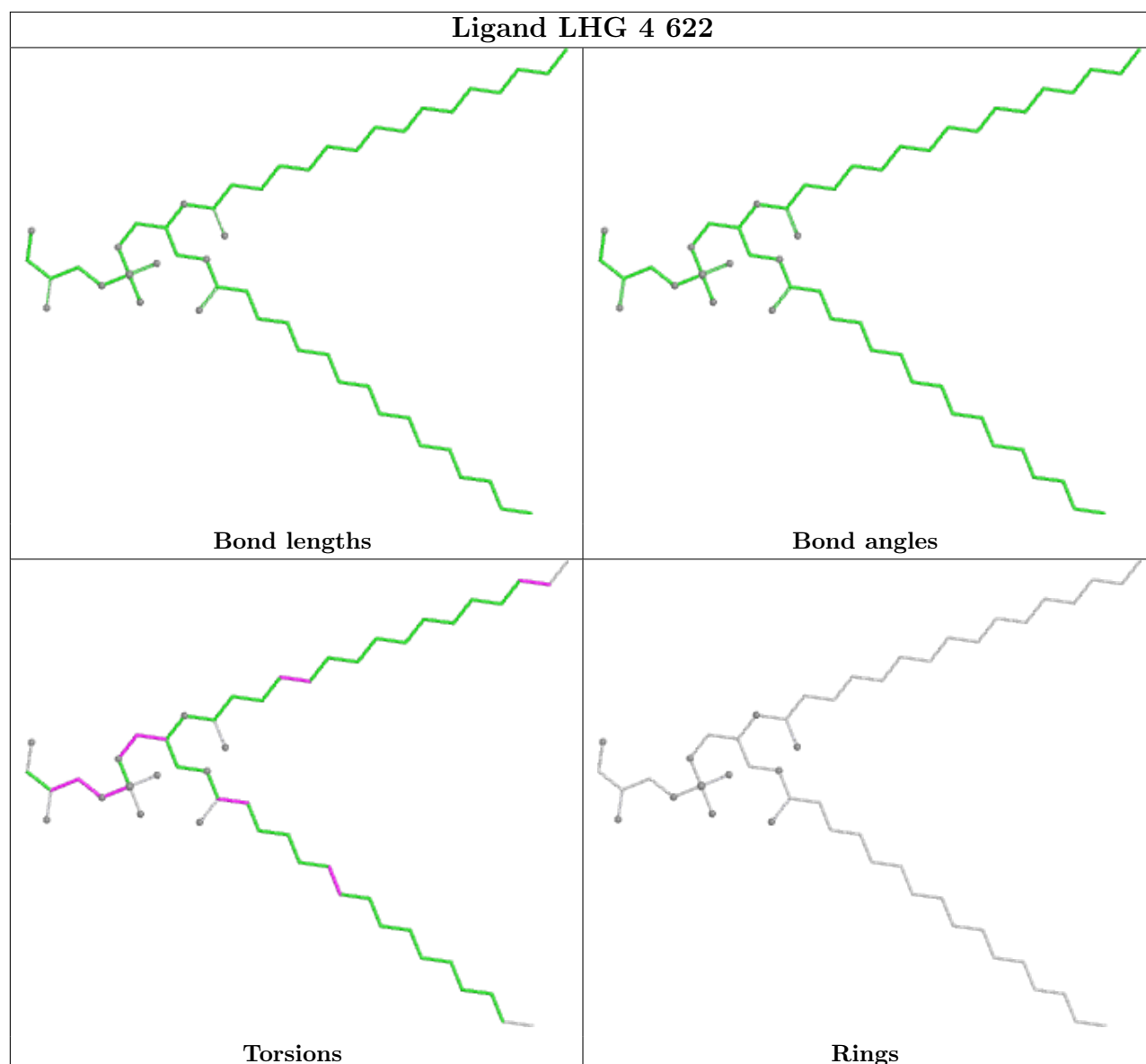
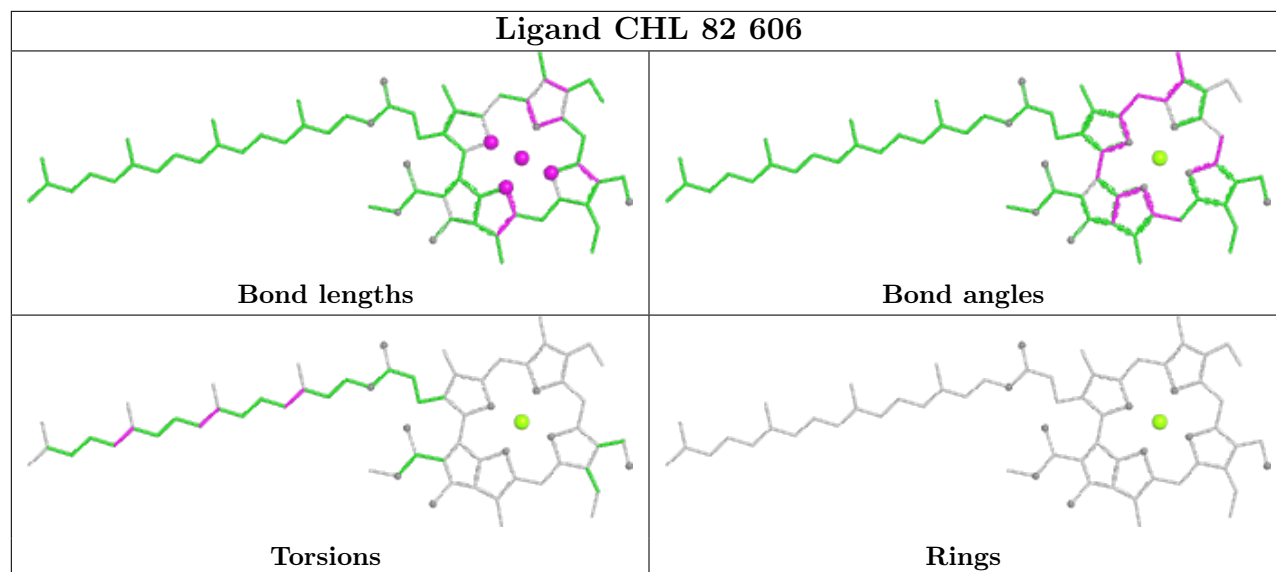


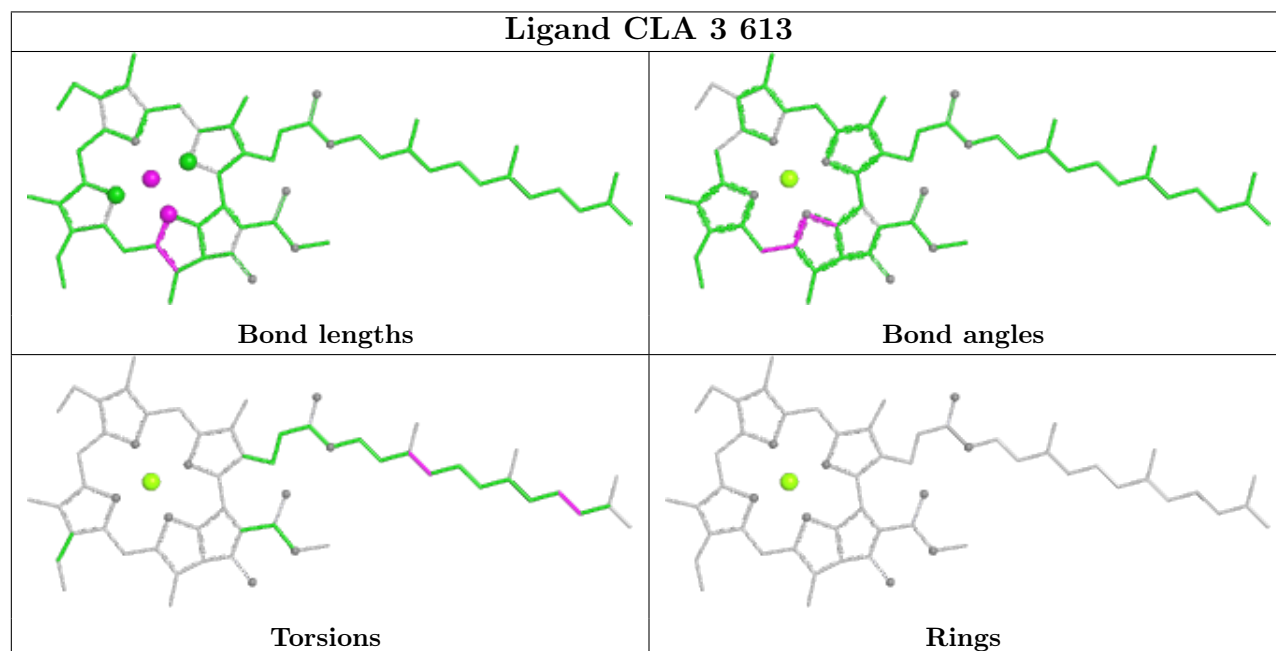
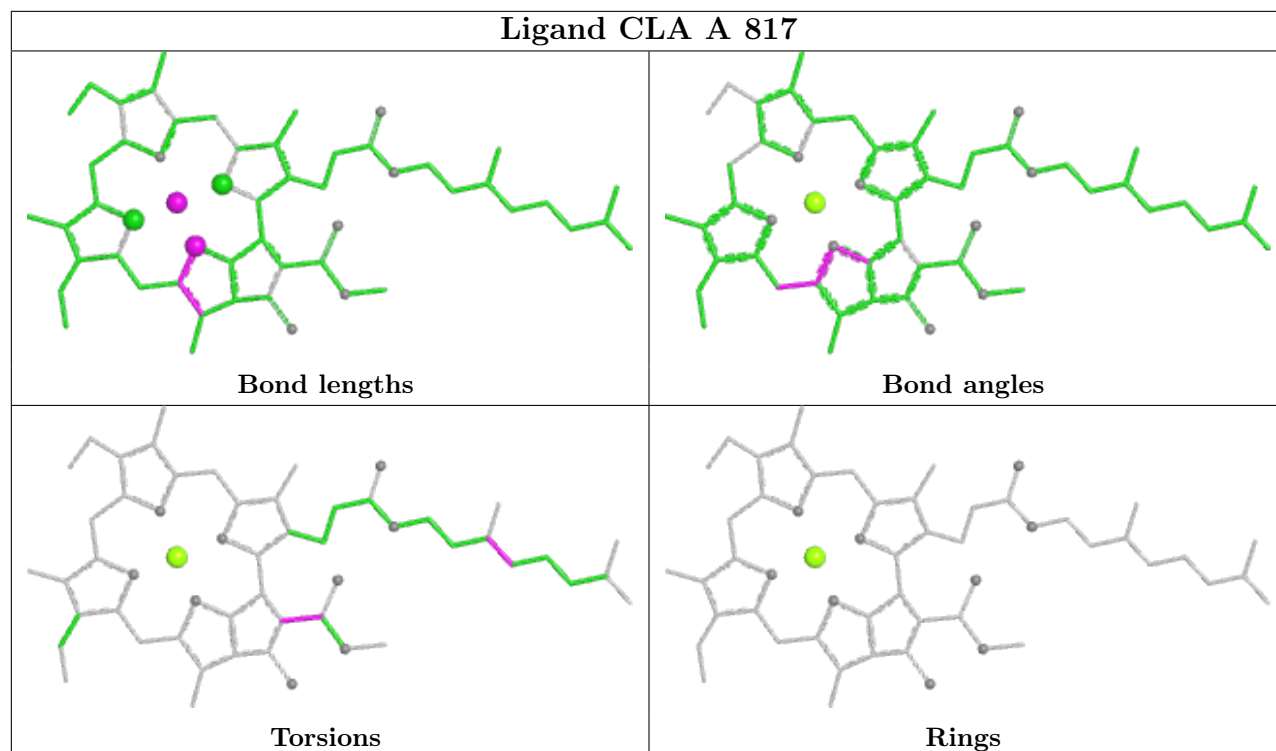


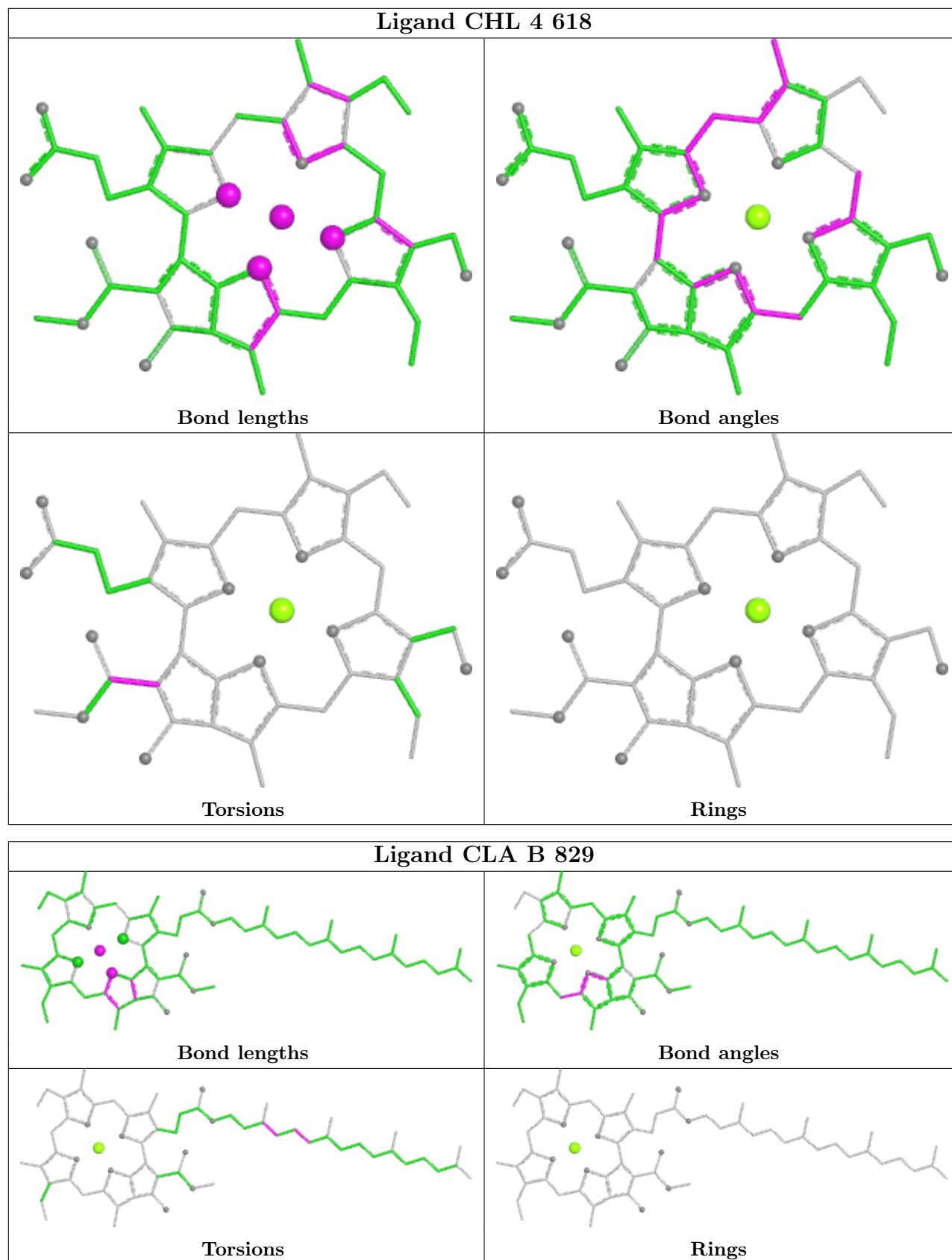


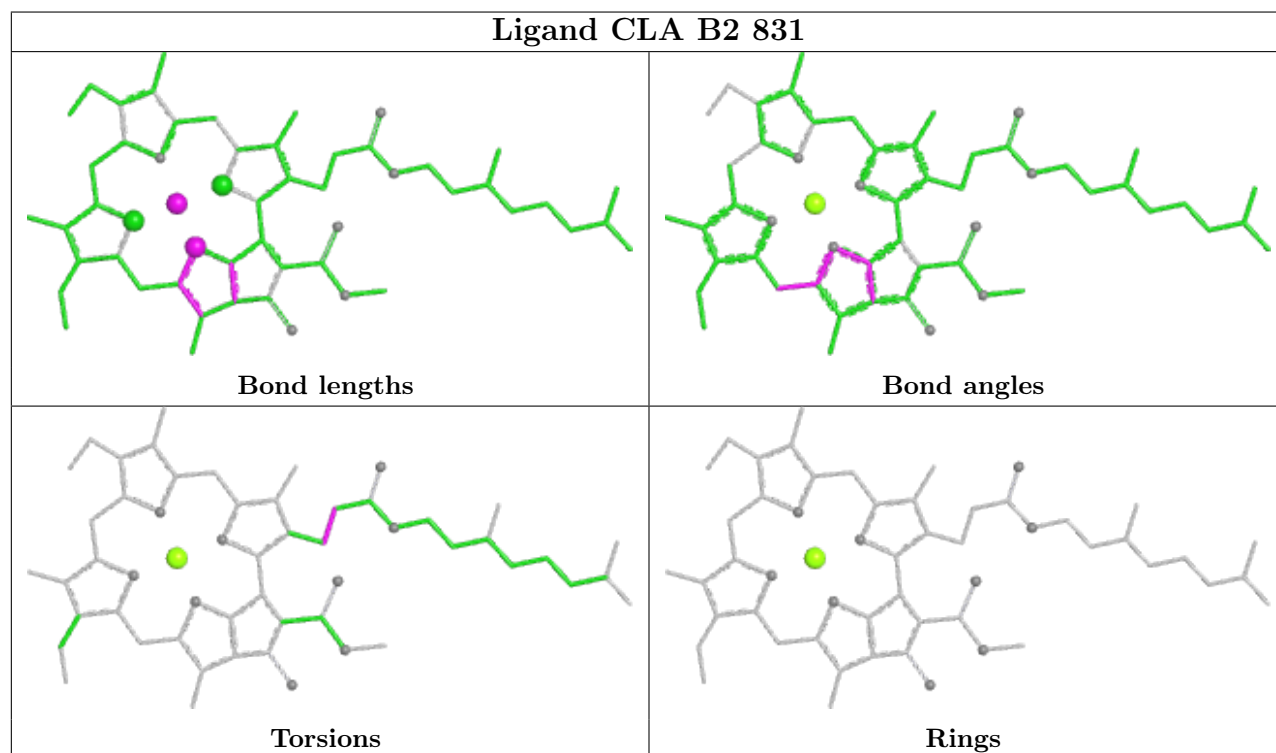
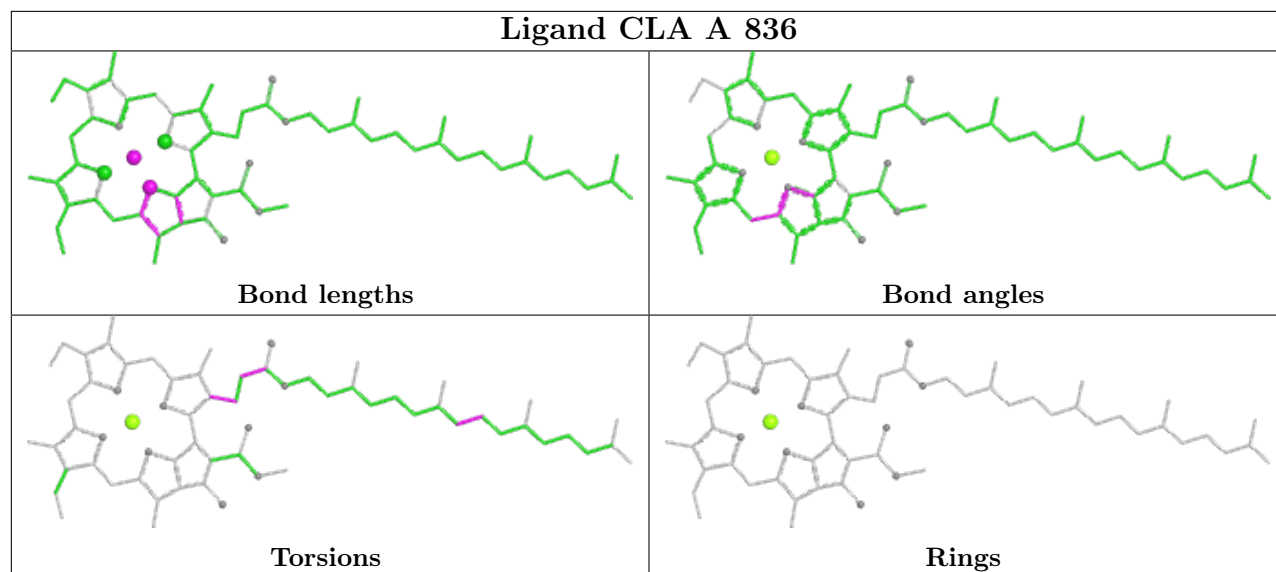


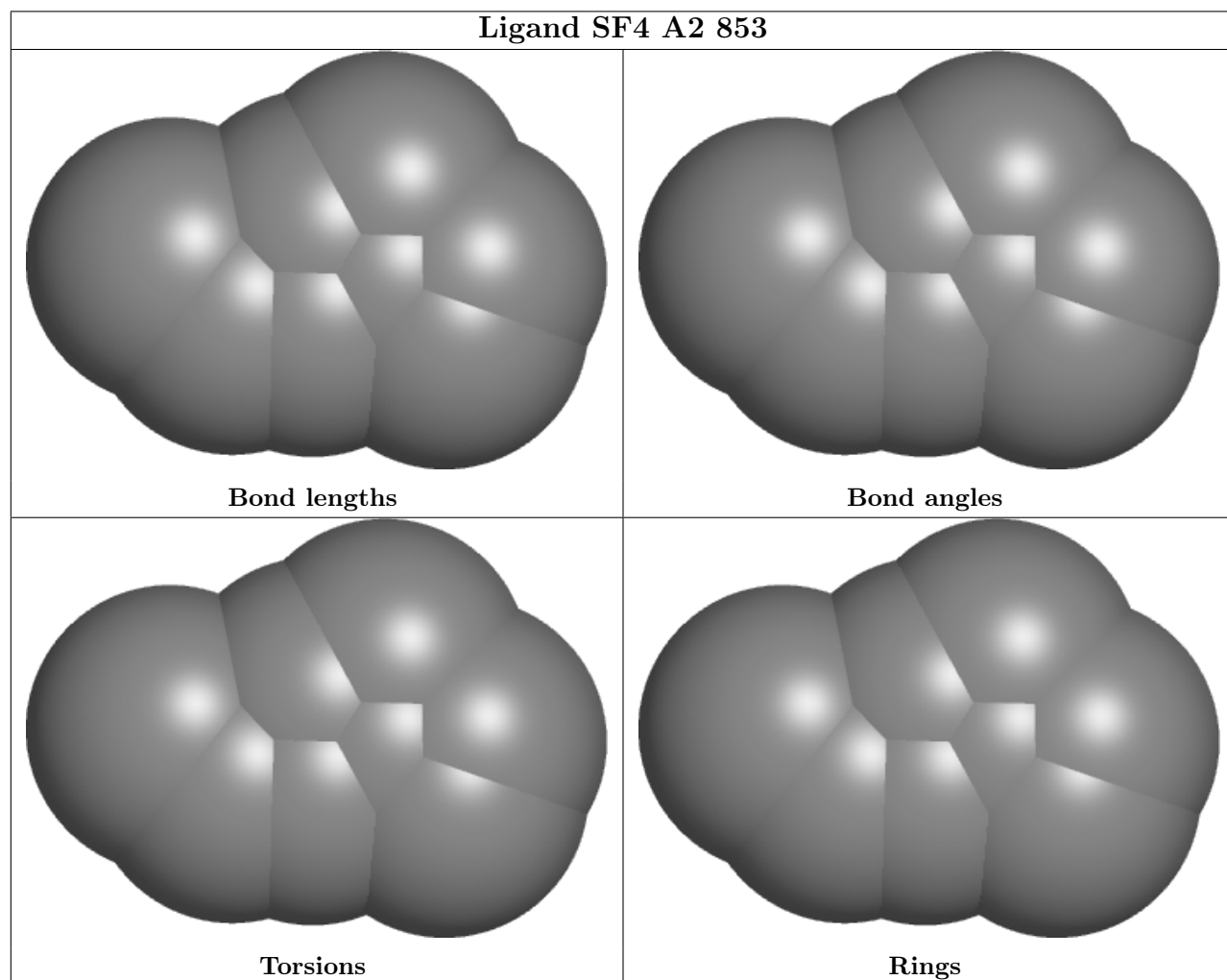
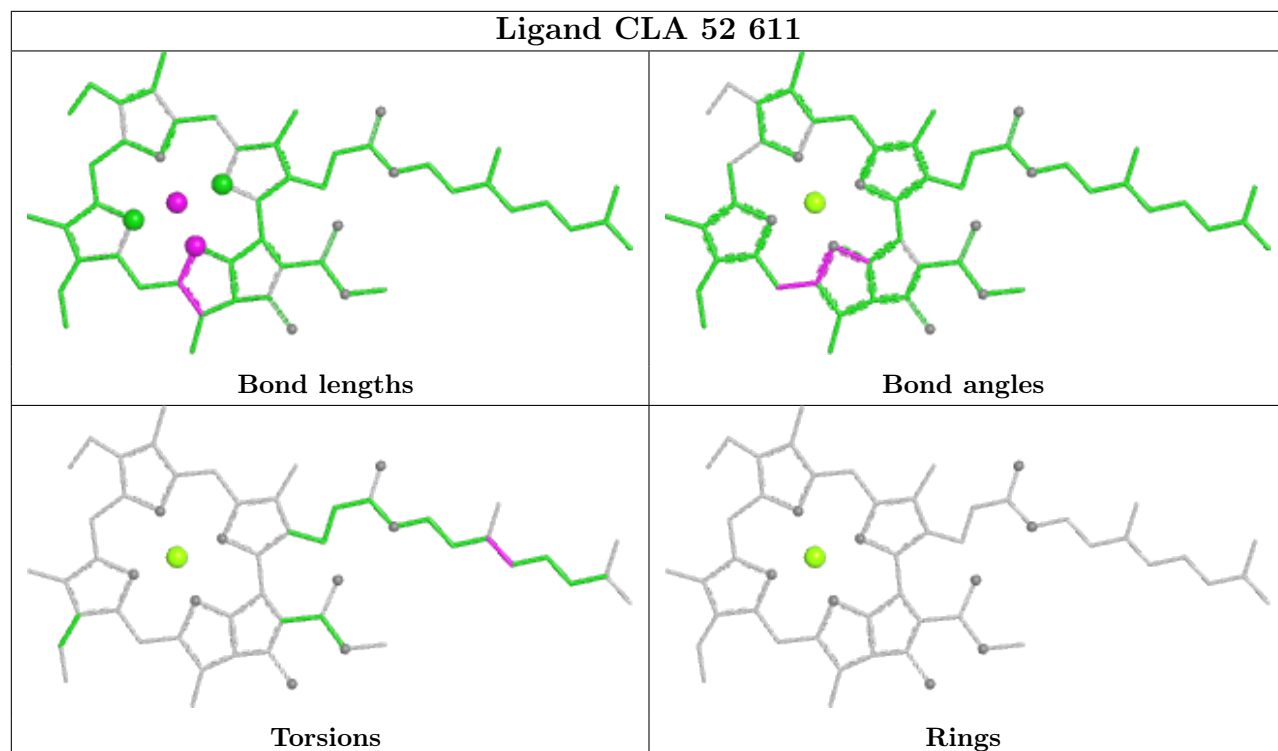


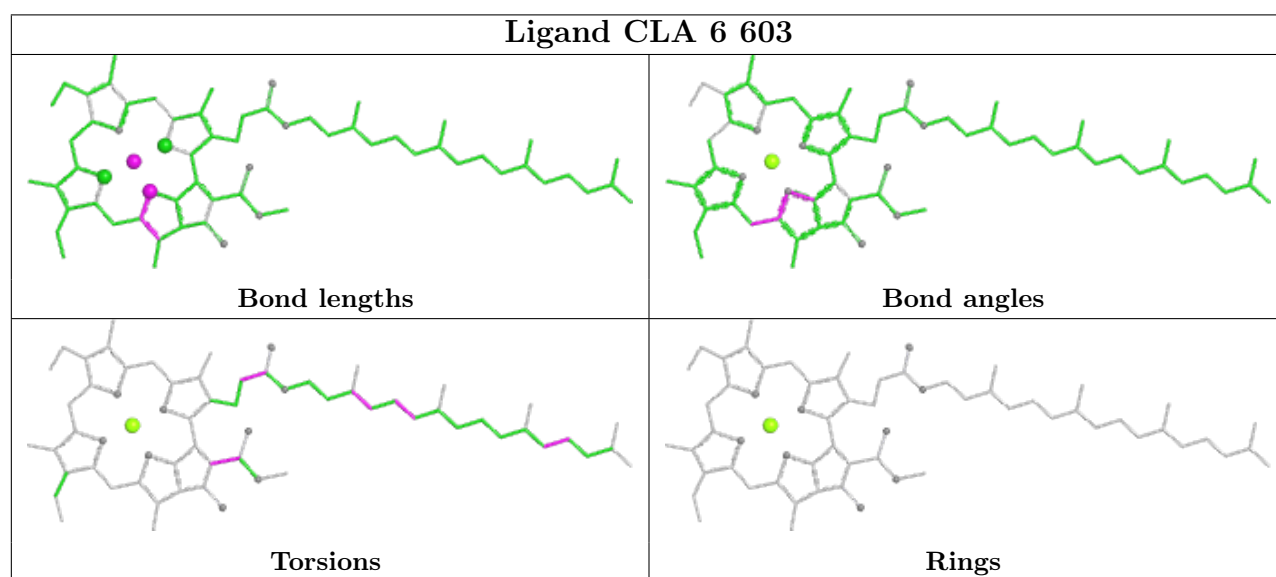
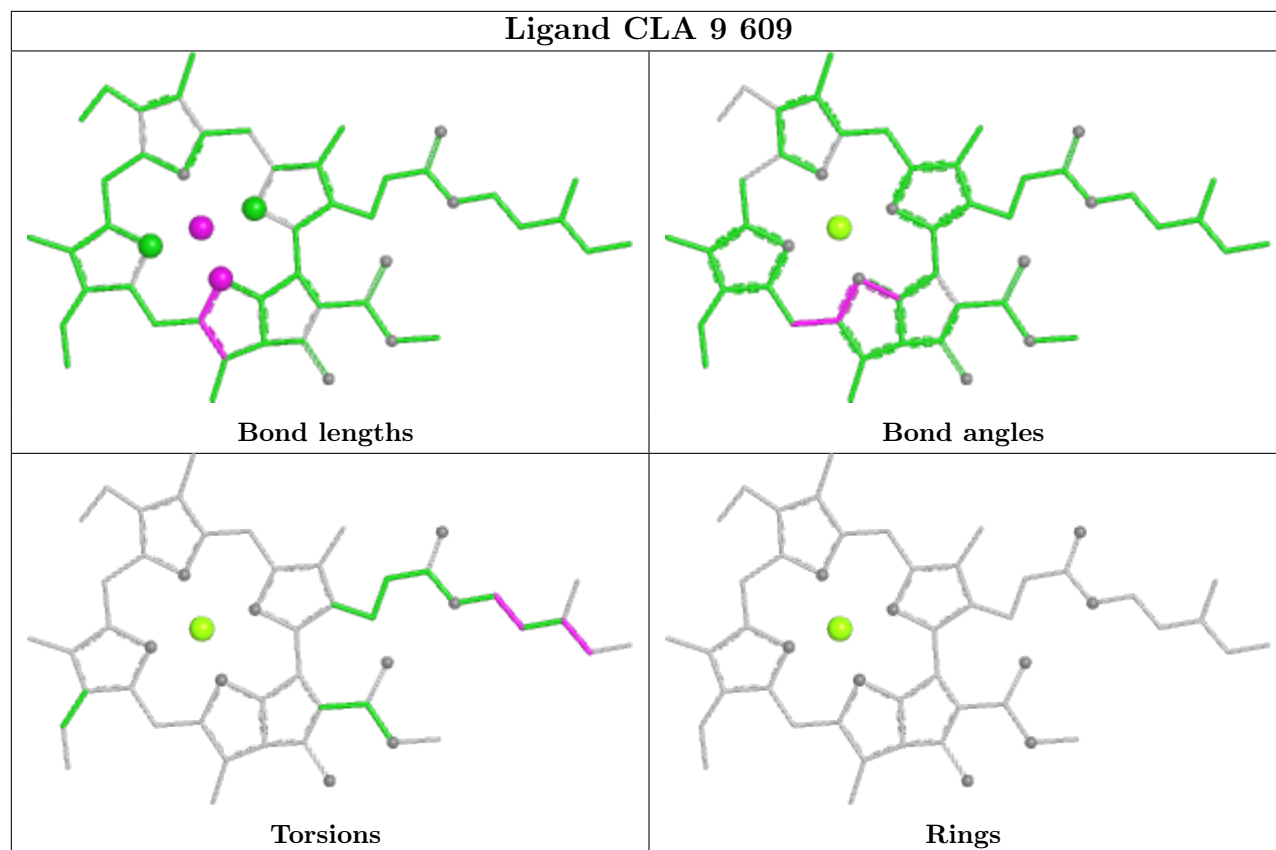


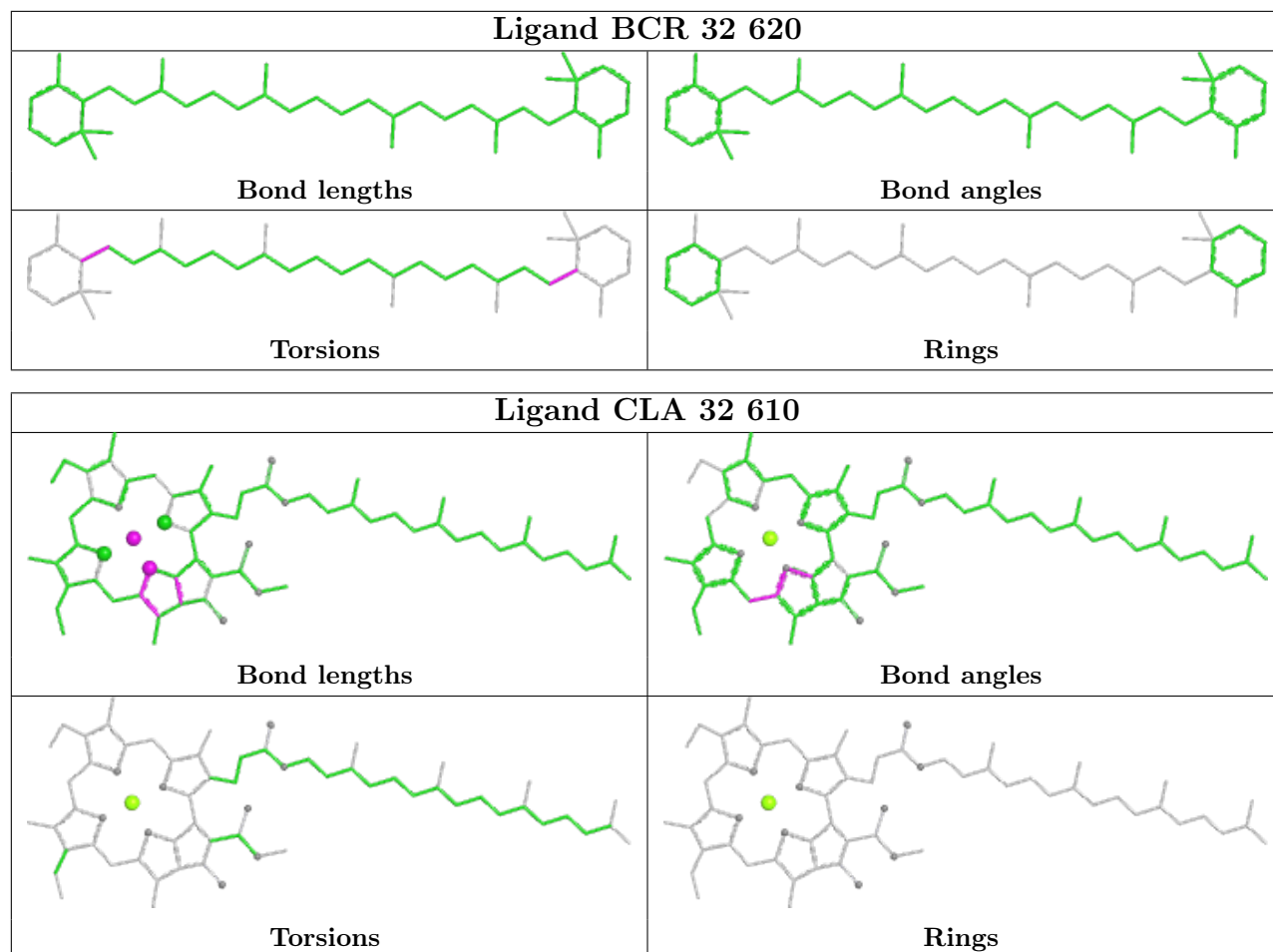


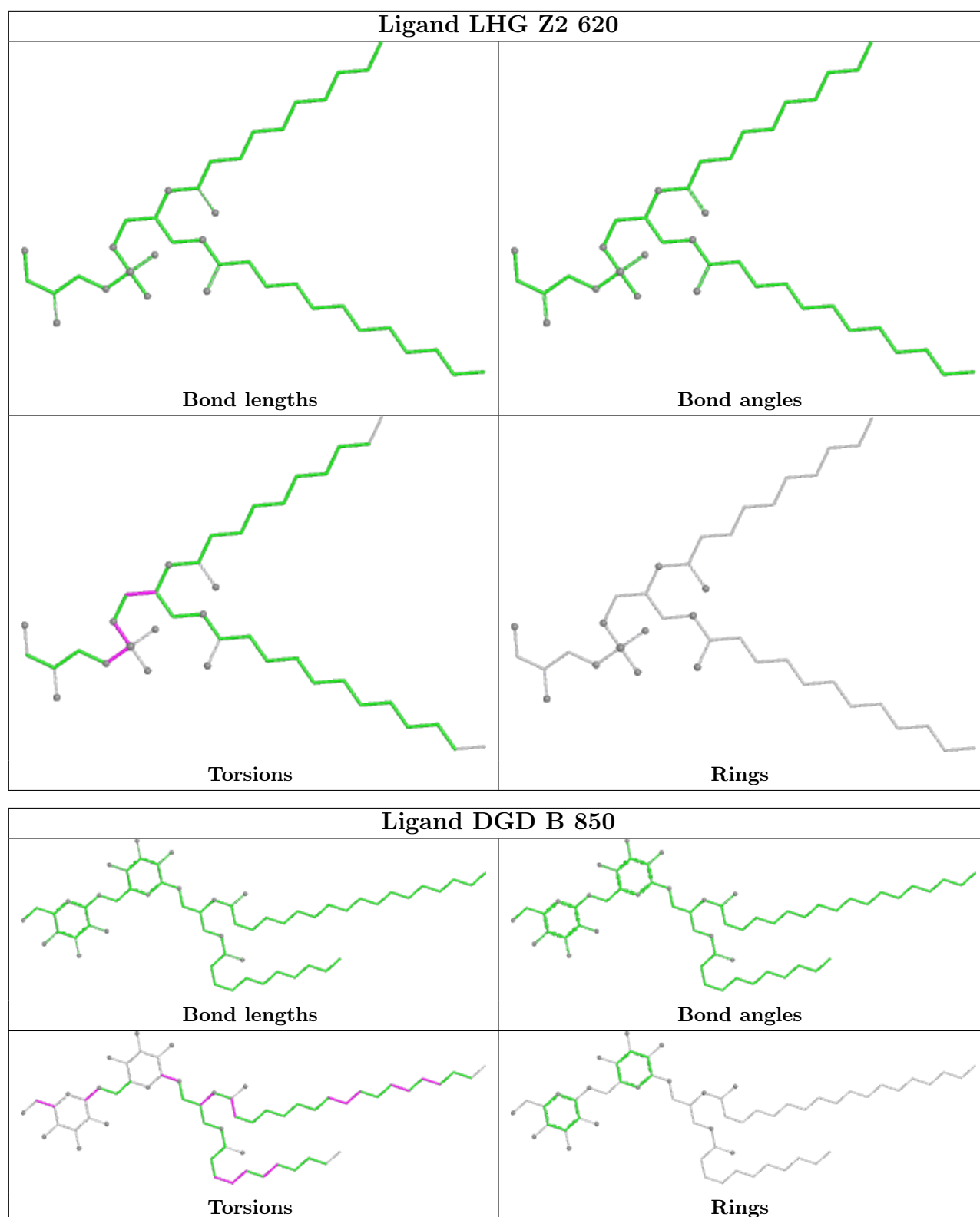


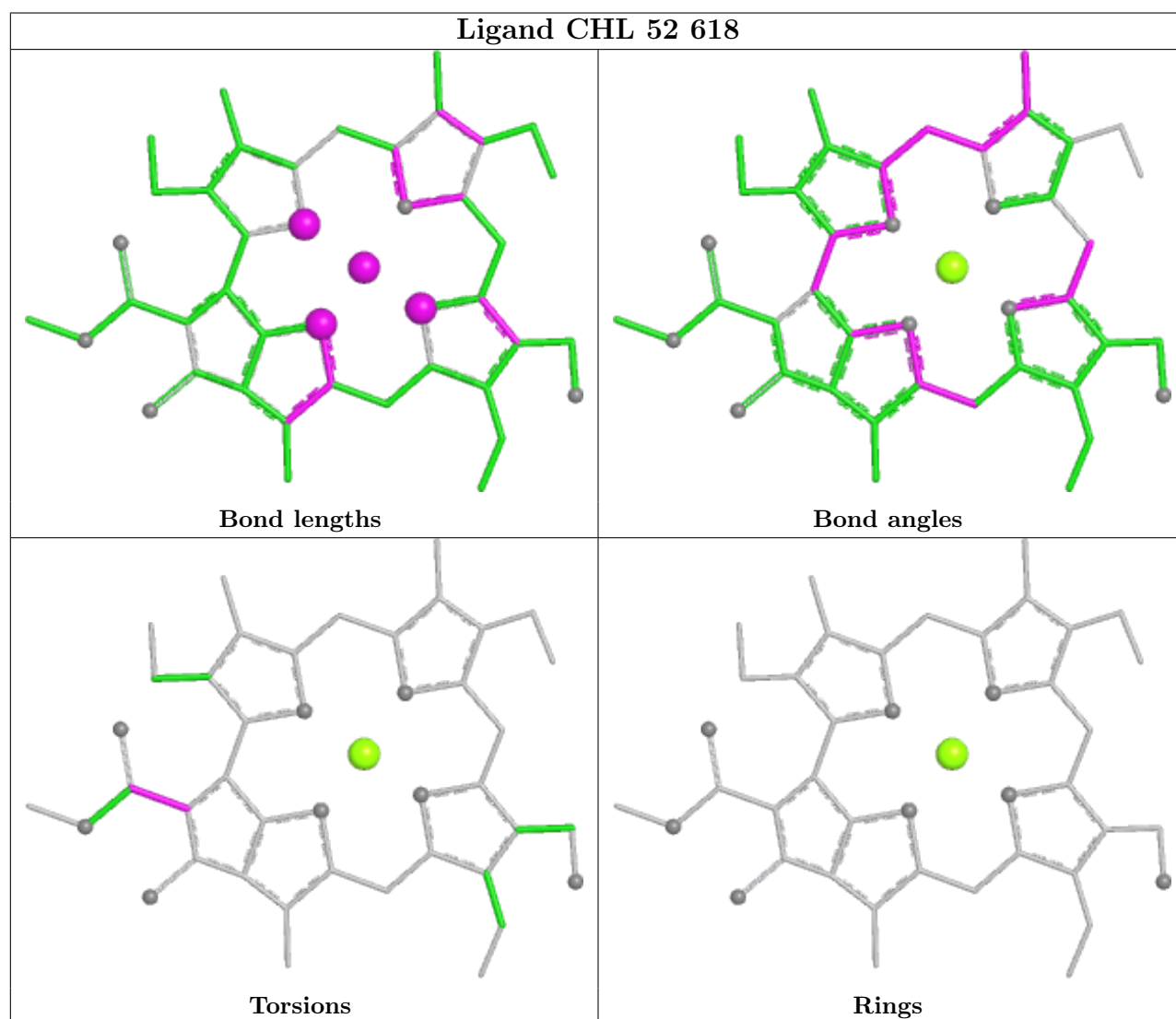
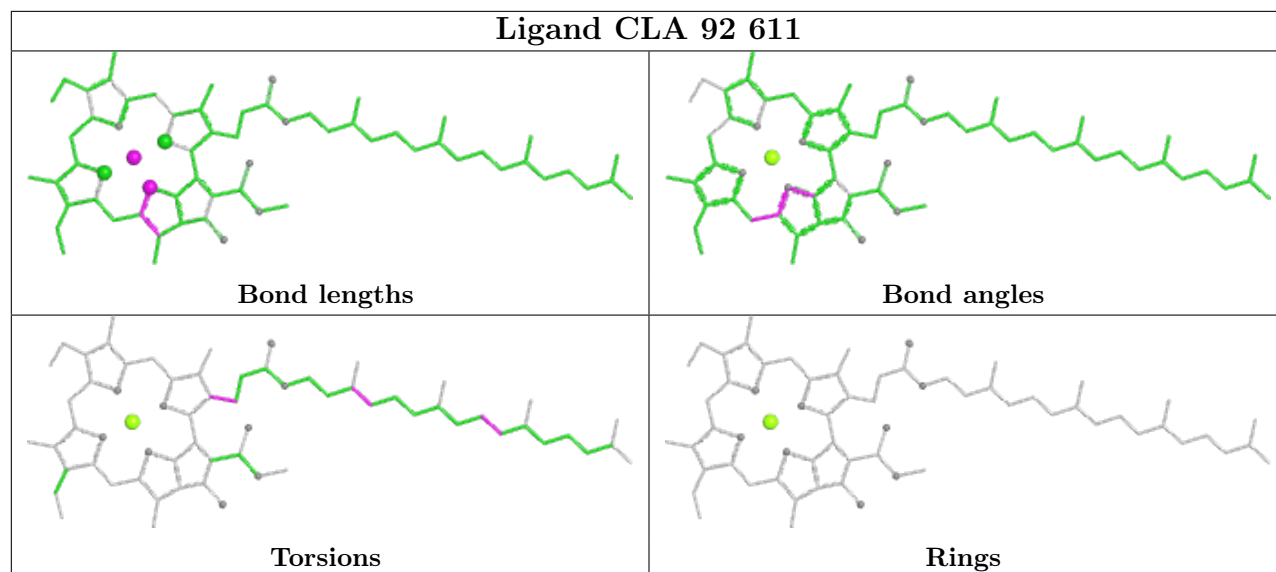


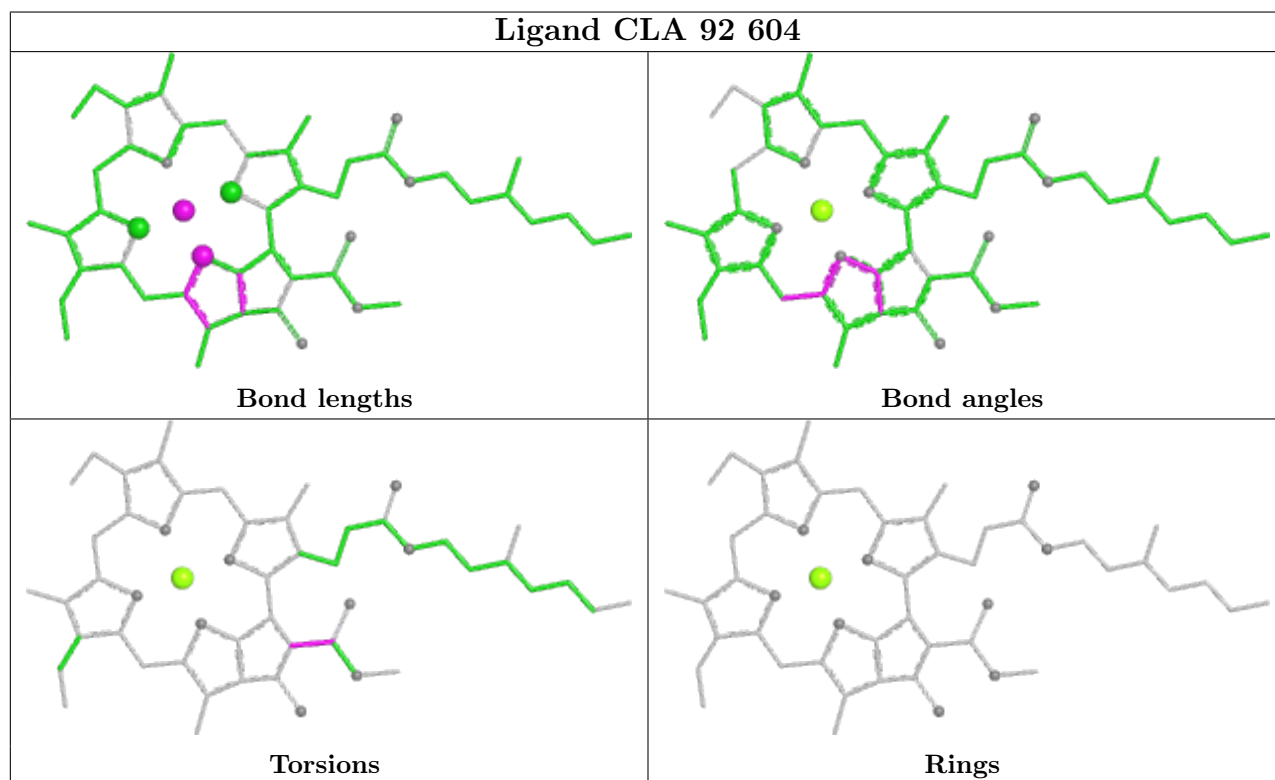
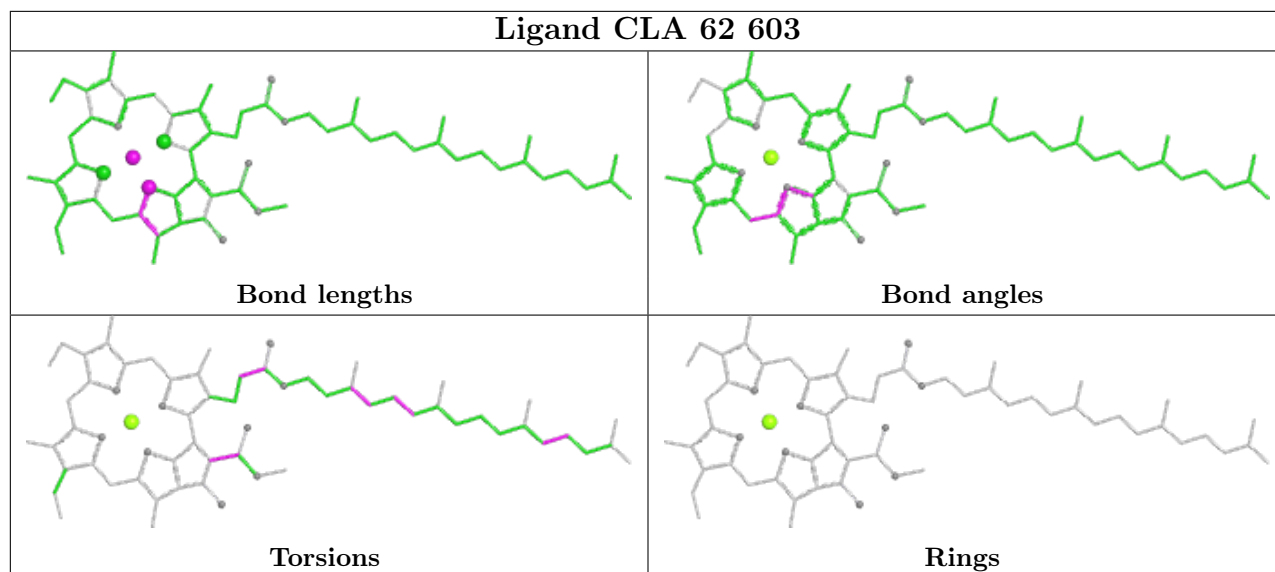


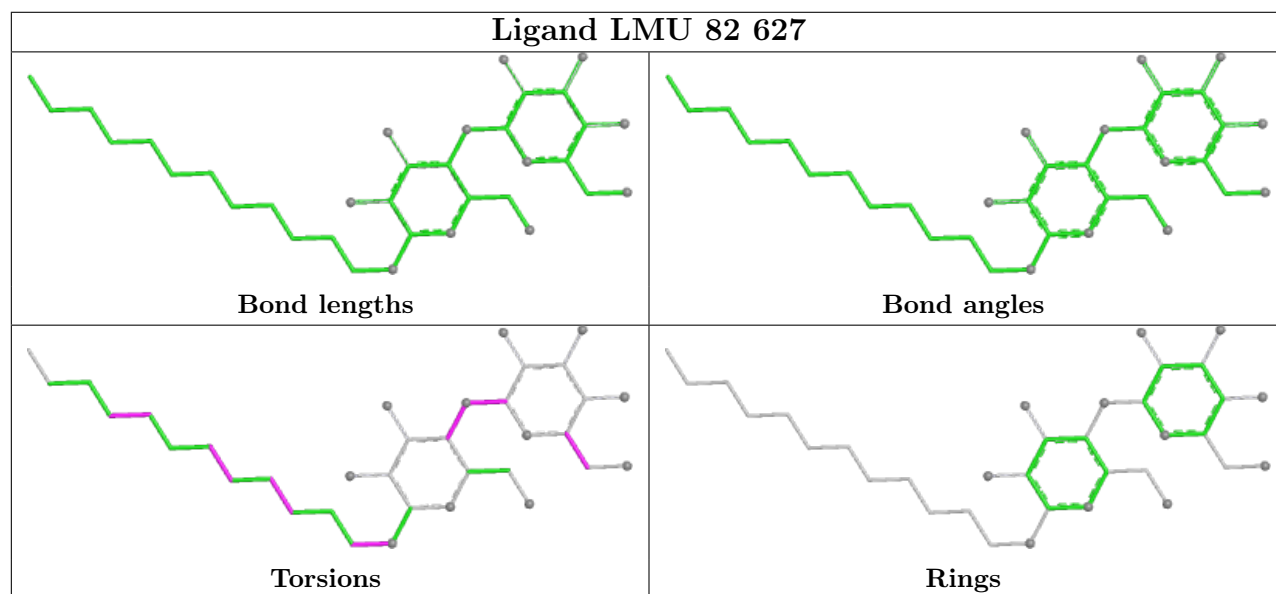
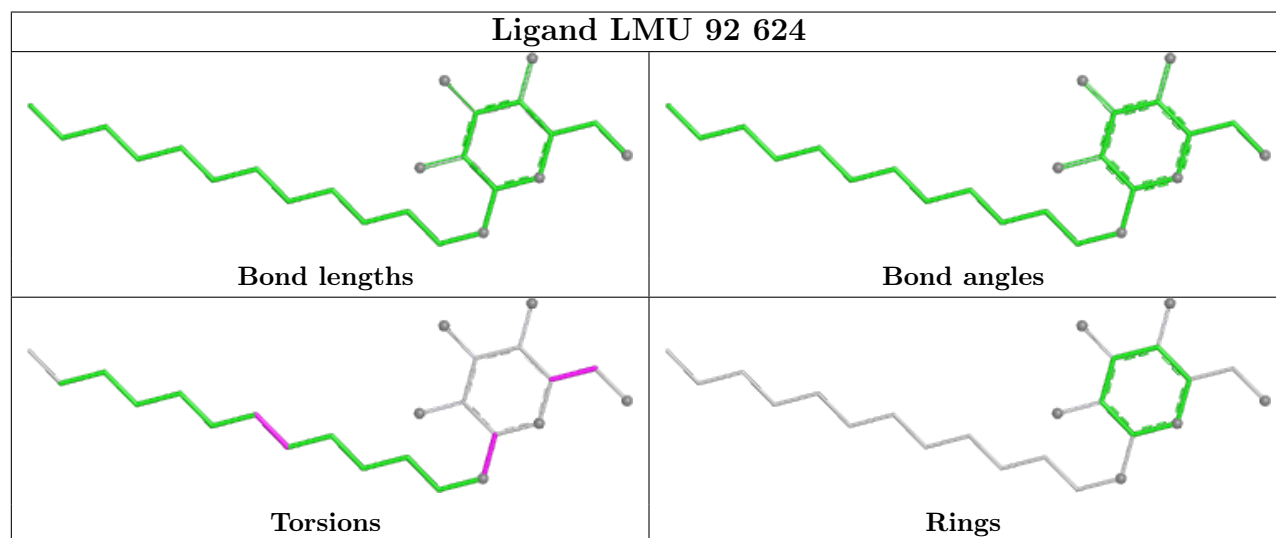
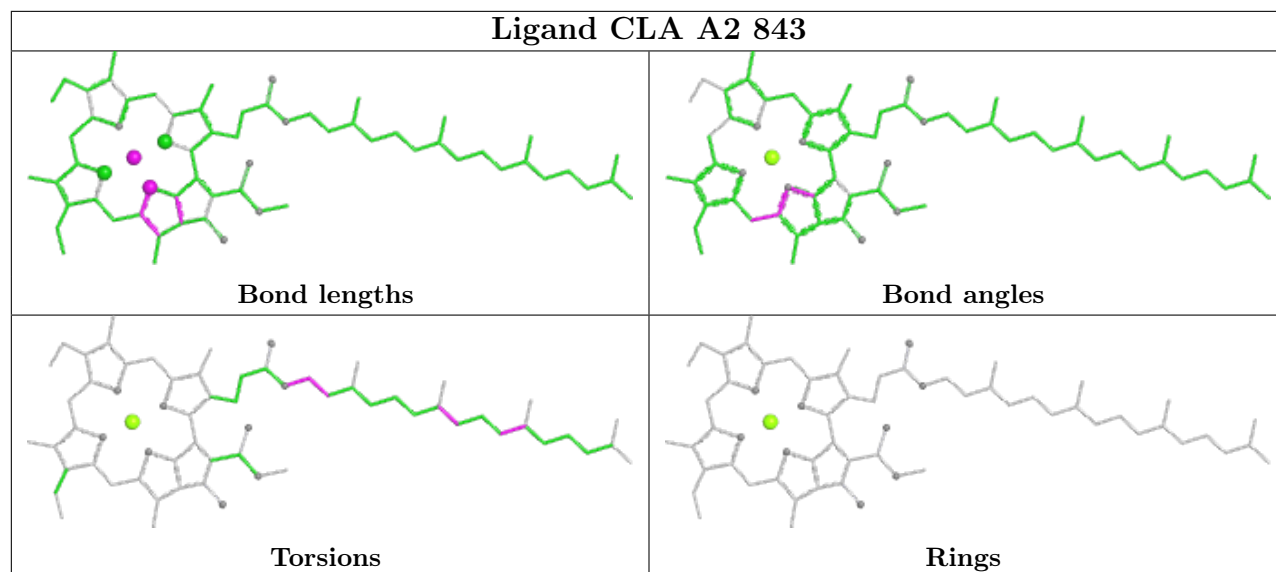


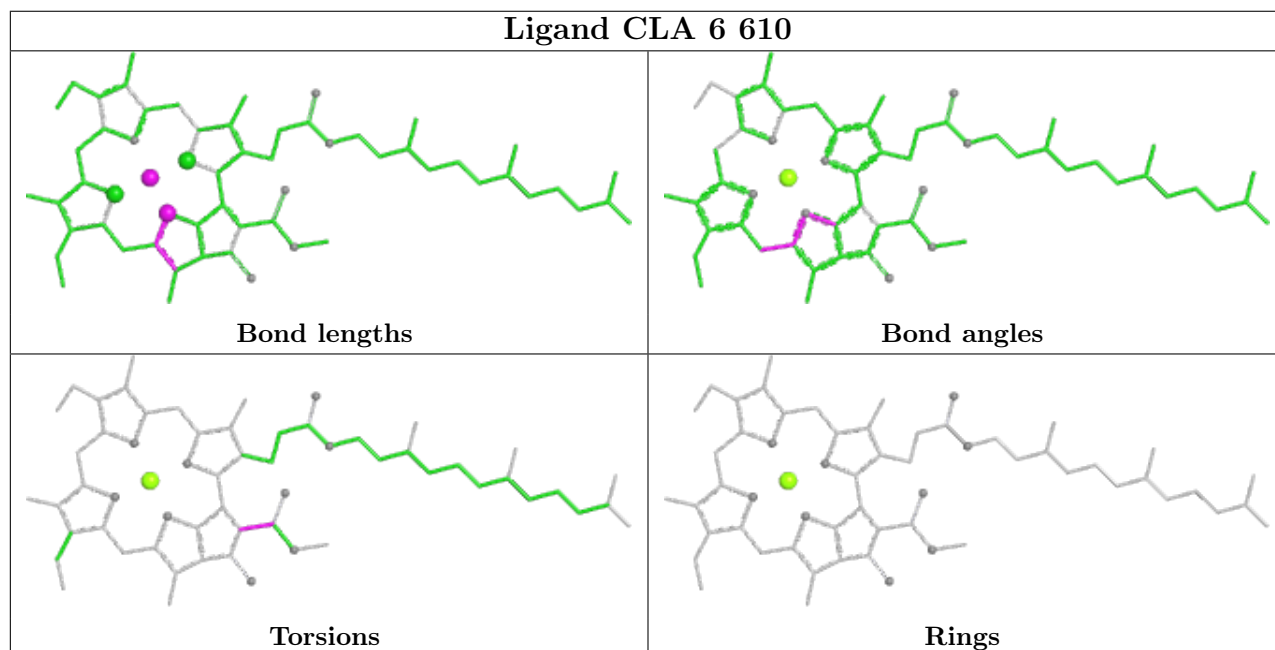
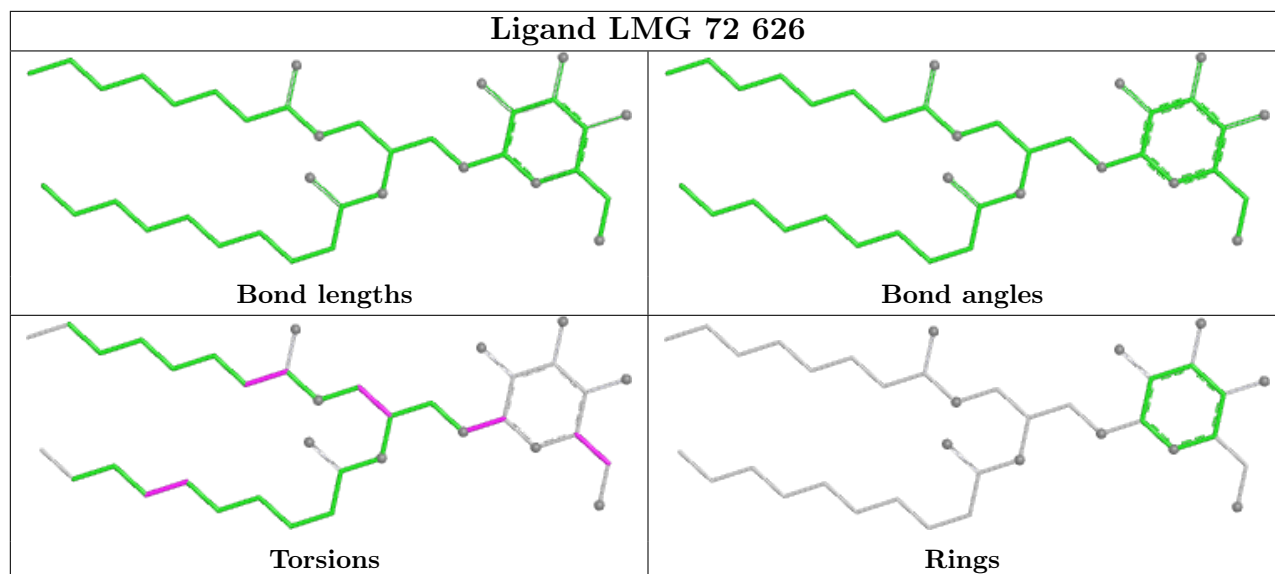


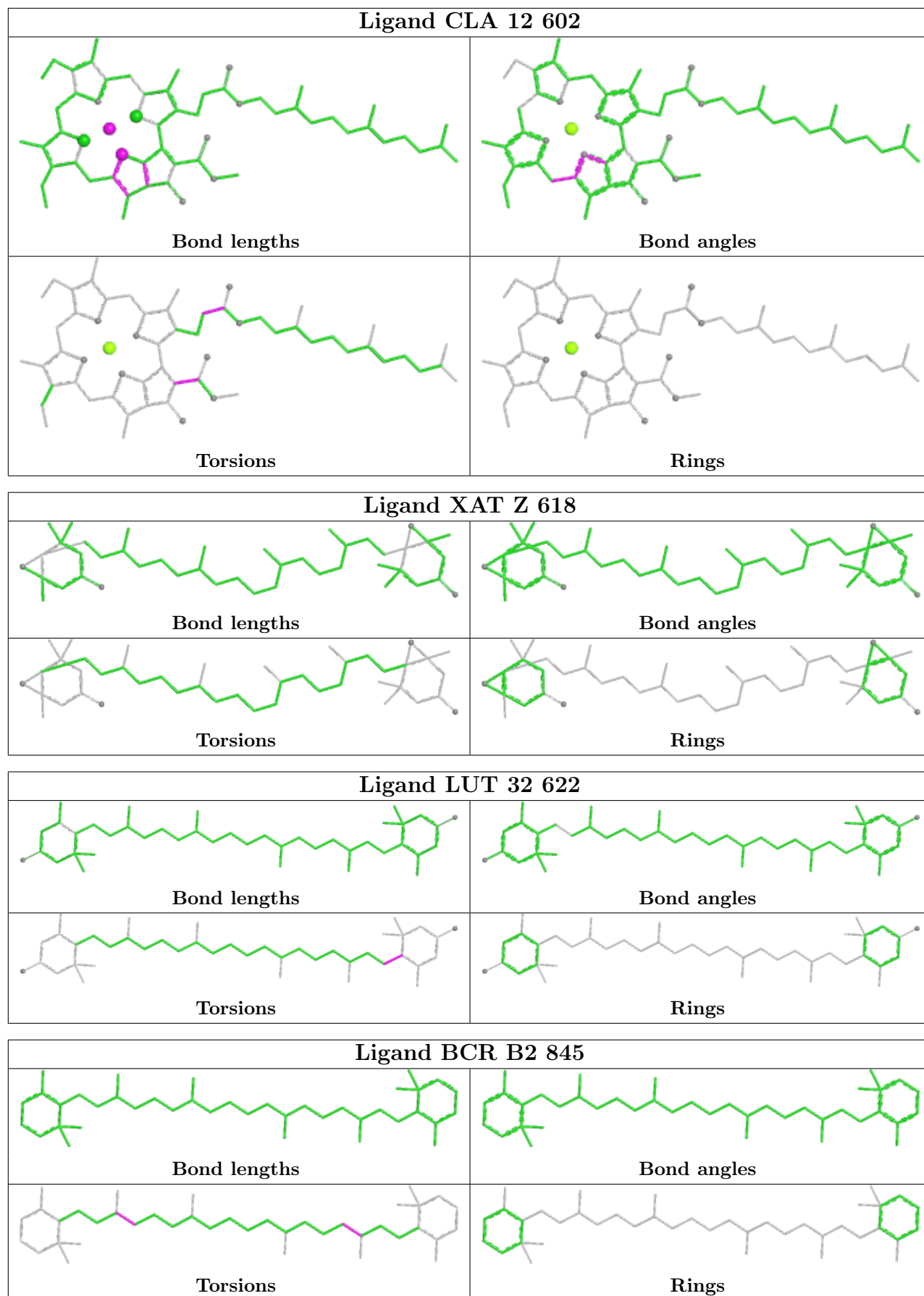


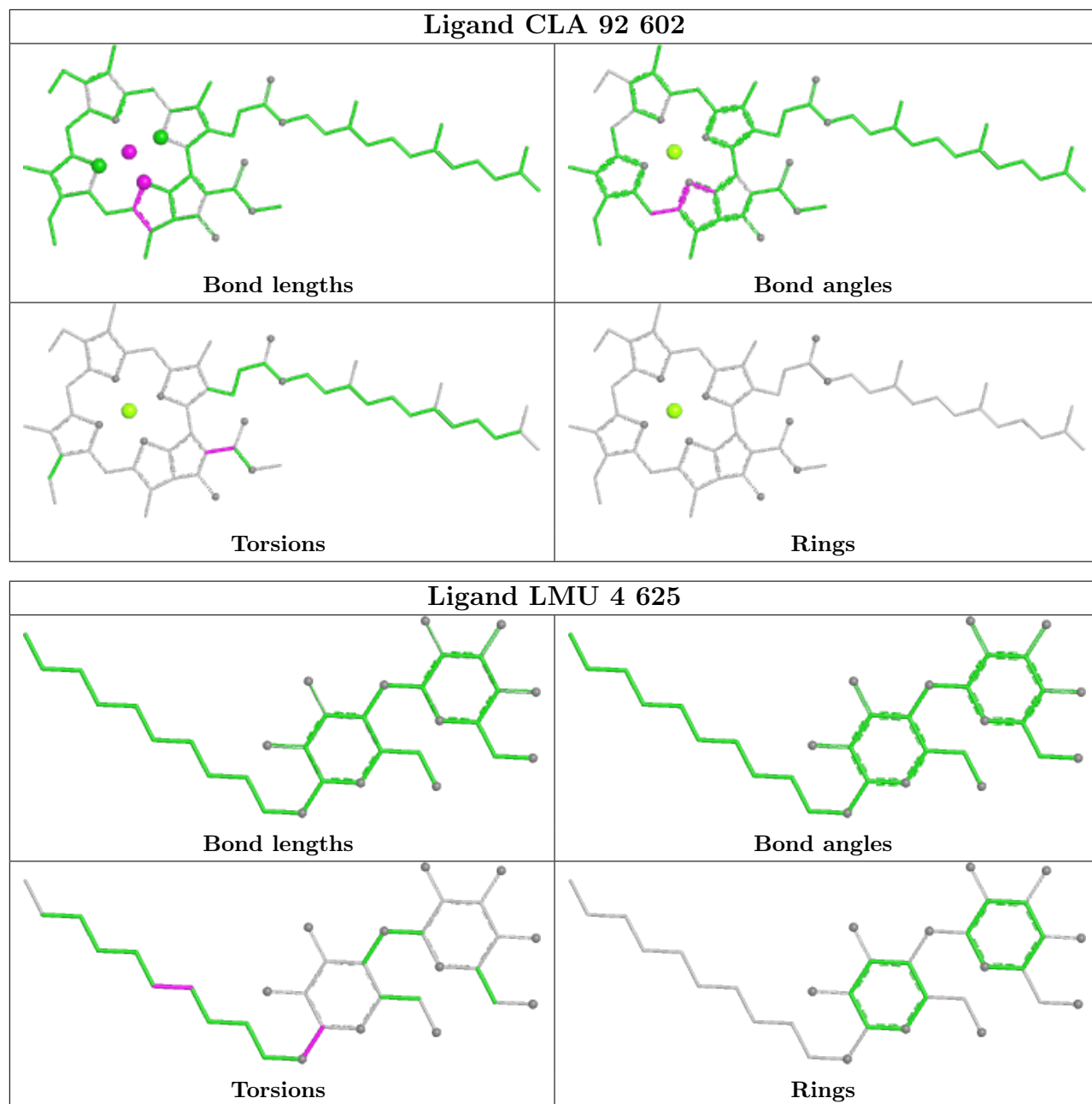


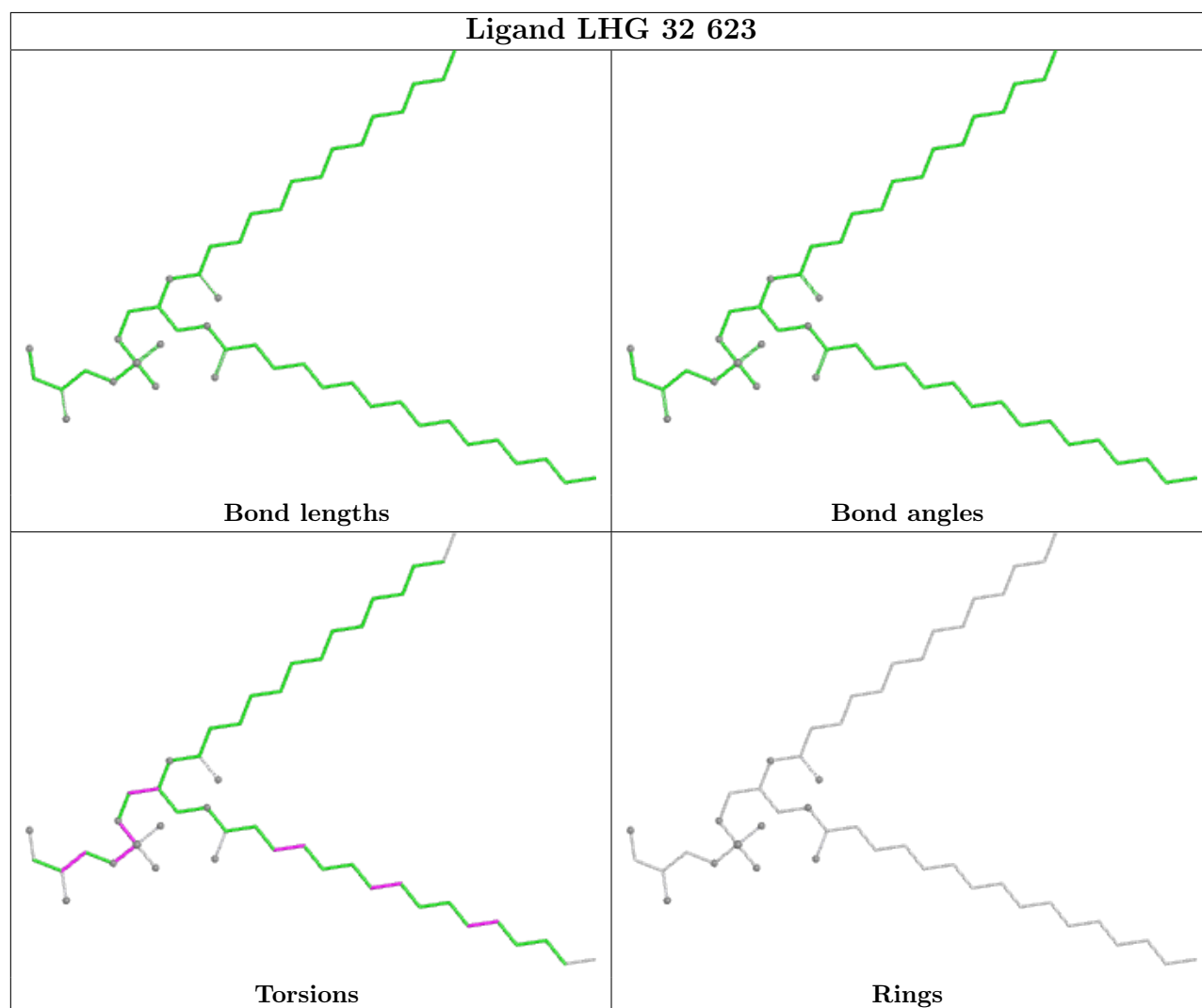
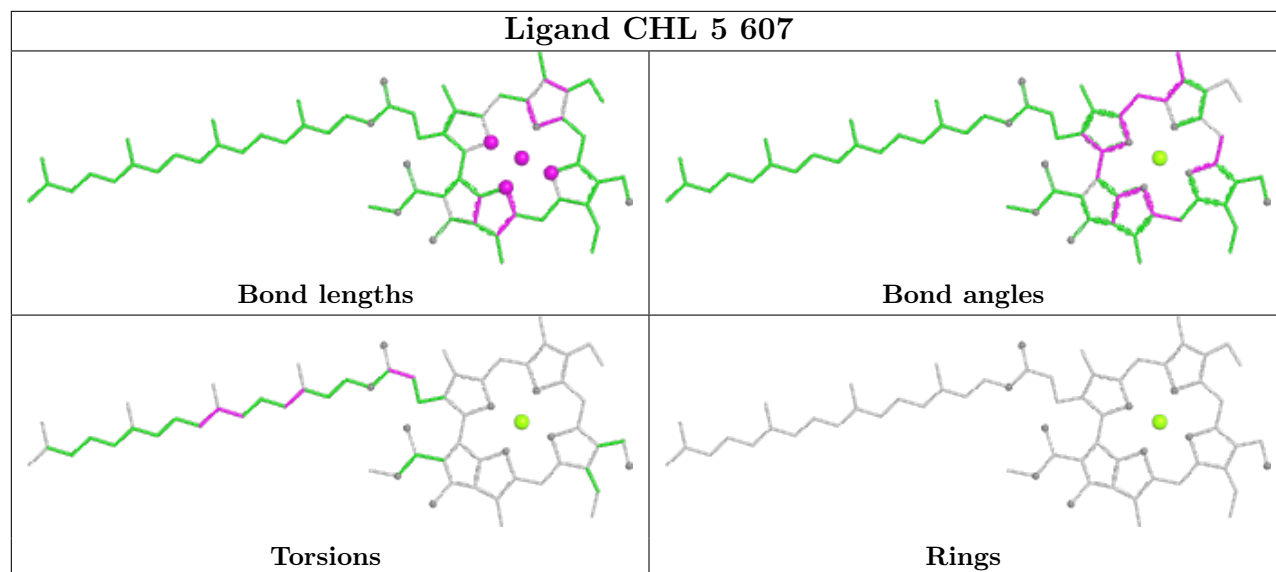


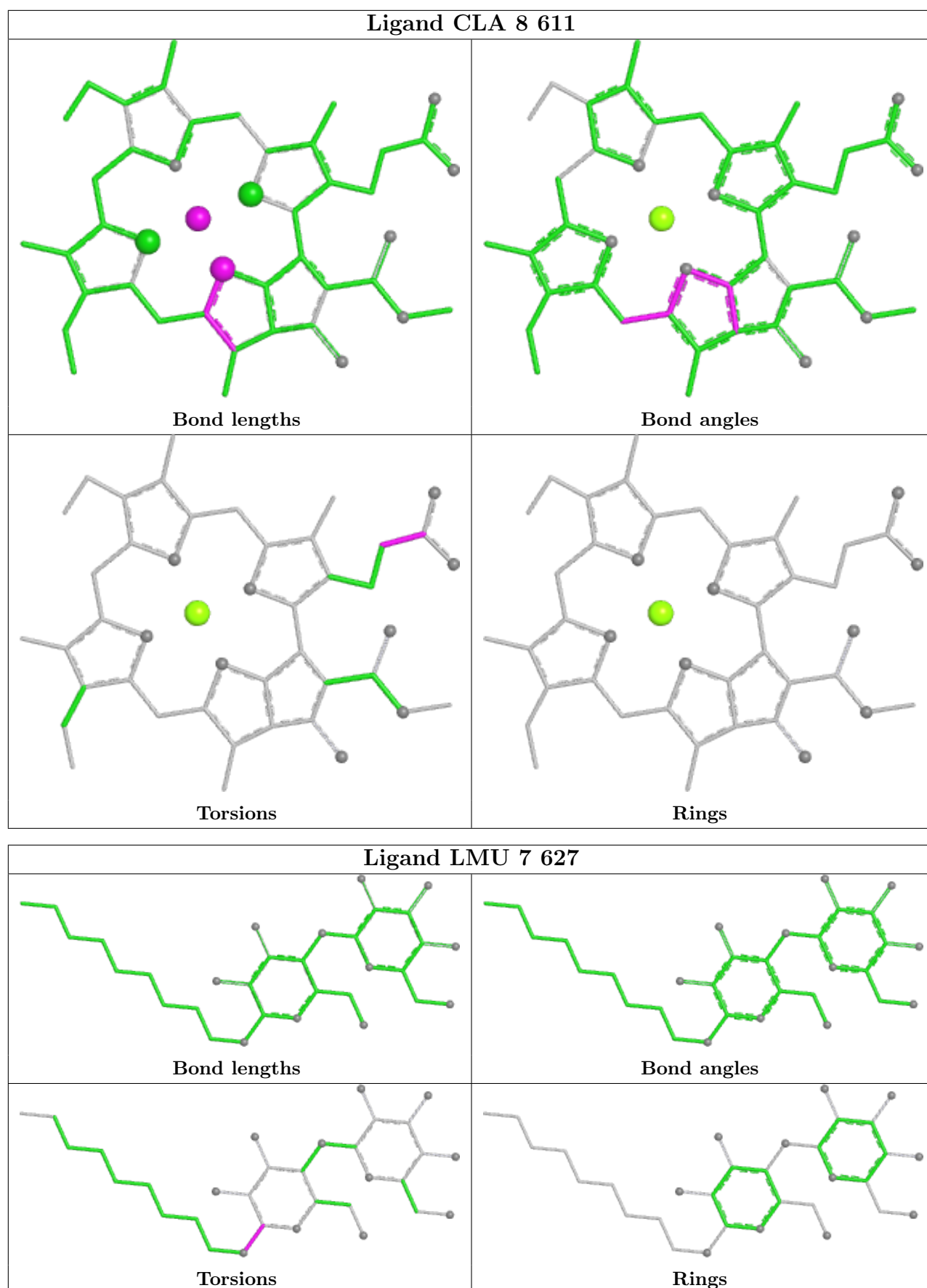


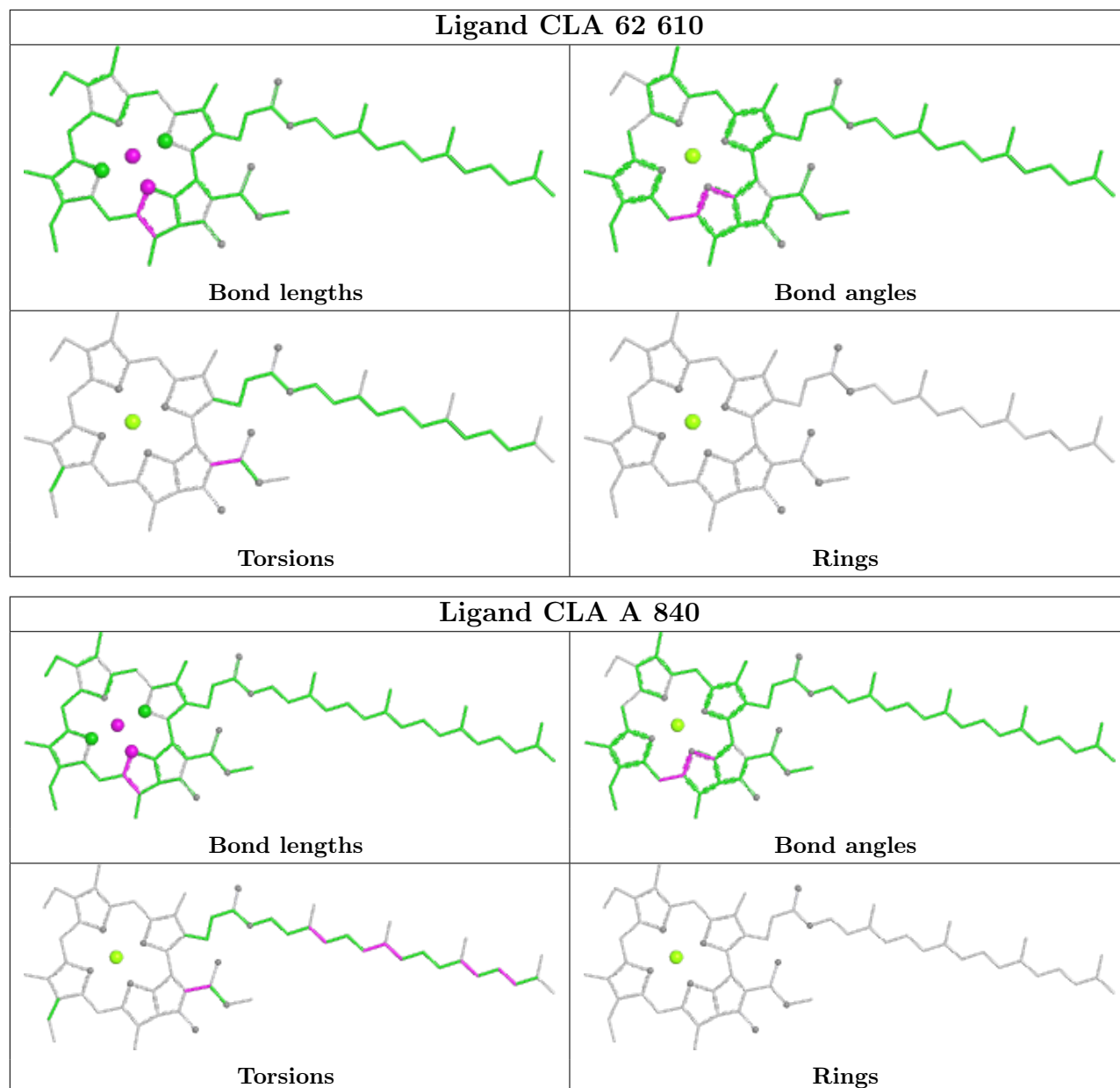


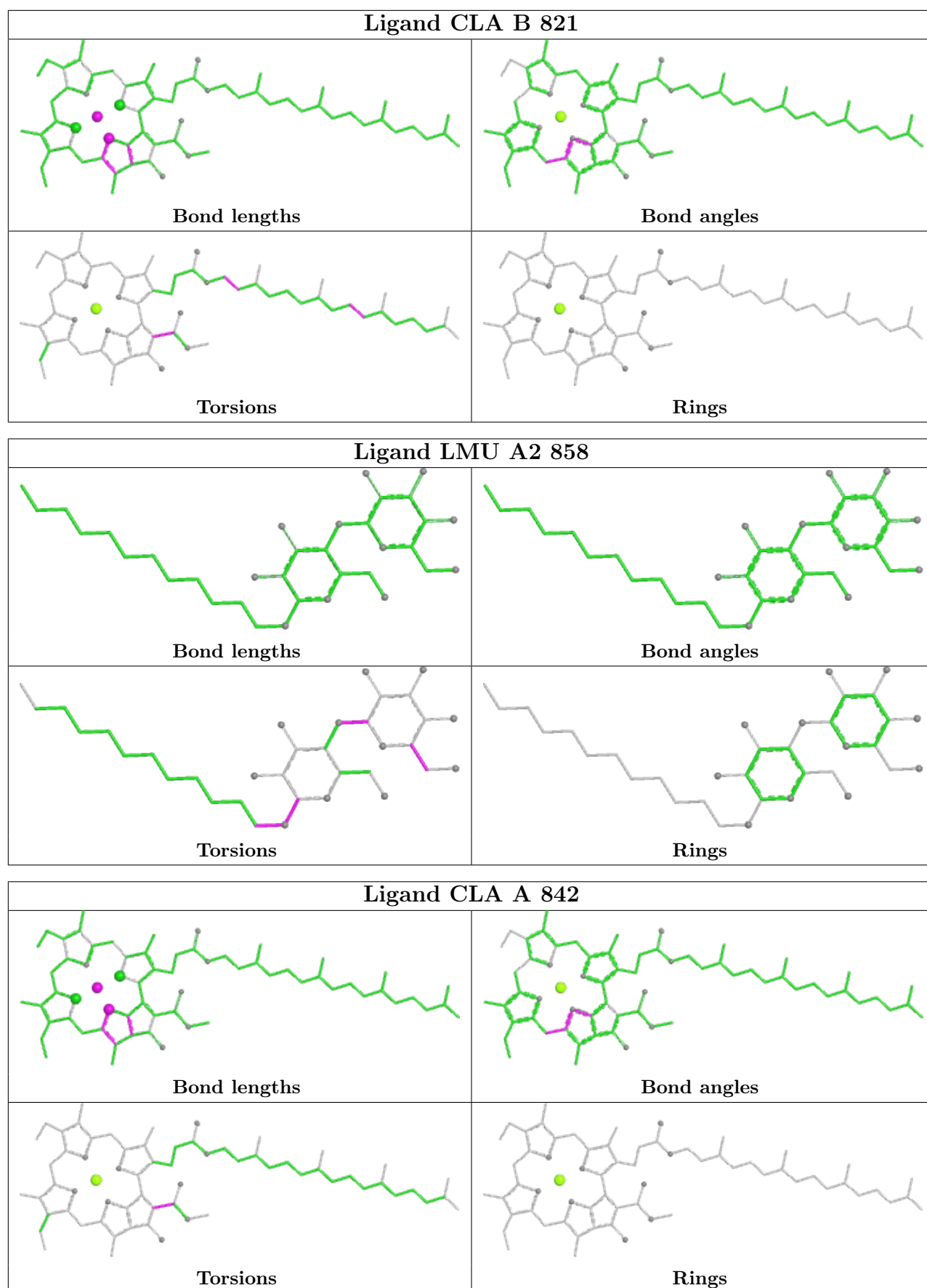


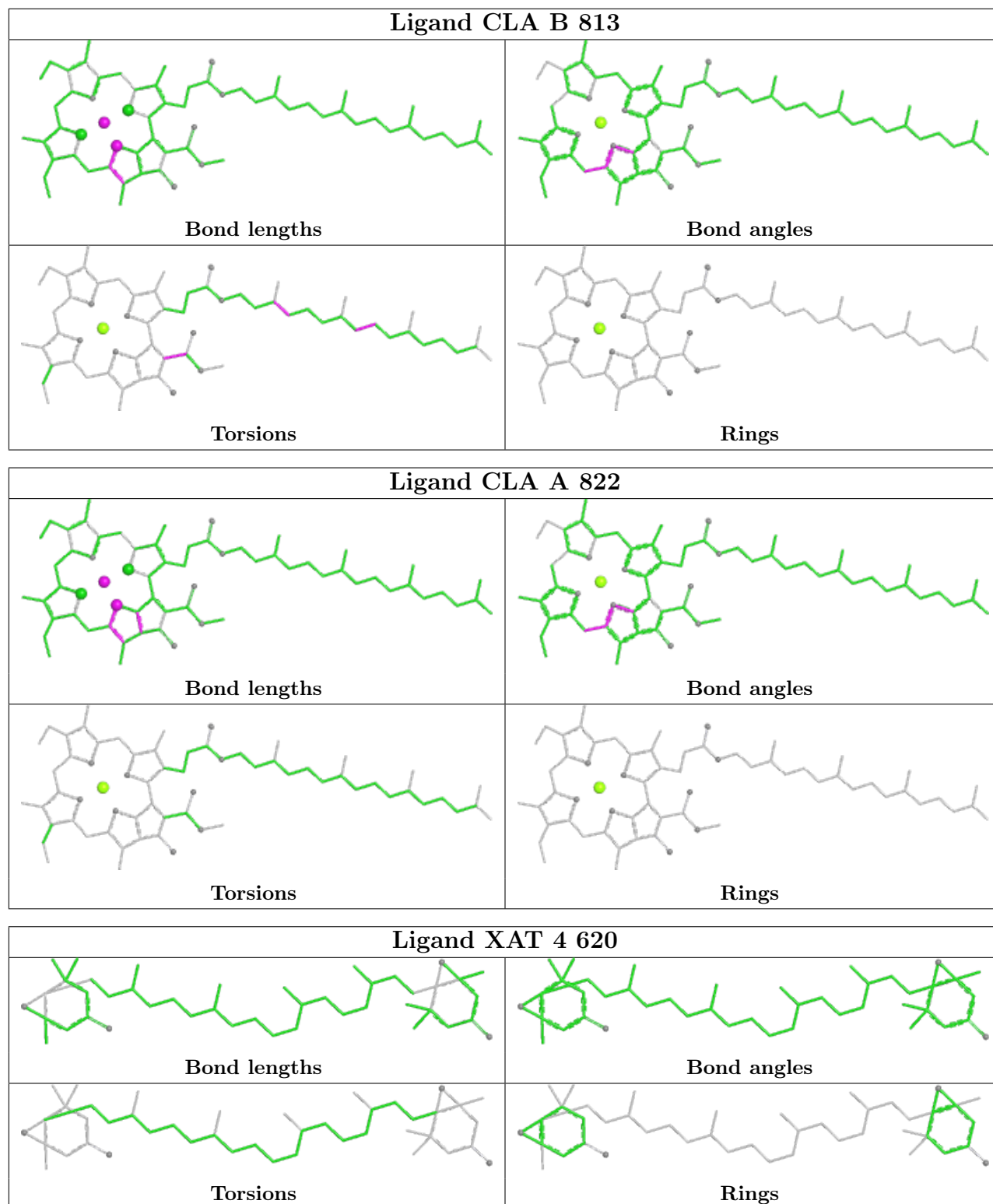


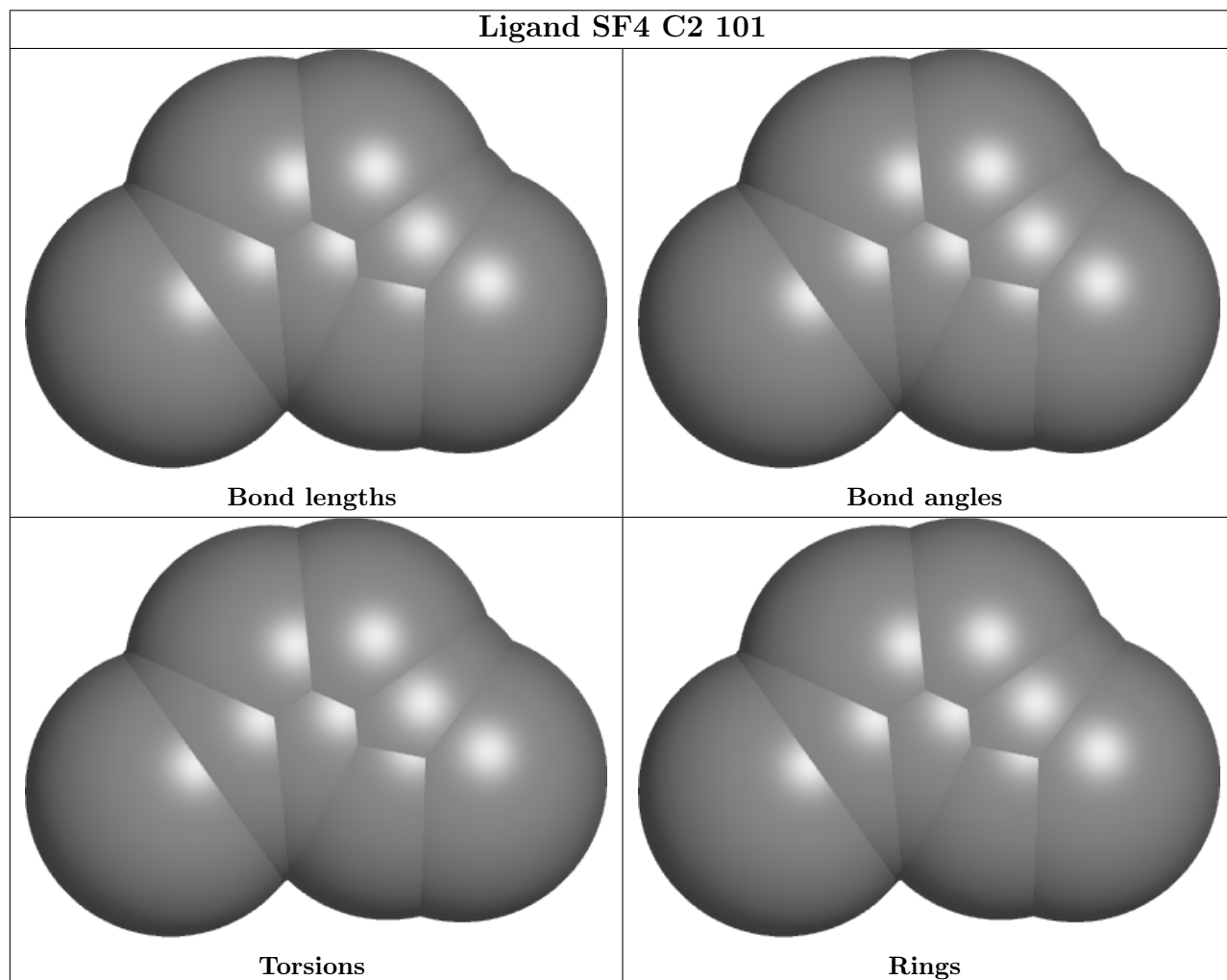
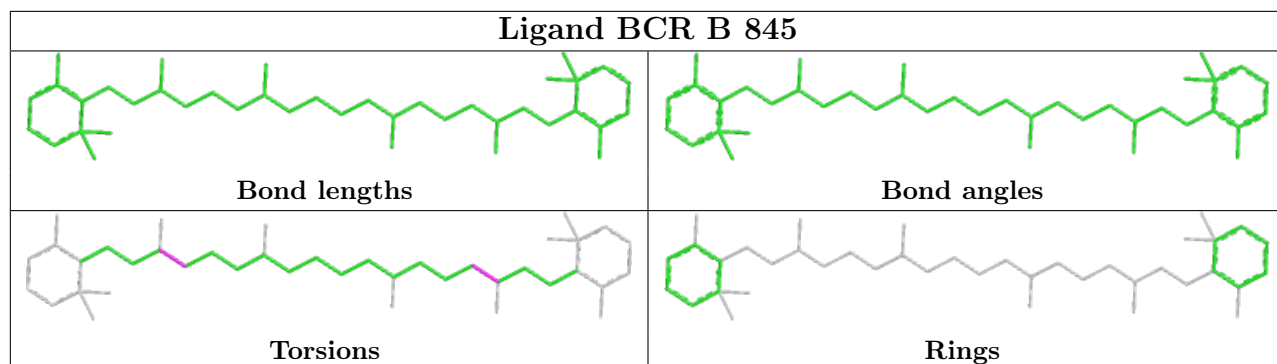


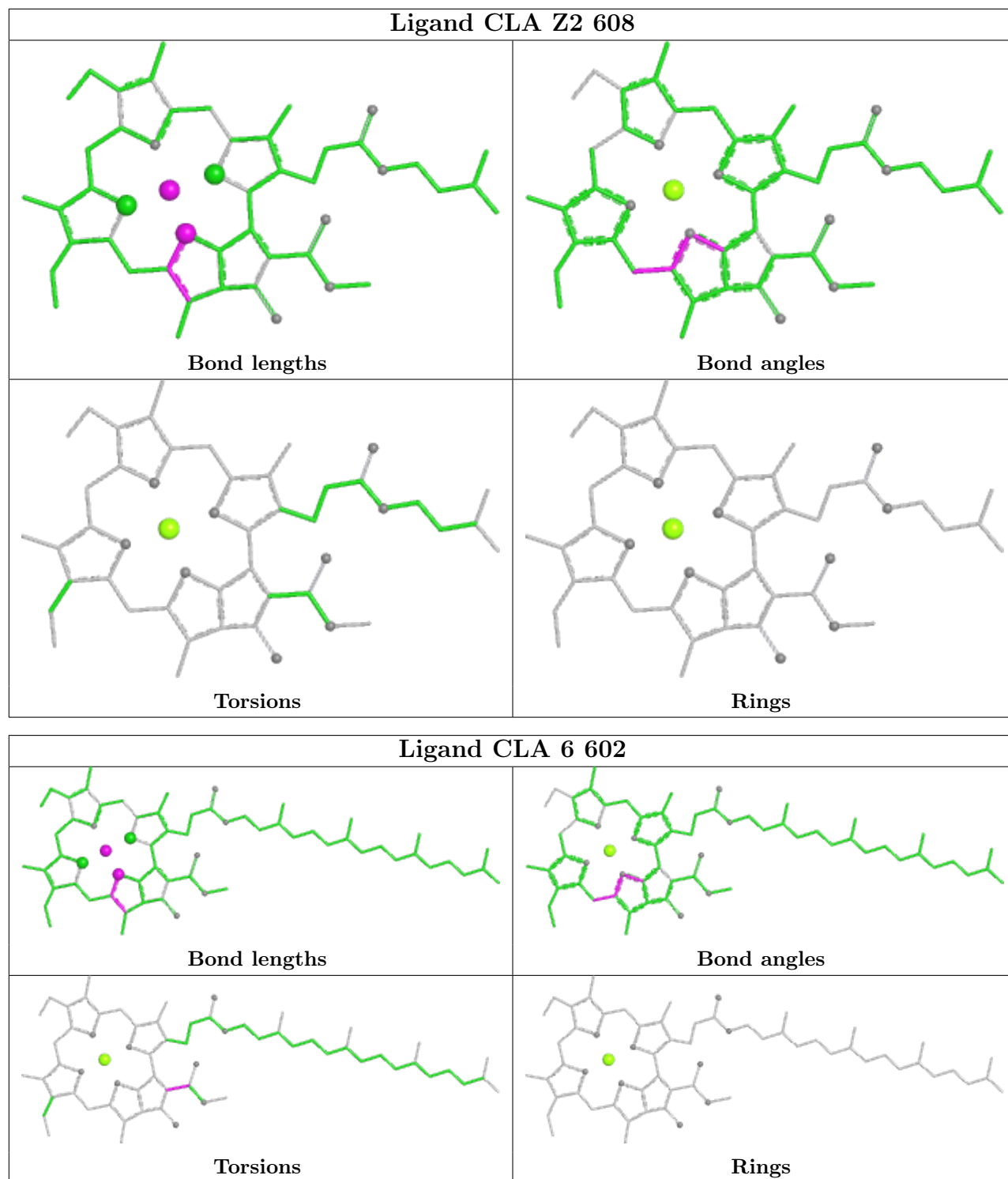


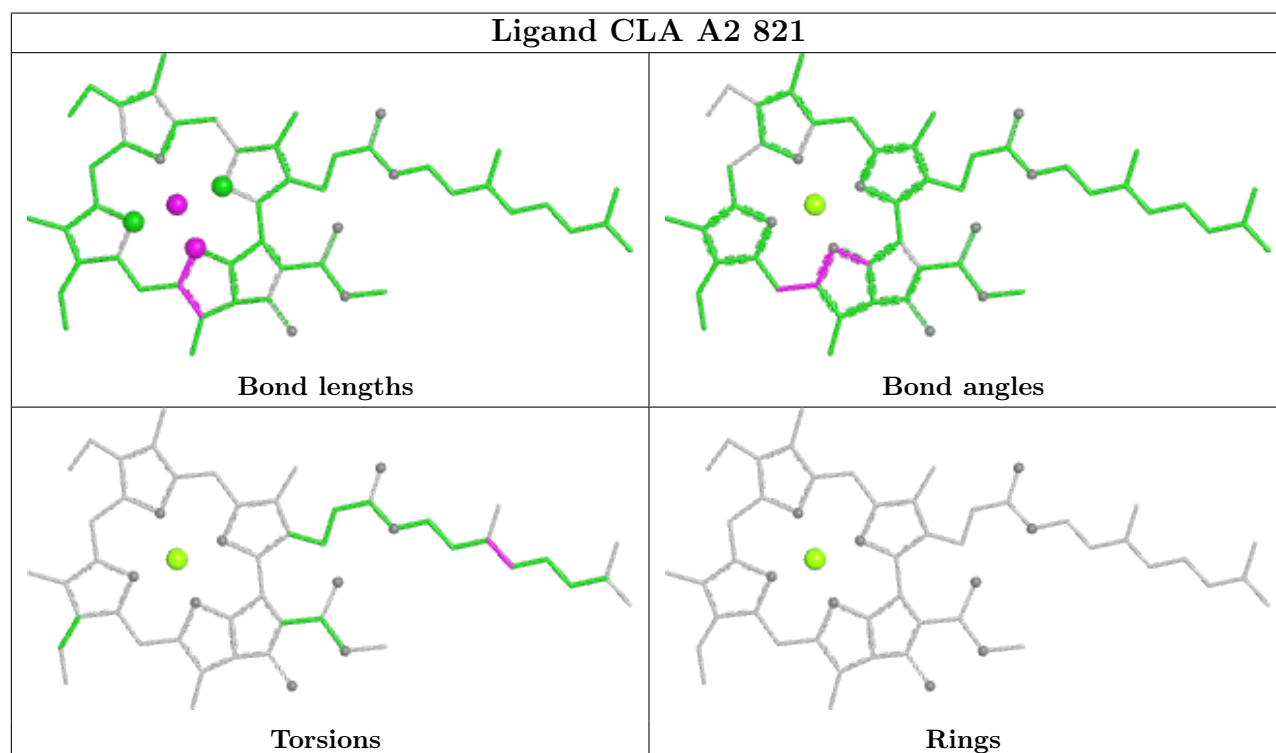
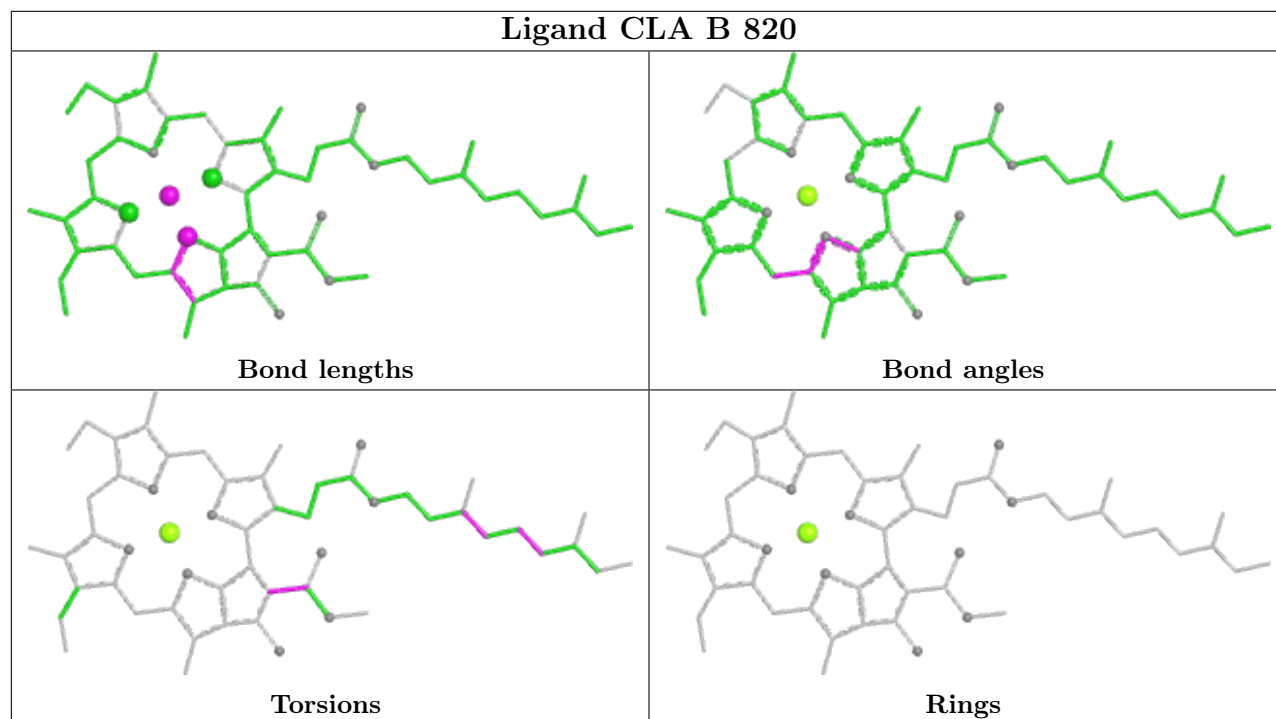


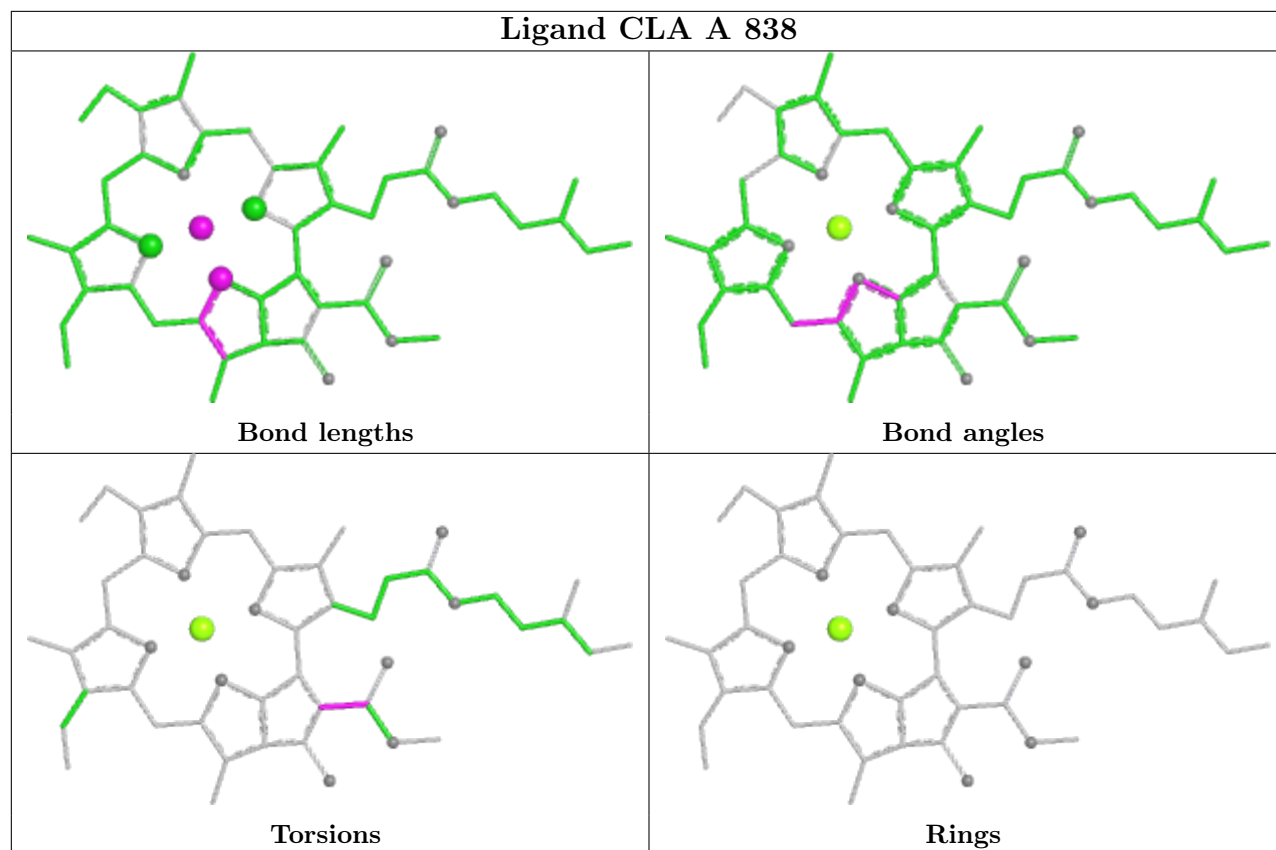


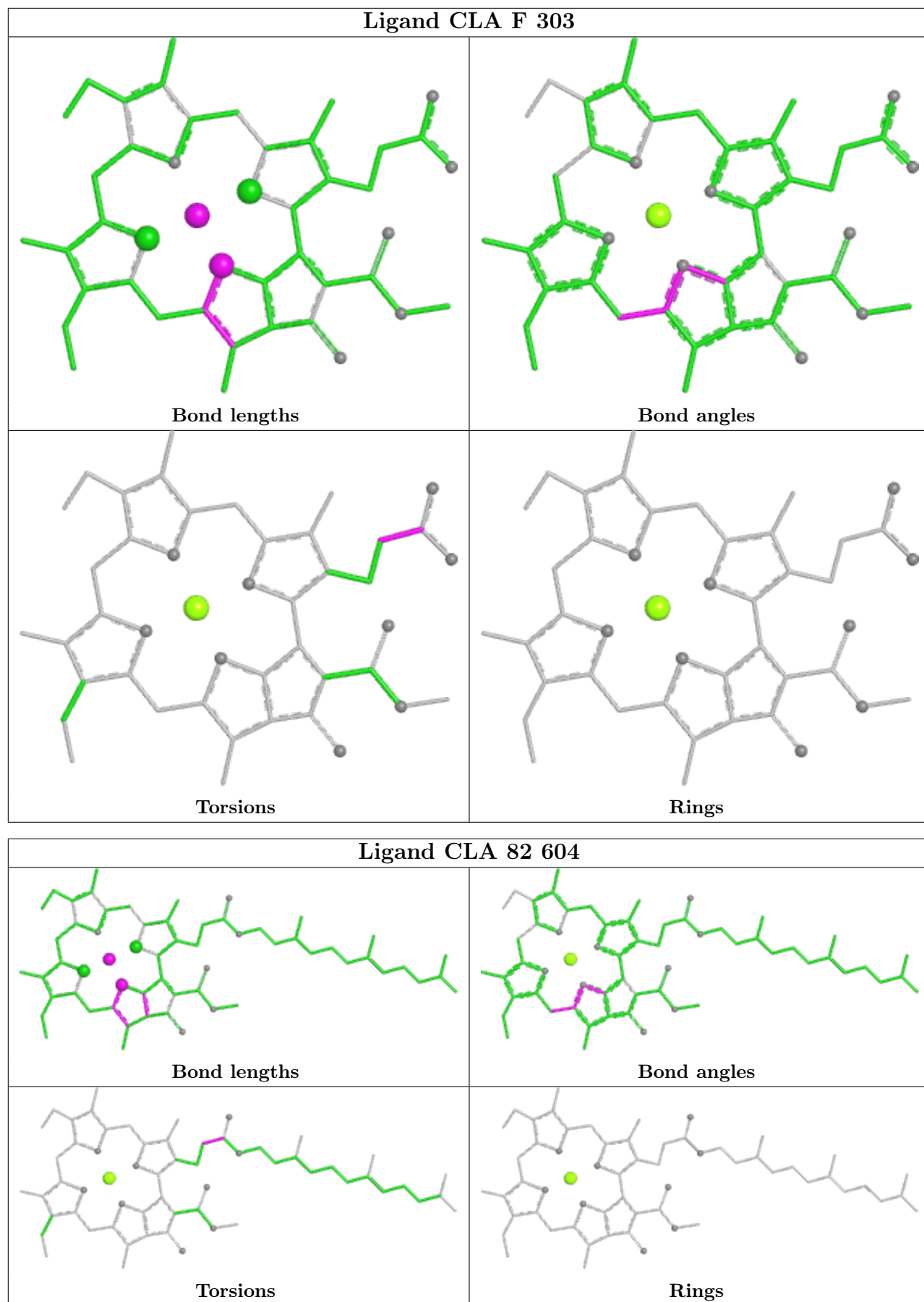


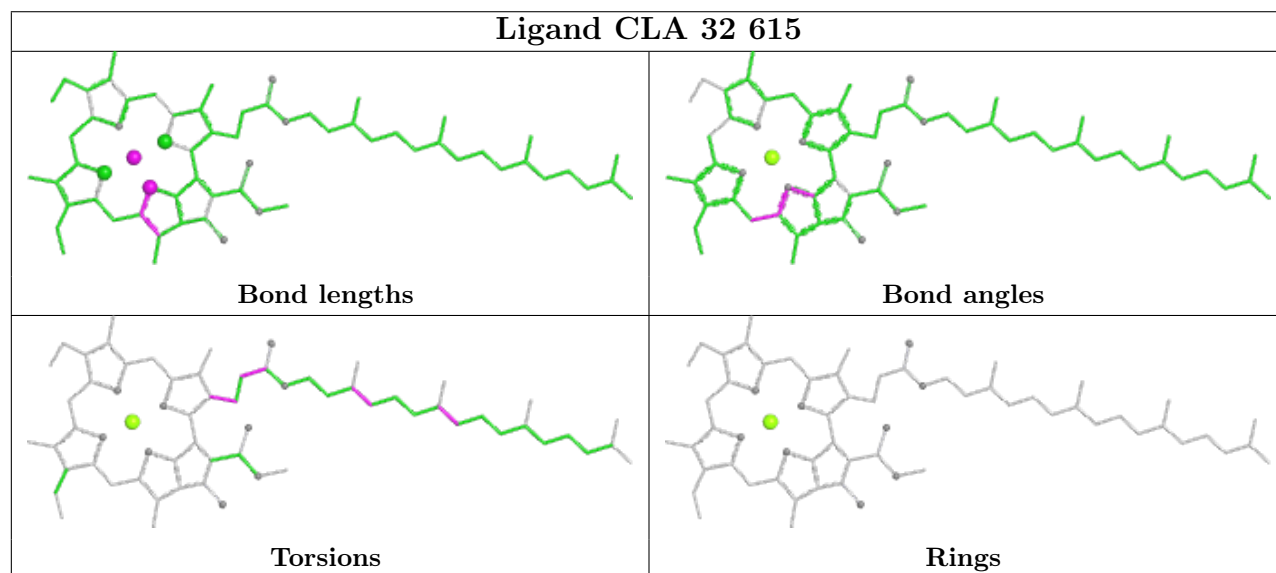
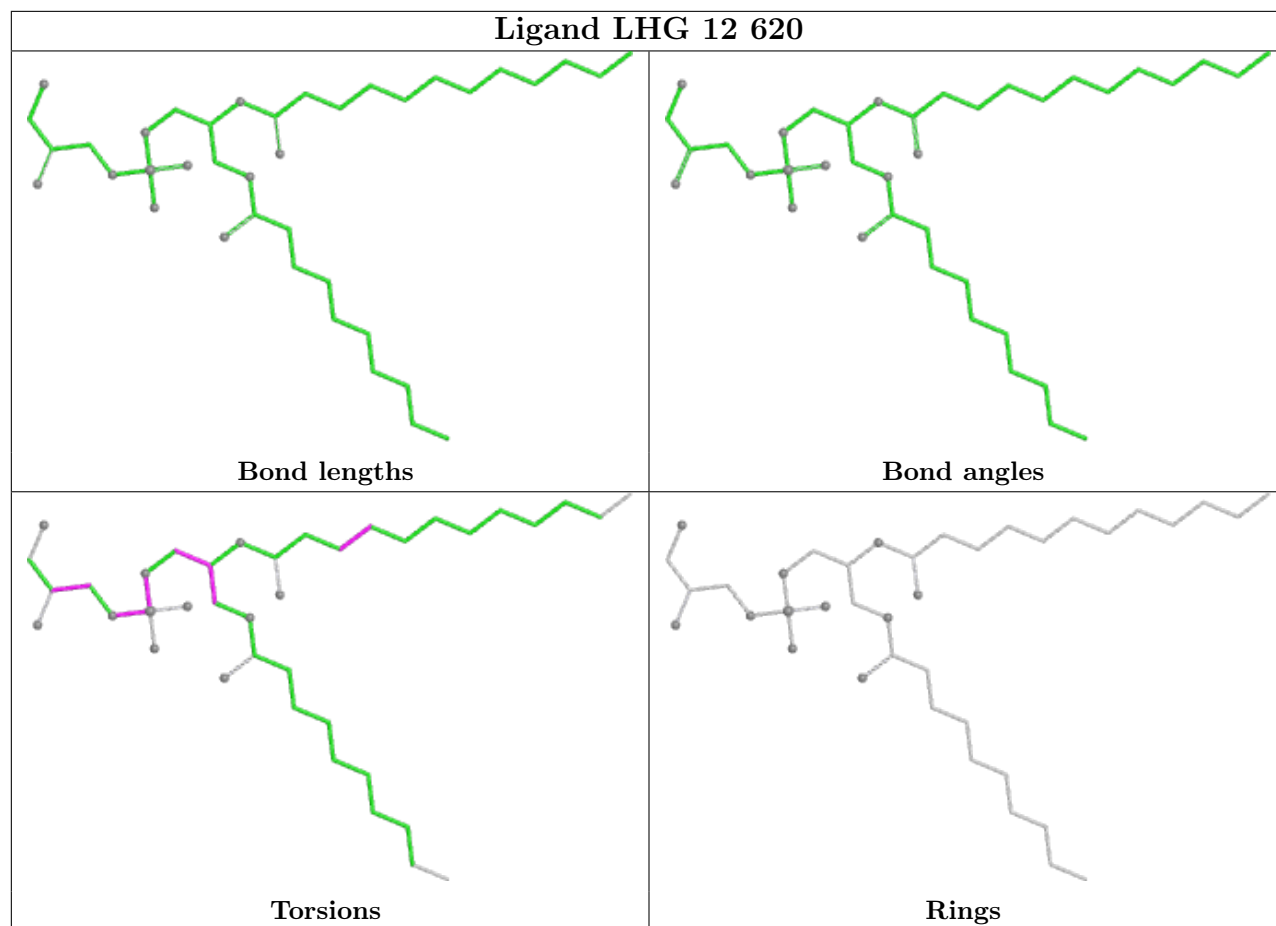


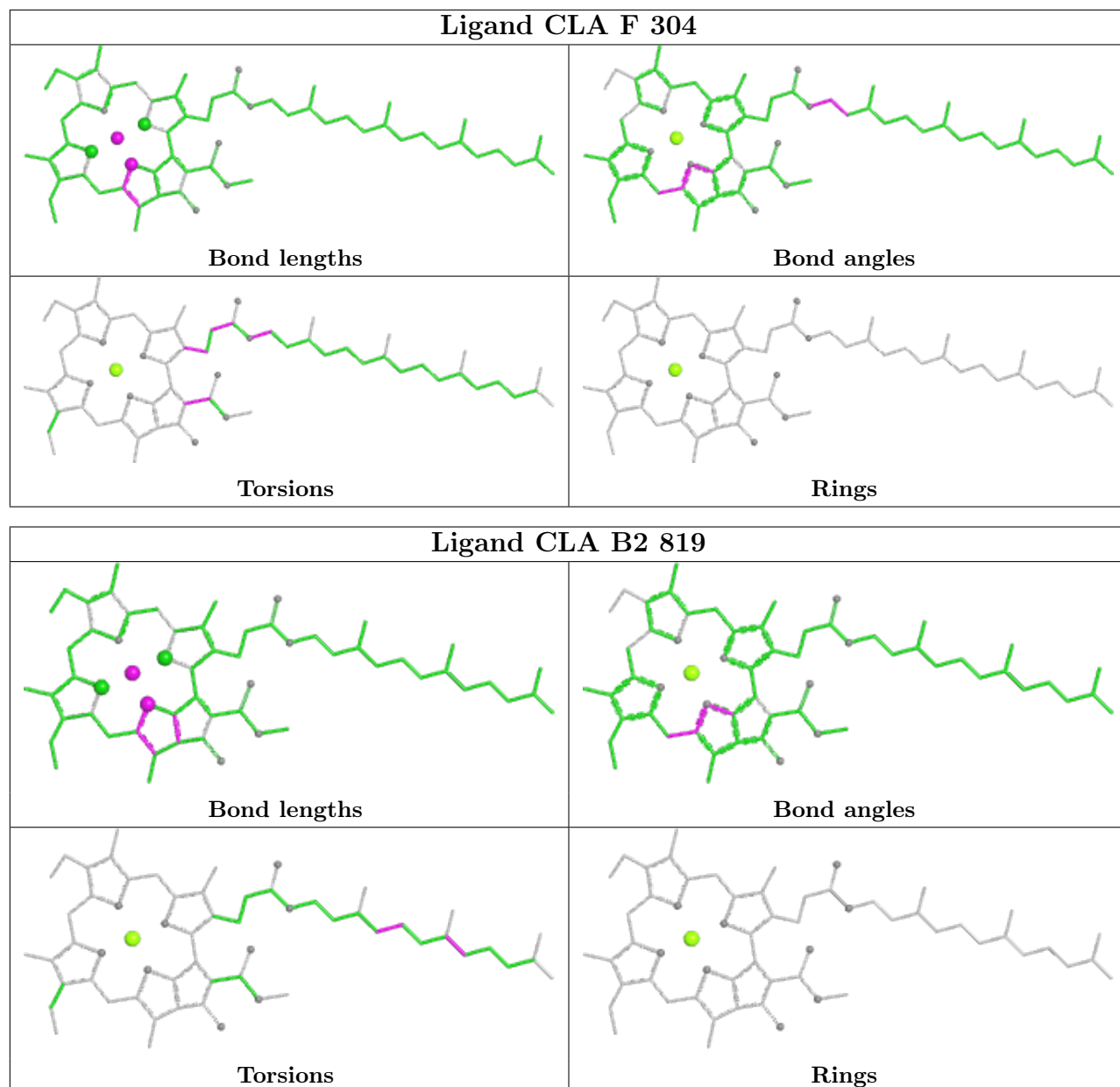


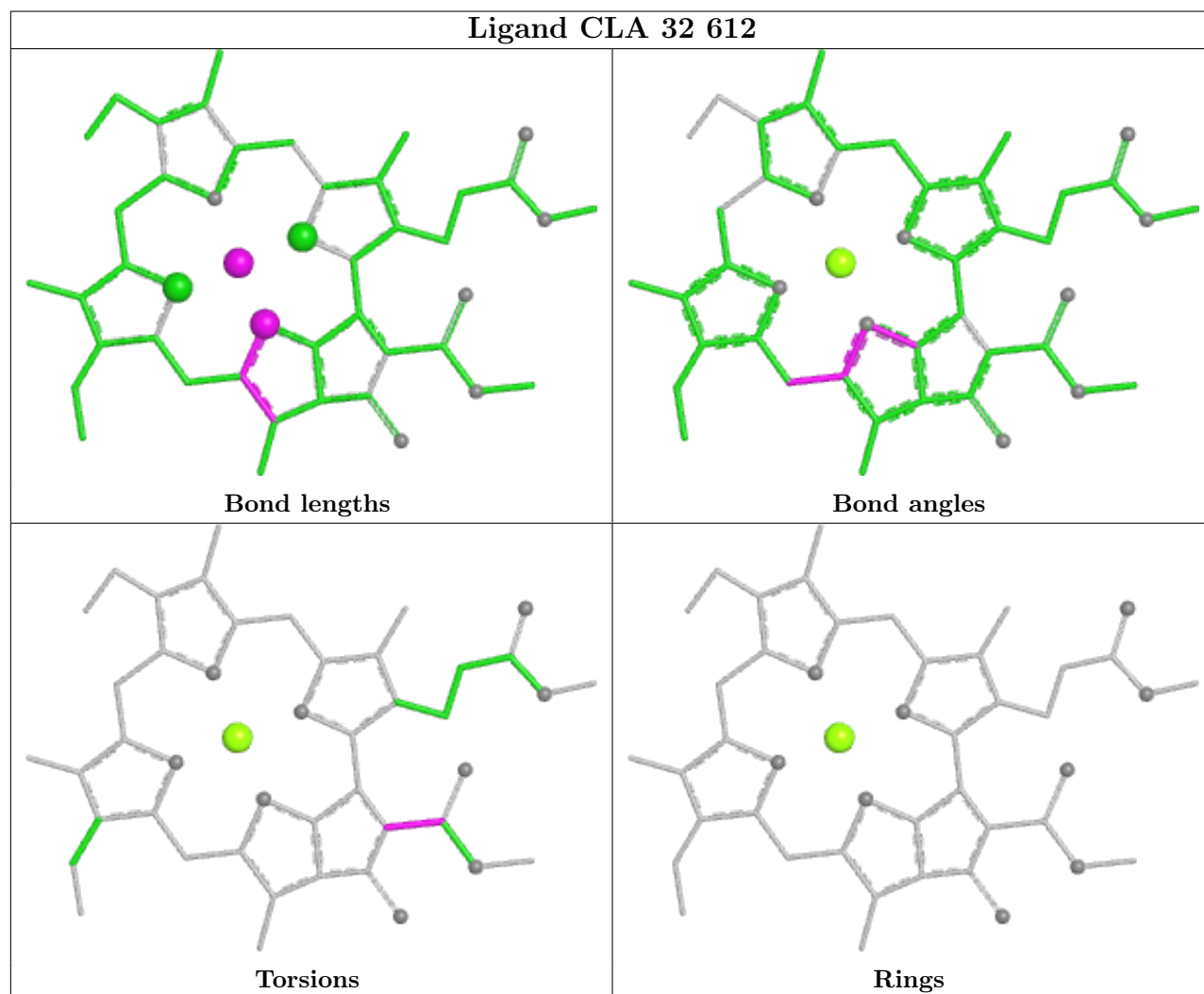
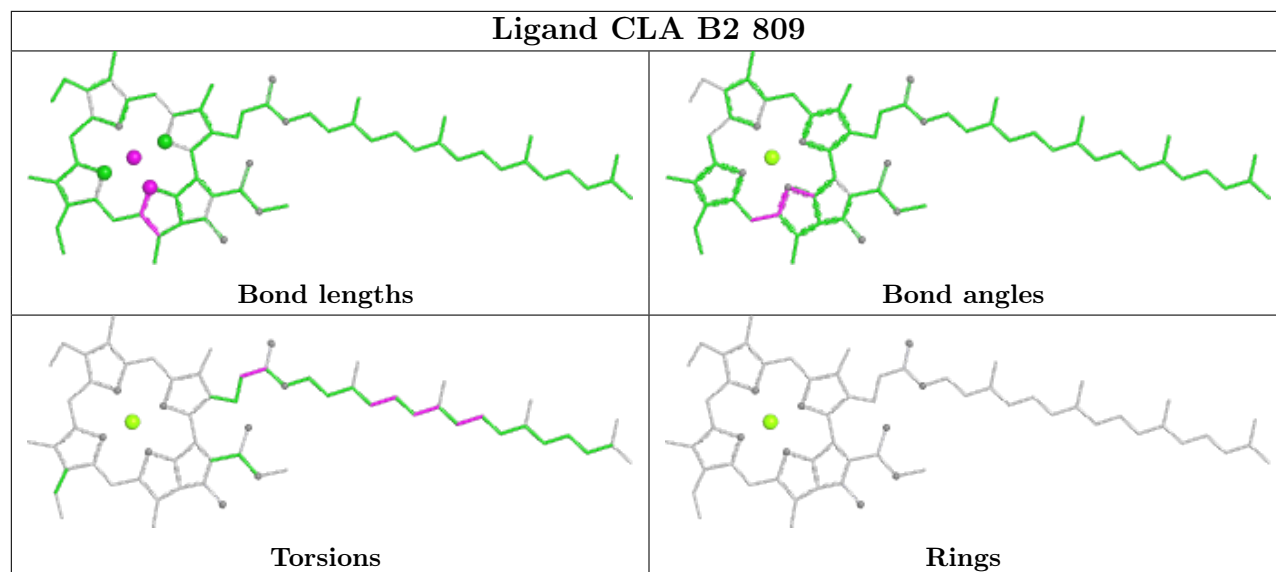


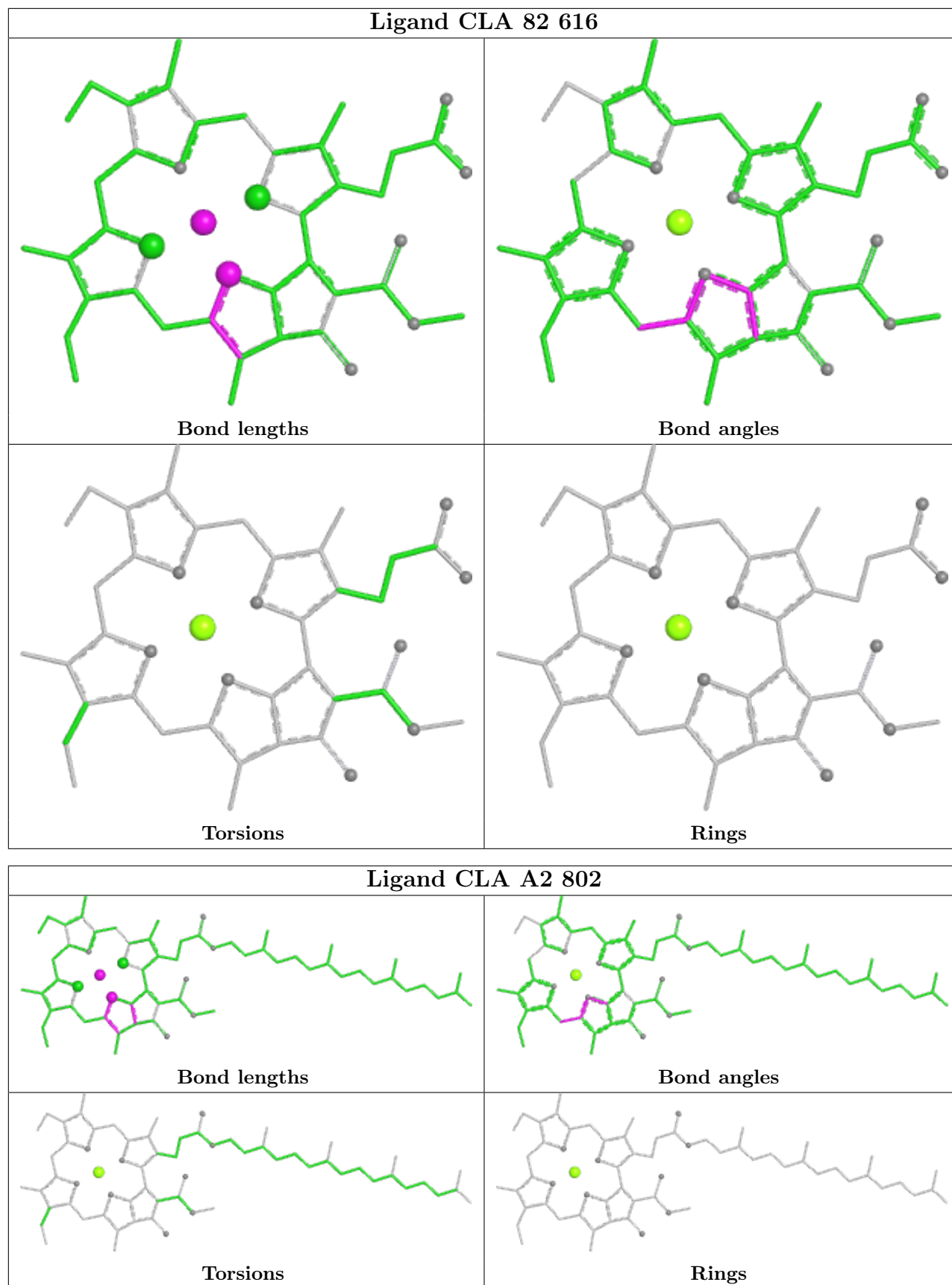


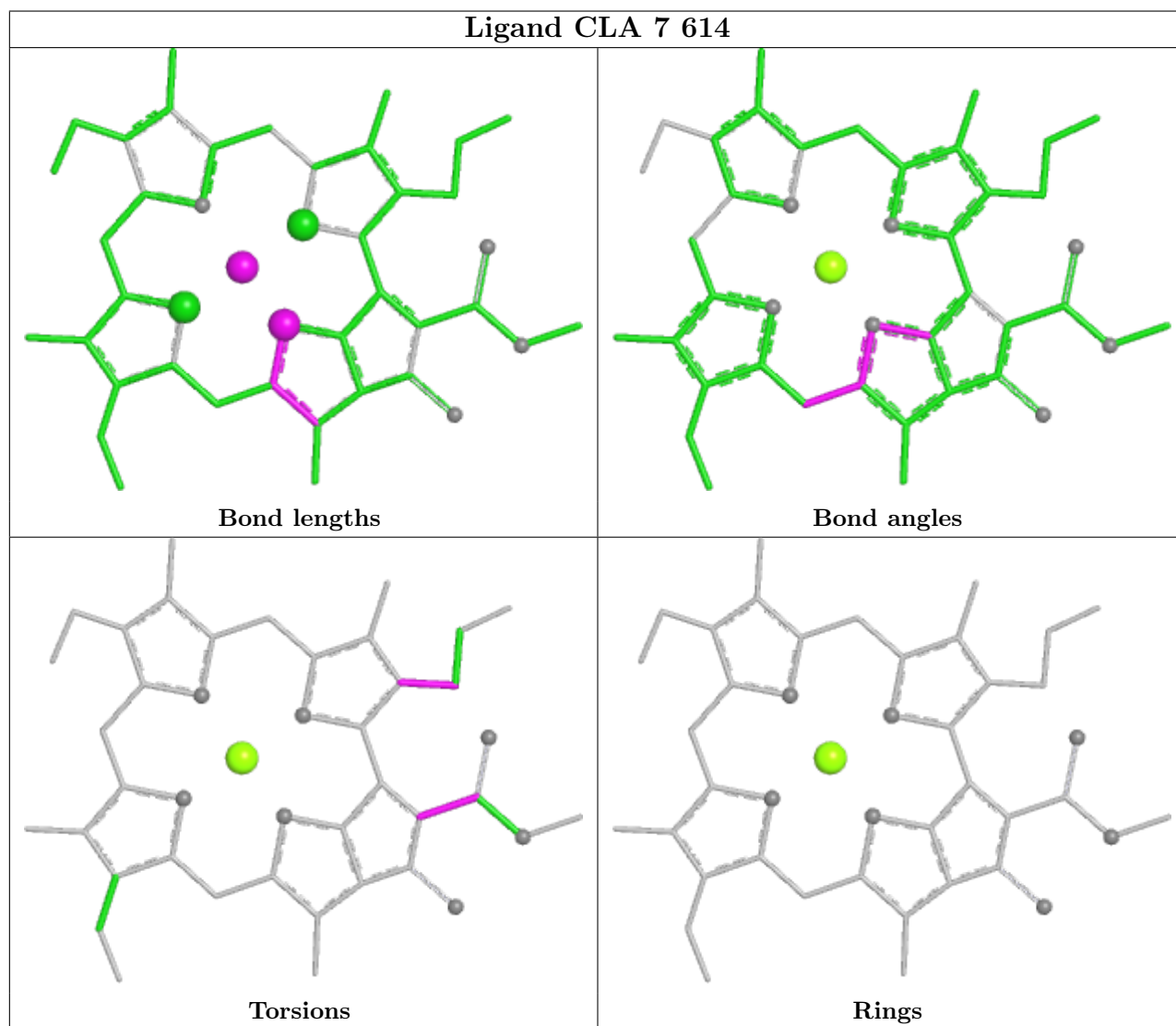
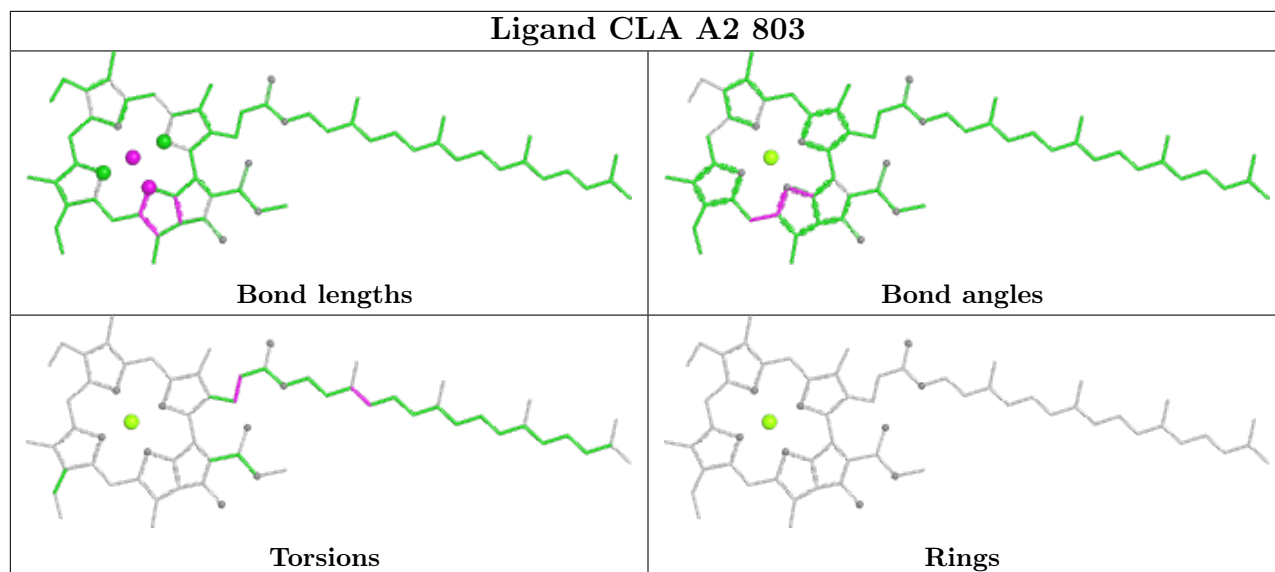


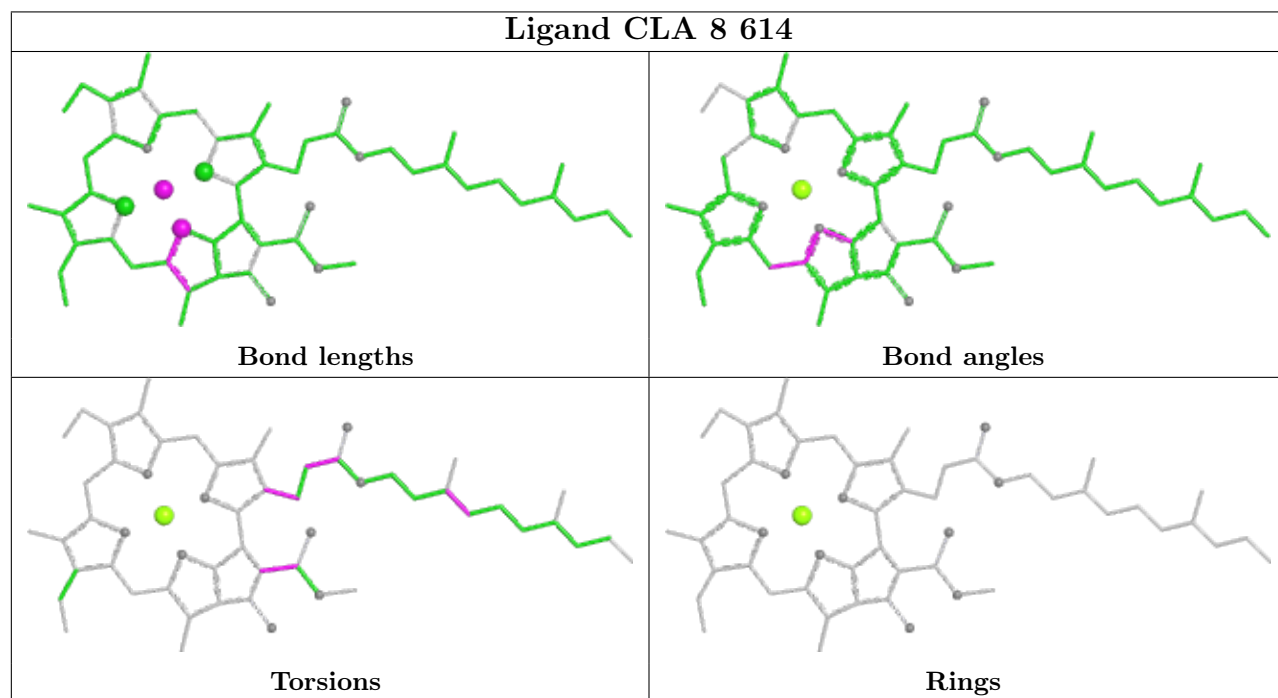
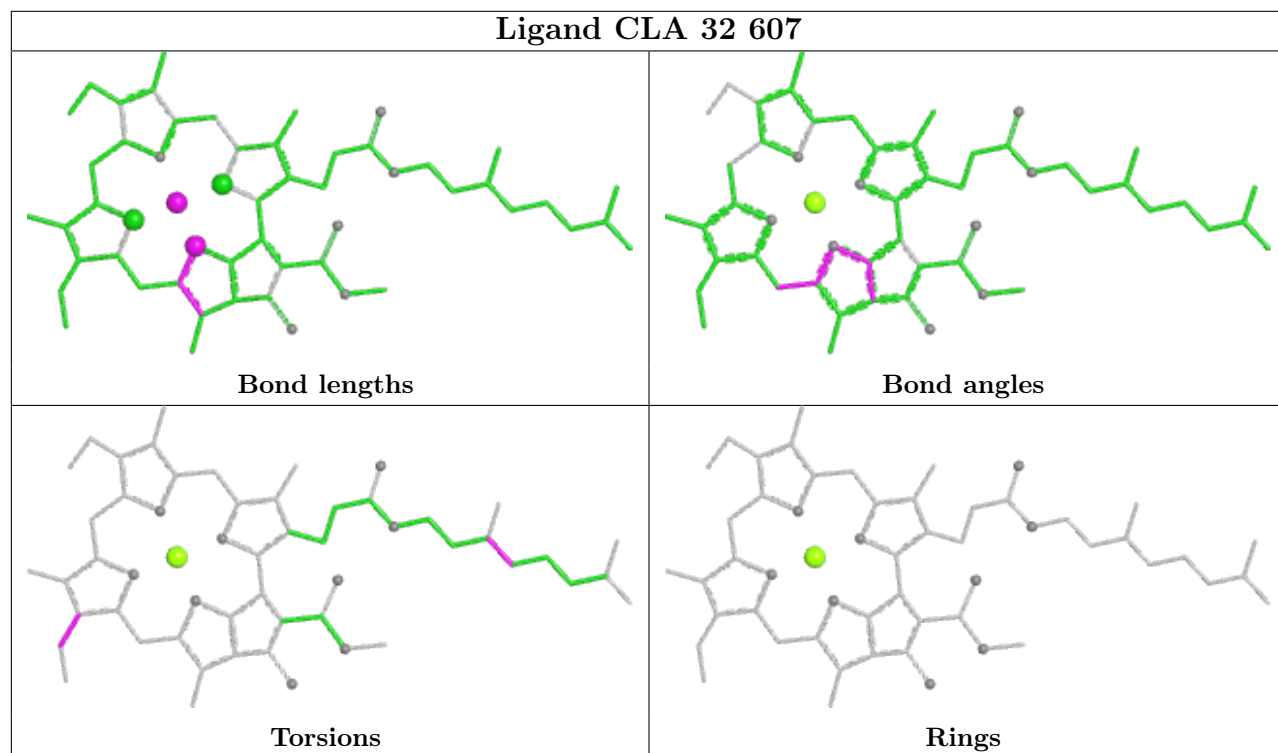


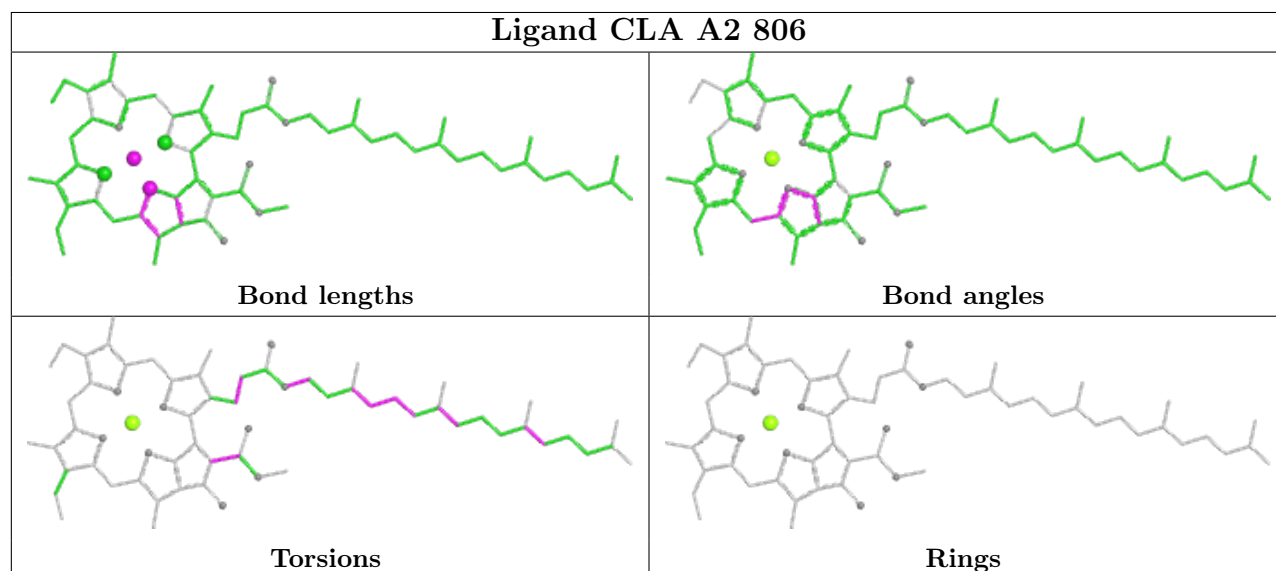
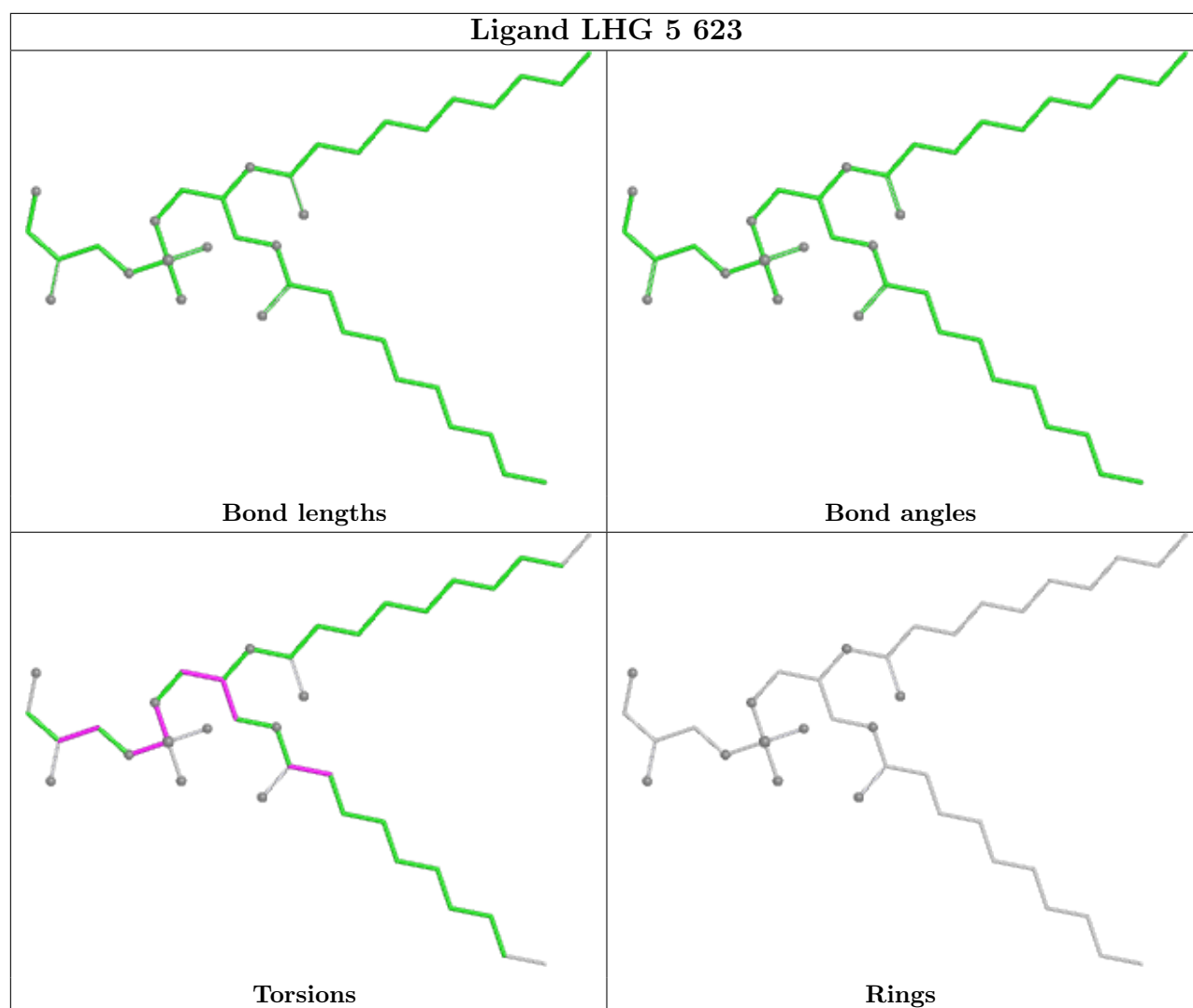


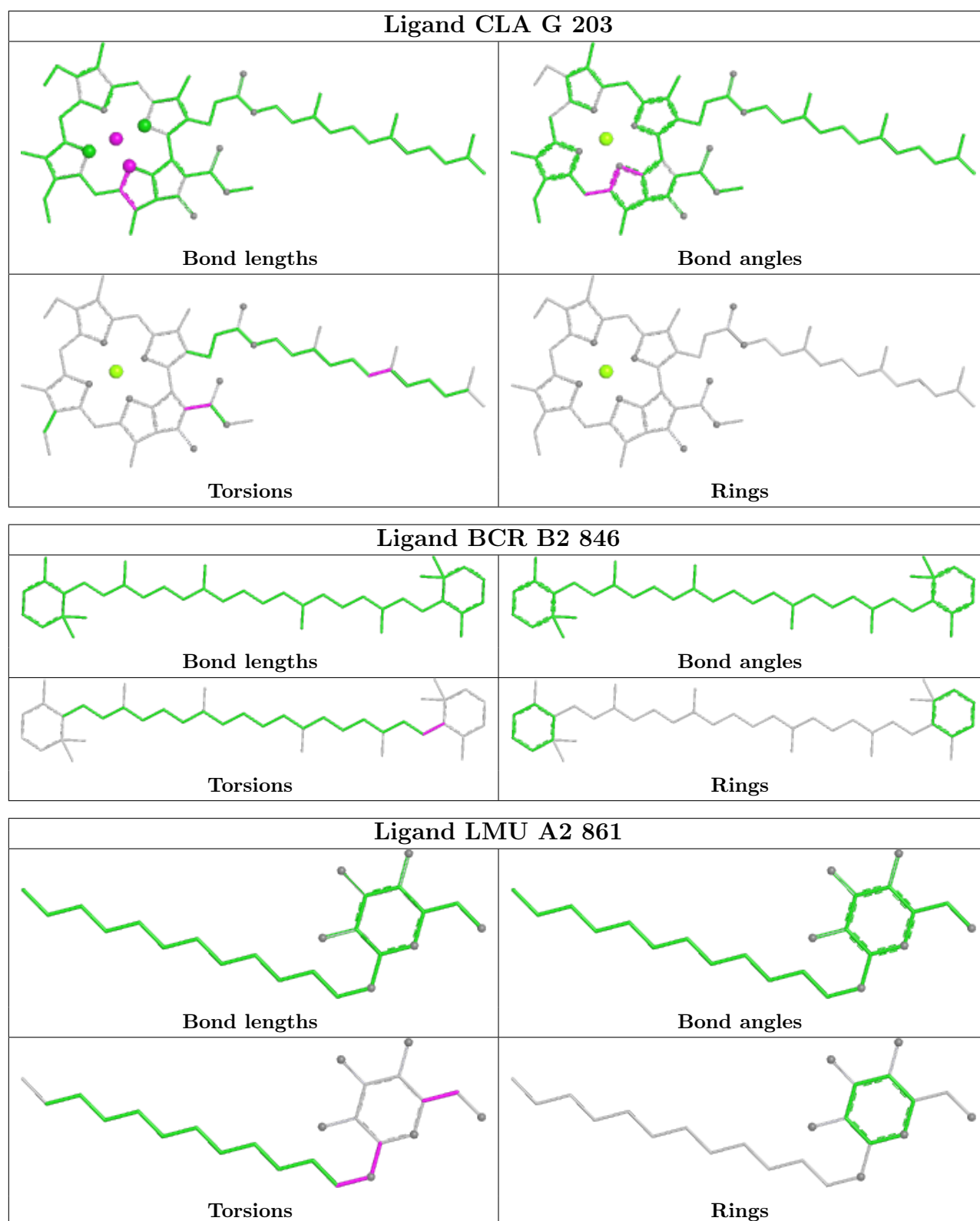


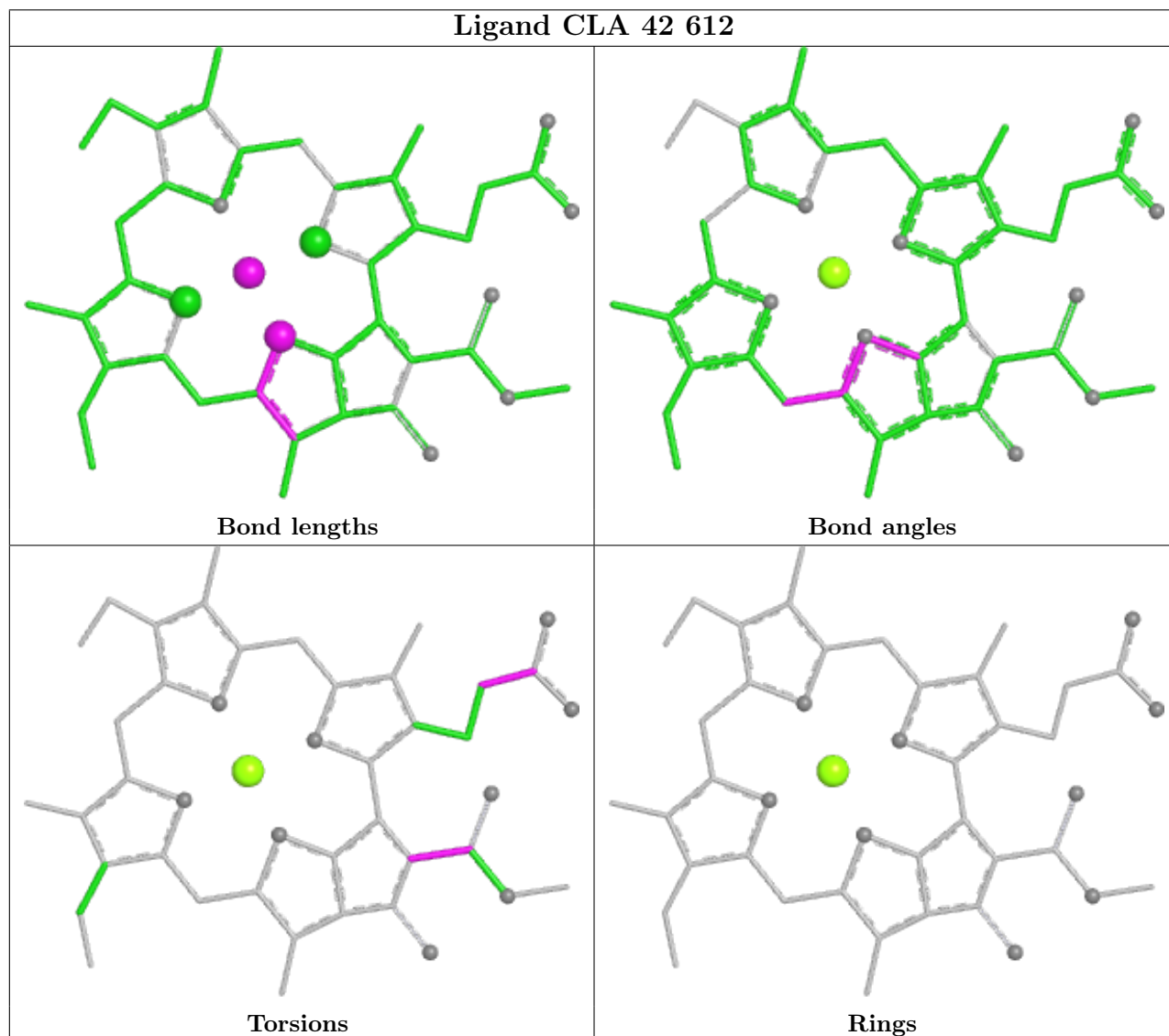
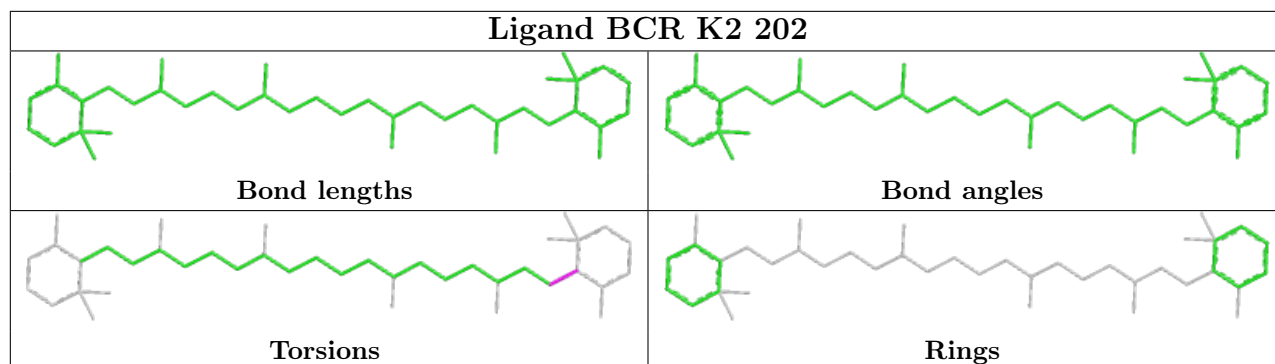


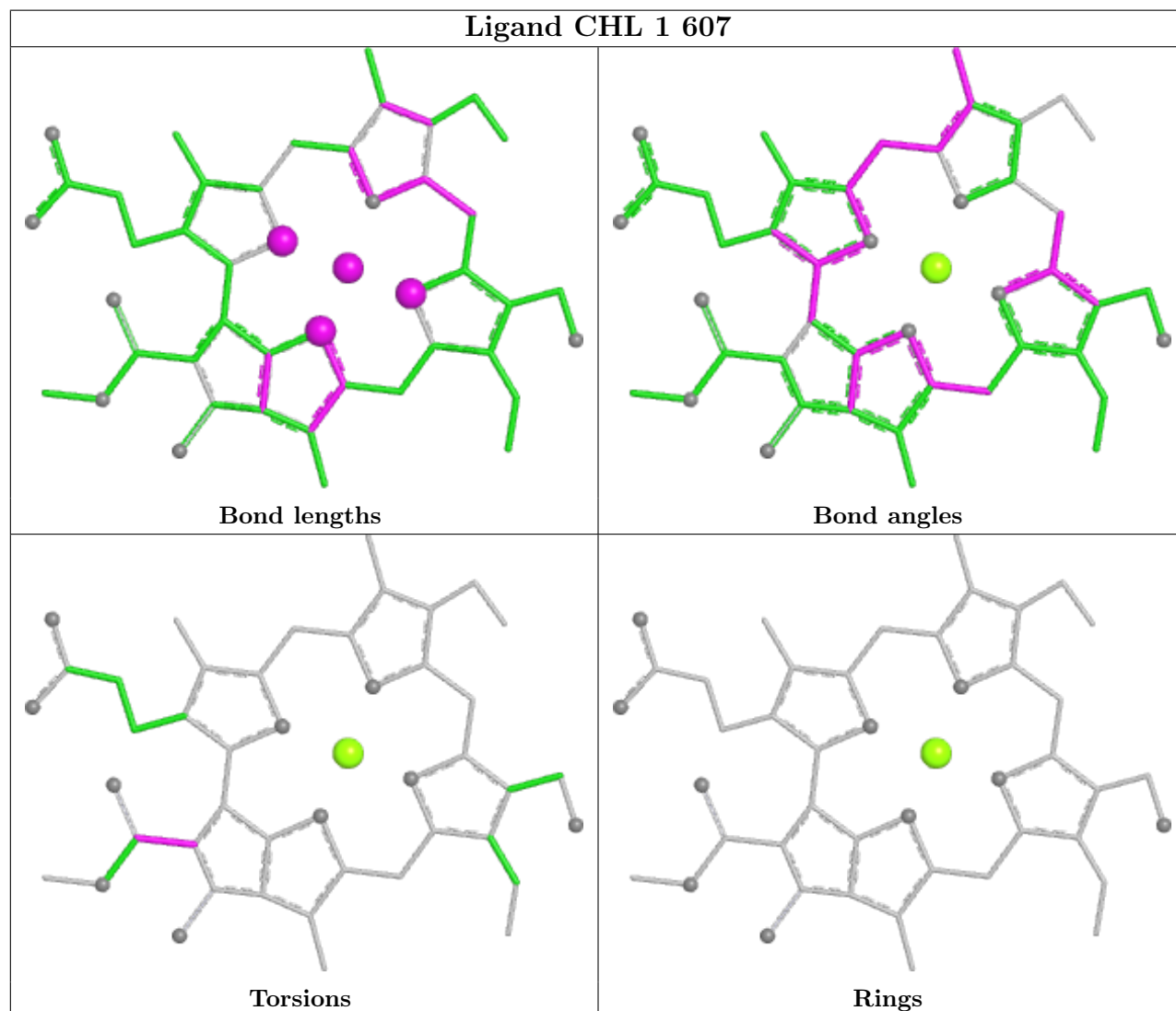
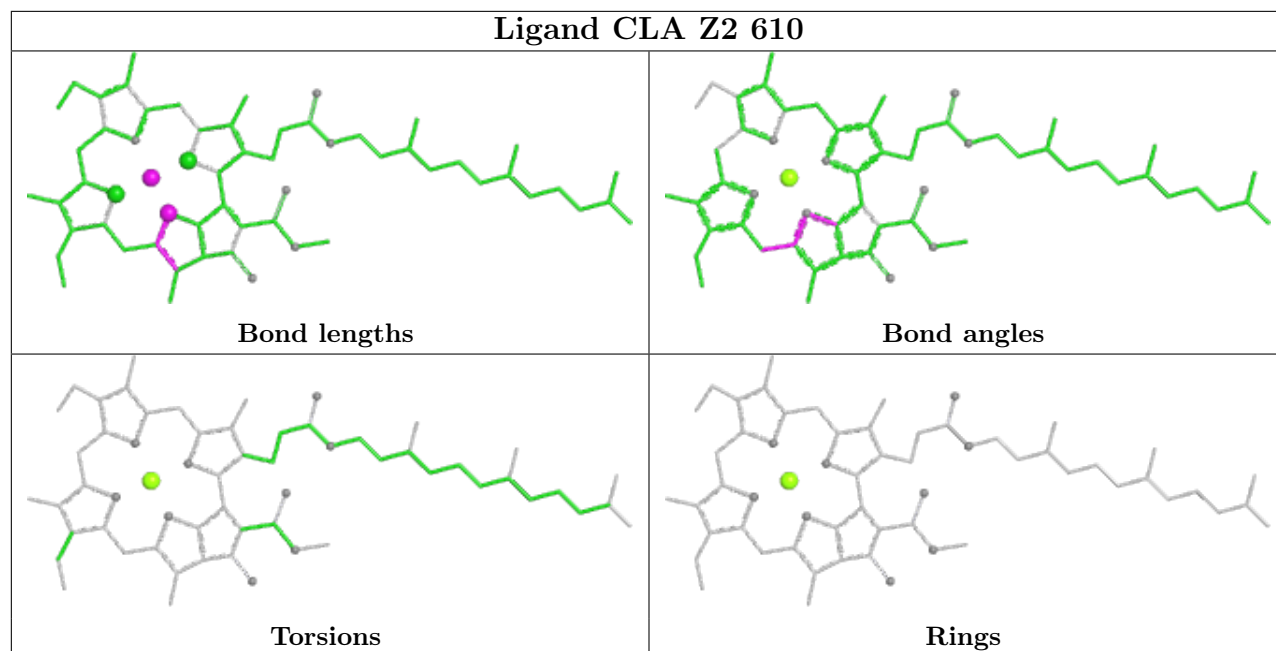


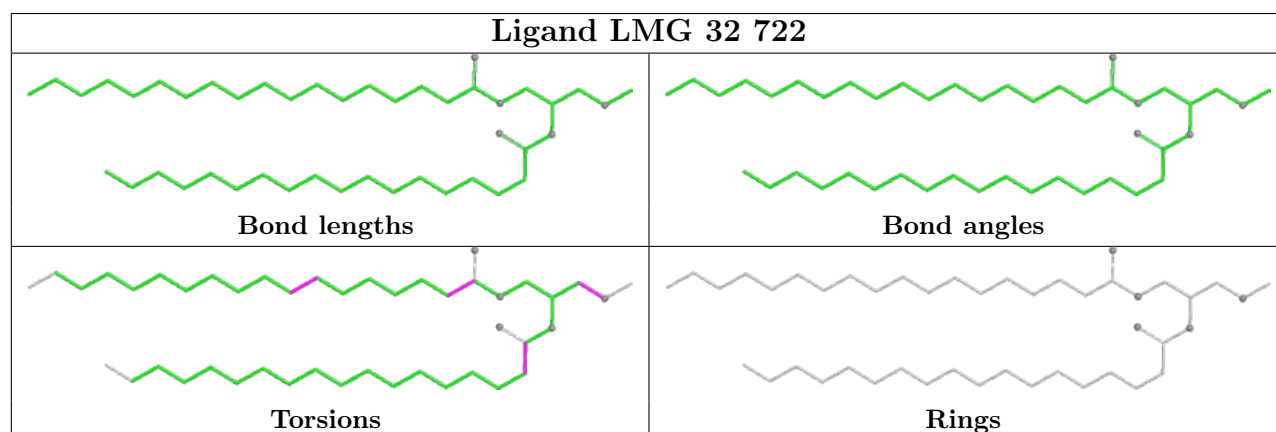
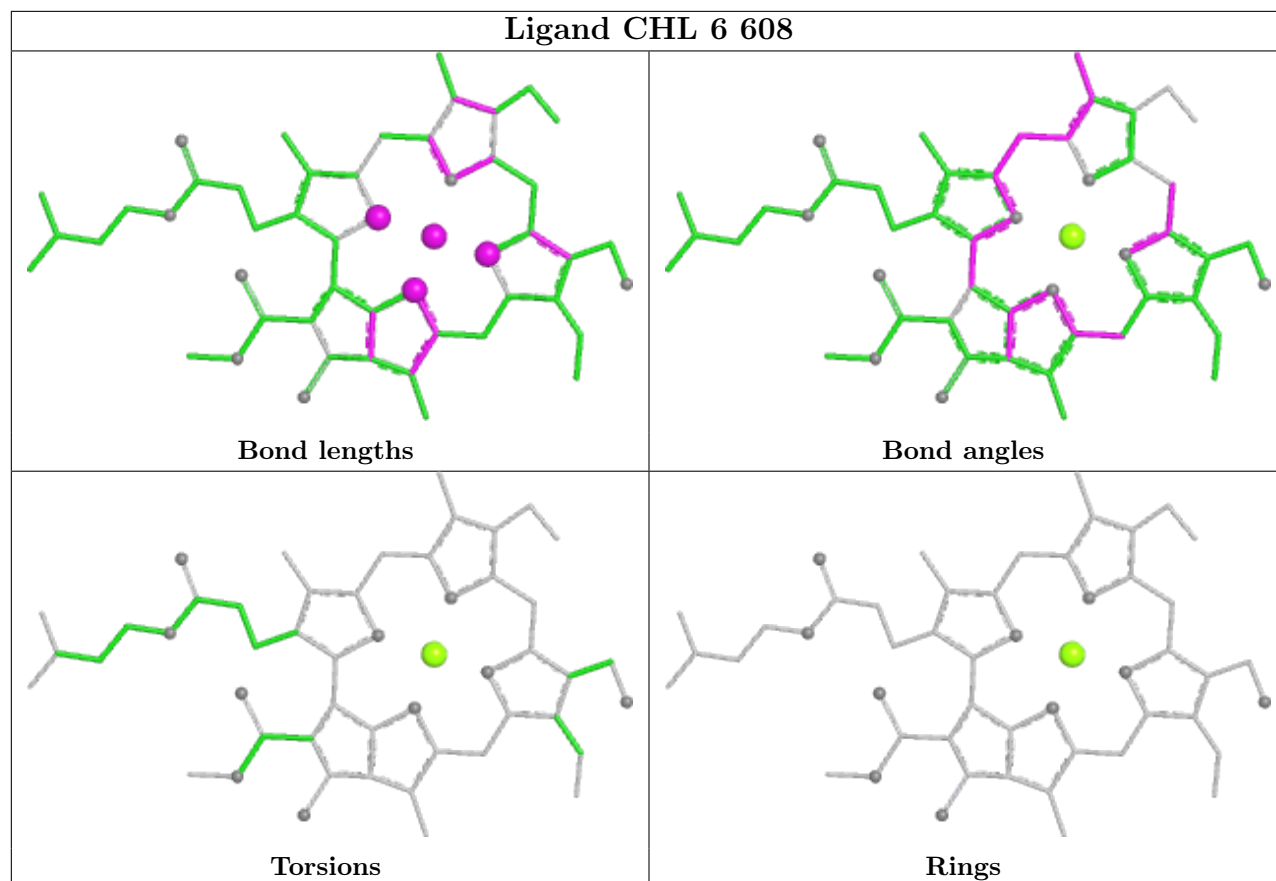


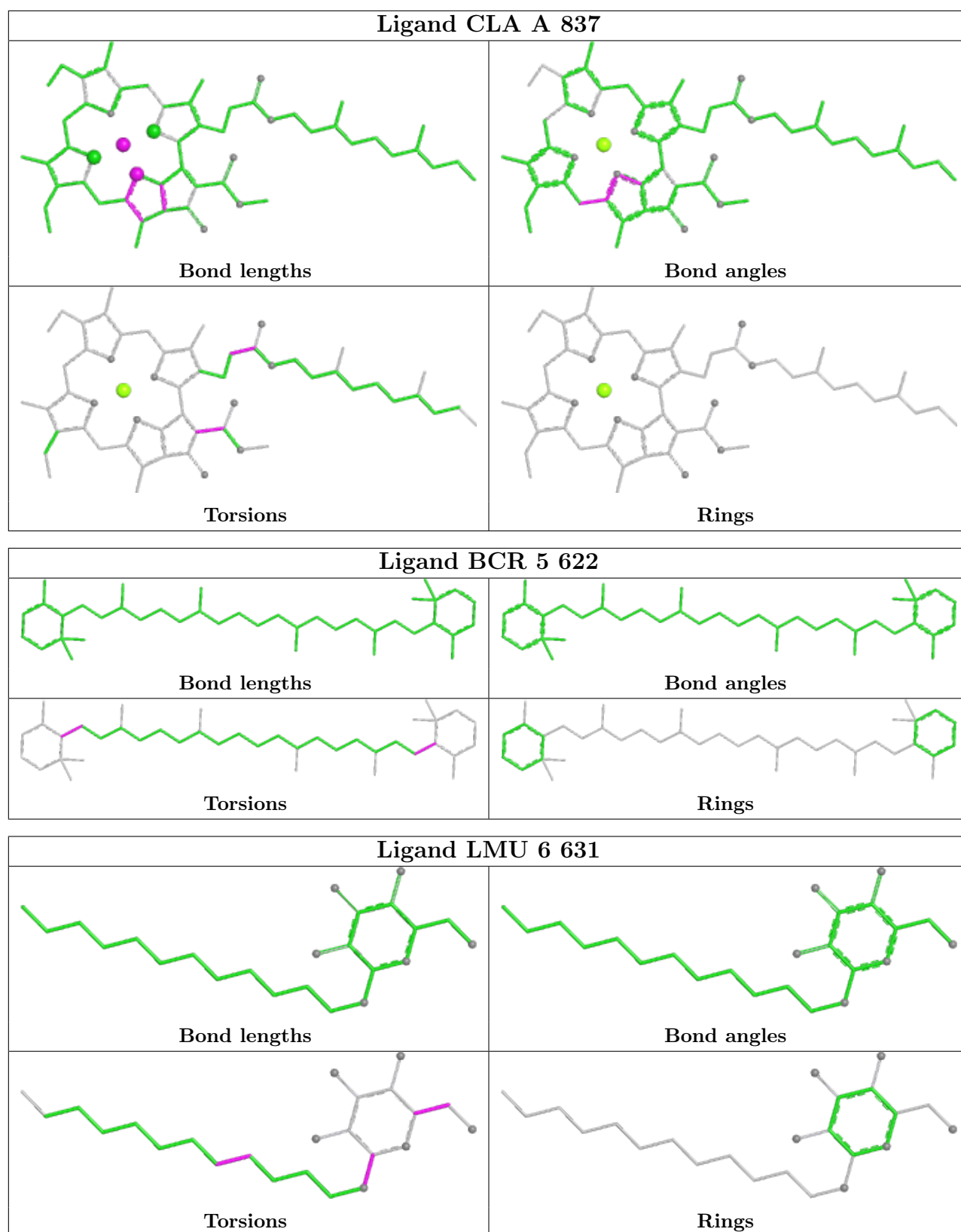


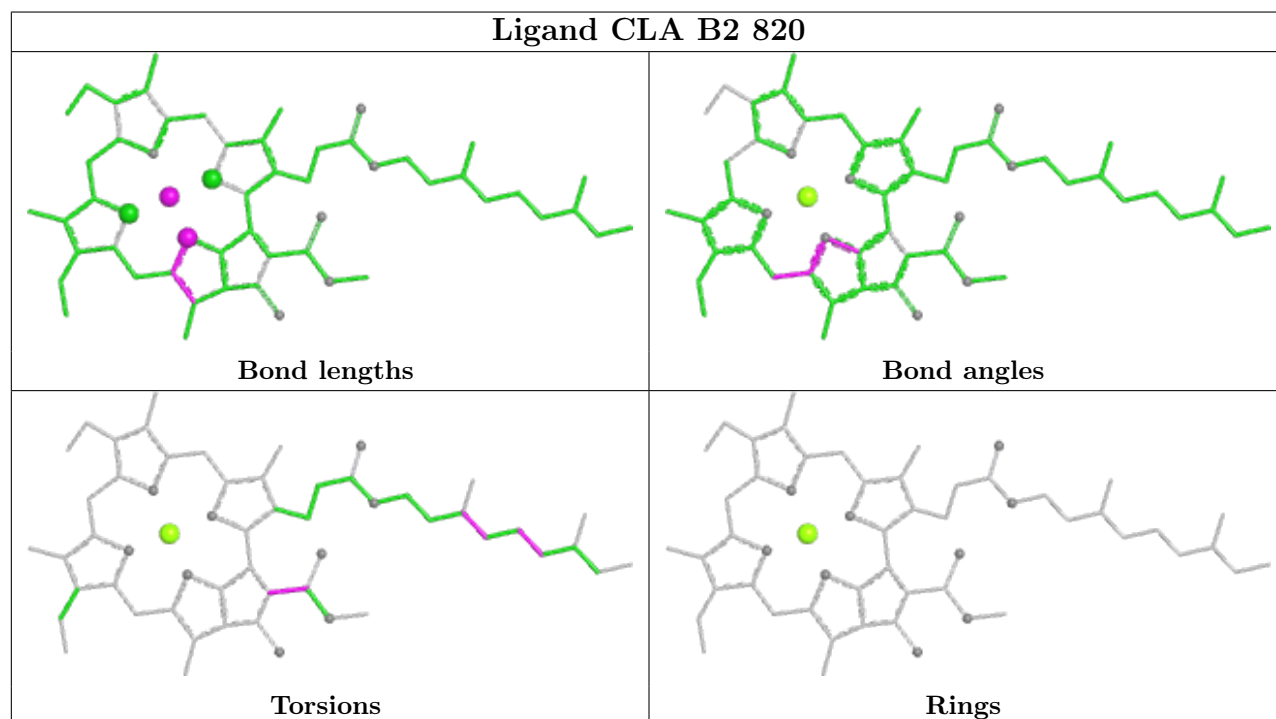
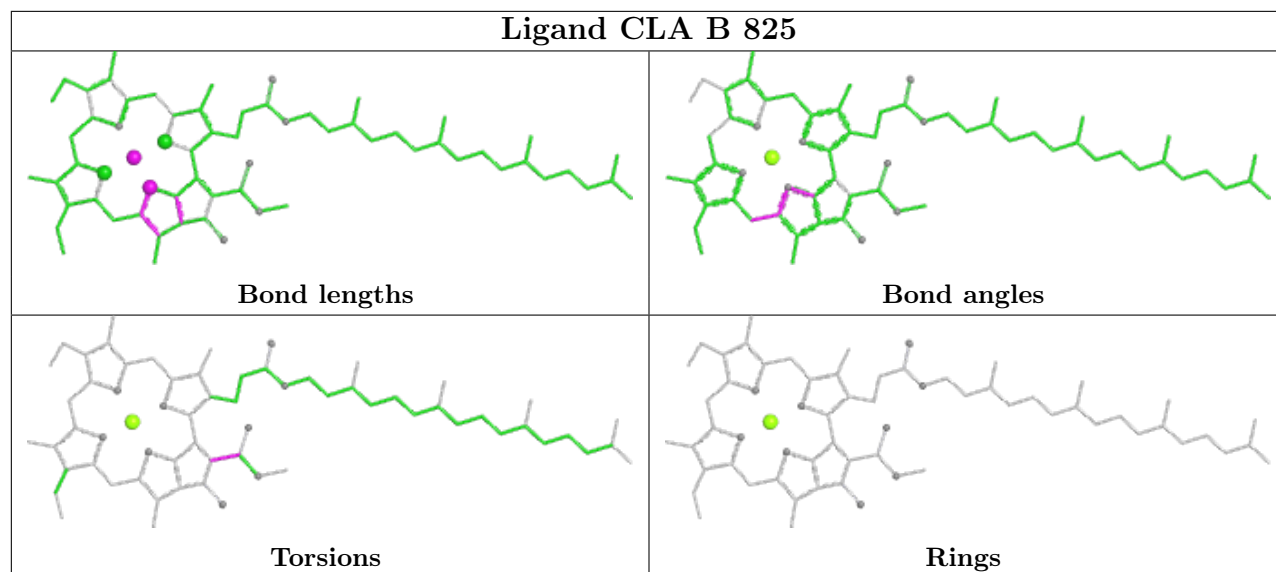


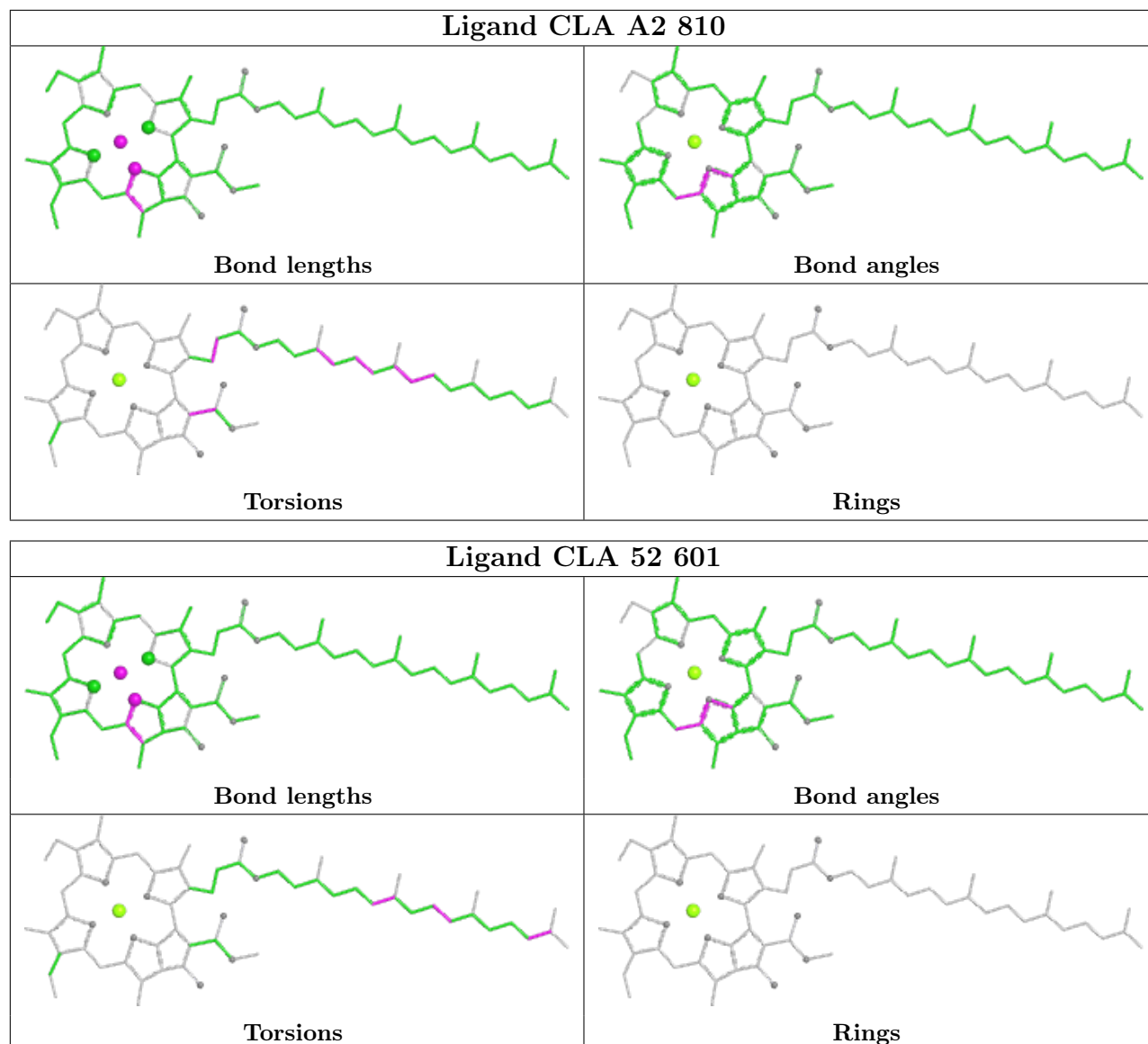


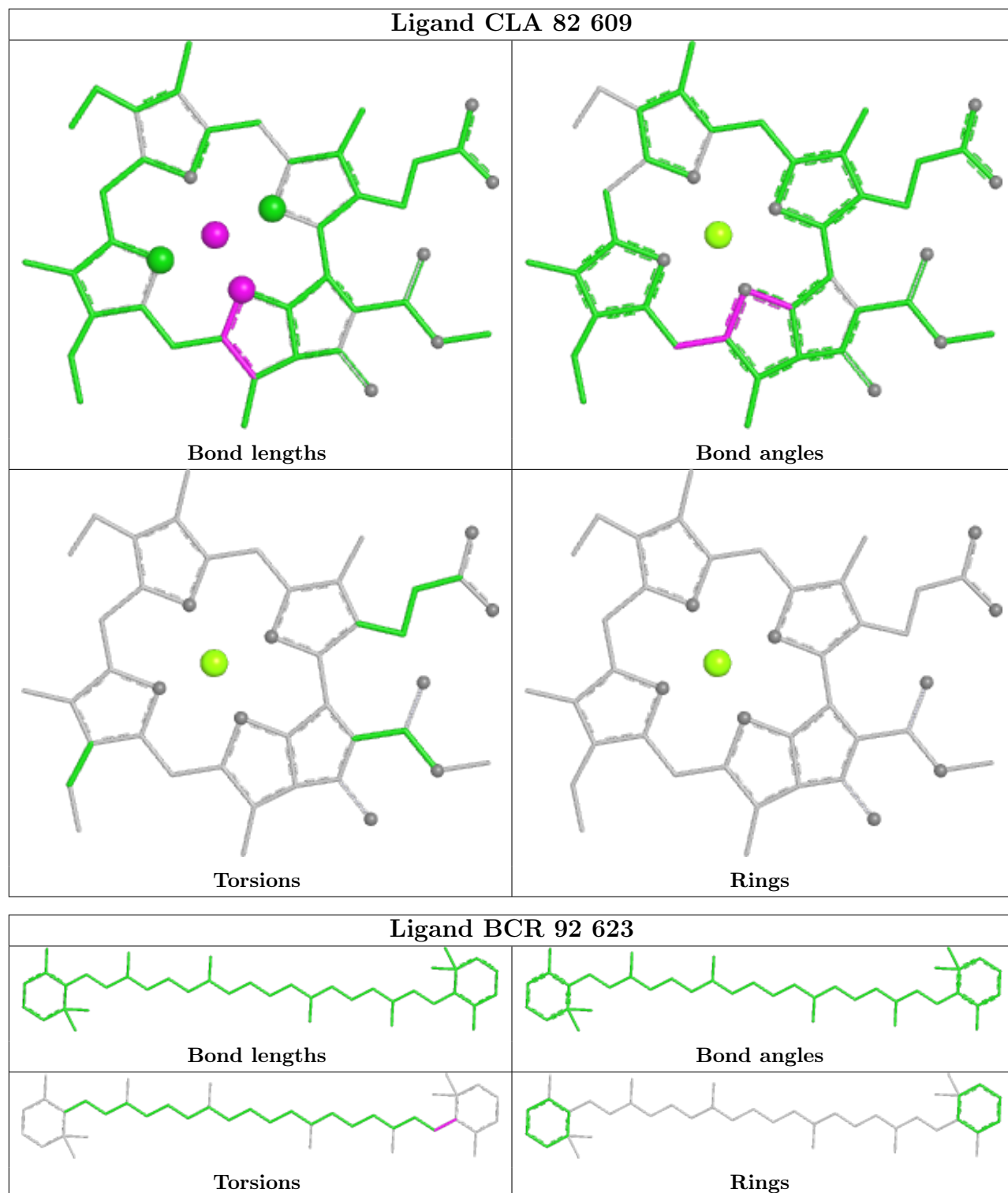


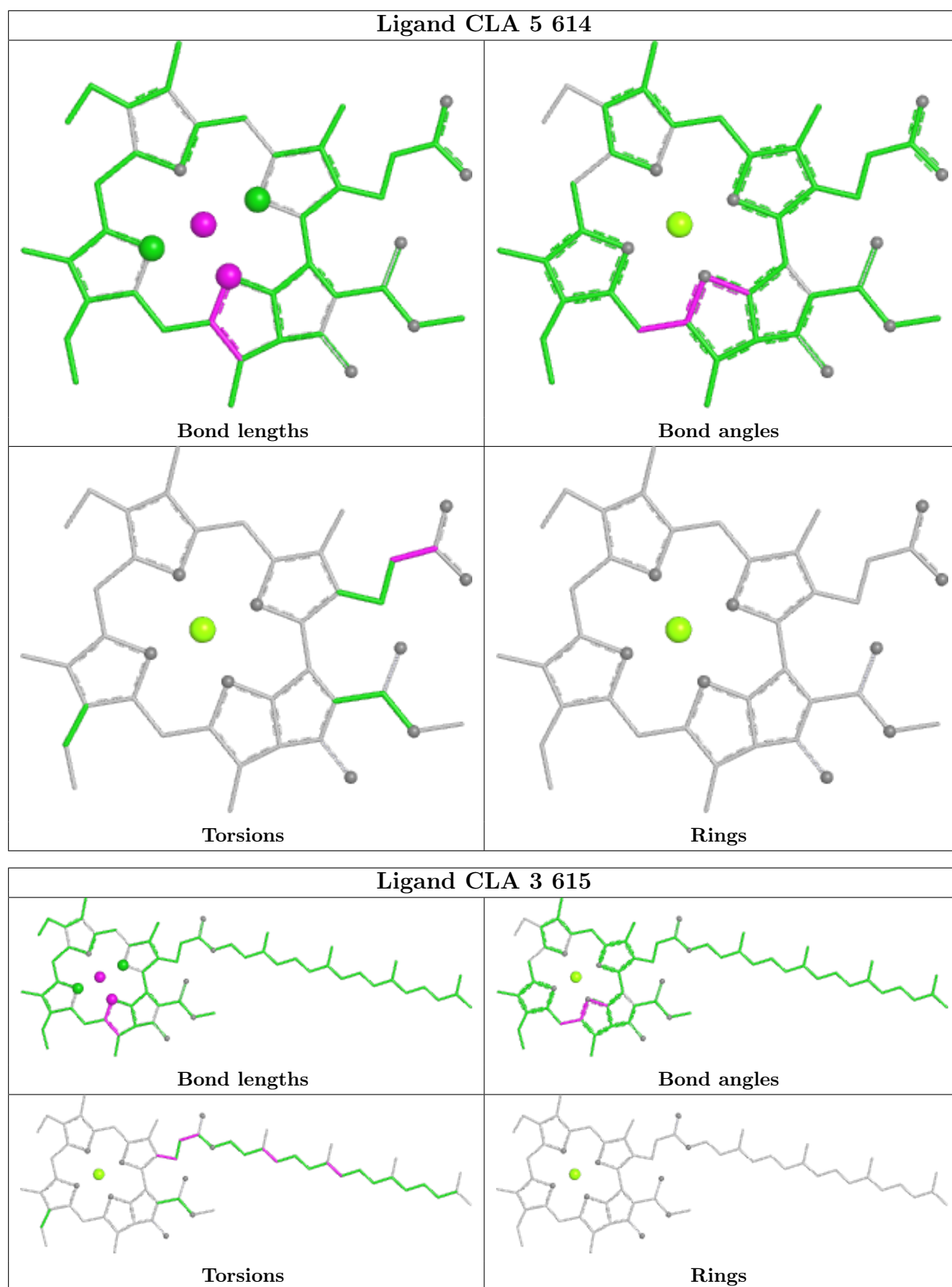


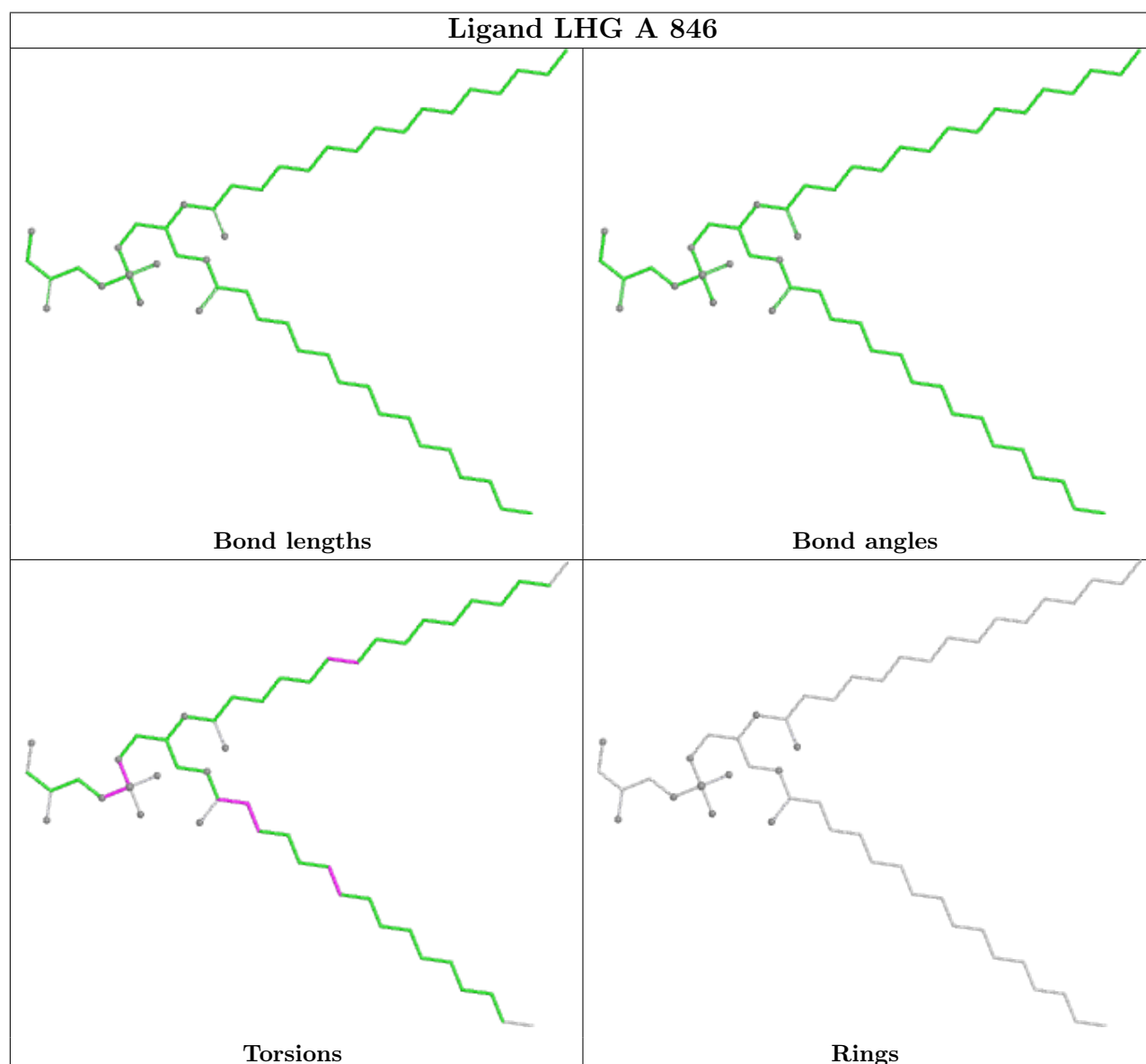
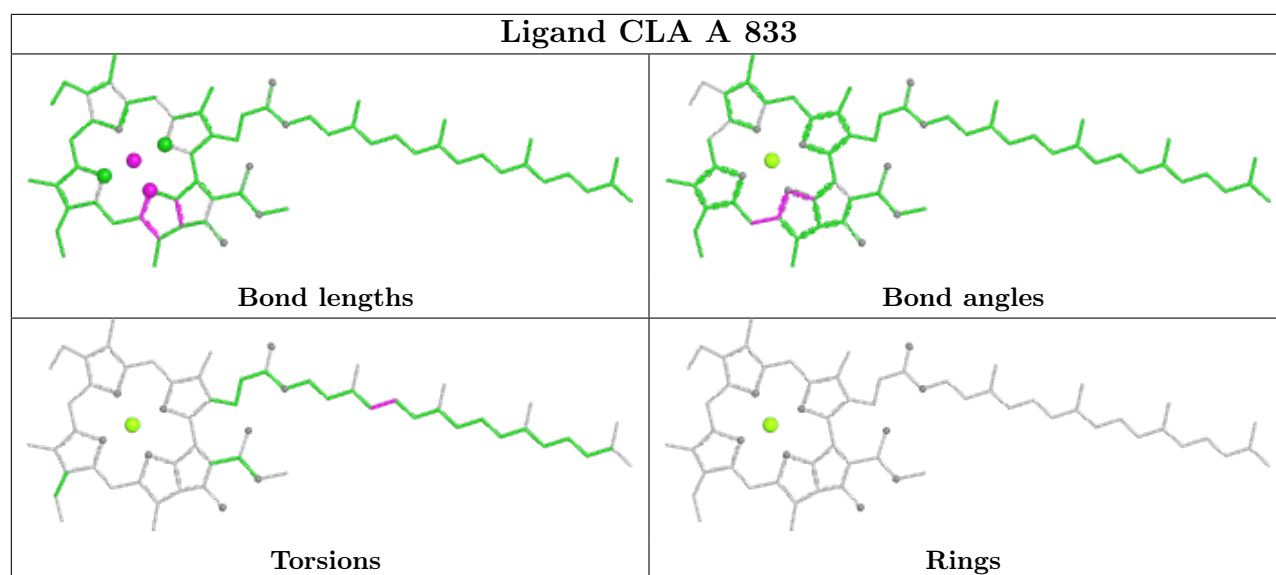


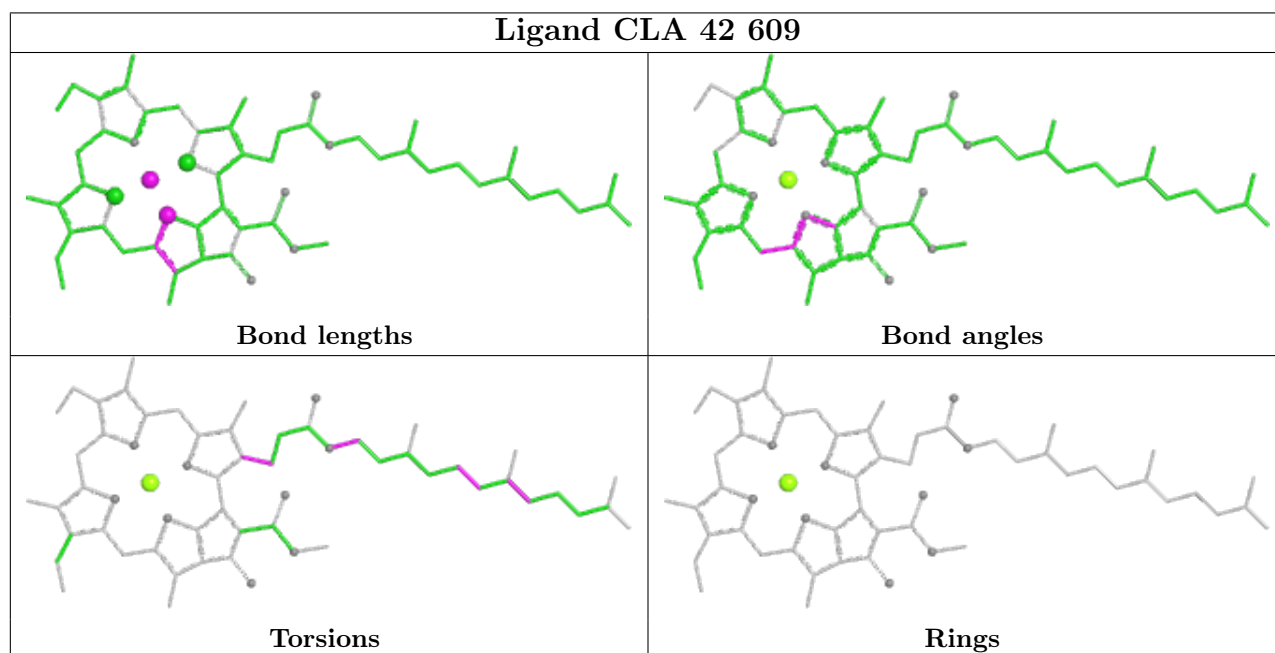
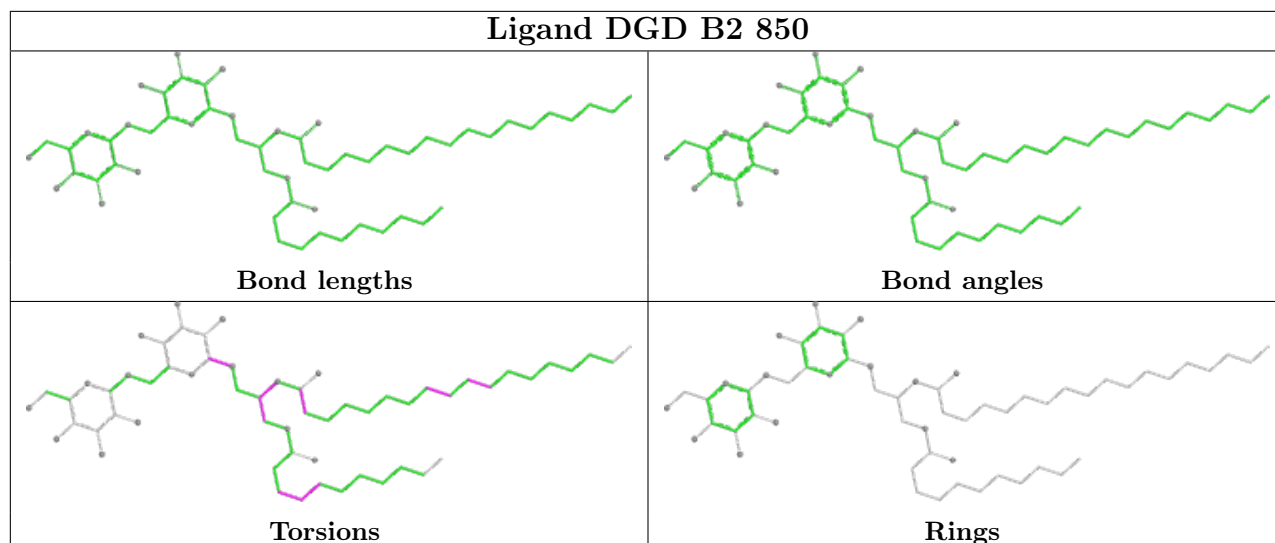


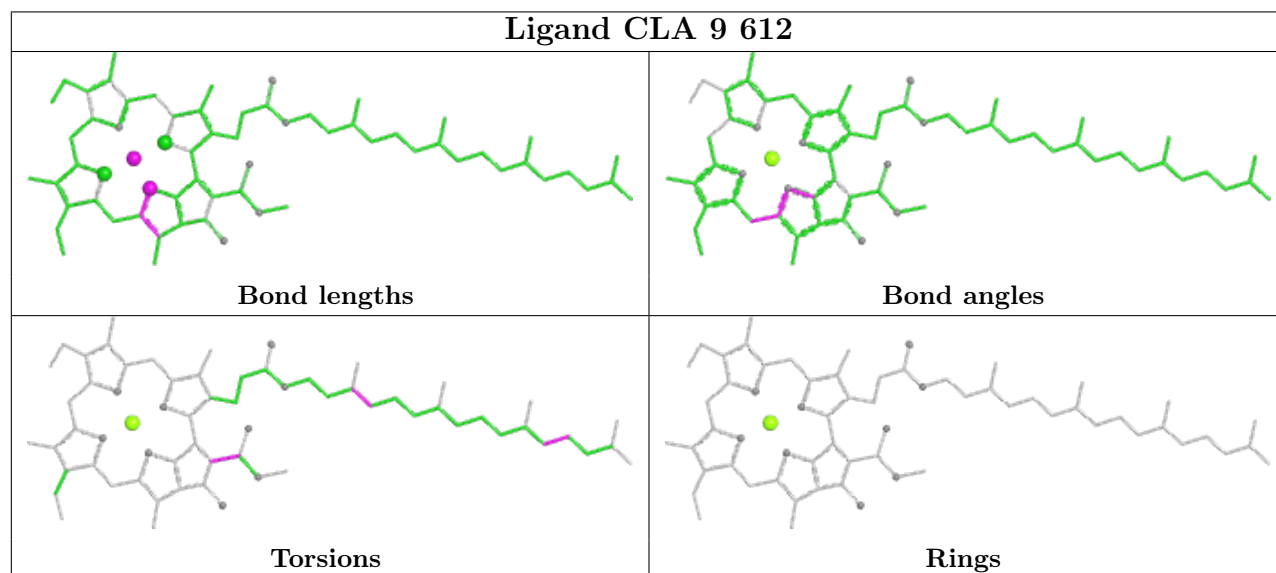
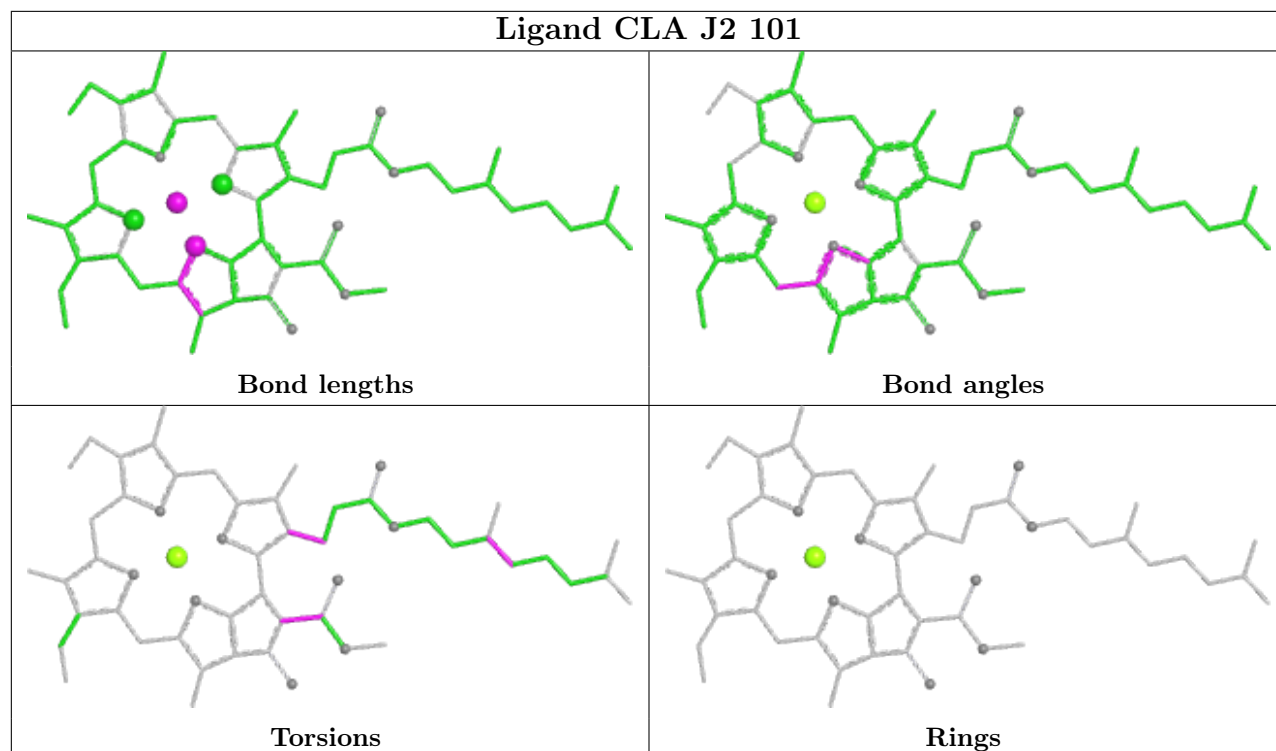


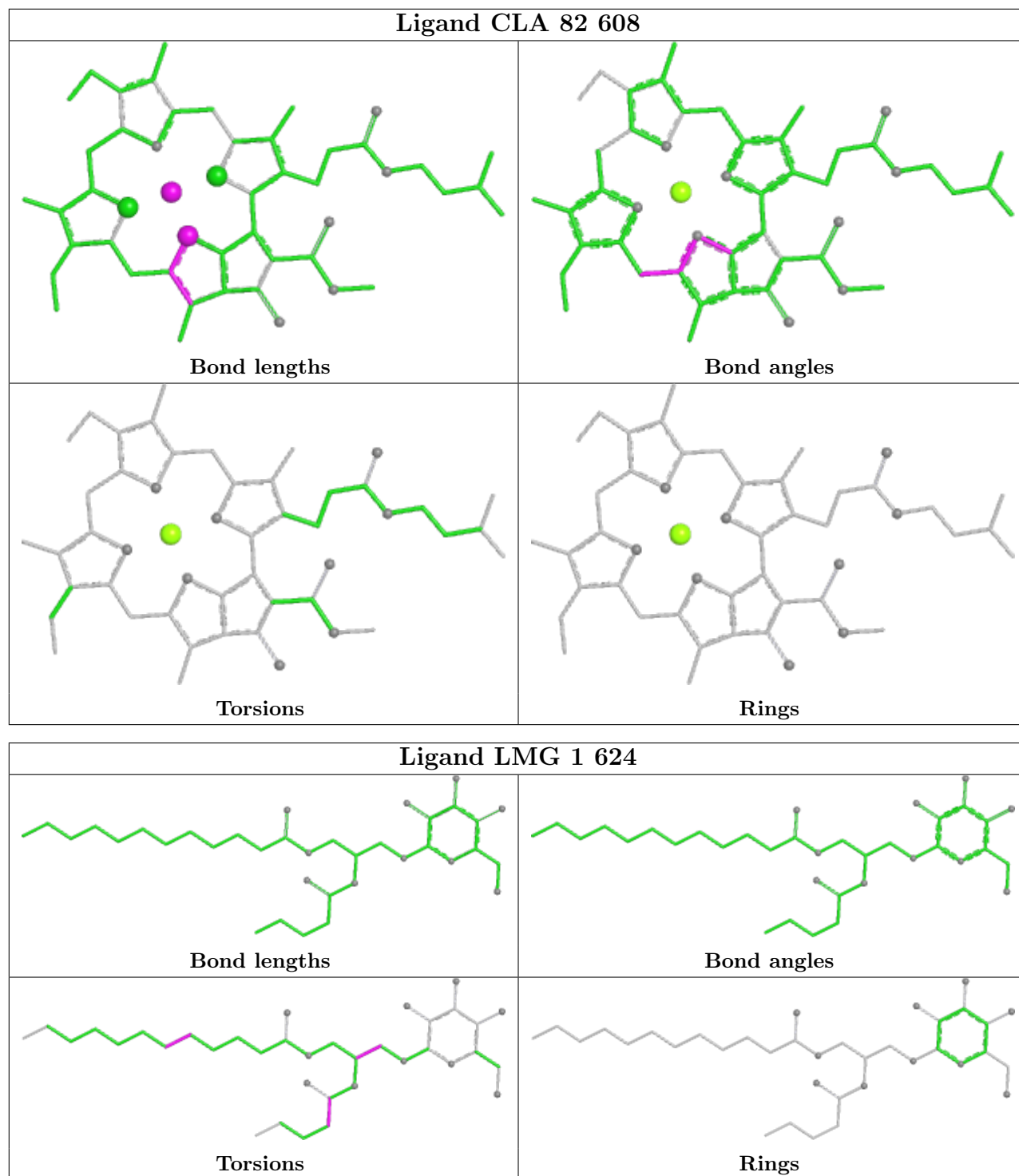


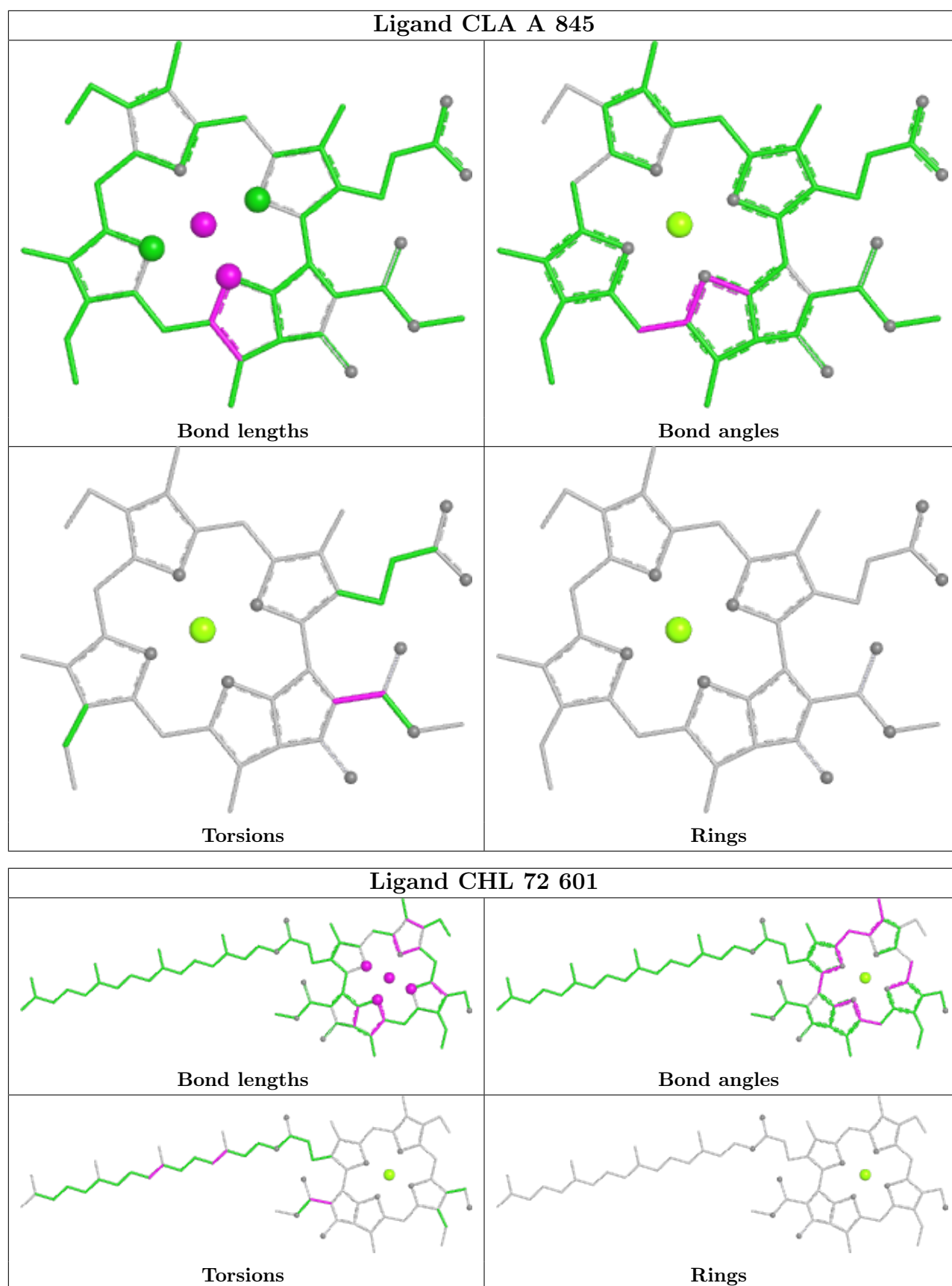


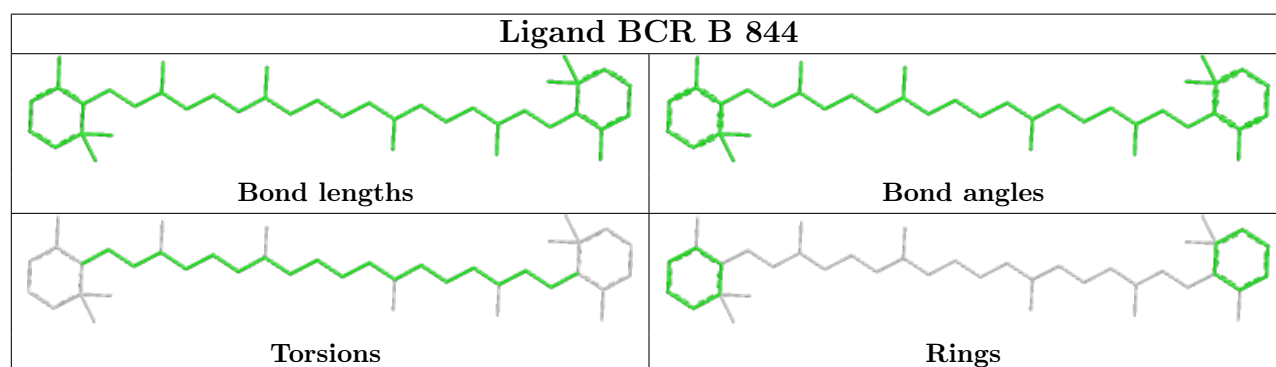
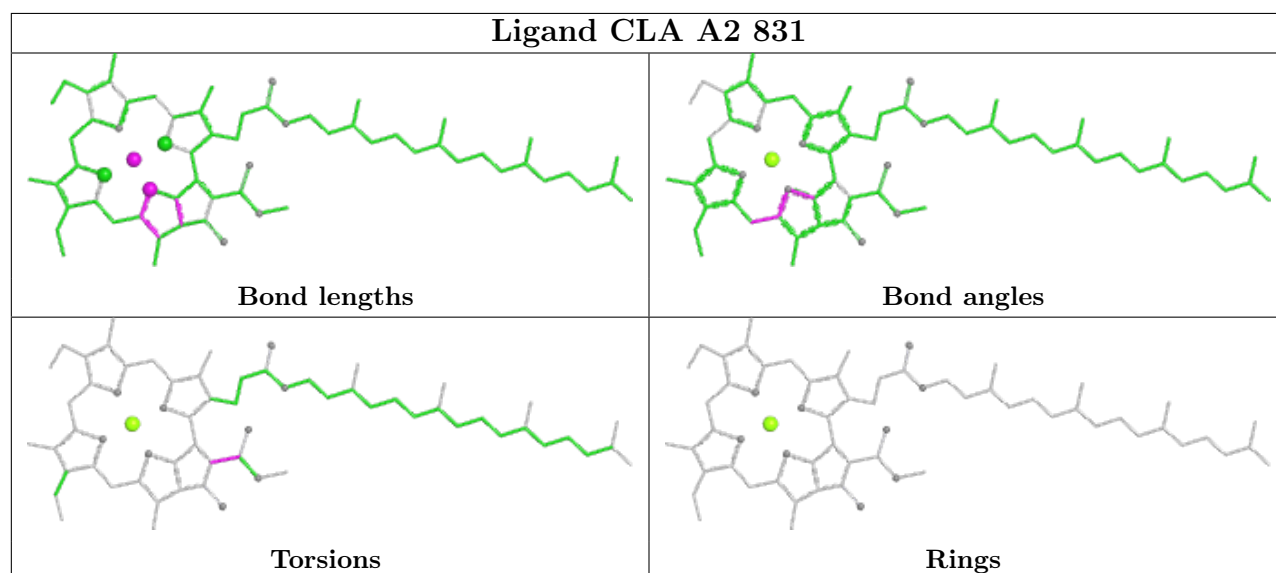
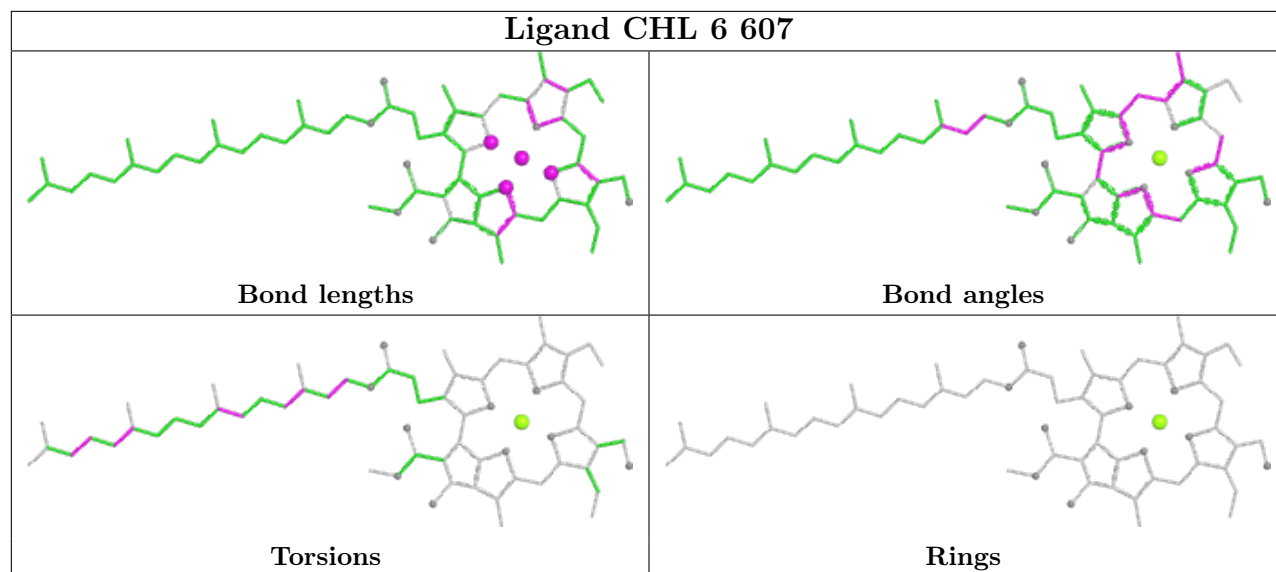


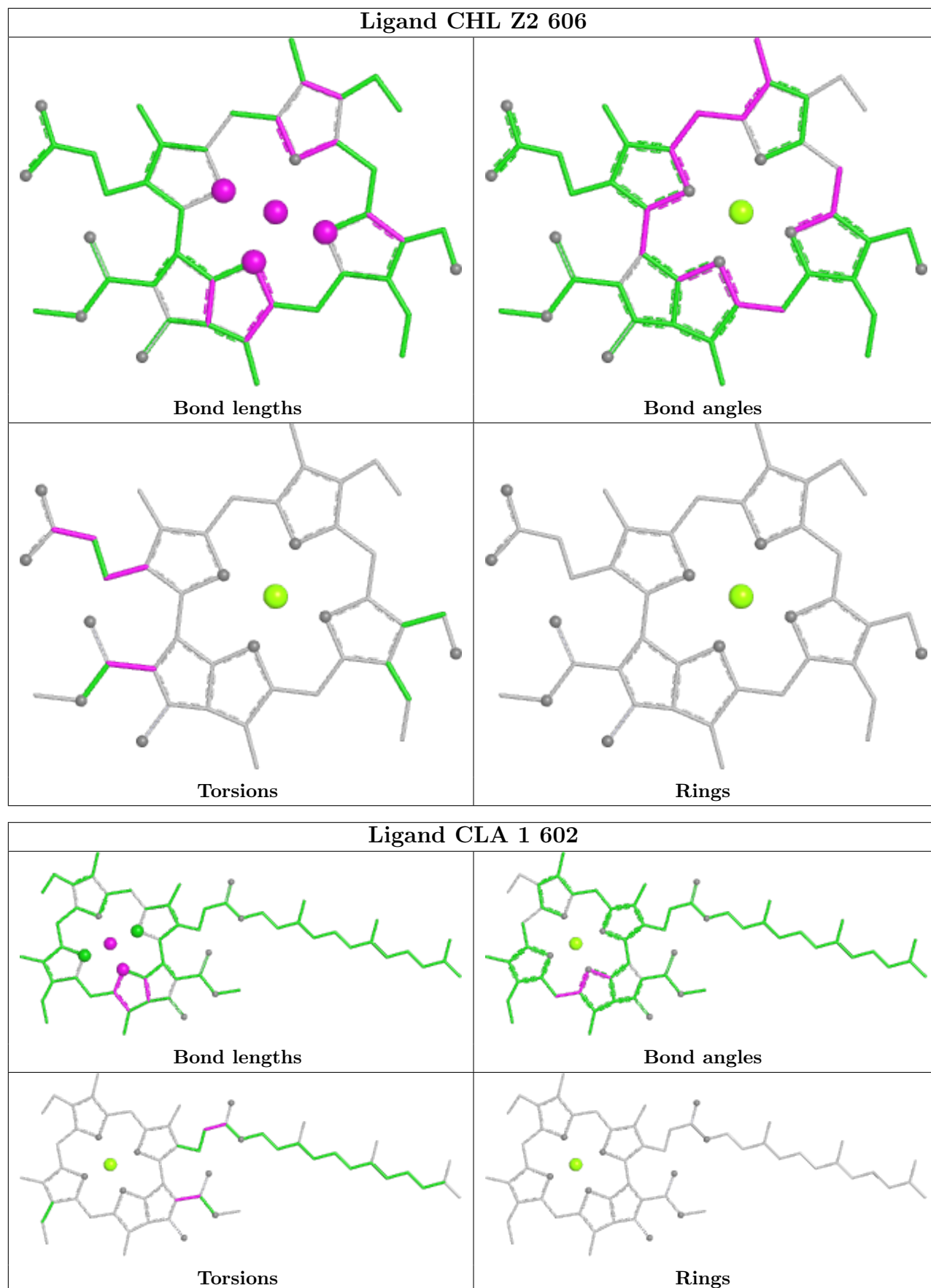


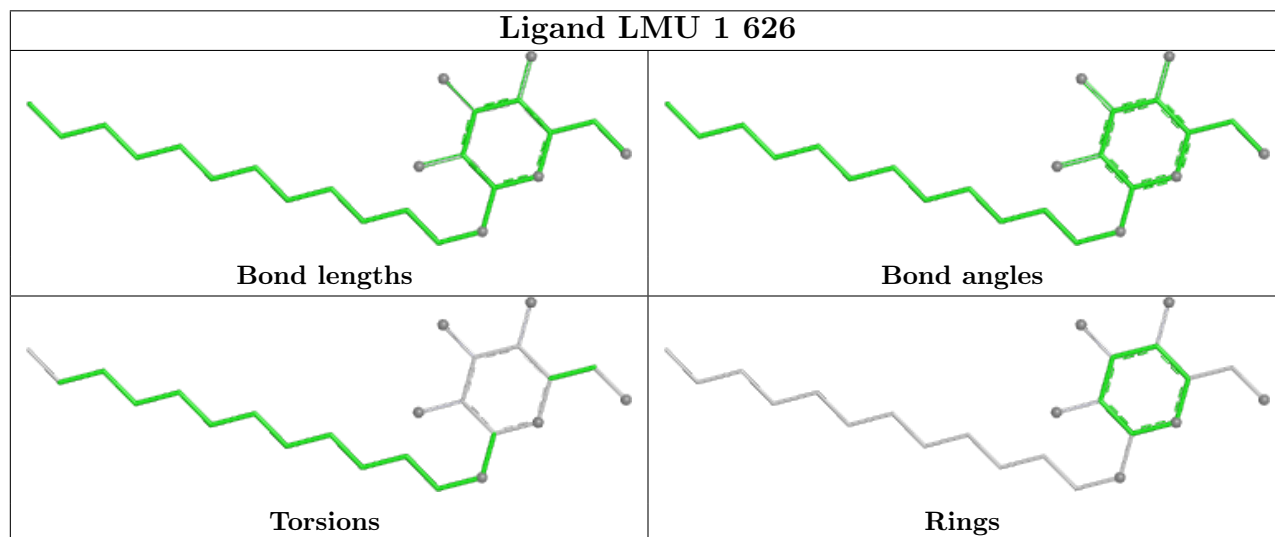
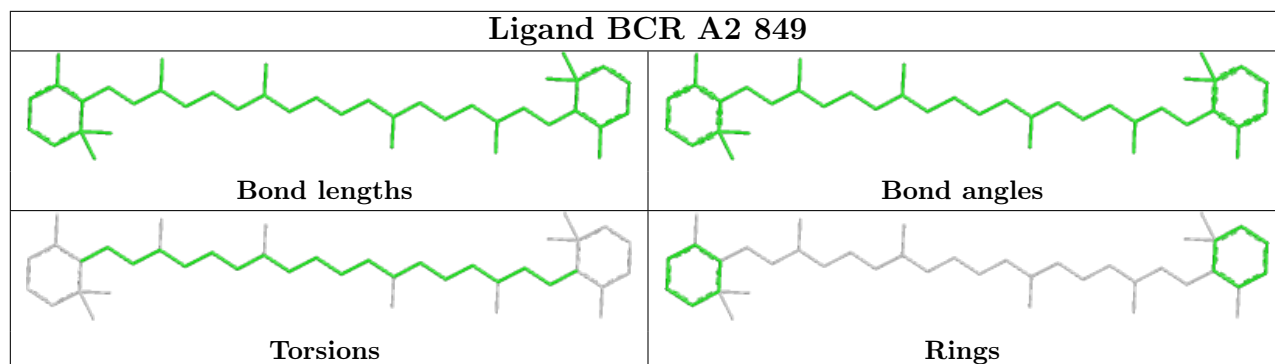


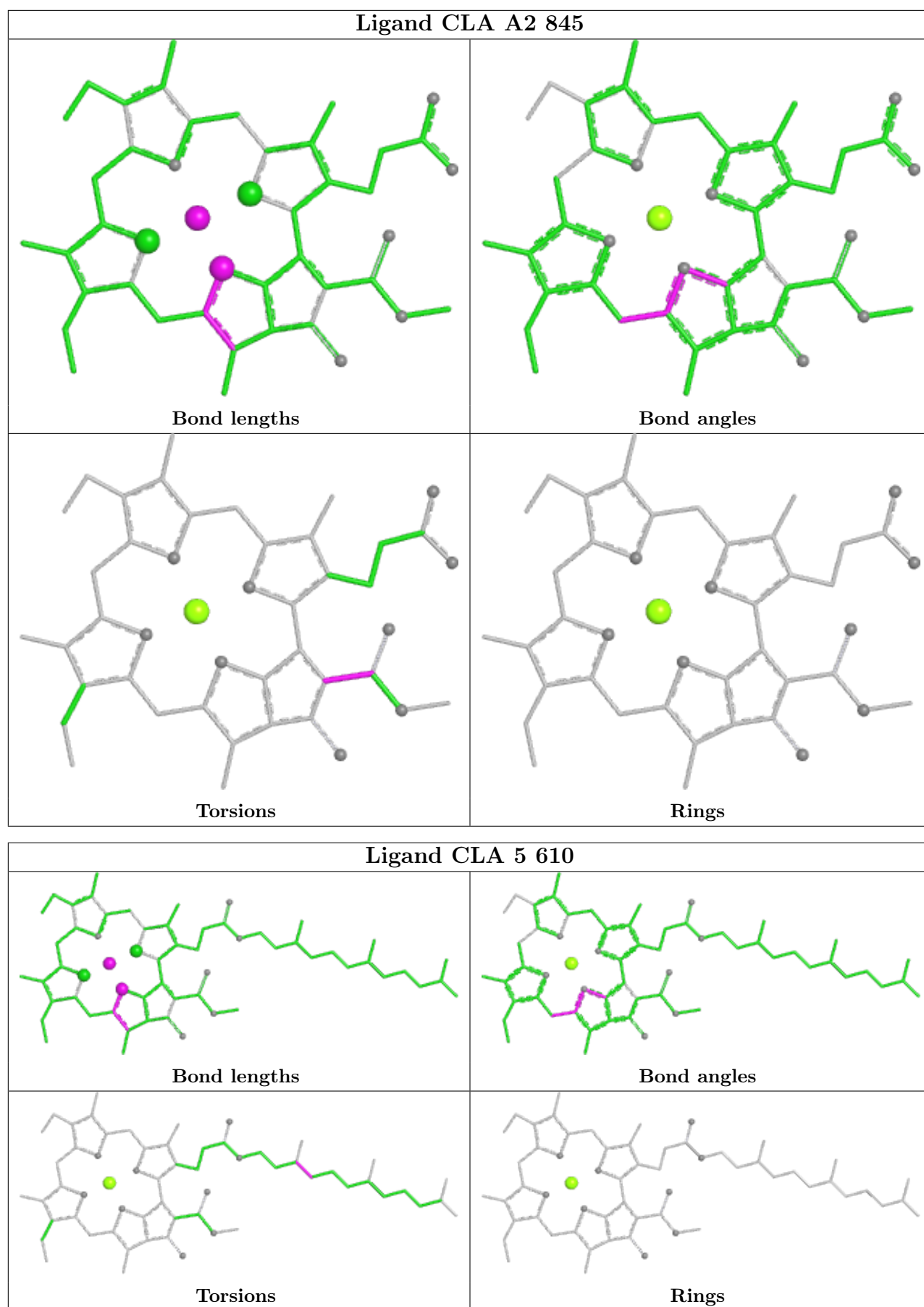


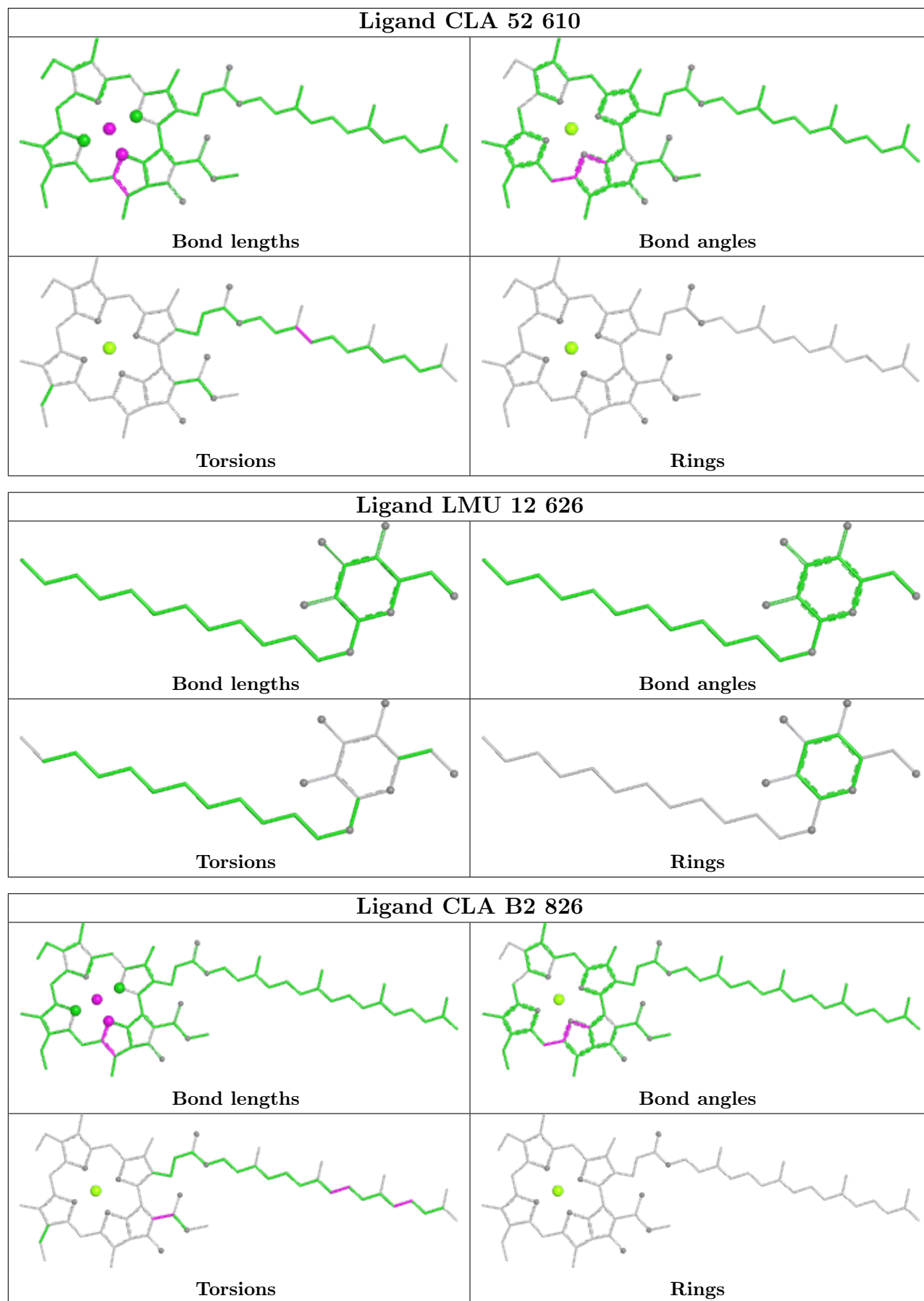


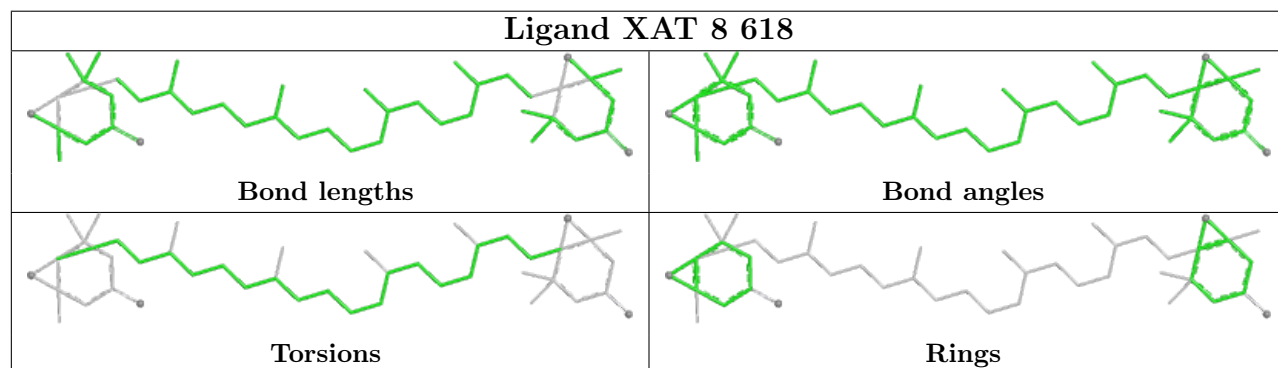
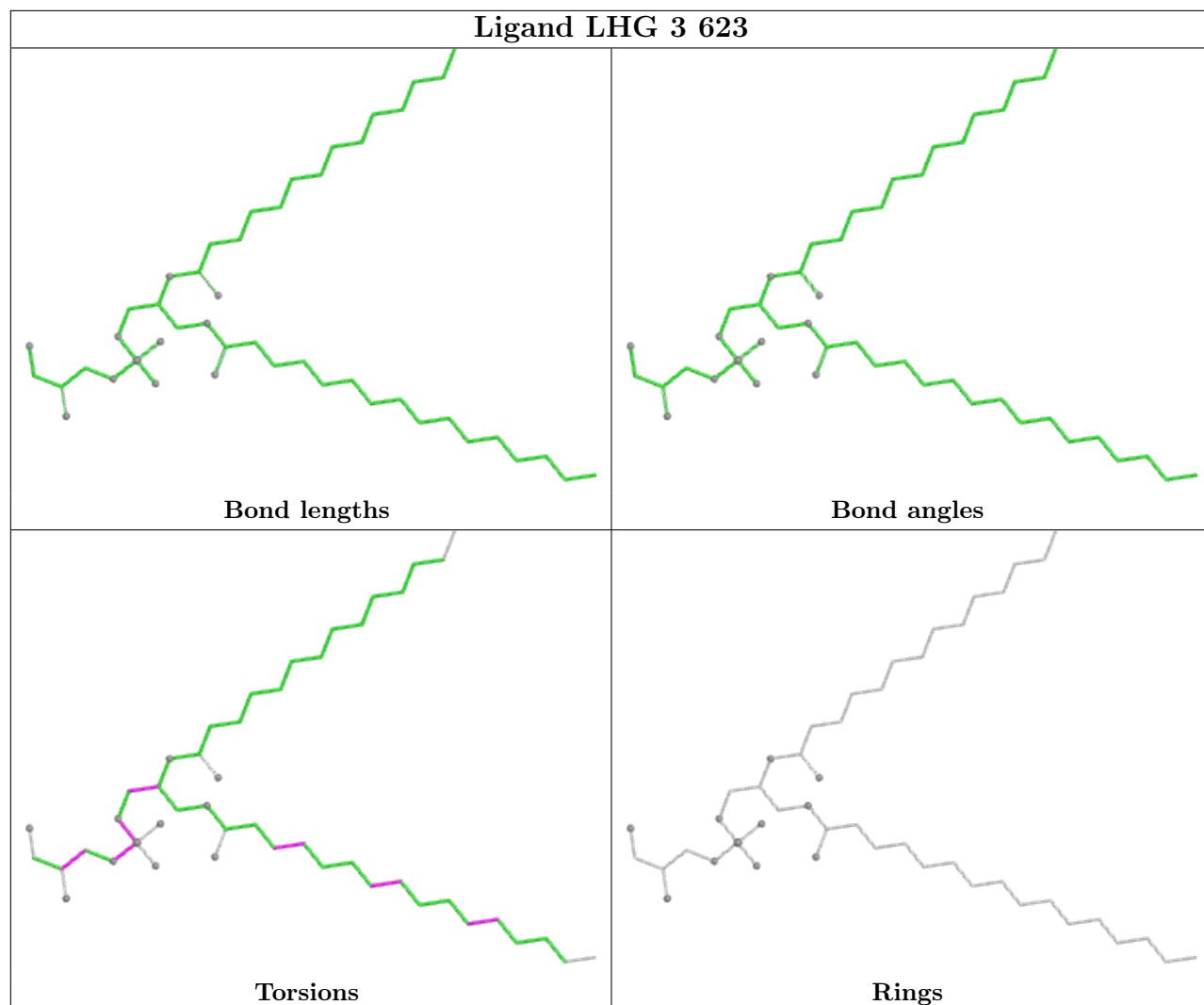


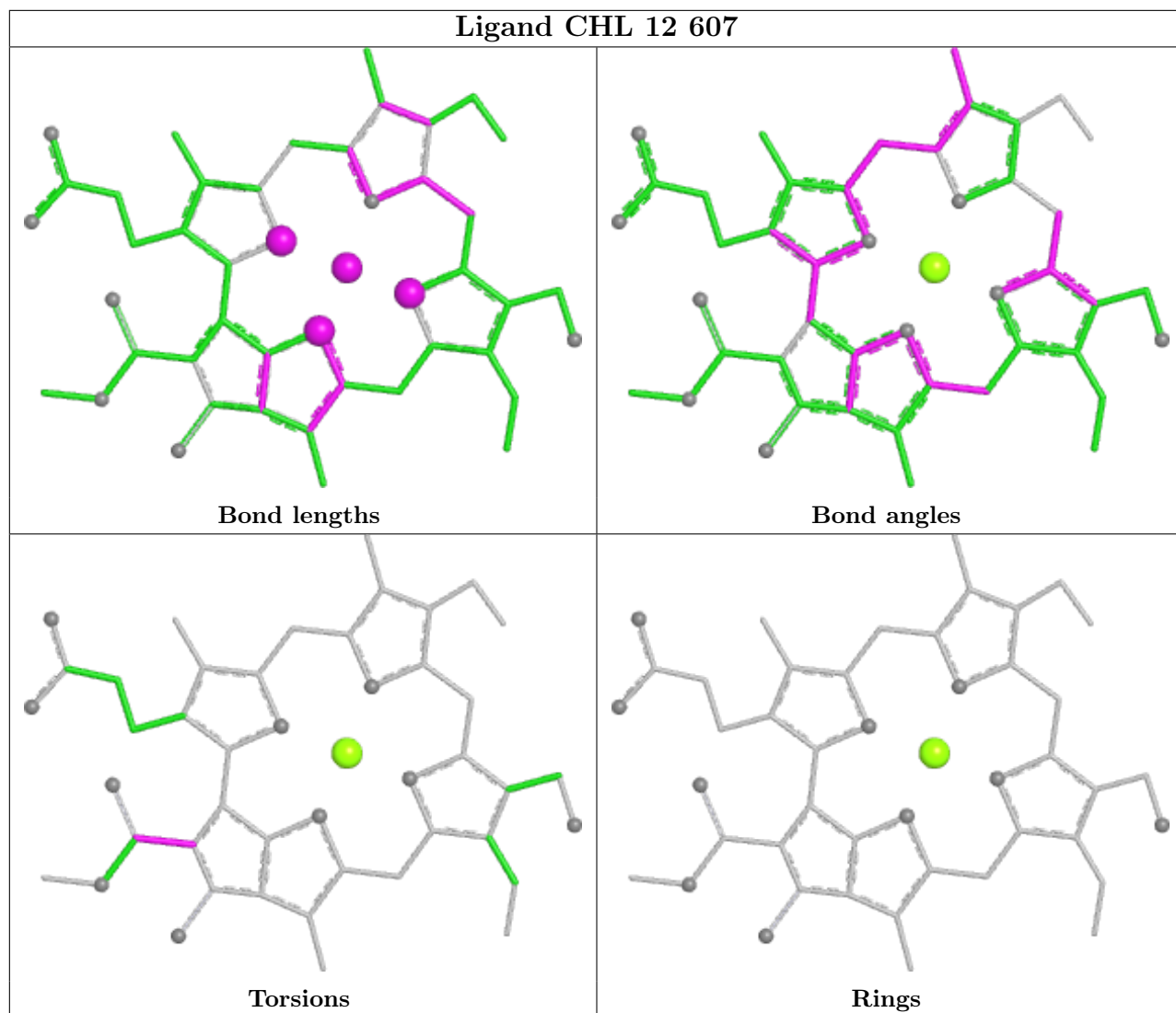


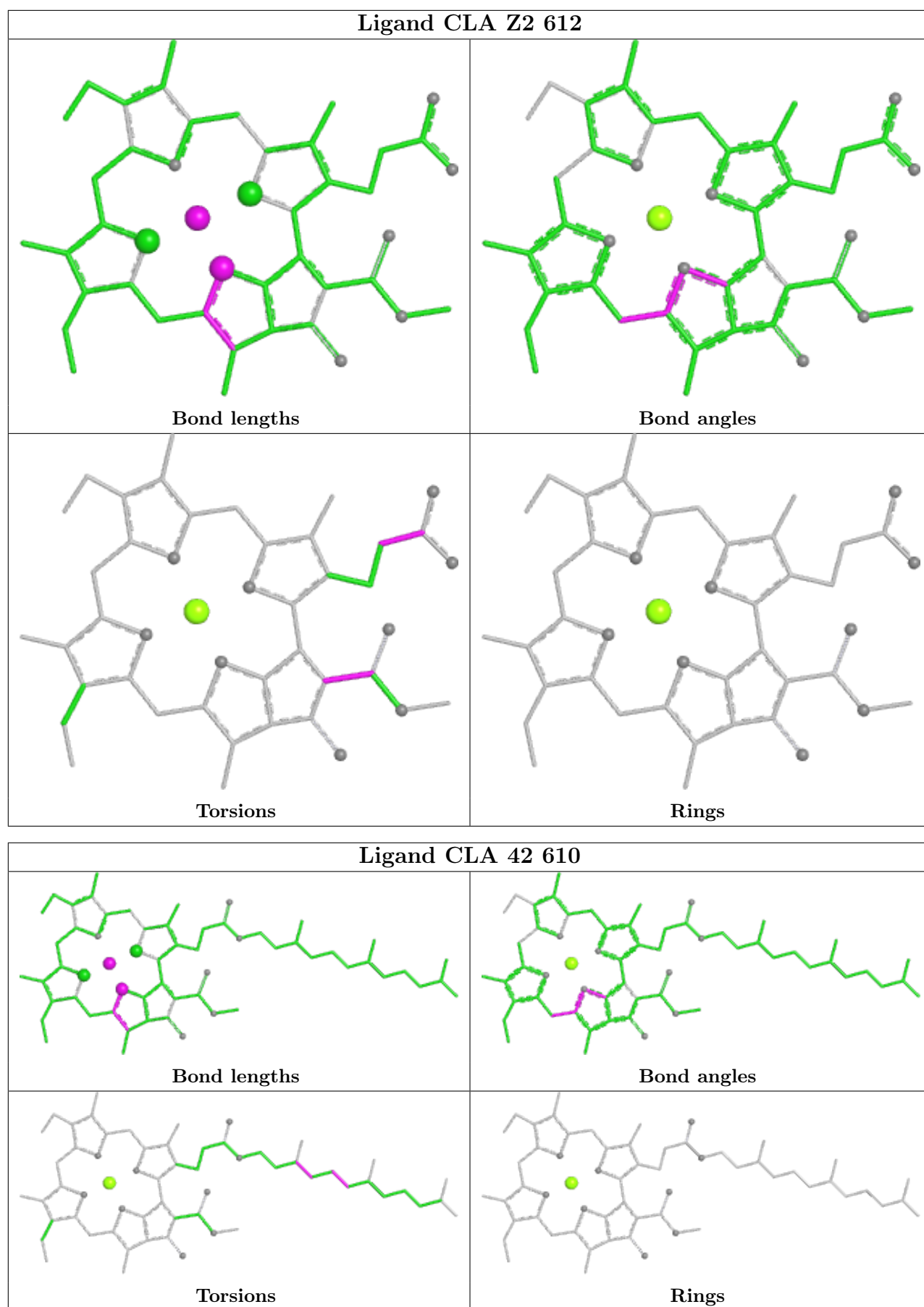


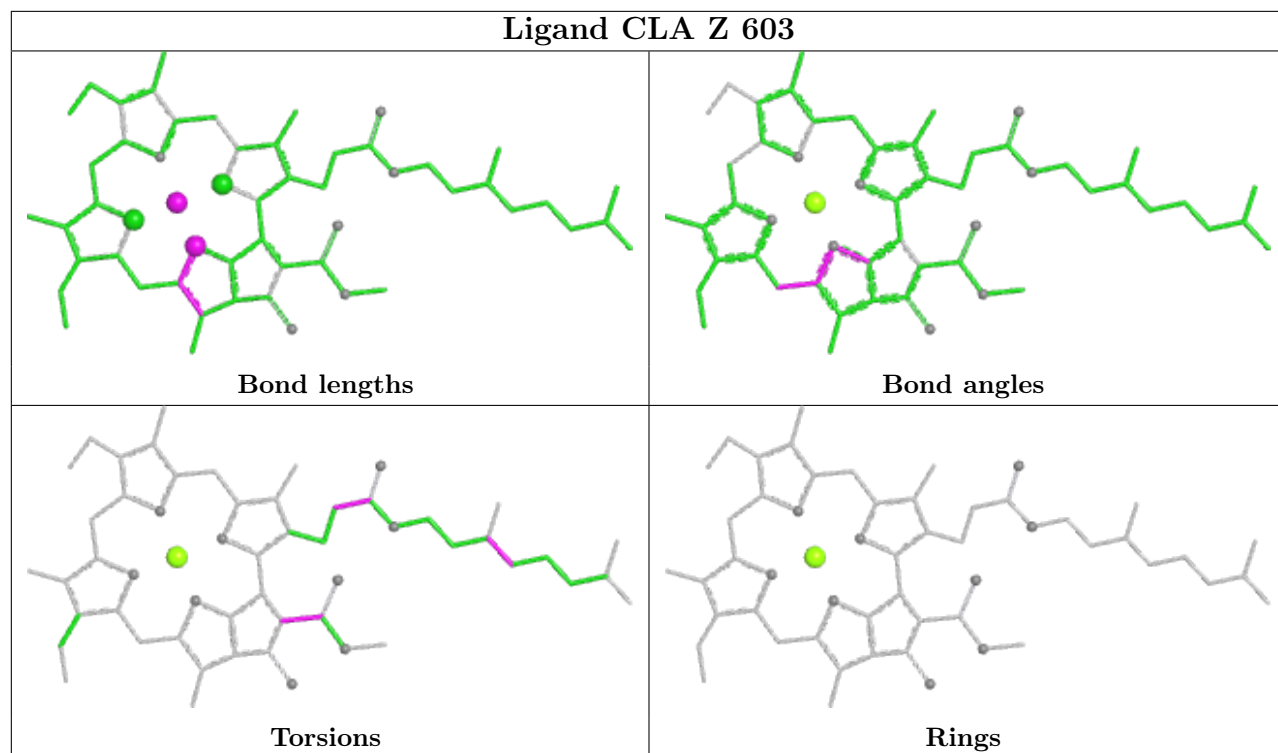


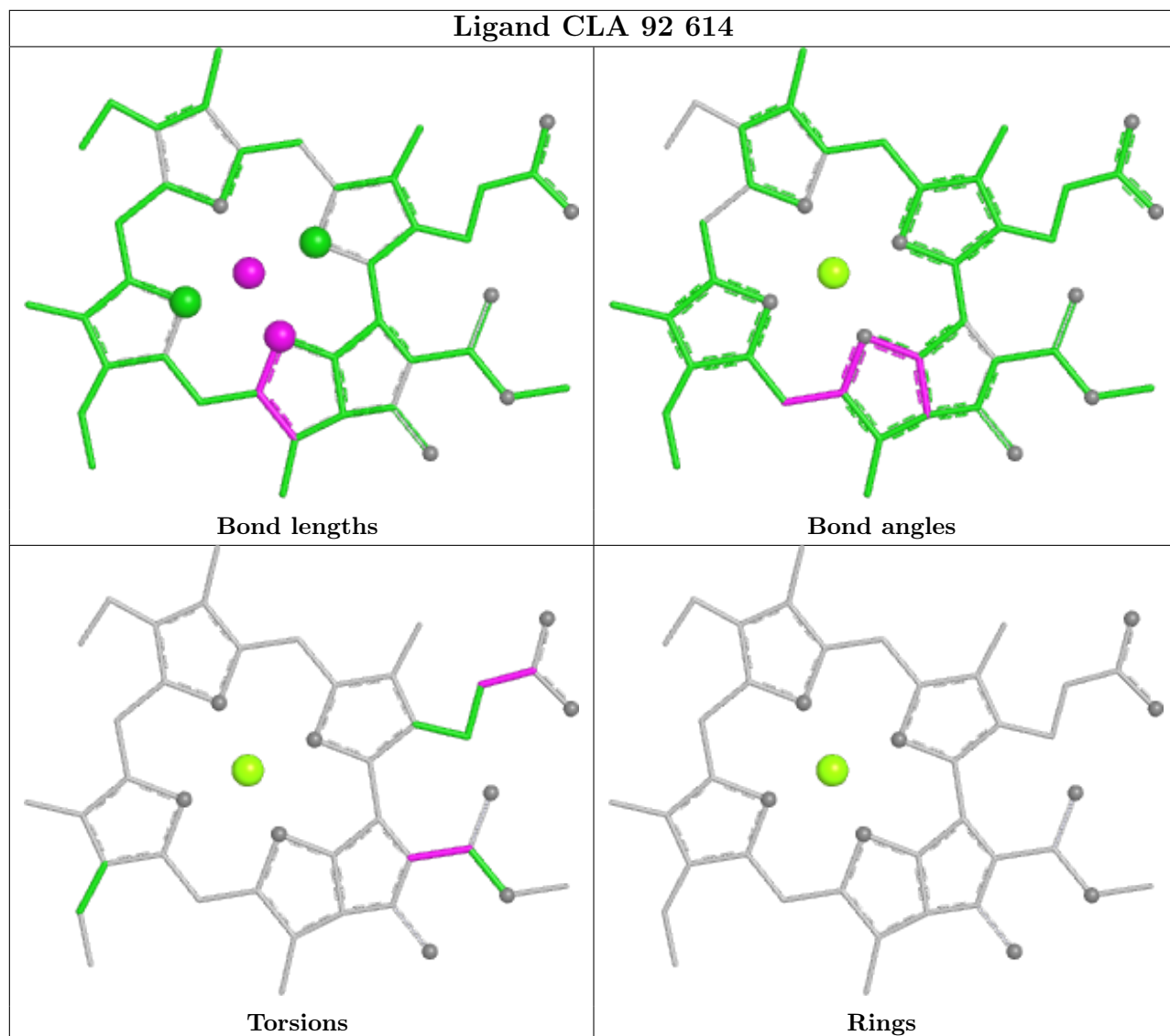


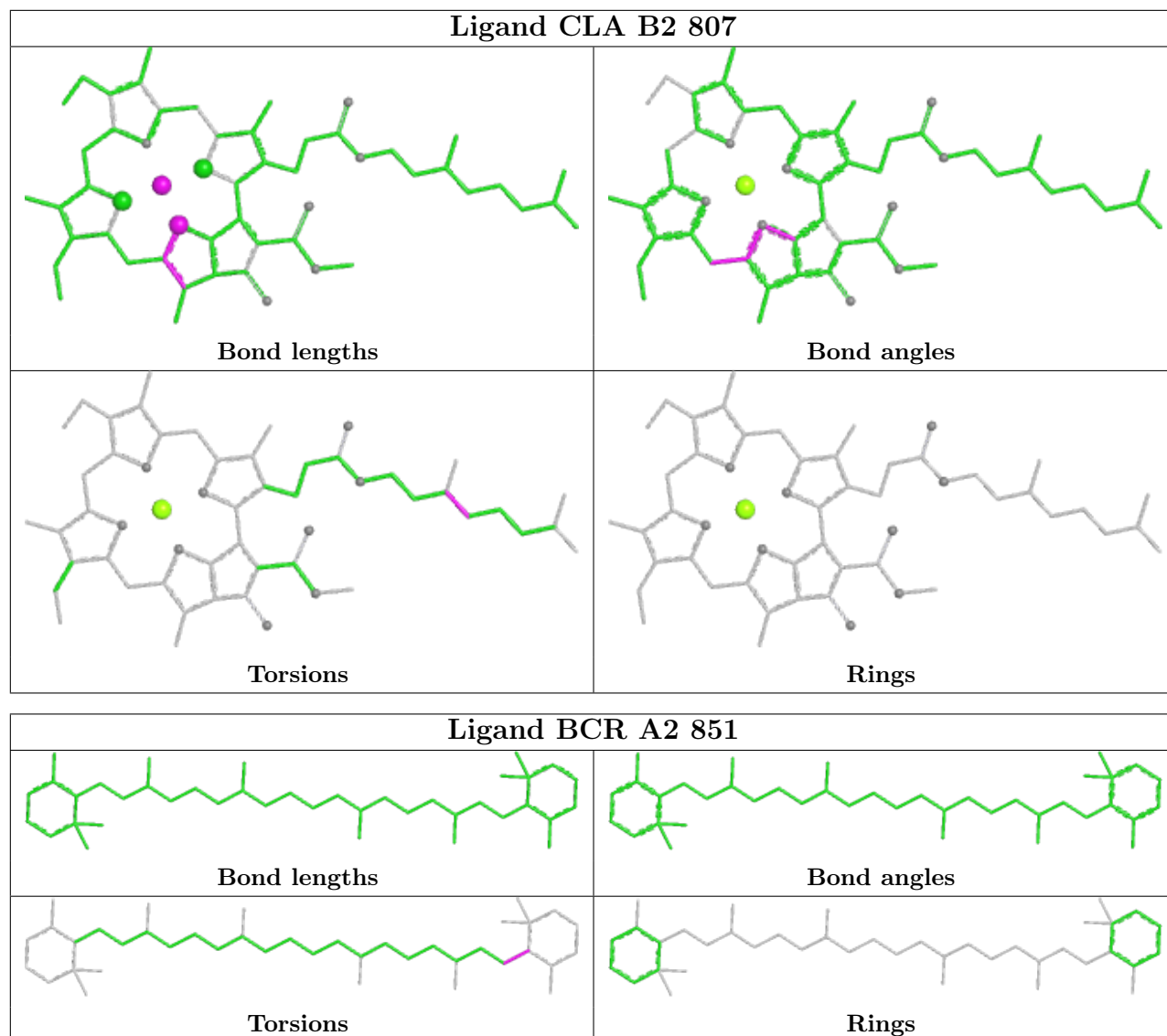


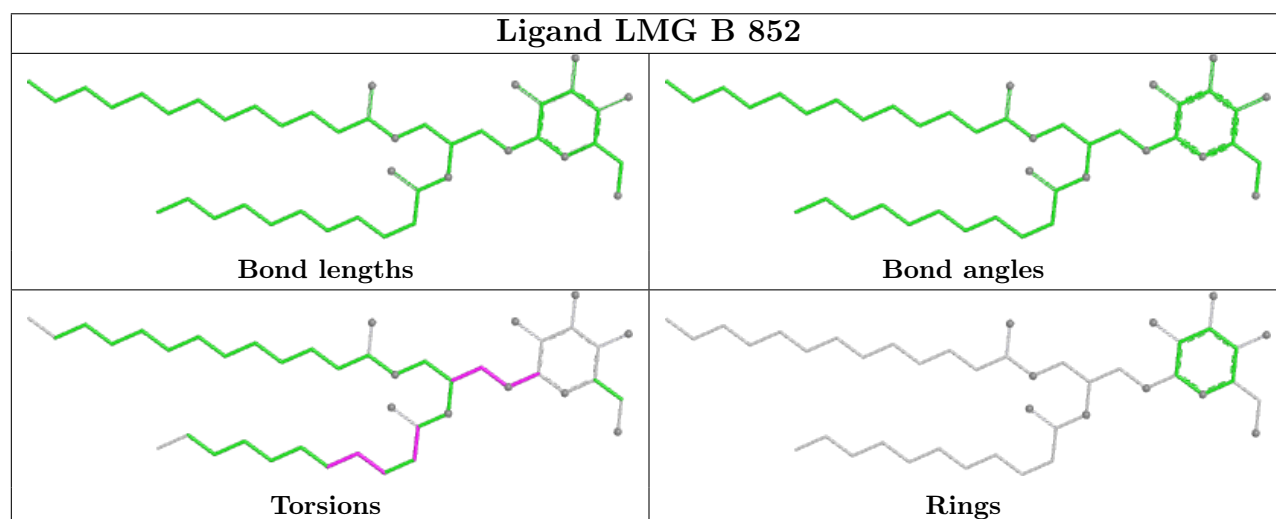
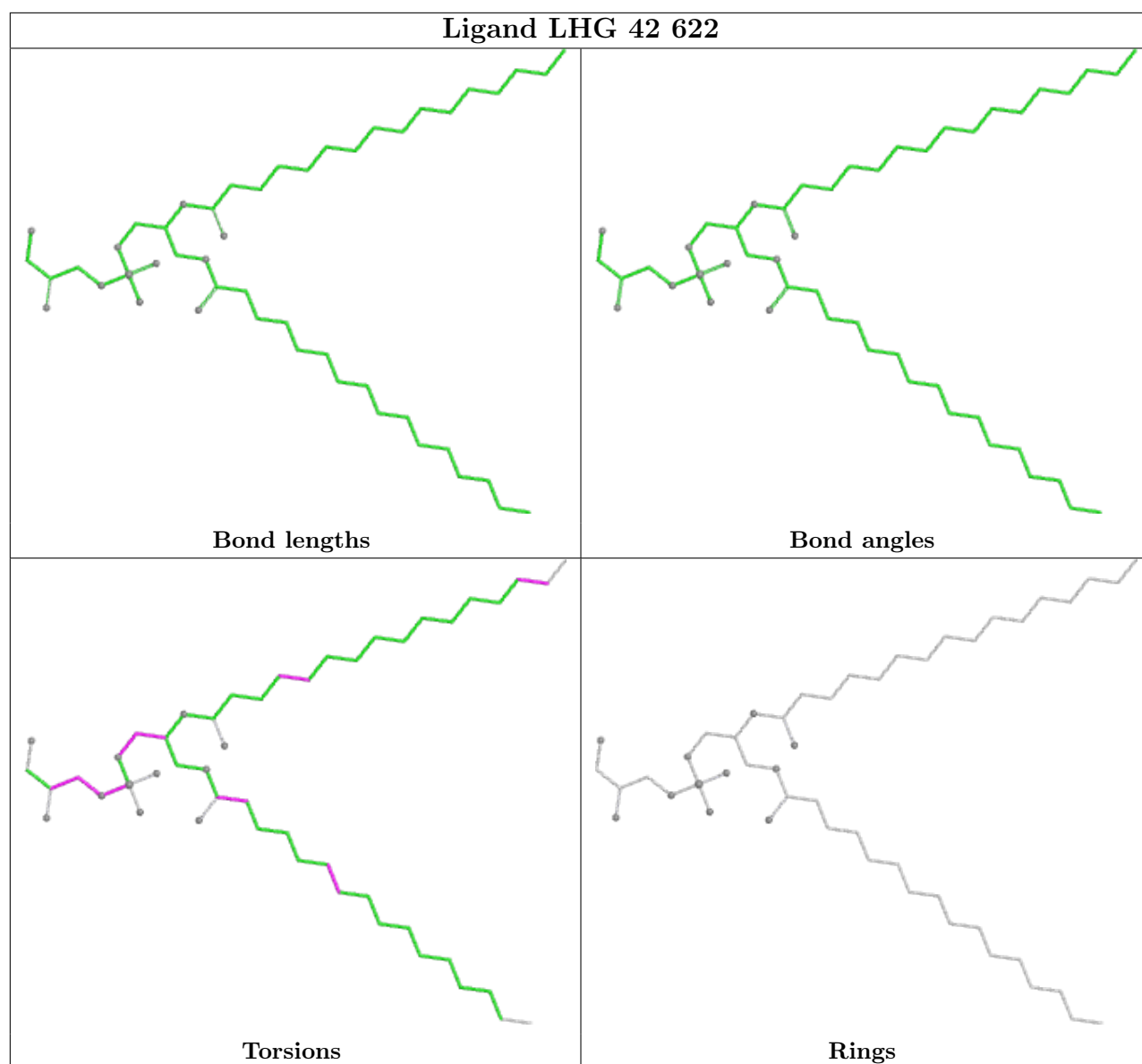


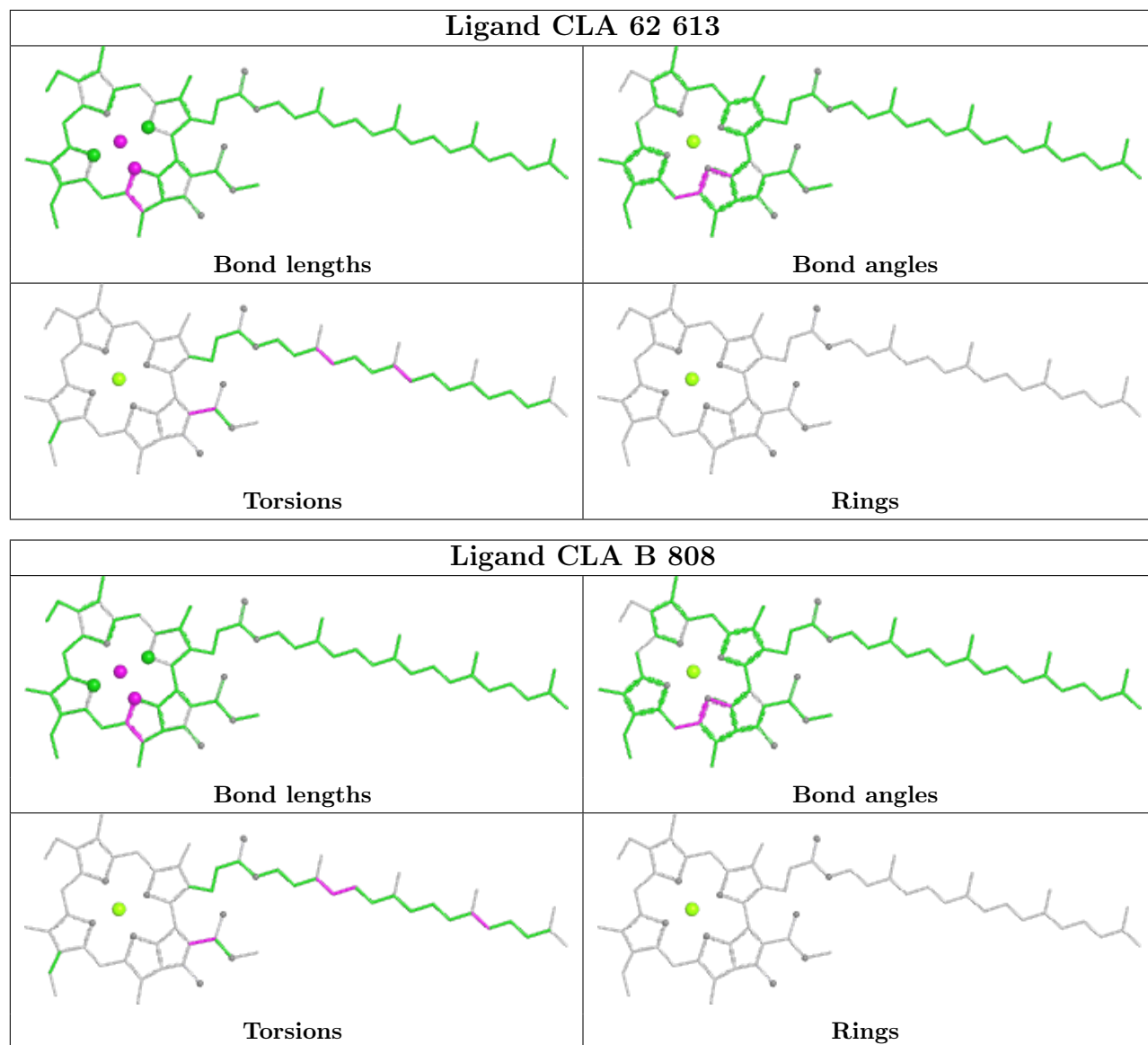


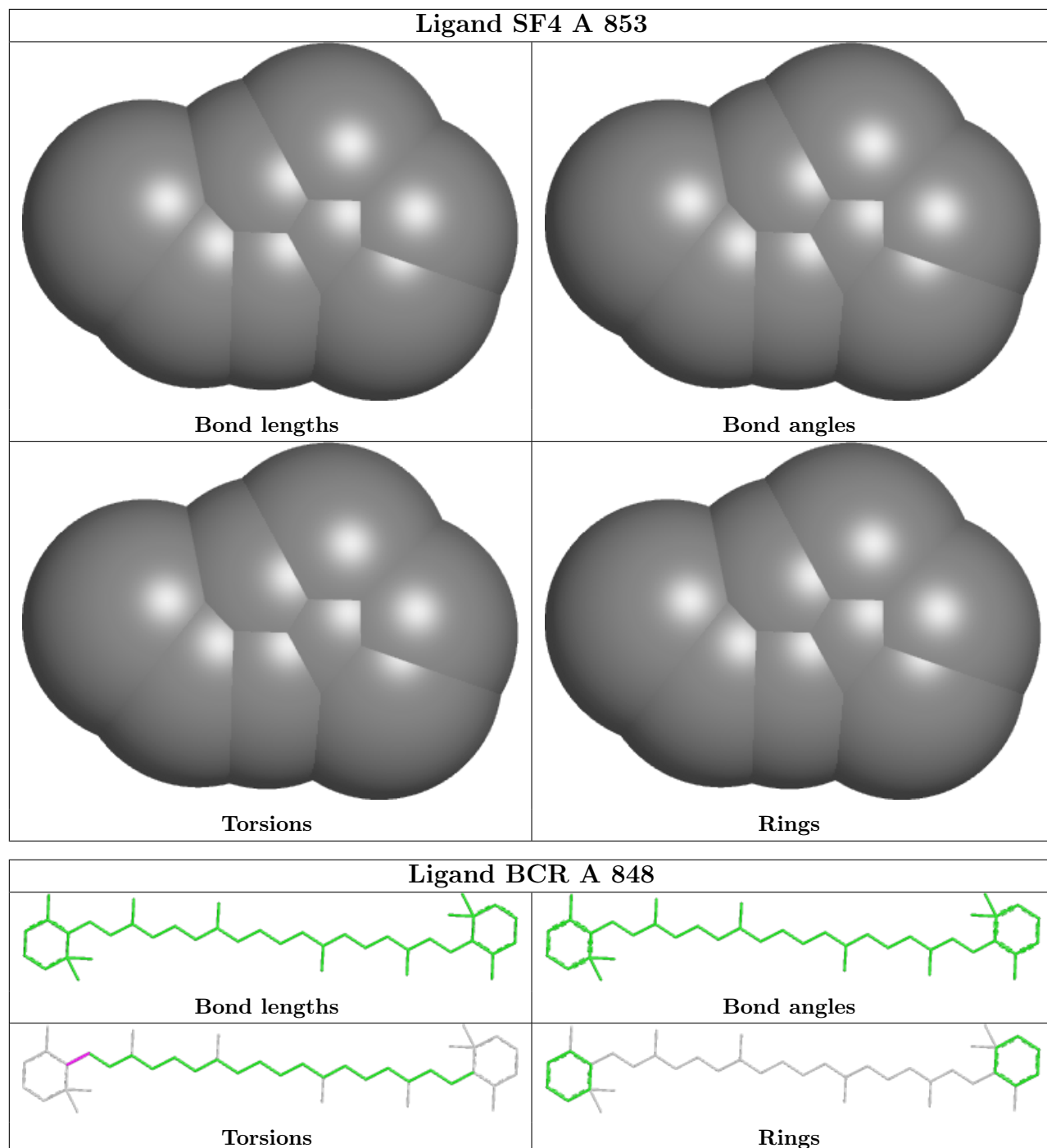


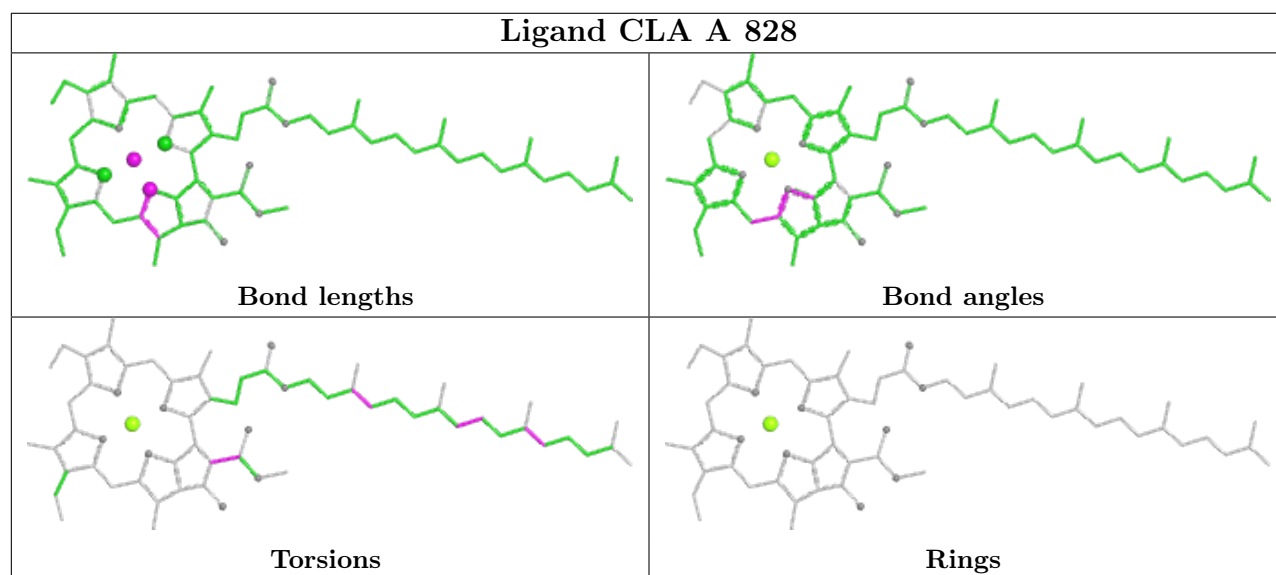
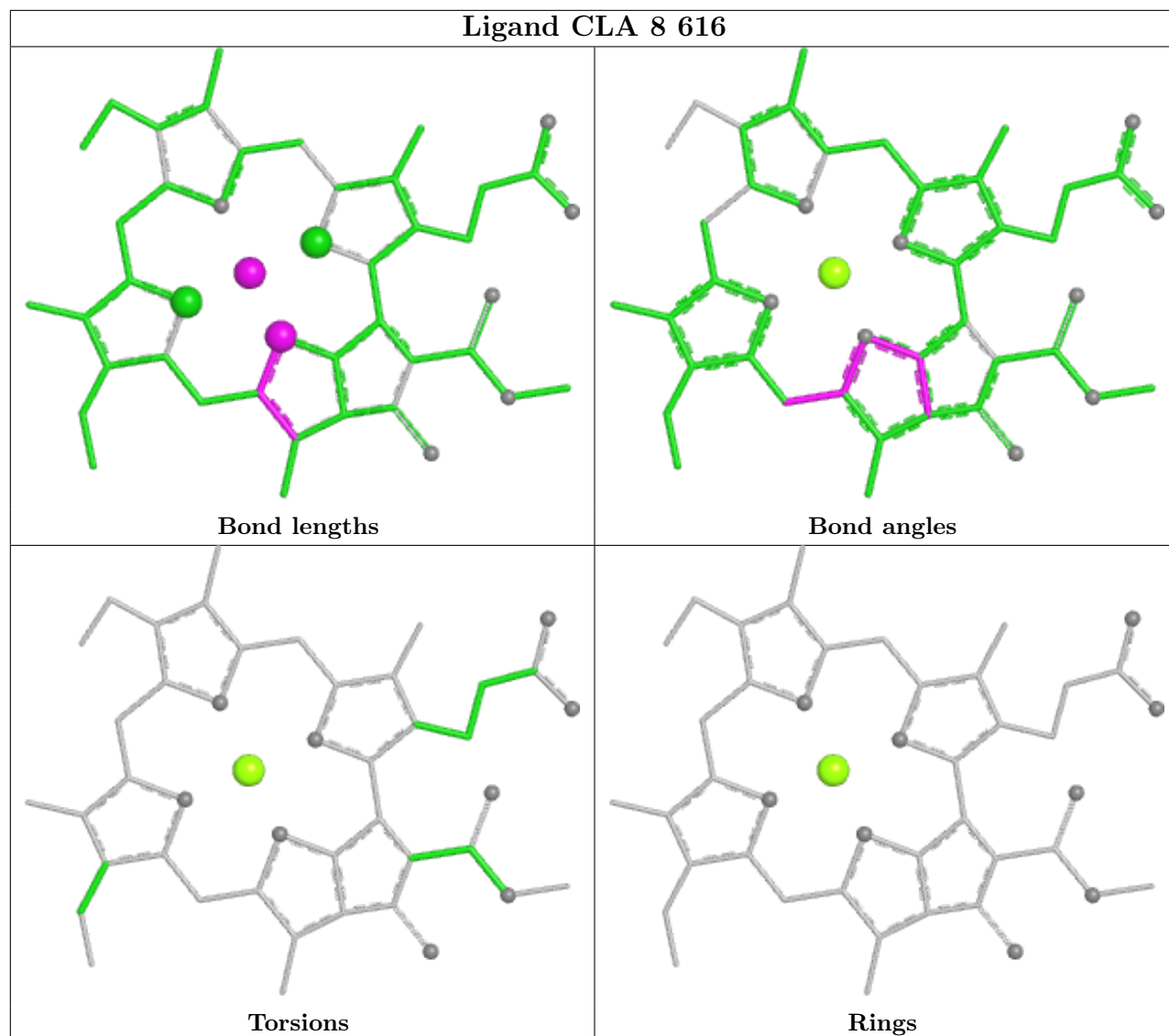


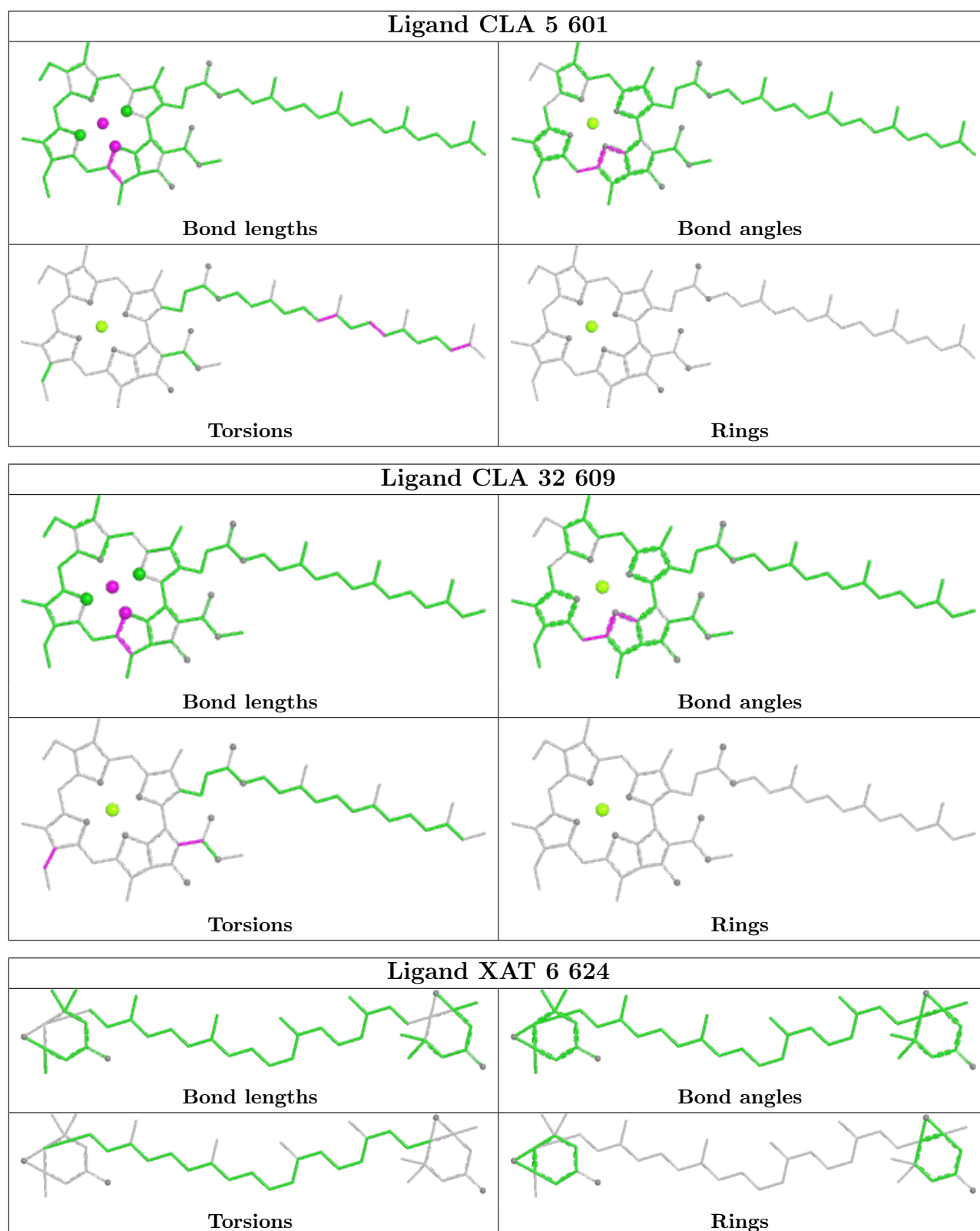


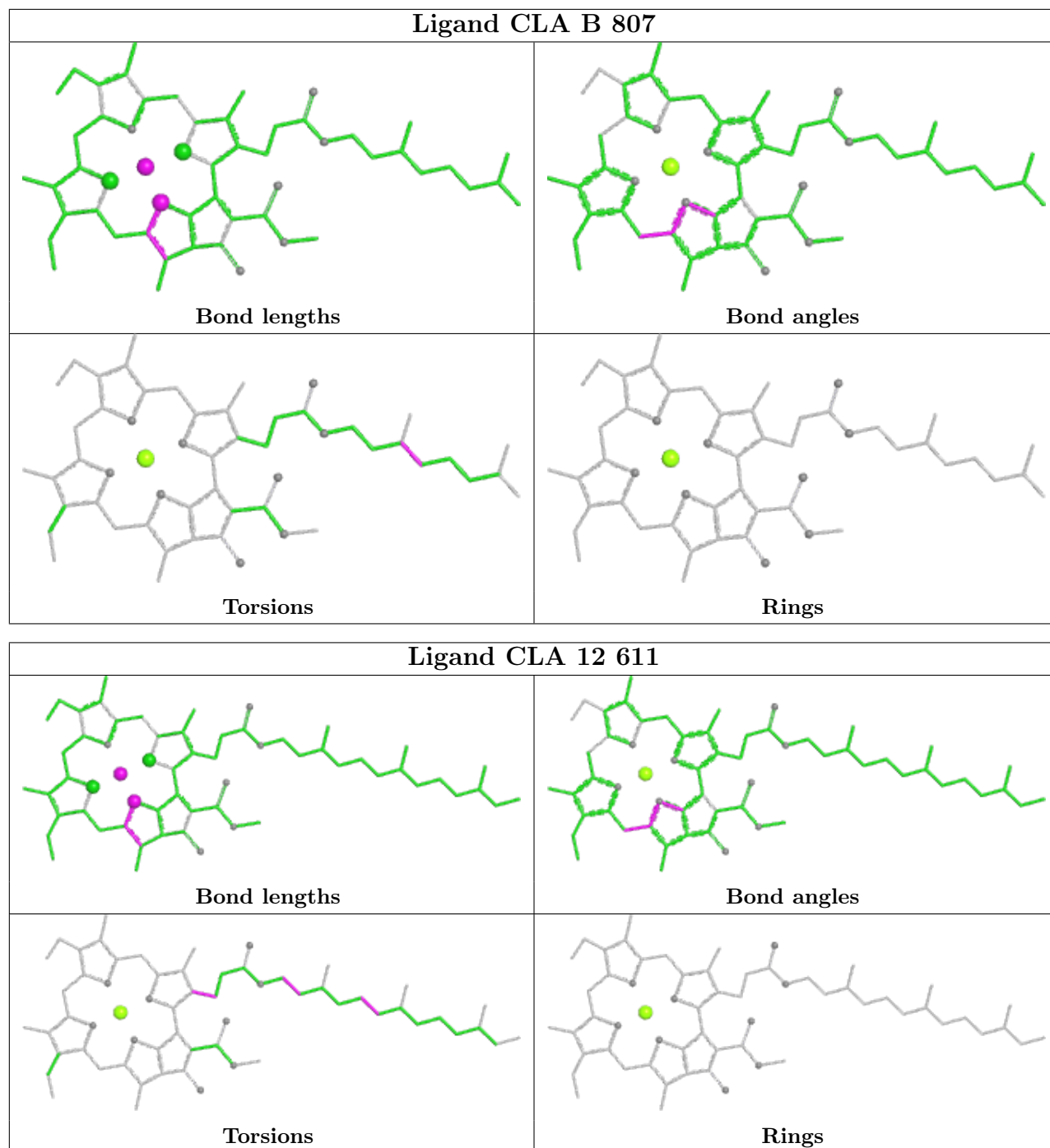


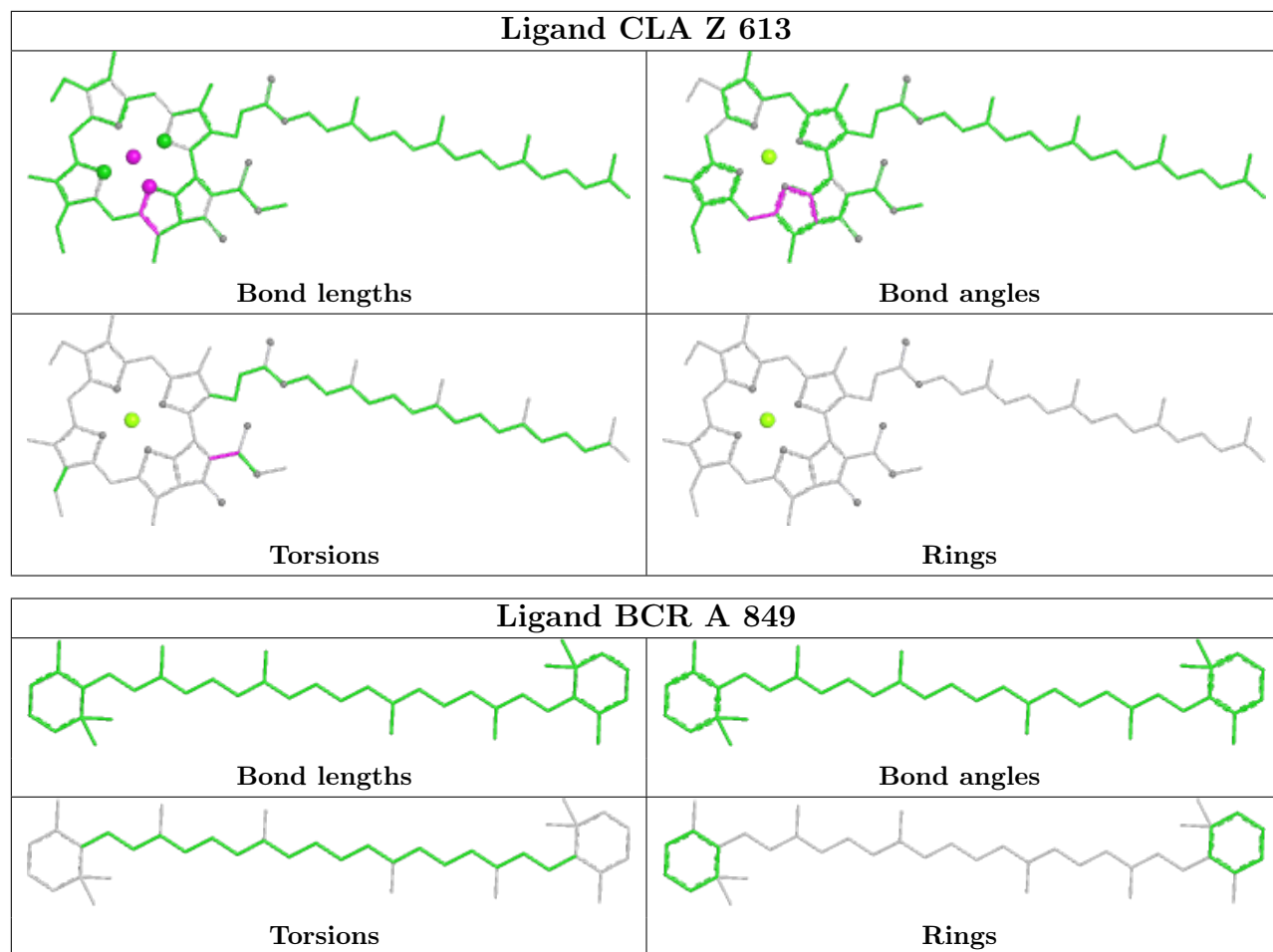


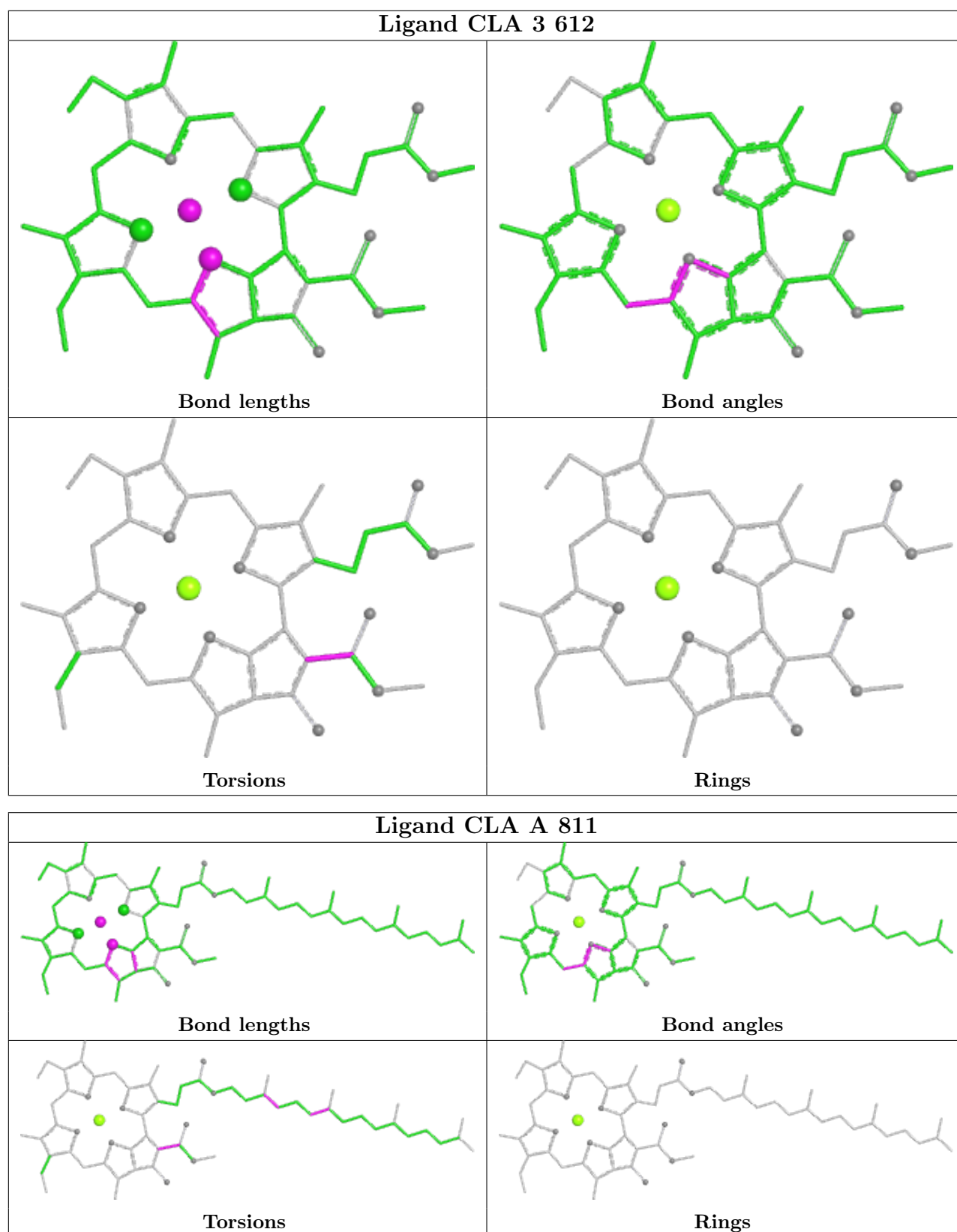


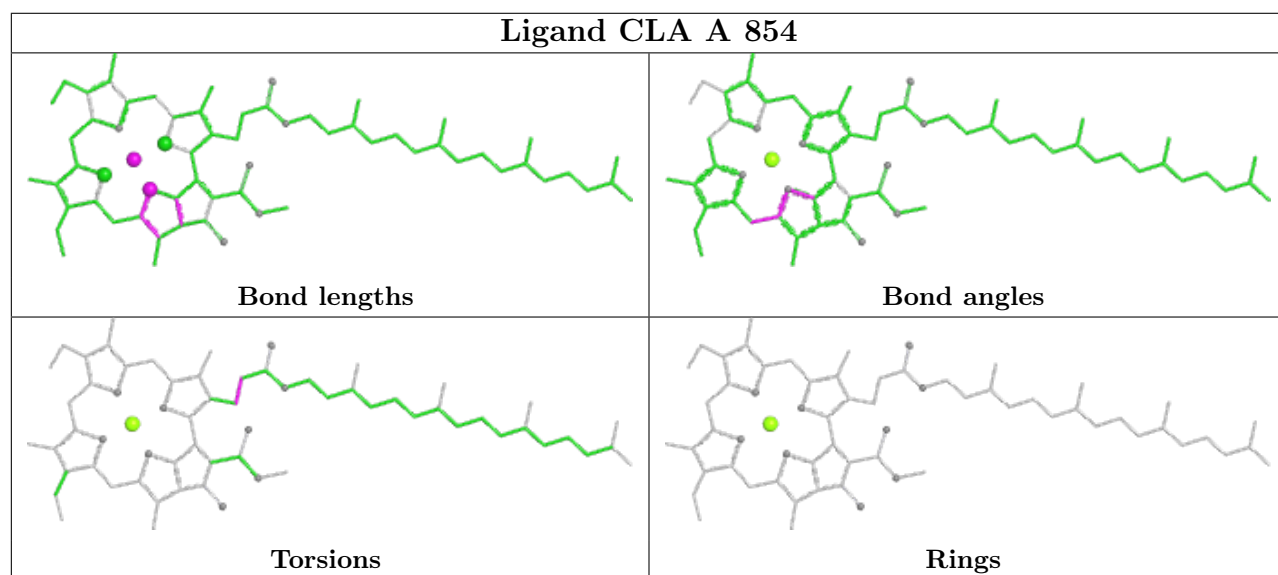
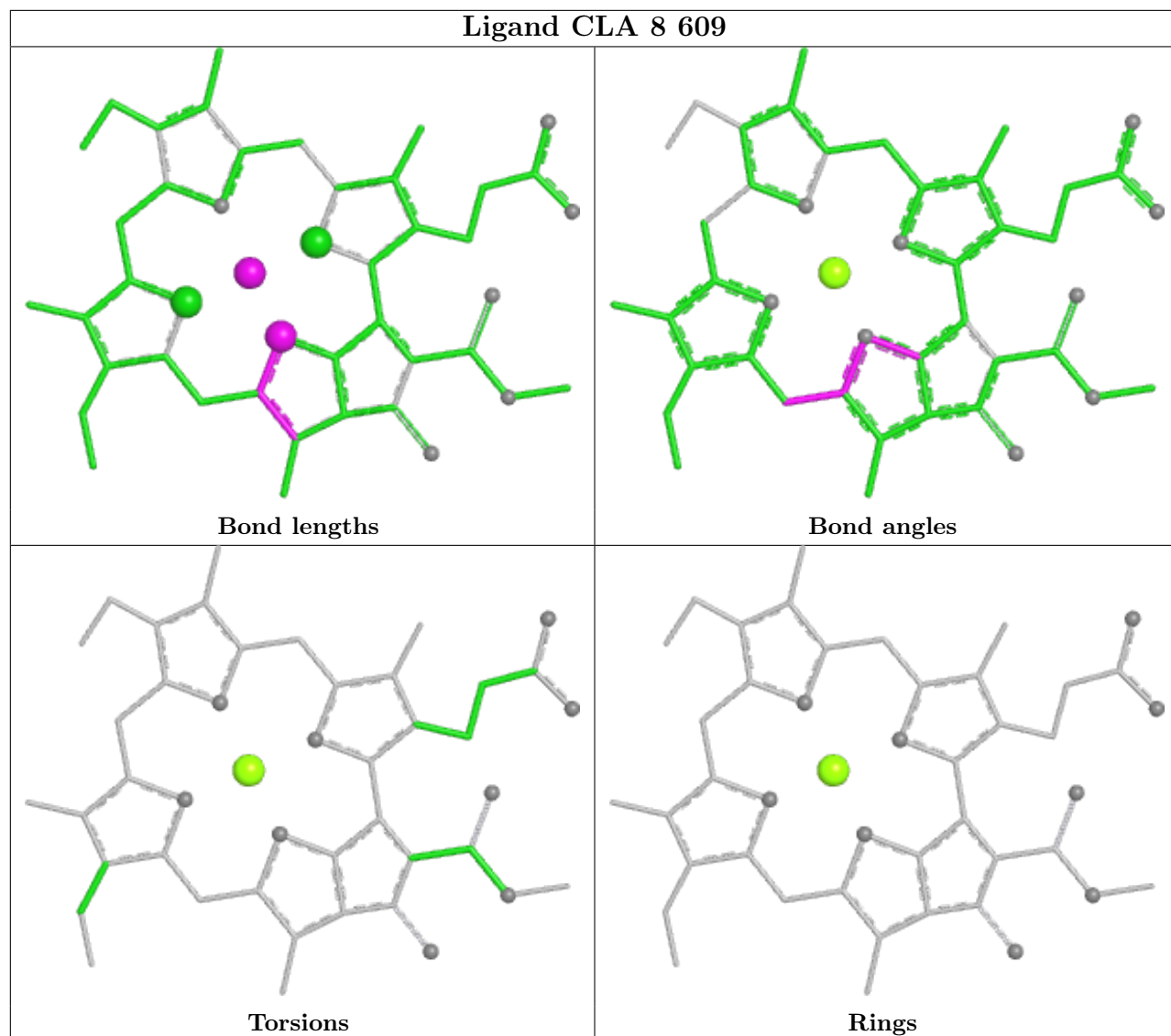


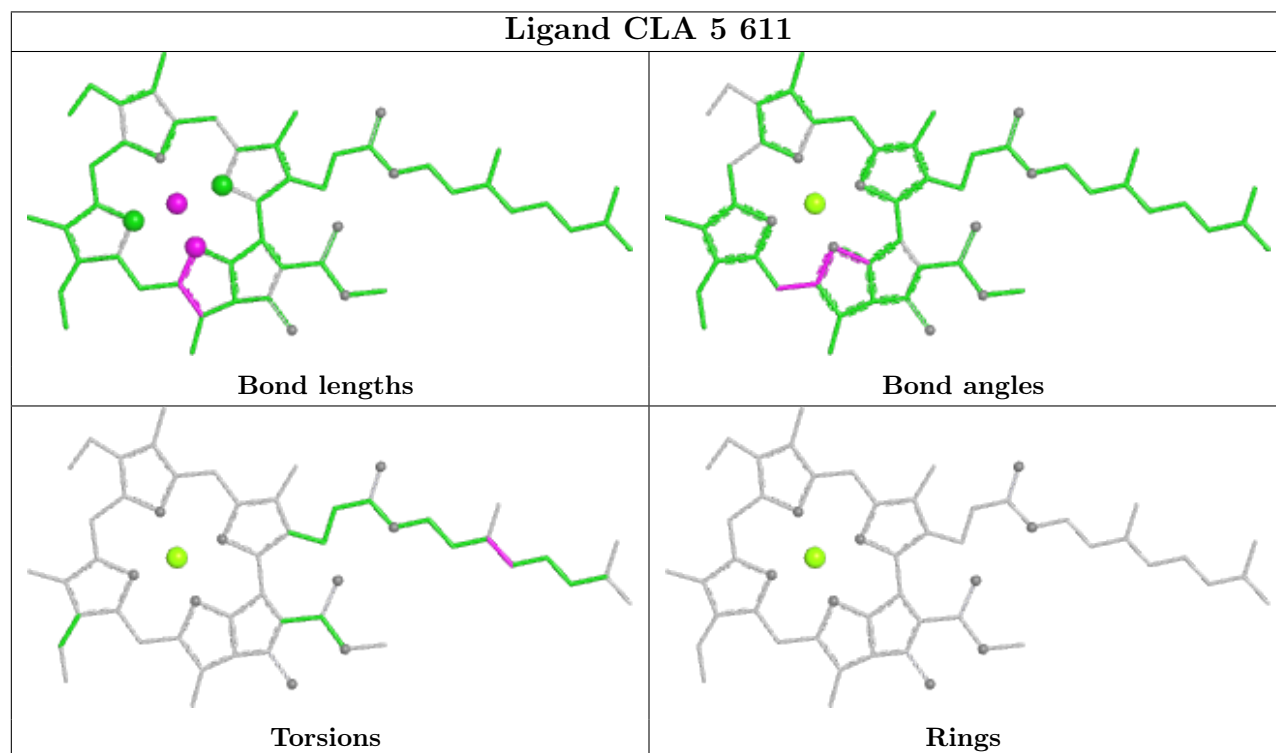
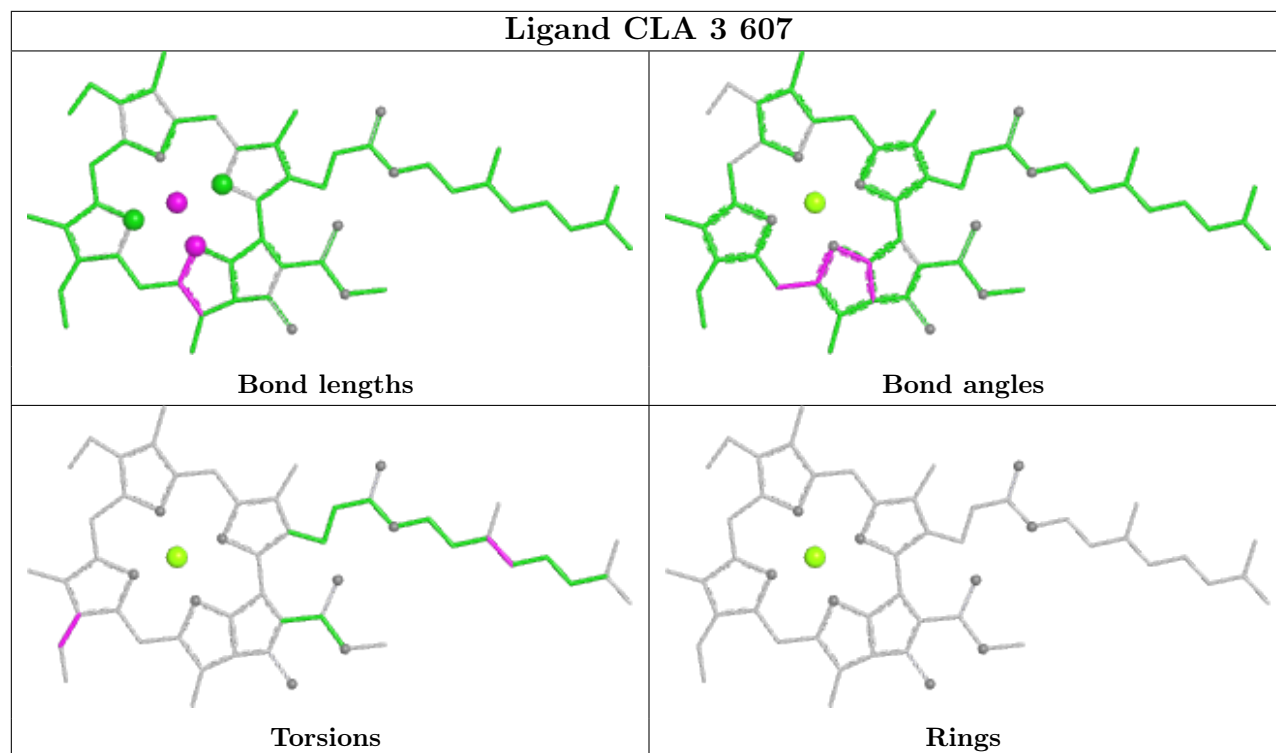


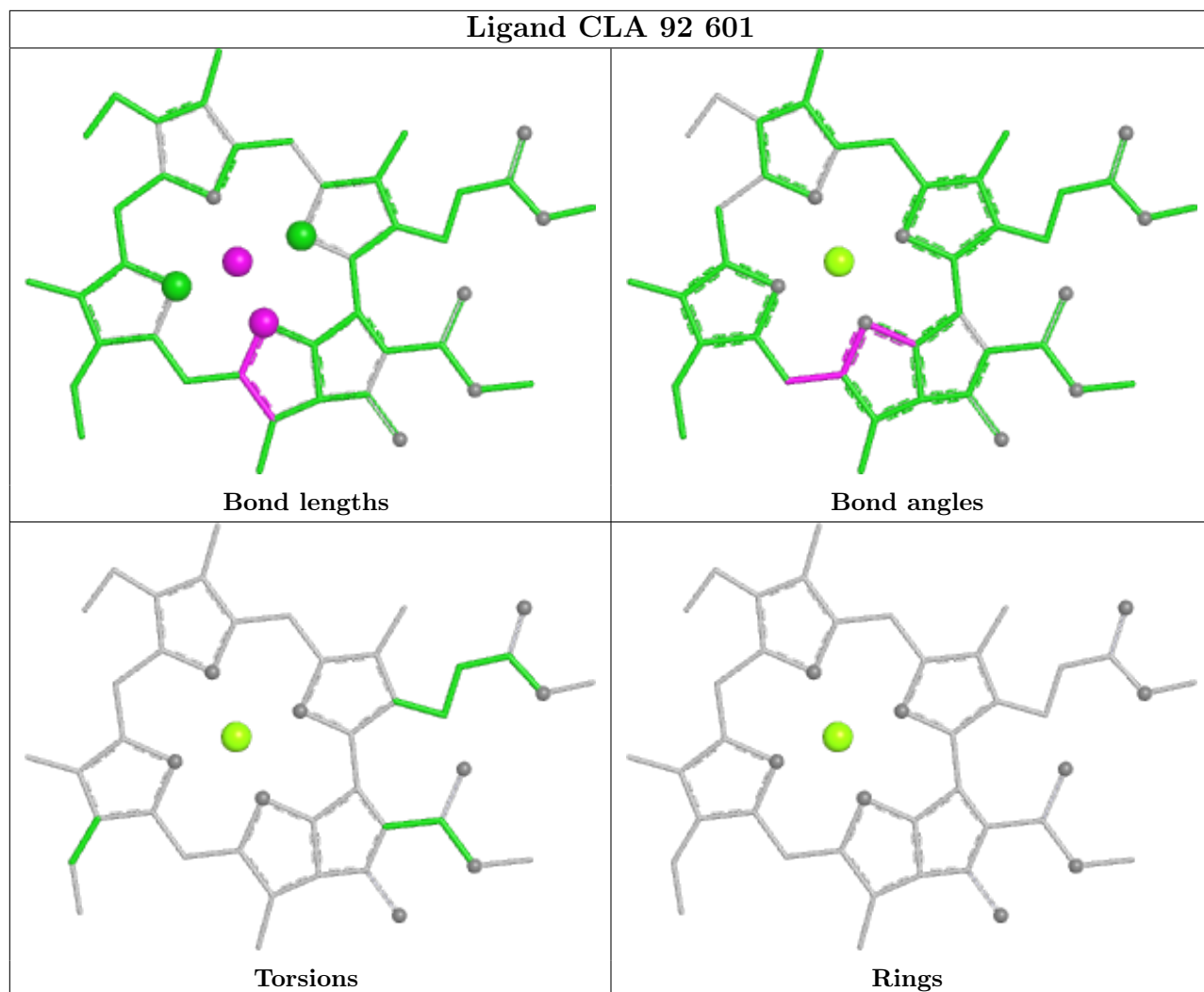


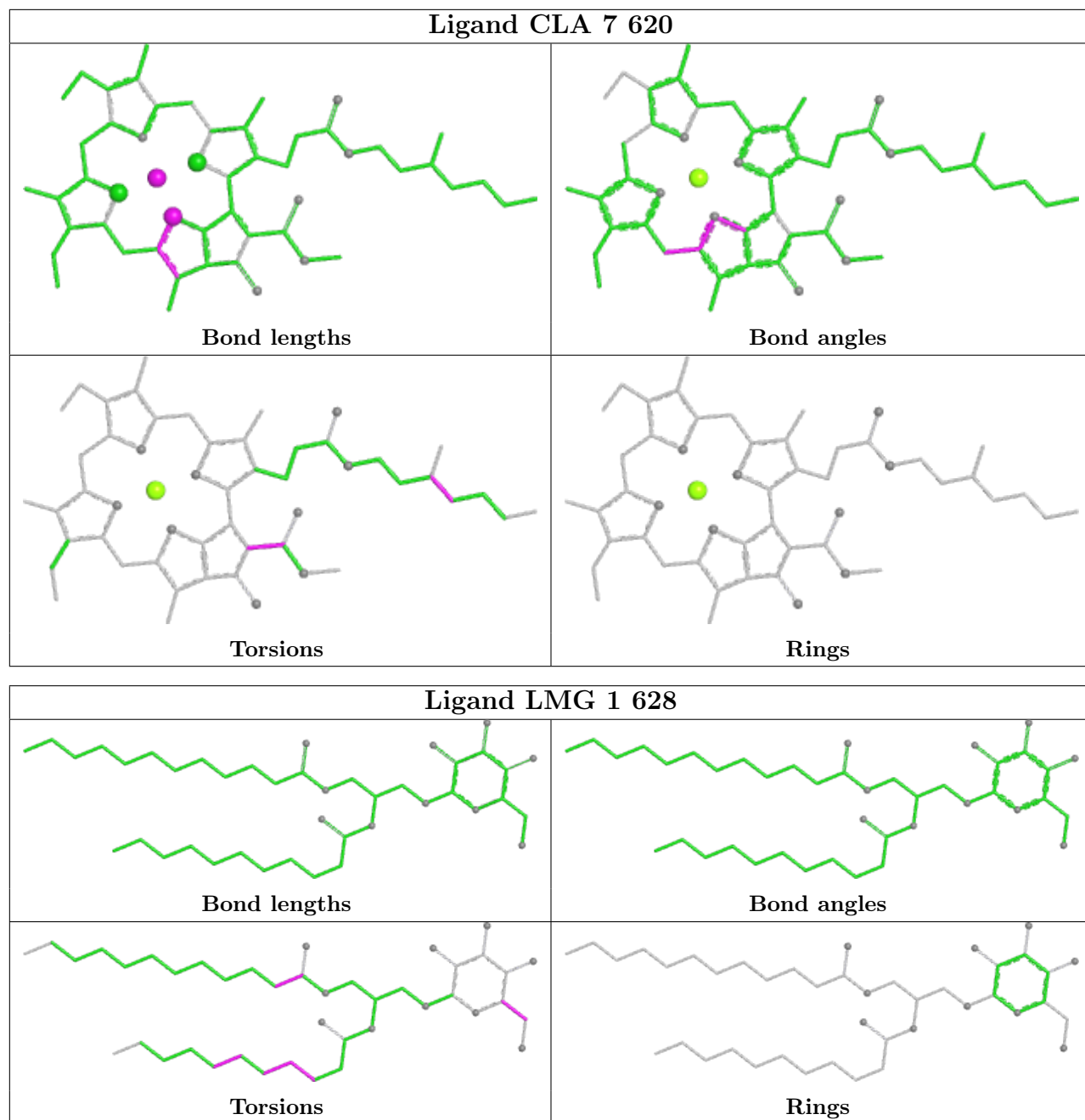


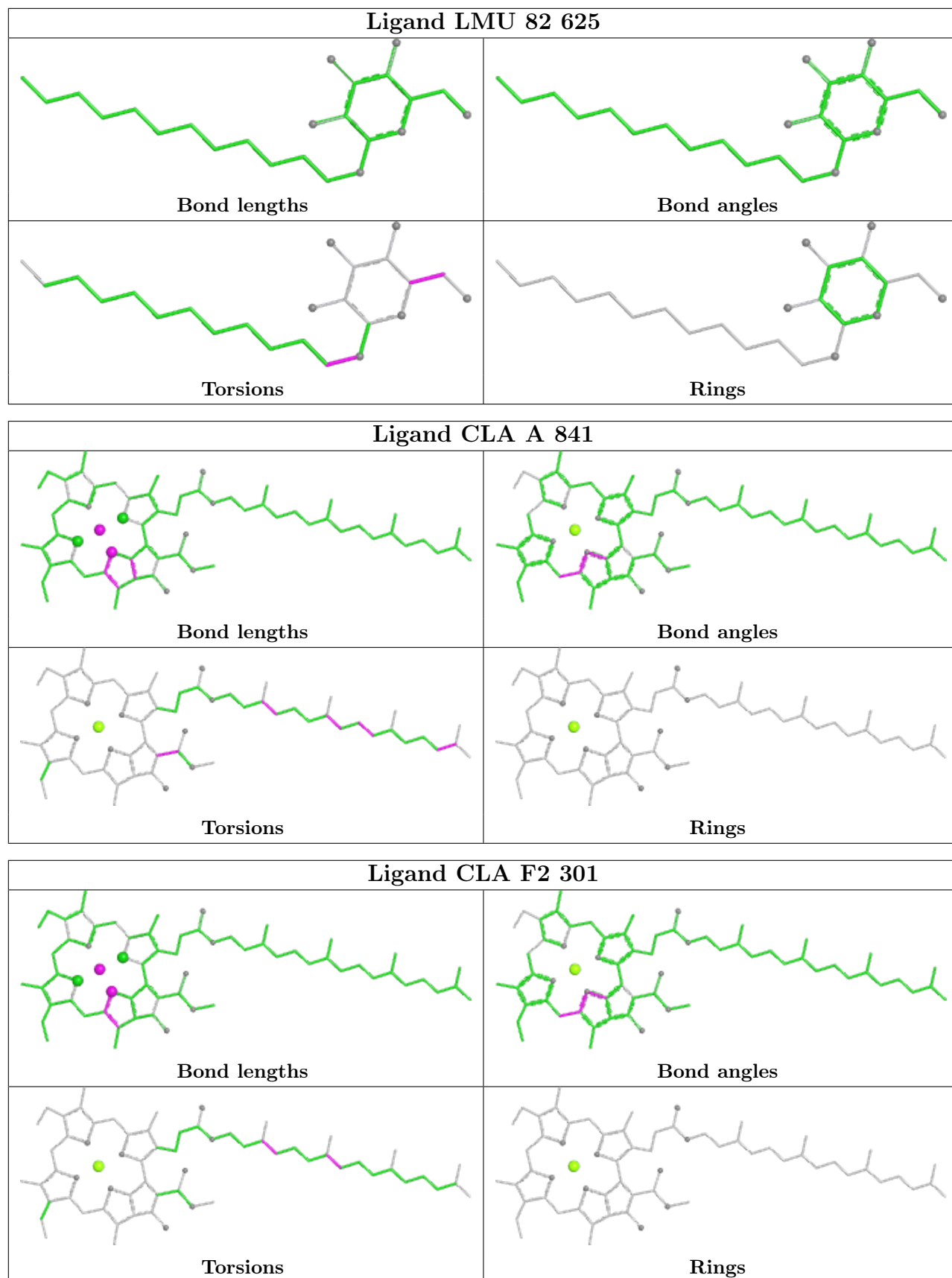


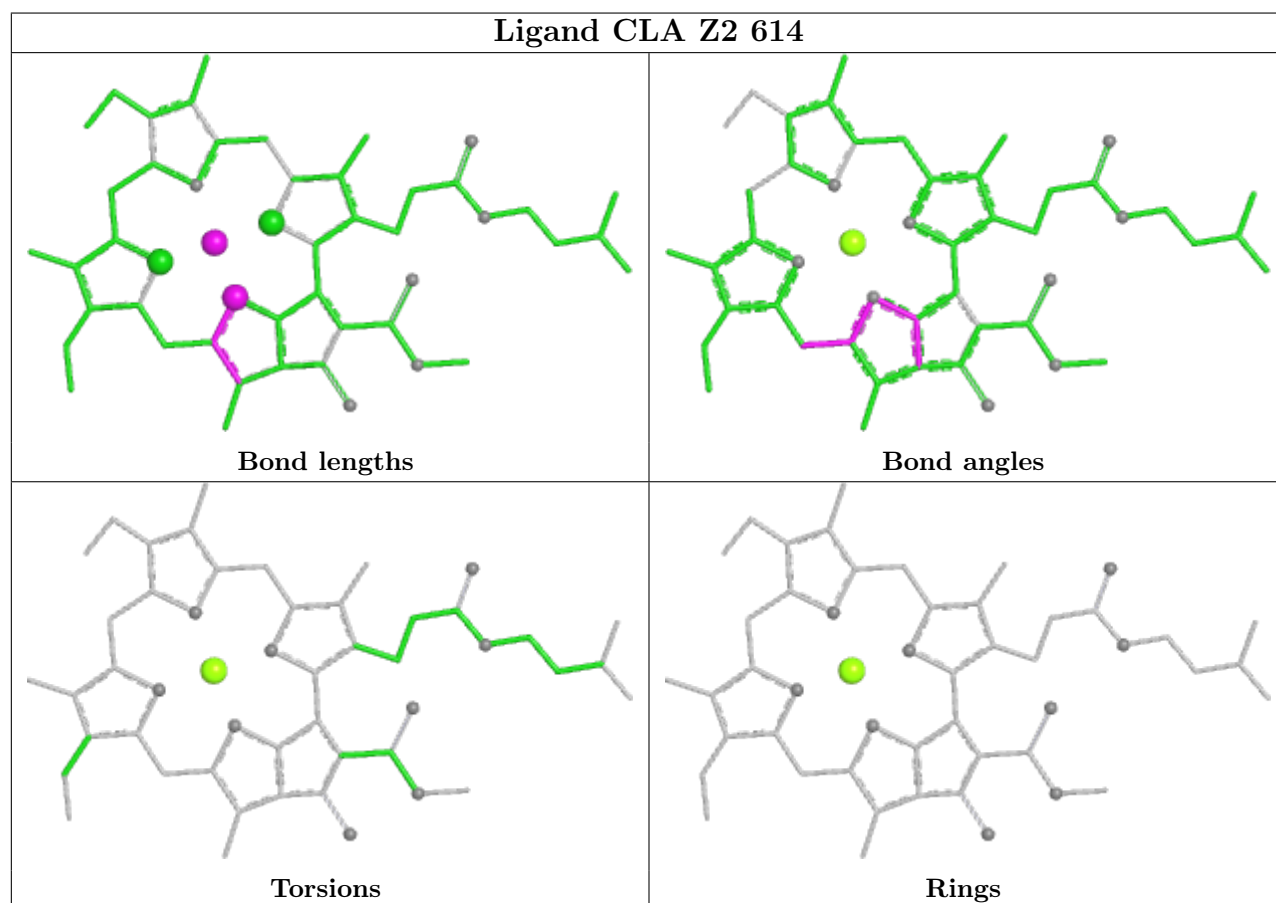
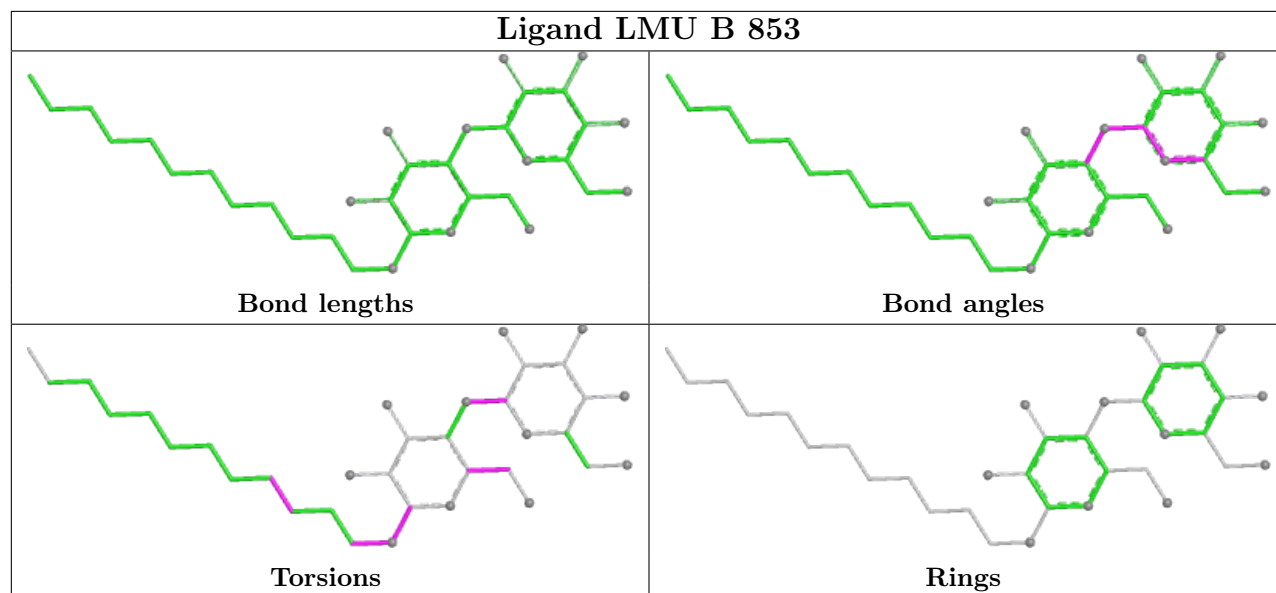


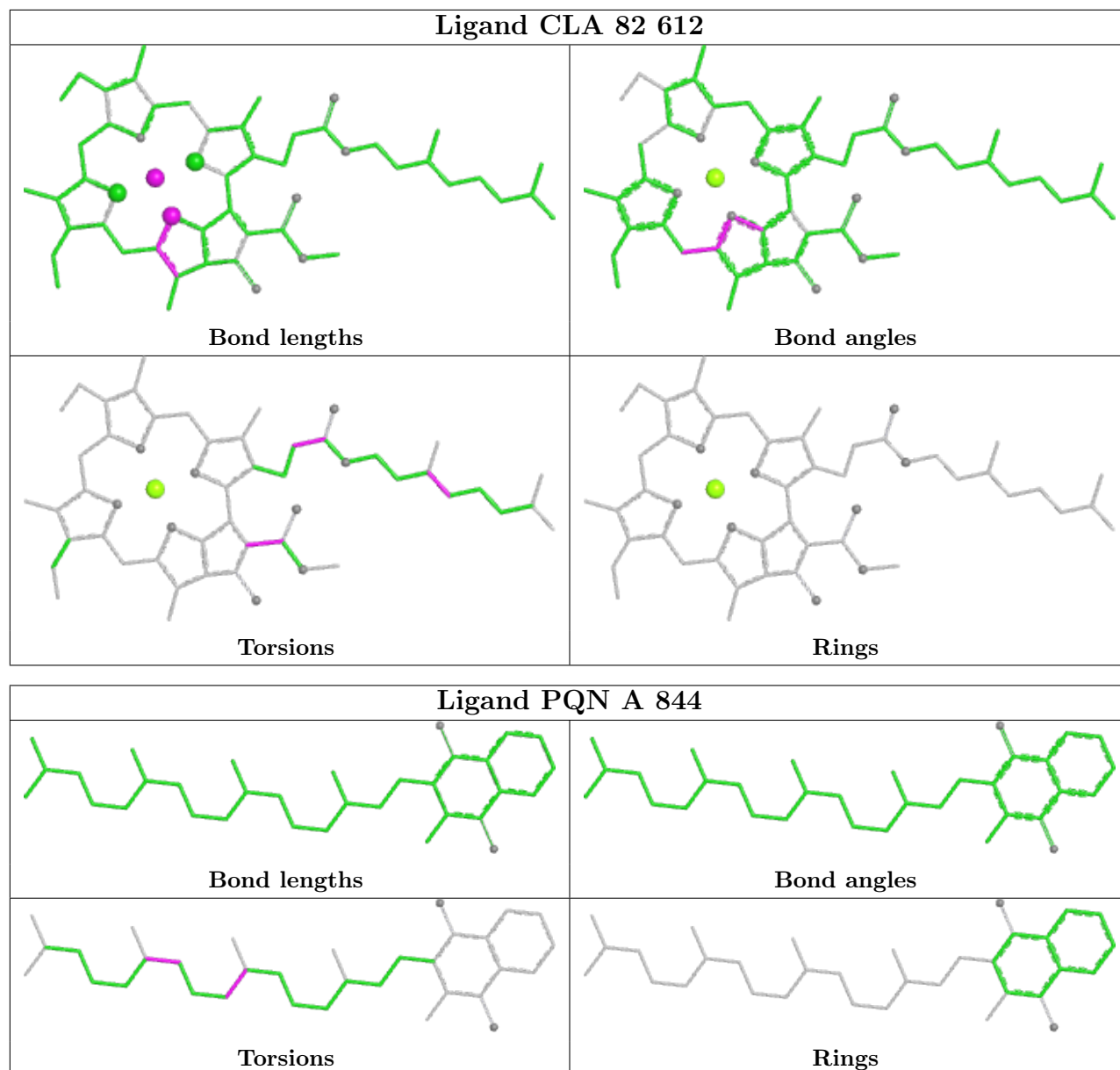


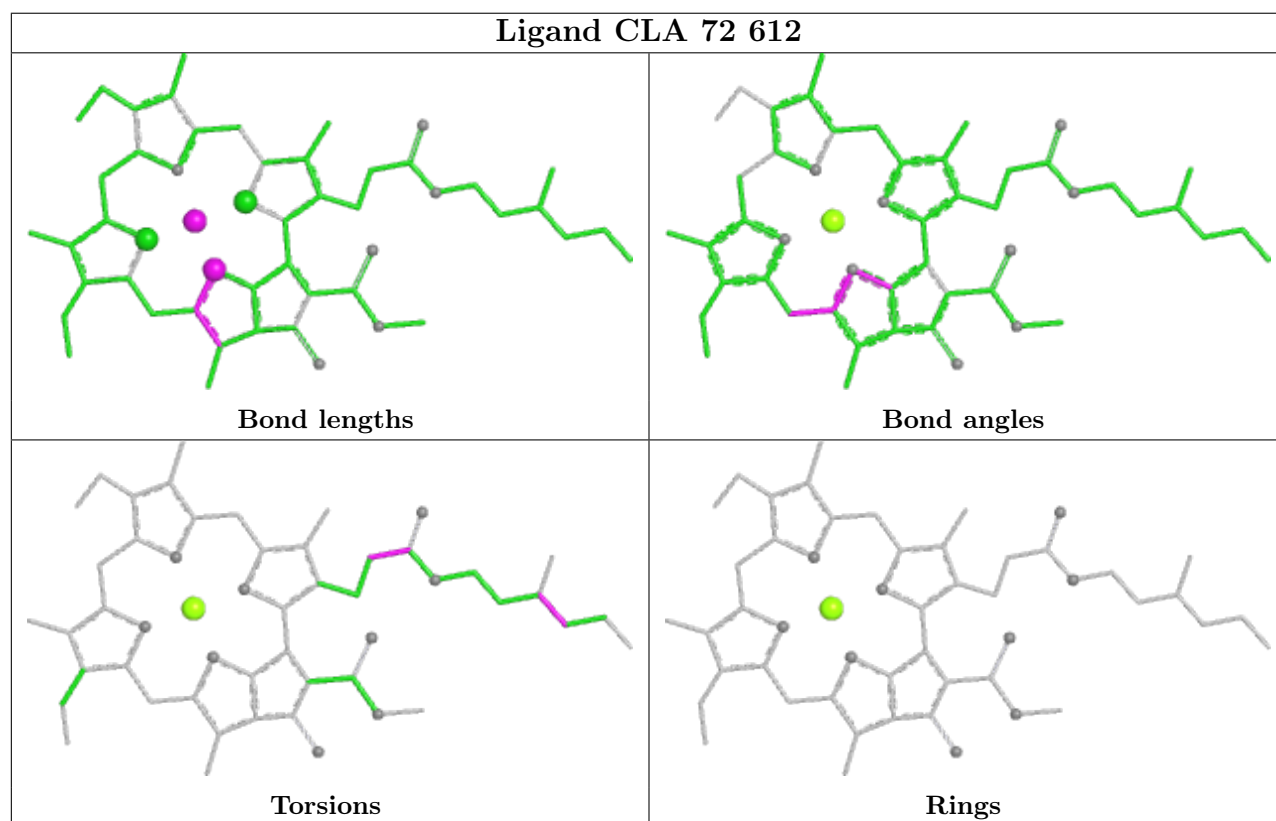
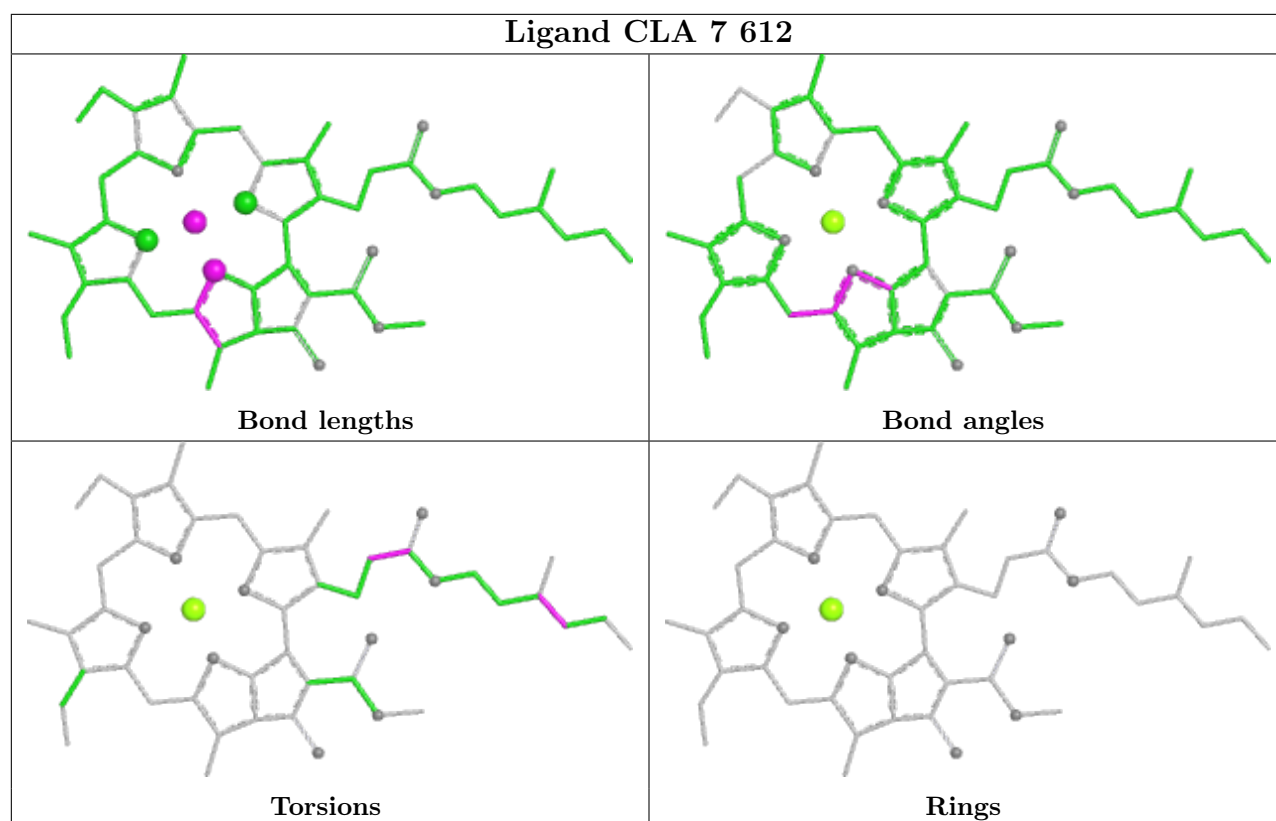


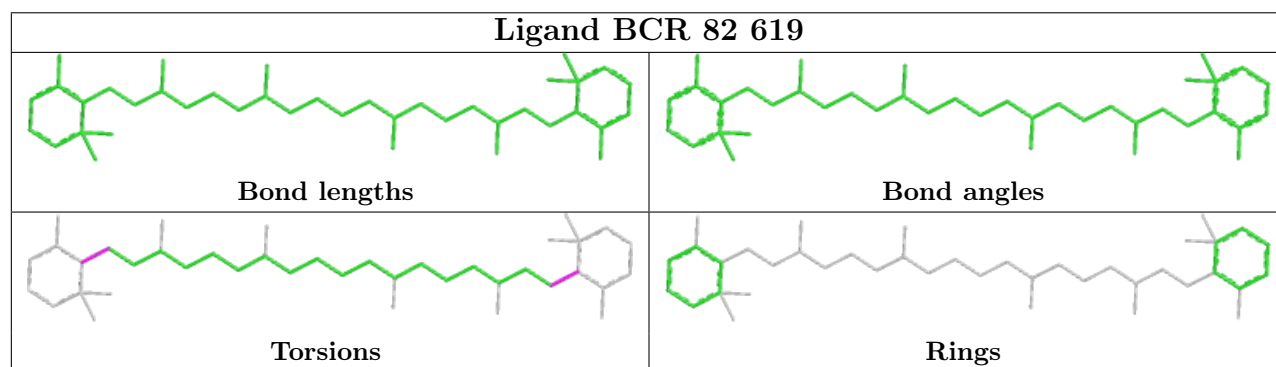
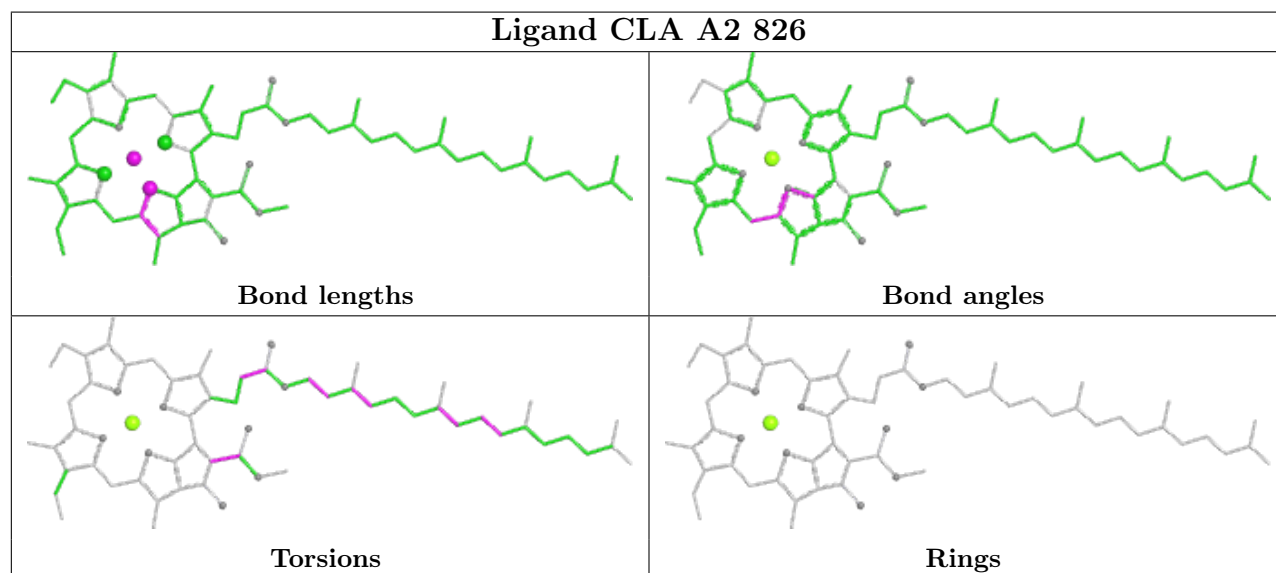
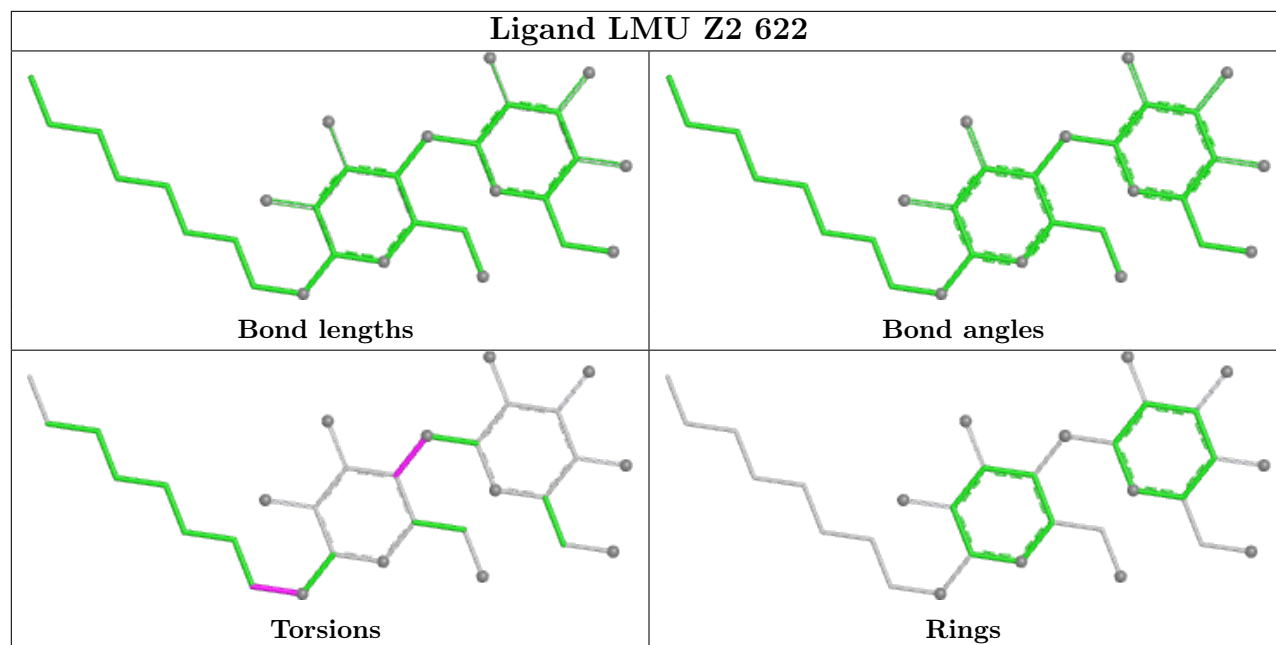


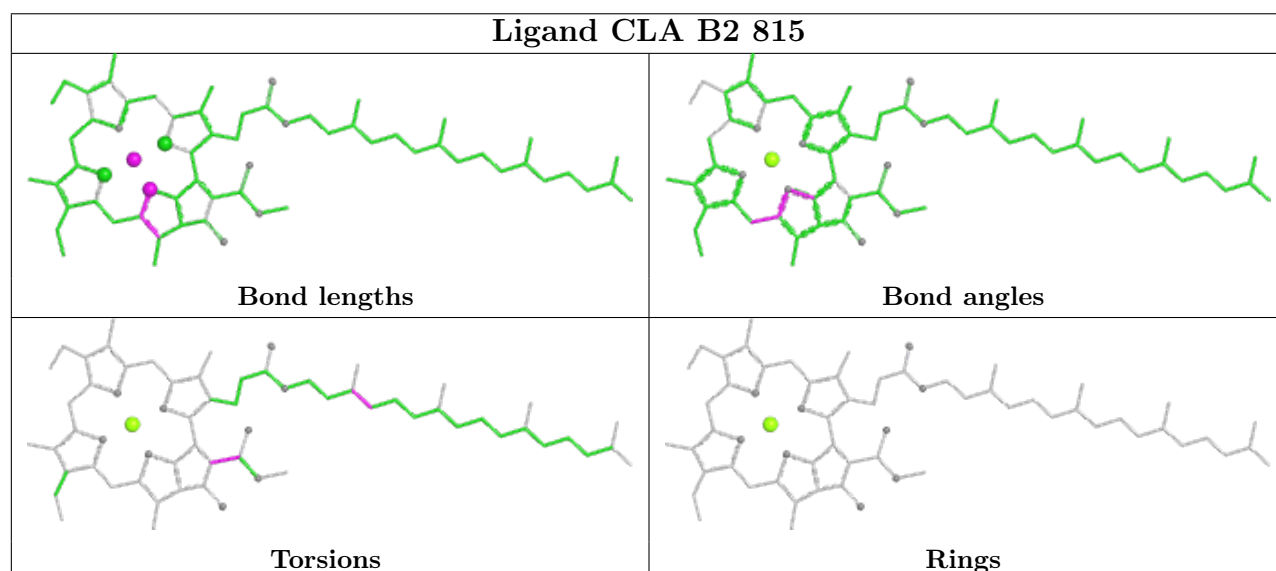
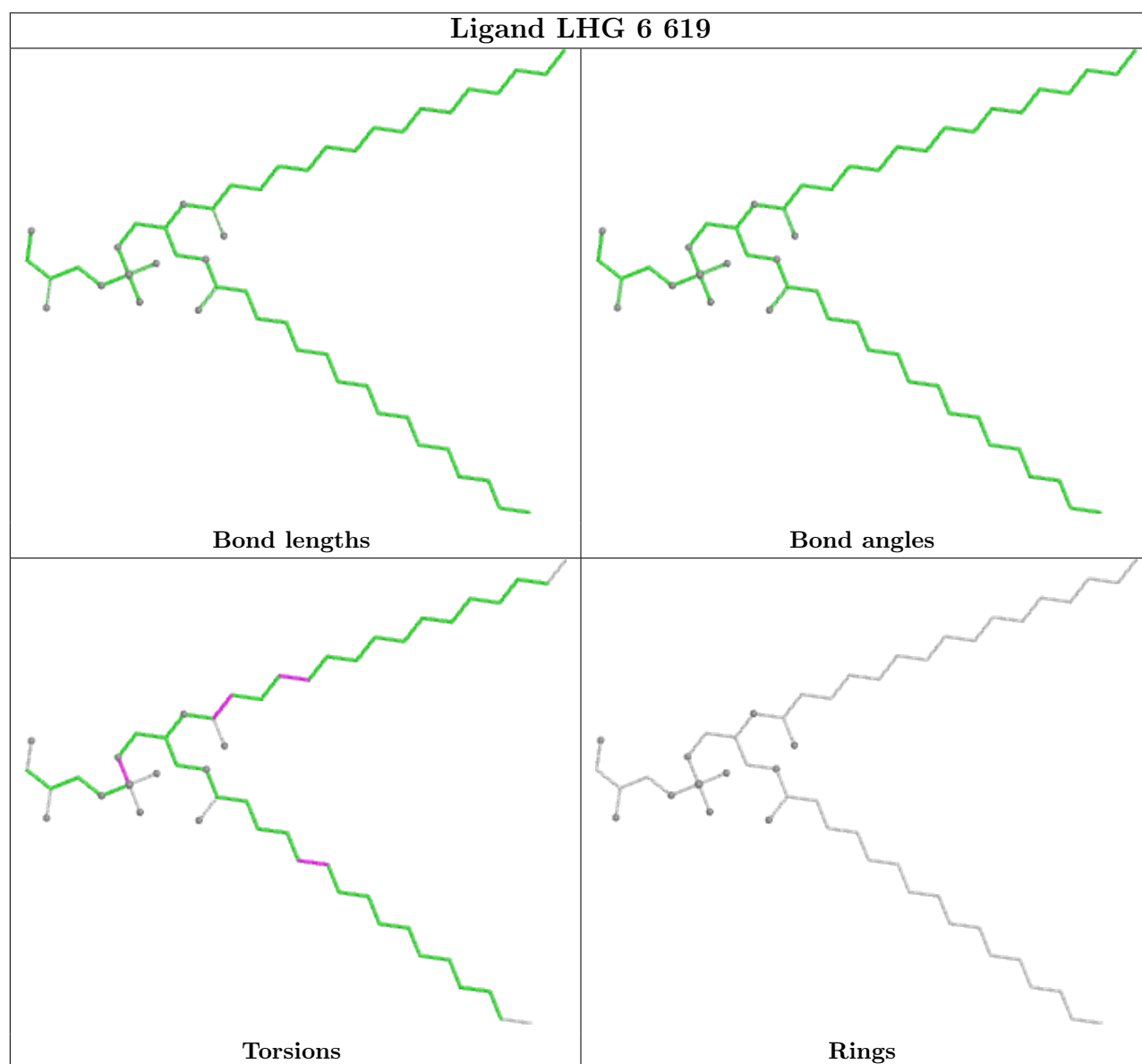


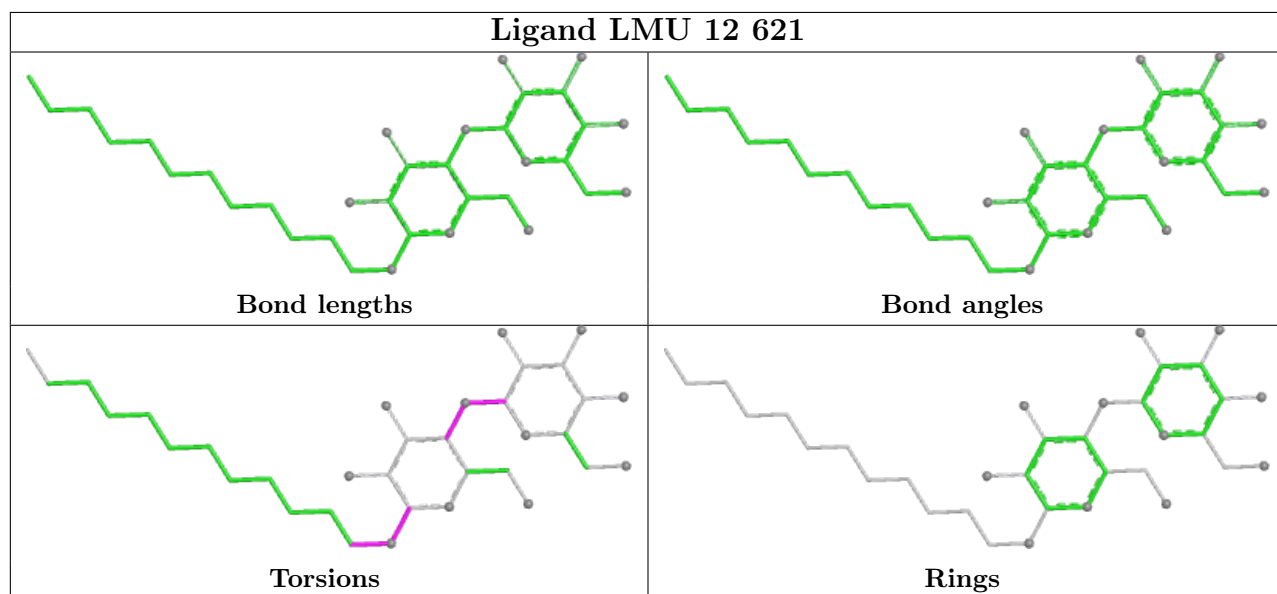
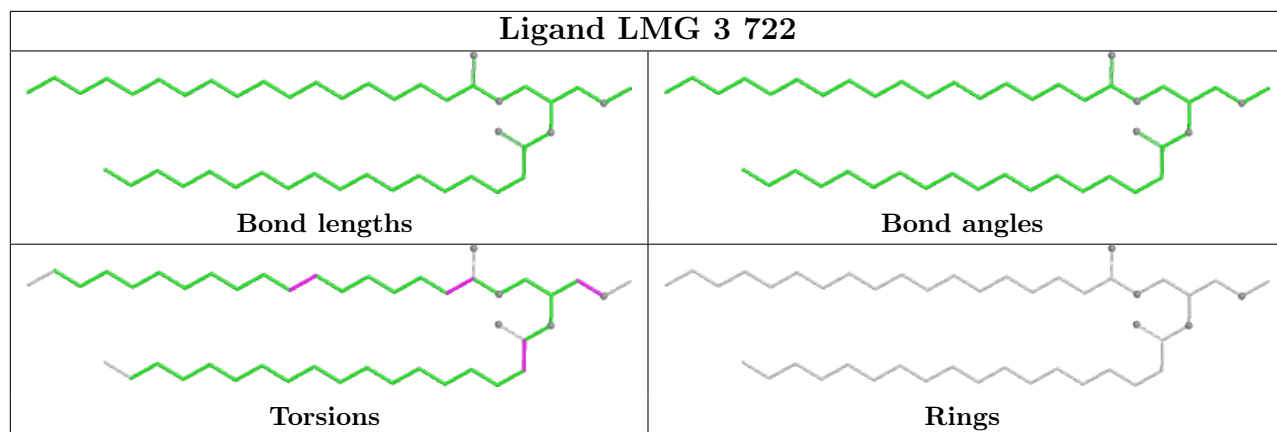


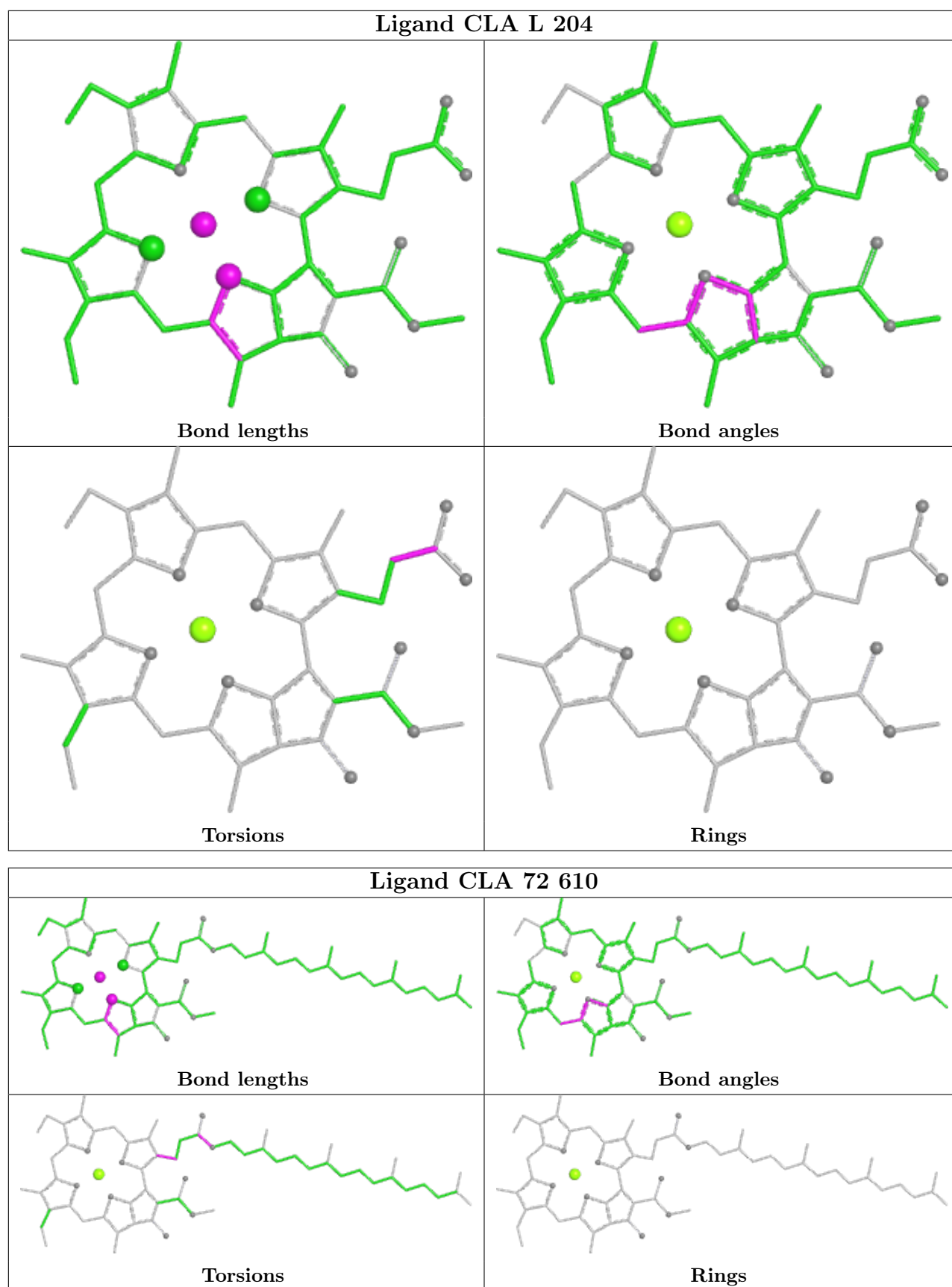


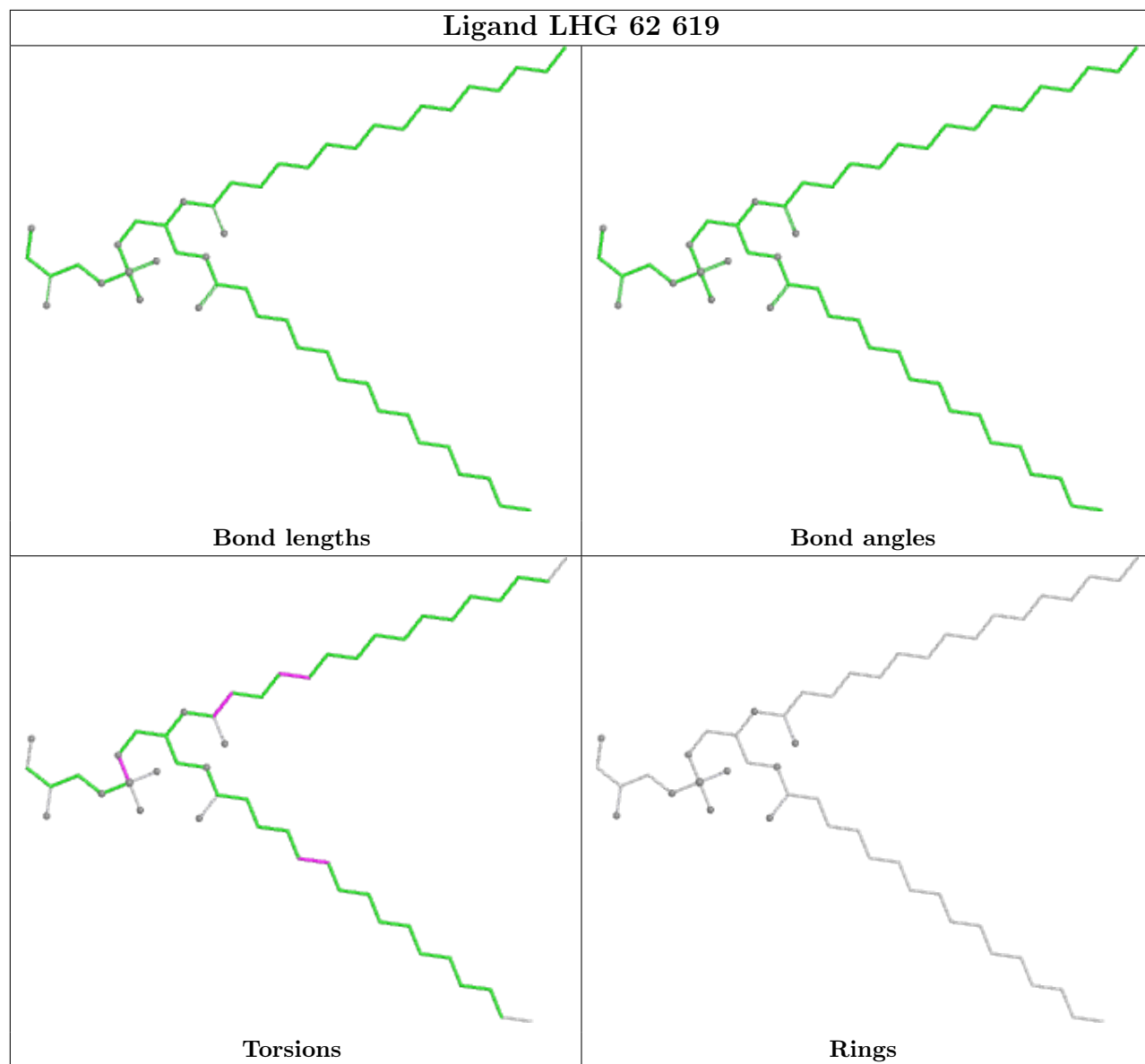


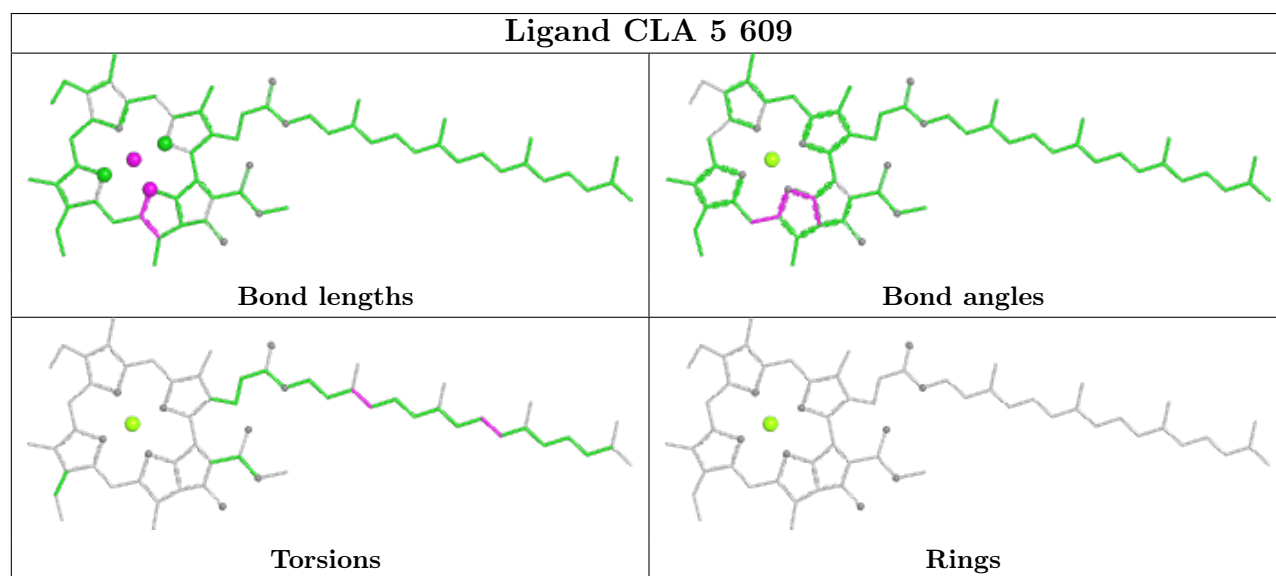
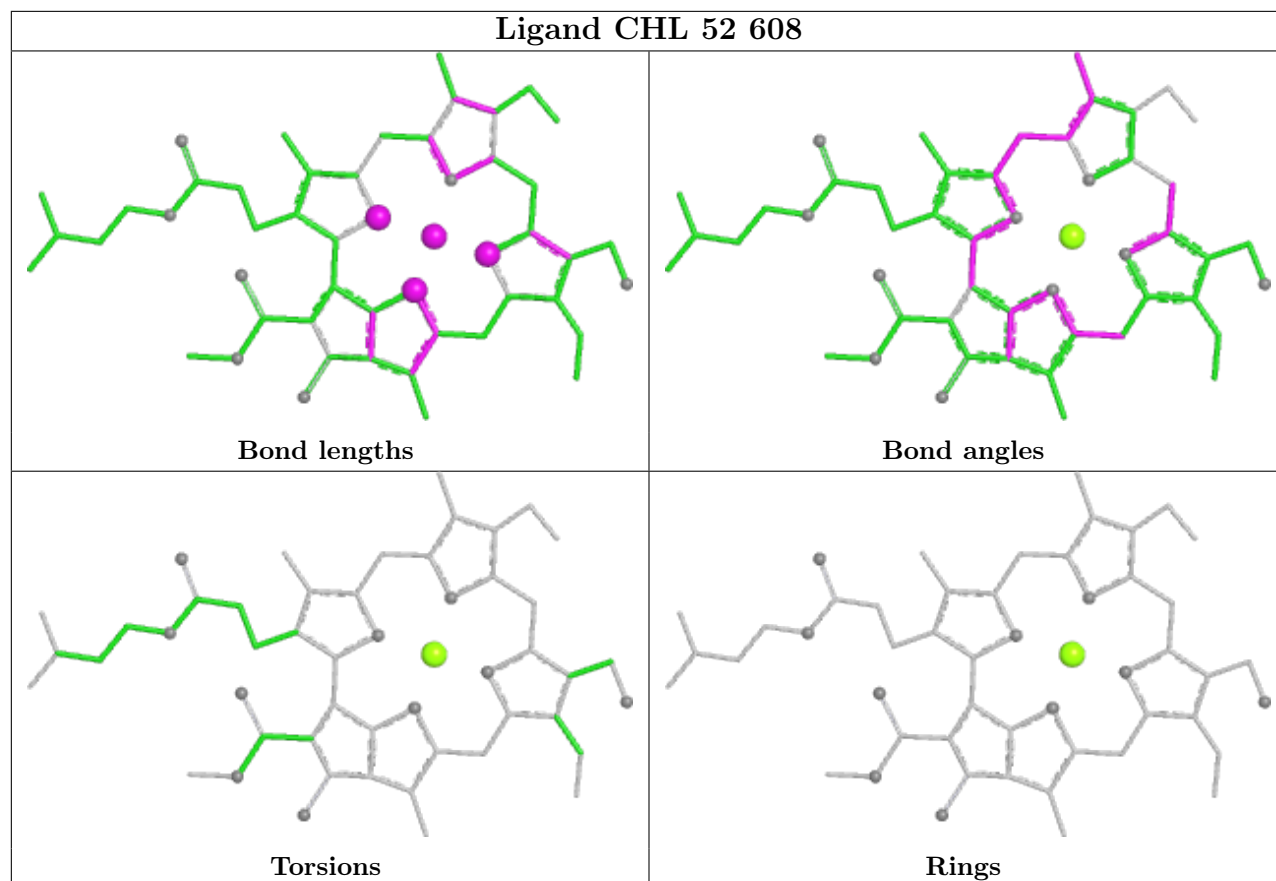


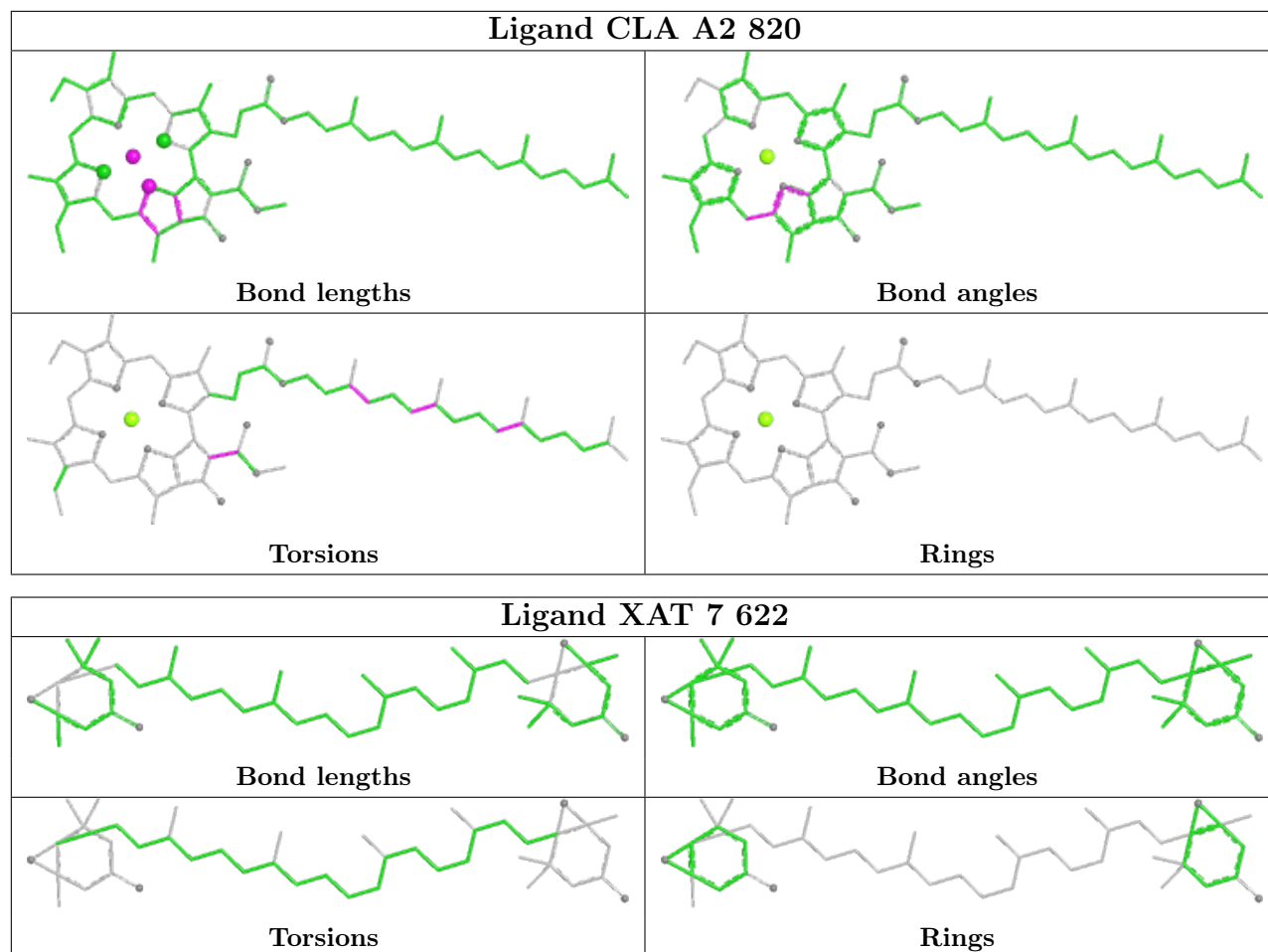


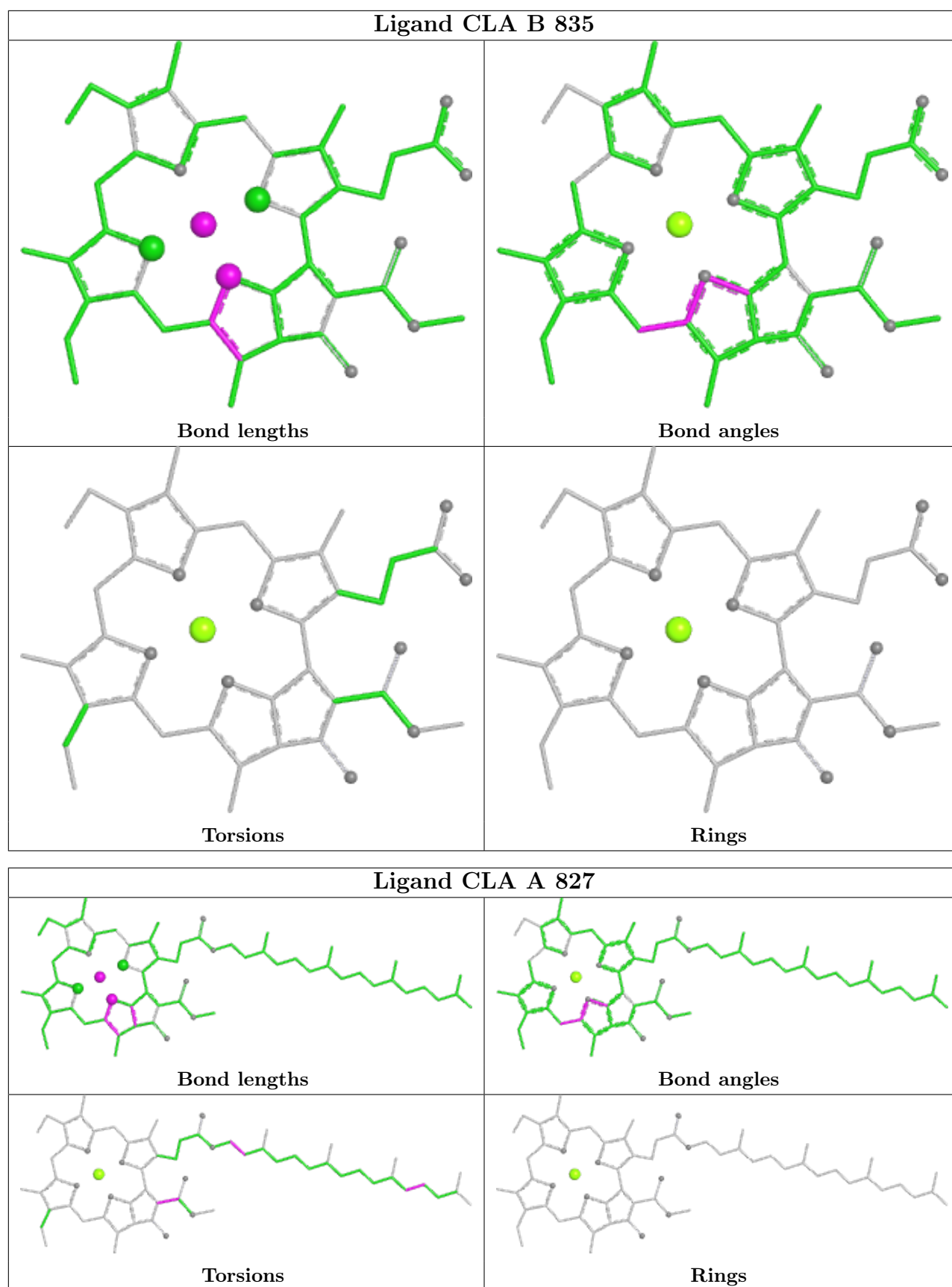


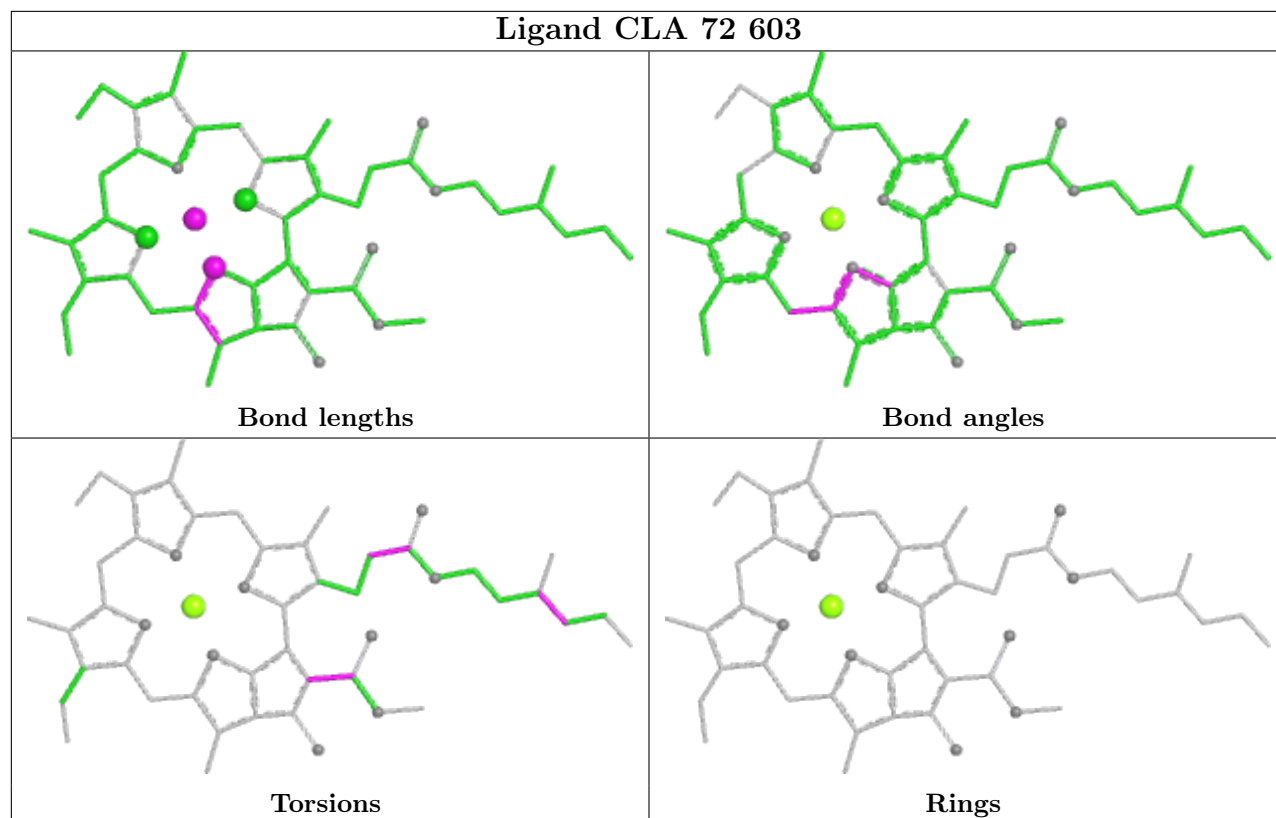


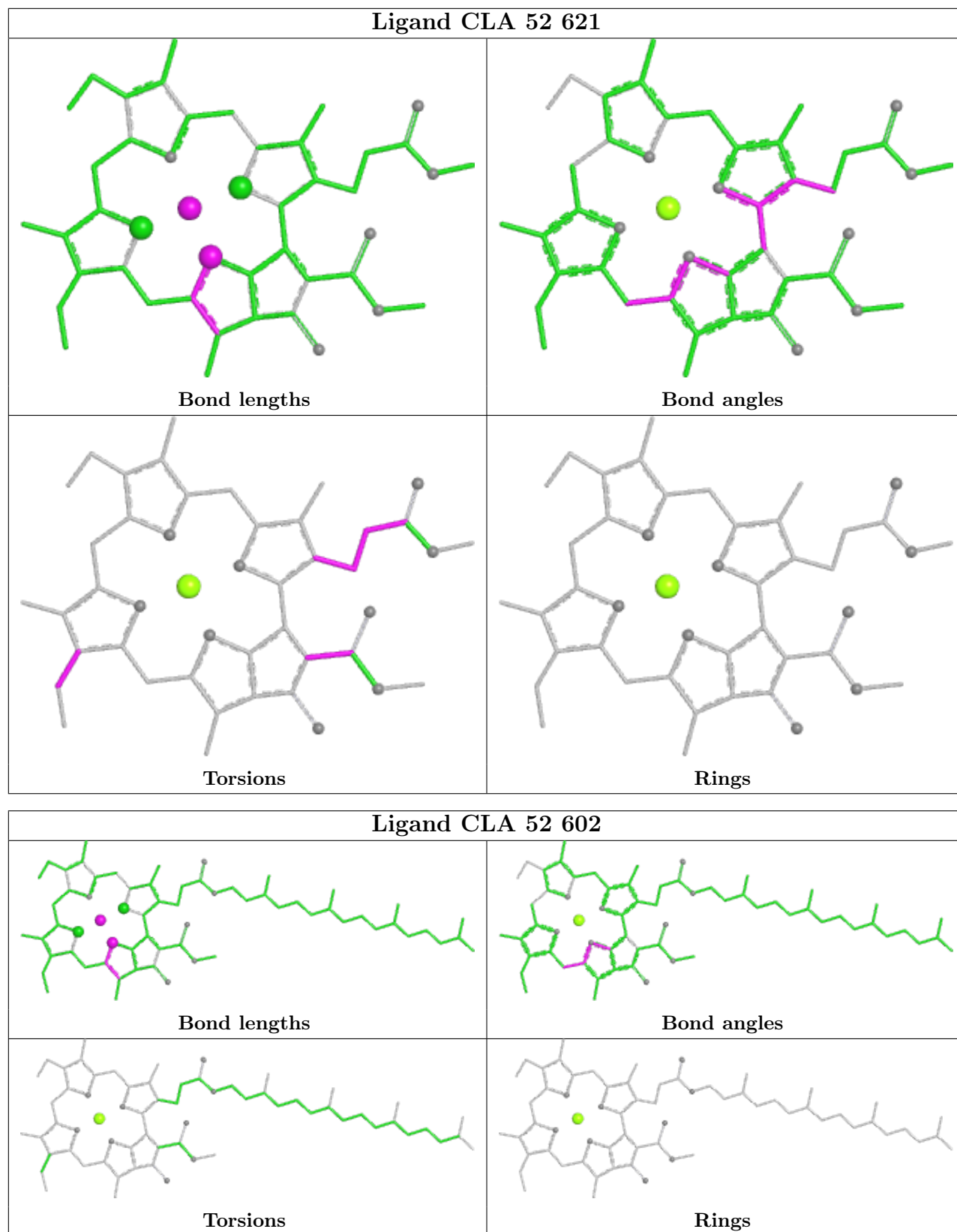


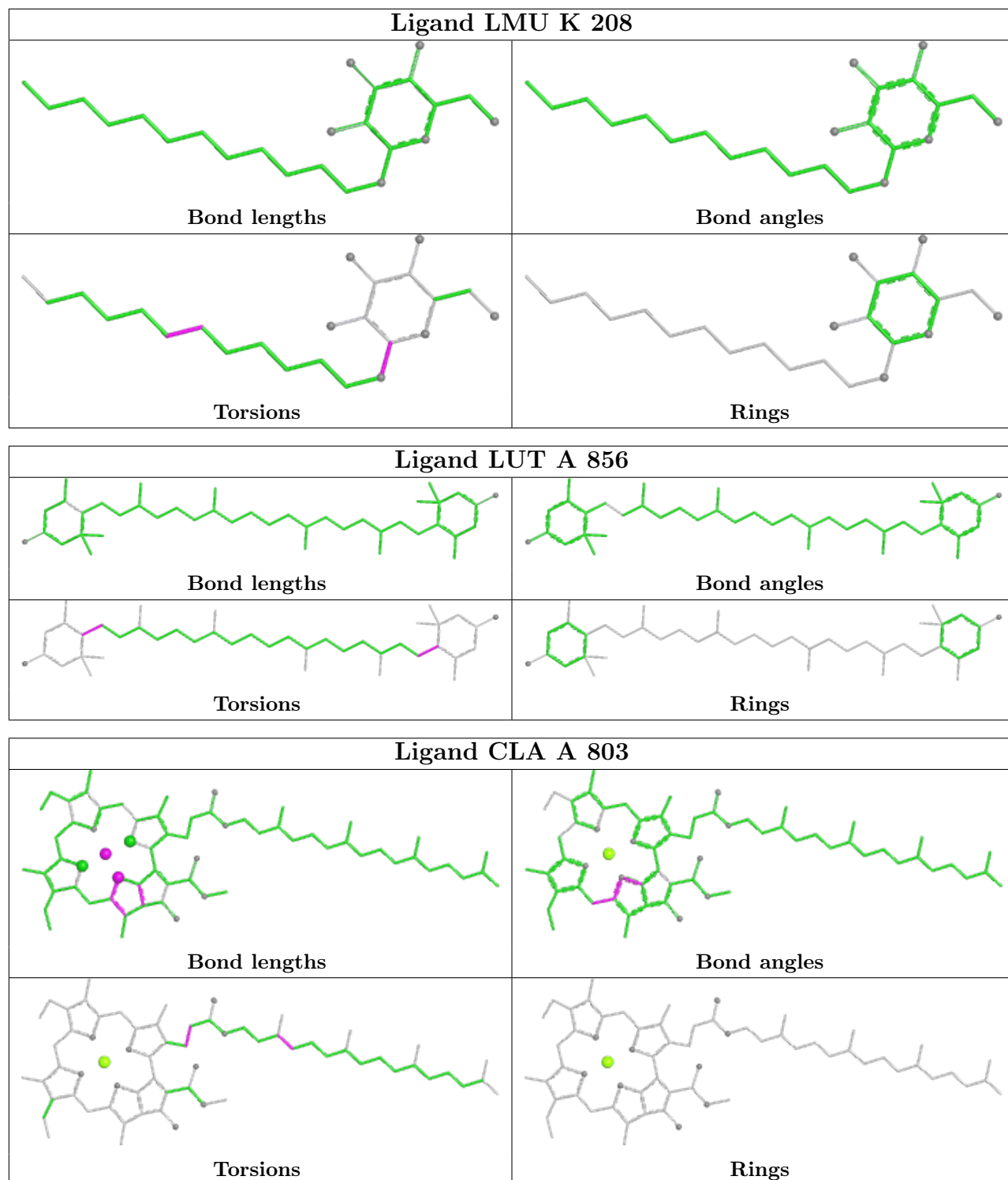


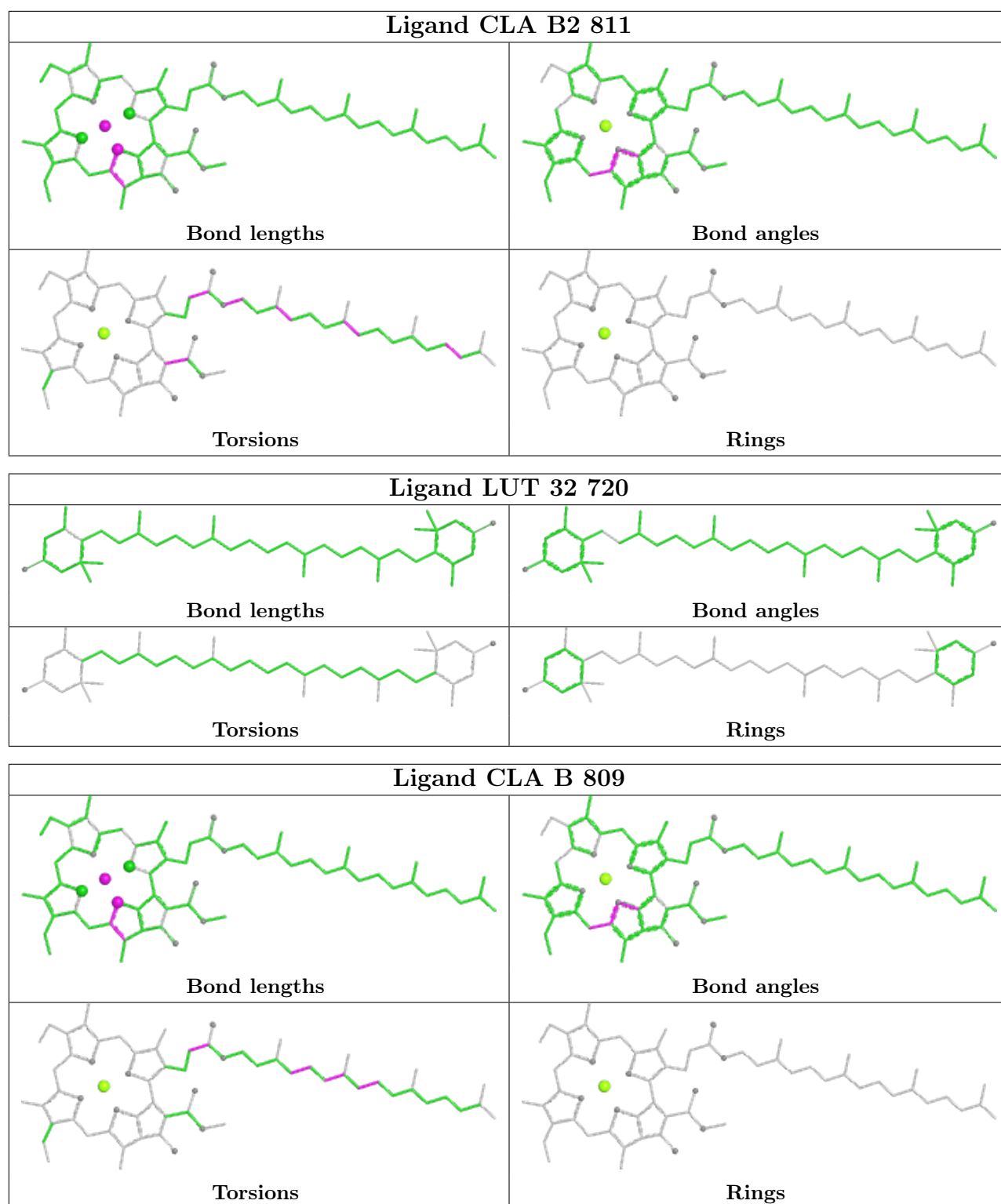


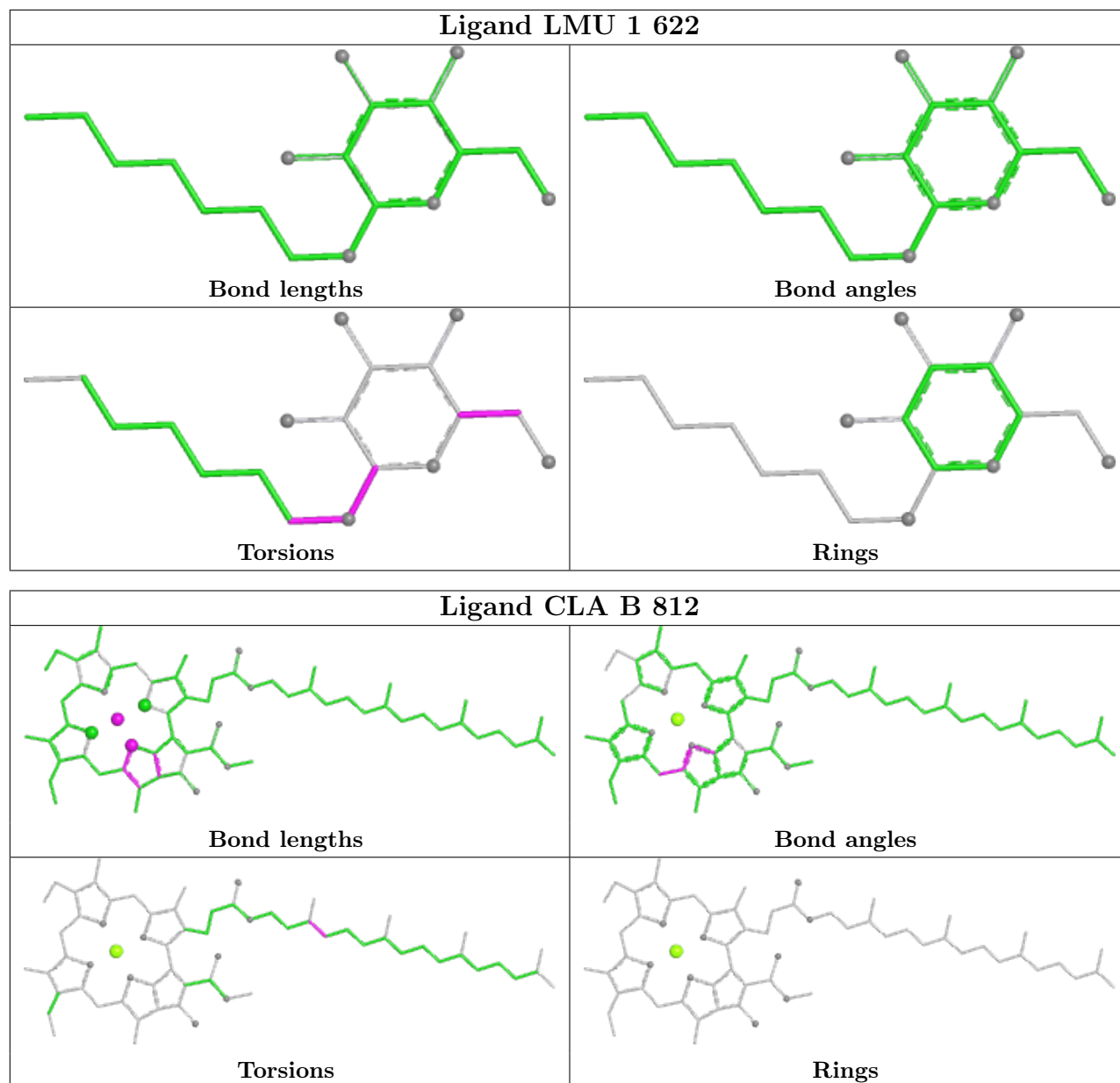


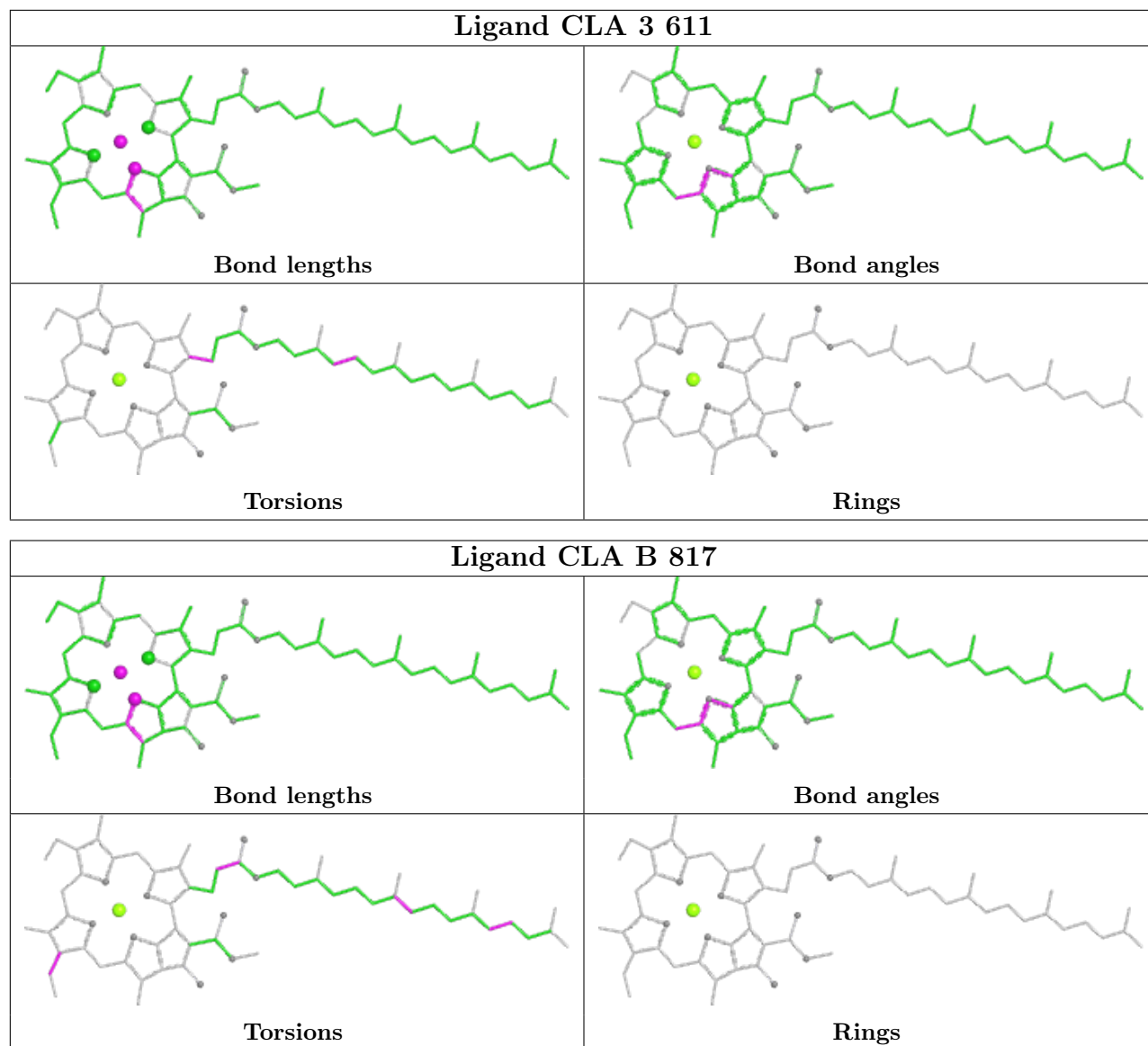


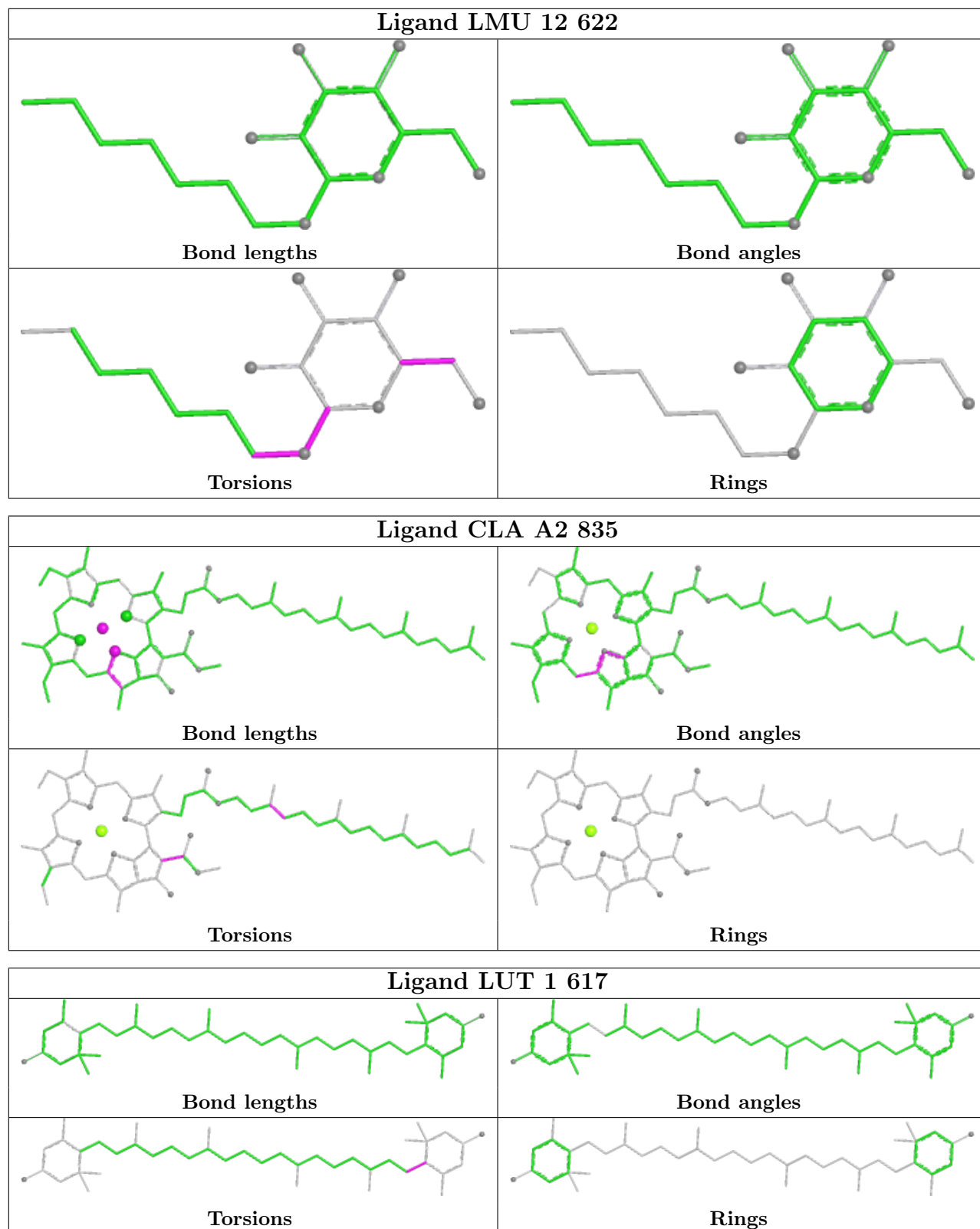


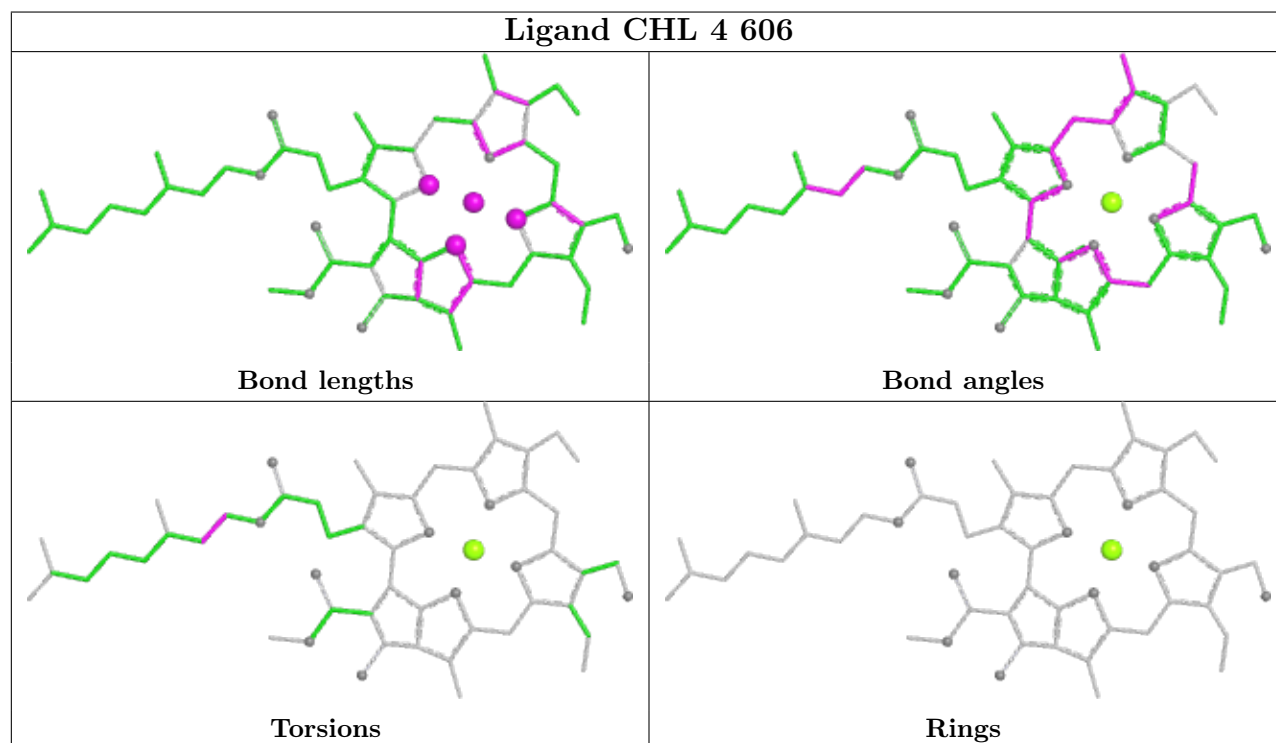
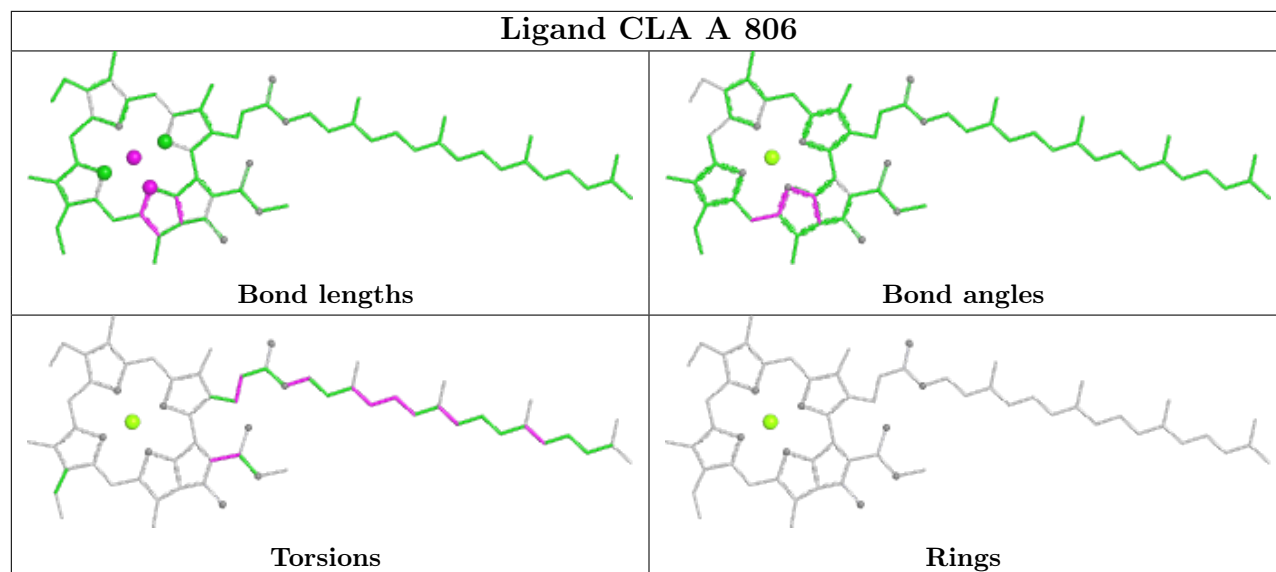


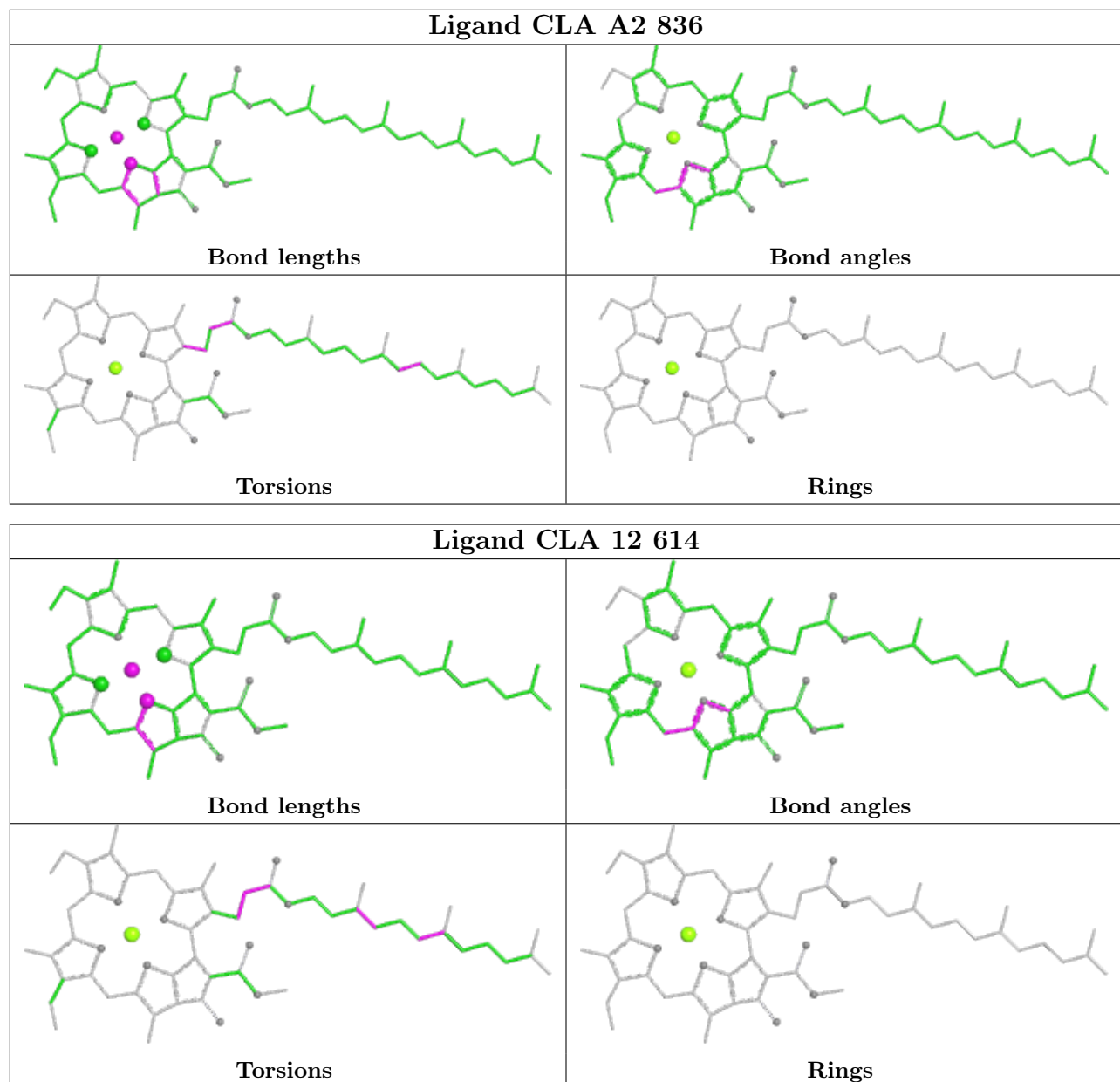


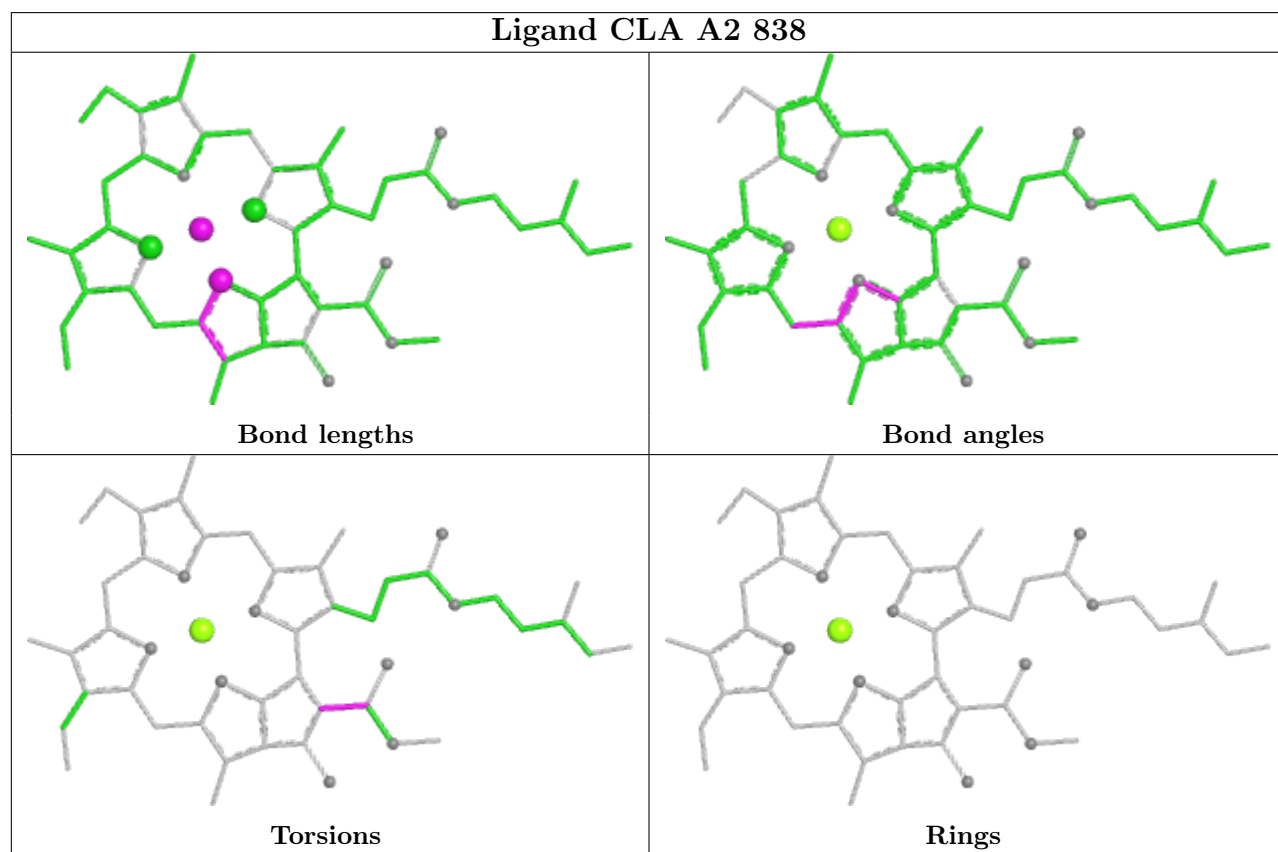
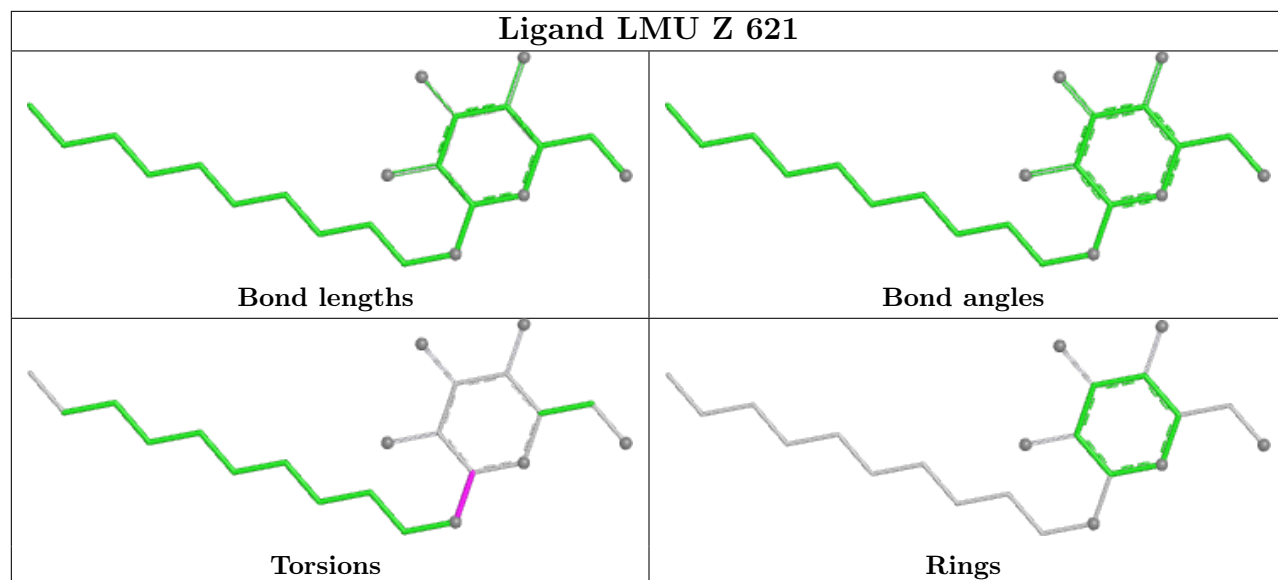


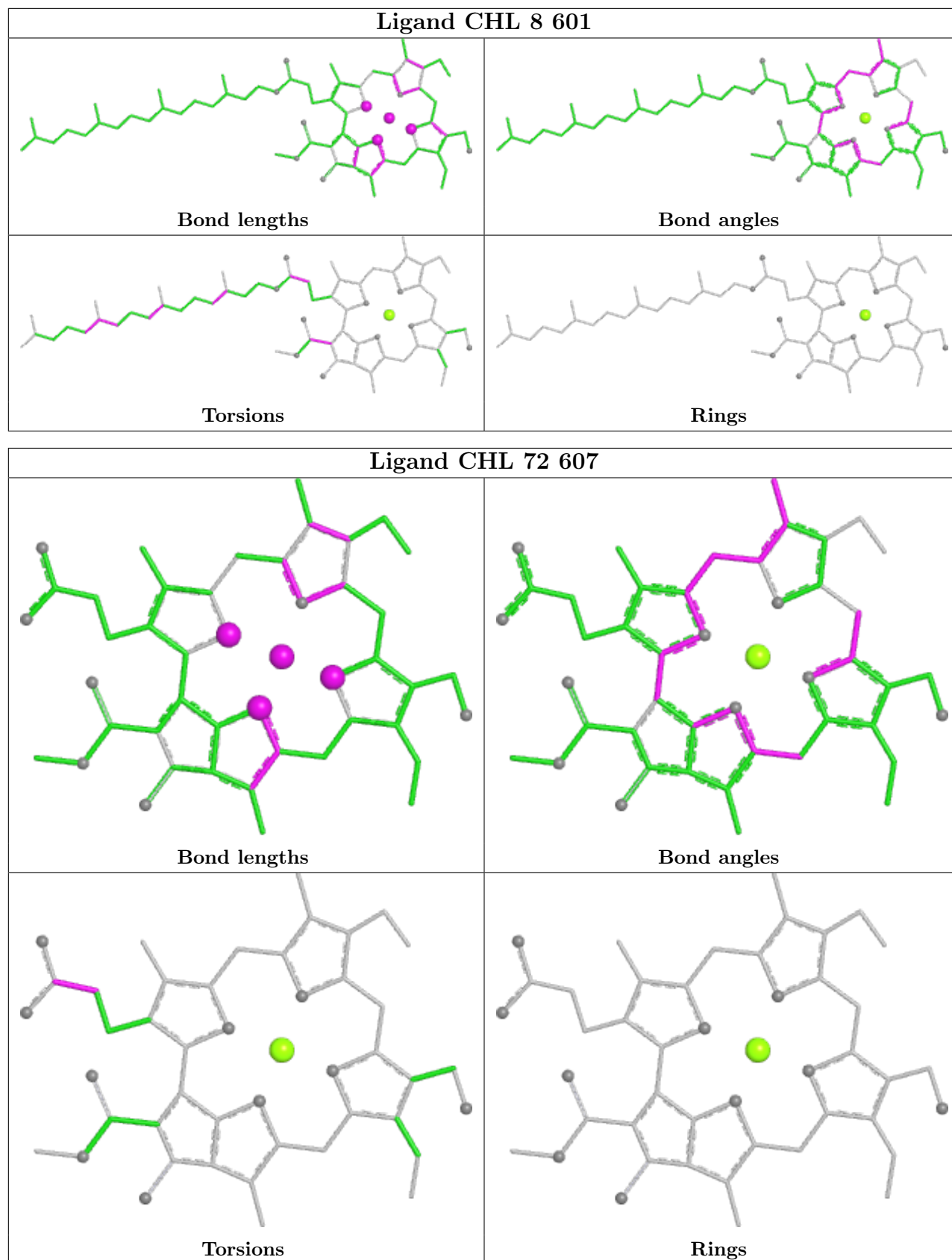


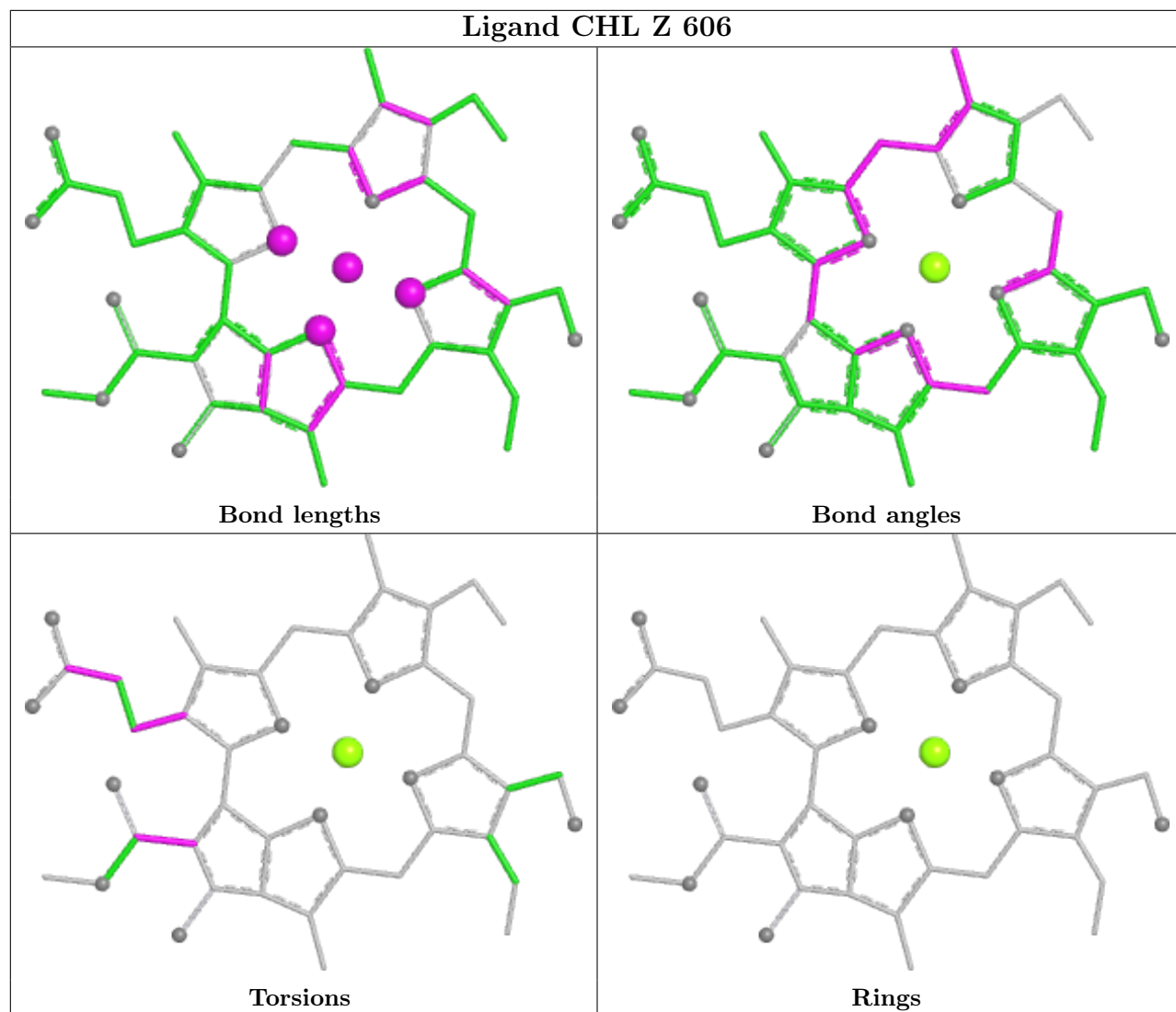


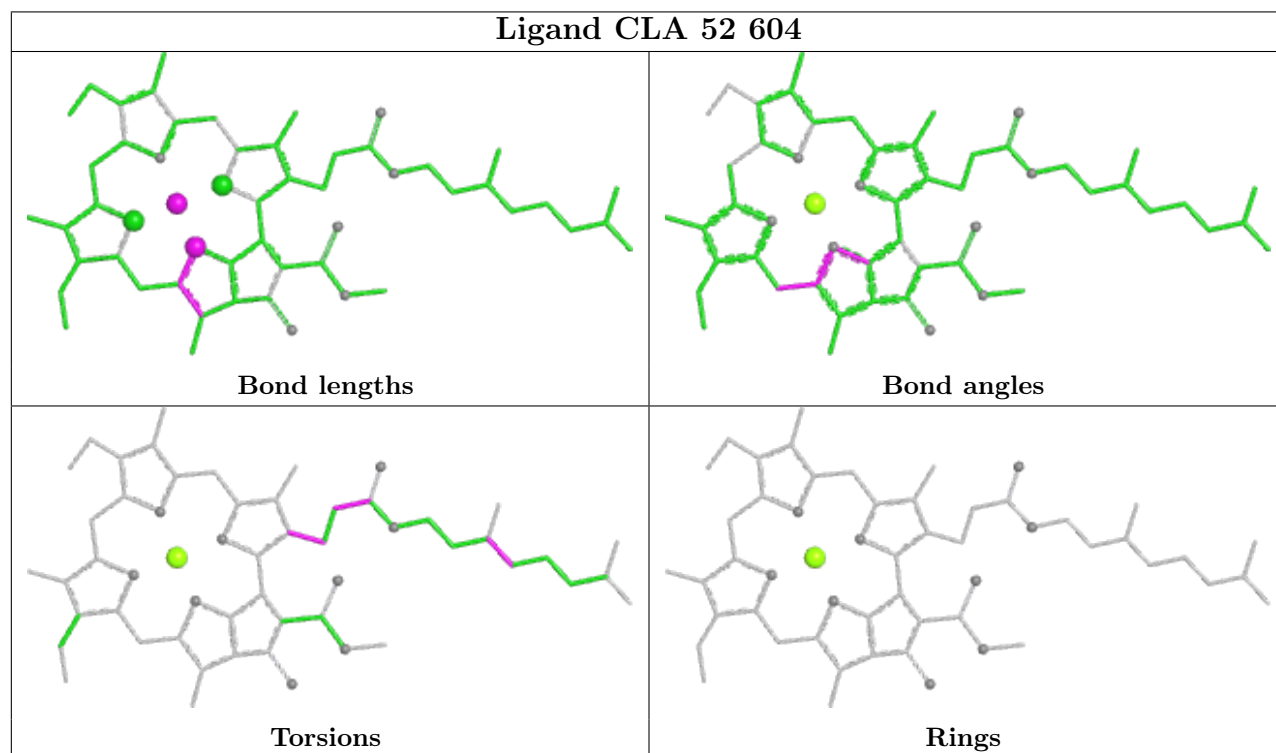
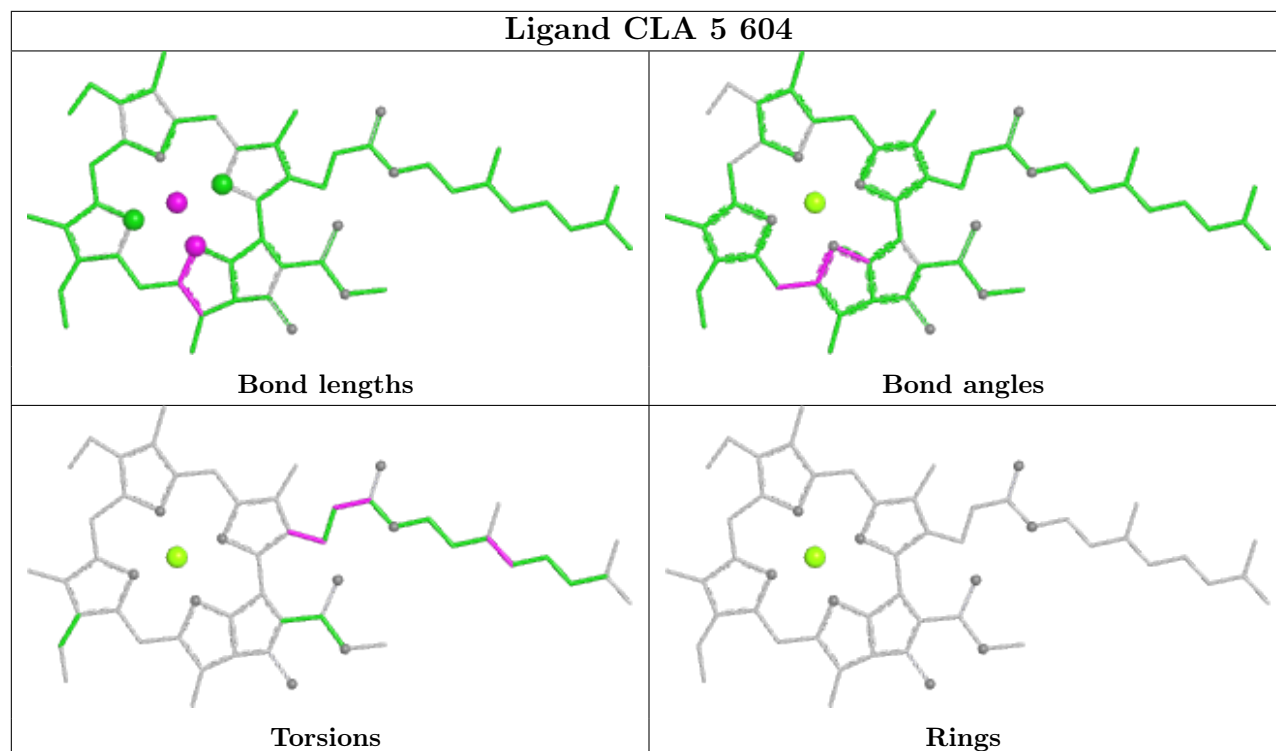


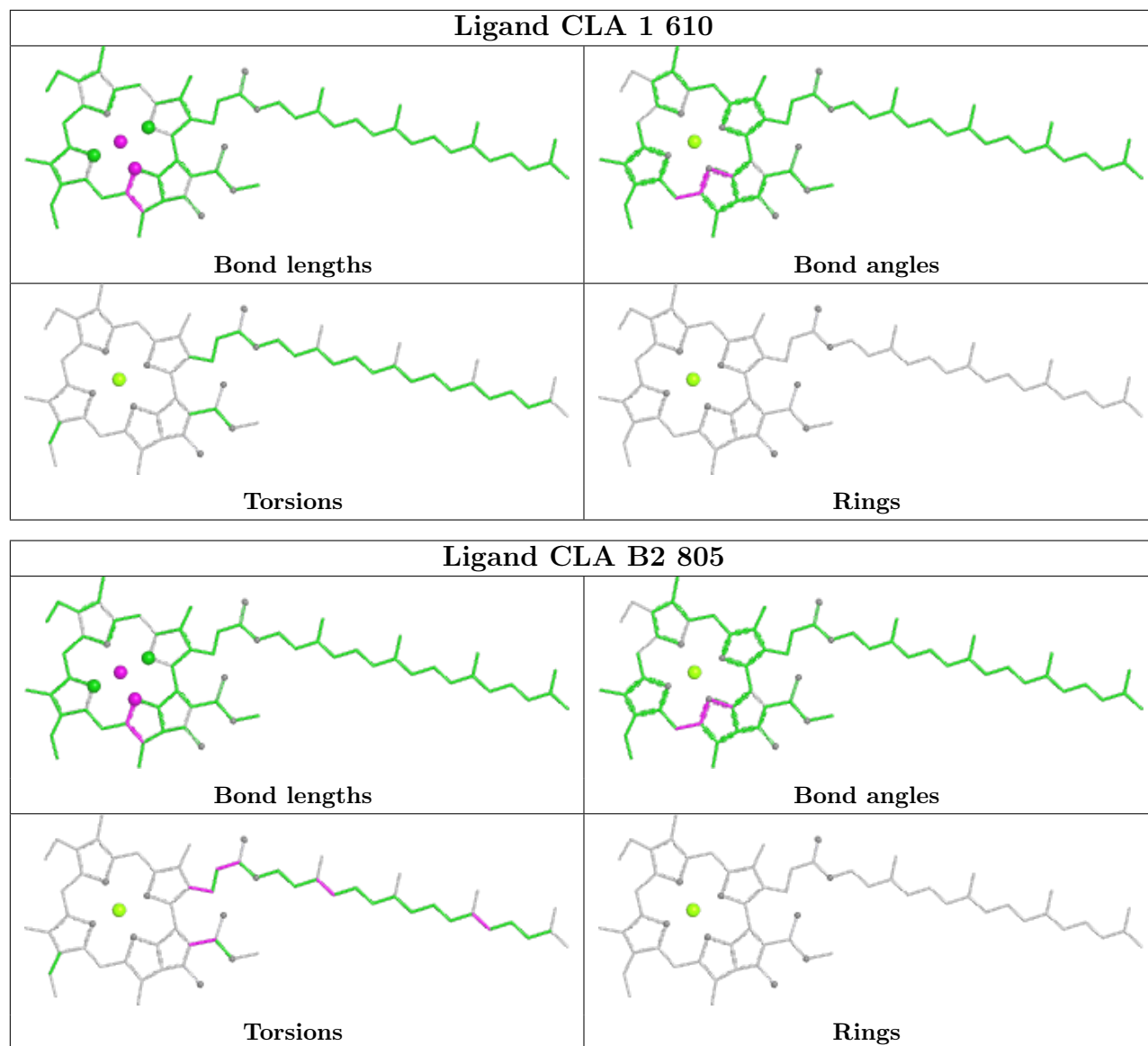


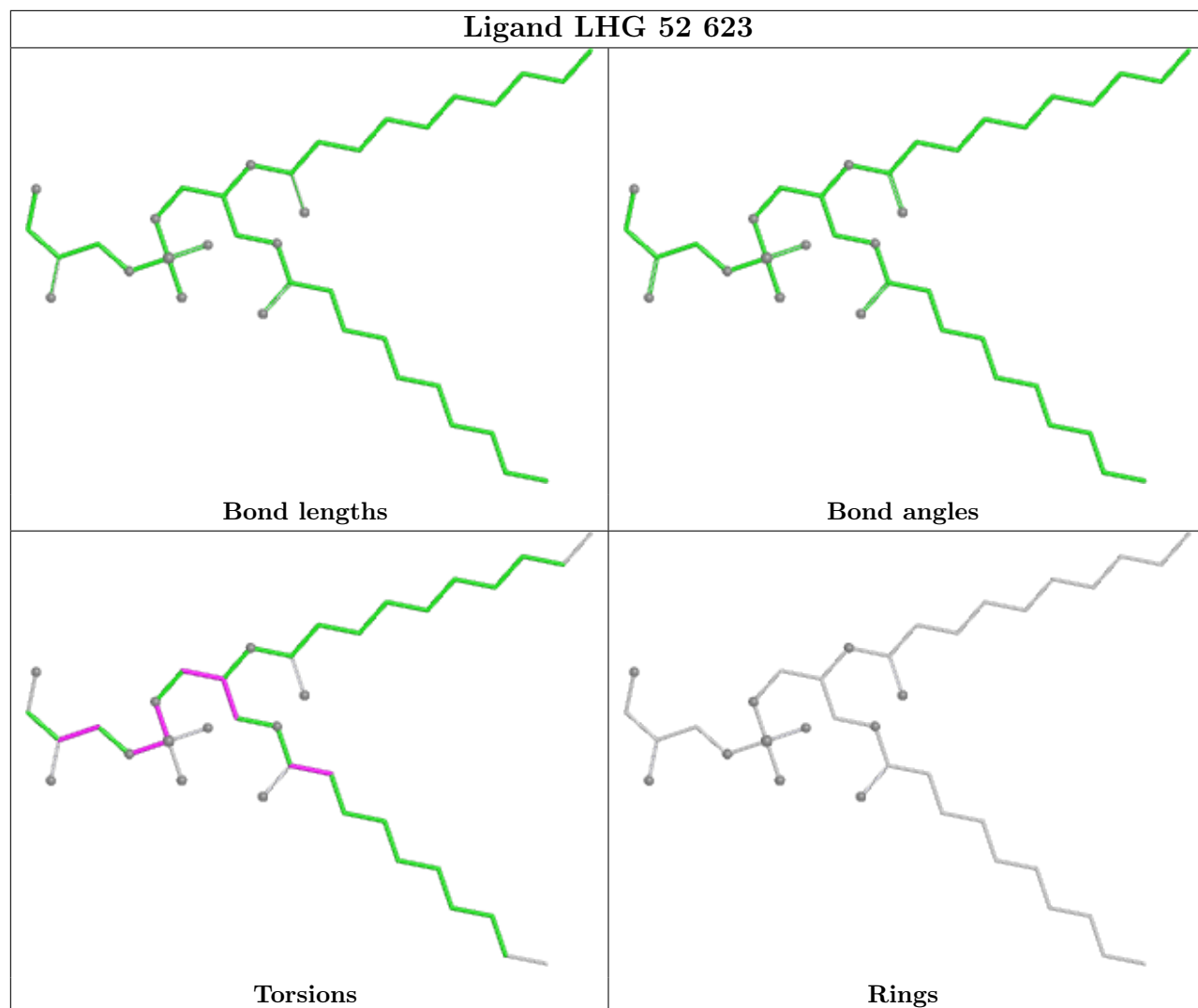


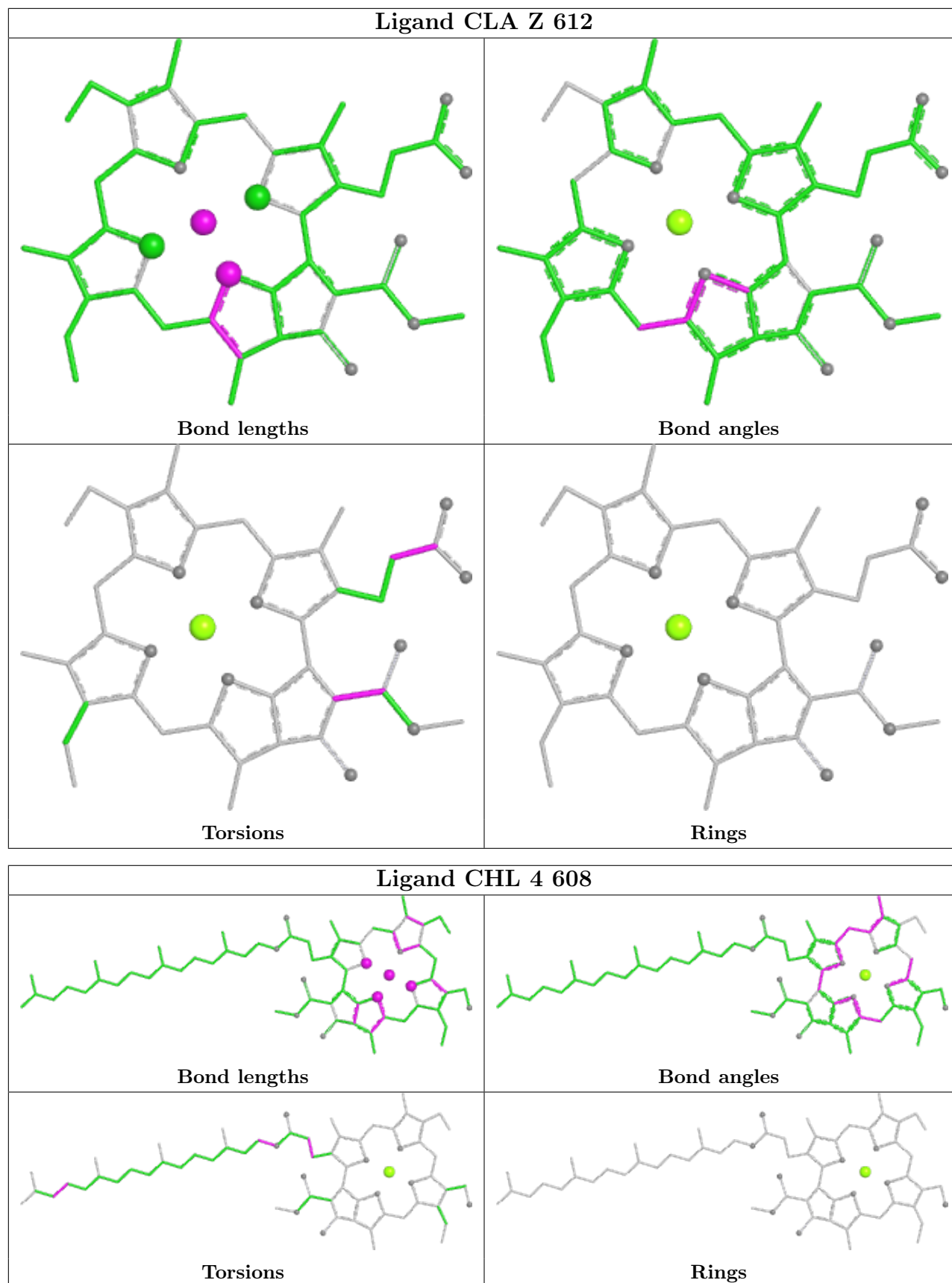


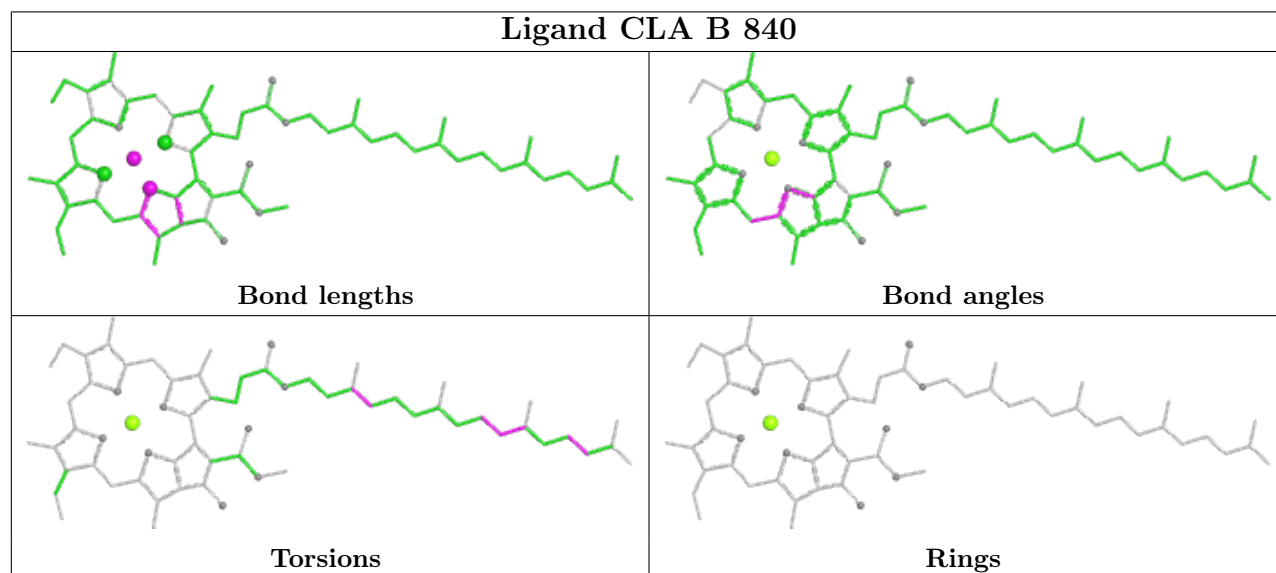
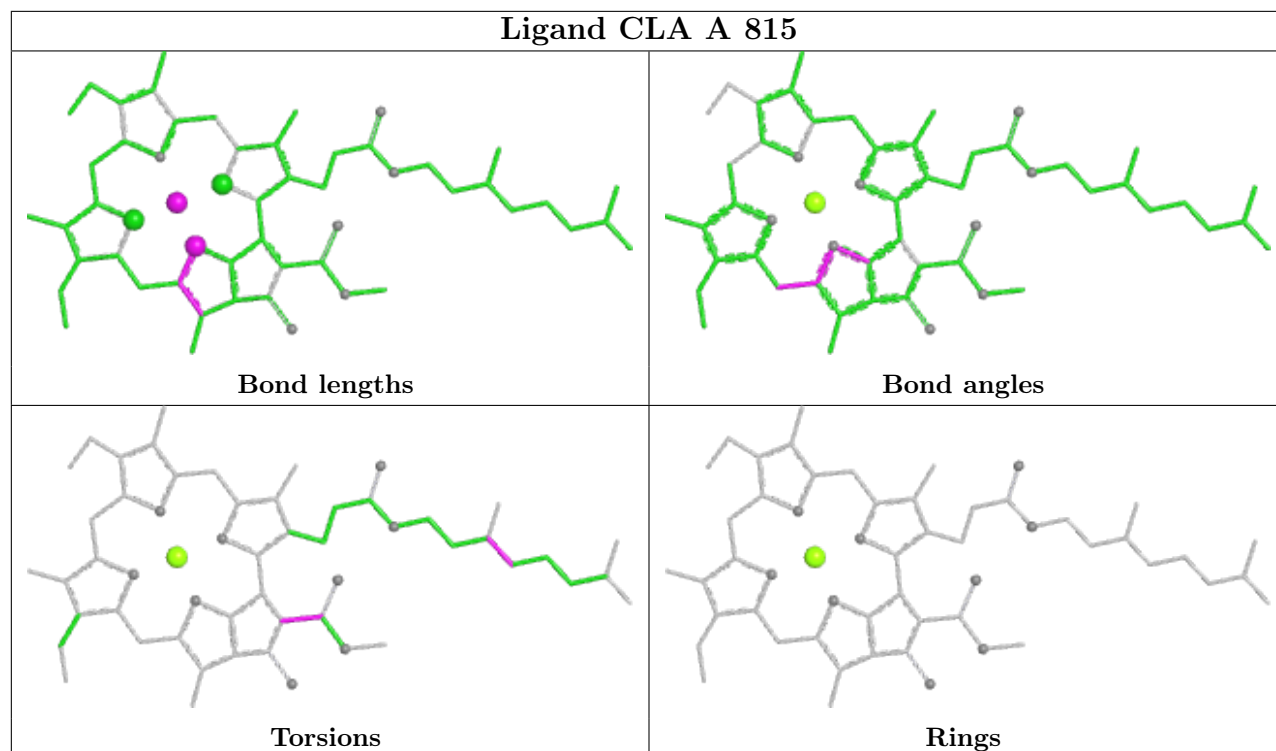


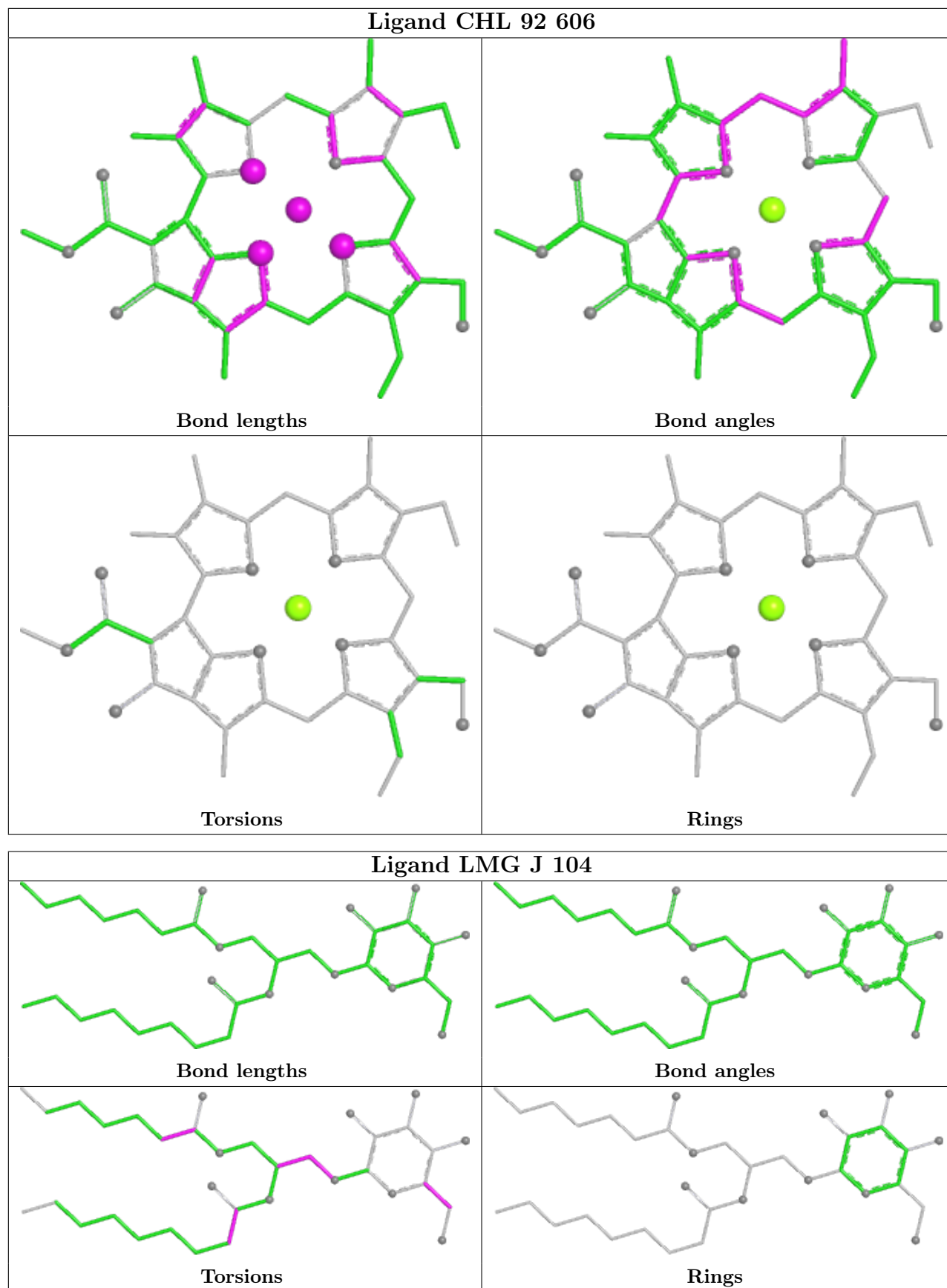


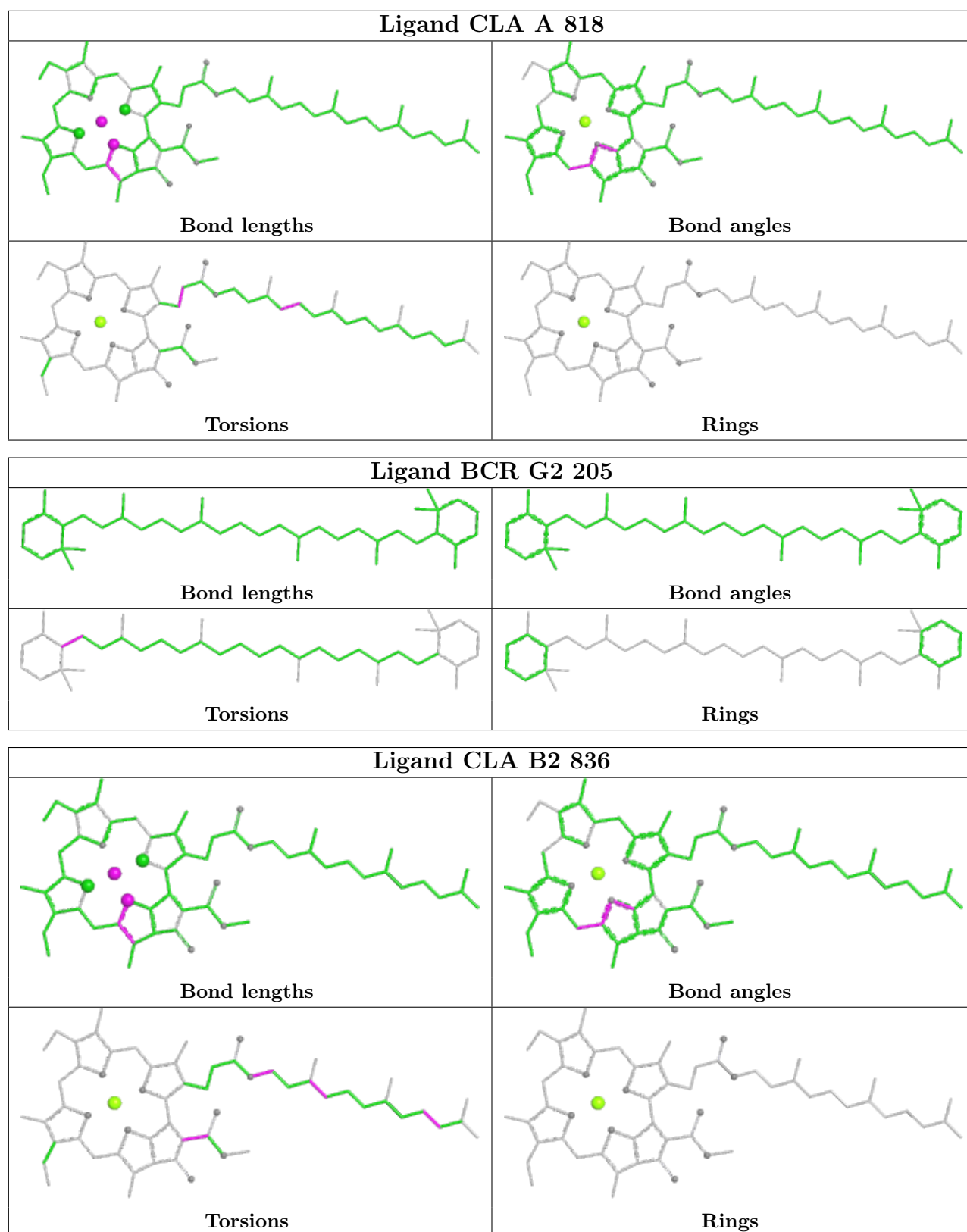


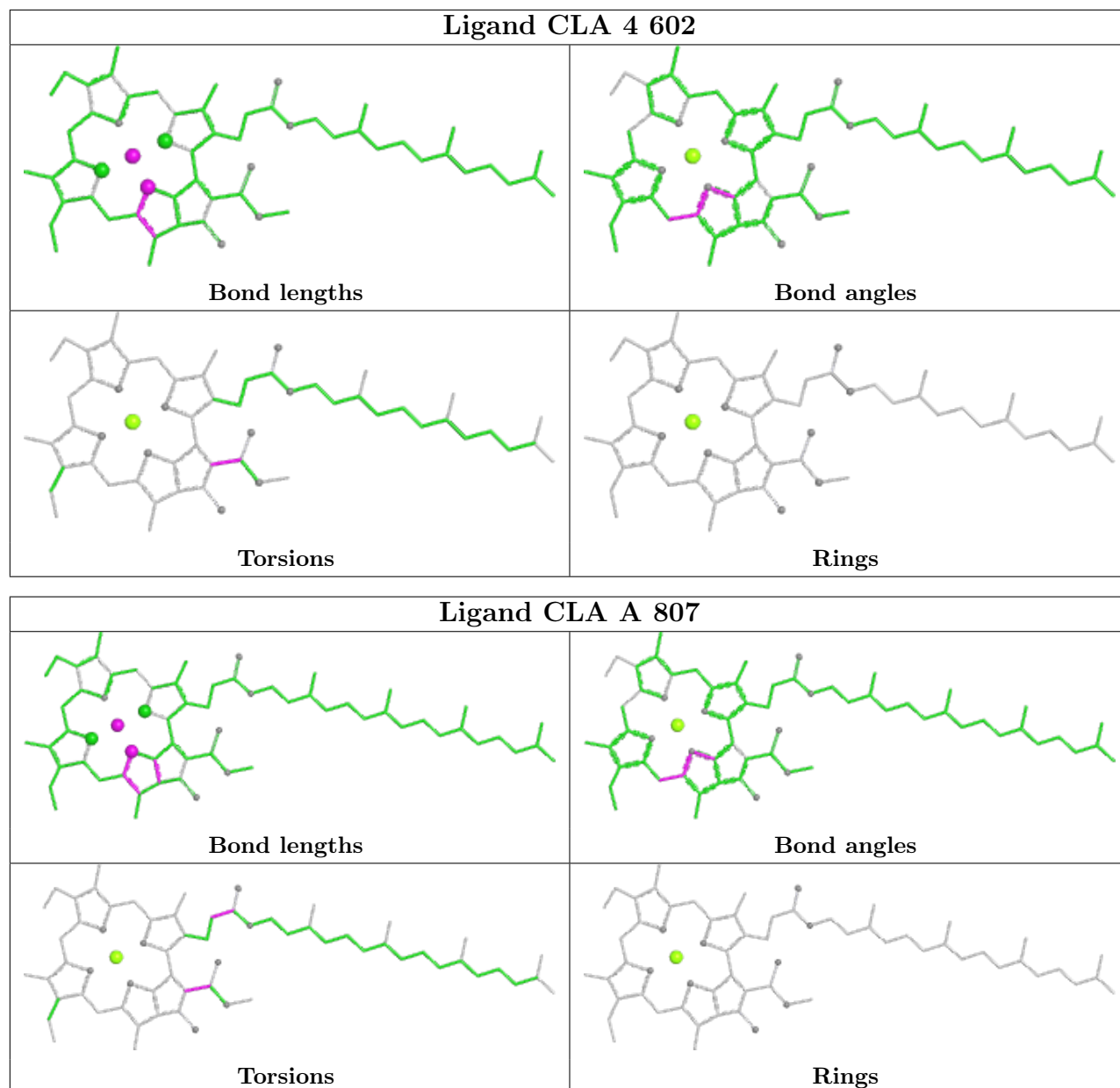


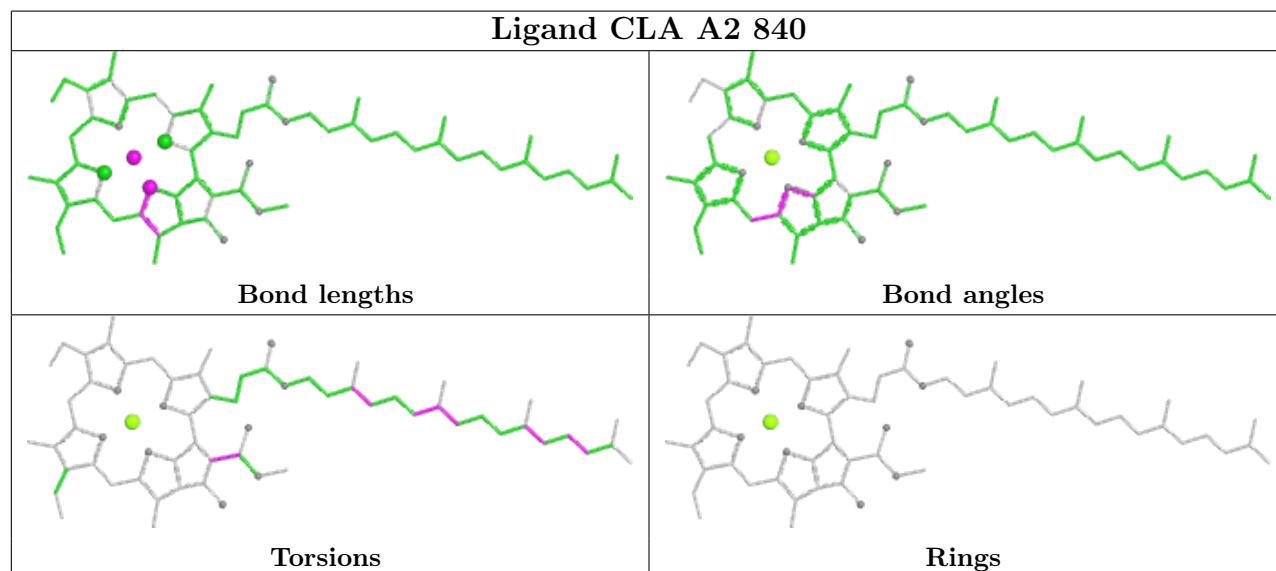
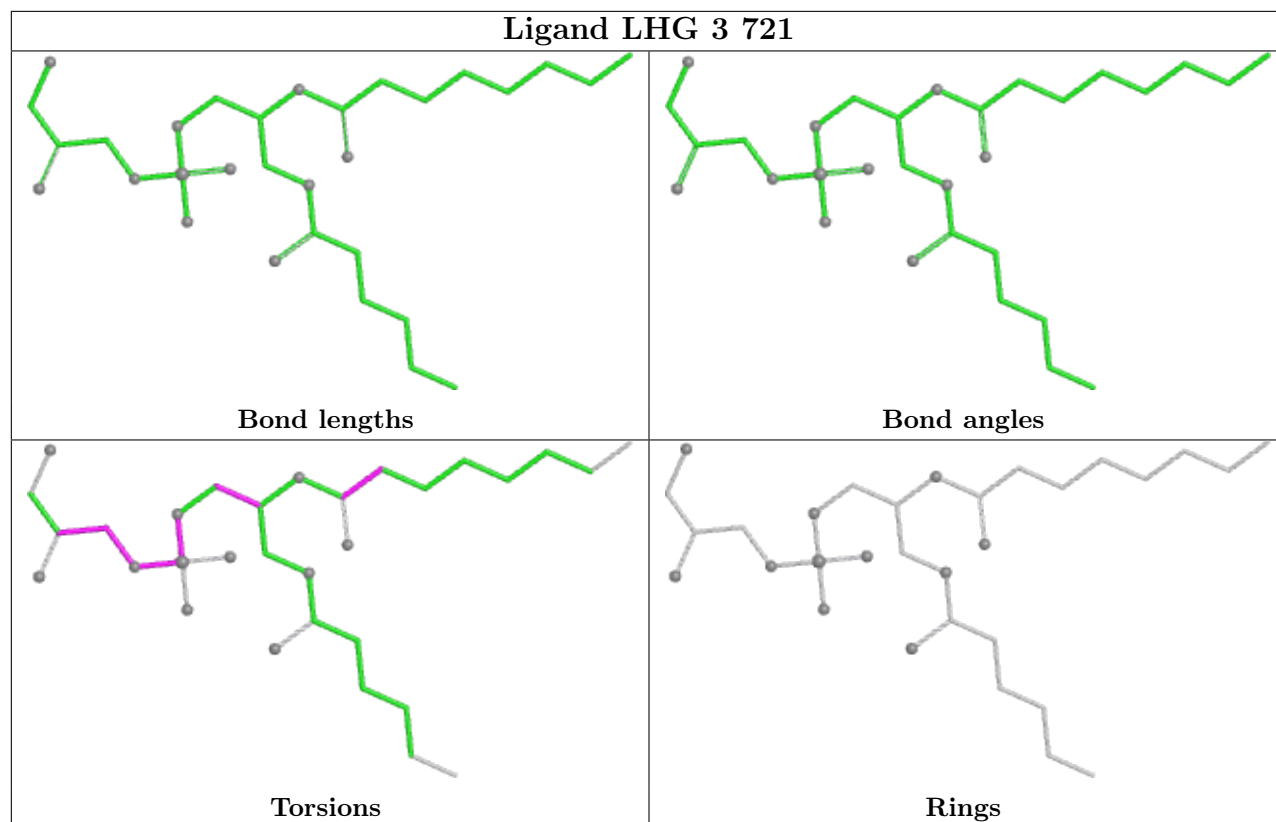


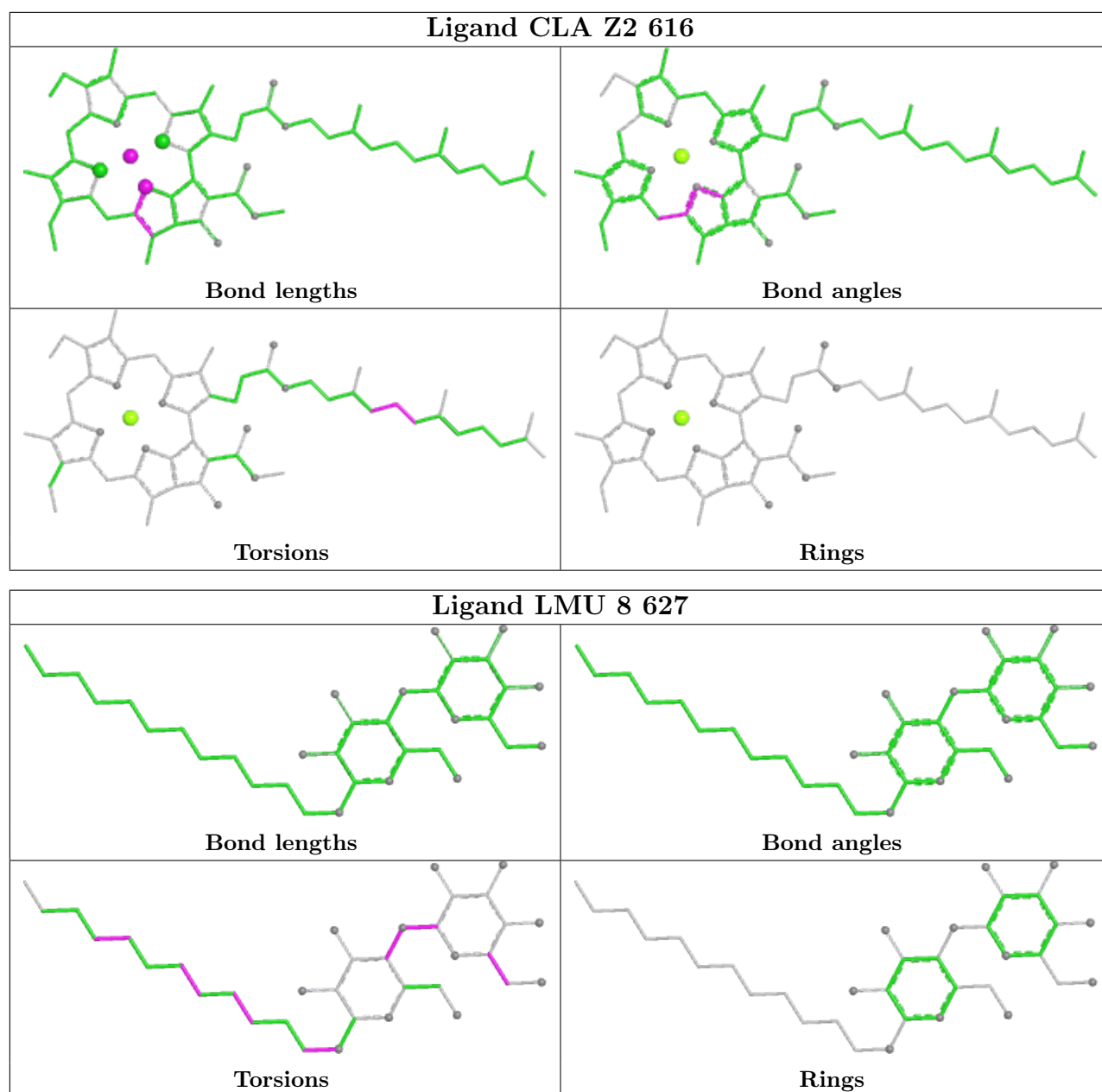


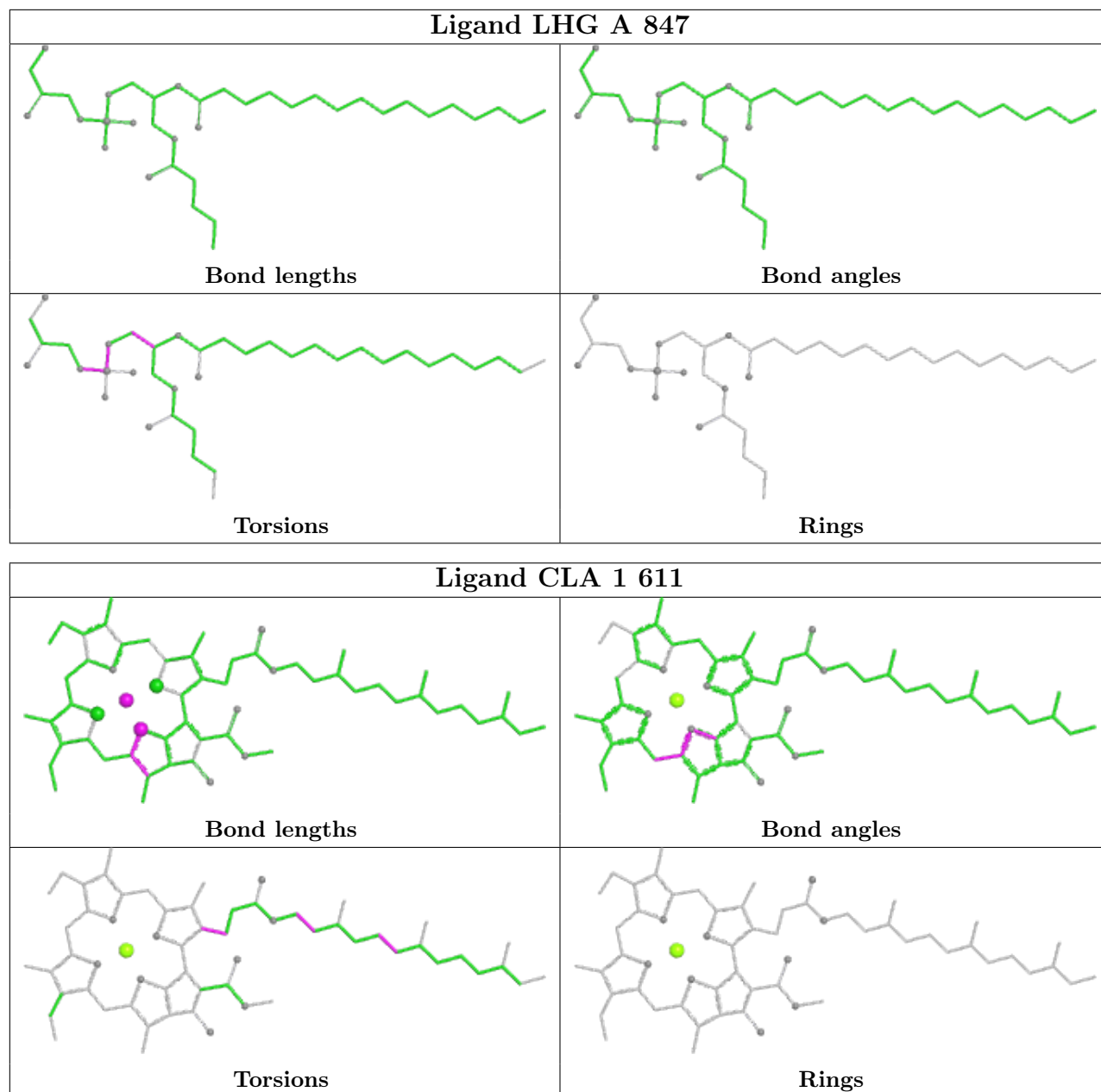


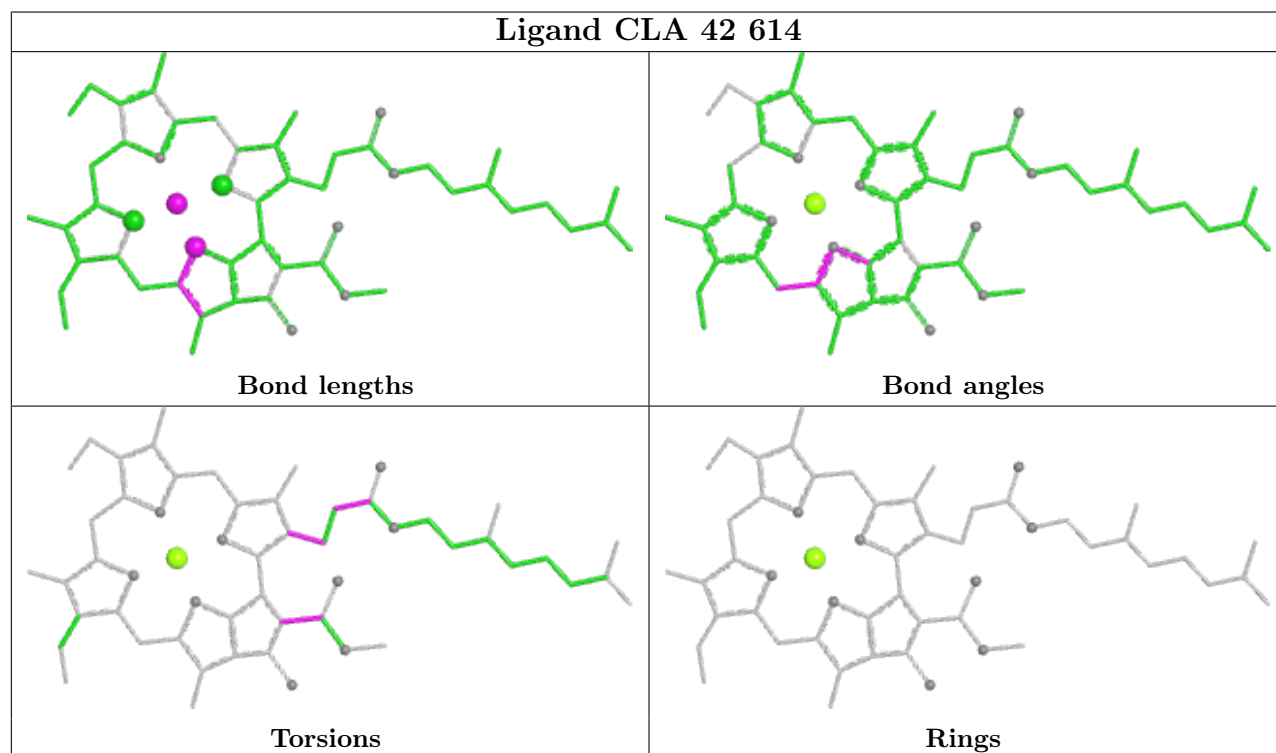
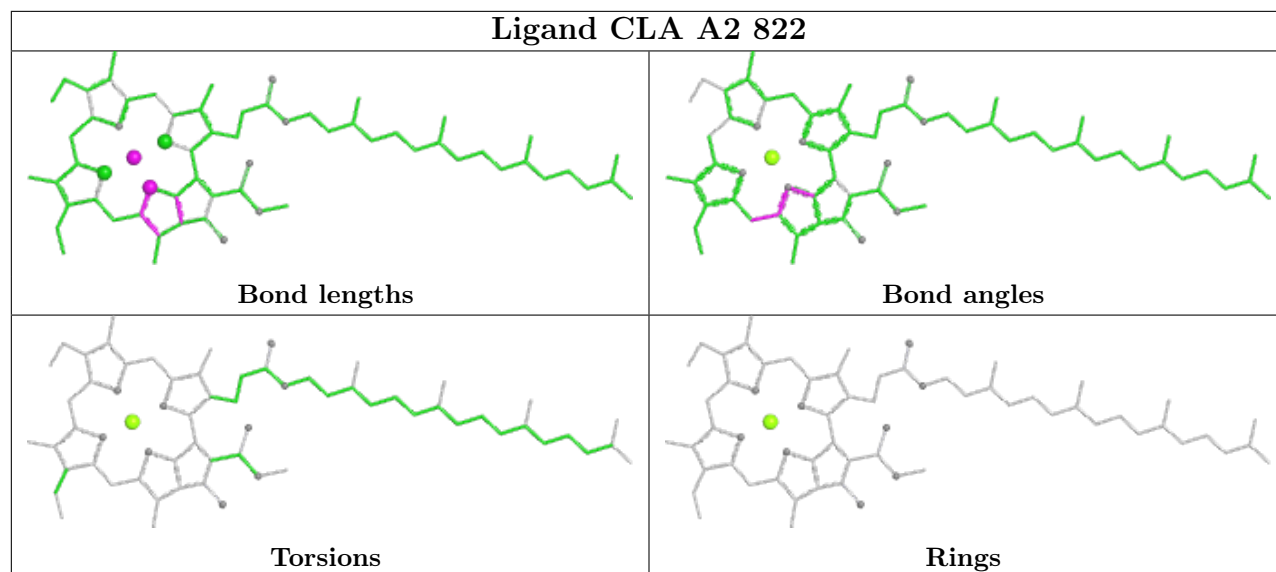


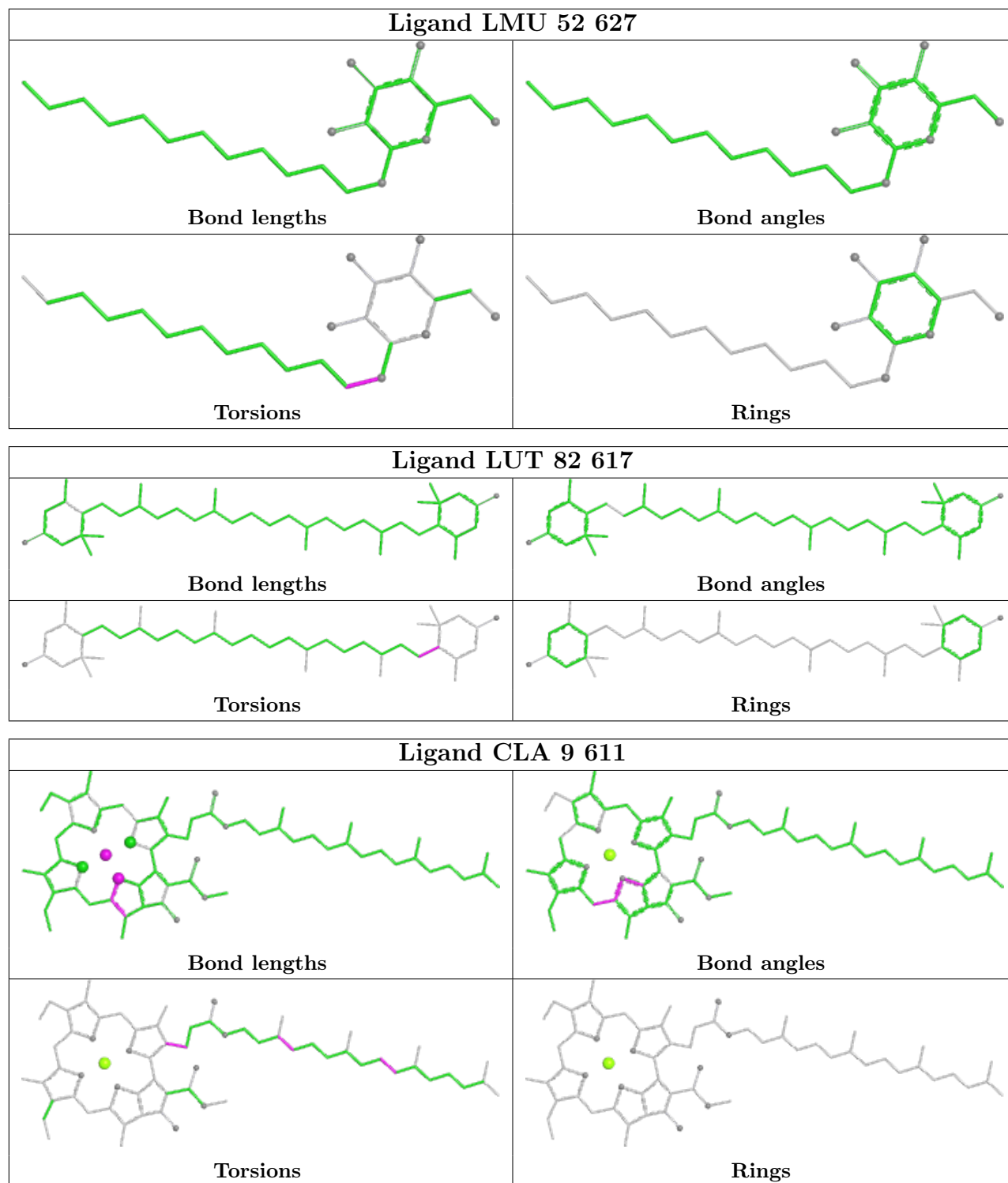


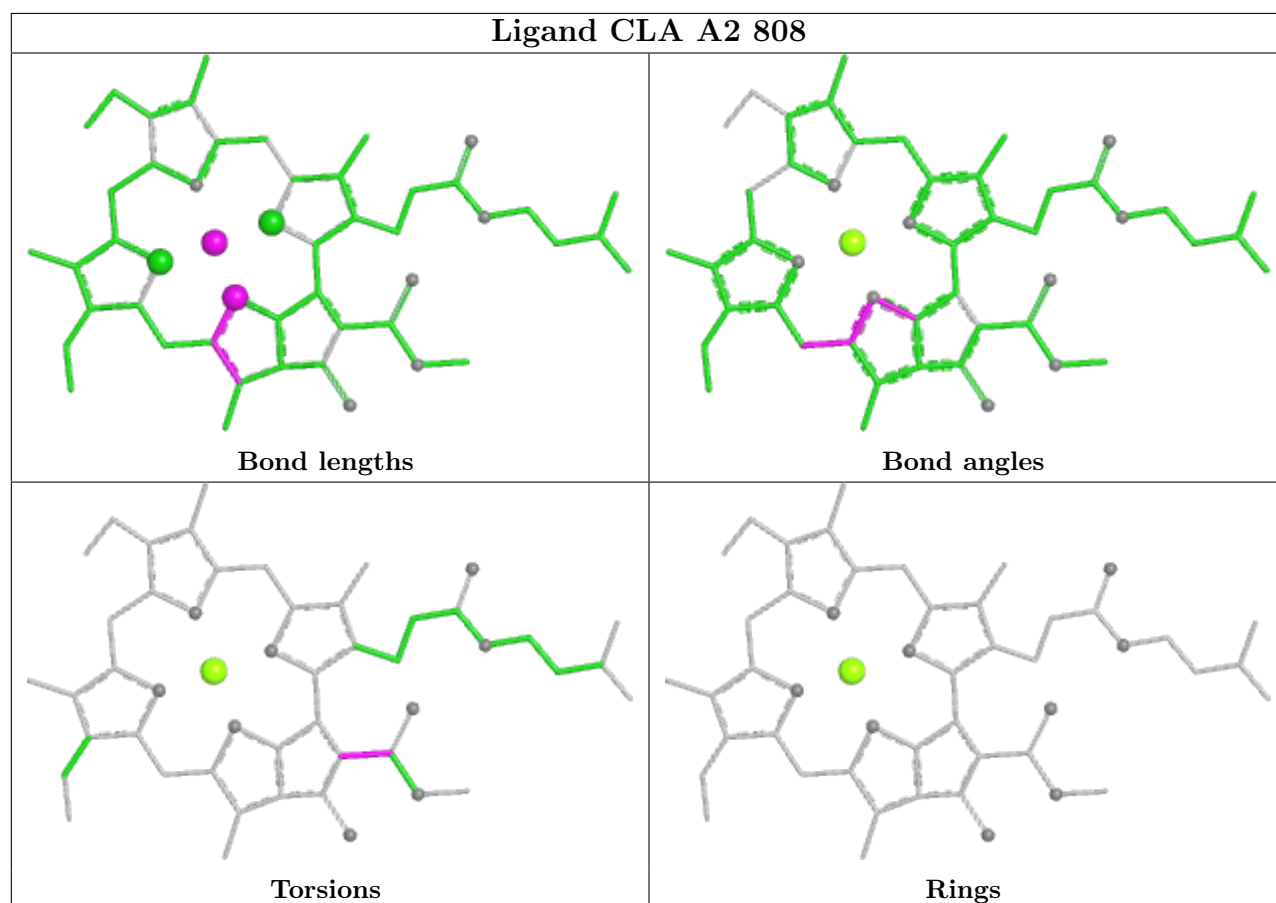
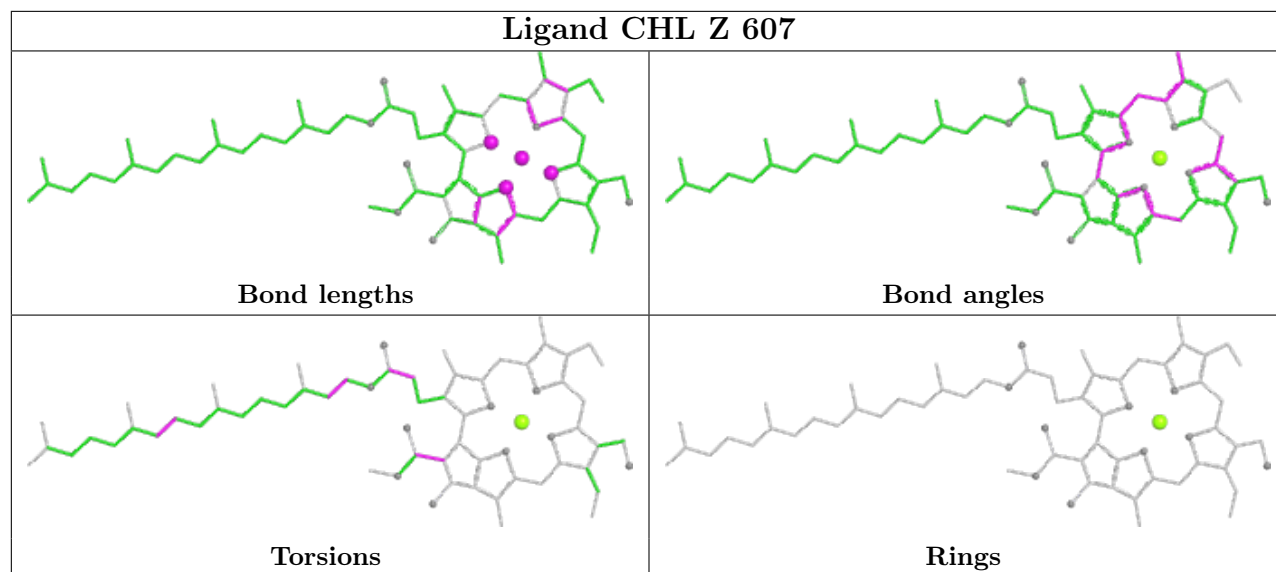


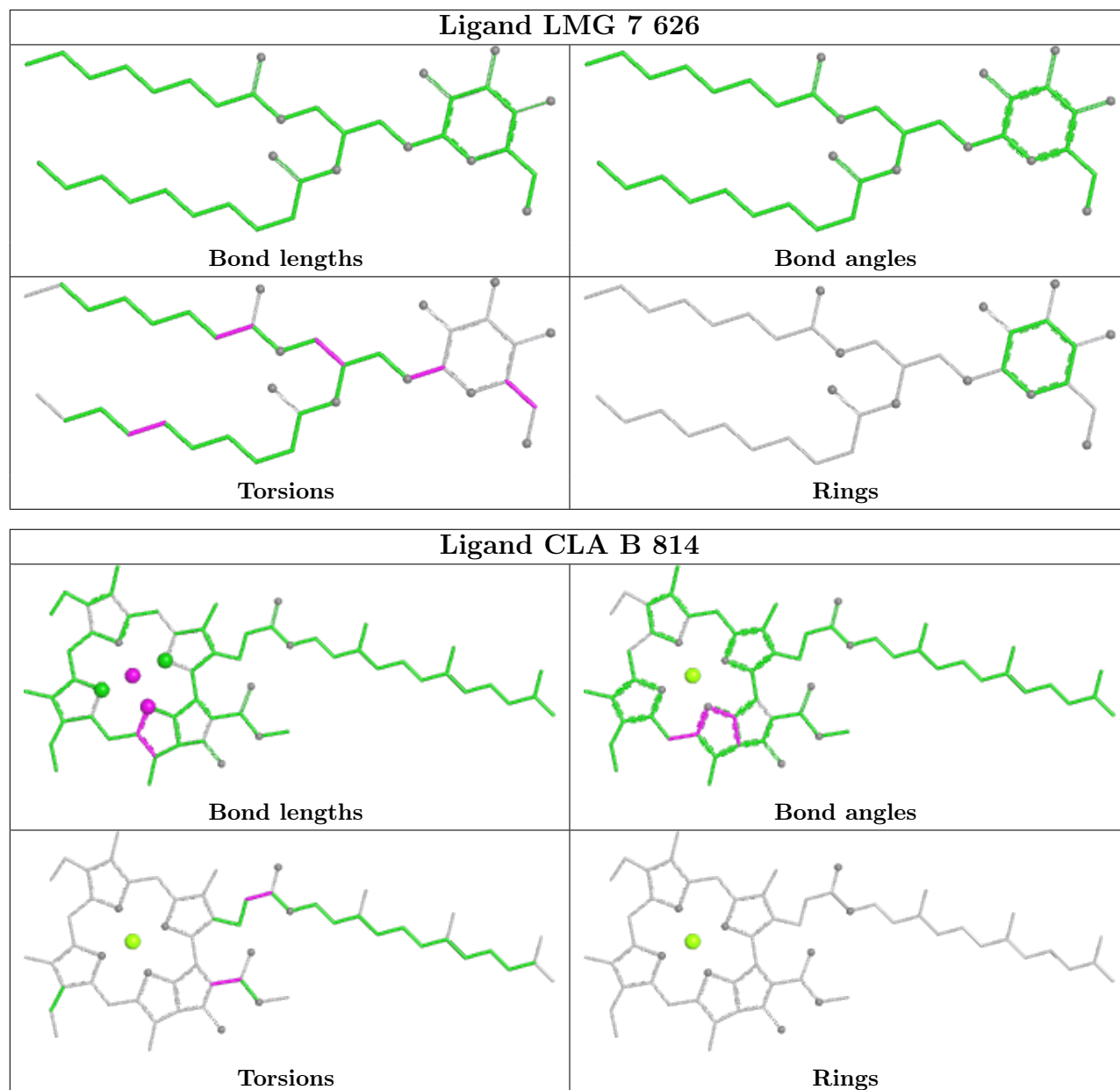


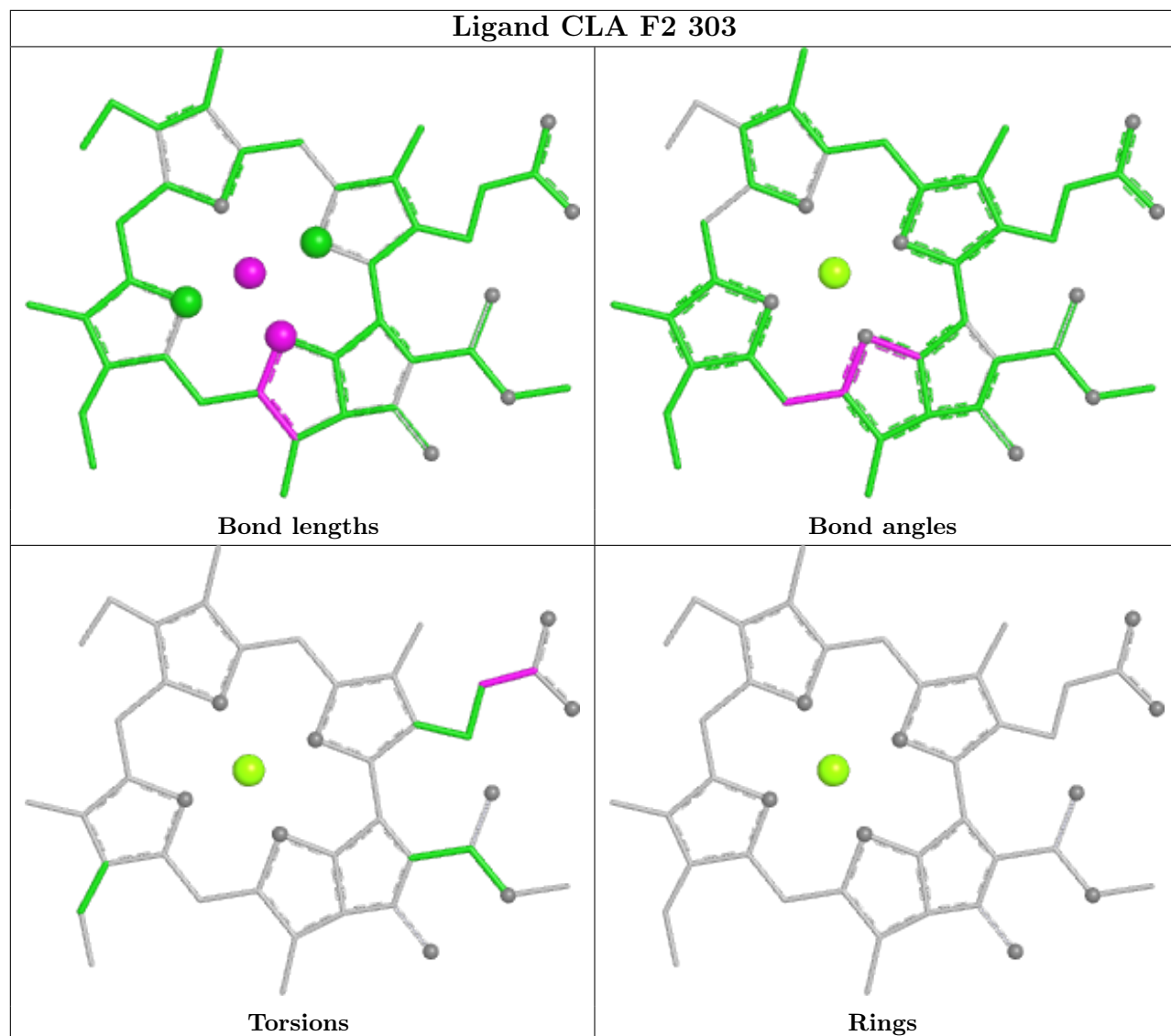


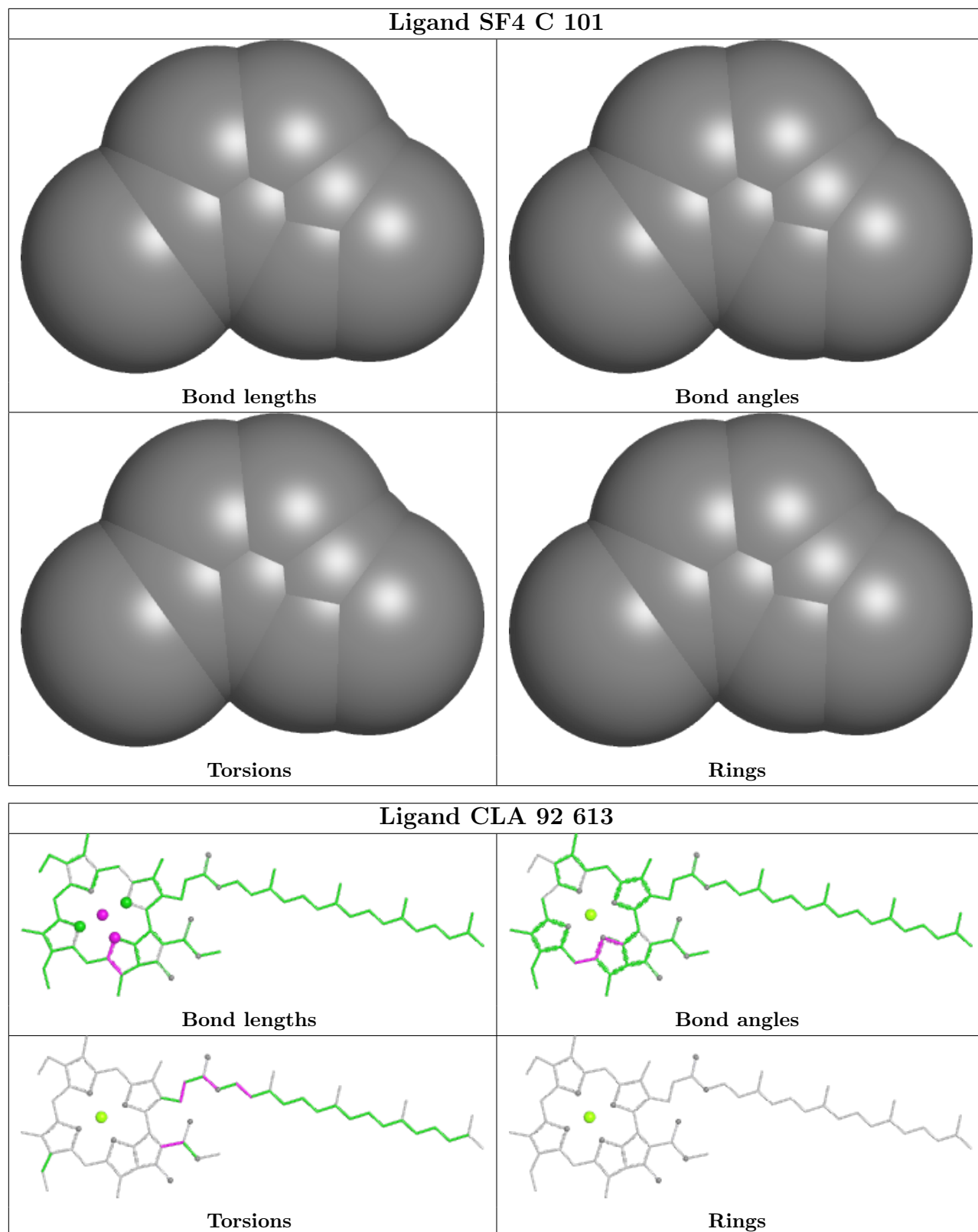


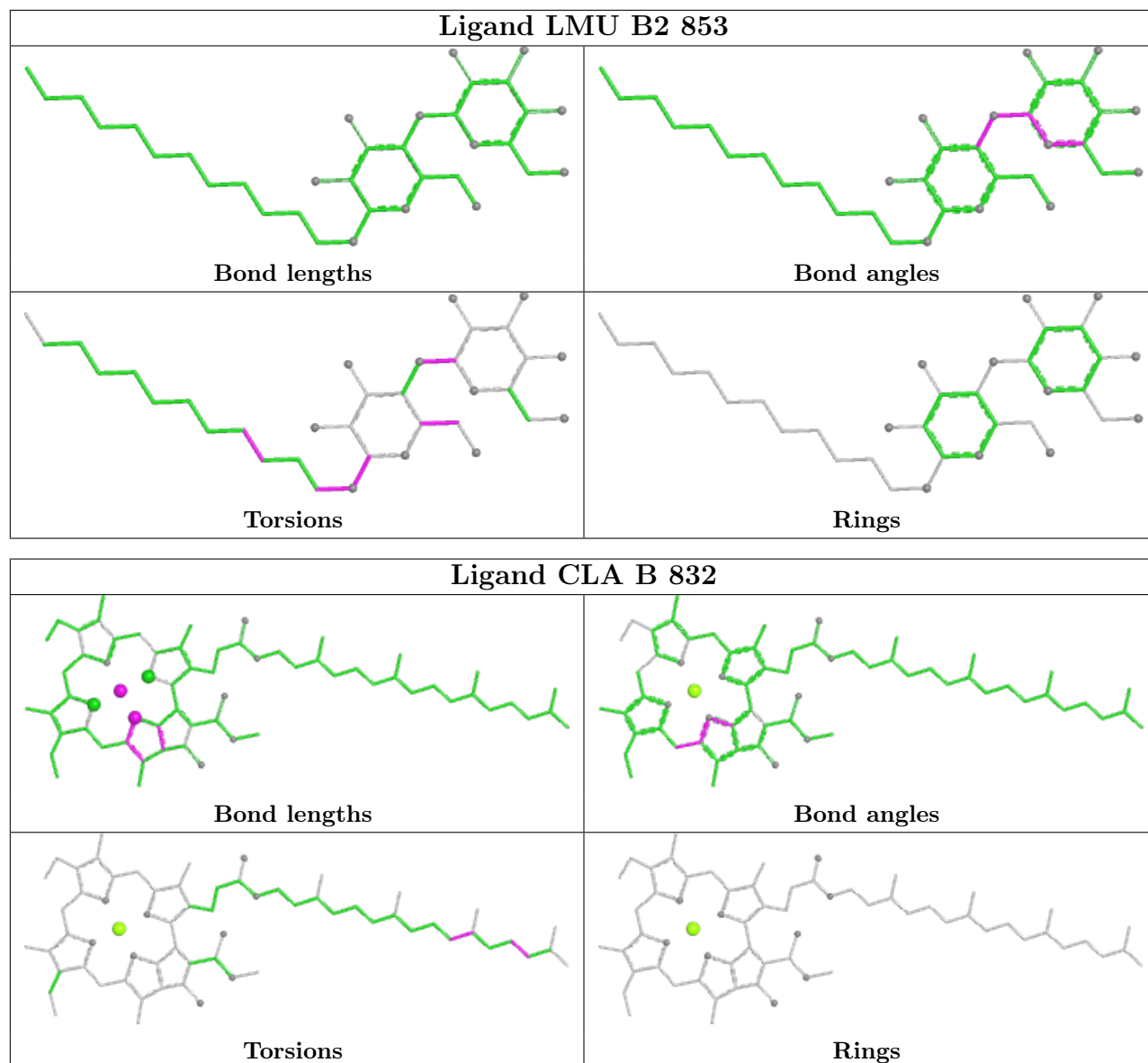


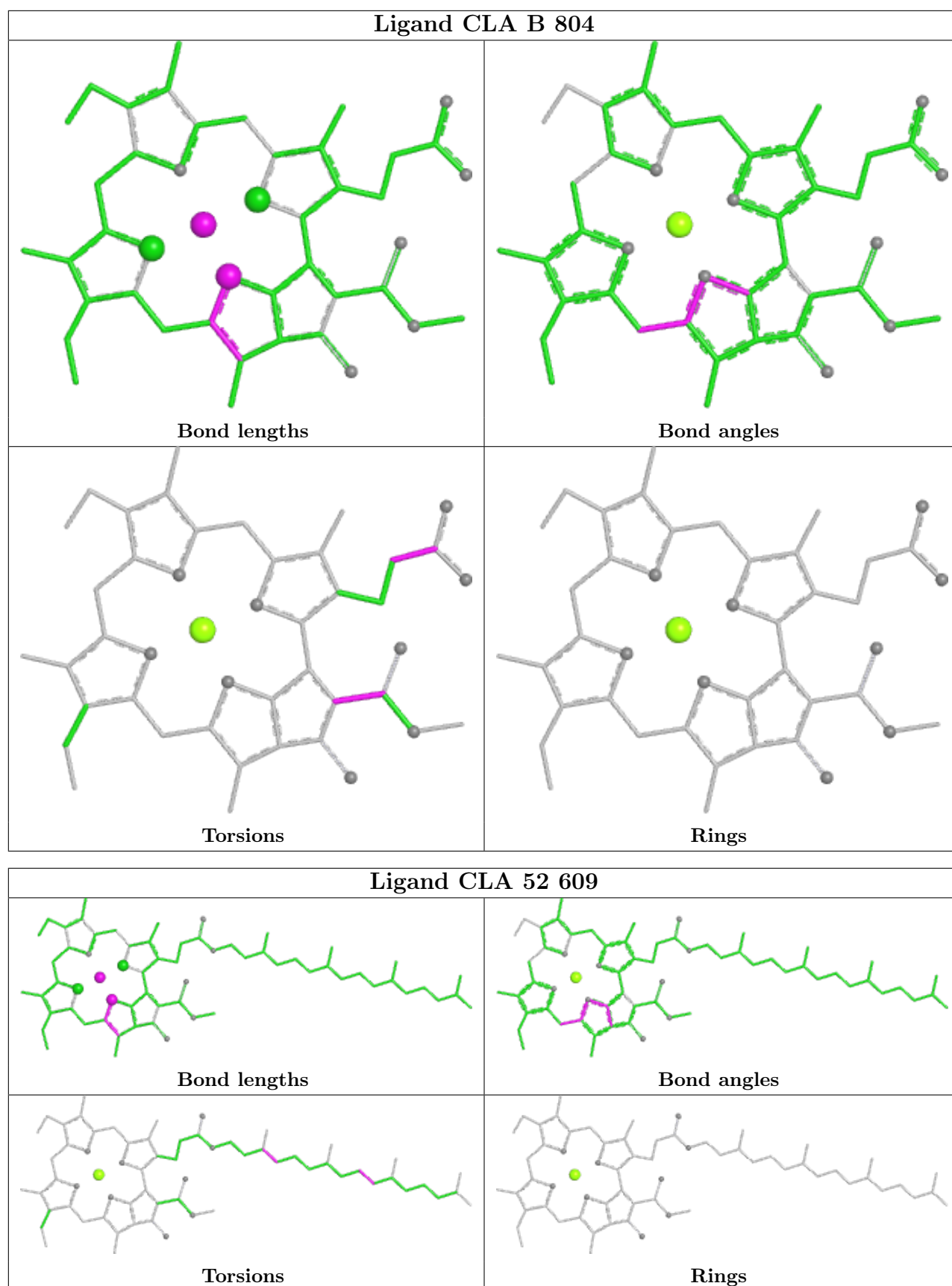


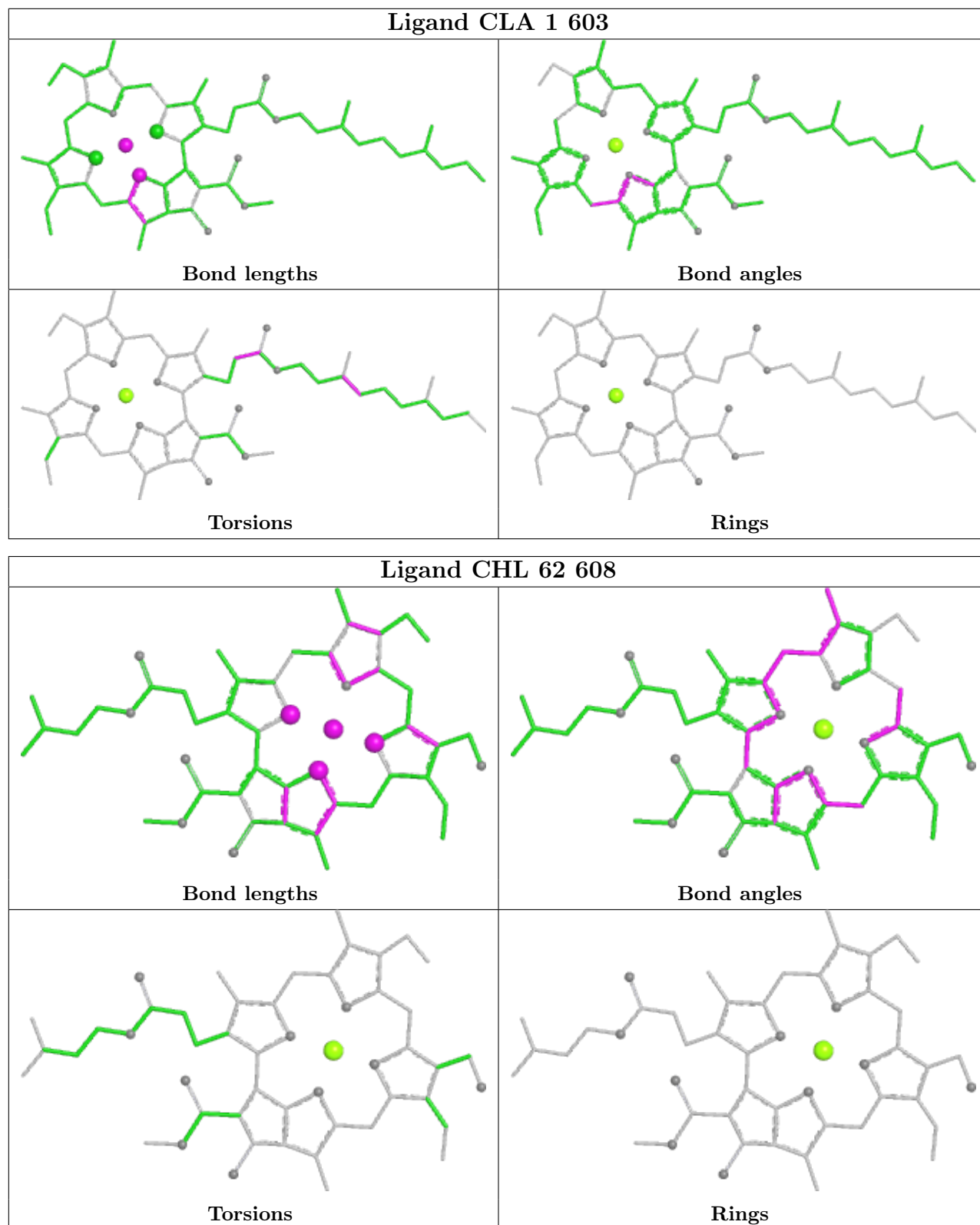


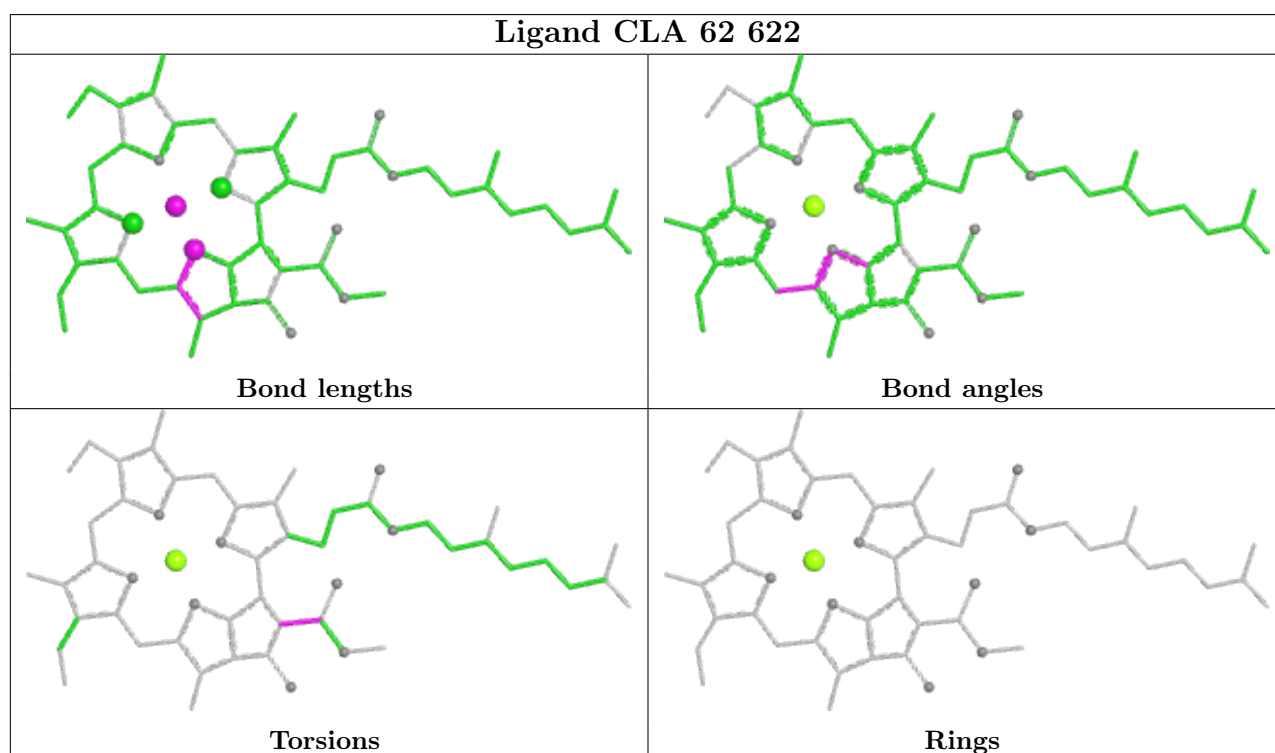
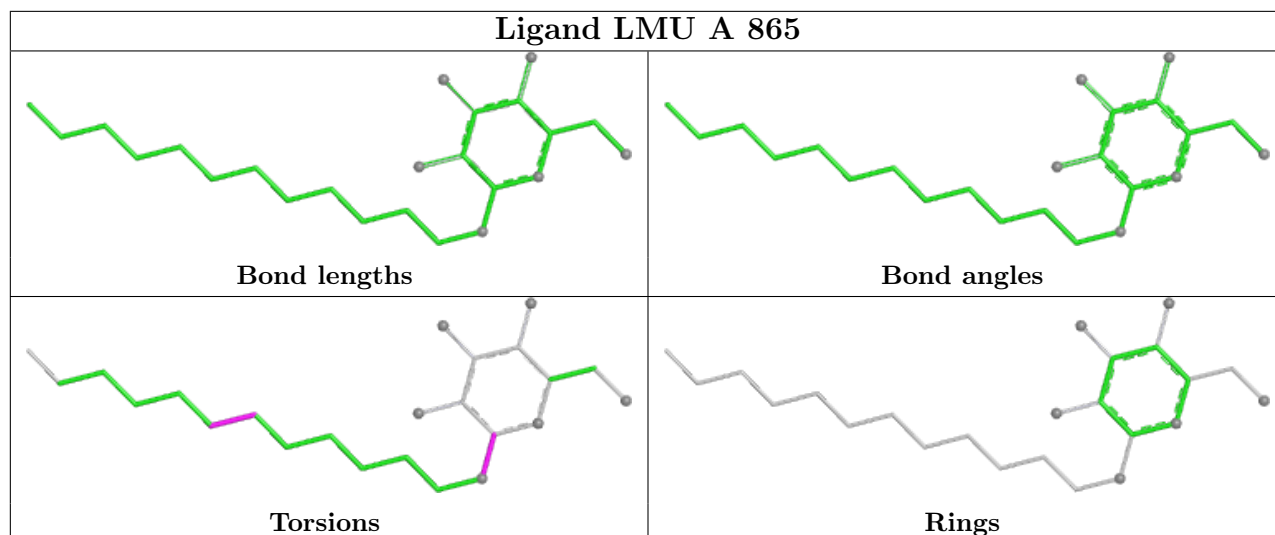


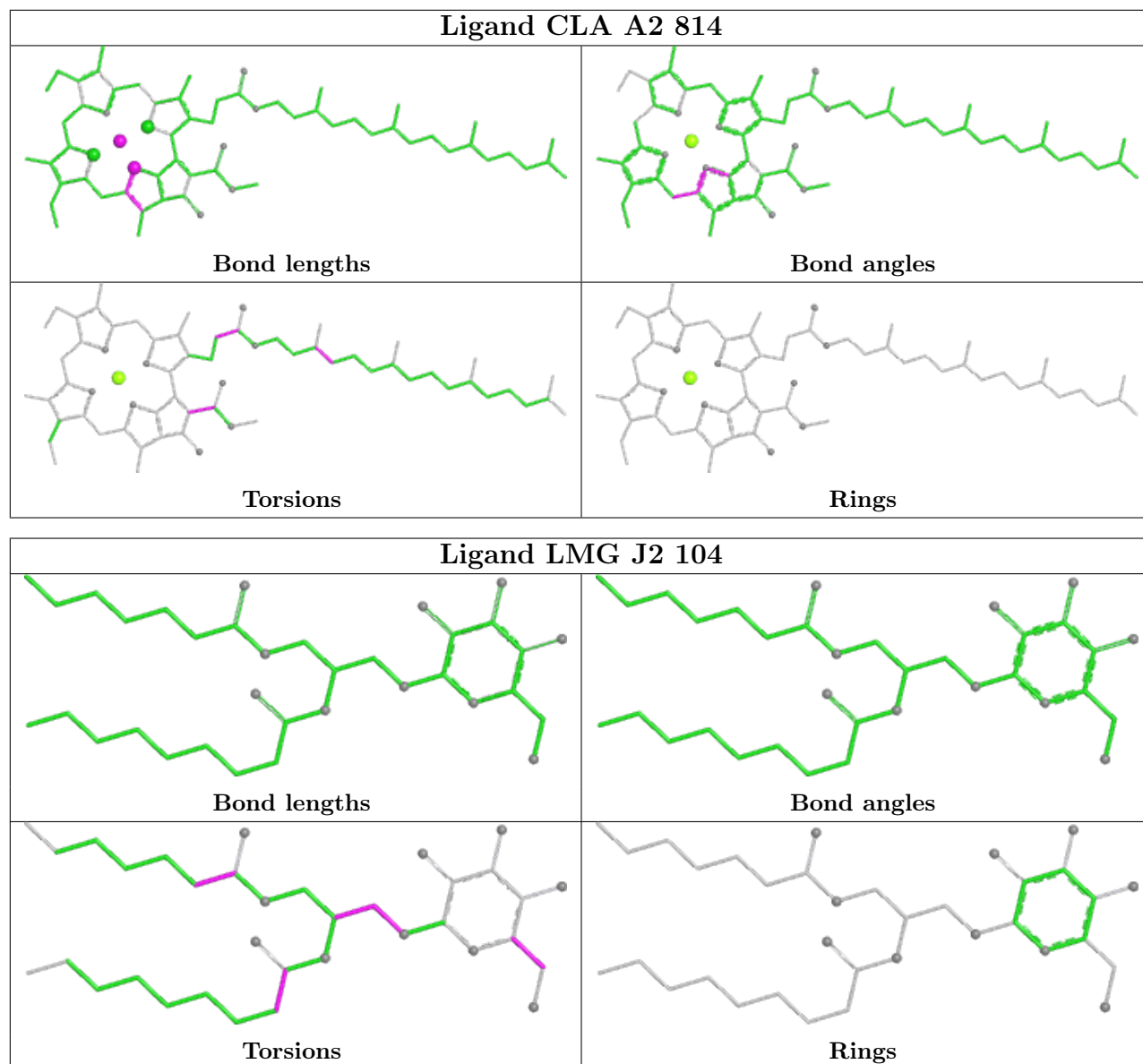


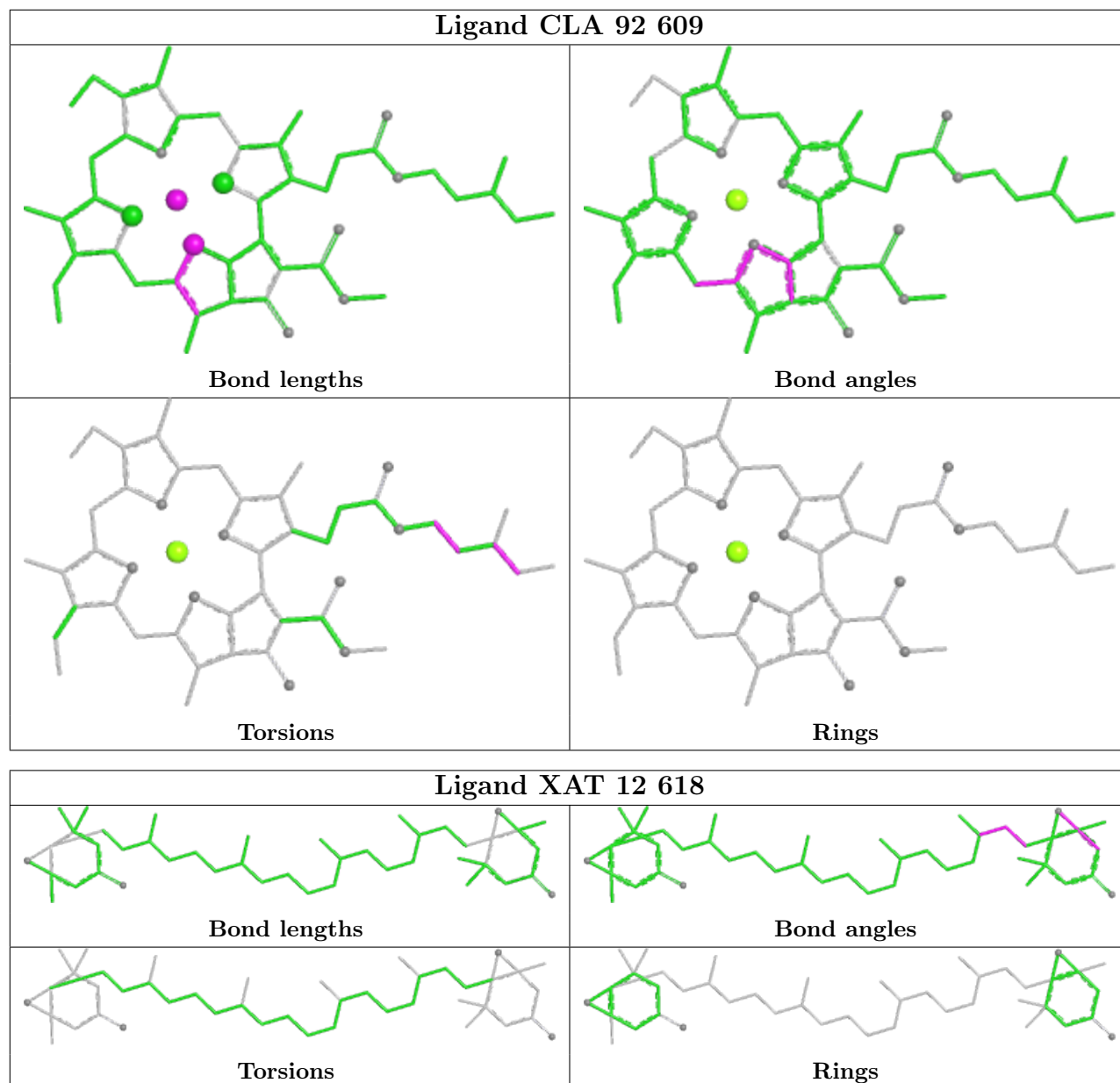


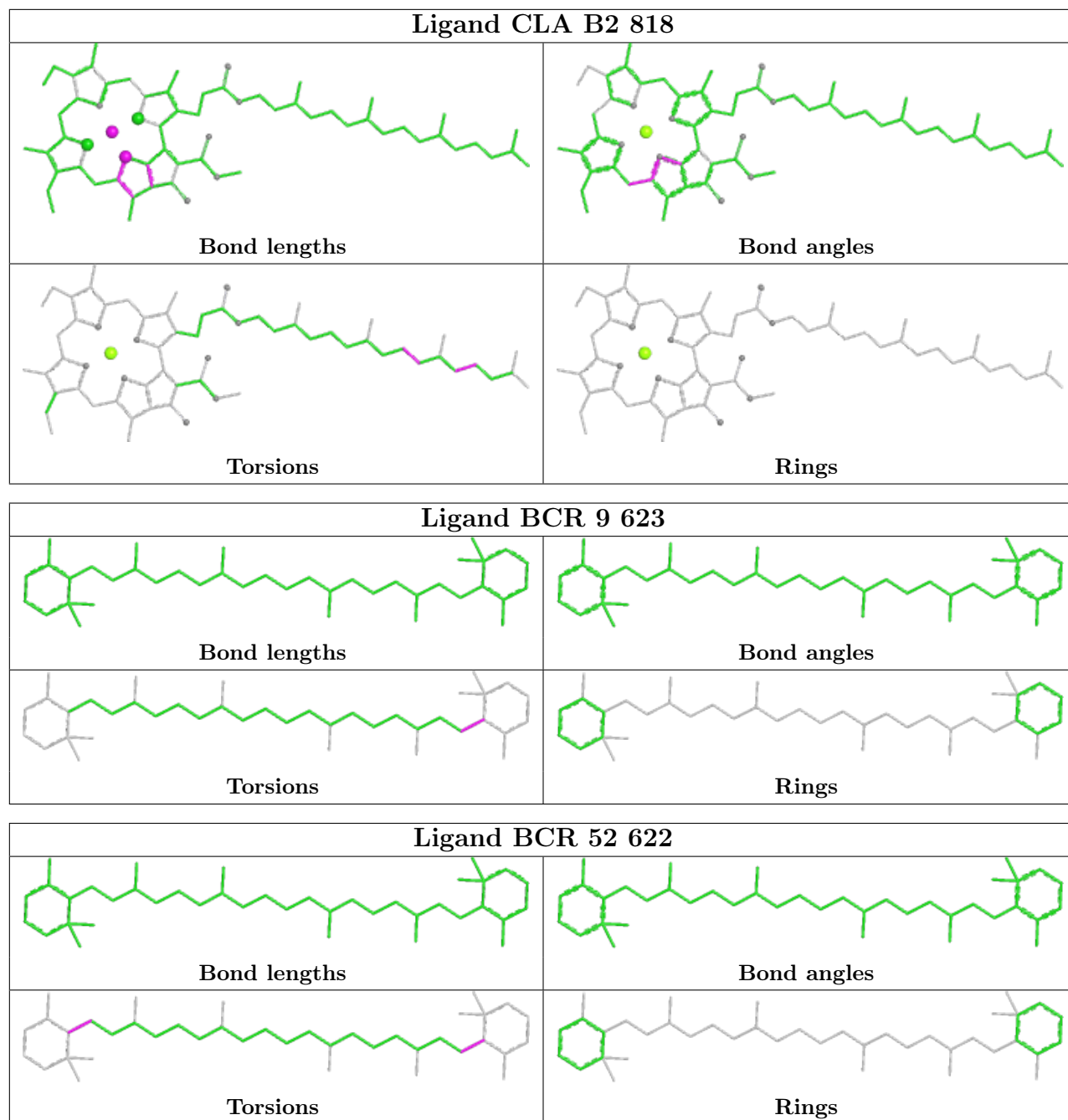


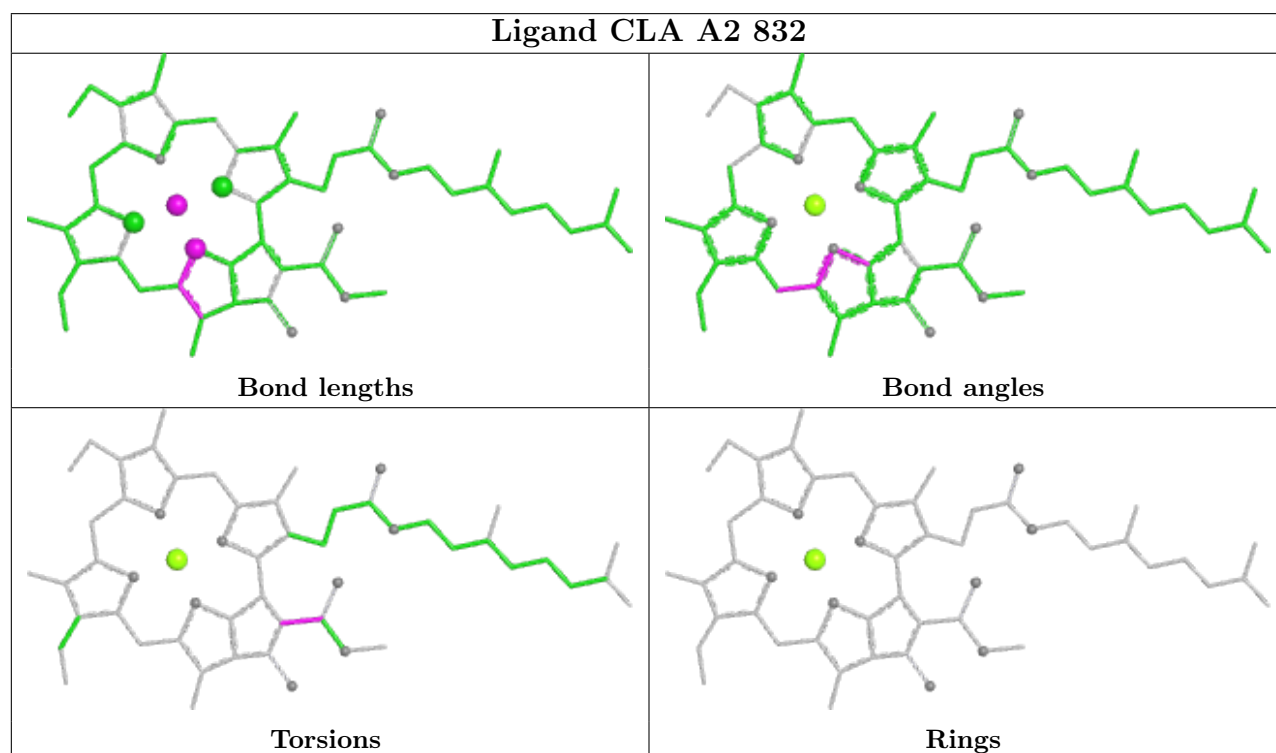
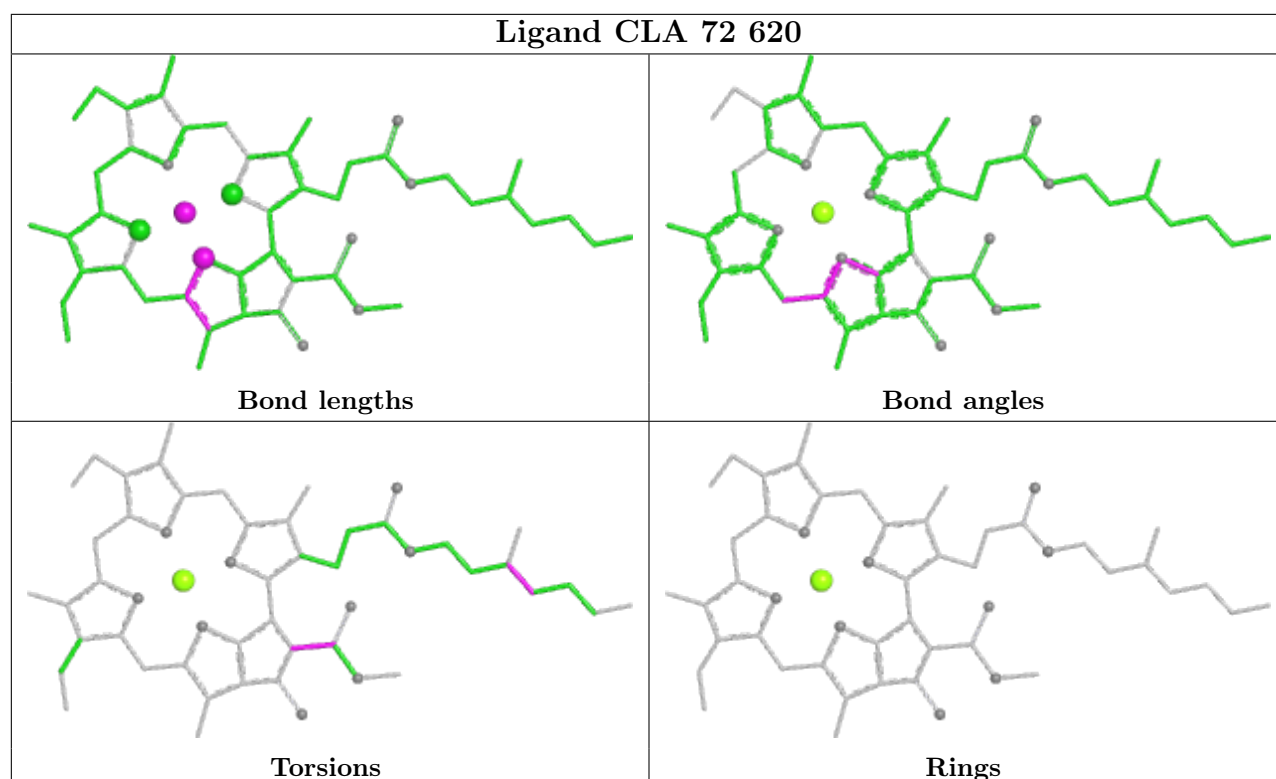


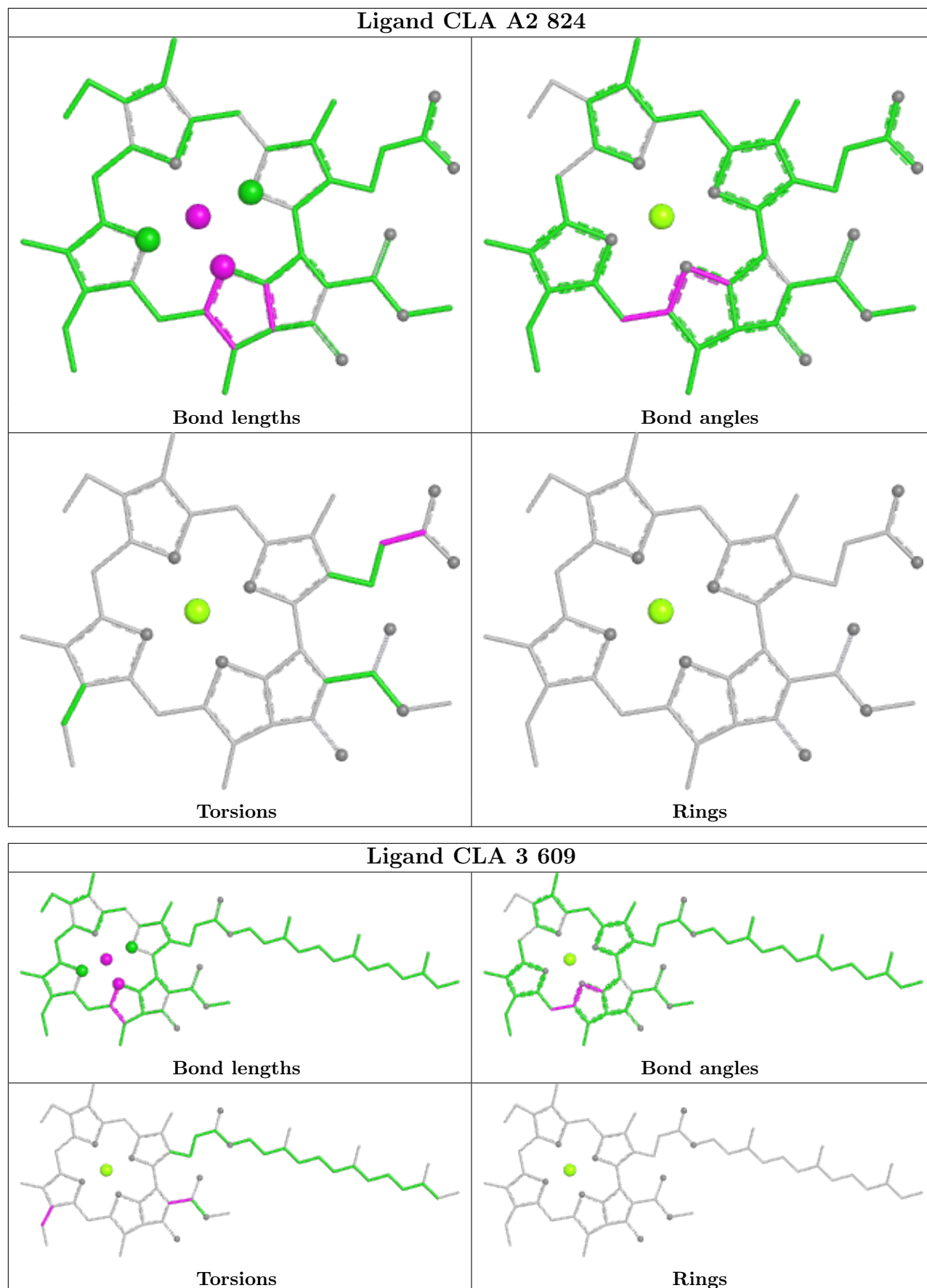


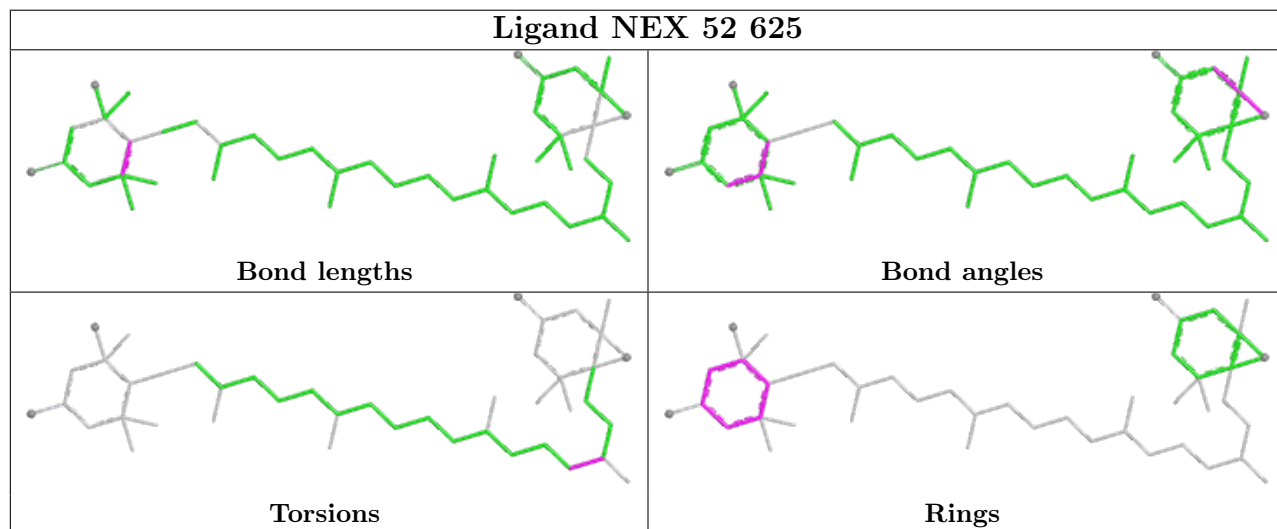
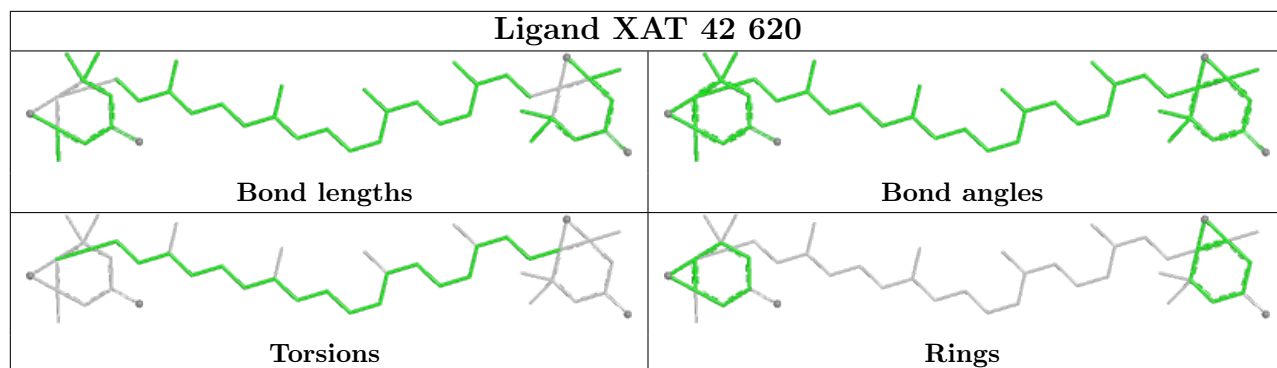


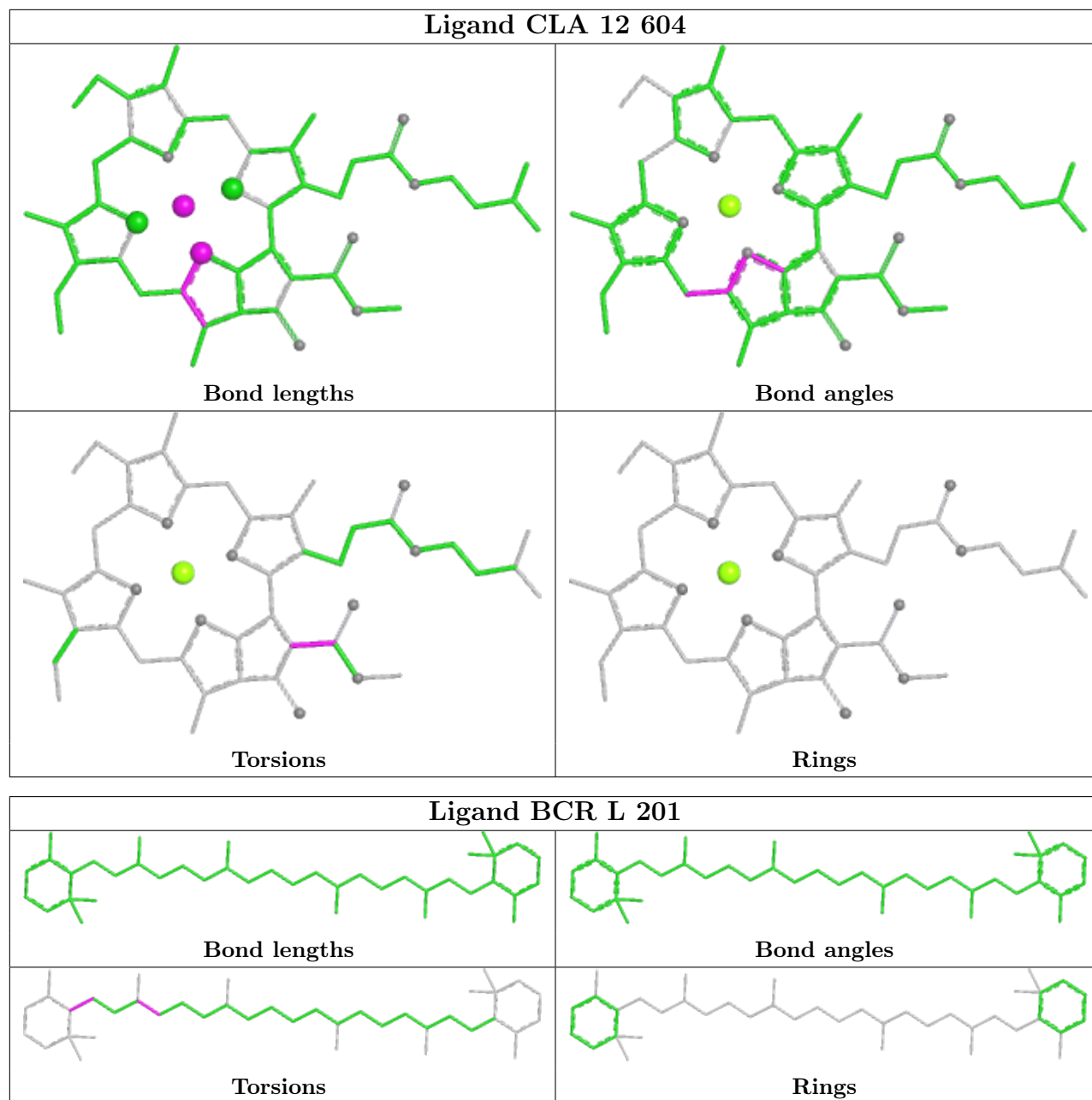


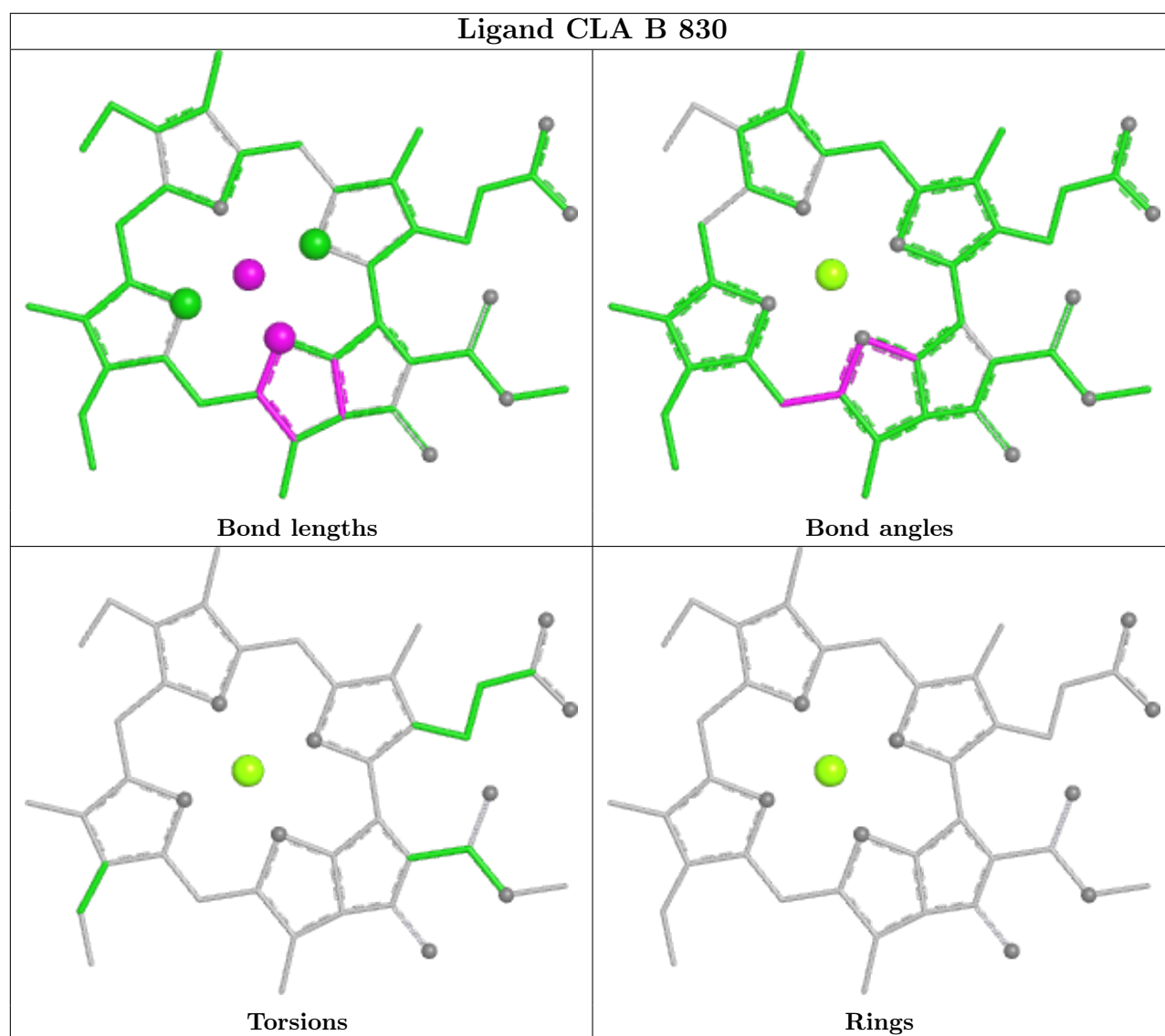
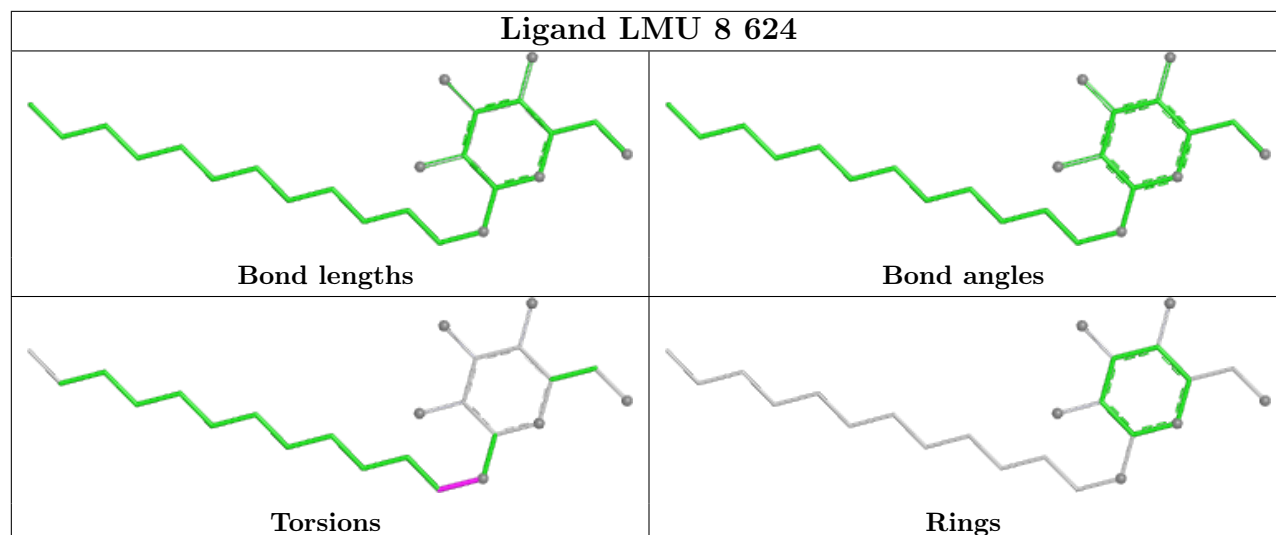


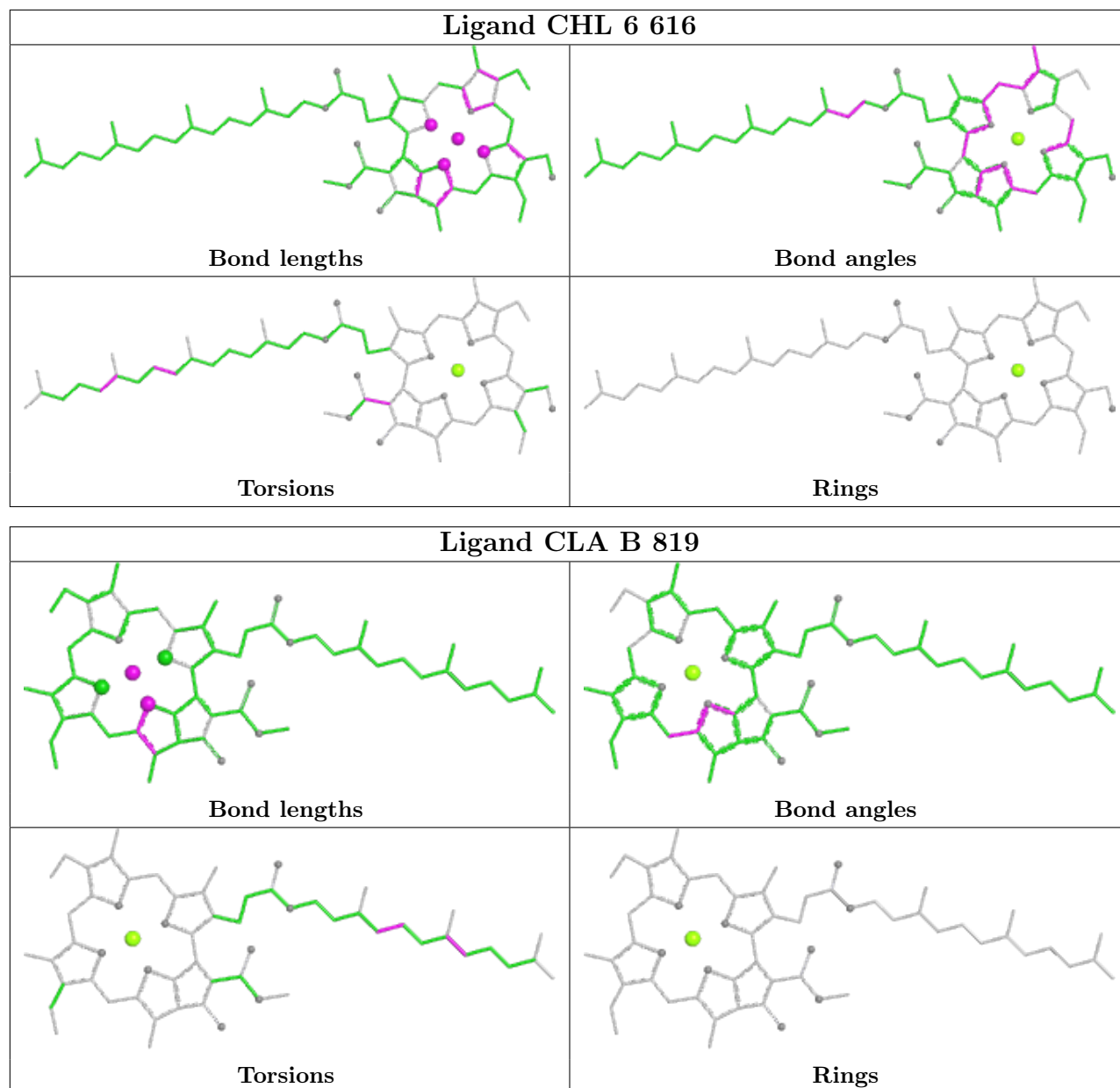


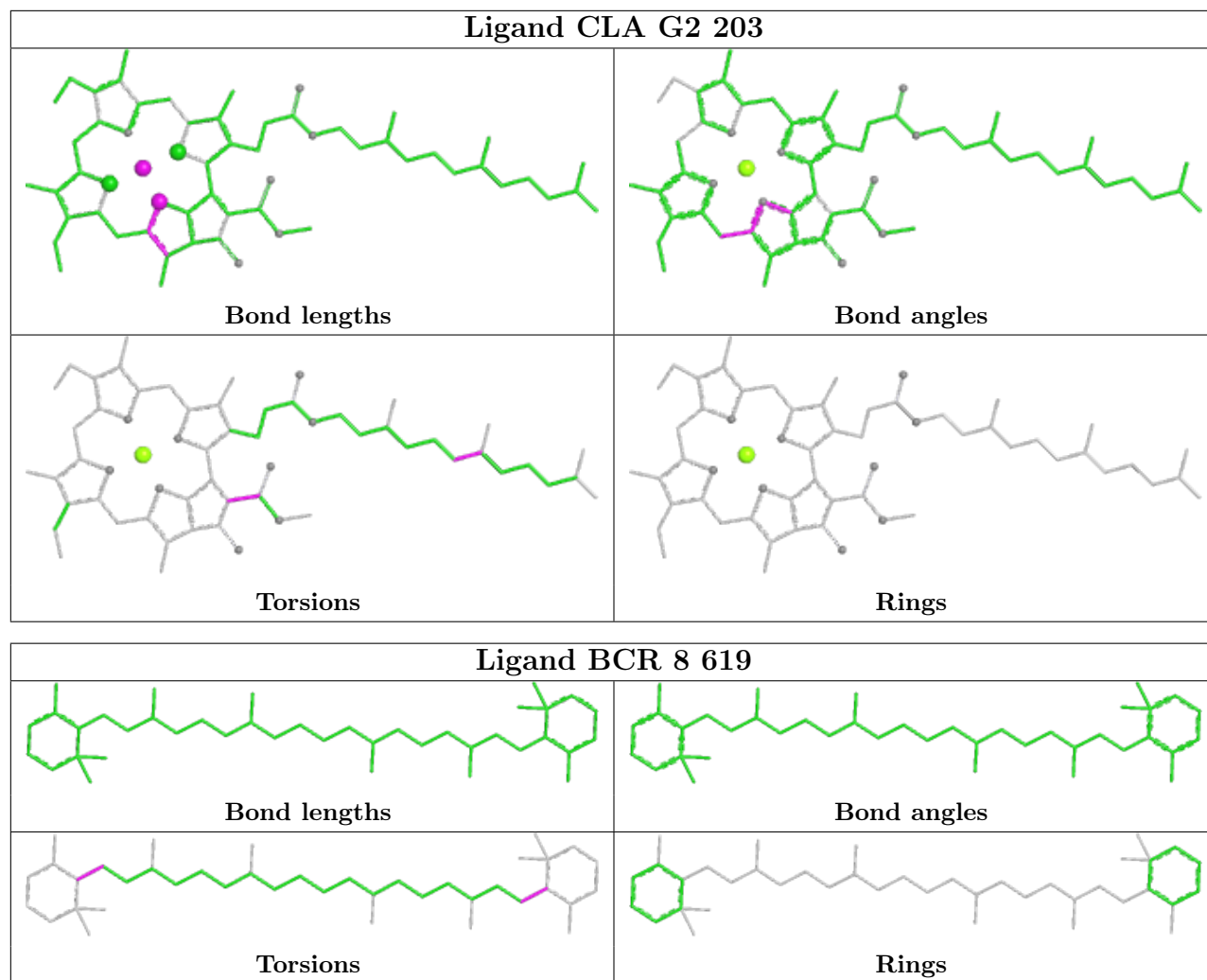


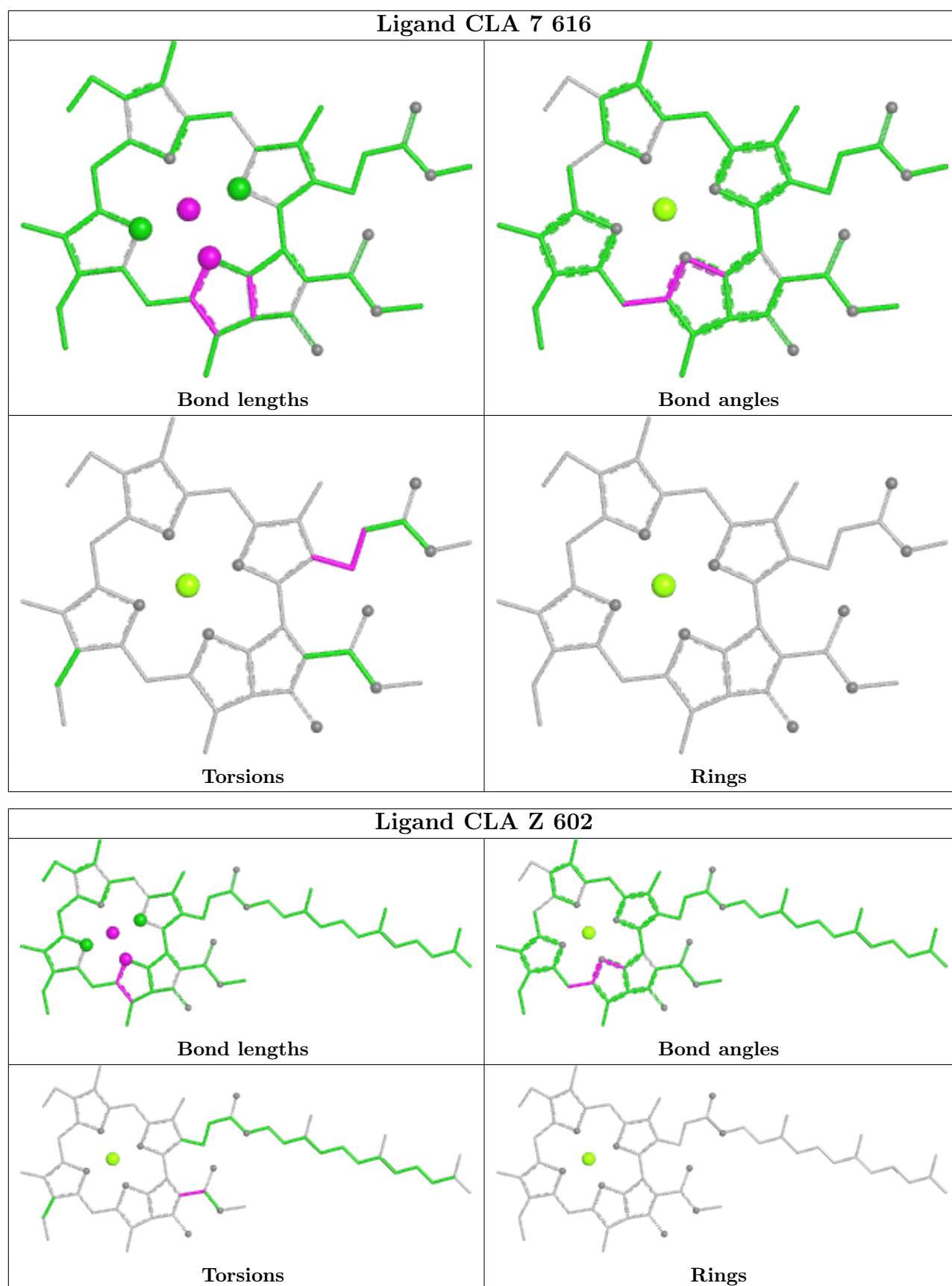


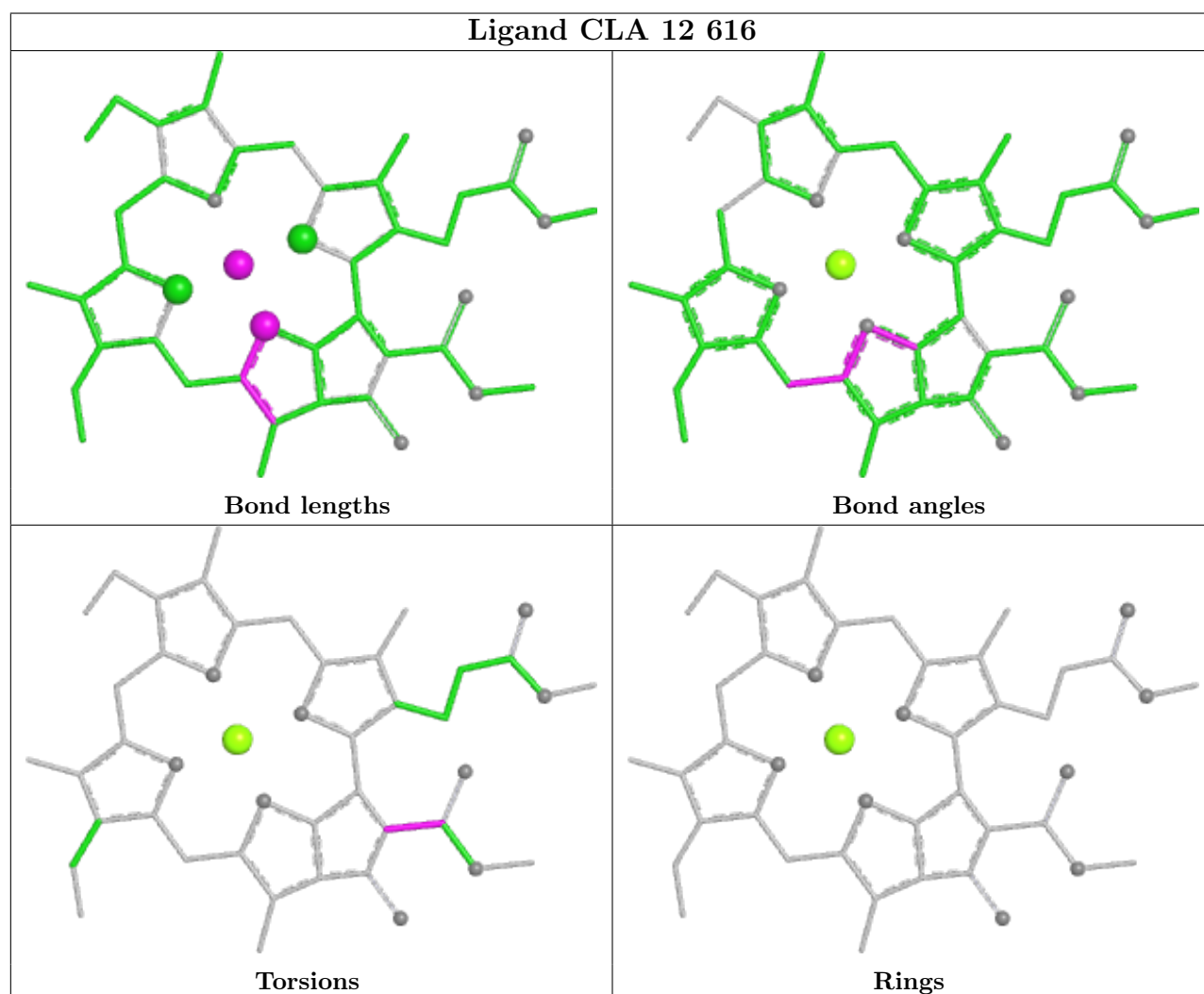
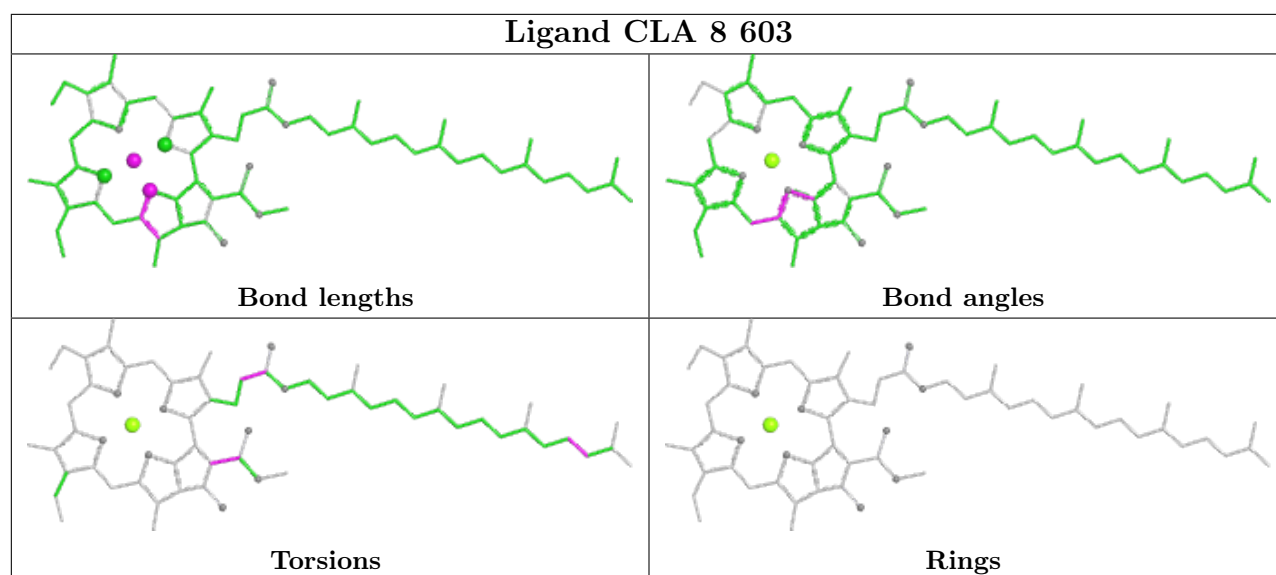


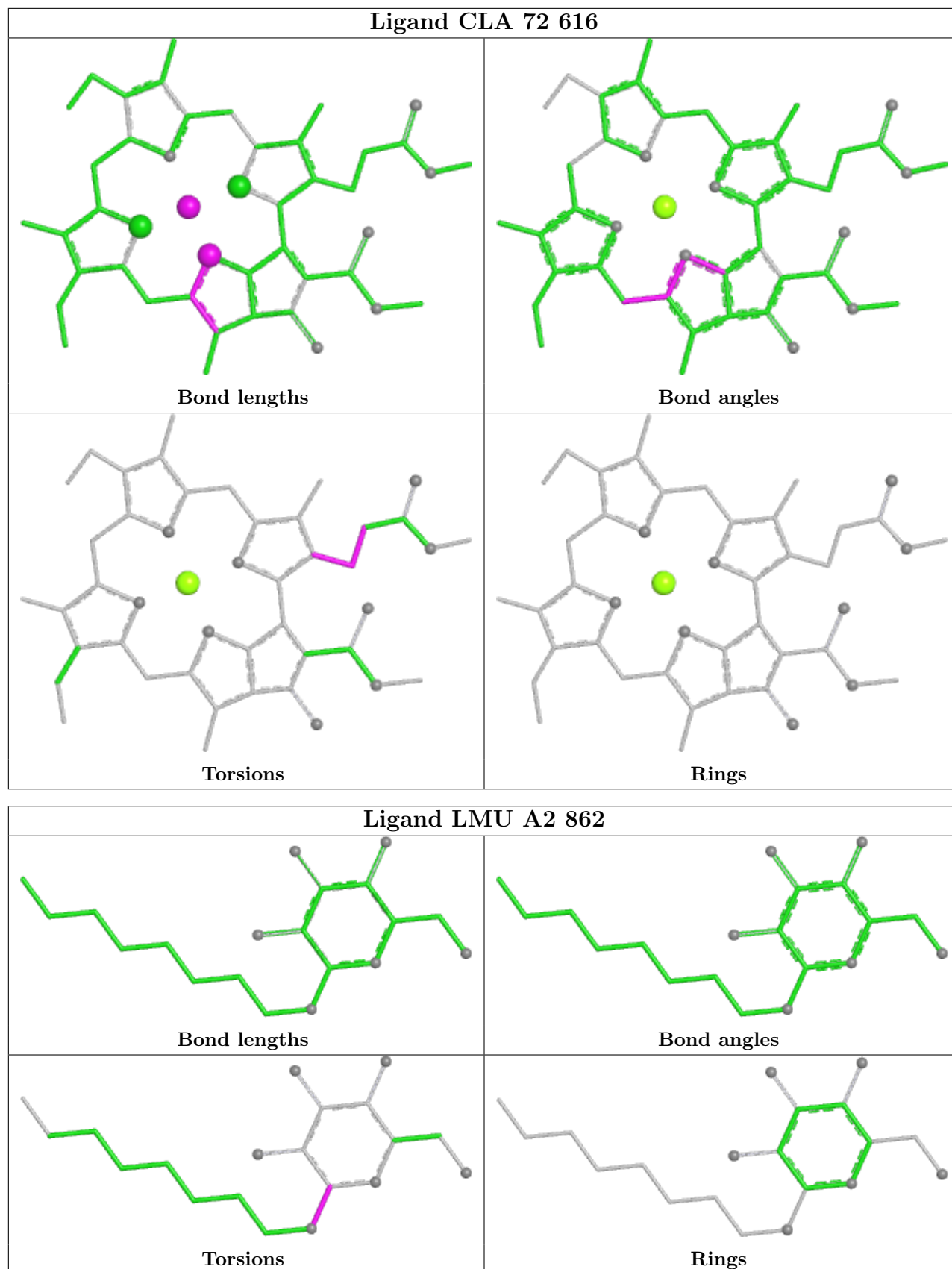


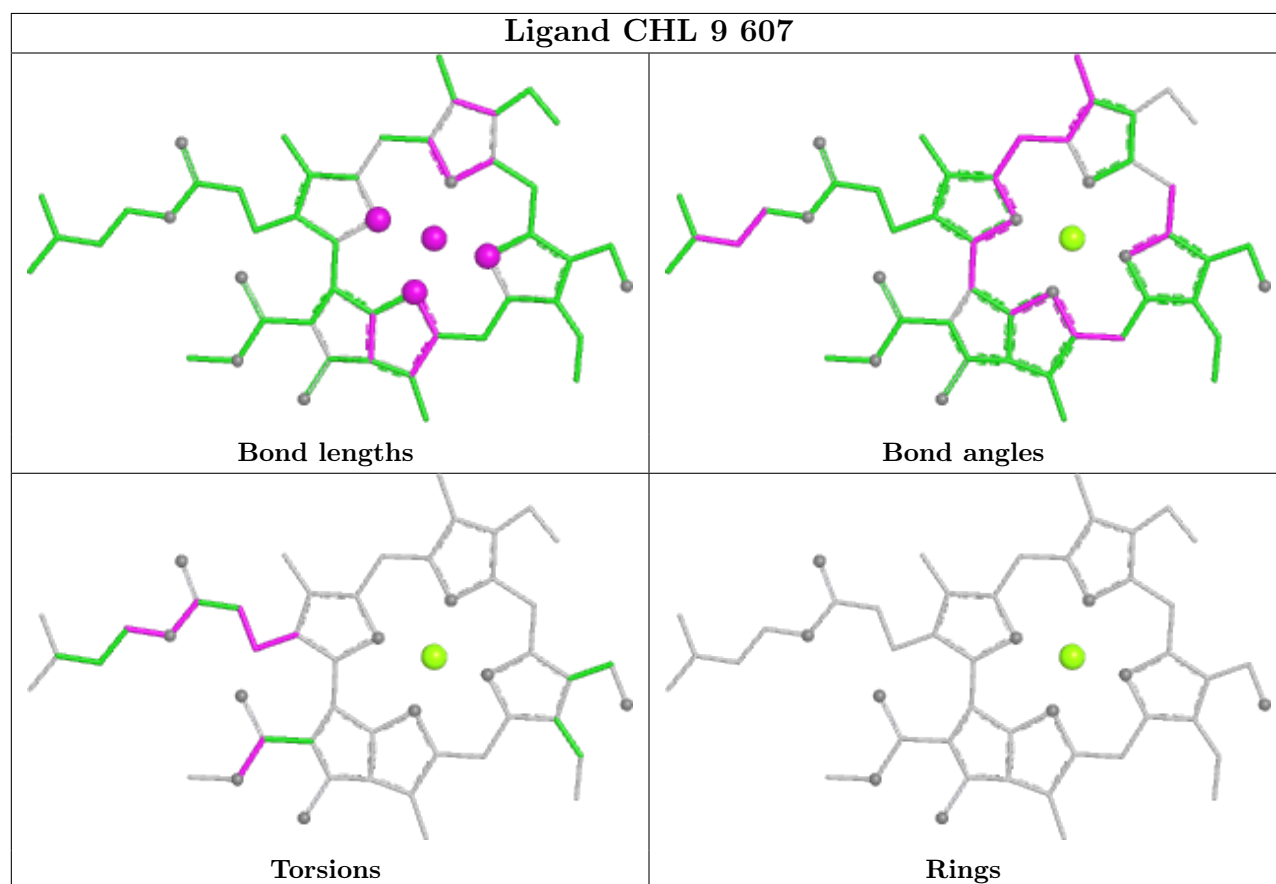
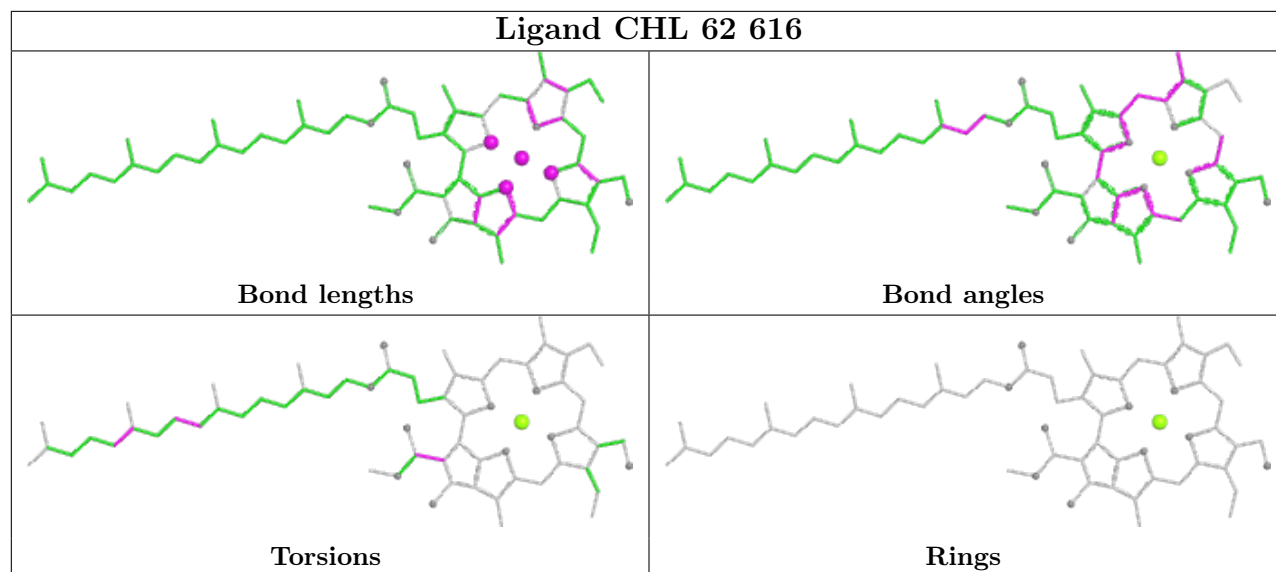


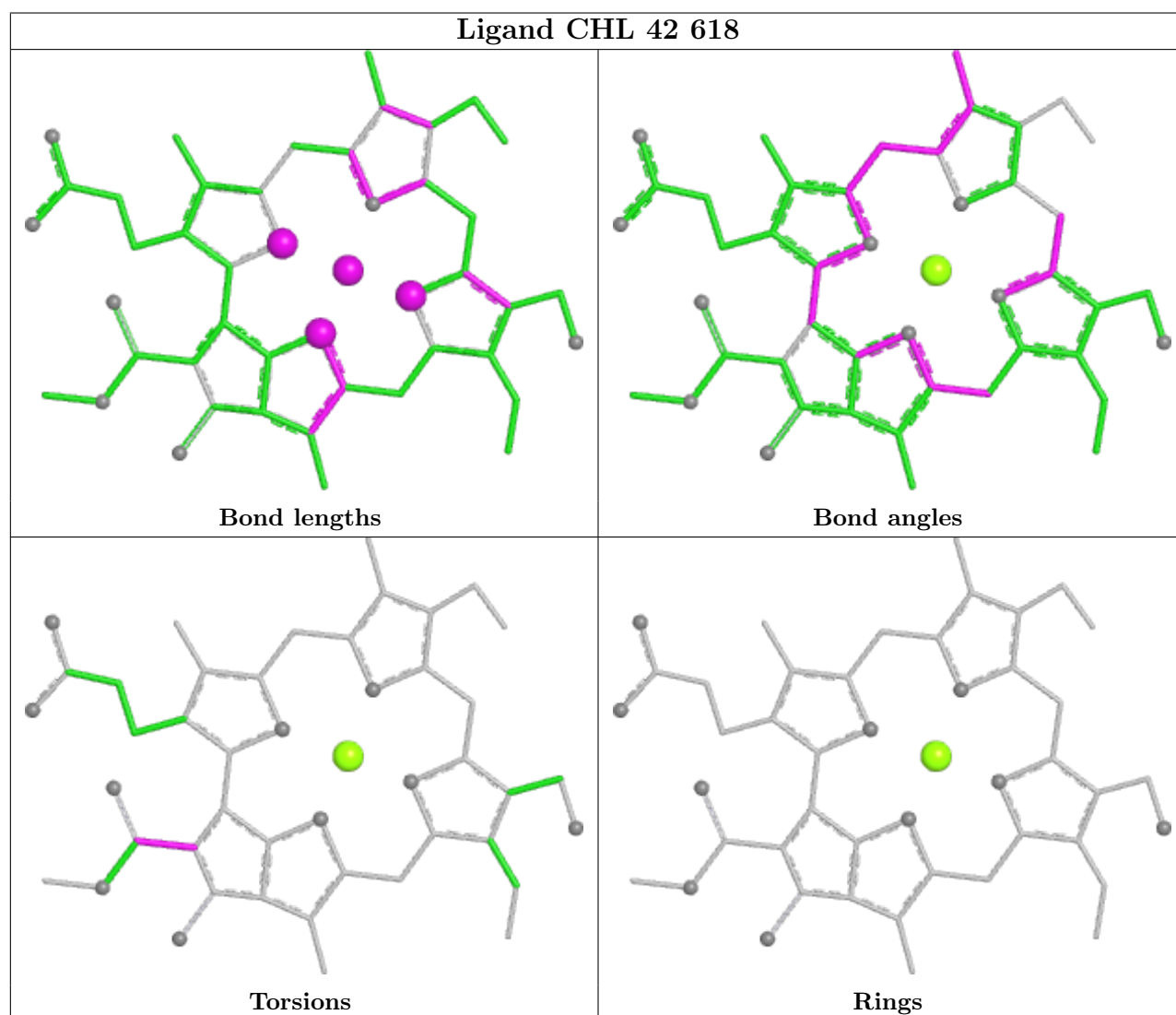
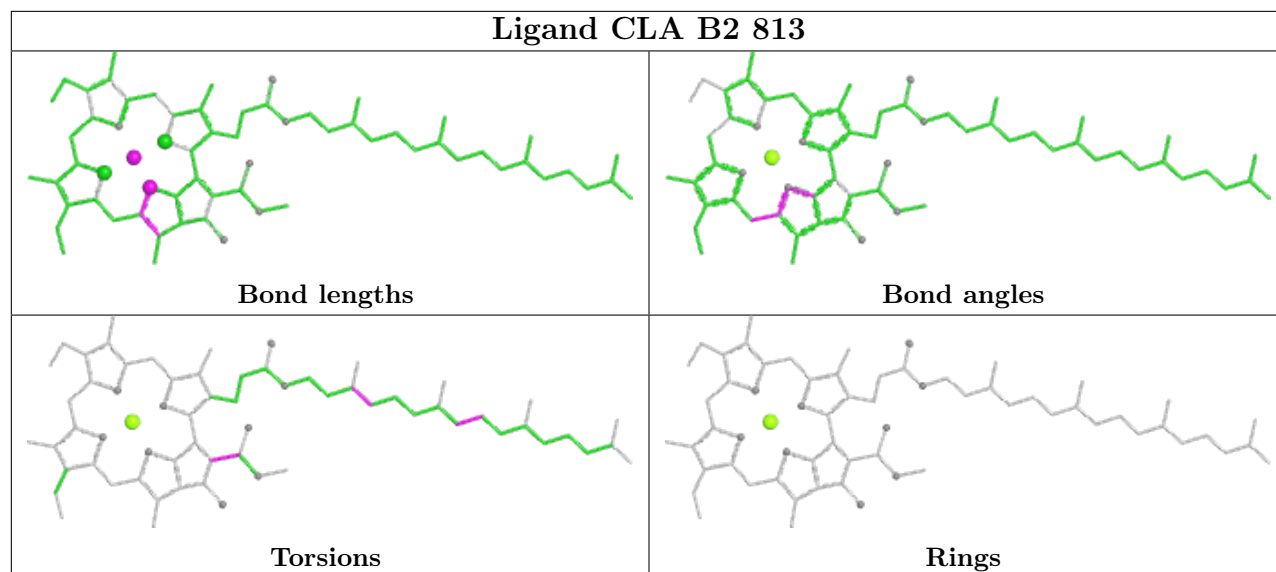


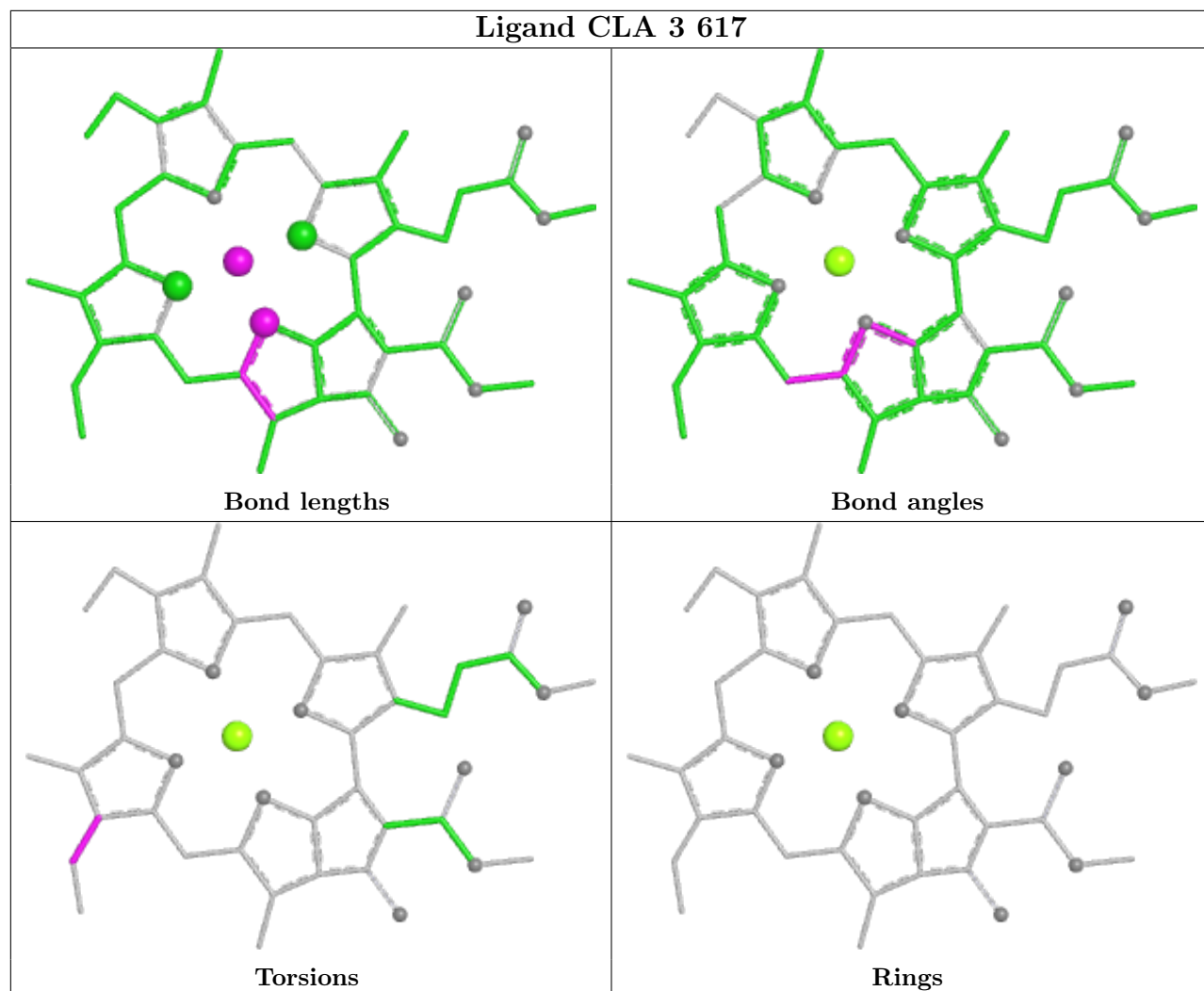


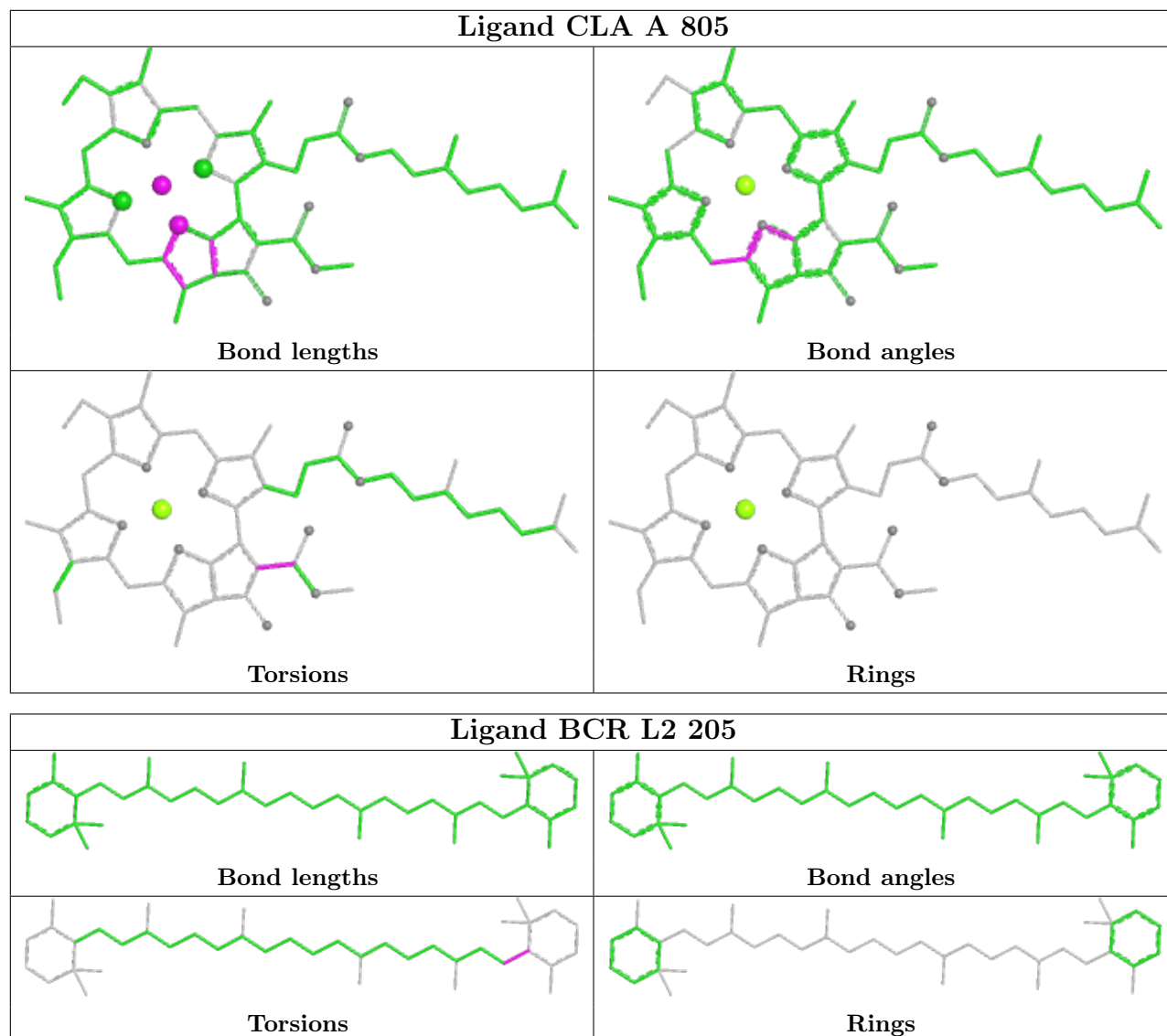


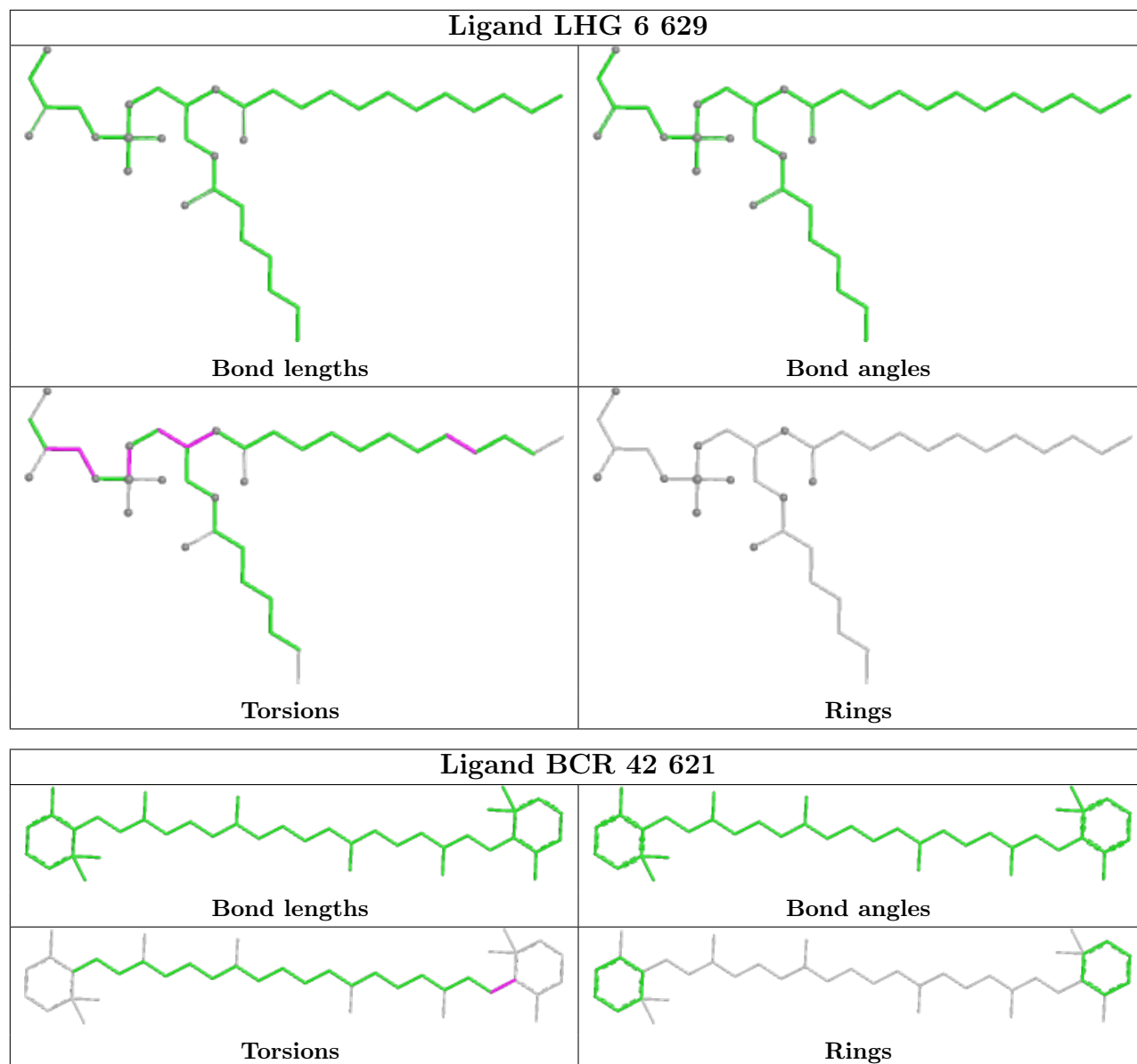


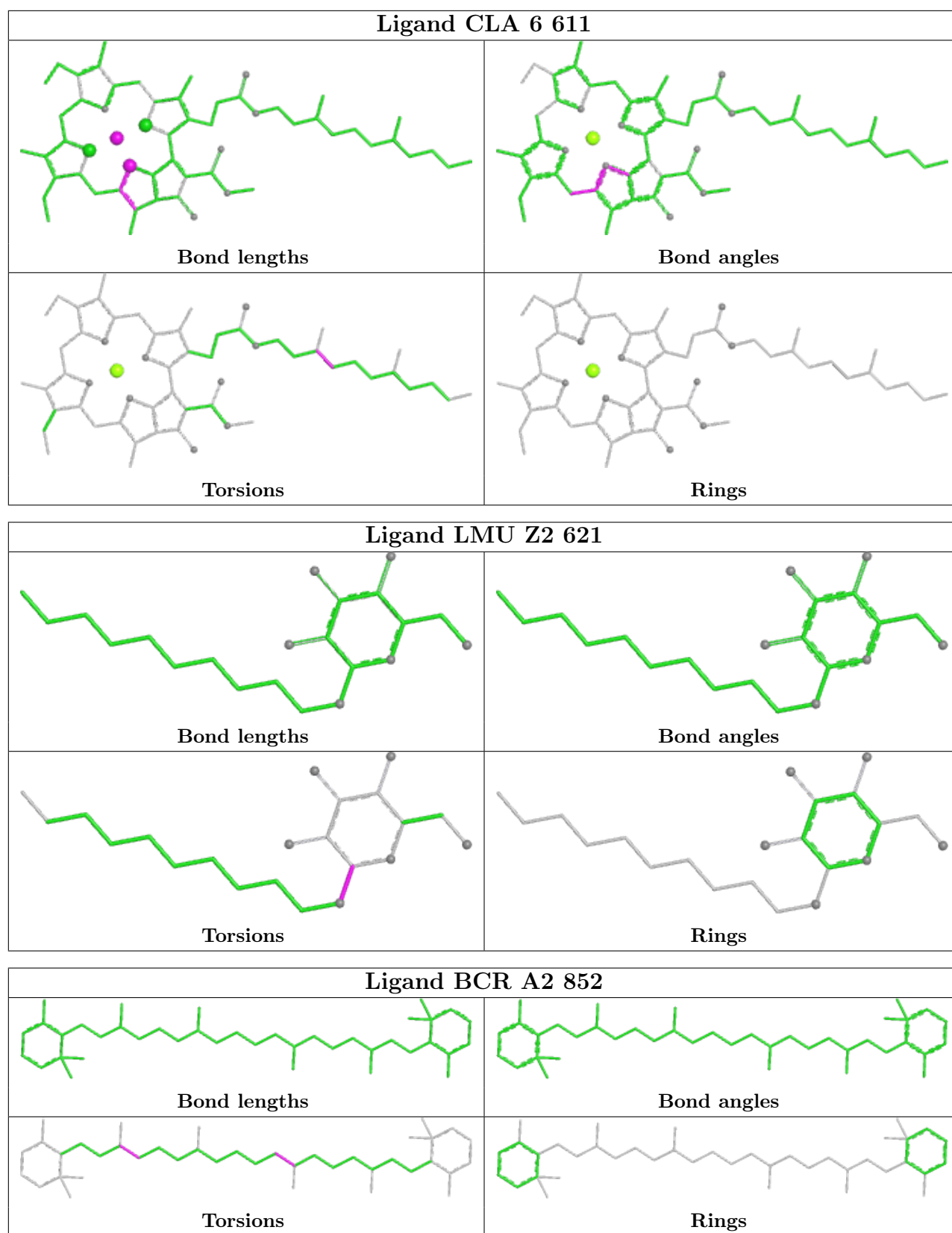


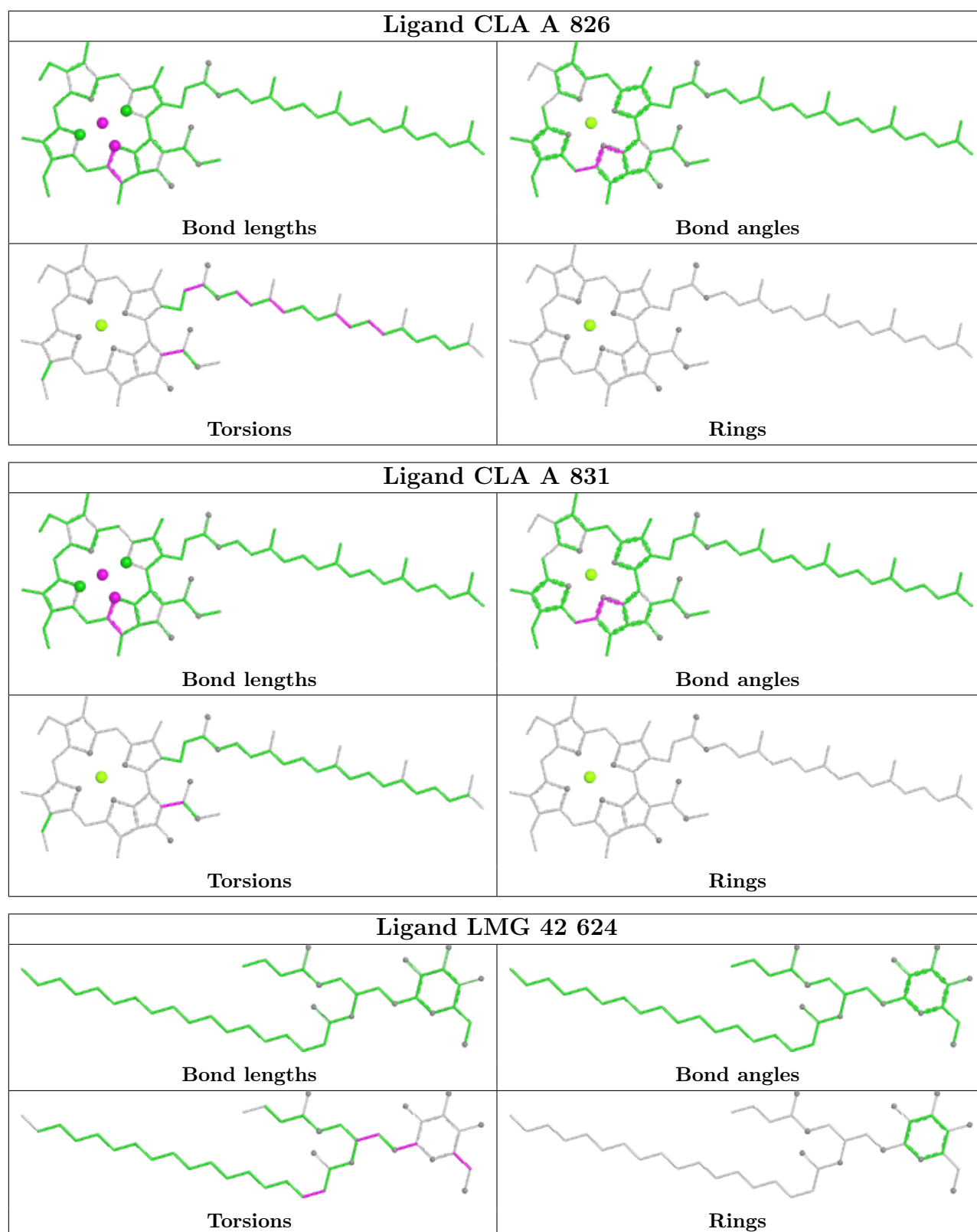


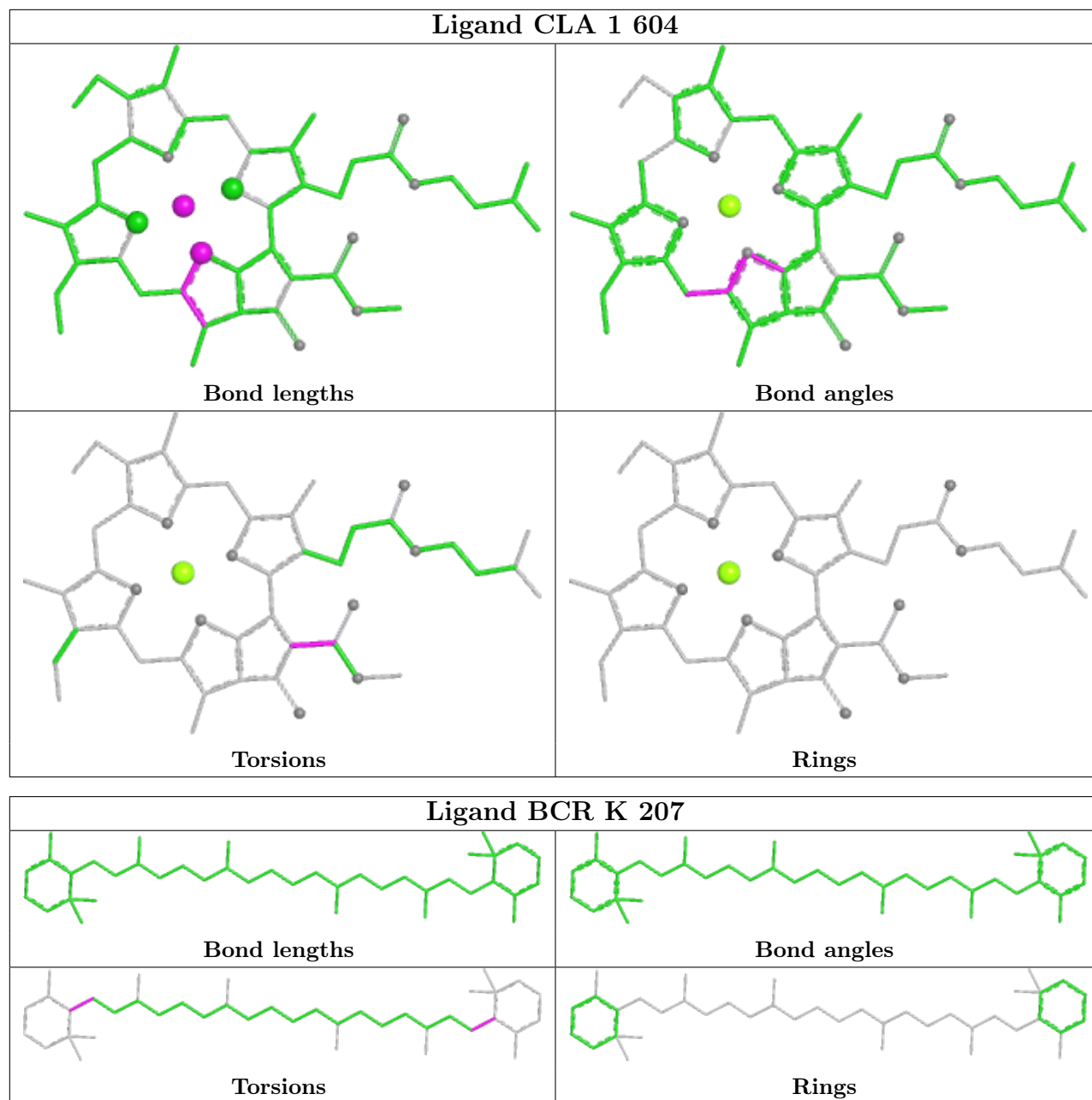


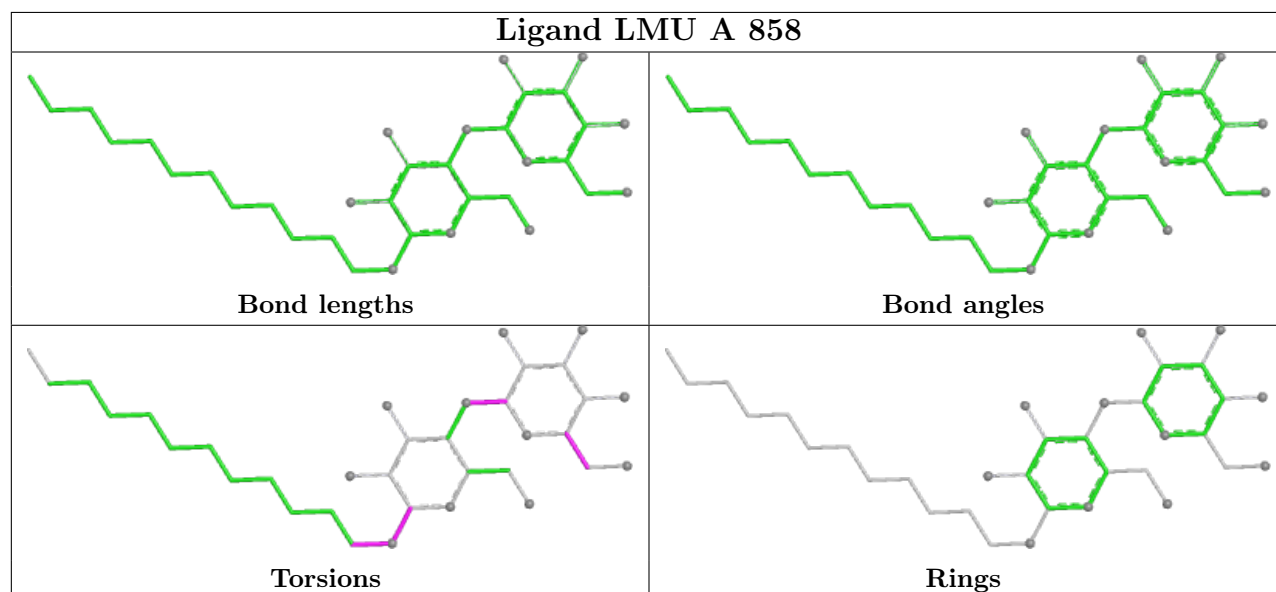
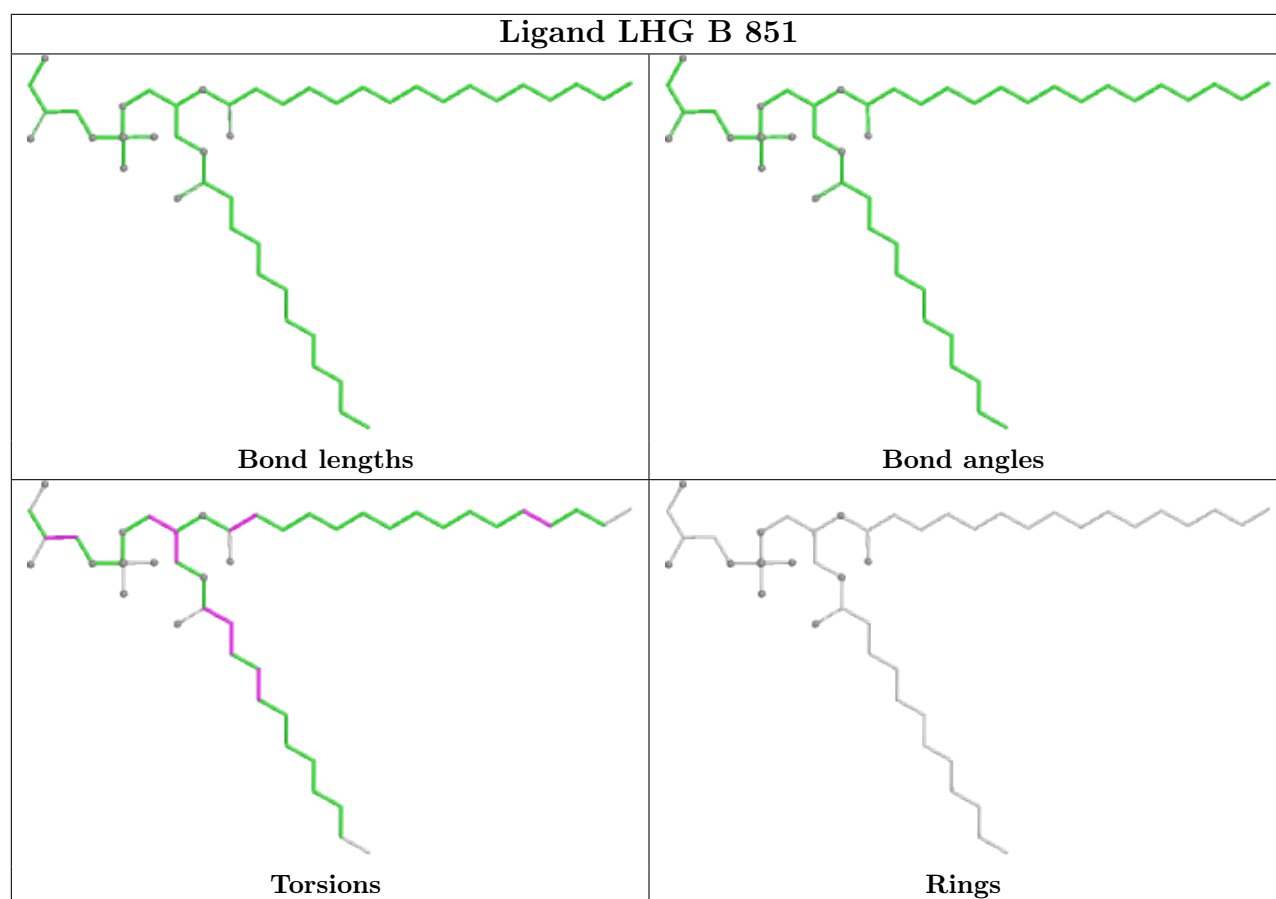


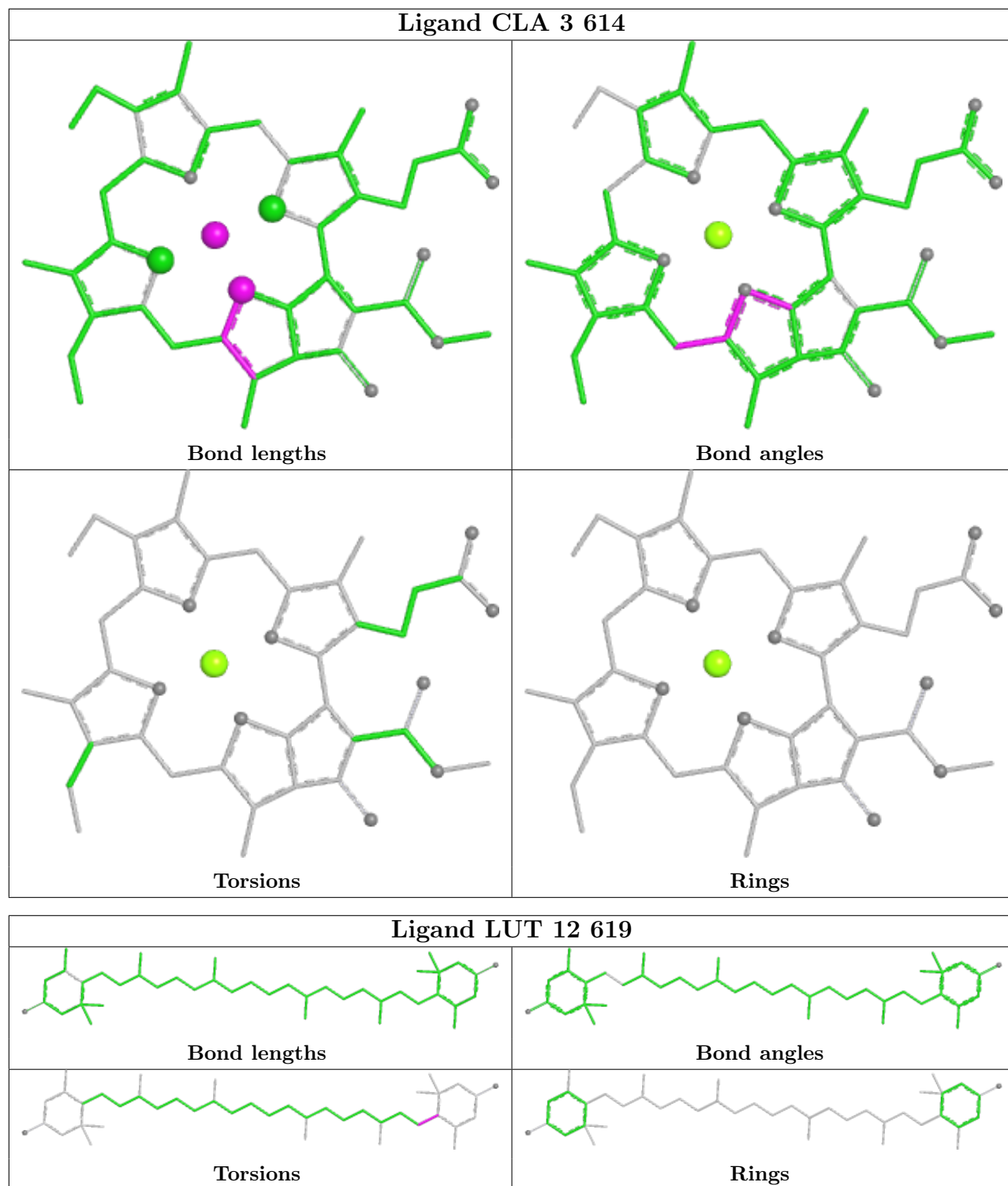


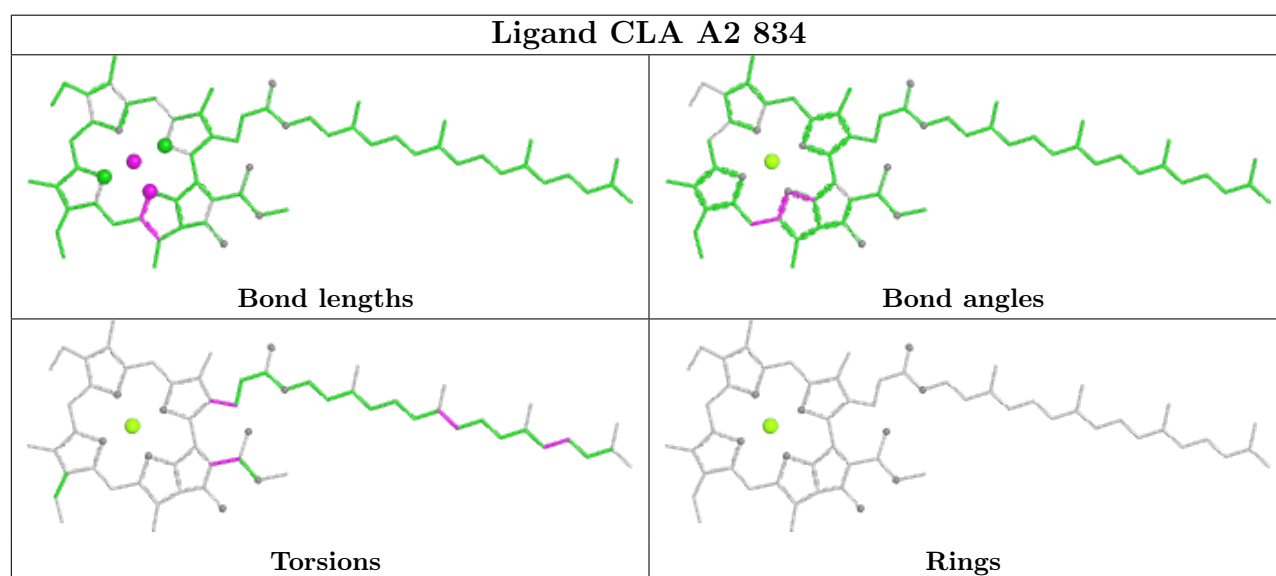
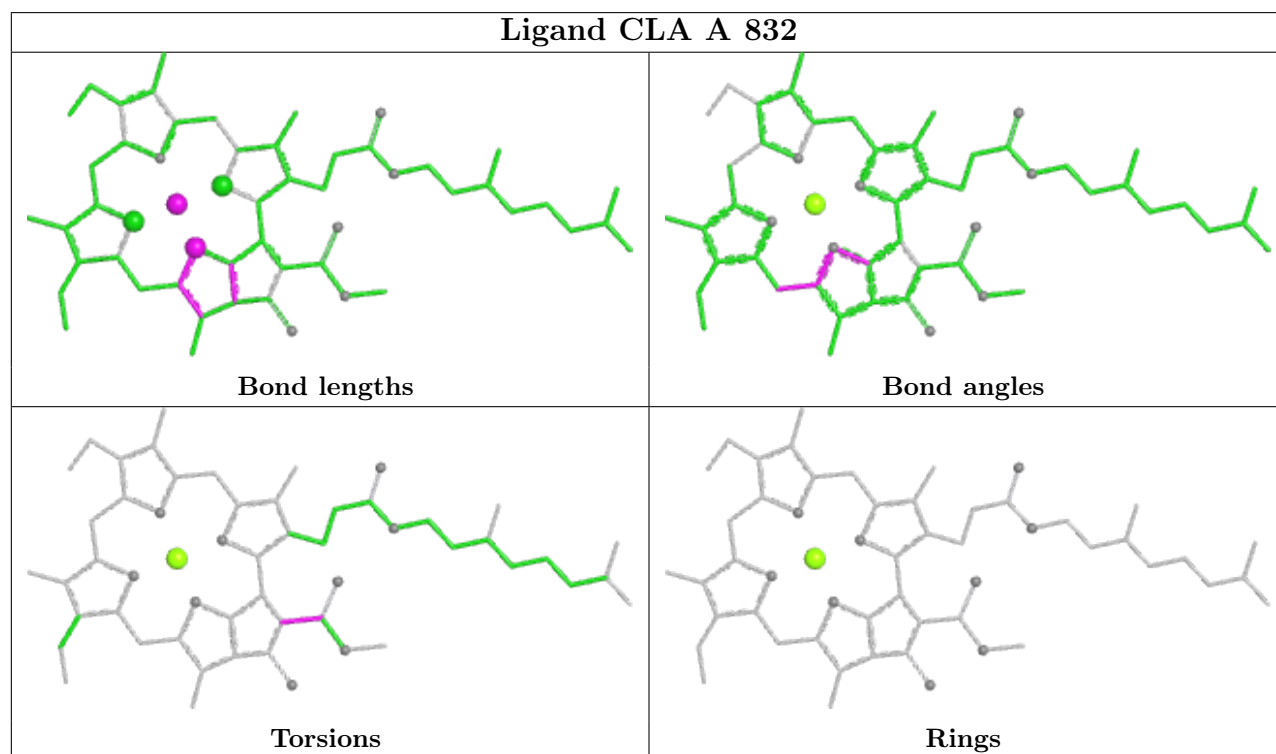
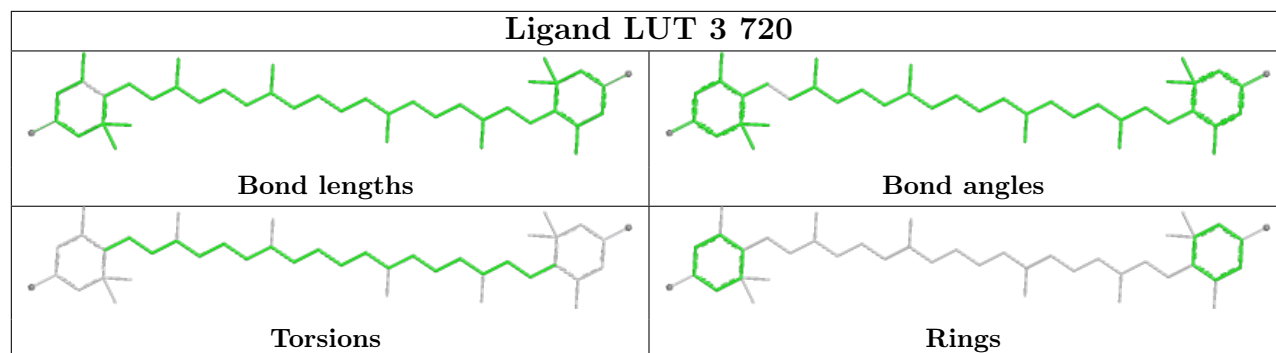


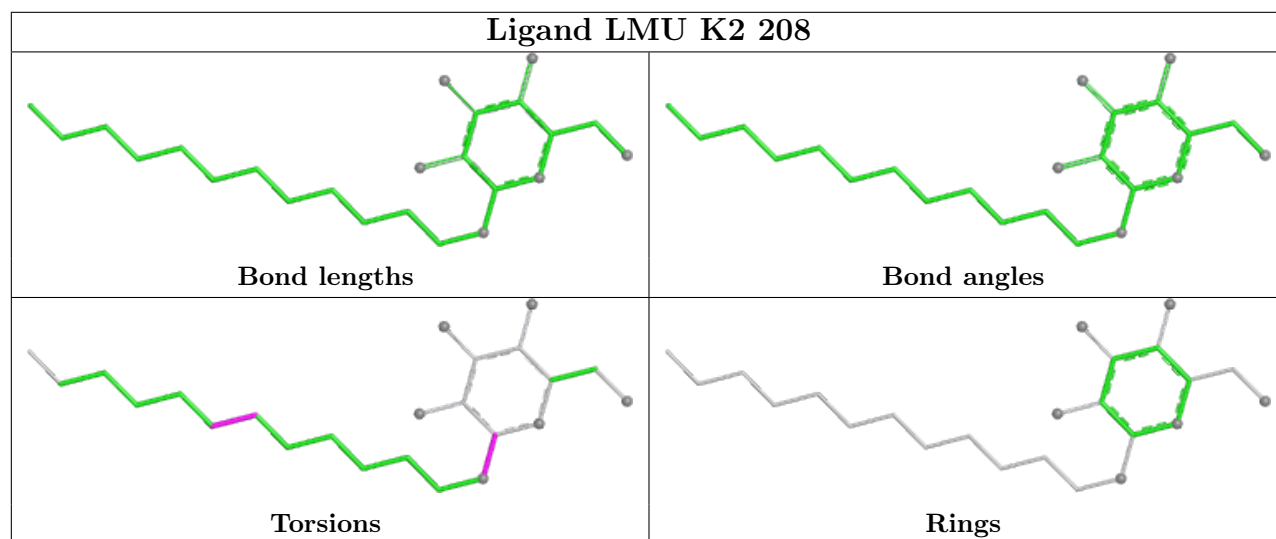
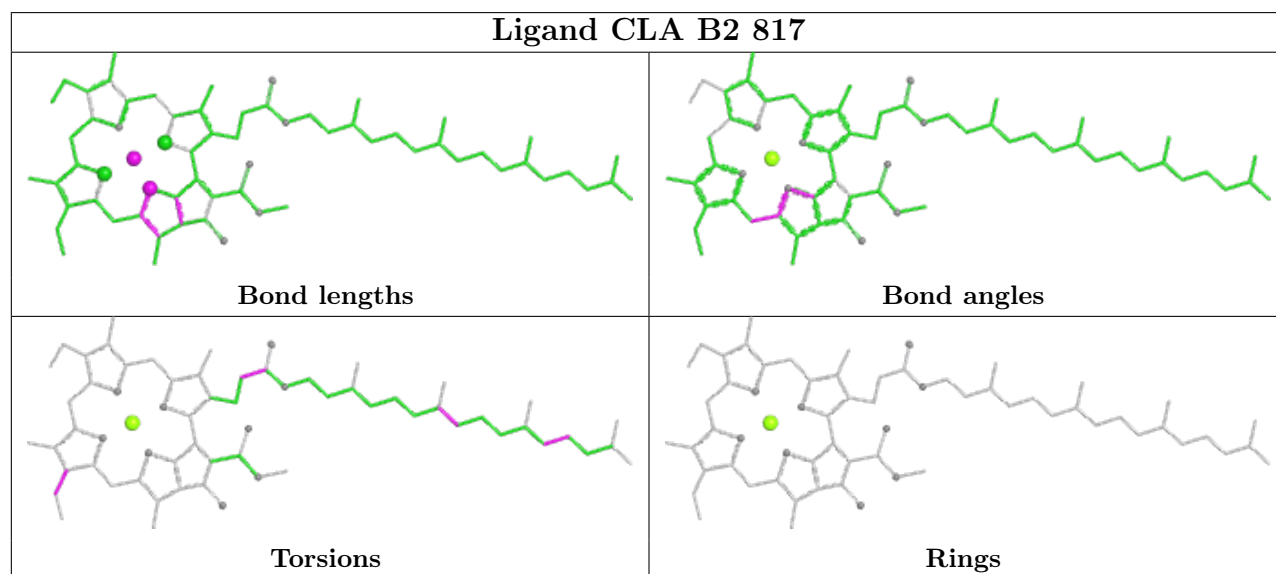
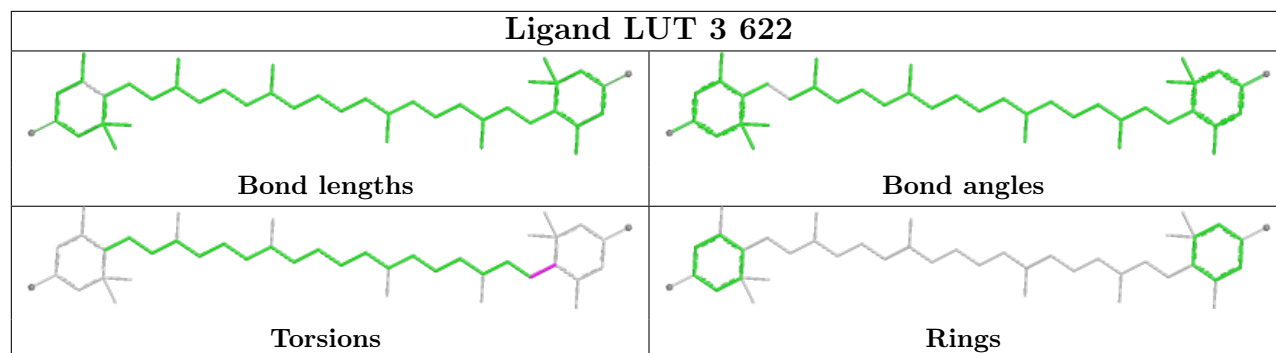


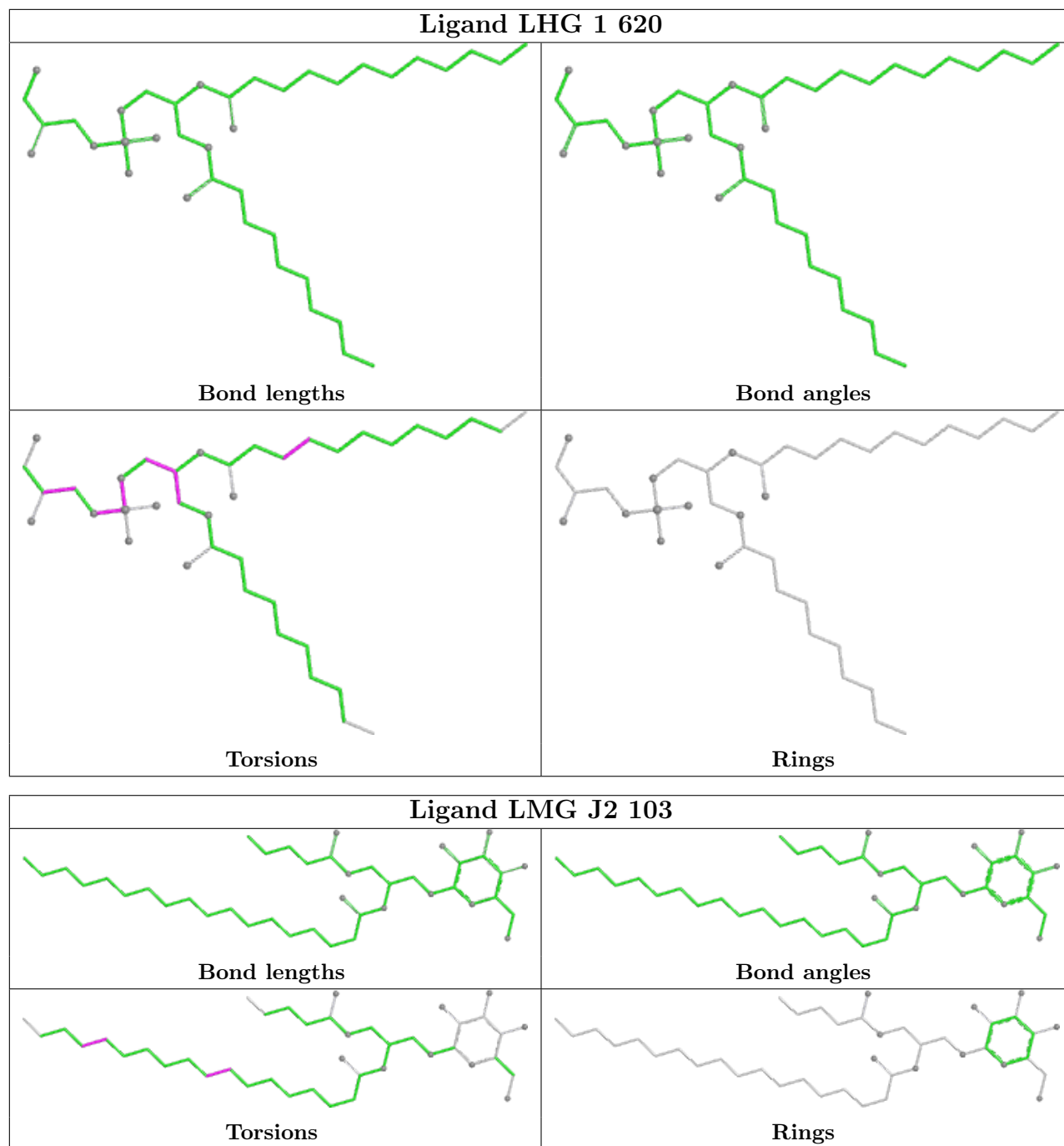


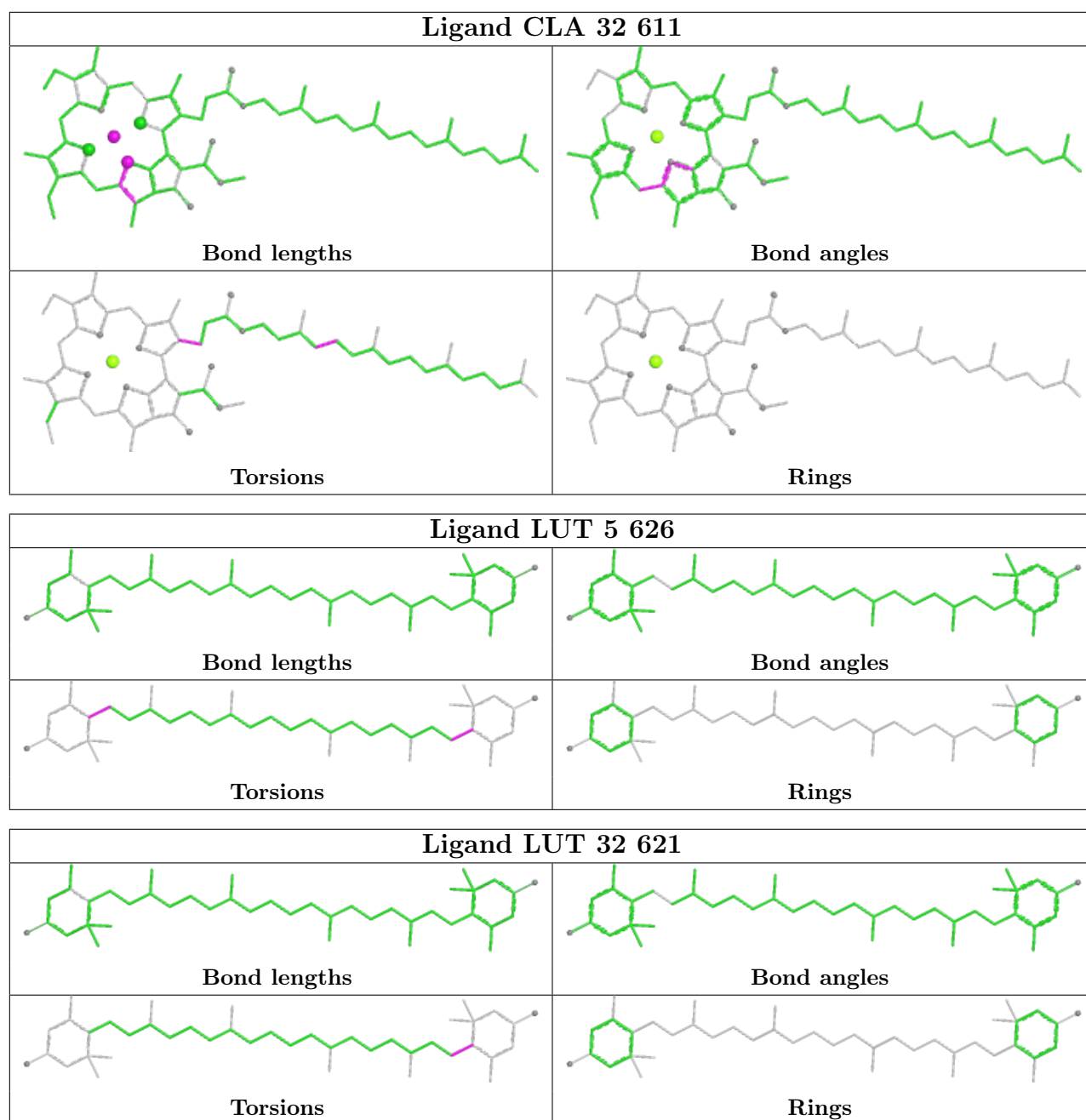


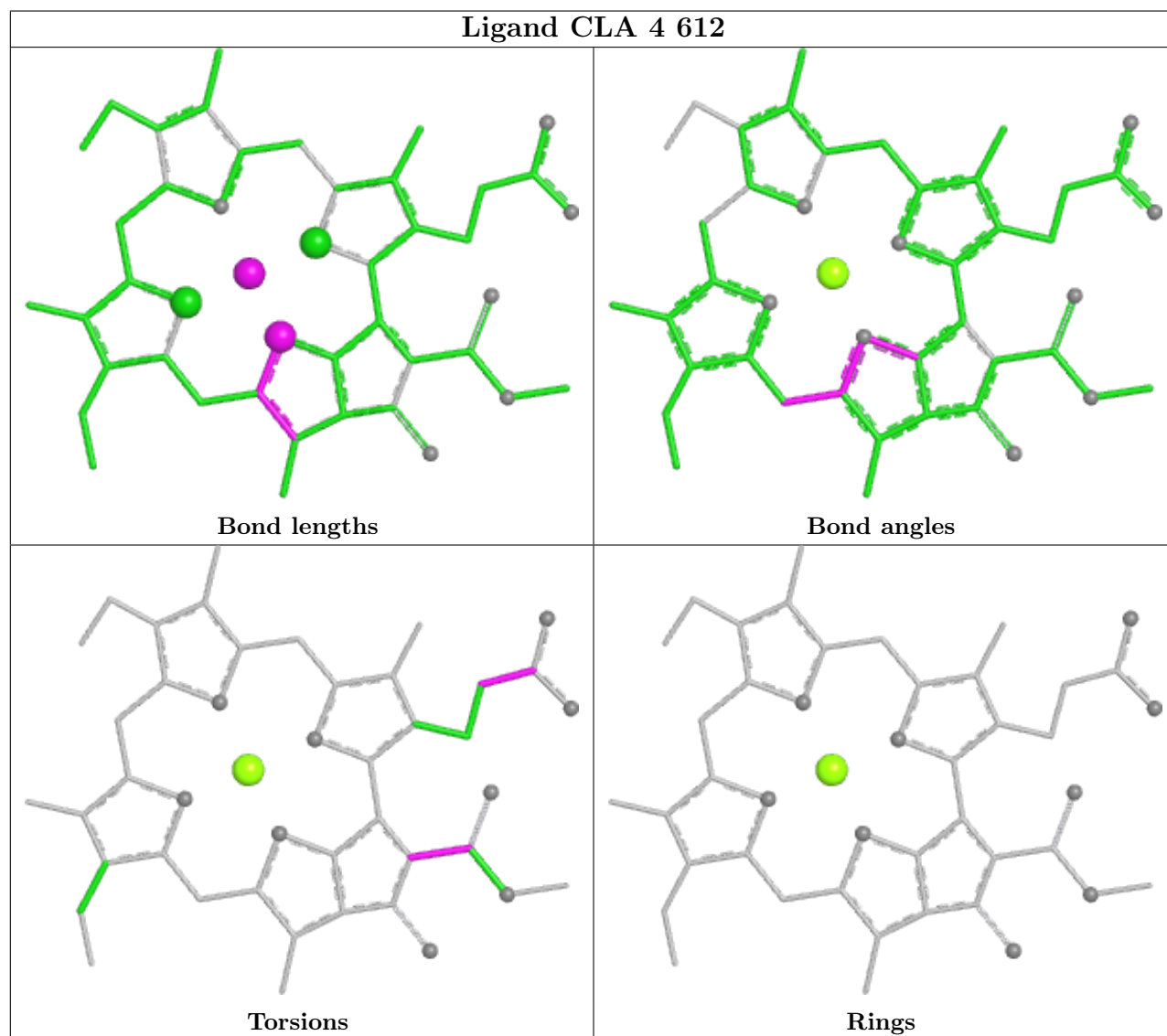
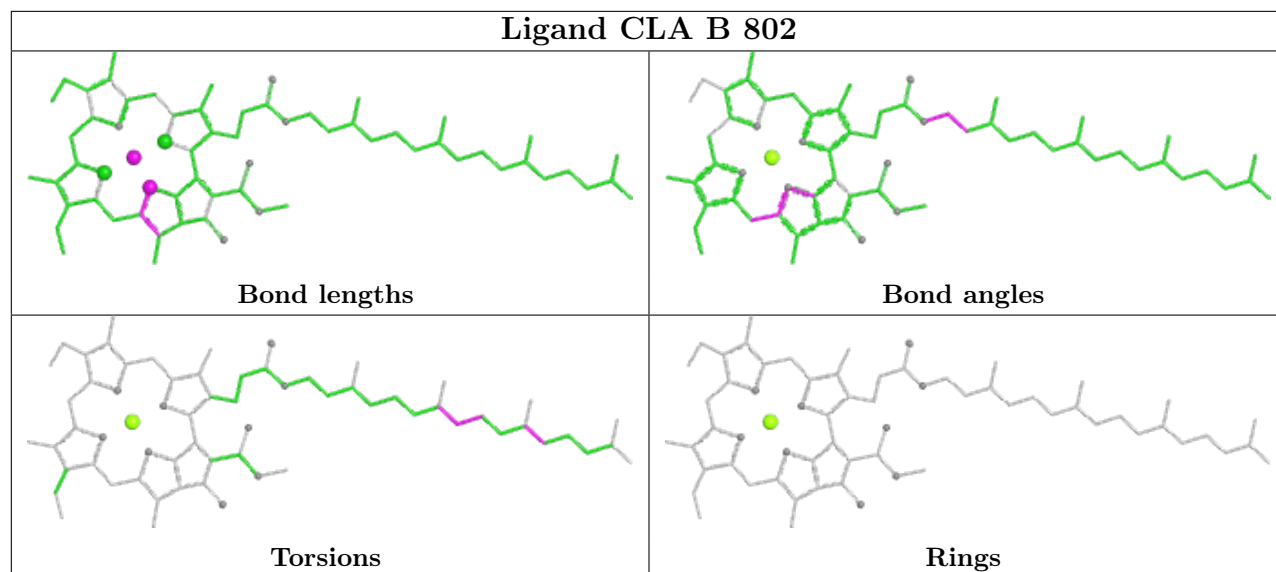


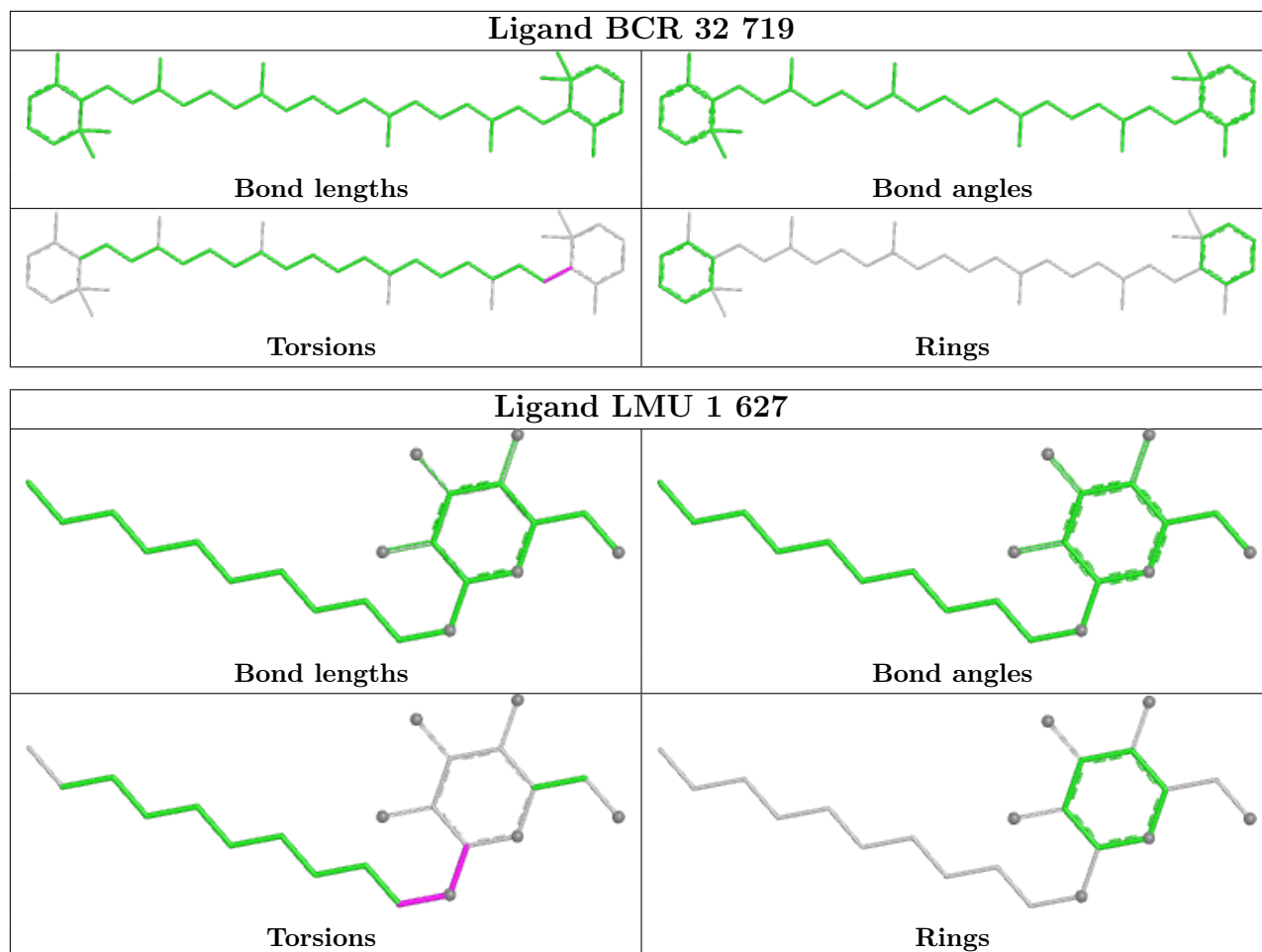


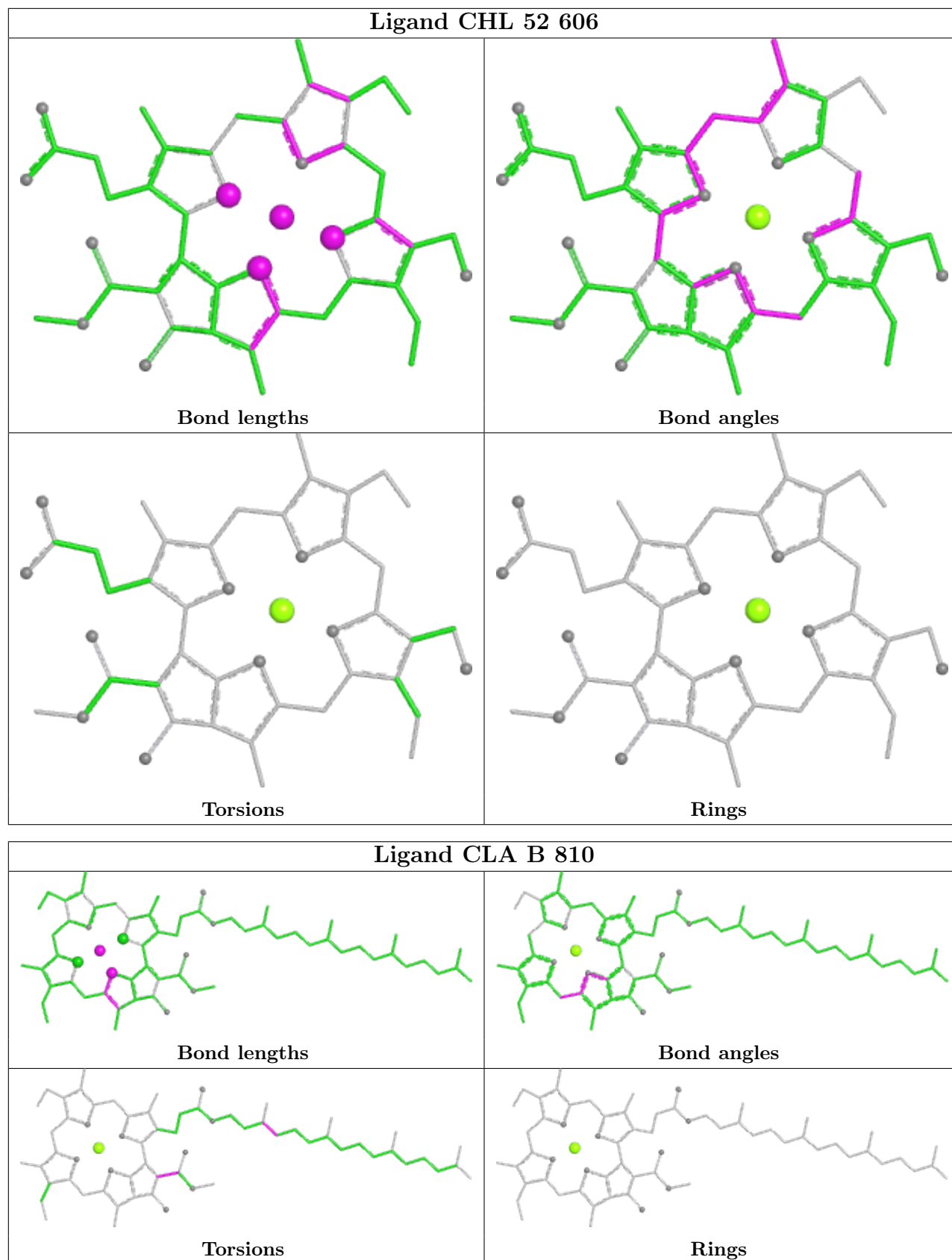


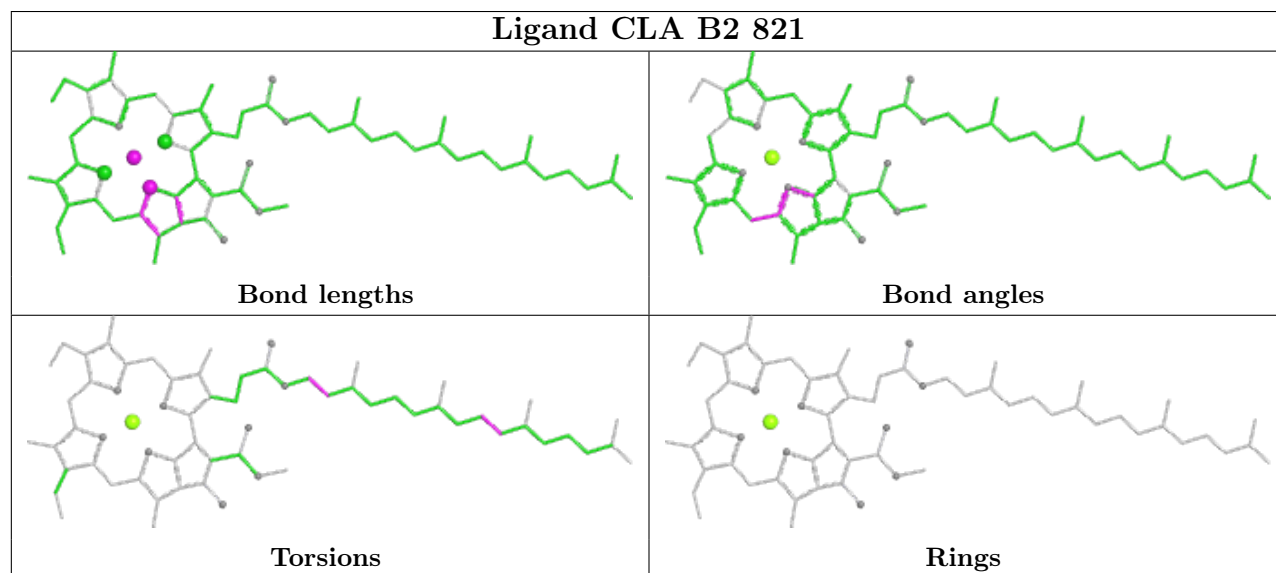
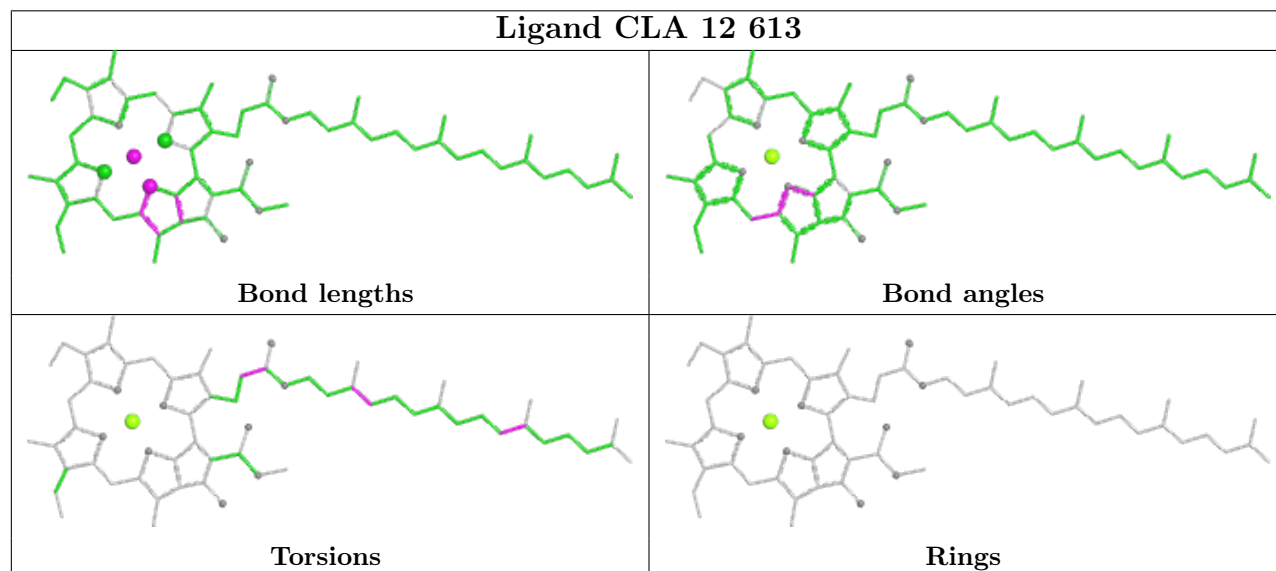
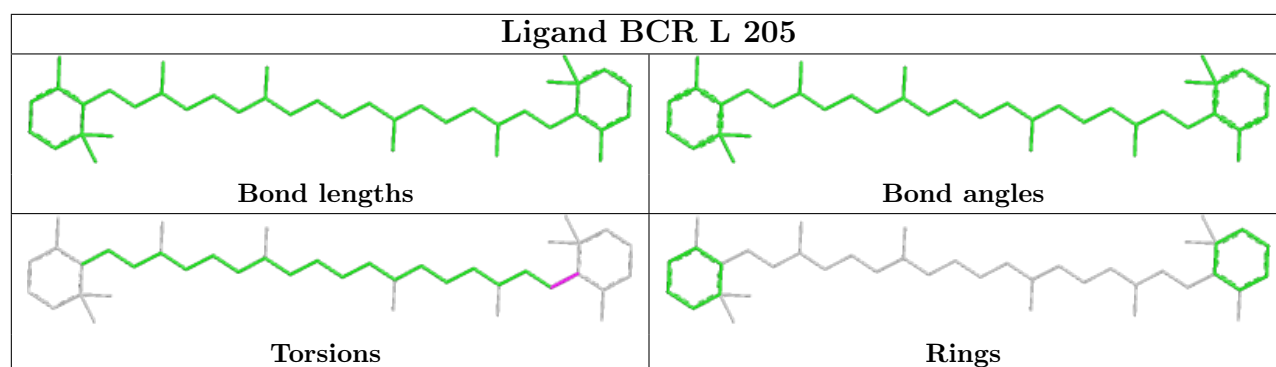


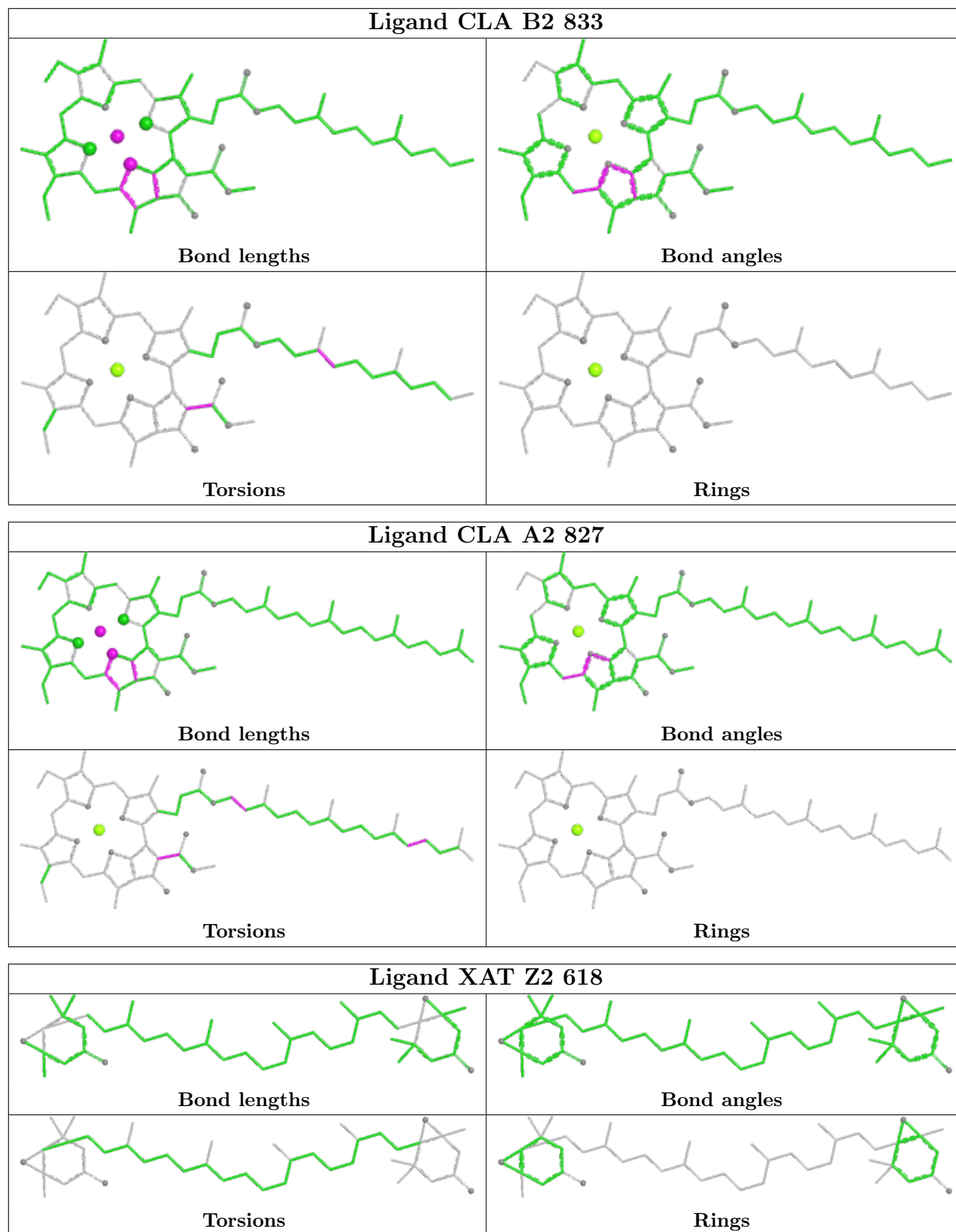


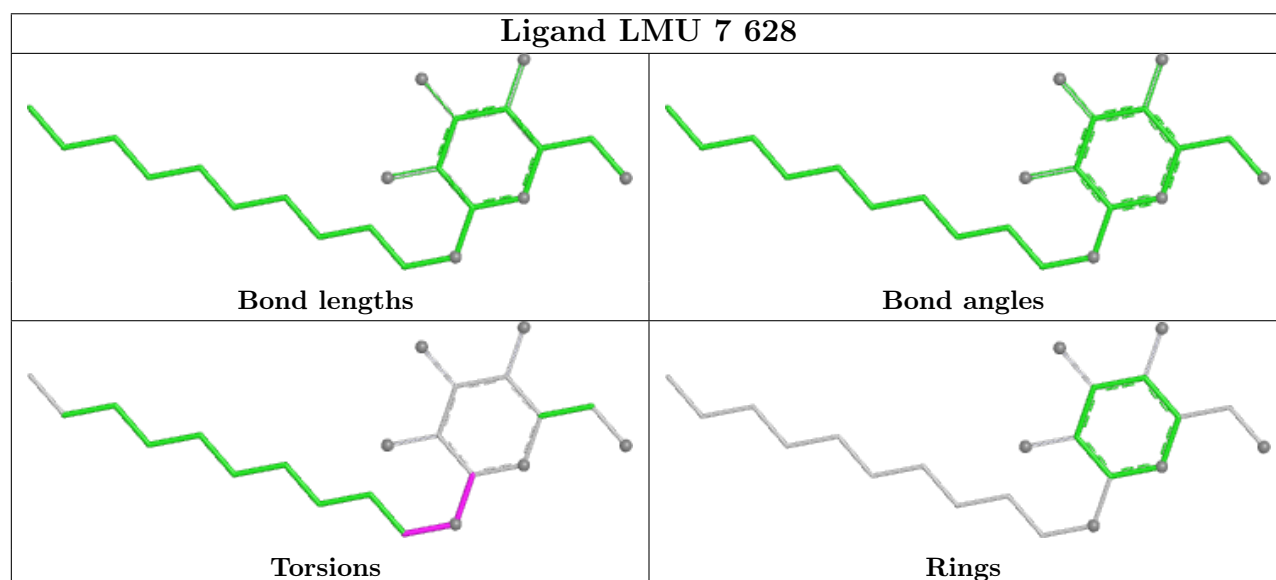
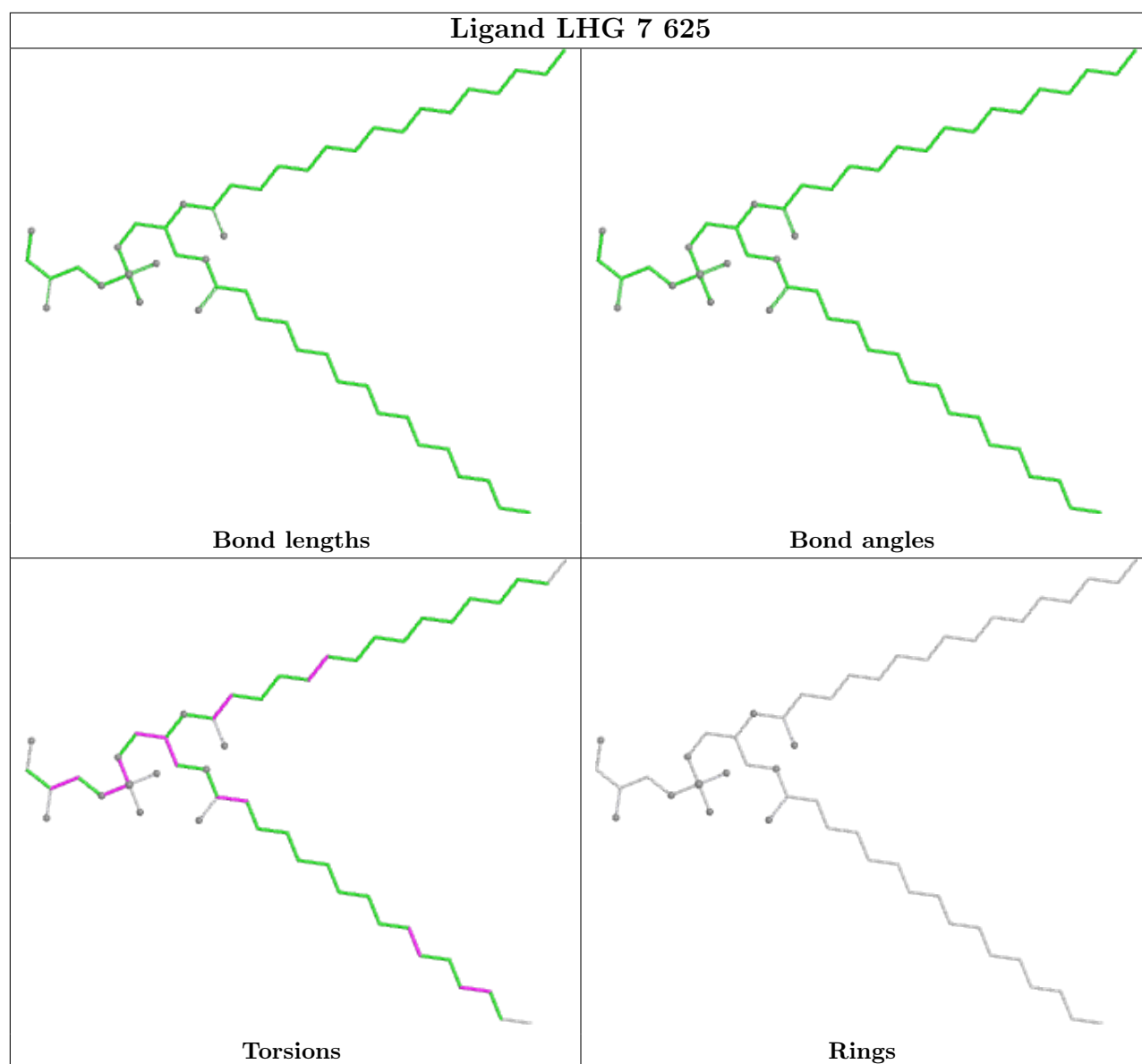


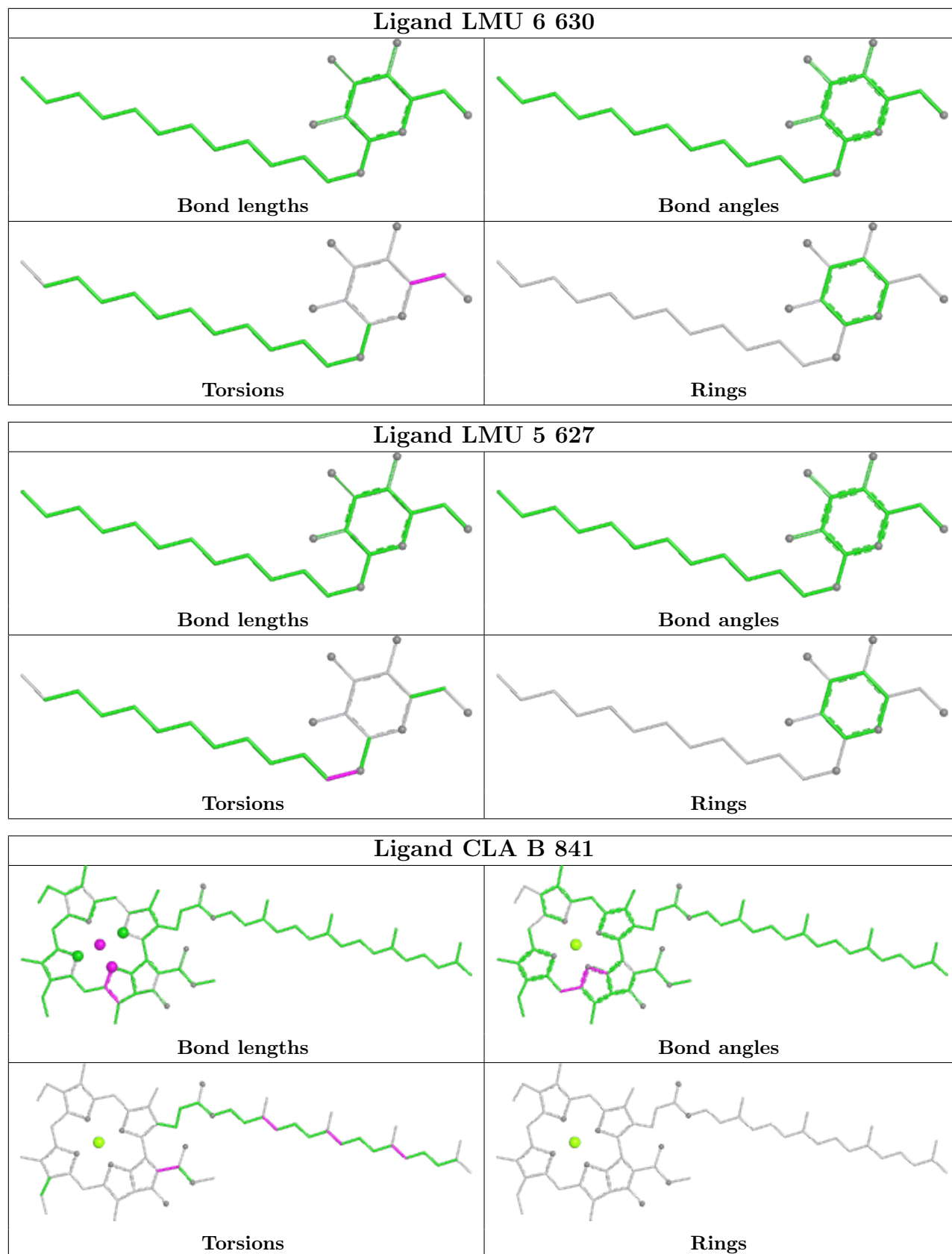


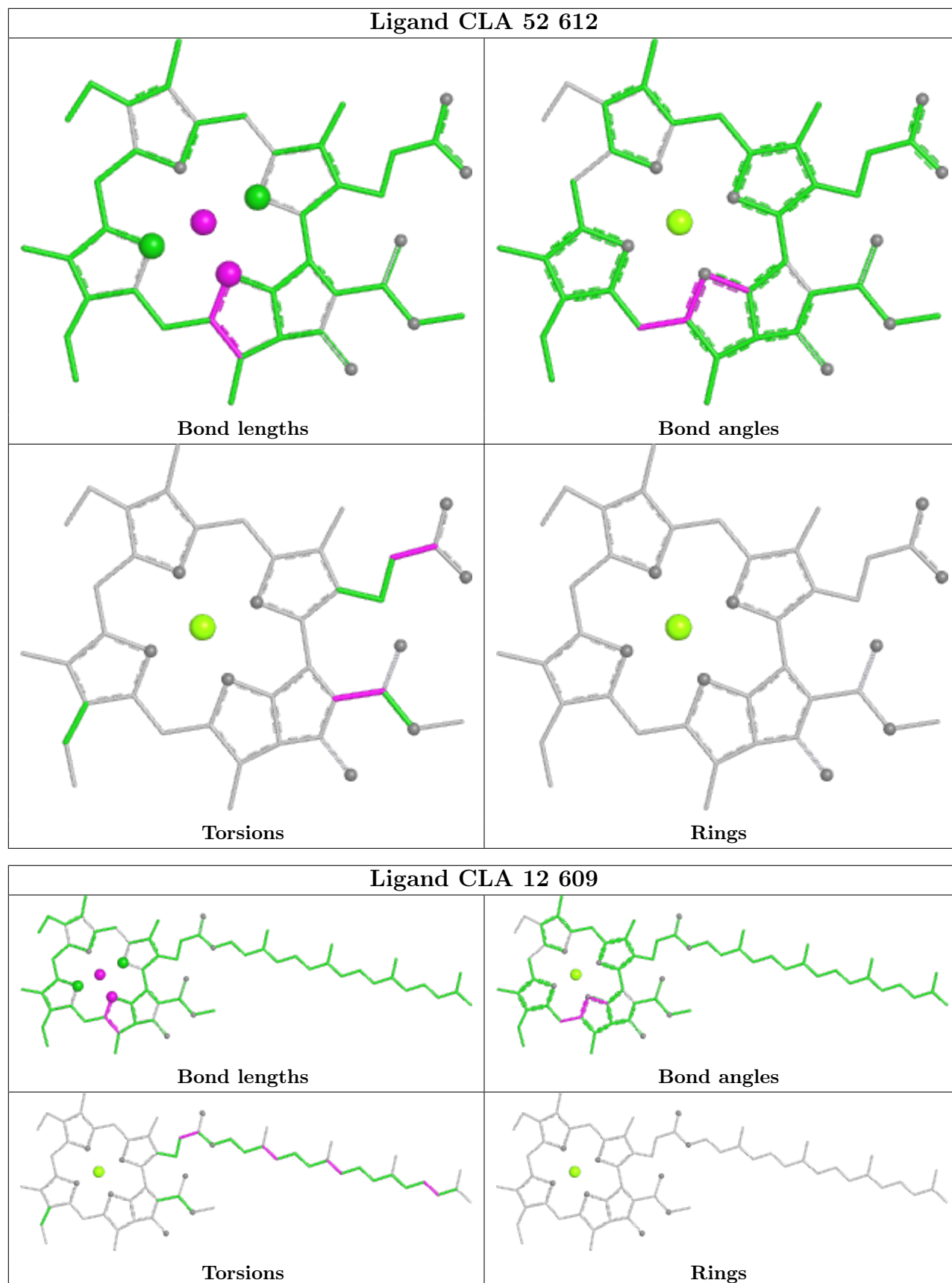


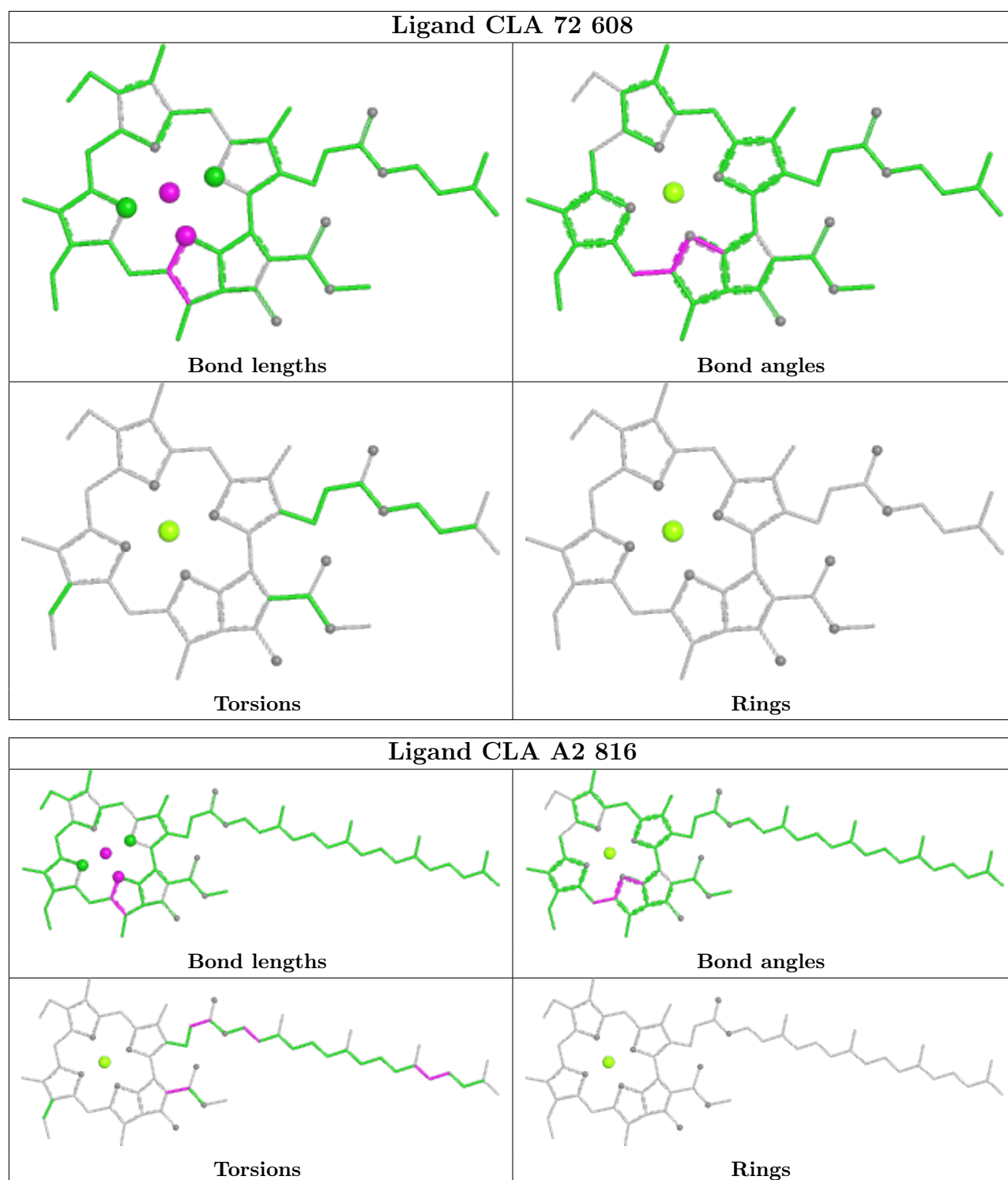


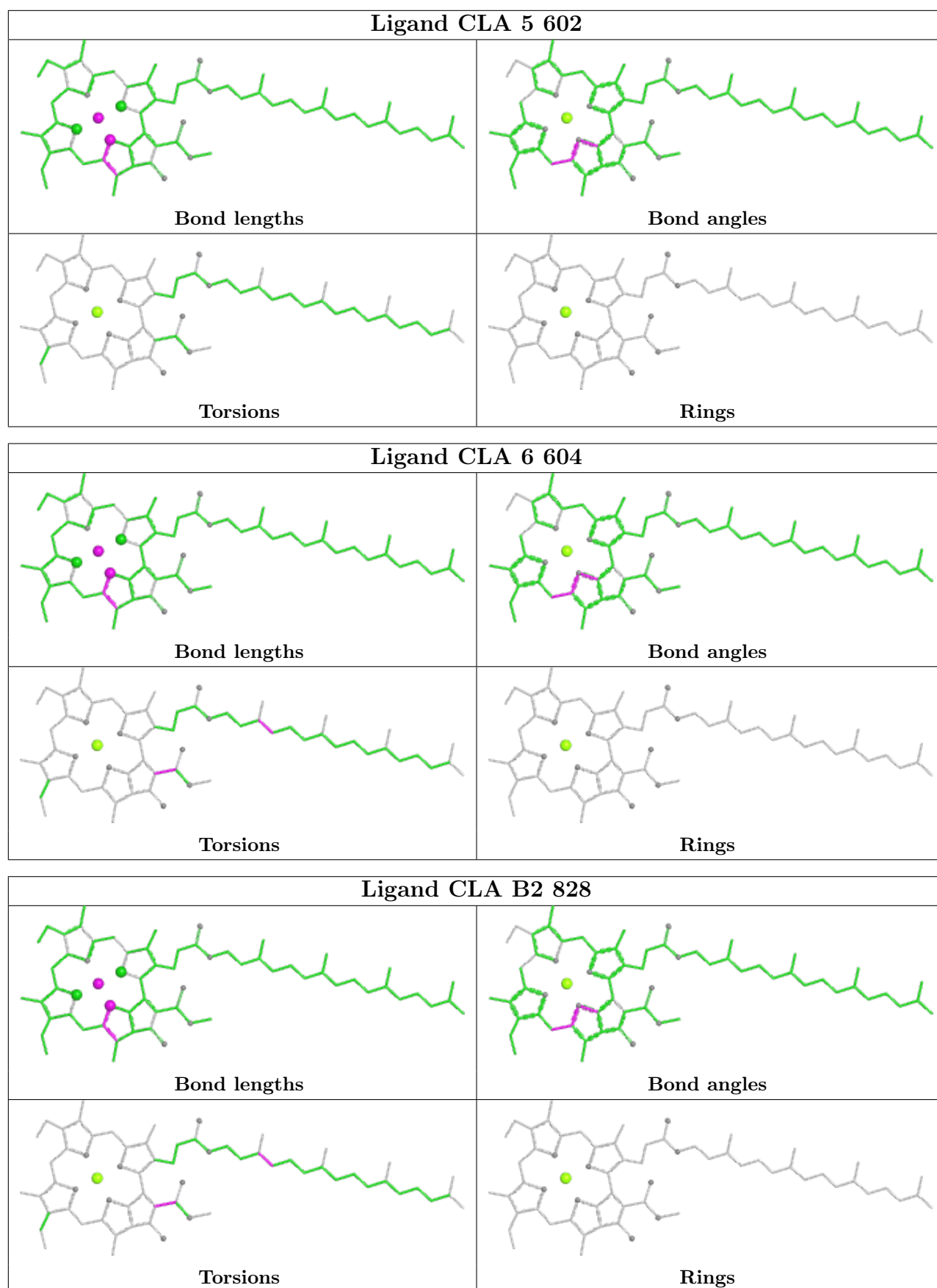


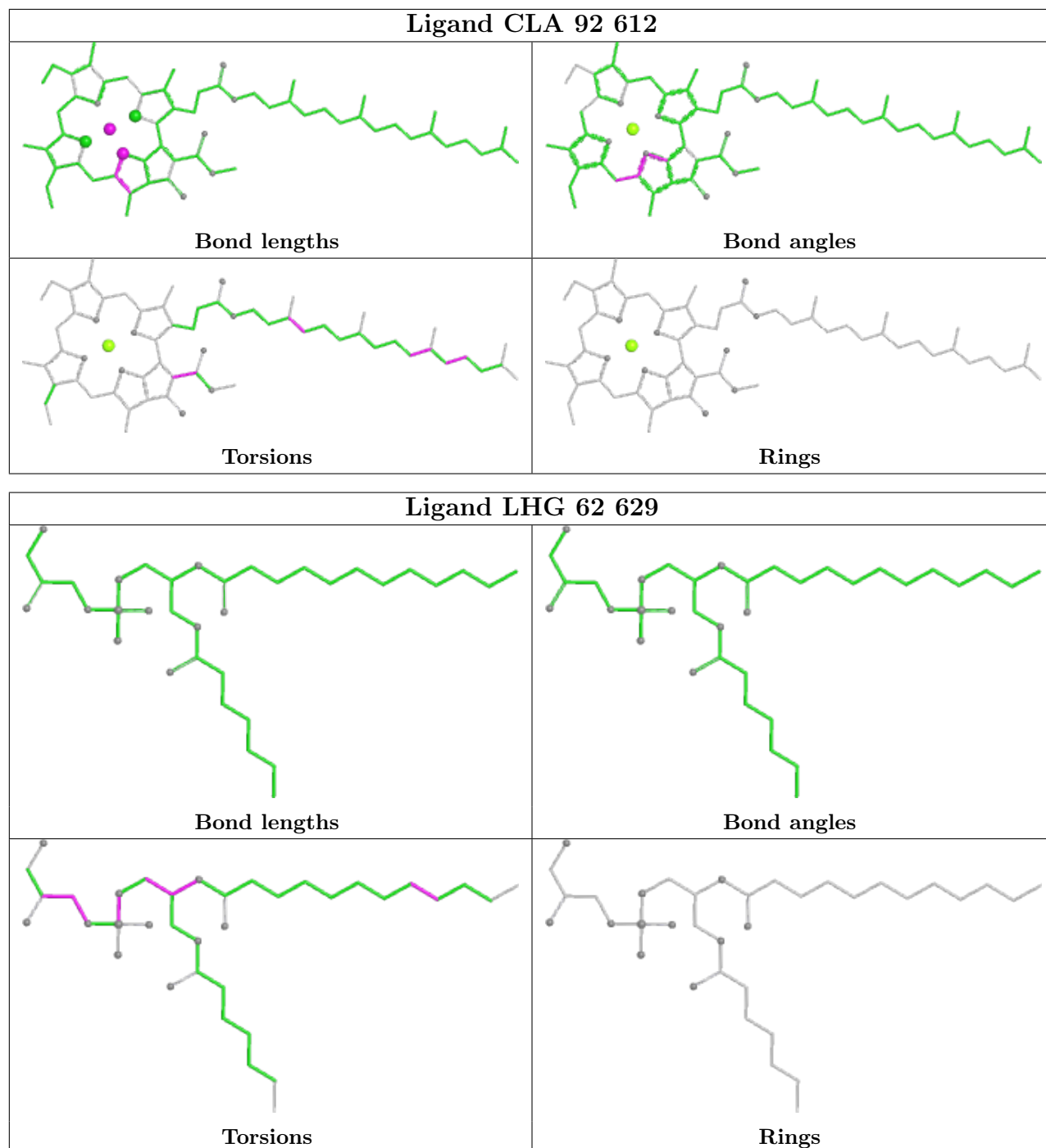


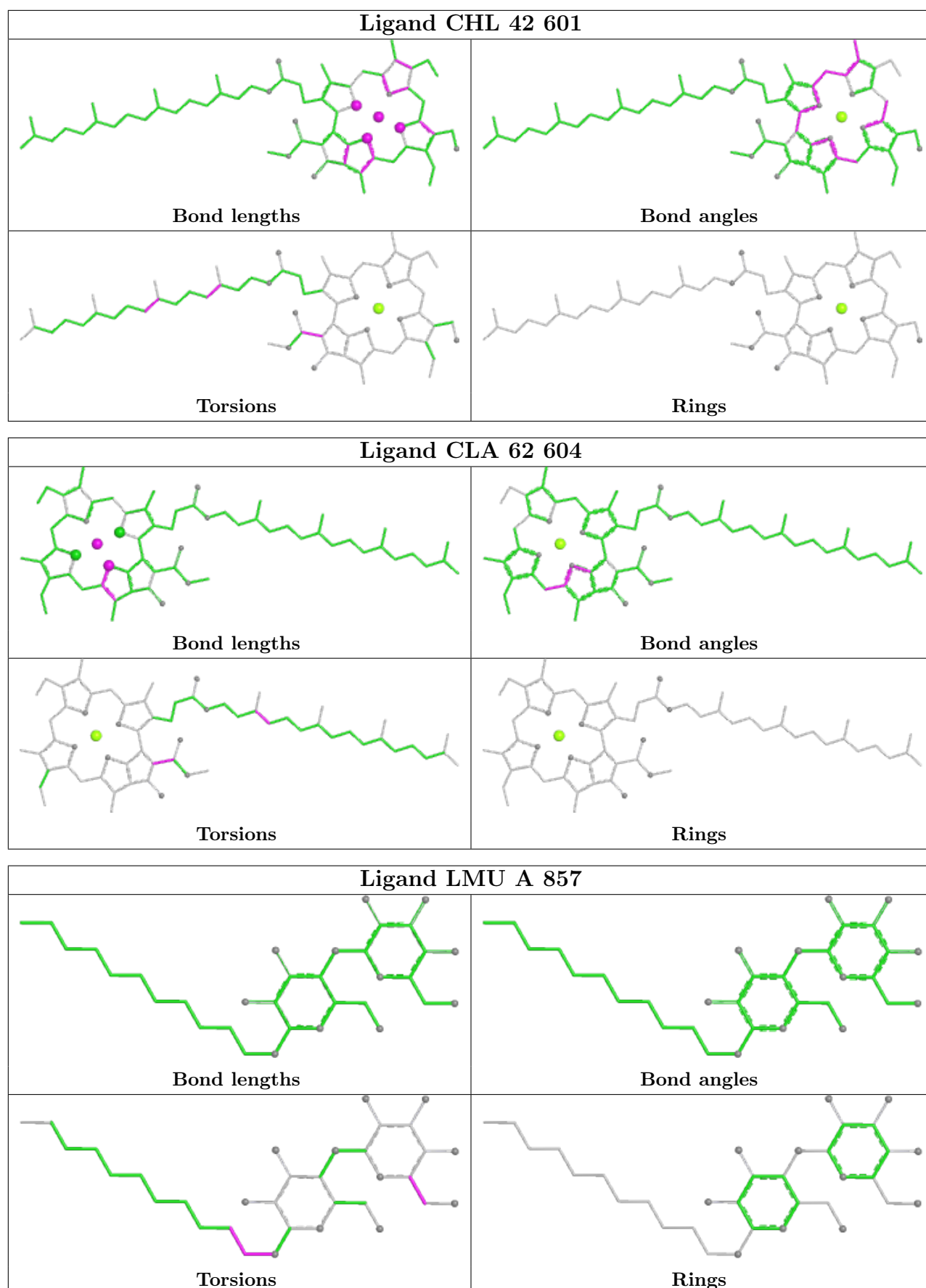


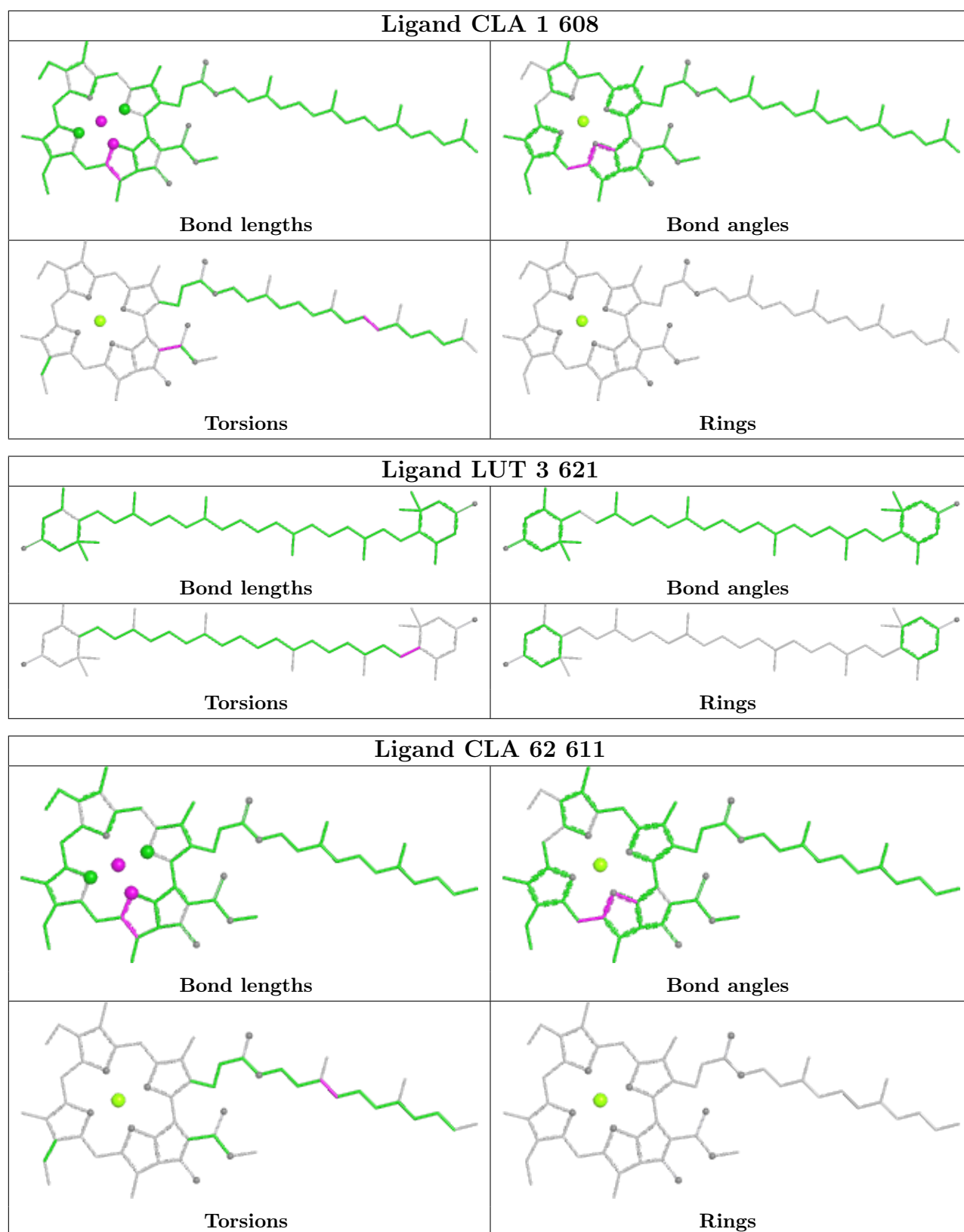


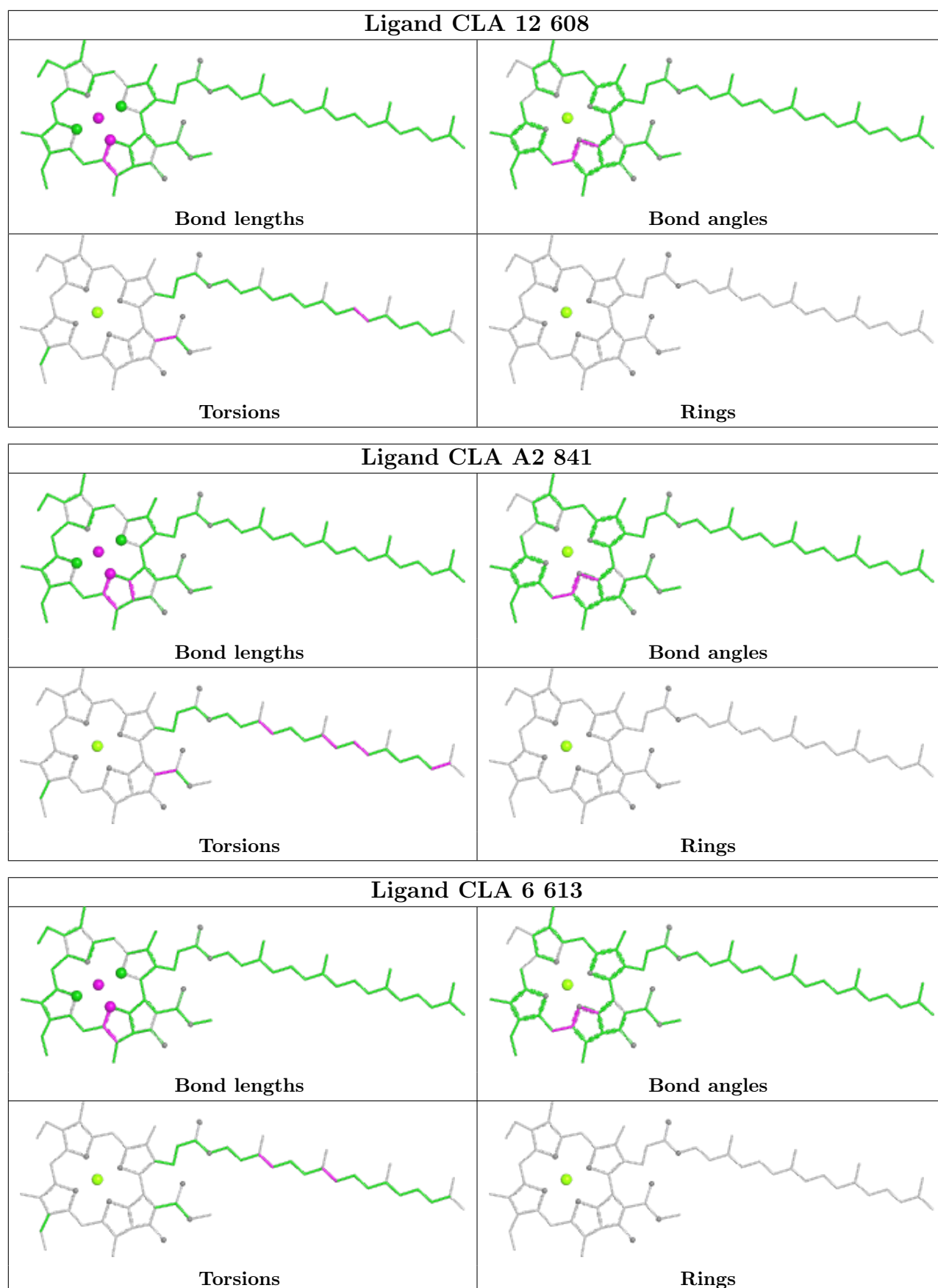


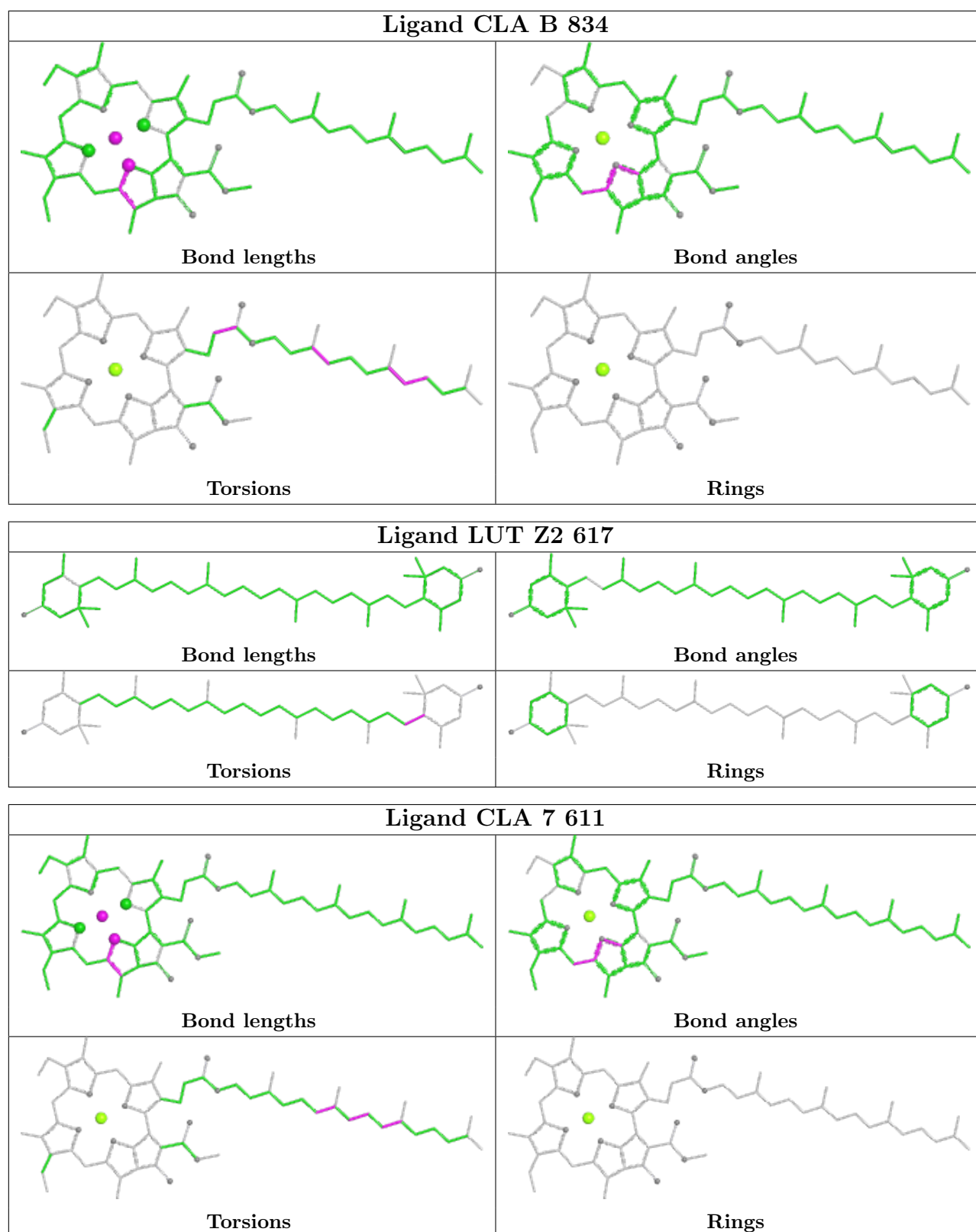


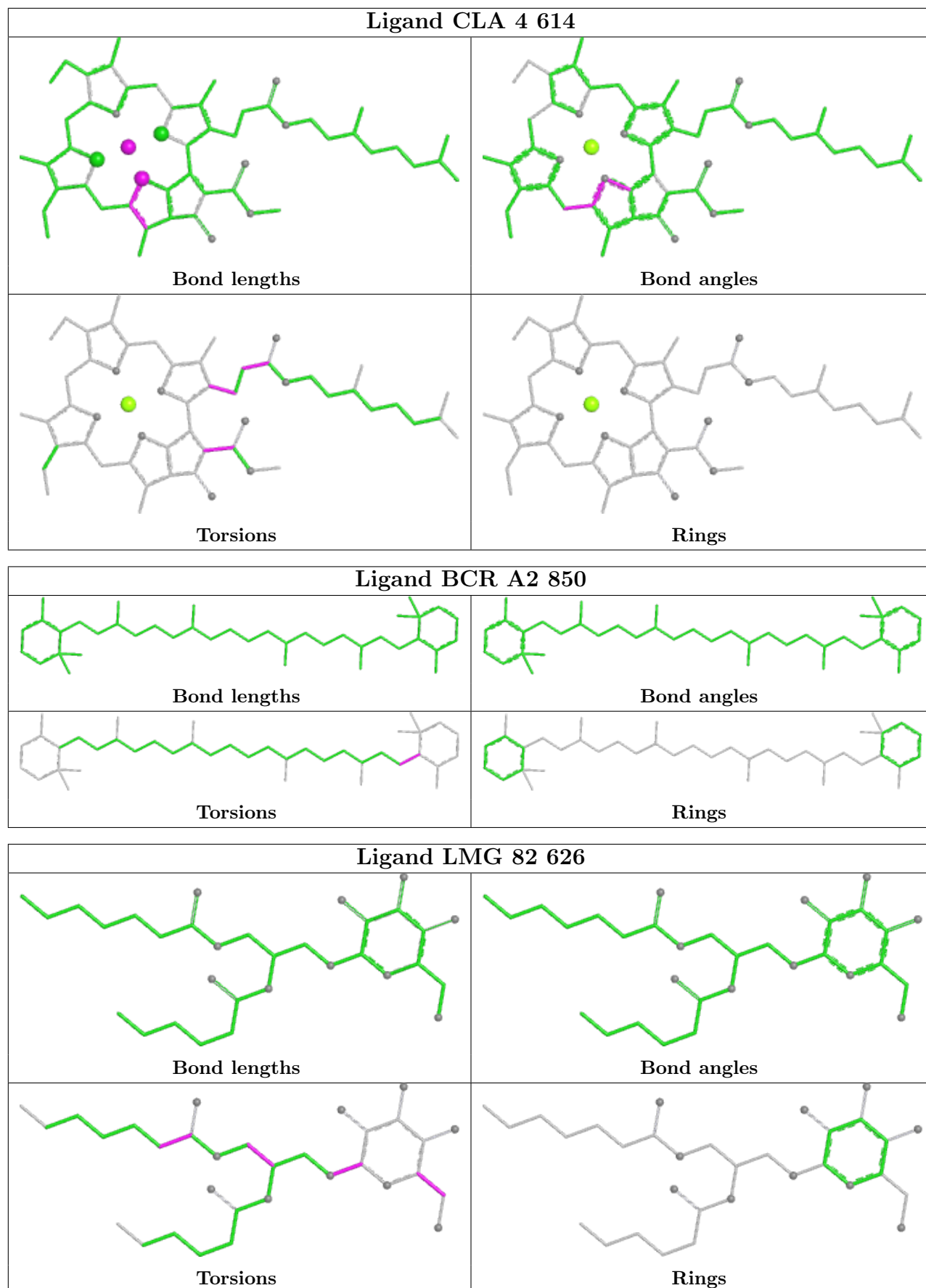


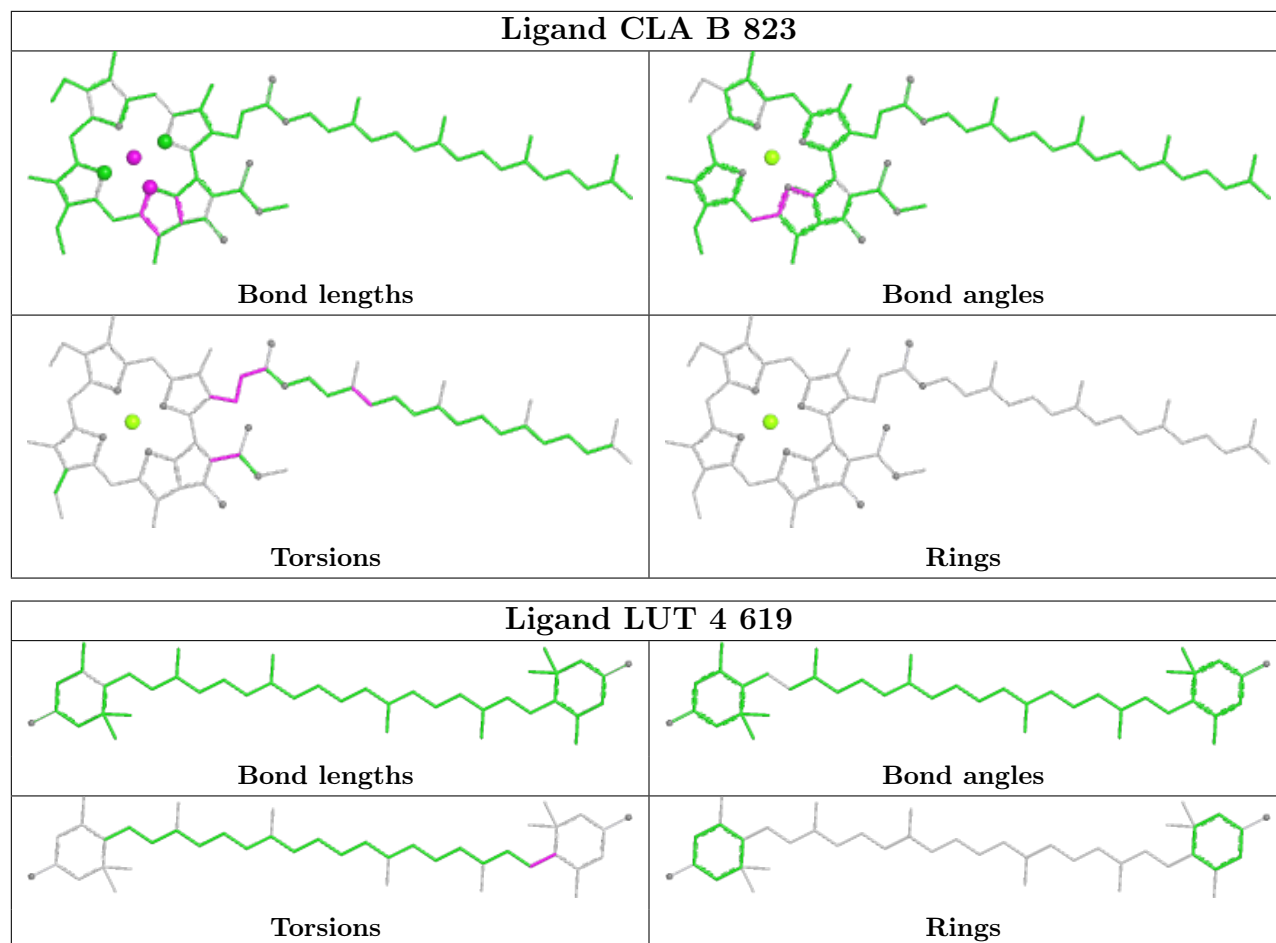


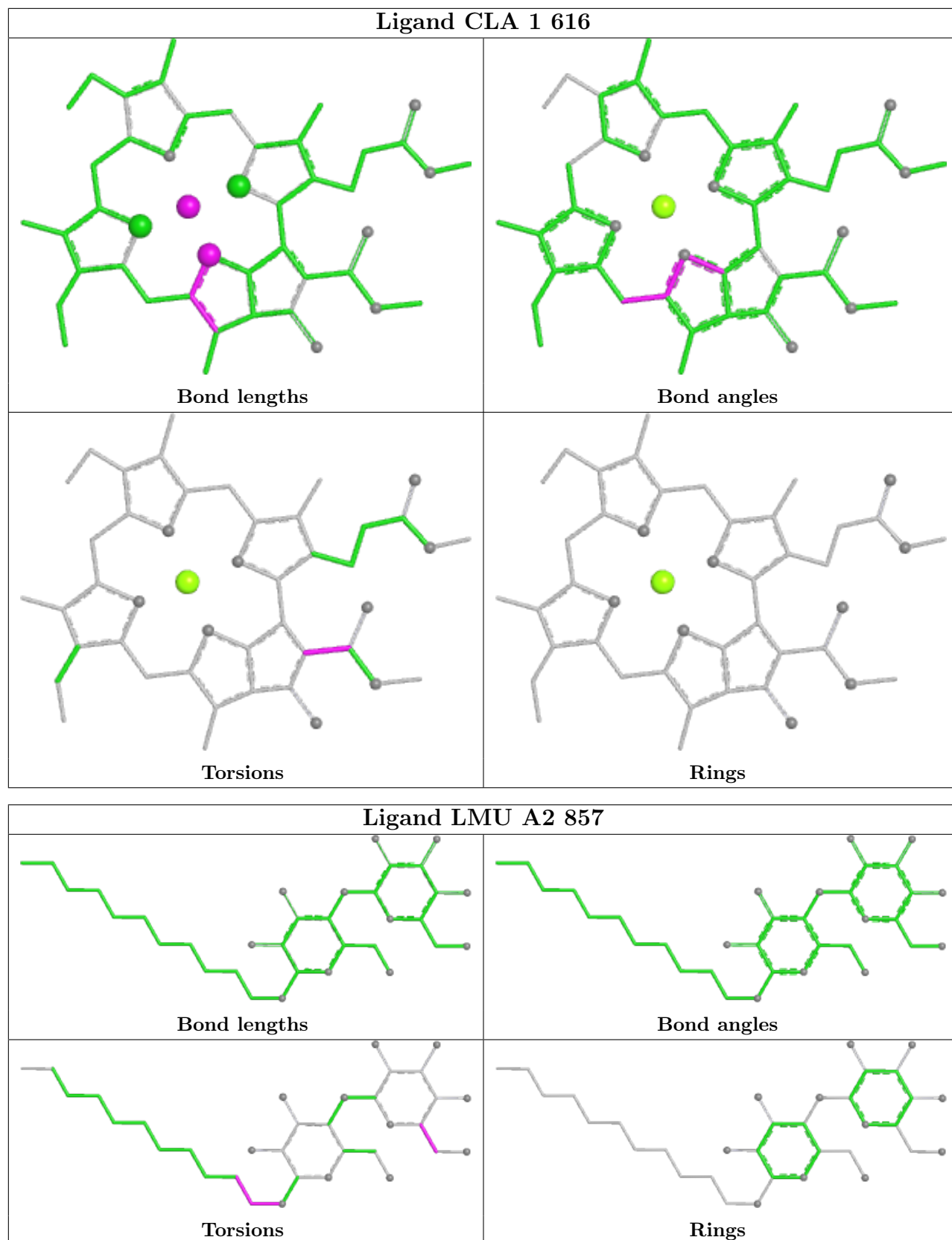


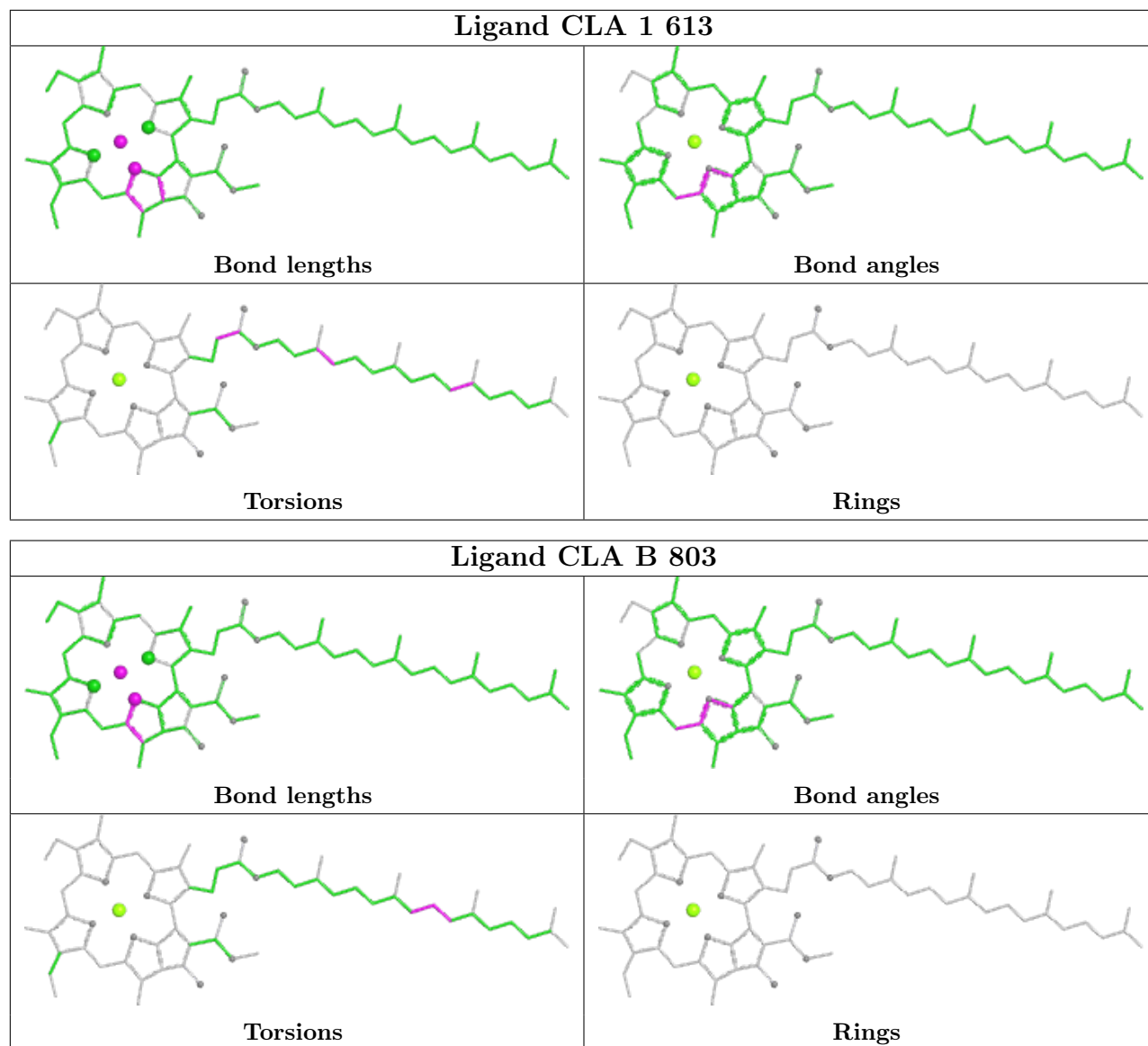


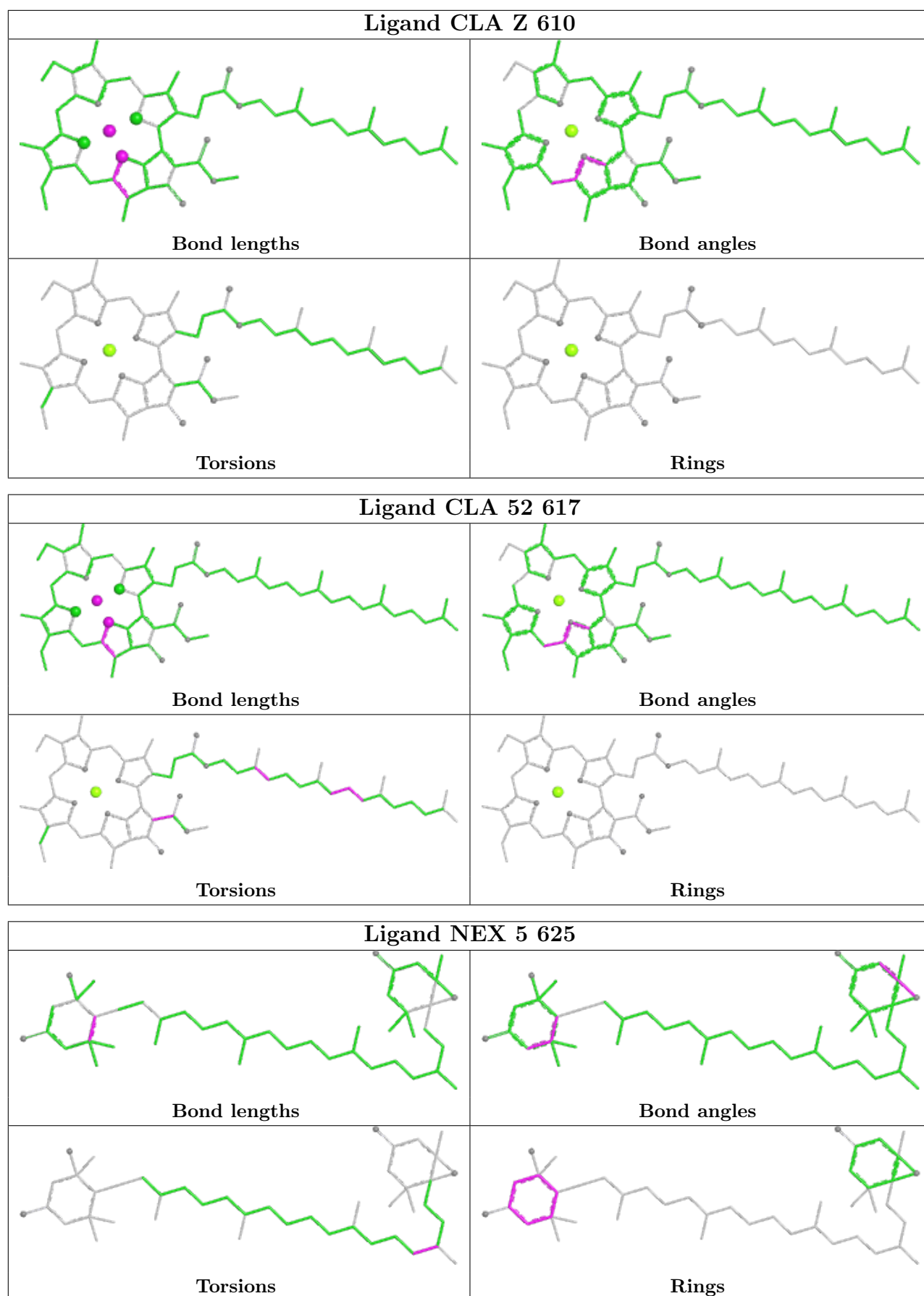


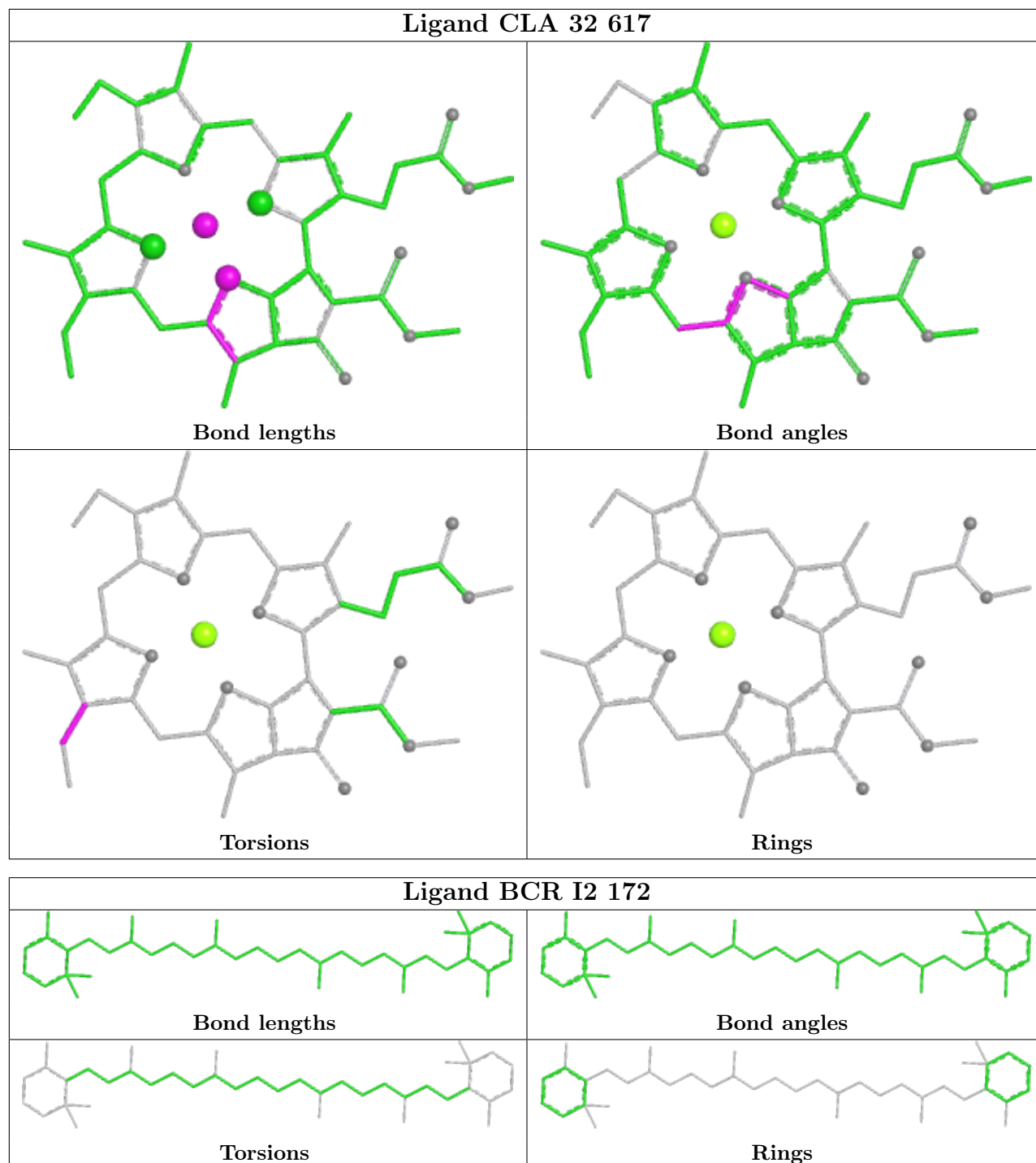


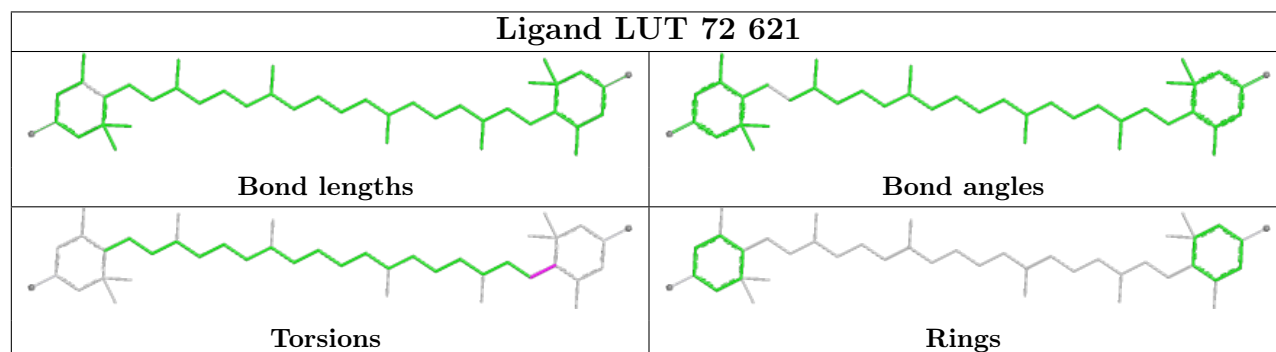
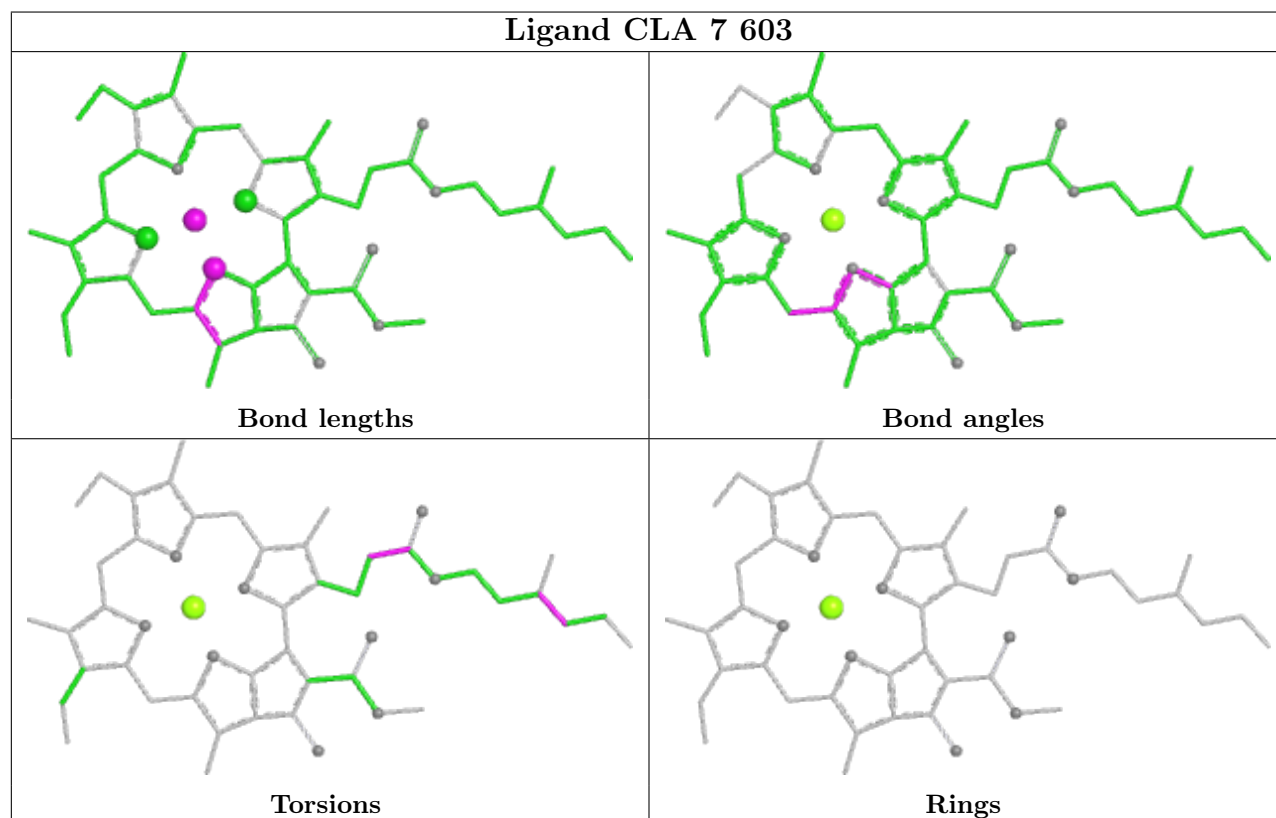
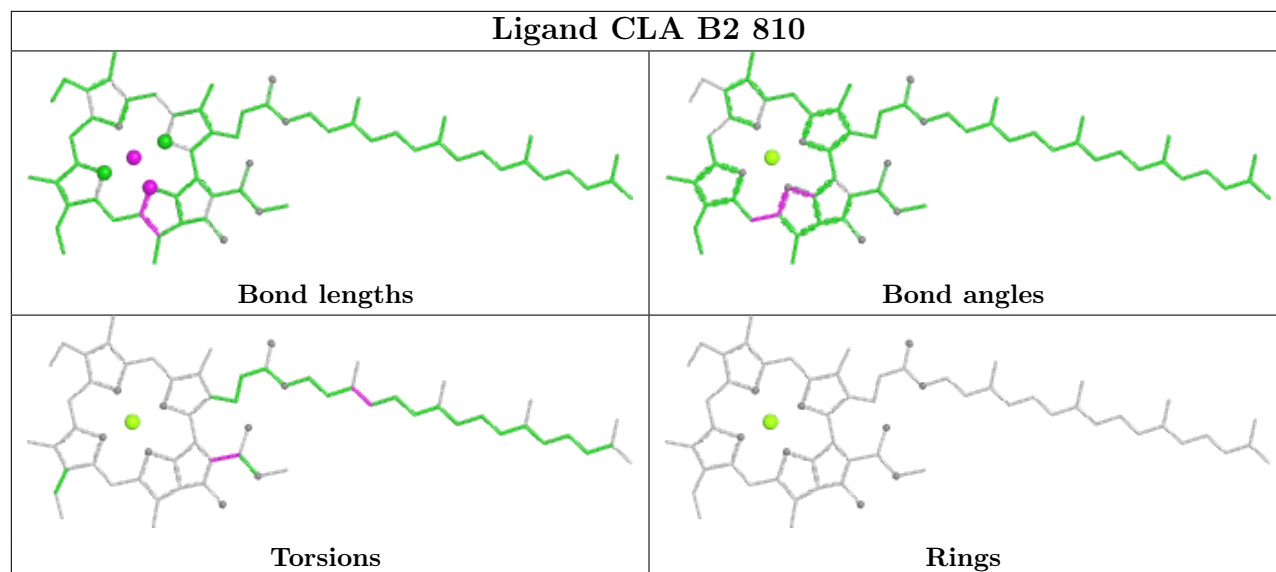


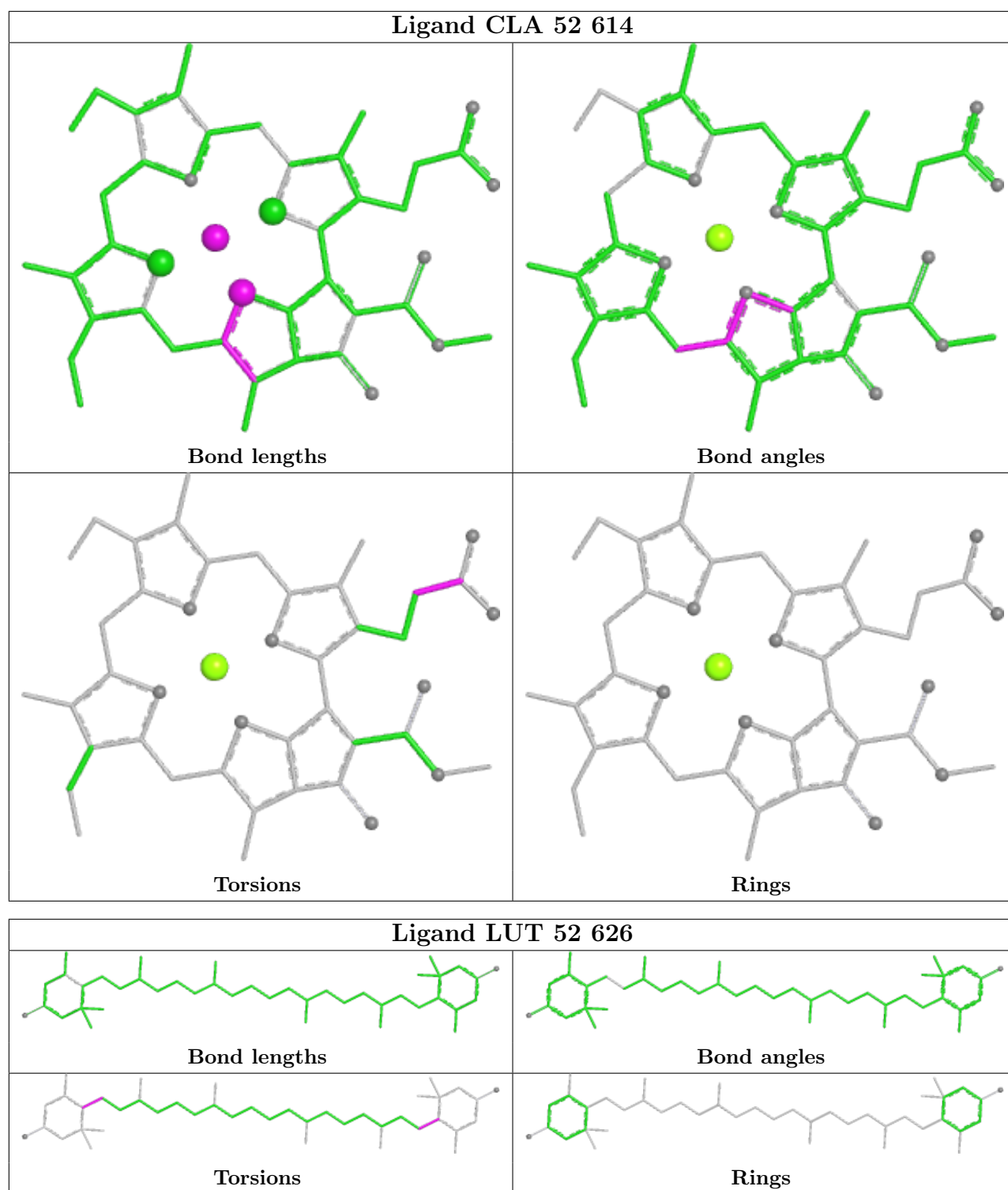


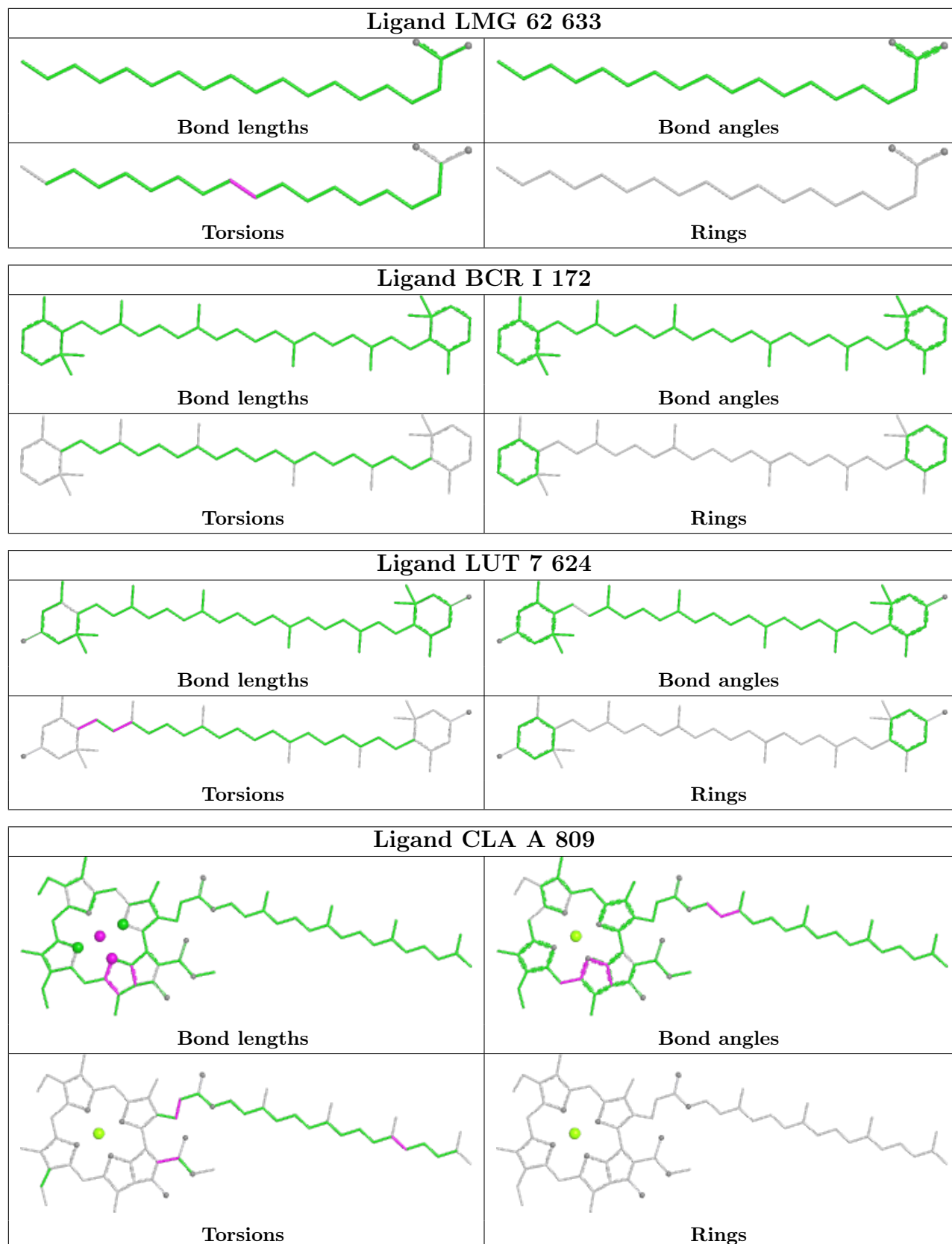


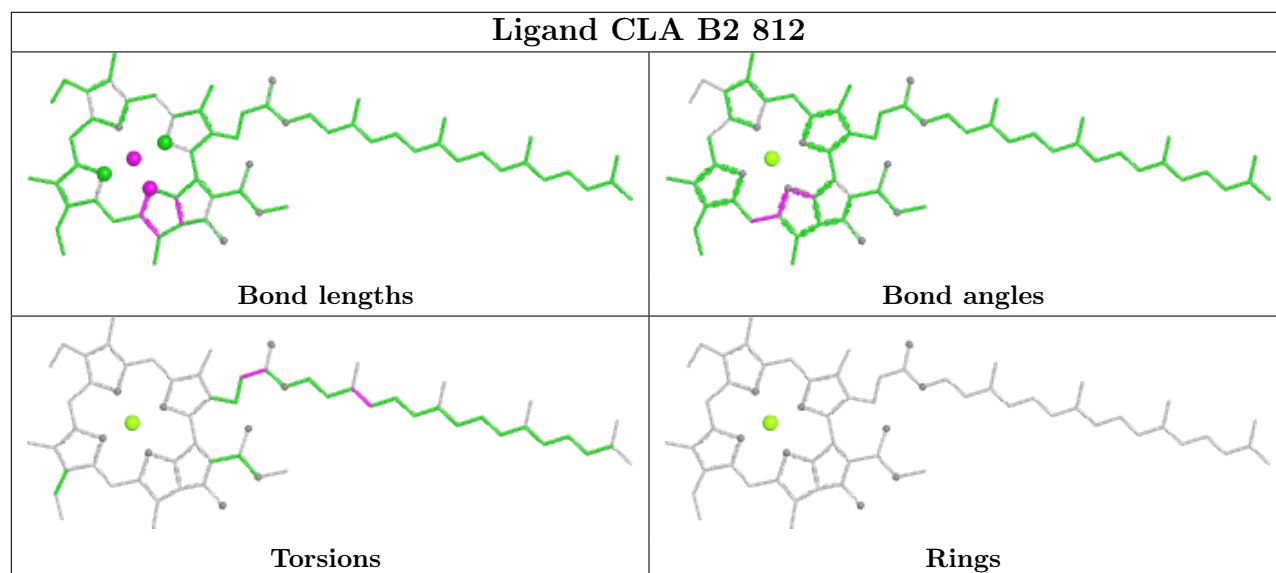
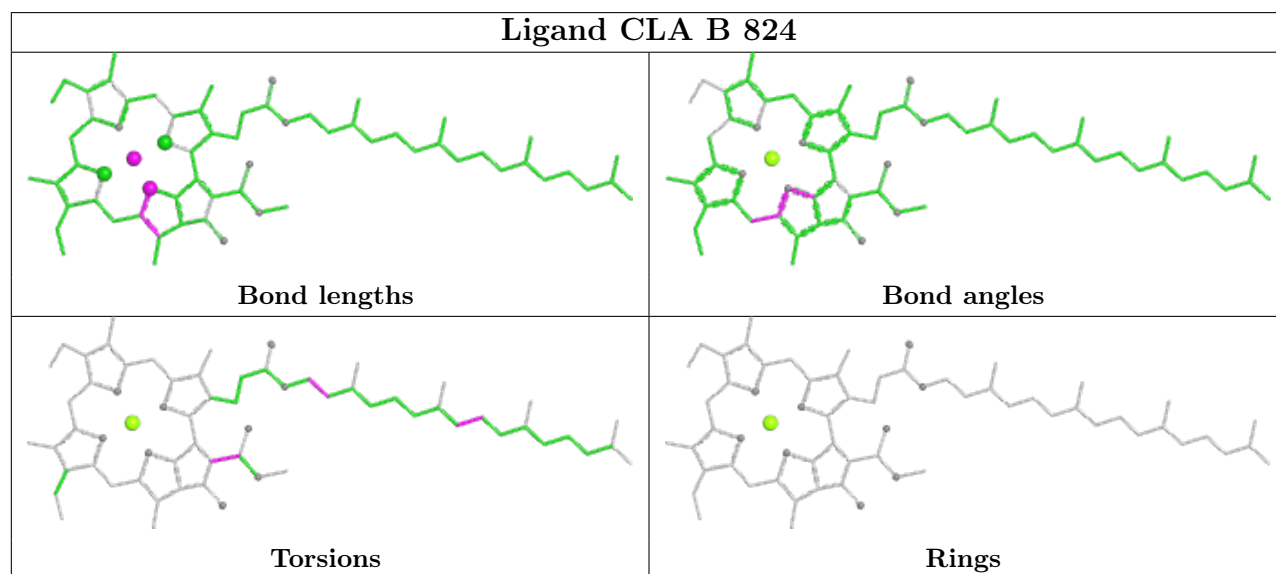
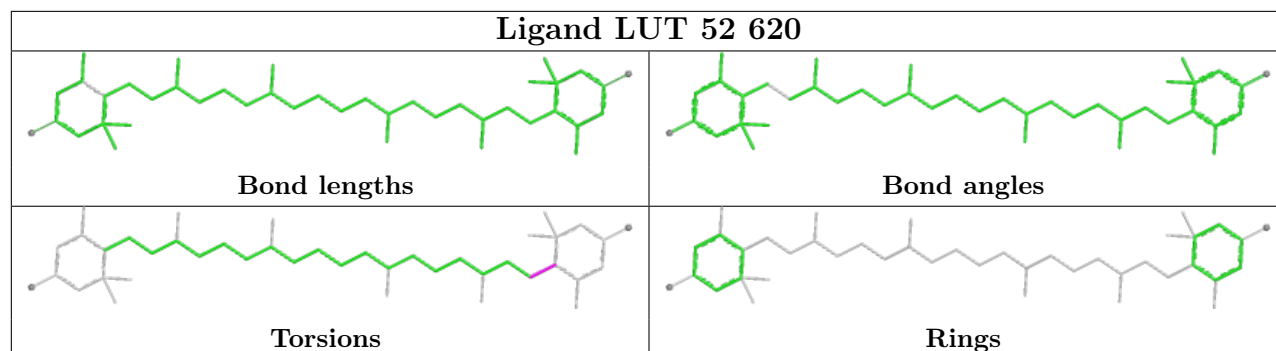


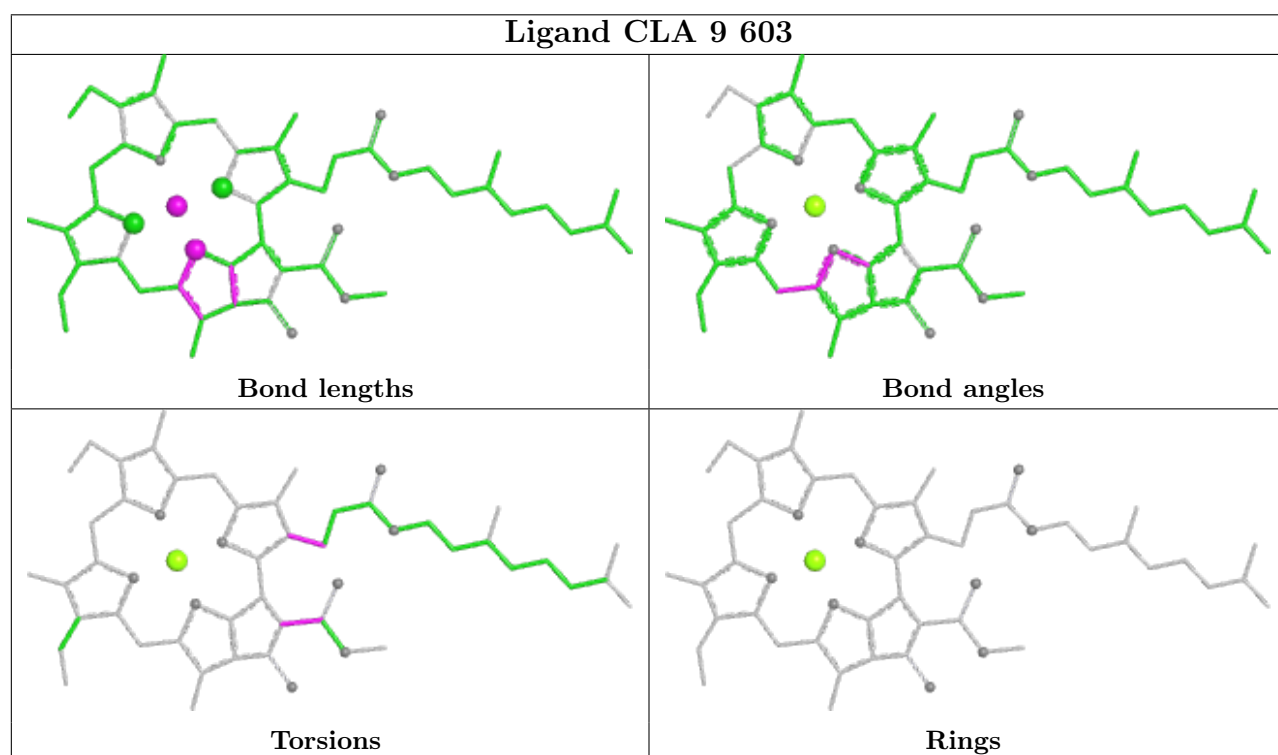
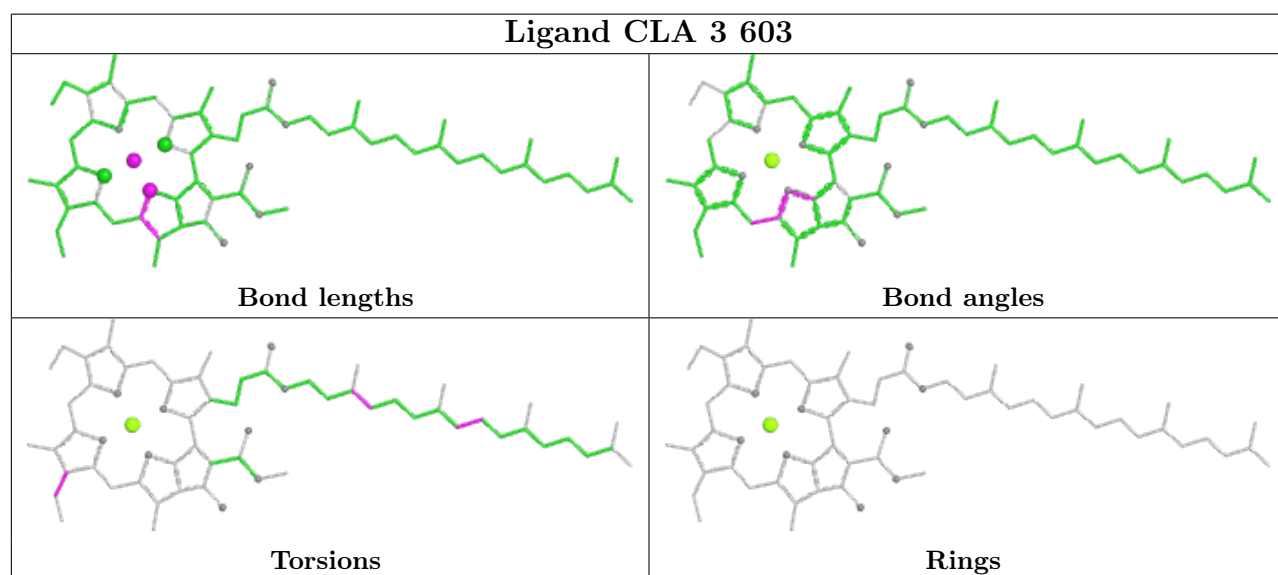
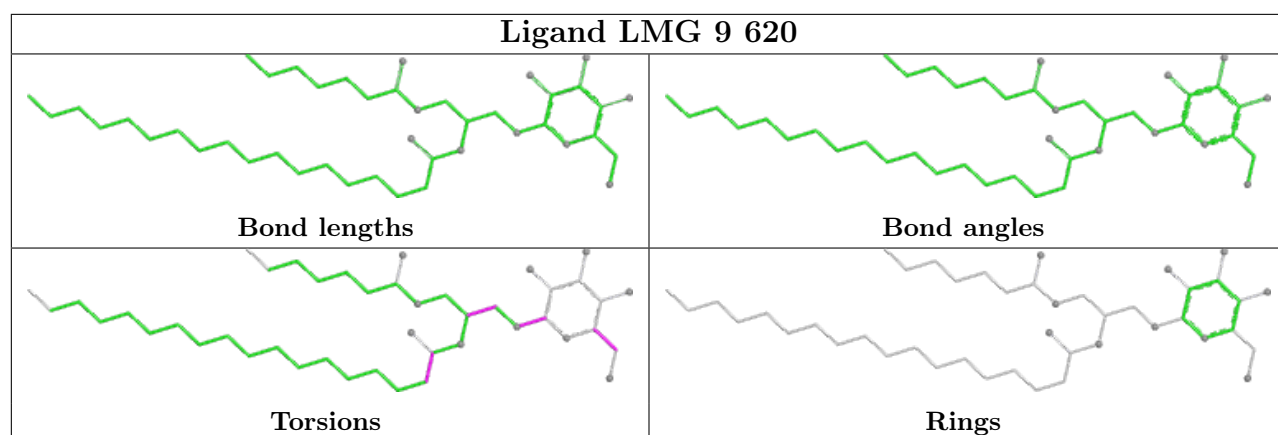


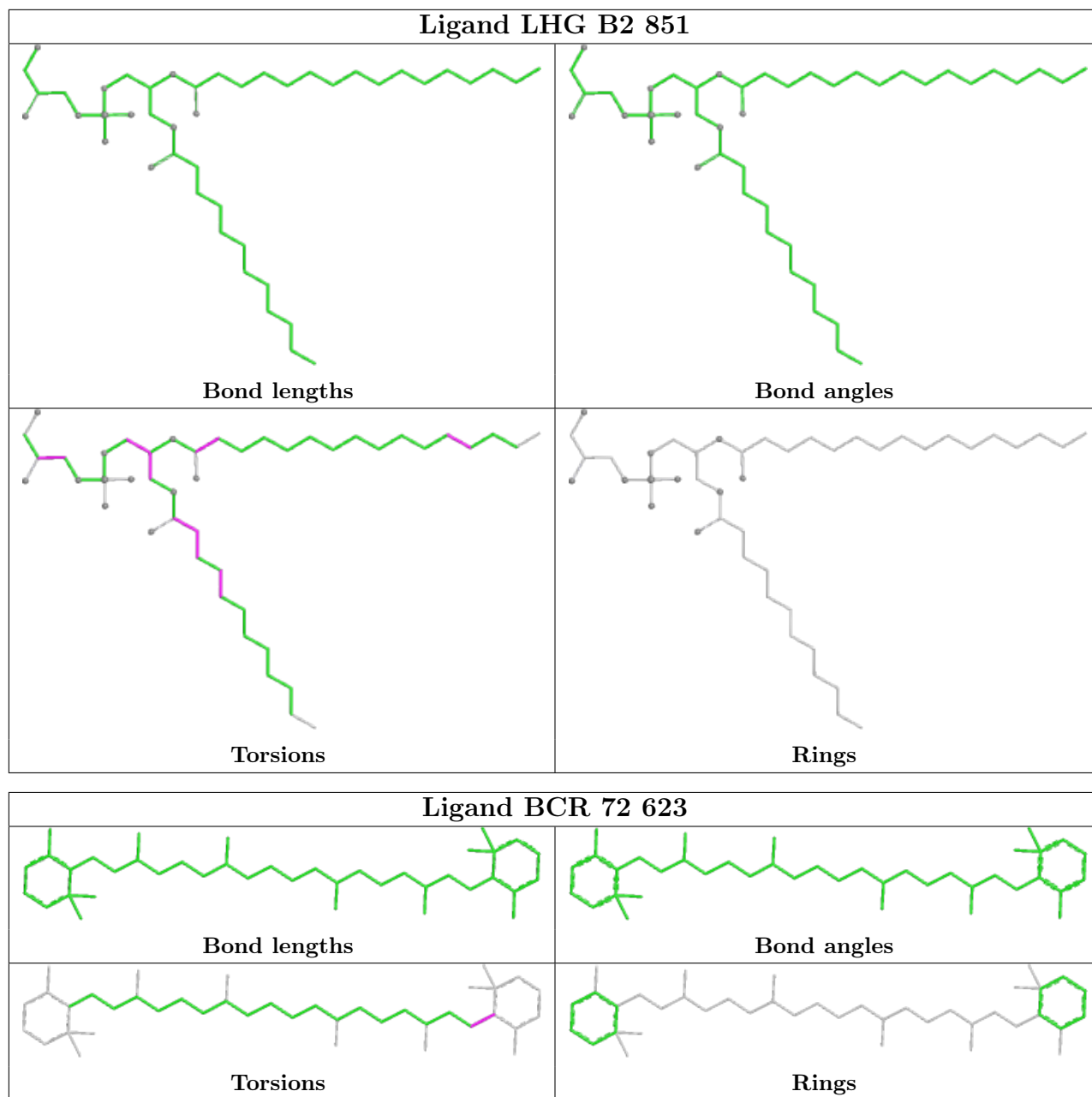


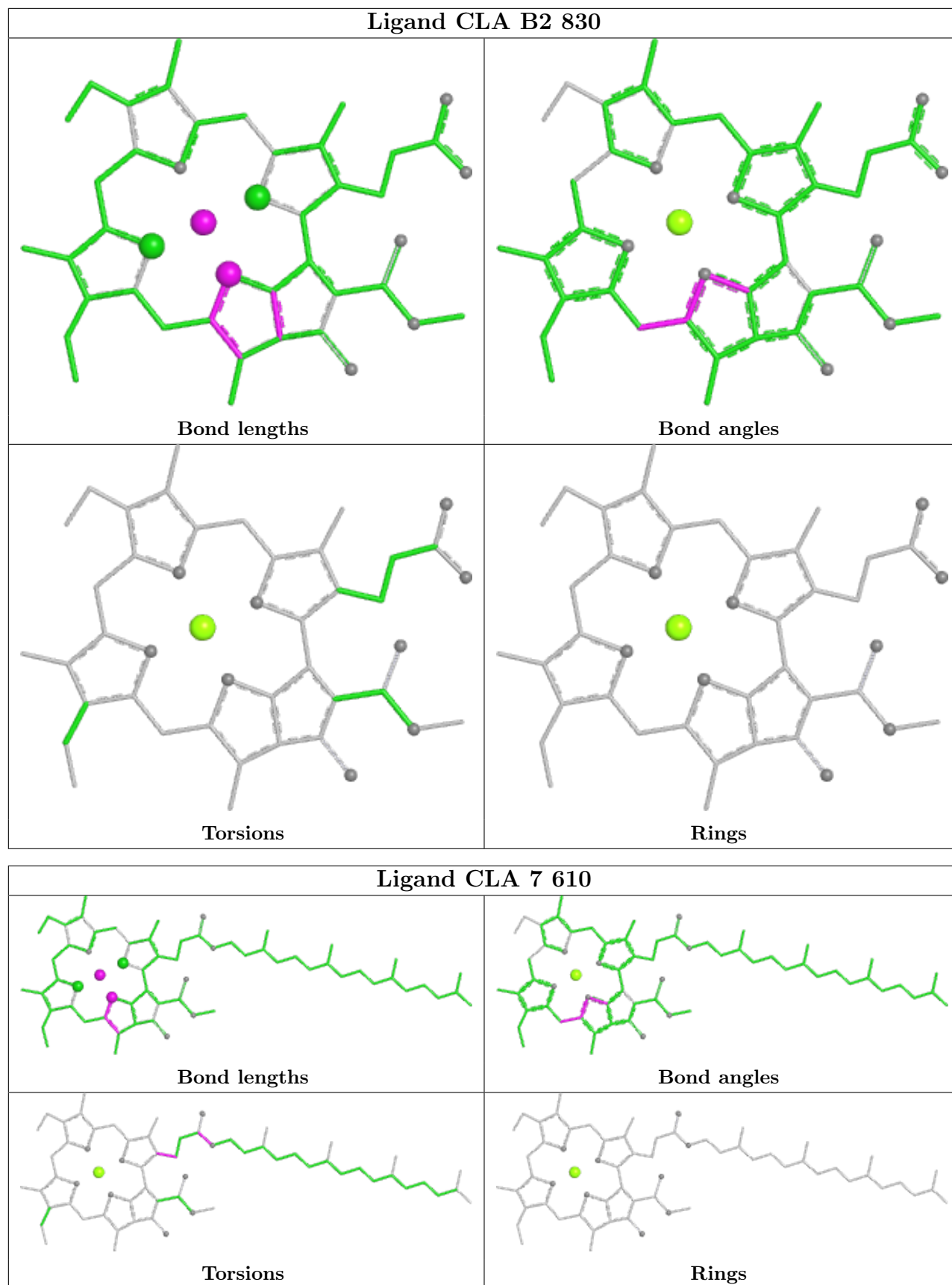


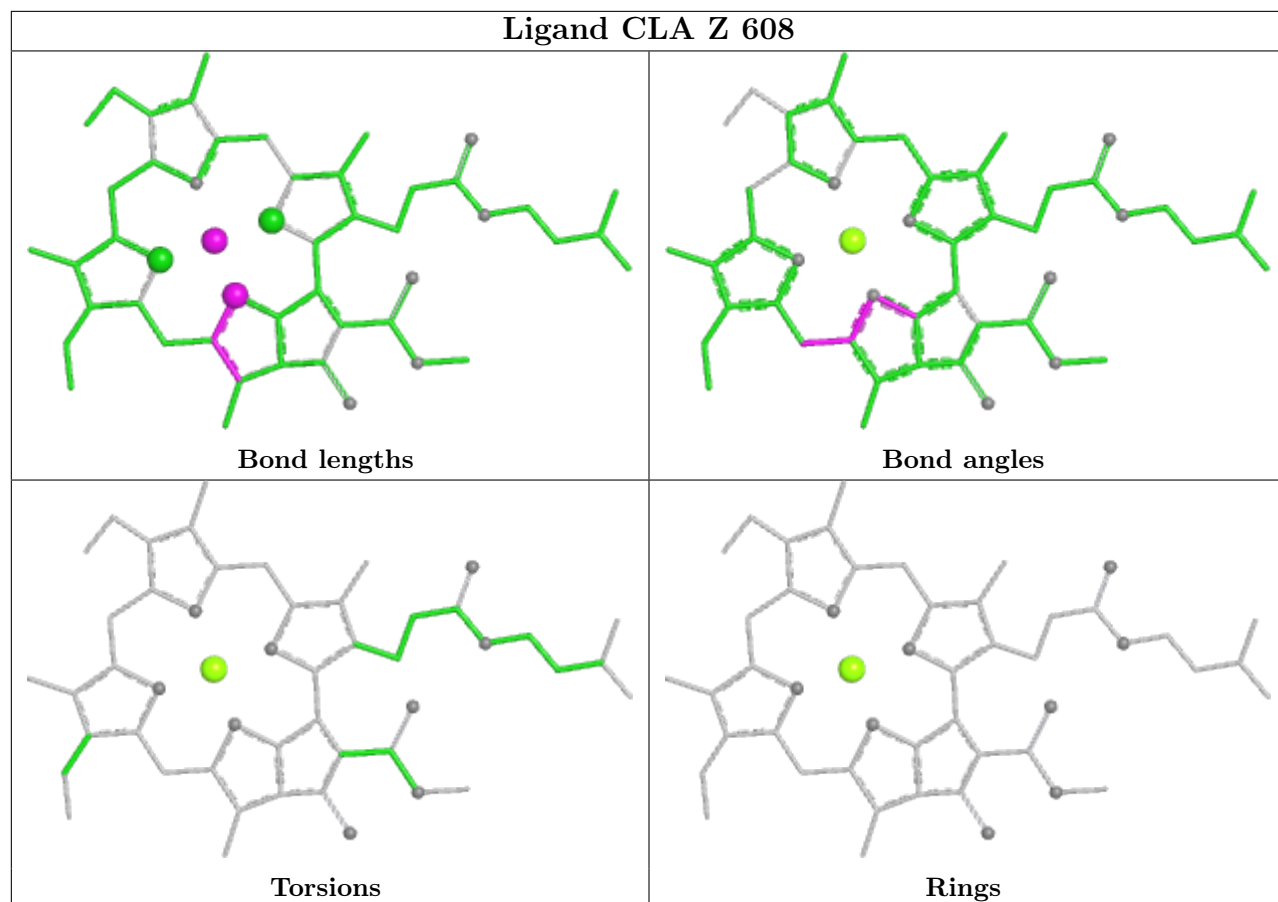


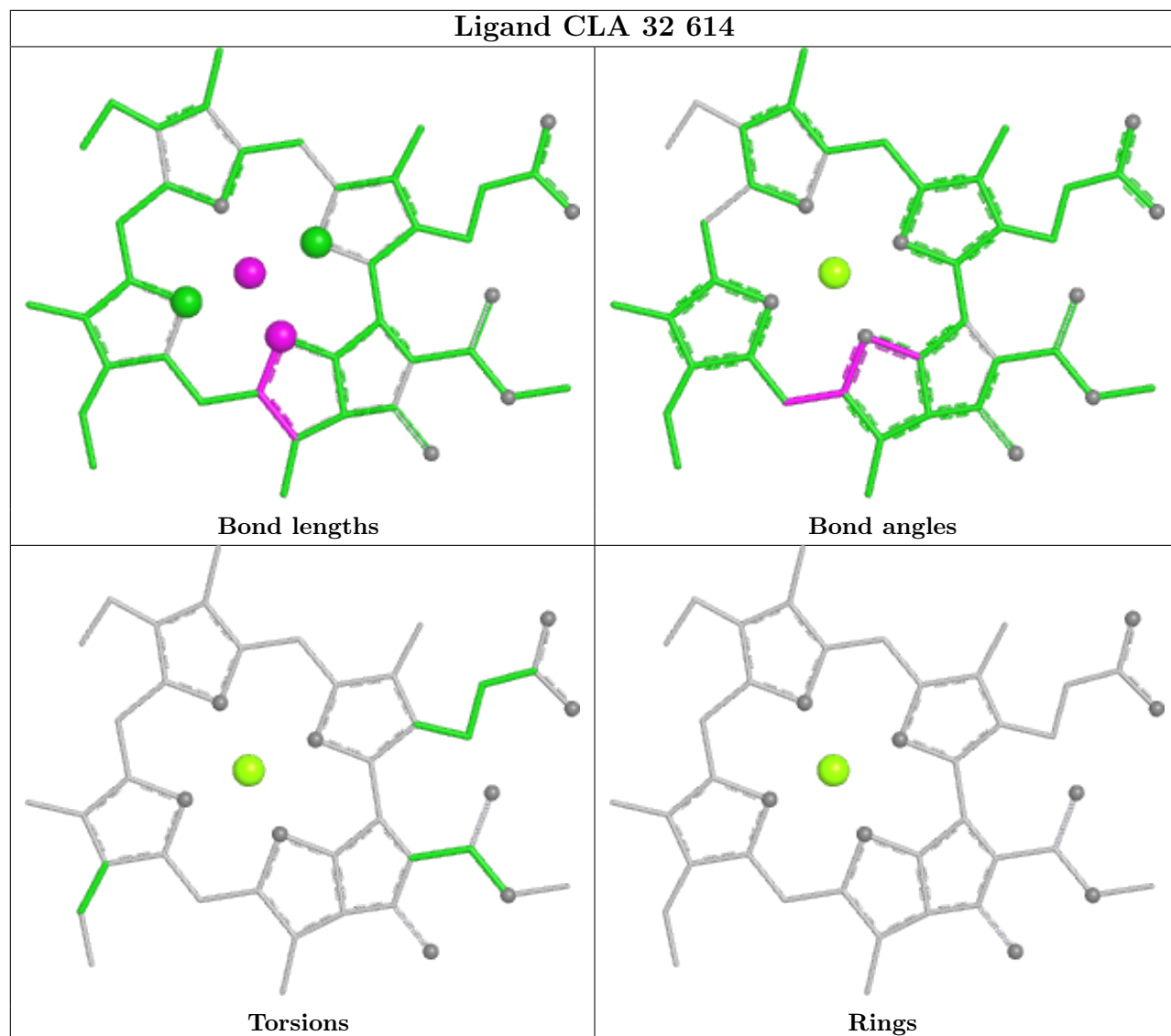


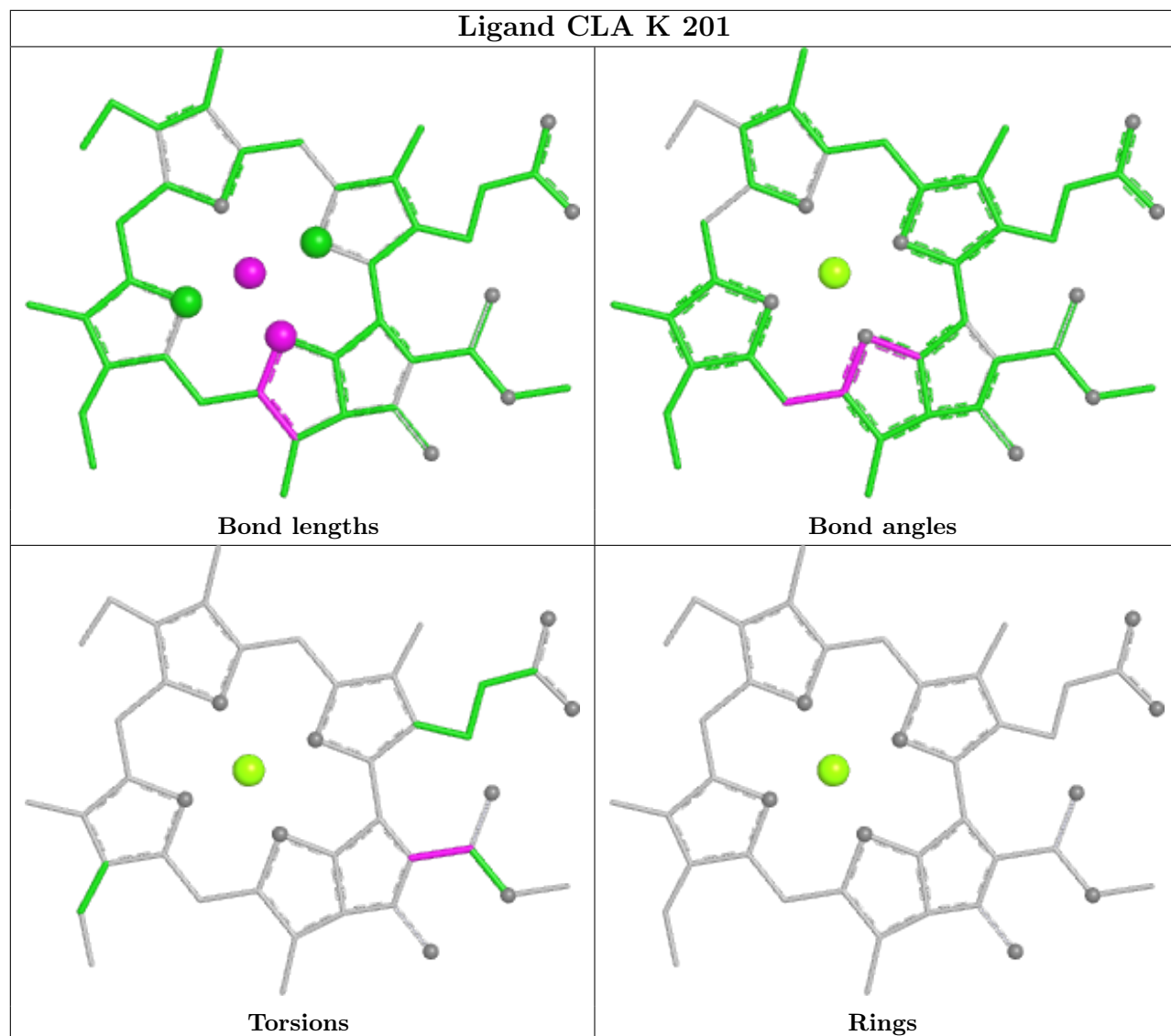


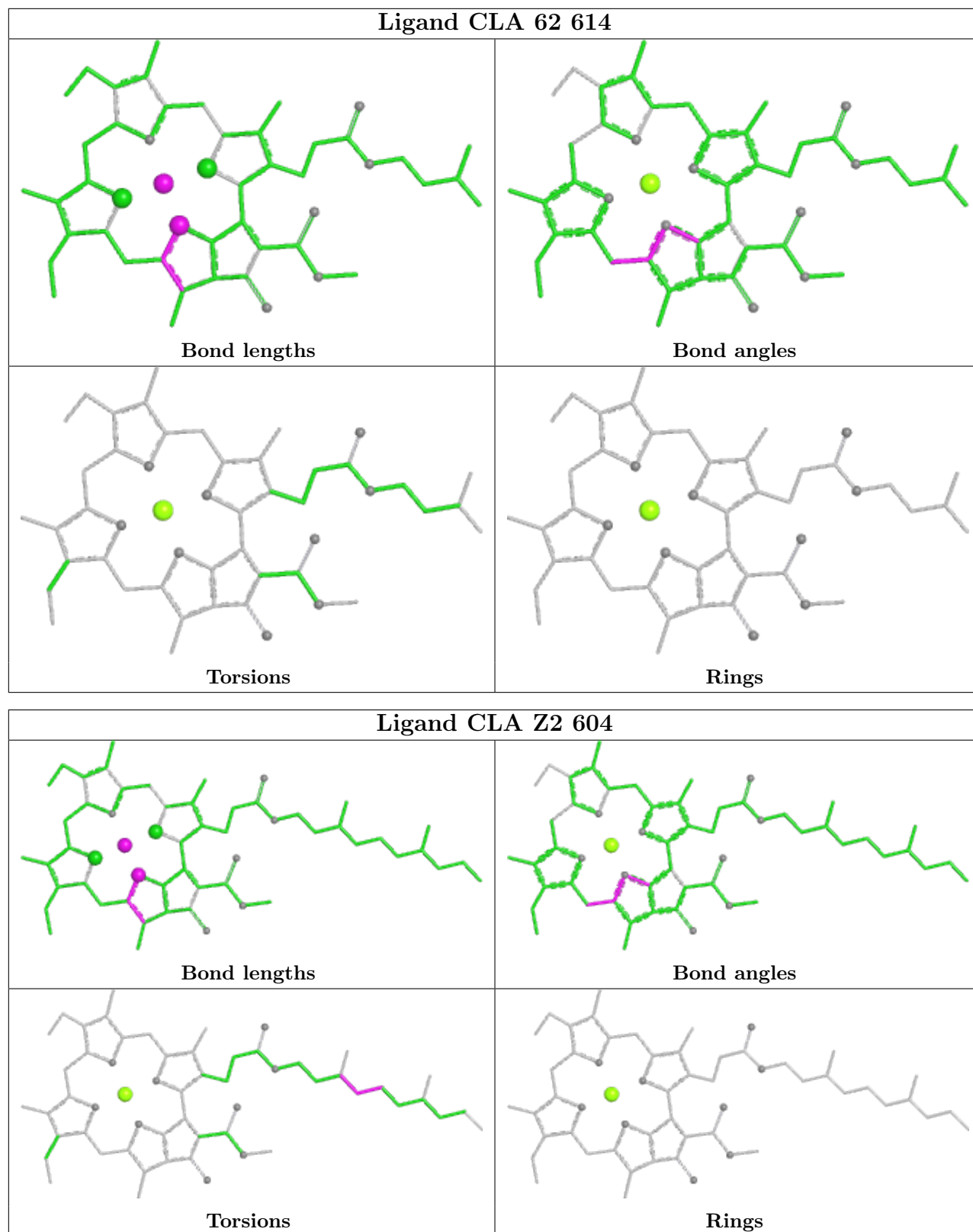


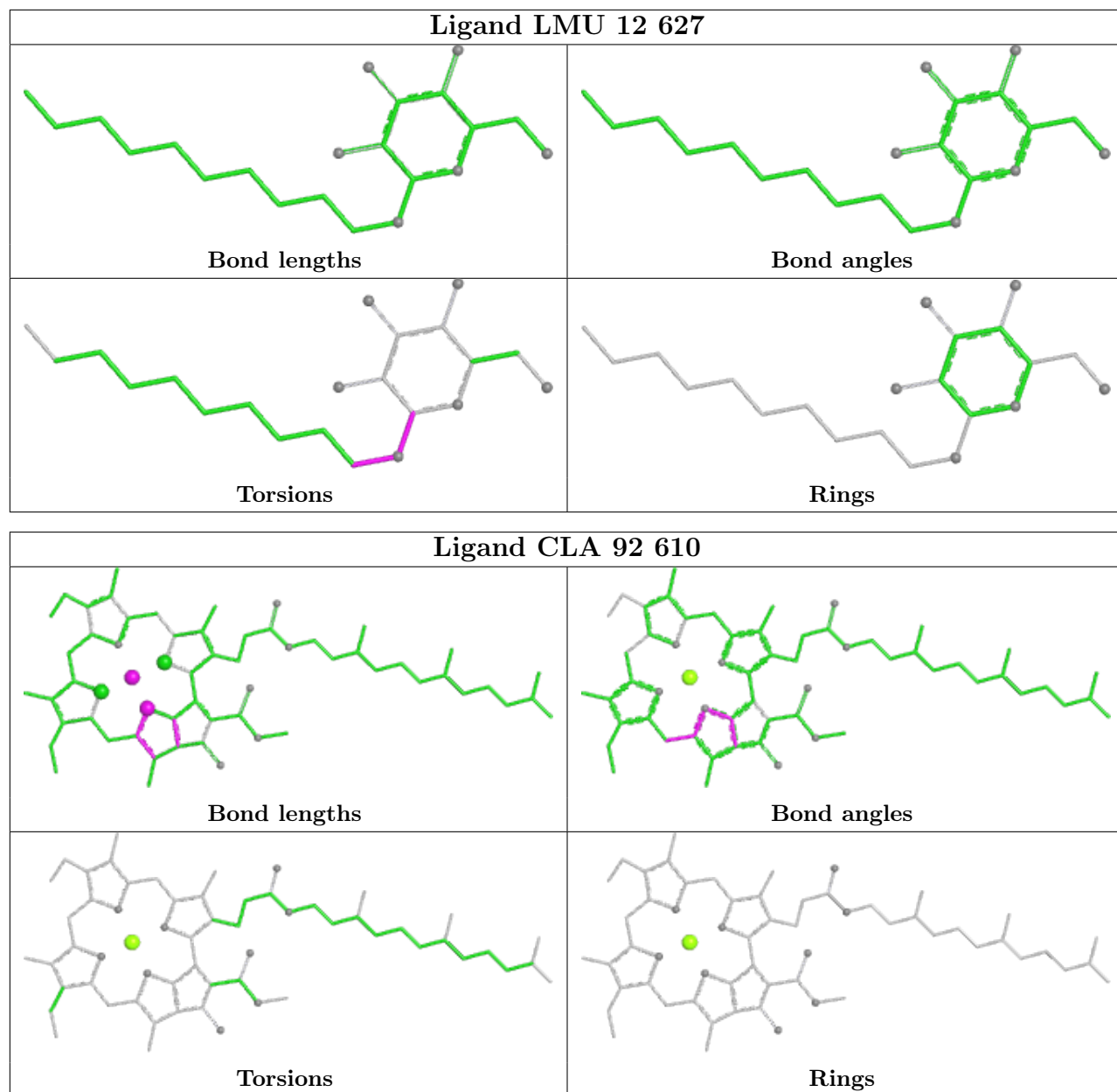


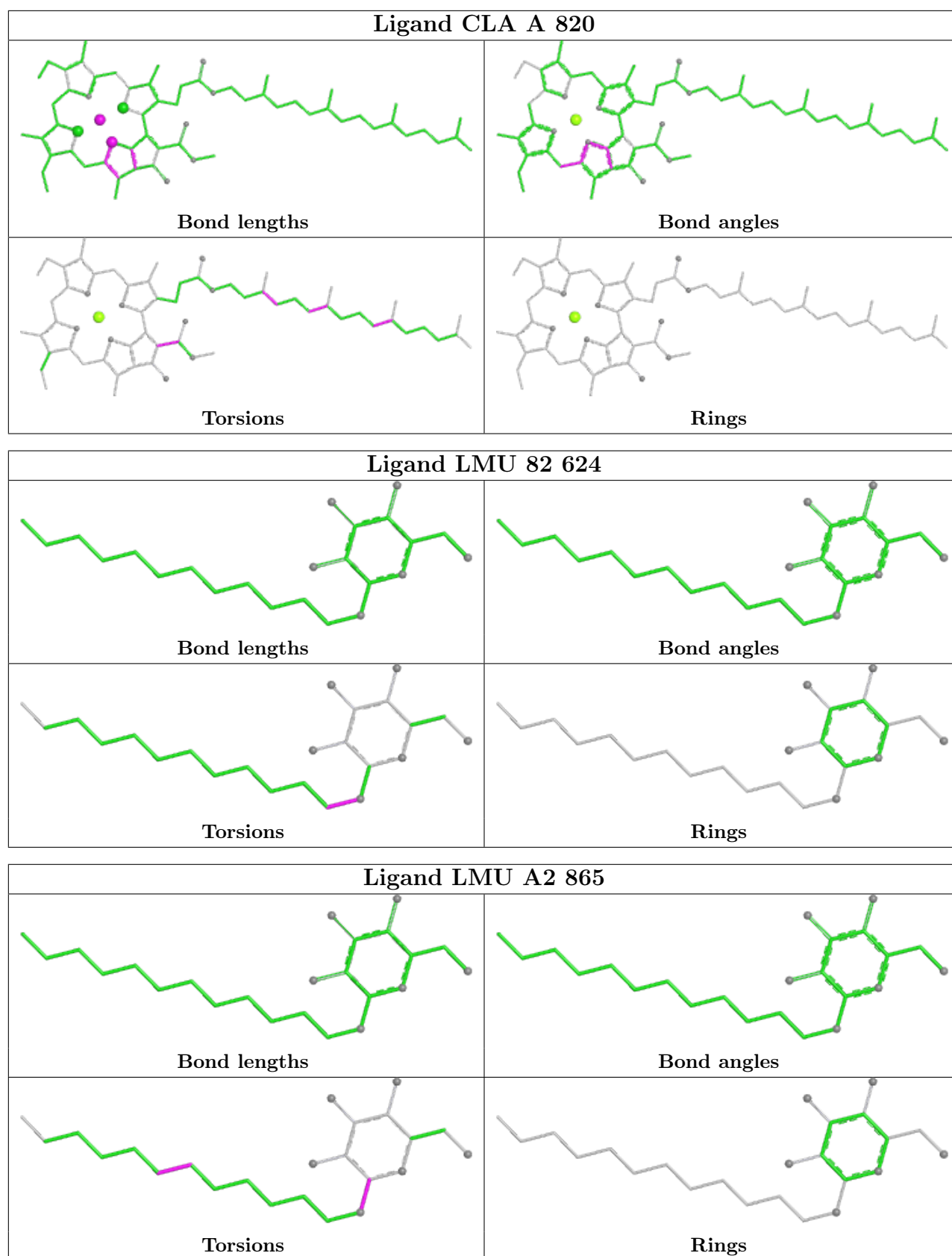


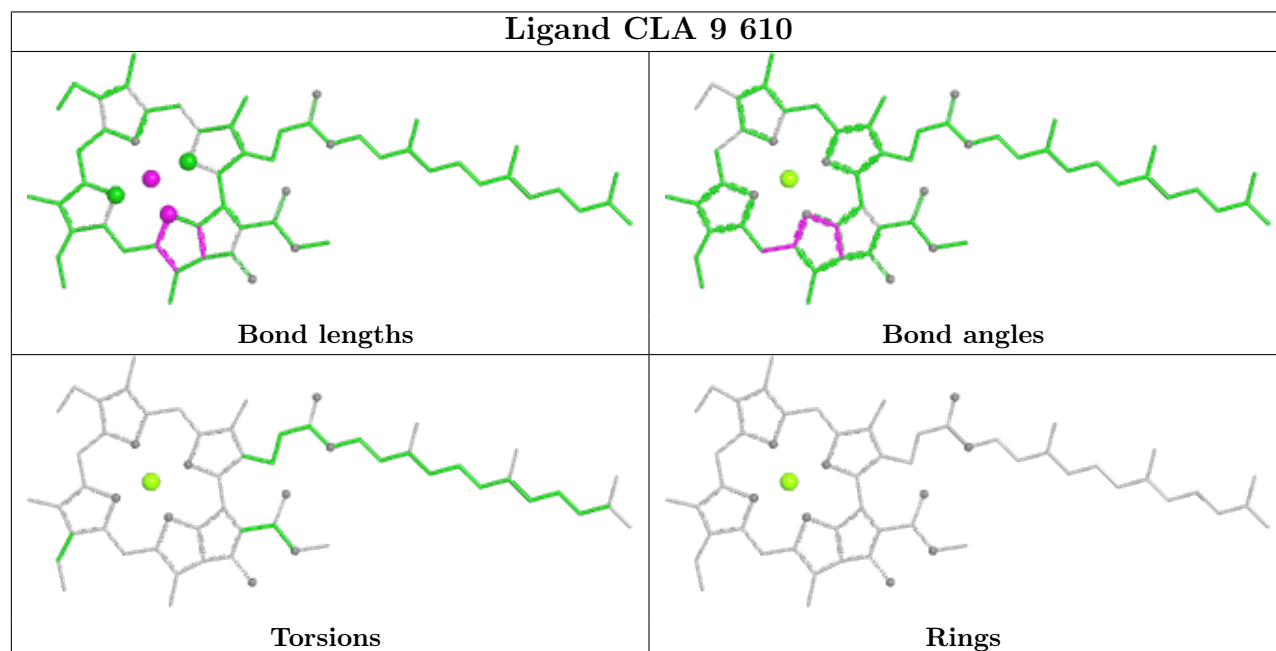
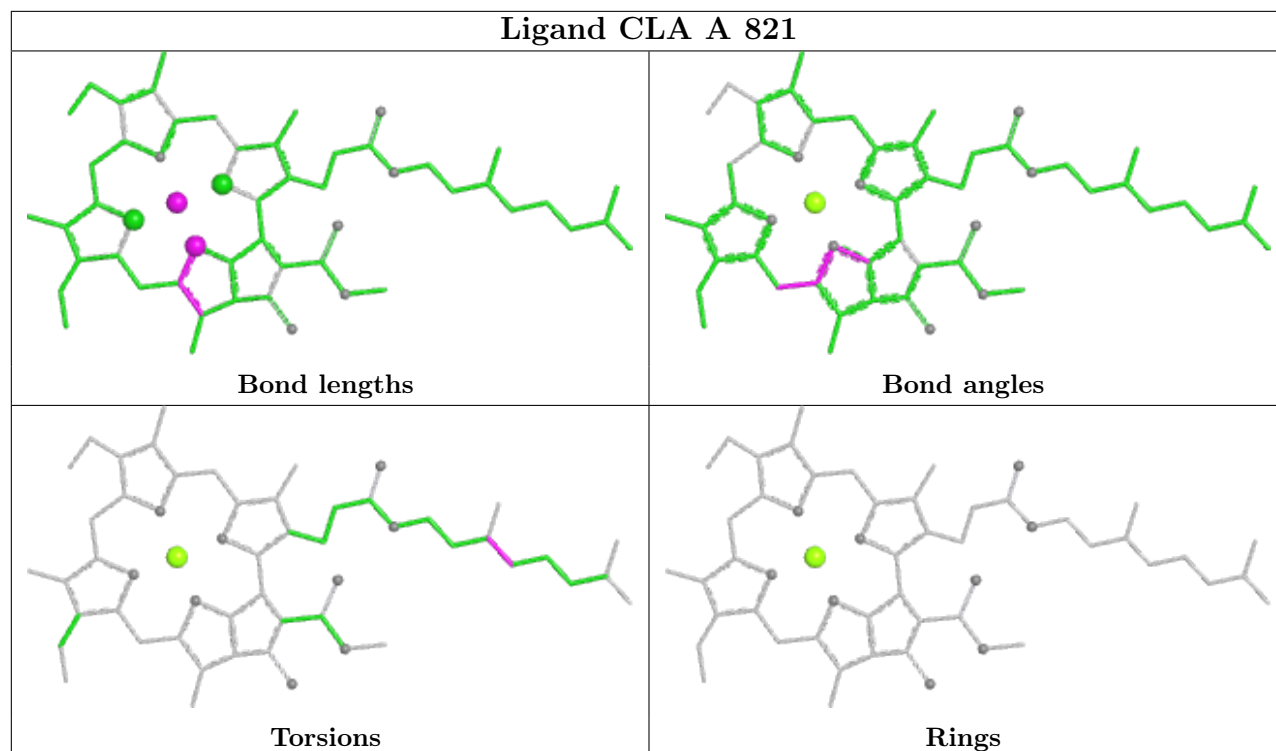


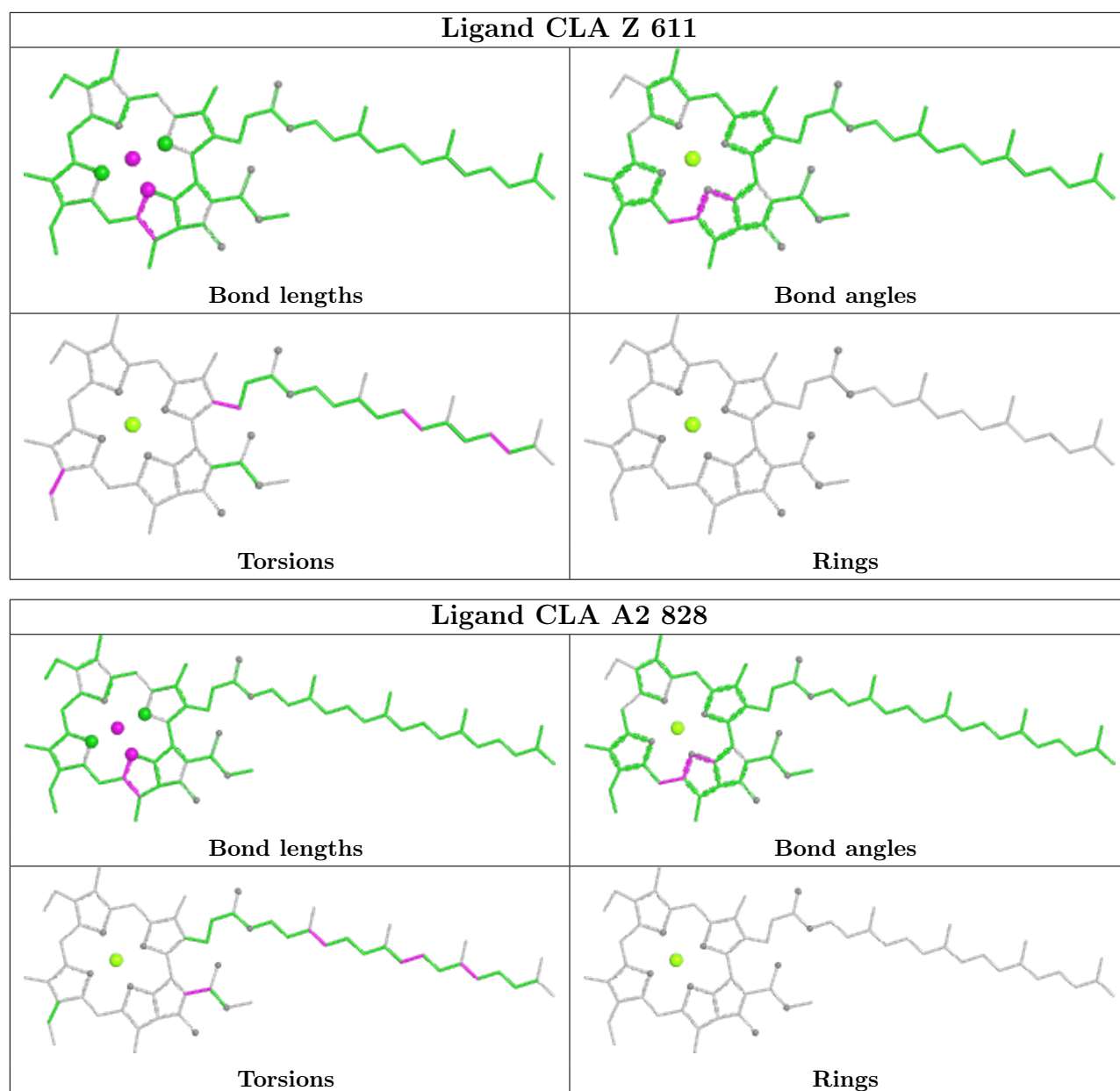


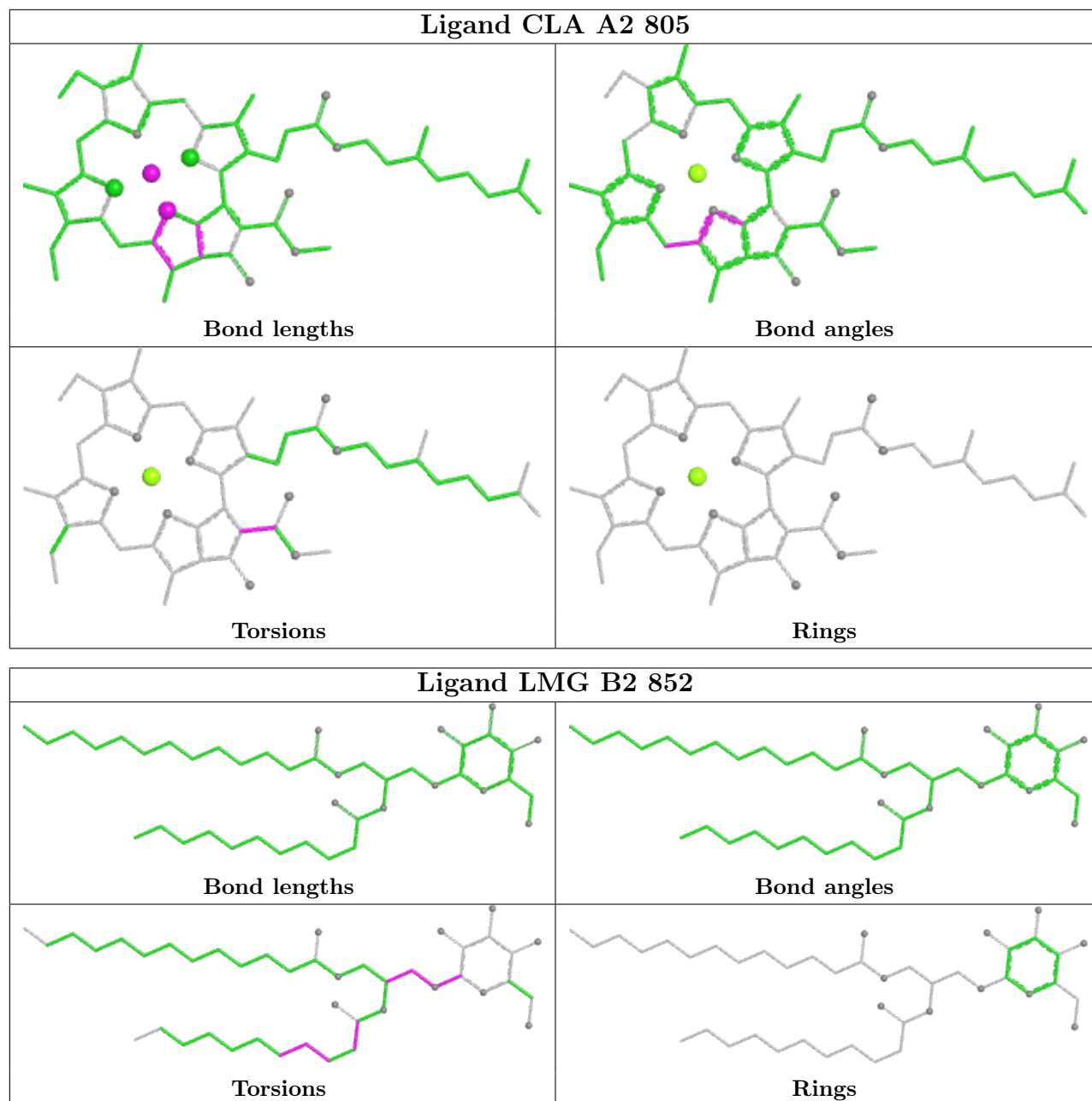


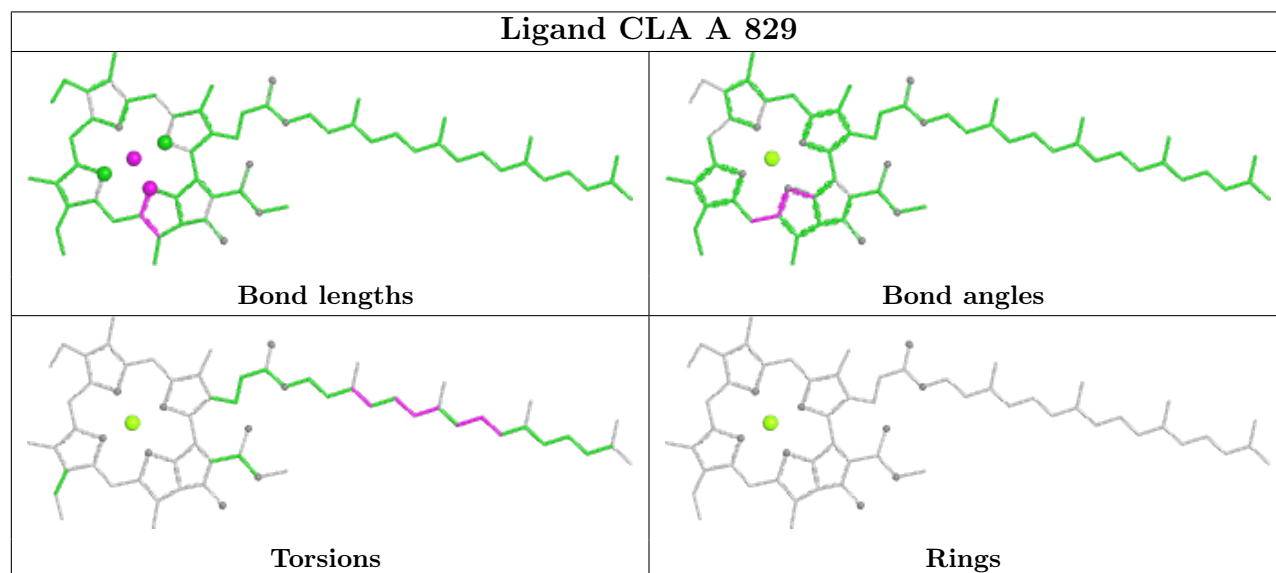
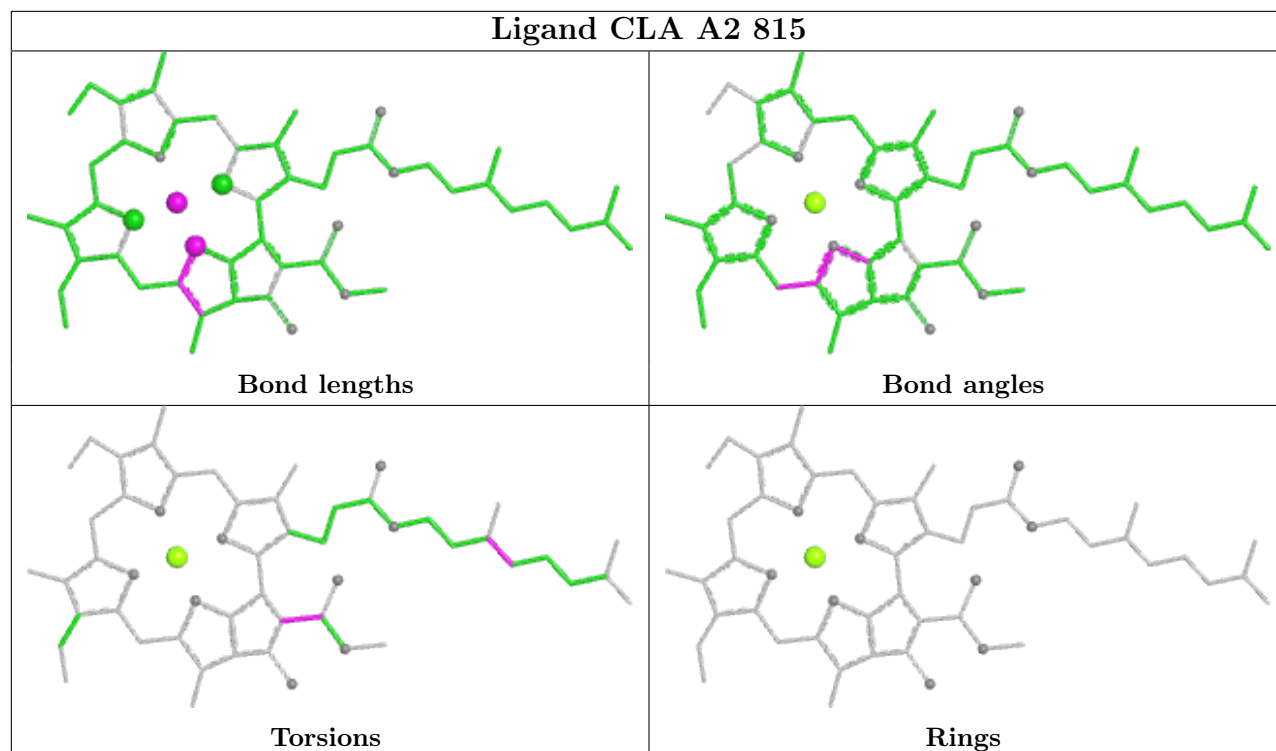


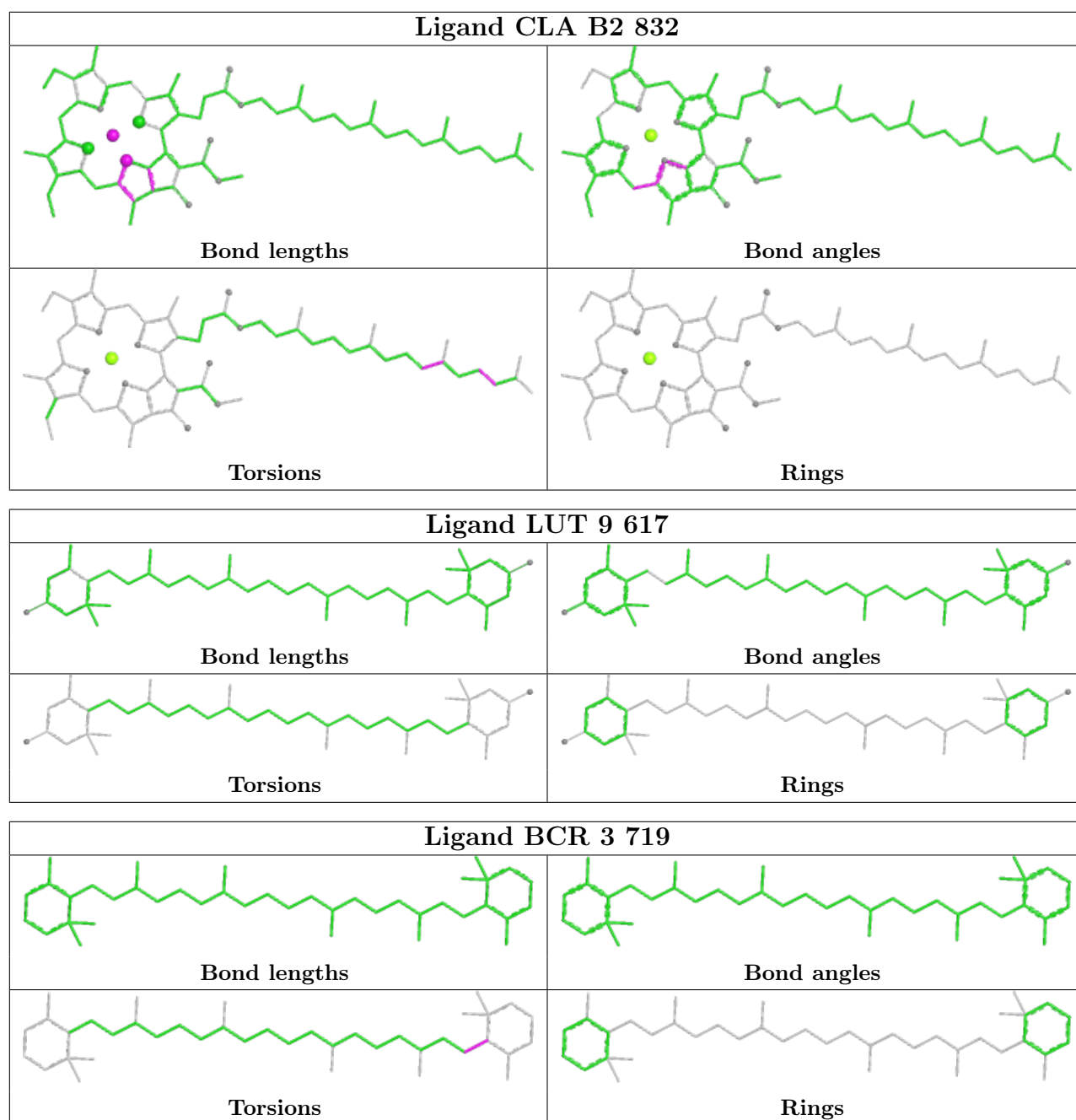


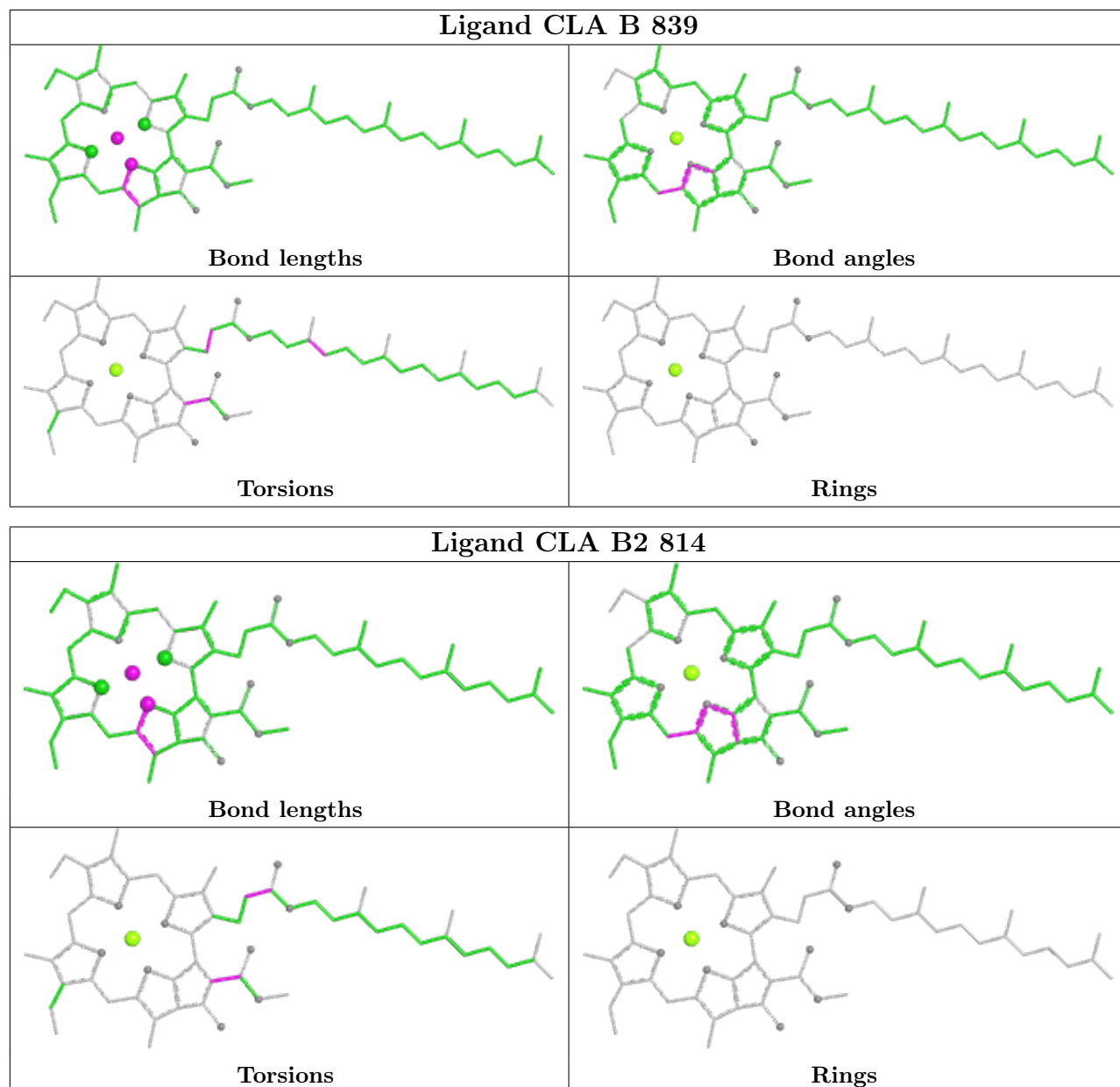


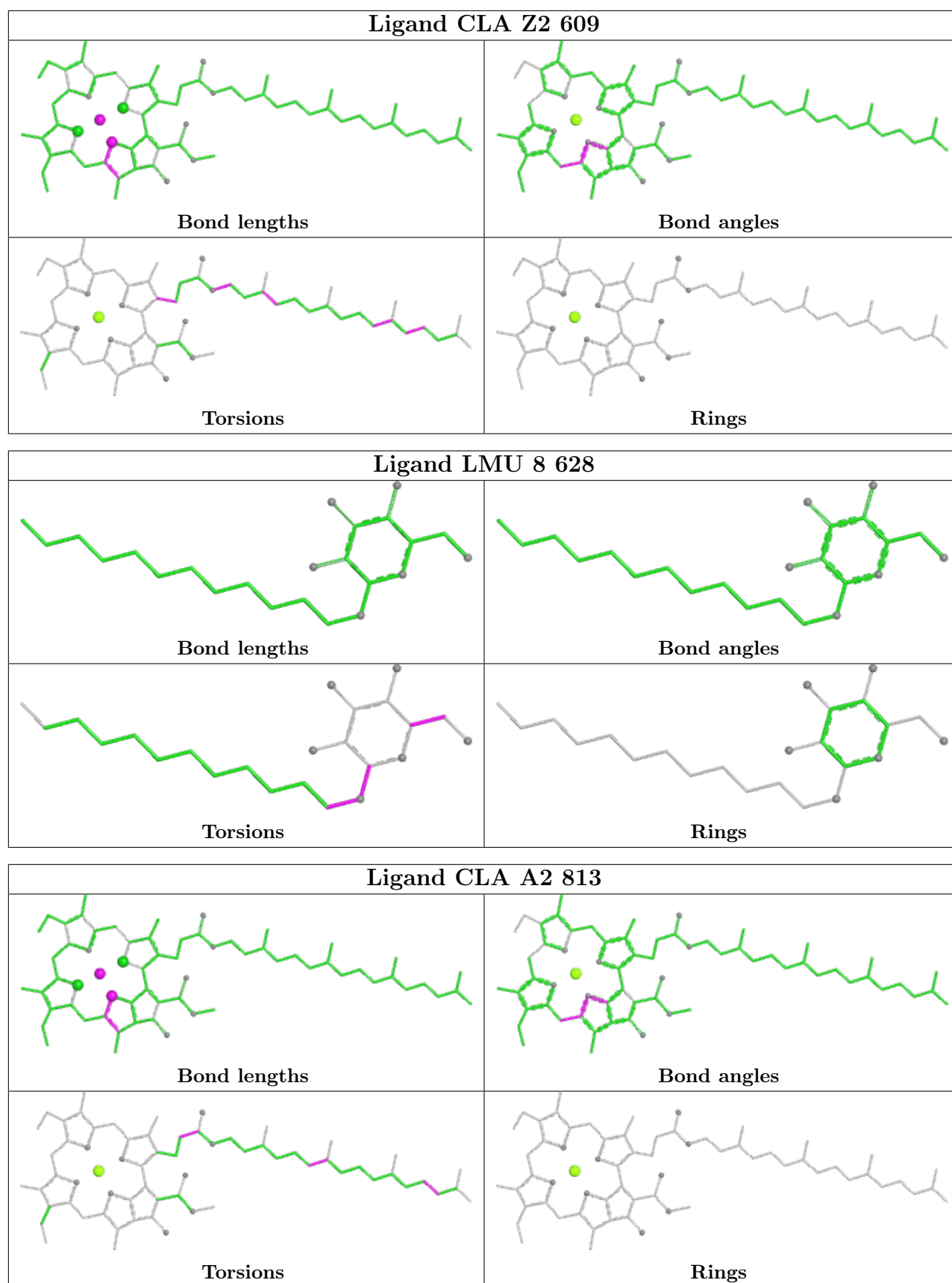


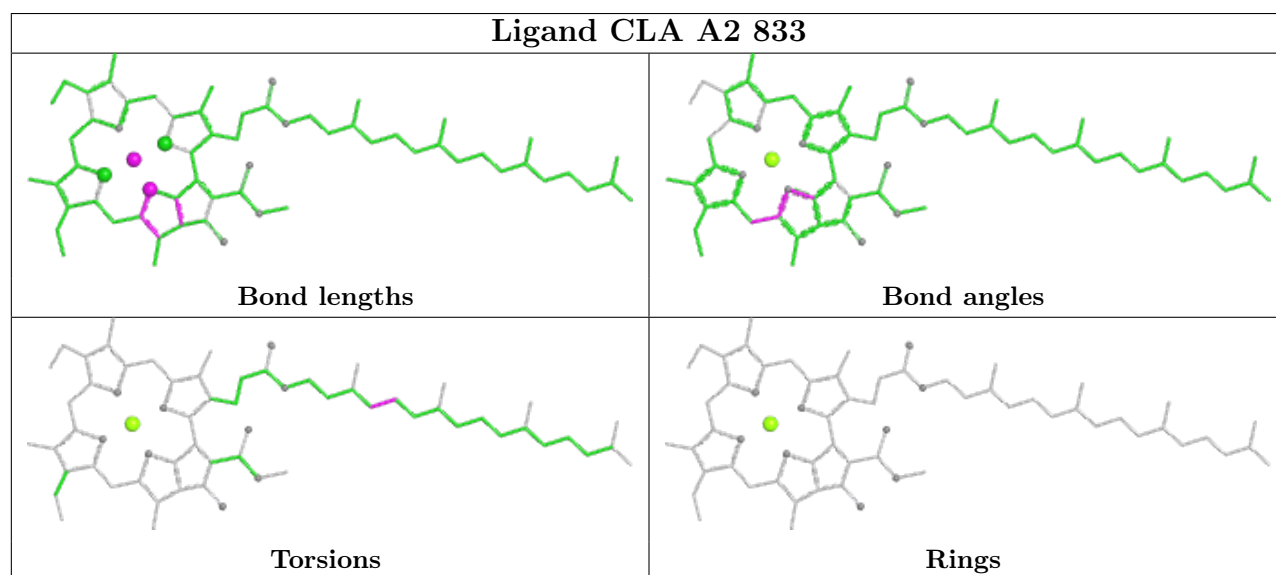
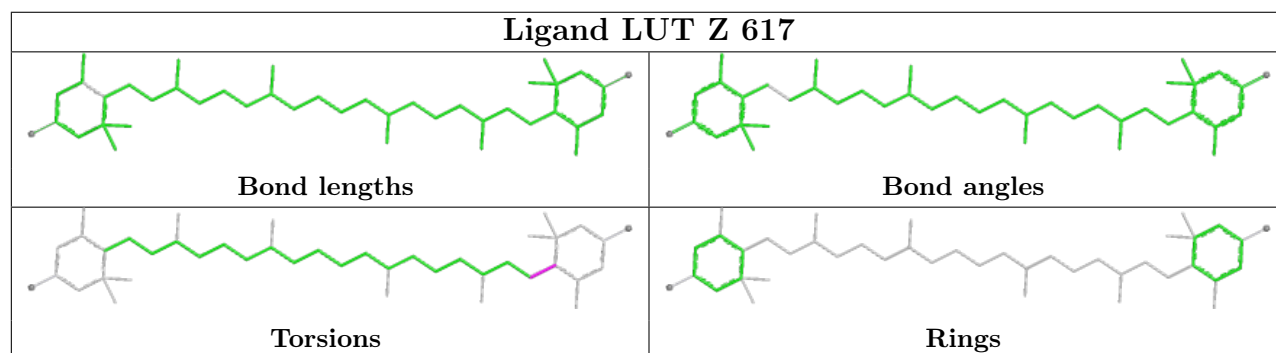
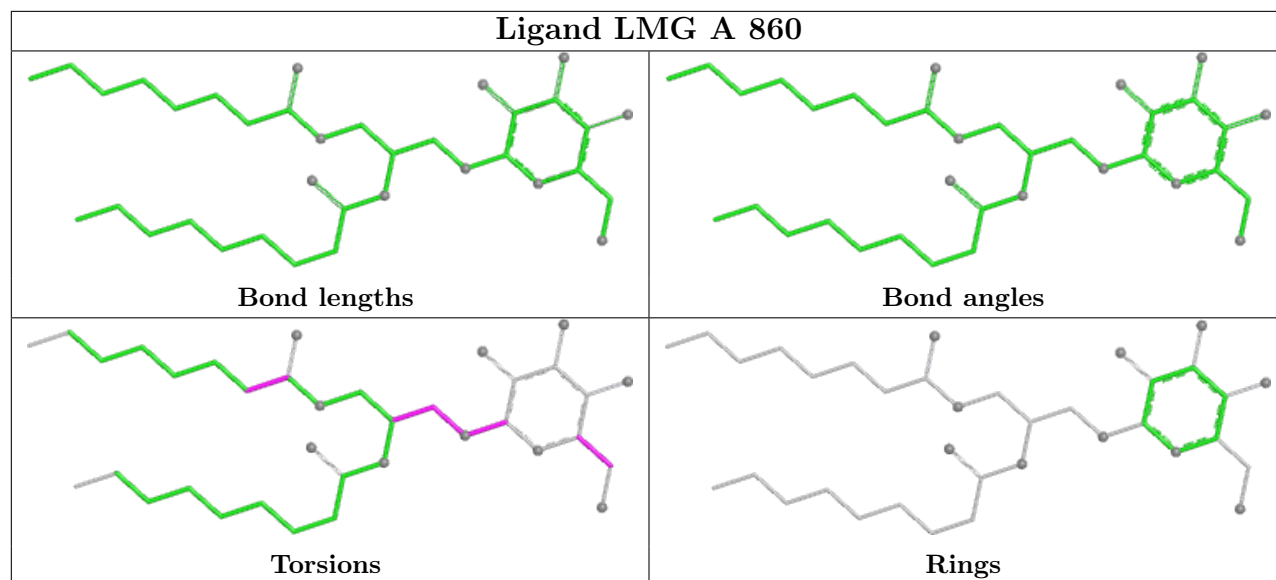


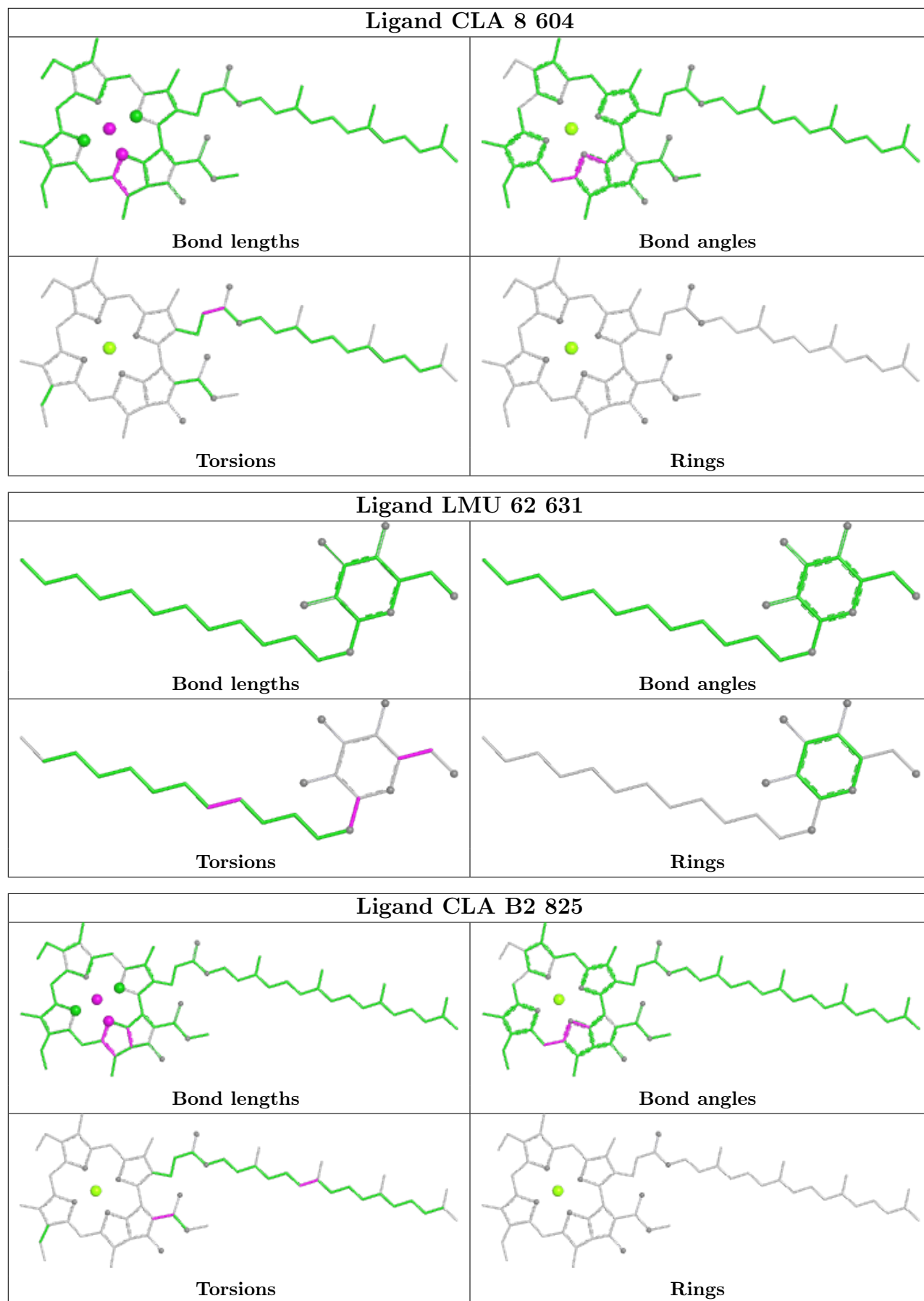


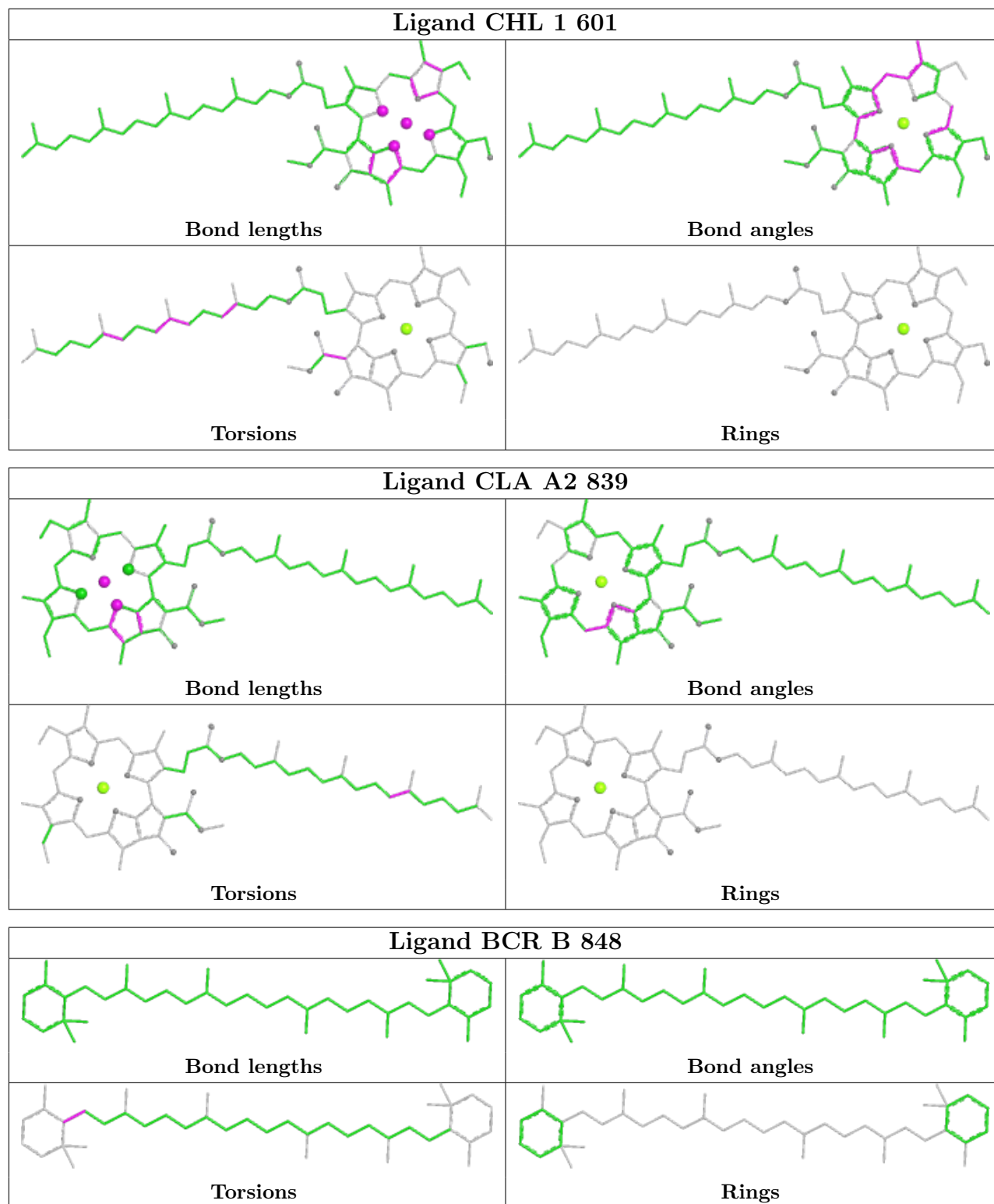


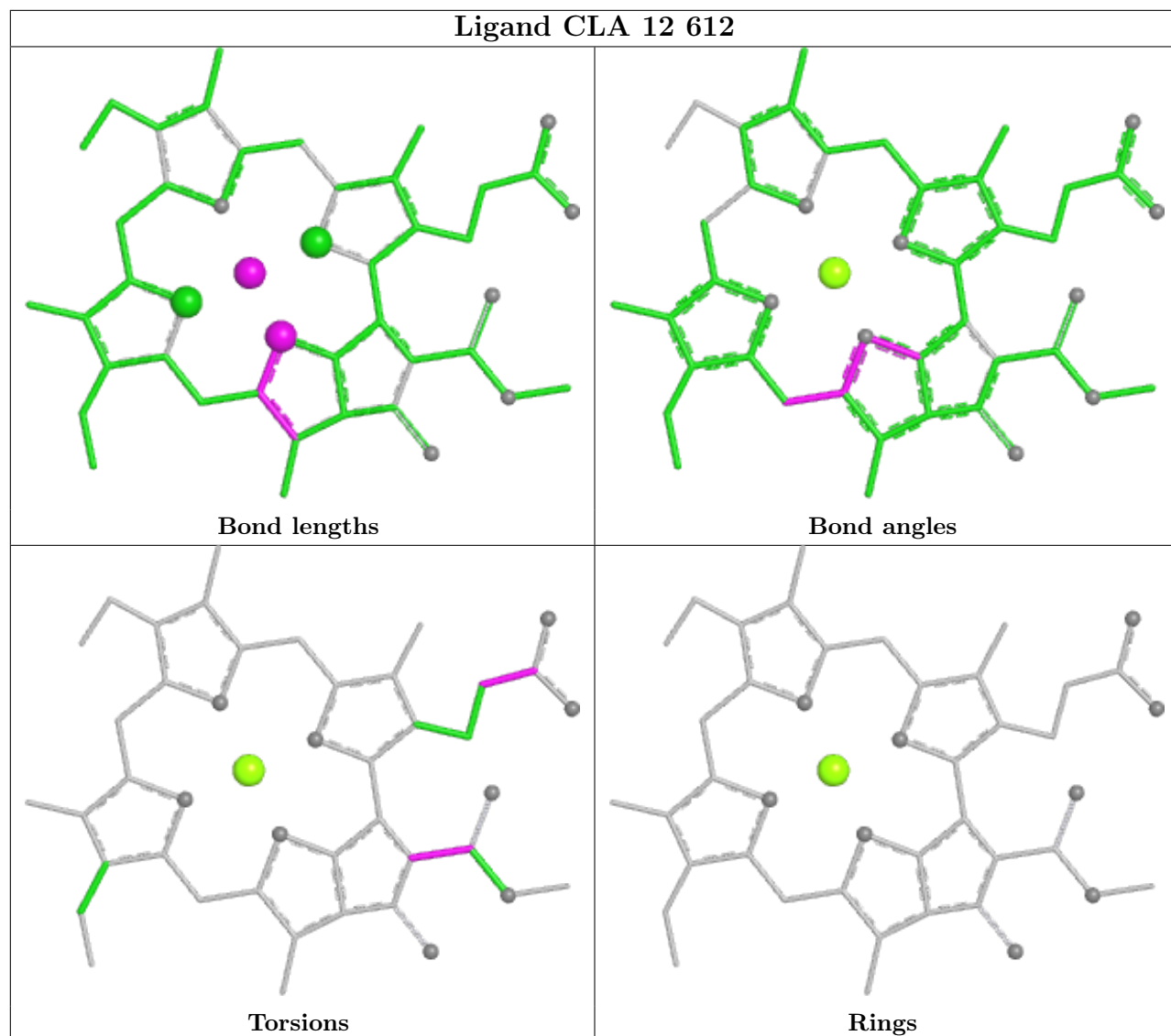


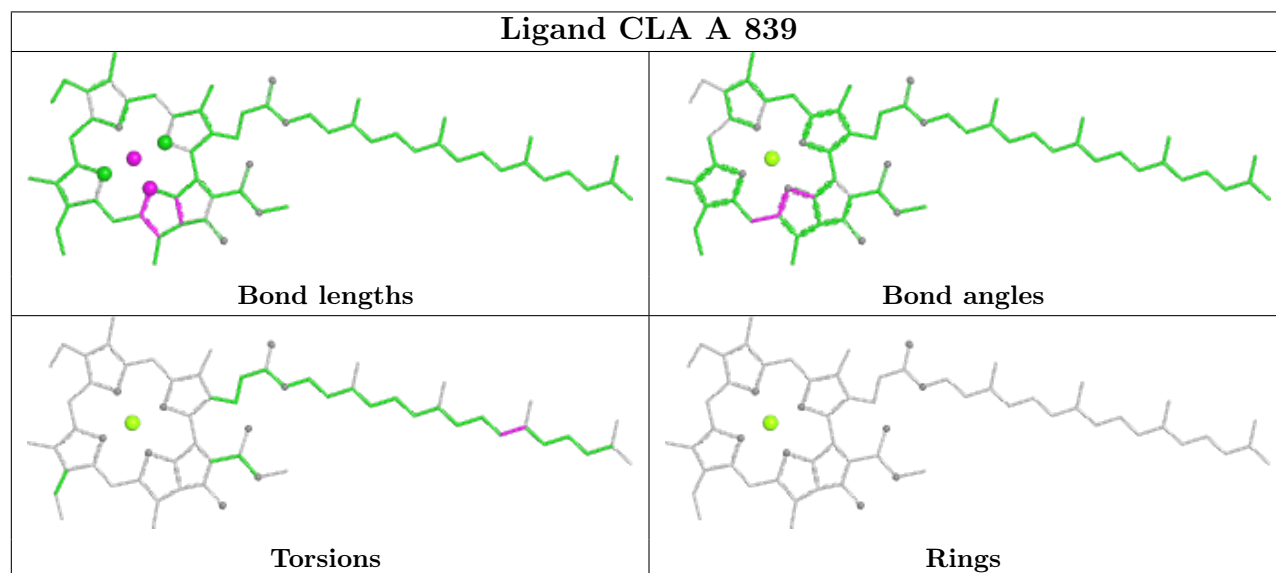
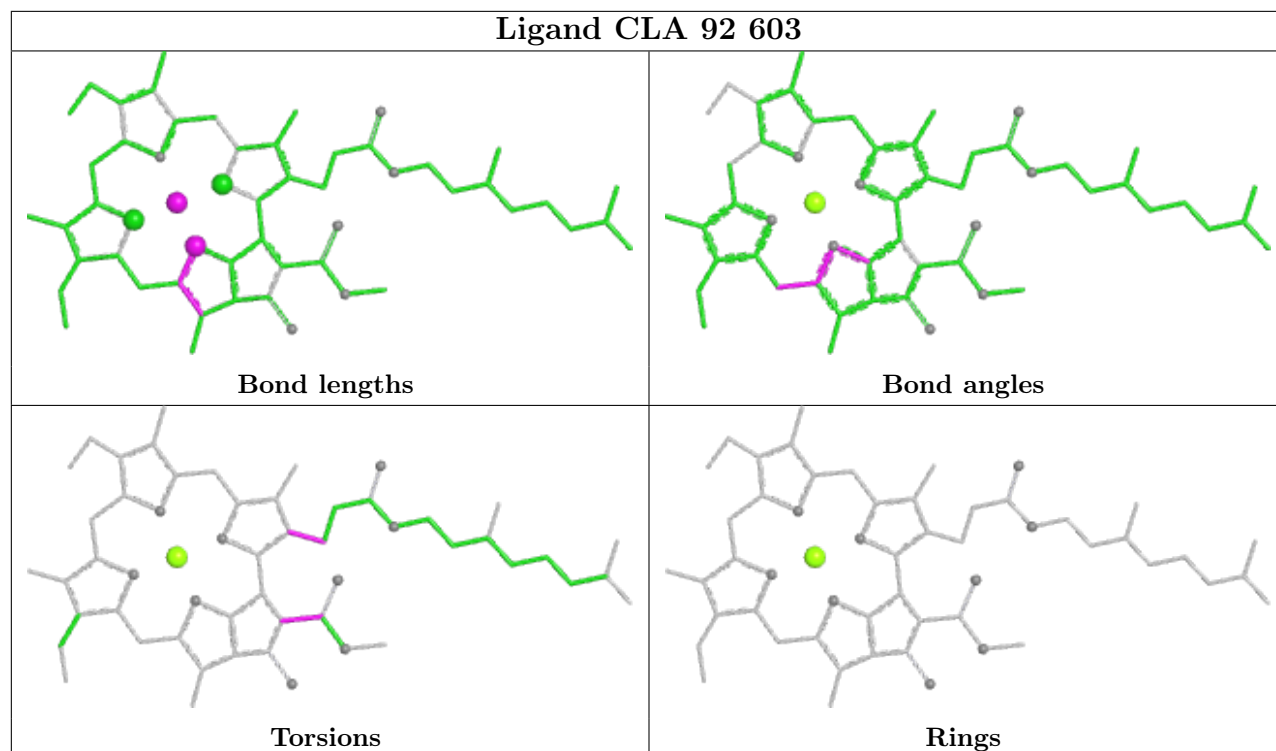


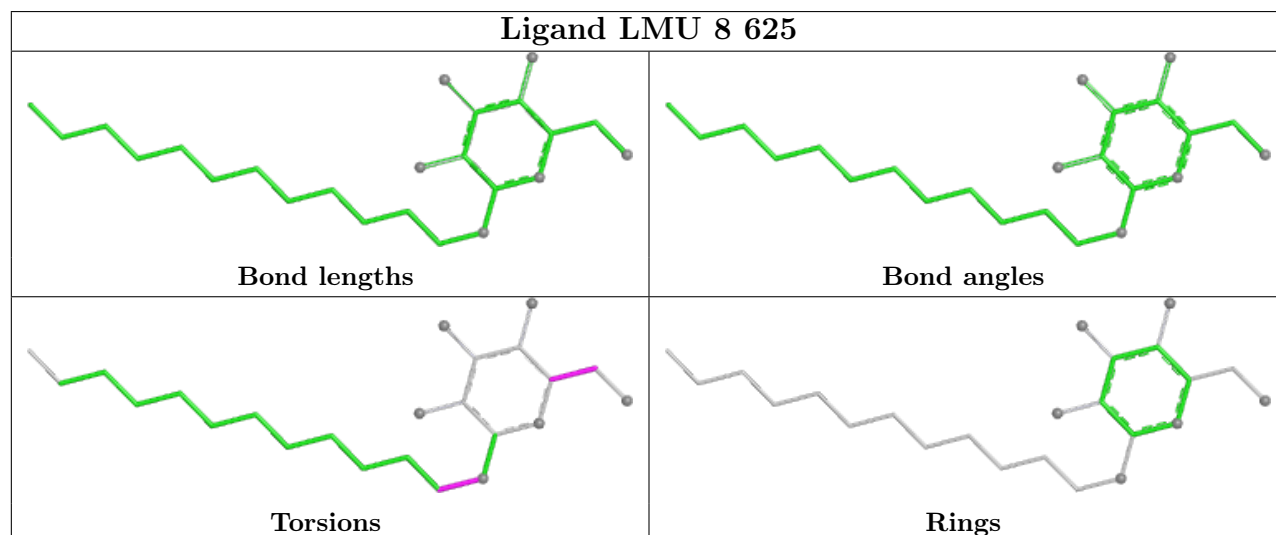
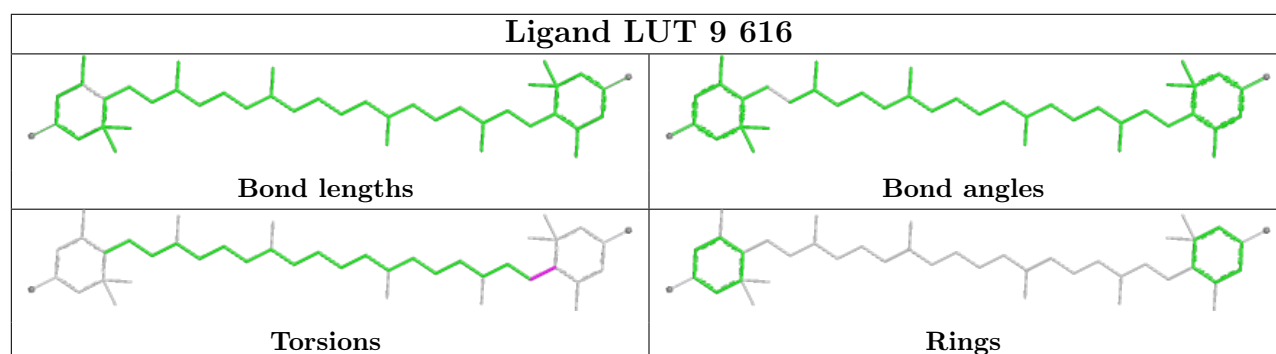
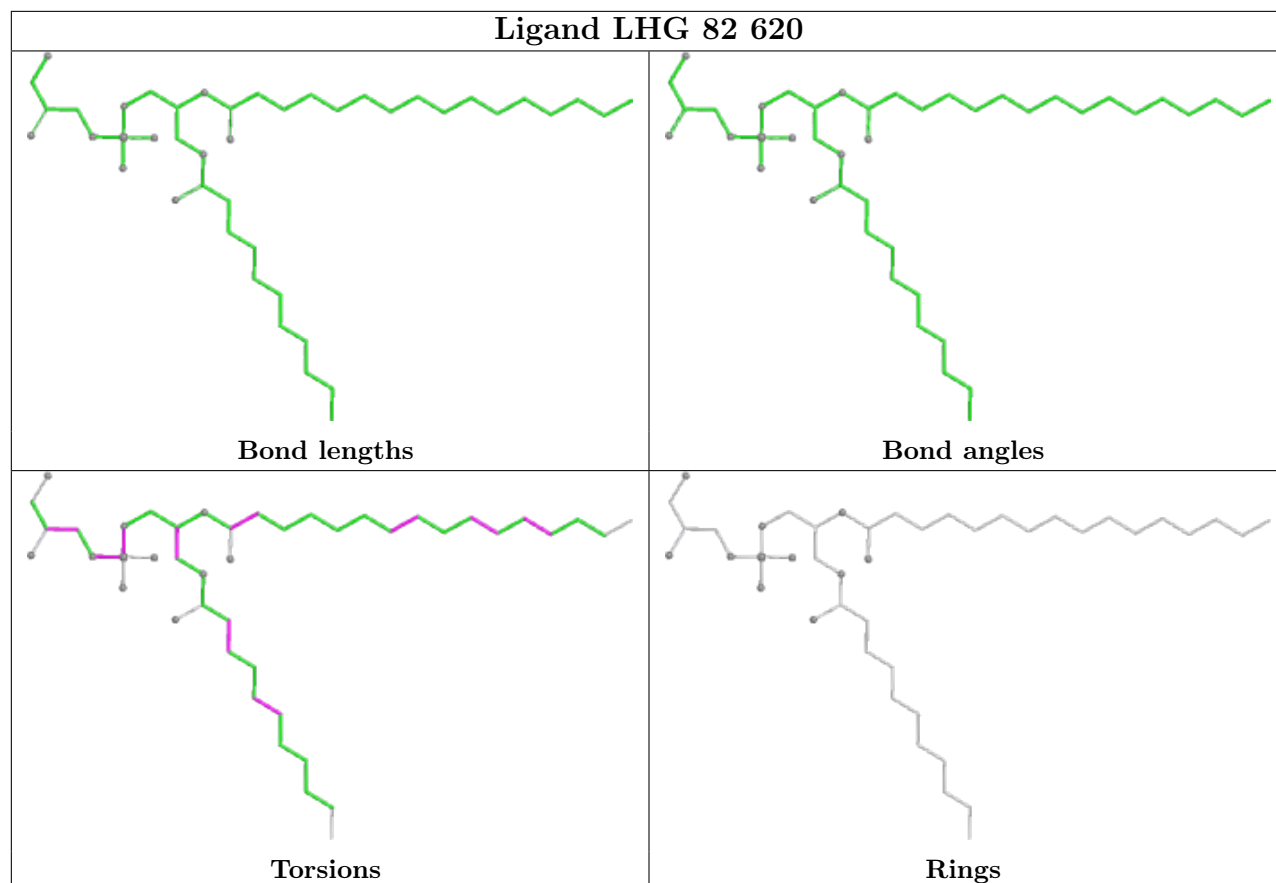


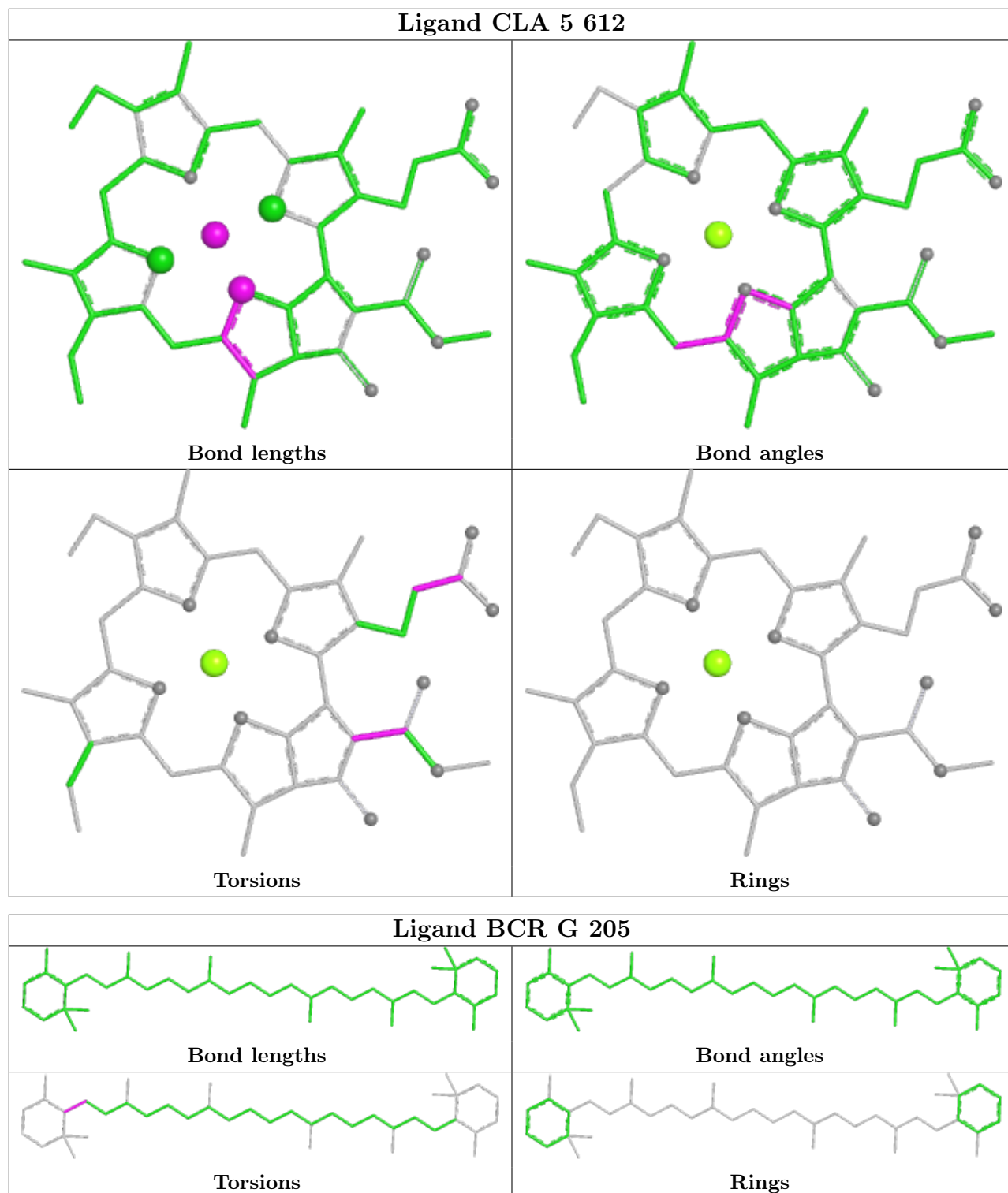


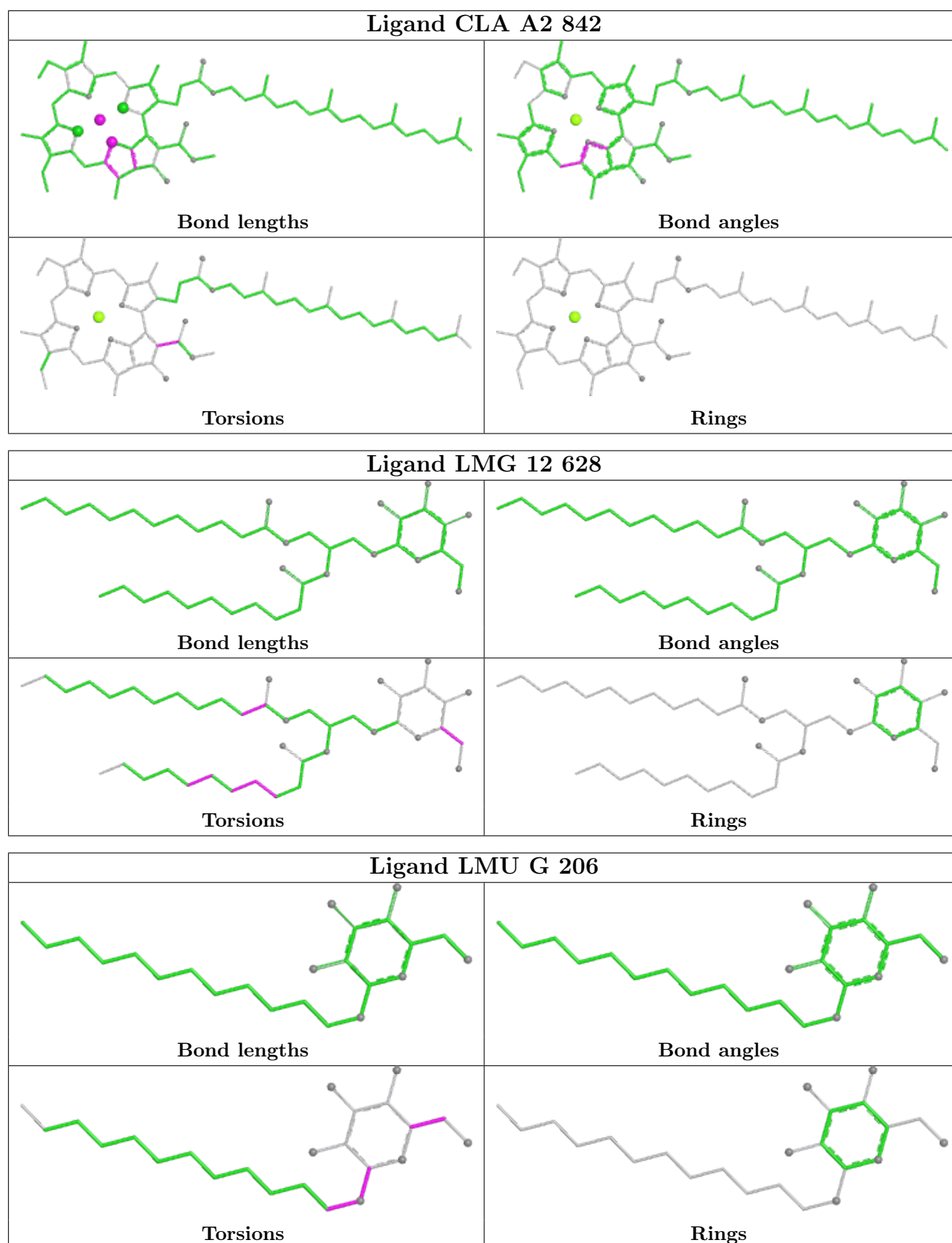


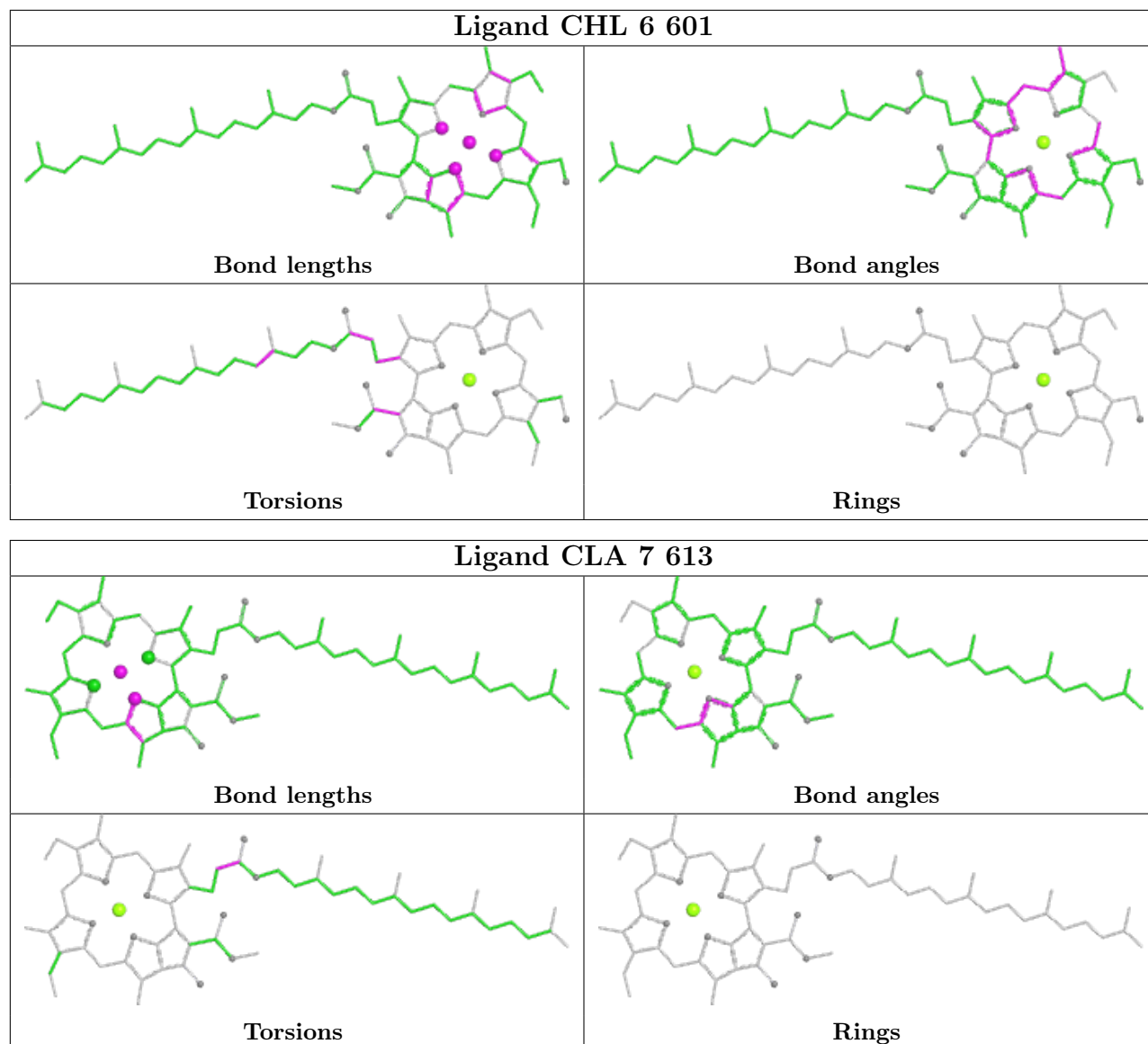


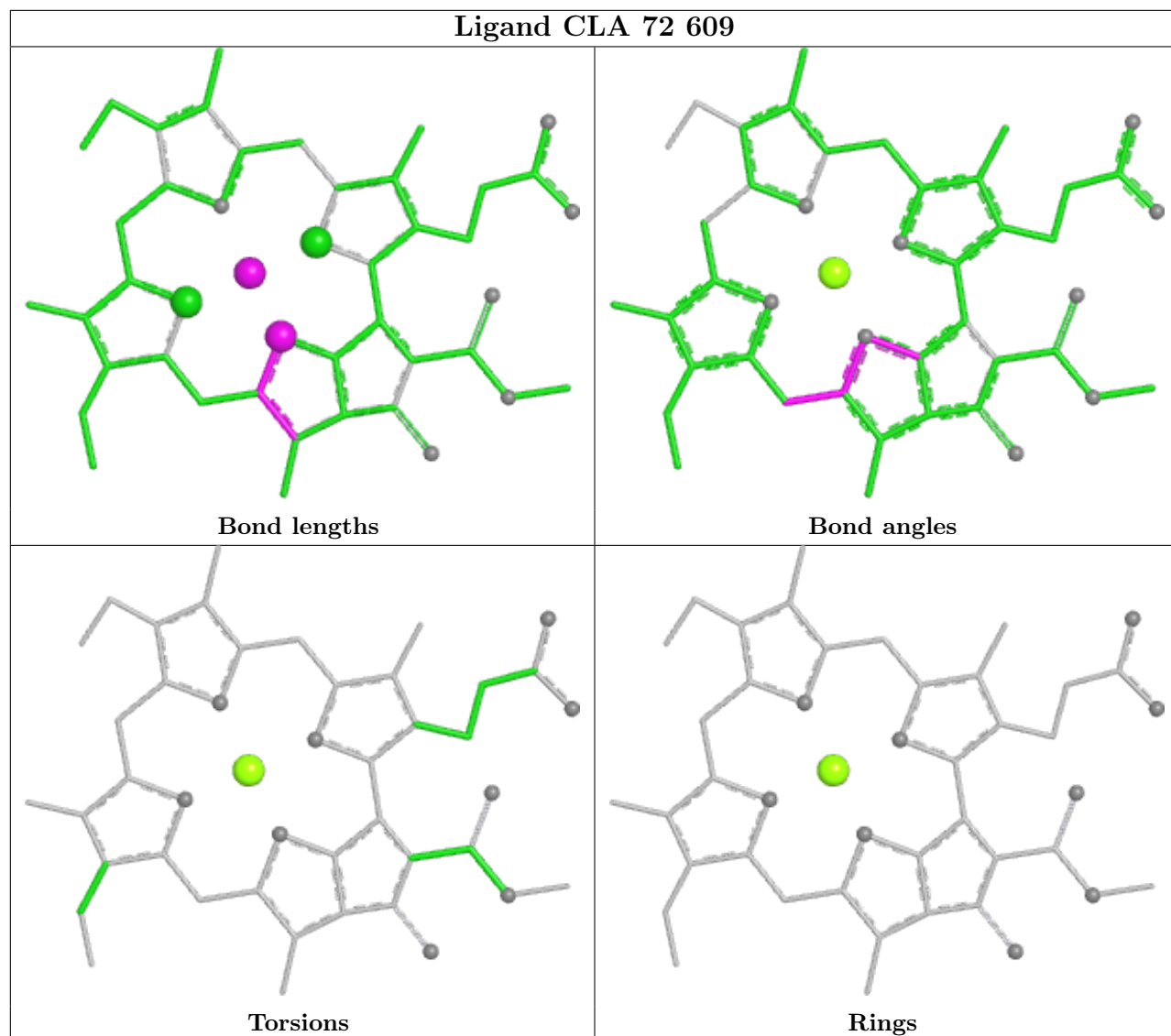


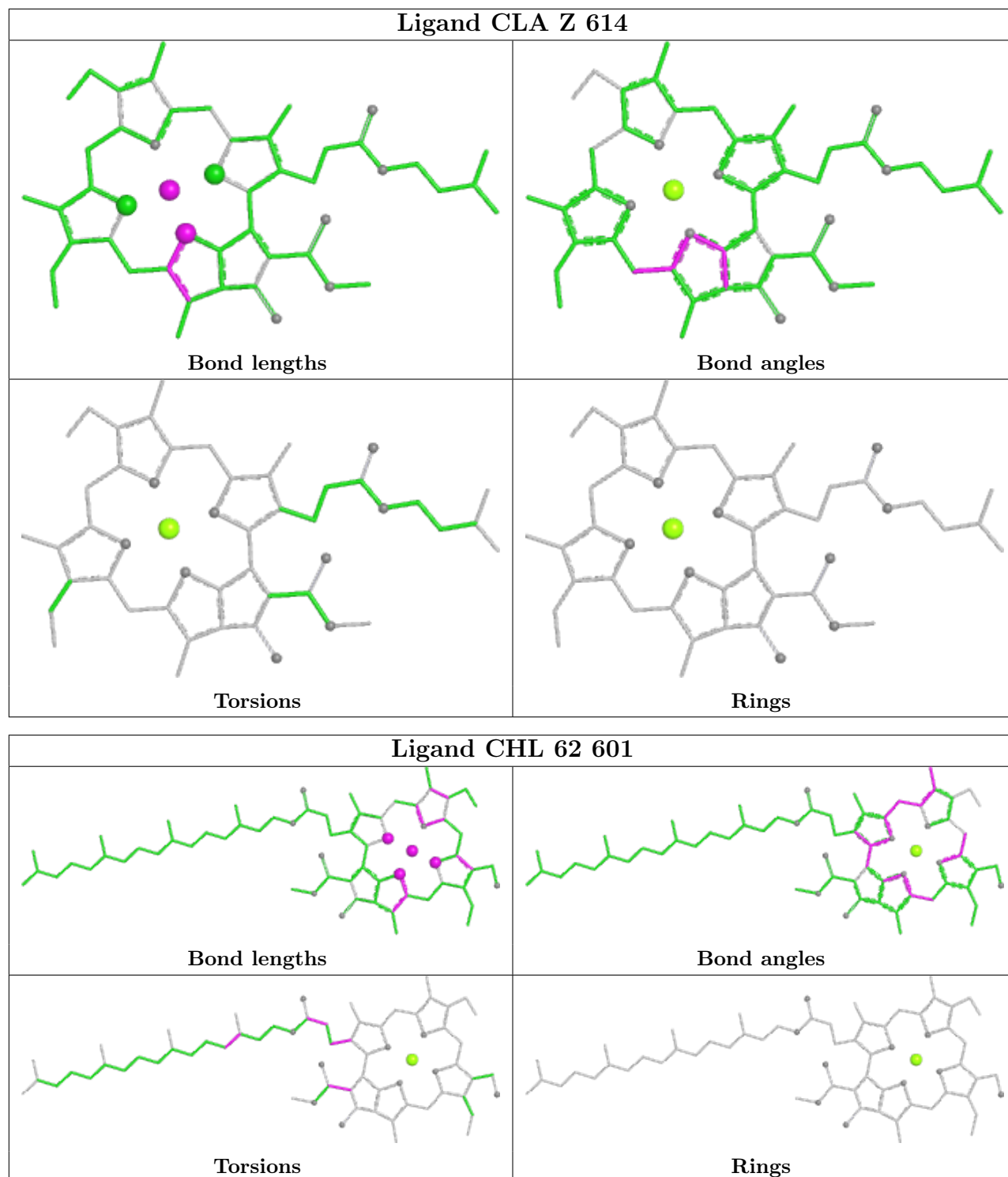


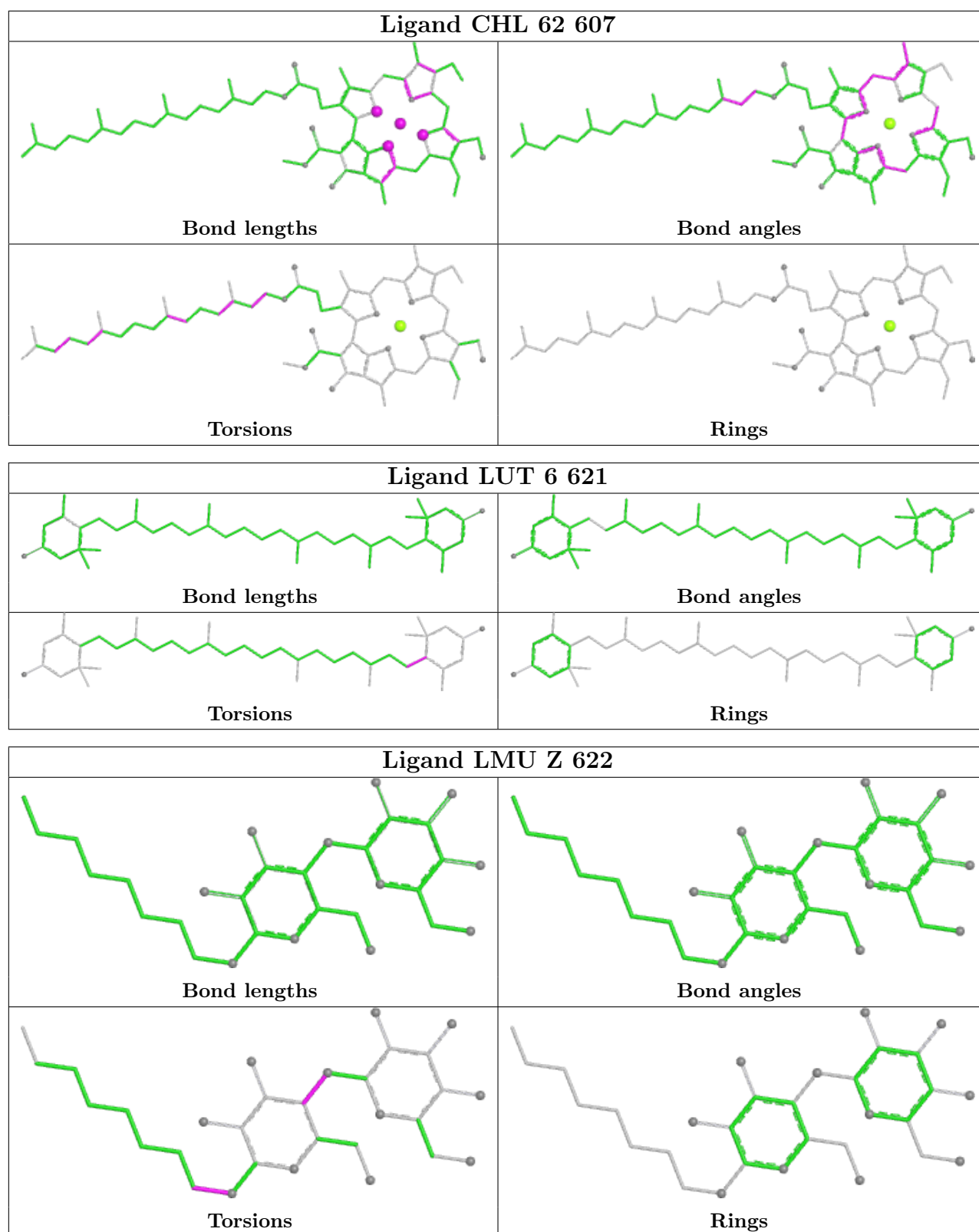


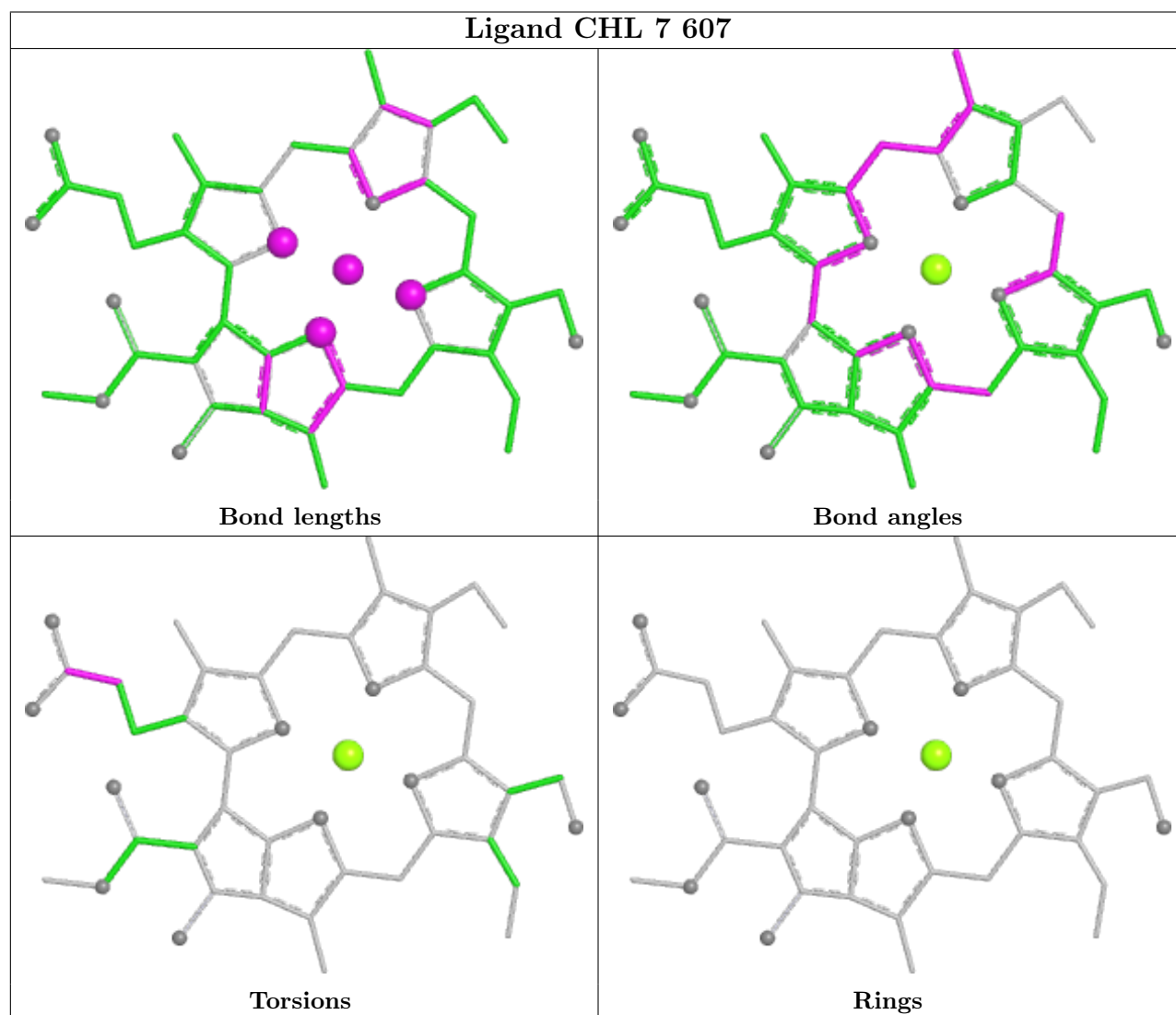
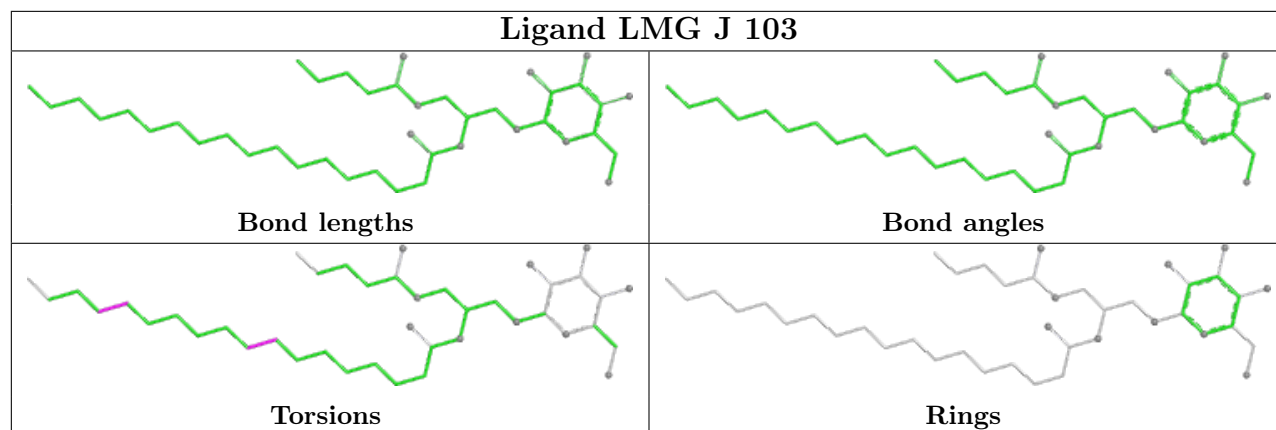


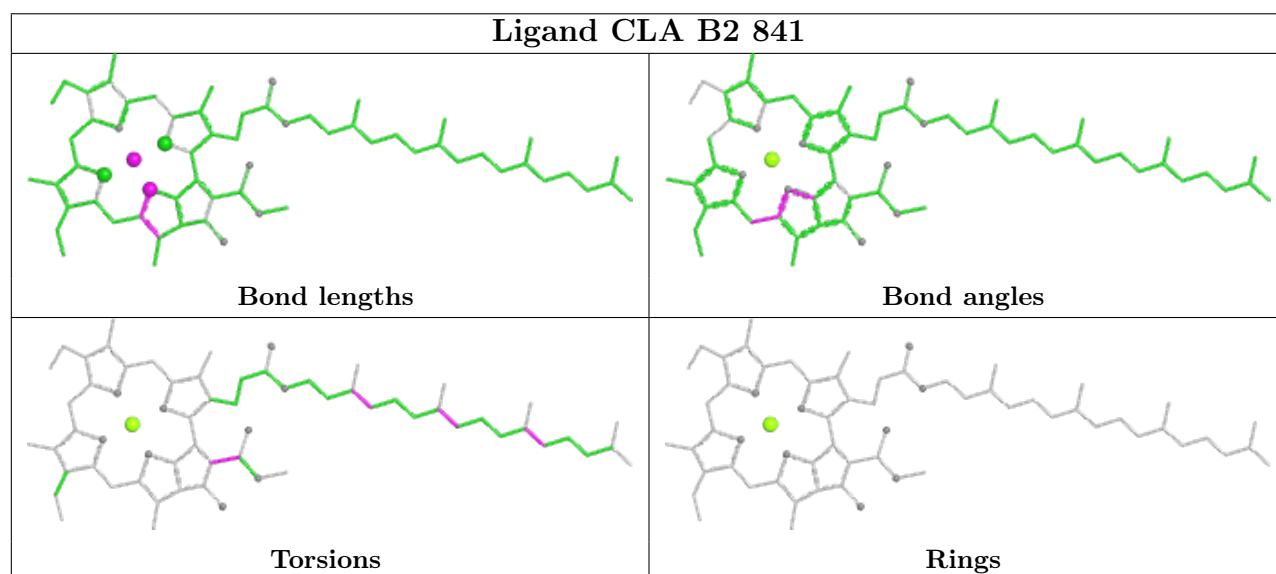
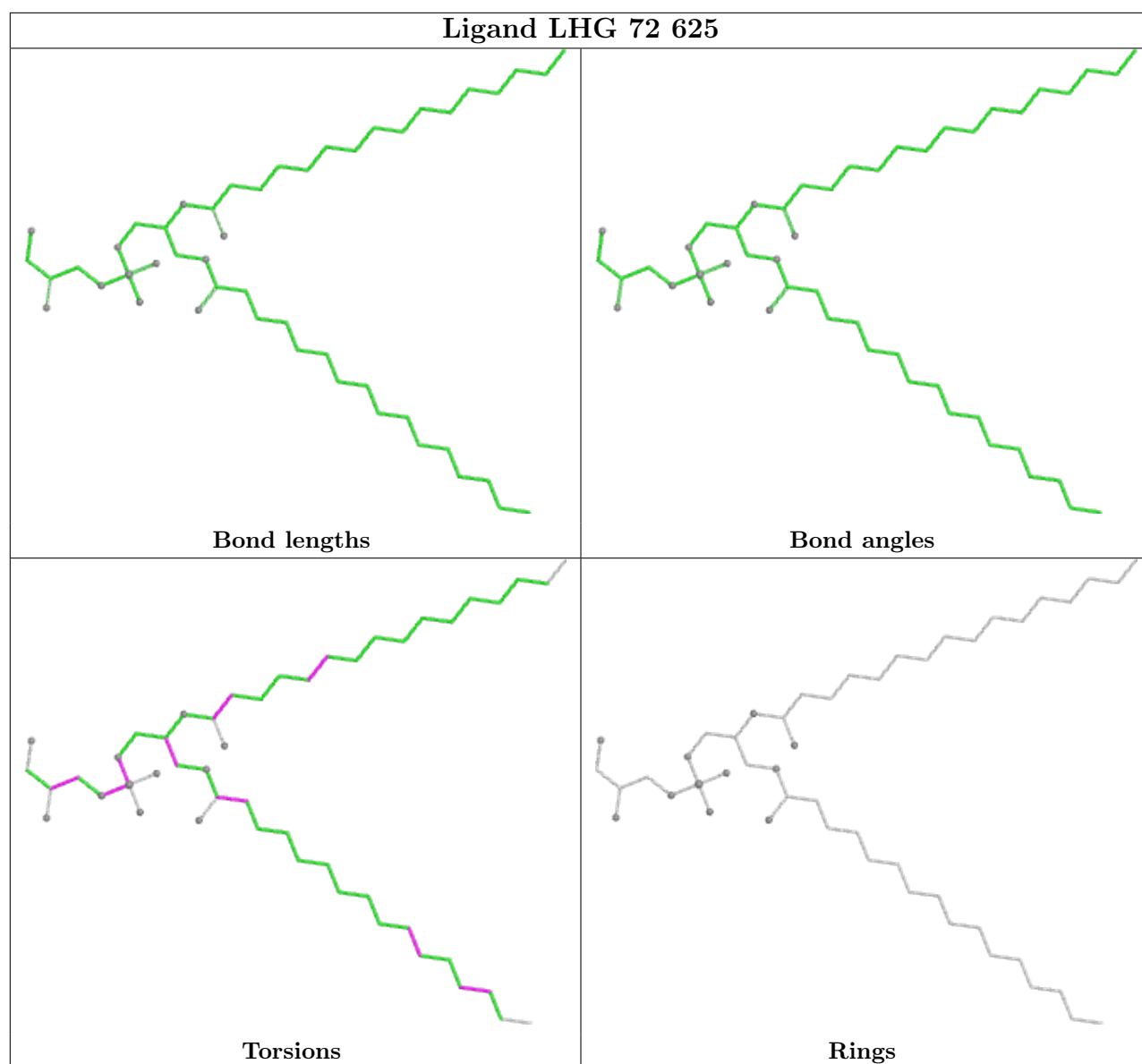


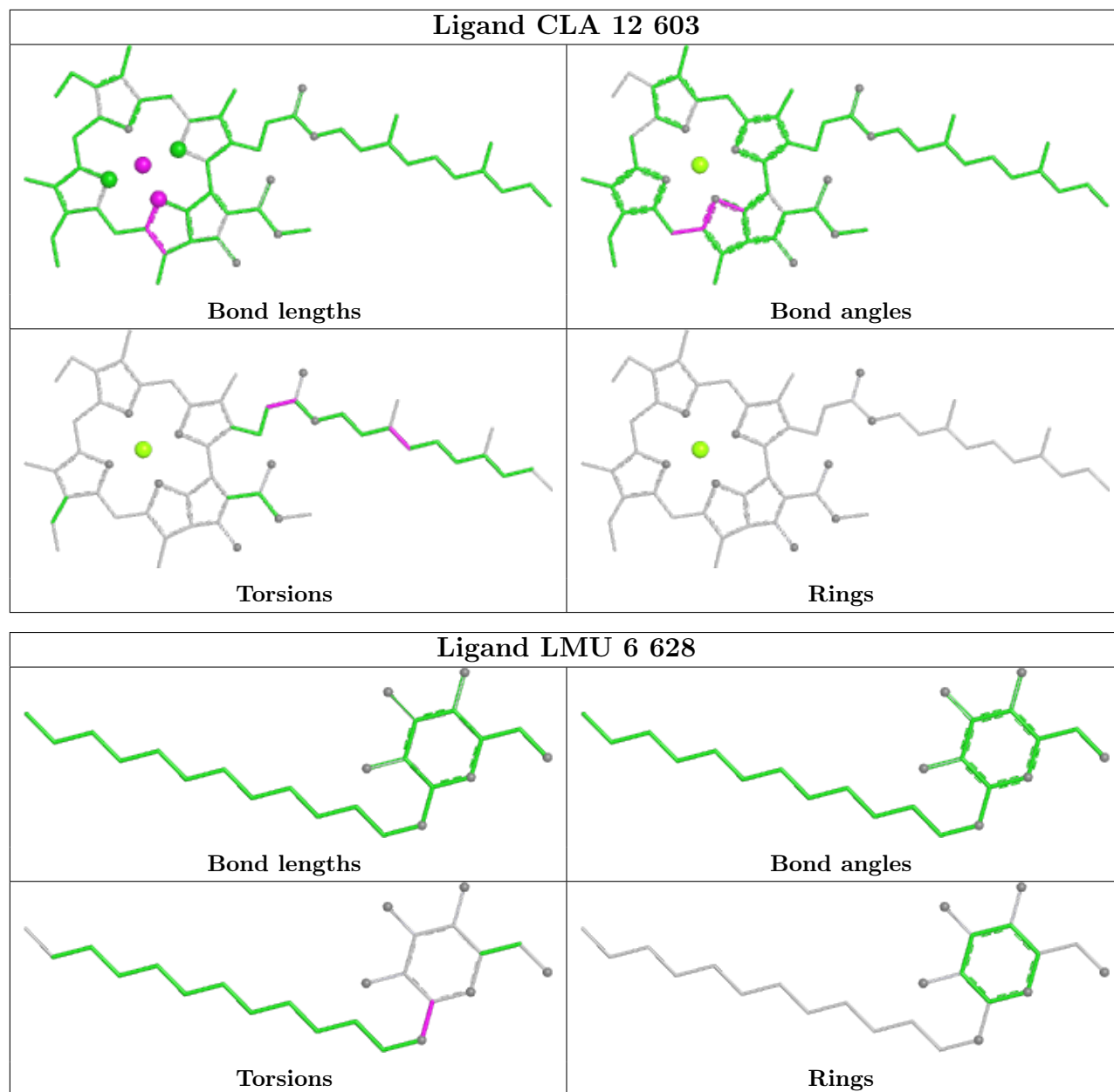


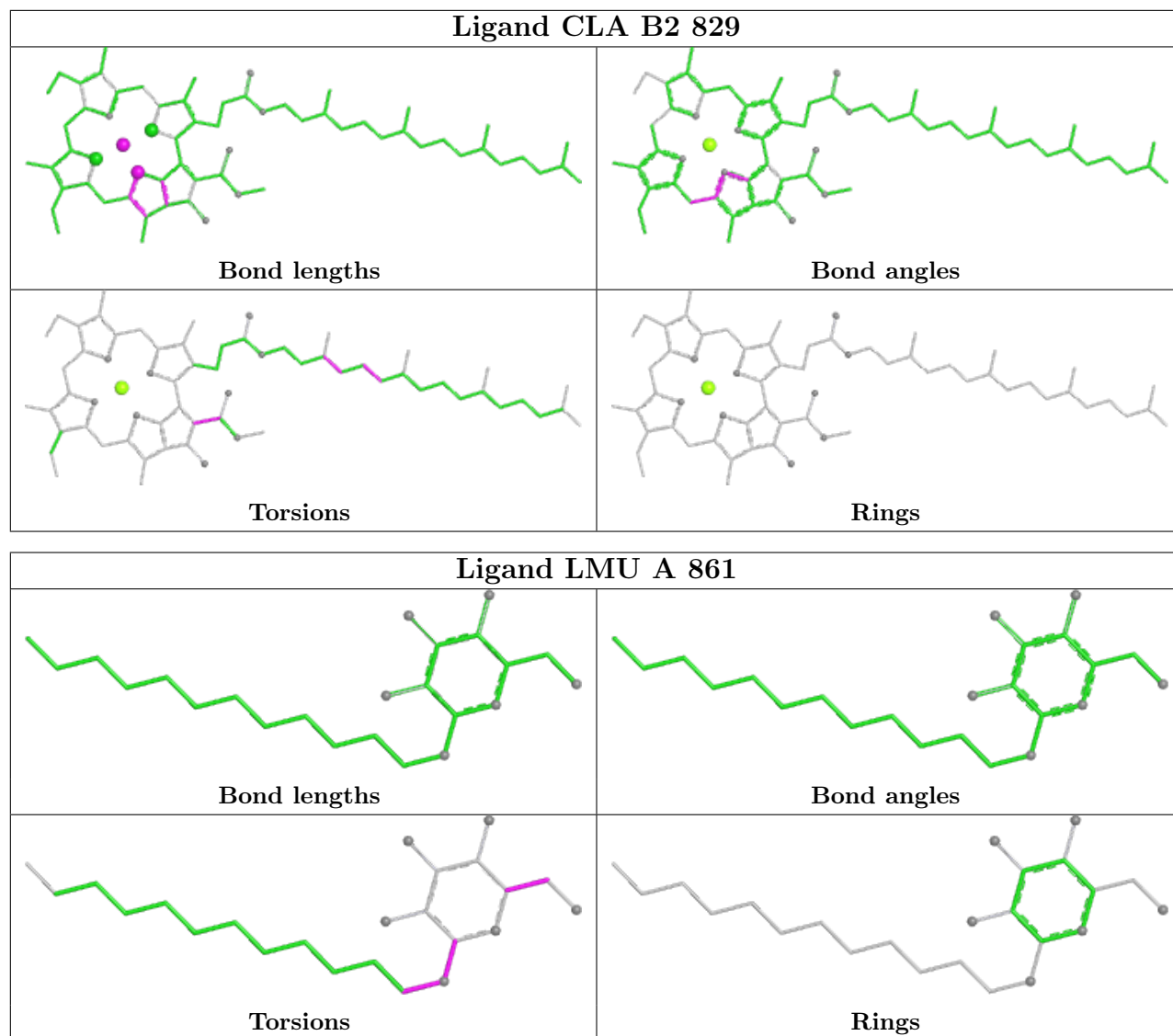


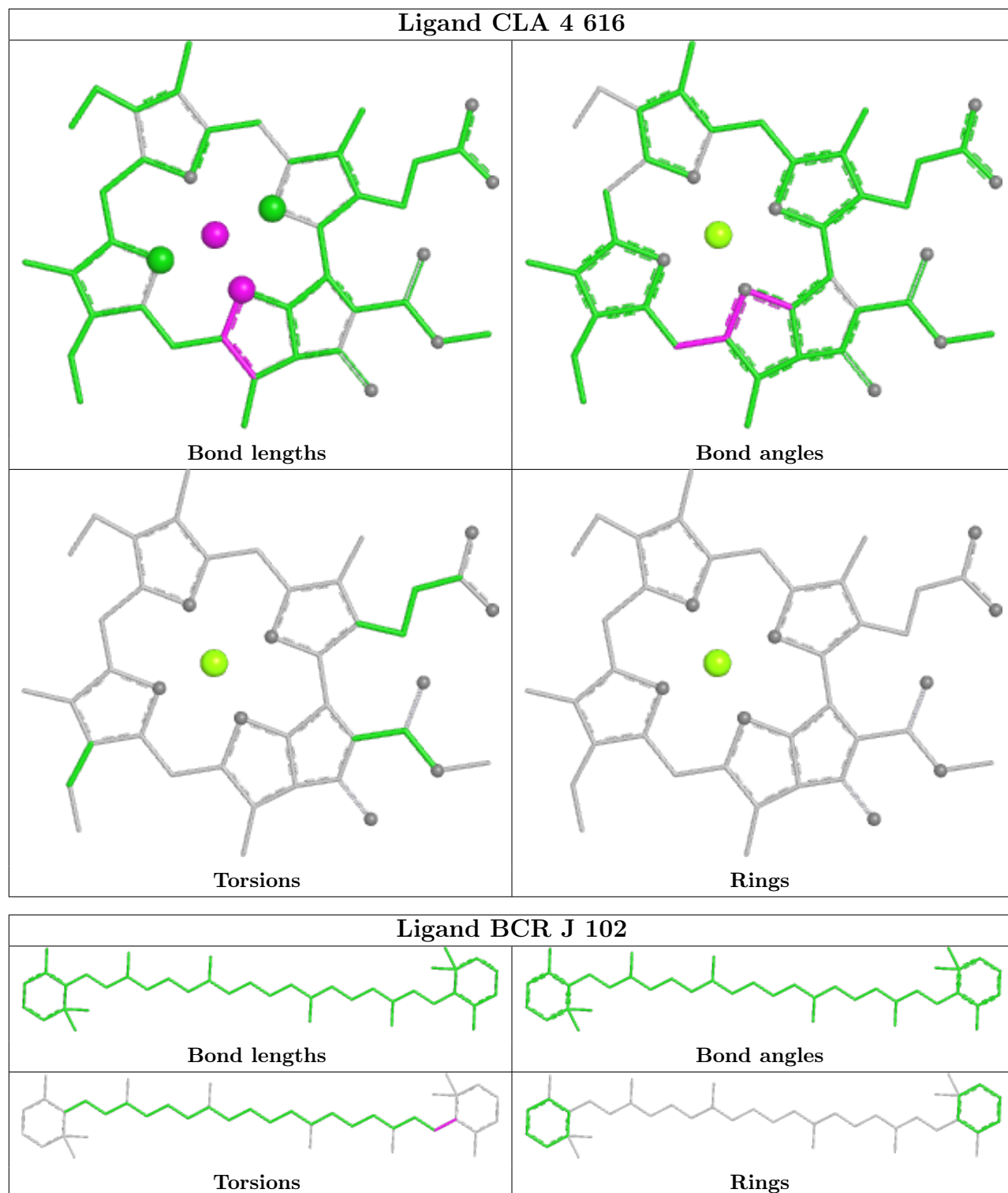


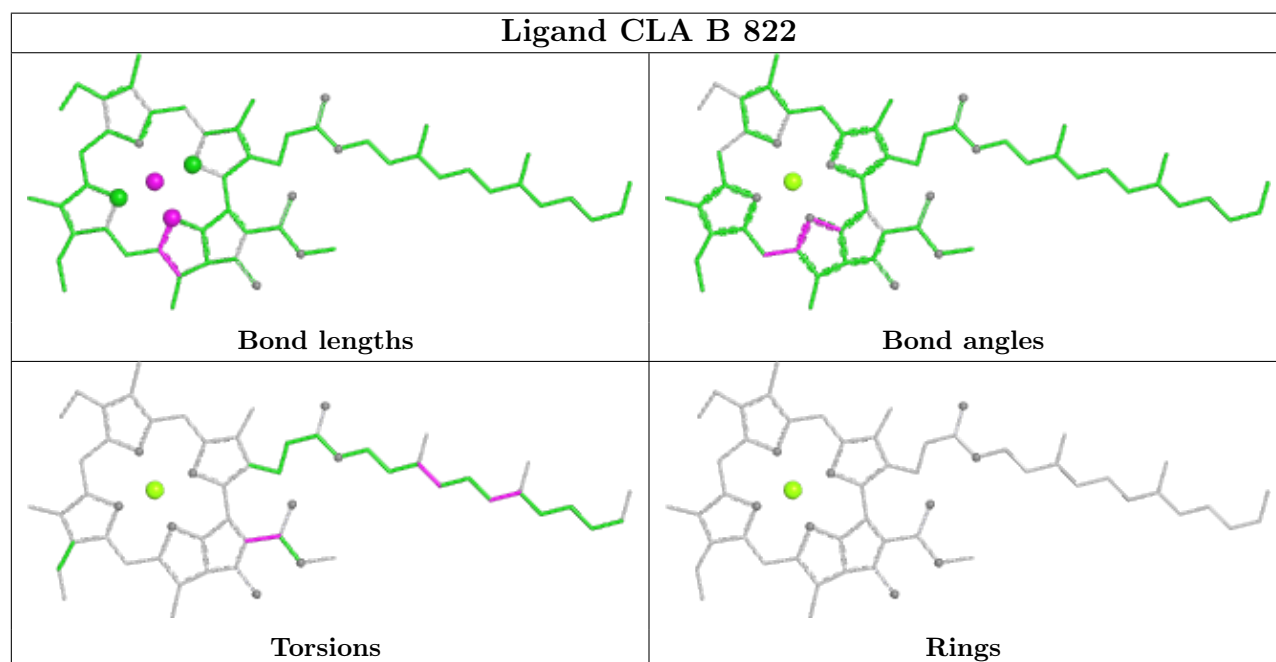
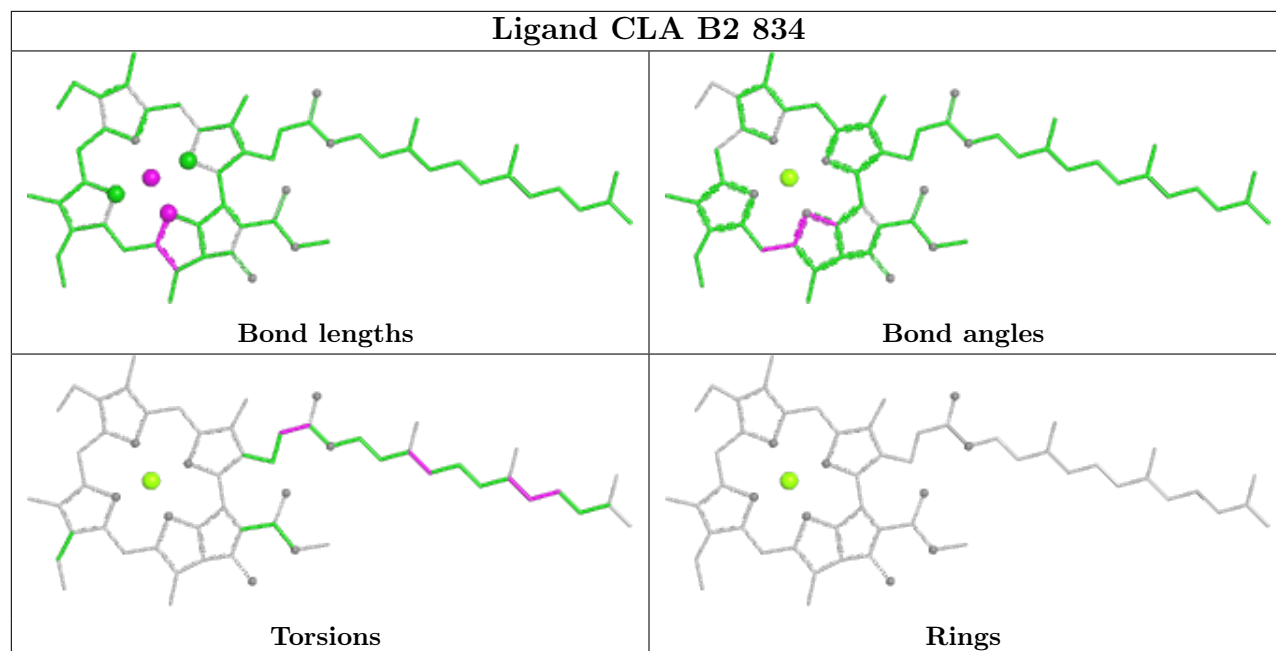


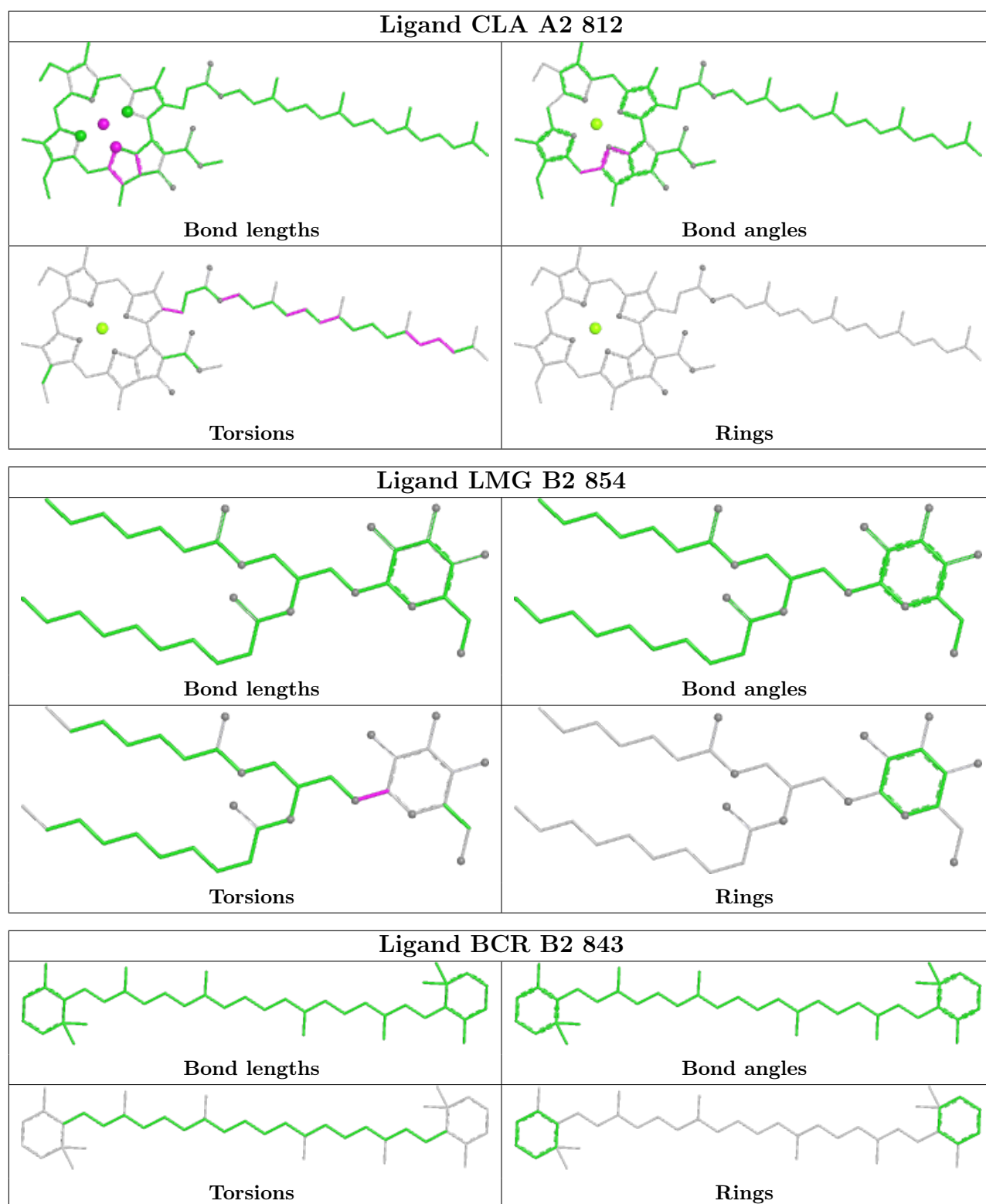


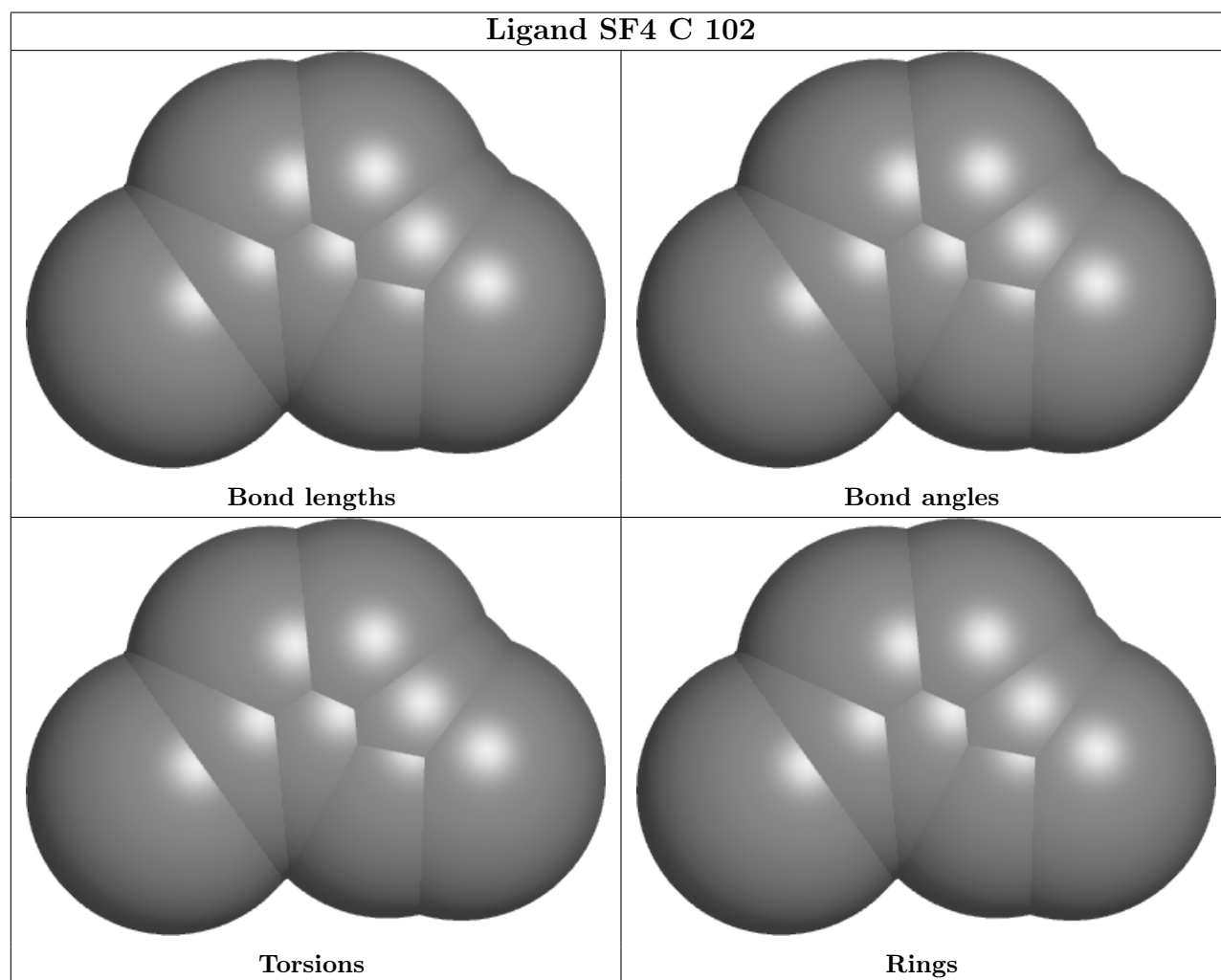
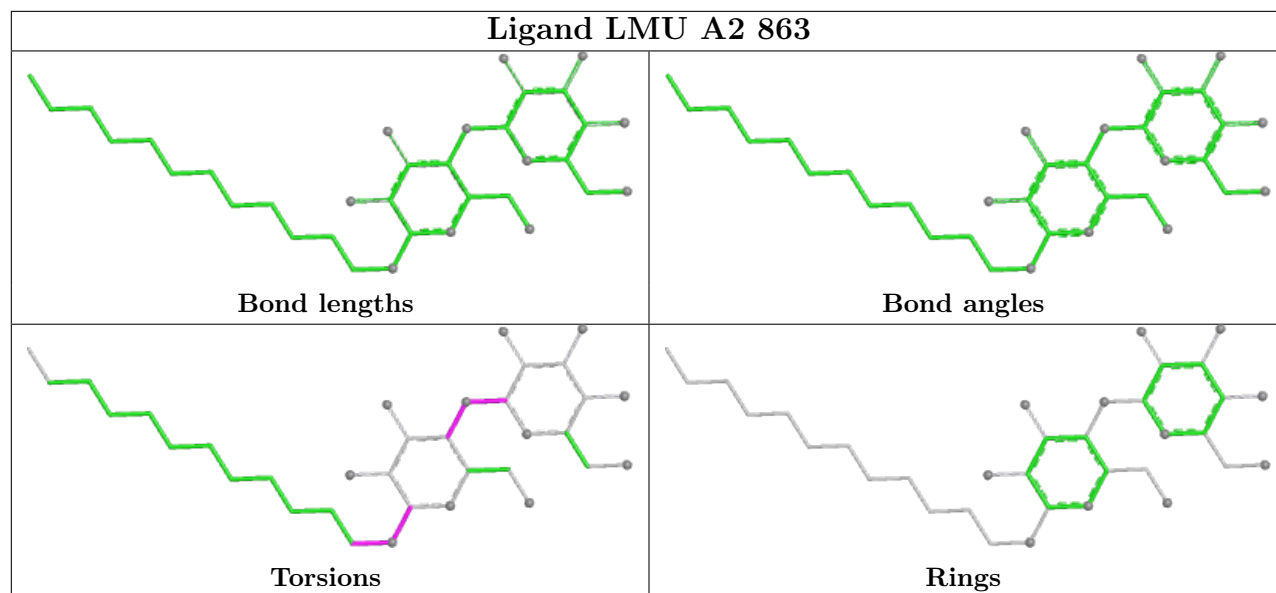


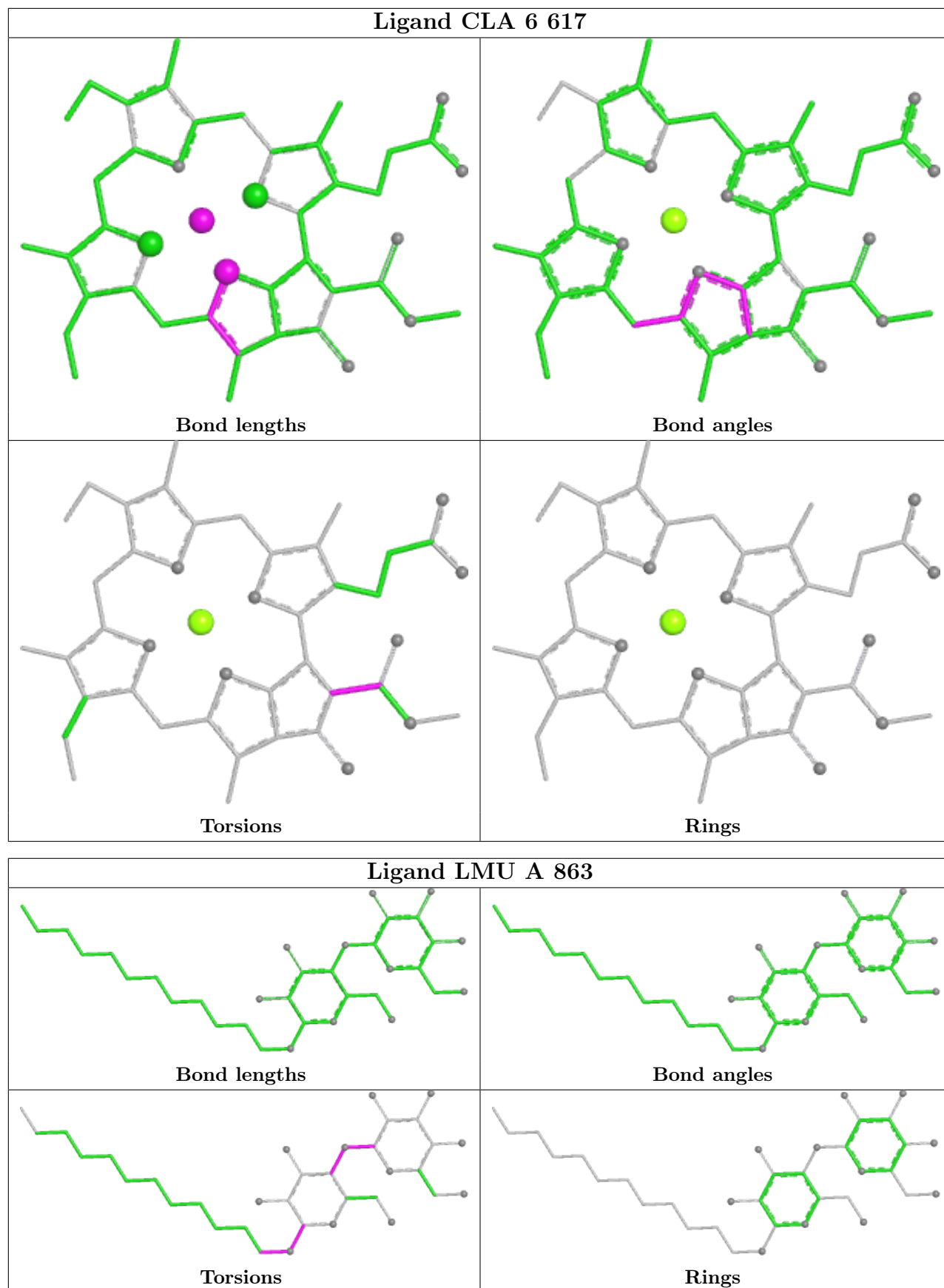


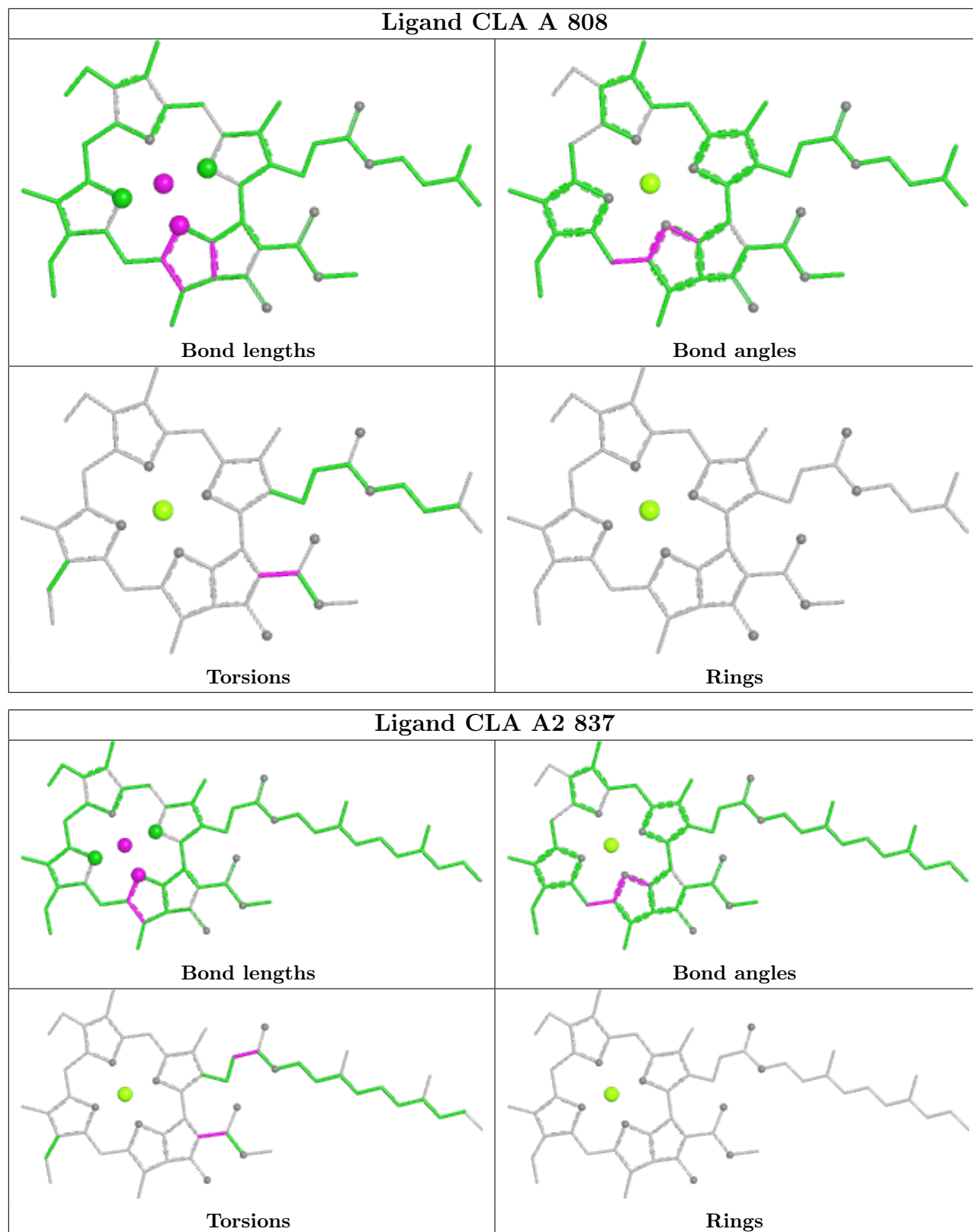


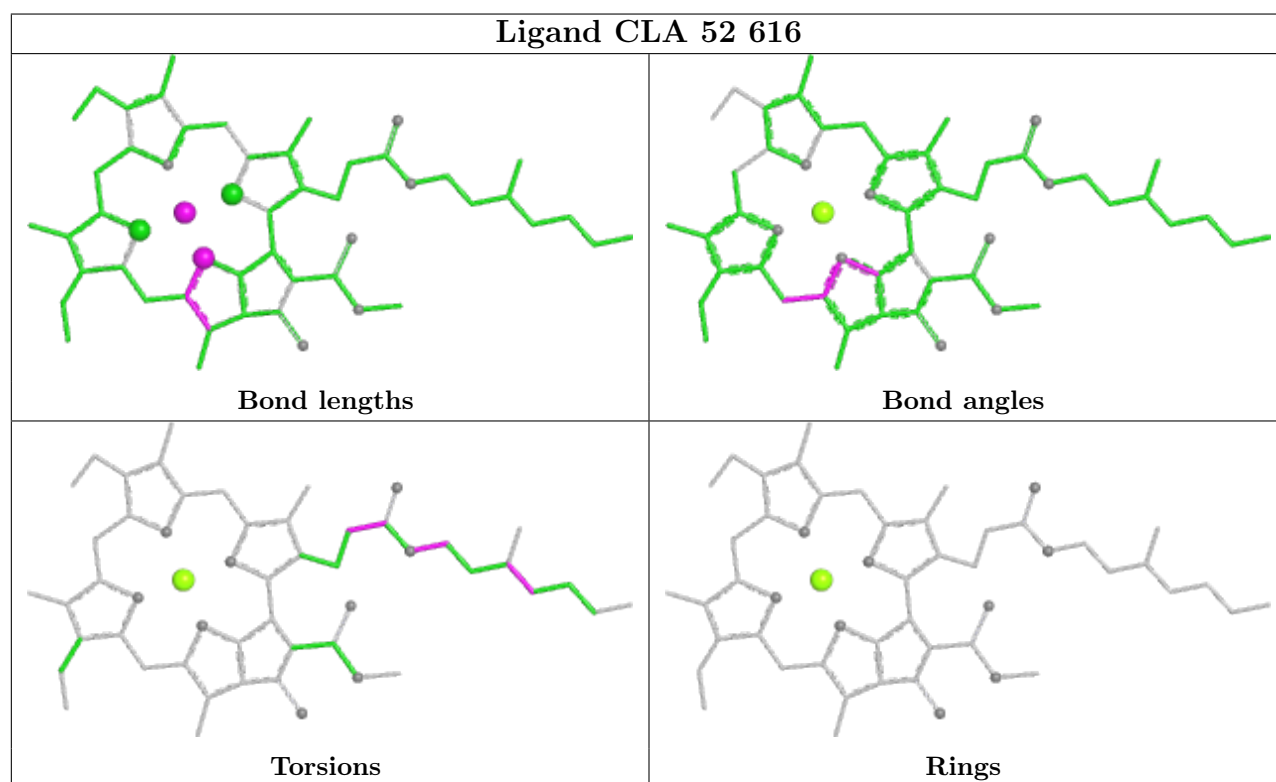
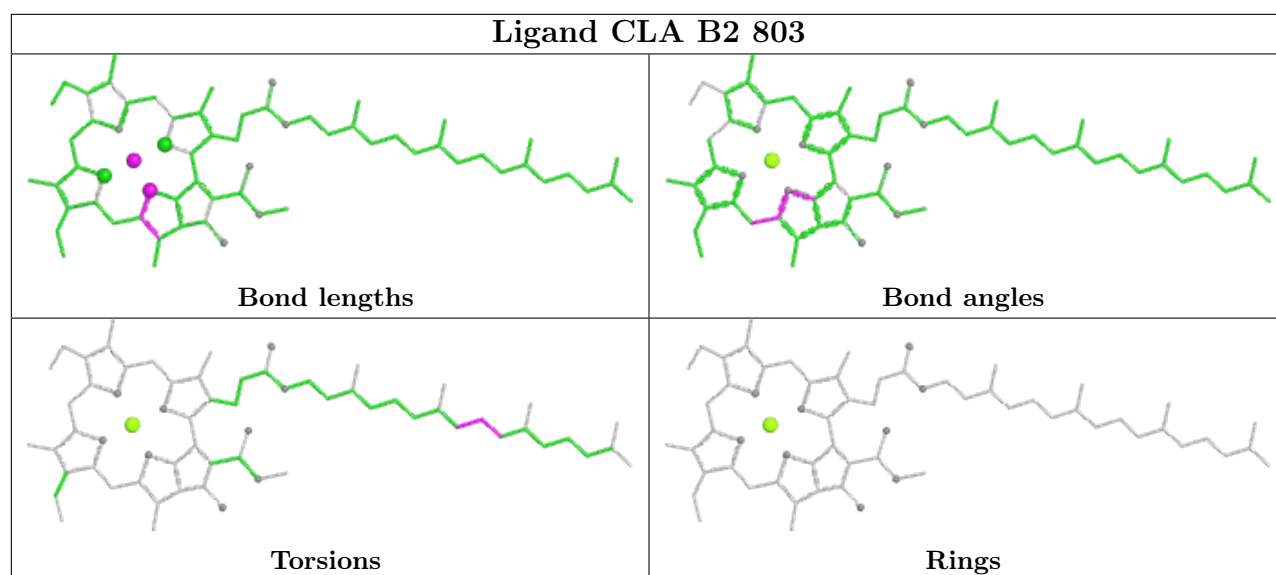


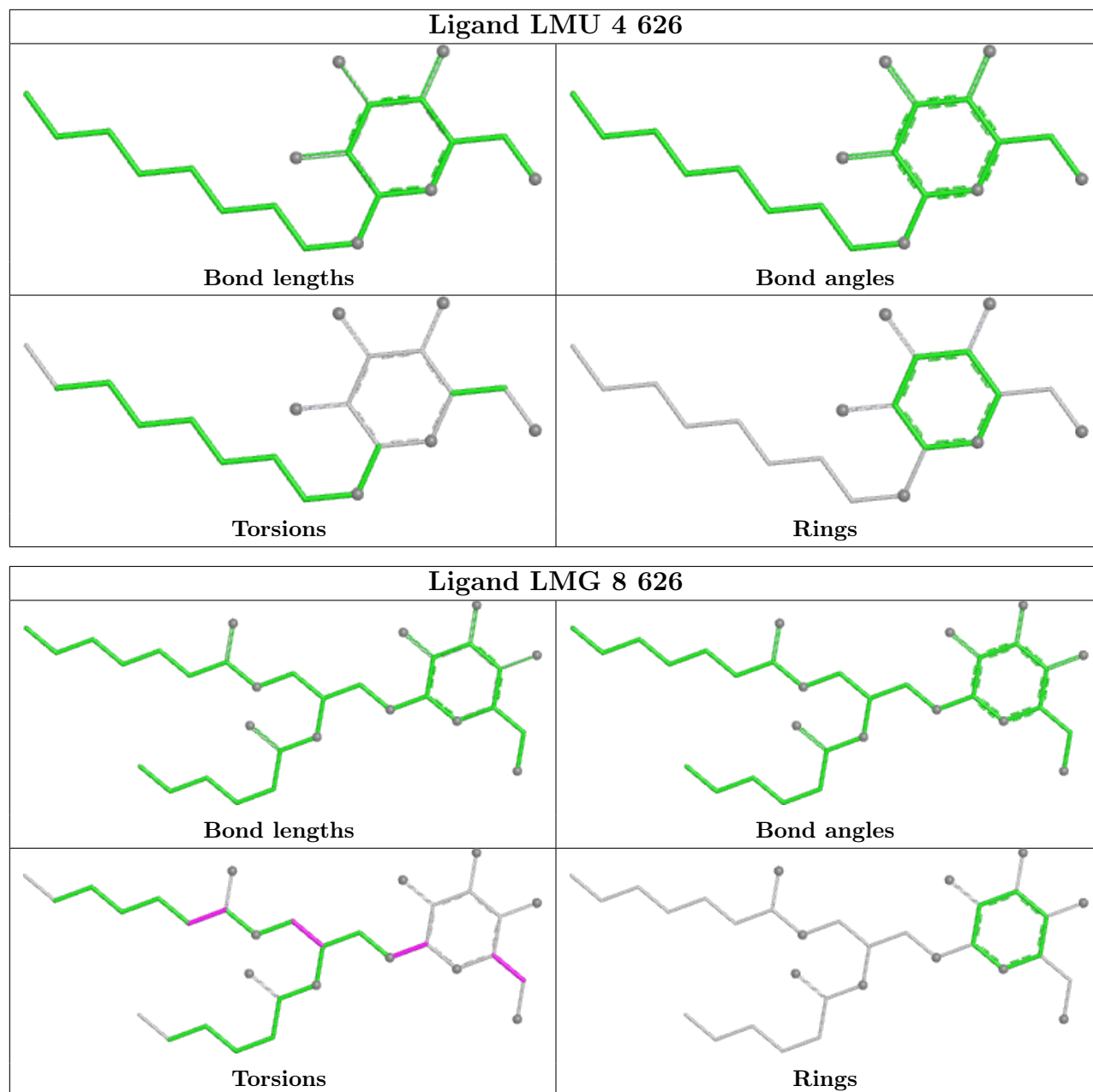


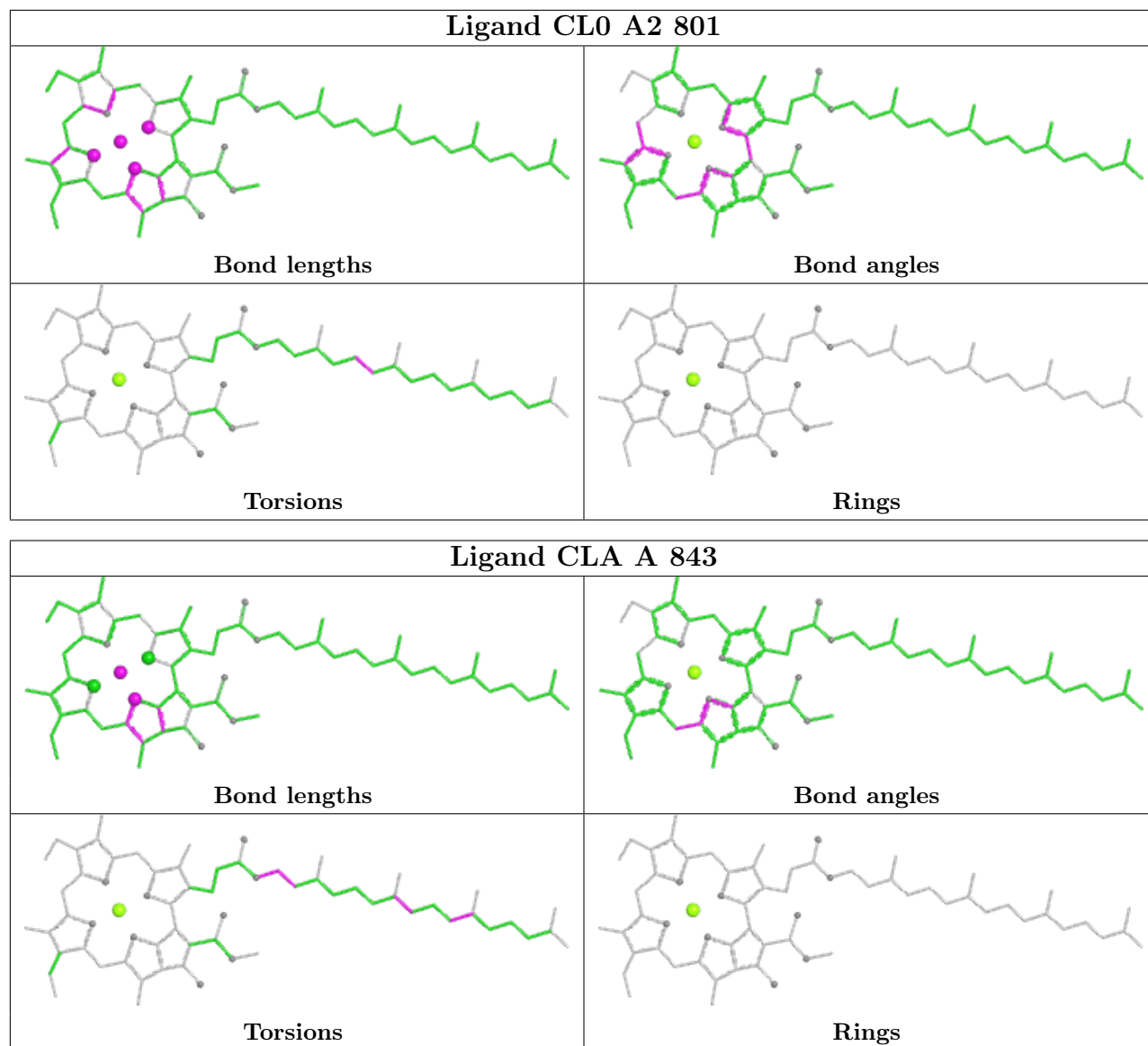


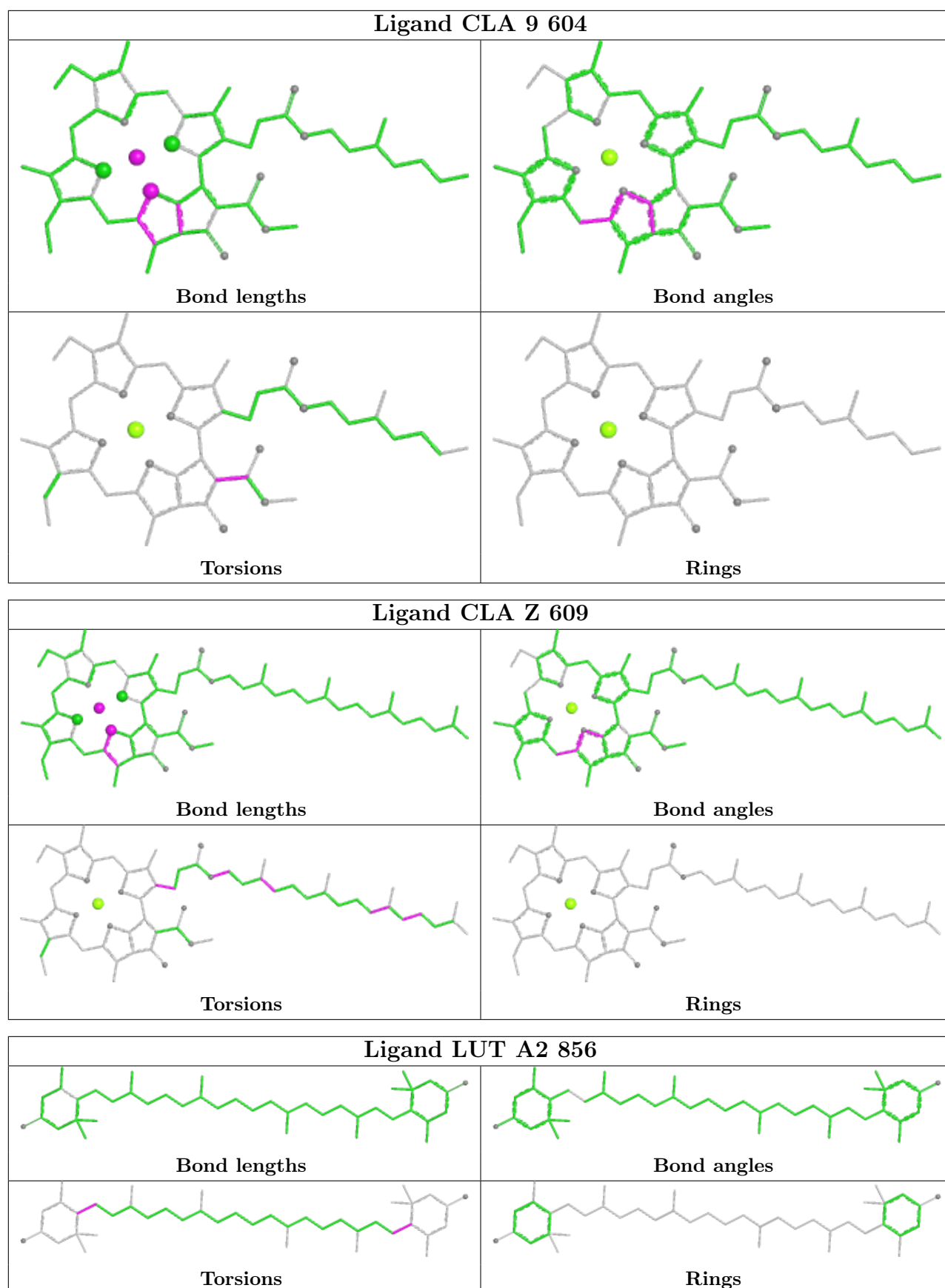


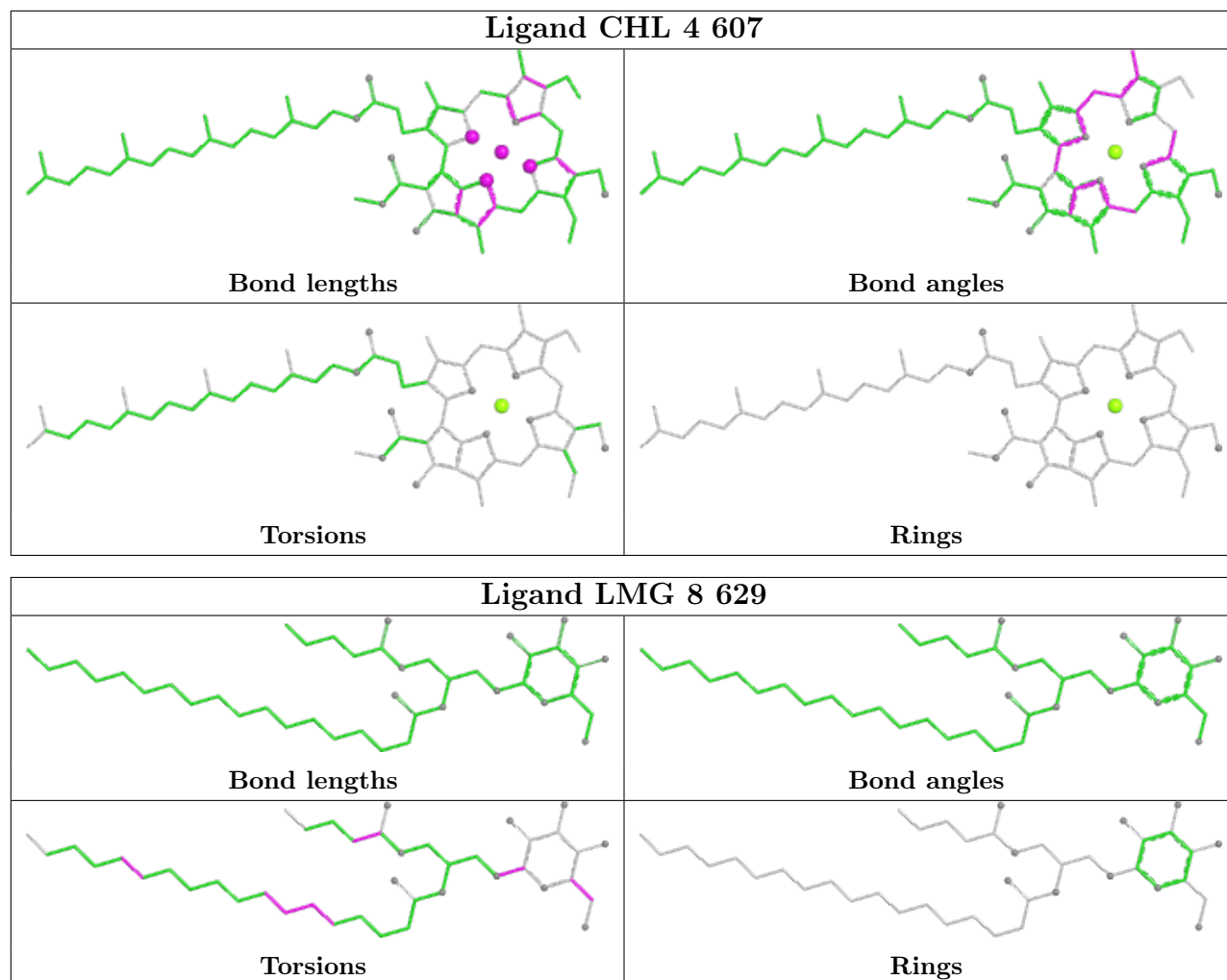


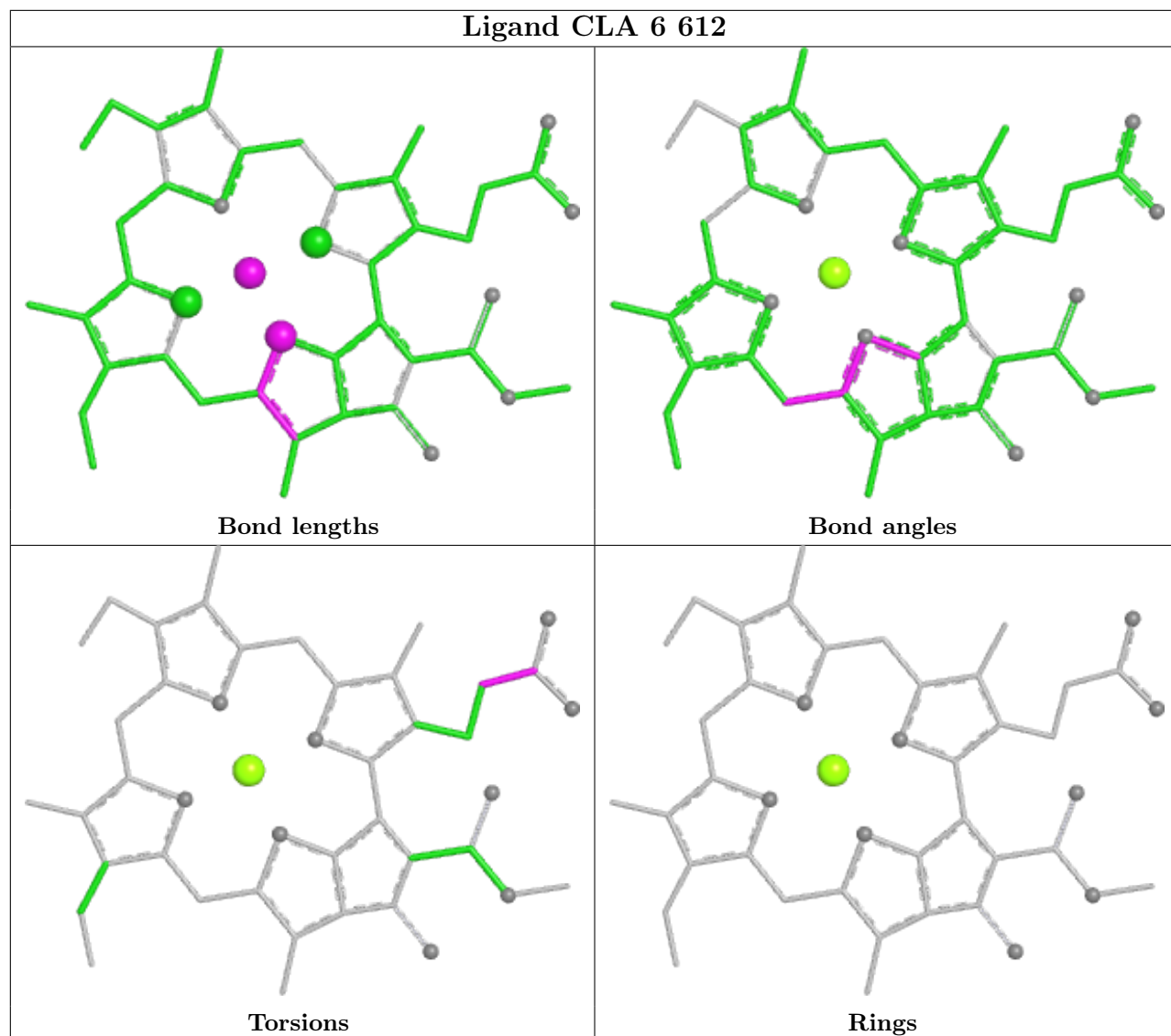


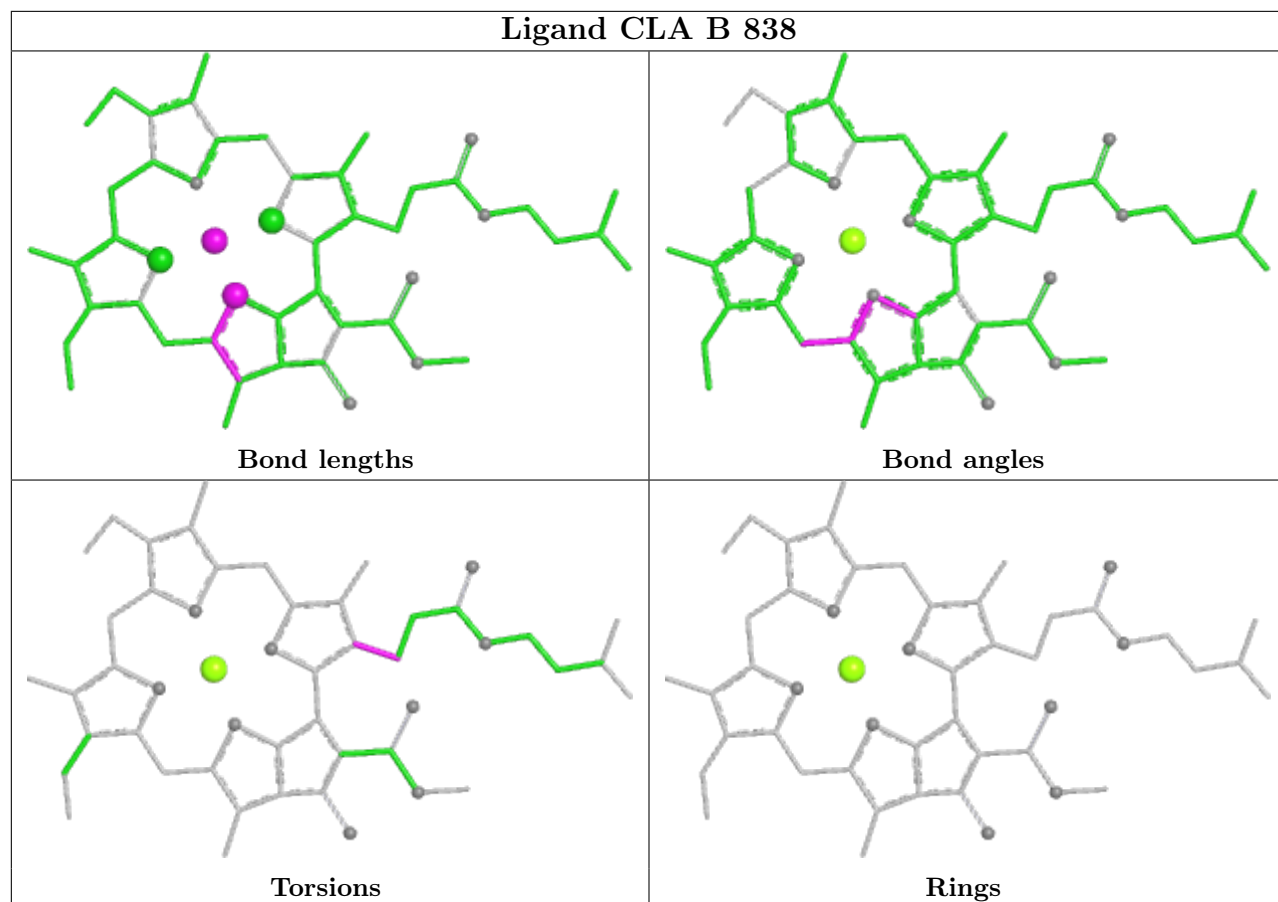


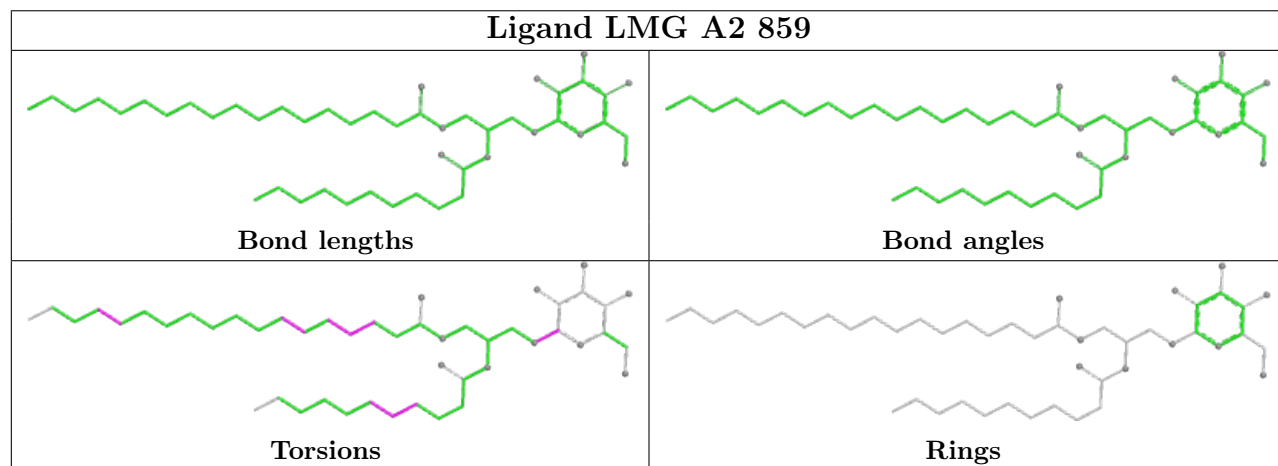
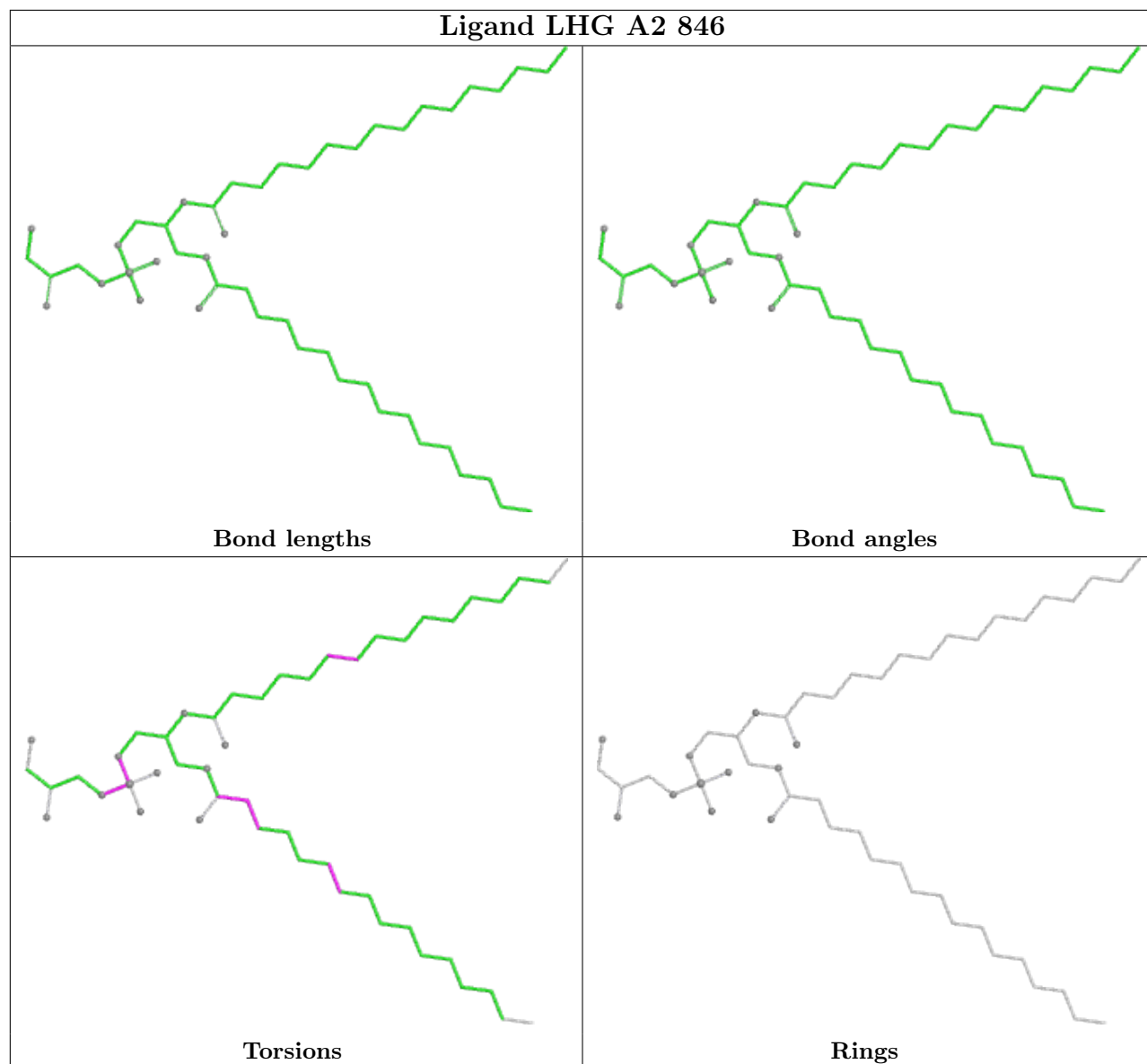


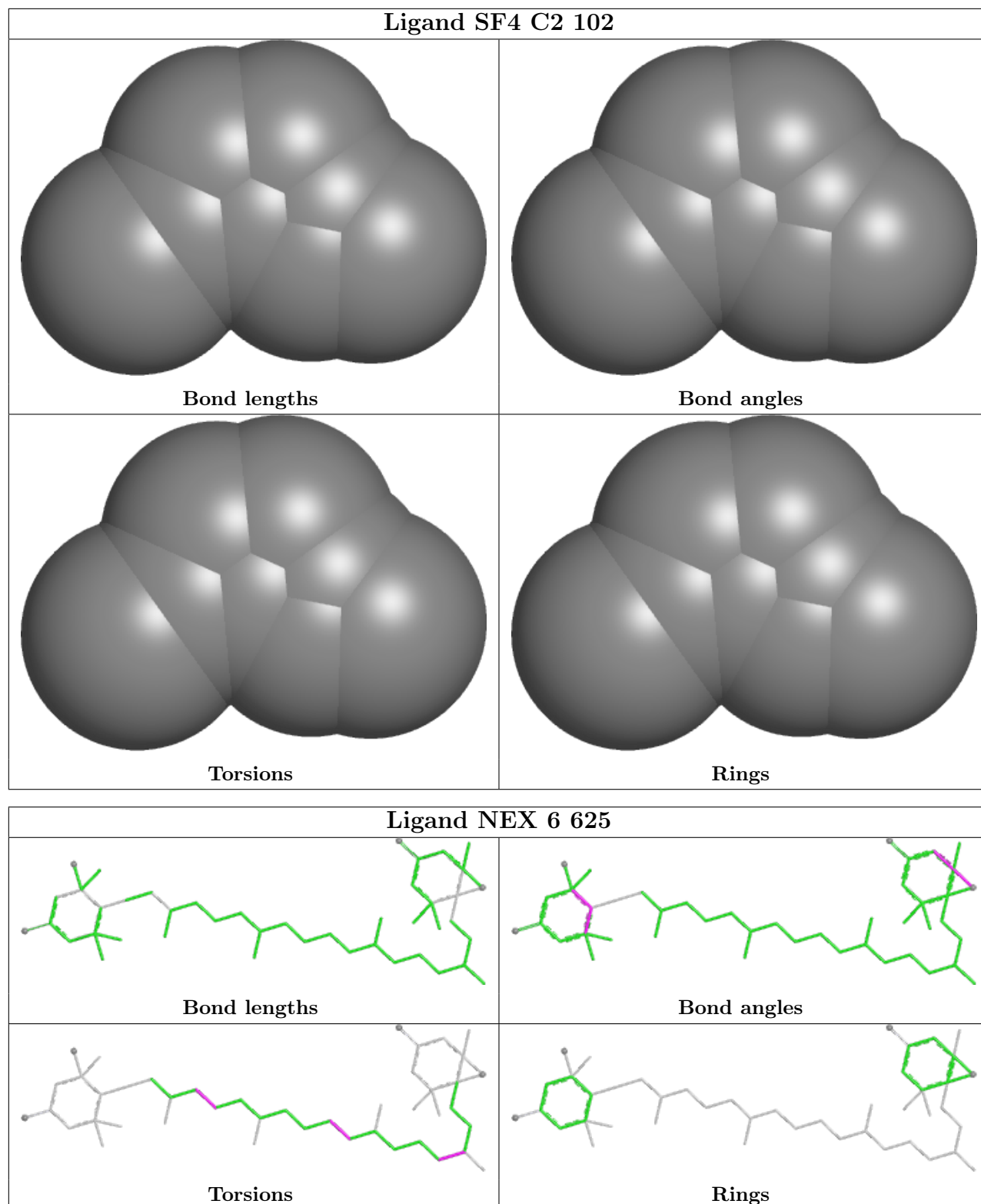


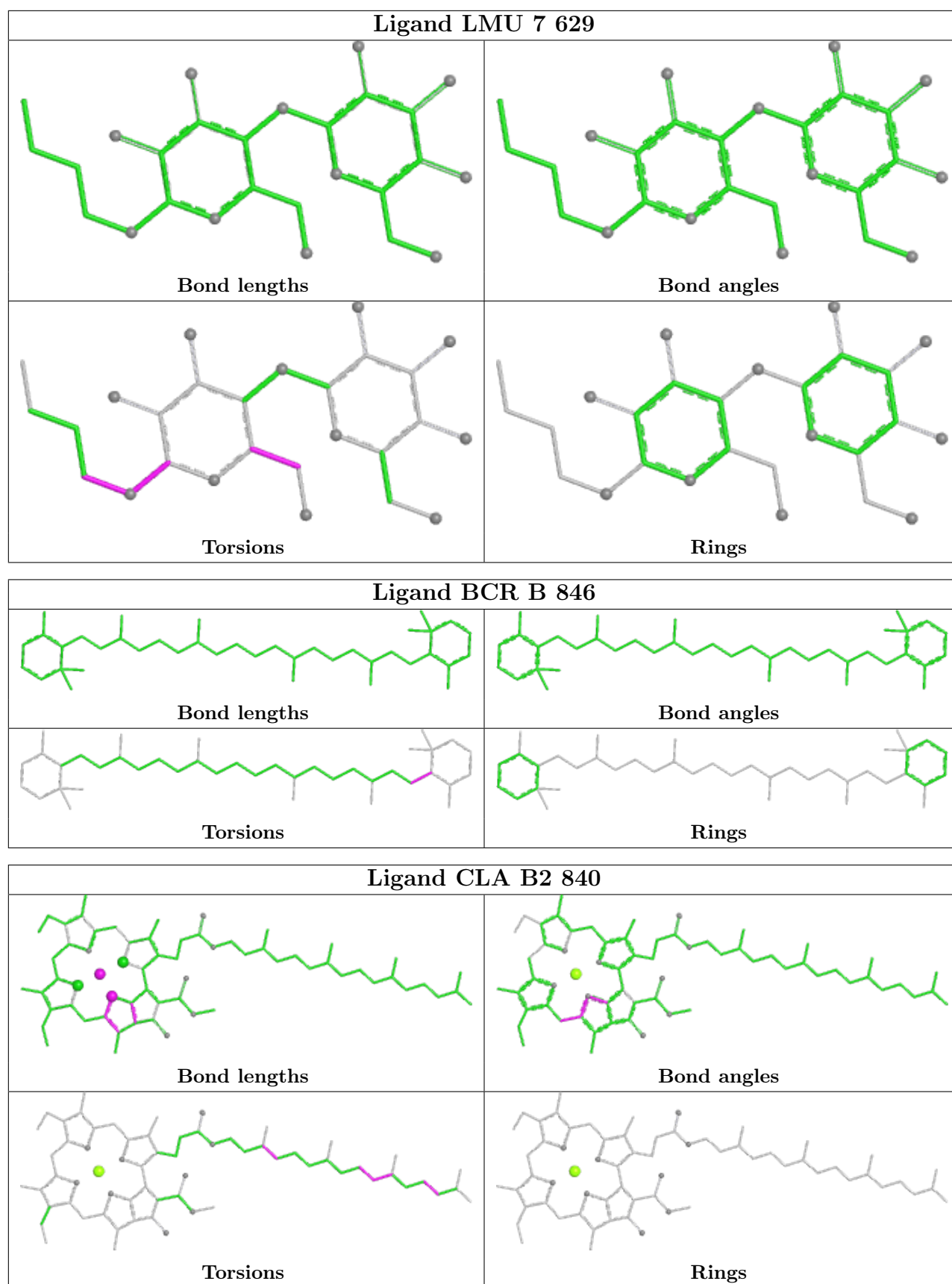


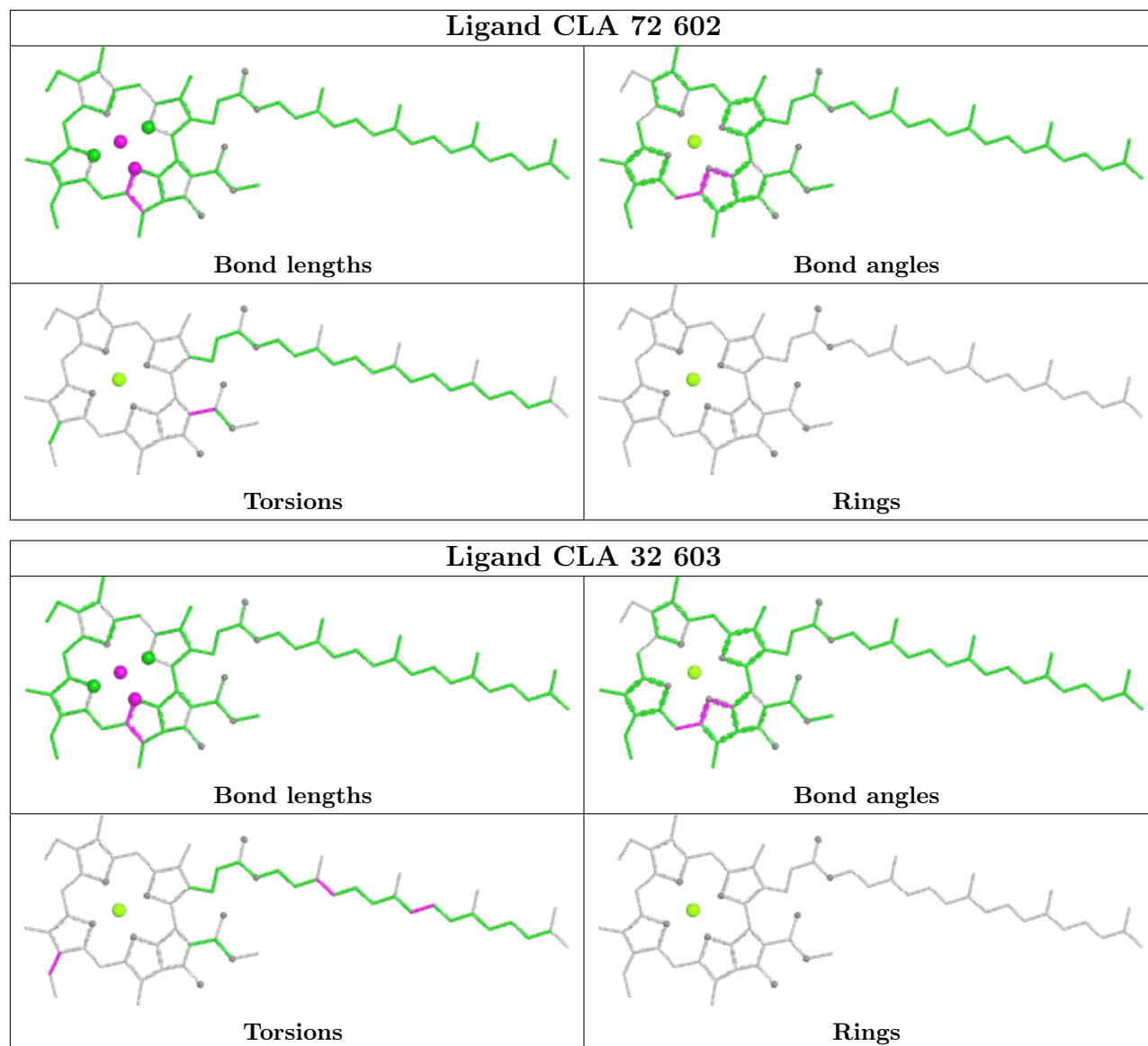


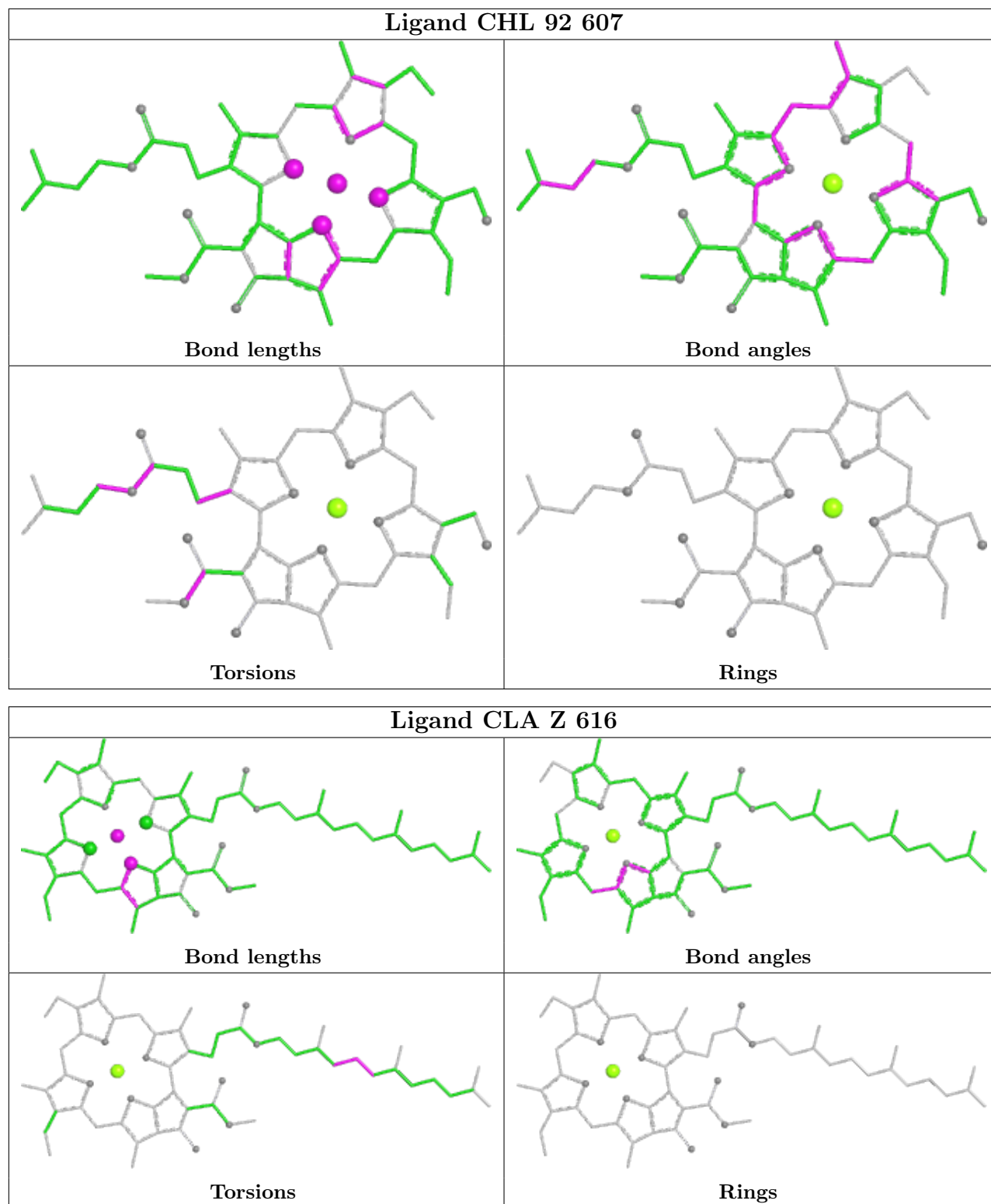


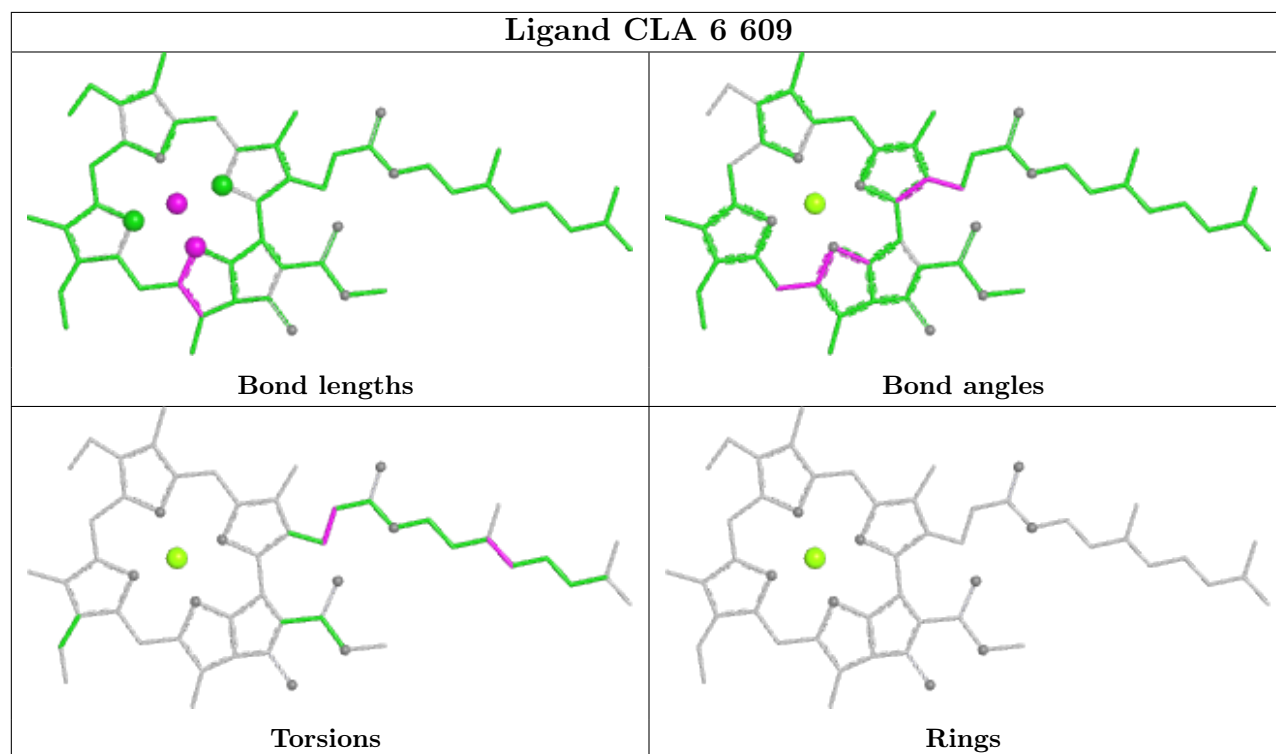
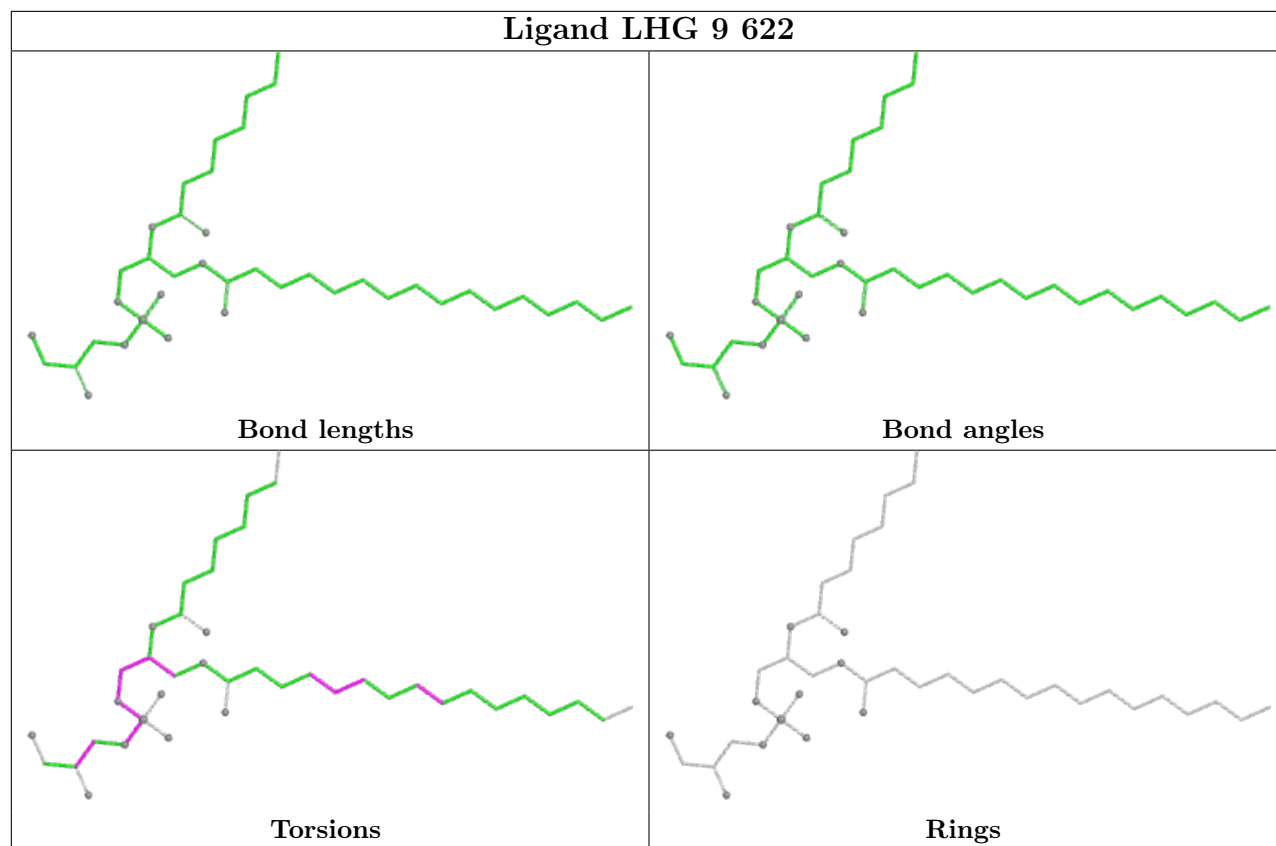


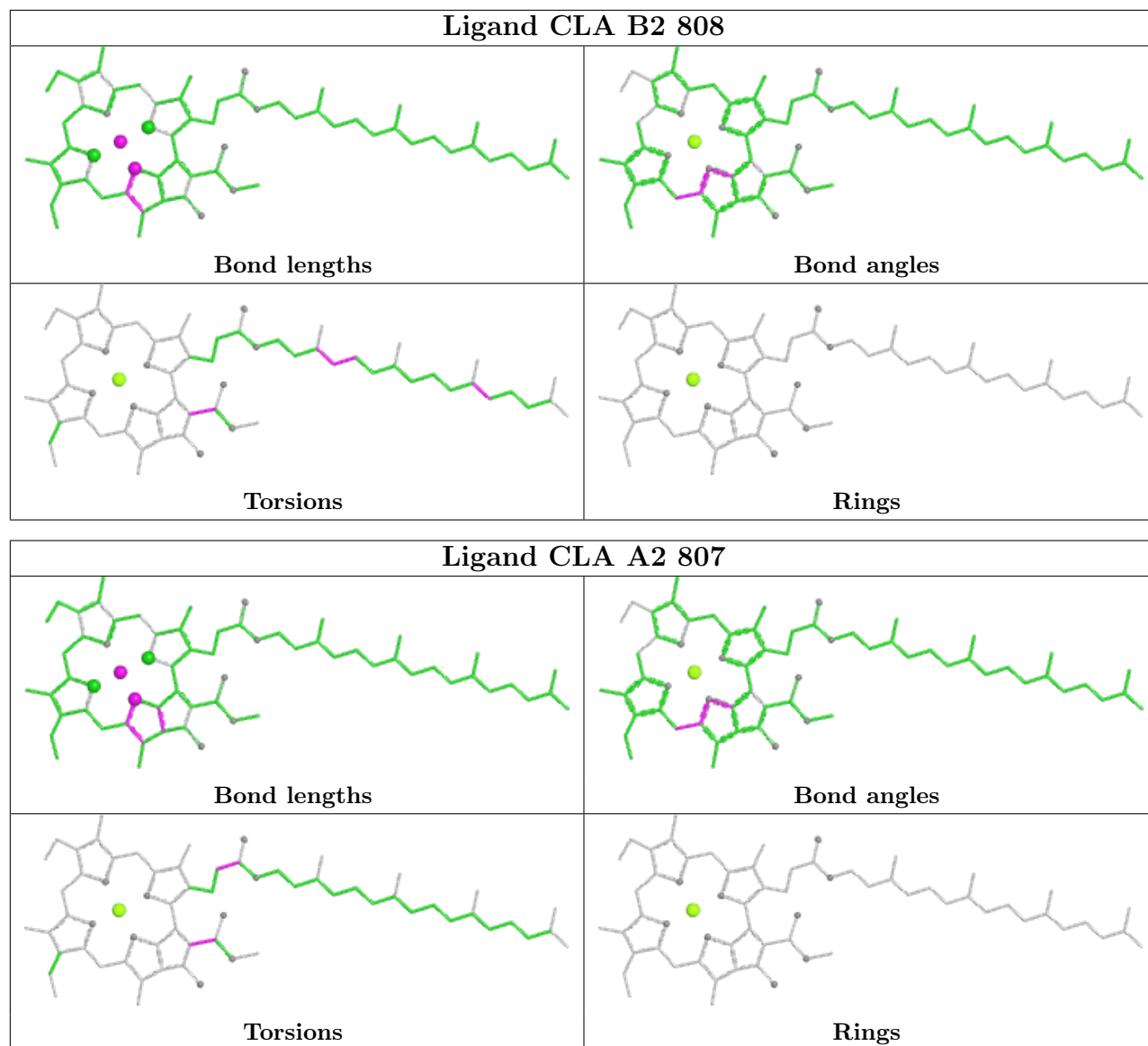


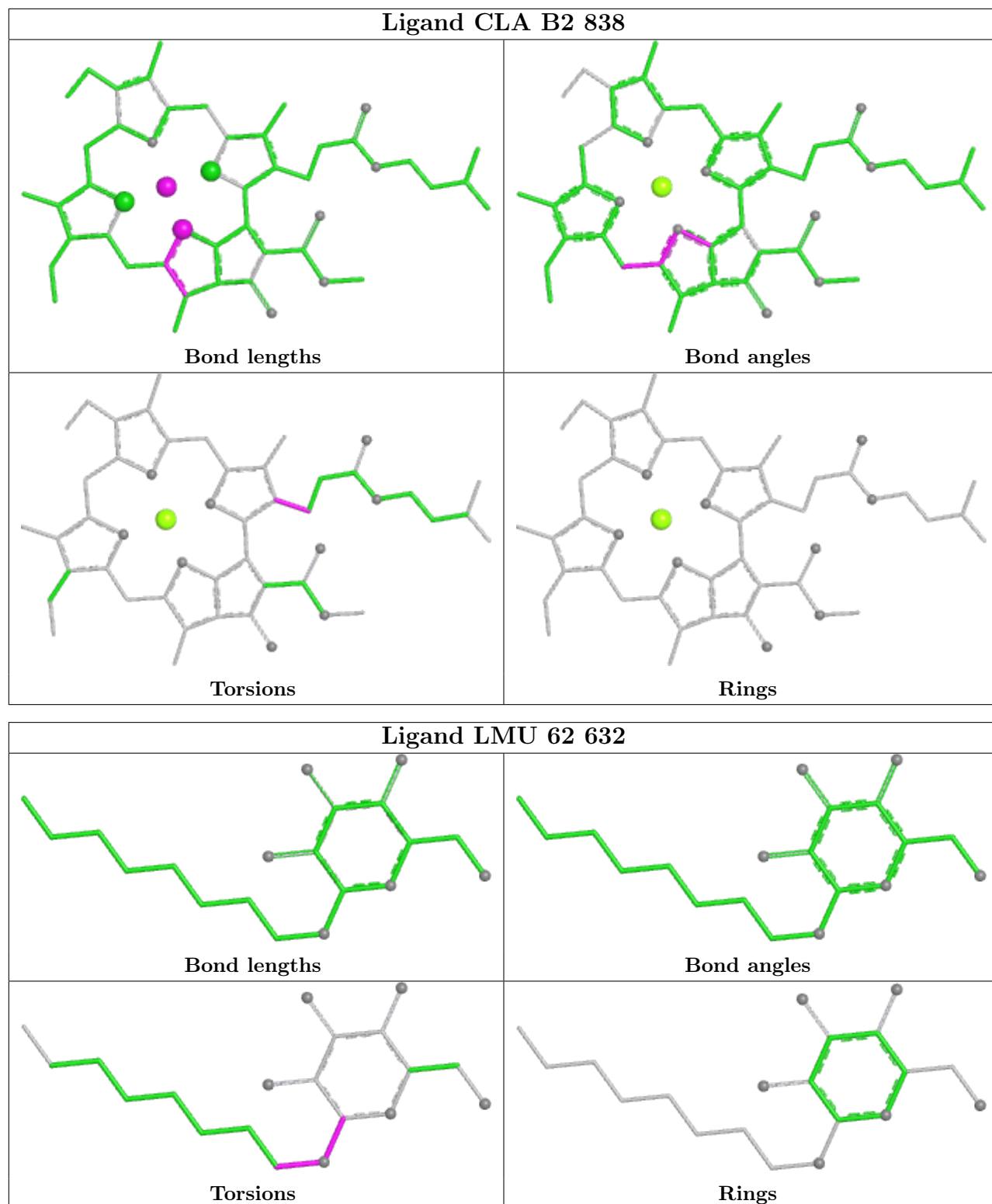


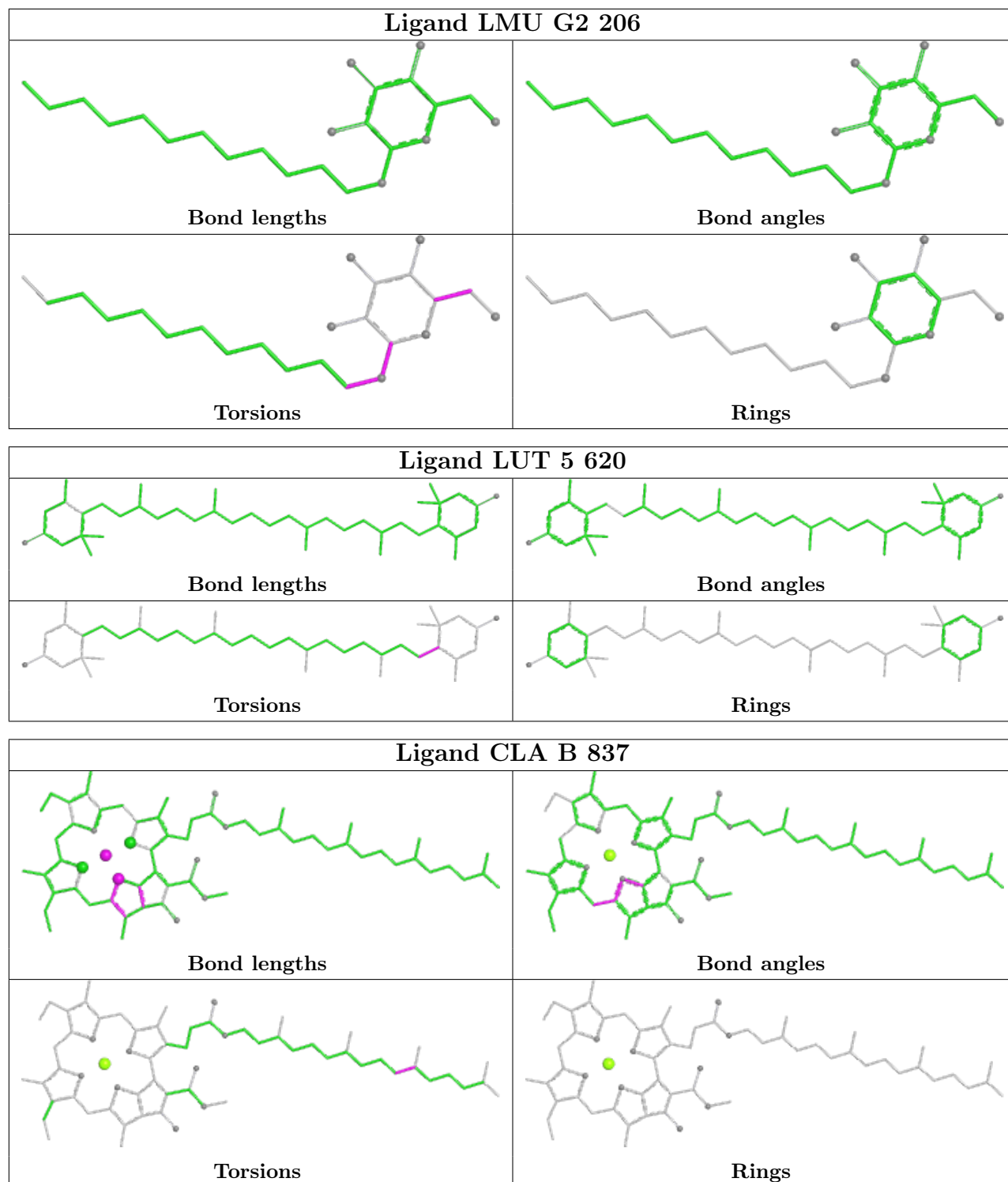


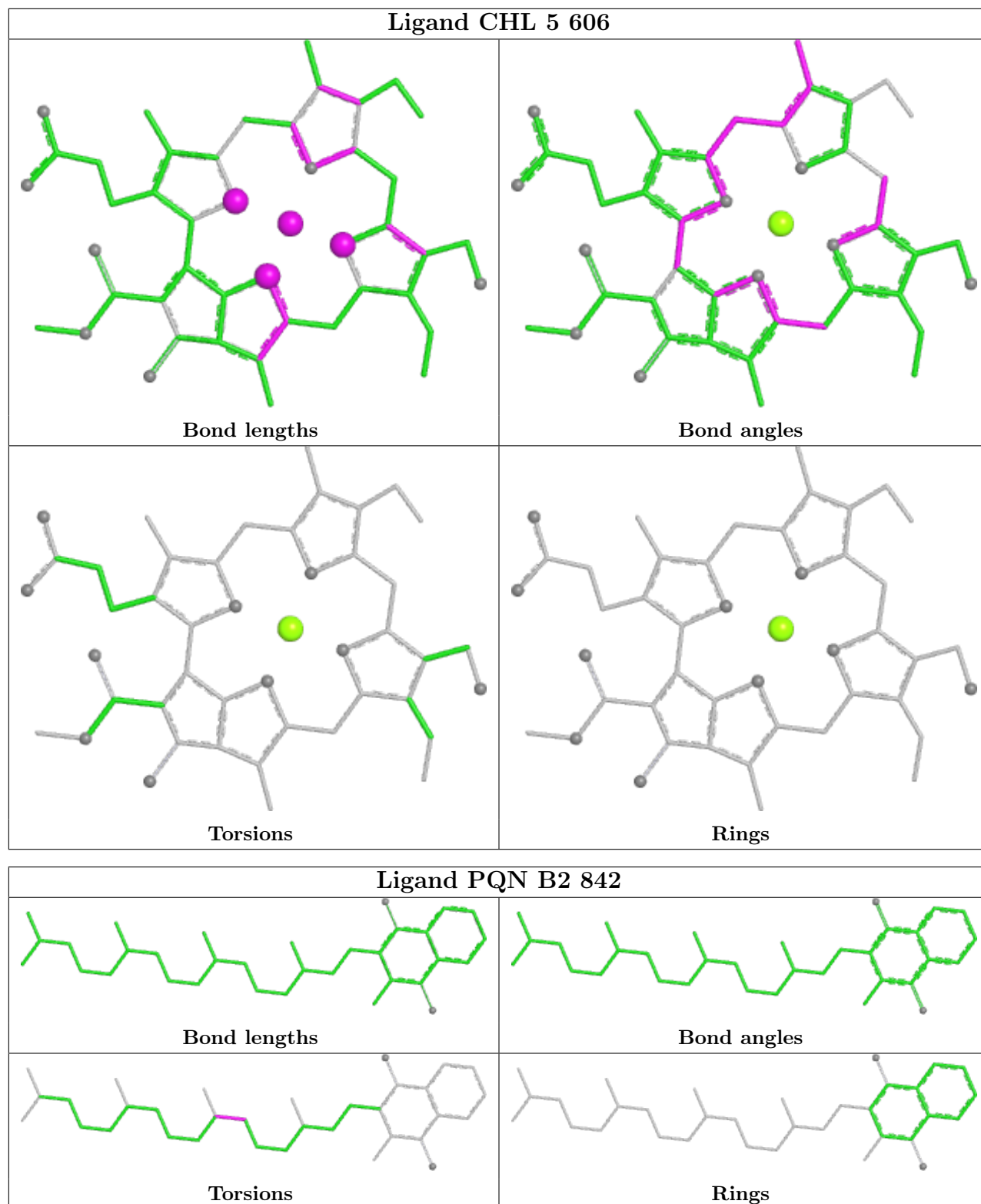


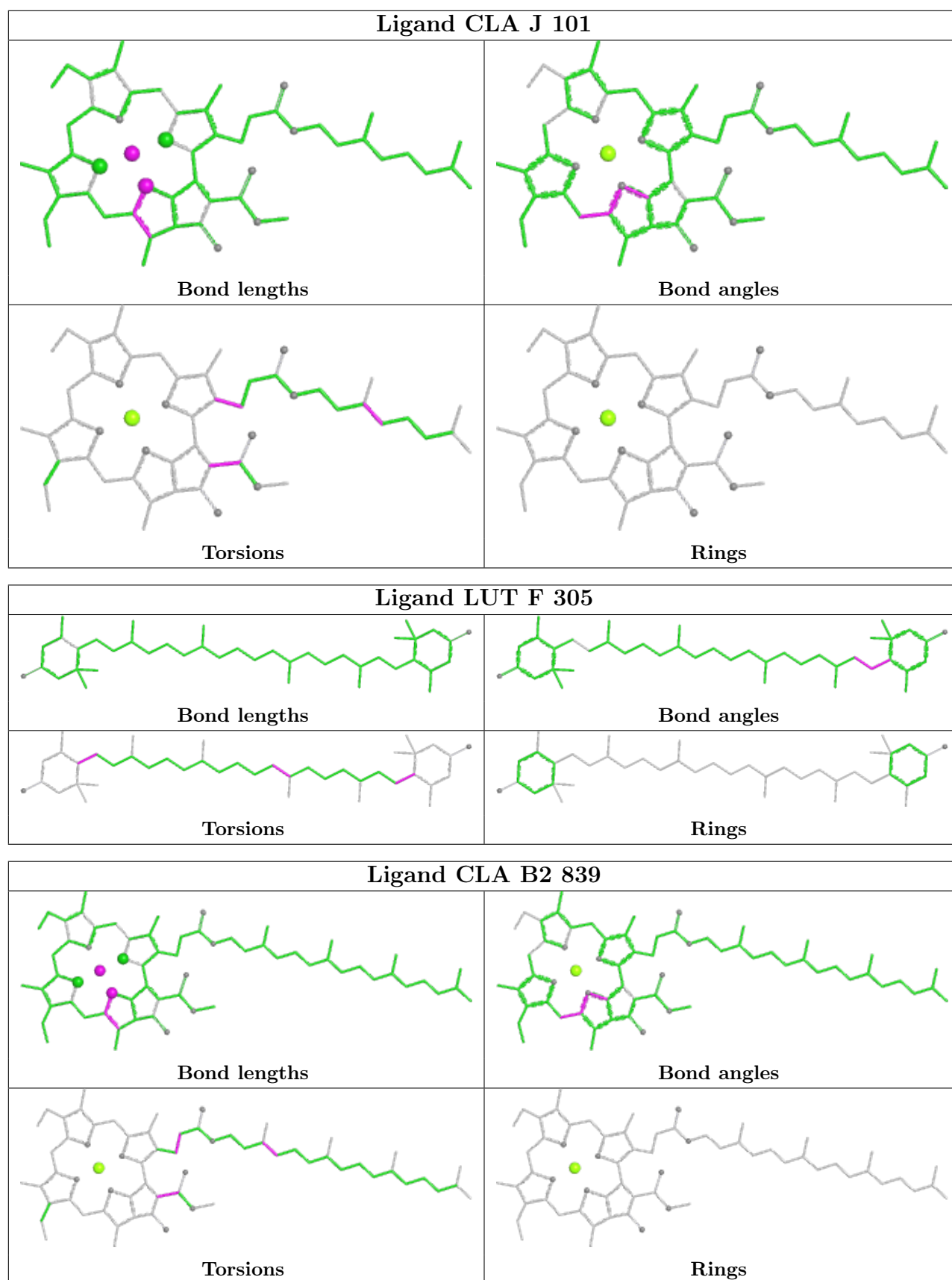


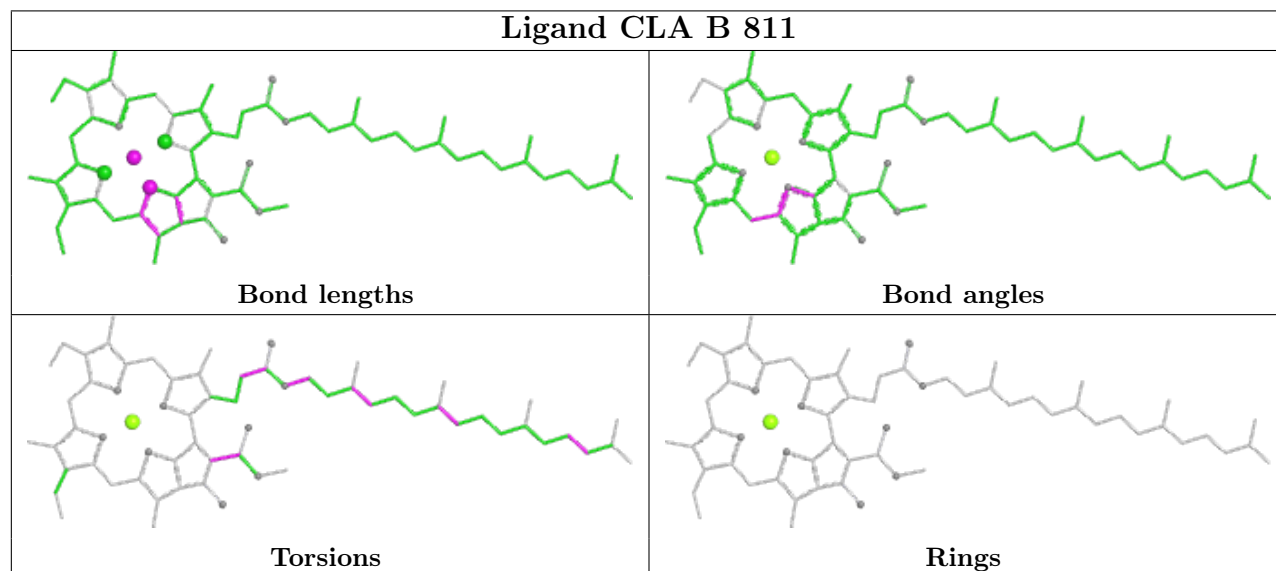
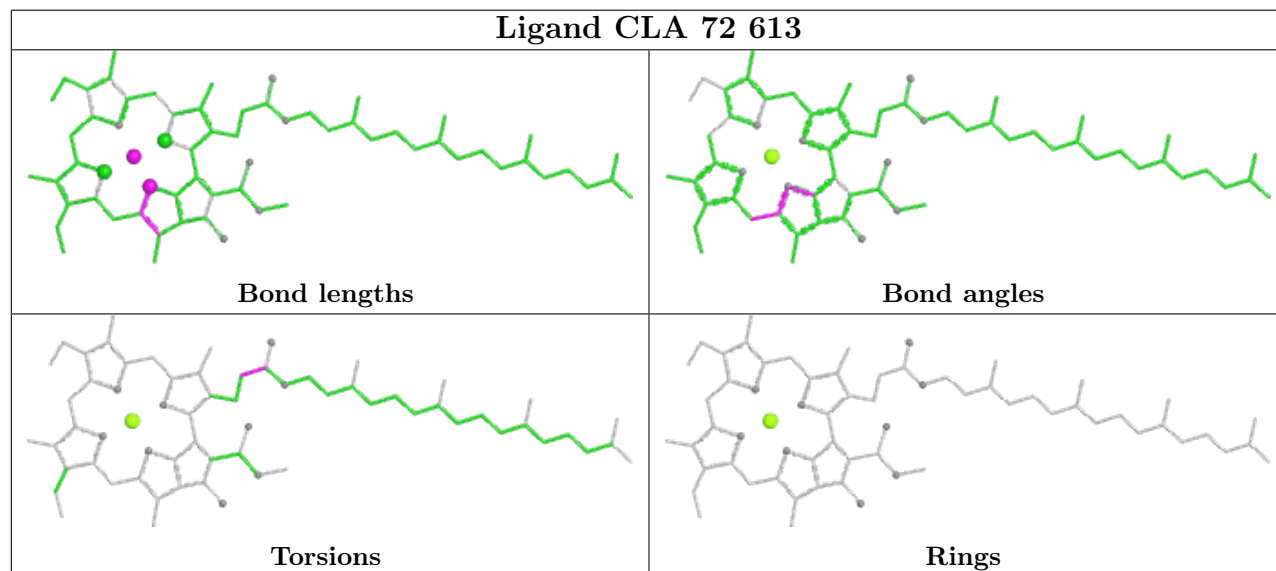
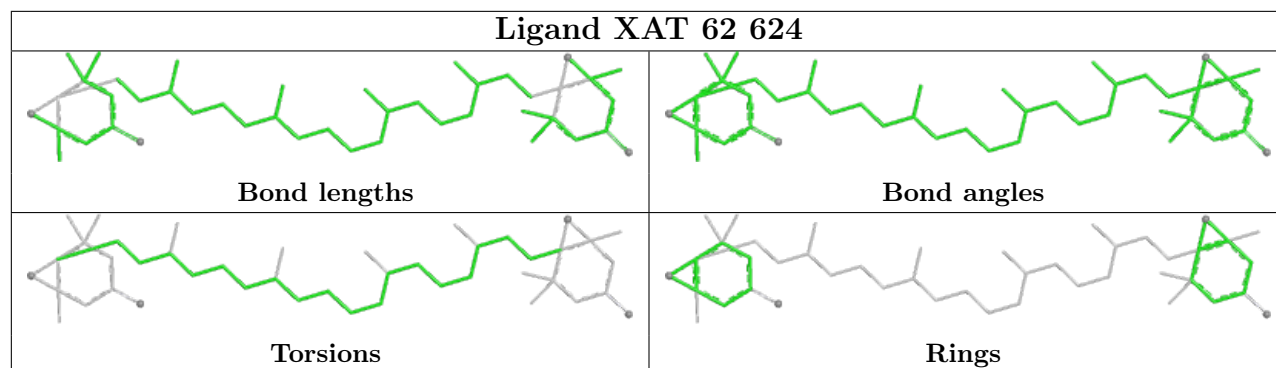


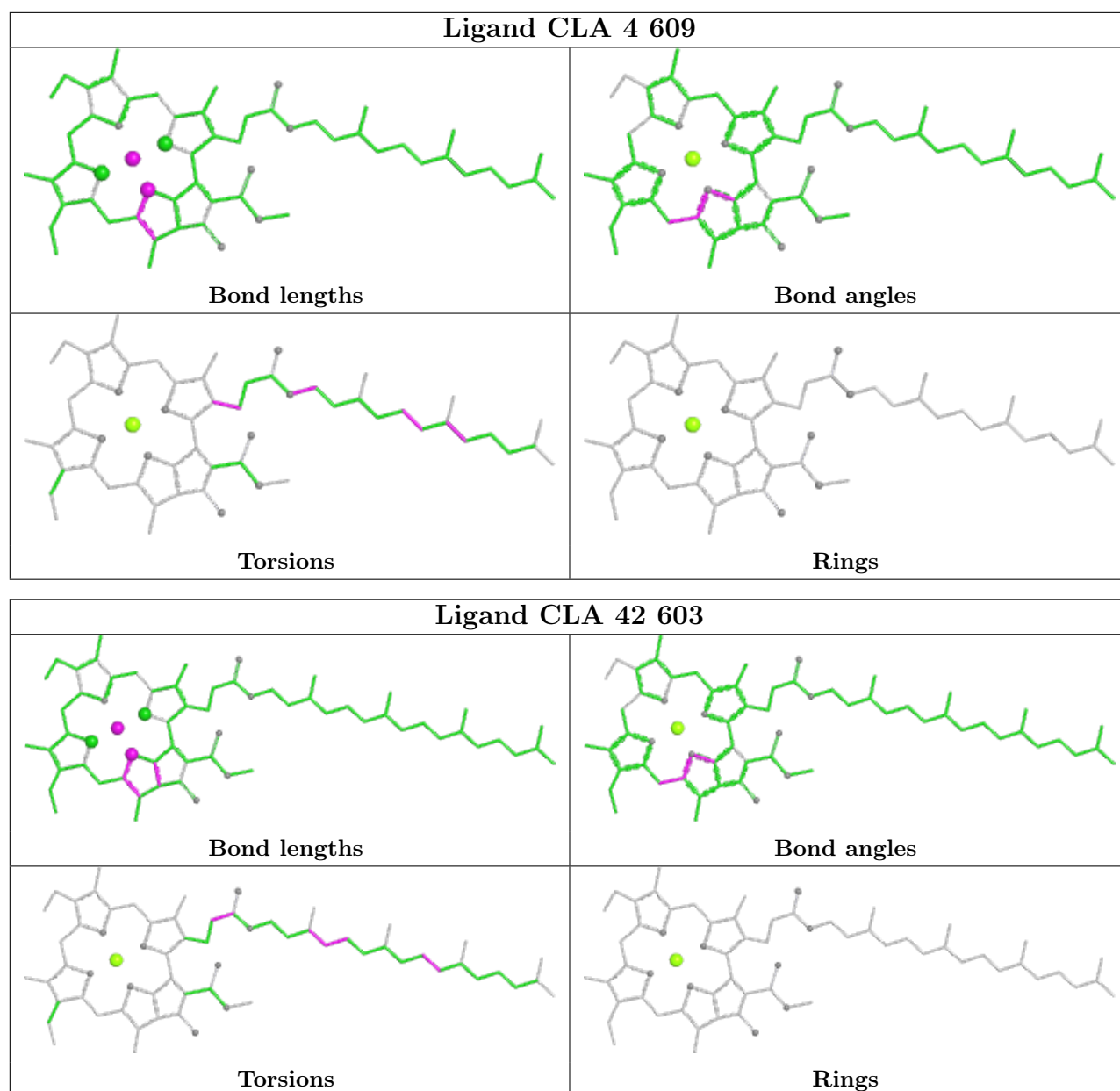


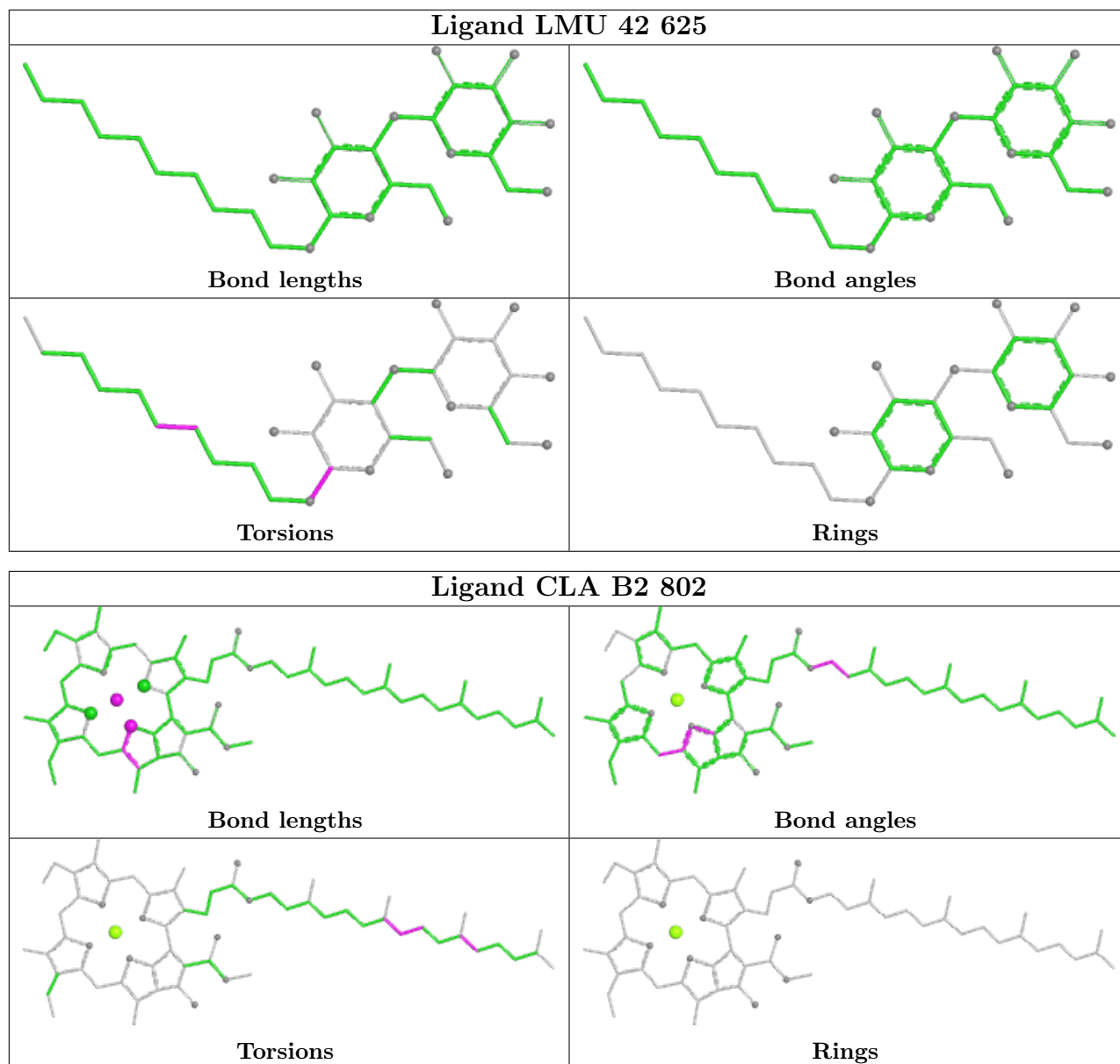


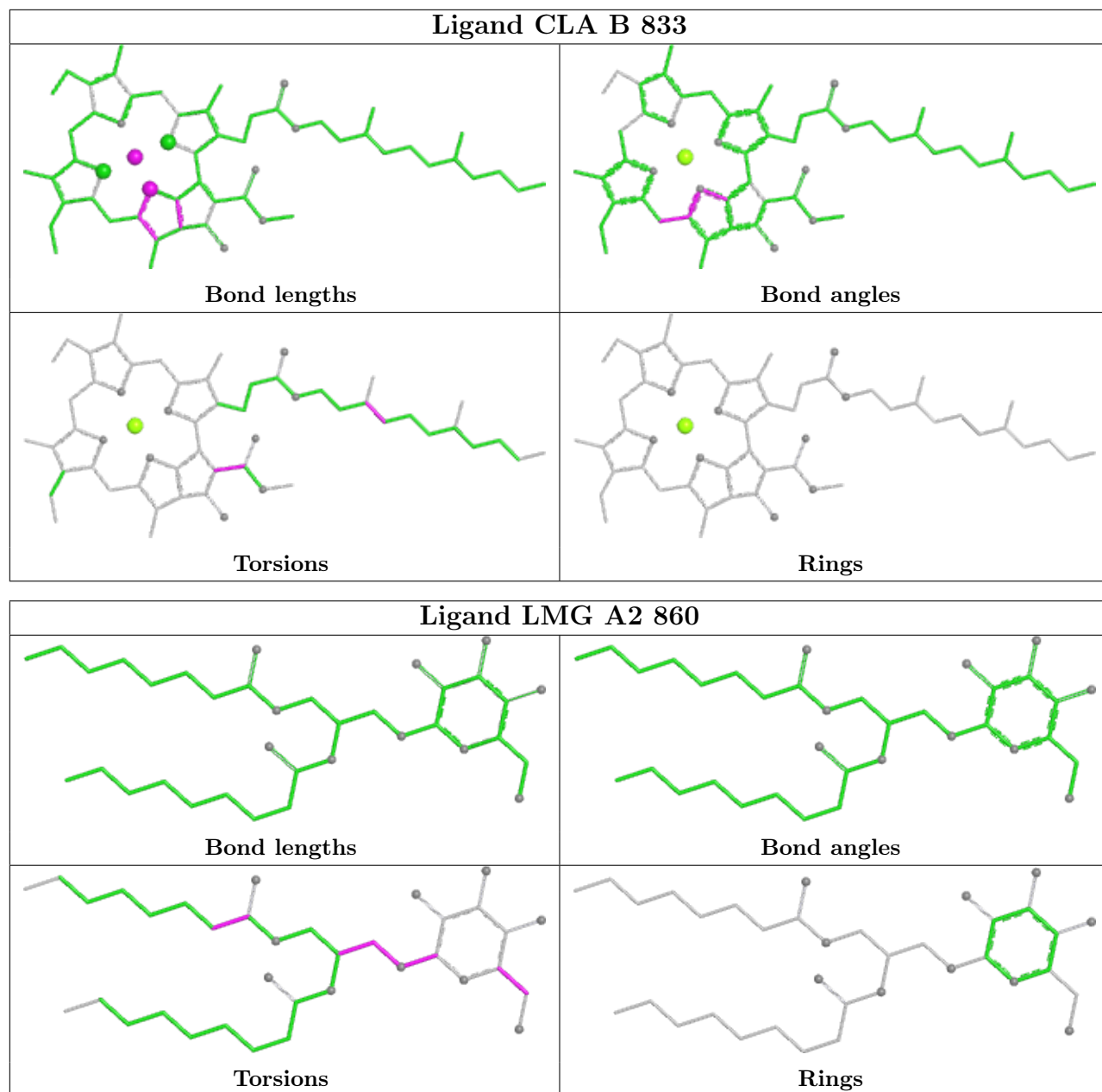


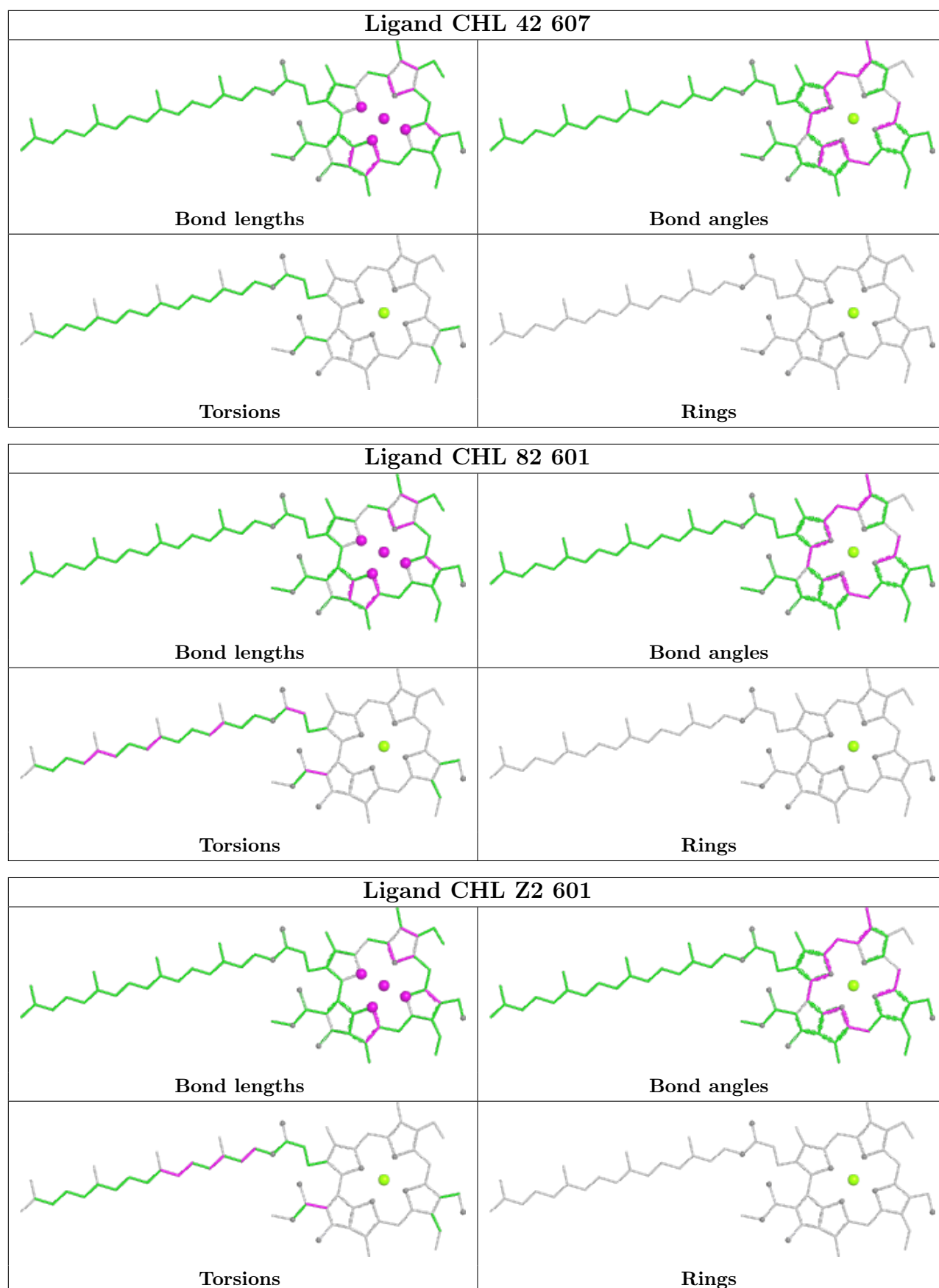


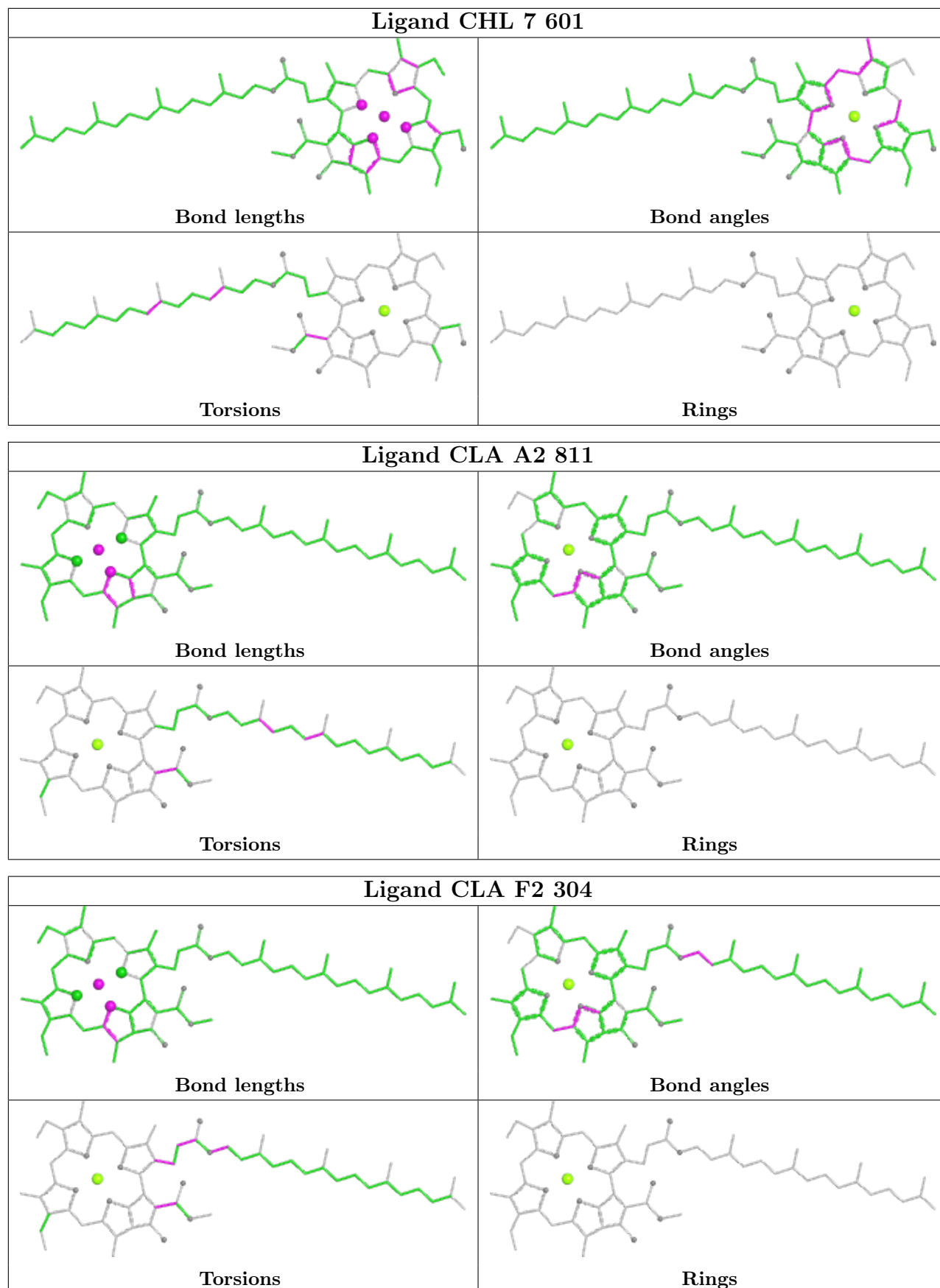


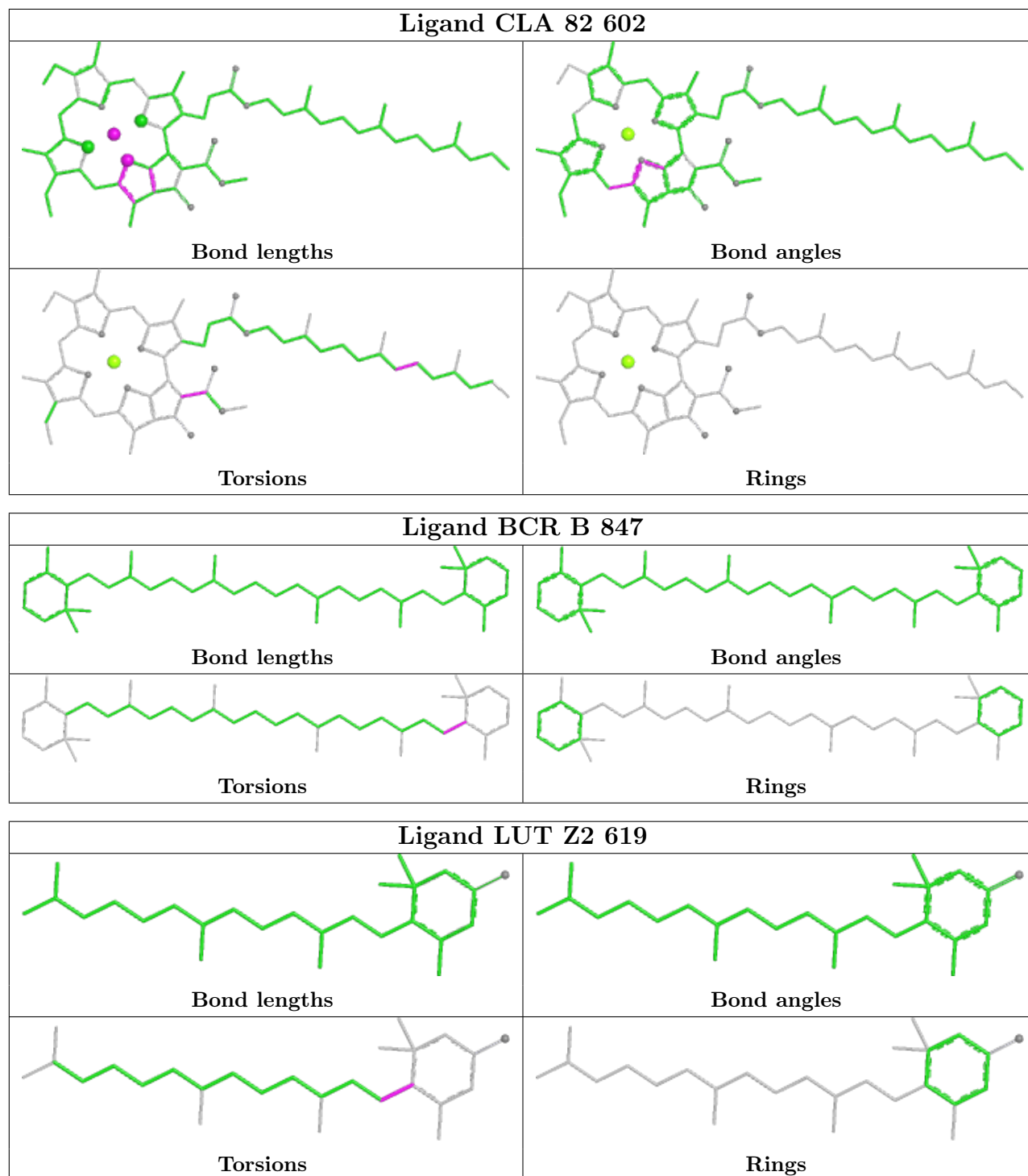


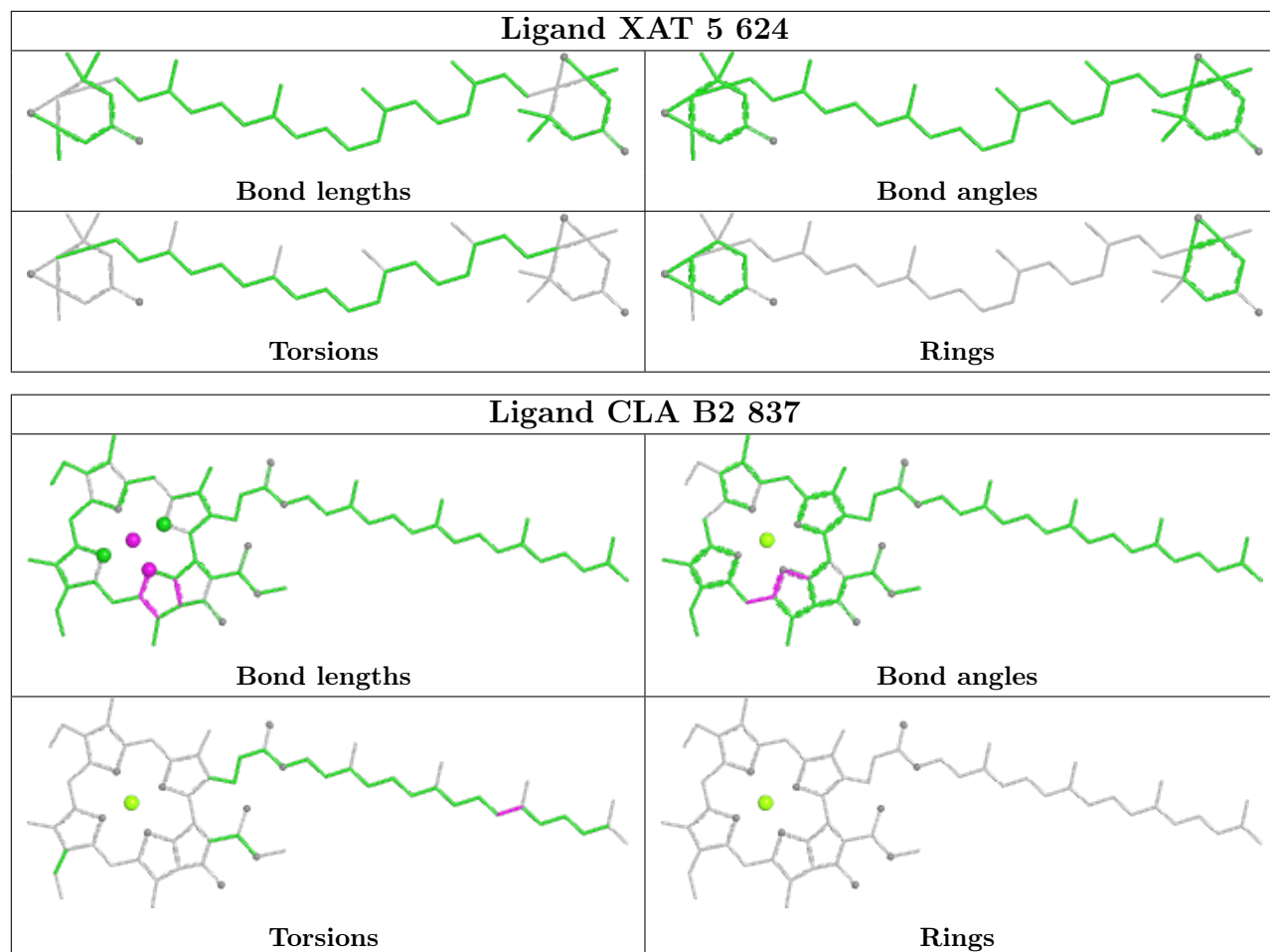


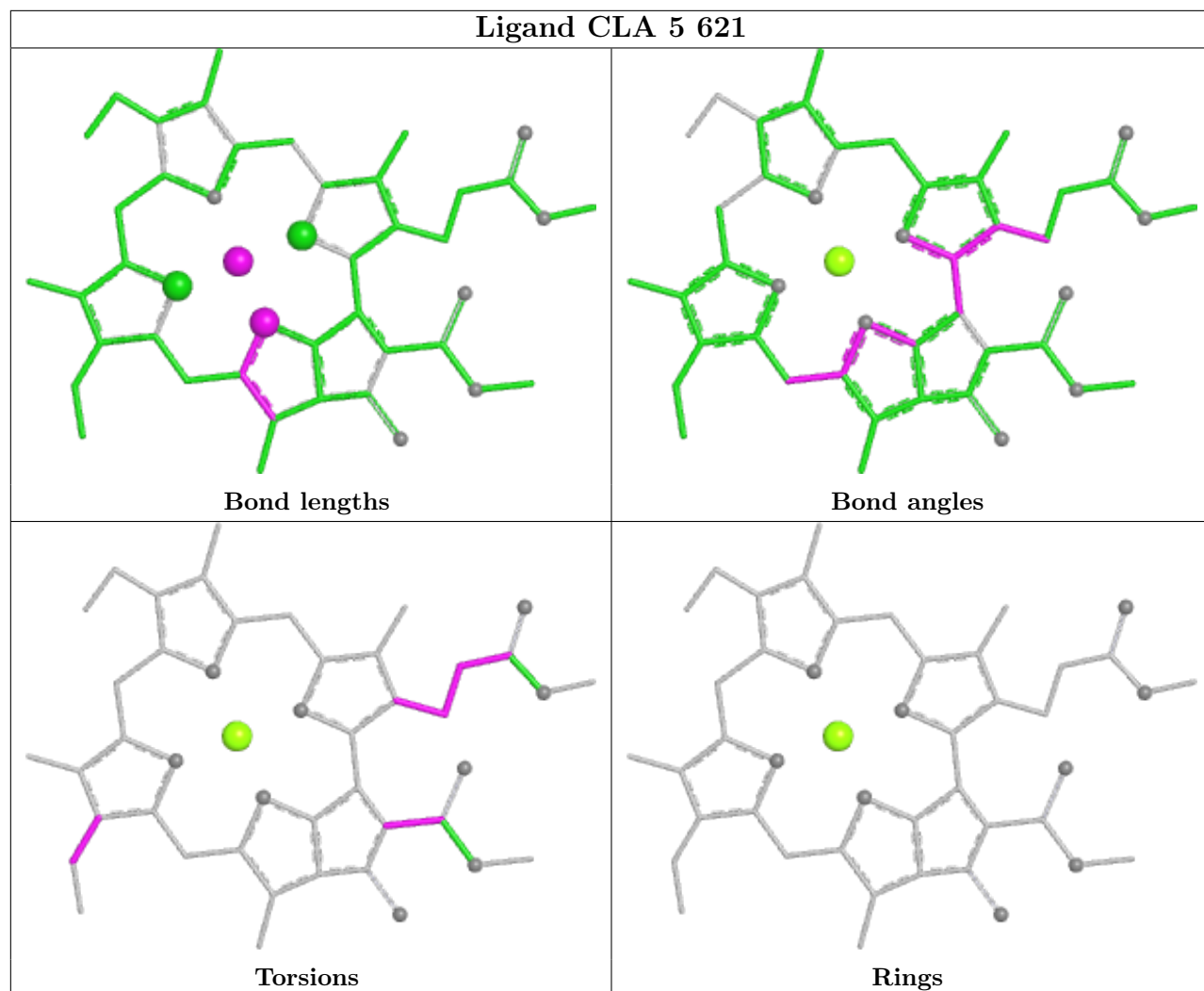


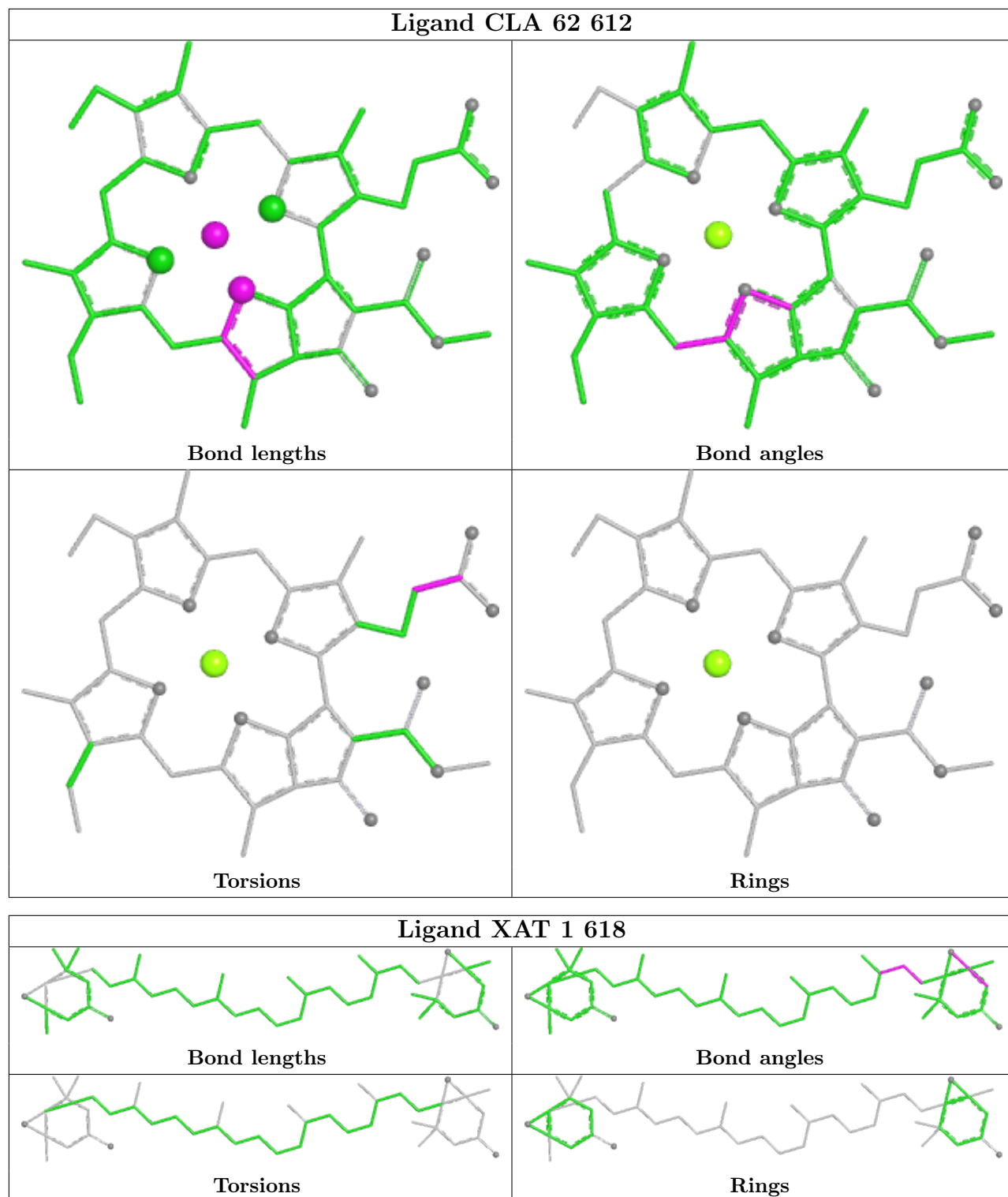


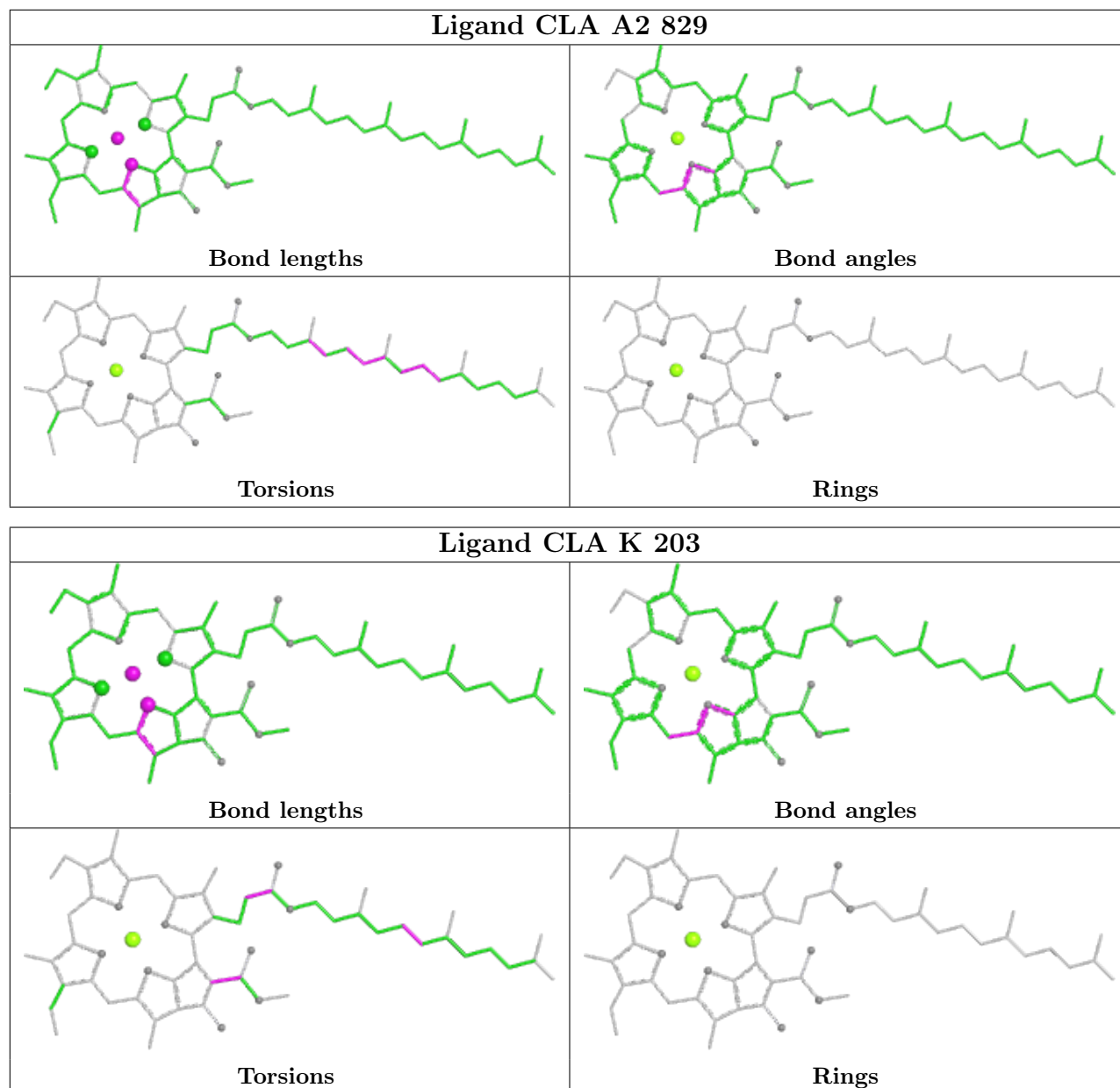


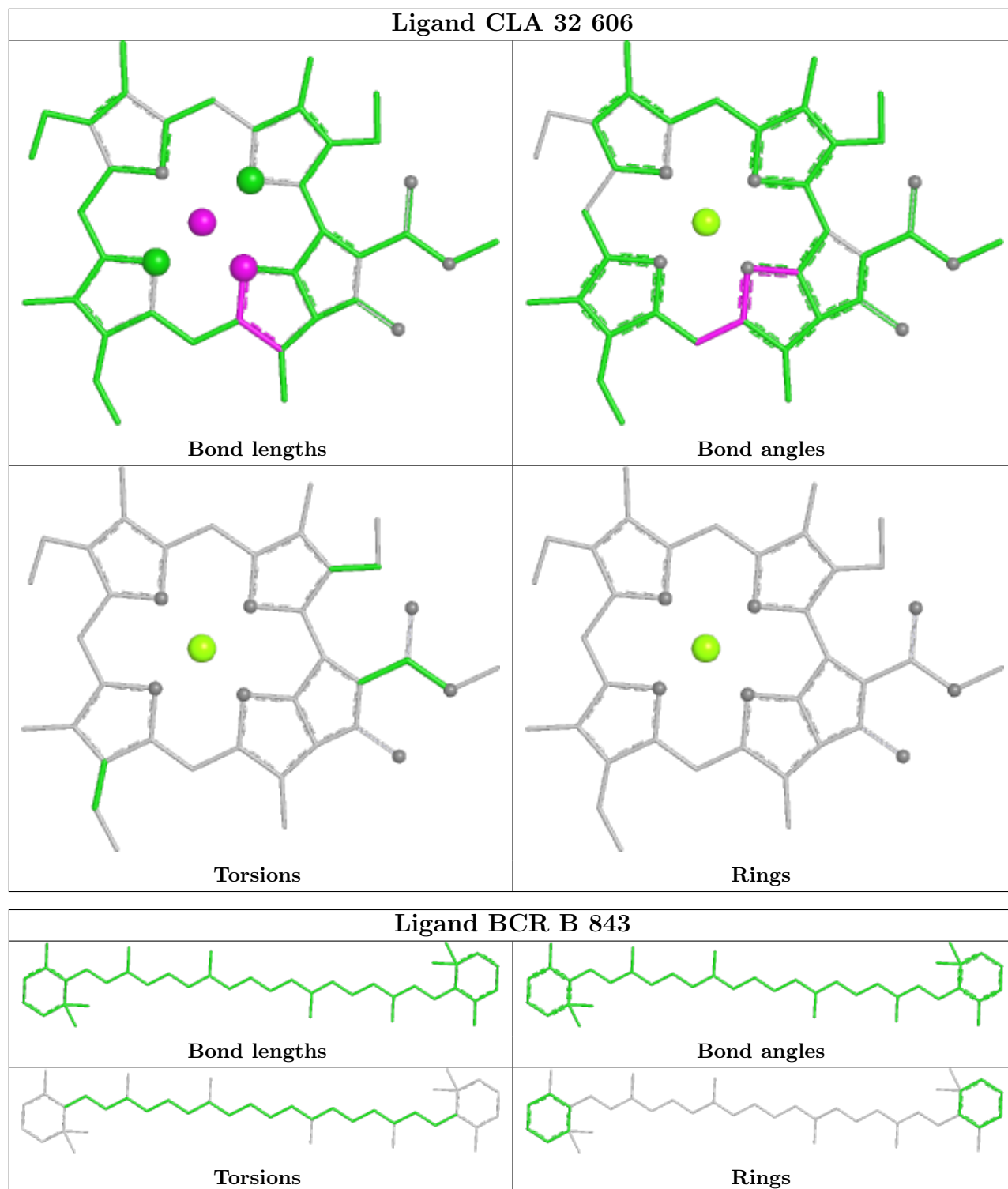


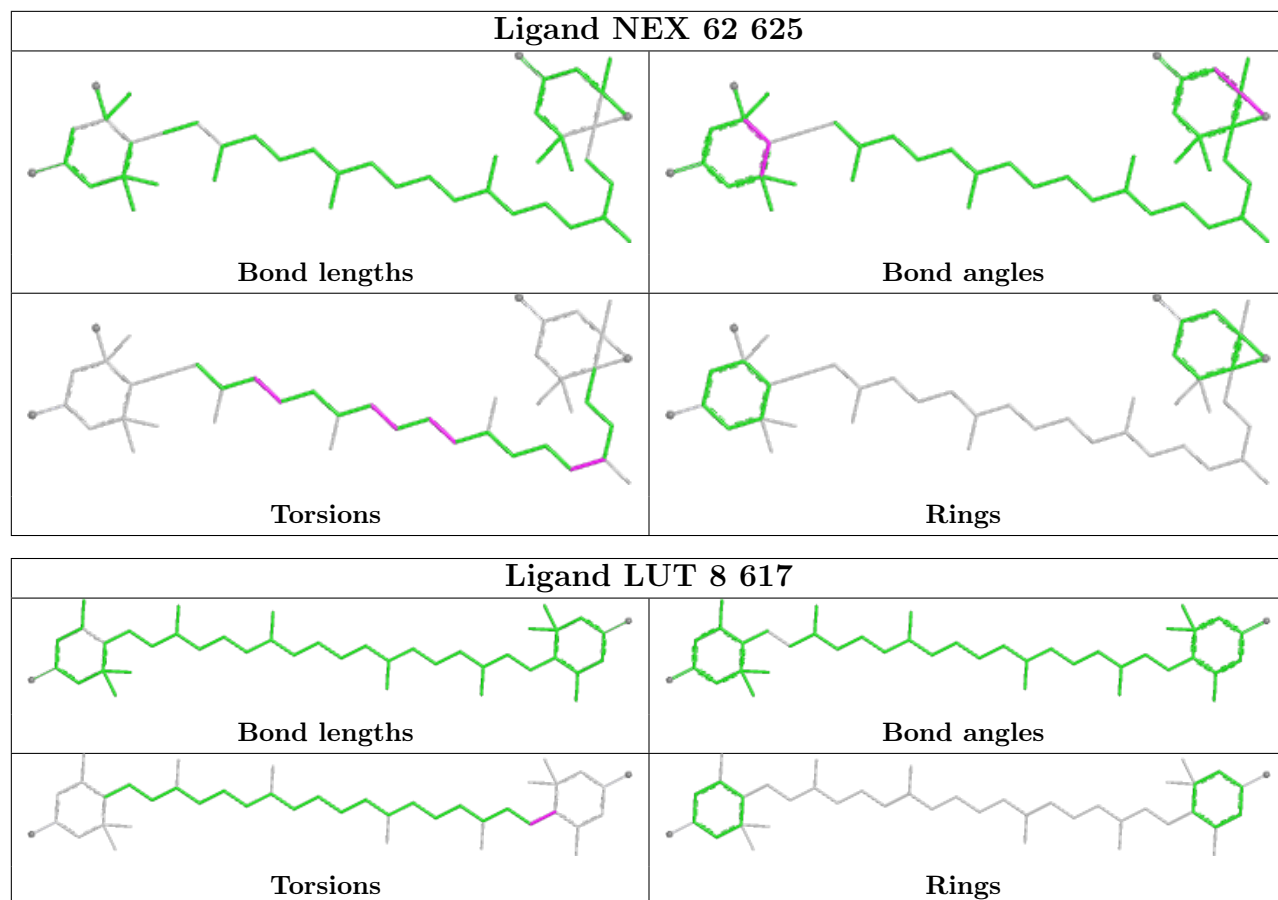


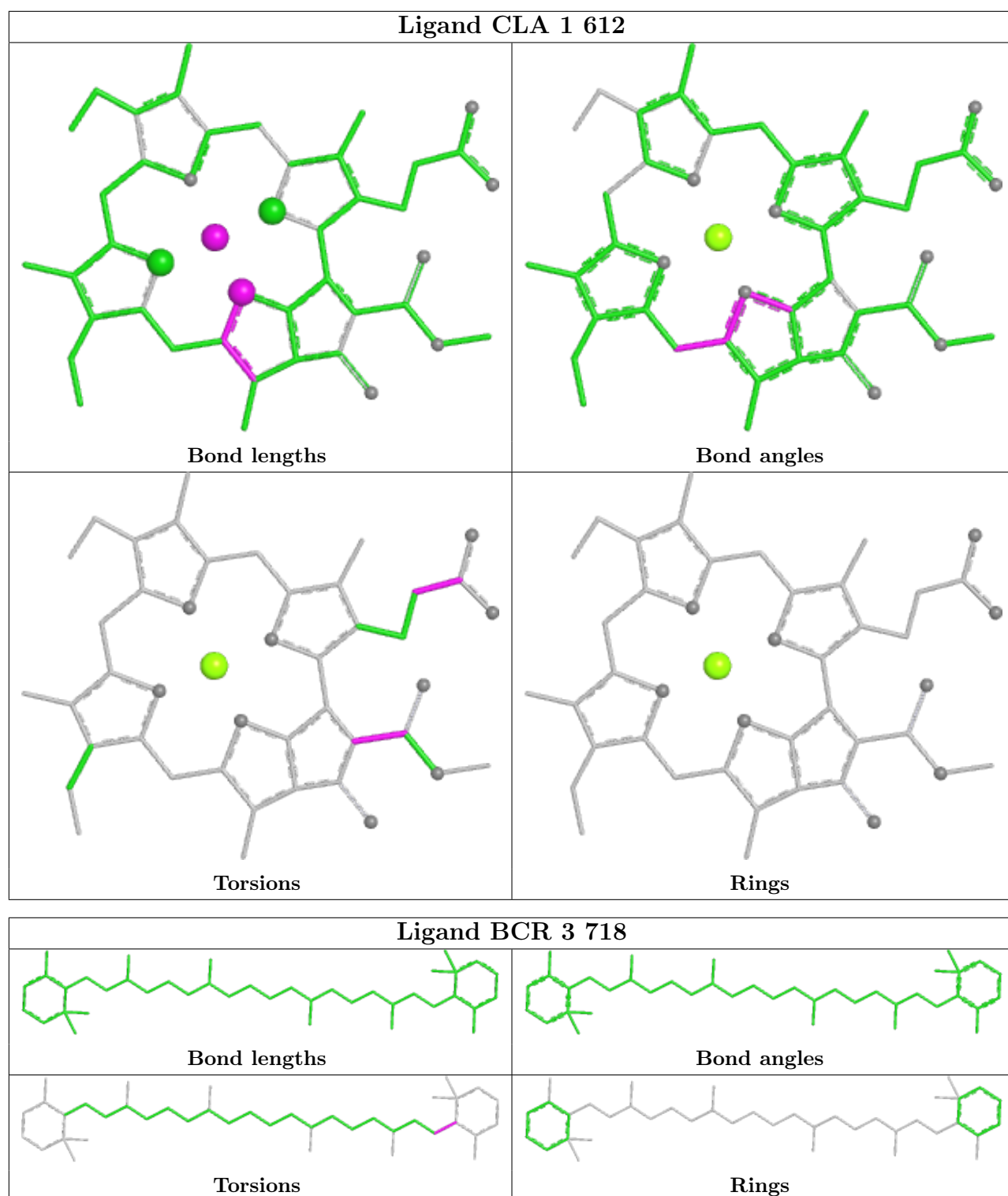


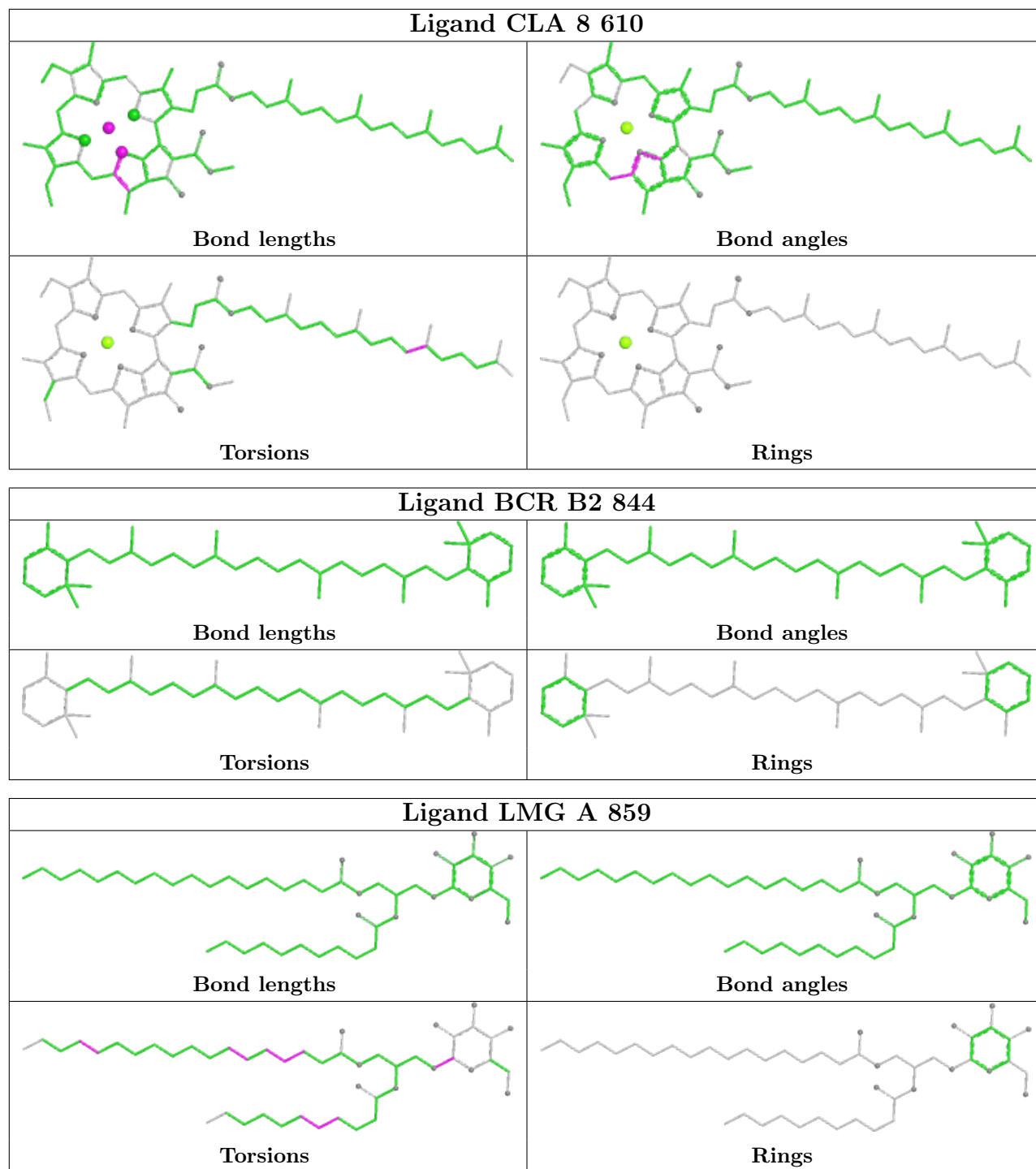


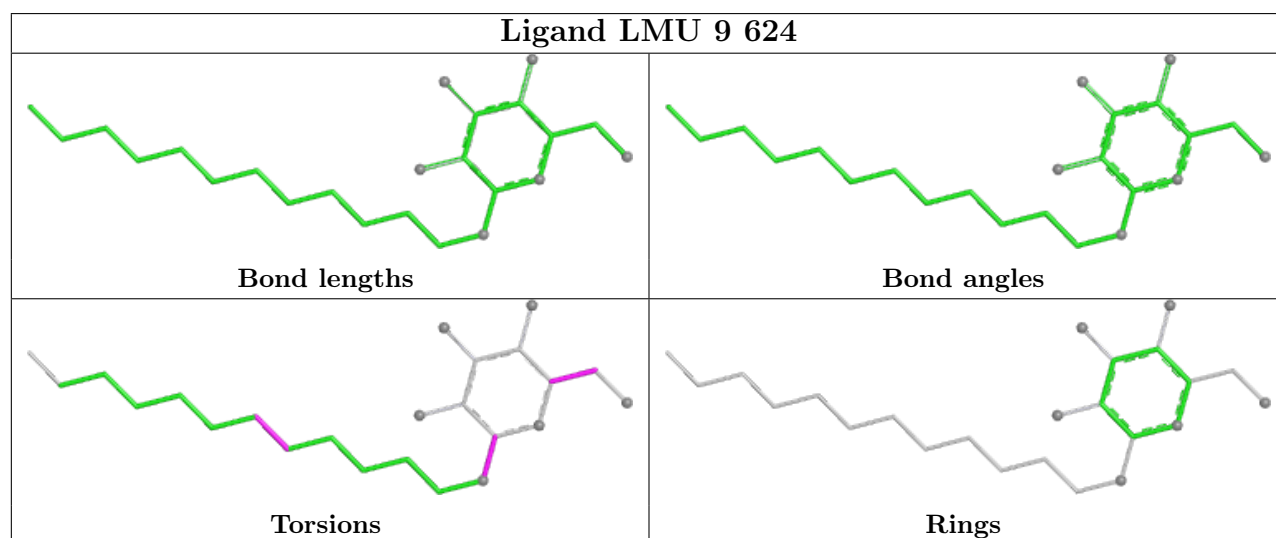
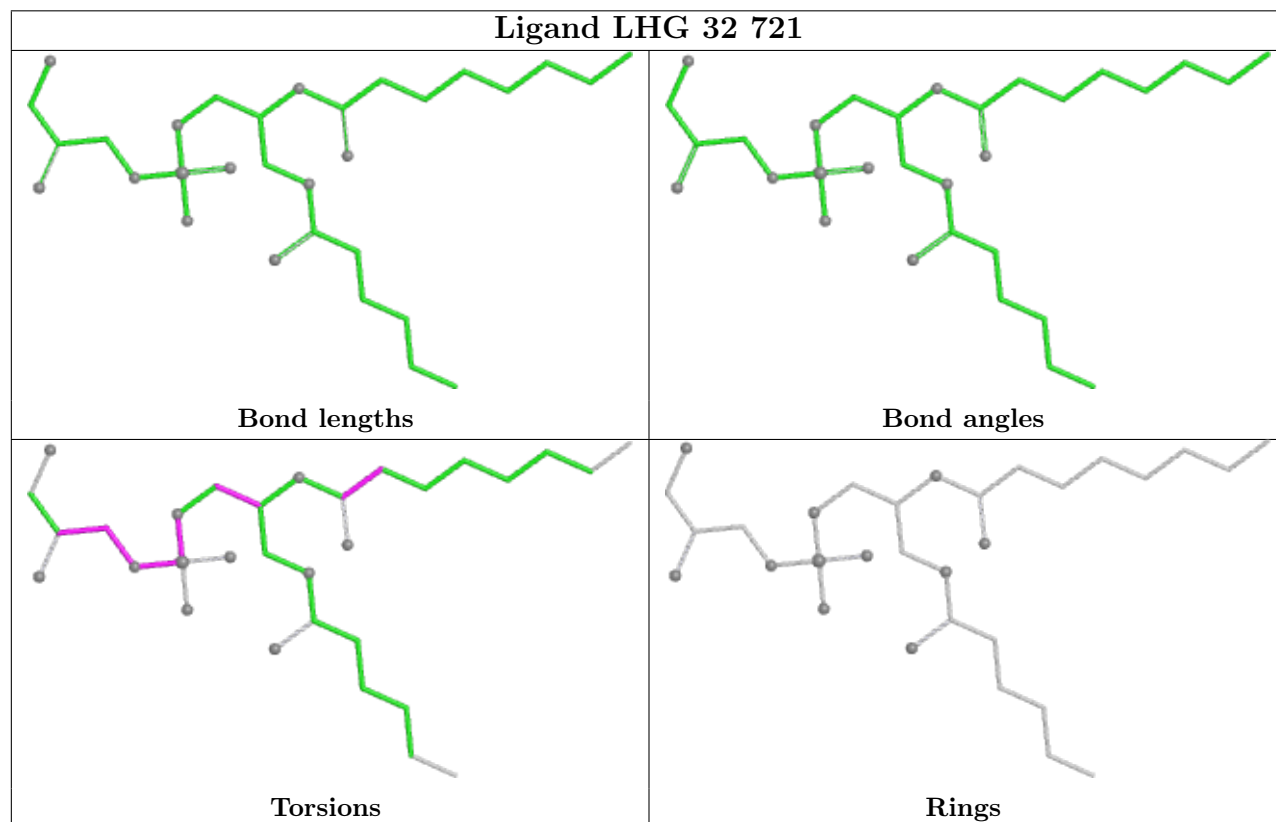
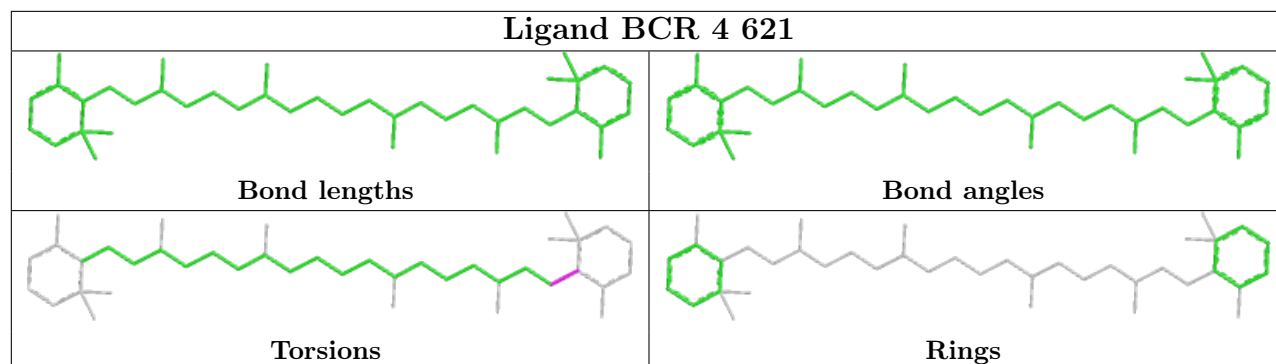


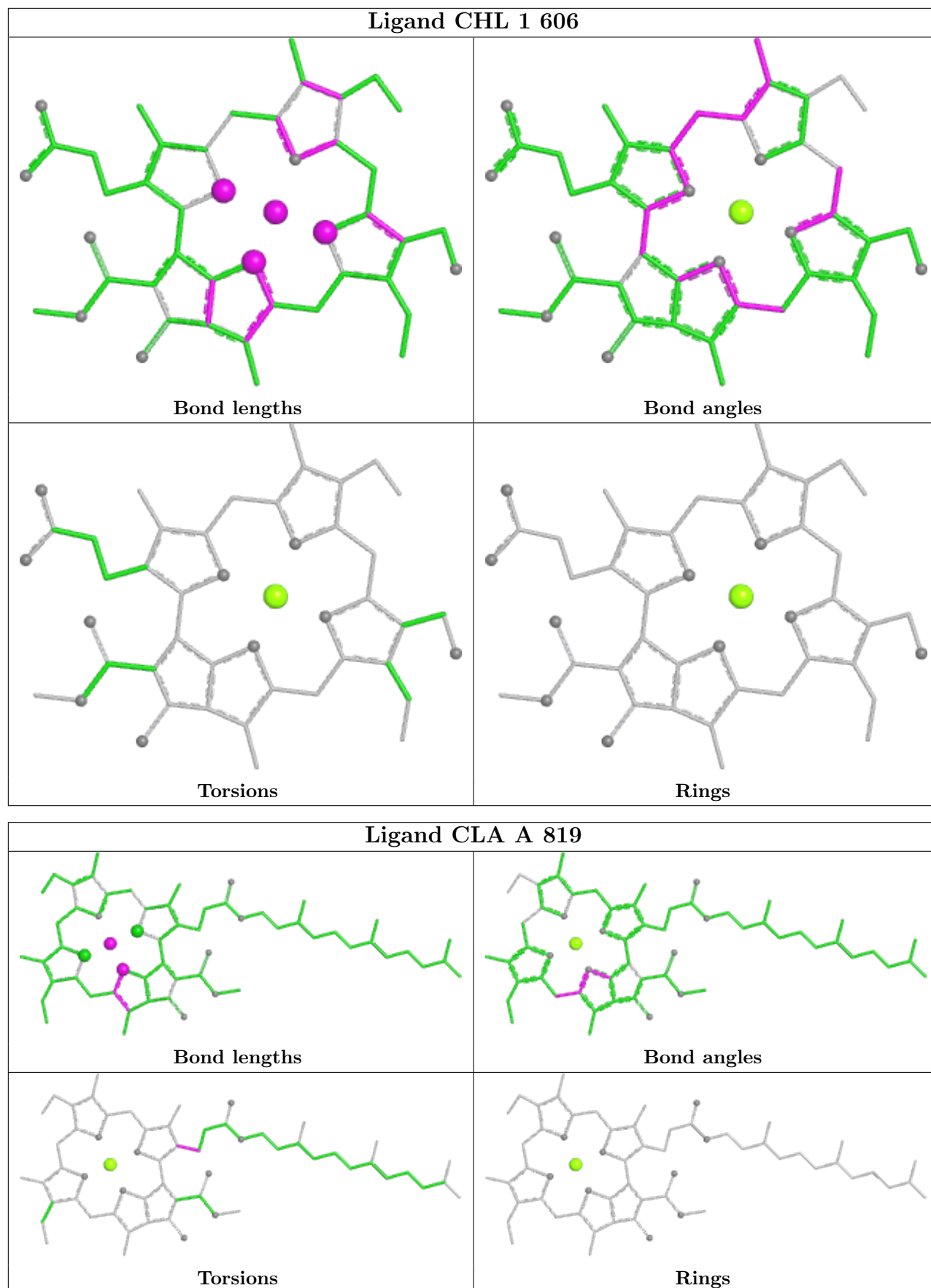


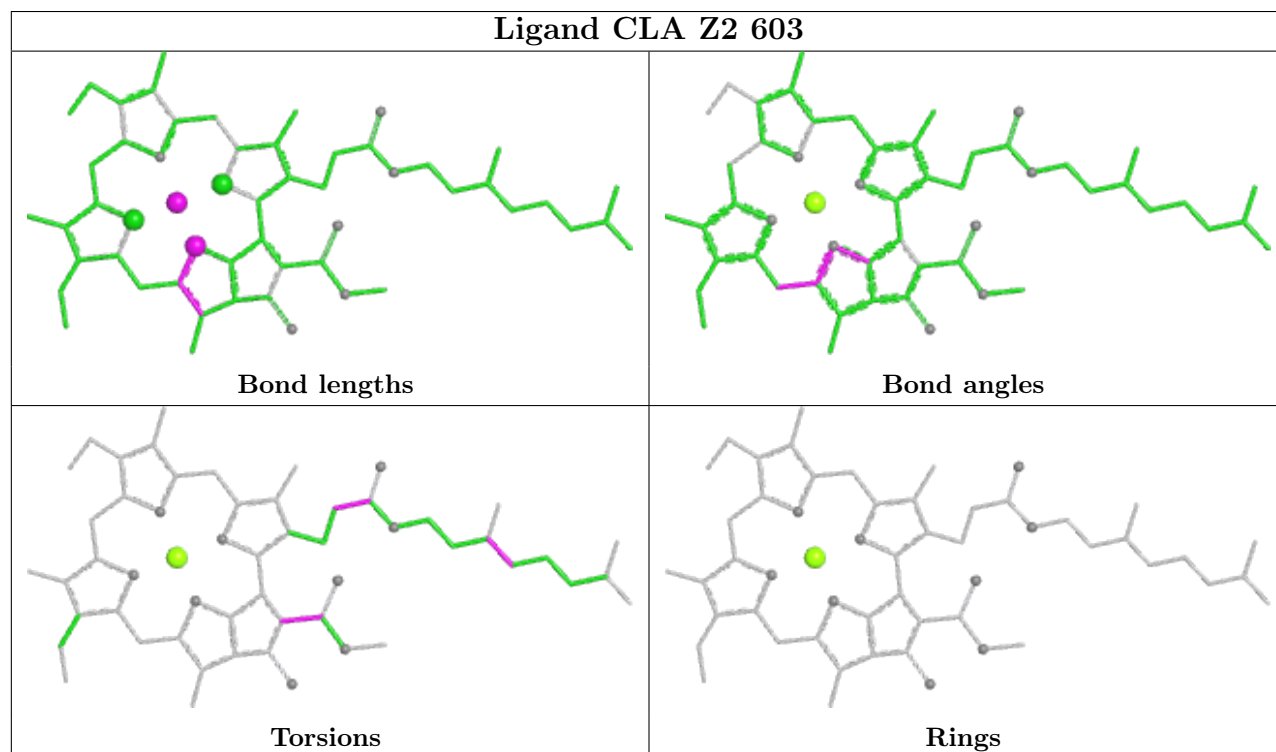
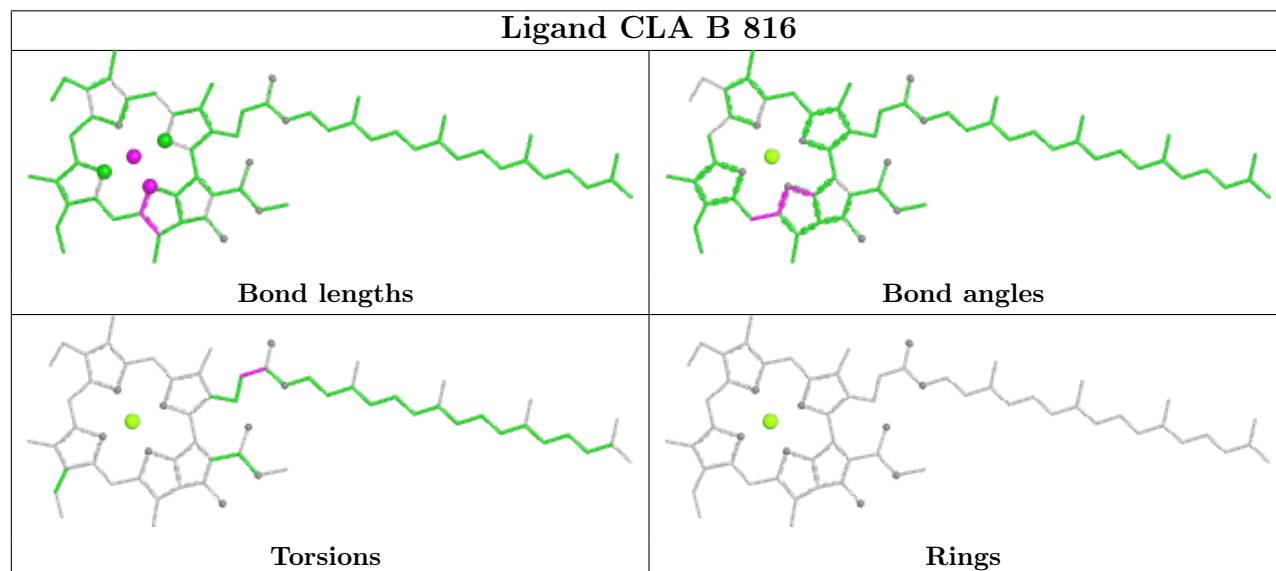
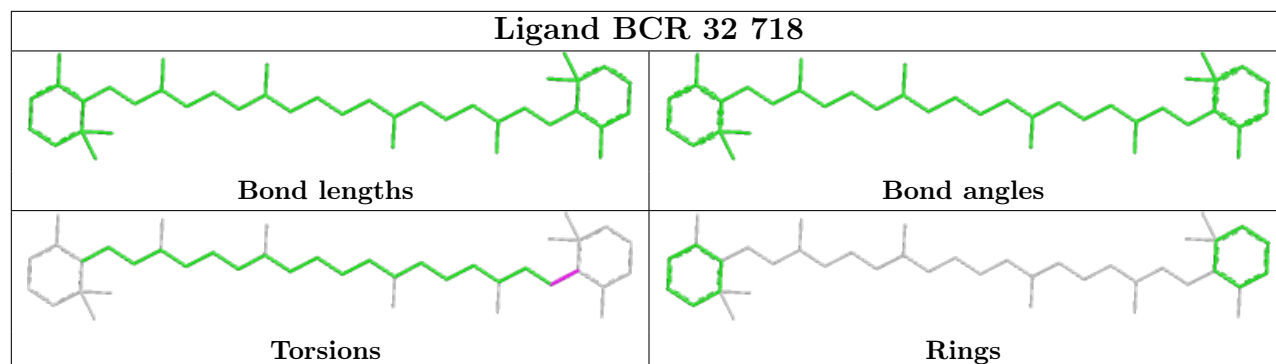


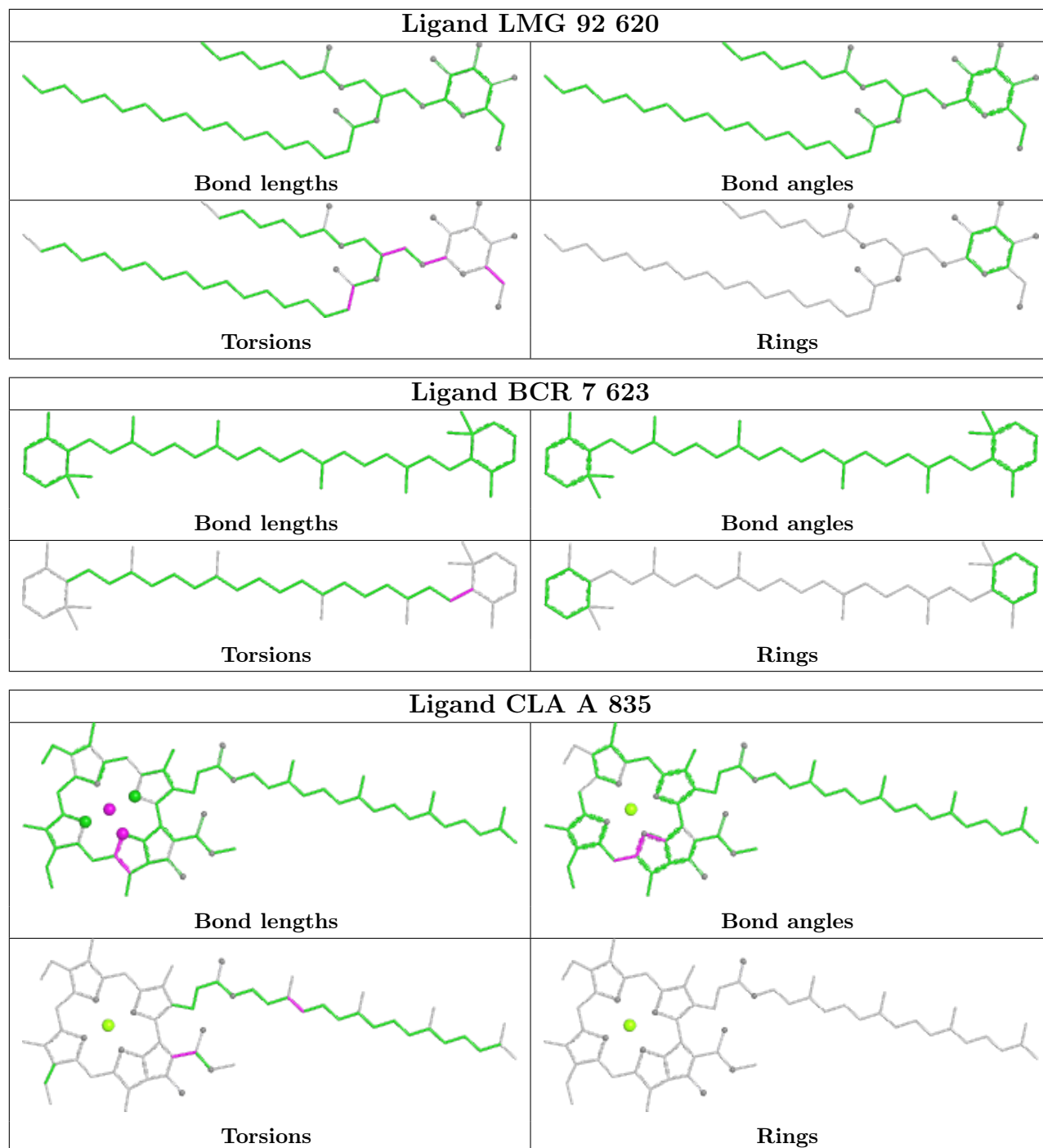


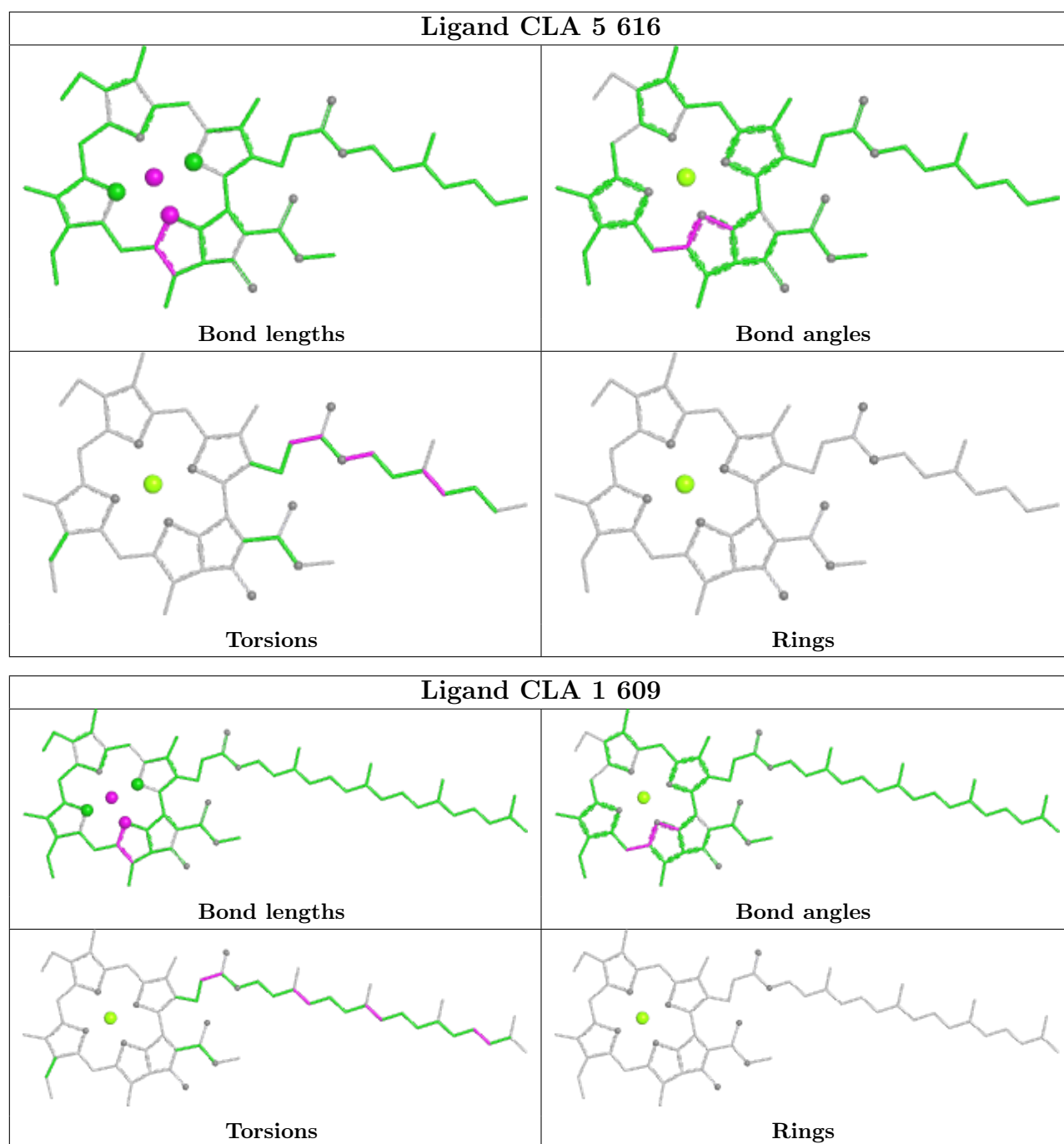


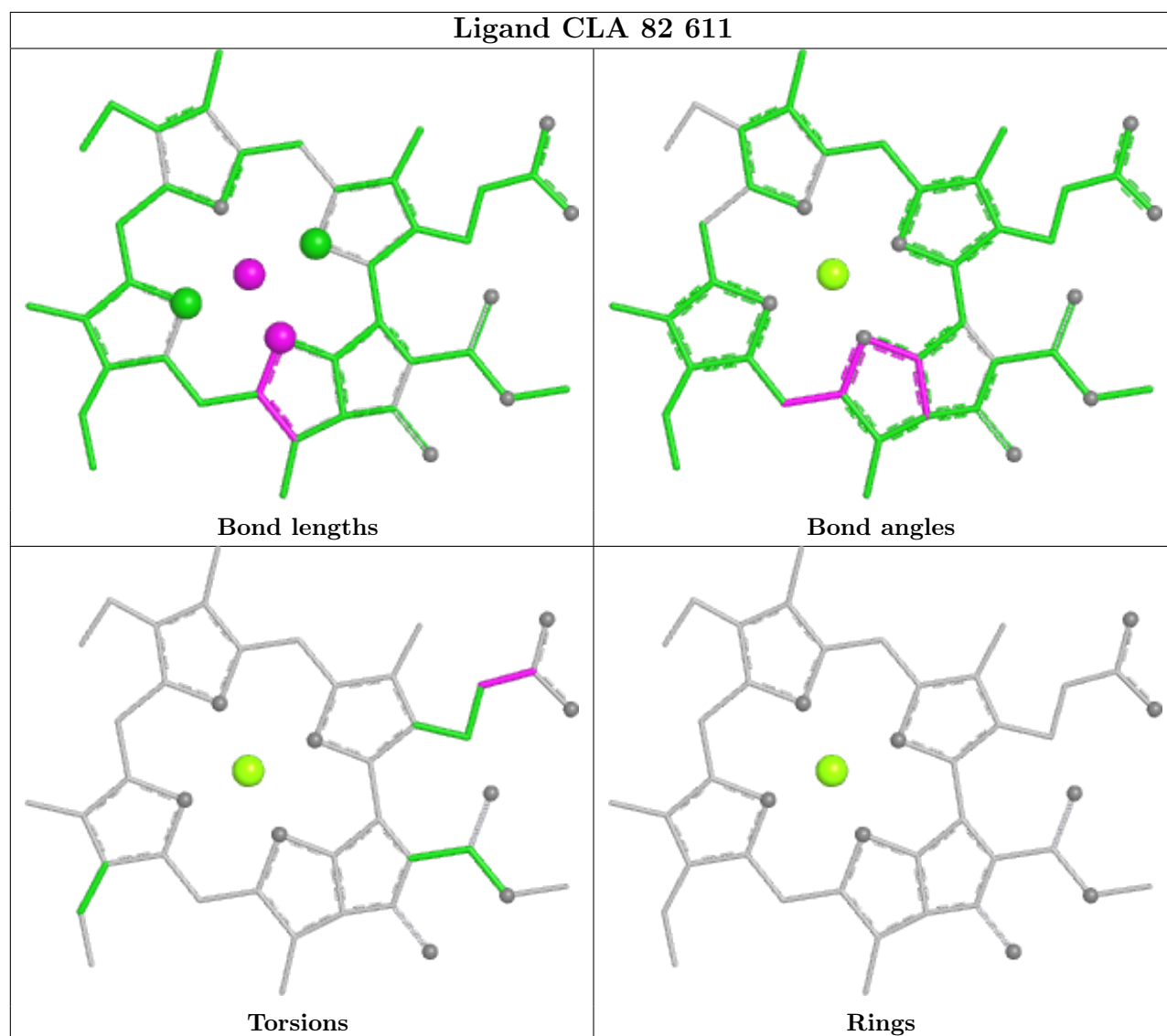
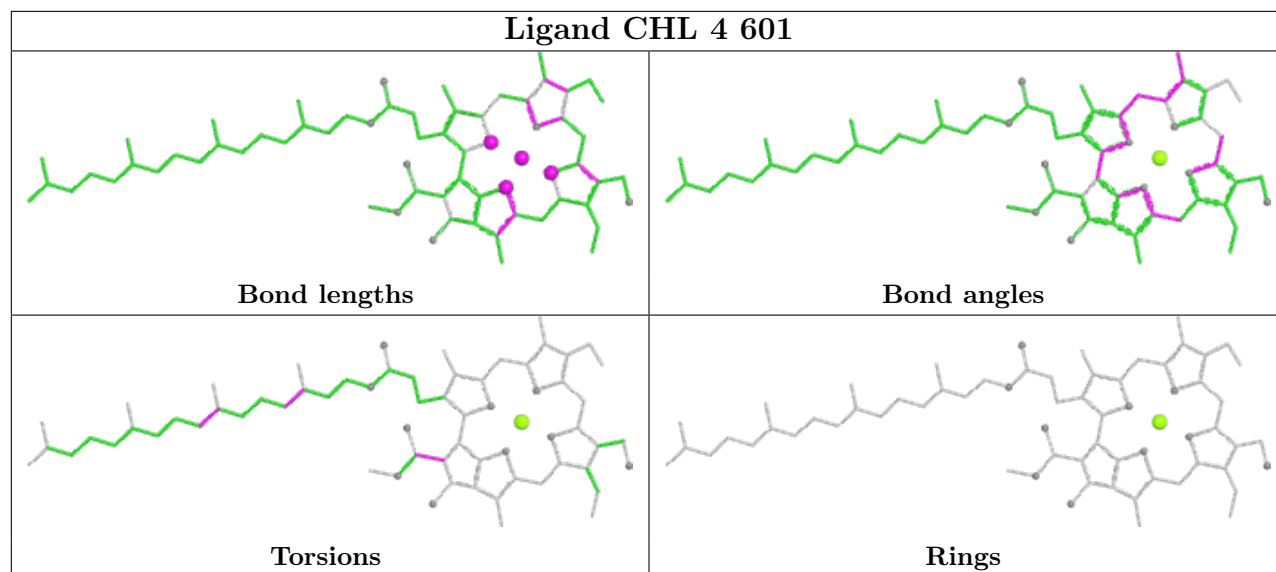




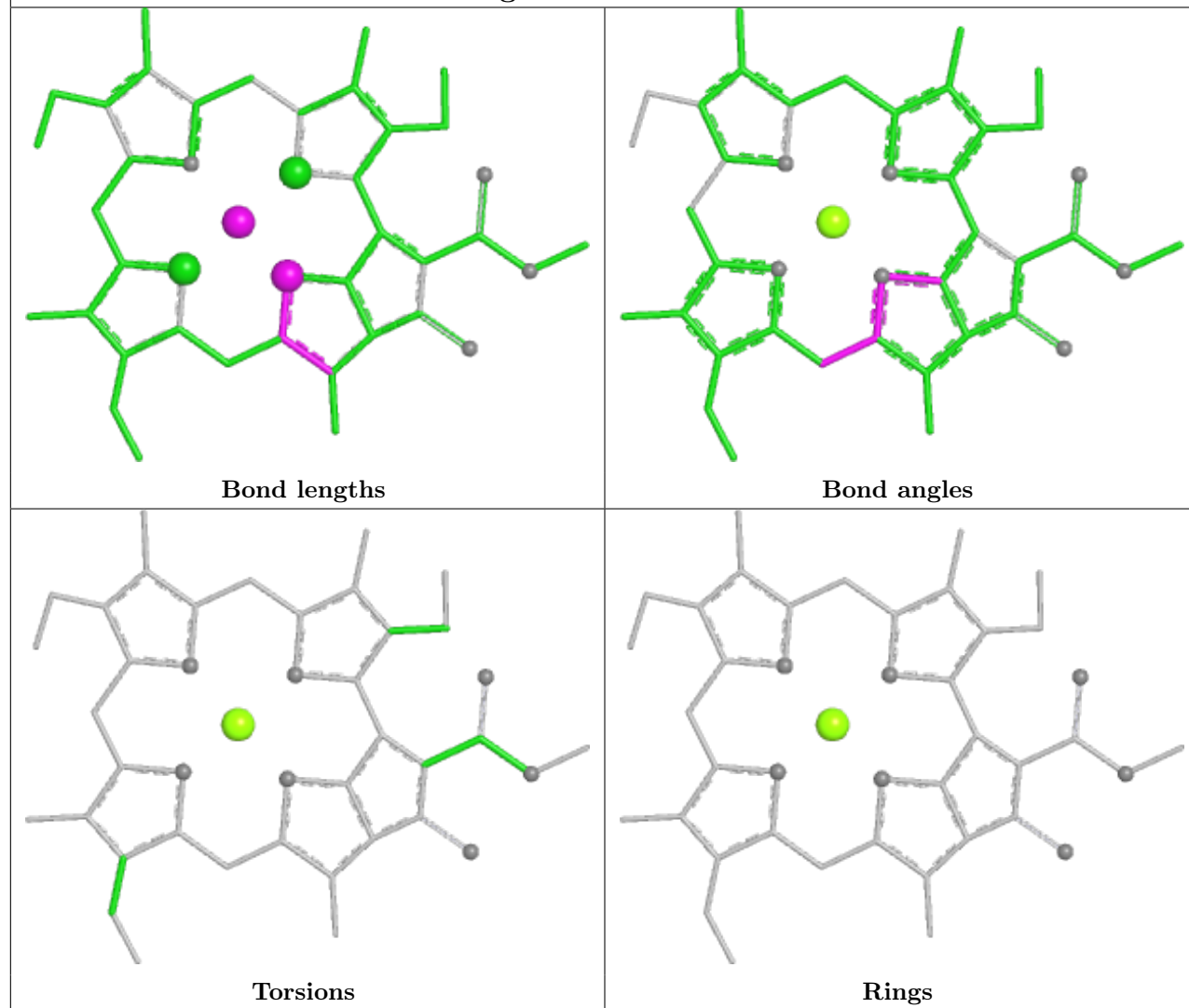




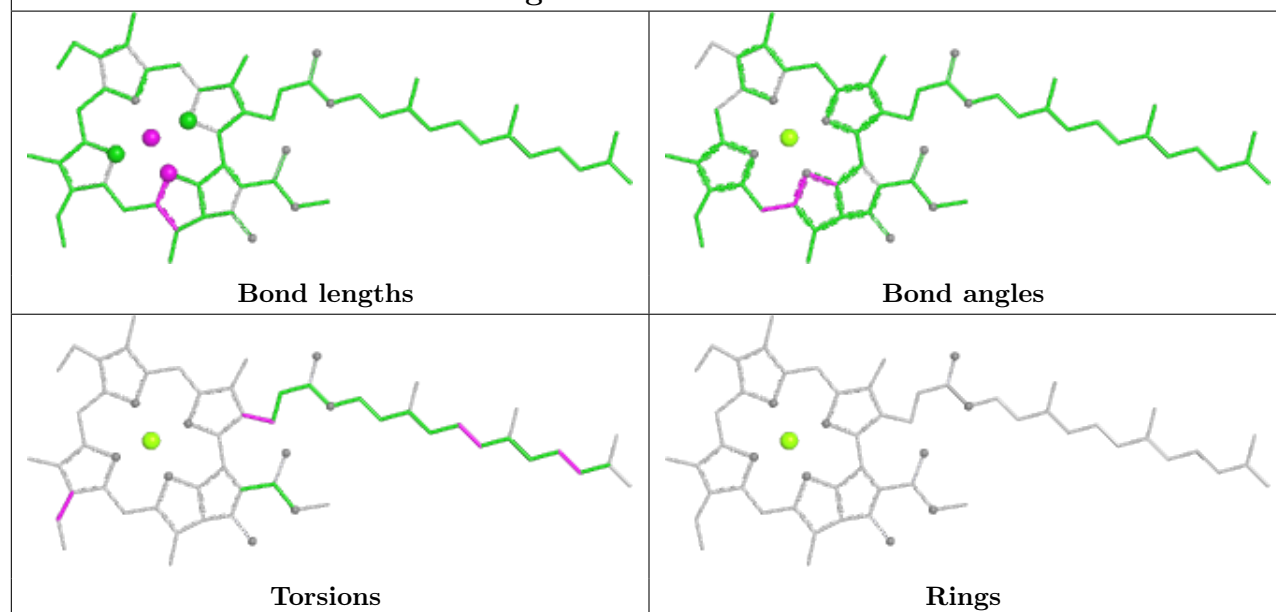


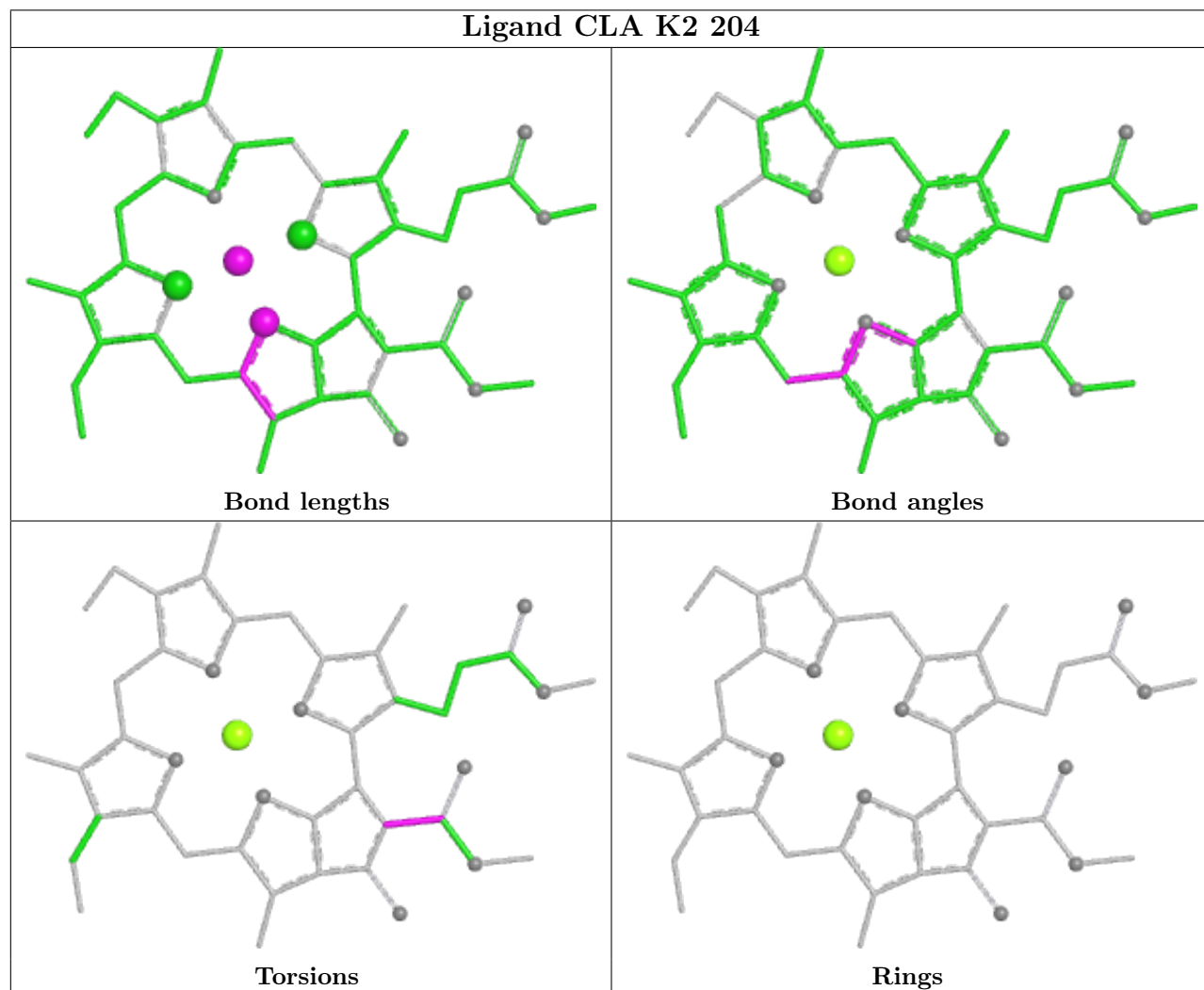
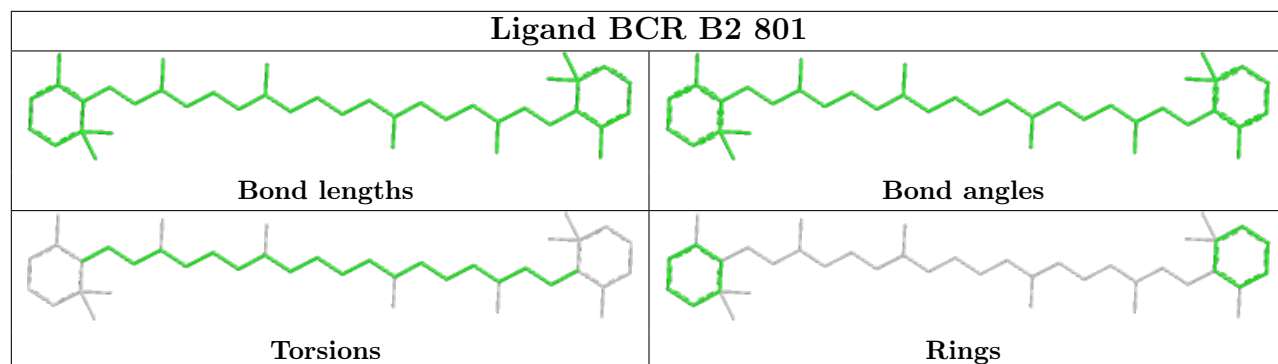


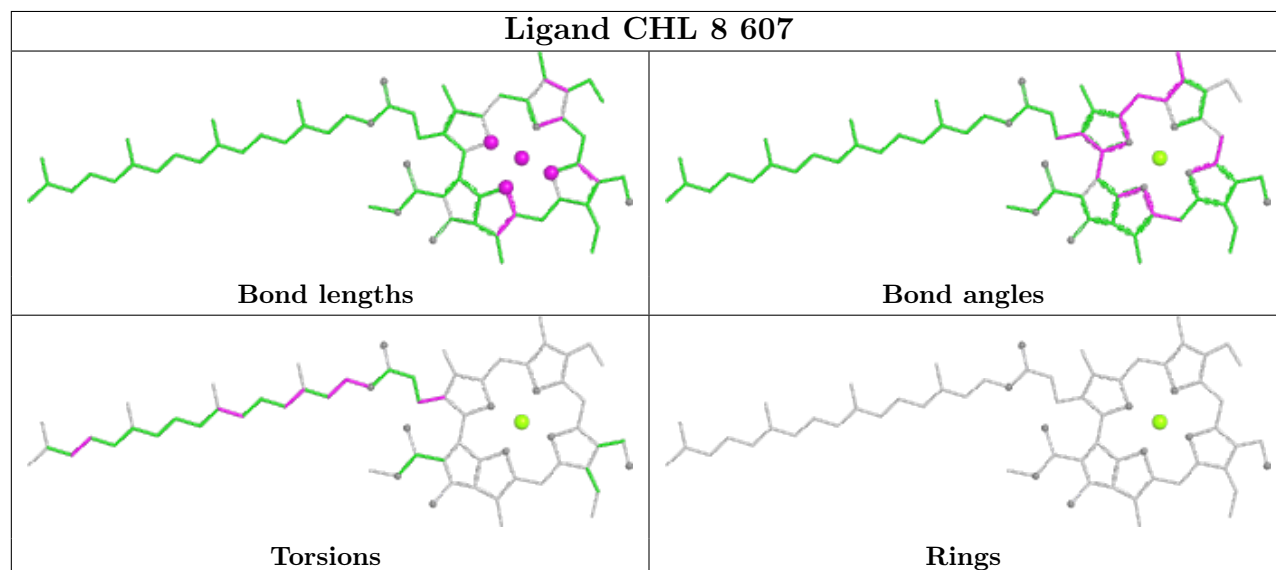
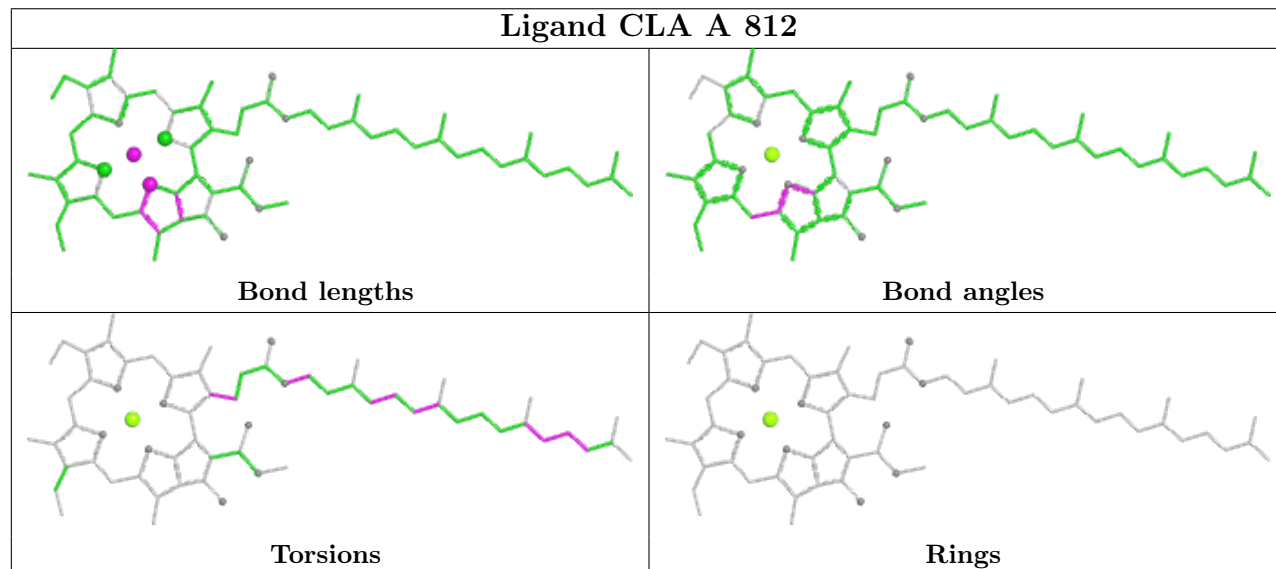
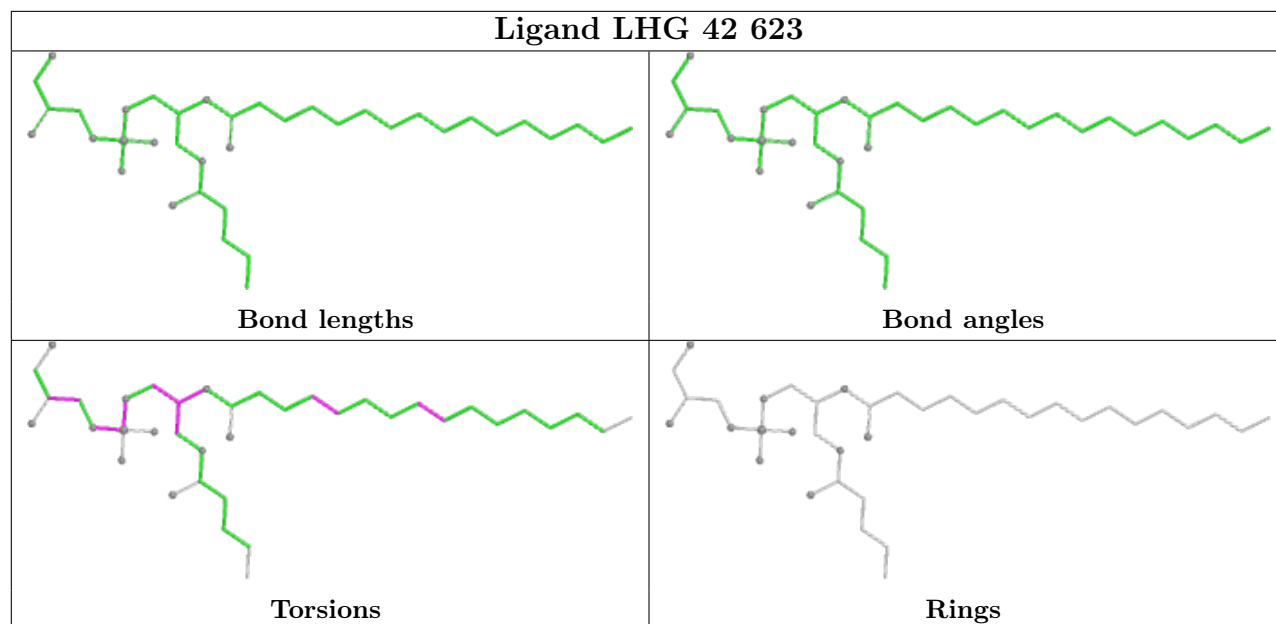
Ligand CLA 3 606

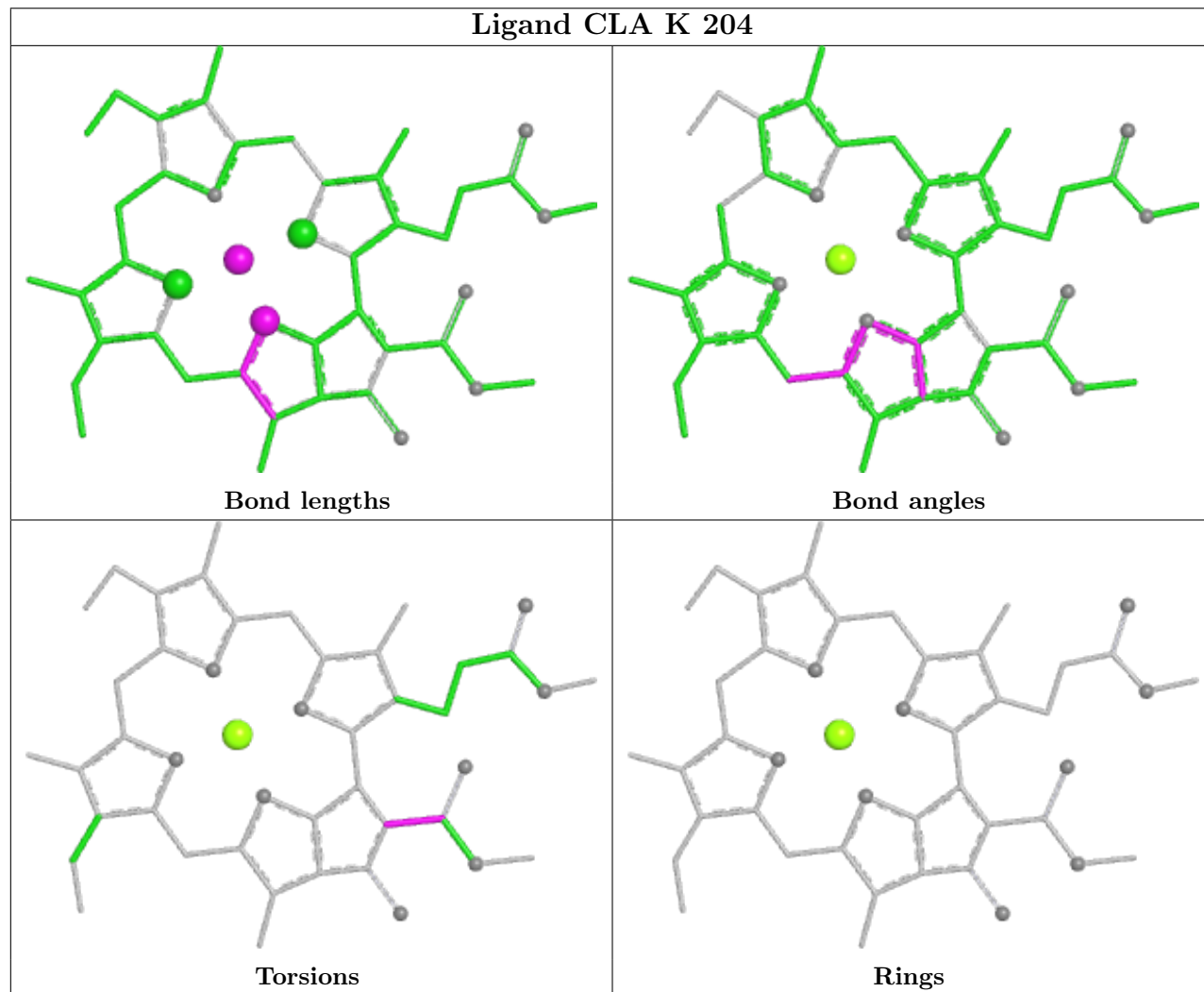
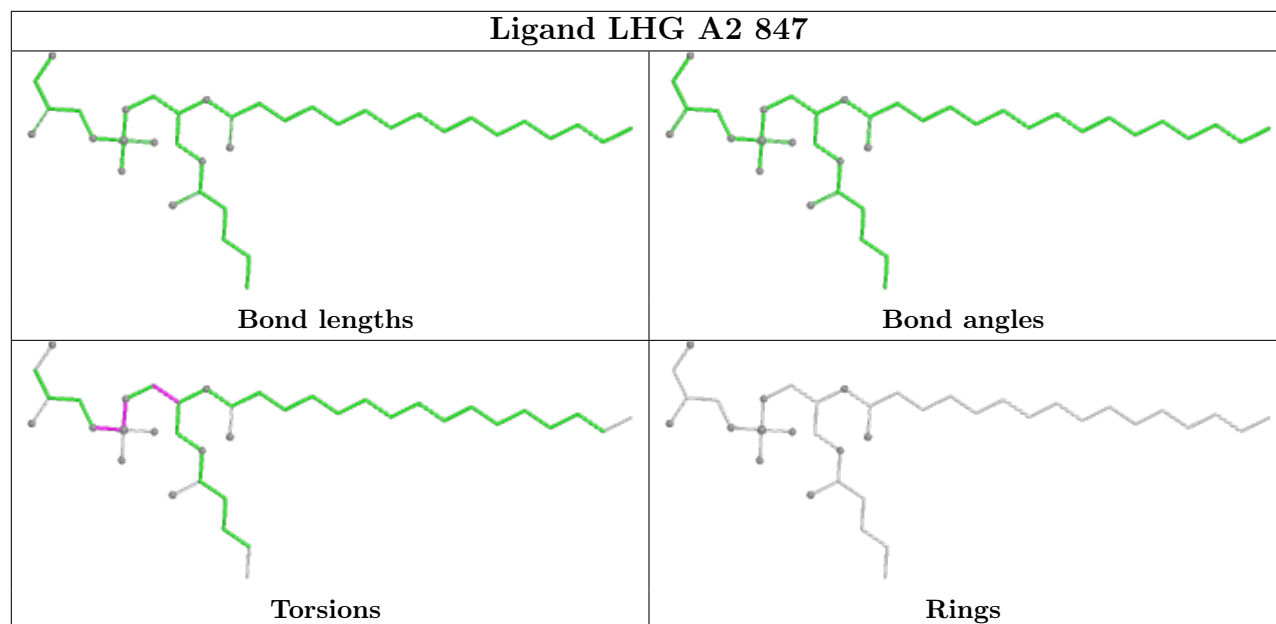


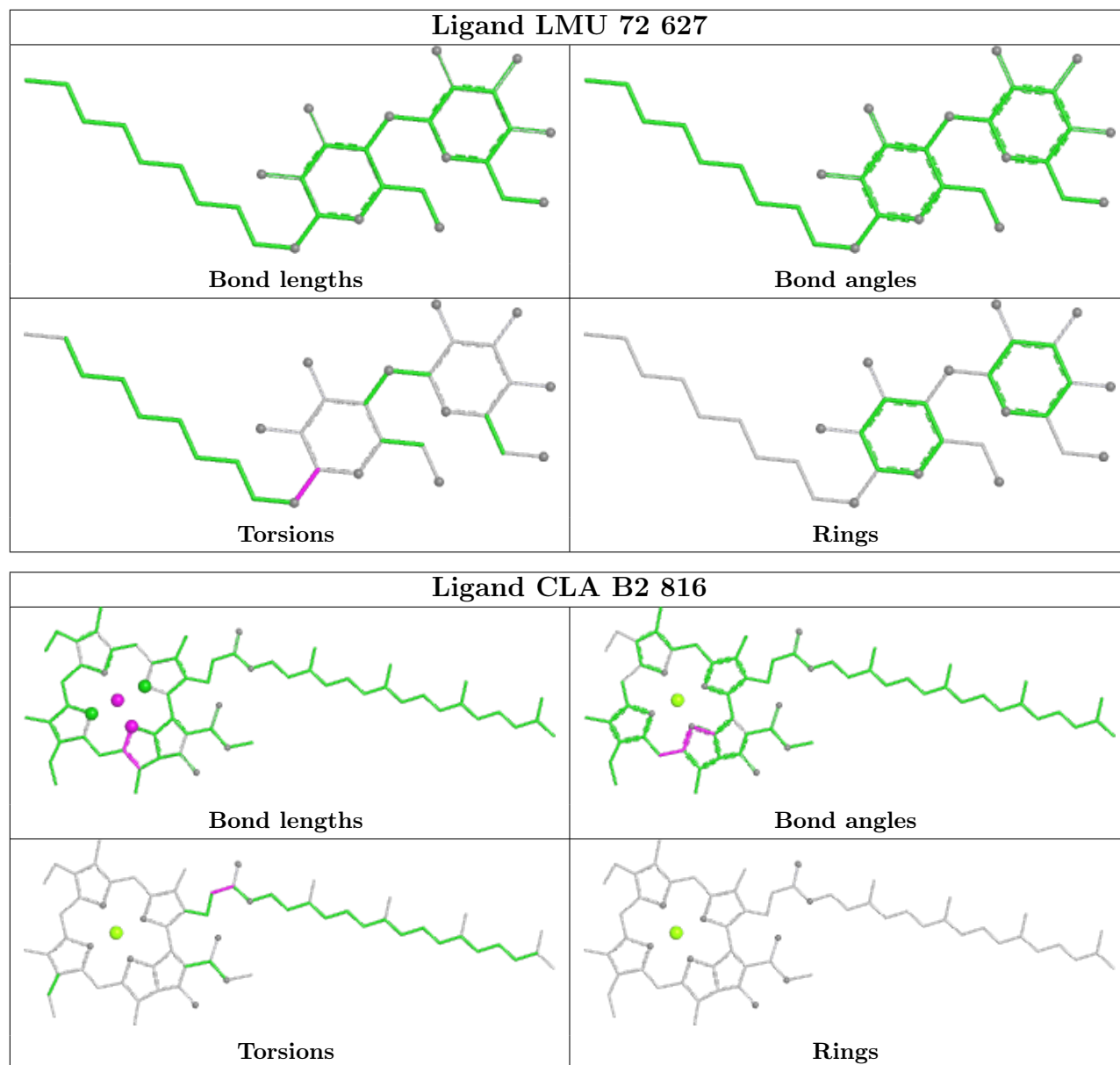
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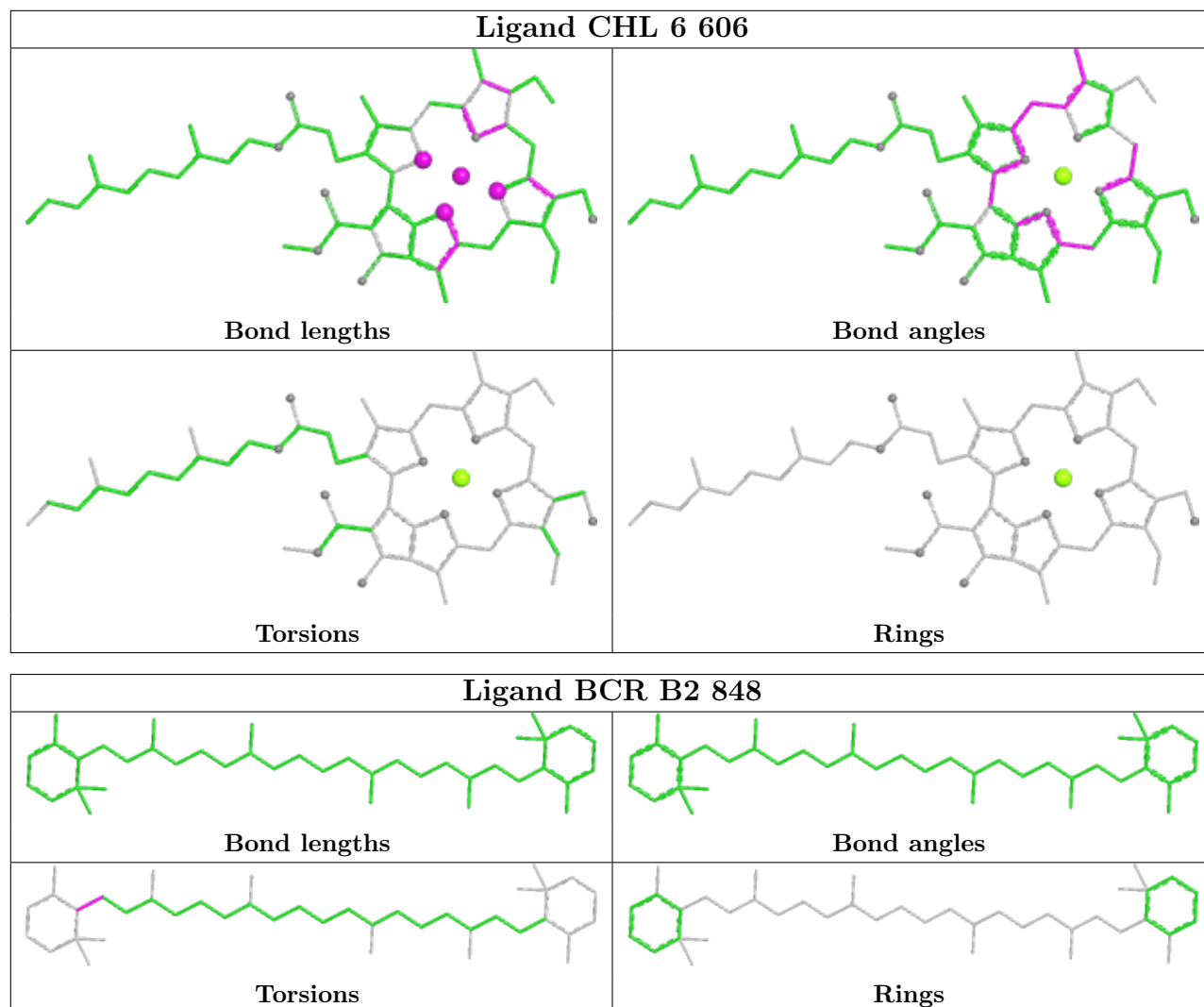


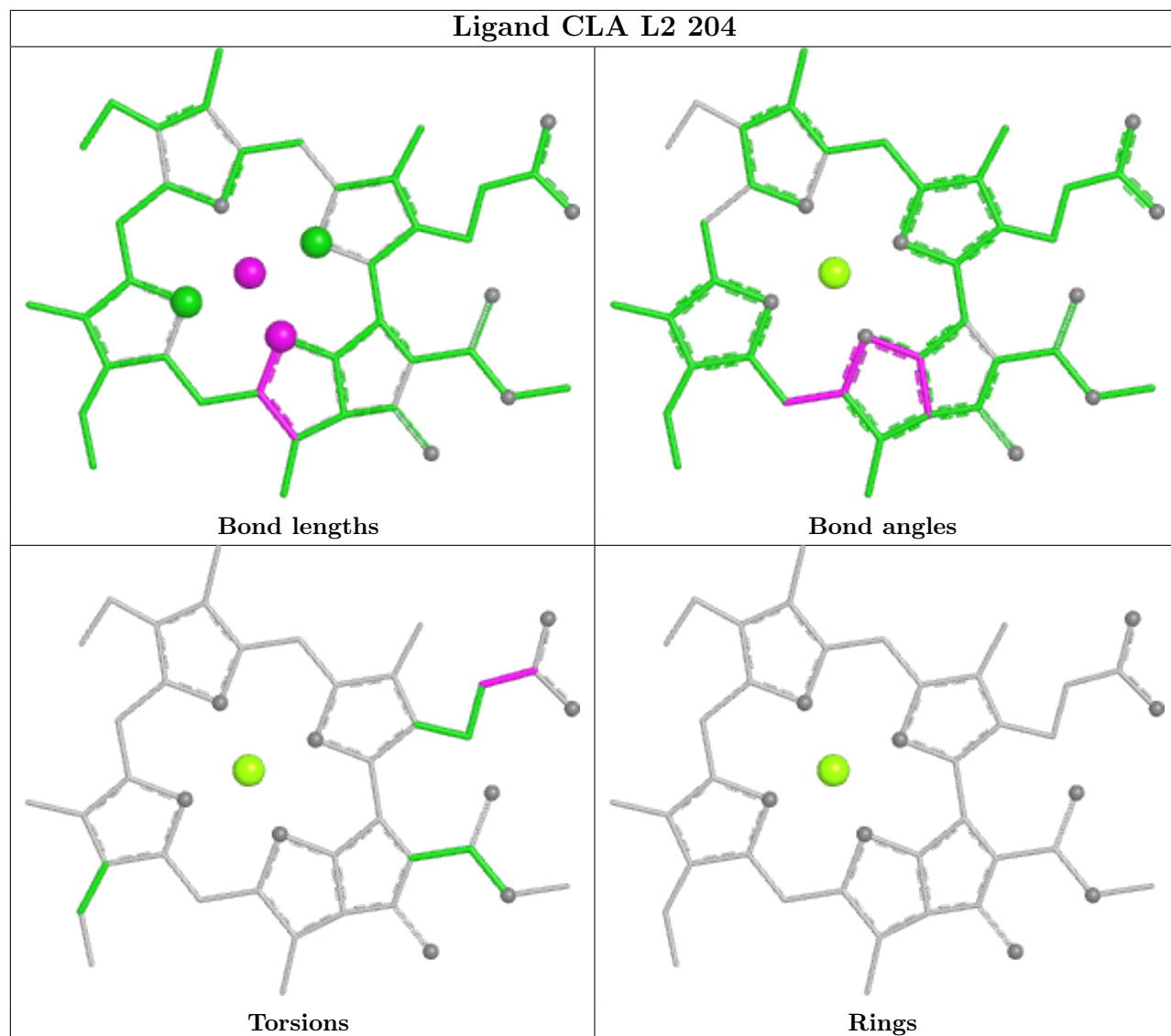


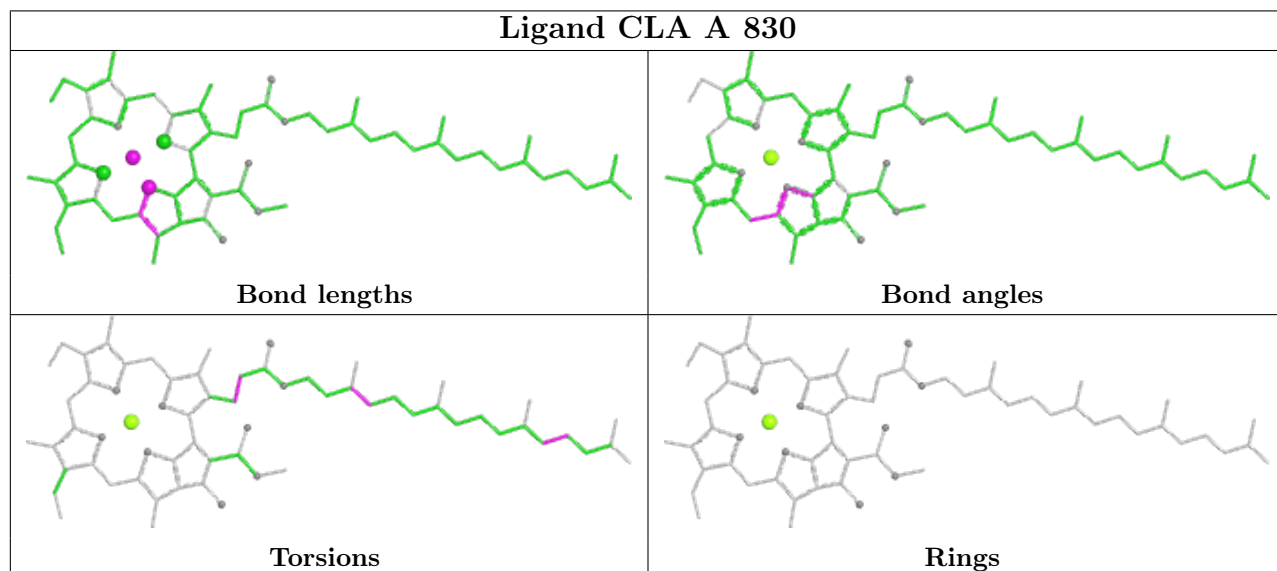
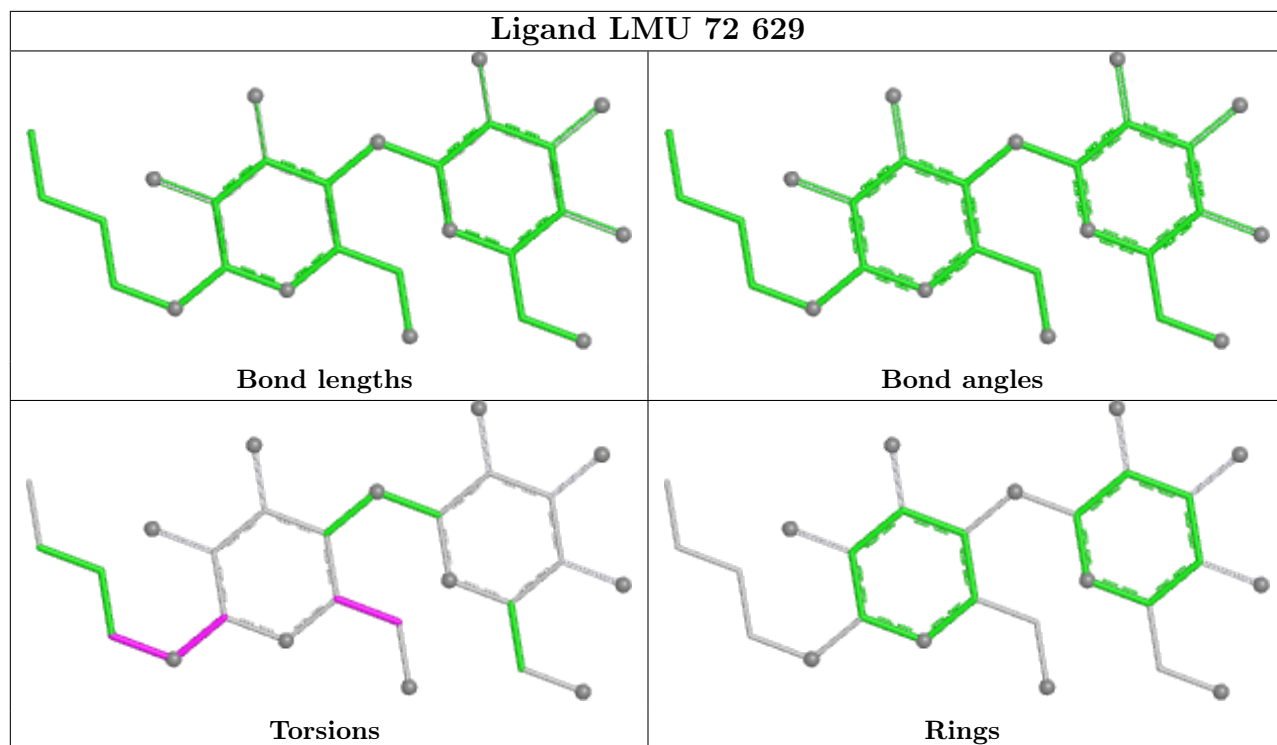


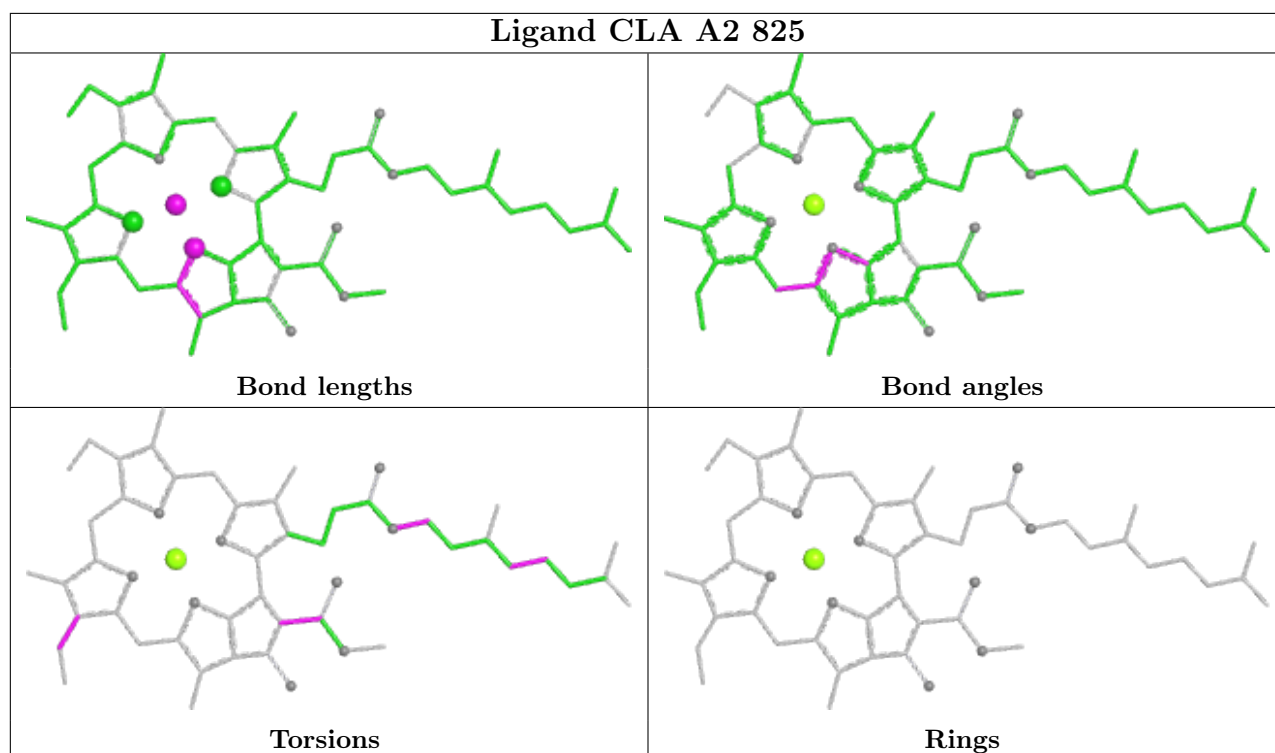
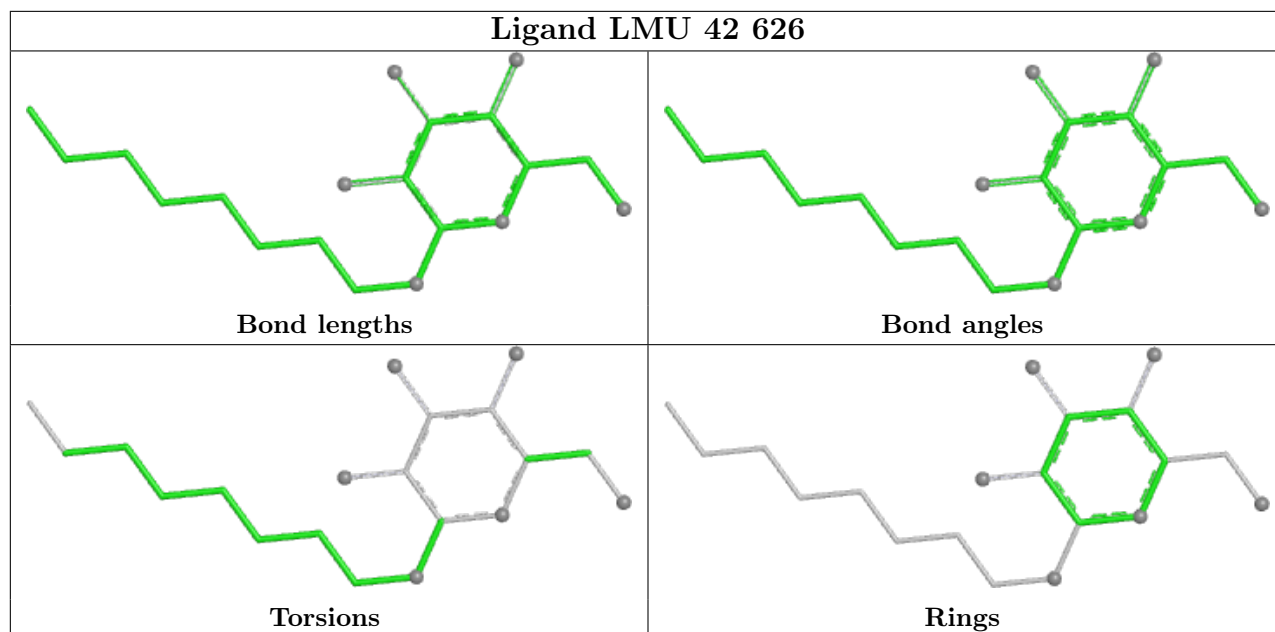


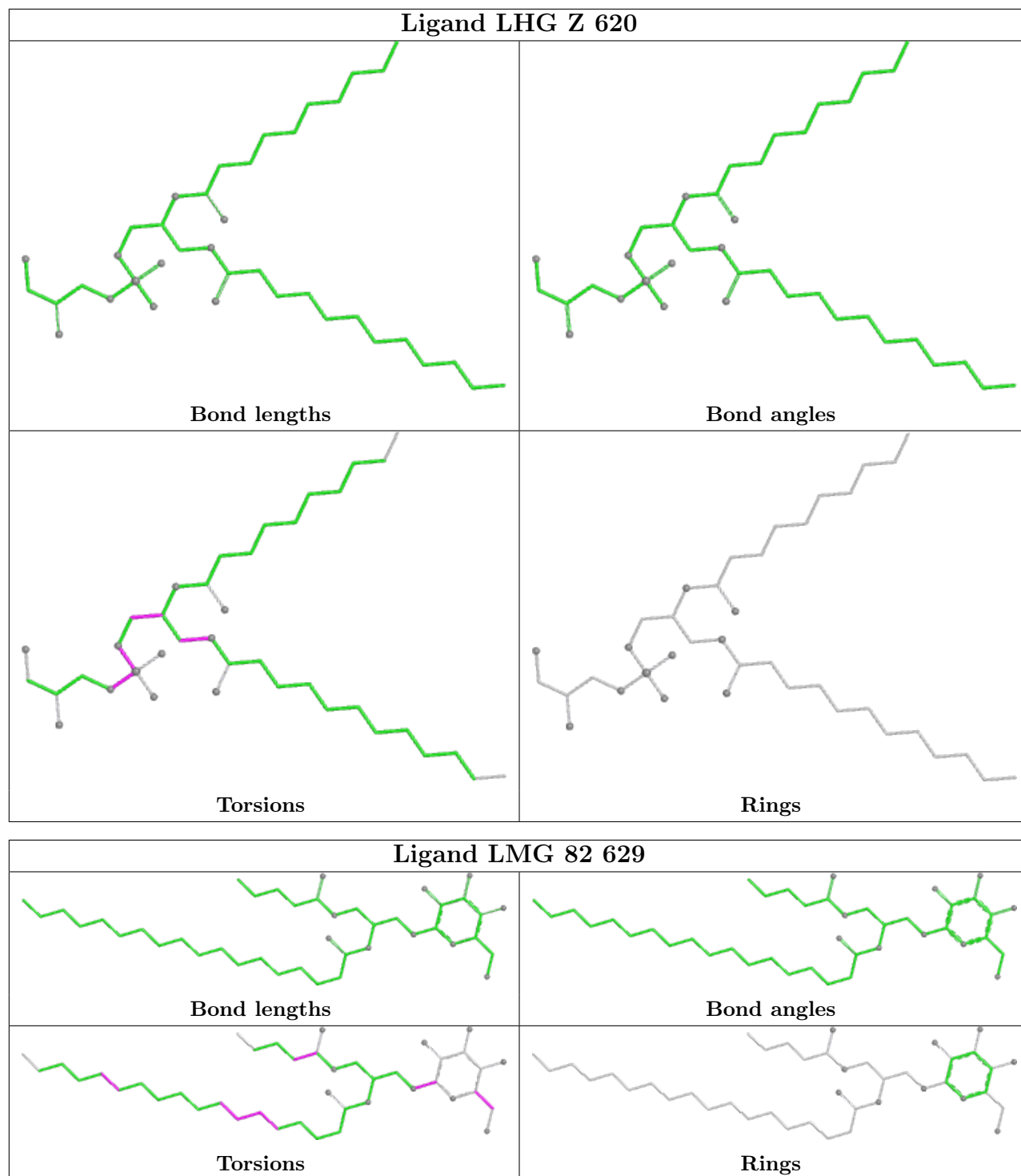


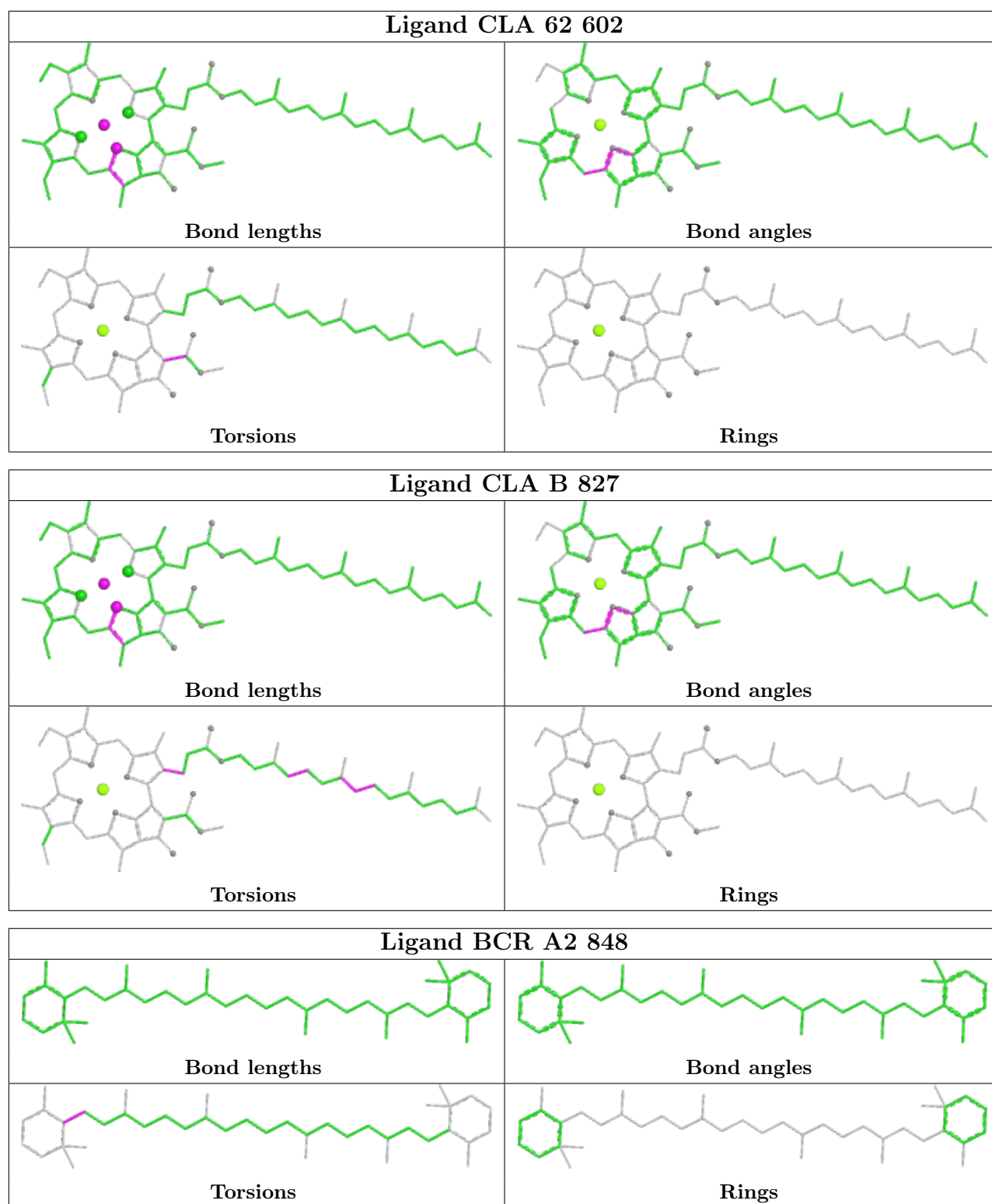


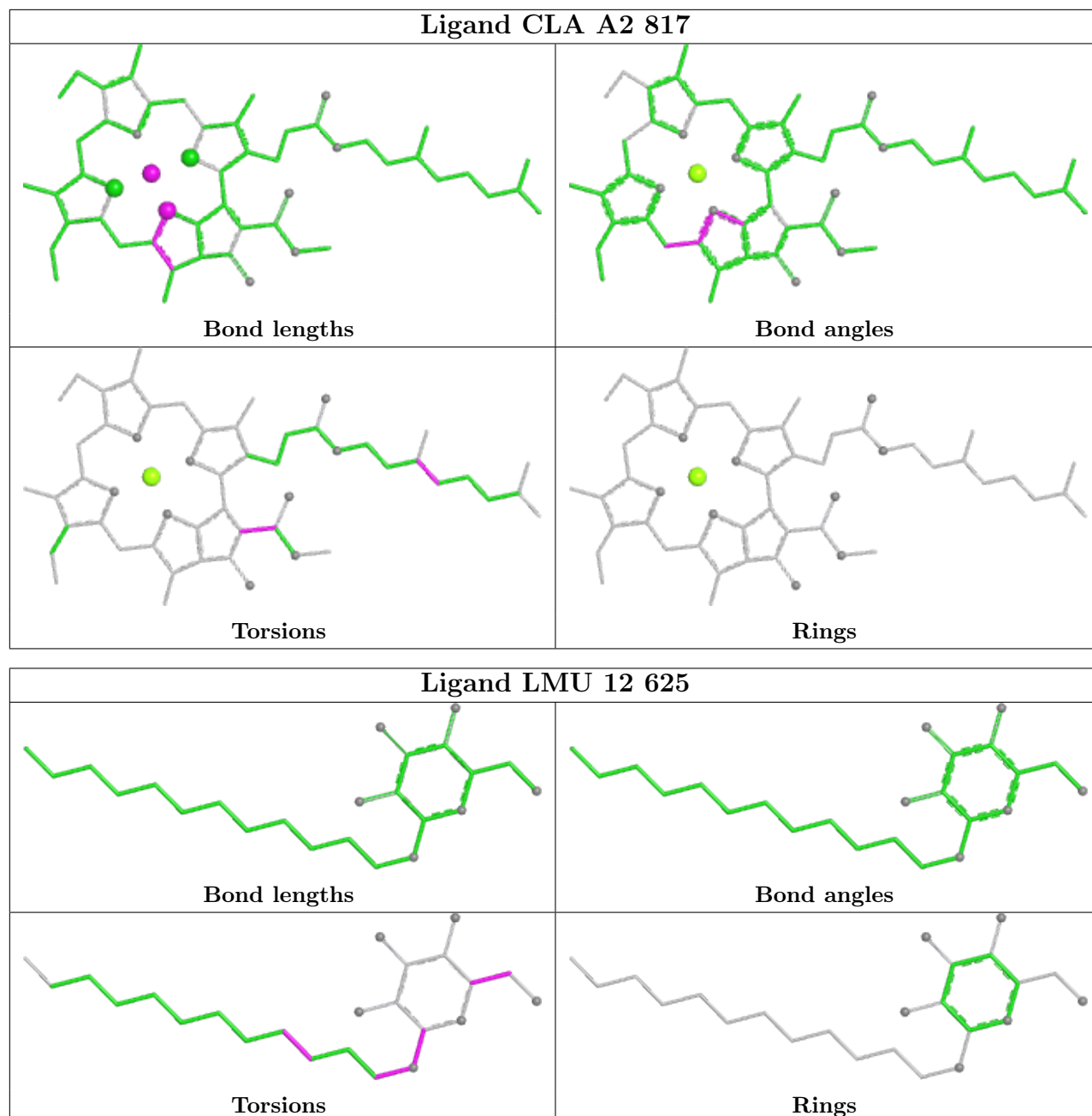


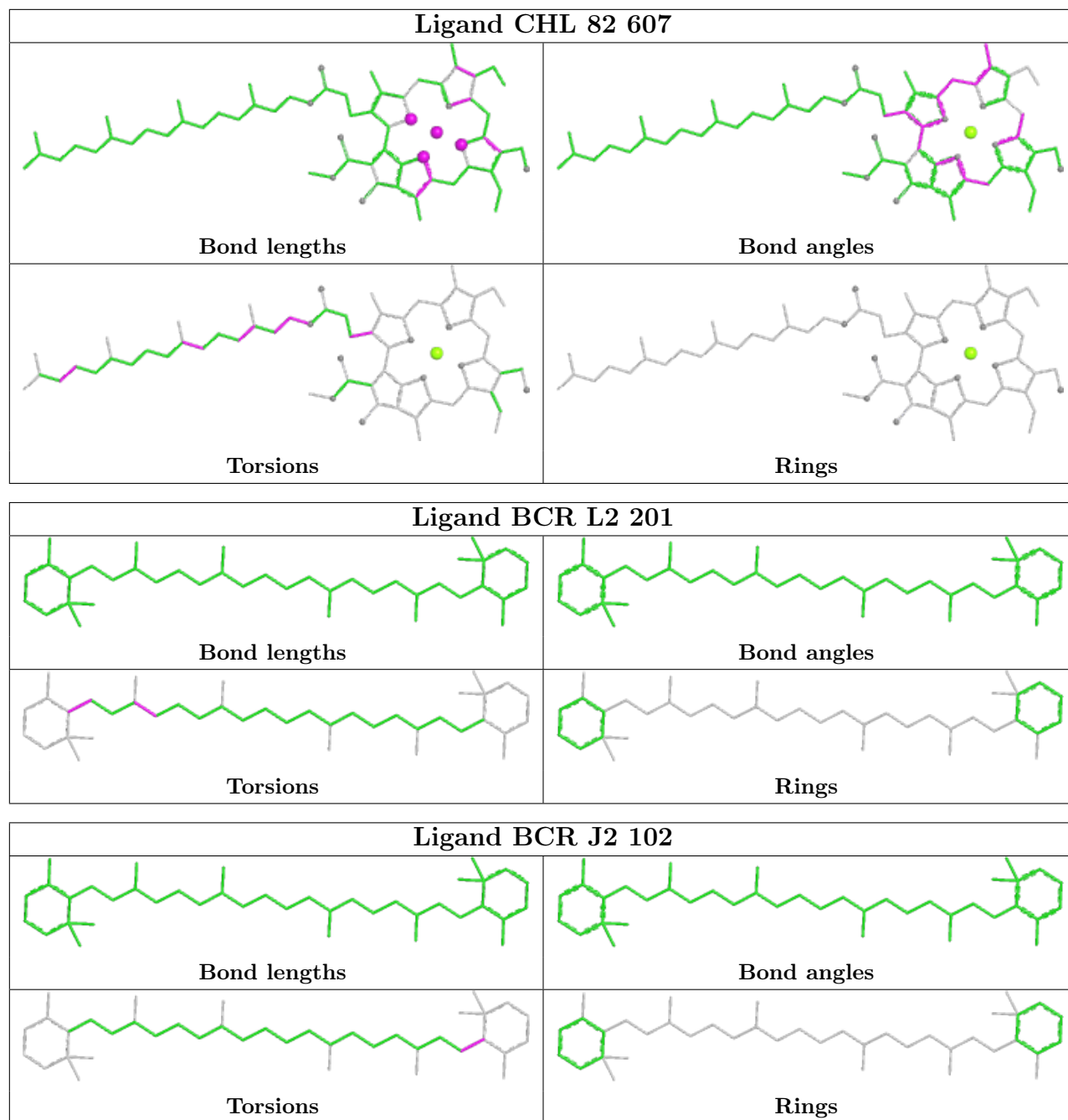


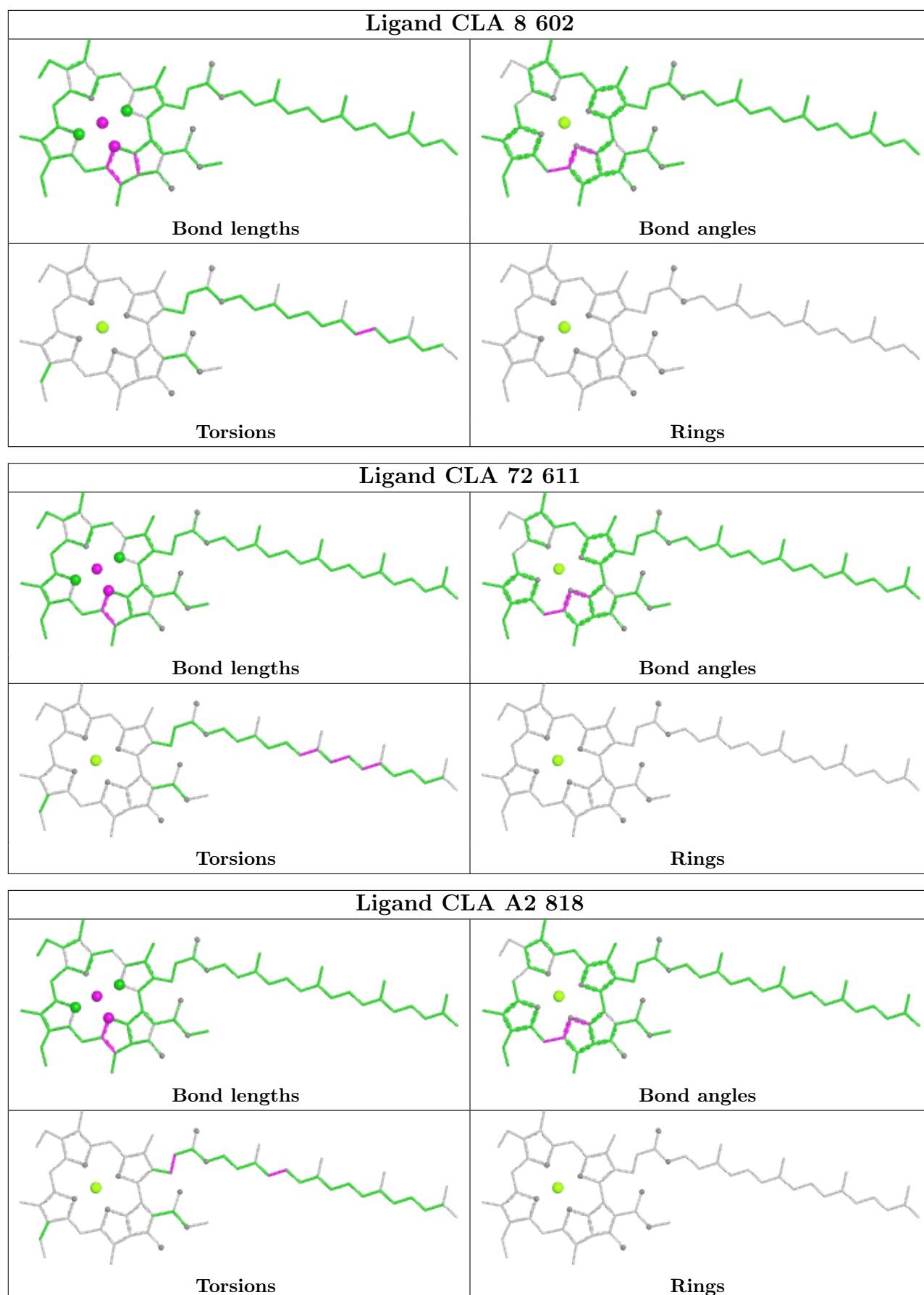


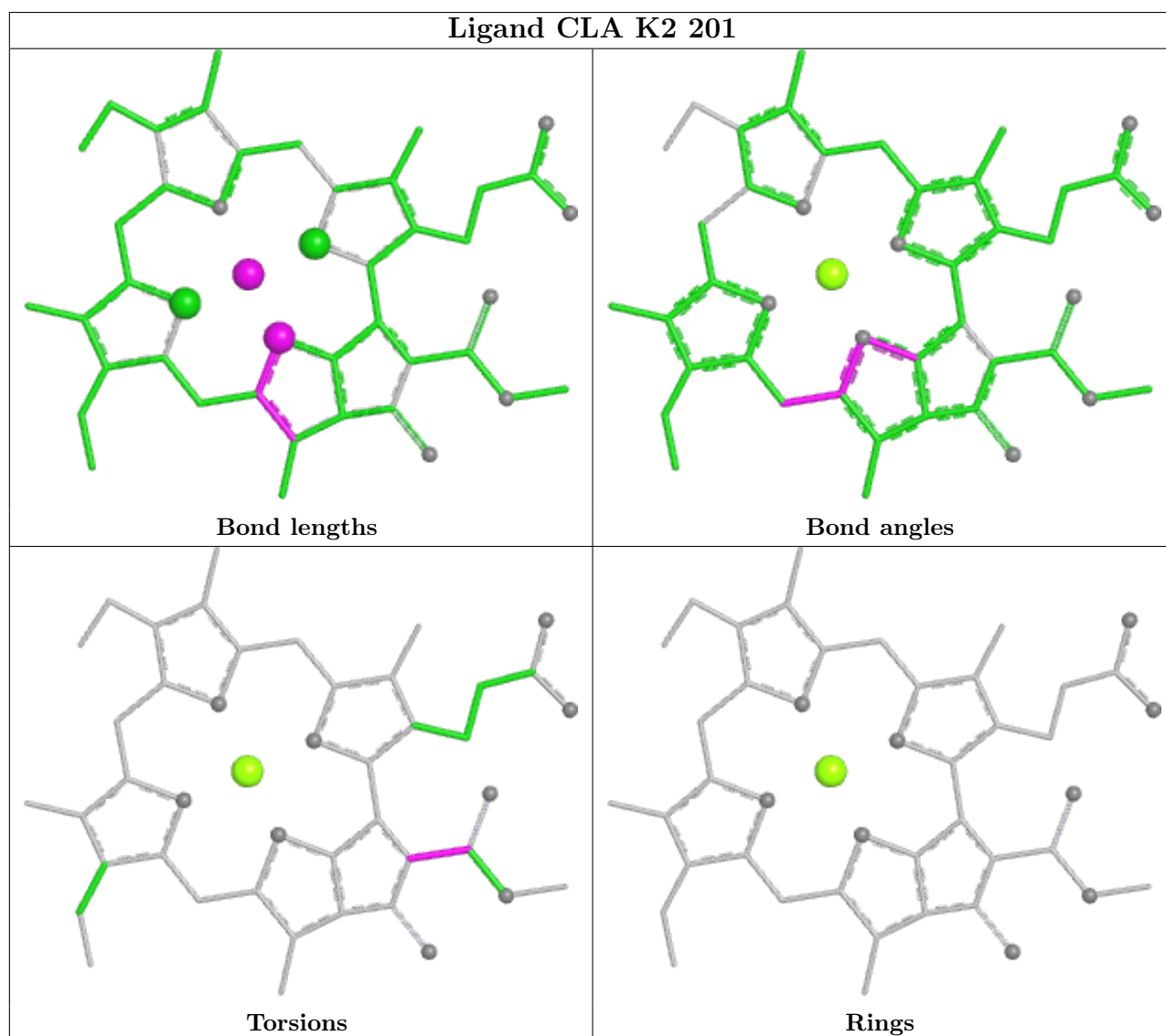
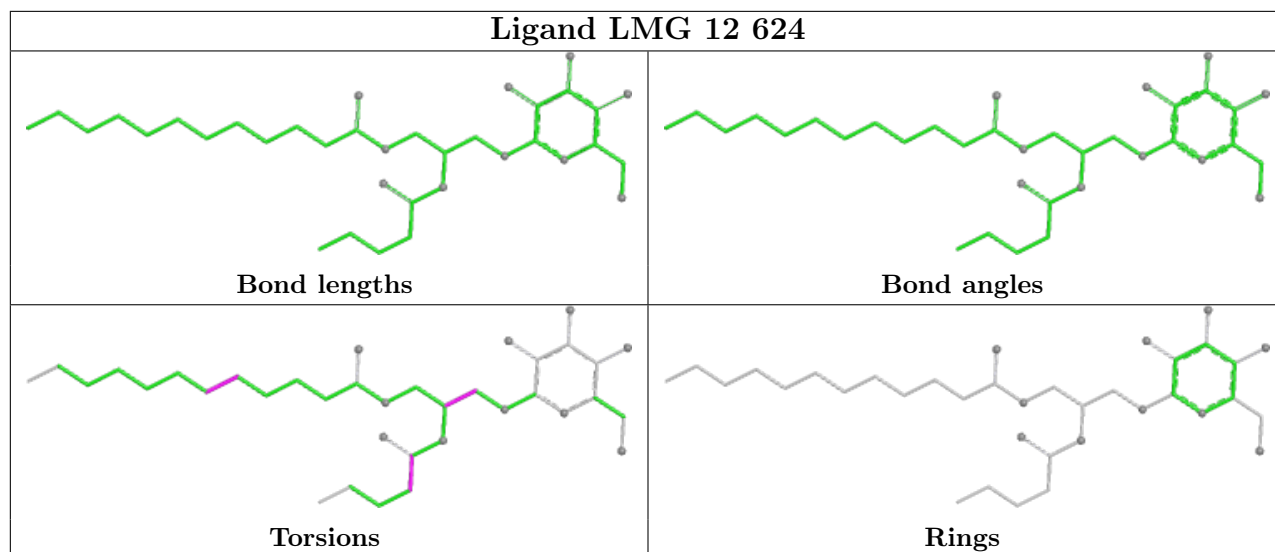


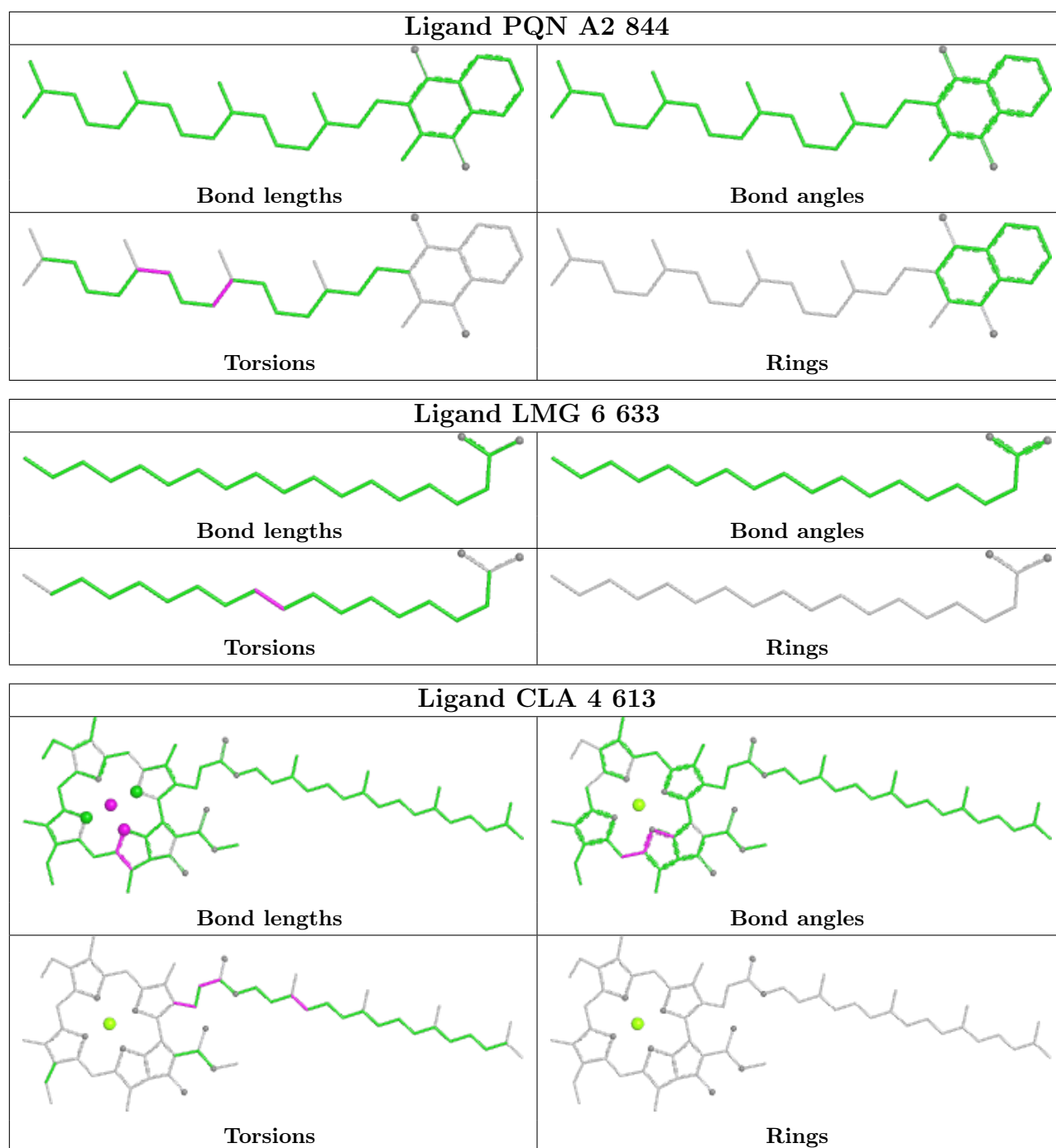


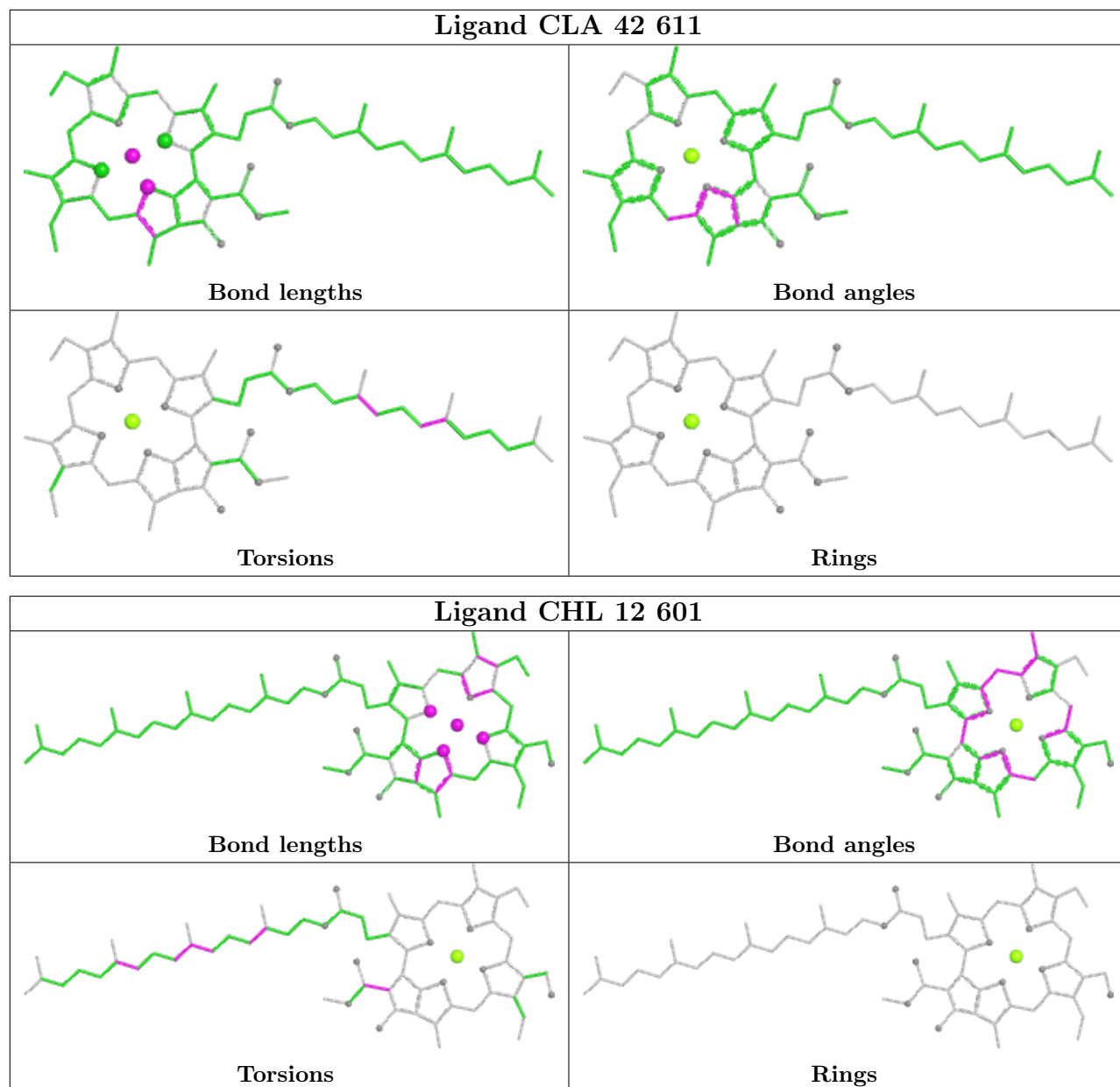


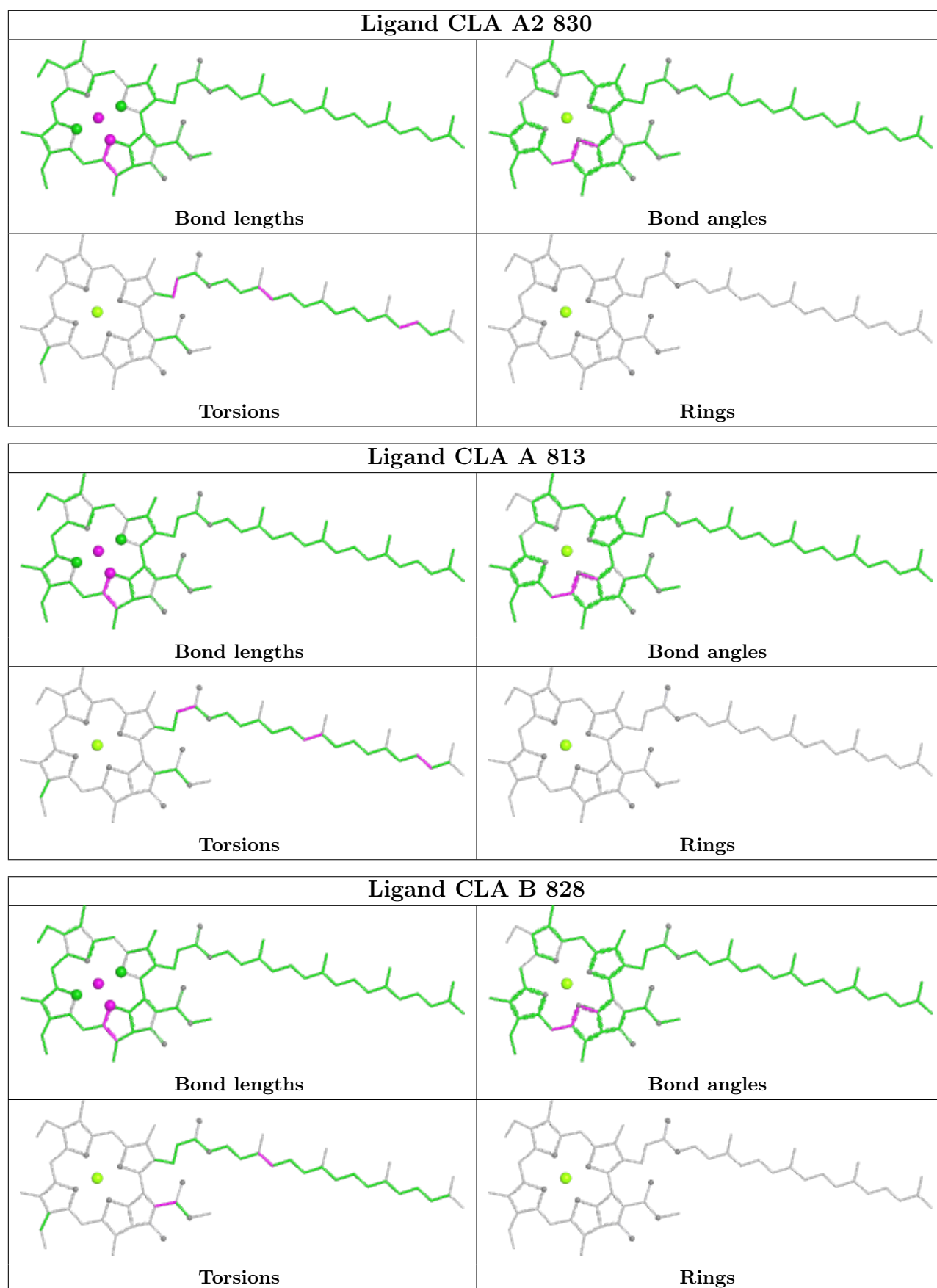


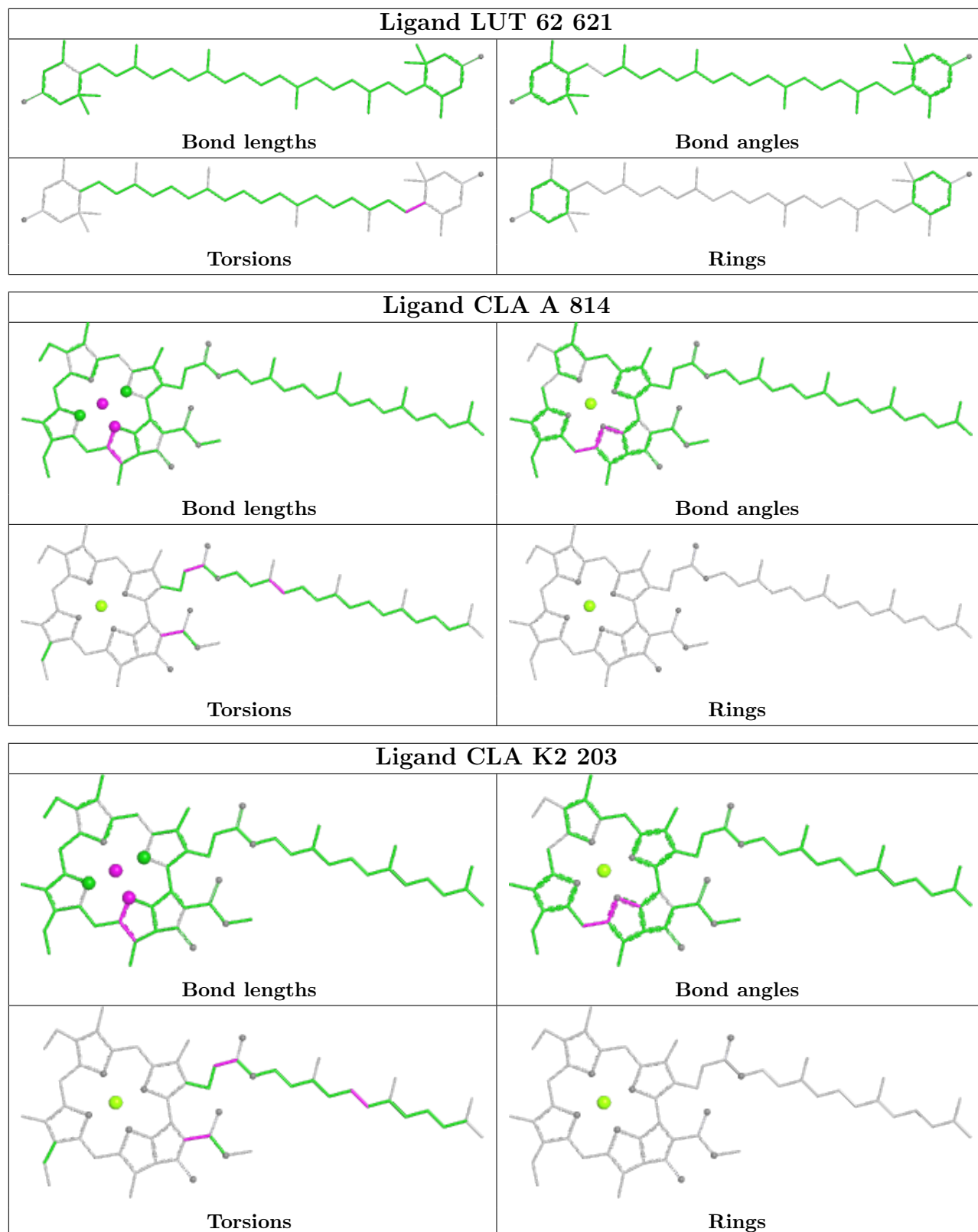


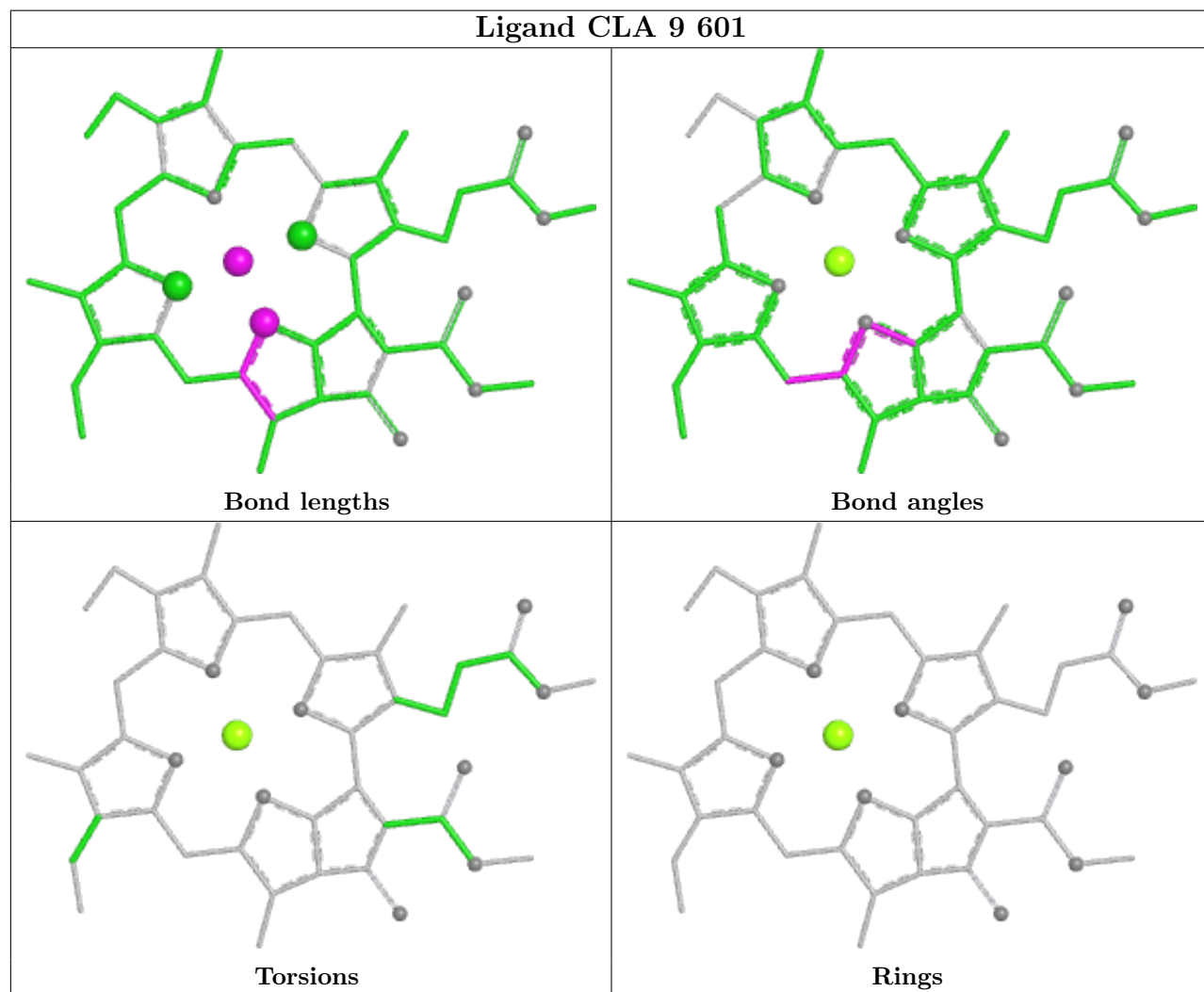
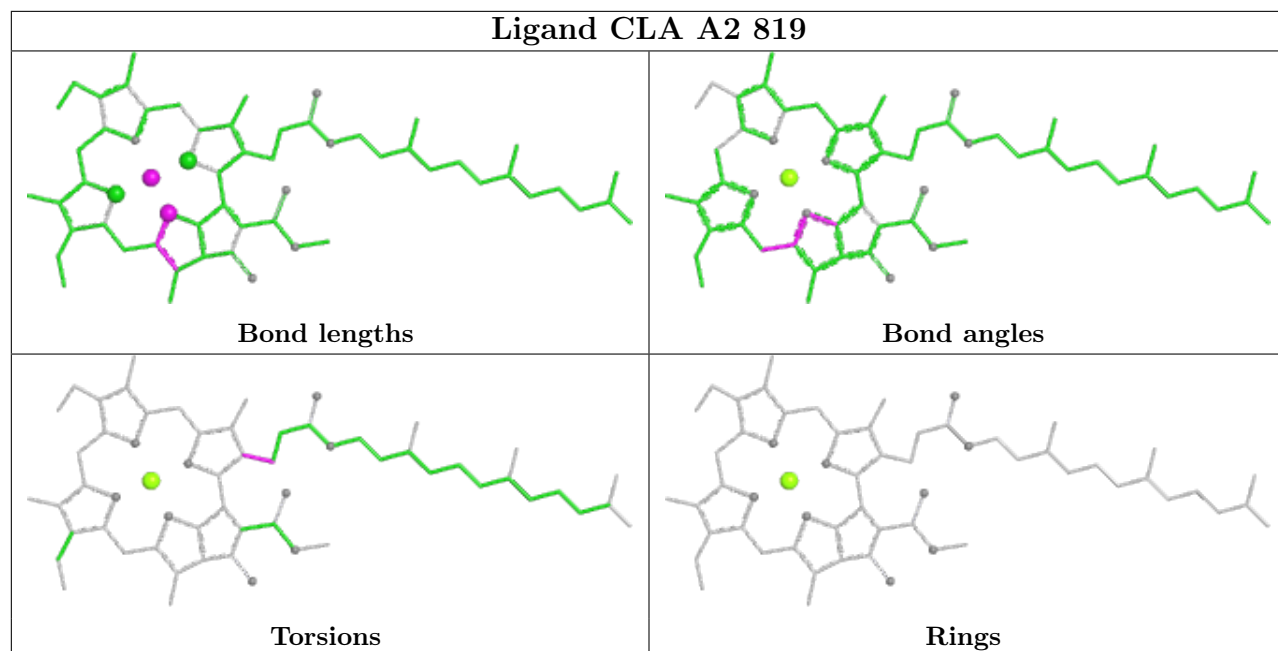


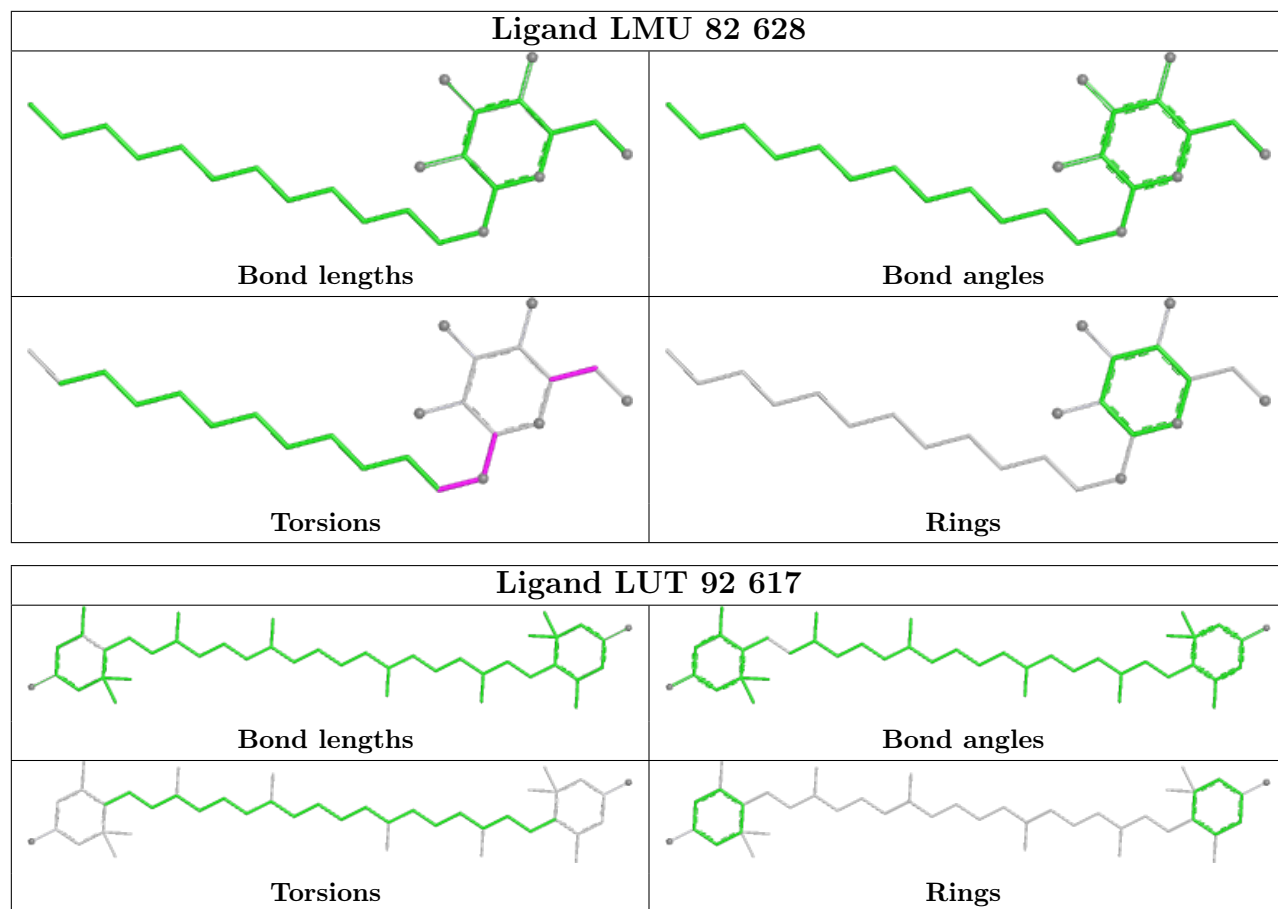


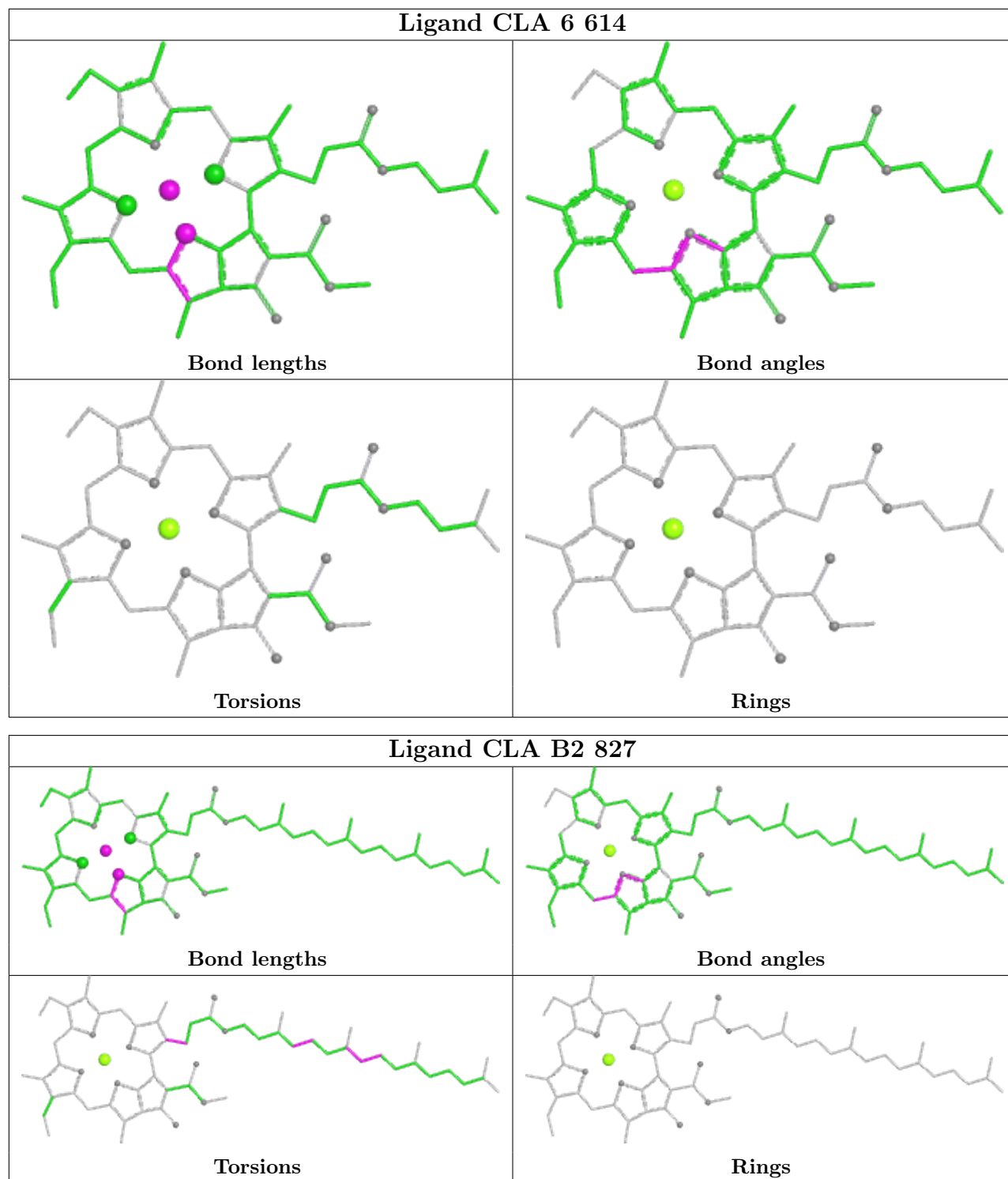


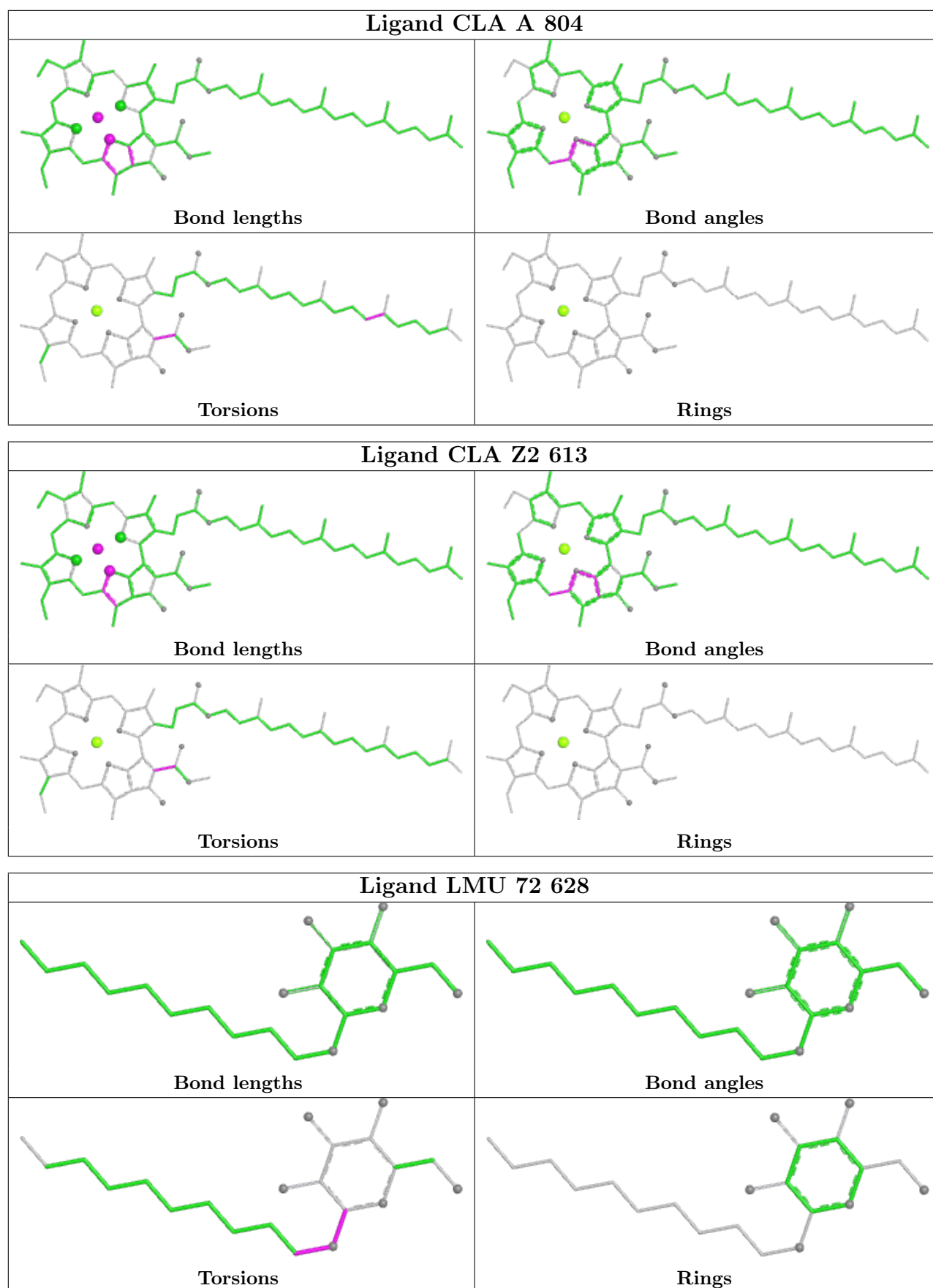


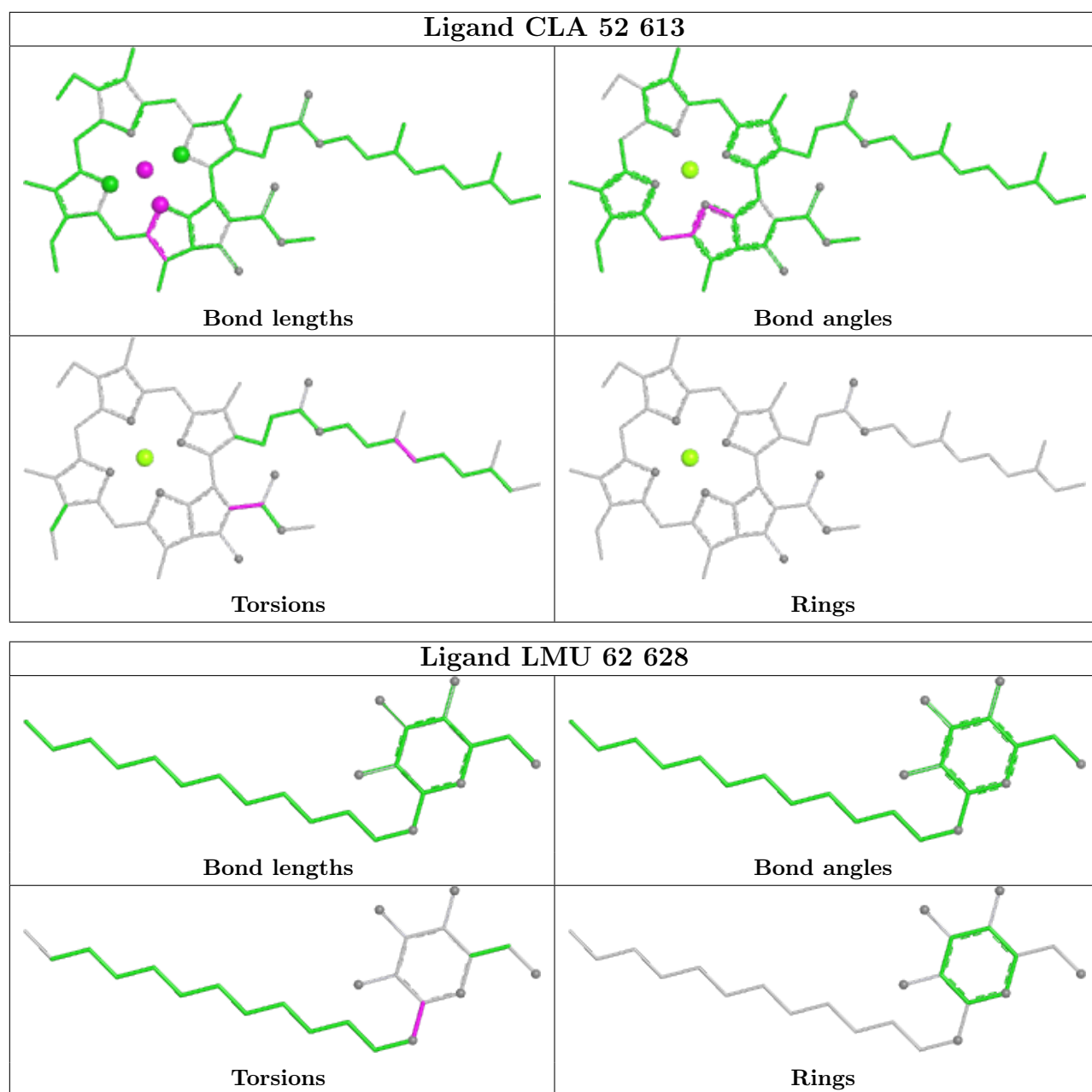


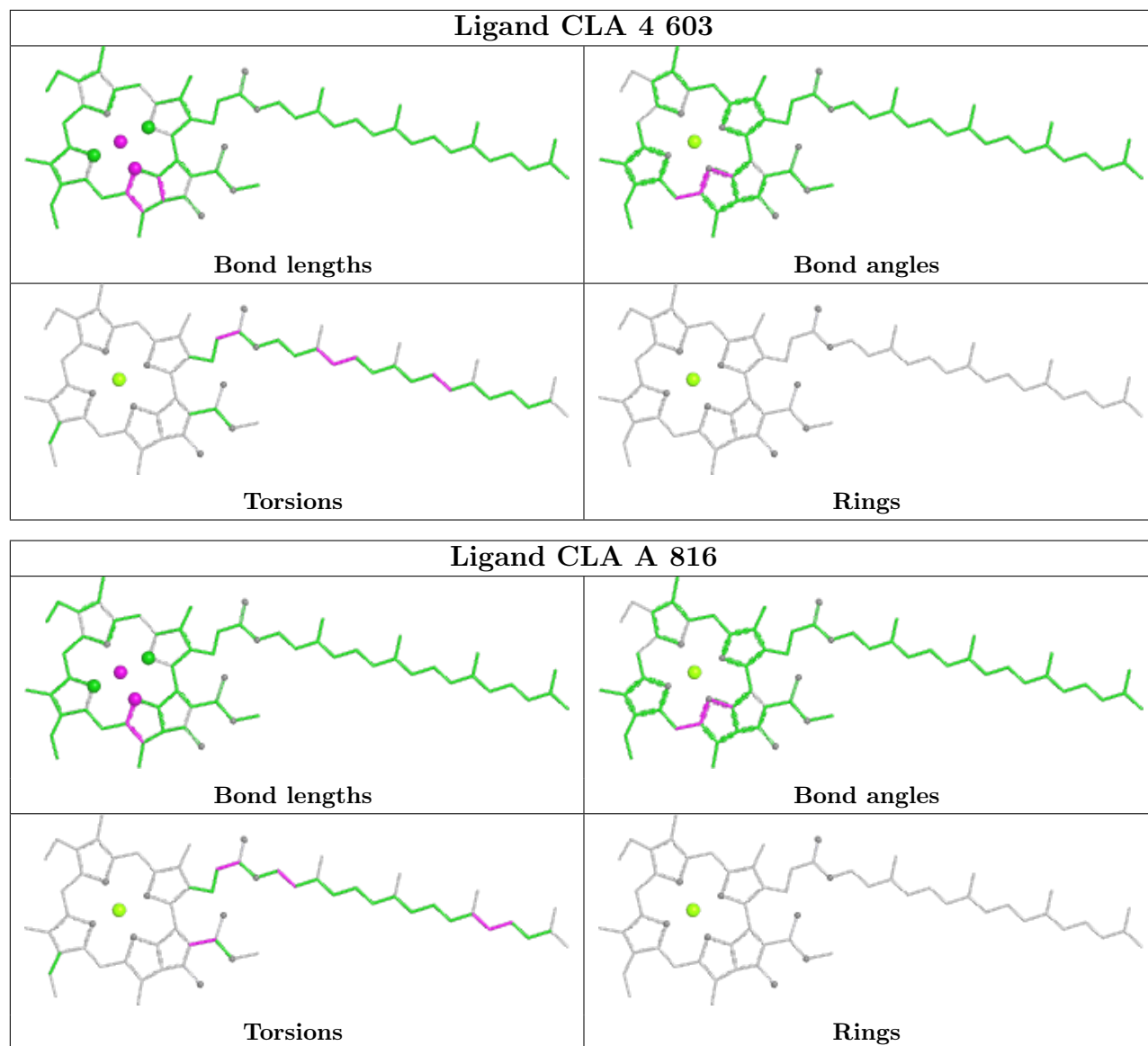


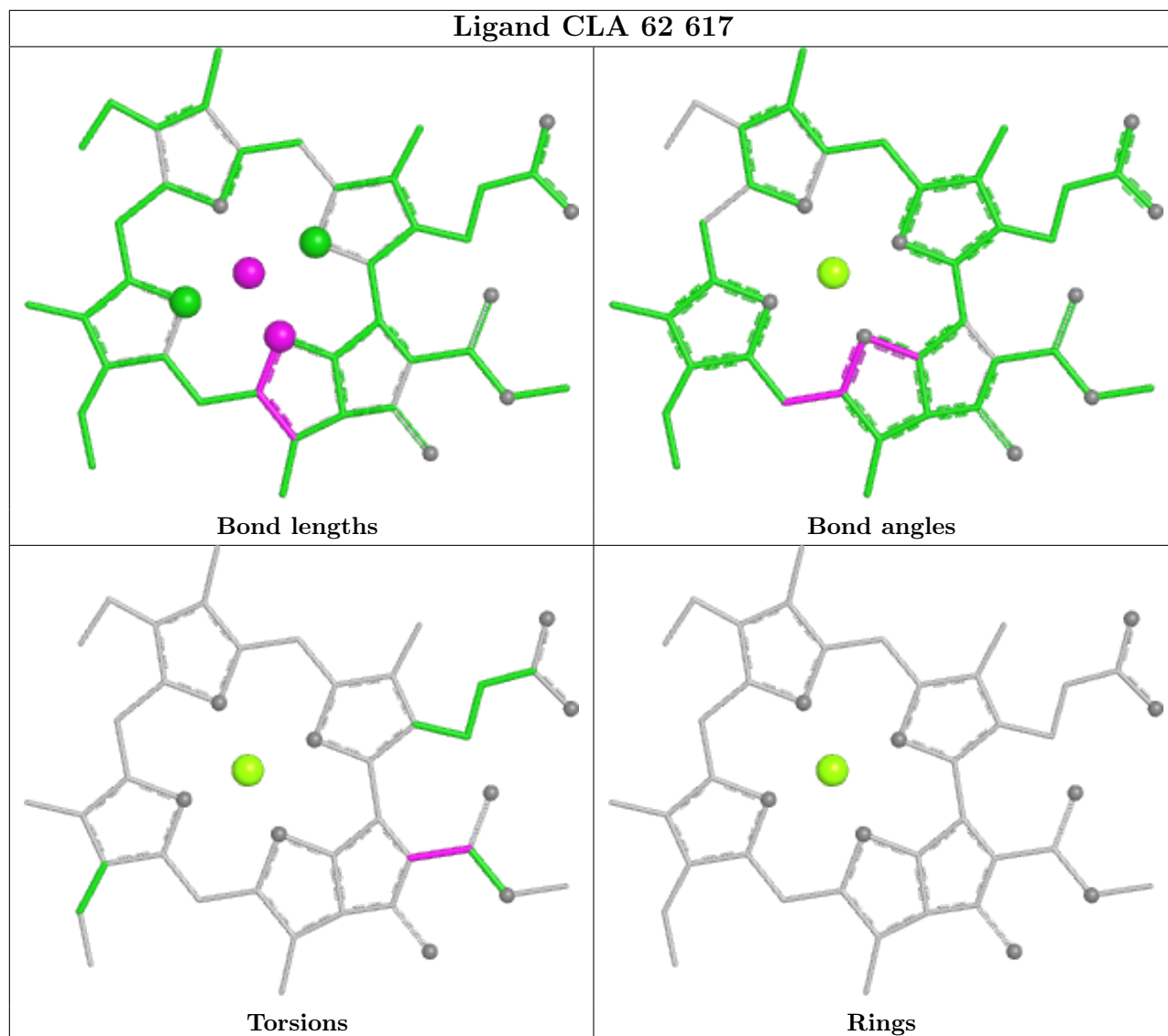
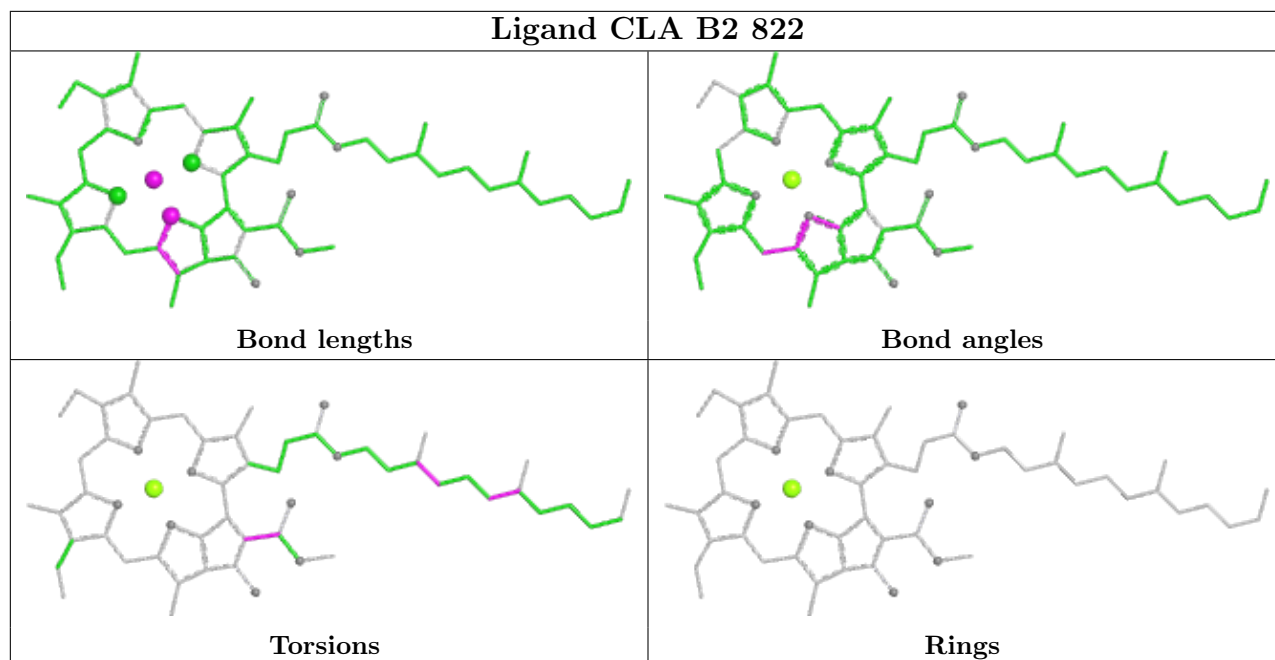


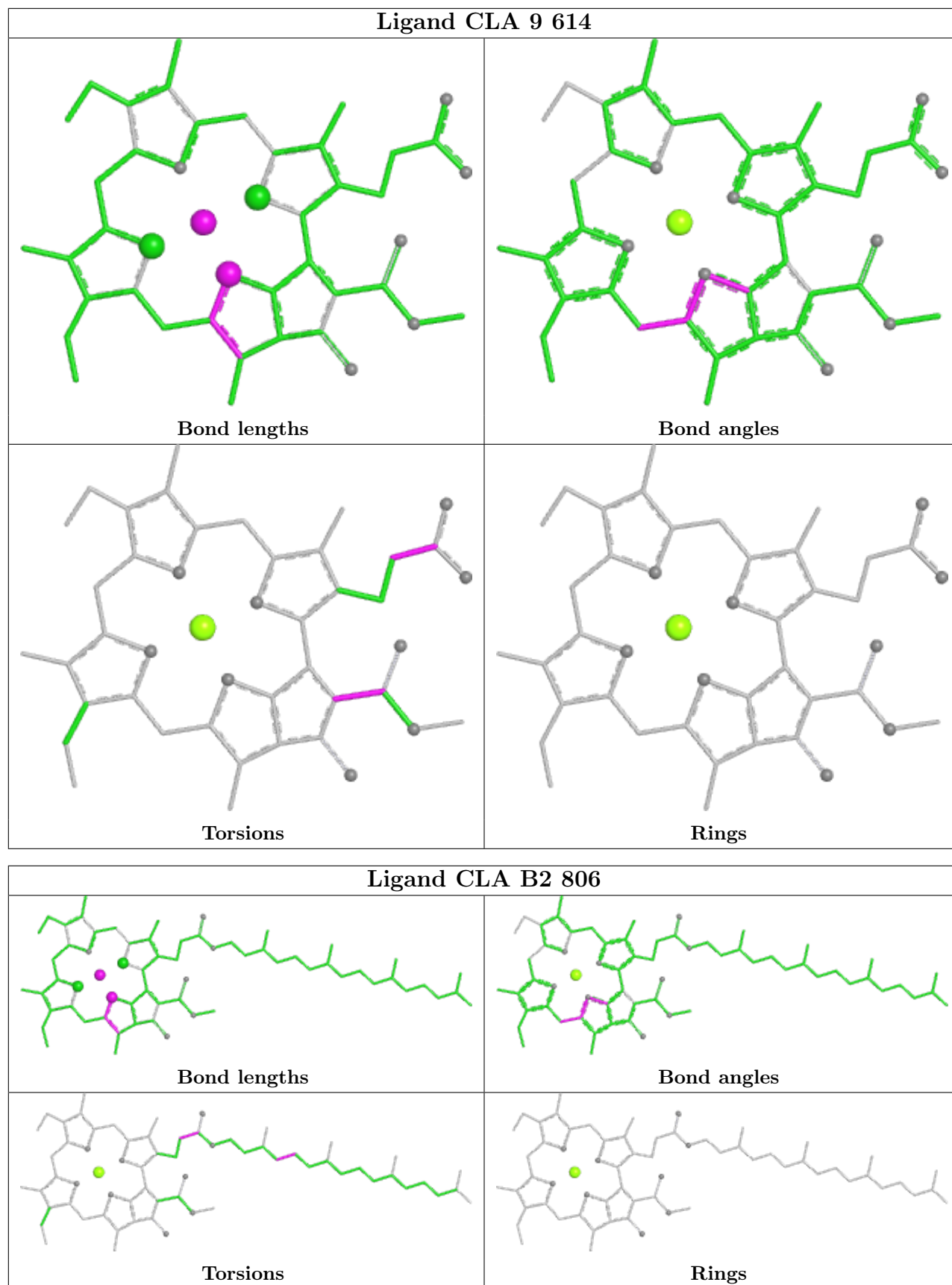


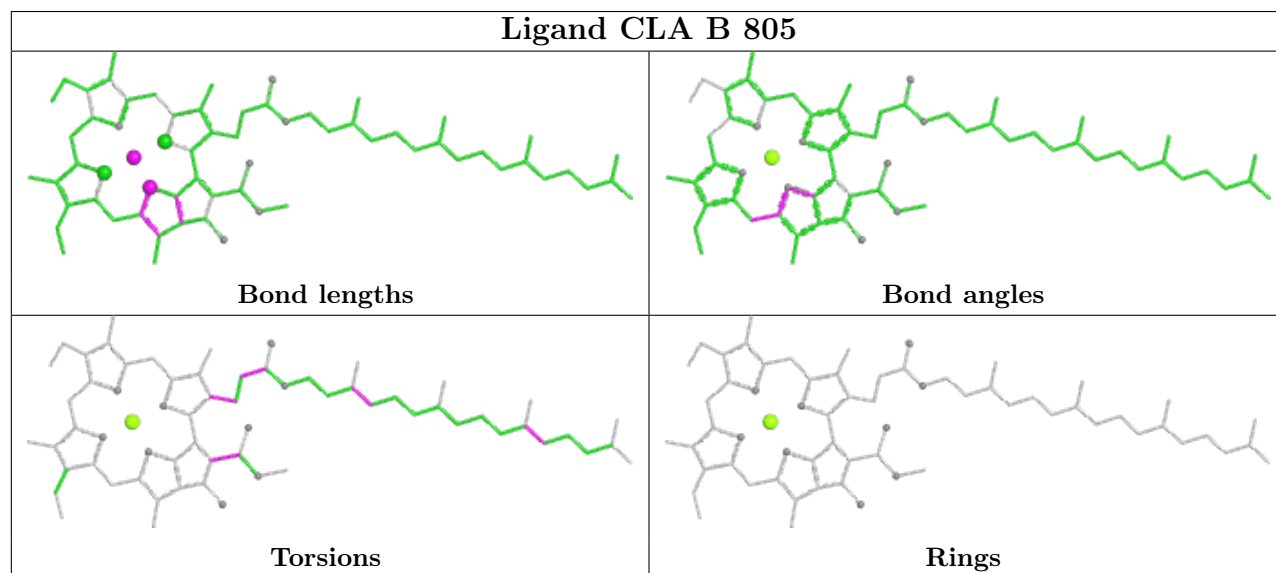
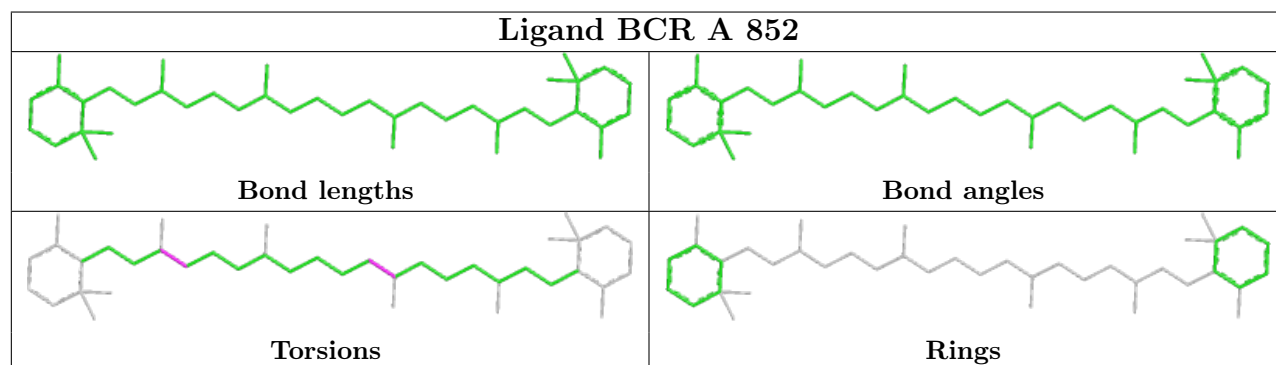
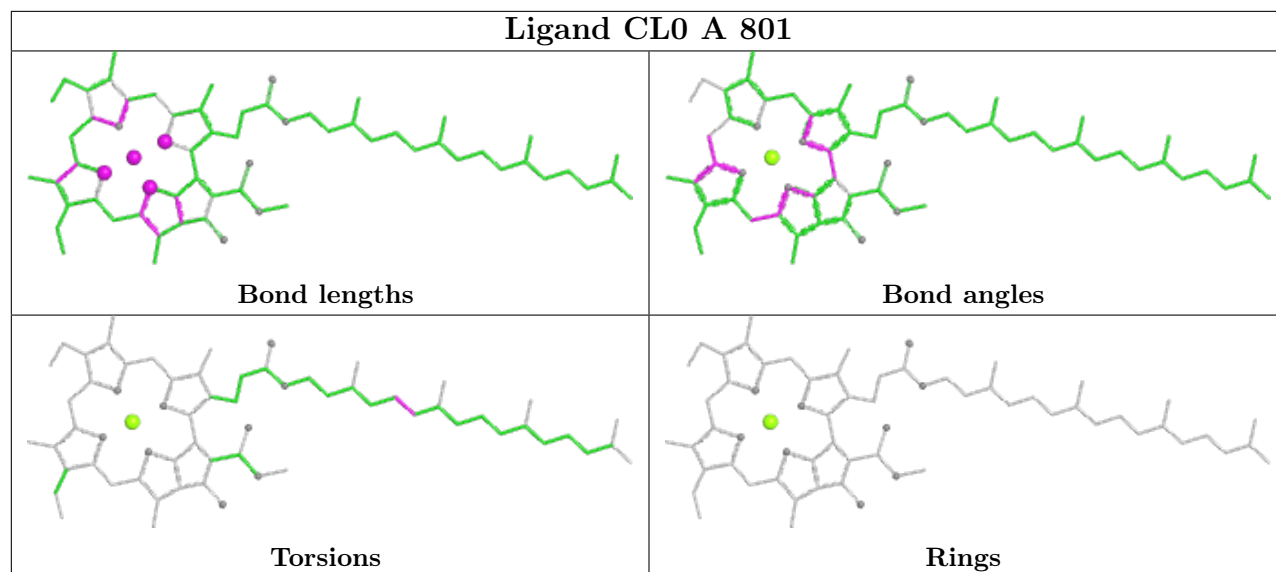


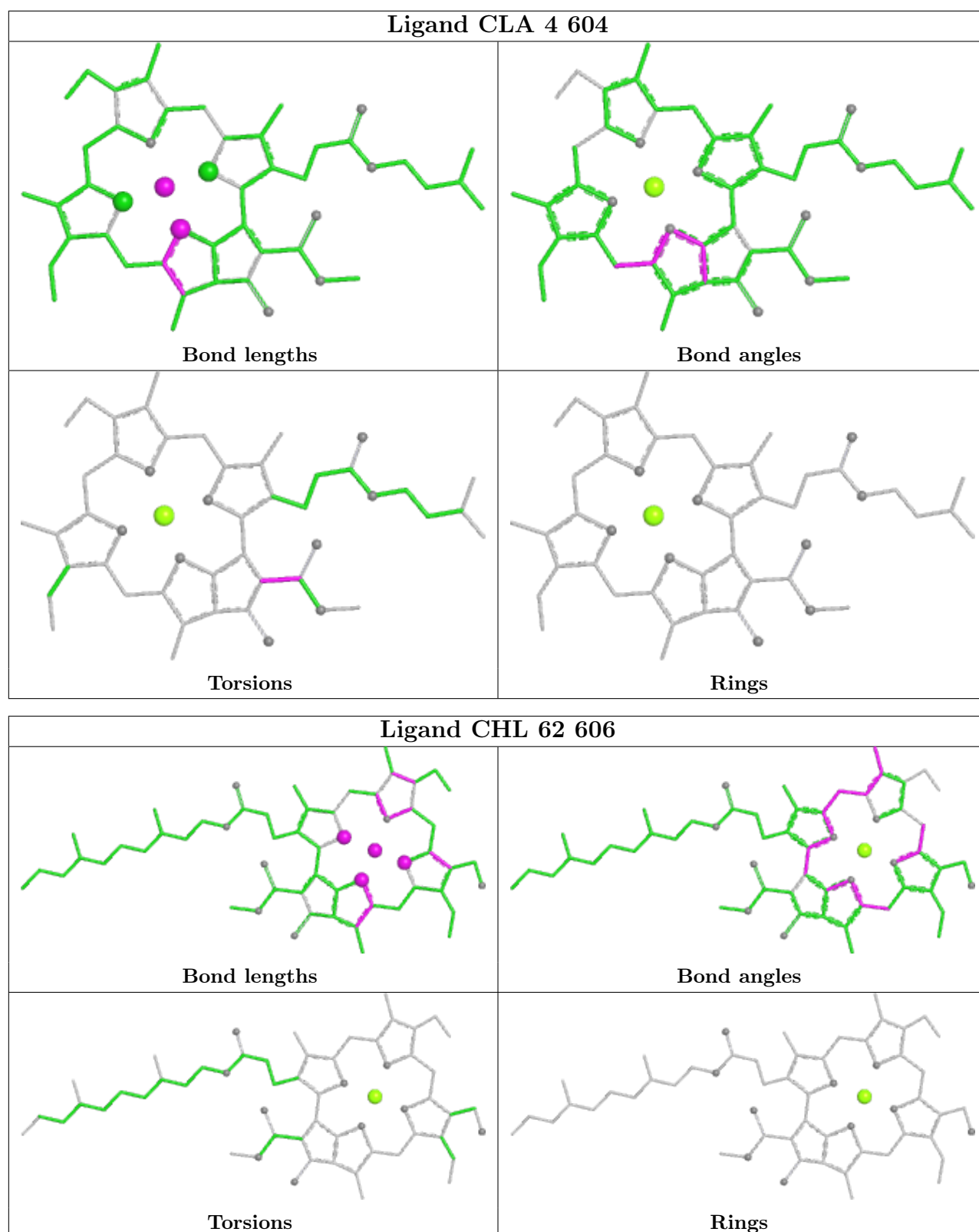


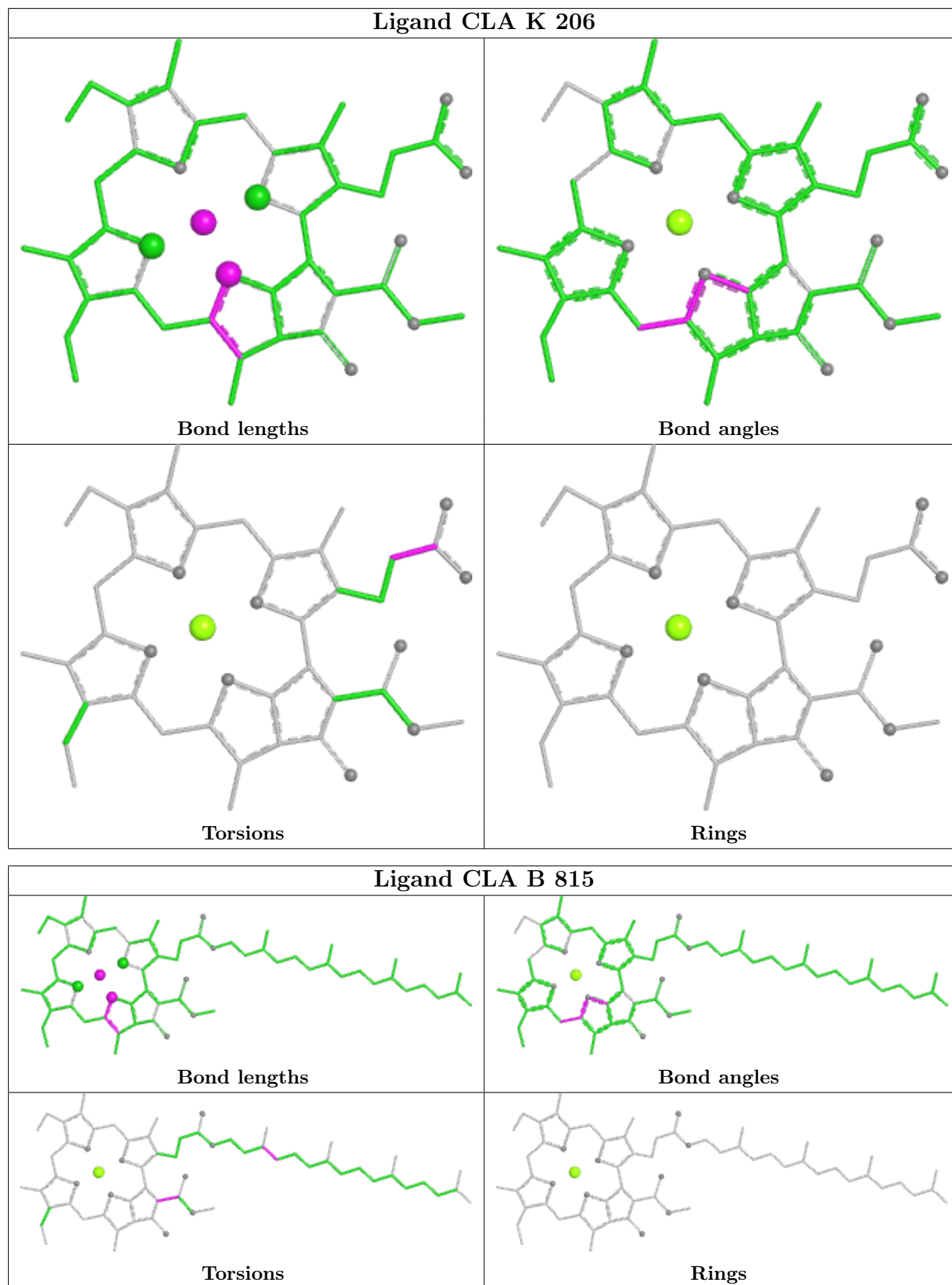


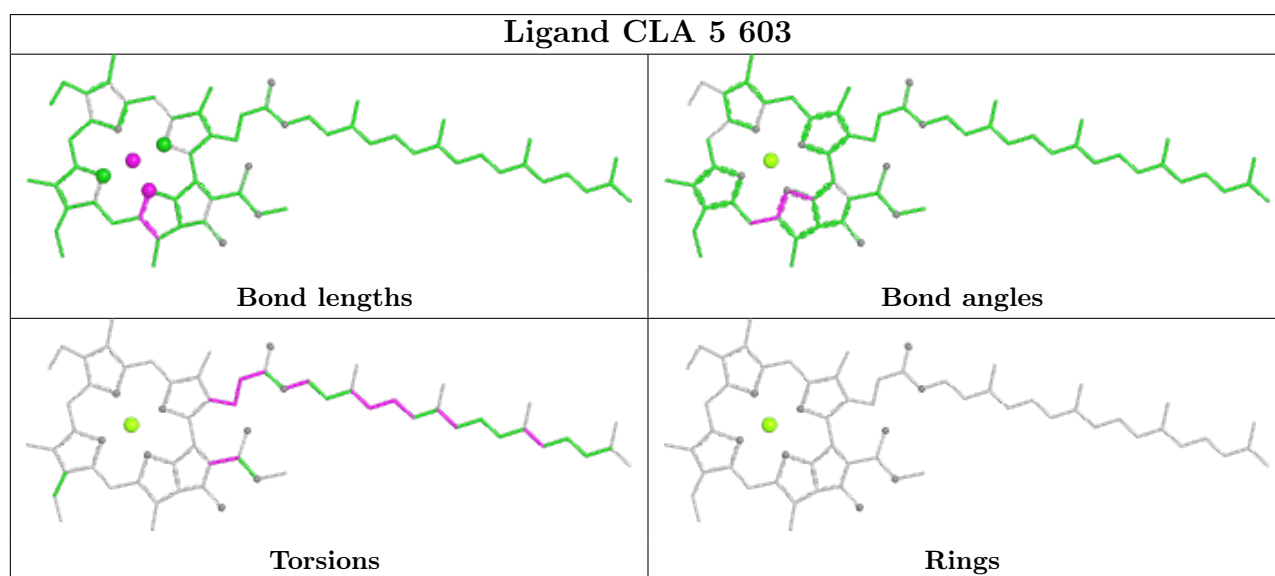
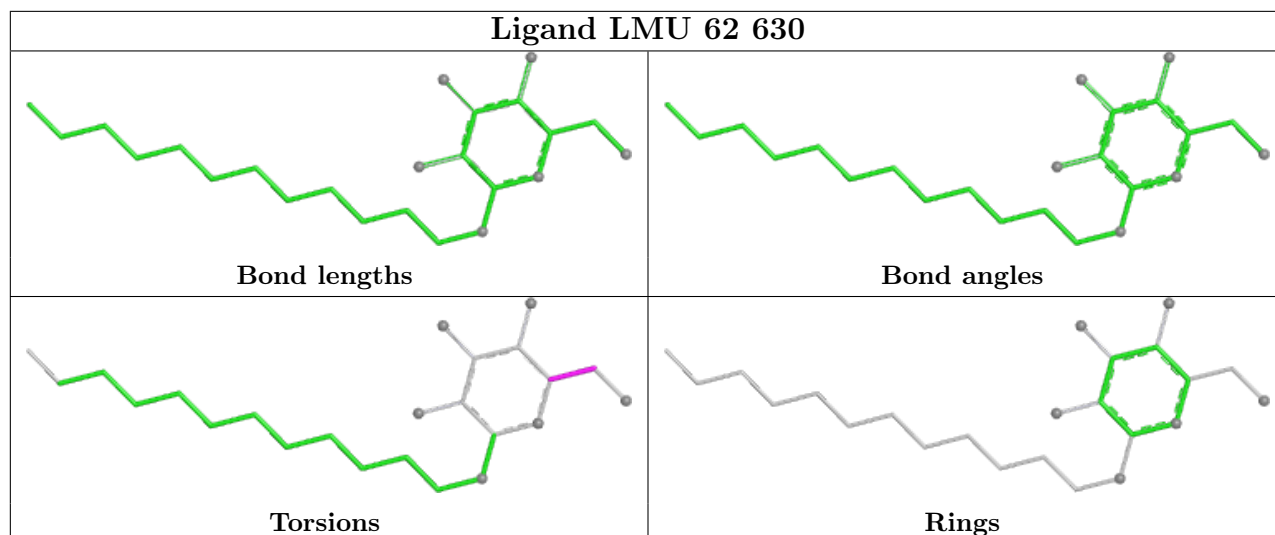


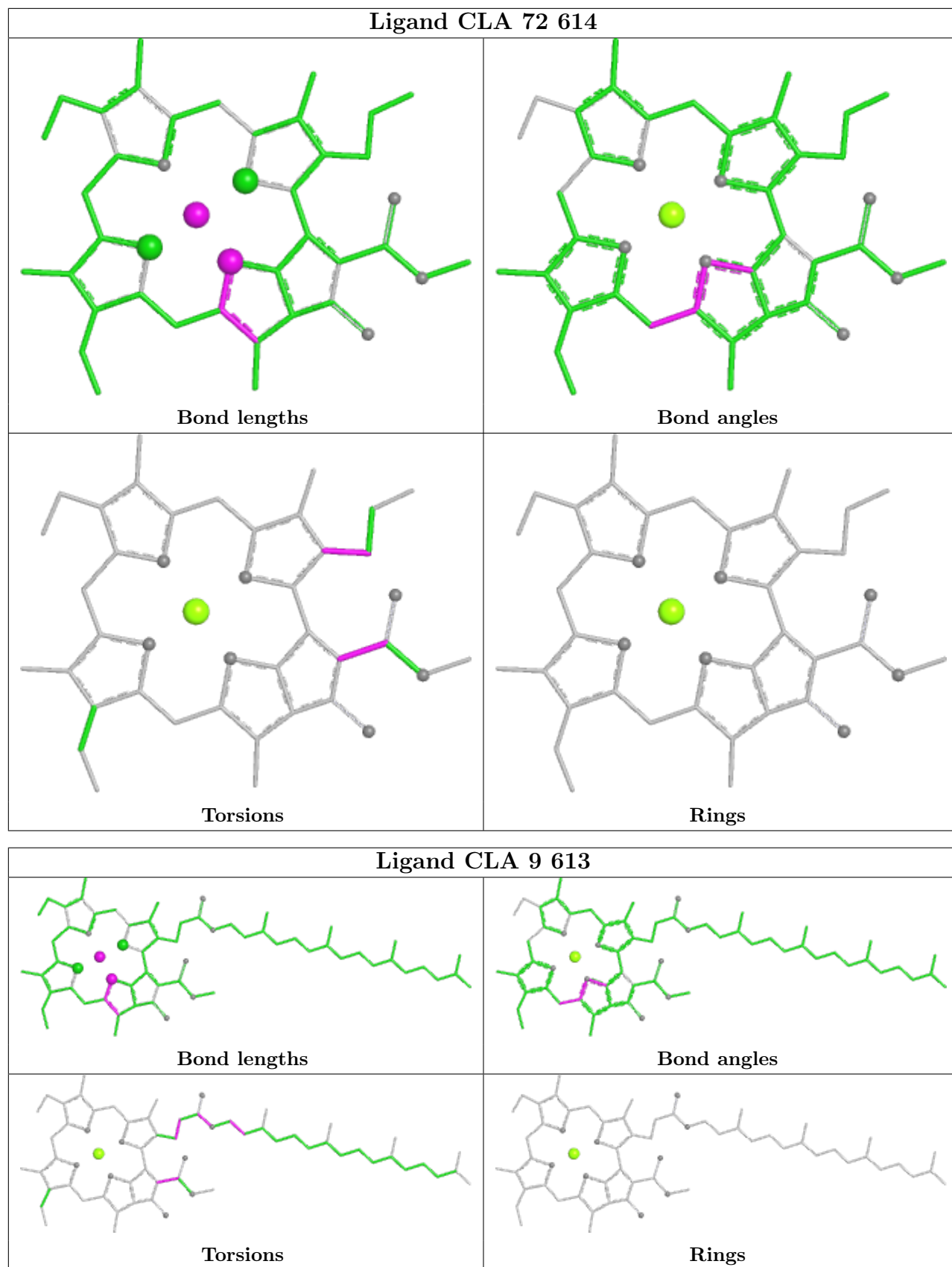


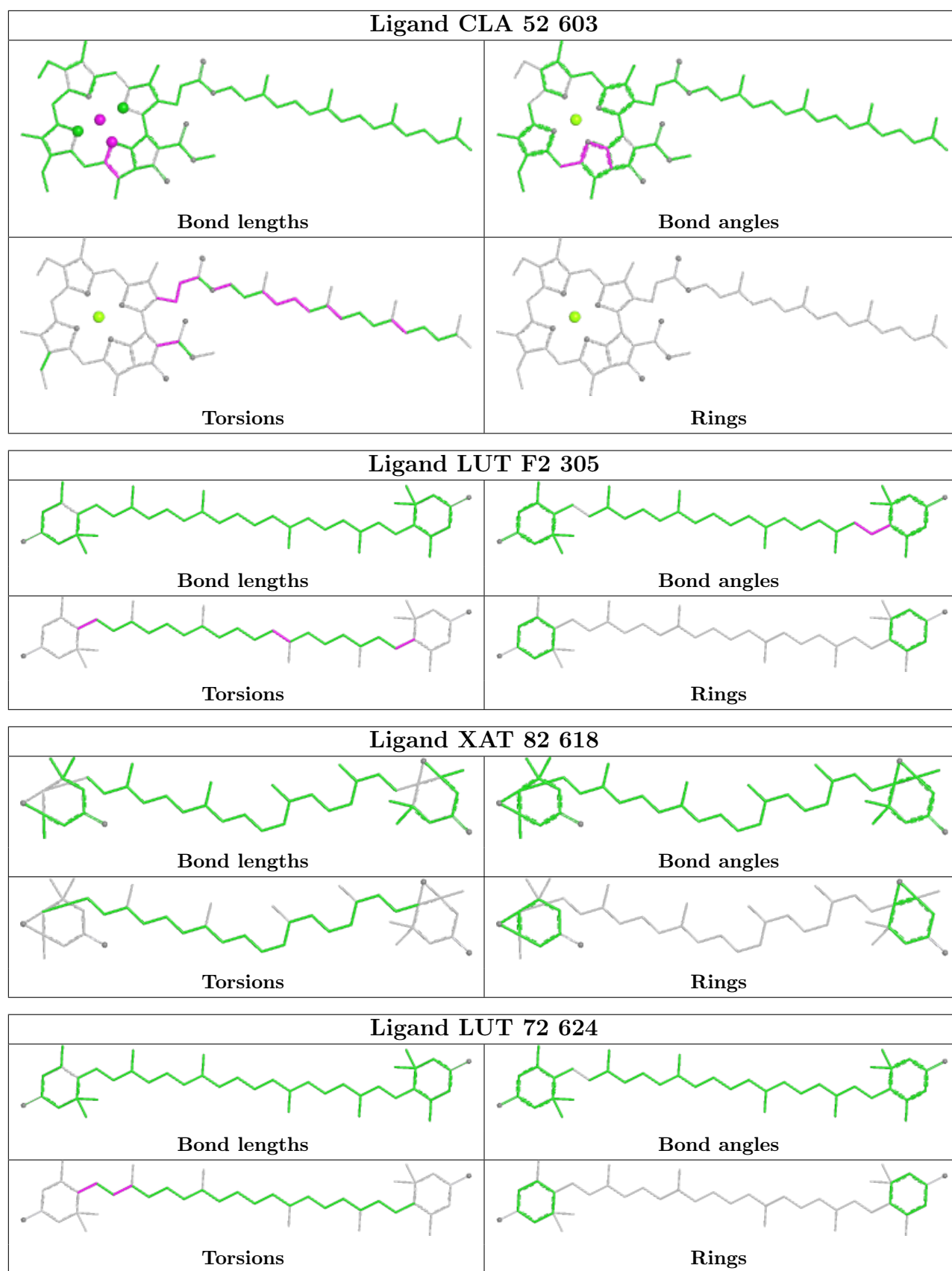


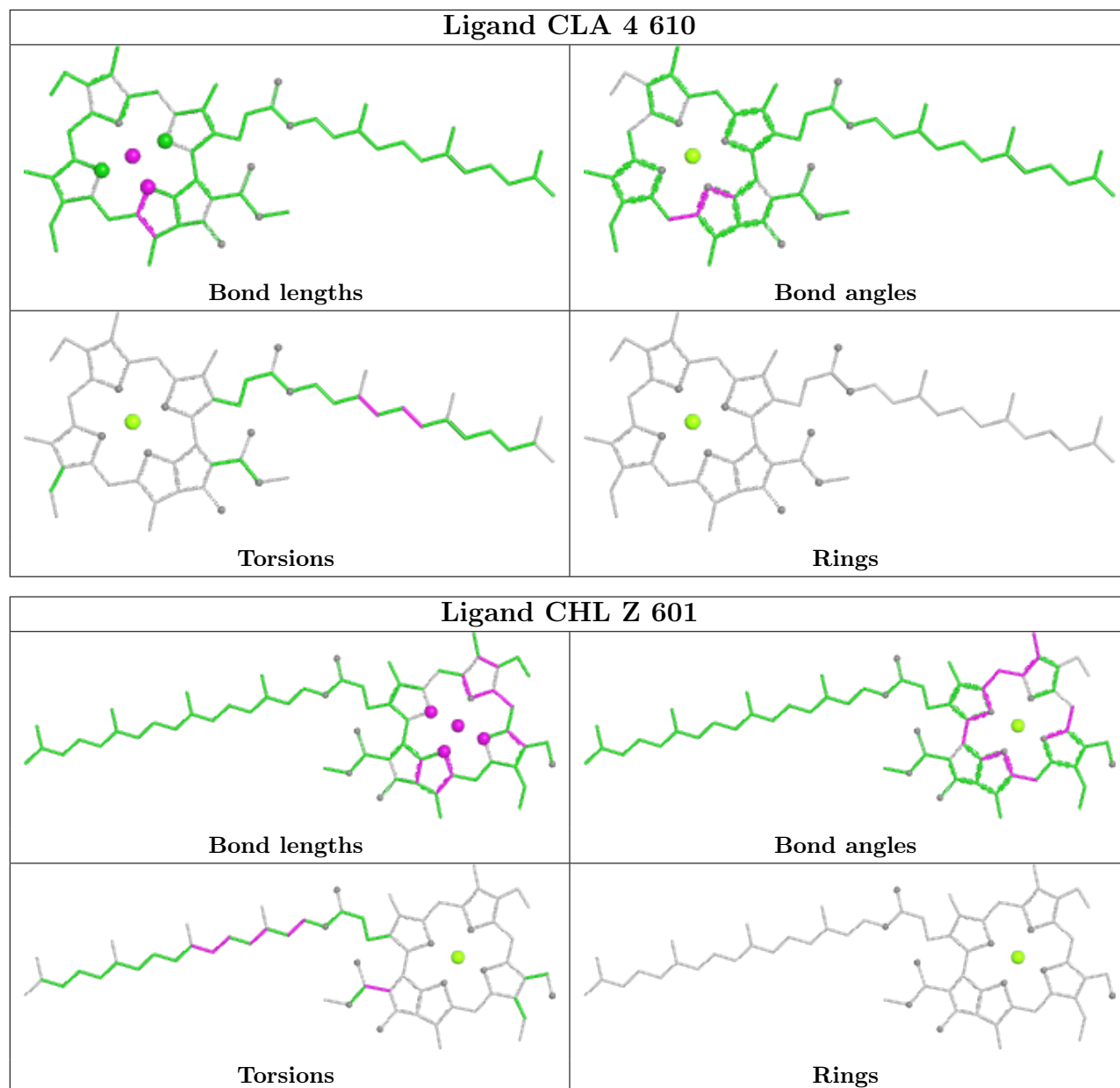


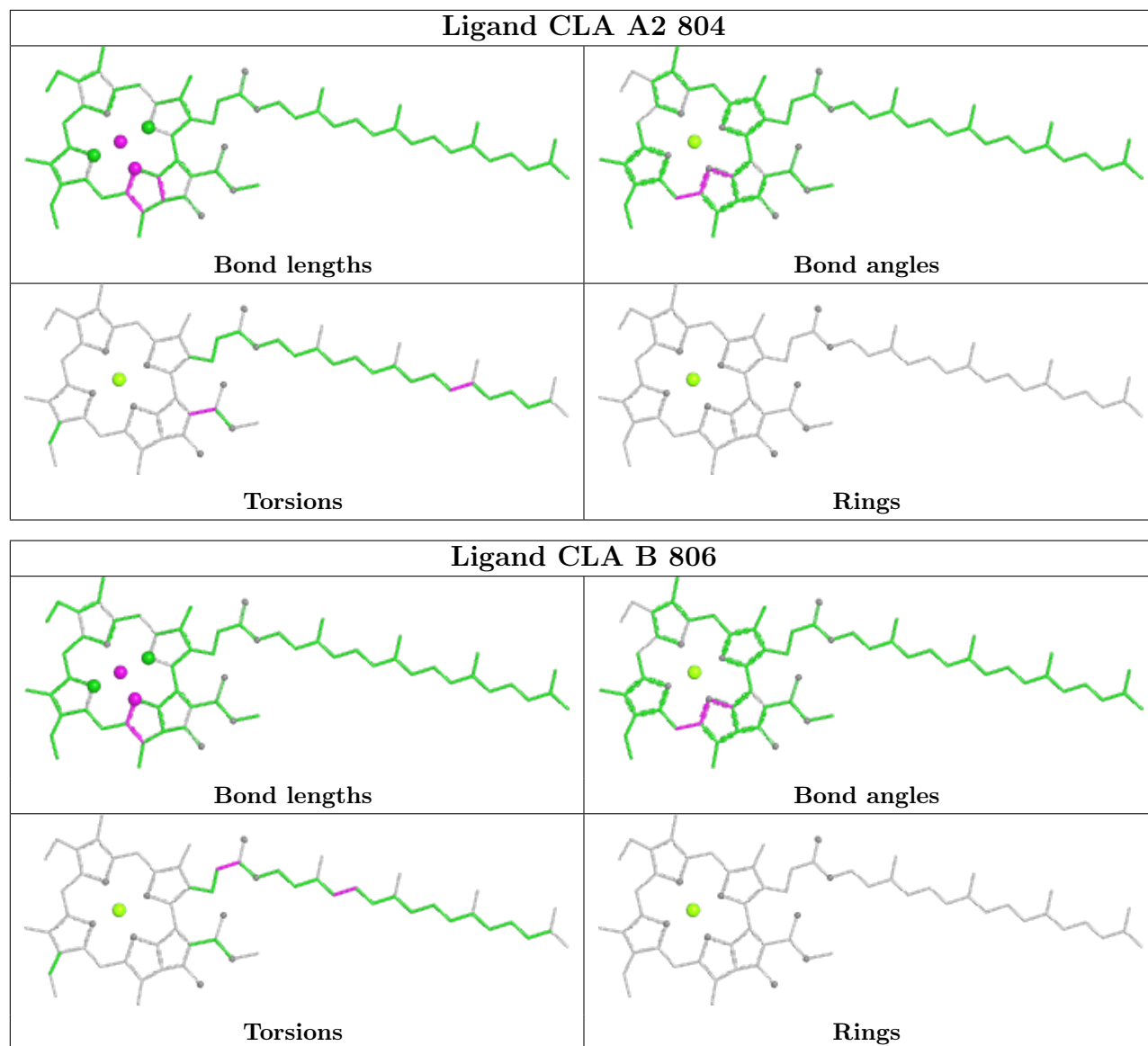


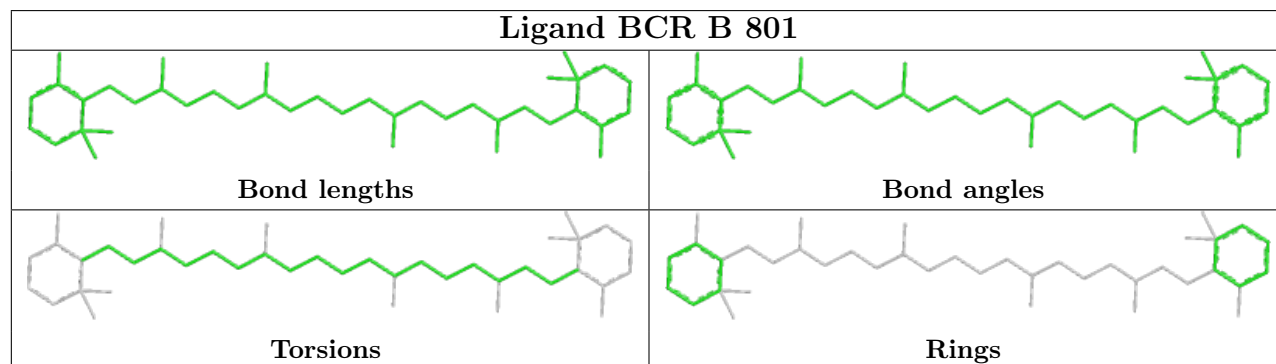
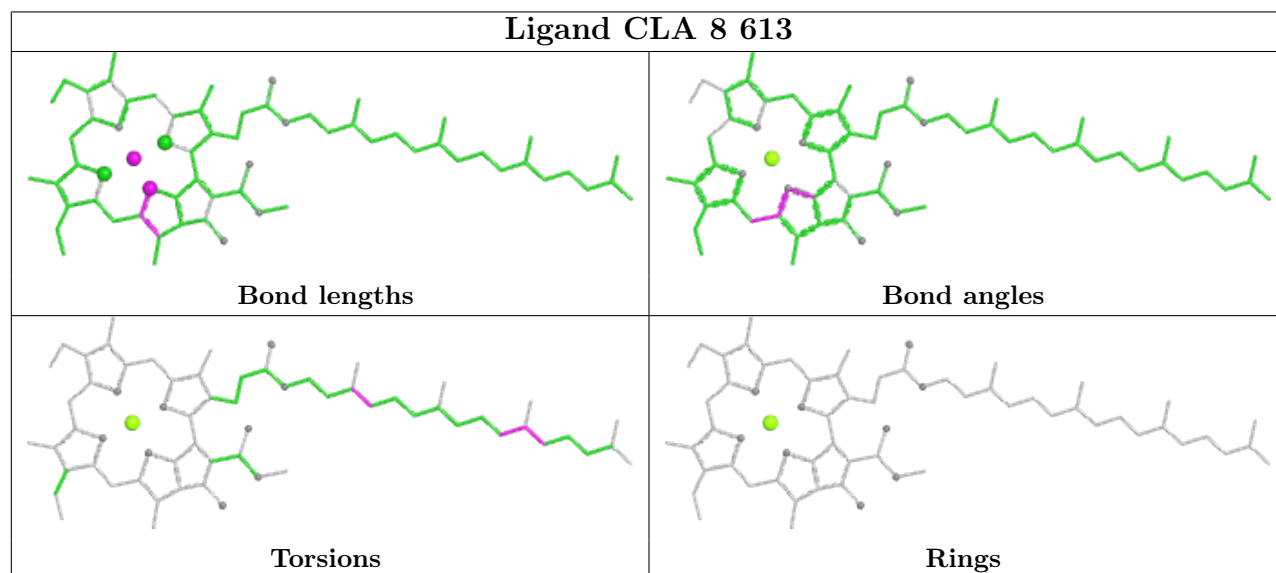
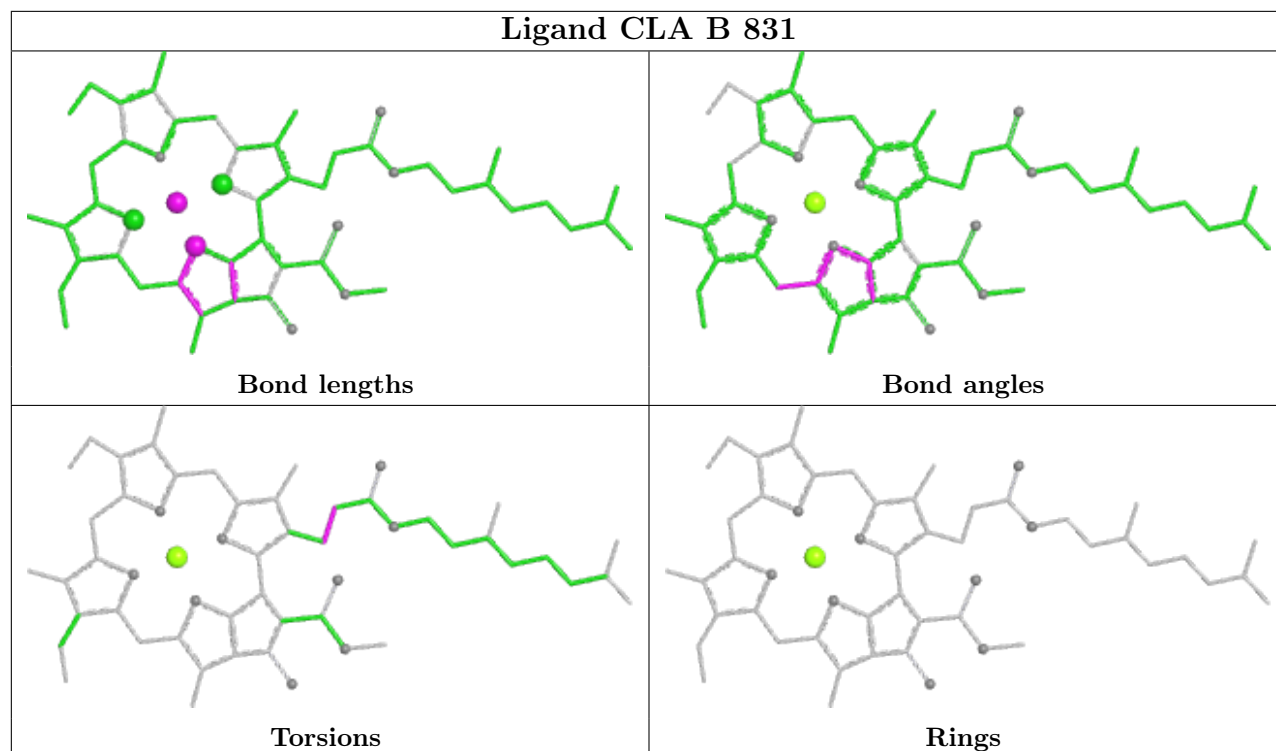


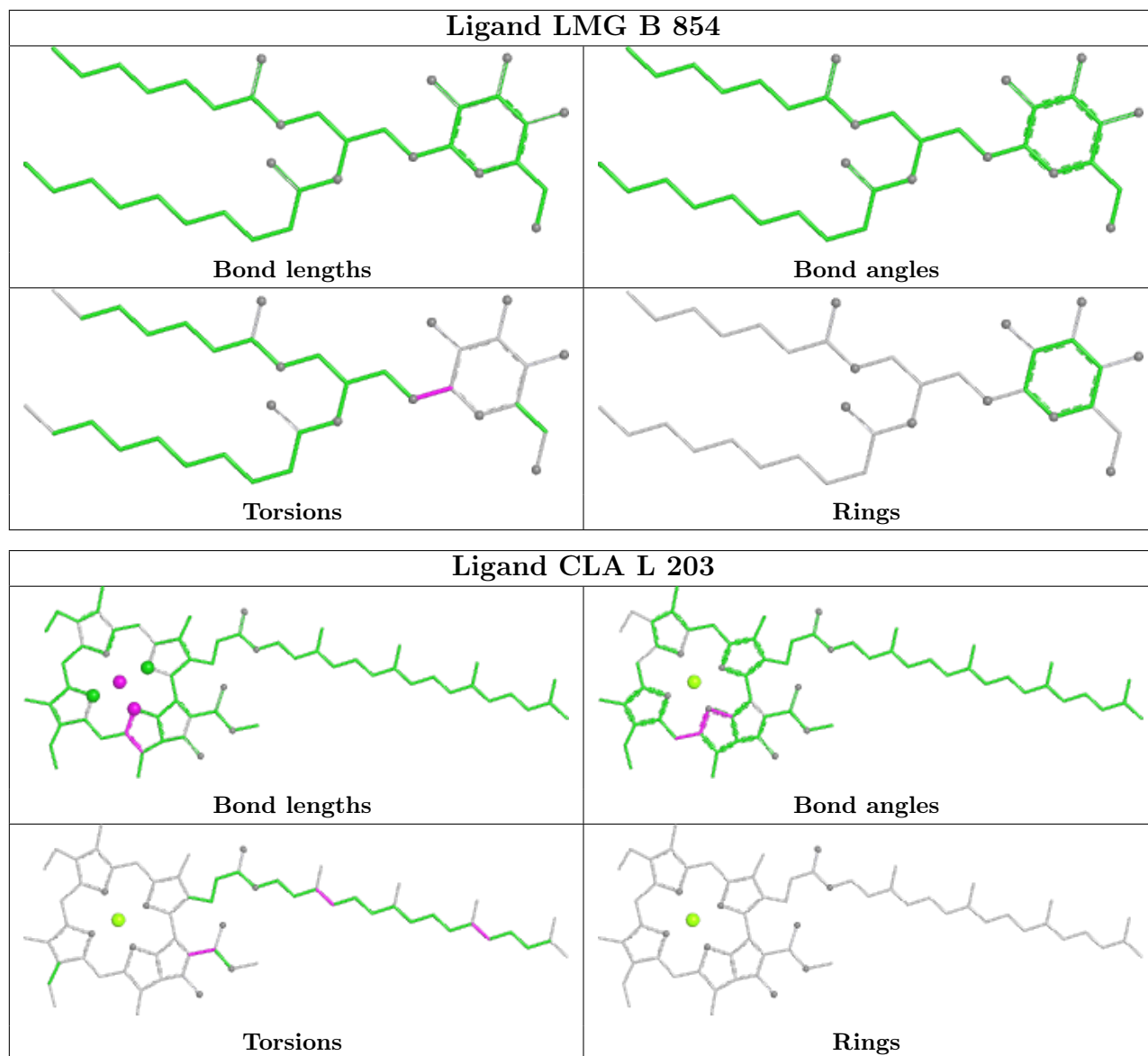


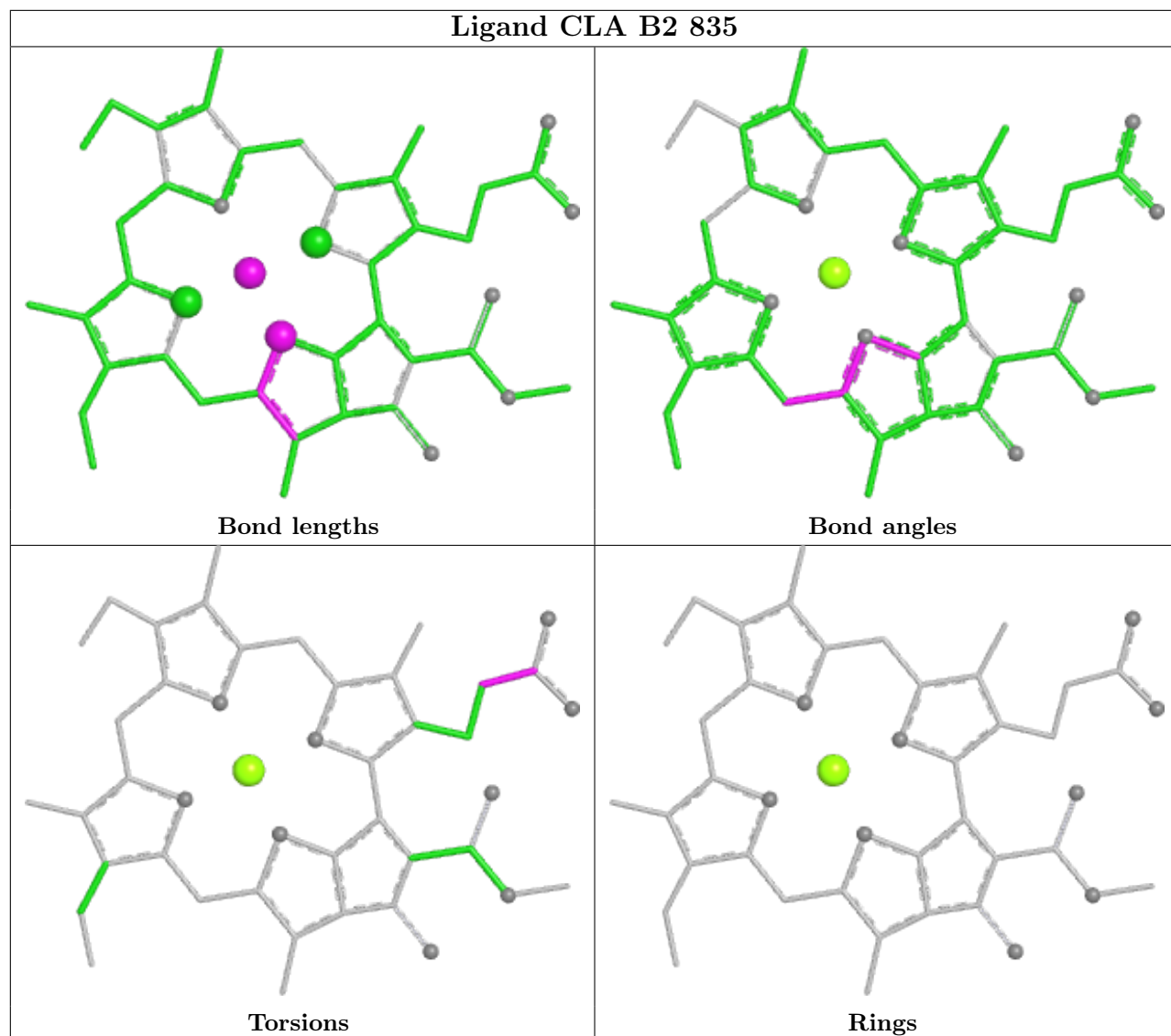


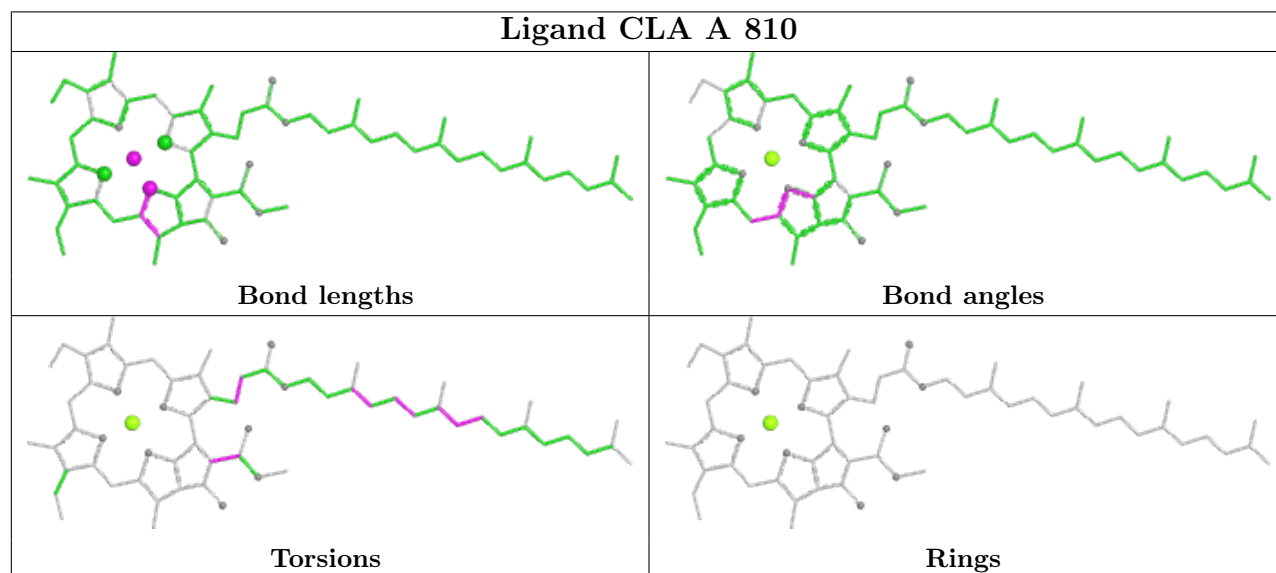
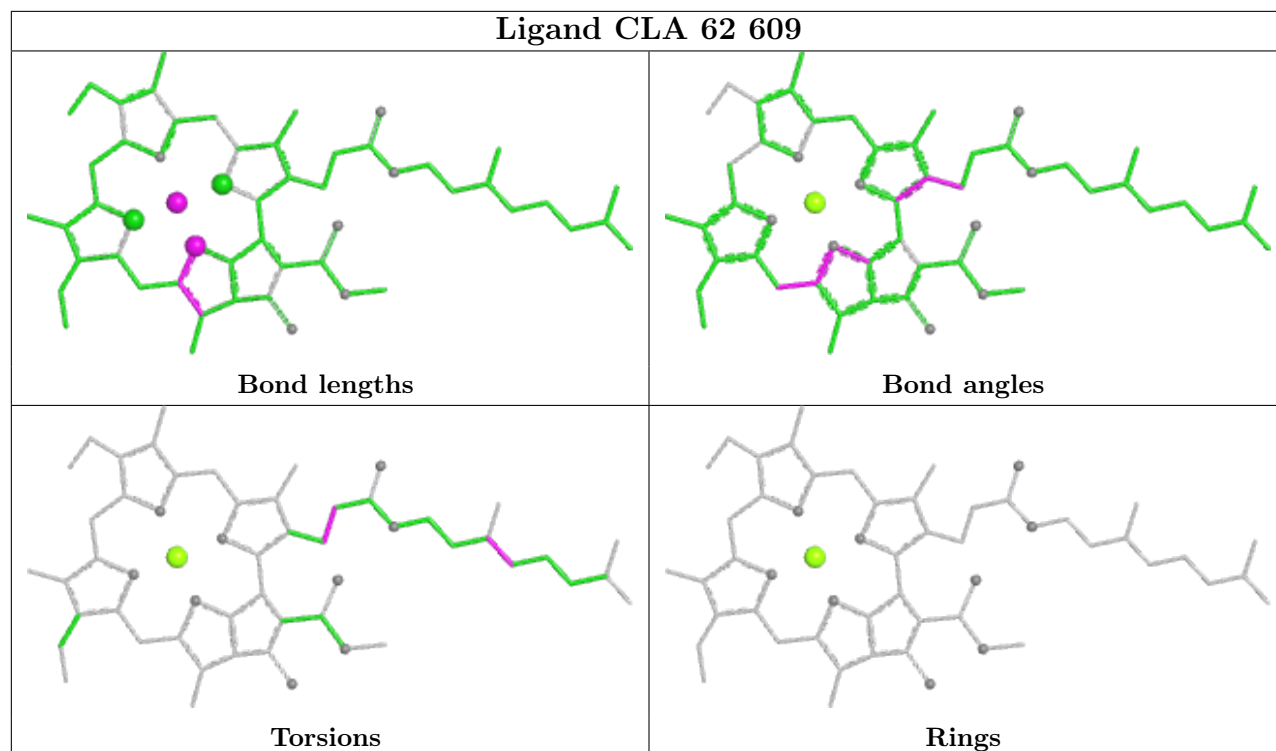


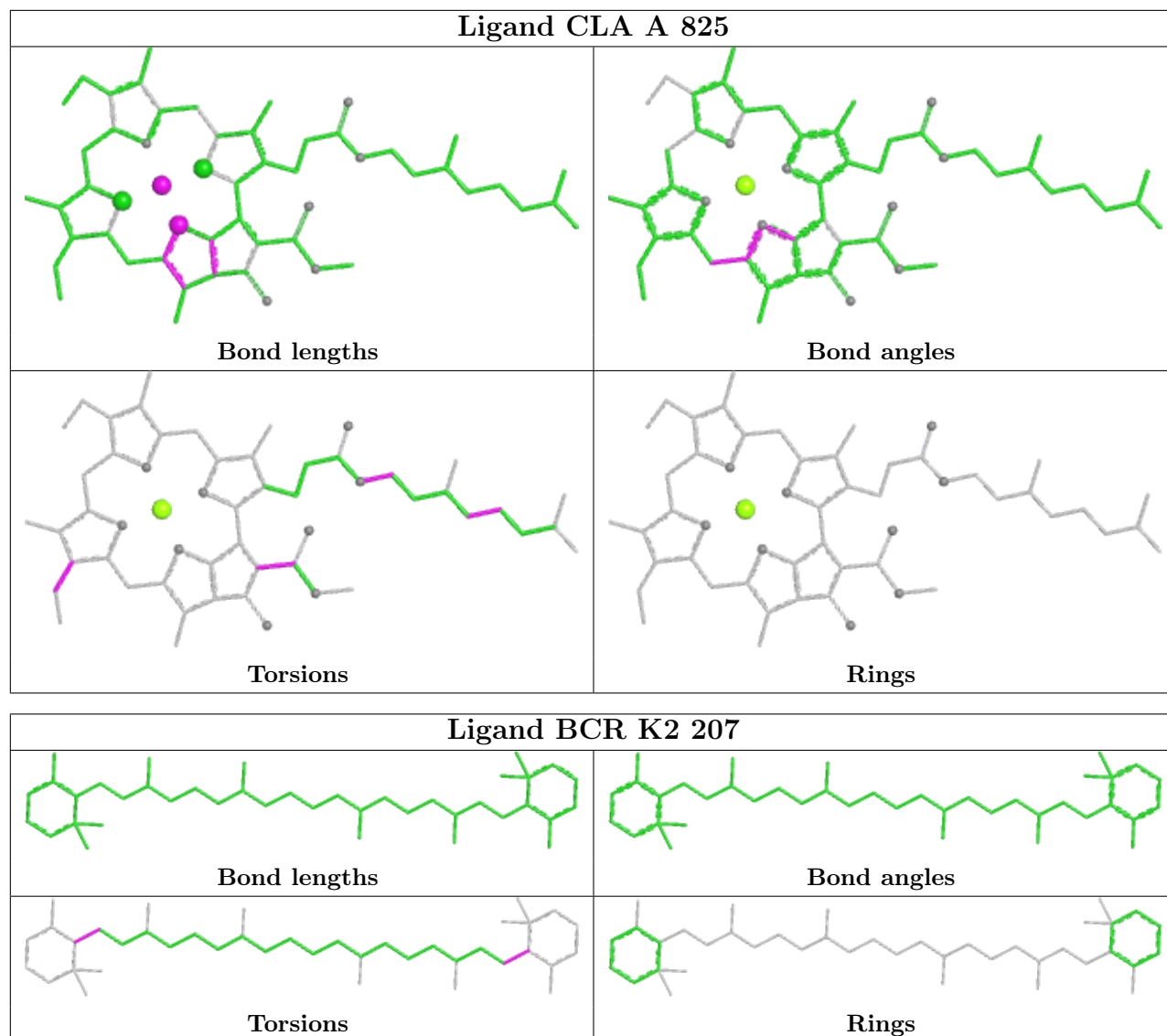


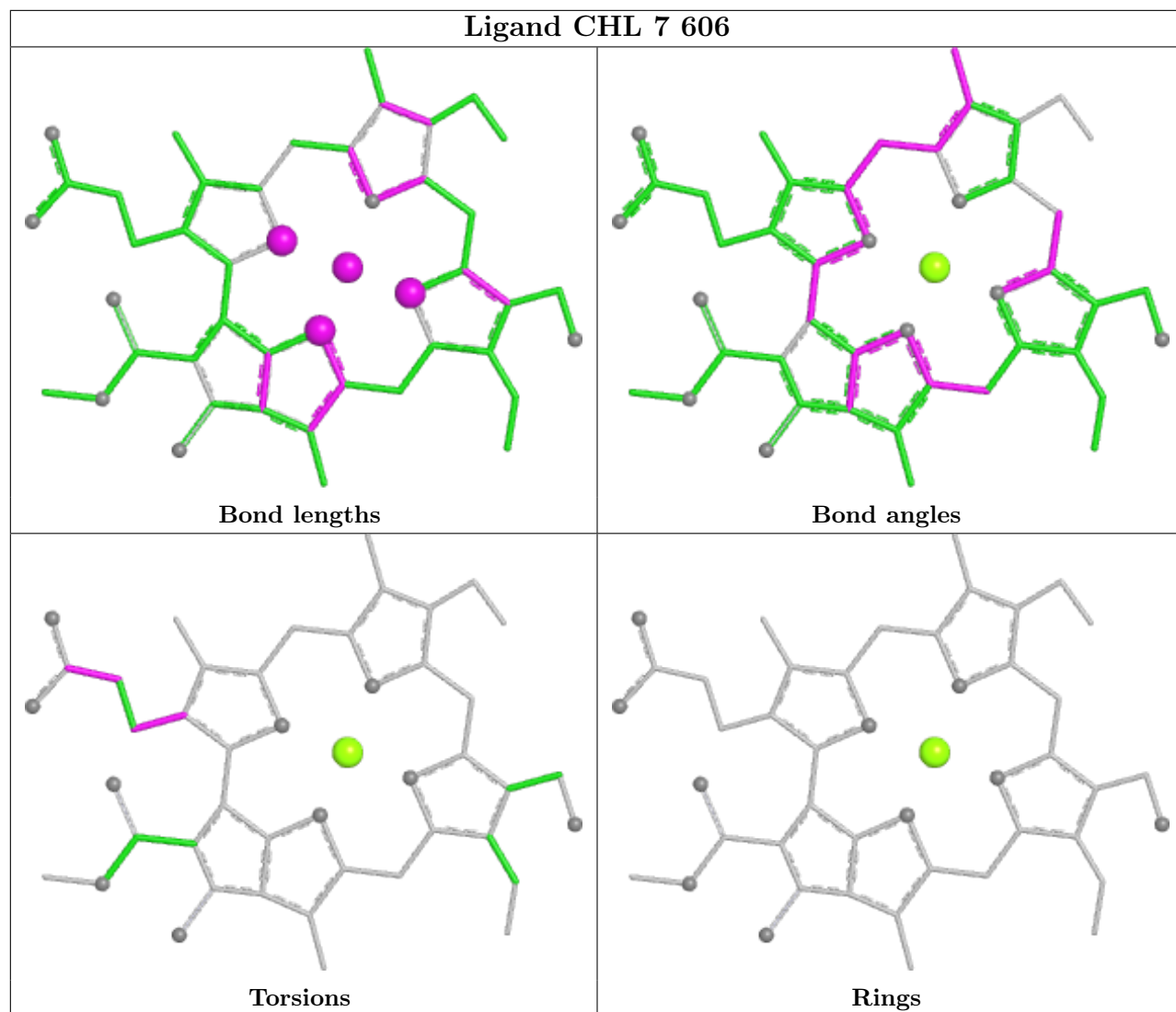


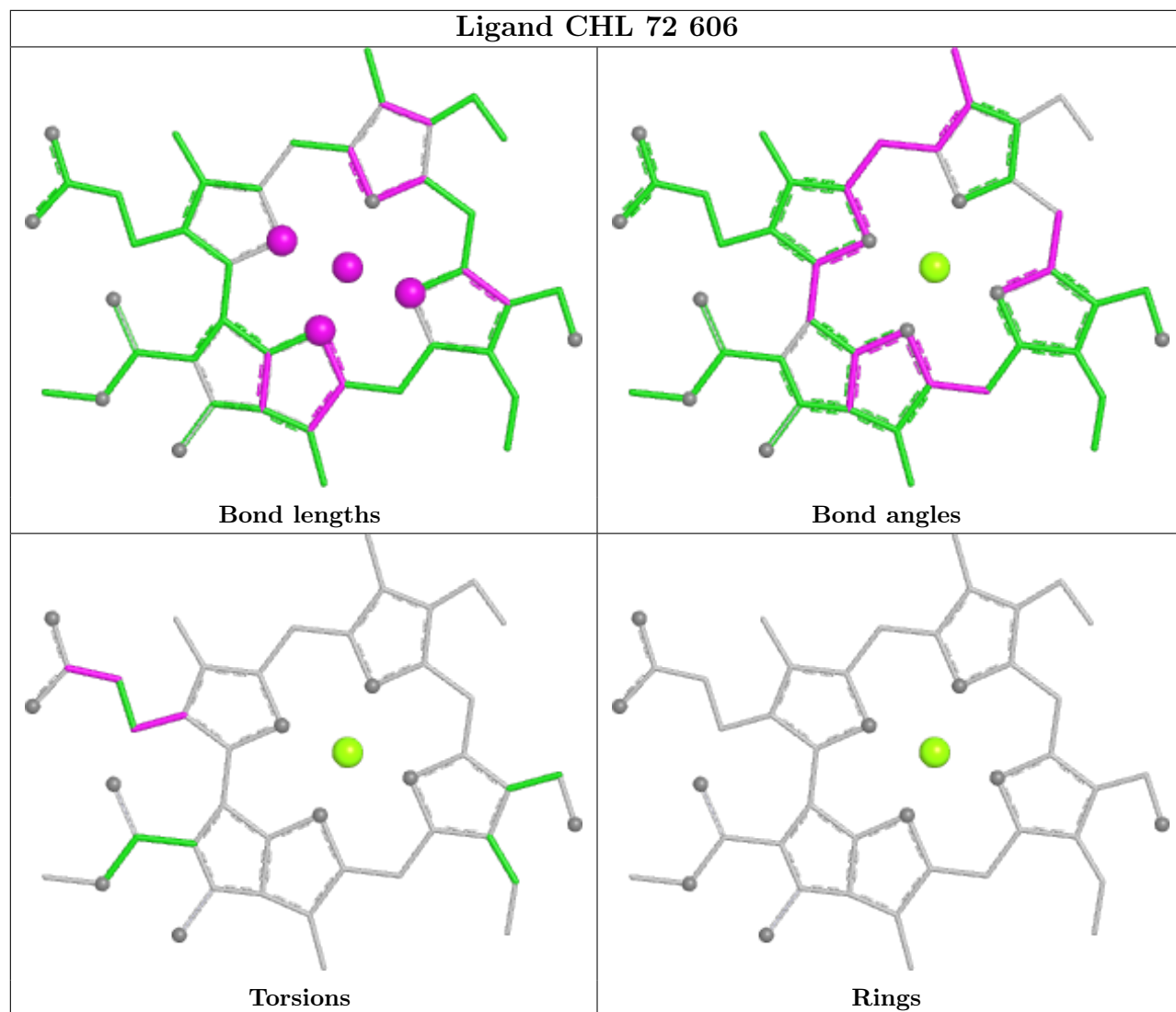


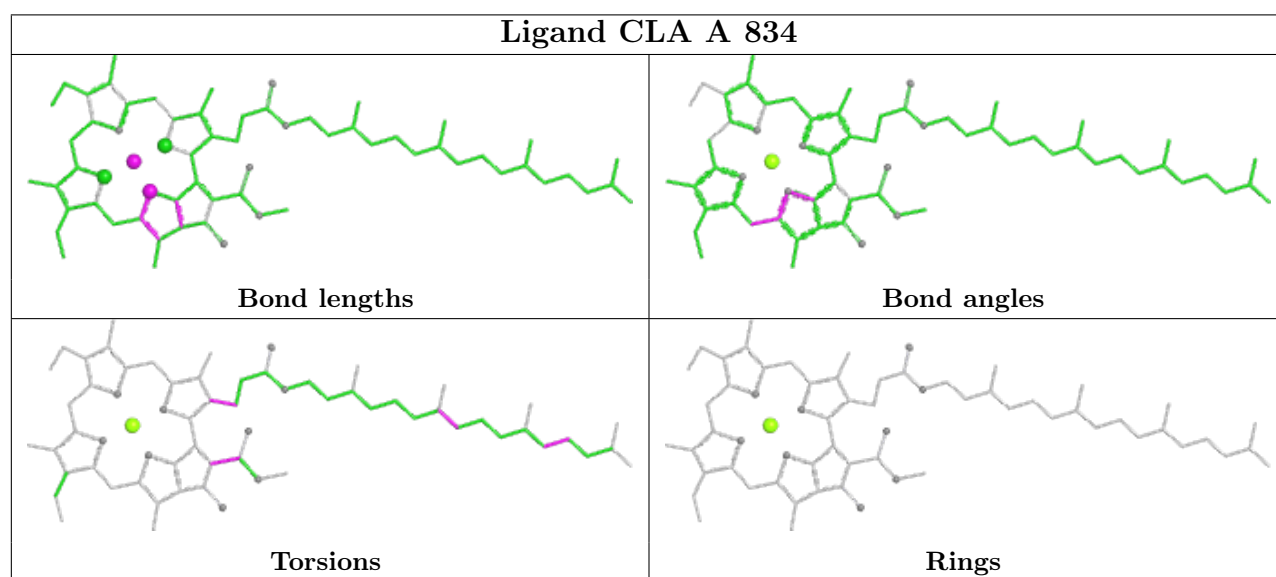
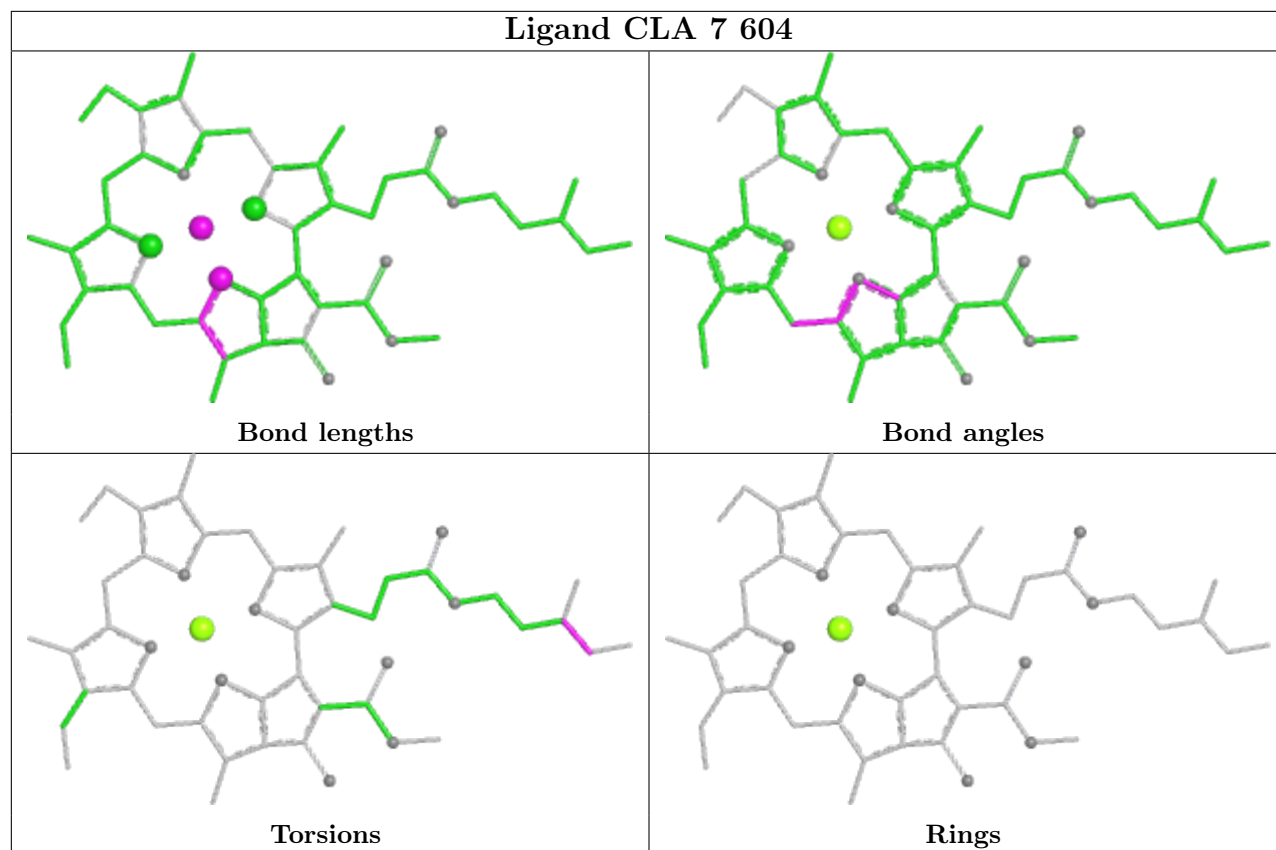


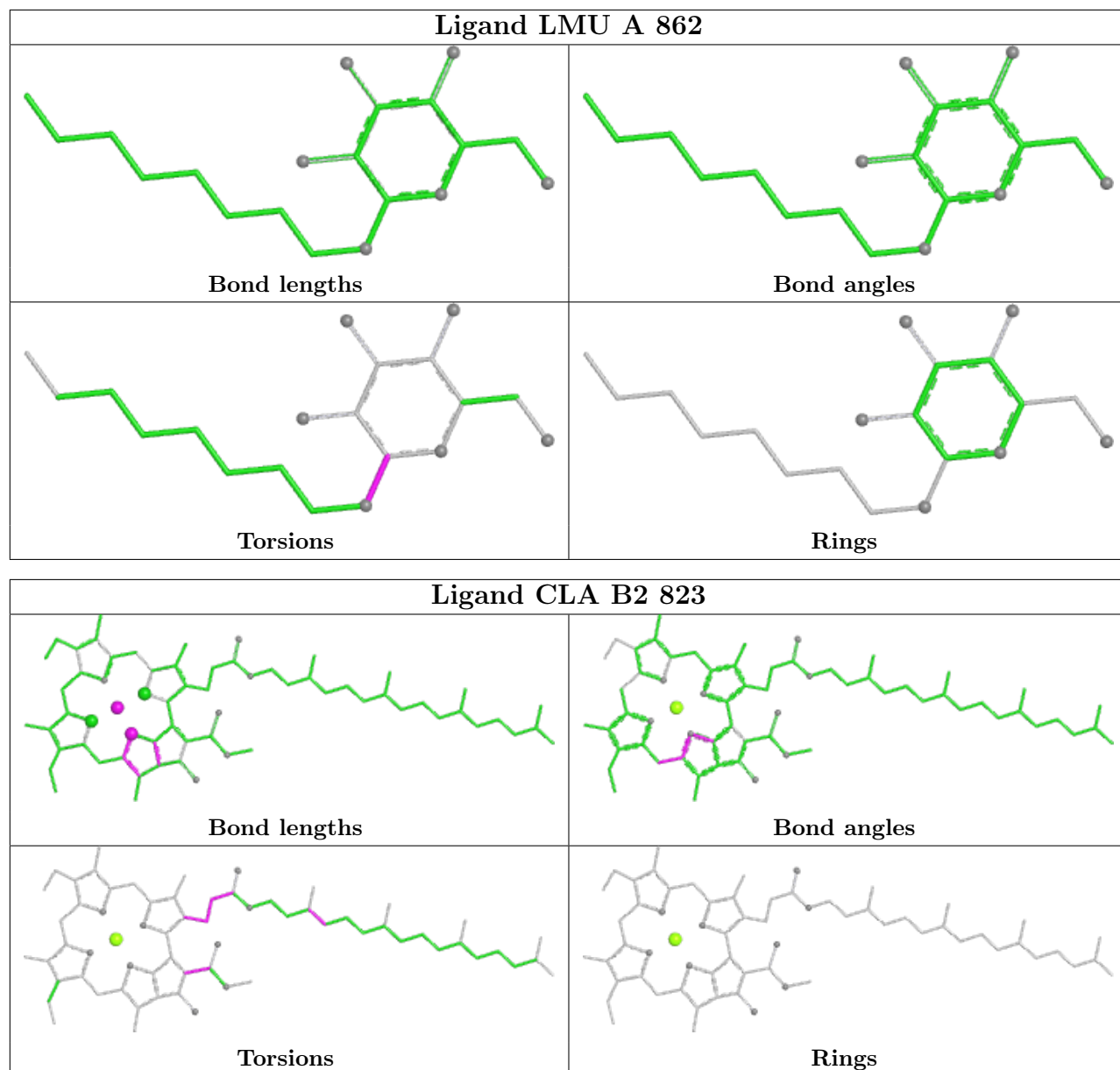


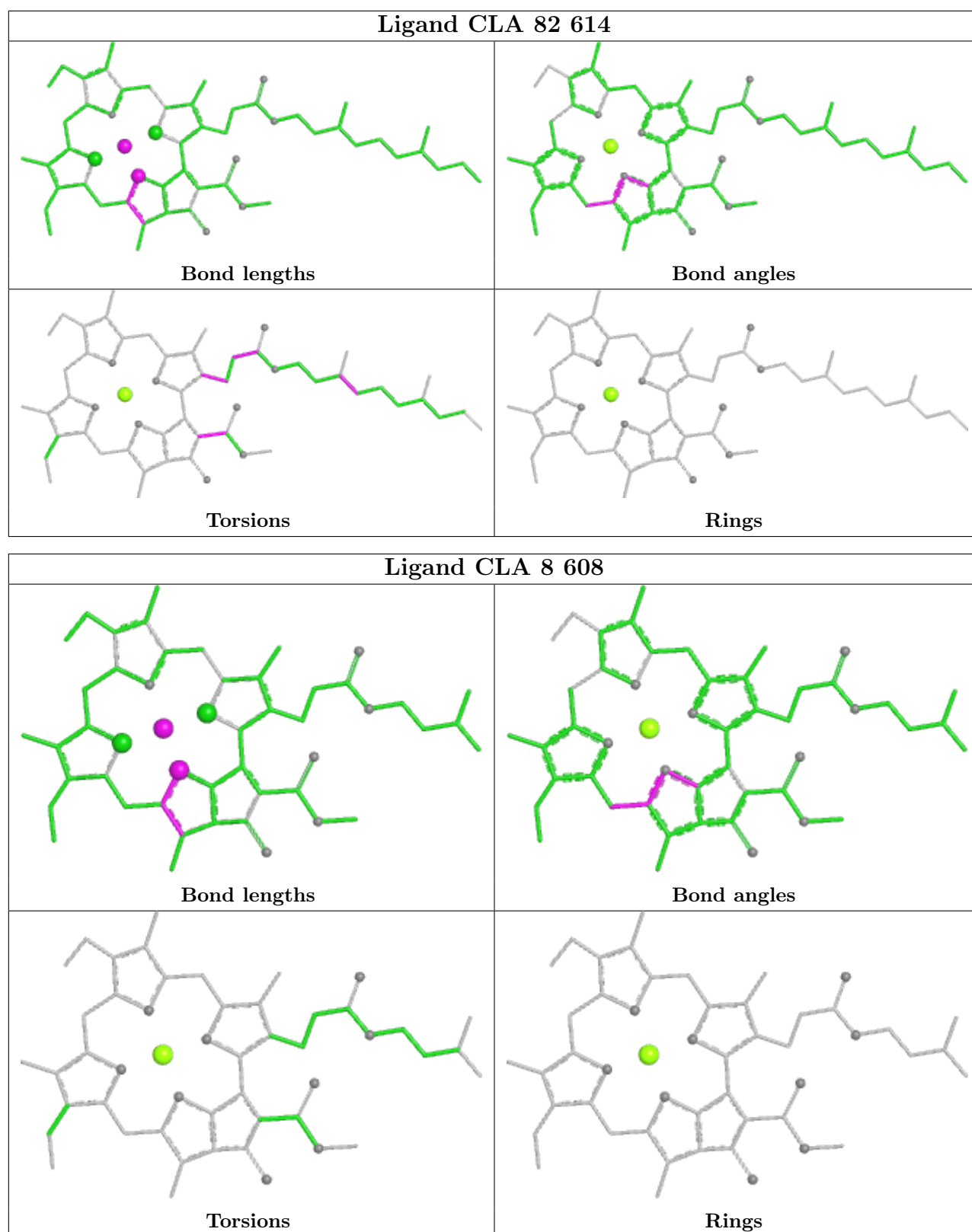


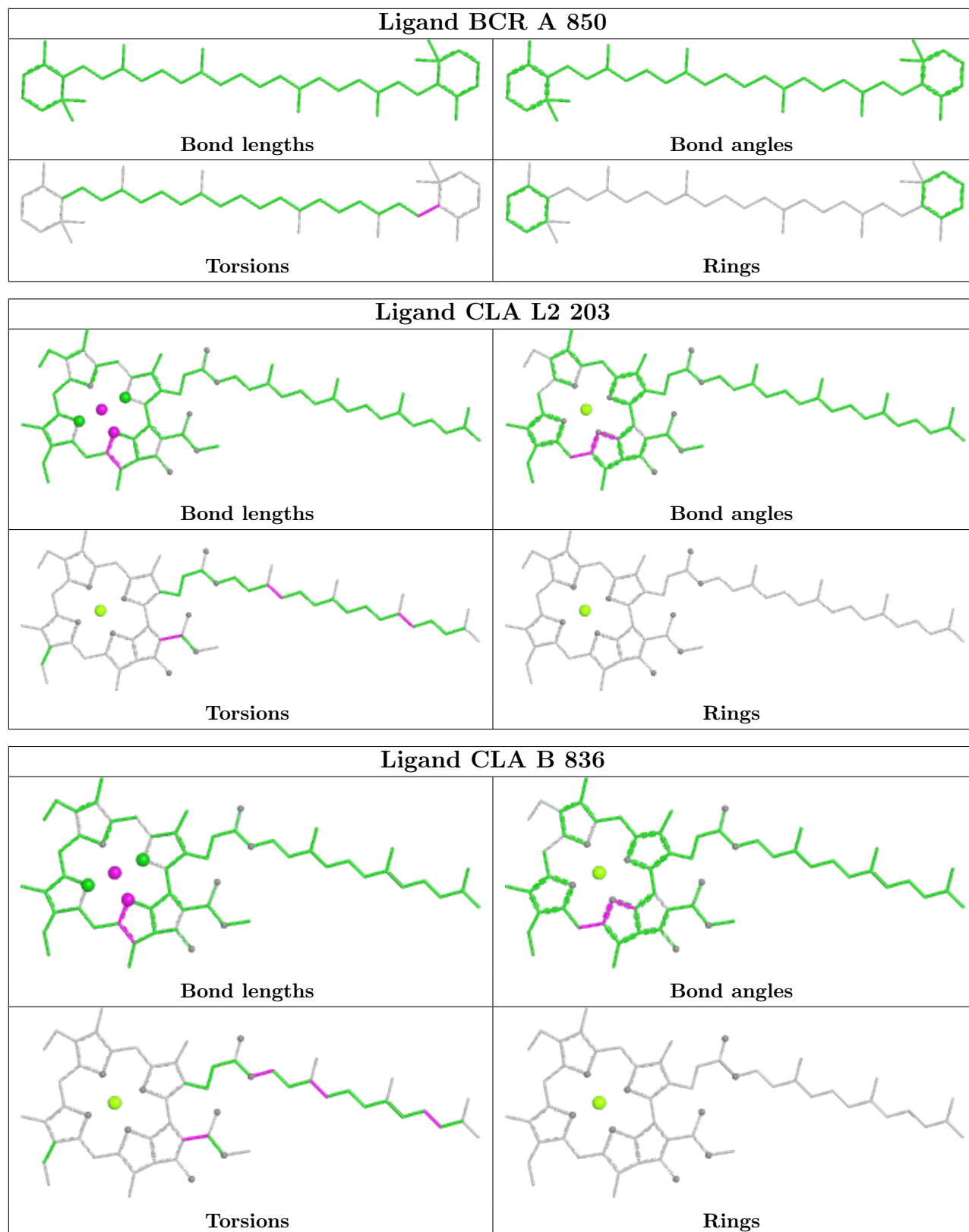


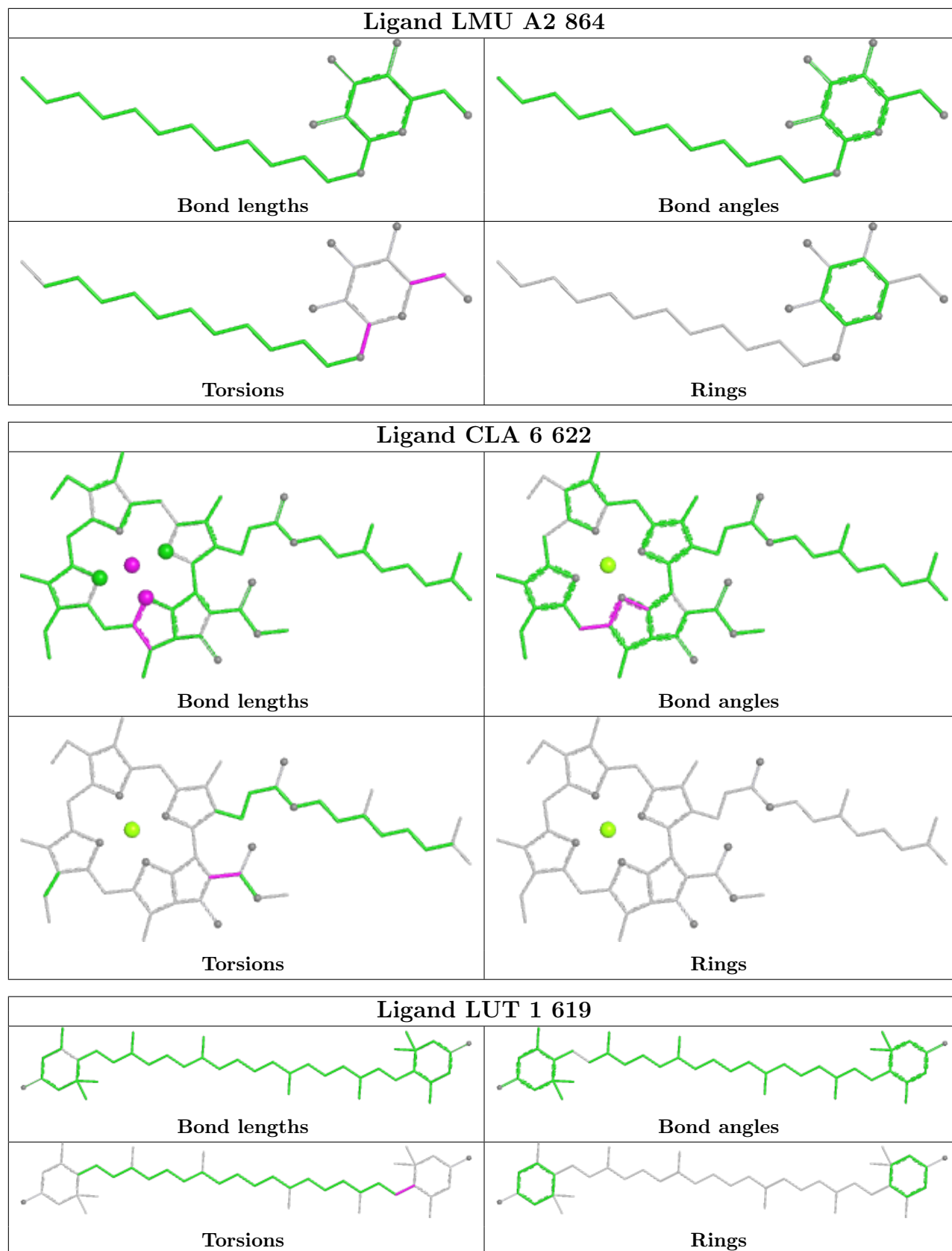


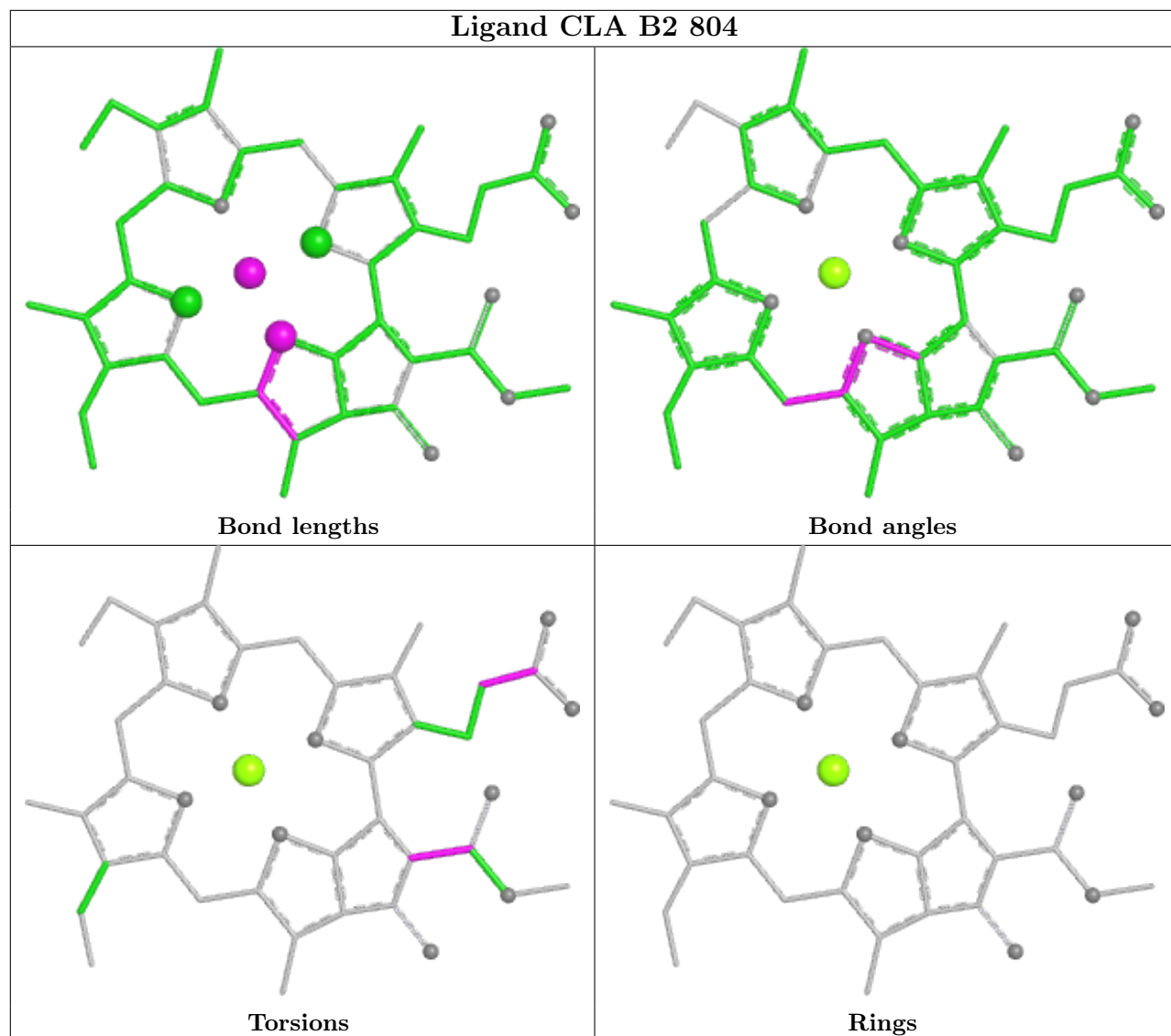


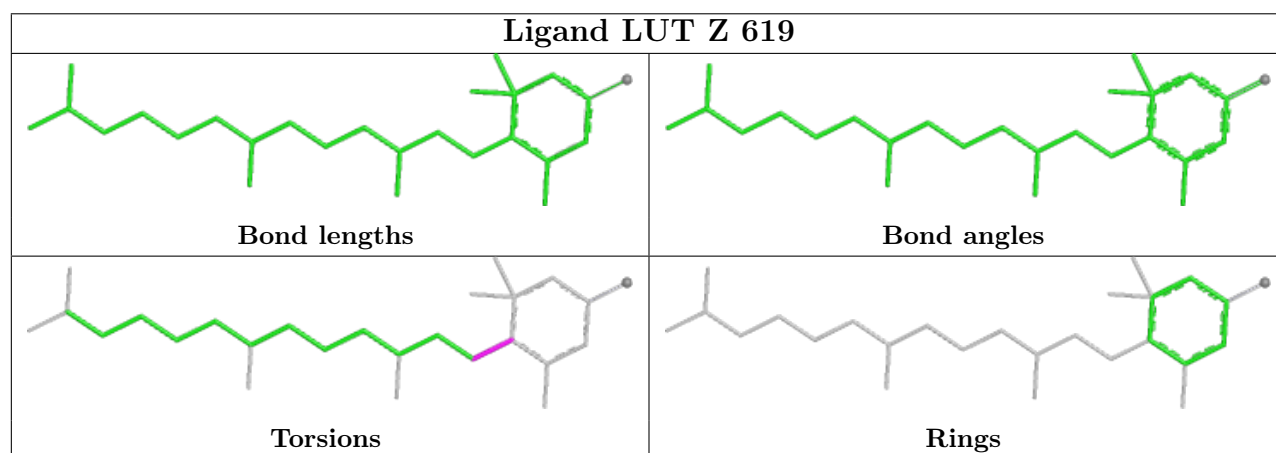
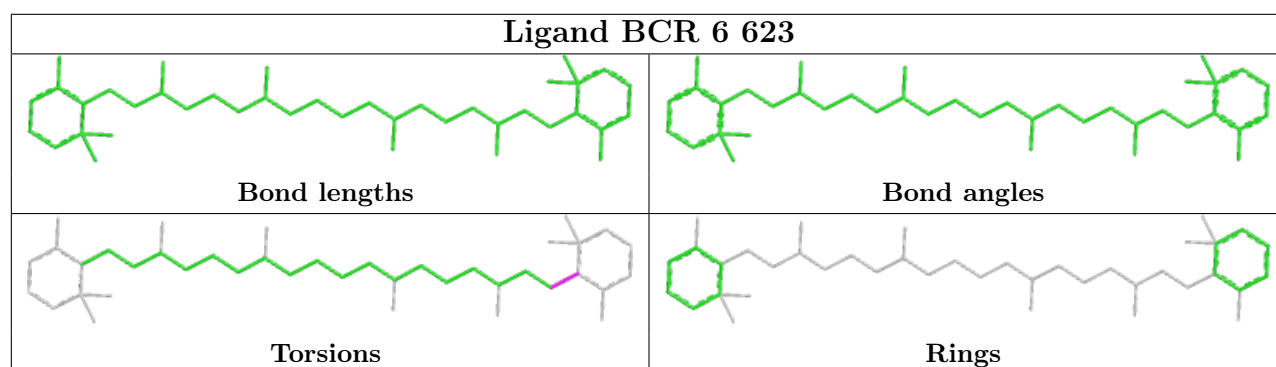
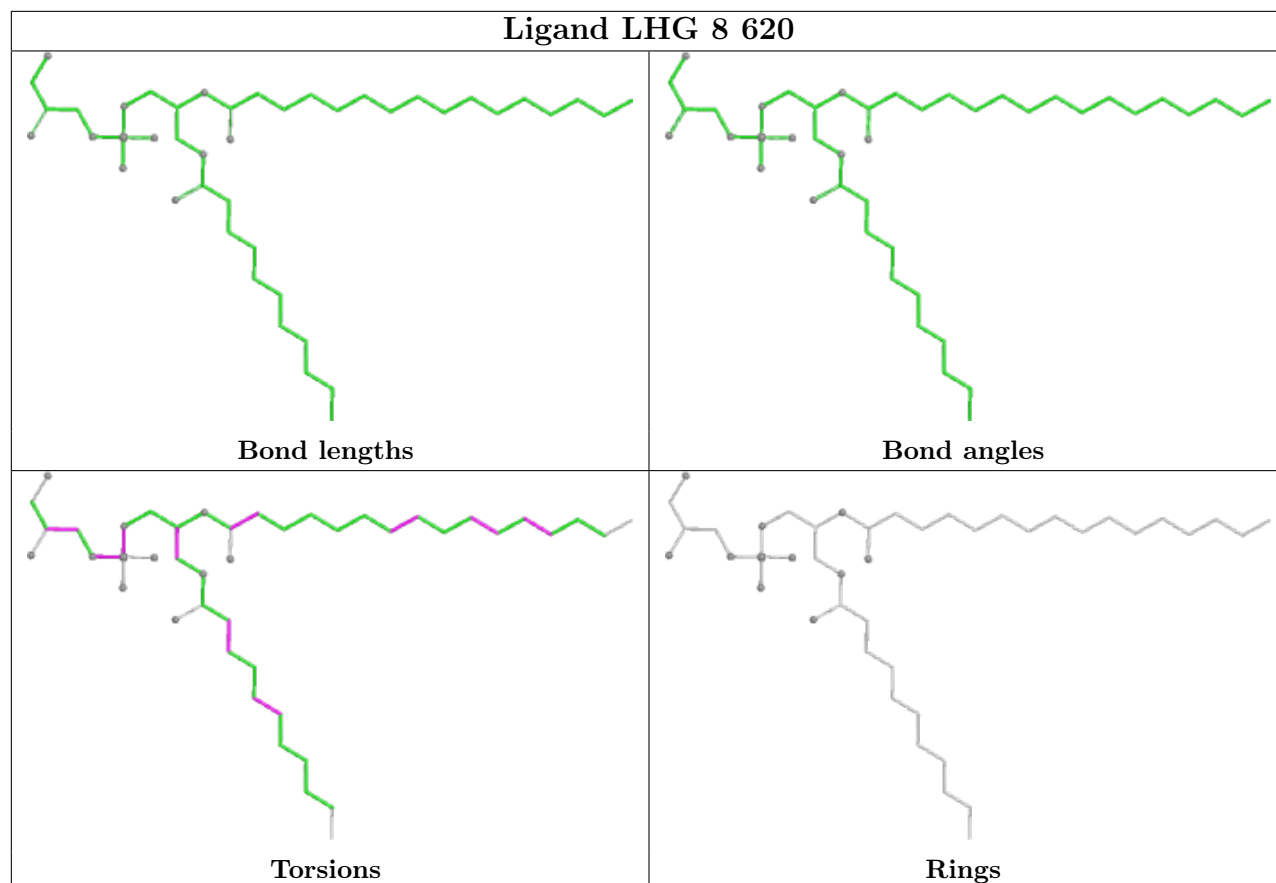


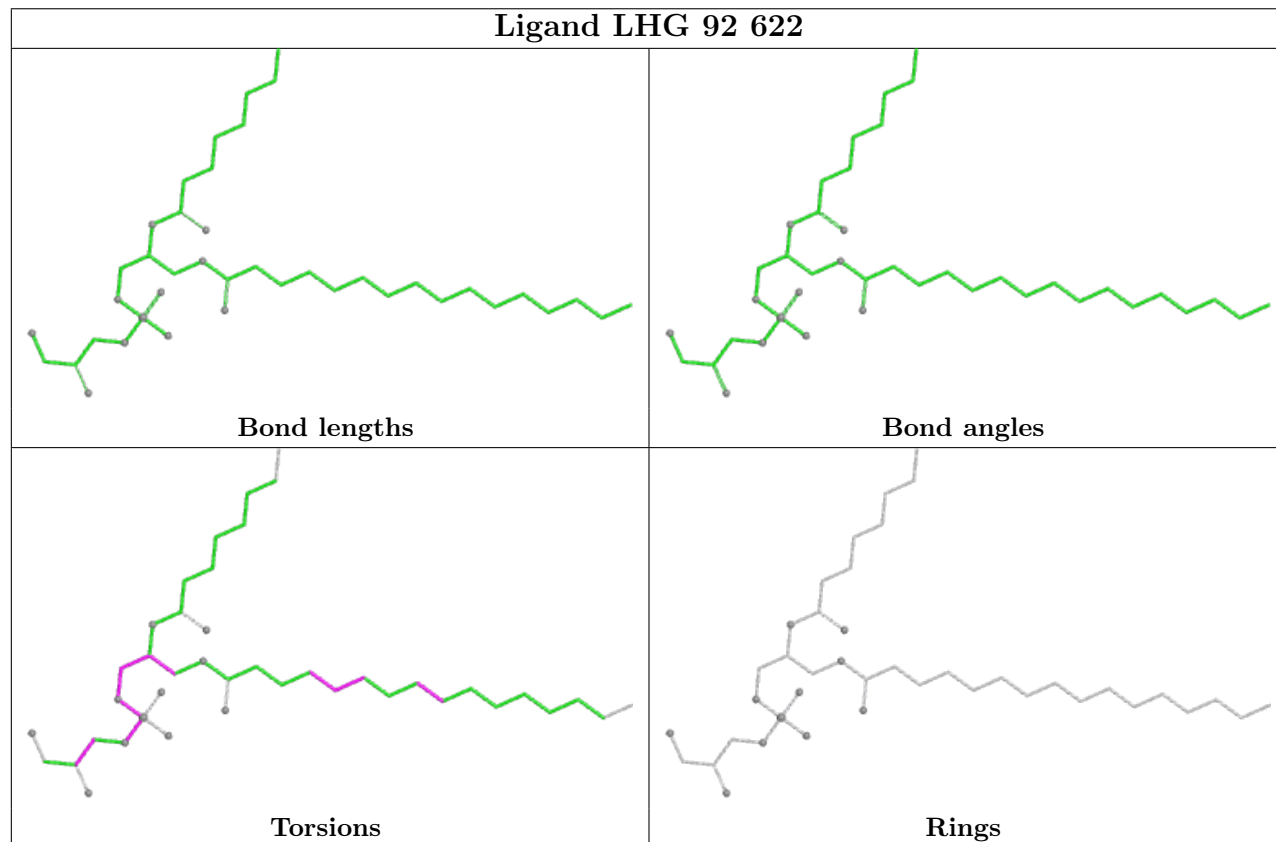
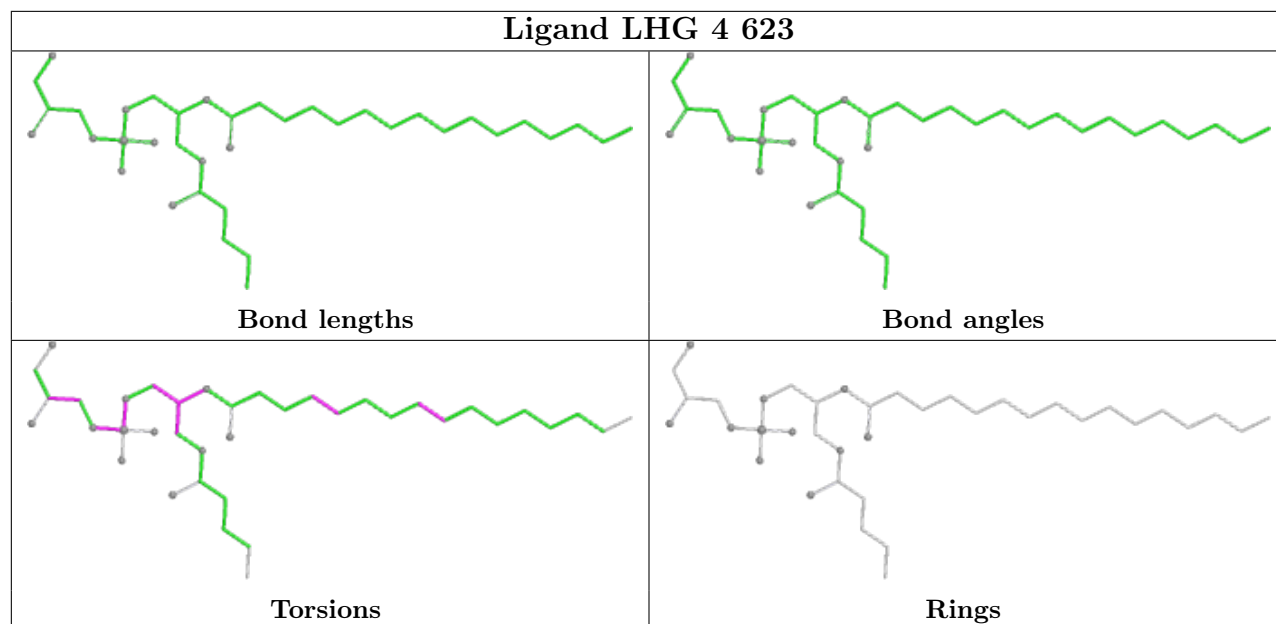


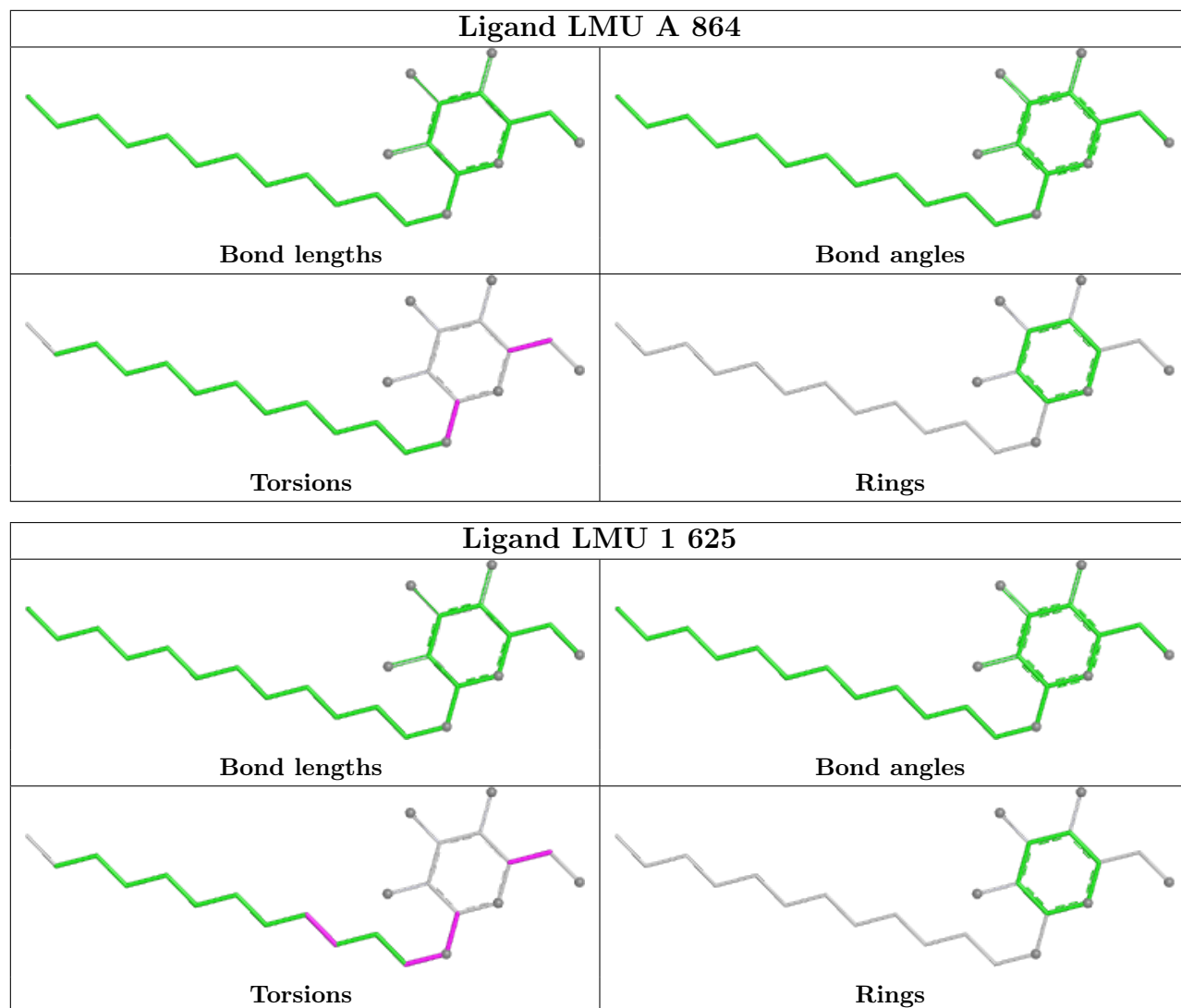


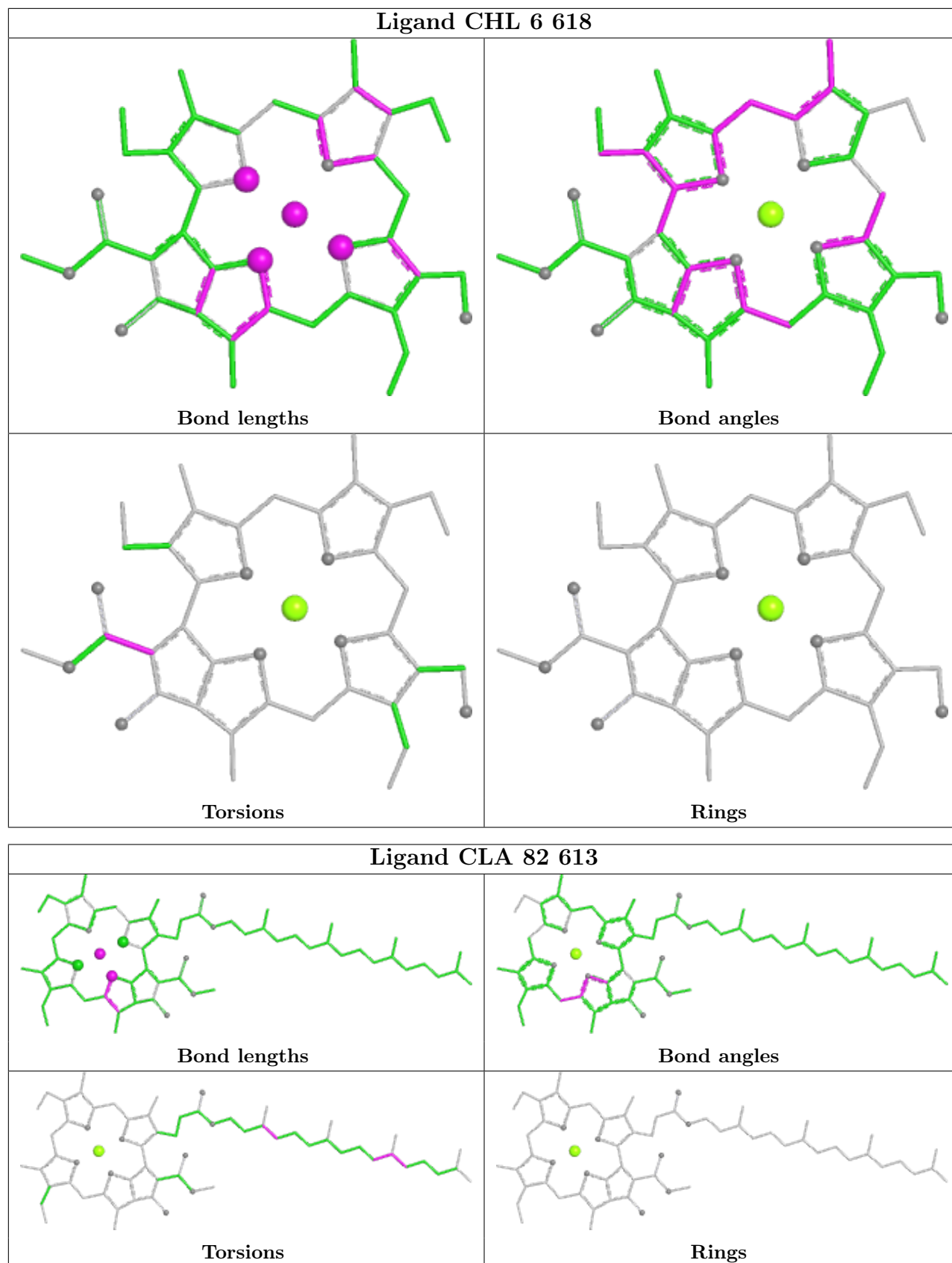


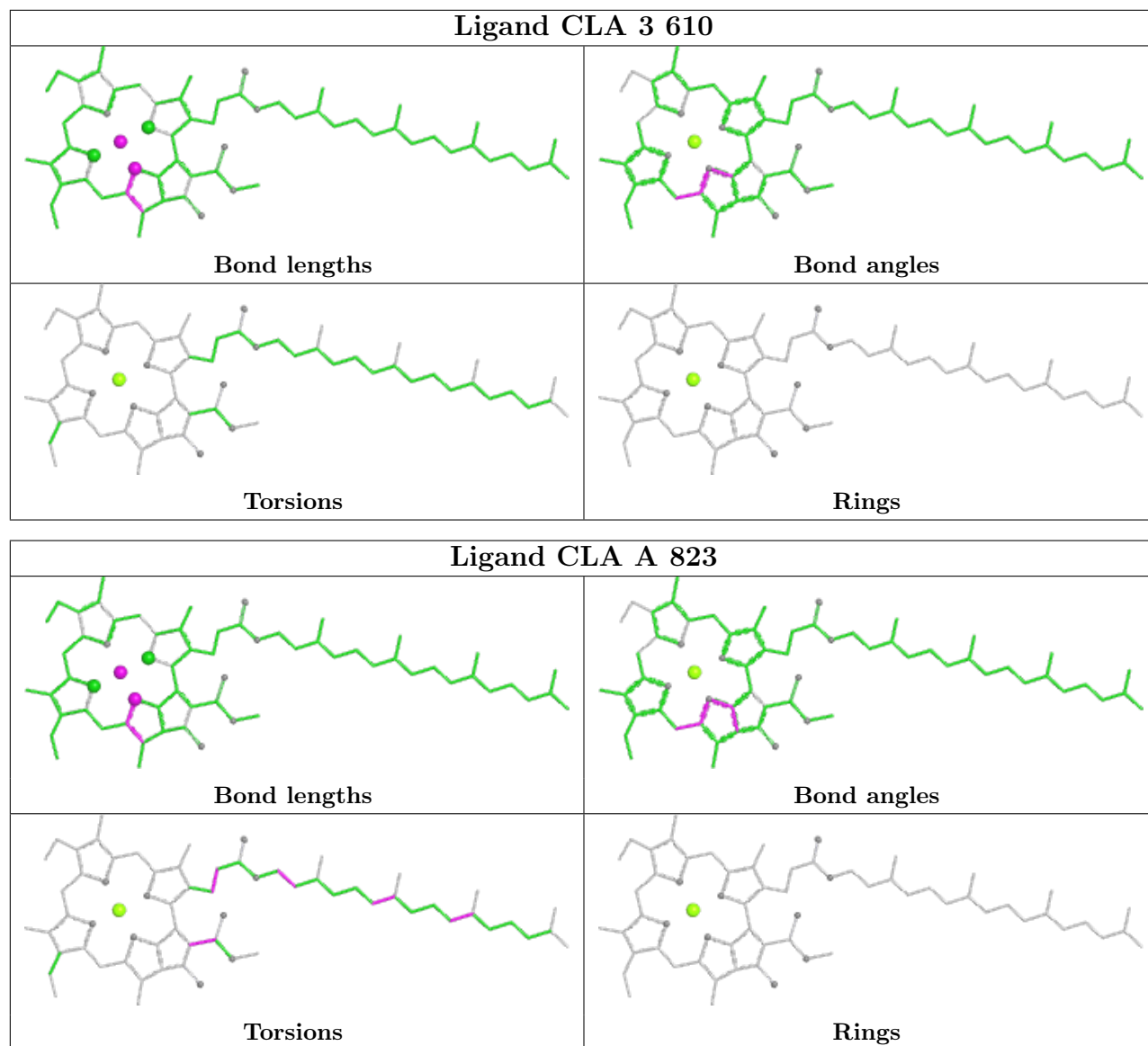


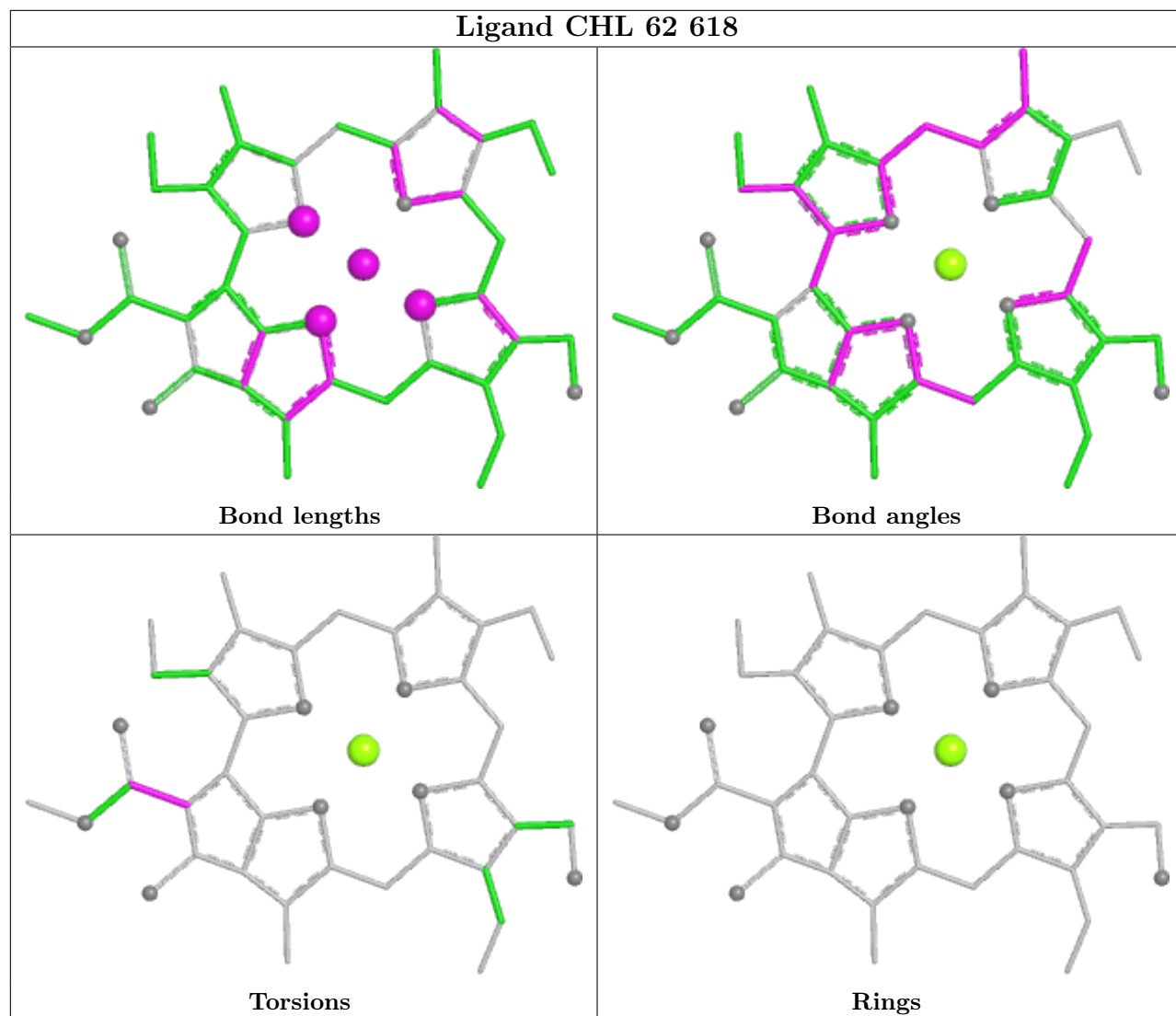




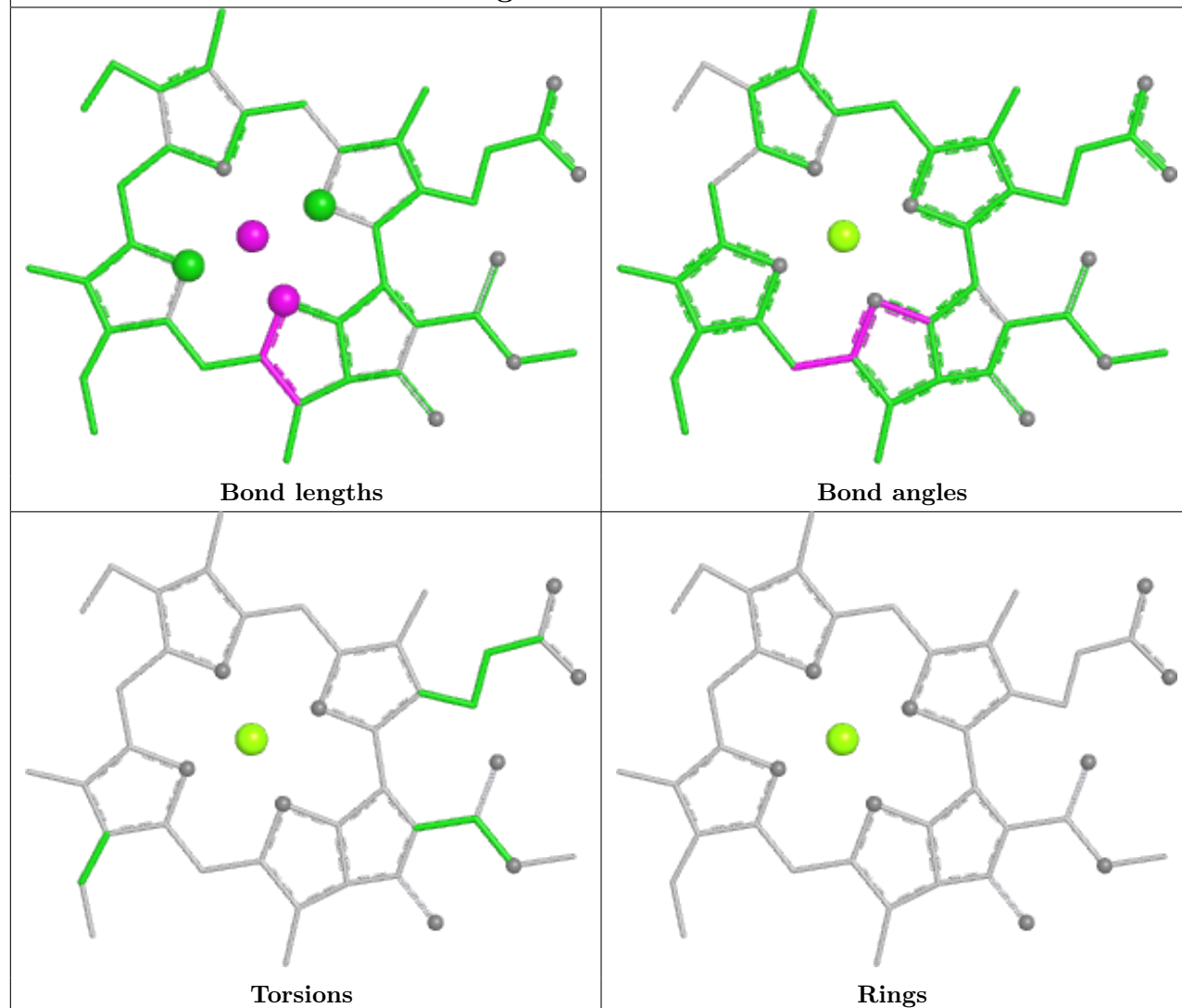




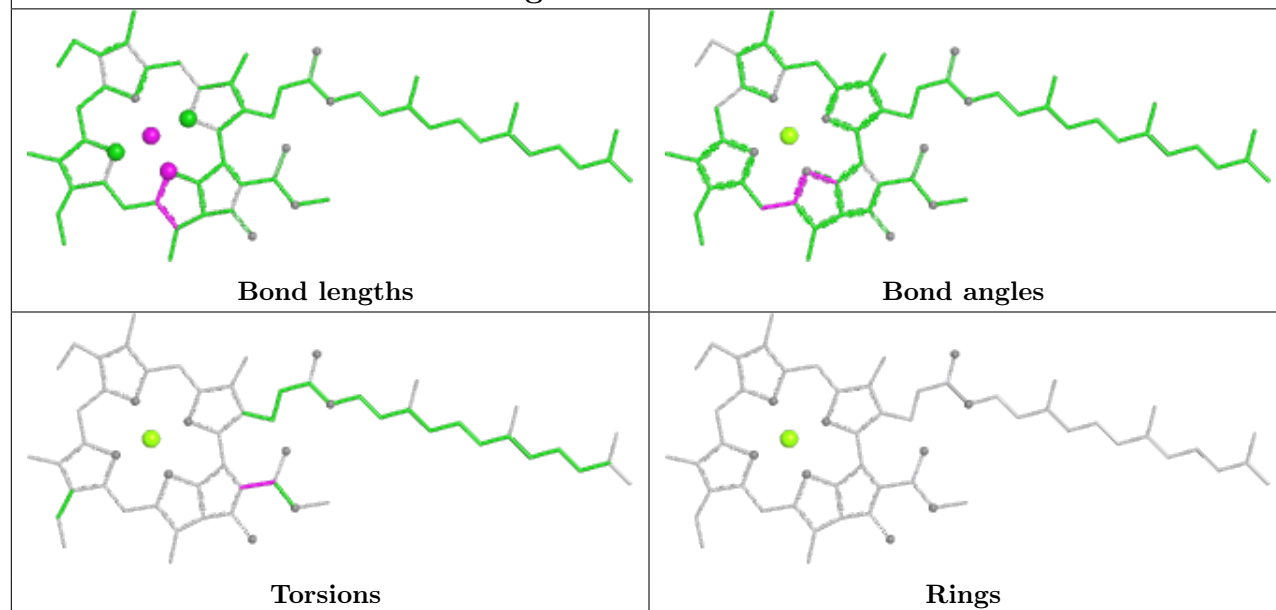


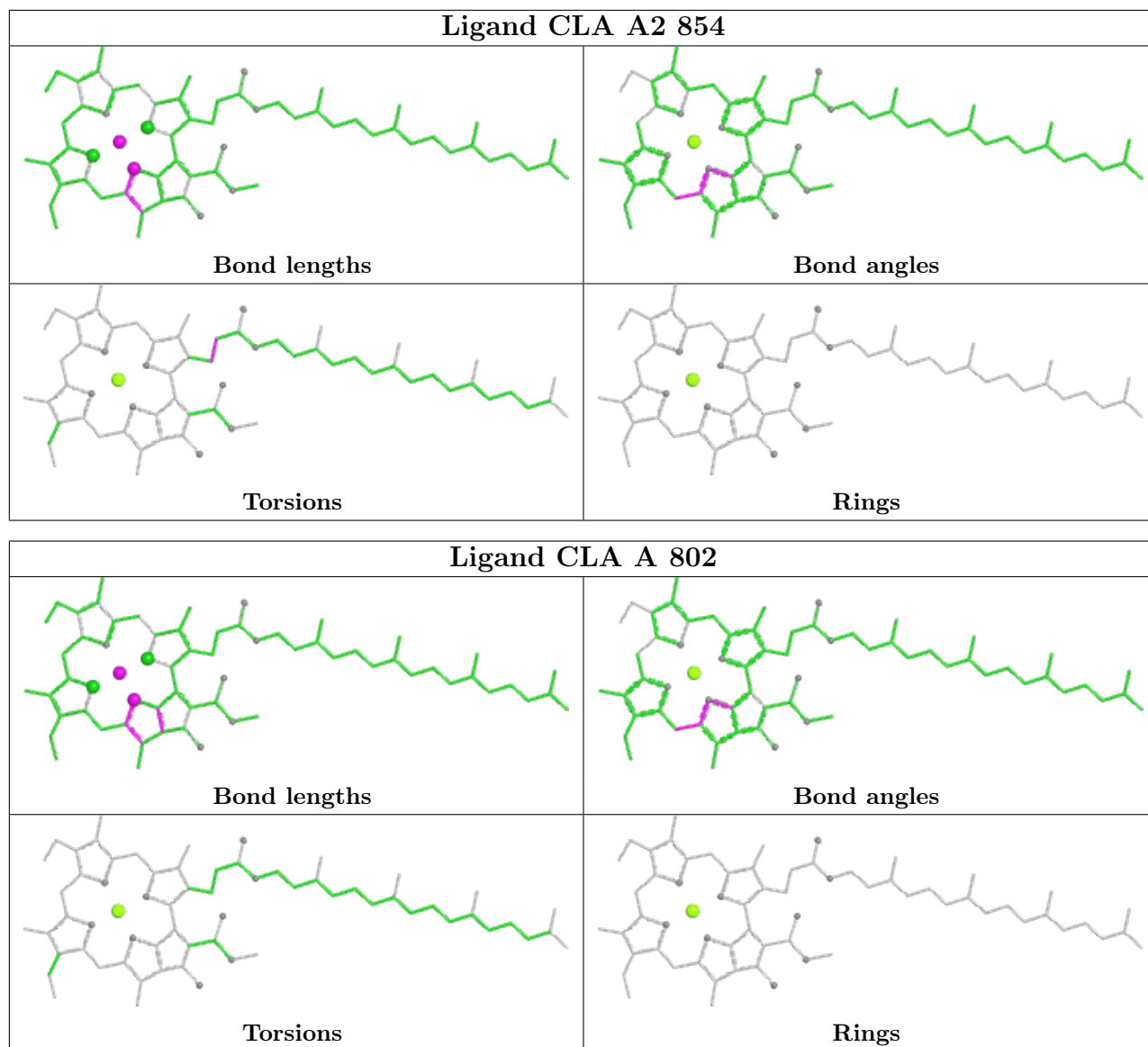


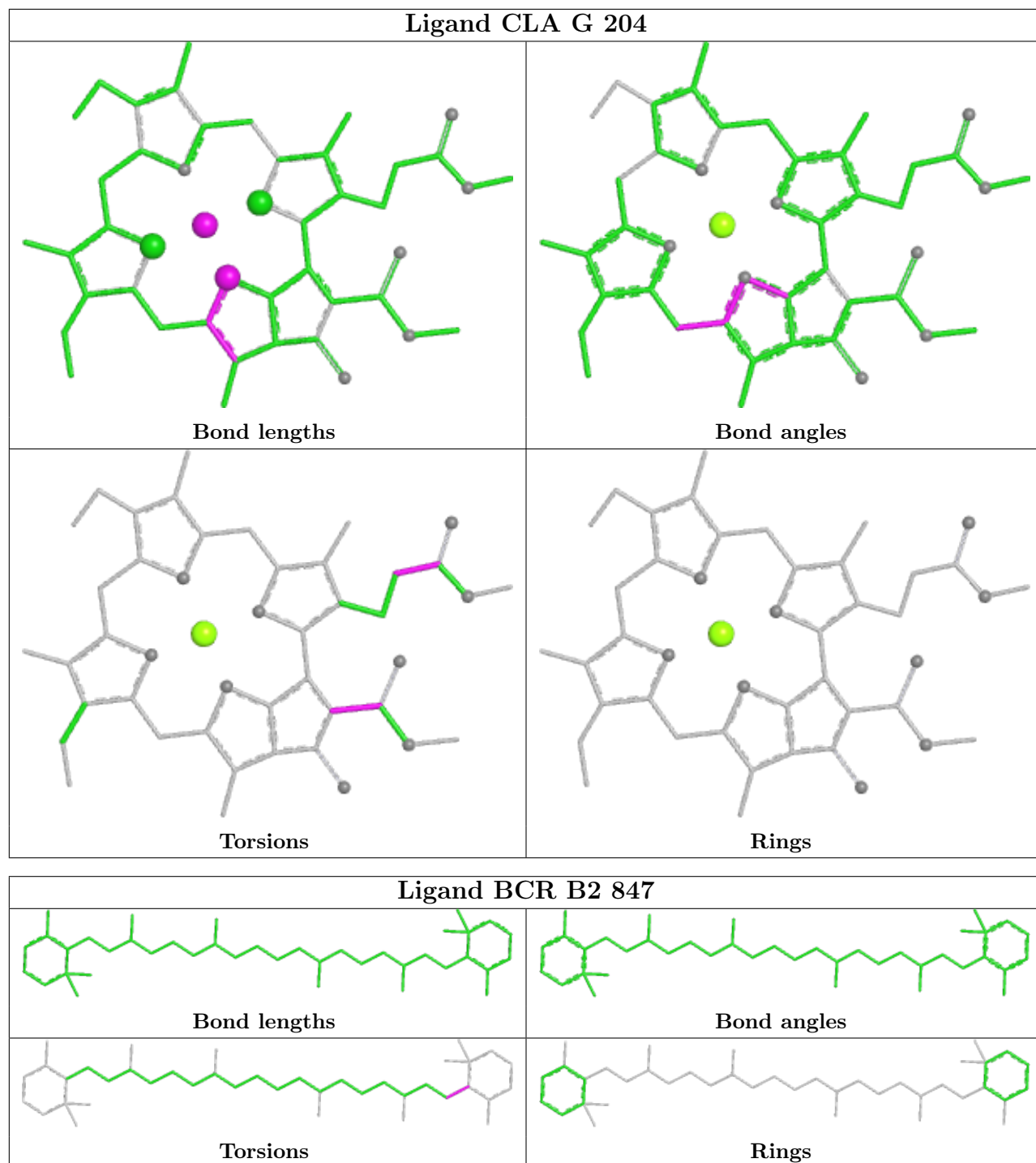
Ligand CLA 7 609

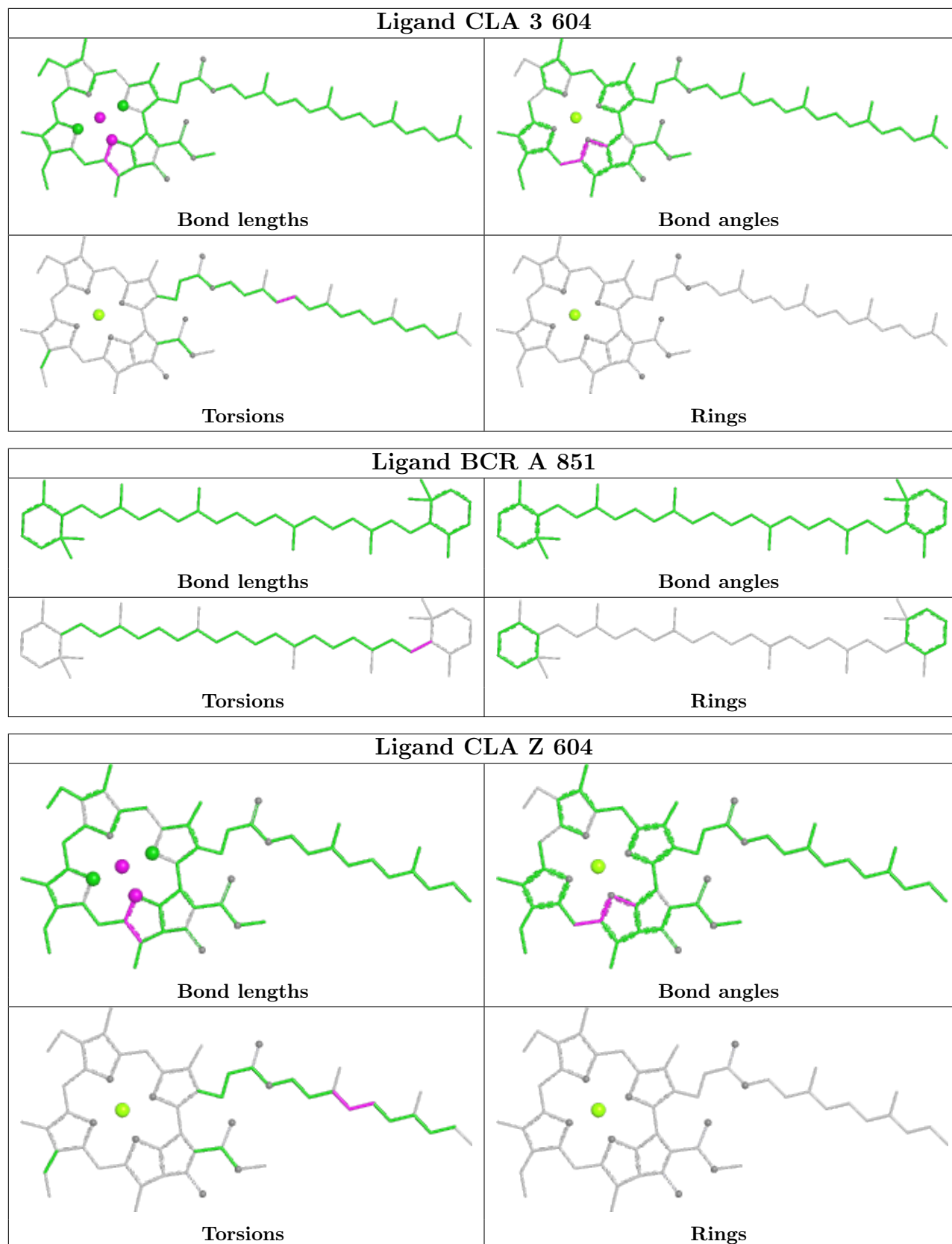


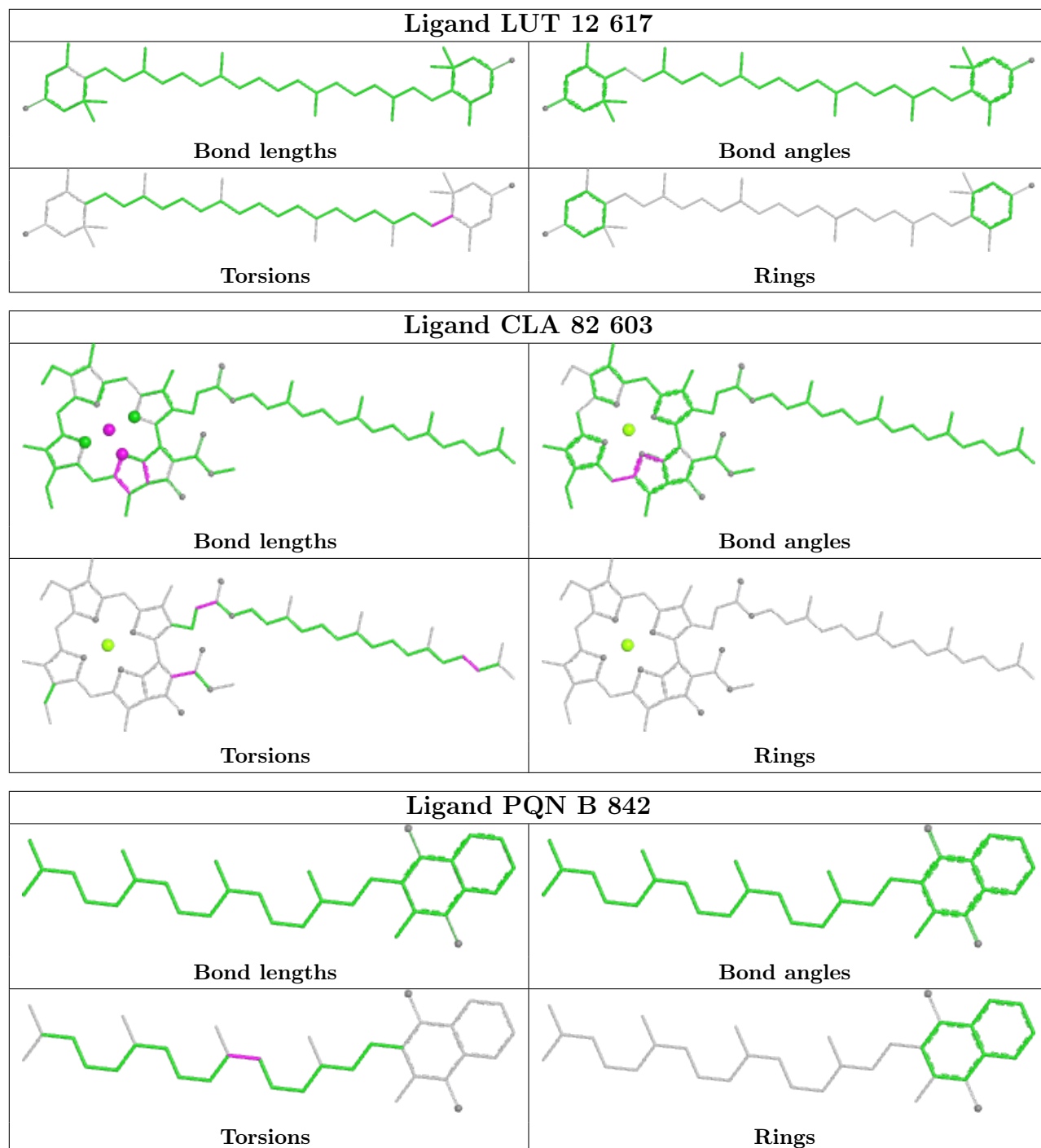
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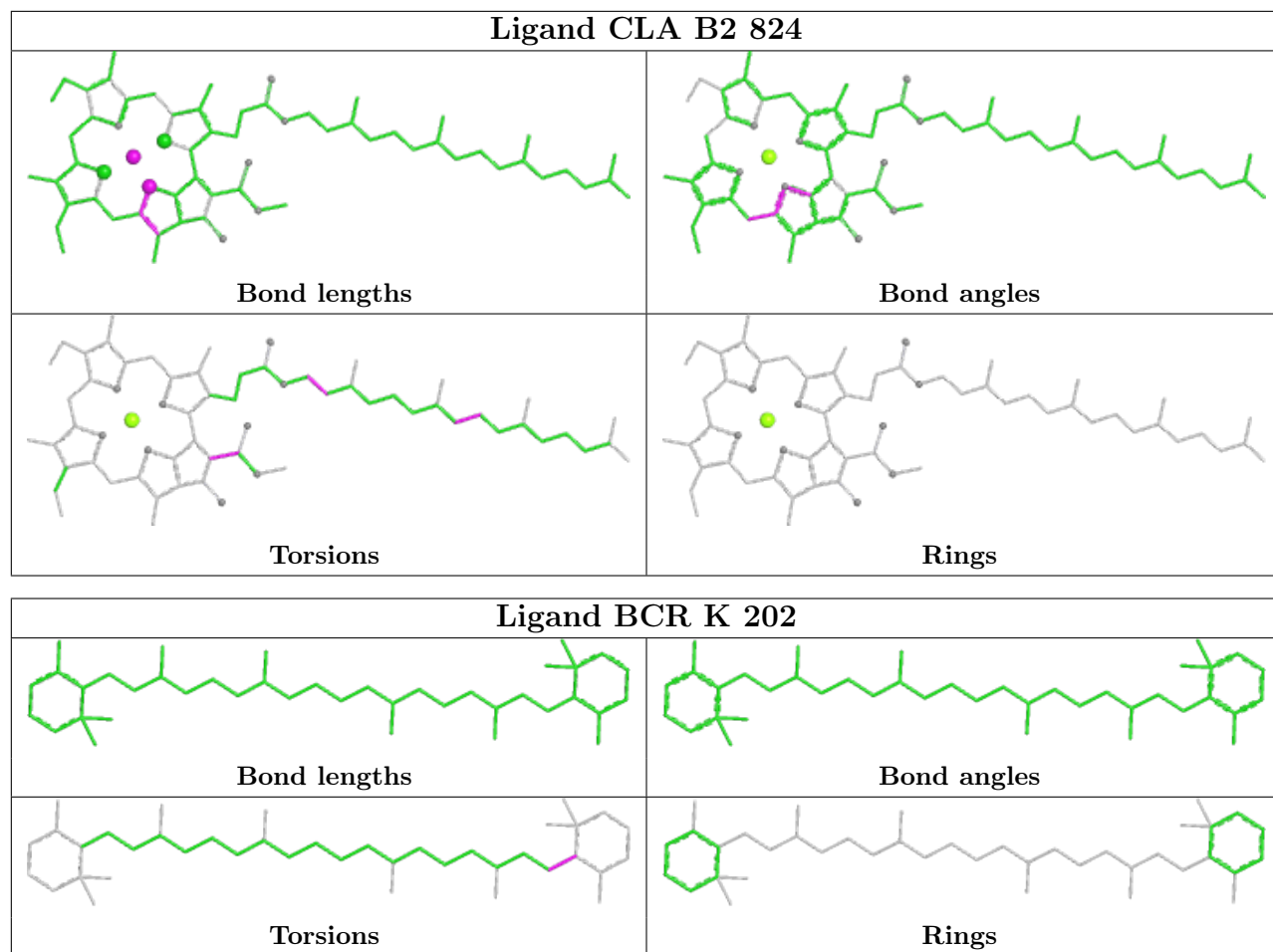


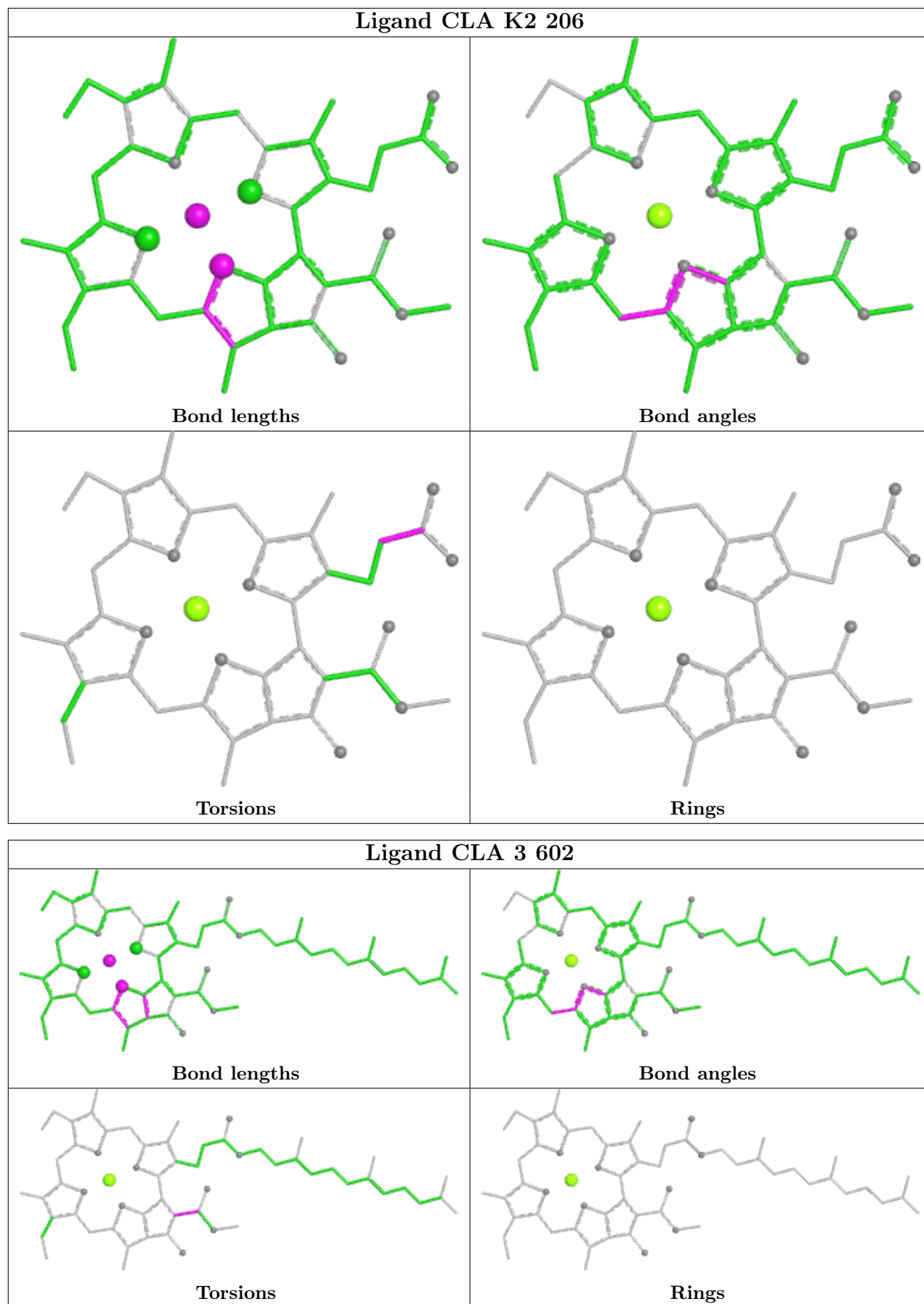


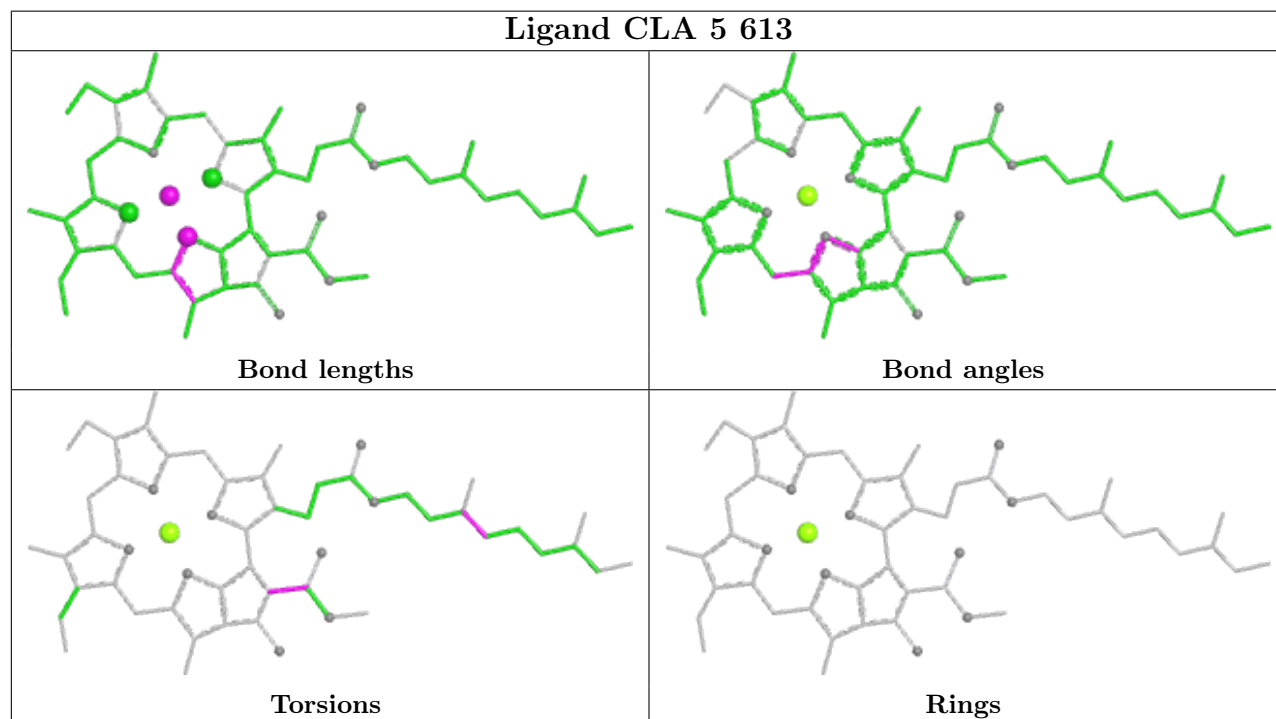
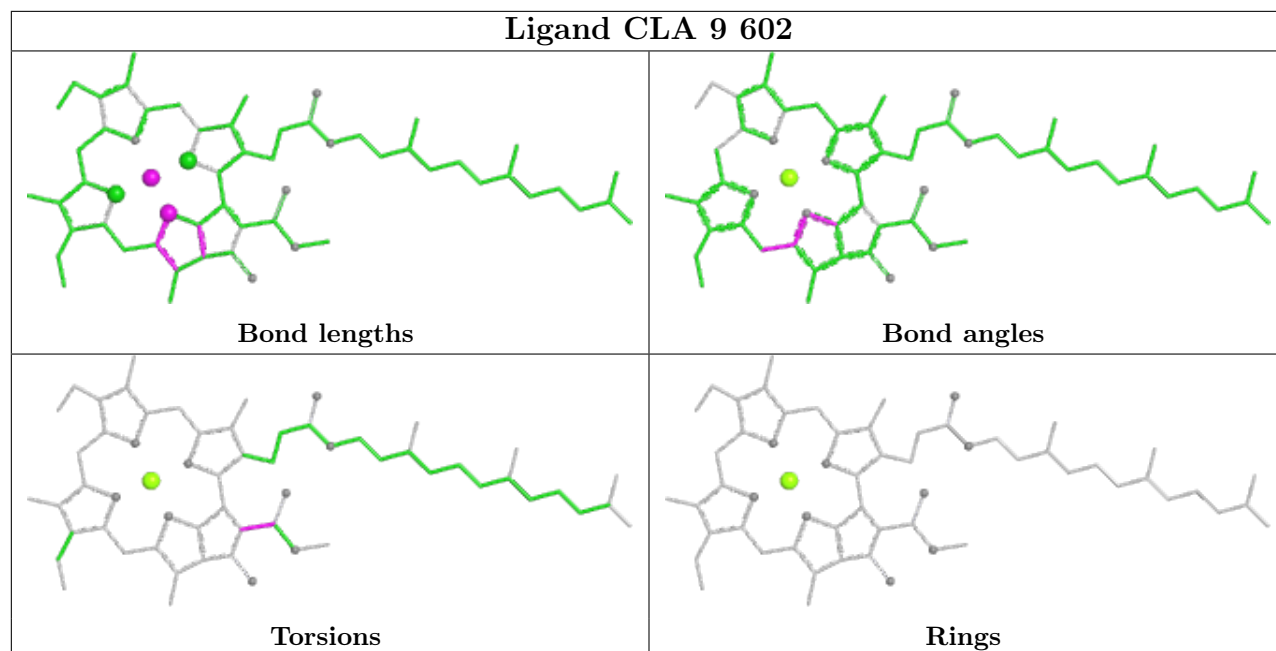


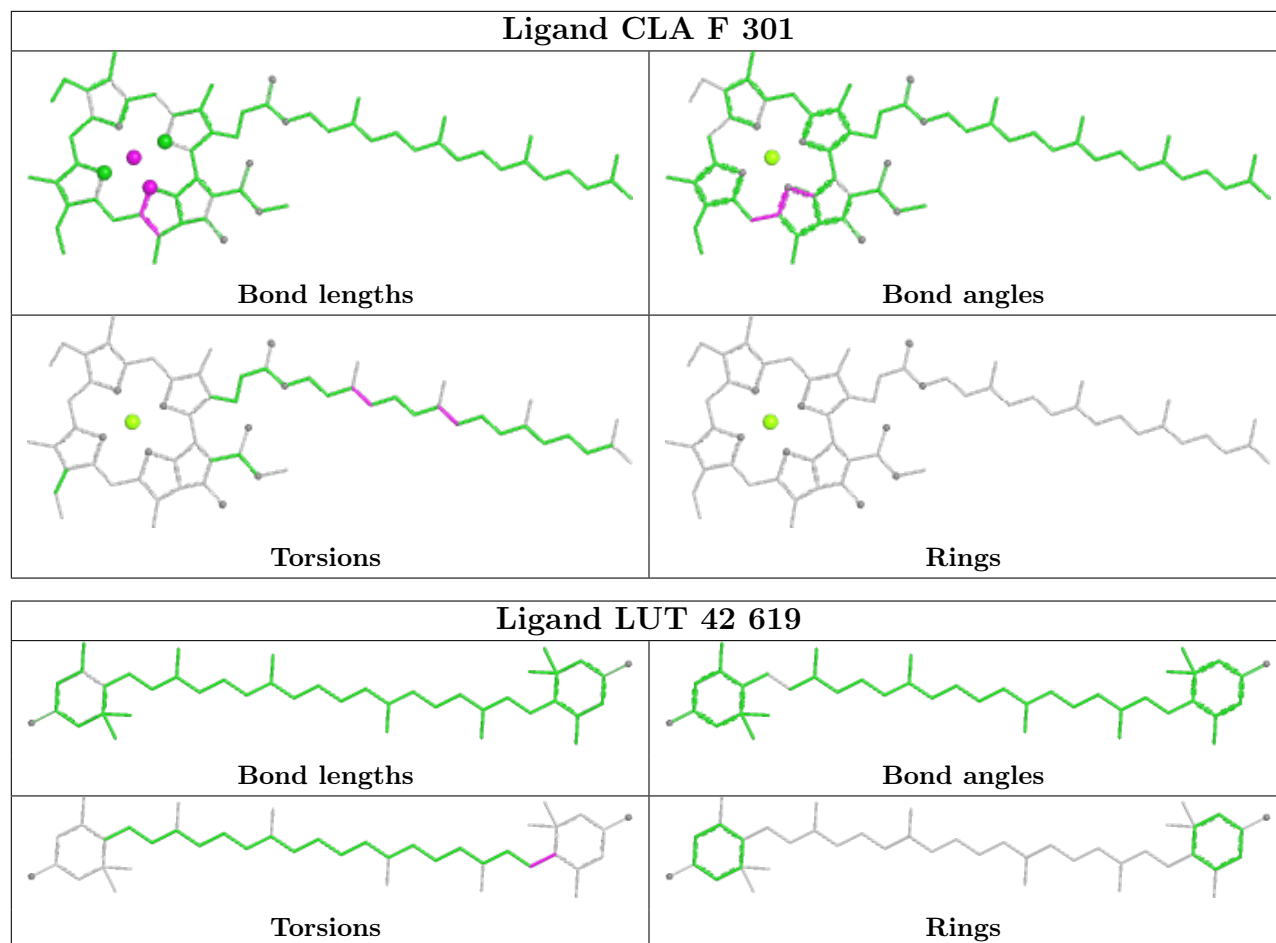


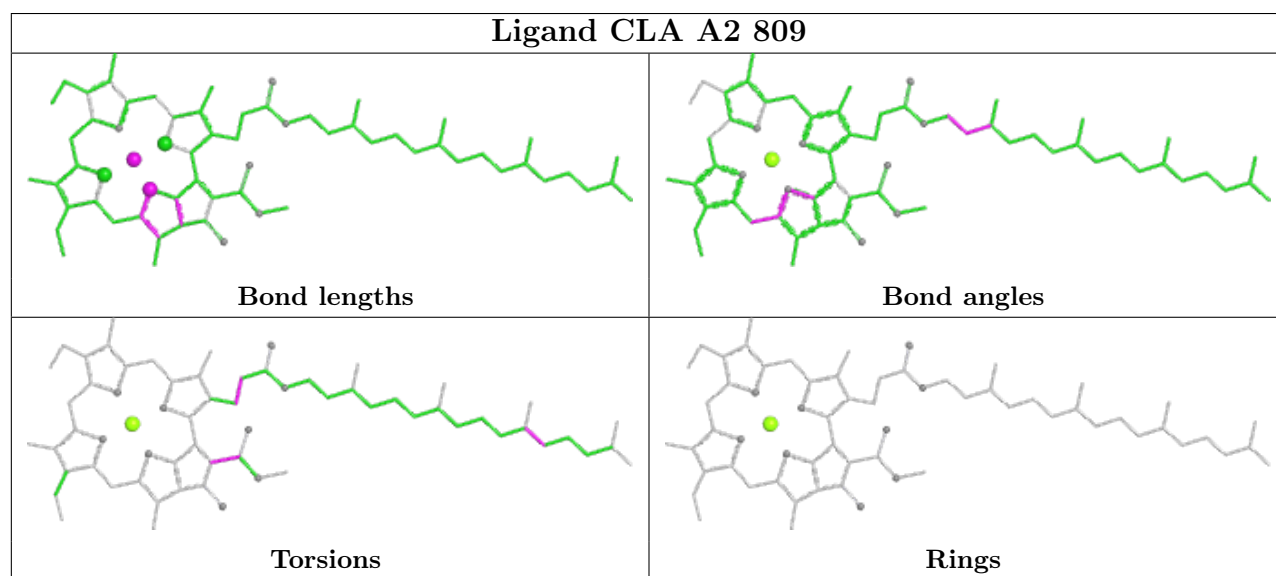
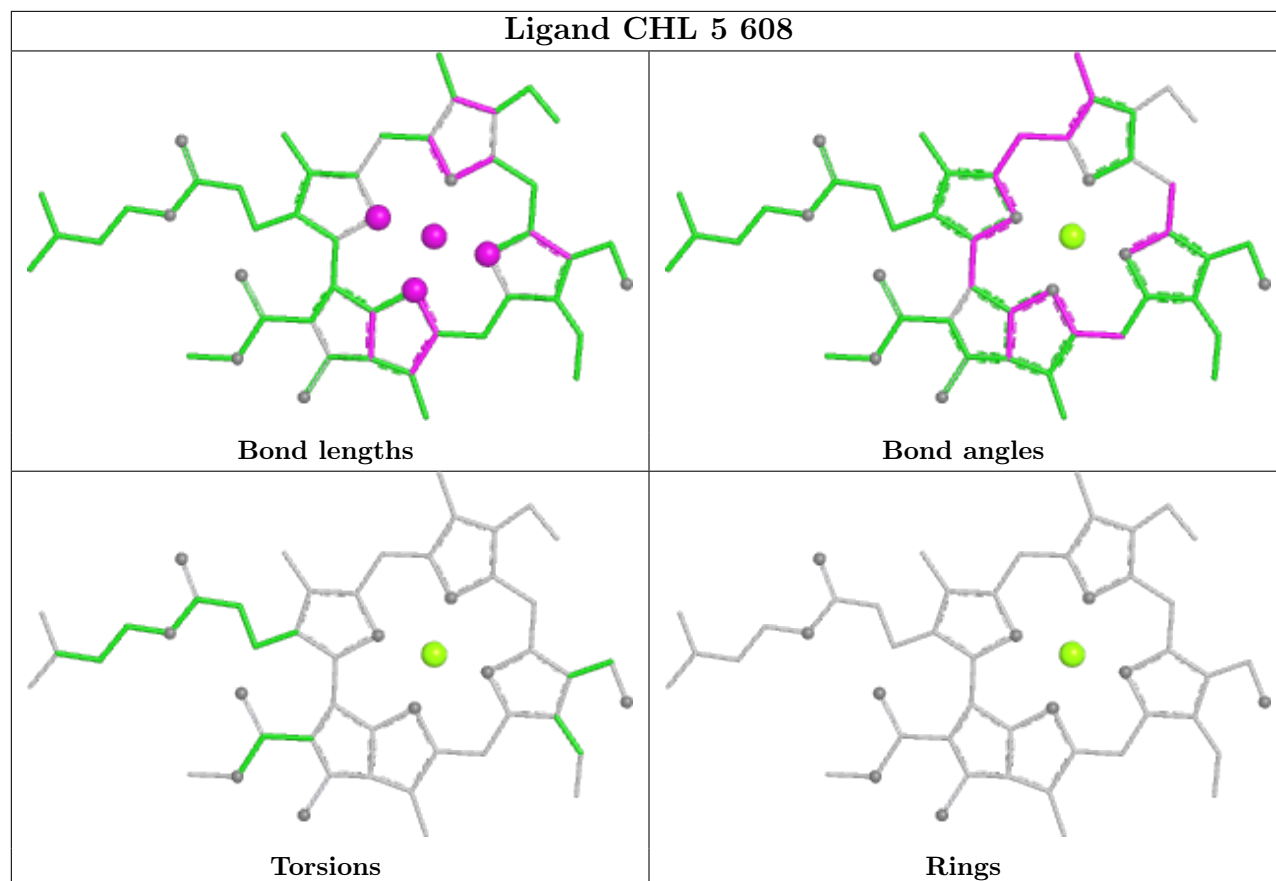


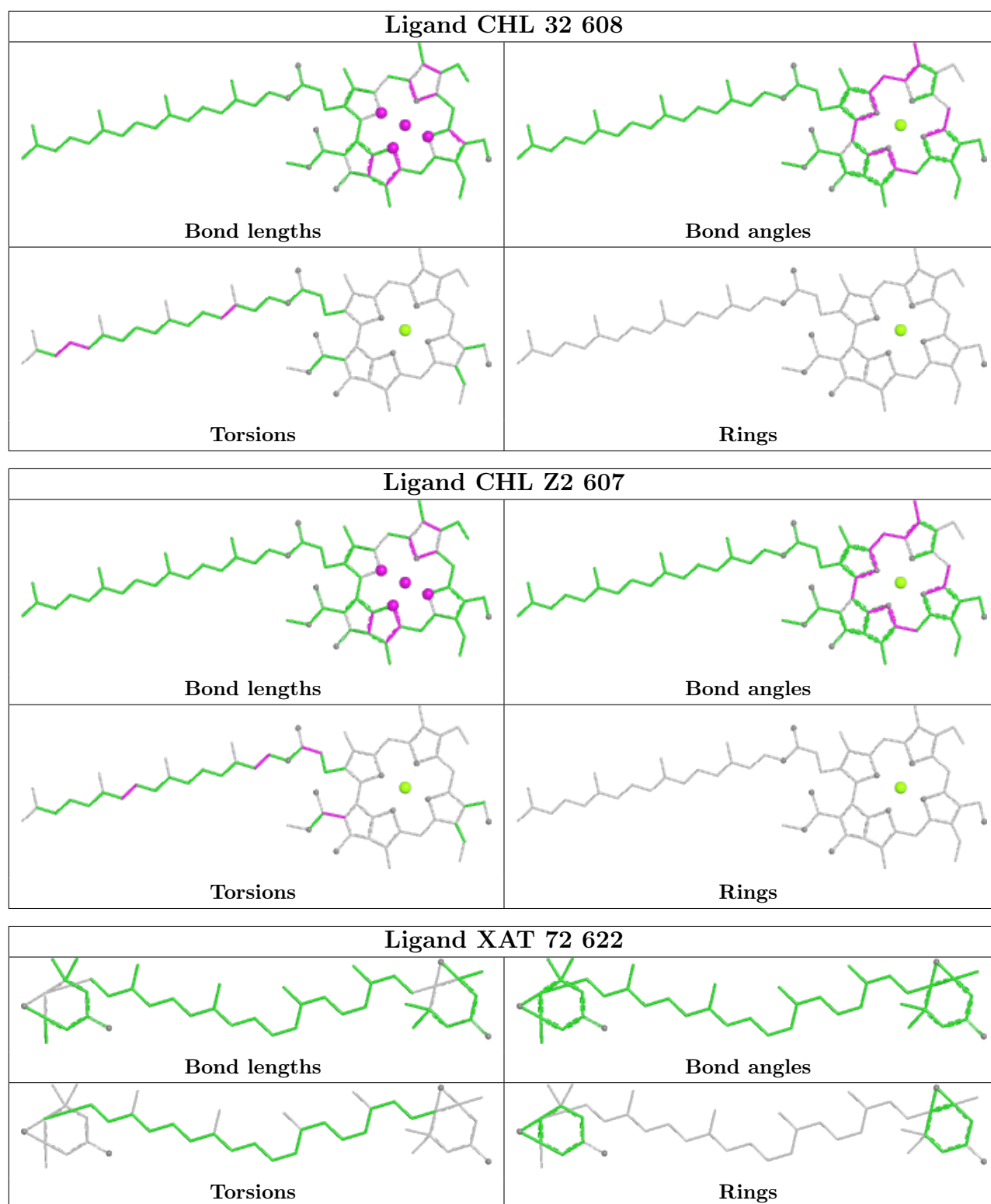


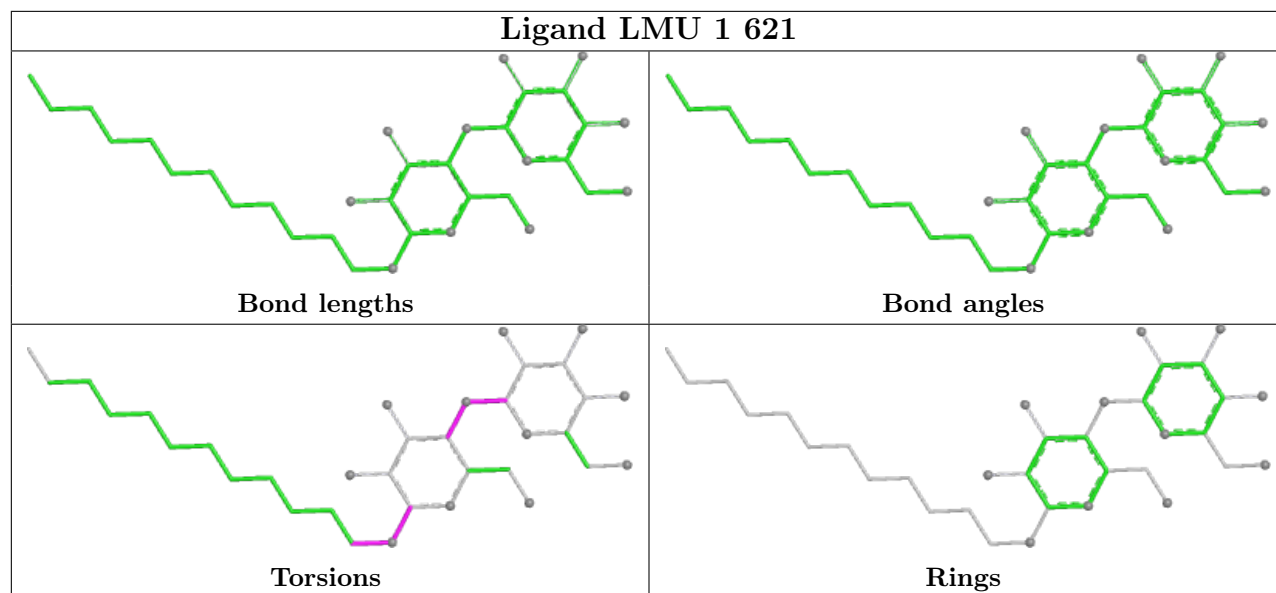












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

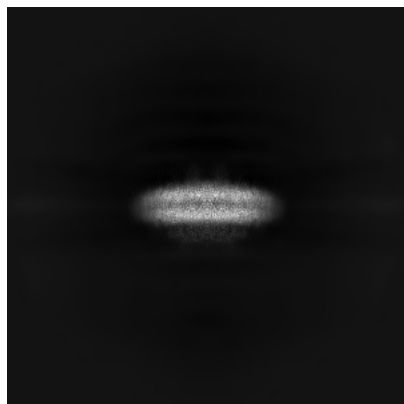
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14871. These allow visual inspection of the internal detail of the map and identification of artifacts.

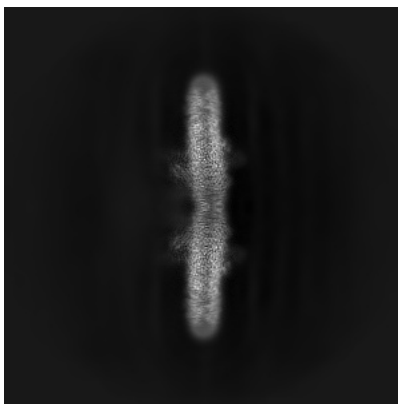
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

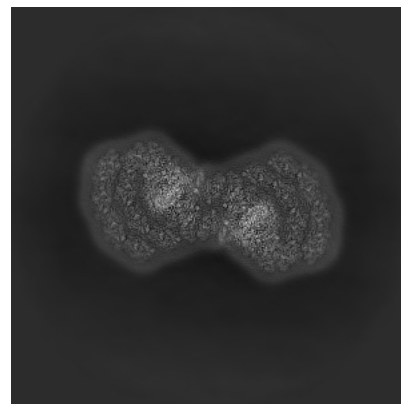
6.1.1 Primary map



X

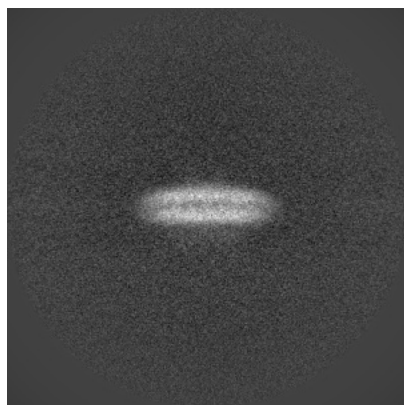


Y

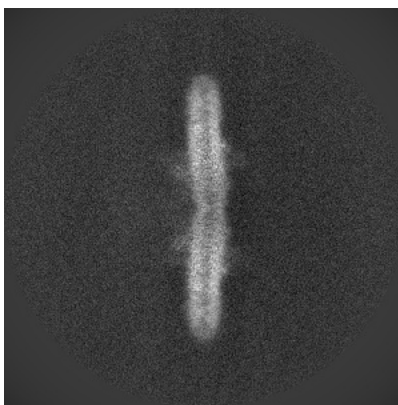


Z

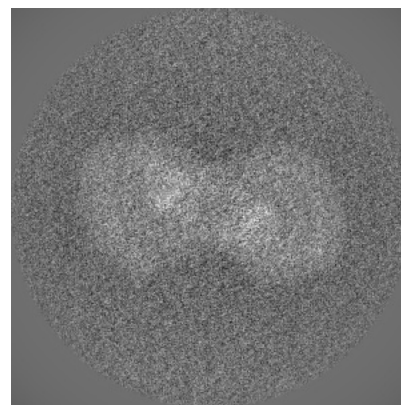
6.1.2 Raw map



X



Y



Z

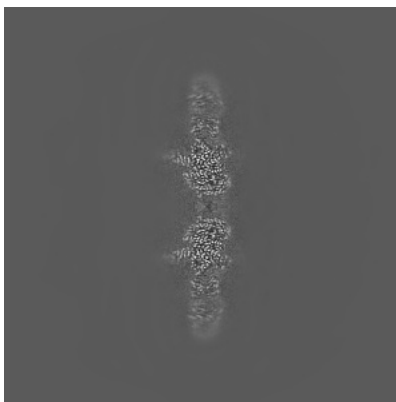
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

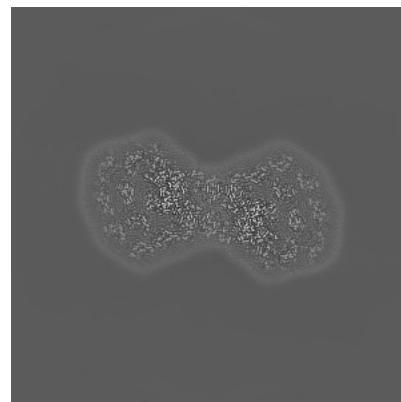
6.2.1 Primary map



X Index: 350

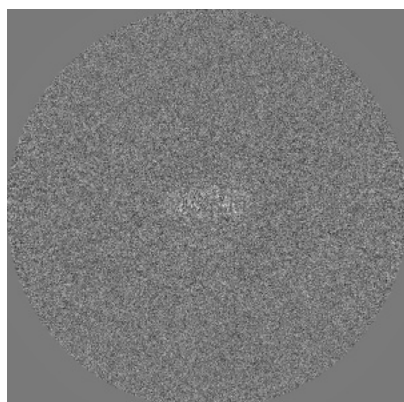


Y Index: 350

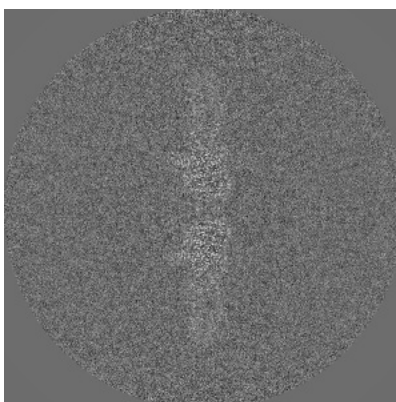


Z Index: 350

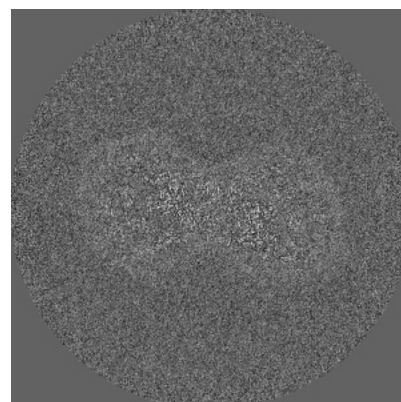
6.2.2 Raw map



X Index: 350



Y Index: 350



Z Index: 350

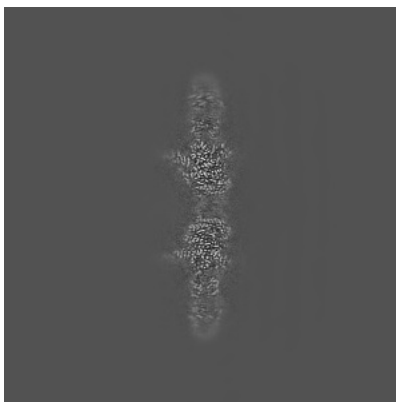
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

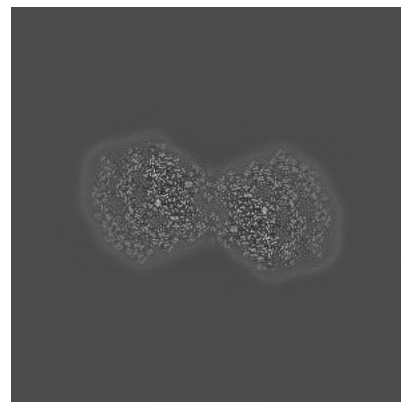
6.3.1 Primary map



X Index: 422

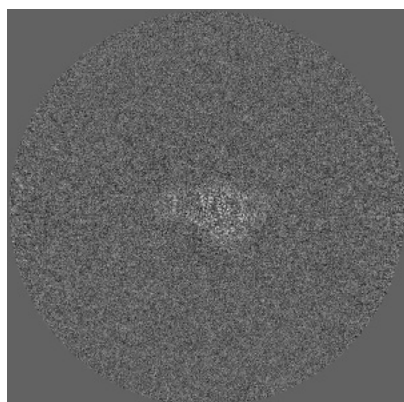


Y Index: 349

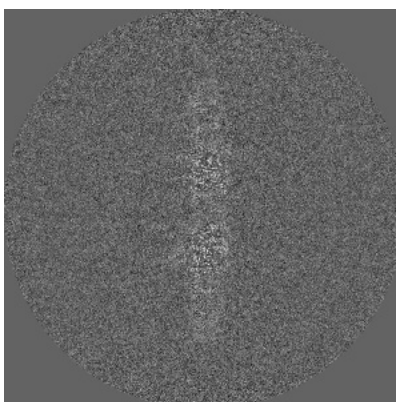


Z Index: 340

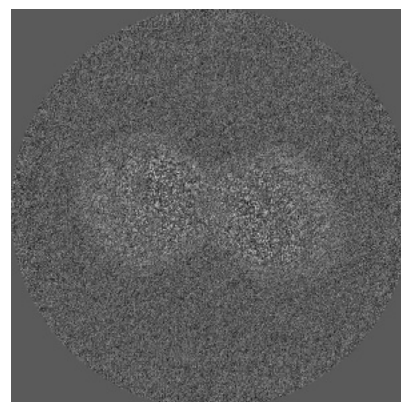
6.3.2 Raw map



X Index: 292



Y Index: 355

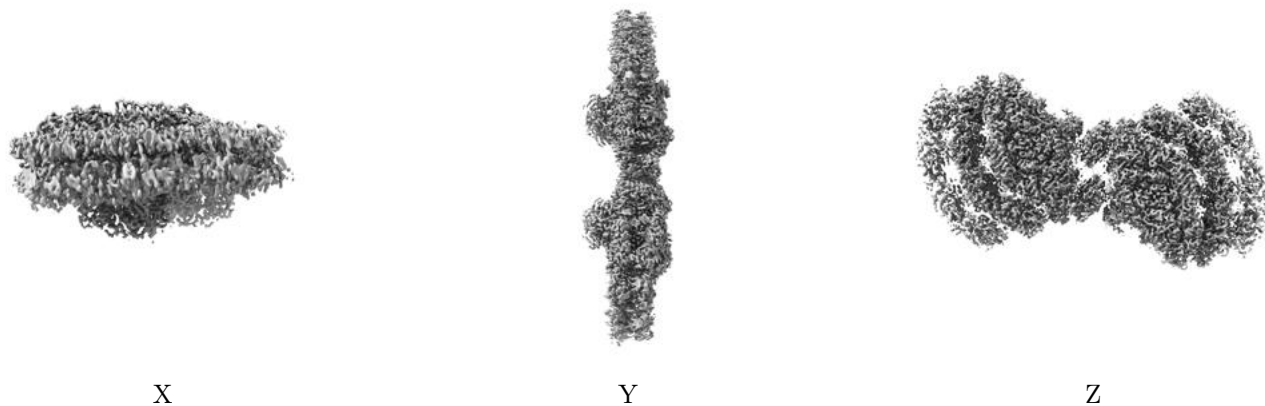


Z Index: 339

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

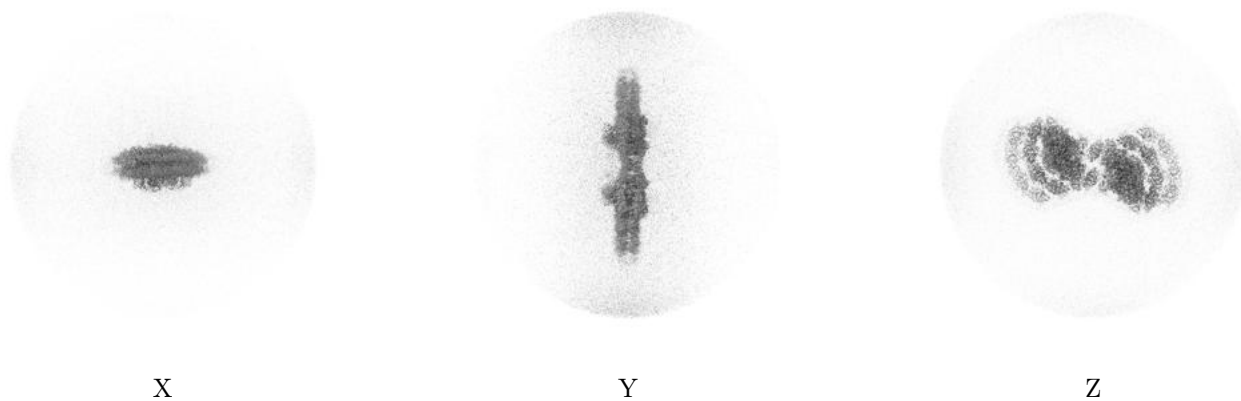
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.036. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

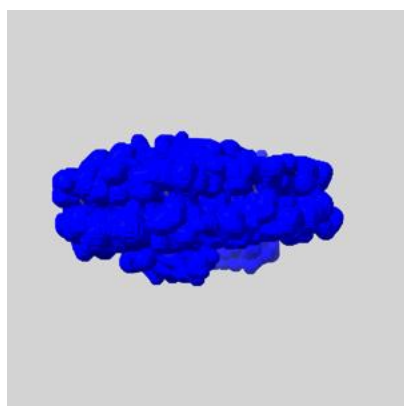
6.5 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

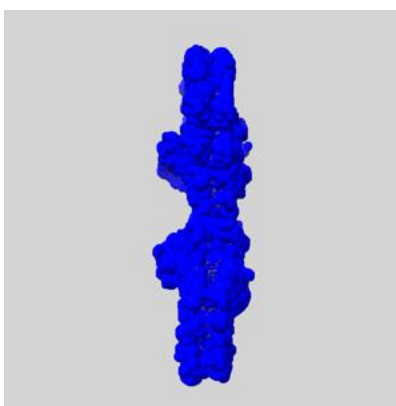
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

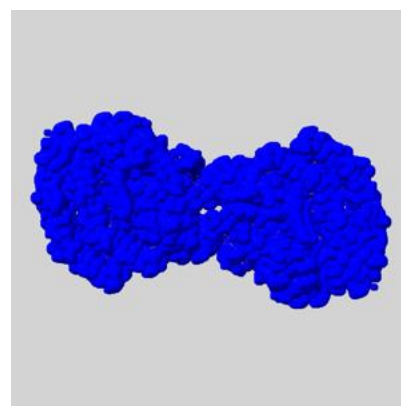
6.5.1 emd_14871_msk_1.map [i](#)



X



Y

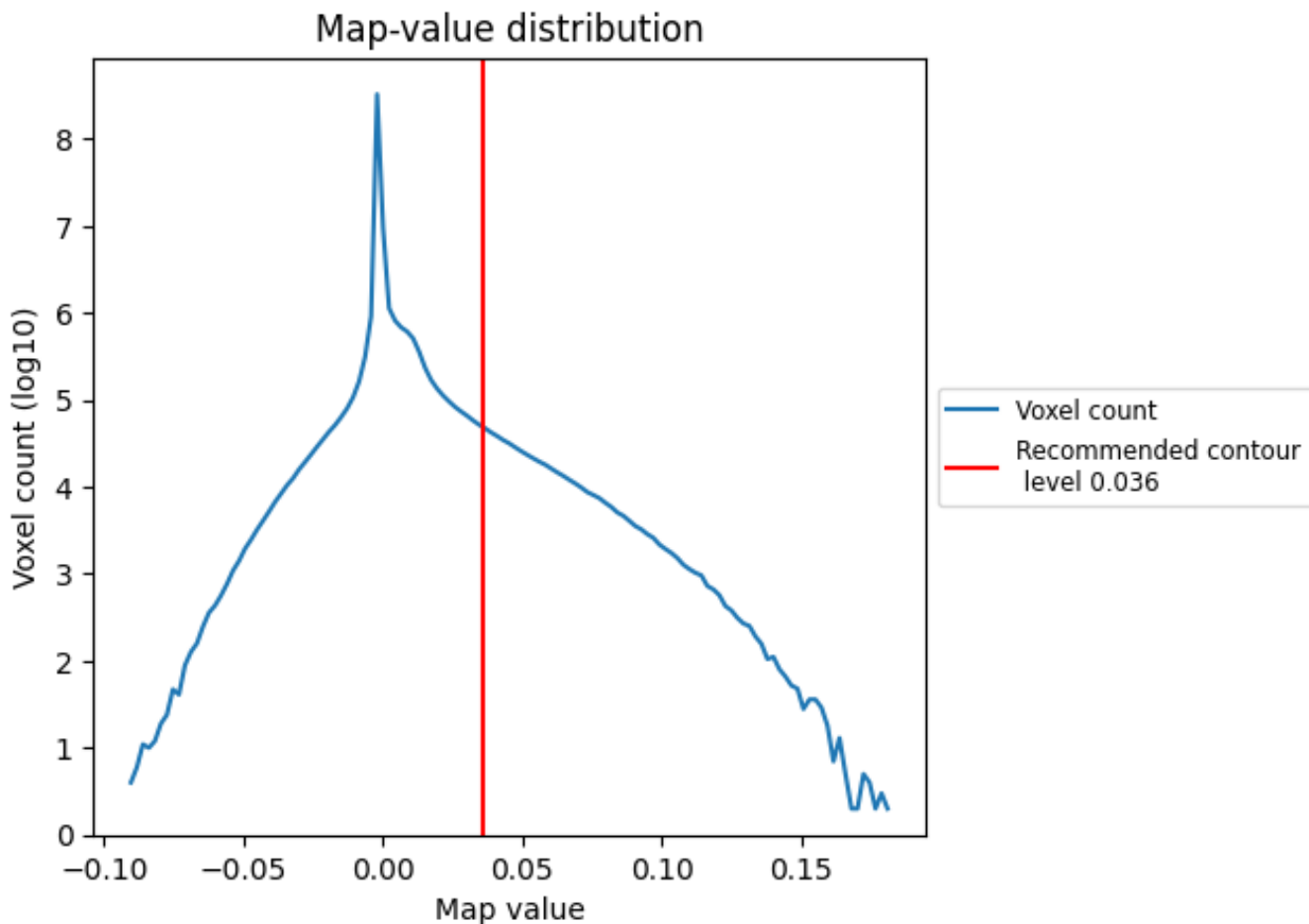


Z

7 Map analysis [i](#)

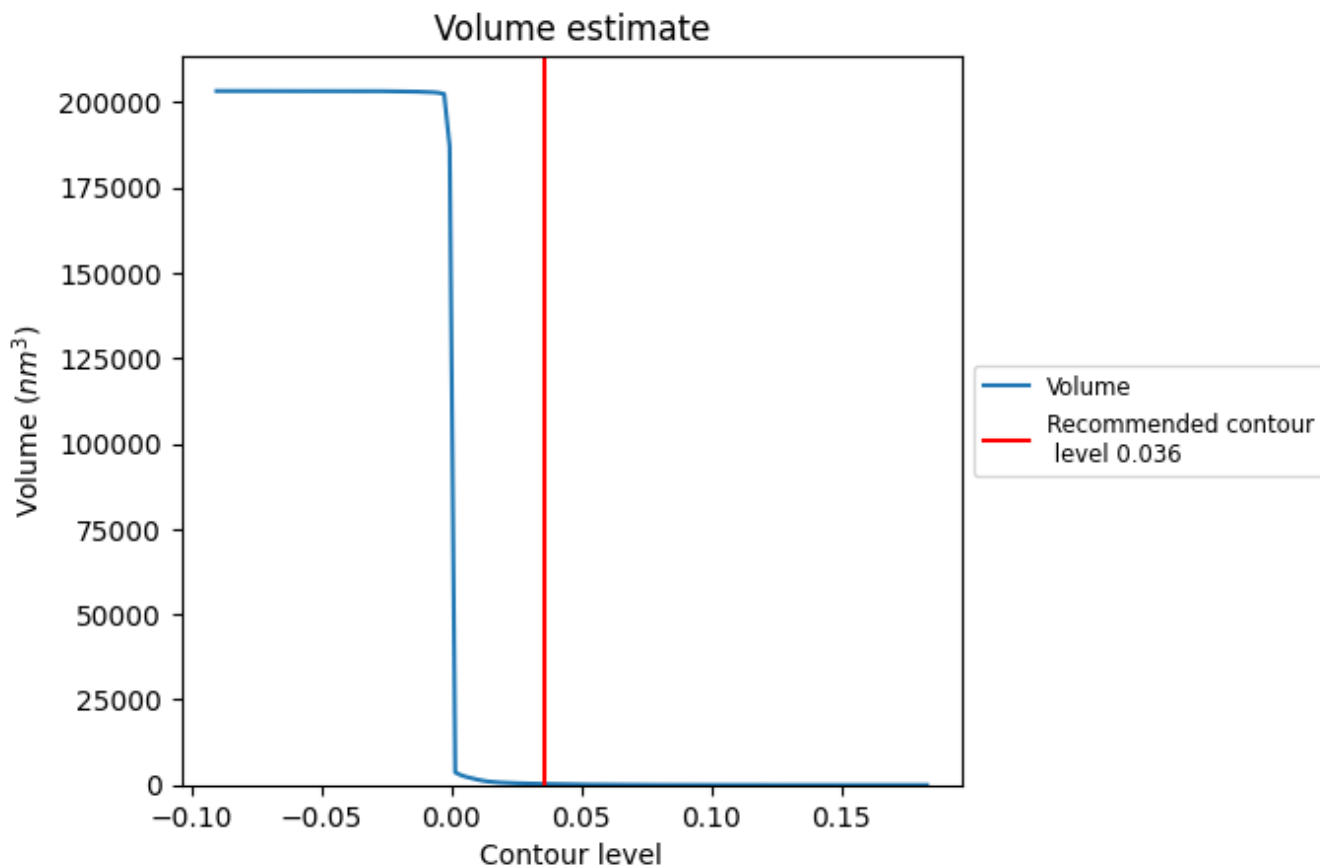
This section contains the results of statistical analysis of the map.

7.1 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.

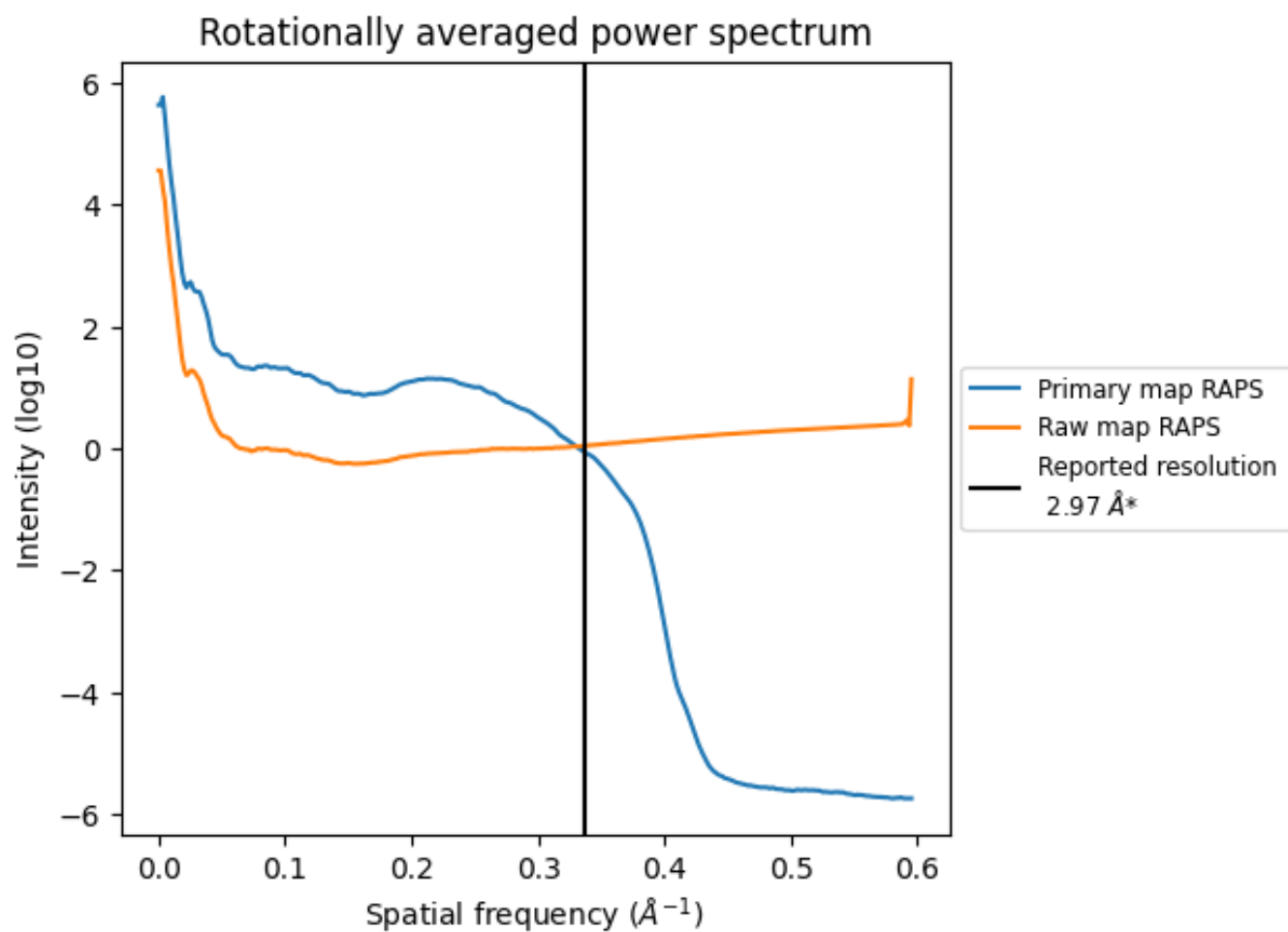
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 297 nm^3 ; this corresponds to an approximate mass of 268 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.

7.3 Rotationally averaged power spectrum i

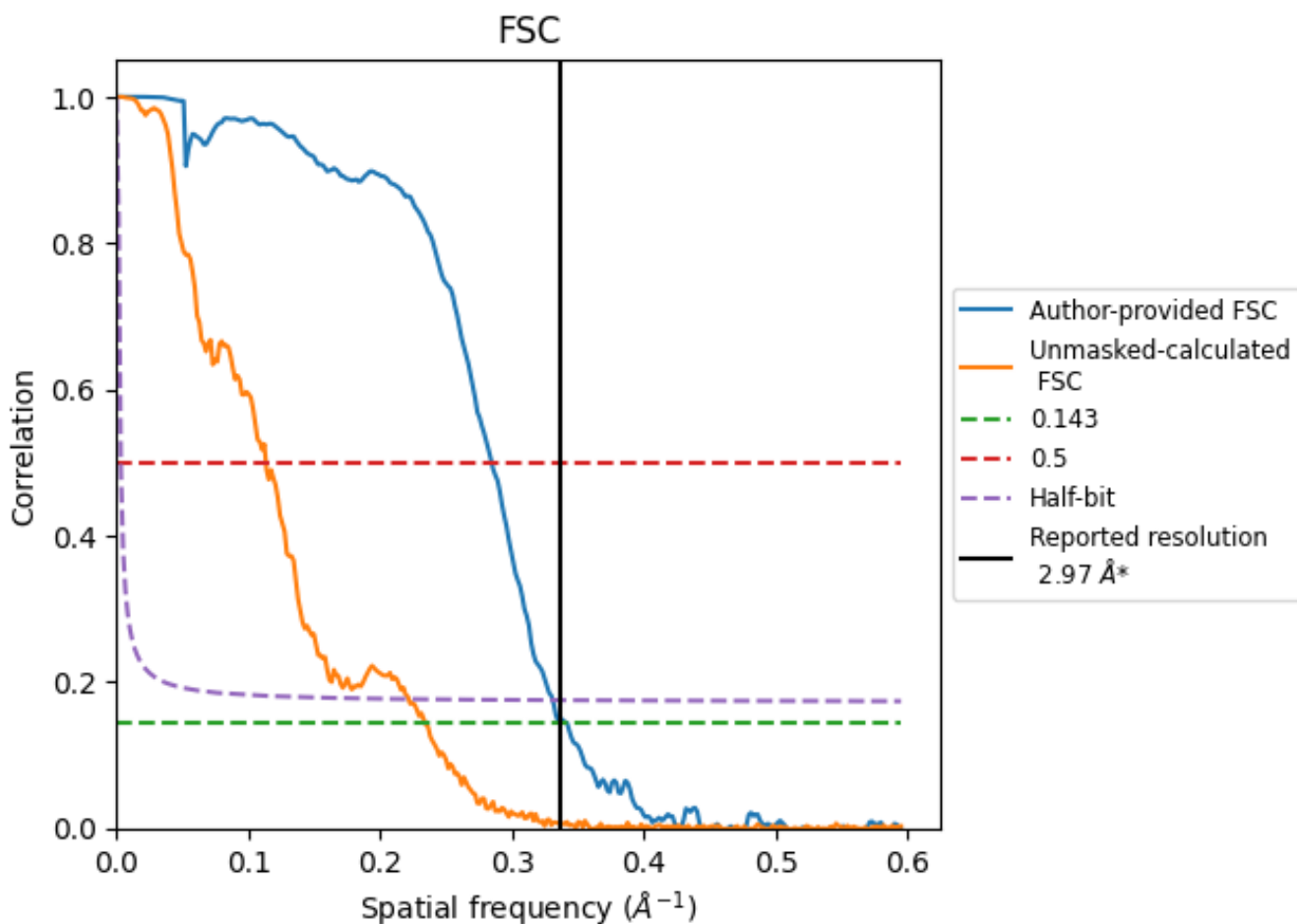


*Reported resolution corresponds to spatial frequency of 0.337 Å⁻¹

8 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.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.337 Å⁻¹

8.2 Resolution estimates [i](#)

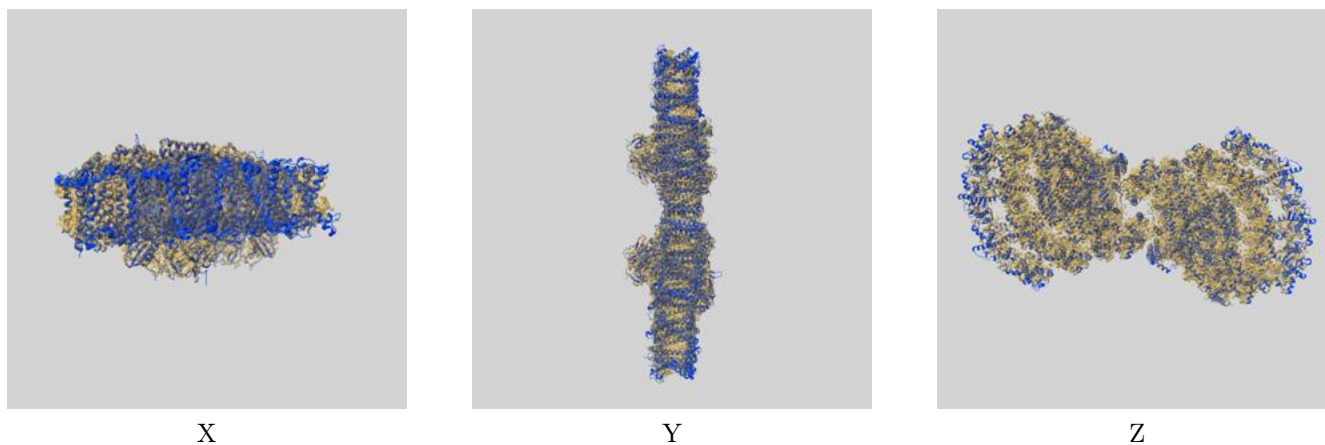
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.97	-	-
Author-provided FSC curve	2.92	3.51	3.02
Unmasked-calculated*	4.27	8.82	4.51

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.27 differs from the reported value 2.97 by more than 10 %

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-14871 and PDB model 7ZQD. Per-residue inclusion information can be found in section 3 on page 62.

9.1 Map-model overlay [i](#)

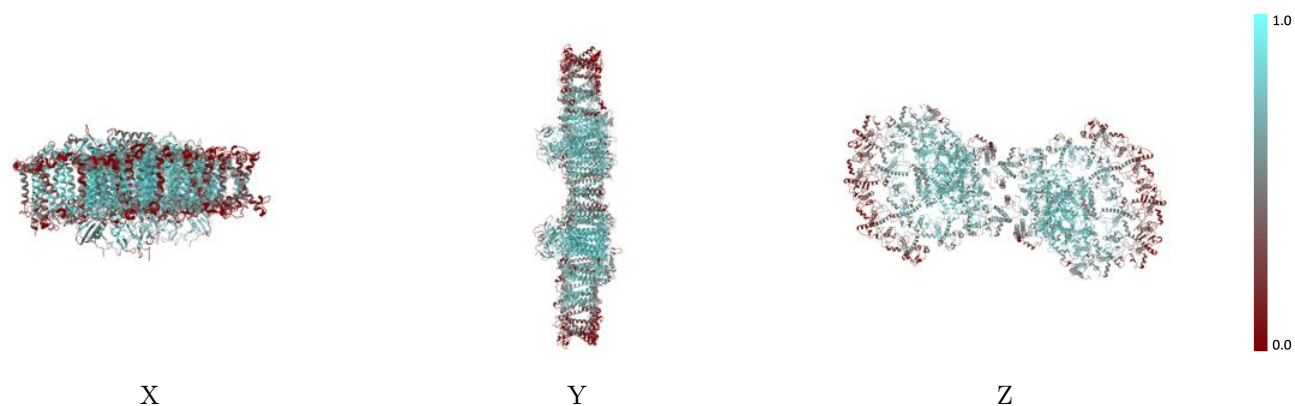


The images above show the 3D surface view of the map at the recommended contour level 0.036 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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

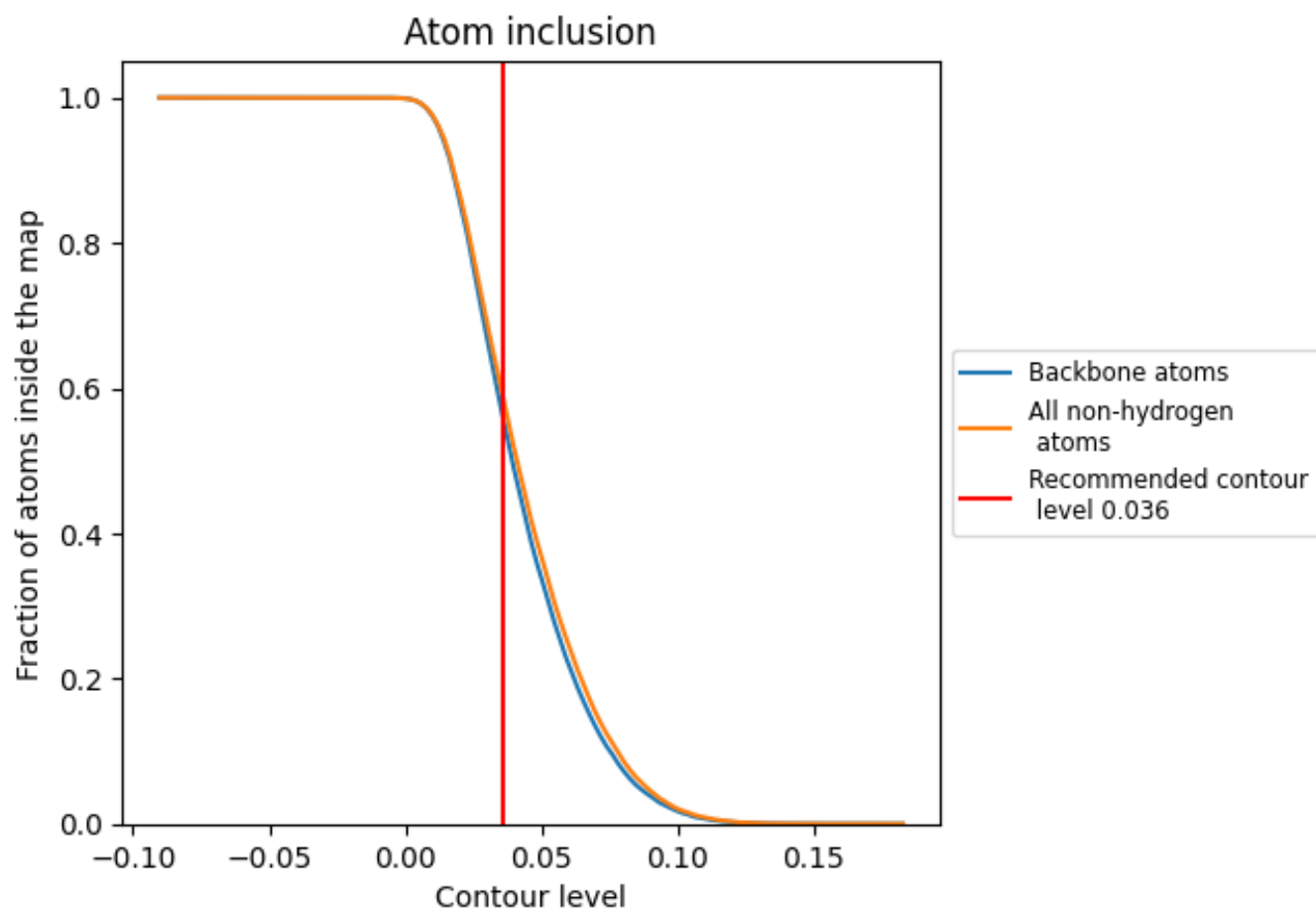
This section was not generated.

9.3 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 (0.036).

9.4 Atom inclusion [i](#)



At the recommended contour level, 56% of all backbone atoms, 59% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary [i](#)







The table lists the average atom inclusion at the recommended contour level (0.036) and Q-score for the entire model and for each chain.

Chain	Atom inclusion
All	0.5861
1	0.5836
12	0.5941
3	0.5550
32	0.5536
4	0.2174
42	0.2182
5	0.2788
52	0.2723
6	0.1972
62	0.2044
7	0.5825
72	0.5770
8	0.6234
82	0.6215
9	0.5399
92	0.5426
A	0.7974
A2	0.7976
B	0.8062
B2	0.8072
C	0.7496
C2	0.7512
D	0.5599
D2	0.5608
E	0.6126
E2	0.6045
F	0.6943
F2	0.6888
G	0.5064
G2	0.5052
I	0.5737
I2	0.5737
J	0.7276
J2	0.7337



Continued on next page...

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Chain	Atom inclusion
K	 0.3468
K2	 0.3191
L	 0.3927
L2	 0.3889
Z	 0.3190
Z2	 0.3190