



Full wwPDB EM Validation Report ⓘ

Nov 14, 2022 – 11:18 pm GMT

PDB ID : 7ZQ9
EMDB ID : EMD-14867
Title : Dimeric PSI of Chlamydomonas reinhardtii at 2.74 Å resolution (symmetry expanded)
Authors : Naschberger, A.; Amunts, A.
Deposited on : 2022-04-29
Resolution : 2.74 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:

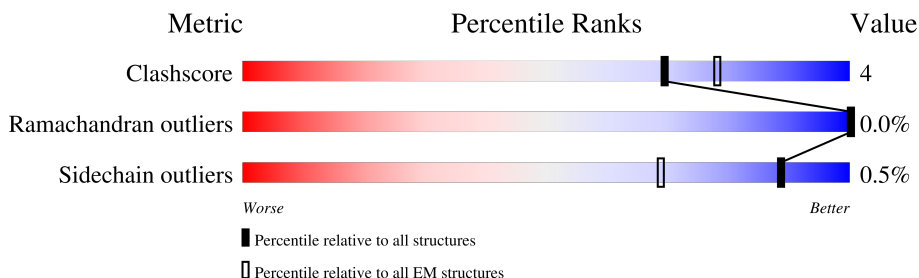
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : 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 2.74 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.



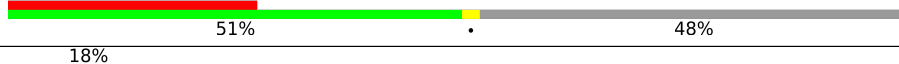

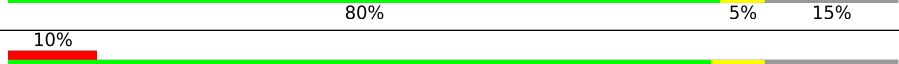
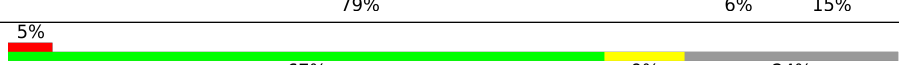
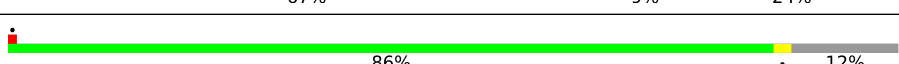
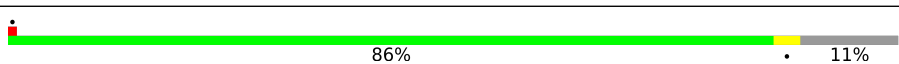

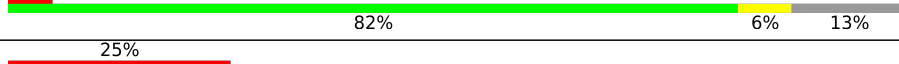
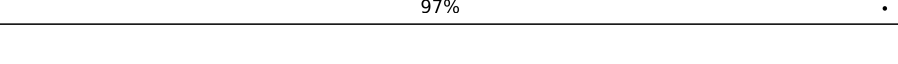
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	
2	B	735	
3	C	81	
4	D	196	
5	E	97	
6	F	227	
7	G	126	
8	I	106	

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Mol	Chain	Length	Quality of chain
8	I2	106	
9	J	40	
10	L	196	
10	L2	196	
11	K	113	
12	1	228	
12	Z	228	
13	3	298	
14	7	241	
15	8	243	
16	4	264	
17	5	257	
18	6	257	
19	9	213	
19	92	213	
20	B2	180	

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
21	CL0	A	801	X	-	-	-
22	CLA	1	602	X	-	-	-
22	CLA	1	603	X	-	-	-
22	CLA	1	604	X	-	-	-
22	CLA	1	608	X	-	-	-
22	CLA	1	609	X	-	-	-
22	CLA	1	610	X	-	-	-
22	CLA	1	611	X	-	-	-
22	CLA	1	612	X	-	-	-
22	CLA	1	613	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	1	614	X	-	-	-
22	CLA	1	616	X	-	-	-
22	CLA	3	602	X	-	-	-
22	CLA	3	603	X	-	-	-
22	CLA	3	604	X	-	-	-
22	CLA	3	606	X	-	-	-
22	CLA	3	607	X	-	-	-
22	CLA	3	609	X	-	-	-
22	CLA	3	610	X	-	-	-
22	CLA	3	611	X	-	-	-
22	CLA	3	612	X	-	-	-
22	CLA	3	613	X	-	-	-
22	CLA	3	614	X	-	-	-
22	CLA	3	615	X	-	-	-
22	CLA	3	617	X	-	-	-
22	CLA	4	602	X	-	-	-
22	CLA	4	603	X	-	-	-
22	CLA	4	604	X	-	-	-
22	CLA	4	609	X	-	-	-
22	CLA	4	610	X	-	-	-
22	CLA	4	611	X	-	-	-
22	CLA	4	612	X	-	-	-
22	CLA	4	613	X	-	-	-
22	CLA	4	614	X	-	-	-
22	CLA	4	616	X	-	-	-
22	CLA	5	601	X	-	-	-
22	CLA	5	602	X	-	-	-
22	CLA	5	603	X	-	-	-
22	CLA	5	604	X	-	-	-
22	CLA	5	609	X	-	-	-
22	CLA	5	610	X	-	-	-
22	CLA	5	611	X	-	-	-
22	CLA	5	612	X	-	-	-
22	CLA	5	613	X	-	-	-
22	CLA	5	614	X	-	-	-
22	CLA	5	616	X	-	-	-
22	CLA	5	617	X	-	-	-
22	CLA	5	621	X	-	-	-
22	CLA	6	602	X	-	-	-
22	CLA	6	603	X	-	-	-
22	CLA	6	604	X	-	-	-
22	CLA	6	609	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	6	610	X	-	-	-
22	CLA	6	611	X	-	-	-
22	CLA	6	612	X	-	-	-
22	CLA	6	613	X	-	-	-
22	CLA	6	614	X	-	-	-
22	CLA	6	617	X	-	-	-
22	CLA	6	622	X	-	-	-
22	CLA	7	602	X	-	-	-
22	CLA	7	603	X	-	-	-
22	CLA	7	604	X	-	-	-
22	CLA	7	608	X	-	-	-
22	CLA	7	609	X	-	-	-
22	CLA	7	610	X	-	-	-
22	CLA	7	611	X	-	-	-
22	CLA	7	612	X	-	-	-
22	CLA	7	613	X	-	-	-
22	CLA	7	614	X	-	-	-
22	CLA	7	616	X	-	-	-
22	CLA	7	620	X	-	-	-
22	CLA	8	602	X	-	-	-
22	CLA	8	603	X	-	-	-
22	CLA	8	604	X	-	-	-
22	CLA	8	608	X	-	-	-
22	CLA	8	609	X	-	-	-
22	CLA	8	610	X	-	-	-
22	CLA	8	611	X	-	-	-
22	CLA	8	612	X	-	-	-
22	CLA	8	613	X	-	-	-
22	CLA	8	614	X	-	-	-
22	CLA	8	616	X	-	-	-
22	CLA	9	601	X	-	-	-
22	CLA	9	602	X	-	-	-
22	CLA	9	603	X	-	-	-
22	CLA	9	604	X	-	-	-
22	CLA	9	609	X	-	-	-
22	CLA	9	610	X	-	-	-
22	CLA	9	611	X	-	-	-
22	CLA	9	612	X	-	-	-
22	CLA	9	613	X	-	-	-
22	CLA	9	614	X	-	-	-
22	CLA	92	601	X	-	-	-
22	CLA	92	602	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	92	603	X	-	-	-
22	CLA	92	604	X	-	-	-
22	CLA	92	609	X	-	-	-
22	CLA	92	610	X	-	-	-
22	CLA	92	611	X	-	-	-
22	CLA	92	612	X	-	-	-
22	CLA	92	613	X	-	-	-
22	CLA	92	614	X	-	-	-
22	CLA	A	802	X	-	-	-
22	CLA	A	803	X	-	-	-
22	CLA	A	804	X	-	-	-
22	CLA	A	805	X	-	-	-
22	CLA	A	806	X	-	-	-
22	CLA	A	807	X	-	-	-
22	CLA	A	808	X	-	-	-
22	CLA	A	809	X	-	-	-
22	CLA	A	810	X	-	-	-
22	CLA	A	811	X	-	-	-
22	CLA	A	812	X	-	-	-
22	CLA	A	813	X	-	-	-
22	CLA	A	814	X	-	-	-
22	CLA	A	815	X	-	-	-
22	CLA	A	816	X	-	-	-
22	CLA	A	817	X	-	-	-
22	CLA	A	818	X	-	-	-
22	CLA	A	819	X	-	-	-
22	CLA	A	820	X	-	-	-
22	CLA	A	821	X	-	-	-
22	CLA	A	822	X	-	-	-
22	CLA	A	823	X	-	-	-
22	CLA	A	824	X	-	-	-
22	CLA	A	825	X	-	-	-
22	CLA	A	826	X	-	-	-
22	CLA	A	827	X	-	-	-
22	CLA	A	828	X	-	-	-
22	CLA	A	829	X	-	-	-
22	CLA	A	830	X	-	-	-
22	CLA	A	831	X	-	-	-
22	CLA	A	832	X	-	-	-
22	CLA	A	833	X	-	-	-
22	CLA	A	834	X	-	-	-
22	CLA	A	835	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	A	836	X	-	-	-
22	CLA	A	837	X	-	-	-
22	CLA	A	838	X	-	-	-
22	CLA	A	839	X	-	-	-
22	CLA	A	840	X	-	-	-
22	CLA	A	841	X	-	-	-
22	CLA	A	842	X	-	-	-
22	CLA	A	843	X	-	-	-
22	CLA	A	845	X	-	-	-
22	CLA	A	854	X	-	-	-
22	CLA	B	802	X	-	-	-
22	CLA	B	803	X	-	-	-
22	CLA	B	804	X	-	-	-
22	CLA	B	805	X	-	-	-
22	CLA	B	806	X	-	-	-
22	CLA	B	807	X	-	-	-
22	CLA	B	808	X	-	-	-
22	CLA	B	809	X	-	-	-
22	CLA	B	810	X	-	-	-
22	CLA	B	811	X	-	-	-
22	CLA	B	812	X	-	-	-
22	CLA	B	813	X	-	-	-
22	CLA	B	814	X	-	-	-
22	CLA	B	815	X	-	-	-
22	CLA	B	816	X	-	-	-
22	CLA	B	817	X	-	-	-
22	CLA	B	818	X	-	-	-
22	CLA	B	819	X	-	-	-
22	CLA	B	820	X	-	-	-
22	CLA	B	821	X	-	-	-
22	CLA	B	822	X	-	-	-
22	CLA	B	823	X	-	-	-
22	CLA	B	824	X	-	-	-
22	CLA	B	825	X	-	-	-
22	CLA	B	826	X	-	-	-
22	CLA	B	827	X	-	-	-
22	CLA	B	828	X	-	-	-
22	CLA	B	829	X	-	-	-
22	CLA	B	830	X	-	-	-
22	CLA	B	831	X	-	-	-
22	CLA	B	832	X	-	-	-
22	CLA	B	833	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	B	834	X	-	-	-
22	CLA	B	835	X	-	-	-
22	CLA	B	836	X	-	-	-
22	CLA	B	837	X	-	-	-
22	CLA	B	838	X	-	-	-
22	CLA	B	839	X	-	-	-
22	CLA	B	840	X	-	-	-
22	CLA	B	841	X	-	-	-
22	CLA	B2	804	X	-	-	-
22	CLA	B2	805	X	-	-	-
22	CLA	B2	806	X	-	-	-
22	CLA	B2	807	X	-	-	-
22	CLA	B2	808	X	-	-	-
22	CLA	B2	809	X	-	-	-
22	CLA	B2	810	X	-	-	-
22	CLA	B2	811	X	-	-	-
22	CLA	B2	812	X	-	-	-
22	CLA	B2	813	X	-	-	-
22	CLA	B2	814	X	-	-	-
22	CLA	B2	815	X	-	-	-
22	CLA	B2	820	X	-	-	-
22	CLA	B2	828	X	-	-	-
22	CLA	B2	829	X	-	-	-
22	CLA	B2	839	X	-	-	-
22	CLA	F	301	X	-	-	-
22	CLA	F	303	X	-	-	-
22	CLA	F	304	X	-	-	-
22	CLA	G	203	X	-	-	-
22	CLA	G	204	X	-	-	-
22	CLA	J	101	X	-	-	-
22	CLA	K	201	X	-	-	-
22	CLA	K	203	X	-	-	-
22	CLA	K	204	X	-	-	-
22	CLA	K	206	X	-	-	-
22	CLA	L	203	X	-	-	-
22	CLA	L	204	X	-	-	-
22	CLA	L2	203	X	-	-	-
22	CLA	L2	204	X	-	-	-
22	CLA	Z	602	X	-	-	-
22	CLA	Z	603	X	-	-	-
22	CLA	Z	604	X	-	-	-
22	CLA	Z	608	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	Z	609	X	-	-	-
22	CLA	Z	610	X	-	-	-
22	CLA	Z	611	X	-	-	-
22	CLA	Z	612	X	-	-	-
22	CLA	Z	613	X	-	-	-
22	CLA	Z	614	X	-	-	-
22	CLA	Z	616	X	-	-	-
31	CHL	1	601	X	-	-	-
31	CHL	1	606	X	-	-	-
31	CHL	1	607	X	-	-	-
31	CHL	3	608	X	-	-	-
31	CHL	4	601	X	-	-	-
31	CHL	4	606	X	-	-	-
31	CHL	4	607	X	-	-	-
31	CHL	4	608	X	-	-	-
31	CHL	4	618	X	-	-	-
31	CHL	5	606	X	-	-	-
31	CHL	5	607	X	-	-	-
31	CHL	5	608	X	-	-	-
31	CHL	5	618	X	-	-	-
31	CHL	6	601	X	-	-	-
31	CHL	6	606	X	-	-	-
31	CHL	6	607	X	-	-	-
31	CHL	6	608	X	-	-	-
31	CHL	6	616	X	-	-	-
31	CHL	6	618	X	-	-	-
31	CHL	7	601	X	-	-	-
31	CHL	7	606	X	-	-	-
31	CHL	7	607	X	-	-	-
31	CHL	8	601	X	-	-	-
31	CHL	8	606	X	-	-	-
31	CHL	8	607	X	-	-	-
31	CHL	9	606	X	-	-	-
31	CHL	9	607	X	-	-	-
31	CHL	92	606	X	-	-	-
31	CHL	92	607	X	-	-	-
31	CHL	Z	601	X	-	-	-
31	CHL	Z	606	X	-	-	-
31	CHL	Z	607	X	-	-	-
32	XAT	1	618	X	-	-	-
32	XAT	5	624	X	-	-	-
33	NEX	6	625	X	-	-	-

2 Entry composition [i](#)

There are 34 unique types of molecules in this entry. The entry contains 113459 atoms, of which 56999 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	11500	3808	5675	994	1001	22	0	0

- 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	11400	3824	5576	977	1005	18	0	0

- 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	1183	369	582	103	117	12	0	0

- 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	2284	725	1151	200	201	7	0	0

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

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

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

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

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

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

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

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

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

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

- Molecule 10 is a protein called PSI subunit V.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
10	L	124	1806	586	907	146	164	3	0	0
10	L2	102	1487	487	748	120	130	2	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

- 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

- 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

- 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

- 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

- 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

- 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

- 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

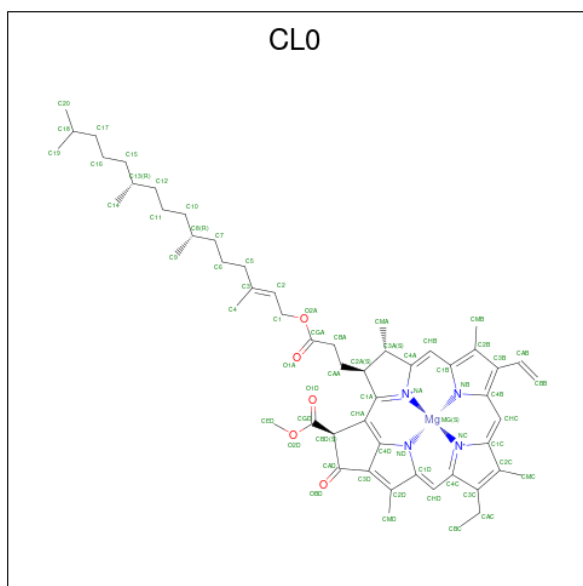
- Molecule 19 is a protein called Chlorophyll a-b binding protein, chloroplastic.

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	184	2802	913	1392	236	254	7	0	0

- Molecule 20 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

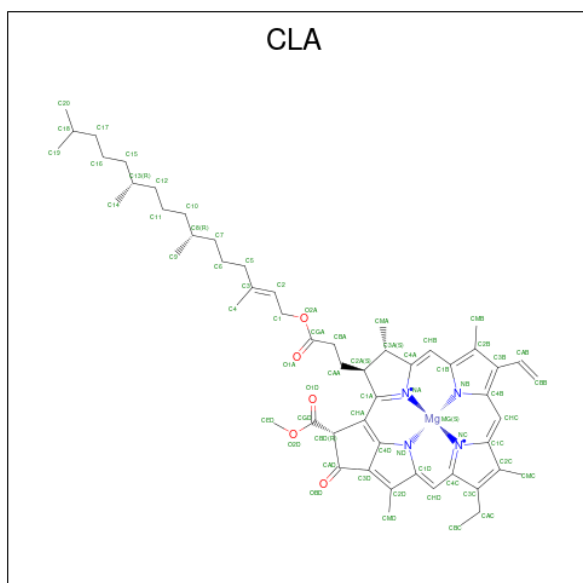
Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
20	B2	180	2865	972	1396	247	247	3	0	0

- Molecule 21 is CHLOROPHYLL A ISOMER (three-letter code: CLO) (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	137	55	72	1	4	5	0

- Molecule 22 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
22	A	1	Total	C	H	Mg	N	O	0
			5574	2278	2856	44	176	220	
22	A	1	Total	C	H	Mg	N	O	0
			5574	2278	2856	44	176	220	
22	A	1	Total	C	H	Mg	N	O	0
			5574	2278	2856	44	176	220	
22	A	1	Total	C	H	Mg	N	O	0
			5574	2278	2856	44	176	220	
22	A	1	Total	C	H	Mg	N	O	0
			5574	2278	2856	44	176	220	
22	A	1	Total	C	H	Mg	N	O	0
			5574	2278	2856	44	176	220	
22	A	1	Total	C	H	Mg	N	O	0
			5574	2278	2856	44	176	220	
22	A	1	Total	C	H	Mg	N	O	0
			5574	2278	2856	44	176	220	
22	A	1	Total	C	H	Mg	N	O	0
			5574	2278	2856	44	176	220	
22	A	1	Total	C	H	Mg	N	O	0
			5574	2278	2856	44	176	220	
22	A	1	Total	C	H	Mg	N	O	0
			5574	2278	2856	44	176	220	
22	A	1	Total	C	H	Mg	N	O	0
			5574	2278	2856	44	176	220	
22	A	1	Total	C	H	Mg	N	O	0
			5574	2278	2856	44	176	220	
22	A	1	Total	C	H	Mg	N	O	0
			5574	2278	2856	44	176	220	
22	A	1	Total	C	H	Mg	N	O	0
			5574	2278	2856	44	176	220	
22	A	1	Total	C	H	Mg	N	O	0
			5574	2278	2856	44	176	220	
22	A	1	Total	C	H	Mg	N	O	0
			5574	2278	2856	44	176	220	

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

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

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Mol	Chain	Residues	Atoms						AltConf
22	B	1	Total	C	H	Mg	N	O	0
			5043	2063	2580	40	160	200	
22	B	1	Total	C	H	Mg	N	O	0
			5043	2063	2580	40	160	200	
22	B	1	Total	C	H	Mg	N	O	0
			5043	2063	2580	40	160	200	
22	B	1	Total	C	H	Mg	N	O	0
			5043	2063	2580	40	160	200	
22	B	1	Total	C	H	Mg	N	O	0
			5043	2063	2580	40	160	200	
22	B	1	Total	C	H	Mg	N	O	0
			5043	2063	2580	40	160	200	
22	B	1	Total	C	H	Mg	N	O	0
			5043	2063	2580	40	160	200	
22	B	1	Total	C	H	Mg	N	O	0
			5043	2063	2580	40	160	200	
22	B	1	Total	C	H	Mg	N	O	0
			5043	2063	2580	40	160	200	
22	B	1	Total	C	H	Mg	N	O	0
			5043	2063	2580	40	160	200	
22	B	1	Total	C	H	Mg	N	O	0
			5043	2063	2580	40	160	200	
22	B	1	Total	C	H	Mg	N	O	0
			5043	2063	2580	40	160	200	
22	B	1	Total	C	H	Mg	N	O	0
			5043	2063	2580	40	160	200	
22	B	1	Total	C	H	Mg	N	O	0
			5043	2063	2580	40	160	200	
22	B	1	Total	C	H	Mg	N	O	0
			5043	2063	2580	40	160	200	
22	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	
22	F	1	Total 352	C 145	H 177	Mg 3	N 12	O 15	0
22	F	1	Total 352	C 145	H 177	Mg 3	N 12	O 15	0
22	G	1	Total 198	C 86	H 92	Mg 2	N 8	O 10	0
22	G	1	Total 198	C 86	H 92	Mg 2	N 8	O 10	0
22	J	1	Total 104	C 45	H 49	Mg 1	N 4	O 5	0
22	L	1	Total 215	C 90	H 105	Mg 2	N 8	O 10	0
22	L	1	Total 215	C 90	H 105	Mg 2	N 8	O 10	0
22	K	1	Total 354	C 156	H 158	Mg 4	N 16	O 20	0
22	K	1	Total 354	C 156	H 158	Mg 4	N 16	O 20	0
22	K	1	Total 354	C 156	H 158	Mg 4	N 16	O 20	0
22	K	1	Total 354	C 156	H 158	Mg 4	N 16	O 20	0
22	1	1	Total 1264	C 529	H 625	Mg 11	N 44	O 55	0
22	1	1	Total 1264	C 529	H 625	Mg 11	N 44	O 55	0
22	1	1	Total 1264	C 529	H 625	Mg 11	N 44	O 55	0
22	1	1	Total 1264	C 529	H 625	Mg 11	N 44	O 55	0
22	1	1	Total 1264	C 529	H 625	Mg 11	N 44	O 55	0
22	1	1	Total 1264	C 529	H 625	Mg 11	N 44	O 55	0
22	1	1	Total 1264	C 529	H 625	Mg 11	N 44	O 55	0
22	1	1	Total 1264	C 529	H 625	Mg 11	N 44	O 55	0
22	1	1	Total 1264	C 529	H 625	Mg 11	N 44	O 55	0
22	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
22	1	1	Total 1264	C 529	H 625	Mg 11	N 44	O 55	0
22	3	1	Total 1458	C 612	H 718	Mg 13	N 52	O 63	0
22	3	1	Total 1458	C 612	H 718	Mg 13	N 52	O 63	0
22	3	1	Total 1458	C 612	H 718	Mg 13	N 52	O 63	0
22	3	1	Total 1458	C 612	H 718	Mg 13	N 52	O 63	0
22	3	1	Total 1458	C 612	H 718	Mg 13	N 52	O 63	0
22	3	1	Total 1458	C 612	H 718	Mg 13	N 52	O 63	0
22	3	1	Total 1458	C 612	H 718	Mg 13	N 52	O 63	0
22	3	1	Total 1458	C 612	H 718	Mg 13	N 52	O 63	0
22	3	1	Total 1458	C 612	H 718	Mg 13	N 52	O 63	0
22	3	1	Total 1458	C 612	H 718	Mg 13	N 52	O 63	0
22	3	1	Total 1458	C 612	H 718	Mg 13	N 52	O 63	0
22	3	1	Total 1458	C 612	H 718	Mg 13	N 52	O 63	0
22	3	1	Total 1458	C 612	H 718	Mg 13	N 52	O 63	0
22	3	1	Total 1458	C 612	H 718	Mg 13	N 52	O 63	0
22	7	1	Total 1250	C 534	H 598	Mg 12	N 48	O 58	0
22	7	1	Total 1250	C 534	H 598	Mg 12	N 48	O 58	0
22	7	1	Total 1250	C 534	H 598	Mg 12	N 48	O 58	0
22	7	1	Total 1250	C 534	H 598	Mg 12	N 48	O 58	0
22	7	1	Total 1250	C 534	H 598	Mg 12	N 48	O 58	0
22	7	1	Total 1250	C 534	H 598	Mg 12	N 48	O 58	0
22	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
22	7	1	Total 1250	C 534	H 598	Mg 12	N 48	O 58	0
22	7	1	Total 1250	C 534	H 598	Mg 12	N 48	O 58	0
22	7	1	Total 1250	C 534	H 598	Mg 12	N 48	O 58	0
22	7	1	Total 1250	C 534	H 598	Mg 12	N 48	O 58	0
22	7	1	Total 1250	C 534	H 598	Mg 12	N 48	O 58	0
22	8	1	Total 1192	C 504	H 578	Mg 11	N 44	O 55	0
22	8	1	Total 1192	C 504	H 578	Mg 11	N 44	O 55	0
22	8	1	Total 1192	C 504	H 578	Mg 11	N 44	O 55	0
22	8	1	Total 1192	C 504	H 578	Mg 11	N 44	O 55	0
22	8	1	Total 1192	C 504	H 578	Mg 11	N 44	O 55	0
22	8	1	Total 1192	C 504	H 578	Mg 11	N 44	O 55	0
22	8	1	Total 1192	C 504	H 578	Mg 11	N 44	O 55	0
22	8	1	Total 1192	C 504	H 578	Mg 11	N 44	O 55	0
22	8	1	Total 1192	C 504	H 578	Mg 11	N 44	O 55	0
22	8	1	Total 1192	C 504	H 578	Mg 11	N 44	O 55	0
22	8	1	Total 1192	C 504	H 578	Mg 11	N 44	O 55	0
22	Z	1	Total 1220	C 517	H 593	Mg 11	N 44	O 55	0
22	Z	1	Total 1220	C 517	H 593	Mg 11	N 44	O 55	0
22	Z	1	Total 1220	C 517	H 593	Mg 11	N 44	O 55	0
22	Z	1	Total 1220	C 517	H 593	Mg 11	N 44	O 55	0
22	Z	1	Total 1220	C 517	H 593	Mg 11	N 44	O 55	0

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Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	Mg	N	O	
22	Z	1	Total 1220	C 517	H 593	Mg 11	N 44	O 55	0
22	Z	1	Total 1220	C 517	H 593	Mg 11	N 44	O 55	0
22	Z	1	Total 1220	C 517	H 593	Mg 11	N 44	O 55	0
22	Z	1	Total 1220	C 517	H 593	Mg 11	N 44	O 55	0
22	Z	1	Total 1220	C 517	H 593	Mg 11	N 44	O 55	0
22	Z	1	Total 1220	C 517	H 593	Mg 11	N 44	O 55	0
22	4	1	Total 1099	C 465	H 534	Mg 10	N 40	O 50	0
22	4	1	Total 1099	C 465	H 534	Mg 10	N 40	O 50	0
22	4	1	Total 1099	C 465	H 534	Mg 10	N 40	O 50	0
22	4	1	Total 1099	C 465	H 534	Mg 10	N 40	O 50	0
22	4	1	Total 1099	C 465	H 534	Mg 10	N 40	O 50	0
22	4	1	Total 1099	C 465	H 534	Mg 10	N 40	O 50	0
22	4	1	Total 1099	C 465	H 534	Mg 10	N 40	O 50	0
22	4	1	Total 1099	C 465	H 534	Mg 10	N 40	O 50	0
22	4	1	Total 1099	C 465	H 534	Mg 10	N 40	O 50	0
22	4	1	Total 1099	C 465	H 534	Mg 10	N 40	O 50	0
22	5	1	Total 1452	C 610	H 712	Mg 13	N 52	O 65	0
22	5	1	Total 1452	C 610	H 712	Mg 13	N 52	O 65	0
22	5	1	Total 1452	C 610	H 712	Mg 13	N 52	O 65	0
22	5	1	Total 1452	C 610	H 712	Mg 13	N 52	O 65	0
22	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
22	5	1	Total 1452	C 610	H 712	Mg 13	N 52	O 65	0
22	5	1	Total 1452	C 610	H 712	Mg 13	N 52	O 65	0
22	5	1	Total 1452	C 610	H 712	Mg 13	N 52	O 65	0
22	5	1	Total 1452	C 610	H 712	Mg 13	N 52	O 65	0
22	5	1	Total 1452	C 610	H 712	Mg 13	N 52	O 65	0
22	5	1	Total 1452	C 610	H 712	Mg 13	N 52	O 65	0
22	5	1	Total 1452	C 610	H 712	Mg 13	N 52	O 65	0
22	5	1	Total 1452	C 610	H 712	Mg 13	N 52	O 65	0
22	5	1	Total 1452	C 610	H 712	Mg 13	N 52	O 65	0
22	6	1	Total 1233	C 518	H 605	Mg 11	N 44	O 55	0
22	6	1	Total 1233	C 518	H 605	Mg 11	N 44	O 55	0
22	6	1	Total 1233	C 518	H 605	Mg 11	N 44	O 55	0
22	6	1	Total 1233	C 518	H 605	Mg 11	N 44	O 55	0
22	6	1	Total 1233	C 518	H 605	Mg 11	N 44	O 55	0
22	6	1	Total 1233	C 518	H 605	Mg 11	N 44	O 55	0
22	6	1	Total 1233	C 518	H 605	Mg 11	N 44	O 55	0
22	6	1	Total 1233	C 518	H 605	Mg 11	N 44	O 55	0
22	6	1	Total 1233	C 518	H 605	Mg 11	N 44	O 55	0
22	6	1	Total 1233	C 518	H 605	Mg 11	N 44	O 55	0
22	6	1	Total 1233	C 518	H 605	Mg 11	N 44	O 55	0
22	6	1	Total 1233	C 518	H 605	Mg 11	N 44	O 55	0
22	9	1	Total 1100	C 465	H 535	Mg 10	N 40	O 50	0
22	9	1	Total 1100	C 465	H 535	Mg 10	N 40	O 50	0

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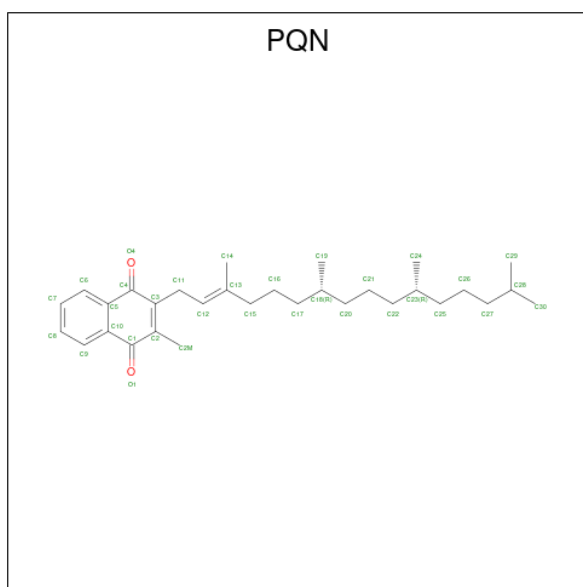
Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	Mg	N	O	
22	9	1	Total	C	H	Mg	N	O	0
			1100	465	535	10	40	50	
22	9	1	Total	C	H	Mg	N	O	0
			1100	465	535	10	40	50	
22	9	1	Total	C	H	Mg	N	O	0
			1100	465	535	10	40	50	
22	9	1	Total	C	H	Mg	N	O	0
			1100	465	535	10	40	50	
22	9	1	Total	C	H	Mg	N	O	0
			1100	465	535	10	40	50	
22	9	1	Total	C	H	Mg	N	O	0
			1100	465	535	10	40	50	
22	B2	1	Total	C	H	Mg	N	O	0
			1810	759	891	16	64	80	
22	B2	1	Total	C	H	Mg	N	O	0
			1810	759	891	16	64	80	
22	B2	1	Total	C	H	Mg	N	O	0
			1810	759	891	16	64	80	
22	B2	1	Total	C	H	Mg	N	O	0
			1810	759	891	16	64	80	
22	B2	1	Total	C	H	Mg	N	O	0
			1810	759	891	16	64	80	
22	B2	1	Total	C	H	Mg	N	O	0
			1810	759	891	16	64	80	
22	B2	1	Total	C	H	Mg	N	O	0
			1810	759	891	16	64	80	
22	B2	1	Total	C	H	Mg	N	O	0
			1810	759	891	16	64	80	
22	B2	1	Total	C	H	Mg	N	O	0
			1810	759	891	16	64	80	
22	B2	1	Total	C	H	Mg	N	O	0
			1810	759	891	16	64	80	
22	B2	1	Total	C	H	Mg	N	O	0
			1810	759	891	16	64	80	

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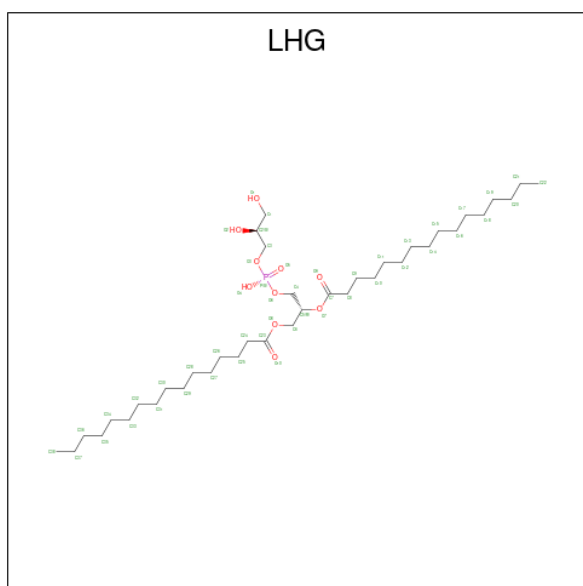
Mol	Chain	Residues	Atoms					AltConf	
			Total	C	H	Mg	N		O
22	B2	1	Total 1810	C 759	H 891	Mg 16	N 64	O 80	0
22	B2	1	Total 1810	C 759	H 891	Mg 16	N 64	O 80	0
22	B2	1	Total 1810	C 759	H 891	Mg 16	N 64	O 80	0
22	L2	1	Total 156	C 70	H 66	Mg 2	N 8	O 10	0
22	L2	1	Total 156	C 70	H 66	Mg 2	N 8	O 10	0
22	92	1	Total 1050	C 445	H 505	Mg 10	N 40	O 50	0
22	92	1	Total 1050	C 445	H 505	Mg 10	N 40	O 50	0
22	92	1	Total 1050	C 445	H 505	Mg 10	N 40	O 50	0
22	92	1	Total 1050	C 445	H 505	Mg 10	N 40	O 50	0
22	92	1	Total 1050	C 445	H 505	Mg 10	N 40	O 50	0
22	92	1	Total 1050	C 445	H 505	Mg 10	N 40	O 50	0
22	92	1	Total 1050	C 445	H 505	Mg 10	N 40	O 50	0
22	92	1	Total 1050	C 445	H 505	Mg 10	N 40	O 50	0
22	92	1	Total 1050	C 445	H 505	Mg 10	N 40	O 50	0
22	92	1	Total 1050	C 445	H 505	Mg 10	N 40	O 50	0
22	92	1	Total 1050	C 445	H 505	Mg 10	N 40	O 50	0

- Molecule 23 is PHYLLOQUINONE (three-letter code: PQN) (formula: C₃₁H₄₆O₂) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 24 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).



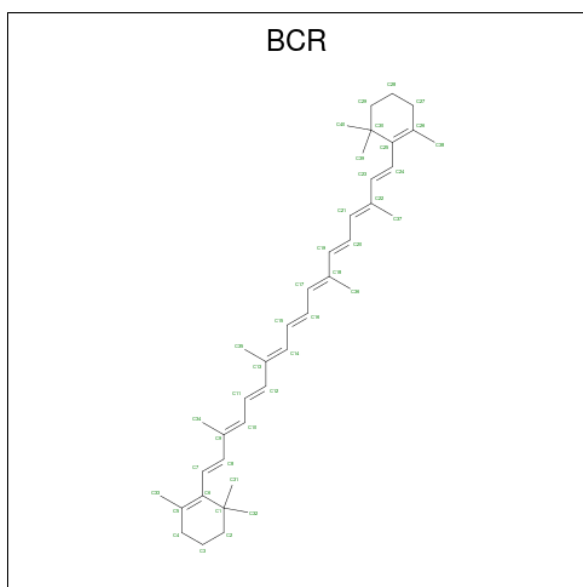
Mol	Chain	Residues	Atoms					AltConf
			Total	C	H	O	P	
24	A	1	210	65	123	20	2	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	H	O	P	
24	A	1	210	65	123	20	2	0
24	B	1	108	34	63	10	1	0
24	1	1	87	28	48	10	1	0
24	3	1	177	56	99	20	2	0
24	3	1	177	56	99	20	2	0
24	7	1	123	38	74	10	1	0
24	8	1	105	33	61	10	1	0
24	Z	1	87	28	48	10	1	0
24	4	1	210	65	123	20	2	0
24	4	1	210	65	123	20	2	0
24	5	1	81	26	44	10	1	0
24	6	1	201	63	116	20	2	0
24	6	1	201	63	116	20	2	0
24	9	1	96	30	55	10	1	0
24	92	1	57	18	28	10	1	0

- Molecule 25 is BETA-CAROTENE (three-letter code: BCR) (formula: C₄₀H₅₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	H	
25	A	1	480	200	280	0
25	A	1	480	200	280	0
25	A	1	480	200	280	0
25	A	1	480	200	280	0
25	A	1	480	200	280	0
25	B	1	672	280	392	0
25	B	1	672	280	392	0
25	B	1	672	280	392	0
25	B	1	672	280	392	0
25	B	1	672	280	392	0
25	B	1	672	280	392	0
25	B	1	672	280	392	0
25	B	1	672	280	392	0
25	G	1	96	40	56	0
25	I	1	96	40	56	0

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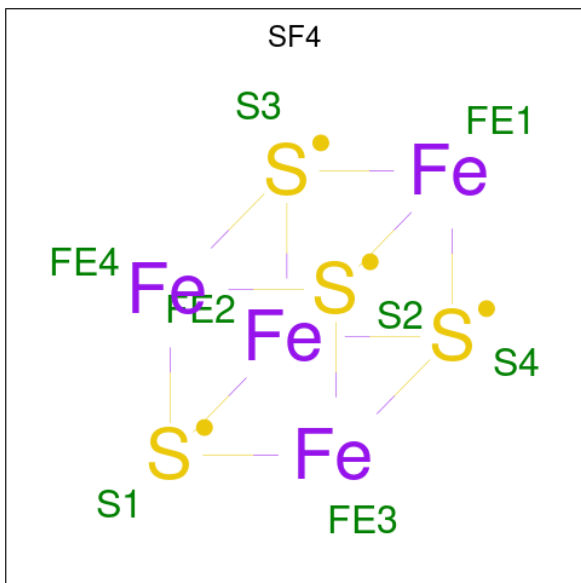
Mol	Chain	Residues	Atoms			AltConf
			Total	C	H	
25	J	1	96	40	56	0
25	L	1	192	80	112	0
25	L	1	192	80	112	0
25	K	1	192	80	112	0
25	K	1	192	80	112	0
25	3	1	288	120	168	0
25	3	1	288	120	168	0
25	3	1	288	120	168	0
25	7	1	96	40	56	0
25	8	1	96	40	56	0
25	4	1	96	40	56	0
25	5	1	96	40	56	0
25	6	1	96	40	56	0
25	9	1	96	40	56	0
25	B2	1	273	114	159	0
25	B2	1	273	114	159	0
25	B2	1	273	114	159	0
25	B2	1	273	114	159	0
25	I2	1	96	40	56	0
25	L2	1	192	80	112	0
25	L2	1	192	80	112	0

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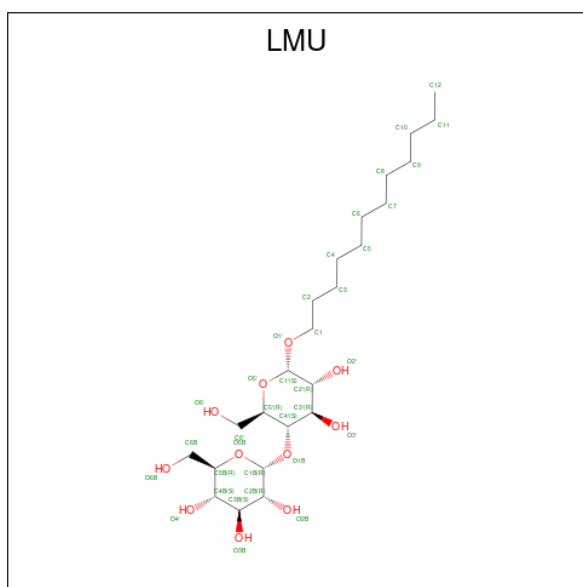
Mol	Chain	Residues	Atoms			AltConf
			Total	C	H	
25	92	1	96	40	56	0

- Molecule 26 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
26	A	1	8	4	4	0
26	C	1	16	8	8	0
26	C	1	16	8	8	0

- Molecule 27 is DODECYL-ALPHA-D-MALTOSE (three-letter code: LMU) (formula: C₂₄H₄₆O₁₁) (labeled as "Ligand of Interest" by depositor).



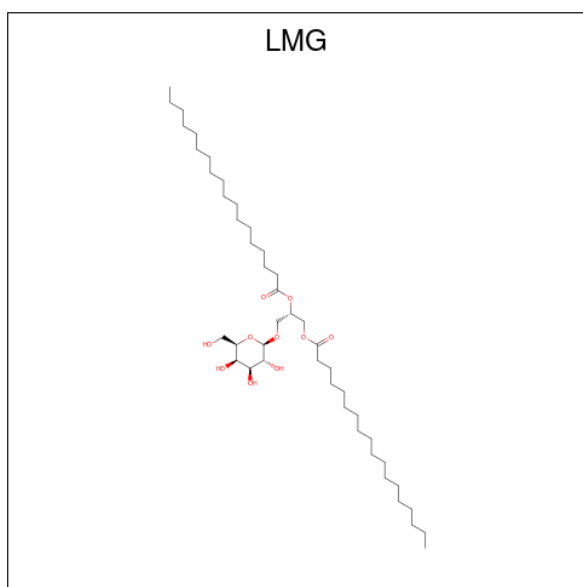
Mol	Chain	Residues	Atoms			AltConf	
			Total	C	H		O
27	A	1	458	139	262	57	0
27	A	1	458	139	262	57	0
27	A	1	458	139	262	57	0
27	A	1	458	139	262	57	0
27	A	1	458	139	262	57	0
27	A	1	458	139	262	57	0
27	A	1	458	139	262	57	0
27	A	1	458	139	262	57	0
27	B	1	81	24	46	11	0
27	G	1	59	18	35	6	0
27	K	1	59	18	35	6	0
27	1	1	349	107	201	41	0
27	1	1	349	107	201	41	0
27	1	1	349	107	201	41	0
27	1	1	349	107	201	41	0

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Mol	Chain	Residues	Atoms				AltConf
27	1	1	Total	C	H	O	0
			349	107	201	41	
27	1	1	Total	C	H	O	0
			349	107	201	41	
27	7	1	Total	C	H	O	0
			173	53	92	28	
27	7	1	Total	C	H	O	0
			173	53	92	28	
27	7	1	Total	C	H	O	0
			173	53	92	28	
27	8	1	Total	C	H	O	0
			258	78	151	29	
27	8	1	Total	C	H	O	0
			258	78	151	29	
27	8	1	Total	C	H	O	0
			258	78	151	29	
27	8	1	Total	C	H	O	0
			258	78	151	29	
27	Z	1	Total	C	H	O	0
			116	36	63	17	
27	Z	1	Total	C	H	O	0
			116	36	63	17	
27	4	1	Total	C	H	O	0
			116	36	63	17	
27	4	1	Total	C	H	O	0
			116	36	63	17	
27	5	1	Total	C	H	O	0
			59	18	35	6	
27	6	1	Total	C	H	O	0
			221	68	129	24	
27	6	1	Total	C	H	O	0
			221	68	129	24	
27	6	1	Total	C	H	O	0
			221	68	129	24	
27	6	1	Total	C	H	O	0
			221	68	129	24	
27	9	1	Total	C	H	O	0
			59	18	35	6	
27	92	1	Total	C	H	O	0
			81	24	46	11	

- Molecule 28 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C₄₅H₈₆O₁₀) (labeled as "Ligand of Interest" by depositor).



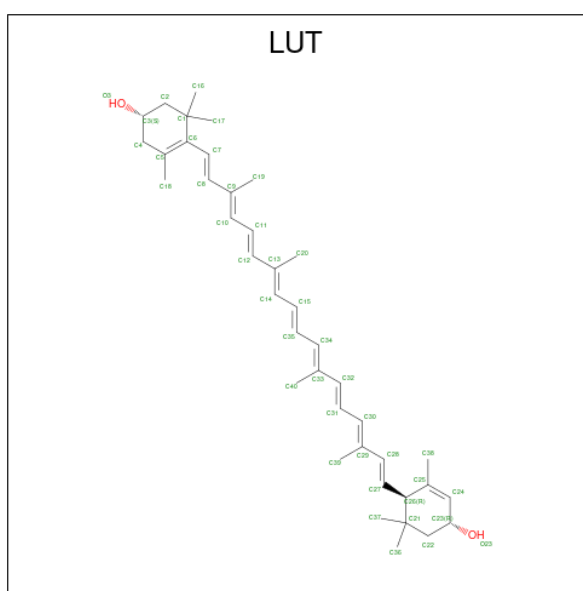
Mol	Chain	Residues	Atoms				AltConf
			Total	C	H	O	
28	A	1	195	64	111	20	0
28	A	1	195	64	111	20	0
28	B	1	177	59	98	20	0
28	B	1	177	59	98	20	0
28	J	1	174	57	97	20	0
28	J	1	174	57	97	20	0
28	1	1	174	58	96	20	0
28	1	1	174	58	96	20	0
28	3	1	120	40	75	5	0
28	7	1	81	27	44	10	0
28	8	1	165	54	91	20	0
28	8	1	165	54	91	20	0
28	4	1	96	31	55	10	0
28	6	1	55	18	35	2	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	H	O	
28	9	1	Total	C	H	O	0
			105	34	61	10	
28	B2	1	Total	C	H	O	0
			162	54	88	20	
28	B2	1	Total	C	H	O	0
			162	54	88	20	

- Molecule 29 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).



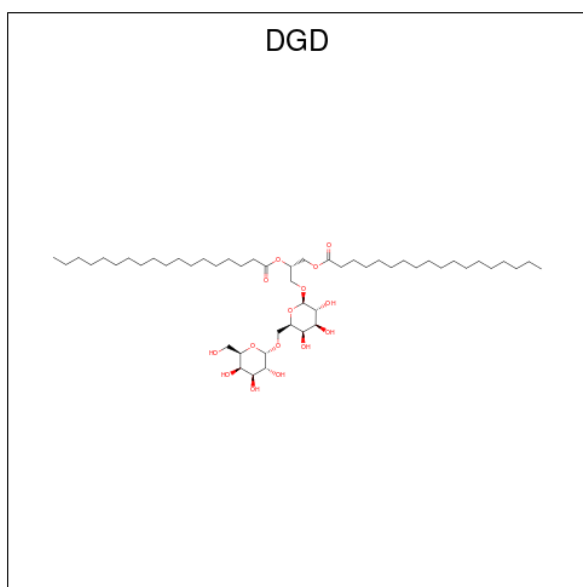
Mol	Chain	Residues	Atoms				AltConf
			Total	C	H	O	
29	A	1	Total	C	H	O	0
			98	40	56	2	
29	F	1	Total	C	H	O	0
			98	40	56	2	
29	1	1	Total	C	H	O	0
			196	80	112	4	
29	1	1	Total	C	H	O	0
			196	80	112	4	
29	3	1	Total	C	H	O	0
			294	120	168	6	
29	3	1	Total	C	H	O	0
			294	120	168	6	
29	3	1	Total	C	H	O	0
			294	120	168	6	

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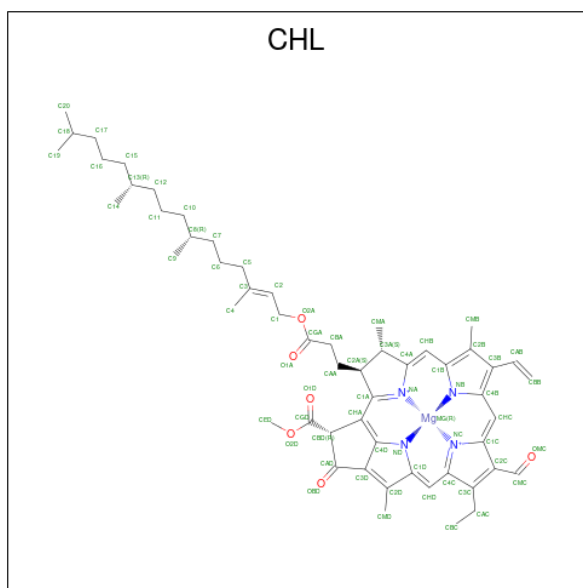
Mol	Chain	Residues	Atoms				AltConf
			Total	C	H	O	
29	7	1	Total 196	C 80	H 112	O 4	0
29	7	1	Total 196	C 80	H 112	O 4	0
29	8	1	Total 98	C 40	H 56	O 2	0
29	Z	1	Total 157	C 65	H 89	O 3	0
29	Z	1	Total 157	C 65	H 89	O 3	0
29	4	1	Total 98	C 40	H 56	O 2	0
29	5	1	Total 196	C 80	H 112	O 4	0
29	5	1	Total 196	C 80	H 112	O 4	0
29	6	1	Total 98	C 40	H 56	O 2	0
29	9	1	Total 196	C 80	H 112	O 4	0
29	9	1	Total 196	C 80	H 112	O 4	0
29	92	1	Total 196	C 80	H 112	O 4	0
29	92	1	Total 196	C 80	H 112	O 4	0

- Molecule 30 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: C₅₁H₉₆O₁₅) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 31 is CHLOROPHYLL B (three-letter code: CHL) (formula: $C_{55}H_{70}MgN_4O_6$).



Mol	Chain	Residues	Atoms					AltConf	
			Total	C	H	Mg	N		O
31	1	1	290	125	132	3	12	18	0
31	1	1	290	125	132	3	12	18	0
31	1	1	290	125	132	3	12	18	0

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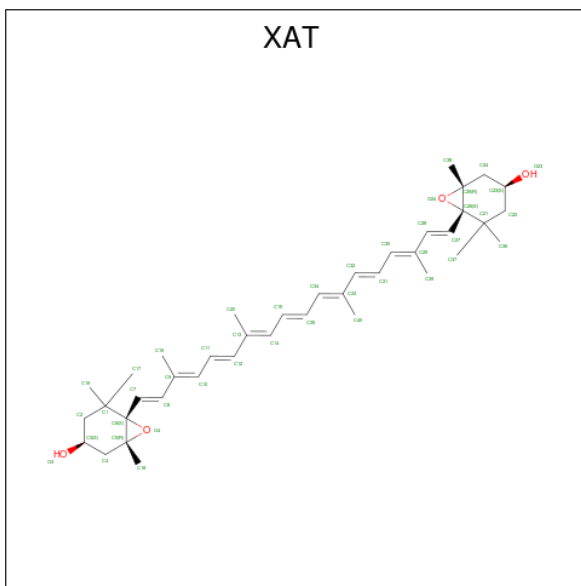
Mol	Chain	Residues	Atoms					AltConf	
			Total	C	H	Mg	N		O
31	3	1	Total 136	C 55	H 70	Mg 1	N 4	O 6	0
31	7	1	Total 290	C 125	H 132	Mg 3	N 12	O 18	0
31	7	1	Total 290	C 125	H 132	Mg 3	N 12	O 18	0
31	7	1	Total 290	C 125	H 132	Mg 3	N 12	O 18	0
31	8	1	Total 408	C 165	H 210	Mg 3	N 12	O 18	0
31	8	1	Total 408	C 165	H 210	Mg 3	N 12	O 18	0
31	8	1	Total 408	C 165	H 210	Mg 3	N 12	O 18	0
31	Z	1	Total 349	C 145	H 171	Mg 3	N 12	O 18	0
31	Z	1	Total 349	C 145	H 171	Mg 3	N 12	O 18	0
31	Z	1	Total 349	C 145	H 171	Mg 3	N 12	O 18	0
31	4	1	Total 588	C 245	H 288	Mg 5	N 20	O 30	0
31	4	1	Total 588	C 245	H 288	Mg 5	N 20	O 30	0
31	4	1	Total 588	C 245	H 288	Mg 5	N 20	O 30	0
31	4	1	Total 588	C 245	H 288	Mg 5	N 20	O 30	0
31	4	1	Total 588	C 245	H 288	Mg 5	N 20	O 30	0
31	5	1	Total 373	C 164	H 167	Mg 4	N 16	O 22	0
31	5	1	Total 373	C 164	H 167	Mg 4	N 16	O 22	0
31	5	1	Total 373	C 164	H 167	Mg 4	N 16	O 22	0
31	5	1	Total 373	C 164	H 167	Mg 4	N 16	O 22	0
31	6	1	Total 677	C 286	H 327	Mg 6	N 24	O 34	0
31	6	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	
31	6	1	Total 677	C 286	H 327	Mg 6	N 24	O 34	0
31	6	1	Total 677	C 286	H 327	Mg 6	N 24	O 34	0
31	6	1	Total 677	C 286	H 327	Mg 6	N 24	O 34	0
31	6	1	Total 677	C 286	H 327	Mg 6	N 24	O 34	0
31	9	1	Total 157	C 73	H 64	Mg 2	N 8	O 10	0
31	9	1	Total 157	C 73	H 64	Mg 2	N 8	O 10	0
31	92	1	Total 146	C 68	H 58	Mg 2	N 8	O 10	0
31	92	1	Total 146	C 68	H 58	Mg 2	N 8	O 10	0

- Molecule 32 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).



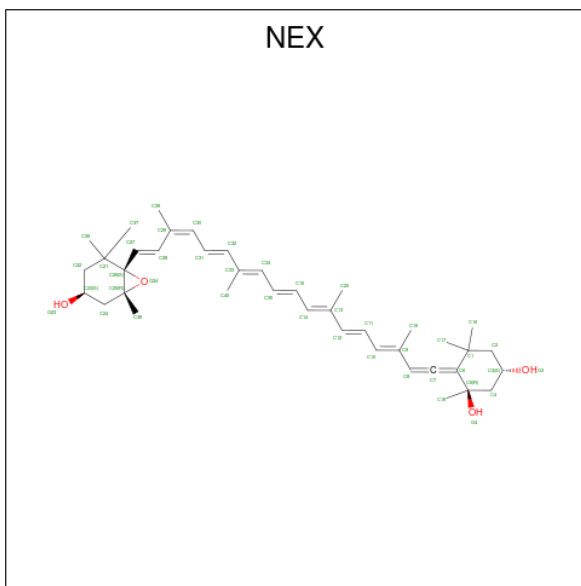
Mol	Chain	Residues	Atoms				AltConf
			Total	C	H	O	
32	1	1	Total 100	C 40	H 56	O 4	0
32	7	1	Total 100	C 40	H 56	O 4	0

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Mol	Chain	Residues	Atoms				AltConf
32	8	1	Total	C	H	O	0
			100	40	56	4	
32	Z	1	Total	C	H	O	0
			100	40	56	4	
32	4	1	Total	C	H	O	0
			100	40	56	4	
32	5	1	Total	C	H	O	0
			100	40	56	4	
32	6	1	Total	C	H	O	0
			100	40	56	4	

- Molecule 33 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-TETRAMETHYLOCTA DECA-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
33	5	1	Total	C	H	O	0
			100	40	56	4	
33	6	1	Total	C	H	O	0
			100	40	56	4	

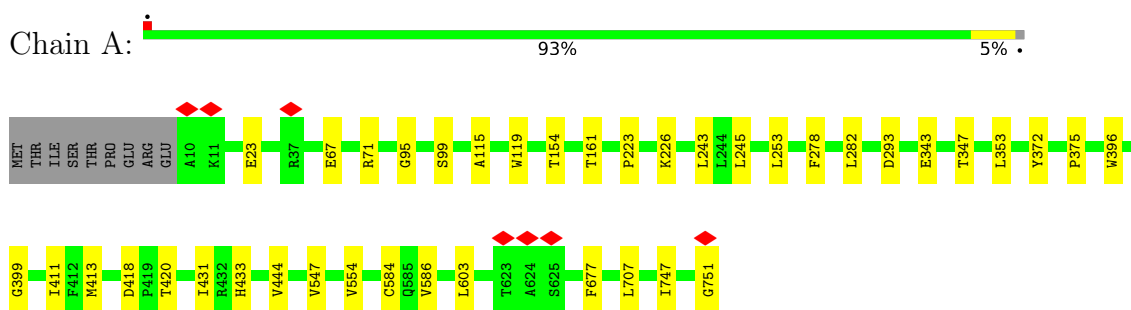
- Molecule 34 is water.

Mol	Chain	Residues	Atoms	AltConf
34	H	11	Total O 88 88	0
34	H	20	Total O 88 88	0
34	H	1	Total O 88 88	0
34	H	1	Total O 88 88	0
34	H	4	Total O 88 88	0
34	H	2	Total O 88 88	0
34	H	7	Total O 88 88	0
34	H	6	Total O 88 88	0
34	H	7	Total O 88 88	0
34	H	7	Total O 88 88	0
34	H	5	Total O 88 88	0
34	H	4	Total O 88 88	0
34	H	7	Total O 88 88	0
34	H	5	Total O 88 88	0
34	H	1	Total O 88 88	0

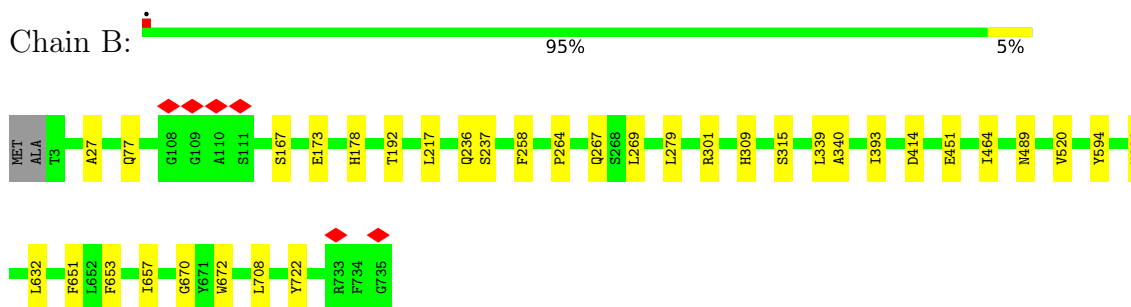
3 Residue-property plots [i](#)

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.

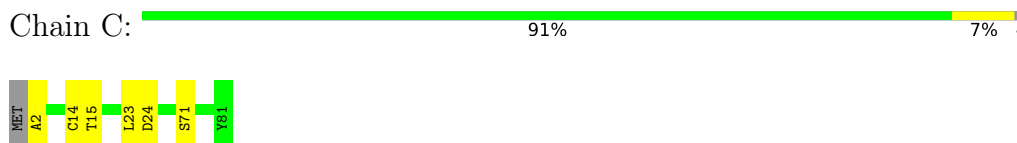
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



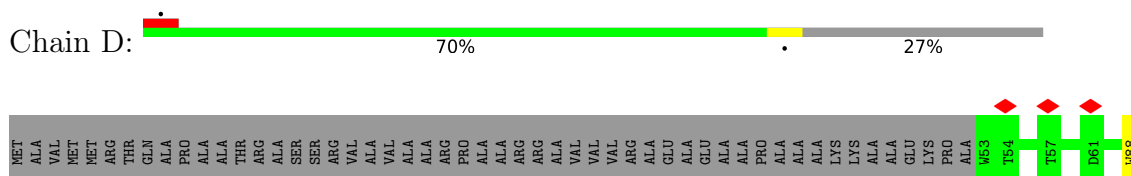
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

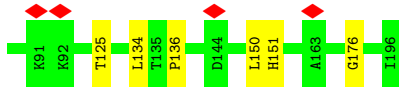


- Molecule 3: Photosystem I iron-sulfur center

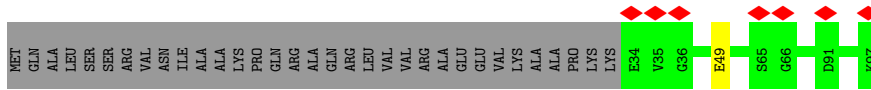


- Molecule 4: Photosystem I reaction center subunit II, chloroplastic

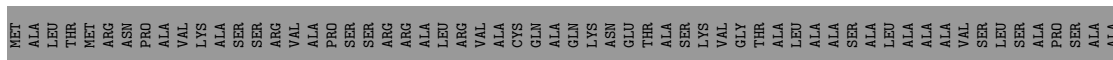




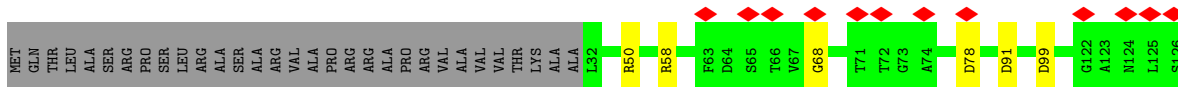
• Molecule 5: Photosystem I reaction center subunit IV, chloroplastic



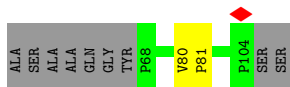
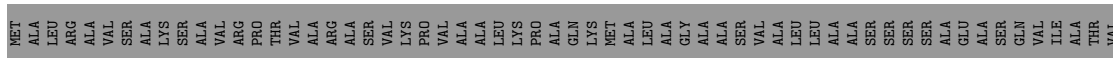
• Molecule 6: Photosystem I reaction center subunit III, chloroplastic



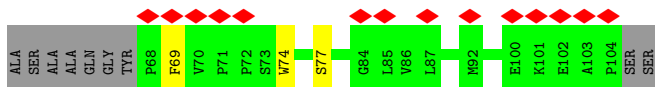
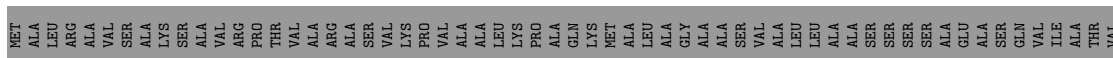
• Molecule 7: Photosystem I reaction center subunit V, chloroplastic



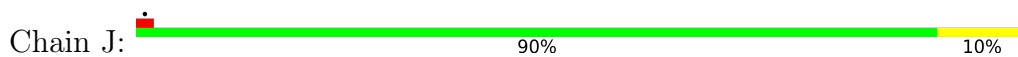
• Molecule 8: Photosystem I reaction center subunit VIII



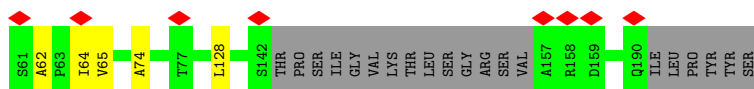
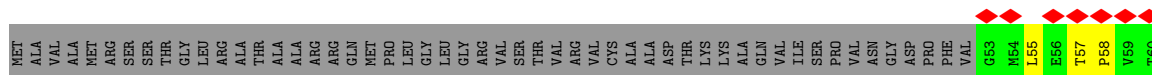
• Molecule 8: Photosystem I reaction center subunit VIII



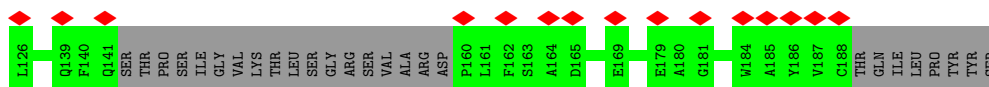
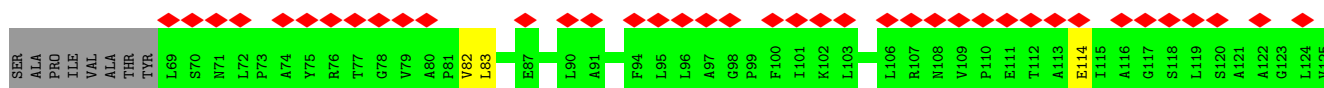
• Molecule 9: Photosystem I reaction center subunit IX



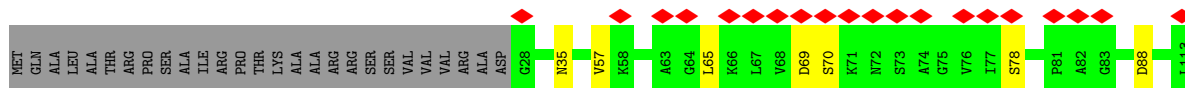
- Molecule 10: PSI subunit V



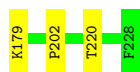
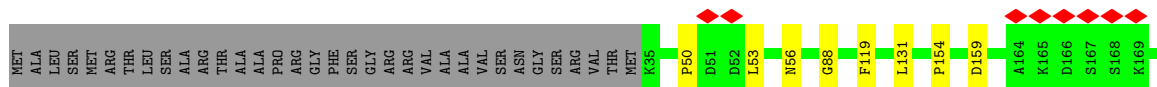
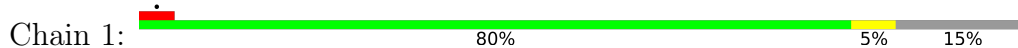
- Molecule 10: PSI subunit V



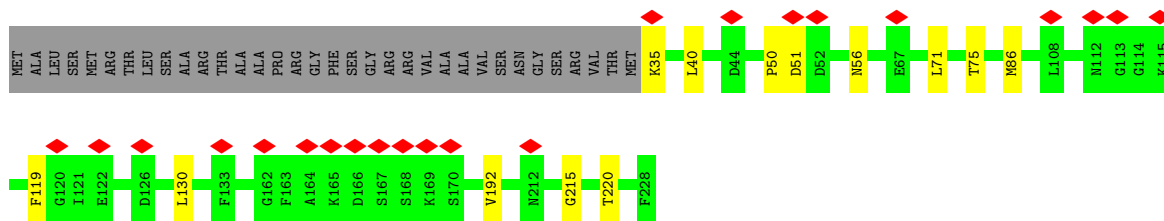
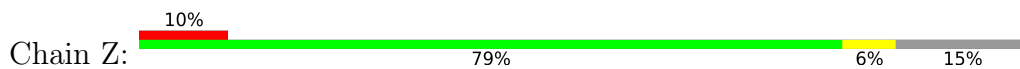
- Molecule 11: Photosystem I reaction center subunit psaK, chloroplastic



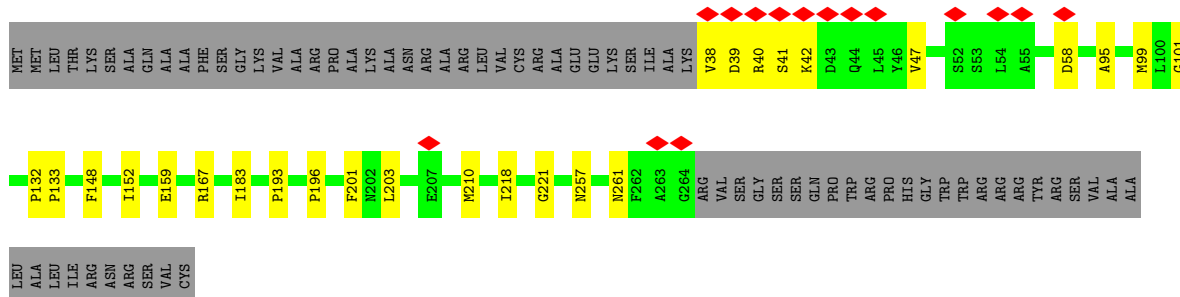
- Molecule 12: Chlorophyll a-b binding protein, chloroplastic



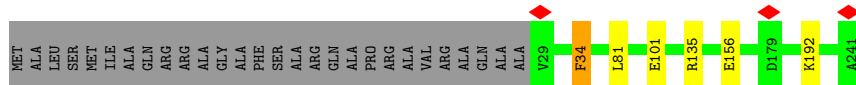
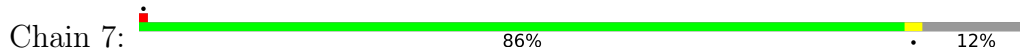
- Molecule 12: Chlorophyll a-b binding protein, chloroplastic



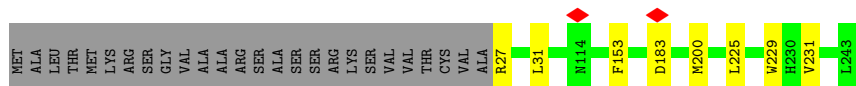
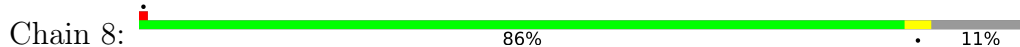
- Molecule 13: Chlorophyll a-b binding protein, chloroplastic



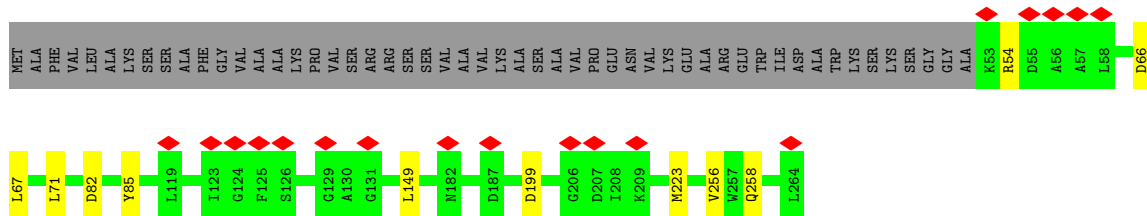
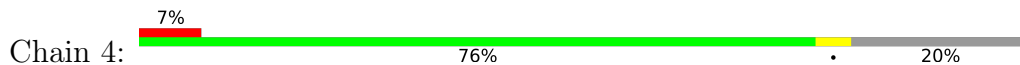
- Molecule 14: Chlorophyll a-b binding protein, chloroplastic



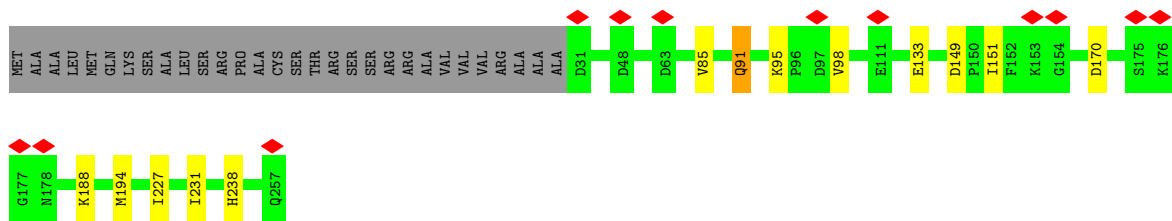
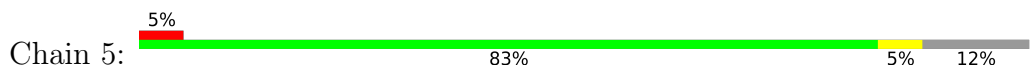
- Molecule 15: Chlorophyll a-b binding protein, chloroplastic



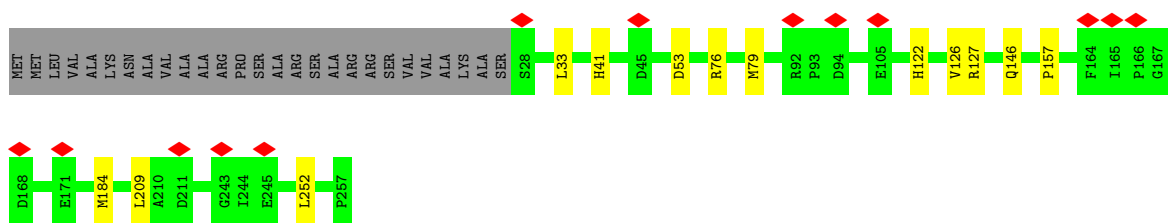
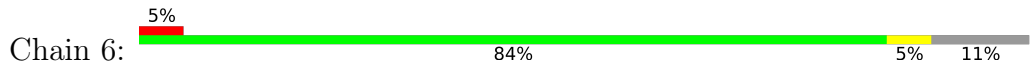
- Molecule 16: Chlorophyll a-b binding protein, chloroplastic (Lhca4)



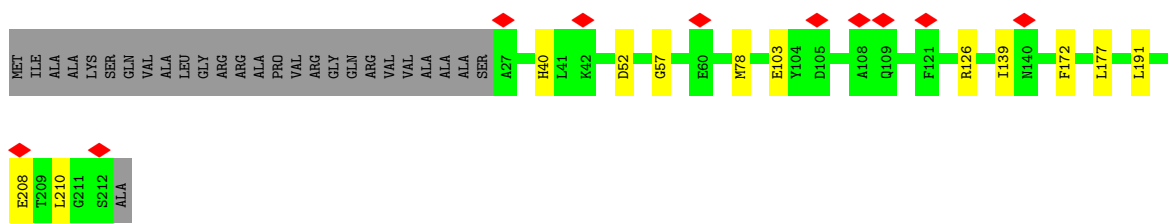
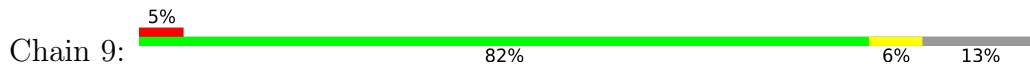
- Molecule 17: Chlorophyll a-b binding protein, chloroplastic



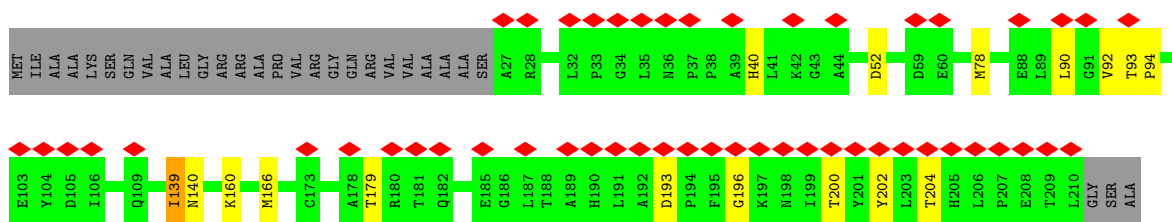
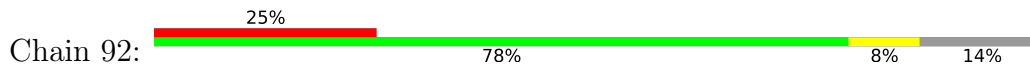
• Molecule 18: Chlorophyll a-b binding protein, chloroplastic



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

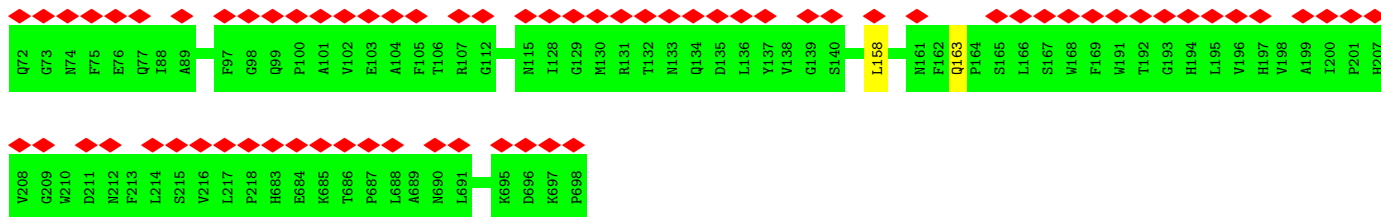


• Molecule 19: Chlorophyll a-b binding protein, chloroplastic



• Molecule 20: Photosystem I P700 chlorophyll a apoprotein A2





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	28346	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	0.175	Depositor
Minimum map value	-0.075	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.031	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: AME, NEX, DGD, CL0, XAT, LMU, SF4, LUT, PQN, CHL, BCR, LMG, CLA, LHG

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	0.28	0/6021	0.43	0/8208
2	B	0.29	0/6036	0.43	0/8240
3	C	0.28	0/611	0.51	0/826
4	D	0.28	0/1161	0.48	0/1567
5	E	0.30	0/516	0.48	0/700
6	F	0.27	0/1292	0.44	0/1747
7	G	0.27	0/721	0.43	0/980
8	I	0.28	0/293	0.38	0/406
8	I2	0.26	0/293	0.38	0/406
9	J	0.30	0/329	0.42	0/452
10	L	0.28	0/920	0.42	0/1257
10	L2	0.25	0/757	0.39	0/1031
11	K	0.26	0/588	0.43	0/795
12	1	0.28	0/1491	0.42	0/2028
12	Z	0.26	0/1491	0.40	0/2028
13	3	0.29	0/1784	0.43	0/2420
14	7	0.29	0/1702	0.42	0/2310
15	8	0.28	0/1701	0.43	0/2315
16	4	0.27	0/1703	0.41	0/2321
17	5	0.27	0/1830	0.42	0/2492
18	6	0.27	0/1834	0.42	0/2505
19	9	0.27	0/1461	0.42	0/1987
19	92	0.26	0/1451	0.43	0/1974
20	B2	0.24	0/1522	0.39	0/2071
All	All	0.28	0/37508	0.43	0/51066

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	28	0
2	B	5824	5576	5577	33	0
3	C	601	582	581	3	0
4	D	1133	1151	1150	4	0
5	E	506	505	504	1	0
6	F	1266	1302	1301	10	0
7	G	706	687	686	4	0
8	I	281	292	292	1	0
8	I2	281	292	292	1	0
9	J	329	328	328	2	0
10	L	899	907	905	8	0
10	L2	739	748	747	2	0
11	K	583	620	620	6	0
12	1	1445	1397	1396	11	0
12	Z	1445	1397	1396	11	0
13	3	1736	1695	1694	17	0
14	7	1650	1590	1589	7	0
15	8	1650	1630	1629	7	0
16	4	1648	1603	1602	9	0
17	5	1775	1747	1746	13	0
18	6	1772	1770	1770	13	0
19	9	1420	1400	1399	11	0
19	92	1410	1392	1391	12	0
20	B2	1469	1396	1395	4	0
21	A	65	72	72	1	0
22	1	639	625	625	14	0
22	3	740	718	718	20	0
22	4	565	534	534	10	0
22	5	740	712	712	11	0
22	6	628	605	605	9	0
22	7	652	598	598	7	0
22	8	614	578	578	13	0
22	9	565	535	535	7	0
22	92	545	505	505	11	0
22	A	2718	2856	2856	44	0
22	B	2463	2580	2580	46	0
22	B2	919	891	891	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	F	175	177	177	1	0
22	G	106	92	92	0	0
22	J	55	49	49	1	0
22	K	196	158	158	2	0
22	L	110	105	105	2	0
22	L2	90	66	66	0	0
22	Z	627	593	593	12	0
23	A	33	46	46	0	0
23	B	33	46	46	1	0
24	1	39	48	48	1	0
24	3	78	99	99	1	0
24	4	87	123	123	1	0
24	5	37	44	44	1	0
24	6	85	116	116	1	0
24	7	49	74	74	1	0
24	8	44	61	61	0	0
24	9	41	55	55	0	0
24	92	29	28	28	1	0
24	A	87	123	123	0	0
24	B	45	63	63	0	0
24	Z	39	48	48	0	0
25	3	120	168	168	7	0
25	4	40	56	56	0	0
25	5	40	56	56	0	0
25	6	40	56	56	3	0
25	7	40	56	56	0	0
25	8	40	56	56	2	0
25	9	40	56	56	2	0
25	92	40	56	56	3	0
25	A	200	280	280	12	0
25	B	280	392	392	12	0
25	B2	114	159	159	6	0
25	G	40	56	56	0	0
25	I	40	56	56	1	0
25	I2	40	56	56	0	0
25	J	40	56	56	1	0
25	K	80	112	112	6	0
25	L	80	112	112	5	0
25	L2	80	112	112	3	0
26	A	8	0	0	0	0
26	C	16	0	0	0	0
27	1	148	201	201	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	4	53	63	63	0	0
27	5	24	35	35	0	0
27	6	92	129	129	1	0
27	7	81	92	92	1	0
27	8	107	151	151	2	0
27	9	24	35	35	1	0
27	92	35	46	46	2	0
27	A	196	262	262	4	0
27	B	35	46	46	3	0
27	G	24	35	35	0	0
27	K	24	35	35	0	0
27	Z	53	63	63	1	0
28	1	78	96	96	0	0
28	3	45	75	75	1	0
28	4	41	55	55	0	0
28	6	20	35	35	0	0
28	7	37	44	44	0	0
28	8	74	91	91	0	0
28	9	44	61	61	2	0
28	A	84	111	111	1	0
28	B	79	98	98	1	0
28	B2	74	88	88	0	0
28	J	77	97	97	2	0
29	1	84	112	112	4	0
29	3	126	168	168	6	0
29	4	42	56	56	2	0
29	5	84	112	112	4	0
29	6	42	56	56	2	0
29	7	84	112	112	5	0
29	8	42	56	56	0	0
29	9	84	112	112	5	0
29	92	84	112	112	2	0
29	A	42	56	56	1	0
29	F	42	56	56	4	0
29	Z	68	89	89	1	0
30	B	59	79	79	1	0
31	1	158	132	132	1	0
31	3	66	70	70	1	0
31	4	300	288	288	6	0
31	5	206	167	167	2	0
31	6	350	327	327	9	0
31	7	158	132	132	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	8	198	210	210	5	0
31	9	93	64	64	0	0
31	92	88	58	58	0	0
31	Z	178	171	171	4	0
32	1	44	56	56	2	0
32	4	44	56	56	1	0
32	5	44	56	56	1	0
32	6	44	56	56	1	0
32	7	44	56	56	1	0
32	8	44	56	56	1	0
32	Z	44	56	56	1	0
33	5	44	56	56	0	0
33	6	44	56	56	1	0
34	H	88	0	0	12	0
All	All	56460	56999	56982	423	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 (423) 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)
29:7:624:LUT:H381	29:7:624:LUT:H28	1.51	0.92
27:B:853:LMU:H2O1	27:B:853:LMU:H6'	1.13	0.87
1:A:95:GLY:O	1:A:99:SER:OG	1.94	0.83
17:5:170:ASP:OD1	29:5:620:LUT:O23	1.96	0.82
2:B:301:ARG:NH1	7:G:68:GLY:O	2.15	0.80
2:B:628:ASN:O	34:H:14:HOH:O	2.00	0.79
2:B:167:SER:OG	7:G:78:ASP:OD1	2.00	0.78
19:92:40:HIS:NE2	19:92:52:ASP:OD2	2.17	0.78
31:8:606:CHL:O1D	34:H:91:HOH:O	2.03	0.77
6:F:184:GLU:OE1	34:H:88:HOH:O	2.03	0.76
7:G:58:ARG:NH2	7:G:99:ASP:OD2	2.21	0.73
27:7:628:LMU:O6'	34:H:81:HOH:O	2.05	0.73
13:3:40:ARG:O	13:3:41:SER:OG	2.06	0.73
12:1:179:LYS:NZ	24:1:620:LHG:O5	2.21	0.73
31:4:601:CHL:OBD	18:6:127:ARG:NH1	2.22	0.72
1:A:226:LYS:NZ	1:A:253:LEU:O	2.22	0.72
2:B:269:LEU:O	34:H:12:HOH:O	2.07	0.71
12:Z:130:LEU:HD11	31:Z:606:CHL:HMD3	1.74	0.70
1:A:23:GLU:OE2	28:A:860:LMG:O5	2.07	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:7:624:LUT:H381	29:7:624:LUT:C28	2.19	0.69
6:F:63:ASP:N	6:F:67:LEU:O	2.26	0.69
19:9:191:LEU:HD21	22:9:614:CLA:HMC3	1.74	0.68
31:6:606:CHL:OMC	34:H:73:HOH:O	2.12	0.68
13:3:159:GLU:OE2	34:H:37:HOH:O	2.12	0.67
2:B:27:ALA:HA	22:B:829:CLA:H43	1.77	0.66
22:A:803:CLA:HMB1	22:A:803:CLA:HBB1	1.77	0.66
22:7:608:CLA:O1A	22:7:610:CLA:HMD2	1.96	0.66
22:5:621:CLA:HBC3	22:5:621:CLA:HMC1	1.78	0.65
29:5:626:LUT:H1	27:6:628:LMU:H6'	1.40	0.65
22:A:811:CLA:H11	22:A:813:CLA:H42	1.79	0.64
22:A:854:CLA:HMB3	22:B:802:CLA:H193	1.79	0.64
2:B:217:LEU:CD1	19:9:210:LEU:HD23	2.28	0.64
11:K:78:SER:OG	22:K:201:CLA:O1D	2.16	0.64
19:9:208:GLU:N	19:9:208:GLU:OE1	2.31	0.64
22:5:621:CLA:HED2	22:5:621:CLA:O1A	1.98	0.63
22:Z:616:CLA:H72	22:Z:616:CLA:H41	1.79	0.63
13:3:148:PHE:CE2	13:3:152:ILE:HD11	2.32	0.63
22:Z:616:CLA:H41	22:Z:616:CLA:C7	2.29	0.63
2:B:315:SER:OG	22:B:841:CLA:O1A	2.07	0.62
31:6:607:CHL:H42	33:6:625:NEX:H403	1.79	0.62
22:8:604:CLA:O1A	31:8:606:CHL:HMD2	1.98	0.62
22:Z:603:CLA:HED2	22:Z:603:CLA:H43	1.80	0.62
22:6:602:CLA:HMC2	32:6:624:XAT:C11	2.29	0.62
14:7:192:LYS:NZ	24:7:625:LHG:O5	2.33	0.62
12:Z:40:LEU:HD13	31:Z:601:CHL:HMA3	1.81	0.61
18:6:146:GLN:OE1	18:6:146:GLN:N	2.33	0.61
22:3:607:CLA:H93	25:3:719:BCR:H392	1.83	0.61
12:Z:50:PRO:O	12:Z:56:ASN:ND2	2.33	0.60
28:9:620:LMG:HO2	28:9:620:LMG:C10	2.14	0.60
19:92:160:LYS:NZ	24:92:622:LHG:O5	2.35	0.60
22:7:620:CLA:O1A	18:6:252:LEU:N	2.35	0.60
16:4:54:ARG:NH1	16:4:71:LEU:O	2.35	0.59
13:3:257:ASN:O	13:3:261:ASN:ND2	2.36	0.59
13:3:193:PRO:CG	31:3:608:CHL:HMD2	2.32	0.59
1:A:396:TRP:HB3	22:A:829:CLA:HMC3	1.83	0.58
18:6:41:HIS:NE2	18:6:53:ASP:OD2	2.31	0.58
22:B:816:CLA:H101	22:B:816:CLA:H142	1.86	0.58
2:B:708:LEU:HD23	30:B:850:DGD:HA22	1.85	0.58
22:A:810:CLA:HAB	22:B:833:CLA:HMD2	1.86	0.58
13:3:167:ARG:NH1	28:3:722:LMG:O1	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:7:101:GLU:N	14:7:101:GLU:OE1	2.37	0.57
22:A:838:CLA:HBB1	22:A:838:CLA:HMB1	1.87	0.57
2:B:393:ILE:HD13	22:B:829:CLA:HED1	1.87	0.57
22:B:823:CLA:HAB	22:B:830:CLA:HMD2	1.86	0.57
1:A:161:THR:HG21	22:A:817:CLA:HBA1	1.85	0.57
22:B:838:CLA:HBB1	22:B:838:CLA:HMB1	1.85	0.57
31:8:606:CHL:OMC	34:H:55:HOH:O	2.18	0.57
2:B:339:LEU:HD21	22:B:829:CLA:HAB	1.86	0.57
22:1:603:CLA:HED2	22:1:603:CLA:H43	1.84	0.57
25:A:851:BCR:H23C	25:A:851:BCR:H403	1.87	0.57
12:1:220:THR:O	12:1:220:THR:HG22	2.05	0.57
22:5:602:CLA:H41	22:5:603:CLA:O1A	2.05	0.57
22:A:822:CLA:HMB2	22:A:826:CLA:HMA3	1.86	0.56
22:4:602:CLA:HMC2	32:4:620:XAT:C11	2.36	0.56
20:B2:33:GLU:OE1	20:B2:33:GLU:N	2.37	0.56
19:92:139:ILE:HG22	19:92:140:ASN:ND2	2.21	0.56
12:1:53:LEU:HD23	22:1:602:CLA:HED2	1.87	0.56
13:3:95:ALA:HB1	13:3:221:GLY:HA3	1.88	0.56
16:4:256:VAL:N	22:4:613:CLA:O1A	2.38	0.56
22:A:840:CLA:H42	22:A:840:CLA:O1A	2.07	0.55
31:4:606:CHL:C4A	34:H:64:HOH:O	2.26	0.55
4:D:125:THR:HG23	4:D:136:PRO:HG2	1.88	0.55
29:7:624:LUT:H383	15:8:229:TRP:CE2	2.42	0.55
10:L2:114:GLU:N	10:L2:114:GLU:OE1	2.40	0.55
22:1:613:CLA:H102	22:1:613:CLA:H143	1.87	0.55
19:92:90:LEU:HD12	22:92:604:CLA:HMD3	1.89	0.55
22:3:606:CLA:HMC2	29:3:622:LUT:H363	1.88	0.55
31:4:608:CHL:O1A	22:4:610:CLA:HMD2	2.06	0.55
19:92:179:THR:HG21	22:92:613:CLA:O1D	2.07	0.55
22:Z:603:CLA:H43	22:Z:603:CLA:CED	2.36	0.55
22:A:829:CLA:HBB1	22:A:829:CLA:HMB1	1.88	0.54
12:1:119:PHE:CE1	22:1:604:CLA:HMD2	2.42	0.54
14:7:156:GLU:N	14:7:156:GLU:OE1	2.39	0.54
22:3:615:CLA:H193	17:5:227:ILE:HG21	1.89	0.54
18:6:184:MET:HE3	22:6:602:CLA:HMC3	1.89	0.54
2:B:722:TYR:HB2	22:B:802:CLA:HED2	1.90	0.54
22:1:608:CLA:HMA1	29:1:619:LUT:H203	1.89	0.54
16:4:149:LEU:HD13	31:4:606:CHL:HMD3	1.90	0.54
22:92:610:CLA:HMC2	29:92:616:LUT:C31	2.38	0.54
22:3:602:CLA:HMC2	29:3:622:LUT:C11	2.38	0.54
19:92:92:VAL:HG12	19:92:94:PRO:HD2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:92:603:CLA:HMD2	22:92:609:CLA:CHD	2.38	0.54
22:A:833:CLA:OBD	10:L:57:THR:HG21	2.07	0.54
6:F:64:ILE:HD11	6:F:143:TYR:CD2	2.43	0.54
22:1:603:CLA:H43	22:1:603:CLA:CED	2.38	0.54
12:1:159:ASP:OD1	29:1:617:LUT:O23	2.23	0.54
2:B:217:LEU:HD13	19:9:210:LEU:HD23	1.90	0.54
2:B:464:ILE:HD11	22:B:836:CLA:H12	1.90	0.54
25:L2:205:BCR:C23	25:L2:205:BCR:H403	2.38	0.54
27:B:853:LMU:O6'	27:B:853:LMU:O2B	1.99	0.53
25:B2:844:BCR:H331	25:B2:844:BCR:C8	2.38	0.53
22:B:836:CLA:HBB1	22:B:836:CLA:HMB1	1.89	0.53
25:L:205:BCR:C23	25:L:205:BCR:H403	2.39	0.53
22:8:602:CLA:HMC2	32:8:618:XAT:C11	2.37	0.53
2:B:653:PHE:CZ	2:B:657:ILE:HD11	2.43	0.53
2:B:393:ILE:HG21	22:B:829:CLA:HED1	1.90	0.53
31:5:606:CHL:C4C	34:H:67:HOH:O	2.34	0.53
22:Z:608:CLA:H12	29:Z:617:LUT:H383	1.90	0.52
13:3:99:MET:HE3	22:3:610:CLA:HMC3	1.91	0.52
25:B:843:BCR:H331	25:B:843:BCR:C8	2.39	0.52
12:Z:71:LEU:O	12:Z:75:THR:HG23	2.09	0.52
31:6:608:CHL:H11	29:6:621:LUT:H383	1.91	0.52
27:A:858:LMU:H2O1	27:A:858:LMU:H3O2	1.58	0.52
22:3:610:CLA:HMC2	29:3:621:LUT:C31	2.40	0.52
20:B2:158:LEU:O	20:B2:163:GLN:NE2	2.43	0.52
6:F:208:GLN:OE1	6:F:212:ARG:NH2	2.43	0.52
22:B:834:CLA:H141	28:B:854:LMG:C34	2.39	0.52
22:F:304:CLA:O1A	22:F:304:CLA:C2	2.58	0.52
25:A:848:BCR:H362	25:A:849:BCR:H21C	1.92	0.51
16:4:149:LEU:CD1	31:4:606:CHL:HMD3	2.40	0.51
31:4:606:CHL:C1A	34:H:64:HOH:O	2.34	0.51
25:B:801:BCR:H331	25:B:801:BCR:C8	2.40	0.51
25:J:102:BCR:H331	25:J:102:BCR:C8	2.40	0.51
31:8:601:CHL:CBB	22:8:602:CLA:HMD2	2.40	0.51
22:9:610:CLA:HBB1	22:9:610:CLA:HMB1	1.92	0.51
22:3:615:CLA:H42	17:5:231:ILE:CG1	2.40	0.51
7:G:50:ARG:NH2	7:G:91:ASP:OD1	2.43	0.51
13:3:210:MET:CE	22:3:610:CLA:HED3	2.41	0.51
22:3:602:CLA:HBA1	29:3:622:LUT:H182	1.93	0.51
6:F:204:LEU:HA	22:8:603:CLA:H42	1.92	0.51
22:1:610:CLA:HMC2	29:1:617:LUT:C31	2.41	0.51
22:3:603:CLA:HMD3	25:3:719:BCR:H403	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:86:MET:HE3	22:Z:610:CLA:HMC3	1.93	0.51
24:3:623:LHG:HC62	22:5:616:CLA:HMD3	1.93	0.51
16:4:82:ASP:OD1	16:4:85:TYR:N	2.44	0.51
22:A:818:CLA:H91	25:K:207:BCR:HC21	1.93	0.51
18:6:33:LEU:HD13	31:6:601:CHL:HMA3	1.91	0.51
25:L2:205:BCR:C8	25:L2:205:BCR:H331	2.41	0.50
22:A:802:CLA:H141	22:A:804:CLA:H191	1.93	0.50
1:A:444:VAL:HG21	22:A:840:CLA:HMC3	1.94	0.50
22:4:610:CLA:HBB1	22:4:610:CLA:HMB1	1.92	0.50
22:4:613:CLA:H43	22:4:614:CLA:OBD	2.11	0.50
22:5:602:CLA:HMC2	32:5:624:XAT:C11	2.41	0.50
1:A:67:GLU:OE2	1:A:71:ARG:NH2	2.45	0.50
22:A:825:CLA:H41	22:A:825:CLA:H72	1.94	0.50
22:9:602:CLA:HMC2	29:9:617:LUT:C31	2.42	0.50
2:B:520:VAL:HG11	2:B:594:TYR:CG	2.47	0.49
22:B:841:CLA:HMC3	22:1:603:CLA:H12	1.95	0.49
1:A:547:VAL:HG11	22:A:840:CLA:HMB3	1.93	0.49
25:A:852:BCR:H331	25:A:852:BCR:C8	2.42	0.49
22:B2:828:CLA:H141	22:B2:828:CLA:H171	1.93	0.49
22:6:613:CLA:CHB	22:6:614:CLA:HMD3	2.42	0.49
10:L:128:LEU:HD22	25:L:205:BCR:H401	1.95	0.49
22:A:854:CLA:HBB1	22:A:854:CLA:HMB1	1.94	0.49
18:6:76:ARG:NH1	31:6:608:CHL:OBD	2.39	0.49
22:A:843:CLA:H93	22:A:843:CLA:H121	1.93	0.49
13:3:39:ASP:HB2	13:3:47:VAL:HG23	1.95	0.48
1:A:413:MET:HE3	1:A:431:ILE:HD11	1.96	0.48
25:B:844:BCR:H382	25:B:844:BCR:H23C	1.94	0.48
22:8:604:CLA:H43	25:8:619:BCR:H272	1.94	0.48
19:9:40:HIS:ND1	19:9:57:GLY:O	2.46	0.48
22:A:820:CLA:HMB1	22:A:820:CLA:HBB1	1.95	0.48
15:8:31:LEU:HD13	31:8:601:CHL:HMA3	1.94	0.48
22:B:834:CLA:H2	22:B:835:CLA:HMB2	1.95	0.48
13:3:201:PHE:O	13:3:203:LEU:N	2.46	0.48
19:9:103:GLU:N	19:9:103:GLU:OE1	2.46	0.48
22:B:839:CLA:H93	25:I:172:BCR:H333	1.96	0.48
22:3:611:CLA:H41	22:3:611:CLA:H71	1.95	0.48
15:8:183:ASP:N	15:8:183:ASP:OD1	2.44	0.48
18:6:79:MET:HE3	22:6:610:CLA:HMC3	1.94	0.48
22:92:602:CLA:HMC2	29:92:617:LUT:C31	2.43	0.48
29:F:305:LUT:C28	29:F:305:LUT:H381	2.41	0.48
27:92:624:LMU:H82	25:92:623:BCR:H362	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:A:826:CLA:C14	22:A:826:CLA:HMD2	2.43	0.47
2:B:489:ASN:ND2	22:B:835:CLA:HMD1	2.28	0.47
25:L:205:BCR:H331	25:L:205:BCR:C8	2.43	0.47
18:6:157:PRO:HD3	31:6:608:CHL:HMD2	1.96	0.47
12:Z:130:LEU:CD1	31:Z:606:CHL:HMD3	2.43	0.47
16:4:199:ASP:OD1	29:4:619:LUT:O23	2.29	0.47
17:5:194:MET:HE3	22:5:602:CLA:HMC3	1.96	0.47
2:B:309:HIS:HA	22:B:841:CLA:HMD1	1.96	0.47
22:7:610:CLA:HMC2	29:7:621:LUT:C31	2.44	0.47
22:Z:602:CLA:HMC2	32:Z:618:XAT:C11	2.43	0.47
22:92:611:CLA:H93	22:92:611:CLA:H121	1.96	0.47
2:B:340:ALA:HB2	25:B:847:BCR:H372	1.96	0.47
1:A:399:GLY:HA3	1:A:603:LEU:HD11	1.95	0.47
2:B:192:THR:HG21	2:B:279:LEU:HB2	1.96	0.47
22:B:806:CLA:H2	22:B:806:CLA:HED3	1.96	0.47
22:3:606:CLA:HMC3	22:3:607:CLA:O1D	2.13	0.47
22:6:610:CLA:HMC2	29:6:621:LUT:C31	2.45	0.47
21:A:801:CL0:H13	22:A:854:CLA:OBD	2.15	0.47
3:C:14:CYS:O	3:C:15:THR:OG1	2.27	0.47
22:8:611:CLA:HMB2	27:8:625:LMU:H41	1.97	0.47
17:5:85:VAL:HG11	29:5:620:LUT:H12	1.95	0.47
19:92:179:THR:HG22	19:92:202:TYR:CG	2.50	0.47
22:A:854:CLA:HMD3	22:B:802:CLA:O1A	2.14	0.47
22:A:817:CLA:HMD2	13:3:133:PRO:HG3	1.97	0.47
4:D:176:GLY:N	5:E:49:GLU:OE1	2.48	0.47
22:8:604:CLA:H142	22:Z:616:CLA:HMB2	1.96	0.47
28:9:620:LMG:O9	28:9:620:LMG:O2	2.29	0.47
20:B2:27:ALA:HA	22:B2:829:CLA:H42	1.97	0.47
20:B2:60:LEU:O	20:B2:63:SER:OG	2.24	0.46
1:A:353:LEU:HB2	22:A:806:CLA:HMD3	1.96	0.46
10:L:58:PRO:O	10:L:62:ALA:HB2	2.15	0.46
11:K:57:VAL:HG23	11:K:88:ASP:OD1	2.14	0.46
12:1:88:GLY:HA2	32:1:618:XAT:H181	1.98	0.46
17:5:188:LYS:NZ	24:5:623:LHG:O5	2.48	0.46
22:5:617:CLA:HED1	24:6:619:LHG:H311	1.98	0.46
1:A:433:HIS:HB3	10:L:55:LEU:HD22	1.96	0.46
22:B:841:CLA:HBC1	27:B:853:LMU:H2'	1.97	0.46
2:B:236:GLN:O	2:B:237:SER:OG	2.32	0.46
2:B:269:LEU:HD13	22:B:817:CLA:HMA2	1.97	0.46
2:B:632:LEU:HD21	2:B:651:PHE:CD1	2.51	0.46
22:A:802:CLA:HMC2	22:A:854:CLA:CAC	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:7:81:LEU:HD22	22:7:610:CLA:H201	1.98	0.46
25:9:623:BCR:H362	27:9:624:LMU:H82	1.97	0.46
22:92:609:CLA:HBC2	22:92:609:CLA:HMC1	1.97	0.46
1:A:677:PHE:CG	25:A:852:BCR:H363	2.51	0.46
6:F:165:TYR:HD1	29:F:305:LUT:HO3	1.64	0.46
10:L:57:THR:HG22	10:L:58:PRO:HD2	1.98	0.46
22:6:609:CLA:HMB2	22:6:617:CLA:C2C	2.46	0.46
19:92:166:MET:HE3	22:92:602:CLA:HMC3	1.98	0.46
22:A:803:CLA:OBD	22:B:802:CLA:HMB3	2.15	0.46
1:A:223:PRO:HB2	1:A:243:LEU:HD13	1.98	0.45
22:B:829:CLA:HBB1	22:B:829:CLA:HMB1	1.96	0.45
25:B:845:BCR:H331	25:B:845:BCR:C8	2.46	0.45
22:4:611:CLA:C1D	22:4:612:CLA:HMD2	2.46	0.45
12:1:202:PRO:O	29:1:617:LUT:O3	2.33	0.45
31:Z:601:CHL:CBB	22:Z:602:CLA:HMD2	2.46	0.45
25:6:623:BCR:H331	25:6:623:BCR:C8	2.45	0.45
22:4:612:CLA:HMC2	29:4:619:LUT:C11	2.46	0.45
22:A:802:CLA:HBB1	22:A:802:CLA:HMB1	1.98	0.45
14:7:135:ARG:NH1	22:7:609:CLA:O1D	2.46	0.45
8:I2:74:TRP:O	8:I2:77:SER:OG	2.26	0.45
25:B:845:BCR:H342	19:9:177:LEU:HD21	1.99	0.45
25:K:202:BCR:H392	25:K:202:BCR:C23	2.46	0.45
1:A:282:LEU:HD21	1:A:375:PRO:HD2	1.98	0.45
15:8:200:MET:HE3	22:8:602:CLA:HMC3	1.97	0.45
22:B:811:CLA:C9	22:B:813:CLA:HMB3	2.47	0.45
22:1:603:CLA:H61	22:1:603:CLA:H41	1.87	0.45
22:B:832:CLA:CAB	22:B:833:CLA:HMB2	2.46	0.45
22:3:612:CLA:HMC2	29:3:621:LUT:C11	2.46	0.45
27:92:624:LMU:C8	25:92:623:BCR:H362	2.47	0.45
22:A:809:CLA:H91	22:A:812:CLA:H201	1.99	0.45
22:B:821:CLA:H191	12:1:131:LEU:HD22	1.99	0.45
25:B:844:BCR:H331	25:B:844:BCR:C8	2.46	0.45
19:9:52:ASP:OD1	29:9:617:LUT:O23	2.34	0.45
8:I:80:VAL:HB	8:I:81:PRO:HD3	1.98	0.44
25:K:202:BCR:H331	25:K:202:BCR:C8	2.47	0.44
29:7:624:LUT:H383	15:8:229:TRP:CZ2	2.52	0.44
2:B:414:ASP:O	6:F:227:ARG:NH1	2.51	0.44
2:B:451:GLU:OE2	6:F:114:ARG:NH1	2.50	0.44
22:B:819:CLA:HMB2	22:B:824:CLA:HMA3	1.99	0.44
22:3:615:CLA:H42	17:5:231:ILE:HG13	1.98	0.44
22:Z:603:CLA:HMD2	22:Z:609:CLA:C1D	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:418:ASP:OD2	1:A:420:THR:OG1	2.30	0.44
2:B:632:LEU:HD21	2:B:651:PHE:CG	2.52	0.44
12:1:154:PRO:CG	22:1:608:CLA:HMD2	2.48	0.44
1:A:413:MET:CE	1:A:431:ILE:HD11	2.47	0.44
22:3:603:CLA:HBB1	22:3:603:CLA:HMB1	2.00	0.44
22:3:603:CLA:HBC1	22:3:609:CLA:CBC	2.48	0.44
22:8:604:CLA:HMB1	22:8:604:CLA:HBB1	1.99	0.44
19:92:93:THR:OG1	19:92:94:PRO:HD3	2.17	0.44
19:92:200:THR:O	19:92:204:THR:OG1	2.29	0.44
1:A:119:TRP:CD2	22:A:810:CLA:HED3	2.53	0.44
12:1:119:PHE:CZ	22:1:604:CLA:HMD2	2.52	0.44
27:A:862:LMU:O2'	27:A:863:LMU:O6B	2.04	0.44
10:L:74:ALA:HB2	22:L:203:CLA:HMD1	1.98	0.44
2:B:173:GLU:OE1	2:B:173:GLU:N	2.49	0.44
3:C:2:ALA:N	3:C:71:SER:O	2.51	0.44
12:Z:35:LYS:N	12:Z:51:ASP:OD1	2.51	0.44
22:5:621:CLA:CBD	22:5:621:CLA:HAA2	2.48	0.44
18:6:122:HIS:O	18:6:126:VAL:HG23	2.17	0.44
25:9:623:BCR:H20C	25:9:623:BCR:H361	1.86	0.44
22:A:826:CLA:HBB1	22:A:826:CLA:HMB1	2.00	0.44
22:B:827:CLA:H141	22:B:829:CLA:H143	2.00	0.44
3:C:24:ASP:OD2	4:D:151:HIS:ND1	2.46	0.44
15:8:231:VAL:HG12	22:8:613:CLA:HED1	1.99	0.44
25:K:202:BCR:H23C	25:K:202:BCR:H403	1.99	0.43
25:A:850:BCR:C8	25:A:850:BCR:H331	2.48	0.43
22:B:837:CLA:HBB1	22:B:837:CLA:HMB1	2.00	0.43
25:L:201:BCR:H24C	25:L:201:BCR:H371	1.90	0.43
22:1:609:CLA:HMB1	22:1:609:CLA:HBB1	2.00	0.43
13:3:101:GLY:HA2	29:3:622:LUT:H381	1.99	0.43
17:5:95:LYS:HB3	17:5:98:VAL:HG13	1.99	0.43
17:5:149:ASP:OD1	17:5:151:ILE:N	2.51	0.43
22:B:816:CLA:H142	22:B:816:CLA:C10	2.49	0.43
6:F:193:THR:HG21	28:J:104:LMG:H142	1.99	0.43
2:B:77:GLN:OE1	2:B:77:GLN:N	2.48	0.43
22:A:833:CLA:H42	10:L:65:VAL:HG13	2.00	0.43
22:B:808:CLA:HMB2	22:B:808:CLA:H142	2.00	0.43
13:3:183:ILE:HG22	13:3:196:PRO:HG2	2.00	0.43
1:A:343:GLU:O	1:A:347:THR:OG1	2.28	0.43
1:A:554:VAL:HG11	22:A:822:CLA:H203	2.01	0.43
22:B:806:CLA:HMC2	25:B:844:BCR:H401	2.00	0.43
22:L:203:CLA:H62	22:L:203:CLA:H41	1.89	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:3:719:BCR:C8	25:3:719:BCR:H331	2.47	0.43
25:B2:845:BCR:H24C	25:B2:845:BCR:H371	1.87	0.43
22:B:840:CLA:H122	22:B:840:CLA:H91	2.01	0.43
18:6:33:LEU:HD13	31:6:601:CHL:CMA	2.48	0.43
1:A:411:ILE:HD13	22:A:831:CLA:CED	2.49	0.43
25:A:849:BCR:H331	25:A:849:BCR:C8	2.49	0.43
25:K:207:BCR:H24C	25:K:207:BCR:H371	1.88	0.43
22:1:602:CLA:HMC2	32:1:618:XAT:C31	2.48	0.43
22:7:610:CLA:H13	22:6:603:CLA:H142	2.00	0.43
12:Z:215:GLY:O	12:Z:220:THR:HG21	2.19	0.43
2:B:264:PRO:O	2:B:267:GLN:NE2	2.51	0.42
31:1:601:CHL:H62	31:1:601:CHL:H41	1.77	0.42
22:B:808:CLA:CGA	22:B:808:CLA:C1A	2.97	0.42
22:3:615:CLA:C19	17:5:227:ILE:HG21	2.49	0.42
22:7:602:CLA:HMC2	32:7:622:XAT:C11	2.49	0.42
15:8:225:LEU:HD21	22:8:614:CLA:HMC3	2.01	0.42
1:A:586:VAL:HG13	2:B:670:GLY:HA3	2.00	0.42
1:A:707:LEU:HD23	6:F:216:LEU:HD23	2.01	0.42
25:B:848:BCR:H24C	25:B:848:BCR:H371	1.91	0.42
25:3:719:BCR:H20C	25:3:719:BCR:H361	1.90	0.42
14:7:34:PHE:HE1	31:7:601:CHL:HED2	1.85	0.42
22:4:603:CLA:HMD2	22:4:609:CLA:C1D	2.48	0.42
17:5:133:GLU:OE2	34:H:86:HOH:O	2.21	0.42
19:9:126:ARG:NH2	22:9:609:CLA:O1D	2.53	0.42
22:B2:828:CLA:H101	25:B2:845:BCR:H372	2.00	0.42
22:A:802:CLA:CGA	22:A:802:CLA:H3A	2.50	0.42
27:A:858:LMU:O3'	27:A:858:LMU:O2B	2.27	0.42
16:4:54:ARG:HD3	16:4:67:LEU:HD12	2.00	0.42
22:9:612:CLA:HBB1	22:9:612:CLA:HMB1	2.02	0.42
2:B:672:TRP:CZ2	23:B:842:PQN:H2M3	2.54	0.42
22:3:615:CLA:HAA2	22:5:616:CLA:HED2	2.01	0.42
22:8:610:CLA:HBB1	22:8:610:CLA:HMB1	2.02	0.42
16:4:66:ASP:O	24:4:623:LHG:O4	2.38	0.42
22:5:616:CLA:H62	22:5:616:CLA:H41	1.92	0.42
29:9:617:LUT:C28	29:9:617:LUT:H381	2.48	0.42
22:A:823:CLA:H42	11:K:65:LEU:HD21	2.01	0.42
22:A:840:CLA:HMB1	22:A:840:CLA:HBB1	2.01	0.42
22:A:843:CLA:H61	22:A:843:CLA:H41	1.87	0.42
13:3:210:MET:HE2	22:3:610:CLA:HED3	2.02	0.42
25:3:718:BCR:H24C	25:3:718:BCR:H371	1.90	0.42
19:9:78:MET:HE3	22:9:610:CLA:HMC3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:92:602:CLA:H62	22:92:602:CLA:H41	1.82	0.42
22:A:843:CLA:H52	22:B:839:CLA:H43	2.01	0.42
13:3:58:ASP:OD1	13:3:58:ASP:N	2.53	0.42
12:Z:119:PHE:CZ	22:Z:604:CLA:HMD2	2.54	0.42
22:92:613:CLA:C1A	22:92:613:CLA:CGA	2.98	0.42
14:7:34:PHE:CE1	31:7:601:CHL:HED2	2.54	0.42
22:5:617:CLA:H61	22:5:617:CLA:H41	1.90	0.42
28:J:103:LMG:HC61	28:J:103:LMG:O1	2.20	0.42
11:K:69:ASP:OD1	11:K:70:SER:N	2.53	0.42
22:Z:613:CLA:CGA	22:Z:613:CLA:C1A	2.98	0.42
25:92:623:BCR:H361	25:92:623:BCR:H20C	1.84	0.42
25:A:848:BCR:H24C	25:A:848:BCR:H371	1.87	0.42
22:B:837:CLA:H41	29:F:305:LUT:C37	2.50	0.42
25:B:843:BCR:H24C	25:B:843:BCR:H371	1.92	0.42
4:D:88:TRP:CD1	4:D:134:LEU:HD13	2.55	0.42
25:L:205:BCR:H403	25:L:205:BCR:H23C	2.02	0.42
22:B2:828:CLA:H142	25:B2:844:BCR:C15	2.50	0.42
22:A:820:CLA:CAD	22:A:830:CLA:H41	2.50	0.41
18:6:33:LEU:HD12	31:6:601:CHL:HED2	2.01	0.41
22:A:829:CLA:H72	22:A:829:CLA:C12	2.50	0.41
29:A:856:LUT:H171	29:A:856:LUT:H8	2.02	0.41
25:3:620:BCR:H24C	25:3:620:BCR:H371	1.92	0.41
31:5:608:CHL:H12	29:5:620:LUT:H383	2.01	0.41
25:B2:844:BCR:H20C	25:B2:844:BCR:H361	1.95	0.41
1:A:245:LEU:O	27:A:857:LMU:O2B	2.35	0.41
25:A:851:BCR:H371	25:A:851:BCR:H24C	1.89	0.41
22:9:610:CLA:HMC2	29:9:616:LUT:C31	2.50	0.41
22:B:834:CLA:HMD2	22:B:835:CLA:CHC	2.50	0.41
11:K:65:LEU:N	11:K:65:LEU:HD12	2.36	0.41
12:Z:220:THR:HG22	12:Z:220:THR:O	2.21	0.41
19:9:172:PHE:CE1	29:9:616:LUT:H182	2.55	0.41
1:A:584:CYS:O	2:B:670:GLY:N	2.53	0.41
1:A:747:ILE:O	1:A:751:GLY:N	2.52	0.41
22:A:811:CLA:C1	22:A:813:CLA:H42	2.49	0.41
2:B:178:HIS:CG	22:B:813:CLA:HMC2	2.55	0.41
25:3:719:BCR:H24C	25:3:719:BCR:H371	1.86	0.41
1:A:343:GLU:OE1	1:A:343:GLU:N	2.48	0.41
11:K:35:ASN:ND2	22:K:204:CLA:OBD	2.53	0.41
22:3:607:CLA:HBC2	22:3:607:CLA:HMC1	2.02	0.41
25:L2:205:BCR:H20C	25:L2:205:BCR:H361	1.92	0.41
25:8:619:BCR:HC8	25:8:619:BCR:H311	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A:848:BCR:H20C	25:A:848:BCR:H361	1.85	0.41
22:B:840:CLA:H91	22:B:840:CLA:C12	2.51	0.41
9:J:32:TYR:OH	22:J:101:CLA:HED3	2.21	0.41
18:6:209:LEU:HD21	22:6:614:CLA:HMC3	2.03	0.41
19:92:78:MET:HE3	22:92:610:CLA:HMC3	2.03	0.41
1:A:115:ALA:HB3	22:A:809:CLA:HED3	2.03	0.41
25:A:851:BCR:H20C	25:A:851:BCR:H361	1.94	0.41
25:A:852:BCR:H20C	25:A:852:BCR:H361	1.87	0.41
22:B:817:CLA:HBC3	22:B:817:CLA:HMC1	2.01	0.41
22:1:613:CLA:H2	22:1:614:CLA:HMD1	2.02	0.41
31:7:601:CHL:H61	31:7:601:CHL:H41	1.83	0.41
16:4:223:MET:HE3	22:4:602:CLA:HMC3	2.03	0.41
31:6:606:CHL:HMB2	25:6:623:BCR:H373	2.03	0.41
22:6:613:CLA:C1B	22:6:614:CLA:HMD3	2.50	0.41
19:92:193:ASP:OD2	19:92:196:GLY:N	2.53	0.41
22:A:833:CLA:C4	10:L:65:VAL:HG13	2.51	0.41
25:A:852:BCR:H24C	25:A:852:BCR:H371	1.91	0.41
22:B:837:CLA:H41	29:F:305:LUT:H371	2.03	0.41
17:5:91:GLN:CD	17:5:98:VAL:HG21	2.41	0.41
25:6:623:BCR:H20C	25:6:623:BCR:H361	1.96	0.41
12:1:50:PRO:O	12:1:56:ASN:ND2	2.54	0.40
9:J:8:LEU:HA	9:J:13:VAL:HG11	2.03	0.40
22:8:612:CLA:H43	22:4:609:CLA:H11	2.03	0.40
27:8:627:LMU:H2'	27:8:627:LMU:H6D	2.03	0.40
22:B2:828:CLA:H142	25:B2:844:BCR:H15C	2.04	0.40
22:B:823:CLA:H3A	22:B:841:CLA:HED3	2.04	0.40
22:B:832:CLA:HBB1	25:B:801:BCR:H323	2.02	0.40
25:B:845:BCR:H24C	25:B:845:BCR:H371	1.84	0.40
22:A:839:CLA:C1A	22:A:839:CLA:CGA	3.00	0.40
22:B:808:CLA:HMB2	22:B:808:CLA:C14	2.51	0.40
12:Z:192:VAL:HG13	27:Z:622:LMU:O2'	2.20	0.40
25:K:207:BCR:H20C	25:K:207:BCR:H361	1.90	0.40
13:3:132:PRO:N	13:3:133:PRO:CD	2.84	0.40
17:5:95:LYS:O	17:5:98:VAL:HG22	2.21	0.40
10:L2:82:VAL:HG13	10:L2:83:LEU:N	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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%)	729 (98%)	11 (2%)	0	100	100
2	B	731/735 (100%)	718 (98%)	13 (2%)	0	100	100
3	C	78/81 (96%)	76 (97%)	2 (3%)	0	100	100
4	D	142/196 (72%)	138 (97%)	4 (3%)	0	100	100
5	E	62/97 (64%)	61 (98%)	1 (2%)	0	100	100
6	F	163/227 (72%)	162 (99%)	1 (1%)	0	100	100
7	G	93/126 (74%)	93 (100%)	0	0	100	100
8	I	35/106 (33%)	35 (100%)	0	0	100	100
8	I2	35/106 (33%)	34 (97%)	1 (3%)	0	100	100
9	J	38/40 (95%)	37 (97%)	1 (3%)	0	100	100
10	L	120/196 (61%)	117 (98%)	3 (2%)	0	100	100
10	L2	98/196 (50%)	95 (97%)	3 (3%)	0	100	100
11	K	84/113 (74%)	82 (98%)	2 (2%)	0	100	100
12	1	192/228 (84%)	192 (100%)	0	0	100	100
12	Z	192/228 (84%)	189 (98%)	3 (2%)	0	100	100
13	3	225/298 (76%)	218 (97%)	7 (3%)	0	100	100
14	7	211/241 (88%)	210 (100%)	1 (0%)	0	100	100
15	8	215/243 (88%)	213 (99%)	2 (1%)	0	100	100
16	4	210/264 (80%)	207 (99%)	3 (1%)	0	100	100
17	5	225/257 (88%)	220 (98%)	5 (2%)	0	100	100
18	6	228/257 (89%)	225 (99%)	3 (1%)	0	100	100
19	9	184/213 (86%)	179 (97%)	4 (2%)	1 (0%)	29	48
19	92	182/213 (85%)	178 (98%)	3 (2%)	1 (0%)	29	48
20	B2	166/180 (92%)	164 (99%)	2 (1%)	0	100	100
All	All	4649/5592 (83%)	4572 (98%)	75 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
19	92	139	ILE
19	9	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	90
2	B	596/597 (100%)	595 (100%)	1 (0%)	93	96
3	C	69/70 (99%)	68 (99%)	1 (1%)	67	80
4	D	121/152 (80%)	120 (99%)	1 (1%)	81	89
5	E	55/81 (68%)	55 (100%)	0	100	100
6	F	127/169 (75%)	126 (99%)	1 (1%)	81	89
7	G	71/94 (76%)	71 (100%)	0	100	100
8	I	31/76 (41%)	31 (100%)	0	100	100
8	I2	31/76 (41%)	30 (97%)	1 (3%)	39	59
9	J	35/35 (100%)	35 (100%)	0	100	100
10	L	90/148 (61%)	89 (99%)	1 (1%)	73	84
10	L2	72/148 (49%)	72 (100%)	0	100	100
11	K	59/80 (74%)	59 (100%)	0	100	100
12	1	137/162 (85%)	137 (100%)	0	100	100
12	Z	137/162 (85%)	137 (100%)	0	100	100
13	3	174/230 (76%)	171 (98%)	3 (2%)	60	76
14	7	164/181 (91%)	163 (99%)	1 (1%)	86	91
15	8	163/183 (89%)	161 (99%)	2 (1%)	71	83
16	4	166/205 (81%)	165 (99%)	1 (1%)	86	91
17	5	184/206 (89%)	182 (99%)	2 (1%)	73	84
18	6	184/203 (91%)	184 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	9	142/159 (89%)	142 (100%)	0	100	100
19	92	141/159 (89%)	141 (100%)	0	100	100
20	B2	153/153 (100%)	153 (100%)	0	100	100
All	All	3703/4339 (85%)	3684 (100%)	19 (0%)	89	92

All (19) 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
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
16	4	258	GLN
17	5	91	GLN
17	5	238	HIS
8	I2	69	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	369	HIS
12	1	195	HIS
13	3	256	ASN
19	9	109	GLN
19	92	140	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	J	1	9	9,10,11	0.51	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	J	1	9	-	2/9/10/12	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	J	1	AME	O-C-CA	-2.53	118.15	124.78

There are no chirality outliers.

All (2) 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

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](#)

397 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$
22	CLA	8	604	34	60,68,73	1.10	4 (6%)	70,107,113	0.92	2 (2%)
22	CLA	B2	809	20	52,60,73	1.16	3 (5%)	60,97,113	0.94	2 (3%)
32	XAT	4	620	-	39,47,47	0.12	0	54,74,74	0.66	0
22	CLA	92	602	19	65,73,73	1.02	4 (6%)	76,113,113	0.89	3 (3%)
31	CHL	4	618	16	46,54,74	2.40	10 (21%)	49,90,114	1.38	7 (14%)
22	CLA	B	837	-	65,73,73	1.01	4 (6%)	76,113,113	0.85	2 (2%)
22	CLA	B	828	-	65,73,73	1.02	4 (6%)	76,113,113	0.83	2 (2%)
22	CLA	5	610	17	60,68,73	1.04	3 (5%)	70,107,113	0.87	2 (2%)
22	CLA	8	611	24	45,53,73	1.26	4 (8%)	52,89,113	1.04	2 (3%)
25	BCR	L2	201	-	41,41,41	0.14	0	56,56,56	0.37	0
22	CLA	4	611	24	60,68,73	1.08	3 (5%)	70,107,113	0.89	2 (2%)
25	BCR	B	845	-	41,41,41	0.15	0	56,56,56	0.37	0
31	CHL	6	601	18	66,74,74	2.00	10 (15%)	73,114,114	1.18	9 (12%)
29	LUT	5	626	-	42,43,43	0.24	0	51,60,60	0.36	0
22	CLA	7	613	14	65,73,73	1.03	4 (6%)	76,113,113	0.87	2 (2%)
28	LMG	A	859	-	48,48,55	0.18	0	56,56,63	0.18	0
25	BCR	3	620	-	41,41,41	0.21	0	56,56,56	0.36	0
31	CHL	6	616	18	66,74,74	2.00	10 (15%)	73,114,114	1.15	9 (12%)
22	CLA	Z	610	12	60,68,73	1.07	4 (6%)	70,107,113	0.89	2 (2%)
22	CLA	B	833	-	58,66,73	1.07	4 (6%)	67,104,113	0.95	2 (2%)
25	BCR	3	718	-	41,41,41	0.17	0	56,56,56	0.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	CHL	6	618	18	43,51,74	2.48	9 (20%)	45,86,114	1.46	7 (15%)
22	CLA	L2	203	-	45,53,73	1.24	3 (6%)	52,89,113	1.03	3 (5%)
22	CLA	B	830	-	45,53,73	1.21	4 (8%)	52,89,113	1.02	2 (3%)
25	BCR	B2	844	-	41,41,41	0.14	0	56,56,56	0.30	0
28	LMG	3	722	-	44,44,55	0.21	0	46,46,63	0.26	0
22	CLA	A	840	-	65,73,73	1.01	3 (4%)	76,113,113	0.86	2 (2%)
29	LUT	7	621	-	42,43,43	0.27	0	51,60,60	0.38	0
22	CLA	B	808	-	65,73,73	1.03	4 (6%)	76,113,113	0.83	2 (2%)
33	NEX	5	625	-	38,46,46	0.46	1 (2%)	50,70,70	0.77	3 (6%)
29	LUT	Z	617	-	42,43,43	0.29	0	51,60,60	0.41	0
22	CLA	6	614	-	50,58,73	1.19	4 (8%)	58,95,113	0.98	2 (3%)
22	CLA	7	610	14	65,73,73	1.03	4 (6%)	76,113,113	0.90	2 (2%)
28	LMG	B2	852	-	43,43,55	0.18	0	51,51,63	0.18	0
26	SF4	C	101	3	0,12,12	-	-	-	-	-
22	CLA	A	812	-	65,73,73	1.00	4 (6%)	76,113,113	0.84	2 (2%)
22	CLA	A	803	34	65,73,73	1.05	4 (6%)	76,113,113	0.87	2 (2%)
28	LMG	A	860	-	36,36,55	0.20	0	44,44,63	0.24	0
28	LMG	7	626	-	37,37,55	0.19	0	45,45,63	0.26	0
22	CLA	A	809	1	65,73,73	1.02	4 (6%)	76,113,113	0.94	3 (3%)
22	CLA	6	612	18	45,53,73	1.24	3 (6%)	52,89,113	1.02	2 (3%)
32	XAT	5	624	-	39,47,47	0.12	0	54,74,74	0.60	0
29	LUT	4	619	-	42,43,43	0.27	0	51,60,60	0.43	0
22	CLA	L	204	-	45,53,73	1.27	3 (6%)	52,89,113	1.06	3 (5%)
22	CLA	A	825	-	55,63,73	1.13	4 (7%)	64,101,113	0.94	2 (3%)
22	CLA	B	817	-	65,73,73	1.01	4 (6%)	76,113,113	0.87	2 (2%)
22	CLA	B2	814	-	60,68,73	1.08	3 (5%)	70,107,113	0.89	2 (2%)
22	CLA	B2	813	-	65,73,73	1.05	3 (4%)	76,113,113	0.86	2 (2%)
29	LUT	1	617	-	42,43,43	0.28	0	51,60,60	0.40	0
25	BCR	B	843	-	41,41,41	0.17	0	56,56,56	0.32	0
27	LMU	A	858	-	36,36,36	0.09	0	47,47,47	0.19	0
27	LMU	4	625	-	34,34,36	0.10	0	45,45,47	0.19	0
25	BCR	3	719	-	41,41,41	0.12	0	56,56,56	0.40	0
22	CLA	K	201	11	45,53,73	1.28	3 (6%)	52,89,113	1.01	2 (3%)
26	SF4	C	102	3	0,12,12	-	-	-	-	-
22	CLA	1	614	-	60,68,73	1.07	4 (6%)	70,107,113	0.93	2 (2%)
29	LUT	9	616	-	42,43,43	0.28	0	51,60,60	0.36	0
31	CHL	4	601	16	66,74,74	1.99	10 (15%)	73,114,114	1.15	7 (9%)
22	CLA	B2	808	-	45,53,73	1.26	3 (6%)	52,89,113	1.02	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	B	812	-	65,73,73	1.04	4 (6%)	76,113,113	0.87	2 (2%)
28	LMG	B2	855	-	31,31,55	0.21	0	39,39,63	0.17	0
22	CLA	7	616	14	46,54,73	1.21	4 (8%)	53,90,113	1.01	2 (3%)
29	LUT	3	720	-	42,43,43	0.22	0	51,60,60	0.34	0
31	CHL	1	606	34	46,54,74	2.38	10 (21%)	49,90,114	1.37	7 (14%)
27	LMU	A	864	-	24,24,36	0.12	0	29,29,47	0.31	0
22	CLA	3	617	13	46,54,73	1.21	3 (6%)	53,90,113	1.03	2 (3%)
25	BCR	L	201	-	41,41,41	0.18	0	56,56,56	0.35	0
24	LHG	9	622	22	40,40,48	0.25	0	43,46,54	0.28	0
22	CLA	B	825	34	65,73,73	1.01	4 (6%)	76,113,113	0.81	2 (2%)
25	BCR	L2	205	-	41,41,41	0.14	0	56,56,56	0.34	0
22	CLA	6	604	-	65,73,73	1.03	3 (4%)	76,113,113	0.85	2 (2%)
27	LMU	8	625	-	24,24,36	0.12	0	29,29,47	0.29	0
24	LHG	7	625	22	48,48,48	0.25	0	51,54,54	0.22	0
27	LMU	K	208	-	24,24,36	0.11	0	29,29,47	0.31	0
27	LMU	1	622	-	19,19,36	0.14	0	24,24,47	0.30	0
22	CLA	5	611	24	55,63,73	1.10	4 (7%)	64,101,113	0.92	2 (3%)
27	LMU	6	632	-	20,20,36	0.16	0	25,25,47	0.26	0
29	LUT	8	617	-	42,43,43	0.31	0	51,60,60	0.42	0
25	BCR	B2	845	-	41,41,41	0.14	0	56,56,56	0.33	0
22	CLA	5	601	17	65,73,73	1.05	3 (4%)	76,113,113	0.87	2 (2%)
28	LMG	8	626	-	32,32,55	0.20	0	40,40,63	0.19	0
31	CHL	6	608	34	51,59,74	2.30	9 (17%)	55,96,114	1.33	8 (14%)
31	CHL	7	607	34	46,54,74	2.35	9 (19%)	49,90,114	1.40	7 (14%)
27	LMU	8	628	-	24,24,36	0.16	0	29,29,47	0.33	0
31	CHL	1	601	12	66,74,74	1.95	9 (13%)	73,114,114	1.12	7 (9%)
27	LMU	Z	621	-	22,22,36	0.14	0	27,27,47	0.27	0
25	BCR	I	172	-	41,41,41	0.20	0	56,56,56	0.37	0
22	CLA	4	612	16	45,53,73	1.27	3 (6%)	52,89,113	1.01	2 (3%)
22	CLA	Z	602	12	60,68,73	1.07	4 (6%)	70,107,113	0.93	2 (2%)
22	CLA	6	609	18	55,63,73	1.11	4 (7%)	64,101,113	0.96	3 (4%)
22	CLA	1	616	12	46,54,73	1.22	3 (6%)	53,90,113	1.03	2 (3%)
25	BCR	B2	843	-	20,20,41	0.75	1 (5%)	27,27,56	0.25	0
22	CLA	A	828	-	65,73,73	1.04	4 (6%)	76,113,113	0.79	2 (2%)
25	BCR	B	846	-	41,41,41	0.13	0	56,56,56	0.34	0
22	CLA	Z	609	12	65,73,73	1.06	3 (4%)	76,113,113	0.86	2 (2%)
22	CLA	B2	812	-	60,68,73	1.06	3 (5%)	70,107,113	0.90	2 (2%)
28	LMG	B	852	-	43,43,55	0.17	0	51,51,63	0.23	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	F	304	6	65,73,73	1.03	3 (4%)	76,113,113	0.95	3 (3%)
22	CLA	5	603	-	65,73,73	1.01	4 (6%)	76,113,113	0.87	3 (3%)
25	BCR	L	205	-	41,41,41	0.15	0	56,56,56	0.37	0
22	CLA	3	602	13	60,68,73	1.05	4 (6%)	70,107,113	0.89	2 (2%)
22	CLA	L2	204	-	45,53,73	1.25	3 (6%)	52,89,113	1.05	3 (5%)
27	LMU	1	626	-	24,24,36	0.13	0	29,29,47	0.27	0
22	CLA	A	837	1	57,65,73	1.12	3 (5%)	66,103,113	0.93	2 (3%)
22	CLA	B	822	-	59,67,73	1.09	4 (6%)	68,105,113	0.92	2 (2%)
28	LMG	6	633	-	19,19,55	0.31	0	19,19,63	0.29	0
22	CLA	4	604	34	50,58,73	1.18	4 (8%)	58,95,113	0.99	3 (5%)
31	CHL	92	607	-	46,54,74	2.41	9 (19%)	49,90,114	1.38	7 (14%)
22	CLA	A	836	-	65,73,73	1.04	4 (6%)	76,113,113	0.86	2 (2%)
29	LUT	92	616	-	42,43,43	0.26	0	51,60,60	0.29	0
24	LHG	1	620	22	38,38,48	0.28	0	41,44,54	0.30	0
24	LHG	4	623	-	37,37,48	0.25	0	40,43,54	0.30	0
27	LMU	5	627	-	24,24,36	0.12	0	29,29,47	0.26	0
24	LHG	A	846	-	48,48,48	0.24	0	51,54,54	0.30	0
22	CLA	A	820	-	65,73,73	1.01	4 (6%)	76,113,113	0.88	3 (3%)
31	CHL	1	607	34	46,54,74	2.34	9 (19%)	49,90,114	1.41	9 (18%)
22	CLA	A	835	-	65,73,73	1.02	3 (4%)	76,113,113	0.86	2 (2%)
22	CLA	B	821	-	65,73,73	1.02	4 (6%)	76,113,113	0.84	2 (2%)
22	CLA	6	617	-	45,53,73	1.25	3 (6%)	52,89,113	1.02	3 (5%)
22	CLA	B2	807	-	55,63,73	1.12	3 (5%)	64,101,113	0.92	2 (3%)
32	XAT	7	622	-	39,47,47	0.14	0	54,74,74	0.59	0
22	CLA	92	611	24	65,73,73	1.05	3 (4%)	76,113,113	0.86	2 (2%)
22	CLA	8	609	15	45,53,73	1.23	4 (8%)	52,89,113	1.01	2 (3%)
27	LMU	G	206	-	24,24,36	0.14	0	29,29,47	0.24	0
22	CLA	3	610	13	65,73,73	1.00	4 (6%)	76,113,113	0.86	2 (2%)
27	LMU	6	630	-	24,24,36	0.15	0	29,29,47	0.29	0
22	CLA	92	614	-	45,53,73	1.27	3 (6%)	52,89,113	1.04	2 (3%)
22	CLA	Z	613	34	65,73,73	1.03	4 (6%)	76,113,113	0.89	3 (3%)
22	CLA	B	835	34	45,53,73	1.25	3 (6%)	52,89,113	1.02	2 (3%)
25	BCR	8	619	-	41,41,41	0.15	0	56,56,56	0.31	0
22	CLA	92	609	19	45,53,73	1.26	3 (6%)	52,89,113	1.05	2 (3%)
31	CHL	Z	601	12	66,74,74	1.95	10 (15%)	73,114,114	1.15	7 (9%)
33	NEX	6	625	-	38,46,46	0.31	0	50,70,70	0.84	2 (4%)
31	CHL	9	606	-	42,50,74	2.59	11 (26%)	44,85,114	1.44	7 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	Z	616	12	60,68,73	1.08	3 (5%)	70,107,113	0.89	2 (2%)
27	LMU	7	627	-	33,33,36	0.11	0	44,44,47	0.17	0
22	CLA	K	204	-	46,54,73	1.22	4 (8%)	53,90,113	1.05	2 (3%)
25	BCR	A	851	-	41,41,41	0.15	0	56,56,56	0.33	0
22	CLA	8	616	15	45,53,73	1.21	4 (8%)	52,89,113	1.04	2 (3%)
22	CLA	8	610	15	65,73,73	1.00	3 (4%)	76,113,113	0.84	2 (2%)
27	LMU	6	631	-	24,24,36	0.14	0	29,29,47	0.28	0
22	CLA	9	612	19	65,73,73	1.03	3 (4%)	76,113,113	0.83	2 (2%)
31	CHL	4	607	34	66,74,74	1.98	10 (15%)	73,114,114	1.13	8 (10%)
22	CLA	K	206	11	45,53,73	1.25	3 (6%)	52,89,113	1.03	2 (3%)
22	CLA	G	204	7	46,54,73	1.22	3 (6%)	53,90,113	1.01	2 (3%)
22	CLA	A	845	24	45,53,73	1.23	3 (6%)	52,89,113	0.99	2 (3%)
27	LMU	6	628	-	24,24,36	0.13	0	29,29,47	0.30	0
22	CLA	7	611	24	65,73,73	1.03	4 (6%)	76,113,113	0.84	2 (2%)
22	CLA	7	603	-	52,60,73	1.13	4 (7%)	60,97,113	0.98	2 (3%)
32	XAT	Z	618	-	39,47,47	0.16	0	54,74,74	0.57	0
22	CLA	92	601	19	45,53,73	1.24	3 (6%)	52,89,113	1.00	2 (3%)
27	LMU	4	626	-	20,20,36	0.15	0	25,25,47	0.28	0
22	CLA	1	602	12	60,68,73	1.05	4 (6%)	70,107,113	0.91	2 (2%)
23	PQN	A	844	-	34,34,34	0.31	0	42,45,45	0.37	0
22	CLA	7	620	34	53,61,73	1.15	3 (5%)	61,98,113	0.94	2 (3%)
22	CLA	Z	614	-	50,58,73	1.17	3 (6%)	58,95,113	0.99	3 (5%)
31	CHL	4	606	34	56,64,74	2.14	9 (16%)	61,102,114	1.32	8 (13%)
29	LUT	F	305	-	42,43,43	0.39	0	51,60,60	0.77	1 (1%)
25	BCR	J	102	-	41,41,41	0.15	0	56,56,56	0.30	0
22	CLA	92	603	19	45,53,73	1.26	4 (8%)	52,89,113	1.02	2 (3%)
22	CLA	4	603	16	65,73,73	1.05	4 (6%)	76,113,113	0.85	2 (2%)
22	CLA	7	612	14	52,60,73	1.16	4 (7%)	60,97,113	0.94	2 (3%)
24	LHG	92	622	22	28,28,48	0.29	0	31,34,54	0.29	0
27	LMU	B	853	-	36,36,36	0.12	0	47,47,47	0.68	2 (4%)
25	BCR	9	623	-	41,41,41	0.12	0	56,56,56	0.35	0
24	LHG	Z	620	22	38,38,48	0.27	0	41,44,54	0.30	0
22	CLA	9	614	-	45,53,73	1.25	3 (6%)	52,89,113	1.03	2 (3%)
27	LMU	1	627	-	22,22,36	0.14	0	27,27,47	0.30	0
22	CLA	92	613	19	60,68,73	1.07	3 (5%)	70,107,113	0.90	2 (2%)
25	BCR	A	848	-	41,41,41	0.15	0	56,56,56	0.30	0
31	CHL	Z	607	34	66,74,74	1.97	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
22	CLA	A	811	-	65,73,73	1.00	4 (6%)	76,113,113	0.87	2 (2%)
22	CLA	B	841	24	65,73,73	1.02	4 (6%)	76,113,113	0.88	3 (3%)
22	CLA	A	817	34	55,63,73	1.12	3 (5%)	64,101,113	0.92	2 (3%)
22	CLA	3	609	13	61,69,73	1.03	4 (6%)	71,108,113	0.87	2 (2%)
28	LMG	1	624	-	36,36,55	0.20	0	44,44,63	0.18	0
22	CLA	1	603	-	57,65,73	1.09	4 (7%)	66,103,113	0.92	2 (3%)
22	CLA	3	614	-	45,53,73	1.23	4 (8%)	52,89,113	1.03	3 (5%)
22	CLA	9	604	19	53,61,73	1.13	4 (7%)	61,98,113	0.96	3 (4%)
22	CLA	A	854	34	65,73,73	1.04	4 (6%)	76,113,113	0.81	2 (2%)
22	CLA	3	615	34	65,73,73	1.04	3 (4%)	76,113,113	0.87	2 (2%)
22	CLA	A	829	-	65,73,73	1.03	3 (4%)	76,113,113	0.83	2 (2%)
29	LUT	92	617	-	42,43,43	0.21	0	51,60,60	0.37	0
22	CLA	5	609	17	65,73,73	1.03	4 (6%)	76,113,113	0.84	2 (2%)
22	CLA	4	616	16	45,53,73	1.25	3 (6%)	52,89,113	1.02	2 (3%)
22	CLA	A	843	34	65,73,73	1.02	4 (6%)	76,113,113	0.89	2 (2%)
28	LMG	B	854	-	36,36,55	0.20	0	44,44,63	0.17	0
22	CLA	Z	611	24	60,68,73	1.07	3 (5%)	70,107,113	0.89	2 (2%)
22	CLA	A	833	-	65,73,73	1.04	4 (6%)	76,113,113	0.85	2 (2%)
22	CLA	1	613	34	65,73,73	1.01	4 (6%)	76,113,113	0.88	3 (3%)
25	BCR	K	202	-	41,41,41	0.16	0	56,56,56	0.35	0
29	LUT	1	619	-	42,43,43	0.21	0	51,60,60	0.40	0
22	CLA	B	839	34	65,73,73	1.03	4 (6%)	76,113,113	0.87	2 (2%)
31	CHL	4	608	-	66,74,74	2.00	10 (15%)	73,114,114	1.13	7 (9%)
24	LHG	6	619	22	48,48,48	0.23	0	51,54,54	0.24	0
22	CLA	92	612	19	65,73,73	1.02	3 (4%)	76,113,113	0.85	2 (2%)
22	CLA	A	813	-	65,73,73	1.02	4 (6%)	76,113,113	0.91	2 (2%)
22	CLA	A	834	-	65,73,73	1.02	4 (6%)	76,113,113	0.87	2 (2%)
22	CLA	8	614	-	57,65,73	1.10	3 (5%)	66,103,113	0.91	2 (3%)
22	CLA	B	805	-	65,73,73	0.99	4 (6%)	76,113,113	0.89	2 (2%)
22	CLA	92	610	19	60,68,73	1.07	4 (6%)	70,107,113	0.92	3 (4%)
27	LMU	7	629	-	28,28,36	0.11	0	39,39,47	0.27	0
32	XAT	1	618	-	39,47,47	0.14	0	54,74,74	0.69	2 (3%)
22	CLA	B	829	-	65,73,73	0.98	4 (6%)	76,113,113	0.86	2 (2%)
22	CLA	3	607	13	55,63,73	1.12	4 (7%)	64,101,113	0.94	2 (3%)
24	LHG	5	623	22	36,36,48	0.27	0	39,42,54	0.28	0
22	CLA	A	832	-	55,63,73	1.12	4 (7%)	64,101,113	0.95	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	A	826	34	65,73,73	1.03	3 (4%)	76,113,113	0.83	2 (2%)
22	CLA	A	821	-	55,63,73	1.11	4 (7%)	64,101,113	0.89	2 (3%)
22	CLA	1	612	12	45,53,73	1.24	3 (6%)	52,89,113	1.01	2 (3%)
22	CLA	5	616	17	53,61,73	1.14	4 (7%)	61,98,113	0.96	2 (3%)
27	LMU	A	861	-	24,24,36	0.13	0	29,29,47	0.30	0
31	CHL	8	606	34	66,74,74	1.96	9 (13%)	73,114,114	1.13	8 (10%)
31	CHL	8	601	15	66,74,74	1.99	9 (13%)	73,114,114	1.10	7 (9%)
25	BCR	4	621	-	41,41,41	0.15	0	56,56,56	0.35	0
22	CLA	B	819	34	60,68,73	1.06	4 (6%)	70,107,113	0.89	2 (2%)
22	CLA	6	613	34	65,73,73	1.02	3 (4%)	76,113,113	0.87	2 (2%)
25	BCR	B	847	-	41,41,41	0.21	0	56,56,56	0.41	0
22	CLA	F	301	34	65,73,73	0.98	3 (4%)	76,113,113	0.83	2 (2%)
22	CLA	5	612	17	45,53,73	1.25	3 (6%)	52,89,113	1.00	2 (3%)
22	CLA	B	818	-	65,73,73	1.00	4 (6%)	76,113,113	0.85	2 (2%)
22	CLA	A	810	1	65,73,73	1.01	3 (4%)	76,113,113	0.87	2 (2%)
22	CLA	5	604	34	55,63,73	1.13	3 (5%)	64,101,113	0.94	2 (3%)
22	CLA	B	834	-	60,68,73	1.06	3 (5%)	70,107,113	0.89	2 (2%)
22	CLA	1	608	34	65,73,73	1.03	4 (6%)	76,113,113	0.86	2 (2%)
22	CLA	B	832	-	65,73,73	1.02	4 (6%)	76,113,113	0.86	2 (2%)
22	CLA	A	824	-	45,53,73	1.21	4 (8%)	52,89,113	1.04	2 (3%)
22	CLA	A	814	-	65,73,73	1.03	4 (6%)	76,113,113	0.84	2 (2%)
22	CLA	3	613	13	60,68,73	1.07	4 (6%)	70,107,113	0.87	2 (2%)
31	CHL	5	606	34	46,54,74	2.37	10 (21%)	49,90,114	1.37	7 (14%)
24	LHG	4	622	22	48,48,48	0.24	0	51,54,54	0.28	0
22	CLA	B	815	-	65,73,73	1.03	3 (4%)	76,113,113	0.84	2 (2%)
22	CLA	8	608	34	50,58,73	1.17	4 (8%)	58,95,113	0.97	2 (3%)
25	BCR	A	850	-	41,41,41	0.16	0	56,56,56	0.24	0
29	LUT	3	621	-	42,43,43	0.32	0	51,60,60	0.37	0
31	CHL	3	608	34	66,74,74	1.95	9 (13%)	73,114,114	1.15	7 (9%)
27	LMU	9	624	-	24,24,36	0.14	0	29,29,47	0.29	0
29	LUT	9	617	-	42,43,43	0.21	0	51,60,60	0.39	0
24	LHG	B	851	22	44,44,48	0.26	0	47,50,54	0.32	0
22	CLA	A	806	-	65,73,73	1.00	4 (6%)	76,113,113	0.88	3 (3%)
28	LMG	J	103	-	42,42,55	0.18	0	50,50,63	0.40	0
27	LMU	8	624	-	24,24,36	0.14	0	29,29,47	0.27	0
22	CLA	1	604	34	50,58,73	1.17	4 (8%)	58,95,113	0.99	2 (3%)
22	CLA	6	610	18	60,68,73	1.06	4 (6%)	70,107,113	0.88	2 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	L	203	-	65,73,73	1.01	4 (6%)	76,113,113	0.84	2 (2%)
31	CHL	5	618	17	43,51,74	2.49	10 (23%)	45,86,114	1.44	7 (15%)
25	BCR	B2	848	-	14,14,41	0.36	0	19,20,56	0.33	0
22	CLA	B	824	34	65,73,73	1.02	3 (4%)	76,113,113	0.85	2 (2%)
22	CLA	F	303	34	45,53,73	1.25	4 (8%)	52,89,113	1.03	2 (3%)
22	CLA	3	603	-	65,73,73	1.00	3 (4%)	76,113,113	0.83	2 (2%)
22	CLA	4	614	-	55,63,73	1.13	3 (5%)	64,101,113	0.92	2 (3%)
22	CLA	4	609	16	60,68,73	1.09	3 (5%)	70,107,113	0.90	2 (2%)
22	CLA	B	814	-	60,68,73	1.05	4 (6%)	70,107,113	0.90	3 (4%)
22	CLA	6	602	18	65,73,73	1.01	4 (6%)	76,113,113	0.86	2 (2%)
24	LHG	8	620	22	43,43,48	0.27	0	46,49,54	0.26	0
22	CLA	3	606	34	42,50,73	1.27	4 (9%)	48,85,113	1.06	2 (4%)
22	CLA	B	826	-	65,73,73	1.01	4 (6%)	76,113,113	0.84	2 (2%)
22	CLA	B	809	2	65,73,73	1.03	3 (4%)	76,113,113	0.82	2 (2%)
31	CHL	8	607	34	66,74,74	1.98	10 (15%)	73,114,114	1.17	8 (10%)
22	CLA	5	614	-	45,53,73	1.24	3 (6%)	52,89,113	1.02	2 (3%)
27	LMU	A	862	-	20,20,36	0.13	0	25,25,47	0.28	0
21	CL0	A	801	-	65,73,73	1.92	9 (13%)	76,113,113	1.09	6 (7%)
22	CLA	B	806	2	65,73,73	1.02	4 (6%)	76,113,113	0.81	2 (2%)
22	CLA	4	602	16	60,68,73	1.07	4 (6%)	70,107,113	0.87	2 (2%)
22	CLA	8	613	15	65,73,73	1.01	4 (6%)	76,113,113	0.85	2 (2%)
27	LMU	8	627	-	36,36,36	0.11	0	47,47,47	0.37	0
27	LMU	A	857	-	35,35,36	0.10	0	46,46,47	0.18	0
28	LMG	4	624	-	41,41,55	0.19	0	49,49,63	0.26	0
22	CLA	6	603	-	65,73,73	1.03	4 (6%)	76,113,113	0.82	2 (2%)
22	CLA	B	836	-	60,68,73	1.06	3 (5%)	70,107,113	0.91	2 (2%)
27	LMU	Z	622	-	32,32,36	0.10	0	43,43,47	0.18	0
25	BCR	I2	172	-	41,41,41	0.12	0	56,56,56	0.32	0
25	BCR	7	623	-	41,41,41	0.16	0	56,56,56	0.38	0
25	BCR	A	849	-	41,41,41	0.18	0	56,56,56	0.32	0
22	CLA	3	604	34	65,73,73	1.01	4 (6%)	76,113,113	0.85	2 (2%)
22	CLA	7	614	-	43,51,73	1.29	4 (9%)	49,86,113	1.07	2 (4%)
22	CLA	1	611	24	61,69,73	1.07	4 (6%)	71,108,113	0.86	2 (2%)
22	CLA	B2	810	-	65,73,73	1.04	3 (4%)	76,113,113	0.85	2 (2%)
25	BCR	B	801	-	41,41,41	0.17	0	56,56,56	0.38	0
22	CLA	Z	603	-	55,63,73	1.13	3 (5%)	64,101,113	0.91	2 (3%)
22	CLA	B	813	-	65,73,73	1.02	4 (6%)	76,113,113	0.84	2 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	LMU	1	623	-	24,24,36	0.14	0	29,29,47	0.26	0
22	CLA	A	842	-	65,73,73	1.00	4 (6%)	76,113,113	0.84	2 (2%)
31	CHL	Z	606	34	46,54,74	2.37	10 (21%)	49,90,114	1.36	8 (16%)
25	BCR	92	623	-	41,41,41	0.14	0	56,56,56	0.33	0
22	CLA	7	604	34	51,59,73	1.14	4 (7%)	59,96,113	0.96	2 (3%)
22	CLA	B2	828	-	65,73,73	1.05	3 (4%)	76,113,113	0.84	2 (2%)
30	DGD	B	850	-	60,60,67	0.17	0	74,74,81	0.35	0
25	BCR	G	205	-	41,41,41	0.15	0	56,56,56	0.32	0
22	CLA	K	203	34	60,68,73	1.09	3 (5%)	70,107,113	0.90	2 (2%)
22	CLA	B2	804	-	45,53,73	1.25	3 (6%)	52,89,113	1.04	2 (3%)
31	CHL	5	607	34	66,74,74	1.99	9 (13%)	73,114,114	1.18	8 (10%)
22	CLA	5	617	-	65,73,73	1.04	3 (4%)	76,113,113	0.85	2 (2%)
25	BCR	K	207	-	41,41,41	0.14	0	56,56,56	0.28	0
26	SF4	A	853	2,1	0,12,12	-	-	-	-	-
29	LUT	Z	619	-	26,26,43	0.36	0	34,35,60	0.38	0
22	CLA	A	827	34	65,73,73	1.03	4 (6%)	76,113,113	0.87	2 (2%)
22	CLA	J	101	9	55,63,73	1.13	3 (5%)	64,101,113	0.92	2 (3%)
27	LMU	A	865	-	24,24,36	0.13	0	29,29,47	0.46	0
22	CLA	A	805	-	55,63,73	1.11	4 (7%)	64,101,113	0.90	2 (3%)
22	CLA	B2	839	-	45,53,73	1.26	3 (6%)	52,89,113	1.07	2 (3%)
22	CLA	8	602	15	62,70,73	1.06	4 (6%)	72,109,113	0.89	2 (2%)
22	CLA	B2	806	20	65,73,73	1.03	3 (4%)	76,113,113	0.83	2 (2%)
22	CLA	3	612	13	46,54,73	1.23	4 (8%)	53,90,113	1.00	2 (3%)
28	LMG	8	629	-	42,42,55	0.19	0	50,50,63	0.16	0
28	LMG	1	628	-	42,42,55	0.19	0	50,50,63	0.29	0
28	LMG	9	620	22	44,44,55	0.18	0	52,52,63	0.37	0
22	CLA	A	819	-	60,68,73	1.08	3 (5%)	70,107,113	0.92	2 (2%)
22	CLA	5	621	34	46,54,73	1.28	3 (6%)	53,90,113	1.12	5 (9%)
25	BCR	5	622	-	41,41,41	0.17	0	56,56,56	0.31	0
22	CLA	B	803	-	65,73,73	1.00	3 (4%)	76,113,113	0.82	2 (2%)
22	CLA	B	827	-	65,73,73	1.01	3 (4%)	76,113,113	0.85	2 (2%)
24	LHG	6	629	-	35,35,48	0.26	0	38,41,54	0.28	0
31	CHL	6	606	34	58,66,74	2.13	9 (15%)	63,104,114	1.22	7 (11%)
22	CLA	A	838	-	51,59,73	1.15	3 (5%)	59,96,113	0.97	2 (3%)
22	CLA	Z	608	34	50,58,73	1.18	4 (8%)	58,95,113	0.99	2 (3%)
31	CHL	6	607	34	66,74,74	2.04	10 (15%)	73,114,114	1.16	7 (9%)
22	CLA	A	815	-	55,63,73	1.11	3 (5%)	64,101,113	0.92	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	8	603	-	65,73,73	1.05	4 (6%)	76,113,113	0.82	2 (2%)
25	BCR	6	623	-	41,41,41	0.18	0	56,56,56	0.34	0
22	CLA	4	610	16	60,68,73	1.06	3 (5%)	70,107,113	0.87	2 (2%)
22	CLA	4	613	16	65,73,73	1.05	4 (6%)	76,113,113	0.88	2 (2%)
22	CLA	A	841	-	65,73,73	1.00	4 (6%)	76,113,113	0.85	2 (2%)
31	CHL	5	608	34	51,59,74	2.26	10 (19%)	55,96,114	1.35	8 (14%)
22	CLA	7	608	34	50,58,73	1.17	3 (6%)	58,95,113	0.95	2 (3%)
22	CLA	B2	820	-	56,64,73	1.13	3 (5%)	65,102,113	0.93	2 (3%)
22	CLA	A	823	-	65,73,73	1.02	4 (6%)	76,113,113	0.85	3 (3%)
22	CLA	Z	604	34	57,65,73	1.09	4 (7%)	66,103,113	0.93	2 (3%)
22	CLA	5	613	17	56,64,73	1.11	4 (7%)	65,102,113	0.93	2 (3%)
29	LUT	5	620	-	42,43,43	0.28	0	51,60,60	0.45	0
25	BCR	A	852	-	41,41,41	0.14	0	56,56,56	0.39	0
22	CLA	B	811	-	65,73,73	1.00	4 (6%)	76,113,113	0.86	2 (2%)
22	CLA	5	602	17	65,73,73	1.03	3 (4%)	76,113,113	0.85	2 (2%)
22	CLA	A	804	-	65,73,73	1.02	4 (6%)	76,113,113	0.86	3 (3%)
28	LMG	J	104	-	35,35,55	0.20	0	43,43,63	0.20	0
22	CLA	A	802	-	65,73,73	1.00	4 (6%)	76,113,113	0.82	2 (2%)
22	CLA	A	807	1	65,73,73	1.02	4 (6%)	76,113,113	0.82	2 (2%)
22	CLA	B	838	-	50,58,73	1.19	3 (6%)	58,95,113	0.98	2 (3%)
22	CLA	9	602	19	60,68,73	1.06	3 (5%)	70,107,113	0.89	2 (2%)
22	CLA	A	831	-	65,73,73	1.02	4 (6%)	76,113,113	0.85	2 (2%)
22	CLA	B	810	-	65,73,73	1.01	4 (6%)	76,113,113	0.86	2 (2%)
22	CLA	A	839	-	65,73,73	1.02	4 (6%)	76,113,113	0.86	2 (2%)
29	LUT	7	624	-	42,43,43	0.22	0	51,60,60	0.41	0
32	XAT	8	618	-	39,47,47	0.17	0	54,74,74	0.57	0
32	XAT	6	624	-	39,47,47	0.13	0	54,74,74	0.61	0
22	CLA	1	610	12	65,73,73	1.01	4 (6%)	76,113,113	0.85	2 (2%)
22	CLA	B	823	-	65,73,73	1.02	4 (6%)	76,113,113	0.88	2 (2%)
22	CLA	9	611	24	65,73,73	1.04	4 (6%)	76,113,113	0.85	2 (2%)
31	CHL	7	606	34	46,54,74	2.35	10 (21%)	49,90,114	1.36	7 (14%)
22	CLA	9	609	19	51,59,73	1.16	4 (7%)	59,96,113	0.96	2 (3%)
22	CLA	8	612	15	55,63,73	1.12	4 (7%)	64,101,113	0.89	2 (3%)
22	CLA	B	840	-	65,73,73	0.98	4 (6%)	76,113,113	0.85	2 (2%)
27	LMU	92	624	-	36,36,36	0.10	0	47,47,47	0.22	0
22	CLA	B	804	-	45,53,73	1.23	3 (6%)	52,89,113	0.99	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	PQN	B	842	-	34,34,34	0.31	0	42,45,45	0.37	0
29	LUT	A	856	-	42,43,43	0.29	0	51,60,60	0.36	0
22	CLA	B2	805	-	65,73,73	1.05	3 (4%)	76,113,113	0.85	2 (2%)
22	CLA	B	807	-	55,63,73	1.12	4 (7%)	64,101,113	0.93	2 (3%)
29	LUT	3	622	-	42,43,43	0.31	0	51,60,60	0.36	0
22	CLA	9	601	19	46,54,73	1.23	3 (6%)	53,90,113	1.04	2 (3%)
24	LHG	3	623	-	46,46,48	0.24	0	49,52,54	0.27	0
22	CLA	A	818	-	65,73,73	1.01	4 (6%)	76,113,113	0.84	2 (2%)
22	CLA	B	831	-	55,63,73	1.08	4 (7%)	64,101,113	0.92	2 (3%)
24	LHG	3	721	-	30,30,48	0.27	0	33,36,54	0.35	0
22	CLA	3	611	-	65,73,73	1.03	4 (6%)	76,113,113	0.86	2 (2%)
22	CLA	6	611	24	58,66,73	1.10	3 (5%)	67,104,113	0.91	2 (2%)
22	CLA	B2	811	-	54,62,73	1.16	4 (7%)	67,100,113	1.08	4 (5%)
31	CHL	7	601	14	66,74,74	1.99	10 (15%)	73,114,114	1.14	7 (9%)
22	CLA	A	816	-	65,73,73	1.03	3 (4%)	76,113,113	0.87	2 (2%)
22	CLA	A	822	34	65,73,73	1.01	4 (6%)	76,113,113	0.84	2 (2%)
27	LMU	A	863	-	36,36,36	0.10	0	47,47,47	0.27	0
22	CLA	B	802	-	65,73,73	0.99	4 (6%)	76,113,113	0.86	3 (3%)
27	LMU	7	628	-	22,22,36	0.14	0	27,27,47	0.32	0
22	CLA	G	203	-	60,68,73	1.08	3 (5%)	70,107,113	0.84	2 (2%)
22	CLA	B2	815	-	57,65,73	1.11	3 (5%)	66,103,113	0.91	2 (3%)
24	LHG	A	847	22	37,37,48	0.28	0	40,43,54	0.30	0
22	CLA	9	603	28,19	55,63,73	1.13	4 (7%)	64,101,113	0.94	2 (3%)
31	CHL	92	606	-	42,50,74	2.62	11 (26%)	44,85,114	1.48	7 (15%)
22	CLA	Z	612	12	45,53,73	1.25	3 (6%)	52,89,113	1.01	2 (3%)
29	LUT	6	621	-	42,43,43	0.26	0	51,60,60	0.39	0
22	CLA	92	604	19	50,58,73	1.19	3 (6%)	58,95,113	0.99	2 (3%)
22	CLA	B	820	-	56,64,73	1.10	4 (7%)	65,102,113	0.90	2 (3%)
25	BCR	B	848	-	41,41,41	0.13	0	56,56,56	0.46	0
22	CLA	B	816	-	65,73,73	1.01	4 (6%)	76,113,113	0.87	2 (2%)
27	LMU	1	625	-	24,24,36	0.11	0	29,29,47	0.31	0
22	CLA	7	602	14	65,73,73	1.02	4 (6%)	76,113,113	0.85	2 (2%)
22	CLA	7	609	14	45,53,73	1.25	4 (8%)	52,89,113	1.00	2 (3%)
31	CHL	9	607	34	51,59,74	2.26	9 (17%)	55,96,114	1.31	8 (14%)
22	CLA	6	622	34	55,63,73	1.12	3 (5%)	64,101,113	0.92	2 (3%)
22	CLA	9	613	19	65,73,73	1.01	4 (6%)	76,113,113	0.89	2 (2%)
27	LMU	1	621	-	36,36,36	0.10	0	47,47,47	0.29	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	B2	829	-	65,73,73	1.04	3 (4%)	76,113,113	0.86	2 (2%)
22	CLA	A	830	-	65,73,73	1.02	4 (6%)	76,113,113	0.84	2 (2%)
25	BCR	B	844	-	41,41,41	0.14	0	56,56,56	0.45	0
22	CLA	9	610	19	60,68,73	1.06	4 (6%)	70,107,113	0.95	3 (4%)
22	CLA	A	808	-	50,58,73	1.17	4 (8%)	58,95,113	0.95	2 (3%)
22	CLA	1	609	12	65,73,73	1.03	4 (6%)	76,113,113	0.86	2 (2%)

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
22	CLA	8	604	34	1/1/19/20	2/31/109/115	-
22	CLA	B2	809	20	1/1/17/20	0/22/100/115	-
32	XAT	4	620	-	-	0/31/93/93	0/4/4/4
22	CLA	92	602	19	1/1/20/20	8/37/115/115	-
31	CHL	4	618	16	3/3/21/26	1/15/113/137	-
22	CLA	B	837	-	1/1/20/20	1/37/115/115	-
22	CLA	B	828	-	1/1/20/20	4/37/115/115	-
22	CLA	5	610	17	1/1/19/20	2/31/109/115	-
22	CLA	8	611	24	1/1/15/20	2/13/91/115	-
25	BCR	L2	201	-	-	4/29/63/63	0/2/2/2
22	CLA	4	611	24	1/1/19/20	4/31/109/115	-
25	BCR	B	845	-	-	4/29/63/63	0/2/2/2
31	CHL	6	601	18	3/3/26/26	8/39/137/137	-
29	LUT	5	626	-	-	4/29/67/67	0/2/2/2
22	CLA	7	613	14	1/1/20/20	1/37/115/115	-
28	LMG	A	859	-	-	8/43/63/70	0/1/1/1
25	BCR	3	620	-	-	4/29/63/63	0/2/2/2
31	CHL	6	616	18	3/3/26/26	5/39/137/137	-
22	CLA	Z	610	12	1/1/19/20	0/31/109/115	-
22	CLA	B	833	-	1/1/18/20	4/29/107/115	-
25	BCR	3	718	-	-	2/29/63/63	0/2/2/2
31	CHL	6	618	18	3/3/20/26	2/12/110/137	-
22	CLA	L2	203	-	1/1/15/20	2/13/91/115	-
22	CLA	B	830	-	1/1/15/20	0/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	BCR	B2	844	-	-	0/29/63/63	0/2/2/2
28	LMG	3	722	-	-	6/46/46/70	-
22	CLA	A	840	-	1/1/20/20	8/37/115/115	-
29	LUT	7	621	-	-	2/29/67/67	0/2/2/2
22	CLA	B	808	-	1/1/20/20	7/37/115/115	-
33	NEX	5	625	-	-	2/27/83/83	1/3/3/3
29	LUT	Z	617	-	-	2/29/67/67	0/2/2/2
22	CLA	6	614	-	1/1/17/20	0/19/97/115	-
22	CLA	7	610	14	1/1/20/20	5/37/115/115	-
28	LMG	B2	852	-	-	3/38/58/70	0/1/1/1
26	SF4	C	101	3	-	-	0/6/5/5
22	CLA	A	812	-	1/1/20/20	8/37/115/115	-
22	CLA	A	803	34	1/1/20/20	2/37/115/115	-
28	LMG	A	860	-	-	7/31/51/70	0/1/1/1
28	LMG	7	626	-	-	8/32/52/70	0/1/1/1
22	CLA	A	809	1	1/1/20/20	5/37/115/115	-
22	CLA	6	612	18	1/1/15/20	2/13/91/115	-
32	XAT	5	624	-	1/1/26/26	0/31/93/93	0/4/4/4
29	LUT	4	619	-	-	2/29/67/67	0/2/2/2
22	CLA	L	204	-	1/1/15/20	2/13/91/115	-
22	CLA	A	825	-	1/1/18/20	7/25/103/115	-
22	CLA	B	817	-	1/1/20/20	6/37/115/115	-
22	CLA	B2	814	-	1/1/19/20	3/31/109/115	-
22	CLA	B2	813	-	1/1/20/20	4/37/115/115	-
29	LUT	1	617	-	-	2/29/67/67	0/2/2/2
25	BCR	B	843	-	-	0/29/63/63	0/2/2/2
27	LMU	A	858	-	-	6/21/61/61	0/2/2/2
27	LMU	4	625	-	-	3/19/59/61	0/2/2/2
25	BCR	3	719	-	-	2/29/63/63	0/2/2/2
22	CLA	K	201	11	1/1/15/20	1/13/91/115	-
26	SF4	C	102	3	-	-	0/6/5/5
22	CLA	1	614	-	1/1/19/20	4/31/109/115	-
31	CHL	4	601	16	3/3/26/26	6/39/137/137	-
29	LUT	9	616	-	-	2/29/67/67	0/2/2/2
22	CLA	B2	808	-	1/1/15/20	2/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	B	812	-	1/1/20/20	2/37/115/115	-
28	LMG	B2	855	-	-	3/26/46/70	0/1/1/1
22	CLA	7	616	14	1/1/15/20	3/15/93/115	-
29	LUT	3	720	-	-	0/29/67/67	0/2/2/2
31	CHL	1	606	34	3/3/21/26	0/15/113/137	-
27	LMU	A	864	-	-	2/15/35/61	0/1/1/2
22	CLA	3	617	13	1/1/15/20	2/15/93/115	-
25	BCR	L	201	-	-	4/29/63/63	0/2/2/2
24	LHG	9	622	22	-	13/45/45/53	-
22	CLA	B	825	34	1/1/20/20	2/37/115/115	-
25	BCR	L2	205	-	-	2/29/63/63	0/2/2/2
22	CLA	6	604	-	1/1/20/20	4/37/115/115	-
27	LMU	8	625	-	-	2/15/35/61	0/1/1/2
24	LHG	7	625	22	-	17/53/53/53	-
27	LMU	K	208	-	-	3/15/35/61	0/1/1/2
27	LMU	1	622	-	-	4/10/30/61	0/1/1/2
22	CLA	5	611	24	1/1/18/20	2/25/103/115	-
27	LMU	6	632	-	-	3/11/31/61	0/1/1/2
29	LUT	8	617	-	-	2/29/67/67	0/2/2/2
25	BCR	B2	845	-	-	4/29/63/63	0/2/2/2
22	CLA	5	601	17	1/1/20/20	5/37/115/115	-
28	LMG	8	626	-	-	6/27/47/70	0/1/1/1
31	CHL	6	608	34	3/3/23/26	0/21/119/137	-
31	CHL	7	607	34	3/3/21/26	0/15/113/137	-
31	CHL	1	601	12	3/3/26/26	9/39/137/137	-
27	LMU	8	628	-	-	4/15/35/61	0/1/1/2
27	LMU	Z	621	-	-	2/13/33/61	0/1/1/2
25	BCR	I	172	-	-	0/29/63/63	0/2/2/2
22	CLA	4	612	16	1/1/15/20	4/13/91/115	-
22	CLA	Z	602	12	1/1/19/20	2/31/109/115	-
22	CLA	6	609	18	1/1/18/20	2/25/103/115	-
22	CLA	1	616	12	1/1/15/20	2/15/93/115	-
25	BCR	B2	843	-	-	0/13/30/63	0/1/1/2
22	CLA	A	828	-	1/1/20/20	6/37/115/115	-
25	BCR	B	846	-	-	2/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	Z	609	12	1/1/20/20	7/37/115/115	-
22	CLA	B2	812	-	1/1/19/20	3/31/109/115	-
28	LMG	B	852	-	-	7/38/58/70	0/1/1/1
22	CLA	F	304	6	1/1/20/20	8/37/115/115	-
22	CLA	5	603	-	1/1/20/20	15/37/115/115	-
25	BCR	L	205	-	-	2/29/63/63	0/2/2/2
22	CLA	3	602	13	1/1/19/20	1/31/109/115	-
22	CLA	L2	204	-	1/1/15/20	4/13/91/115	-
27	LMU	1	626	-	-	0/15/35/61	0/1/1/2
22	CLA	A	837	1	1/1/18/20	4/28/106/115	-
22	CLA	B	822	-	1/1/18/20	5/30/108/115	-
28	LMG	6	633	-	-	1/17/17/70	-
22	CLA	4	604	34	1/1/17/20	1/19/97/115	-
31	CHL	92	607	-	3/3/21/26	4/15/113/137	-
22	CLA	A	836	-	1/1/20/20	4/37/115/115	-
29	LUT	92	616	-	-	2/29/67/67	0/2/2/2
24	LHG	1	620	22	-	10/43/43/53	-
24	LHG	4	623	-	-	15/42/42/53	-
27	LMU	5	627	-	-	1/15/35/61	0/1/1/2
24	LHG	A	846	-	-	10/53/53/53	-
22	CLA	A	820	-	1/1/20/20	8/37/115/115	-
31	CHL	1	607	34	3/3/21/26	3/15/113/137	-
22	CLA	A	835	-	1/1/20/20	4/37/115/115	-
22	CLA	B	821	-	1/1/20/20	3/37/115/115	-
22	CLA	6	617	-	1/1/15/20	0/13/91/115	-
22	CLA	B2	807	-	1/1/18/20	0/25/103/115	-
32	XAT	7	622	-	-	0/31/93/93	0/4/4/4
22	CLA	92	611	24	1/1/20/20	2/37/115/115	-
22	CLA	8	609	15	1/1/15/20	0/13/91/115	-
27	LMU	G	206	-	-	4/15/35/61	0/1/1/2
22	CLA	3	610	13	1/1/20/20	0/37/115/115	-
27	LMU	6	630	-	-	1/15/35/61	0/1/1/2
22	CLA	92	614	-	1/1/15/20	2/13/91/115	-
22	CLA	Z	613	34	1/1/20/20	2/37/115/115	-
22	CLA	B	835	34	1/1/15/20	2/13/91/115	-
25	BCR	8	619	-	-	4/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	92	609	19	1/1/15/20	6/13/91/115	-
31	CHL	Z	601	12	3/3/26/26	7/39/137/137	-
33	NEX	6	625	-	1/1/25/25	4/27/83/83	0/3/3/3
31	CHL	9	606	-	3/3/20/26	0/10/108/137	-
22	CLA	Z	616	12	1/1/19/20	1/31/109/115	-
27	LMU	7	627	-	-	2/18/58/61	0/2/2/2
22	CLA	K	204	-	1/1/15/20	1/15/93/115	-
25	BCR	A	851	-	-	2/29/63/63	0/2/2/2
22	CLA	8	616	15	1/1/15/20	0/13/91/115	-
22	CLA	8	610	15	1/1/20/20	2/37/115/115	-
27	LMU	6	631	-	-	4/15/35/61	0/1/1/2
22	CLA	9	612	19	1/1/20/20	6/37/115/115	-
31	CHL	4	607	34	3/3/26/26	0/39/137/137	-
22	CLA	K	206	11	1/1/15/20	2/13/91/115	-
22	CLA	G	204	7	1/1/15/20	4/15/93/115	-
22	CLA	A	845	24	1/1/15/20	4/13/91/115	-
27	LMU	6	628	-	-	2/15/35/61	0/1/1/2
22	CLA	7	611	24	1/1/20/20	5/37/115/115	-
22	CLA	7	603	-	1/1/17/20	5/22/100/115	-
32	XAT	Z	618	-	-	0/31/93/93	0/4/4/4
22	CLA	92	601	19	1/1/15/20	2/13/91/115	-
27	LMU	4	626	-	-	0/11/31/61	0/1/1/2
22	CLA	1	602	12	1/1/19/20	2/31/109/115	-
23	PQN	A	844	-	-	3/23/43/43	0/2/2/2
22	CLA	7	620	34	1/1/17/20	5/23/101/115	-
22	CLA	Z	614	-	1/1/17/20	0/19/97/115	-
31	CHL	4	606	34	3/3/24/26	1/27/125/137	-
29	LUT	F	305	-	-	5/29/67/67	0/2/2/2
25	BCR	J	102	-	-	2/29/63/63	0/2/2/2
22	CLA	92	603	19	1/1/15/20	2/13/91/115	-
22	CLA	4	603	16	1/1/20/20	6/37/115/115	-
22	CLA	7	612	14	1/1/17/20	3/22/100/115	-
24	LHG	92	622	22	-	10/33/33/53	-
27	LMU	B	853	-	-	7/21/61/61	0/2/2/2
25	BCR	9	623	-	-	2/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	LHG	Z	620	22	-	7/43/43/53	-
22	CLA	9	614	-	1/1/15/20	2/13/91/115	-
27	LMU	1	627	-	-	3/13/33/61	0/1/1/2
22	CLA	92	613	19	1/1/19/20	4/31/109/115	-
25	BCR	A	848	-	-	2/29/63/63	0/2/2/2
31	CHL	Z	607	34	3/3/26/26	3/39/137/137	-
22	CLA	A	811	-	1/1/20/20	4/37/115/115	-
22	CLA	B	841	24	1/1/20/20	6/37/115/115	-
22	CLA	A	817	34	1/1/18/20	4/25/103/115	-
22	CLA	3	609	13	1/1/19/20	3/33/111/115	-
28	LMG	1	624	-	-	4/31/51/70	0/1/1/1
22	CLA	1	603	-	1/1/18/20	5/28/106/115	-
22	CLA	3	614	-	1/1/15/20	0/13/91/115	-
22	CLA	9	604	19	1/1/17/20	1/23/101/115	-
22	CLA	A	854	34	1/1/20/20	1/37/115/115	-
22	CLA	3	615	34	1/1/20/20	6/37/115/115	-
22	CLA	A	829	-	1/1/20/20	8/37/115/115	-
29	LUT	92	617	-	-	0/29/67/67	0/2/2/2
22	CLA	5	609	17	1/1/20/20	2/37/115/115	-
22	CLA	4	616	16	1/1/15/20	0/13/91/115	-
22	CLA	A	843	34	1/1/20/20	7/37/115/115	-
28	LMG	B	854	-	-	2/31/51/70	0/1/1/1
22	CLA	Z	611	24	1/1/19/20	4/31/109/115	-
22	CLA	A	833	-	1/1/20/20	1/37/115/115	-
22	CLA	1	613	34	1/1/20/20	4/37/115/115	-
25	BCR	K	202	-	-	2/29/63/63	0/2/2/2
29	LUT	1	619	-	-	2/29/67/67	0/2/2/2
22	CLA	B	839	34	1/1/20/20	4/37/115/115	-
31	CHL	4	608	-	3/3/26/26	3/39/137/137	-
24	LHG	6	619	22	-	7/53/53/53	-
22	CLA	92	612	19	1/1/20/20	6/37/115/115	-
22	CLA	A	813	-	1/1/20/20	5/37/115/115	-
22	CLA	A	834	-	1/1/20/20	5/37/115/115	-
22	CLA	8	614	-	1/1/18/20	8/28/106/115	-
22	CLA	B	805	-	1/1/20/20	9/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	92	610	19	1/1/19/20	0/31/109/115	-
32	XAT	1	618	-	1/1/26/26	0/31/93/93	0/4/4/4
27	LMU	7	629	-	-	4/13/53/61	0/2/2/2
22	CLA	B	829	-	1/1/20/20	4/37/115/115	-
22	CLA	3	607	13	1/1/18/20	4/25/103/115	-
24	LHG	5	623	22	-	12/41/41/53	-
22	CLA	A	832	-	1/1/18/20	1/25/103/115	-
22	CLA	A	826	34	1/1/20/20	9/37/115/115	-
22	CLA	A	821	-	1/1/18/20	2/25/103/115	-
22	CLA	1	612	12	1/1/15/20	2/13/91/115	-
22	CLA	5	616	17	1/1/17/20	5/23/101/115	-
31	CHL	8	606	34	3/3/26/26	3/39/137/137	-
27	LMU	A	861	-	-	3/15/35/61	0/1/1/2
31	CHL	8	601	15	3/3/26/26	10/39/137/137	-
25	BCR	4	621	-	-	2/29/63/63	0/2/2/2
22	CLA	B	819	34	1/1/19/20	3/31/109/115	-
22	CLA	6	613	34	1/1/20/20	3/37/115/115	-
25	BCR	B	847	-	-	2/29/63/63	0/2/2/2
22	CLA	F	301	34	1/1/20/20	3/37/115/115	-
22	CLA	5	612	17	1/1/15/20	3/13/91/115	-
22	CLA	B	818	-	1/1/20/20	2/37/115/115	-
22	CLA	A	810	1	1/1/20/20	8/37/115/115	-
22	CLA	5	604	34	1/1/18/20	5/25/103/115	-
22	CLA	B	834	-	1/1/19/20	6/31/109/115	-
22	CLA	1	608	34	1/1/20/20	2/37/115/115	-
22	CLA	B	832	-	1/1/20/20	3/37/115/115	-
22	CLA	A	824	-	1/1/15/20	2/13/91/115	-
22	CLA	A	814	-	1/1/20/20	5/37/115/115	-
22	CLA	3	613	13	1/1/19/20	3/31/109/115	-
31	CHL	5	606	34	3/3/21/26	0/15/113/137	-
24	LHG	4	622	22	-	13/53/53/53	-
22	CLA	B	815	-	1/1/20/20	4/37/115/115	-
22	CLA	8	608	34	1/1/17/20	0/19/97/115	-
25	BCR	A	850	-	-	0/29/63/63	0/2/2/2
29	LUT	3	621	-	-	2/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CHL	3	608	34	3/3/26/26	3/39/137/137	-
27	LMU	9	624	-	-	4/15/35/61	0/1/1/2
29	LUT	9	617	-	-	0/29/67/67	0/2/2/2
24	LHG	B	851	22	-	13/49/49/53	-
22	CLA	A	806	-	1/1/20/20	12/37/115/115	-
28	LMG	J	103	-	-	2/37/57/70	0/1/1/1
27	LMU	8	624	-	-	1/15/35/61	0/1/1/2
22	CLA	1	604	34	1/1/17/20	1/19/97/115	-
22	CLA	6	610	18	1/1/19/20	3/31/109/115	-
22	CLA	L	203	-	1/1/20/20	6/37/115/115	-
31	CHL	5	618	17	3/3/20/26	2/12/110/137	-
25	BCR	B2	848	-	-	2/5/22/63	0/1/1/2
22	CLA	B	824	34	1/1/20/20	4/37/115/115	-
22	CLA	F	303	34	1/1/15/20	1/13/91/115	-
22	CLA	3	603	-	1/1/20/20	5/37/115/115	-
22	CLA	4	614	-	1/1/18/20	4/25/103/115	-
22	CLA	4	609	16	1/1/19/20	5/31/109/115	-
22	CLA	B	814	-	1/1/19/20	3/31/109/115	-
22	CLA	6	602	18	1/1/20/20	2/37/115/115	-
24	LHG	8	620	22	-	15/48/48/53	-
22	CLA	3	606	34	1/1/14/20	0/10/88/115	-
22	CLA	B	826	-	1/1/20/20	3/37/115/115	-
22	CLA	B	809	2	1/1/20/20	5/37/115/115	-
31	CHL	8	607	34	3/3/26/26	8/39/137/137	-
22	CLA	5	614	-	1/1/15/20	2/13/91/115	-
27	LMU	A	862	-	-	2/11/31/61	0/1/1/2
21	CL0	A	801	-	3/3/25/25	1/37/135/135	-
22	CLA	B	806	2	1/1/20/20	3/37/115/115	-
22	CLA	4	602	16	1/1/19/20	2/31/109/115	-
22	CLA	8	613	15	1/1/20/20	5/37/115/115	-
27	LMU	8	627	-	-	9/21/61/61	0/2/2/2
27	LMU	A	857	-	-	3/20/60/61	0/2/2/2
28	LMG	4	624	-	-	5/36/56/70	0/1/1/1
22	CLA	6	603	-	1/1/20/20	6/37/115/115	-
22	CLA	B	836	-	1/1/19/20	5/31/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	LMU	Z	622	-	-	3/17/57/61	0/2/2/2
25	BCR	I2	172	-	-	0/29/63/63	0/2/2/2
25	BCR	7	623	-	-	2/29/63/63	0/2/2/2
25	BCR	A	849	-	-	0/29/63/63	0/2/2/2
22	CLA	3	604	34	1/1/20/20	1/37/115/115	-
22	CLA	7	614	-	1/1/14/20	4/11/89/115	-
22	CLA	1	611	24	1/1/19/20	3/33/111/115	-
22	CLA	B2	810	-	1/1/20/20	4/37/115/115	-
25	BCR	B	801	-	-	0/29/63/63	0/2/2/2
22	CLA	Z	603	-	1/1/18/20	5/25/103/115	-
22	CLA	B	813	-	1/1/20/20	3/37/115/115	-
27	LMU	1	623	-	-	1/15/35/61	0/1/1/2
22	CLA	A	842	-	1/1/20/20	1/37/115/115	-
31	CHL	Z	606	34	3/3/21/26	5/15/113/137	-
25	BCR	92	623	-	-	4/29/63/63	0/2/2/2
22	CLA	7	604	34	1/1/17/20	1/21/99/115	-
22	CLA	B2	828	-	1/1/20/20	3/37/115/115	-
30	DGD	B	850	-	-	10/48/88/95	0/2/2/2
25	BCR	G	205	-	-	2/29/63/63	0/2/2/2
22	CLA	K	203	34	1/1/19/20	4/31/109/115	-
22	CLA	B2	804	-	1/1/15/20	2/13/91/115	-
31	CHL	5	607	34	3/3/26/26	8/39/137/137	-
22	CLA	5	617	-	1/1/20/20	6/37/115/115	-
25	BCR	K	207	-	-	4/29/63/63	0/2/2/2
26	SF4	A	853	2,1	-	-	0/6/5/5
29	LUT	Z	619	-	-	2/18/37/67	0/1/1/2
22	CLA	A	827	34	1/1/20/20	3/37/115/115	-
22	CLA	J	101	9	1/1/18/20	5/25/103/115	-
27	LMU	A	865	-	-	3/15/35/61	0/1/1/2
22	CLA	A	805	-	1/1/18/20	1/25/103/115	-
22	CLA	B2	839	-	1/1/15/20	3/13/91/115	-
22	CLA	8	602	15	1/1/19/20	2/34/112/115	-
22	CLA	B2	806	20	1/1/20/20	4/37/115/115	-
22	CLA	3	612	13	1/1/15/20	1/15/93/115	-
28	LMG	8	629	-	-	8/37/57/70	0/1/1/1
28	LMG	1	628	-	-	5/37/57/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	LMG	9	620	22	-	7/39/59/70	0/1/1/1
22	CLA	A	819	-	1/1/19/20	1/31/109/115	-
22	CLA	5	621	34	1/1/15/20	8/15/93/115	-
25	BCR	5	622	-	-	3/29/63/63	0/2/2/2
22	CLA	B	803	-	1/1/20/20	2/37/115/115	-
22	CLA	B	827	-	1/1/20/20	5/37/115/115	-
24	LHG	6	629	-	-	10/40/40/53	-
31	CHL	6	606	34	3/3/24/26	0/30/128/137	-
22	CLA	A	838	-	1/1/17/20	1/21/99/115	-
22	CLA	Z	608	34	1/1/17/20	0/19/97/115	-
31	CHL	6	607	34	3/3/26/26	9/39/137/137	-
22	CLA	A	815	-	1/1/18/20	3/25/103/115	-
22	CLA	8	603	-	1/1/20/20	5/37/115/115	-
25	BCR	6	623	-	-	2/29/63/63	0/2/2/2
22	CLA	4	610	16	1/1/19/20	3/31/109/115	-
22	CLA	4	613	16	1/1/20/20	5/37/115/115	-
22	CLA	A	841	-	1/1/20/20	6/37/115/115	-
31	CHL	5	608	34	3/3/23/26	0/21/119/137	-
22	CLA	7	608	34	1/1/17/20	0/19/97/115	-
22	CLA	B2	820	-	1/1/18/20	6/27/105/115	-
22	CLA	A	823	-	1/1/20/20	6/37/115/115	-
22	CLA	Z	604	34	1/1/18/20	2/28/106/115	-
22	CLA	5	613	17	1/1/18/20	4/27/105/115	-
29	LUT	5	620	-	-	2/29/67/67	0/2/2/2
25	BCR	A	852	-	-	4/29/63/63	0/2/2/2
22	CLA	B	811	-	1/1/20/20	8/37/115/115	-
22	CLA	5	602	17	1/1/20/20	1/37/115/115	-
22	CLA	A	804	-	1/1/20/20	5/37/115/115	-
28	LMG	J	104	-	-	8/30/50/70	0/1/1/1
22	CLA	A	802	-	1/1/20/20	0/37/115/115	-
22	CLA	A	807	1	1/1/20/20	4/37/115/115	-
22	CLA	B	838	-	1/1/17/20	1/19/97/115	-
22	CLA	9	602	19	1/1/19/20	2/31/109/115	-
22	CLA	A	831	-	1/1/20/20	2/37/115/115	-
22	CLA	B	810	-	1/1/20/20	3/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	A	839	-	1/1/20/20	2/37/115/115	-
29	LUT	7	624	-	-	4/29/67/67	0/2/2/2
32	XAT	8	618	-	-	0/31/93/93	0/4/4/4
32	XAT	6	624	-	-	0/31/93/93	0/4/4/4
22	CLA	1	610	12	1/1/20/20	0/37/115/115	-
22	CLA	B	823	-	1/1/20/20	7/37/115/115	-
22	CLA	9	611	24	1/1/20/20	4/37/115/115	-
31	CHL	7	606	34	3/3/21/26	3/15/113/137	-
22	CLA	9	609	19	1/1/17/20	2/21/99/115	-
22	CLA	8	612	15	1/1/18/20	6/25/103/115	-
22	CLA	B	840	-	1/1/20/20	5/37/115/115	-
27	LMU	92	624	-	-	1/21/61/61	0/2/2/2
22	CLA	B	804	-	1/1/15/20	4/13/91/115	-
23	PQN	B	842	-	-	1/23/43/43	0/2/2/2
29	LUT	A	856	-	-	4/29/67/67	0/2/2/2
22	CLA	B2	805	-	1/1/20/20	3/37/115/115	-
22	CLA	B	807	-	1/1/18/20	2/25/103/115	-
29	LUT	3	622	-	-	2/29/67/67	0/2/2/2
22	CLA	9	601	19	1/1/15/20	0/15/93/115	-
24	LHG	3	623	-	-	13/51/51/53	-
22	CLA	A	818	-	1/1/20/20	2/37/115/115	-
22	CLA	B	831	-	1/1/18/20	1/25/103/115	-
24	LHG	3	721	-	-	12/35/35/53	-
22	CLA	3	611	-	1/1/20/20	4/37/115/115	-
22	CLA	6	611	24	1/1/18/20	2/29/107/115	-
22	CLA	B2	811	-	1/1/17/20	3/25/101/115	-
31	CHL	7	601	14	3/3/26/26	5/39/137/137	-
22	CLA	A	816	-	1/1/20/20	5/37/115/115	-
22	CLA	A	822	34	1/1/20/20	0/37/115/115	-
27	LMU	A	863	-	-	7/21/61/61	0/2/2/2
22	CLA	B	802	-	1/1/20/20	4/37/115/115	-
27	LMU	7	628	-	-	3/13/33/61	0/1/1/2
22	CLA	G	203	-	1/1/19/20	3/31/109/115	-
22	CLA	B2	815	-	1/1/18/20	2/28/106/115	-
24	LHG	A	847	22	-	6/42/42/53	-
22	CLA	9	603	28,19	1/1/18/20	4/25/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CHL	92	606	-	3/3/20/26	0/10/108/137	-
22	CLA	Z	612	12	1/1/15/20	3/13/91/115	-
29	LUT	6	621	-	-	2/29/67/67	0/2/2/2
22	CLA	92	604	19	1/1/17/20	2/19/97/115	-
22	CLA	B	820	-	1/1/18/20	4/27/105/115	-
25	BCR	B	848	-	-	2/29/63/63	0/2/2/2
22	CLA	B	816	-	1/1/20/20	1/37/115/115	-
22	CLA	7	602	14	1/1/20/20	2/37/115/115	-
22	CLA	7	609	14	1/1/15/20	0/13/91/115	-
27	LMU	1	625	-	-	5/15/35/61	0/1/1/2
31	CHL	9	607	34	3/3/23/26	0/21/119/137	-
22	CLA	6	622	34	1/1/18/20	3/25/103/115	-
22	CLA	9	613	19	1/1/20/20	3/37/115/115	-
27	LMU	1	621	-	-	6/21/61/61	0/2/2/2
22	CLA	B2	829	-	1/1/20/20	0/37/115/115	-
22	CLA	A	830	-	1/1/20/20	4/37/115/115	-
25	BCR	B	844	-	-	0/29/63/63	0/2/2/2
22	CLA	9	610	19	1/1/19/20	0/31/109/115	-
22	CLA	A	808	-	1/1/17/20	1/19/97/115	-
22	CLA	1	609	12	1/1/20/20	5/37/115/115	-

All (1129) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	92	606	CHL	C4B-NB	11.96	1.45	1.35
31	6	607	CHL	C4B-NB	11.95	1.45	1.35
31	9	606	CHL	C4B-NB	11.93	1.45	1.35
31	6	608	CHL	C4B-NB	11.81	1.45	1.35
31	5	618	CHL	C4B-NB	11.77	1.45	1.35
31	6	618	CHL	C4B-NB	11.64	1.45	1.35
31	6	606	CHL	C4B-NB	11.63	1.45	1.35
31	6	616	CHL	C4B-NB	11.62	1.45	1.35
31	4	608	CHL	C4B-NB	11.57	1.45	1.35
31	4	618	CHL	C4B-NB	11.57	1.45	1.35
31	1	606	CHL	C4B-NB	11.54	1.45	1.35
31	92	607	CHL	C4B-NB	11.51	1.45	1.35
31	7	601	CHL	C4B-NB	11.49	1.45	1.35
31	8	601	CHL	C4B-NB	11.49	1.45	1.35
31	8	607	CHL	C4B-NB	11.48	1.45	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	4	601	CHL	C4B-NB	11.45	1.45	1.35
31	5	608	CHL	C4B-NB	11.40	1.45	1.35
31	Z	606	CHL	C4B-NB	11.38	1.45	1.35
31	5	606	CHL	C4B-NB	11.37	1.45	1.35
31	Z	607	CHL	C4B-NB	11.36	1.45	1.35
31	6	601	CHL	C4B-NB	11.36	1.45	1.35
31	4	607	CHL	C4B-NB	11.35	1.45	1.35
31	4	606	CHL	C4B-NB	11.34	1.45	1.35
31	7	606	CHL	C4B-NB	11.33	1.45	1.35
31	7	607	CHL	C4B-NB	11.32	1.45	1.35
31	8	606	CHL	C4B-NB	11.27	1.45	1.35
31	9	607	CHL	C4B-NB	11.24	1.45	1.35
31	1	601	CHL	C4B-NB	11.22	1.45	1.35
31	5	607	CHL	C4B-NB	11.20	1.45	1.35
31	1	607	CHL	C4B-NB	11.01	1.45	1.35
31	Z	601	CHL	C4B-NB	10.95	1.45	1.35
31	3	608	CHL	C4B-NB	10.95	1.45	1.35
21	A	801	CL0	C4B-NB	9.42	1.43	1.35
21	A	801	CL0	C1B-NB	6.34	1.40	1.35
31	3	608	CHL	MG-ND	-6.13	1.93	2.05
31	6	601	CHL	MG-ND	-6.10	1.93	2.05
31	Z	601	CHL	MG-ND	-6.08	1.93	2.05
31	Z	607	CHL	MG-ND	-6.06	1.93	2.05
31	4	607	CHL	MG-ND	-6.04	1.93	2.05
31	4	601	CHL	MG-ND	-6.04	1.93	2.05
31	5	606	CHL	MG-ND	-6.02	1.93	2.05
31	5	608	CHL	MG-ND	-6.01	1.93	2.05
31	1	607	CHL	MG-ND	-6.01	1.93	2.05
31	8	601	CHL	MG-ND	-6.01	1.93	2.05
31	8	607	CHL	MG-ND	-6.00	1.93	2.05
31	4	606	CHL	MG-ND	-6.00	1.93	2.05
31	92	606	CHL	MG-ND	-6.00	1.93	2.05
31	7	601	CHL	MG-ND	-5.99	1.93	2.05
31	7	607	CHL	MG-ND	-5.99	1.93	2.05
31	4	608	CHL	MG-ND	-5.98	1.93	2.05
31	6	606	CHL	MG-ND	-5.97	1.93	2.05
31	1	606	CHL	MG-ND	-5.97	1.94	2.05
31	6	616	CHL	MG-ND	-5.96	1.94	2.05
31	9	607	CHL	MG-ND	-5.94	1.94	2.05
31	6	607	CHL	MG-ND	-5.94	1.94	2.05
31	6	608	CHL	MG-ND	-5.92	1.94	2.05
31	7	606	CHL	MG-ND	-5.87	1.94	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	5	607	CHL	MG-ND	-5.87	1.94	2.05
31	92	607	CHL	MG-ND	-5.85	1.94	2.05
31	6	618	CHL	MG-ND	-5.84	1.94	2.05
31	9	606	CHL	MG-ND	-5.84	1.94	2.05
31	Z	606	CHL	MG-ND	-5.83	1.94	2.05
31	1	601	CHL	MG-ND	-5.82	1.94	2.05
31	5	618	CHL	MG-ND	-5.81	1.94	2.05
22	B2	820	CLA	C1D-ND	5.77	1.44	1.37
31	8	606	CHL	MG-ND	-5.73	1.94	2.05
31	4	618	CHL	MG-ND	-5.71	1.94	2.05
22	B2	828	CLA	C1D-ND	5.67	1.44	1.37
22	92	614	CLA	C1D-ND	5.66	1.44	1.37
22	5	621	CLA	C1D-ND	5.64	1.44	1.37
22	L	204	CLA	C1D-ND	5.64	1.44	1.37
22	B2	804	CLA	C1D-ND	5.61	1.44	1.37
22	B2	808	CLA	C1D-ND	5.60	1.44	1.37
22	B2	813	CLA	C1D-ND	5.59	1.44	1.37
22	B2	815	CLA	C1D-ND	5.58	1.44	1.37
22	B2	805	CLA	C1D-ND	5.56	1.44	1.37
22	Z	612	CLA	C1D-ND	5.55	1.44	1.37
22	6	614	CLA	C1D-ND	5.52	1.44	1.37
22	4	612	CLA	C1D-ND	5.51	1.44	1.37
22	K	203	CLA	C1D-ND	5.46	1.44	1.37
22	B2	809	CLA	C1D-ND	5.46	1.44	1.37
31	5	607	CHL	MG-NA	-5.45	1.93	2.06
22	K	206	CLA	C1D-ND	5.44	1.44	1.37
22	B2	829	CLA	C1D-ND	5.44	1.44	1.37
22	4	603	CLA	C1D-ND	5.43	1.44	1.37
22	7	620	CLA	C1D-ND	5.43	1.44	1.37
22	92	603	CLA	C1D-ND	5.42	1.44	1.37
22	6	612	CLA	C1D-ND	5.41	1.44	1.37
22	G	204	CLA	C1D-ND	5.40	1.44	1.37
31	1	607	CHL	MG-NA	-5.40	1.93	2.06
22	B	835	CLA	C1D-ND	5.40	1.44	1.37
22	B2	806	CLA	C1D-ND	5.40	1.44	1.37
31	6	601	CHL	MG-NA	-5.39	1.93	2.06
22	B	822	CLA	C1D-ND	5.38	1.44	1.37
22	5	601	CLA	C1D-ND	5.38	1.44	1.37
31	Z	601	CHL	MG-NA	-5.37	1.93	2.06
22	5	612	CLA	C1D-ND	5.37	1.44	1.37
22	6	611	CLA	C1D-ND	5.37	1.44	1.37
22	8	612	CLA	C1D-ND	5.36	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	1	612	CLA	C1D-ND	5.36	1.44	1.37
22	K	201	CLA	C1D-ND	5.36	1.44	1.37
22	Z	603	CLA	C1D-ND	5.35	1.44	1.37
22	J	101	CLA	C1D-ND	5.35	1.44	1.37
22	F	303	CLA	C1D-ND	5.35	1.44	1.37
22	9	601	CLA	C1D-ND	5.34	1.44	1.37
22	Z	609	CLA	C1D-ND	5.34	1.44	1.37
22	B2	810	CLA	C1D-ND	5.34	1.44	1.37
22	92	613	CLA	C1D-ND	5.34	1.44	1.37
22	9	603	CLA	C1D-ND	5.33	1.44	1.37
22	92	604	CLA	C1D-ND	5.32	1.44	1.37
22	4	616	CLA	C1D-ND	5.31	1.44	1.37
22	7	612	CLA	C1D-ND	5.31	1.44	1.37
22	Z	602	CLA	C1D-ND	5.31	1.44	1.37
22	6	604	CLA	C1D-ND	5.30	1.44	1.37
22	8	608	CLA	C1D-ND	5.30	1.44	1.37
31	9	607	CHL	MG-NA	-5.29	1.93	2.06
22	3	612	CLA	C1D-ND	5.29	1.44	1.37
22	5	614	CLA	C1D-ND	5.29	1.44	1.37
22	L2	204	CLA	C1D-ND	5.29	1.44	1.37
22	B2	807	CLA	C1D-ND	5.29	1.44	1.37
22	B	824	CLA	C1D-ND	5.28	1.44	1.37
22	B	812	CLA	C1D-ND	5.28	1.44	1.37
22	9	612	CLA	C1D-ND	5.28	1.44	1.37
22	B2	814	CLA	C1D-ND	5.28	1.44	1.37
22	B2	811	CLA	C1D-ND	5.27	1.44	1.37
22	A	826	CLA	C1D-ND	5.27	1.44	1.37
22	5	602	CLA	C1D-ND	5.27	1.44	1.37
31	3	608	CHL	MG-NA	-5.27	1.93	2.06
22	3	606	CLA	C1D-ND	5.26	1.44	1.37
22	8	603	CLA	C1D-ND	5.26	1.44	1.37
22	8	611	CLA	C1D-ND	5.26	1.44	1.37
22	7	614	CLA	C1D-ND	5.25	1.44	1.37
22	92	601	CLA	C1D-ND	5.25	1.44	1.37
22	A	817	CLA	C1D-ND	5.25	1.44	1.37
22	5	613	CLA	C1D-ND	5.25	1.44	1.37
22	7	613	CLA	C1D-ND	5.25	1.44	1.37
22	F	304	CLA	C1D-ND	5.25	1.44	1.37
22	9	614	CLA	C1D-ND	5.25	1.44	1.37
22	3	615	CLA	C1D-ND	5.24	1.44	1.37
22	A	832	CLA	C1D-ND	5.24	1.44	1.37
22	6	622	CLA	C1D-ND	5.23	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	Z	616	CLA	C1D-ND	5.23	1.44	1.37
22	B	815	CLA	C1D-ND	5.23	1.44	1.37
22	B2	839	CLA	C1D-ND	5.23	1.44	1.37
22	4	604	CLA	C1D-ND	5.22	1.44	1.37
22	4	611	CLA	C1D-ND	5.22	1.44	1.37
22	7	611	CLA	C1D-ND	5.21	1.44	1.37
31	92	606	CHL	MG-NA	-5.21	1.93	2.06
22	B	827	CLA	C1D-ND	5.21	1.44	1.37
22	Z	611	CLA	C1D-ND	5.21	1.44	1.37
22	Z	614	CLA	C1D-ND	5.20	1.44	1.37
22	K	204	CLA	C1D-ND	5.20	1.44	1.37
22	A	819	CLA	C1D-ND	5.20	1.44	1.37
22	3	607	CLA	C1D-ND	5.20	1.44	1.37
22	7	602	CLA	C1D-ND	5.20	1.44	1.37
22	1	609	CLA	C1D-ND	5.20	1.44	1.37
22	B	839	CLA	C1D-ND	5.19	1.44	1.37
31	1	601	CHL	MG-NA	-5.19	1.93	2.06
22	A	816	CLA	C1D-ND	5.19	1.44	1.37
22	4	614	CLA	C1D-ND	5.19	1.44	1.37
22	92	612	CLA	C1D-ND	5.19	1.44	1.37
22	A	845	CLA	C1D-ND	5.19	1.44	1.37
22	6	613	CLA	C1D-ND	5.19	1.44	1.37
22	9	604	CLA	C1D-ND	5.19	1.44	1.37
31	7	601	CHL	MG-NA	-5.18	1.94	2.06
22	8	602	CLA	C1D-ND	5.18	1.44	1.37
22	5	616	CLA	C1D-ND	5.18	1.44	1.37
22	A	835	CLA	C1D-ND	5.18	1.44	1.37
22	3	613	CLA	C1D-ND	5.17	1.44	1.37
22	4	613	CLA	C1D-ND	5.17	1.44	1.37
22	B	832	CLA	C1D-ND	5.17	1.44	1.37
31	8	601	CHL	MG-NA	-5.16	1.94	2.06
22	B2	812	CLA	C1D-ND	5.16	1.44	1.37
22	1	614	CLA	C1D-ND	5.16	1.44	1.37
22	A	828	CLA	C1D-ND	5.16	1.44	1.37
22	B	808	CLA	C1D-ND	5.16	1.44	1.37
22	6	617	CLA	C1D-ND	5.16	1.44	1.37
31	4	601	CHL	MG-NA	-5.16	1.94	2.06
22	1	611	CLA	C1D-ND	5.15	1.44	1.37
31	8	606	CHL	MG-NA	-5.15	1.94	2.06
22	A	814	CLA	C1D-ND	5.15	1.44	1.37
31	92	607	CHL	MG-NA	-5.14	1.94	2.06
22	5	617	CLA	C1D-ND	5.14	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	5	604	CLA	C1D-ND	5.14	1.44	1.37
22	A	831	CLA	C1D-ND	5.14	1.44	1.37
22	1	608	CLA	C1D-ND	5.14	1.44	1.37
22	Z	604	CLA	C1D-ND	5.14	1.44	1.37
31	4	618	CHL	MG-NA	-5.14	1.94	2.06
22	B	809	CLA	C1D-ND	5.13	1.44	1.37
22	5	603	CLA	C1D-ND	5.13	1.44	1.37
22	G	203	CLA	C1D-ND	5.13	1.44	1.37
22	1	603	CLA	C1D-ND	5.13	1.44	1.37
22	8	613	CLA	C1D-ND	5.13	1.44	1.37
22	A	839	CLA	C1D-ND	5.13	1.44	1.37
22	3	614	CLA	C1D-ND	5.12	1.44	1.37
22	9	609	CLA	C1D-ND	5.12	1.44	1.37
22	L2	203	CLA	C1D-ND	5.12	1.44	1.37
22	A	815	CLA	C1D-ND	5.11	1.44	1.37
22	B	804	CLA	C1D-ND	5.11	1.44	1.37
31	Z	606	CHL	MG-NA	-5.11	1.94	2.06
31	4	606	CHL	MG-NA	-5.11	1.94	2.06
22	B	841	CLA	C1D-ND	5.11	1.44	1.37
22	3	611	CLA	C1D-ND	5.10	1.44	1.37
22	A	825	CLA	C1D-ND	5.10	1.44	1.37
22	A	830	CLA	C1D-ND	5.10	1.44	1.37
22	A	840	CLA	C1D-ND	5.10	1.44	1.37
22	8	604	CLA	C1D-ND	5.09	1.44	1.37
22	92	611	CLA	C1D-ND	5.09	1.44	1.37
22	Z	613	CLA	C1D-ND	5.09	1.44	1.37
22	4	610	CLA	C1D-ND	5.09	1.44	1.37
22	A	803	CLA	C1D-ND	5.08	1.44	1.37
22	A	838	CLA	C1D-ND	5.08	1.44	1.37
22	8	614	CLA	C1D-ND	5.08	1.44	1.37
22	6	602	CLA	C1D-ND	5.08	1.44	1.37
22	B	838	CLA	C1D-ND	5.08	1.44	1.37
22	6	603	CLA	C1D-ND	5.07	1.44	1.37
31	7	607	CHL	MG-NA	-5.07	1.94	2.06
22	B	820	CLA	C1D-ND	5.07	1.44	1.37
22	B	836	CLA	C1D-ND	5.06	1.44	1.37
22	A	854	CLA	C1D-ND	5.06	1.44	1.37
22	A	829	CLA	C1D-ND	5.06	1.44	1.37
22	6	610	CLA	C1D-ND	5.06	1.44	1.37
31	4	607	CHL	MG-NA	-5.06	1.94	2.06
22	92	609	CLA	C1D-ND	5.06	1.44	1.37
31	6	608	CHL	MG-NA	-5.05	1.94	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	6	616	CHL	MG-NA	-5.05	1.94	2.06
22	A	833	CLA	C1D-ND	5.05	1.44	1.37
22	3	604	CLA	C1D-ND	5.05	1.44	1.37
31	6	607	CHL	MG-NA	-5.05	1.94	2.06
31	5	608	CHL	MG-NA	-5.05	1.94	2.06
22	4	609	CLA	C1D-ND	5.05	1.44	1.37
31	5	618	CHL	MG-NA	-5.04	1.94	2.06
22	B	811	CLA	C1D-ND	5.03	1.44	1.37
22	3	617	CLA	C1D-ND	5.03	1.44	1.37
22	Z	610	CLA	C1D-ND	5.03	1.44	1.37
22	8	609	CLA	C1D-ND	5.03	1.44	1.37
22	4	602	CLA	C1D-ND	5.03	1.44	1.37
31	4	608	CHL	MG-NA	-5.03	1.94	2.06
22	1	604	CLA	C1D-ND	5.03	1.44	1.37
22	5	609	CLA	C1D-ND	5.03	1.44	1.37
22	B	837	CLA	C1D-ND	5.02	1.44	1.37
22	A	808	CLA	C1D-ND	5.02	1.44	1.37
22	7	603	CLA	C1D-ND	5.01	1.43	1.37
31	6	618	CHL	MG-NA	-5.01	1.94	2.06
22	A	821	CLA	C1D-ND	5.01	1.43	1.37
22	9	602	CLA	C1D-ND	5.01	1.43	1.37
22	B	816	CLA	C1D-ND	5.00	1.43	1.37
22	7	604	CLA	C1D-ND	5.00	1.43	1.37
22	7	608	CLA	C1D-ND	5.00	1.43	1.37
22	1	613	CLA	C1D-ND	4.99	1.43	1.37
22	5	611	CLA	C1D-ND	4.99	1.43	1.37
22	A	805	CLA	C1D-ND	4.98	1.43	1.37
22	A	837	CLA	C1D-ND	4.98	1.43	1.37
31	5	606	CHL	MG-NA	-4.97	1.94	2.06
22	B	813	CLA	C1D-ND	4.97	1.43	1.37
22	B	810	CLA	C1D-ND	4.97	1.43	1.37
22	A	804	CLA	C1D-ND	4.97	1.43	1.37
22	A	843	CLA	C1D-ND	4.97	1.43	1.37
22	1	616	CLA	C1D-ND	4.97	1.43	1.37
22	A	813	CLA	C1D-ND	4.96	1.43	1.37
22	A	834	CLA	C1D-ND	4.96	1.43	1.37
22	7	609	CLA	C1D-ND	4.95	1.43	1.37
31	7	606	CHL	MG-NA	-4.95	1.94	2.06
22	B	828	CLA	C1D-ND	4.95	1.43	1.37
22	Z	608	CLA	C1D-ND	4.95	1.43	1.37
22	A	818	CLA	C1D-ND	4.95	1.43	1.37
22	B	814	CLA	C1D-ND	4.95	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	7	616	CLA	C1D-ND	4.93	1.43	1.37
22	B	807	CLA	C1D-ND	4.93	1.43	1.37
31	9	606	CHL	MG-NA	-4.92	1.94	2.06
22	A	841	CLA	C1D-ND	4.92	1.43	1.37
22	9	610	CLA	C1D-ND	4.92	1.43	1.37
22	9	613	CLA	C1D-ND	4.92	1.43	1.37
22	B	826	CLA	C1D-ND	4.92	1.43	1.37
22	B	819	CLA	C1D-ND	4.92	1.43	1.37
31	Z	607	CHL	MG-NA	-4.92	1.94	2.06
22	6	609	CLA	C1D-ND	4.91	1.43	1.37
22	A	807	CLA	C1D-ND	4.91	1.43	1.37
22	A	820	CLA	C1D-ND	4.91	1.43	1.37
22	A	836	CLA	C1D-ND	4.90	1.43	1.37
22	9	611	CLA	C1D-ND	4.90	1.43	1.37
22	A	812	CLA	C1D-ND	4.90	1.43	1.37
22	92	602	CLA	C1D-ND	4.89	1.43	1.37
22	3	602	CLA	C1D-ND	4.88	1.43	1.37
31	6	606	CHL	MG-NA	-4.88	1.94	2.06
31	1	606	CHL	MG-NA	-4.88	1.94	2.06
22	B	802	CLA	C1D-ND	4.88	1.43	1.37
22	A	827	CLA	C1D-ND	4.88	1.43	1.37
22	B	834	CLA	C1D-ND	4.87	1.43	1.37
22	A	811	CLA	C1D-ND	4.87	1.43	1.37
22	A	822	CLA	C1D-ND	4.87	1.43	1.37
22	A	809	CLA	C1D-ND	4.85	1.43	1.37
22	8	616	CLA	C1D-ND	4.85	1.43	1.37
22	5	610	CLA	C1D-ND	4.85	1.43	1.37
22	B	805	CLA	C1D-ND	4.84	1.43	1.37
22	A	824	CLA	C1D-ND	4.84	1.43	1.37
21	A	801	CL0	MG-NA	-4.84	1.94	2.06
22	B	806	CLA	C1D-ND	4.83	1.43	1.37
22	B	818	CLA	C1D-ND	4.83	1.43	1.37
22	1	602	CLA	C1D-ND	4.83	1.43	1.37
22	A	842	CLA	C1D-ND	4.83	1.43	1.37
22	8	610	CLA	C1D-ND	4.83	1.43	1.37
22	B	830	CLA	C1D-ND	4.81	1.43	1.37
22	L	203	CLA	C1D-ND	4.80	1.43	1.37
22	A	810	CLA	C1D-ND	4.79	1.43	1.37
22	7	610	CLA	C1D-ND	4.78	1.43	1.37
22	B	821	CLA	C1D-ND	4.78	1.43	1.37
22	92	610	CLA	C1D-ND	4.78	1.43	1.37
22	B	831	CLA	C1D-ND	4.78	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	803	CLA	MG-ND	-4.78	1.96	2.05
22	B	833	CLA	C1D-ND	4.77	1.43	1.37
22	1	610	CLA	C1D-ND	4.77	1.43	1.37
22	3	610	CLA	C1D-ND	4.73	1.43	1.37
31	8	607	CHL	MG-NA	-4.73	1.95	2.06
22	3	609	CLA	C1D-ND	4.72	1.43	1.37
22	F	301	CLA	C1D-ND	4.71	1.43	1.37
22	A	806	CLA	C1D-ND	4.71	1.43	1.37
22	B	840	CLA	C1D-ND	4.71	1.43	1.37
22	3	603	CLA	C1D-ND	4.71	1.43	1.37
22	A	823	CLA	C1D-ND	4.68	1.43	1.37
22	B	817	CLA	C1D-ND	4.67	1.43	1.37
22	B	825	CLA	C1D-ND	4.66	1.43	1.37
22	A	837	CLA	MG-ND	-4.65	1.96	2.05
22	K	201	CLA	MG-ND	-4.65	1.96	2.05
22	B	821	CLA	MG-ND	-4.63	1.96	2.05
22	A	810	CLA	MG-ND	-4.63	1.96	2.05
21	A	801	CL0	MG-ND	-4.60	1.96	2.05
22	7	610	CLA	MG-ND	-4.59	1.96	2.05
22	B	838	CLA	MG-ND	-4.57	1.96	2.05
22	5	621	CLA	MG-ND	-4.54	1.96	2.05
22	A	854	CLA	MG-ND	-4.53	1.96	2.05
22	B	803	CLA	C1D-ND	4.52	1.43	1.37
22	A	823	CLA	MG-ND	-4.50	1.96	2.05
22	B	803	CLA	MG-ND	-4.50	1.96	2.05
22	1	616	CLA	MG-ND	-4.50	1.96	2.05
22	A	829	CLA	MG-ND	-4.46	1.96	2.05
22	A	825	CLA	MG-ND	-4.46	1.96	2.05
22	A	833	CLA	MG-ND	-4.46	1.96	2.05
22	A	802	CLA	C1D-ND	4.46	1.43	1.37
22	7	609	CLA	MG-ND	-4.45	1.97	2.05
22	B	829	CLA	C1D-ND	4.44	1.43	1.37
22	B	839	CLA	MG-ND	-4.43	1.97	2.05
22	B	823	CLA	C1D-ND	4.43	1.43	1.37
22	92	610	CLA	MG-ND	-4.42	1.97	2.05
22	B	807	CLA	MG-ND	-4.42	1.97	2.05
22	7	608	CLA	MG-ND	-4.41	1.97	2.05
22	7	614	CLA	MG-ND	-4.41	1.97	2.05
22	B	806	CLA	MG-ND	-4.41	1.97	2.05
22	4	602	CLA	MG-ND	-4.41	1.97	2.05
22	Z	608	CLA	MG-ND	-4.40	1.97	2.05
22	3	617	CLA	MG-ND	-4.40	1.97	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	802	CLA	MG-ND	-4.40	1.97	2.05
22	A	843	CLA	MG-ND	-4.39	1.97	2.05
22	8	611	CLA	MG-ND	-4.38	1.97	2.05
22	Z	609	CLA	MG-ND	-4.37	1.97	2.05
22	B	812	CLA	MG-ND	-4.37	1.97	2.05
22	A	819	CLA	MG-ND	-4.36	1.97	2.05
22	4	613	CLA	MG-ND	-4.36	1.97	2.05
22	1	611	CLA	MG-ND	-4.36	1.97	2.05
22	A	824	CLA	MG-ND	-4.36	1.97	2.05
22	1	602	CLA	MG-ND	-4.35	1.97	2.05
22	B	819	CLA	MG-ND	-4.35	1.97	2.05
22	92	609	CLA	MG-ND	-4.35	1.97	2.05
22	1	608	CLA	MG-ND	-4.34	1.97	2.05
22	Z	616	CLA	MG-ND	-4.34	1.97	2.05
22	G	203	CLA	MG-ND	-4.34	1.97	2.05
22	B	820	CLA	MG-ND	-4.34	1.97	2.05
22	3	603	CLA	MG-ND	-4.33	1.97	2.05
22	8	603	CLA	MG-ND	-4.33	1.97	2.05
22	92	602	CLA	MG-ND	-4.33	1.97	2.05
22	B	833	CLA	MG-ND	-4.33	1.97	2.05
22	B	829	CLA	MG-ND	-4.33	1.97	2.05
22	B	823	CLA	MG-ND	-4.32	1.97	2.05
22	A	836	CLA	MG-ND	-4.32	1.97	2.05
22	4	611	CLA	MG-ND	-4.32	1.97	2.05
22	A	807	CLA	MG-ND	-4.32	1.97	2.05
22	7	611	CLA	MG-ND	-4.32	1.97	2.05
22	3	611	CLA	MG-ND	-4.32	1.97	2.05
22	9	602	CLA	MG-ND	-4.31	1.97	2.05
22	B	809	CLA	MG-ND	-4.31	1.97	2.05
22	A	817	CLA	MG-ND	-4.31	1.97	2.05
22	8	604	CLA	MG-ND	-4.31	1.97	2.05
22	9	613	CLA	MG-ND	-4.31	1.97	2.05
22	A	813	CLA	MG-ND	-4.31	1.97	2.05
22	8	602	CLA	MG-ND	-4.31	1.97	2.05
22	3	609	CLA	MG-ND	-4.30	1.97	2.05
22	A	808	CLA	MG-ND	-4.30	1.97	2.05
22	6	617	CLA	MG-ND	-4.30	1.97	2.05
22	5	611	CLA	MG-ND	-4.30	1.97	2.05
22	B	813	CLA	MG-ND	-4.30	1.97	2.05
21	A	801	CL0	C1D-ND	4.30	1.43	1.37
22	4	609	CLA	MG-ND	-4.30	1.97	2.05
22	92	611	CLA	MG-ND	-4.30	1.97	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	7	613	CLA	MG-ND	-4.29	1.97	2.05
22	L	203	CLA	MG-ND	-4.29	1.97	2.05
22	3	615	CLA	MG-ND	-4.29	1.97	2.05
22	8	609	CLA	MG-ND	-4.29	1.97	2.05
22	3	613	CLA	MG-ND	-4.29	1.97	2.05
22	9	611	CLA	MG-ND	-4.29	1.97	2.05
22	A	828	CLA	MG-ND	-4.28	1.97	2.05
22	5	602	CLA	MG-ND	-4.28	1.97	2.05
22	A	815	CLA	MG-ND	-4.28	1.97	2.05
22	9	601	CLA	MG-ND	-4.28	1.97	2.05
22	A	805	CLA	MG-ND	-4.28	1.97	2.05
22	B	815	CLA	MG-ND	-4.28	1.97	2.05
22	3	607	CLA	MG-ND	-4.27	1.97	2.05
22	1	614	CLA	MG-ND	-4.27	1.97	2.05
22	4	616	CLA	MG-ND	-4.27	1.97	2.05
22	1	604	CLA	MG-ND	-4.27	1.97	2.05
22	6	613	CLA	MG-ND	-4.27	1.97	2.05
22	1	603	CLA	MG-ND	-4.27	1.97	2.05
22	B	834	CLA	MG-ND	-4.26	1.97	2.05
22	4	604	CLA	MG-ND	-4.26	1.97	2.05
22	L2	203	CLA	MG-ND	-4.26	1.97	2.05
22	J	101	CLA	MG-ND	-4.26	1.97	2.05
22	4	614	CLA	MG-ND	-4.26	1.97	2.05
22	4	603	CLA	MG-ND	-4.26	1.97	2.05
22	A	826	CLA	MG-ND	-4.25	1.97	2.05
22	5	601	CLA	MG-ND	-4.25	1.97	2.05
22	B2	829	CLA	MG-ND	-4.25	1.97	2.05
22	6	603	CLA	MG-ND	-4.25	1.97	2.05
22	9	614	CLA	MG-ND	-4.25	1.97	2.05
22	5	604	CLA	MG-ND	-4.25	1.97	2.05
22	6	622	CLA	MG-ND	-4.25	1.97	2.05
22	B	826	CLA	MG-ND	-4.25	1.97	2.05
22	92	603	CLA	MG-ND	-4.25	1.97	2.05
22	Z	613	CLA	MG-ND	-4.24	1.97	2.05
22	B	830	CLA	MG-ND	-4.24	1.97	2.05
22	92	601	CLA	MG-ND	-4.24	1.97	2.05
22	B2	807	CLA	MG-ND	-4.24	1.97	2.05
22	92	604	CLA	MG-ND	-4.24	1.97	2.05
22	B	817	CLA	MG-ND	-4.24	1.97	2.05
22	B2	810	CLA	MG-ND	-4.24	1.97	2.05
22	B2	839	CLA	MG-ND	-4.23	1.97	2.05
22	A	814	CLA	MG-ND	-4.23	1.97	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	1	610	CLA	MG-ND	-4.23	1.97	2.05
22	A	845	CLA	MG-ND	-4.23	1.97	2.05
22	K	203	CLA	MG-ND	-4.22	1.97	2.05
22	7	612	CLA	MG-ND	-4.22	1.97	2.05
22	A	821	CLA	MG-ND	-4.22	1.97	2.05
22	3	606	CLA	MG-ND	-4.22	1.97	2.05
22	Z	610	CLA	MG-ND	-4.22	1.97	2.05
22	A	839	CLA	MG-ND	-4.22	1.97	2.05
22	A	822	CLA	MG-ND	-4.22	1.97	2.05
22	Z	603	CLA	MG-ND	-4.22	1.97	2.05
22	8	610	CLA	MG-ND	-4.21	1.97	2.05
22	6	604	CLA	MG-ND	-4.21	1.97	2.05
22	B	837	CLA	MG-ND	-4.21	1.97	2.05
22	3	610	CLA	MG-ND	-4.21	1.97	2.05
22	7	616	CLA	MG-ND	-4.21	1.97	2.05
22	4	612	CLA	MG-ND	-4.20	1.97	2.05
22	5	616	CLA	MG-ND	-4.20	1.97	2.05
22	B	841	CLA	MG-ND	-4.20	1.97	2.05
22	6	611	CLA	MG-ND	-4.20	1.97	2.05
22	A	831	CLA	MG-ND	-4.20	1.97	2.05
22	B2	812	CLA	MG-ND	-4.19	1.97	2.05
22	1	613	CLA	MG-ND	-4.19	1.97	2.05
22	A	818	CLA	MG-ND	-4.19	1.97	2.05
22	5	617	CLA	MG-ND	-4.19	1.97	2.05
22	B	818	CLA	MG-ND	-4.19	1.97	2.05
22	B	824	CLA	MG-ND	-4.19	1.97	2.05
22	B2	814	CLA	MG-ND	-4.18	1.97	2.05
22	B2	809	CLA	MG-ND	-4.18	1.97	2.05
22	6	610	CLA	MG-ND	-4.18	1.97	2.05
22	92	612	CLA	MG-ND	-4.18	1.97	2.05
22	B	835	CLA	MG-ND	-4.18	1.97	2.05
22	K	206	CLA	MG-ND	-4.18	1.97	2.05
22	A	834	CLA	MG-ND	-4.18	1.97	2.05
22	B	825	CLA	MG-ND	-4.18	1.97	2.05
22	Z	614	CLA	MG-ND	-4.18	1.97	2.05
22	1	609	CLA	MG-ND	-4.18	1.97	2.05
22	B	828	CLA	MG-ND	-4.18	1.97	2.05
22	3	604	CLA	MG-ND	-4.18	1.97	2.05
22	A	832	CLA	MG-ND	-4.18	1.97	2.05
22	3	614	CLA	MG-ND	-4.18	1.97	2.05
22	F	303	CLA	MG-ND	-4.17	1.97	2.05
22	6	609	CLA	MG-ND	-4.17	1.97	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	811	CLA	MG-ND	-4.17	1.97	2.05
22	B	810	CLA	MG-ND	-4.17	1.97	2.05
22	9	609	CLA	MG-ND	-4.17	1.97	2.05
22	5	610	CLA	MG-ND	-4.17	1.97	2.05
22	3	602	CLA	MG-ND	-4.16	1.97	2.05
22	Z	602	CLA	MG-ND	-4.16	1.97	2.05
22	B	832	CLA	MG-ND	-4.16	1.97	2.05
22	8	614	CLA	MG-ND	-4.16	1.97	2.05
22	5	614	CLA	MG-ND	-4.16	1.97	2.05
22	B	816	CLA	MG-ND	-4.16	1.97	2.05
22	F	304	CLA	MG-ND	-4.15	1.97	2.05
22	A	816	CLA	MG-ND	-4.15	1.97	2.05
22	K	204	CLA	MG-ND	-4.15	1.97	2.05
22	7	604	CLA	MG-ND	-4.15	1.97	2.05
22	9	604	CLA	MG-ND	-4.15	1.97	2.05
22	B2	806	CLA	MG-ND	-4.15	1.97	2.05
22	7	603	CLA	MG-ND	-4.14	1.97	2.05
22	A	804	CLA	MG-ND	-4.14	1.97	2.05
22	3	612	CLA	MG-ND	-4.14	1.97	2.05
22	6	602	CLA	MG-ND	-4.14	1.97	2.05
22	Z	611	CLA	MG-ND	-4.14	1.97	2.05
22	9	612	CLA	MG-ND	-4.14	1.97	2.05
22	7	620	CLA	MG-ND	-4.14	1.97	2.05
22	92	613	CLA	MG-ND	-4.14	1.97	2.05
22	7	602	CLA	MG-ND	-4.14	1.97	2.05
22	9	610	CLA	MG-ND	-4.14	1.97	2.05
22	B	831	CLA	MG-ND	-4.14	1.97	2.05
22	B2	813	CLA	MG-ND	-4.13	1.97	2.05
22	A	811	CLA	MG-ND	-4.13	1.97	2.05
22	5	609	CLA	MG-ND	-4.13	1.97	2.05
22	A	827	CLA	MG-ND	-4.13	1.97	2.05
22	A	840	CLA	MG-ND	-4.13	1.97	2.05
22	Z	604	CLA	MG-ND	-4.13	1.97	2.05
22	B	822	CLA	MG-ND	-4.12	1.97	2.05
22	A	820	CLA	MG-ND	-4.12	1.97	2.05
22	B	804	CLA	MG-ND	-4.12	1.97	2.05
22	L2	204	CLA	MG-ND	-4.12	1.97	2.05
22	A	841	CLA	MG-ND	-4.12	1.97	2.05
22	A	830	CLA	MG-ND	-4.12	1.97	2.05
22	5	613	CLA	MG-ND	-4.12	1.97	2.05
22	B	814	CLA	MG-ND	-4.11	1.97	2.05
22	4	610	CLA	MG-ND	-4.11	1.97	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	842	CLA	MG-ND	-4.11	1.97	2.05
22	G	204	CLA	MG-ND	-4.11	1.97	2.05
22	B	836	CLA	MG-ND	-4.11	1.97	2.05
22	B2	815	CLA	MG-ND	-4.11	1.97	2.05
22	5	612	CLA	MG-ND	-4.10	1.97	2.05
22	A	838	CLA	MG-ND	-4.09	1.97	2.05
22	B2	811	CLA	MG-ND	-4.09	1.97	2.05
22	1	612	CLA	MG-ND	-4.09	1.97	2.05
22	8	608	CLA	MG-ND	-4.09	1.97	2.05
22	8	613	CLA	MG-ND	-4.08	1.97	2.05
22	8	616	CLA	MG-ND	-4.08	1.97	2.05
22	A	812	CLA	MG-ND	-4.07	1.97	2.05
22	A	835	CLA	MG-ND	-4.07	1.97	2.05
22	A	806	CLA	MG-ND	-4.07	1.97	2.05
22	A	809	CLA	MG-ND	-4.06	1.97	2.05
22	6	612	CLA	MG-ND	-4.06	1.97	2.05
22	9	603	CLA	MG-ND	-4.05	1.97	2.05
22	B	808	CLA	MG-ND	-4.05	1.97	2.05
22	B2	828	CLA	MG-ND	-4.05	1.97	2.05
22	B	805	CLA	MG-ND	-4.03	1.97	2.05
22	92	614	CLA	MG-ND	-4.02	1.97	2.05
22	6	614	CLA	MG-ND	-4.02	1.97	2.05
22	F	301	CLA	MG-ND	-4.01	1.97	2.05
22	B2	805	CLA	MG-ND	-4.01	1.97	2.05
21	A	801	CL0	MG-NC	-4.00	1.96	2.06
22	B2	808	CLA	MG-ND	-4.00	1.97	2.05
22	L	204	CLA	MG-ND	-3.99	1.97	2.05
22	5	603	CLA	MG-ND	-3.99	1.97	2.05
22	B	827	CLA	MG-ND	-3.97	1.97	2.05
22	B2	820	CLA	MG-ND	-3.96	1.97	2.05
22	Z	612	CLA	MG-ND	-3.93	1.98	2.05
22	B	840	CLA	MG-ND	-3.90	1.98	2.05
22	8	612	CLA	MG-ND	-3.88	1.98	2.05
22	B2	804	CLA	MG-ND	-3.87	1.98	2.05
22	B	802	CLA	MG-ND	-3.85	1.98	2.05
31	92	606	CHL	C3A-C2A	-3.76	1.51	1.54
31	92	607	CHL	C1D-ND	3.61	1.42	1.37
31	9	606	CHL	C3A-C2A	-3.59	1.51	1.54
31	8	607	CHL	C1D-ND	3.51	1.42	1.37
31	92	606	CHL	C1D-ND	3.49	1.42	1.37
31	6	618	CHL	C1D-ND	3.42	1.42	1.37
31	5	618	CHL	C1D-ND	3.42	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	4	618	CHL	C1D-ND	3.41	1.42	1.37
31	6	607	CHL	C1D-ND	3.40	1.42	1.37
31	5	606	CHL	C1D-ND	3.39	1.42	1.37
31	9	606	CHL	C1D-ND	3.37	1.41	1.37
31	9	607	CHL	C1D-ND	3.36	1.41	1.37
31	Z	606	CHL	C1D-ND	3.35	1.41	1.37
31	6	606	CHL	C1D-ND	3.35	1.41	1.37
31	4	606	CHL	C1D-ND	3.34	1.41	1.37
31	5	608	CHL	C1D-ND	3.31	1.41	1.37
31	6	608	CHL	C1D-ND	3.30	1.41	1.37
31	92	606	CHL	MG-NC	-3.26	1.98	2.06
31	8	601	CHL	C1D-ND	3.24	1.41	1.37
31	4	601	CHL	C1D-ND	3.23	1.41	1.37
31	8	606	CHL	C1D-ND	3.21	1.41	1.37
31	5	606	CHL	C3B-C2B	-3.21	1.35	1.40
31	6	601	CHL	MG-NC	-3.19	1.98	2.06
31	4	608	CHL	C1D-ND	3.19	1.41	1.37
31	5	607	CHL	MG-NC	-3.18	1.98	2.06
31	92	607	CHL	MG-NC	-3.17	1.98	2.06
31	1	601	CHL	C3B-C2B	-3.17	1.36	1.40
31	8	607	CHL	C3B-C2B	-3.17	1.36	1.40
31	1	606	CHL	C1D-ND	3.16	1.41	1.37
31	9	607	CHL	C3B-C2B	-3.14	1.36	1.40
31	Z	606	CHL	C3B-C2B	-3.14	1.36	1.40
31	6	601	CHL	C1D-ND	3.13	1.41	1.37
31	Z	607	CHL	C3B-C2B	-3.12	1.36	1.40
31	1	607	CHL	C3B-C2B	-3.12	1.36	1.40
31	1	607	CHL	MG-NC	-3.11	1.98	2.06
31	7	606	CHL	C1D-ND	3.11	1.41	1.37
31	5	607	CHL	C1D-ND	3.10	1.41	1.37
31	1	606	CHL	C3B-C2B	-3.10	1.36	1.40
31	7	607	CHL	C3B-C2B	-3.10	1.36	1.40
31	5	607	CHL	C3B-C2B	-3.10	1.36	1.40
31	6	608	CHL	MG-NC	-3.09	1.98	2.06
31	6	607	CHL	MG-NC	-3.08	1.98	2.06
31	3	608	CHL	C3B-C2B	-3.08	1.36	1.40
31	6	608	CHL	C3B-C2B	-3.08	1.36	1.40
31	6	616	CHL	C1D-ND	3.07	1.41	1.37
31	5	618	CHL	C3B-C2B	-3.07	1.36	1.40
31	4	618	CHL	C3B-C2B	-3.07	1.36	1.40
31	6	618	CHL	C3B-C2B	-3.06	1.36	1.40
31	6	606	CHL	C3B-C2B	-3.06	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	5	608	CHL	C3B-C2B	-3.05	1.36	1.40
31	6	607	CHL	C3B-C2B	-3.05	1.36	1.40
31	9	607	CHL	MG-NC	-3.05	1.99	2.06
31	4	607	CHL	C1D-ND	3.04	1.41	1.37
31	Z	607	CHL	C1D-ND	3.04	1.41	1.37
31	4	618	CHL	MG-NC	-3.04	1.99	2.06
31	92	607	CHL	C3B-C2B	-3.03	1.36	1.40
31	9	606	CHL	C3B-C2B	-3.03	1.36	1.40
31	4	607	CHL	C3B-C2B	-3.02	1.36	1.40
31	7	607	CHL	C1D-ND	3.02	1.41	1.37
31	7	606	CHL	MG-NC	-3.01	1.99	2.06
31	6	616	CHL	C3B-C2B	-3.01	1.36	1.40
31	8	601	CHL	C3B-C2B	-3.00	1.36	1.40
31	1	601	CHL	C1D-ND	3.00	1.41	1.37
31	8	606	CHL	C3B-C2B	-3.00	1.36	1.40
31	5	608	CHL	MG-NC	-3.00	1.99	2.06
31	Z	601	CHL	MG-NC	-2.99	1.99	2.06
31	7	601	CHL	C1D-ND	2.99	1.41	1.37
31	4	608	CHL	C3B-C2B	-2.97	1.36	1.40
31	4	606	CHL	C3B-C2B	-2.97	1.36	1.40
31	5	618	CHL	MG-NC	-2.96	1.99	2.06
31	4	606	CHL	MG-NC	-2.96	1.99	2.06
31	7	601	CHL	C3B-C2B	-2.95	1.36	1.40
31	Z	601	CHL	C3B-C2B	-2.95	1.36	1.40
31	7	601	CHL	MG-NC	-2.95	1.99	2.06
31	7	606	CHL	C3B-C2B	-2.95	1.36	1.40
31	8	606	CHL	MG-NC	-2.93	1.99	2.06
31	4	601	CHL	C3B-C2B	-2.93	1.36	1.40
31	1	601	CHL	MG-NC	-2.91	1.99	2.06
31	1	606	CHL	MG-NC	-2.90	1.99	2.06
25	B2	843	BCR	C17-C18	2.90	1.36	1.33
31	5	607	CHL	C1B-NB	2.89	1.37	1.35
31	9	606	CHL	MG-NC	-2.89	1.99	2.06
31	92	606	CHL	C3B-C2B	-2.88	1.36	1.40
31	6	618	CHL	MG-NC	-2.87	1.99	2.06
31	4	608	CHL	MG-NC	-2.87	1.99	2.06
31	3	608	CHL	C1D-ND	2.87	1.41	1.37
31	6	606	CHL	MG-NC	-2.85	1.99	2.06
31	7	607	CHL	MG-NC	-2.85	1.99	2.06
31	1	607	CHL	C1D-ND	2.85	1.41	1.37
31	6	601	CHL	C3B-C2B	-2.85	1.36	1.40
31	8	607	CHL	MG-NC	-2.84	1.99	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	4	601	CHL	MG-NC	-2.83	1.99	2.06
31	8	601	CHL	MG-NC	-2.83	1.99	2.06
31	6	616	CHL	MG-NC	-2.83	1.99	2.06
31	Z	601	CHL	C1D-ND	2.82	1.41	1.37
31	Z	607	CHL	MG-NC	-2.82	1.99	2.06
31	Z	606	CHL	MG-NC	-2.81	1.99	2.06
31	4	607	CHL	MG-NC	-2.81	1.99	2.06
31	4	608	CHL	C1B-NB	2.80	1.37	1.35
31	5	606	CHL	MG-NC	-2.80	1.99	2.06
31	3	608	CHL	MG-NC	-2.79	1.99	2.06
31	9	606	CHL	C1B-NB	2.76	1.37	1.35
31	92	607	CHL	C1B-NB	2.73	1.37	1.35
33	5	625	NEX	C1-C6	-2.70	1.50	1.54
31	4	607	CHL	C1B-NB	2.68	1.37	1.35
31	4	618	CHL	C1B-NB	2.66	1.37	1.35
31	6	601	CHL	C1B-NB	2.59	1.37	1.35
31	9	607	CHL	C1B-NB	2.58	1.37	1.35
31	6	608	CHL	C1B-NB	2.57	1.37	1.35
22	B	803	CLA	C1D-C2D	-2.57	1.40	1.45
22	B	806	CLA	C1D-C2D	-2.57	1.40	1.45
22	B	802	CLA	C1D-C2D	-2.57	1.40	1.45
22	A	829	CLA	C1D-C2D	-2.55	1.40	1.45
22	A	828	CLA	C1D-C2D	-2.54	1.40	1.45
22	B	809	CLA	C1D-C2D	-2.53	1.40	1.45
22	A	807	CLA	C1D-C2D	-2.52	1.40	1.45
22	A	819	CLA	C1D-C2D	-2.52	1.40	1.45
22	B	808	CLA	C1D-C2D	-2.52	1.40	1.45
22	K	201	CLA	C1D-C2D	-2.51	1.40	1.45
22	7	612	CLA	C1D-C2D	-2.51	1.40	1.45
31	6	618	CHL	C1B-NB	2.51	1.37	1.35
22	A	805	CLA	C1D-C2D	-2.51	1.40	1.45
31	Z	601	CHL	C1B-NB	2.51	1.37	1.35
22	A	854	CLA	C1D-C2D	-2.50	1.40	1.45
31	5	618	CHL	C1B-NB	2.50	1.37	1.35
22	3	603	CLA	C1D-C2D	-2.50	1.40	1.45
22	8	610	CLA	C1D-C2D	-2.49	1.40	1.45
22	8	608	CLA	C1D-C2D	-2.49	1.40	1.45
22	B	816	CLA	C1D-C2D	-2.49	1.40	1.45
31	Z	606	CHL	C1B-NB	2.48	1.37	1.35
22	A	802	CLA	C1D-C2D	-2.48	1.40	1.45
22	A	842	CLA	C1D-C2D	-2.48	1.40	1.45
22	B	825	CLA	C1D-C2D	-2.47	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	1	611	CLA	C1D-C2D	-2.47	1.40	1.45
22	A	830	CLA	C1D-C2D	-2.47	1.40	1.45
22	A	808	CLA	C1D-C2D	-2.47	1.40	1.45
22	A	814	CLA	C1D-C2D	-2.46	1.40	1.45
22	4	602	CLA	C1D-C2D	-2.46	1.40	1.45
31	8	607	CHL	C1D-C2D	-2.46	1.40	1.45
22	B	820	CLA	C1D-C2D	-2.46	1.40	1.45
22	B	827	CLA	C1D-C2D	-2.46	1.40	1.45
22	B	838	CLA	C1D-C2D	-2.46	1.40	1.45
22	A	821	CLA	C1D-C2D	-2.46	1.40	1.45
22	F	301	CLA	C1D-C2D	-2.46	1.40	1.45
22	9	603	CLA	C1D-C2D	-2.46	1.40	1.45
22	A	813	CLA	C1D-C2D	-2.46	1.40	1.45
22	5	617	CLA	C1D-C2D	-2.46	1.40	1.45
22	B	821	CLA	C1D-C2D	-2.46	1.40	1.45
22	B	829	CLA	C1D-C2D	-2.46	1.40	1.45
22	J	101	CLA	C1D-C2D	-2.45	1.40	1.45
22	A	812	CLA	C1D-C2D	-2.45	1.40	1.45
22	A	826	CLA	C1D-C2D	-2.45	1.40	1.45
22	B	813	CLA	C1D-C2D	-2.45	1.40	1.45
31	5	606	CHL	C1B-NB	2.45	1.37	1.35
22	B	824	CLA	C1D-C2D	-2.45	1.40	1.45
22	3	606	CLA	C1D-C2D	-2.45	1.40	1.45
22	B	835	CLA	C1D-C2D	-2.45	1.40	1.45
22	5	621	CLA	C1D-C2D	-2.44	1.40	1.45
22	A	815	CLA	C1D-C2D	-2.44	1.40	1.45
22	A	817	CLA	C1D-C2D	-2.44	1.40	1.45
22	A	810	CLA	C1D-C2D	-2.44	1.40	1.45
22	8	612	CLA	C1D-C2D	-2.44	1.40	1.45
22	3	615	CLA	C1D-C2D	-2.44	1.40	1.45
22	7	614	CLA	C1D-C2D	-2.44	1.40	1.45
22	5	601	CLA	C1D-C2D	-2.44	1.40	1.45
22	B	810	CLA	C1D-C2D	-2.44	1.40	1.45
31	1	607	CHL	C1B-NB	2.44	1.37	1.35
22	8	613	CLA	C1D-C2D	-2.44	1.40	1.45
22	3	617	CLA	C1D-C2D	-2.44	1.40	1.45
22	5	612	CLA	C1D-C2D	-2.43	1.40	1.45
22	B	840	CLA	C1D-C2D	-2.43	1.40	1.45
22	1	612	CLA	C1D-C2D	-2.43	1.40	1.45
22	A	822	CLA	C1D-C2D	-2.43	1.40	1.45
22	G	203	CLA	C1D-C2D	-2.43	1.40	1.45
22	92	609	CLA	C1D-C2D	-2.43	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	807	CLA	C1D-C2D	-2.43	1.40	1.45
22	9	612	CLA	C1D-C2D	-2.43	1.40	1.45
22	B	815	CLA	C1D-C2D	-2.42	1.40	1.45
31	92	606	CHL	C1B-NB	2.42	1.37	1.35
22	B	804	CLA	C1D-C2D	-2.42	1.40	1.45
22	A	818	CLA	C1D-C2D	-2.42	1.40	1.45
22	F	304	CLA	C1D-C2D	-2.42	1.40	1.45
22	B	837	CLA	C1D-C2D	-2.42	1.40	1.45
22	A	827	CLA	C1D-C2D	-2.42	1.40	1.45
22	4	613	CLA	C1D-C2D	-2.42	1.40	1.45
22	1	616	CLA	C1D-C2D	-2.42	1.40	1.45
31	6	616	CHL	C1B-NB	2.42	1.37	1.35
22	Z	612	CLA	C1D-C2D	-2.42	1.40	1.45
22	Z	609	CLA	C1D-C2D	-2.42	1.40	1.45
22	A	834	CLA	C1D-C2D	-2.42	1.40	1.45
22	4	603	CLA	C1D-C2D	-2.42	1.40	1.45
22	F	303	CLA	C1D-C2D	-2.42	1.40	1.45
22	7	602	CLA	C1D-C2D	-2.42	1.40	1.45
22	A	839	CLA	C1D-C2D	-2.41	1.40	1.45
22	A	838	CLA	C1D-C2D	-2.41	1.40	1.45
22	8	602	CLA	C1D-C2D	-2.41	1.40	1.45
22	5	613	CLA	C1D-C2D	-2.41	1.40	1.45
22	B	826	CLA	C1D-C2D	-2.41	1.40	1.45
22	6	603	CLA	C1D-C2D	-2.41	1.40	1.45
22	7	608	CLA	C1D-C2D	-2.41	1.40	1.45
22	A	845	CLA	C1D-C2D	-2.41	1.40	1.45
21	A	801	CL0	C1D-C2D	-2.41	1.40	1.45
22	A	832	CLA	C1D-C2D	-2.41	1.40	1.45
22	6	610	CLA	C1D-C2D	-2.41	1.40	1.45
22	B	841	CLA	C1D-C2D	-2.40	1.40	1.45
22	B	812	CLA	C1D-C2D	-2.40	1.40	1.45
22	6	611	CLA	C1D-C2D	-2.40	1.40	1.45
22	B	805	CLA	C1D-C2D	-2.40	1.40	1.45
22	A	806	CLA	C1D-C2D	-2.40	1.40	1.45
22	B	836	CLA	C1D-C2D	-2.40	1.40	1.45
31	8	601	CHL	C1D-C2D	-2.40	1.40	1.45
22	Z	610	CLA	C1D-C2D	-2.40	1.40	1.45
22	1	609	CLA	C1D-C2D	-2.40	1.40	1.45
22	92	603	CLA	C1D-C2D	-2.40	1.40	1.45
22	4	614	CLA	C1D-C2D	-2.39	1.40	1.45
22	6	609	CLA	C1D-C2D	-2.39	1.40	1.45
22	A	816	CLA	C1D-C2D	-2.39	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	7	613	CLA	C1D-C2D	-2.39	1.40	1.45
22	6	604	CLA	C1D-C2D	-2.39	1.40	1.45
22	3	604	CLA	C1D-C2D	-2.39	1.40	1.45
22	4	612	CLA	C1D-C2D	-2.39	1.40	1.45
22	9	611	CLA	C1D-C2D	-2.39	1.40	1.45
22	9	602	CLA	C1D-C2D	-2.39	1.40	1.45
22	5	616	CLA	C1D-C2D	-2.39	1.40	1.45
31	6	607	CHL	C1D-C2D	-2.39	1.40	1.45
31	4	601	CHL	C1B-NB	2.39	1.37	1.35
22	5	609	CLA	C1D-C2D	-2.39	1.40	1.45
22	9	604	CLA	C1D-C2D	-2.39	1.40	1.45
22	8	609	CLA	C1D-C2D	-2.39	1.40	1.45
22	A	837	CLA	C1D-C2D	-2.39	1.40	1.45
22	B	832	CLA	C1D-C2D	-2.39	1.40	1.45
22	8	603	CLA	C1D-C2D	-2.39	1.40	1.45
22	A	833	CLA	C1D-C2D	-2.39	1.40	1.45
22	5	602	CLA	C1D-C2D	-2.38	1.40	1.45
22	A	803	CLA	C1D-C2D	-2.38	1.40	1.45
22	B	831	CLA	C1D-C2D	-2.38	1.40	1.45
22	3	612	CLA	C1D-C2D	-2.38	1.40	1.45
22	B	811	CLA	C1D-C2D	-2.38	1.40	1.45
22	7	620	CLA	C1D-C2D	-2.38	1.40	1.45
22	A	820	CLA	C1D-C2D	-2.38	1.40	1.45
22	B	830	CLA	C1D-C2D	-2.38	1.40	1.45
22	8	616	CLA	C1D-C2D	-2.38	1.40	1.45
22	3	613	CLA	C1D-C2D	-2.38	1.40	1.45
22	Z	616	CLA	C1D-C2D	-2.38	1.40	1.45
22	A	825	CLA	C1D-C2D	-2.38	1.40	1.45
22	3	602	CLA	C1D-C2D	-2.38	1.40	1.45
22	5	611	CLA	C1D-C2D	-2.38	1.40	1.45
22	8	611	CLA	C1D-C2D	-2.38	1.40	1.45
22	6	612	CLA	C1D-C2D	-2.38	1.40	1.45
22	B	834	CLA	C1D-C2D	-2.38	1.40	1.45
22	7	609	CLA	C1D-C2D	-2.38	1.40	1.45
22	1	602	CLA	C1D-C2D	-2.38	1.40	1.45
22	1	614	CLA	C1D-C2D	-2.37	1.40	1.45
22	Z	611	CLA	C1D-C2D	-2.37	1.40	1.45
22	B	818	CLA	C1D-C2D	-2.37	1.40	1.45
22	5	614	CLA	C1D-C2D	-2.37	1.40	1.45
22	B	823	CLA	C1D-C2D	-2.37	1.40	1.45
22	9	613	CLA	C1D-C2D	-2.37	1.40	1.45
22	A	836	CLA	C1D-C2D	-2.37	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	7	601	CHL	C1D-C2D	-2.37	1.40	1.45
22	6	602	CLA	C1D-C2D	-2.37	1.40	1.45
22	1	603	CLA	C1D-C2D	-2.37	1.40	1.45
22	9	609	CLA	C1D-C2D	-2.37	1.40	1.45
22	6	613	CLA	C1D-C2D	-2.36	1.40	1.45
22	A	843	CLA	C1D-C2D	-2.36	1.40	1.45
22	B	833	CLA	C1D-C2D	-2.36	1.40	1.45
22	K	206	CLA	C1D-C2D	-2.36	1.40	1.45
22	A	840	CLA	C1D-C2D	-2.36	1.40	1.45
22	Z	603	CLA	C1D-C2D	-2.36	1.40	1.45
22	92	612	CLA	C1D-C2D	-2.36	1.40	1.45
22	7	611	CLA	C1D-C2D	-2.36	1.40	1.45
22	92	611	CLA	C1D-C2D	-2.36	1.40	1.45
31	7	606	CHL	C1D-C2D	-2.36	1.40	1.45
22	4	610	CLA	C1D-C2D	-2.36	1.40	1.45
22	8	614	CLA	C1D-C2D	-2.36	1.40	1.45
22	6	622	CLA	C1D-C2D	-2.36	1.40	1.45
22	B2	820	CLA	C1D-C2D	-2.36	1.40	1.45
22	B	828	CLA	C1D-C2D	-2.36	1.40	1.45
31	5	607	CHL	C1D-C2D	-2.36	1.40	1.45
22	K	203	CLA	C1D-C2D	-2.36	1.40	1.45
22	1	610	CLA	C1D-C2D	-2.35	1.40	1.45
22	3	611	CLA	C1D-C2D	-2.35	1.40	1.45
22	3	609	CLA	C1D-C2D	-2.35	1.40	1.45
22	3	610	CLA	C1D-C2D	-2.35	1.40	1.45
31	Z	601	CHL	C1D-C2D	-2.35	1.40	1.45
22	7	616	CLA	C1D-C2D	-2.35	1.40	1.45
22	9	614	CLA	C1D-C2D	-2.35	1.40	1.45
22	4	609	CLA	C1D-C2D	-2.35	1.40	1.45
31	4	601	CHL	C1D-C2D	-2.35	1.40	1.45
22	5	604	CLA	C1D-C2D	-2.35	1.40	1.45
31	Z	607	CHL	C1B-NB	2.35	1.37	1.35
22	B	819	CLA	C1D-C2D	-2.35	1.40	1.45
22	A	835	CLA	C1D-C2D	-2.35	1.40	1.45
22	G	204	CLA	C1D-C2D	-2.35	1.40	1.45
22	5	610	CLA	C1D-C2D	-2.35	1.40	1.45
31	1	606	CHL	C1D-C2D	-2.35	1.40	1.45
22	92	601	CLA	C1D-C2D	-2.35	1.40	1.45
31	7	607	CHL	C1D-C2D	-2.34	1.40	1.45
22	B	839	CLA	C1D-C2D	-2.34	1.40	1.45
22	A	809	CLA	C1D-C2D	-2.34	1.40	1.45
22	92	602	CLA	C1D-C2D	-2.34	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B2	808	CLA	C1D-C2D	-2.34	1.40	1.45
22	92	613	CLA	C1D-C2D	-2.34	1.40	1.45
22	A	831	CLA	C1D-C2D	-2.34	1.40	1.45
22	4	604	CLA	C1D-C2D	-2.34	1.40	1.45
22	7	603	CLA	C1D-C2D	-2.34	1.40	1.45
22	A	824	CLA	C1D-C2D	-2.34	1.40	1.45
31	6	607	CHL	C1B-NB	2.34	1.37	1.35
22	K	204	CLA	C1D-C2D	-2.34	1.40	1.45
22	B	814	CLA	C1D-C2D	-2.34	1.40	1.45
22	L	203	CLA	C1D-C2D	-2.34	1.40	1.45
22	4	611	CLA	C1D-C2D	-2.34	1.40	1.45
22	B2	807	CLA	C1D-C2D	-2.34	1.40	1.45
22	6	614	CLA	C1D-C2D	-2.34	1.40	1.45
22	1	613	CLA	C1D-C2D	-2.33	1.40	1.45
22	B2	813	CLA	C1D-C2D	-2.33	1.40	1.45
31	6	618	CHL	C1D-C2D	-2.33	1.40	1.45
22	7	610	CLA	C1D-C2D	-2.33	1.40	1.45
31	6	601	CHL	C1D-C2D	-2.33	1.40	1.45
22	92	610	CLA	C1D-C2D	-2.33	1.40	1.45
22	1	608	CLA	C1D-C2D	-2.33	1.40	1.45
22	B2	806	CLA	C1D-C2D	-2.33	1.40	1.45
22	B2	810	CLA	C1D-C2D	-2.33	1.40	1.45
22	Z	608	CLA	C1D-C2D	-2.33	1.40	1.45
22	8	604	CLA	C1D-C2D	-2.33	1.40	1.45
22	4	616	CLA	C1D-C2D	-2.33	1.40	1.45
22	A	811	CLA	C1D-C2D	-2.33	1.40	1.45
22	7	604	CLA	C1D-C2D	-2.33	1.40	1.45
22	Z	604	CLA	C1D-C2D	-2.33	1.40	1.45
22	B	817	CLA	C1D-C2D	-2.33	1.40	1.45
31	4	608	CHL	C1D-C2D	-2.33	1.40	1.45
31	6	616	CHL	C1D-C2D	-2.33	1.40	1.45
22	A	804	CLA	C1D-C2D	-2.32	1.40	1.45
22	B2	811	CLA	CAB-C3B	-2.32	1.46	1.51
22	A	823	CLA	C1D-C2D	-2.32	1.40	1.45
22	3	614	CLA	C1D-C2D	-2.32	1.40	1.45
22	6	617	CLA	C1D-C2D	-2.32	1.40	1.45
22	B2	812	CLA	C1D-C2D	-2.32	1.40	1.45
22	3	607	CLA	C1D-C2D	-2.31	1.40	1.45
22	Z	602	CLA	C1D-C2D	-2.31	1.40	1.45
22	92	604	CLA	C1D-C2D	-2.31	1.40	1.45
22	9	601	CLA	C1D-C2D	-2.31	1.40	1.45
31	5	608	CHL	C1D-C2D	-2.31	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	841	CLA	C1D-C2D	-2.31	1.40	1.45
22	B2	811	CLA	C1D-C2D	-2.31	1.40	1.45
31	Z	607	CHL	C1D-C2D	-2.31	1.40	1.45
31	9	607	CHL	C1D-C2D	-2.30	1.40	1.45
22	B2	805	CLA	C1D-C2D	-2.30	1.40	1.45
22	B	822	CLA	C1D-C2D	-2.30	1.40	1.45
31	1	601	CHL	C1D-C2D	-2.30	1.40	1.45
31	6	606	CHL	C1D-C2D	-2.30	1.40	1.45
31	92	607	CHL	C1D-C2D	-2.30	1.40	1.45
22	B2	804	CLA	C1D-C2D	-2.29	1.40	1.45
31	5	618	CHL	C1D-C2D	-2.29	1.40	1.45
22	Z	614	CLA	C1D-C2D	-2.29	1.40	1.45
22	B2	839	CLA	C1D-C2D	-2.29	1.40	1.45
22	B2	828	CLA	C1D-C2D	-2.29	1.40	1.45
22	B2	814	CLA	C1D-C2D	-2.29	1.40	1.45
22	92	614	CLA	C1D-C2D	-2.29	1.40	1.45
31	3	608	CHL	C1D-C2D	-2.29	1.40	1.45
22	Z	613	CLA	C1D-C2D	-2.29	1.40	1.45
22	B2	809	CLA	C1D-C2D	-2.29	1.40	1.45
31	1	607	CHL	C1D-C2D	-2.29	1.40	1.45
31	Z	606	CHL	C1D-C2D	-2.28	1.40	1.45
31	4	606	CHL	C1D-C2D	-2.28	1.40	1.45
31	92	606	CHL	C1D-C2D	-2.27	1.40	1.45
22	L2	203	CLA	C1D-C2D	-2.27	1.40	1.45
31	9	606	CHL	C1D-C2D	-2.27	1.40	1.45
22	5	603	CLA	C1D-C2D	-2.27	1.40	1.45
31	5	606	CHL	C1D-C2D	-2.27	1.40	1.45
22	B2	829	CLA	C1D-C2D	-2.27	1.40	1.45
31	6	606	CHL	C1B-NB	2.26	1.37	1.35
31	6	608	CHL	C1D-C2D	-2.26	1.40	1.45
22	L2	204	CLA	C1D-C2D	-2.26	1.40	1.45
22	L	204	CLA	C1D-C2D	-2.26	1.40	1.45
22	9	610	CLA	C1D-C2D	-2.26	1.40	1.45
22	B2	815	CLA	C1D-C2D	-2.26	1.40	1.45
31	4	607	CHL	C1D-C2D	-2.26	1.40	1.45
31	4	618	CHL	C1D-C2D	-2.25	1.40	1.45
22	1	604	CLA	C1D-C2D	-2.25	1.40	1.45
31	8	606	CHL	C1D-C2D	-2.25	1.40	1.45
31	7	606	CHL	C1B-NB	2.23	1.37	1.35
31	3	608	CHL	C1B-NB	2.23	1.37	1.35
31	8	606	CHL	C1B-NB	2.22	1.37	1.35
31	5	608	CHL	C1B-NB	2.21	1.37	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	8	601	CHL	C1B-NB	2.20	1.37	1.35
31	1	606	CHL	C1B-NB	2.20	1.37	1.35
31	7	601	CHL	C1B-NB	2.19	1.37	1.35
31	8	607	CHL	C2C-C1C	2.19	1.49	1.44
31	1	601	CHL	C1B-NB	2.19	1.37	1.35
31	1	606	CHL	C2C-C1C	2.19	1.49	1.44
31	6	616	CHL	C2C-C1C	2.19	1.49	1.44
31	5	607	CHL	C3D-C4D	-2.18	1.39	1.44
31	6	607	CHL	C2C-C1C	2.17	1.49	1.44
31	3	608	CHL	C3D-C4D	-2.16	1.39	1.44
22	B	823	CLA	C3D-C4D	-2.16	1.39	1.44
31	6	616	CHL	C3D-C4D	-2.15	1.39	1.44
31	4	606	CHL	C1B-NB	2.15	1.37	1.35
22	B	840	CLA	C3D-C4D	-2.15	1.39	1.44
22	A	827	CLA	C3D-C4D	-2.14	1.39	1.44
31	7	601	CHL	C3D-C4D	-2.14	1.39	1.44
31	8	606	CHL	C3D-C4D	-2.14	1.39	1.44
31	7	601	CHL	C2C-C1C	2.12	1.49	1.44
31	9	606	CHL	C2C-C1C	2.12	1.49	1.44
31	1	607	CHL	C3D-C4D	-2.12	1.39	1.44
21	A	801	CL0	C3D-C4D	-2.12	1.39	1.44
22	A	806	CLA	C3D-C4D	-2.12	1.39	1.44
31	6	608	CHL	C3D-C4D	-2.11	1.39	1.44
31	4	608	CHL	C3D-C4D	-2.11	1.39	1.44
31	5	608	CHL	C3D-C4D	-2.11	1.39	1.44
31	Z	606	CHL	C2C-C1C	2.11	1.49	1.44
31	8	601	CHL	C3D-C4D	-2.11	1.39	1.44
31	9	607	CHL	C3D-C4D	-2.10	1.39	1.44
22	B	825	CLA	C3D-C4D	-2.10	1.39	1.44
21	A	801	CL0	C1C-C2C	2.10	1.48	1.44
22	3	602	CLA	C3D-C4D	-2.10	1.39	1.44
31	1	601	CHL	C3D-C4D	-2.10	1.39	1.44
22	1	602	CLA	C3D-C4D	-2.10	1.39	1.44
22	B	818	CLA	C3D-C4D	-2.10	1.39	1.44
22	B	808	CLA	C3D-C4D	-2.10	1.39	1.44
31	6	601	CHL	C2C-C1C	2.10	1.49	1.44
22	A	807	CLA	C3D-C4D	-2.10	1.39	1.44
22	A	842	CLA	C3D-C4D	-2.10	1.39	1.44
22	B	831	CLA	C3D-C4D	-2.10	1.39	1.44
31	7	606	CHL	C3D-C4D	-2.10	1.39	1.44
22	A	820	CLA	C3D-C4D	-2.09	1.39	1.44
31	7	607	CHL	C3D-C4D	-2.09	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	Z	613	CLA	C3D-C4D	-2.09	1.39	1.44
22	A	808	CLA	C3D-C4D	-2.09	1.39	1.44
22	A	823	CLA	C3D-C4D	-2.09	1.39	1.44
22	1	613	CLA	C3D-C4D	-2.09	1.39	1.44
22	8	602	CLA	C3D-C4D	-2.09	1.39	1.44
22	B	837	CLA	C3D-C4D	-2.09	1.39	1.44
31	Z	601	CHL	C4B-CHC	-2.08	1.35	1.41
22	B	830	CLA	C3D-C4D	-2.08	1.39	1.44
22	3	610	CLA	C3D-C4D	-2.08	1.39	1.44
31	92	606	CHL	C2C-C1C	2.08	1.49	1.44
31	4	607	CHL	C3D-C4D	-2.08	1.39	1.44
31	8	607	CHL	C3D-C4D	-2.08	1.39	1.44
22	1	610	CLA	C3D-C4D	-2.08	1.39	1.44
22	A	832	CLA	C3D-C4D	-2.08	1.39	1.44
22	A	834	CLA	C3D-C4D	-2.08	1.39	1.44
22	A	803	CLA	C3D-C4D	-2.08	1.39	1.44
22	A	825	CLA	C3D-C4D	-2.08	1.39	1.44
22	B	806	CLA	C3D-C4D	-2.08	1.39	1.44
22	B	802	CLA	C3D-C4D	-2.08	1.39	1.44
22	B	819	CLA	C3D-C4D	-2.08	1.39	1.44
22	B	810	CLA	C3D-C4D	-2.07	1.39	1.44
31	4	606	CHL	C3D-C4D	-2.07	1.39	1.44
22	A	821	CLA	C3D-C4D	-2.07	1.39	1.44
31	Z	607	CHL	C3D-C4D	-2.07	1.39	1.44
22	9	603	CLA	C3D-C4D	-2.07	1.39	1.44
22	92	602	CLA	C3D-C4D	-2.07	1.39	1.44
31	5	618	CHL	C3D-C4D	-2.07	1.39	1.44
31	4	618	CHL	C2C-C1C	2.07	1.49	1.44
22	B	814	CLA	C3D-C4D	-2.07	1.39	1.44
31	6	618	CHL	C2C-C1C	2.07	1.49	1.44
22	A	822	CLA	C3D-C4D	-2.07	1.39	1.44
22	A	841	CLA	C3D-C4D	-2.07	1.39	1.44
22	A	818	CLA	C3D-C4D	-2.07	1.39	1.44
31	6	606	CHL	C3D-C4D	-2.07	1.39	1.44
22	7	616	CLA	C3D-C4D	-2.07	1.39	1.44
22	B	821	CLA	C3D-C4D	-2.07	1.39	1.44
31	5	606	CHL	C3D-C4D	-2.07	1.39	1.44
22	8	616	CLA	C3D-C4D	-2.07	1.39	1.44
31	Z	606	CHL	C3D-C4D	-2.07	1.39	1.44
22	A	809	CLA	C3D-C4D	-2.06	1.39	1.44
22	B	829	CLA	C3D-C4D	-2.06	1.39	1.44
31	4	601	CHL	C3D-C4D	-2.06	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	807	CLA	C3D-C4D	-2.06	1.39	1.44
22	B	817	CLA	C3D-C4D	-2.06	1.39	1.44
22	A	813	CLA	C3D-C4D	-2.06	1.39	1.44
31	Z	601	CHL	C3D-C4D	-2.06	1.39	1.44
22	4	603	CLA	C3D-C4D	-2.06	1.39	1.44
22	9	610	CLA	C3D-C4D	-2.06	1.39	1.44
22	A	836	CLA	C3D-C4D	-2.06	1.39	1.44
31	9	606	CHL	C3D-C4D	-2.06	1.39	1.44
22	A	843	CLA	C3D-C4D	-2.05	1.39	1.44
22	7	603	CLA	C3D-C4D	-2.05	1.39	1.44
22	9	604	CLA	C3D-C4D	-2.05	1.39	1.44
22	92	610	CLA	C3D-C4D	-2.05	1.39	1.44
31	1	606	CHL	C3D-C4D	-2.05	1.39	1.44
22	B	833	CLA	C3D-C4D	-2.05	1.39	1.44
31	5	618	CHL	C2C-C1C	2.05	1.49	1.44
22	A	811	CLA	C3D-C4D	-2.05	1.39	1.44
31	6	601	CHL	C3D-C4D	-2.05	1.39	1.44
22	5	616	CLA	C3D-C4D	-2.05	1.39	1.44
31	7	607	CHL	C1B-NB	2.05	1.37	1.35
22	A	804	CLA	C3D-C4D	-2.05	1.39	1.44
22	L	203	CLA	C3D-C4D	-2.05	1.39	1.44
22	1	608	CLA	C3D-C4D	-2.05	1.39	1.44
22	A	802	CLA	C3D-C4D	-2.05	1.39	1.44
22	B	826	CLA	C3D-C4D	-2.05	1.39	1.44
31	6	607	CHL	C3D-C4D	-2.05	1.39	1.44
22	3	612	CLA	C3D-C4D	-2.04	1.39	1.44
31	8	607	CHL	C1B-NB	2.04	1.37	1.35
31	5	606	CHL	C2C-C1C	2.04	1.48	1.44
22	B	828	CLA	C3D-C4D	-2.04	1.39	1.44
22	5	609	CLA	C3D-C4D	-2.04	1.39	1.44
22	B	813	CLA	C3D-C4D	-2.04	1.39	1.44
22	1	614	CLA	C3D-C4D	-2.04	1.39	1.44
22	7	602	CLA	C3D-C4D	-2.04	1.39	1.44
22	3	604	CLA	C3D-C4D	-2.04	1.39	1.44
22	A	833	CLA	C3D-C4D	-2.04	1.39	1.44
22	8	603	CLA	C3D-C4D	-2.04	1.39	1.44
22	A	839	CLA	C3D-C4D	-2.03	1.39	1.44
31	7	606	CHL	C2C-C1C	2.03	1.48	1.44
22	3	609	CLA	C3D-C4D	-2.03	1.39	1.44
22	3	611	CLA	C3D-C4D	-2.03	1.39	1.44
22	A	828	CLA	C3D-C4D	-2.03	1.39	1.44
22	K	204	CLA	C3D-C4D	-2.03	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	831	CLA	C3D-C4D	-2.03	1.39	1.44
22	B	812	CLA	C3D-C4D	-2.03	1.39	1.44
22	6	610	CLA	C3D-C4D	-2.03	1.39	1.44
22	A	805	CLA	C3D-C4D	-2.03	1.39	1.44
22	3	607	CLA	C3D-C4D	-2.03	1.39	1.44
31	92	607	CHL	C3D-C4D	-2.03	1.39	1.44
22	Z	608	CLA	C3D-C4D	-2.03	1.39	1.44
22	5	611	CLA	C3D-C4D	-2.03	1.39	1.44
22	A	854	CLA	C3D-C4D	-2.03	1.39	1.44
22	B	816	CLA	C3D-C4D	-2.03	1.39	1.44
22	B	841	CLA	C3D-C4D	-2.03	1.39	1.44
22	8	612	CLA	C3D-C4D	-2.03	1.39	1.44
22	7	609	CLA	C3D-C4D	-2.03	1.39	1.44
31	4	618	CHL	C3D-C4D	-2.03	1.39	1.44
22	7	610	CLA	C3D-C4D	-2.03	1.39	1.44
31	4	608	CHL	C2C-C1C	2.03	1.48	1.44
22	9	613	CLA	C3D-C4D	-2.02	1.39	1.44
22	5	613	CLA	C3D-C4D	-2.02	1.39	1.44
22	6	614	CLA	C3D-C4D	-2.02	1.39	1.44
22	9	611	CLA	C3D-C4D	-2.02	1.39	1.44
31	5	608	CHL	C2C-C1C	2.02	1.48	1.44
22	A	814	CLA	C3D-C4D	-2.02	1.39	1.44
22	B	839	CLA	C3D-C4D	-2.02	1.39	1.44
22	8	609	CLA	C3D-C4D	-2.02	1.39	1.44
22	F	303	CLA	C3D-C4D	-2.02	1.39	1.44
22	1	603	CLA	C3D-C4D	-2.02	1.39	1.44
22	6	603	CLA	C3D-C4D	-2.02	1.39	1.44
31	4	601	CHL	C2C-C1C	2.02	1.48	1.44
22	7	613	CLA	C3D-C4D	-2.02	1.39	1.44
22	8	611	CLA	C3D-C4D	-2.02	1.39	1.44
22	B	822	CLA	C3D-C4D	-2.02	1.39	1.44
22	8	608	CLA	C3D-C4D	-2.02	1.39	1.44
31	92	606	CHL	C3D-C4D	-2.02	1.39	1.44
22	A	830	CLA	C3D-C4D	-2.02	1.39	1.44
22	A	812	CLA	C3D-C4D	-2.02	1.39	1.44
22	Z	610	CLA	C3D-C4D	-2.02	1.39	1.44
22	3	614	CLA	C3D-C4D	-2.01	1.39	1.44
22	B	832	CLA	C3D-C4D	-2.01	1.39	1.44
22	1	611	CLA	C3D-C4D	-2.01	1.39	1.44
22	7	604	CLA	C3D-C4D	-2.01	1.39	1.44
22	5	603	CLA	C3D-C4D	-2.01	1.39	1.44
22	B	820	CLA	C3D-C4D	-2.01	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	6	609	CLA	C3D-C4D	-2.01	1.39	1.44
22	1	609	CLA	C3D-C4D	-2.01	1.39	1.44
22	3	606	CLA	C3D-C4D	-2.01	1.39	1.44
22	Z	602	CLA	C3D-C4D	-2.01	1.39	1.44
22	3	613	CLA	C3D-C4D	-2.01	1.39	1.44
22	6	602	CLA	C3D-C4D	-2.01	1.39	1.44
22	7	611	CLA	C3D-C4D	-2.01	1.39	1.44
22	A	824	CLA	C3D-C4D	-2.01	1.39	1.44
22	7	614	CLA	C3D-C4D	-2.01	1.39	1.44
22	Z	604	CLA	C3D-C4D	-2.01	1.39	1.44
22	7	612	CLA	C3D-C4D	-2.00	1.39	1.44
22	8	604	CLA	C3D-C4D	-2.00	1.39	1.44
22	4	604	CLA	C3D-C4D	-2.00	1.39	1.44
22	8	613	CLA	C3D-C4D	-2.00	1.39	1.44
22	4	602	CLA	C3D-C4D	-2.00	1.39	1.44
22	B	811	CLA	C3D-C4D	-2.00	1.39	1.44
22	1	604	CLA	C3D-C4D	-2.00	1.39	1.44
22	9	609	CLA	C3D-C4D	-2.00	1.39	1.44
22	4	613	CLA	C3D-C4D	-2.00	1.39	1.44
31	4	607	CHL	C2C-C1C	2.00	1.48	1.44
22	B	805	CLA	C3D-C4D	-2.00	1.39	1.44
22	92	603	CLA	C3D-C4D	-2.00	1.39	1.44

All (736) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	9	610	CLA	C1D-ND-C4D	-4.48	103.16	106.33
31	3	608	CHL	CHD-C1D-ND	-4.44	120.37	124.45
22	Z	613	CLA	C1D-ND-C4D	-4.42	103.20	106.33
22	9	604	CLA	C1D-ND-C4D	-4.36	103.24	106.33
22	L	204	CLA	C1D-ND-C4D	-4.32	103.27	106.33
22	F	303	CLA	C1D-ND-C4D	-4.31	103.27	106.33
22	1	613	CLA	C1D-ND-C4D	-4.31	103.27	106.33
22	4	604	CLA	C1D-ND-C4D	-4.31	103.27	106.33
22	9	603	CLA	C1D-ND-C4D	-4.30	103.28	106.33
22	6	614	CLA	C1D-ND-C4D	-4.29	103.29	106.33
22	92	614	CLA	C1D-ND-C4D	-4.29	103.29	106.33
22	B	814	CLA	C1D-ND-C4D	-4.29	103.29	106.33
22	B2	804	CLA	C1D-ND-C4D	-4.29	103.29	106.33
22	5	617	CLA	C1D-ND-C4D	-4.28	103.29	106.33
22	5	603	CLA	C1D-ND-C4D	-4.28	103.30	106.33
22	A	816	CLA	C1D-ND-C4D	-4.28	103.30	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	6	608	CHL	CHD-C1D-ND	-4.26	120.53	124.45
22	Z	602	CLA	C1D-ND-C4D	-4.26	103.31	106.33
22	B	822	CLA	C1D-ND-C4D	-4.26	103.31	106.33
22	A	809	CLA	C1D-ND-C4D	-4.26	103.31	106.33
22	K	204	CLA	C1D-ND-C4D	-4.26	103.31	106.33
22	Z	614	CLA	C1D-ND-C4D	-4.25	103.31	106.33
22	92	604	CLA	C1D-ND-C4D	-4.25	103.32	106.33
31	4	606	CHL	CHD-C1D-ND	-4.25	120.55	124.45
31	1	607	CHL	CHD-C1D-ND	-4.24	120.56	124.45
22	92	602	CLA	C1D-ND-C4D	-4.24	103.32	106.33
22	92	613	CLA	C1D-ND-C4D	-4.24	103.33	106.33
22	1	602	CLA	C1D-ND-C4D	-4.22	103.34	106.33
22	5	609	CLA	C1D-ND-C4D	-4.22	103.34	106.33
22	Z	612	CLA	C1D-ND-C4D	-4.21	103.34	106.33
22	A	804	CLA	C1D-ND-C4D	-4.21	103.34	106.33
22	5	613	CLA	C1D-ND-C4D	-4.21	103.34	106.33
22	92	610	CLA	C1D-ND-C4D	-4.20	103.35	106.33
22	6	609	CLA	C1D-ND-C4D	-4.20	103.35	106.33
31	4	618	CHL	CHD-C1D-ND	-4.20	120.60	124.45
22	B2	812	CLA	C1D-ND-C4D	-4.19	103.36	106.33
22	7	614	CLA	C1D-ND-C4D	-4.19	103.36	106.33
22	6	612	CLA	C1D-ND-C4D	-4.19	103.36	106.33
31	5	608	CHL	CHD-C1D-ND	-4.18	120.61	124.45
22	8	616	CLA	C1D-ND-C4D	-4.18	103.37	106.33
31	8	606	CHL	CHD-C1D-ND	-4.17	120.62	124.45
22	B	808	CLA	C1D-ND-C4D	-4.17	103.37	106.33
22	9	601	CLA	C1D-ND-C4D	-4.17	103.37	106.33
22	B2	820	CLA	C1D-ND-C4D	-4.17	103.37	106.33
22	Z	611	CLA	C1D-ND-C4D	-4.17	103.37	106.33
22	L2	204	CLA	C1D-ND-C4D	-4.17	103.37	106.33
22	B	833	CLA	C1D-ND-C4D	-4.17	103.37	106.33
22	B2	814	CLA	C1D-ND-C4D	-4.17	103.37	106.33
22	5	616	CLA	C1D-ND-C4D	-4.17	103.37	106.33
22	B2	815	CLA	C1D-ND-C4D	-4.17	103.37	106.33
31	92	606	CHL	CHD-C1D-ND	-4.17	120.62	124.45
22	3	612	CLA	C1D-ND-C4D	-4.17	103.38	106.33
22	4	612	CLA	C1D-ND-C4D	-4.17	103.38	106.33
22	A	820	CLA	C1D-ND-C4D	-4.16	103.38	106.33
22	9	614	CLA	C1D-ND-C4D	-4.16	103.38	106.33
22	1	614	CLA	C1D-ND-C4D	-4.16	103.38	106.33
22	B2	813	CLA	C1D-ND-C4D	-4.16	103.38	106.33
22	3	614	CLA	C1D-ND-C4D	-4.16	103.38	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	4	611	CLA	C1D-ND-C4D	-4.16	103.38	106.33
22	Z	604	CLA	C1D-ND-C4D	-4.16	103.38	106.33
22	B2	828	CLA	C1D-ND-C4D	-4.15	103.38	106.33
22	3	602	CLA	C1D-ND-C4D	-4.15	103.39	106.33
22	3	607	CLA	C1D-ND-C4D	-4.15	103.39	106.33
22	L2	203	CLA	C1D-ND-C4D	-4.15	103.39	106.33
22	6	610	CLA	C1D-ND-C4D	-4.15	103.39	106.33
22	6	617	CLA	C1D-ND-C4D	-4.15	103.39	106.33
22	4	603	CLA	C1D-ND-C4D	-4.14	103.39	106.33
22	A	831	CLA	C1D-ND-C4D	-4.14	103.39	106.33
31	Z	606	CHL	CHD-C1D-ND	-4.14	120.65	124.45
22	3	611	CLA	C1D-ND-C4D	-4.14	103.39	106.33
22	7	603	CLA	C1D-ND-C4D	-4.14	103.39	106.33
31	92	607	CHL	CHD-C1D-ND	-4.14	120.65	124.45
22	8	611	CLA	C1D-ND-C4D	-4.14	103.39	106.33
22	A	834	CLA	C1D-ND-C4D	-4.14	103.39	106.33
22	7	616	CLA	C1D-ND-C4D	-4.14	103.40	106.33
22	9	609	CLA	C1D-ND-C4D	-4.14	103.40	106.33
22	B2	805	CLA	C1D-ND-C4D	-4.13	103.40	106.33
22	A	835	CLA	C1D-ND-C4D	-4.13	103.40	106.33
22	7	604	CLA	C1D-ND-C4D	-4.13	103.40	106.33
22	6	604	CLA	C1D-ND-C4D	-4.13	103.40	106.33
22	7	602	CLA	C1D-ND-C4D	-4.13	103.40	106.33
22	Z	610	CLA	C1D-ND-C4D	-4.13	103.40	106.33
22	6	602	CLA	C1D-ND-C4D	-4.13	103.40	106.33
22	B2	808	CLA	C1D-ND-C4D	-4.12	103.41	106.33
22	A	839	CLA	C1D-ND-C4D	-4.12	103.41	106.33
22	B	836	CLA	C1D-ND-C4D	-4.12	103.41	106.33
22	B	840	CLA	C1D-ND-C4D	-4.12	103.41	106.33
22	F	304	CLA	C1D-ND-C4D	-4.12	103.41	106.33
22	4	616	CLA	C1D-ND-C4D	-4.12	103.41	106.33
31	4	601	CHL	CHD-C1D-ND	-4.12	120.67	124.45
22	5	611	CLA	C1D-ND-C4D	-4.12	103.41	106.33
22	7	612	CLA	C1D-ND-C4D	-4.11	103.41	106.33
22	A	806	CLA	C1D-ND-C4D	-4.11	103.41	106.33
22	A	830	CLA	C1D-ND-C4D	-4.11	103.41	106.33
22	1	616	CLA	C1D-ND-C4D	-4.11	103.41	106.33
22	B2	811	CLA	C1D-ND-C4D	-4.11	103.41	106.33
22	8	613	CLA	C1D-ND-C4D	-4.11	103.42	106.33
22	5	601	CLA	C1D-ND-C4D	-4.11	103.42	106.33
22	A	813	CLA	C1D-ND-C4D	-4.11	103.42	106.33
22	Z	616	CLA	C1D-ND-C4D	-4.11	103.42	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	1	610	CLA	C1D-ND-C4D	-4.11	103.42	106.33
22	7	620	CLA	C1D-ND-C4D	-4.11	103.42	106.33
22	A	827	CLA	C1D-ND-C4D	-4.10	103.42	106.33
22	1	612	CLA	C1D-ND-C4D	-4.10	103.42	106.33
22	5	614	CLA	C1D-ND-C4D	-4.10	103.42	106.33
22	A	818	CLA	C1D-ND-C4D	-4.10	103.42	106.33
22	6	611	CLA	C1D-ND-C4D	-4.10	103.42	106.33
31	6	618	CHL	CHD-C1D-ND	-4.10	120.69	124.45
22	A	843	CLA	C1D-ND-C4D	-4.10	103.42	106.33
22	B	835	CLA	C1D-ND-C4D	-4.10	103.42	106.33
22	92	603	CLA	C1D-ND-C4D	-4.10	103.42	106.33
22	A	822	CLA	C1D-ND-C4D	-4.09	103.43	106.33
22	A	811	CLA	C1D-ND-C4D	-4.09	103.43	106.33
22	B	831	CLA	C1D-ND-C4D	-4.09	103.43	106.33
22	G	204	CLA	C1D-ND-C4D	-4.09	103.43	106.33
22	3	610	CLA	C1D-ND-C4D	-4.09	103.43	106.33
22	B2	829	CLA	C1D-ND-C4D	-4.09	103.43	106.33
31	7	606	CHL	CHD-C1D-ND	-4.09	120.70	124.45
22	6	613	CLA	C1D-ND-C4D	-4.09	103.43	106.33
22	8	604	CLA	C1D-ND-C4D	-4.08	103.44	106.33
22	9	613	CLA	C1D-ND-C4D	-4.08	103.44	106.33
22	B2	839	CLA	C1D-ND-C4D	-4.08	103.44	106.33
31	1	601	CHL	CHD-C1D-ND	-4.08	120.70	124.45
31	8	601	CHL	CHD-C1D-ND	-4.08	120.70	124.45
22	7	611	CLA	C1D-ND-C4D	-4.08	103.44	106.33
22	7	613	CLA	C1D-ND-C4D	-4.08	103.44	106.33
22	K	203	CLA	C1D-ND-C4D	-4.08	103.44	106.33
22	K	206	CLA	C1D-ND-C4D	-4.07	103.44	106.33
22	1	604	CLA	C1D-ND-C4D	-4.07	103.44	106.33
22	8	614	CLA	C1D-ND-C4D	-4.07	103.44	106.33
22	6	622	CLA	C1D-ND-C4D	-4.07	103.44	106.33
22	B	816	CLA	C1D-ND-C4D	-4.07	103.44	106.33
22	5	612	CLA	C1D-ND-C4D	-4.07	103.44	106.33
22	A	832	CLA	C1D-ND-C4D	-4.07	103.45	106.33
22	A	808	CLA	C1D-ND-C4D	-4.07	103.45	106.33
31	7	601	CHL	CHD-C1D-ND	-4.06	120.72	124.45
22	B	834	CLA	C1D-ND-C4D	-4.06	103.45	106.33
22	B	805	CLA	C1D-ND-C4D	-4.06	103.45	106.33
22	8	609	CLA	C1D-ND-C4D	-4.06	103.45	106.33
22	5	602	CLA	C1D-ND-C4D	-4.06	103.45	106.33
22	B2	807	CLA	C1D-ND-C4D	-4.06	103.45	106.33
22	B2	810	CLA	C1D-ND-C4D	-4.06	103.45	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	1	609	CLA	C1D-ND-C4D	-4.06	103.45	106.33
22	92	612	CLA	C1D-ND-C4D	-4.05	103.46	106.33
22	A	824	CLA	C1D-ND-C4D	-4.05	103.46	106.33
22	8	602	CLA	C1D-ND-C4D	-4.05	103.46	106.33
22	1	608	CLA	C1D-ND-C4D	-4.05	103.46	106.33
22	8	612	CLA	C1D-ND-C4D	-4.05	103.46	106.33
31	5	618	CHL	CHD-C1D-ND	-4.05	120.73	124.45
22	1	611	CLA	C1D-ND-C4D	-4.04	103.46	106.33
22	A	842	CLA	C1D-ND-C4D	-4.04	103.46	106.33
22	L	203	CLA	C1D-ND-C4D	-4.04	103.47	106.33
22	B2	809	CLA	C1D-ND-C4D	-4.04	103.47	106.33
22	92	609	CLA	C1D-ND-C4D	-4.04	103.47	106.33
31	6	607	CHL	CHD-C1D-ND	-4.03	120.75	124.45
22	A	823	CLA	C1D-ND-C4D	-4.03	103.47	106.33
22	B	828	CLA	C1D-ND-C4D	-4.03	103.47	106.33
31	4	608	CHL	CHD-C1D-ND	-4.03	120.75	124.45
22	1	603	CLA	C1D-ND-C4D	-4.03	103.47	106.33
22	5	604	CLA	C1D-ND-C4D	-4.03	103.47	106.33
31	6	601	CHL	CHD-C1D-ND	-4.03	120.75	124.45
22	Z	603	CLA	C1D-ND-C4D	-4.03	103.47	106.33
22	9	602	CLA	C1D-ND-C4D	-4.03	103.47	106.33
22	Z	608	CLA	C1D-ND-C4D	-4.02	103.48	106.33
22	A	838	CLA	C1D-ND-C4D	-4.02	103.48	106.33
22	B	832	CLA	C1D-ND-C4D	-4.02	103.48	106.33
22	B	810	CLA	C1D-ND-C4D	-4.02	103.48	106.33
22	B	837	CLA	C1D-ND-C4D	-4.02	103.48	106.33
22	4	602	CLA	C1D-ND-C4D	-4.02	103.48	106.33
22	B	804	CLA	C1D-ND-C4D	-4.02	103.48	106.33
22	B	807	CLA	C1D-ND-C4D	-4.02	103.48	106.33
22	A	841	CLA	C1D-ND-C4D	-4.01	103.48	106.33
31	Z	601	CHL	CHD-C1D-ND	-4.01	120.77	124.45
31	9	606	CHL	CHD-C1D-ND	-4.01	120.77	124.45
22	3	604	CLA	C1D-ND-C4D	-4.01	103.48	106.33
22	5	610	CLA	C1D-ND-C4D	-4.01	103.48	106.33
22	9	612	CLA	C1D-ND-C4D	-4.01	103.49	106.33
22	B	819	CLA	C1D-ND-C4D	-4.00	103.49	106.33
22	92	601	CLA	C1D-ND-C4D	-4.00	103.49	106.33
22	4	610	CLA	C1D-ND-C4D	-4.00	103.49	106.33
22	A	833	CLA	C1D-ND-C4D	-4.00	103.49	106.33
22	B2	806	CLA	C1D-ND-C4D	-4.00	103.49	106.33
22	3	606	CLA	C1D-ND-C4D	-4.00	103.50	106.33
22	8	603	CLA	C1D-ND-C4D	-3.99	103.50	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	841	CLA	C1D-ND-C4D	-3.99	103.50	106.33
31	9	607	CHL	CHD-C1D-ND	-3.99	120.79	124.45
22	92	611	CLA	C1D-ND-C4D	-3.98	103.51	106.33
31	4	607	CHL	CHD-C1D-ND	-3.98	120.80	124.45
22	A	814	CLA	C1D-ND-C4D	-3.98	103.51	106.33
22	A	845	CLA	C1D-ND-C4D	-3.98	103.51	106.33
22	A	821	CLA	C1D-ND-C4D	-3.98	103.51	106.33
22	8	608	CLA	C1D-ND-C4D	-3.98	103.51	106.33
22	4	614	CLA	C1D-ND-C4D	-3.98	103.51	106.33
31	5	607	CHL	CHD-C1D-ND	-3.98	120.80	124.45
22	A	803	CLA	C1D-ND-C4D	-3.97	103.51	106.33
22	9	611	CLA	C1D-ND-C4D	-3.97	103.51	106.33
22	A	815	CLA	C1D-ND-C4D	-3.97	103.51	106.33
22	B	813	CLA	C1D-ND-C4D	-3.97	103.52	106.33
22	4	613	CLA	C1D-ND-C4D	-3.97	103.52	106.33
22	7	608	CLA	C1D-ND-C4D	-3.97	103.52	106.33
22	J	101	CLA	C1D-ND-C4D	-3.96	103.52	106.33
22	B	812	CLA	C1D-ND-C4D	-3.96	103.52	106.33
22	3	613	CLA	C1D-ND-C4D	-3.96	103.53	106.33
21	A	801	CL0	CHD-C1D-ND	-3.96	120.82	124.45
22	B	839	CLA	C1D-ND-C4D	-3.95	103.53	106.33
22	A	812	CLA	C1D-ND-C4D	-3.95	103.53	106.33
31	6	616	CHL	CHD-C1D-ND	-3.95	120.83	124.45
22	B	826	CLA	C1D-ND-C4D	-3.95	103.53	106.33
22	A	840	CLA	C1D-ND-C4D	-3.95	103.53	106.33
22	6	603	CLA	C1D-ND-C4D	-3.94	103.53	106.33
31	5	606	CHL	CHD-C1D-ND	-3.94	120.83	124.45
31	7	607	CHL	CHD-C1D-ND	-3.94	120.84	124.45
22	3	617	CLA	C1D-ND-C4D	-3.94	103.54	106.33
31	1	606	CHL	CHD-C1D-ND	-3.93	120.84	124.45
22	B	823	CLA	C1D-ND-C4D	-3.93	103.55	106.33
22	B	811	CLA	C1D-ND-C4D	-3.93	103.55	106.33
22	B	827	CLA	C1D-ND-C4D	-3.92	103.55	106.33
22	A	825	CLA	C1D-ND-C4D	-3.92	103.55	106.33
22	7	609	CLA	C1D-ND-C4D	-3.91	103.55	106.33
31	Z	607	CHL	CHD-C1D-ND	-3.91	120.86	124.45
22	B	830	CLA	C1D-ND-C4D	-3.91	103.56	106.33
22	3	615	CLA	C1D-ND-C4D	-3.91	103.56	106.33
22	A	817	CLA	C1D-ND-C4D	-3.90	103.56	106.33
22	A	836	CLA	C1D-ND-C4D	-3.90	103.56	106.33
22	A	805	CLA	C1D-ND-C4D	-3.90	103.57	106.33
22	3	609	CLA	C1D-ND-C4D	-3.90	103.57	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	820	CLA	C1D-ND-C4D	-3.89	103.57	106.33
22	B	818	CLA	C1D-ND-C4D	-3.89	103.57	106.33
22	A	819	CLA	C1D-ND-C4D	-3.88	103.58	106.33
22	B	817	CLA	C1D-ND-C4D	-3.88	103.58	106.33
22	F	301	CLA	C1D-ND-C4D	-3.87	103.59	106.33
22	8	610	CLA	C1D-ND-C4D	-3.87	103.59	106.33
22	4	609	CLA	C1D-ND-C4D	-3.86	103.59	106.33
22	B	825	CLA	C1D-ND-C4D	-3.85	103.60	106.33
22	B	802	CLA	C1D-ND-C4D	-3.84	103.60	106.33
22	G	203	CLA	C1D-ND-C4D	-3.84	103.61	106.33
22	A	854	CLA	C1D-ND-C4D	-3.83	103.61	106.33
31	6	606	CHL	CHD-C1D-ND	-3.81	120.95	124.45
31	8	607	CHL	CHD-C1D-ND	-3.81	120.95	124.45
22	B	829	CLA	C1D-ND-C4D	-3.80	103.63	106.33
22	B	815	CLA	C1D-ND-C4D	-3.79	103.64	106.33
22	Z	609	CLA	C1D-ND-C4D	-3.79	103.64	106.33
22	B	809	CLA	C1D-ND-C4D	-3.79	103.64	106.33
22	A	807	CLA	C1D-ND-C4D	-3.79	103.64	106.33
22	B	838	CLA	C1D-ND-C4D	-3.79	103.64	106.33
22	B	821	CLA	C1D-ND-C4D	-3.78	103.65	106.33
22	B	824	CLA	C1D-ND-C4D	-3.77	103.66	106.33
22	B	833	CLA	CHD-C1D-ND	-3.76	121.00	124.45
22	A	826	CLA	C1D-ND-C4D	-3.74	103.68	106.33
22	A	828	CLA	C1D-ND-C4D	-3.74	103.68	106.33
22	B2	811	CLA	CAB-C3B-C4B	-3.73	122.74	128.46
31	6	608	CHL	C1D-ND-C4D	-3.72	103.69	106.33
33	6	625	NEX	O24-C25-C24	-3.72	110.59	113.38
31	5	608	CHL	C1D-ND-C4D	-3.71	103.70	106.33
22	7	610	CLA	CHD-C1D-ND	-3.69	121.06	124.45
22	A	802	CLA	C1D-ND-C4D	-3.69	103.71	106.33
22	3	603	CLA	C1D-ND-C4D	-3.67	103.73	106.33
22	K	201	CLA	C1D-ND-C4D	-3.67	103.73	106.33
22	A	809	CLA	CHD-C1D-ND	-3.67	121.08	124.45
22	A	837	CLA	C1D-ND-C4D	-3.66	103.73	106.33
22	9	610	CLA	CHD-C1D-ND	-3.65	121.10	124.45
22	5	621	CLA	C1D-ND-C4D	-3.64	103.75	106.33
22	B	806	CLA	C1D-ND-C4D	-3.63	103.75	106.33
21	A	801	CL0	C1D-ND-C4D	-3.63	103.76	106.33
31	5	607	CHL	C1D-ND-C4D	-3.63	103.76	106.33
22	A	810	CLA	C1D-ND-C4D	-3.62	103.76	106.33
22	1	604	CLA	CHD-C1D-ND	-3.62	121.12	124.45
22	7	610	CLA	C1D-ND-C4D	-3.61	103.77	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	801	CL0	CHC-C1C-NC	3.61	129.67	124.20
31	9	607	CHL	C1D-ND-C4D	-3.61	103.77	106.33
31	Z	606	CHL	C1D-ND-C4D	-3.60	103.78	106.33
31	4	601	CHL	C1D-ND-C4D	-3.60	103.78	106.33
22	A	829	CLA	C1D-ND-C4D	-3.59	103.78	106.33
22	B	822	CLA	CHD-C1D-ND	-3.57	121.17	124.45
22	A	823	CLA	CHD-C1D-ND	-3.56	121.18	124.45
31	8	606	CHL	C1D-ND-C4D	-3.56	103.81	106.33
31	7	601	CHL	C1D-ND-C4D	-3.55	103.82	106.33
31	4	608	CHL	C1D-ND-C4D	-3.54	103.82	106.33
31	5	618	CHL	C1D-ND-C4D	-3.54	103.82	106.33
31	9	606	CHL	C1D-ND-C4D	-3.54	103.82	106.33
31	92	607	CHL	C1D-ND-C4D	-3.53	103.83	106.33
22	A	806	CLA	CHD-C1D-ND	-3.53	121.21	124.45
31	6	618	CHL	C1D-ND-C4D	-3.53	103.83	106.33
31	7	606	CHL	C1D-ND-C4D	-3.52	103.83	106.33
22	A	827	CLA	CHD-C1D-ND	-3.52	121.22	124.45
31	4	618	CHL	C1D-ND-C4D	-3.52	103.83	106.33
22	Z	602	CLA	CHD-C1D-ND	-3.51	121.22	124.45
22	5	603	CLA	CHD-C1D-ND	-3.51	121.23	124.45
22	8	602	CLA	CHD-C1D-ND	-3.50	121.24	124.45
22	A	836	CLA	CHD-C1D-ND	-3.50	121.24	124.45
31	92	606	CHL	C1D-ND-C4D	-3.50	103.85	106.33
22	B	803	CLA	CHD-C1D-ND	-3.49	121.24	124.45
22	L2	203	CLA	CHD-C1D-ND	-3.49	121.24	124.45
22	B	841	CLA	CHD-C1D-ND	-3.49	121.24	124.45
31	6	607	CHL	C1D-ND-C4D	-3.49	103.85	106.33
22	92	604	CLA	CHD-C1D-ND	-3.49	121.25	124.45
22	L	203	CLA	CHD-C1D-ND	-3.48	121.25	124.45
22	A	812	CLA	CHD-C1D-ND	-3.48	121.25	124.45
22	B	805	CLA	CHD-C1D-ND	-3.48	121.25	124.45
22	B	819	CLA	CHD-C1D-ND	-3.48	121.25	124.45
22	92	614	CLA	CHD-C1D-ND	-3.48	121.26	124.45
31	4	607	CHL	C1D-ND-C4D	-3.48	103.87	106.33
22	1	610	CLA	CHD-C1D-ND	-3.47	121.26	124.45
22	7	603	CLA	CHD-C1D-ND	-3.47	121.26	124.45
22	B	834	CLA	CHD-C1D-ND	-3.47	121.26	124.45
22	1	608	CLA	CHD-C1D-ND	-3.47	121.26	124.45
22	Z	604	CLA	CHD-C1D-ND	-3.47	121.27	124.45
22	5	616	CLA	CHD-C1D-ND	-3.47	121.27	124.45
22	A	835	CLA	CHD-C1D-ND	-3.47	121.27	124.45
22	8	616	CLA	CHD-C1D-ND	-3.47	121.27	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	804	CLA	CHD-C1D-ND	-3.47	121.27	124.45
22	6	610	CLA	CHD-C1D-ND	-3.46	121.27	124.45
31	4	606	CHL	C1D-ND-C4D	-3.46	103.88	106.33
22	4	610	CLA	CHD-C1D-ND	-3.45	121.28	124.45
22	5	610	CLA	CHD-C1D-ND	-3.45	121.28	124.45
22	Z	610	CLA	CHD-C1D-ND	-3.45	121.28	124.45
31	1	606	CHL	C1D-ND-C4D	-3.45	103.88	106.33
22	A	802	CLA	CHD-C1D-ND	-3.45	121.28	124.45
22	B	829	CLA	CHD-C1D-ND	-3.45	121.28	124.45
22	A	803	CLA	CHD-C1D-ND	-3.45	121.29	124.45
31	6	616	CHL	C1D-ND-C4D	-3.45	103.89	106.33
22	L2	204	CLA	CHD-C1D-ND	-3.44	121.29	124.45
22	8	604	CLA	CHD-C1D-ND	-3.44	121.29	124.45
22	Z	613	CLA	CHD-C1D-ND	-3.44	121.29	124.45
22	6	614	CLA	CHD-C1D-ND	-3.44	121.29	124.45
22	4	604	CLA	CHD-C1D-ND	-3.44	121.30	124.45
33	6	625	NEX	C5-C6-C1	3.43	123.10	119.70
31	1	601	CHL	C1D-ND-C4D	-3.43	103.90	106.33
22	9	604	CLA	CHD-C1D-ND	-3.43	121.30	124.45
22	9	609	CLA	CHD-C1D-ND	-3.43	121.31	124.45
31	5	607	CHL	C1B-CHB-C4A	-3.43	123.33	130.12
22	Z	614	CLA	CHD-C1D-ND	-3.43	121.31	124.45
22	B2	839	CLA	CHD-C1D-ND	-3.43	121.31	124.45
22	A	811	CLA	CHD-C1D-ND	-3.42	121.31	124.45
22	92	610	CLA	CHD-C1D-ND	-3.42	121.31	124.45
22	B	839	CLA	CHD-C1D-ND	-3.42	121.31	124.45
22	9	614	CLA	CHD-C1D-ND	-3.41	121.32	124.45
22	3	602	CLA	CHD-C1D-ND	-3.41	121.32	124.45
22	6	617	CLA	CHD-C1D-ND	-3.41	121.32	124.45
22	7	616	CLA	CHD-C1D-ND	-3.41	121.32	124.45
31	3	608	CHL	C1D-ND-C4D	-3.40	103.92	106.33
22	A	816	CLA	CHD-C1D-ND	-3.40	121.33	124.45
22	5	613	CLA	CHD-C1D-ND	-3.40	121.33	124.45
22	A	833	CLA	CHD-C1D-ND	-3.39	121.33	124.45
22	B2	829	CLA	CHD-C1D-ND	-3.39	121.34	124.45
22	B	826	CLA	CHD-C1D-ND	-3.39	121.34	124.45
22	L	204	CLA	CHD-C1D-ND	-3.39	121.34	124.45
22	A	837	CLA	CHD-C1D-ND	-3.39	121.34	124.45
33	5	625	NEX	O24-C25-C24	-3.38	110.84	113.38
22	Z	603	CLA	CHD-C1D-ND	-3.38	121.34	124.45
22	B	814	CLA	CHD-C1D-ND	-3.38	121.35	124.45
22	92	602	CLA	CHD-C1D-ND	-3.38	121.35	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	830	CLA	CHD-C1D-ND	-3.38	121.35	124.45
22	3	610	CLA	CHD-C1D-ND	-3.38	121.35	124.45
22	6	609	CLA	CHD-C1D-ND	-3.38	121.35	124.45
22	K	204	CLA	CHD-C1D-ND	-3.38	121.35	124.45
22	3	614	CLA	CHD-C1D-ND	-3.38	121.35	124.45
31	5	606	CHL	C1D-ND-C4D	-3.37	103.94	106.33
22	A	841	CLA	CHD-C1D-ND	-3.37	121.35	124.45
22	B	830	CLA	CHD-C1D-ND	-3.37	121.35	124.45
22	A	832	CLA	CHD-C1D-ND	-3.37	121.36	124.45
22	8	614	CLA	CHD-C1D-ND	-3.37	121.36	124.45
22	B	840	CLA	CHD-C1D-ND	-3.37	121.36	124.45
22	8	609	CLA	CHD-C1D-ND	-3.37	121.36	124.45
22	92	613	CLA	CHD-C1D-ND	-3.37	121.36	124.45
22	B2	805	CLA	CHD-C1D-ND	-3.36	121.36	124.45
22	A	820	CLA	CHD-C1D-ND	-3.36	121.37	124.45
22	B	831	CLA	CHD-C1D-ND	-3.36	121.37	124.45
31	8	607	CHL	C1D-ND-C4D	-3.36	103.95	106.33
22	3	611	CLA	CHD-C1D-ND	-3.36	121.37	124.45
22	B	832	CLA	CHD-C1D-ND	-3.35	121.37	124.45
22	A	840	CLA	CHD-C1D-ND	-3.35	121.37	124.45
22	B	807	CLA	CHD-C1D-ND	-3.35	121.37	124.45
22	B2	814	CLA	CHD-C1D-ND	-3.35	121.38	124.45
22	9	613	CLA	CHD-C1D-ND	-3.35	121.38	124.45
22	1	613	CLA	CHD-C1D-ND	-3.35	121.38	124.45
22	5	617	CLA	CHD-C1D-ND	-3.34	121.38	124.45
22	9	611	CLA	CHD-C1D-ND	-3.34	121.39	124.45
22	8	613	CLA	CHD-C1D-ND	-3.34	121.39	124.45
22	B	812	CLA	CHD-C1D-ND	-3.34	121.39	124.45
22	5	604	CLA	CHD-C1D-ND	-3.33	121.39	124.45
22	4	616	CLA	CHD-C1D-ND	-3.33	121.39	124.45
22	B	835	CLA	CHD-C1D-ND	-3.33	121.40	124.45
22	F	303	CLA	CHD-C1D-ND	-3.33	121.40	124.45
22	K	203	CLA	CHD-C1D-ND	-3.33	121.40	124.45
31	9	607	CHL	C1B-CHB-C4A	-3.33	123.53	130.12
31	7	607	CHL	C1D-ND-C4D	-3.32	103.97	106.33
22	B	823	CLA	CHD-C1D-ND	-3.32	121.40	124.45
22	1	602	CLA	CHD-C1D-ND	-3.32	121.40	124.45
22	A	815	CLA	CHD-C1D-ND	-3.32	121.40	124.45
22	1	609	CLA	CHD-C1D-ND	-3.32	121.40	124.45
22	A	831	CLA	CHD-C1D-ND	-3.32	121.41	124.45
22	A	834	CLA	CHD-C1D-ND	-3.32	121.41	124.45
22	6	602	CLA	CHD-C1D-ND	-3.32	121.41	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	7	611	CLA	CHD-C1D-ND	-3.31	121.41	124.45
22	6	622	CLA	CHD-C1D-ND	-3.31	121.41	124.45
22	92	611	CLA	CHD-C1D-ND	-3.31	121.41	124.45
22	8	610	CLA	CHD-C1D-ND	-3.31	121.41	124.45
22	92	601	CLA	CHD-C1D-ND	-3.31	121.41	124.45
22	5	609	CLA	CHD-C1D-ND	-3.31	121.41	124.45
22	B	828	CLA	CHD-C1D-ND	-3.31	121.42	124.45
22	3	604	CLA	CHD-C1D-ND	-3.30	121.42	124.45
22	3	609	CLA	CHD-C1D-ND	-3.30	121.42	124.45
22	B	838	CLA	CHD-C1D-ND	-3.30	121.42	124.45
31	Z	607	CHL	C1D-ND-C4D	-3.30	103.99	106.33
31	6	606	CHL	C1D-ND-C4D	-3.30	103.99	106.33
22	1	603	CLA	CHD-C1D-ND	-3.29	121.43	124.45
22	9	602	CLA	CHD-C1D-ND	-3.29	121.43	124.45
22	B	821	CLA	CHD-C1D-ND	-3.29	121.43	124.45
22	3	607	CLA	CHD-C1D-ND	-3.29	121.43	124.45
22	8	603	CLA	CHD-C1D-ND	-3.29	121.43	124.45
22	Z	608	CLA	CHD-C1D-ND	-3.29	121.43	124.45
22	A	822	CLA	CHD-C1D-ND	-3.29	121.43	124.45
22	7	602	CLA	CHD-C1D-ND	-3.29	121.43	124.45
31	92	607	CHL	C1B-CHB-C4A	-3.28	123.61	130.12
22	6	613	CLA	CHD-C1D-ND	-3.28	121.44	124.45
22	B	818	CLA	CHD-C1D-ND	-3.28	121.44	124.45
22	B2	807	CLA	CHD-C1D-ND	-3.28	121.44	124.45
22	7	608	CLA	CHD-C1D-ND	-3.27	121.45	124.45
22	4	602	CLA	CHD-C1D-ND	-3.27	121.45	124.45
22	A	843	CLA	CHD-C1D-ND	-3.27	121.45	124.45
22	B	810	CLA	CHD-C1D-ND	-3.27	121.45	124.45
22	B2	811	CLA	CHD-C1D-ND	-3.27	121.45	124.45
22	4	613	CLA	CHD-C1D-ND	-3.26	121.45	124.45
22	7	613	CLA	CHD-C1D-ND	-3.26	121.46	124.45
22	B	804	CLA	CHD-C1D-ND	-3.26	121.46	124.45
22	6	611	CLA	CHD-C1D-ND	-3.26	121.46	124.45
22	Z	616	CLA	CHD-C1D-ND	-3.26	121.46	124.45
22	92	609	CLA	CHD-C1D-ND	-3.25	121.46	124.45
22	7	614	CLA	CHD-C1D-ND	-3.25	121.47	124.45
22	B2	804	CLA	CHD-C1D-ND	-3.25	121.47	124.45
31	1	607	CHL	C1D-ND-C4D	-3.25	104.03	106.33
22	A	839	CLA	CHD-C1D-ND	-3.25	121.47	124.45
31	6	601	CHL	C1B-CHB-C4A	-3.24	123.69	130.12
22	B	802	CLA	CHD-C1D-ND	-3.24	121.47	124.45
22	5	614	CLA	CHD-C1D-ND	-3.24	121.47	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	7	609	CLA	CHD-C1D-ND	-3.24	121.48	124.45
22	B2	809	CLA	CHD-C1D-ND	-3.24	121.48	124.45
22	B	803	CLA	C1D-ND-C4D	-3.24	104.04	106.33
22	B	837	CLA	CHD-C1D-ND	-3.24	121.48	124.45
22	4	609	CLA	CHD-C1D-ND	-3.24	121.48	124.45
22	B2	810	CLA	CHD-C1D-ND	-3.24	121.48	124.45
31	8	601	CHL	C1D-ND-C4D	-3.23	104.04	106.33
22	B2	828	CLA	CHD-C1D-ND	-3.23	121.48	124.45
22	8	608	CLA	CHD-C1D-ND	-3.23	121.48	124.45
22	5	602	CLA	CHD-C1D-ND	-3.23	121.48	124.45
22	A	824	CLA	CHD-C1D-ND	-3.23	121.49	124.45
22	B	817	CLA	CHD-C1D-ND	-3.23	121.49	124.45
22	4	611	CLA	CHD-C1D-ND	-3.23	121.49	124.45
22	1	614	CLA	CHD-C1D-ND	-3.23	121.49	124.45
31	1	607	CHL	C1B-CHB-C4A	-3.23	123.73	130.12
22	3	612	CLA	CHD-C1D-ND	-3.22	121.49	124.45
22	A	808	CLA	CHD-C1D-ND	-3.22	121.49	124.45
22	7	604	CLA	CHD-C1D-ND	-3.22	121.50	124.45
22	A	825	CLA	CHD-C1D-ND	-3.22	121.50	124.45
22	4	614	CLA	CHD-C1D-ND	-3.22	121.50	124.45
22	9	601	CLA	CHD-C1D-ND	-3.22	121.50	124.45
22	A	807	CLA	CHD-C1D-ND	-3.21	121.50	124.45
22	A	821	CLA	CHD-C1D-ND	-3.21	121.50	124.45
22	A	805	CLA	CHD-C1D-ND	-3.21	121.50	124.45
22	B	815	CLA	CHD-C1D-ND	-3.21	121.50	124.45
22	K	206	CLA	CHD-C1D-ND	-3.21	121.50	124.45
31	6	601	CHL	C1D-ND-C4D	-3.21	104.06	106.33
22	B2	815	CLA	CHD-C1D-ND	-3.21	121.50	124.45
22	B	836	CLA	CHD-C1D-ND	-3.21	121.51	124.45
22	9	603	CLA	CHD-C1D-ND	-3.20	121.51	124.45
22	A	813	CLA	CHD-C1D-ND	-3.20	121.51	124.45
22	B	811	CLA	CHD-C1D-ND	-3.20	121.51	124.45
22	B2	820	CLA	CHD-C1D-ND	-3.20	121.52	124.45
31	92	606	CHL	C1B-CHB-C4A	-3.19	123.80	130.12
22	6	604	CLA	CHD-C1D-ND	-3.19	121.52	124.45
22	3	606	CLA	CHD-C1D-ND	-3.19	121.53	124.45
22	A	842	CLA	CHD-C1D-ND	-3.18	121.53	124.45
22	B	816	CLA	CHD-C1D-ND	-3.18	121.53	124.45
22	A	818	CLA	CHD-C1D-ND	-3.18	121.53	124.45
22	B2	808	CLA	CHD-C1D-ND	-3.18	121.53	124.45
22	F	301	CLA	CHD-C1D-ND	-3.18	121.53	124.45
22	1	612	CLA	CHD-C1D-ND	-3.18	121.53	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	817	CLA	CHD-C1D-ND	-3.17	121.54	124.45
22	1	611	CLA	CHD-C1D-ND	-3.17	121.54	124.45
22	A	838	CLA	CHD-C1D-ND	-3.17	121.54	124.45
22	1	616	CLA	CHD-C1D-ND	-3.17	121.54	124.45
22	G	203	CLA	CHD-C1D-ND	-3.17	121.54	124.45
22	8	611	CLA	CHD-C1D-ND	-3.17	121.54	124.45
22	A	845	CLA	CHD-C1D-ND	-3.17	121.54	124.45
22	Z	609	CLA	CHD-C1D-ND	-3.17	121.54	124.45
31	4	607	CHL	C1B-CHB-C4A	-3.16	123.85	130.12
22	B2	813	CLA	CHD-C1D-ND	-3.16	121.55	124.45
22	9	612	CLA	CHD-C1D-ND	-3.16	121.55	124.45
22	Z	611	CLA	CHD-C1D-ND	-3.16	121.55	124.45
22	5	601	CLA	CHD-C1D-ND	-3.16	121.55	124.45
22	B	806	CLA	CHD-C1D-ND	-3.15	121.56	124.45
22	B	825	CLA	CHD-C1D-ND	-3.15	121.56	124.45
22	B2	812	CLA	CHD-C1D-ND	-3.15	121.56	124.45
22	4	603	CLA	CHD-C1D-ND	-3.15	121.56	124.45
22	B2	806	CLA	CHD-C1D-ND	-3.14	121.56	124.45
22	7	620	CLA	CHD-C1D-ND	-3.14	121.57	124.45
22	6	603	CLA	CHD-C1D-ND	-3.14	121.57	124.45
22	Z	612	CLA	CHD-C1D-ND	-3.14	121.57	124.45
22	92	612	CLA	CHD-C1D-ND	-3.13	121.58	124.45
22	3	615	CLA	CHD-C1D-ND	-3.13	121.58	124.45
22	8	612	CLA	CHD-C1D-ND	-3.13	121.58	124.45
22	B	808	CLA	CHD-C1D-ND	-3.13	121.58	124.45
22	6	612	CLA	CHD-C1D-ND	-3.13	121.58	124.45
22	A	814	CLA	CHD-C1D-ND	-3.12	121.58	124.45
31	7	601	CHL	C1B-CHB-C4A	-3.12	123.93	130.12
22	A	854	CLA	CHD-C1D-ND	-3.12	121.59	124.45
31	6	608	CHL	C1B-CHB-C4A	-3.12	123.94	130.12
22	G	204	CLA	CHD-C1D-ND	-3.11	121.59	124.45
31	Z	601	CHL	C1D-ND-C4D	-3.11	104.13	106.33
31	Z	607	CHL	C1B-CHB-C4A	-3.11	123.96	130.12
22	3	617	CLA	CHD-C1D-ND	-3.11	121.60	124.45
22	A	826	CLA	CHD-C1D-ND	-3.11	121.60	124.45
31	6	607	CHL	C1B-CHB-C4A	-3.11	123.97	130.12
22	5	611	CLA	CHD-C1D-ND	-3.10	121.60	124.45
22	A	828	CLA	CHD-C1D-ND	-3.10	121.60	124.45
31	6	616	CHL	C1B-CHB-C4A	-3.10	123.97	130.12
22	B	809	CLA	CHD-C1D-ND	-3.10	121.61	124.45
22	7	612	CLA	CHD-C1D-ND	-3.09	121.61	124.45
31	1	601	CHL	C1B-CHB-C4A	-3.09	123.99	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	5	608	CHL	C1B-CHB-C4A	-3.09	123.99	130.12
31	4	608	CHL	C1B-CHB-C4A	-3.09	123.99	130.12
22	B	827	CLA	CHD-C1D-ND	-3.09	121.61	124.45
22	4	612	CLA	CHD-C1D-ND	-3.09	121.61	124.45
31	6	618	CHL	C1B-CHB-C4A	-3.09	124.00	130.12
22	B	820	CLA	CHD-C1D-ND	-3.08	121.62	124.45
22	3	613	CLA	CHD-C1D-ND	-3.08	121.62	124.45
22	5	612	CLA	CHD-C1D-ND	-3.08	121.62	124.45
31	4	618	CHL	C1B-CHB-C4A	-3.08	124.03	130.12
31	5	618	CHL	C1B-CHB-C4A	-3.07	124.04	130.12
22	A	810	CLA	CHD-C1D-ND	-3.05	121.65	124.45
22	J	101	CLA	CHD-C1D-ND	-3.05	121.65	124.45
31	4	606	CHL	C1B-CHB-C4A	-3.05	124.08	130.12
31	6	606	CHL	C1B-CHB-C4A	-3.04	124.09	130.12
22	92	603	CLA	CHD-C1D-ND	-3.04	121.66	124.45
22	A	829	CLA	CHD-C1D-ND	-3.04	121.66	124.45
22	F	304	CLA	CHD-C1D-ND	-3.03	121.67	124.45
31	9	606	CHL	C1B-CHB-C4A	-3.03	124.12	130.12
31	5	606	CHL	C1B-CHB-C4A	-3.03	124.12	130.12
31	7	607	CHL	C1B-CHB-C4A	-3.02	124.13	130.12
22	B	824	CLA	CHD-C1D-ND	-3.01	121.69	124.45
21	A	801	CL0	CHC-C1C-C2C	-3.01	118.39	126.72
31	1	606	CHL	C1B-CHB-C4A	-3.01	124.16	130.12
22	B	813	CLA	CHD-C1D-ND	-2.98	121.72	124.45
31	8	606	CHL	C1B-CHB-C4A	-2.96	124.26	130.12
31	4	606	CHL	CMB-C2B-C1B	-2.96	123.92	128.46
22	3	603	CLA	CHD-C1D-ND	-2.95	121.74	124.45
31	Z	606	CHL	C1B-CHB-C4A	-2.95	124.28	130.12
31	Z	601	CHL	C1B-CHB-C4A	-2.93	124.31	130.12
31	7	601	CHL	CMB-C2B-C1B	-2.93	123.96	128.46
31	7	606	CHL	C1B-CHB-C4A	-2.92	124.34	130.12
31	6	601	CHL	CMB-C2B-C1B	-2.91	123.99	128.46
31	8	607	CHL	C1B-CHB-C4A	-2.91	124.36	130.12
22	B2	811	CLA	CAB-C3B-C2B	2.89	130.35	124.69
22	A	819	CLA	CHD-C1D-ND	-2.88	121.80	124.45
31	6	616	CHL	CMB-C2B-C1B	-2.88	124.04	128.46
31	3	608	CHL	C1B-CHB-C4A	-2.86	124.45	130.12
31	92	606	CHL	CMB-C2B-C1B	-2.84	124.10	128.46
31	5	608	CHL	CMB-C2B-C1B	-2.84	124.10	128.46
31	4	601	CHL	C1B-CHB-C4A	-2.82	124.53	130.12
31	7	607	CHL	CMB-C2B-C1B	-2.82	124.14	128.46
31	8	601	CHL	C1B-CHB-C4A	-2.81	124.55	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	5	621	CLA	CHD-C1D-ND	-2.80	121.88	124.45
22	F	304	CLA	O2A-C1-C2	2.79	115.97	108.64
31	6	607	CHL	CMB-C2B-C1B	-2.77	124.20	128.46
31	6	608	CHL	CMB-C2B-C1B	-2.76	124.22	128.46
31	6	618	CHL	CMB-C2B-C1B	-2.75	124.24	128.46
31	1	606	CHL	CMB-C2B-C1B	-2.74	124.25	128.46
31	8	607	CHL	CMB-C2B-C1B	-2.74	124.26	128.46
31	Z	601	CHL	CMB-C2B-C1B	-2.72	124.28	128.46
31	4	608	CHL	CMB-C2B-C1B	-2.71	124.30	128.46
31	92	607	CHL	CMB-C2B-C1B	-2.70	124.31	128.46
31	1	607	CHL	CMB-C2B-C1B	-2.70	124.31	128.46
31	4	618	CHL	CMB-C2B-C1B	-2.70	124.31	128.46
31	4	607	CHL	CMB-C2B-C1B	-2.69	124.33	128.46
31	5	618	CHL	CMB-C2B-C1B	-2.69	124.33	128.46
31	7	606	CHL	CMB-C2B-C1B	-2.67	124.36	128.46
31	6	606	CHL	CHB-C4A-NA	2.65	128.18	124.51
31	5	607	CHL	CMB-C2B-C1B	-2.65	124.39	128.46
22	K	201	CLA	CHD-C1D-ND	-2.65	122.02	124.45
31	8	607	CHL	CAA-C2A-C1A	2.64	120.62	111.97
31	5	606	CHL	CMB-C2B-C1B	-2.62	124.43	128.46
31	6	606	CHL	CMB-C2B-C1B	-2.62	124.43	128.46
31	6	601	CHL	CHA-C1A-NA	-2.62	120.40	126.40
31	1	607	CHL	CHC-C1C-NC	2.61	128.16	124.20
31	5	606	CHL	CHB-C4A-NA	2.60	128.10	124.51
31	1	601	CHL	CHB-C4A-NA	2.59	128.09	124.51
31	Z	607	CHL	CMB-C2B-C1B	-2.59	124.49	128.46
31	7	607	CHL	CHB-C4A-NA	2.58	128.07	124.51
31	1	601	CHL	CMB-C2B-C1B	-2.57	124.51	128.46
31	Z	606	CHL	CMB-C2B-C1B	-2.57	124.51	128.46
31	4	601	CHL	CMB-C2B-C1B	-2.56	124.52	128.46
31	8	607	CHL	CHB-C4A-NA	2.56	128.06	124.51
31	8	606	CHL	CMB-C2B-C1B	-2.56	124.53	128.46
31	9	607	CHL	CMB-C2B-C1B	-2.55	124.55	128.46
31	8	607	CHL	CHA-C1A-NA	-2.54	120.59	126.40
31	8	601	CHL	CHB-C4A-NA	2.53	128.01	124.51
31	6	618	CHL	CHB-C4A-NA	2.52	128.00	124.51
31	Z	601	CHL	CHB-C4A-NA	2.52	127.99	124.51
31	1	607	CHL	CHA-C1A-NA	-2.51	120.66	126.40
31	92	606	CHL	CHC-C1C-NC	2.50	128.00	124.20
31	4	606	CHL	CHB-C4A-NA	2.50	127.97	124.51
31	Z	601	CHL	CHC-C1C-NC	2.50	128.00	124.20
31	3	608	CHL	CHB-C4A-NA	2.50	127.97	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	5	607	CHL	CHC-C1C-NC	2.49	127.99	124.20
31	4	601	CHL	CHB-C4A-NA	2.49	127.95	124.51
31	4	606	CHL	CHC-C1C-NC	2.48	127.97	124.20
31	3	608	CHL	CMB-C2B-C1B	-2.48	124.65	128.46
22	5	621	CLA	C2A-C1A-CHA	2.48	128.19	123.86
31	4	607	CHL	CHA-C1A-NA	-2.47	120.75	126.40
31	5	608	CHL	CHB-C4A-NA	2.46	127.92	124.51
31	5	618	CHL	CHB-C4A-NA	2.46	127.92	124.51
31	6	606	CHL	CHA-C1A-NA	-2.46	120.77	126.40
27	B	853	LMU	C1B-O5B-C5B	2.46	118.51	113.69
31	1	606	CHL	CHA-C1A-NA	-2.43	120.82	126.40
31	9	607	CHL	CHC-C1C-NC	2.43	127.89	124.20
31	7	607	CHL	CHC-C1C-NC	2.43	127.89	124.20
31	8	601	CHL	CMB-C2B-C1B	-2.43	124.73	128.46
31	4	618	CHL	CHB-C4A-NA	2.43	127.87	124.51
31	8	606	CHL	CHC-C1C-NC	2.42	127.87	124.20
31	Z	607	CHL	CHC-C1C-NC	2.42	127.87	124.20
31	4	607	CHL	CHC-C1C-NC	2.42	127.87	124.20
31	8	601	CHL	CHA-C1A-NA	-2.42	120.86	126.40
31	5	606	CHL	CHA-C1A-NA	-2.42	120.86	126.40
31	6	607	CHL	CHA-C1A-NA	-2.42	120.86	126.40
31	4	601	CHL	CHA-C1A-NA	-2.42	120.86	126.40
33	5	625	NEX	C2-C1-C6	-2.41	106.86	109.21
31	9	606	CHL	CHB-C4A-NA	2.41	127.84	124.51
31	6	608	CHL	CHC-C1C-NC	2.41	127.86	124.20
31	5	608	CHL	CHA-C1A-NA	-2.40	120.90	126.40
31	6	607	CHL	CHB-C4A-NA	2.40	127.83	124.51
31	1	606	CHL	CHB-C4A-NA	2.40	127.83	124.51
31	7	607	CHL	CHA-C1A-NA	-2.40	120.91	126.40
31	92	607	CHL	CHC-C1C-NC	2.39	127.83	124.20
31	6	608	CHL	CHB-C4A-NA	2.39	127.82	124.51
31	6	601	CHL	C2A-C1A-CHA	2.39	128.04	123.86
31	6	618	CHL	CHA-C1A-NA	-2.39	120.93	126.40
31	3	608	CHL	CHC-C1C-NC	2.39	127.83	124.20
31	92	606	CHL	CHA-C1A-NA	-2.38	120.94	126.40
32	1	618	XAT	C7-C8-C9	2.38	129.23	125.53
31	5	618	CHL	CHA-C1A-NA	-2.38	120.95	126.40
31	3	608	CHL	CHA-C1A-NA	-2.38	120.95	126.40
31	9	606	CHL	CMB-C2B-C1B	-2.38	124.81	128.46
31	Z	607	CHL	CHA-C1A-NA	-2.38	120.95	126.40
22	5	621	CLA	CAA-C2A-C1A	2.38	119.77	111.97
31	7	606	CHL	CHB-C4A-NA	2.38	127.80	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	4	608	CHL	CHA-C1A-NA	-2.37	120.97	126.40
31	4	606	CHL	CHA-C1A-NA	-2.37	120.97	126.40
31	5	608	CHL	CHC-C1C-NC	2.37	127.79	124.20
31	6	601	CHL	CHB-C4A-NA	2.36	127.78	124.51
31	4	618	CHL	CHA-C1A-NA	-2.36	120.98	126.40
31	4	601	CHL	CHC-C1C-NC	2.36	127.79	124.20
31	92	607	CHL	CHA-C1A-NA	-2.36	120.98	126.40
31	6	601	CHL	CHC-C1C-NC	2.36	127.79	124.20
31	6	616	CHL	CHB-C4A-NA	2.36	127.77	124.51
31	6	608	CHL	CHA-C1A-NA	-2.36	121.00	126.40
31	8	606	CHL	CHB-C4A-NA	2.36	127.77	124.51
31	9	606	CHL	CHA-C1A-NA	-2.36	121.00	126.40
31	1	601	CHL	CHC-C1C-NC	2.35	127.77	124.20
31	4	618	CHL	CHC-C1C-NC	2.35	127.77	124.20
31	7	601	CHL	CHB-C4A-NA	2.35	127.76	124.51
31	4	608	CHL	CHC-C1C-NC	2.35	127.76	124.20
31	6	616	CHL	CHA-C1A-NA	-2.35	121.03	126.40
31	1	607	CHL	CHB-C4A-NA	2.35	127.75	124.51
31	9	606	CHL	CHC-C1C-NC	2.34	127.75	124.20
31	6	607	CHL	CHC-C1C-NC	2.34	127.75	124.20
31	6	606	CHL	CHC-C1C-NC	2.33	127.74	124.20
31	Z	601	CHL	CHA-C1A-NA	-2.33	121.06	126.40
31	5	618	CHL	CHC-C1C-NC	2.33	127.73	124.20
31	8	601	CHL	CHC-C1C-NC	2.32	127.72	124.20
31	8	607	CHL	CHC-C1C-NC	2.32	127.72	124.20
31	92	607	CHL	CHB-C4A-NA	2.31	127.70	124.51
31	4	608	CHL	CHB-C4A-NA	2.30	127.70	124.51
31	Z	606	CHL	CHC-C1C-NC	2.30	127.70	124.20
31	6	616	CHL	CHC-C1C-NC	2.30	127.69	124.20
31	5	606	CHL	CHC-C1C-NC	2.30	127.69	124.20
31	7	601	CHL	CHA-C1A-NA	-2.30	121.14	126.40
31	6	618	CHL	CHC-C1C-NC	2.29	127.68	124.20
31	Z	606	CHL	CHB-C4A-NA	2.29	127.68	124.51
31	8	606	CHL	CHA-C1A-NA	-2.29	121.15	126.40
31	7	606	CHL	CHA-C1A-NA	-2.28	121.17	126.40
31	1	607	CHL	C2A-C1A-CHA	2.28	127.85	123.86
31	Z	607	CHL	CHB-C4A-NA	2.28	127.67	124.51
22	A	809	CLA	C1-C2-C3	-2.28	122.11	126.04
31	92	606	CHL	CHB-C4A-NA	2.27	127.65	124.51
22	B	802	CLA	O2A-C1-C2	-2.27	102.67	108.64
31	1	601	CHL	CHA-C1A-NA	-2.26	121.21	126.40
31	9	607	CHL	CHB-C4A-NA	2.26	127.64	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	9	607	CHL	CHA-C1A-NA	-2.24	121.28	126.40
31	1	606	CHL	CHC-C1C-NC	2.23	127.59	124.20
31	Z	606	CHL	CHA-C1A-NA	-2.23	121.30	126.40
31	7	606	CHL	CHC-C1C-NC	2.22	127.58	124.20
32	1	618	XAT	O4-C5-C4	-2.21	111.72	113.38
22	9	610	CLA	C3D-C4D-ND	2.18	113.76	110.24
31	7	601	CHL	CHC-C1C-NC	2.16	127.48	124.20
21	A	801	CL0	CHA-C1A-NA	-2.14	121.49	126.40
31	5	607	CHL	CHB-C4A-NA	2.14	127.47	124.51
29	F	305	LUT	C8-C7-C6	2.13	133.19	127.20
31	6	616	CHL	C1-C2-C3	-2.13	122.36	126.04
27	B	853	LMU	C1B-O1B-C4'	2.13	123.24	117.96
22	B	814	CLA	C3D-C4D-ND	2.13	113.68	110.24
22	Z	613	CLA	C3D-C4D-ND	2.12	113.67	110.24
22	6	609	CLA	CAA-C2A-C1A	-2.11	105.07	111.97
31	4	606	CHL	C1-C2-C3	-2.11	122.40	126.04
22	5	621	CLA	CHA-C1A-NA	-2.10	121.59	126.40
21	A	801	CL0	C2C-C1C-NC	2.08	111.92	109.97
22	92	610	CLA	C3D-C4D-ND	2.08	113.60	110.24
22	B	841	CLA	C1-C2-C3	-2.08	122.45	126.04
31	6	608	CHL	C3D-C4D-ND	2.07	113.59	110.24
31	5	607	CHL	CHA-C1A-NA	-2.07	121.65	126.40
31	5	607	CHL	C3D-C4D-ND	2.06	113.57	110.24
22	92	602	CLA	C3D-C4D-ND	2.06	113.57	110.24
31	4	607	CHL	C3D-C4D-ND	2.06	113.57	110.24
31	9	607	CHL	C3D-C4D-ND	2.06	113.57	110.24
22	L	204	CLA	C3D-C4D-ND	2.05	113.56	110.24
31	1	607	CHL	CHC-C1C-C2C	-2.05	118.68	126.11
31	5	608	CHL	C3D-C4D-ND	2.04	113.54	110.24
31	4	607	CHL	CHB-C4A-NA	2.04	127.34	124.51
22	A	806	CLA	C3D-C4D-ND	2.04	113.54	110.24
22	1	613	CLA	C3D-C4D-ND	2.03	113.53	110.24
22	4	604	CLA	C3D-C4D-ND	2.03	113.53	110.24
22	9	604	CLA	C3D-C4D-ND	2.03	113.53	110.24
22	L2	203	CLA	C3D-C4D-ND	2.03	113.53	110.24
31	8	606	CHL	C3D-C4D-ND	2.03	113.52	110.24
22	Z	614	CLA	C3D-C4D-ND	2.03	113.52	110.24
22	A	820	CLA	C3D-C4D-ND	2.02	113.51	110.24
22	L2	204	CLA	C3D-C4D-ND	2.02	113.50	110.24
33	5	625	NEX	O24-C25-C26	-2.02	57.29	58.96
31	6	601	CHL	CAA-C2A-C1A	2.01	118.58	111.97
22	A	823	CLA	C3D-C4D-ND	2.01	113.49	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	804	CLA	C3D-C4D-ND	2.01	113.49	110.24
22	5	603	CLA	C3D-C4D-ND	2.01	113.49	110.24
22	3	614	CLA	C3D-C4D-ND	2.00	113.48	110.24
31	6	616	CHL	C3D-C4D-ND	2.00	113.48	110.24
22	6	617	CLA	C3D-C4D-ND	2.00	113.47	110.24
31	Z	606	CHL	C3D-C4D-ND	2.00	113.47	110.24

All (328) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
21	A	801	CL0	NA
21	A	801	CL0	NC
21	A	801	CL0	ND
22	A	802	CLA	ND
22	A	803	CLA	ND
22	A	804	CLA	ND
22	A	805	CLA	ND
22	A	806	CLA	ND
22	A	807	CLA	ND
22	A	808	CLA	ND
22	A	809	CLA	ND
22	A	810	CLA	ND
22	A	811	CLA	ND
22	A	812	CLA	ND
22	A	813	CLA	ND
22	A	814	CLA	ND
22	A	815	CLA	ND
22	A	816	CLA	ND
22	A	817	CLA	ND
22	A	818	CLA	ND
22	A	819	CLA	ND
22	A	820	CLA	ND
22	A	821	CLA	ND
22	A	822	CLA	ND
22	A	823	CLA	ND
22	A	824	CLA	ND
22	A	825	CLA	ND
22	A	826	CLA	ND
22	A	827	CLA	ND
22	A	828	CLA	ND
22	A	829	CLA	ND
22	A	830	CLA	ND

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Mol	Chain	Res	Type	Atom
22	A	831	CLA	ND
22	A	832	CLA	ND
22	A	833	CLA	ND
22	A	834	CLA	ND
22	A	835	CLA	ND
22	A	836	CLA	ND
22	A	837	CLA	ND
22	A	838	CLA	ND
22	A	839	CLA	ND
22	A	840	CLA	ND
22	A	841	CLA	ND
22	A	842	CLA	ND
22	A	843	CLA	ND
22	A	845	CLA	ND
22	A	854	CLA	ND
22	B	802	CLA	ND
22	B	803	CLA	ND
22	B	804	CLA	ND
22	B	805	CLA	ND
22	B	806	CLA	ND
22	B	807	CLA	ND
22	B	808	CLA	ND
22	B	809	CLA	ND
22	B	810	CLA	ND
22	B	811	CLA	ND
22	B	812	CLA	ND
22	B	813	CLA	ND
22	B	814	CLA	ND
22	B	815	CLA	ND
22	B	816	CLA	ND
22	B	817	CLA	ND
22	B	818	CLA	ND
22	B	819	CLA	ND
22	B	820	CLA	ND
22	B	821	CLA	ND
22	B	822	CLA	ND
22	B	823	CLA	ND
22	B	824	CLA	ND
22	B	825	CLA	ND
22	B	826	CLA	ND
22	B	827	CLA	ND
22	B	828	CLA	ND

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Mol	Chain	Res	Type	Atom
22	B	829	CLA	ND
22	B	830	CLA	ND
22	B	831	CLA	ND
22	B	832	CLA	ND
22	B	833	CLA	ND
22	B	834	CLA	ND
22	B	835	CLA	ND
22	B	836	CLA	ND
22	B	837	CLA	ND
22	B	838	CLA	ND
22	B	839	CLA	ND
22	B	840	CLA	ND
22	B	841	CLA	ND
22	F	301	CLA	ND
22	F	303	CLA	ND
22	F	304	CLA	ND
22	G	203	CLA	ND
22	G	204	CLA	ND
22	J	101	CLA	ND
22	L	203	CLA	ND
22	L	204	CLA	ND
22	K	201	CLA	ND
22	K	203	CLA	ND
22	K	204	CLA	ND
22	K	206	CLA	ND
22	1	602	CLA	ND
22	1	603	CLA	ND
22	1	604	CLA	ND
22	1	608	CLA	ND
22	1	609	CLA	ND
22	1	610	CLA	ND
22	1	611	CLA	ND
22	1	612	CLA	ND
22	1	613	CLA	ND
22	1	614	CLA	ND
22	1	616	CLA	ND
22	3	602	CLA	ND
22	3	603	CLA	ND
22	3	604	CLA	ND
22	3	606	CLA	ND
22	3	607	CLA	ND
22	3	609	CLA	ND

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Mol	Chain	Res	Type	Atom
22	3	610	CLA	ND
22	3	611	CLA	ND
22	3	612	CLA	ND
22	3	613	CLA	ND
22	3	614	CLA	ND
22	3	617	CLA	ND
22	3	615	CLA	ND
22	7	602	CLA	ND
22	7	603	CLA	ND
22	7	604	CLA	ND
22	7	608	CLA	ND
22	7	609	CLA	ND
22	7	610	CLA	ND
22	7	611	CLA	ND
22	7	612	CLA	ND
22	7	613	CLA	ND
22	7	614	CLA	ND
22	7	616	CLA	ND
22	7	620	CLA	ND
22	8	602	CLA	ND
22	8	603	CLA	ND
22	8	604	CLA	ND
22	8	608	CLA	ND
22	8	609	CLA	ND
22	8	610	CLA	ND
22	8	611	CLA	ND
22	8	612	CLA	ND
22	8	613	CLA	ND
22	8	614	CLA	ND
22	8	616	CLA	ND
22	Z	602	CLA	ND
22	Z	603	CLA	ND
22	Z	604	CLA	ND
22	Z	608	CLA	ND
22	Z	609	CLA	ND
22	Z	610	CLA	ND
22	Z	611	CLA	ND
22	Z	612	CLA	ND
22	Z	613	CLA	ND
22	Z	614	CLA	ND
22	Z	616	CLA	ND
22	4	602	CLA	ND

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Mol	Chain	Res	Type	Atom
22	4	603	CLA	ND
22	4	604	CLA	ND
22	4	609	CLA	ND
22	4	610	CLA	ND
22	4	611	CLA	ND
22	4	612	CLA	ND
22	4	613	CLA	ND
22	4	614	CLA	ND
22	4	616	CLA	ND
22	5	601	CLA	ND
22	5	602	CLA	ND
22	5	603	CLA	ND
22	5	604	CLA	ND
22	5	609	CLA	ND
22	5	610	CLA	ND
22	5	611	CLA	ND
22	5	612	CLA	ND
22	5	613	CLA	ND
22	5	614	CLA	ND
22	5	616	CLA	ND
22	5	617	CLA	ND
22	5	621	CLA	ND
22	6	602	CLA	ND
22	6	603	CLA	ND
22	6	604	CLA	ND
22	6	609	CLA	ND
22	6	610	CLA	ND
22	6	611	CLA	ND
22	6	612	CLA	ND
22	6	613	CLA	ND
22	6	614	CLA	ND
22	6	617	CLA	ND
22	6	622	CLA	ND
22	9	601	CLA	ND
22	9	602	CLA	ND
22	9	603	CLA	ND
22	9	604	CLA	ND
22	9	609	CLA	ND
22	9	610	CLA	ND
22	9	611	CLA	ND
22	9	612	CLA	ND
22	9	613	CLA	ND

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Mol	Chain	Res	Type	Atom
22	9	614	CLA	ND
22	B2	804	CLA	ND
22	B2	805	CLA	ND
22	B2	806	CLA	ND
22	B2	807	CLA	ND
22	B2	808	CLA	ND
22	B2	809	CLA	ND
22	B2	810	CLA	ND
22	B2	811	CLA	ND
22	B2	813	CLA	ND
22	B2	814	CLA	ND
22	B2	815	CLA	ND
22	B2	828	CLA	ND
22	B2	829	CLA	ND
22	B2	839	CLA	ND
22	B2	812	CLA	ND
22	B2	820	CLA	ND
22	L2	203	CLA	ND
22	L2	204	CLA	ND
22	92	601	CLA	ND
22	92	602	CLA	ND
22	92	603	CLA	ND
22	92	604	CLA	ND
22	92	609	CLA	ND
22	92	610	CLA	ND
22	92	611	CLA	ND
22	92	612	CLA	ND
22	92	613	CLA	ND
22	92	614	CLA	ND
31	1	601	CHL	NA
31	1	601	CHL	NC
31	1	601	CHL	ND
31	1	606	CHL	NA
31	1	606	CHL	NC
31	1	606	CHL	ND
31	1	607	CHL	NA
31	1	607	CHL	NC
31	1	607	CHL	ND
31	3	608	CHL	NA
31	3	608	CHL	NC
31	3	608	CHL	ND
31	7	601	CHL	NA

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Mol	Chain	Res	Type	Atom
31	7	601	CHL	NC
31	7	601	CHL	ND
31	7	606	CHL	NA
31	7	606	CHL	NC
31	7	606	CHL	ND
31	7	607	CHL	NA
31	7	607	CHL	NC
31	7	607	CHL	ND
31	8	601	CHL	NA
31	8	601	CHL	NC
31	8	601	CHL	ND
31	8	606	CHL	NA
31	8	606	CHL	NC
31	8	606	CHL	ND
31	8	607	CHL	NA
31	8	607	CHL	NC
31	8	607	CHL	ND
31	Z	601	CHL	NA
31	Z	601	CHL	NC
31	Z	601	CHL	ND
31	Z	606	CHL	NA
31	Z	606	CHL	NC
31	Z	606	CHL	ND
31	Z	607	CHL	NA
31	Z	607	CHL	NC
31	Z	607	CHL	ND
31	4	601	CHL	NA
31	4	601	CHL	NC
31	4	601	CHL	ND
31	4	606	CHL	NA
31	4	606	CHL	NC
31	4	606	CHL	ND
31	4	607	CHL	NA
31	4	607	CHL	NC
31	4	607	CHL	ND
31	4	608	CHL	NA
31	4	608	CHL	NC
31	4	608	CHL	ND
31	4	618	CHL	NA
31	4	618	CHL	NC
31	4	618	CHL	ND
31	5	606	CHL	NA

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Mol	Chain	Res	Type	Atom
31	5	606	CHL	NC
31	5	606	CHL	ND
31	5	607	CHL	NA
31	5	607	CHL	NC
31	5	607	CHL	ND
31	5	608	CHL	NA
31	5	608	CHL	NC
31	5	608	CHL	ND
31	5	618	CHL	NA
31	5	618	CHL	NC
31	5	618	CHL	ND
31	6	601	CHL	NA
31	6	601	CHL	NC
31	6	601	CHL	ND
31	6	606	CHL	NA
31	6	606	CHL	NC
31	6	606	CHL	ND
31	6	607	CHL	NA
31	6	607	CHL	NC
31	6	607	CHL	ND
31	6	608	CHL	NA
31	6	608	CHL	NC
31	6	608	CHL	ND
31	6	616	CHL	NA
31	6	616	CHL	NC
31	6	616	CHL	ND
31	6	618	CHL	NA
31	6	618	CHL	NC
31	6	618	CHL	ND
31	9	606	CHL	NA
31	9	606	CHL	NC
31	9	606	CHL	ND
31	9	607	CHL	NA
31	9	607	CHL	NC
31	9	607	CHL	ND
31	92	606	CHL	NA
31	92	606	CHL	NC
31	92	606	CHL	ND
31	92	607	CHL	NA
31	92	607	CHL	NC
31	92	607	CHL	ND
32	1	618	XAT	C6

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Mol	Chain	Res	Type	Atom
32	5	624	XAT	C26
33	6	625	NEX	C25

All (1376) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	A	806	CLA	CHA-CBD-CGD-O1D
22	A	806	CLA	CHA-CBD-CGD-O2D
22	A	806	CLA	CAD-CBD-CGD-O1D
22	A	806	CLA	CAD-CBD-CGD-O2D
22	A	806	CLA	C2-C3-C5-C6
22	A	806	CLA	C4-C3-C5-C6
22	A	809	CLA	CHA-CBD-CGD-O1D
22	A	809	CLA	CHA-CBD-CGD-O2D
22	A	816	CLA	O2A-C1-C2-C3
22	A	825	CLA	CHA-CBD-CGD-O1D
22	A	825	CLA	CHA-CBD-CGD-O2D
22	A	829	CLA	C2-C3-C5-C6
22	A	829	CLA	C4-C3-C5-C6
22	A	835	CLA	CHA-CBD-CGD-O1D
22	A	835	CLA	CHA-CBD-CGD-O2D
22	A	837	CLA	CHA-CBD-CGD-O1D
22	A	837	CLA	CHA-CBD-CGD-O2D
22	A	840	CLA	CHA-CBD-CGD-O1D
22	A	840	CLA	CHA-CBD-CGD-O2D
22	A	841	CLA	CHA-CBD-CGD-O1D
22	A	841	CLA	CHA-CBD-CGD-O2D
22	A	843	CLA	O2A-C1-C2-C3
22	A	845	CLA	CHA-CBD-CGD-O1D
22	A	845	CLA	CHA-CBD-CGD-O2D
22	A	845	CLA	CAD-CBD-CGD-O1D
22	A	845	CLA	CAD-CBD-CGD-O2D
22	B	804	CLA	CHA-CBD-CGD-O2D
22	B	808	CLA	CHA-CBD-CGD-O2D
22	B	822	CLA	C2-C3-C5-C6
22	B	822	CLA	C4-C3-C5-C6
22	B	823	CLA	CHA-CBD-CGD-O1D
22	B	823	CLA	CHA-CBD-CGD-O2D
22	B	825	CLA	CHA-CBD-CGD-O1D
22	B	825	CLA	CHA-CBD-CGD-O2D
22	B	833	CLA	CHA-CBD-CGD-O1D
22	B	833	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
22	B	840	CLA	C4-C3-C5-C6
22	F	304	CLA	C1A-C2A-CAA-CBA
22	F	304	CLA	C2-C1-O2A-CGA
22	F	304	CLA	CHA-CBD-CGD-O1D
22	F	304	CLA	CHA-CBD-CGD-O2D
22	G	204	CLA	CHA-CBD-CGD-O1D
22	G	204	CLA	CHA-CBD-CGD-O2D
22	J	101	CLA	CHA-CBD-CGD-O1D
22	J	101	CLA	CHA-CBD-CGD-O2D
22	J	101	CLA	C2-C3-C5-C6
22	J	101	CLA	C4-C3-C5-C6
22	L	203	CLA	CHA-CBD-CGD-O1D
22	L	203	CLA	C4-C3-C5-C6
22	K	203	CLA	CHA-CBD-CGD-O1D
22	K	203	CLA	CHA-CBD-CGD-O2D
22	1	603	CLA	C2-C3-C5-C6
22	1	603	CLA	C4-C3-C5-C6
22	7	610	CLA	C1A-C2A-CAA-CBA
22	7	610	CLA	C3A-C2A-CAA-CBA
22	Z	609	CLA	C1A-C2A-CAA-CBA
22	Z	613	CLA	CHA-CBD-CGD-O1D
22	4	610	CLA	C4-C3-C5-C6
22	4	613	CLA	C2-C3-C5-C6
22	4	613	CLA	C4-C3-C5-C6
22	5	603	CLA	CHA-CBD-CGD-O1D
22	5	603	CLA	CHA-CBD-CGD-O2D
22	5	611	CLA	C2-C3-C5-C6
22	5	611	CLA	C4-C3-C5-C6
22	5	617	CLA	CHA-CBD-CGD-O1D
22	5	617	CLA	CHA-CBD-CGD-O2D
22	5	617	CLA	C2-C3-C5-C6
22	5	617	CLA	C4-C3-C5-C6
22	9	609	CLA	C4-C3-C5-C6
22	9	613	CLA	O2A-C1-C2-C3
22	B2	808	CLA	CHA-CBD-CGD-O1D
22	B2	808	CLA	CHA-CBD-CGD-O2D
22	B2	810	CLA	C1A-C2A-CAA-CBA
22	B2	814	CLA	CAD-CBD-CGD-O1D
22	L2	204	CLA	CHA-CBD-CGD-O1D
22	L2	204	CLA	CHA-CBD-CGD-O2D
22	92	601	CLA	CHA-CBD-CGD-O2D
22	92	602	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
22	92	602	CLA	C4-C3-C5-C6
22	92	609	CLA	C1A-C2A-CAA-CBA
22	92	613	CLA	CHA-CBD-CGD-O1D
22	92	613	CLA	CHA-CBD-CGD-O2D
24	A	846	LHG	C3-O3-P-O5
24	A	846	LHG	C4-O6-P-O5
24	3	721	LHG	C2-C3-O3-P
24	3	721	LHG	C3-O3-P-O4
24	3	721	LHG	C4-O6-P-O5
24	3	623	LHG	O2-C2-C3-O3
24	3	623	LHG	C3-O3-P-O5
24	3	623	LHG	O6-C4-C5-O7
24	7	625	LHG	C1-C2-C3-O3
24	7	625	LHG	C3-O3-P-O4
24	7	625	LHG	C3-O3-P-O5
24	7	625	LHG	C3-O3-P-O6
24	8	620	LHG	C3-O3-P-O5
24	8	620	LHG	C4-O6-P-O3
24	8	620	LHG	C4-O6-P-O4
24	4	622	LHG	C2-C3-O3-P
24	4	622	LHG	C3-O3-P-O4
24	4	623	LHG	C3-O3-P-O4
24	4	623	LHG	C3-O3-P-O5
24	4	623	LHG	C4-O6-P-O3
24	4	623	LHG	C4-O6-P-O4
24	4	623	LHG	C4-O6-P-O5
24	5	623	LHG	C3-O3-P-O5
24	5	623	LHG	C3-O3-P-O6
24	5	623	LHG	C4-O6-P-O3
24	5	623	LHG	C4-O6-P-O4
24	5	623	LHG	C4-O6-P-O5
24	6	629	LHG	C1-C2-C3-O3
24	6	629	LHG	C4-O6-P-O4
24	6	629	LHG	C4-O6-P-O5
24	9	622	LHG	C1-C2-C3-O3
24	9	622	LHG	C3-O3-P-O5
24	9	622	LHG	C4-O6-P-O4
24	92	622	LHG	C1-C2-C3-O3
24	92	622	LHG	C4-O6-P-O3
24	92	622	LHG	C4-O6-P-O4
25	A	848	BCR	C1-C6-C7-C8
25	A	851	BCR	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
25	A	851	BCR	C23-C24-C25-C30
25	B	847	BCR	C23-C24-C25-C30
25	J	102	BCR	C23-C24-C25-C26
25	L	201	BCR	C1-C6-C7-C8
25	3	620	BCR	C1-C6-C7-C8
25	3	620	BCR	C5-C6-C7-C8
25	3	718	BCR	C23-C24-C25-C30
25	8	619	BCR	C1-C6-C7-C8
25	8	619	BCR	C5-C6-C7-C8
25	9	623	BCR	C23-C24-C25-C26
25	B2	848	BCR	C1-C6-C7-C8
25	L2	201	BCR	C1-C6-C7-C8
25	92	623	BCR	C23-C24-C25-C26
27	A	858	LMU	O5'-C1'-O1'-C1
27	A	865	LMU	C2'-C1'-O1'-C1
27	A	865	LMU	O5'-C1'-O1'-C1
27	B	853	LMU	O5'-C1'-O1'-C1
27	G	206	LMU	C2'-C1'-O1'-C1
27	G	206	LMU	O5'-C1'-O1'-C1
27	1	622	LMU	C2'-C1'-O1'-C1
27	1	622	LMU	O5'-C1'-O1'-C1
27	1	622	LMU	C2-C1-O1'-C1'
27	1	627	LMU	C2'-C1'-O1'-C1
27	1	627	LMU	O5'-C1'-O1'-C1
27	1	627	LMU	C2-C1-O1'-C1'
27	7	627	LMU	C2'-C1'-O1'-C1
27	7	627	LMU	O5'-C1'-O1'-C1
27	7	628	LMU	C2'-C1'-O1'-C1
27	7	628	LMU	O5'-C1'-O1'-C1
27	7	628	LMU	C2-C1-O1'-C1'
27	7	629	LMU	C2'-C1'-O1'-C1
27	7	629	LMU	O5'-C1'-O1'-C1
27	8	628	LMU	C2'-C1'-O1'-C1
27	Z	622	LMU	C2-C1-O1'-C1'
27	Z	621	LMU	C2'-C1'-O1'-C1
27	Z	621	LMU	O5'-C1'-O1'-C1
27	4	625	LMU	C2'-C1'-O1'-C1
27	4	625	LMU	O5'-C1'-O1'-C1
27	5	627	LMU	C2-C1-O1'-C1'
27	6	632	LMU	C2'-C1'-O1'-C1
27	6	632	LMU	O5'-C1'-O1'-C1
27	6	632	LMU	C2-C1-O1'-C1'

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Mol	Chain	Res	Type	Atoms
27	6	628	LMU	C2'-C1'-O1'-C1
27	6	628	LMU	O5'-C1'-O1'-C1
27	6	631	LMU	C2'-C1'-O1'-C1
27	6	631	LMU	O5'-C1'-O1'-C1
28	A	859	LMG	C2-C1-O1-C7
28	A	859	LMG	O6-C1-O1-C7
28	A	860	LMG	C2-C1-O1-C7
28	A	860	LMG	O6-C1-O1-C7
28	B	854	LMG	C2-C1-O1-C7
28	B	854	LMG	O6-C1-O1-C7
28	7	626	LMG	C2-C1-O1-C7
28	7	626	LMG	O6-C1-O1-C7
28	8	626	LMG	C2-C1-O1-C7
28	8	626	LMG	O6-C1-O1-C7
28	8	629	LMG	C2-C1-O1-C7
28	8	629	LMG	O6-C1-O1-C7
28	9	620	LMG	C2-C1-O1-C7
28	9	620	LMG	O6-C1-O1-C7
28	B2	852	LMG	O6-C1-O1-C7
29	A	856	LUT	C5-C6-C7-C8
29	A	856	LUT	C21-C26-C27-C28
29	A	856	LUT	C25-C26-C27-C28
29	F	305	LUT	C1-C6-C7-C8
29	F	305	LUT	C5-C6-C7-C8
29	F	305	LUT	C25-C26-C27-C28
29	3	621	LUT	C1-C6-C7-C8
29	7	624	LUT	C21-C26-C27-C28
29	7	624	LUT	C25-C26-C27-C28
29	7	624	LUT	C27-C28-C29-C30
29	7	624	LUT	C27-C28-C29-C39
29	5	620	LUT	C1-C6-C7-C8
29	5	626	LUT	C21-C26-C27-C28
29	6	621	LUT	C1-C6-C7-C8
30	B	850	DGD	C2D-C1D-O3G-C3G
30	B	850	DGD	O6D-C1D-O3G-C3G
31	1	601	CHL	C2-C3-C5-C6
31	1	601	CHL	C4-C3-C5-C6
31	8	601	CHL	CHA-CBD-CGD-O1D
31	8	601	CHL	CHA-CBD-CGD-O2D
31	8	601	CHL	CAD-CBD-CGD-O1D
31	8	607	CHL	C2-C3-C5-C6
31	8	607	CHL	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
31	Z	606	CHL	C1A-C2A-CAA-CBA
31	6	616	CHL	CHA-CBD-CGD-O1D
31	6	616	CHL	CHA-CBD-CGD-O2D
31	92	607	CHL	CHA-CBD-CGD-O1D
27	A	858	LMU	O5B-C1B-O1B-C4'
27	A	858	LMU	C2B-C1B-O1B-C4'
27	8	627	LMU	O5B-C1B-O1B-C4'
22	B	806	CLA	C3-C5-C6-C7
27	A	863	LMU	O5B-C1B-O1B-C4'
27	A	863	LMU	C2B-C1B-O1B-C4'
31	7	601	CHL	C4-C3-C5-C6
22	B	840	CLA	C2-C3-C5-C6
22	4	610	CLA	C2-C3-C5-C6
22	B	839	CLA	C2A-CAA-CBA-CGA
22	5	603	CLA	C2A-CAA-CBA-CGA
27	8	627	LMU	C2B-C1B-O1B-C4'
22	5	621	CLA	C2C-C3C-CAC-CBC
27	B	853	LMU	C2B-C1B-O1B-C4'
24	3	721	LHG	O2-C2-C3-O3
24	7	625	LHG	O2-C2-C3-O3
24	4	623	LHG	O2-C2-C3-O3
24	6	629	LHG	O2-C2-C3-O3
24	9	622	LHG	O2-C2-C3-O3
24	92	622	LHG	O2-C2-C3-O3
22	B	808	CLA	C3-C5-C6-C7
24	6	629	LHG	C2-C3-O3-P
22	B	833	CLA	C4-C3-C5-C6
22	7	612	CLA	C4-C3-C5-C6
22	8	612	CLA	C4-C3-C5-C6
22	Z	603	CLA	C4-C3-C5-C6
22	B	833	CLA	C2-C3-C5-C6
22	L	203	CLA	C2-C3-C5-C6
22	7	612	CLA	C2-C3-C5-C6
22	8	612	CLA	C2-C3-C5-C6
22	Z	603	CLA	C2-C3-C5-C6
22	A	830	CLA	C2A-CAA-CBA-CGA
27	A	861	LMU	O5'-C1'-O1'-C1
27	A	864	LMU	O5'-C1'-O1'-C1
27	8	628	LMU	O5'-C1'-O1'-C1
24	1	620	LHG	C1-C2-C3-O3
24	3	623	LHG	C1-C2-C3-O3
27	8	627	LMU	C5'-C4'-O1B-C1B

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Mol	Chain	Res	Type	Atoms
24	1	620	LHG	O2-C2-C3-O3
27	A	858	LMU	C2'-C1'-O1'-C1
27	B	853	LMU	C2'-C1'-O1'-C1
31	7	601	CHL	C2-C3-C5-C6
22	A	806	CLA	C11-C10-C8-C9
22	B	808	CLA	C14-C13-C15-C16
22	B	809	CLA	C6-C7-C8-C9
22	G	203	CLA	C6-C7-C8-C9
22	1	609	CLA	C11-C10-C8-C9
22	4	609	CLA	C11-C10-C8-C9
22	5	603	CLA	C11-C10-C8-C9
22	5	603	CLA	C14-C13-C15-C16
31	1	601	CHL	C6-C7-C8-C9
28	4	624	LMG	C10-C11-C12-C13
31	6	616	CHL	C8-C10-C11-C12
22	B	803	CLA	C10-C11-C12-C13
22	B	818	CLA	C13-C15-C16-C17
22	5	609	CLA	C10-C11-C12-C13
27	B	853	LMU	O5B-C1B-O1B-C4'
27	8	627	LMU	C3'-C4'-O1B-C1B
22	A	840	CLA	C12-C13-C15-C16
22	B	817	CLA	C11-C10-C8-C7
22	7	611	CLA	C6-C7-C8-C10
22	5	601	CLA	C6-C7-C8-C10
22	B2	806	CLA	C11-C12-C13-C15
31	5	607	CHL	C11-C10-C8-C7
22	5	617	CLA	C8-C10-C11-C12
27	A	862	LMU	O5'-C1'-O1'-C1
22	A	840	CLA	C15-C16-C17-C18
24	8	620	LHG	O2-C2-C3-O3
22	5	621	CLA	C4C-C3C-CAC-CBC
22	A	813	CLA	C15-C16-C17-C18
24	A	846	LHG	C4-O6-P-O3
24	A	847	LHG	C4-O6-P-O3
24	1	620	LHG	C3-O3-P-O6
24	3	721	LHG	C4-O6-P-O3
24	3	623	LHG	C3-O3-P-O6
24	3	623	LHG	C4-O6-P-O3
24	4	622	LHG	C3-O3-P-O6
24	6	629	LHG	C4-O6-P-O3
22	4	603	CLA	C3-C5-C6-C7
24	8	620	LHG	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
24	4	623	LHG	C1-C2-C3-O3
22	B2	810	CLA	C4-C3-C5-C6
22	B	823	CLA	C2A-CAA-CBA-CGA
22	7	616	CLA	C2A-CAA-CBA-CGA
22	B2	805	CLA	C2A-CAA-CBA-CGA
22	A	818	CLA	C3-C5-C6-C7
28	6	633	LMG	C17-C18-C19-C20
24	B	851	LHG	O2-C2-C3-O3
27	A	862	LMU	C2'-C1'-O1'-C1
27	A	863	LMU	C2'-C1'-O1'-C1
27	K	208	LMU	C2'-C1'-O1'-C1
22	3	603	CLA	C8-C10-C11-C12
24	6	619	LHG	C26-C27-C28-C29
22	B2	810	CLA	C2-C3-C5-C6
22	A	813	CLA	C6-C7-C8-C9
22	A	820	CLA	C11-C12-C13-C14
22	A	826	CLA	C11-C10-C8-C9
22	A	839	CLA	C11-C12-C13-C14
22	A	843	CLA	C11-C12-C13-C14
22	L	203	CLA	C14-C13-C15-C16
22	7	611	CLA	C11-C12-C13-C14
22	6	613	CLA	C11-C10-C8-C9
22	92	602	CLA	C14-C13-C15-C16
31	Z	607	CHL	C10-C11-C12-C13
22	1	614	CLA	C2A-CAA-CBA-CGA
27	7	629	LMU	O5'-C5'-C6'-O6'
27	92	624	LMU	O5'-C5'-C6'-O6'
22	B	820	CLA	C5-C6-C7-C8
22	A	825	CLA	C3-C5-C6-C7
22	A	834	CLA	C3A-C2A-CAA-CBA
22	B	823	CLA	C3A-C2A-CAA-CBA
22	3	611	CLA	C3A-C2A-CAA-CBA
22	7	616	CLA	C3A-C2A-CAA-CBA
22	9	603	CLA	C3A-C2A-CAA-CBA
22	B2	810	CLA	C3A-C2A-CAA-CBA
31	Z	606	CHL	C3A-C2A-CAA-CBA
27	B	853	LMU	C2-C1-O1'-C1'
27	1	621	LMU	C2-C1-O1'-C1'
27	1	625	LMU	C2-C1-O1'-C1'
27	8	624	LMU	C2-C1-O1'-C1'
22	9	612	CLA	C13-C15-C16-C17
22	A	826	CLA	O2A-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
22	9	609	CLA	O2A-C1-C2-C3
31	Z	601	CHL	O2A-C1-C2-C3
24	8	620	LHG	C23-C24-C25-C26
22	1	611	CLA	C5-C6-C7-C8
22	B	820	CLA	C4-C3-C5-C6
22	B	828	CLA	C4-C3-C5-C6
22	B2	806	CLA	C4-C3-C5-C6
31	6	607	CHL	C4-C3-C5-C6
22	A	835	CLA	C2-C3-C5-C6
22	B	820	CLA	C2-C3-C5-C6
22	B	828	CLA	C2-C3-C5-C6
22	Z	609	CLA	C2-C3-C5-C6
31	6	607	CHL	C2-C3-C5-C6
22	A	806	CLA	C5-C6-C7-C8
24	B	851	LHG	C1-C2-C3-O3
22	B	829	CLA	C5-C6-C7-C8
24	4	622	LHG	C9-C10-C11-C12
24	A	846	LHG	C23-C24-C25-C26
25	A	848	BCR	C5-C6-C7-C8
25	B	846	BCR	C23-C24-C25-C26
25	B	846	BCR	C23-C24-C25-C30
25	B	847	BCR	C23-C24-C25-C26
25	B	848	BCR	C1-C6-C7-C8
25	B	848	BCR	C5-C6-C7-C8
25	J	102	BCR	C23-C24-C25-C30
25	K	202	BCR	C23-C24-C25-C26
25	K	202	BCR	C23-C24-C25-C30
25	K	207	BCR	C23-C24-C25-C26
25	K	207	BCR	C23-C24-C25-C30
25	3	620	BCR	C23-C24-C25-C26
25	3	620	BCR	C23-C24-C25-C30
25	3	719	BCR	C23-C24-C25-C26
25	3	719	BCR	C23-C24-C25-C30
25	7	623	BCR	C23-C24-C25-C26
25	7	623	BCR	C23-C24-C25-C30
25	8	619	BCR	C23-C24-C25-C26
25	8	619	BCR	C23-C24-C25-C30
25	4	621	BCR	C23-C24-C25-C26
25	4	621	BCR	C23-C24-C25-C30
25	5	622	BCR	C23-C24-C25-C26
25	5	622	BCR	C23-C24-C25-C30
25	6	623	BCR	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
25	6	623	BCR	C23-C24-C25-C30
25	9	623	BCR	C23-C24-C25-C30
25	92	623	BCR	C1-C6-C7-C8
25	92	623	BCR	C5-C6-C7-C8
25	92	623	BCR	C23-C24-C25-C30
29	A	856	LUT	C1-C6-C7-C8
29	1	617	LUT	C1-C6-C7-C8
29	1	617	LUT	C5-C6-C7-C8
29	1	619	LUT	C1-C6-C7-C8
29	1	619	LUT	C5-C6-C7-C8
29	3	621	LUT	C5-C6-C7-C8
29	3	622	LUT	C1-C6-C7-C8
29	8	617	LUT	C1-C6-C7-C8
29	8	617	LUT	C5-C6-C7-C8
29	Z	617	LUT	C1-C6-C7-C8
29	Z	617	LUT	C5-C6-C7-C8
29	Z	619	LUT	C1-C6-C7-C8
29	Z	619	LUT	C5-C6-C7-C8
29	5	620	LUT	C5-C6-C7-C8
29	5	626	LUT	C1-C6-C7-C8
29	5	626	LUT	C5-C6-C7-C8
29	6	621	LUT	C5-C6-C7-C8
29	9	616	LUT	C1-C6-C7-C8
29	9	616	LUT	C5-C6-C7-C8
29	92	616	LUT	C1-C6-C7-C8
29	92	616	LUT	C5-C6-C7-C8
24	8	620	LHG	C17-C18-C19-C20
28	B	852	LMG	C11-C12-C13-C14
22	9	611	CLA	C10-C11-C12-C13
22	A	826	CLA	C4-C3-C5-C6
22	A	835	CLA	C4-C3-C5-C6
22	9	611	CLA	C4-C3-C5-C6
22	A	810	CLA	C11-C10-C8-C7
22	A	820	CLA	C11-C12-C13-C15
22	A	823	CLA	C11-C12-C13-C15
22	A	839	CLA	C11-C12-C13-C15
22	B	808	CLA	C12-C13-C15-C16
22	B	839	CLA	C2-C3-C5-C6
22	G	203	CLA	C6-C7-C8-C10
22	L	203	CLA	C12-C13-C15-C16
22	3	615	CLA	C11-C10-C8-C7
22	7	611	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
22	8	610	CLA	C11-C12-C13-C15
22	6	613	CLA	C2-C3-C5-C6
31	5	607	CHL	C6-C7-C8-C10
27	1	621	LMU	O5B-C1B-O1B-C4'
22	A	854	CLA	C2A-CAA-CBA-CGA
27	9	624	LMU	C4-C5-C6-C7
22	Z	604	CLA	C3-C5-C6-C7
27	A	863	LMU	O5'-C1'-O1'-C1
27	K	208	LMU	O5'-C1'-O1'-C1
22	Z	609	CLA	C13-C15-C16-C17
22	4	609	CLA	C5-C6-C7-C8
22	B	817	CLA	C2C-C3C-CAC-CBC
24	B	851	LHG	C17-C18-C19-C20
22	A	826	CLA	C10-C11-C12-C13
22	1	608	CLA	C10-C11-C12-C13
22	3	607	CLA	C2C-C3C-CAC-CBC
24	5	623	LHG	O7-C5-C6-O8
27	A	864	LMU	O5'-C5'-C6'-O6'
27	B	853	LMU	O5'-C5'-C6'-O6'
27	6	630	LMU	O5'-C5'-C6'-O6'
28	1	628	LMG	O6-C5-C6-O5
28	7	626	LMG	O6-C5-C6-O5
22	B	839	CLA	C4-C3-C5-C6
22	Z	609	CLA	C4-C3-C5-C6
22	6	613	CLA	C4-C3-C5-C6
22	A	817	CLA	C2-C3-C5-C6
22	A	826	CLA	C2-C3-C5-C6
22	9	611	CLA	C2-C3-C5-C6
22	B2	806	CLA	C2-C3-C5-C6
22	A	810	CLA	C11-C10-C8-C9
22	A	823	CLA	C11-C12-C13-C14
22	A	828	CLA	C14-C13-C15-C16
22	A	840	CLA	C14-C13-C15-C16
22	B	802	CLA	C11-C10-C8-C9
22	B	805	CLA	C14-C13-C15-C16
22	B	817	CLA	C11-C10-C8-C9
22	3	615	CLA	C11-C10-C8-C9
22	7	611	CLA	C6-C7-C8-C9
22	8	610	CLA	C11-C12-C13-C14
22	5	601	CLA	C6-C7-C8-C9
22	B2	806	CLA	C11-C12-C13-C14
31	5	607	CHL	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
31	5	607	CHL	C11-C10-C8-C9
28	B2	855	LMG	O6-C5-C6-O5
31	6	607	CHL	C15-C16-C17-C18
22	5	603	CLA	C3-C5-C6-C7
27	1	622	LMU	O5'-C5'-C6'-O6'
28	A	860	LMG	O6-C5-C6-O5
28	8	626	LMG	O6-C5-C6-O5
22	A	812	CLA	C1A-C2A-CAA-CBA
22	A	834	CLA	C1A-C2A-CAA-CBA
22	B	823	CLA	C1A-C2A-CAA-CBA
22	B	838	CLA	C1A-C2A-CAA-CBA
22	J	101	CLA	C1A-C2A-CAA-CBA
22	1	611	CLA	C1A-C2A-CAA-CBA
22	3	611	CLA	C1A-C2A-CAA-CBA
22	9	603	CLA	C1A-C2A-CAA-CBA
28	J	104	LMG	O6-C5-C6-O5
28	8	629	LMG	O6-C5-C6-O5
22	A	836	CLA	C8-C10-C11-C12
22	B	840	CLA	C15-C16-C17-C18
22	K	203	CLA	C5-C6-C7-C8
24	Z	620	LHG	C4-O6-P-O3
24	4	623	LHG	C3-O3-P-O6
27	1	625	LMU	O5'-C5'-C6'-O6'
22	A	834	CLA	C13-C15-C16-C17
22	B	836	CLA	C10-C11-C12-C13
31	4	608	CHL	C15-C16-C17-C18
28	9	620	LMG	O6-C5-C6-O5
24	A	847	LHG	O6-C4-C5-C6
24	3	721	LHG	O6-C4-C5-C6
24	5	623	LHG	O6-C4-C5-C6
27	A	861	LMU	O5'-C5'-C6'-O6'
22	B	827	CLA	C3-C5-C6-C7
28	4	624	LMG	O6-C5-C6-O5
22	A	817	CLA	C4-C3-C5-C6
22	A	828	CLA	C4-C3-C5-C6
22	A	841	CLA	C4-C3-C5-C6
22	7	603	CLA	C2-C3-C5-C6
22	B	824	CLA	C8-C10-C11-C12
27	8	627	LMU	O5B-C5B-C6B-O6B
28	J	103	LMG	C16-C17-C18-C19
28	3	722	LMG	C33-C34-C35-C36
31	8	607	CHL	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
27	8	625	LMU	O5'-C5'-C6'-O6'
24	7	625	LHG	C4-C5-C6-O8
28	J	104	LMG	O1-C7-C8-C9
28	4	624	LMG	O1-C7-C8-C9
27	A	857	LMU	O5B-C5B-C6B-O6B
28	A	860	LMG	C8-C7-O1-C1
28	J	104	LMG	C8-C7-O1-C1
22	Z	611	CLA	C10-C11-C12-C13
27	A	858	LMU	O5B-C5B-C6B-O6B
22	A	833	CLA	C3-C5-C6-C7
27	G	206	LMU	O5'-C5'-C6'-O6'
27	8	628	LMU	O5'-C5'-C6'-O6'
22	A	830	CLA	C4-C3-C5-C6
22	A	840	CLA	C4-C3-C5-C6
22	1	609	CLA	C4-C3-C5-C6
22	7	603	CLA	C4-C3-C5-C6
22	9	612	CLA	C4-C3-C5-C6
31	6	601	CHL	C4-C3-C5-C6
22	A	830	CLA	C2-C3-C5-C6
22	A	843	CLA	C2-C3-C5-C6
27	9	624	LMU	O5'-C5'-C6'-O6'
22	5	601	CLA	C10-C11-C12-C13
22	6	603	CLA	C5-C6-C7-C8
27	1	623	LMU	C11-C10-C9-C8
27	6	631	LMU	O5'-C5'-C6'-O6'
22	A	806	CLA	C2A-CAA-CBA-CGA
22	A	810	CLA	C2A-CAA-CBA-CGA
22	A	806	CLA	C2-C1-O2A-CGA
22	5	603	CLA	C2-C1-O2A-CGA
24	A	847	LHG	O6-C4-C5-O7
24	9	622	LHG	C25-C26-C27-C28
22	8	602	CLA	C8-C10-C11-C12
27	9	624	LMU	C2'-C1'-O1'-C1
24	B	851	LHG	O7-C7-C8-C9
31	5	607	CHL	CAA-CBA-CGA-O2A
24	B	851	LHG	O7-C5-C6-O8
22	B	811	CLA	C15-C16-C17-C18
22	B	821	CLA	C10-C11-C12-C13
22	5	603	CLA	C5-C6-C7-C8
22	3	603	CLA	C4-C3-C5-C6
22	A	828	CLA	C2-C3-C5-C6
22	A	828	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
22	A	834	CLA	C11-C10-C8-C7
22	A	841	CLA	C2-C3-C5-C6
22	B	802	CLA	C11-C10-C8-C7
22	F	301	CLA	C11-C10-C8-C7
22	1	609	CLA	C2-C3-C5-C6
22	1	614	CLA	C2-C3-C5-C6
22	1	614	CLA	C6-C7-C8-C10
22	5	603	CLA	C11-C10-C8-C7
23	A	844	PQN	C17-C18-C20-C21
31	1	601	CHL	C11-C12-C13-C15
31	Z	601	CHL	C6-C7-C8-C10
31	6	601	CHL	C2-C3-C5-C6
22	A	812	CLA	C6-C7-C8-C9
22	B	827	CLA	C11-C10-C8-C9
22	B	834	CLA	C11-C10-C8-C9
22	Z	609	CLA	C11-C12-C13-C14
23	A	844	PQN	C19-C18-C20-C21
31	Z	601	CHL	C6-C7-C8-C9
24	4	622	LHG	C1-C2-C3-O3
22	8	603	CLA	C15-C16-C17-C18
22	A	829	CLA	C5-C6-C7-C8
22	B	817	CLA	C13-C15-C16-C17
22	92	609	CLA	C4C-C3C-CAC-CBC
28	A	859	LMG	C40-C41-C42-C43
24	B	851	LHG	O6-C4-C5-C6
24	Z	620	LHG	O6-C4-C5-C6
24	92	622	LHG	O6-C4-C5-C6
22	A	816	CLA	C13-C15-C16-C17
22	92	611	CLA	C15-C16-C17-C18
22	A	820	CLA	C4-C3-C5-C6
22	B	807	CLA	C4-C3-C5-C6
22	B	808	CLA	C4-C3-C5-C6
22	B	812	CLA	C4-C3-C5-C6
22	B	829	CLA	C4-C3-C5-C6
22	1	614	CLA	C4-C3-C5-C6
22	92	612	CLA	C4-C3-C5-C6
22	A	840	CLA	C2-C3-C5-C6
22	B	808	CLA	C2-C3-C5-C6
22	B	829	CLA	C2-C3-C5-C6
22	9	612	CLA	C2-C3-C5-C6
22	A	828	CLA	C8-C10-C11-C12
22	B	826	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
22	7	611	CLA	C8-C10-C11-C12
24	4	623	LHG	C13-C14-C15-C16
22	B	805	CLA	C3A-C2A-CAA-CBA
27	A	857	LMU	C2-C1-O1'-C1'
27	A	858	LMU	C2-C1-O1'-C1'
27	G	206	LMU	C2-C1-O1'-C1'
27	7	629	LMU	C2-C1-O1'-C1'
27	8	628	LMU	C2-C1-O1'-C1'
27	8	627	LMU	C2-C1-O1'-C1'
27	8	625	LMU	C2-C1-O1'-C1'
24	8	620	LHG	C26-C27-C28-C29
22	A	823	CLA	O2A-C1-C2-C3
22	A	827	CLA	O2A-C1-C2-C3
31	8	607	CHL	O2A-C1-C2-C3
31	4	606	CHL	O2A-C1-C2-C3
22	A	810	CLA	C4-C3-C5-C6
22	A	815	CLA	C4-C3-C5-C6
22	5	610	CLA	C4-C3-C5-C6
22	3	603	CLA	C2-C3-C5-C6
22	92	612	CLA	C2-C3-C5-C6
24	8	620	LHG	C15-C16-C17-C18
24	8	620	LHG	C3-O3-P-O6
22	A	812	CLA	C15-C16-C17-C18
24	B	851	LHG	O6-C4-C5-O7
24	6	629	LHG	O6-C4-C5-O7
24	A	846	LHG	C27-C28-C29-C30
28	1	628	LMG	C11-C12-C13-C14
28	7	626	LMG	O8-C28-C29-C30
24	5	623	LHG	O2-C2-C3-O3
30	B	850	DGD	C2A-C3A-C4A-C5A
22	3	603	CLA	C2C-C3C-CAC-CBC
27	B	853	LMU	C2-C3-C4-C5
31	3	608	CHL	C15-C16-C17-C18
22	A	812	CLA	C2-C1-O2A-CGA
22	A	825	CLA	C2-C1-O2A-CGA
22	B	807	CLA	C2-C3-C5-C6
22	B	812	CLA	C2-C3-C5-C6
22	1	609	CLA	C15-C16-C17-C18
22	92	612	CLA	C13-C15-C16-C17
22	7	604	CLA	C4-C3-C5-C6
22	A	803	CLA	C2A-CAA-CBA-CGA
25	L	201	BCR	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
25	K	207	BCR	C5-C6-C7-C8
25	3	718	BCR	C23-C24-C25-C26
25	B2	848	BCR	C5-C6-C7-C8
25	L2	201	BCR	C5-C6-C7-C8
29	3	622	LUT	C5-C6-C7-C8
29	7	621	LUT	C1-C6-C7-C8
29	7	621	LUT	C5-C6-C7-C8
28	3	722	LMG	O8-C28-C29-C30
24	1	620	LHG	O6-C4-C5-C6
22	A	804	CLA	C11-C12-C13-C15
22	A	811	CLA	C6-C7-C8-C10
22	A	815	CLA	C2-C3-C5-C6
22	A	820	CLA	C2-C3-C5-C6
22	A	829	CLA	C6-C7-C8-C10
22	B	819	CLA	C11-C10-C8-C7
22	B	827	CLA	C11-C10-C8-C7
22	B	834	CLA	C11-C10-C8-C7
22	8	613	CLA	C12-C13-C15-C16
22	Z	609	CLA	C11-C12-C13-C15
22	92	602	CLA	C12-C13-C15-C16
31	6	616	CHL	C12-C13-C15-C16
27	4	625	LMU	C3-C4-C5-C6
22	A	809	CLA	C2A-CAA-CBA-CGA
22	B	831	CLA	C2A-CAA-CBA-CGA
22	A	836	CLA	CAA-CBA-CGA-O2A
22	A	805	CLA	CAD-CBD-CGD-O2D
22	A	808	CLA	CAD-CBD-CGD-O2D
22	A	810	CLA	CAD-CBD-CGD-O2D
22	A	823	CLA	CAD-CBD-CGD-O2D
22	A	826	CLA	CAD-CBD-CGD-O2D
22	A	827	CLA	CAD-CBD-CGD-O2D
22	A	838	CLA	CAD-CBD-CGD-O2D
22	A	842	CLA	CAD-CBD-CGD-O2D
22	B	810	CLA	CAD-CBD-CGD-O2D
22	B	811	CLA	CAD-CBD-CGD-O2D
22	B	814	CLA	CAD-CBD-CGD-O2D
22	B	826	CLA	CAD-CBD-CGD-O2D
22	B	829	CLA	CAD-CBD-CGD-O2D
22	B	839	CLA	CAD-CBD-CGD-O2D
22	K	201	CLA	CAD-CBD-CGD-O2D
22	1	604	CLA	CAD-CBD-CGD-O2D
22	1	608	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
22	3	612	CLA	CAD-CBD-CGD-O2D
22	4	604	CLA	CAD-CBD-CGD-O2D
22	4	614	CLA	CAD-CBD-CGD-O2D
22	5	602	CLA	CAD-CBD-CGD-O2D
22	5	612	CLA	CAD-CBD-CGD-O2D
22	9	613	CLA	CAD-CBD-CGD-O2D
22	B2	814	CLA	CAD-CBD-CGD-O2D
22	B2	839	CLA	CAD-CBD-CGD-O2D
22	92	609	CLA	CAD-CBD-CGD-O2D
28	3	722	LMG	C8-C7-O1-C1
27	1	621	LMU	O5'-C1'-O1'-C1
28	B	852	LMG	O6-C1-O1-C7
22	A	810	CLA	C2-C3-C5-C6
28	7	626	LMG	C7-C8-C9-O8
24	Z	620	LHG	O6-C4-C5-O7
24	4	623	LHG	O6-C4-C5-O7
24	92	622	LHG	O6-C4-C5-O7
22	A	804	CLA	CHA-CBD-CGD-O1D
22	A	807	CLA	CHA-CBD-CGD-O1D
22	A	817	CLA	CHA-CBD-CGD-O1D
22	A	817	CLA	CHA-CBD-CGD-O2D
22	A	831	CLA	CHA-CBD-CGD-O1D
22	A	831	CLA	CHA-CBD-CGD-O2D
22	B	804	CLA	CHA-CBD-CGD-O1D
22	B	805	CLA	CHA-CBD-CGD-O1D
22	B	808	CLA	CHA-CBD-CGD-O1D
22	B	815	CLA	CHA-CBD-CGD-O1D
22	B	815	CLA	CHA-CBD-CGD-O2D
22	B	841	CLA	CHA-CBD-CGD-O1D
22	L	203	CLA	CHA-CBD-CGD-O2D
22	7	602	CLA	CHA-CBD-CGD-O1D
22	7	602	CLA	CHA-CBD-CGD-O2D
22	7	614	CLA	CHA-CBD-CGD-O1D
22	7	614	CLA	CHA-CBD-CGD-O2D
22	7	620	CLA	CHA-CBD-CGD-O1D
22	4	602	CLA	CHA-CBD-CGD-O1D
22	4	602	CLA	CHA-CBD-CGD-O2D
22	B2	815	CLA	CHA-CBD-CGD-O1D
22	B2	815	CLA	CHA-CBD-CGD-O2D
22	B2	820	CLA	CHA-CBD-CGD-O1D
22	B2	820	CLA	CHA-CBD-CGD-O2D
22	92	601	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
22	92	602	CLA	CHA-CBD-CGD-O1D
22	92	602	CLA	CHA-CBD-CGD-O2D
22	92	604	CLA	CHA-CBD-CGD-O1D
22	92	604	CLA	CHA-CBD-CGD-O2D
31	1	601	CHL	CHA-CBD-CGD-O1D
31	1	601	CHL	CHA-CBD-CGD-O2D
31	1	607	CHL	CHA-CBD-CGD-O1D
31	5	618	CHL	CHA-CBD-CGD-O1D
31	5	618	CHL	CHA-CBD-CGD-O2D
31	6	601	CHL	CHA-CBD-CGD-O1D
31	92	607	CHL	CHA-CBD-CGD-O2D
22	B	817	CLA	C4C-C3C-CAC-CBC
24	7	625	LHG	O7-C5-C6-O8
28	8	626	LMG	O7-C8-C9-O8
22	A	812	CLA	C13-C15-C16-C17
28	A	859	LMG	C32-C33-C34-C35
22	A	811	CLA	C4-C3-C5-C6
22	A	821	CLA	C4-C3-C5-C6
22	B	813	CLA	C4-C3-C5-C6
22	B	815	CLA	C4-C3-C5-C6
22	1	613	CLA	C4-C3-C5-C6
24	4	622	LHG	C19-C20-C21-C22
22	B	813	CLA	C2-C3-C5-C6
22	B	815	CLA	C2-C3-C5-C6
27	8	627	LMU	C7-C8-C9-C10
22	A	811	CLA	C6-C7-C8-C9
22	A	829	CLA	C6-C7-C8-C9
24	4	623	LHG	C9-C10-C11-C12
22	Z	611	CLA	C5-C6-C7-C8
22	92	609	CLA	C2C-C3C-CAC-CBC
22	9	613	CLA	C2A-CAA-CBA-CGA
22	5	617	CLA	C10-C11-C12-C13
22	3	607	CLA	C4C-C3C-CAC-CBC
24	7	625	LHG	C34-C35-C36-C37
22	B	805	CLA	C1A-C2A-CAA-CBA
22	B	827	CLA	C1A-C2A-CAA-CBA
22	7	616	CLA	C1A-C2A-CAA-CBA
22	B2	820	CLA	C1A-C2A-CAA-CBA
22	7	610	CLA	CBA-CGA-O2A-C1
24	A	846	LHG	C3-O3-P-O6
24	A	847	LHG	C3-O3-P-O6
24	92	622	LHG	C3-O3-P-O6

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Mol	Chain	Res	Type	Atoms
24	A	846	LHG	C4-O6-P-O4
24	3	721	LHG	C3-O3-P-O5
24	3	721	LHG	C4-O6-P-O4
24	3	623	LHG	C3-O3-P-O4
24	3	623	LHG	C4-O6-P-O4
24	3	623	LHG	C4-O6-P-O5
24	8	620	LHG	C3-O3-P-O4
24	8	620	LHG	C4-O6-P-O5
24	Z	620	LHG	C4-O6-P-O4
24	Z	620	LHG	C4-O6-P-O5
24	9	622	LHG	C4-O6-P-O5
24	92	622	LHG	C4-O6-P-O5
28	1	628	LMG	C14-C15-C16-C17
30	B	850	DGD	C3A-C4A-C5A-C6A
27	9	624	LMU	O5'-C1'-O1'-C1
22	Z	616	CLA	C5-C6-C7-C8
24	3	623	LHG	O6-C4-C5-C6
24	4	623	LHG	O6-C4-C5-C6
24	6	629	LHG	O6-C4-C5-C6
24	9	622	LHG	O6-C4-C5-C6
22	A	806	CLA	C3-C5-C6-C7
22	B	819	CLA	C3-C5-C6-C7
22	A	841	CLA	C16-C17-C18-C20
22	A	804	CLA	CAD-CBD-CGD-O1D
22	A	814	CLA	CAD-CBD-CGD-O1D
22	B	805	CLA	CAD-CBD-CGD-O1D
22	B	841	CLA	CAD-CBD-CGD-O1D
22	7	614	CLA	CAD-CBD-CGD-O1D
22	7	620	CLA	CAD-CBD-CGD-O1D
22	6	603	CLA	CAD-CBD-CGD-O1D
22	6	622	CLA	CAD-CBD-CGD-O1D
22	B2	820	CLA	CAD-CBD-CGD-O1D
31	1	601	CHL	CAD-CBD-CGD-O1D
31	1	607	CHL	CAD-CBD-CGD-O1D
31	7	601	CHL	CAD-CBD-CGD-O1D
31	Z	601	CHL	CAD-CBD-CGD-O1D
31	4	601	CHL	CAD-CBD-CGD-O1D
31	6	601	CHL	CAD-CBD-CGD-O1D
24	7	625	LHG	C31-C32-C33-C34
28	A	859	LMG	C12-C13-C14-C15
24	3	721	LHG	C1-C2-C3-O3
22	3	613	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
22	7	620	CLA	C4-C3-C5-C6
22	A	809	CLA	C12-C13-C15-C16
22	A	816	CLA	C12-C13-C15-C16
22	A	820	CLA	C6-C7-C8-C10
22	A	843	CLA	C11-C12-C13-C15
22	B	832	CLA	C11-C12-C13-C15
22	4	609	CLA	C11-C10-C8-C7
24	1	620	LHG	O6-C4-C5-O7
24	3	721	LHG	O6-C4-C5-O7
24	5	623	LHG	O6-C4-C5-O7
29	5	626	LUT	C25-C26-C27-C28
31	8	607	CHL	C6-C7-C8-C10
31	4	601	CHL	C11-C10-C8-C7
31	6	607	CHL	C12-C13-C15-C16
24	3	623	LHG	C32-C33-C34-C35
27	A	863	LMU	C2-C1-O1'-C1'
31	Z	607	CHL	CAA-CBA-CGA-O2A
22	B2	828	CLA	C5-C6-C7-C8
31	4	608	CHL	C2A-CAA-CBA-CGA
27	A	863	LMU	C5'-C4'-O1B-C1B
22	B	805	CLA	CAA-CBA-CGA-O2A
30	B	850	DGD	O2G-C1B-C2B-C3B
28	7	626	LMG	O7-C8-C9-O8
28	4	624	LMG	O1-C7-C8-O7
28	B	852	LMG	C8-C7-O1-C1
28	B2	855	LMG	C8-C7-O1-C1
22	B	818	CLA	C10-C11-C12-C13
22	B	805	CLA	C4-C3-C5-C6
22	B2	812	CLA	C4-C3-C5-C6
22	92	613	CLA	C4-C3-C5-C6
22	3	615	CLA	CAA-CBA-CGA-O2A
22	A	830	CLA	C13-C15-C16-C17
22	A	804	CLA	C11-C12-C13-C14
22	B	819	CLA	C11-C10-C8-C9
22	B	841	CLA	C14-C13-C15-C16
22	8	613	CLA	C11-C12-C13-C14
31	8	601	CHL	C14-C13-C15-C16
31	8	607	CHL	C6-C7-C8-C9
31	6	607	CHL	C6-C7-C8-C9
22	3	611	CLA	C3-C5-C6-C7
24	6	629	LHG	C13-C14-C15-C16
22	3	607	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
22	A	811	CLA	C2-C3-C5-C6
22	B	832	CLA	C15-C16-C17-C18
22	B	826	CLA	C13-C15-C16-C17
24	4	623	LHG	C6-C5-O7-C7
22	5	621	CLA	C2A-CAA-CBA-CGA
22	6	609	CLA	C2A-CAA-CBA-CGA
22	A	843	CLA	C2-C1-O2A-CGA
22	B2	805	CLA	C2-C1-O2A-CGA
22	A	812	CLA	C3-C5-C6-C7
28	8	629	LMG	C14-C15-C16-C17
24	9	622	LHG	O6-C4-C5-O7
27	A	863	LMU	C3'-C4'-O1B-C1B
22	6	604	CLA	C4-C3-C5-C6
25	G	205	BCR	C1-C6-C7-C8
25	K	207	BCR	C1-C6-C7-C8
29	4	619	LUT	C1-C6-C7-C8
22	A	829	CLA	C8-C10-C11-C12
22	A	823	CLA	C2A-CAA-CBA-CGA
28	B	852	LMG	O1-C7-C8-O7
28	J	104	LMG	O1-C7-C8-O7
24	1	620	LHG	C4-O6-P-O3
24	Z	620	LHG	C3-O3-P-O6
24	6	619	LHG	C4-O6-P-O3
24	5	623	LHG	C4-C5-C6-O8
22	B	834	CLA	C4-C3-C5-C6
22	5	613	CLA	C4-C3-C5-C6
31	8	601	CHL	C4-C3-C5-C6
22	92	603	CLA	C2C-C3C-CAC-CBC
22	A	812	CLA	C6-C7-C8-C10
22	A	813	CLA	C6-C7-C8-C10
22	A	826	CLA	C11-C10-C8-C7
22	B	805	CLA	C2-C3-C5-C6
31	8	601	CHL	CAA-CBA-CGA-O2A
22	A	809	CLA	C14-C13-C15-C16
22	F	301	CLA	C11-C10-C8-C9
22	8	613	CLA	C14-C13-C15-C16
31	1	601	CHL	C11-C12-C13-C14
31	6	616	CHL	C14-C13-C15-C16
22	5	601	CLA	C16-C17-C18-C20
24	4	622	LHG	C27-C28-C29-C30
22	B	840	CLA	C10-C11-C12-C13
27	8	627	LMU	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
22	1	609	CLA	CAA-CBA-CGA-O2A
27	A	857	LMU	O1'-C1-C2-C3
24	6	619	LHG	C2-C3-O3-P
24	9	622	LHG	C5-C4-O6-P
28	1	628	LMG	C12-C13-C14-C15
24	5	623	LHG	C1-C2-C3-O3
22	5	601	CLA	C16-C17-C18-C19
22	3	603	CLA	C4C-C3C-CAC-CBC
22	4	603	CLA	C10-C11-C12-C13
24	4	622	LHG	O6-C4-C5-C6
22	L2	203	CLA	CAA-CBA-CGA-O1A
24	4	622	LHG	O6-C4-C5-O7
22	A	843	CLA	C4-C3-C5-C6
22	6	603	CLA	C4-C3-C5-C6
31	4	601	CHL	C4-C3-C5-C6
28	8	629	LMG	C13-C14-C15-C16
22	8	611	CLA	CAA-CBA-CGA-O1A
22	B	836	CLA	C2-C1-O2A-CGA
31	4	608	CHL	C2-C1-O2A-CGA
27	1	625	LMU	C2'-C1'-O1'-C1
22	A	841	CLA	C10-C11-C12-C13
22	B	804	CLA	CAA-CBA-CGA-O1A
28	8	629	LMG	C15-C16-C17-C18
24	B	851	LHG	O9-C7-C8-C9
31	5	607	CHL	CAA-CBA-CGA-O1A
22	4	609	CLA	C3A-C2A-CAA-CBA
22	5	621	CLA	C3A-C2A-CAA-CBA
22	B2	839	CLA	CAA-CBA-CGA-O1A
22	1	613	CLA	C2-C3-C5-C6
22	7	620	CLA	C2-C3-C5-C6
22	A	812	CLA	C14-C13-C15-C16
22	A	820	CLA	C6-C7-C8-C9
22	A	840	CLA	C11-C10-C8-C9
22	B	802	CLA	C14-C13-C15-C16
22	B	811	CLA	C11-C10-C8-C9
22	B	840	CLA	C11-C12-C13-C14
22	B	841	CLA	C11-C10-C8-C9
31	4	601	CHL	C11-C10-C8-C9
22	Z	612	CLA	CAA-CBA-CGA-O1A
25	A	852	BCR	C11-C10-C9-C34
25	A	852	BCR	C16-C17-C18-C36
25	B	845	BCR	C11-C10-C9-C34

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Mol	Chain	Res	Type	Atoms
25	B	845	BCR	C20-C21-C22-C37
25	L	201	BCR	C11-C10-C9-C34
25	B2	845	BCR	C11-C10-C9-C34
25	B2	845	BCR	C20-C21-C22-C37
25	L2	201	BCR	C11-C10-C9-C34
28	B	852	LMG	O1-C7-C8-C9
28	8	626	LMG	C7-C8-C9-O8
29	F	305	LUT	C20-C13-C14-C15
33	5	625	NEX	C39-C29-C30-C31
33	6	625	NEX	C39-C29-C30-C31
22	K	206	CLA	CAA-CBA-CGA-O1A
31	92	607	CHL	CAA-CBA-CGA-O1A
22	B	824	CLA	O2A-C1-C2-C3
31	Z	607	CHL	O2A-C1-C2-C3
24	4	622	LHG	O2-C2-C3-O3
27	1	625	LMU	O5'-C1'-O1'-C1
22	8	611	CLA	CAA-CBA-CGA-O2A
22	6	612	CLA	CAA-CBA-CGA-O1A
31	7	606	CHL	CAA-CBA-CGA-O2A
27	Z	622	LMU	C5'-C4'-O1B-C1B
22	1	612	CLA	CAA-CBA-CGA-O2A
24	4	623	LHG	C4-C5-O7-C7
24	6	629	LHG	C4-C5-O7-C7
30	B	850	DGD	C1G-C2G-O2G-C1B
22	A	827	CLA	C13-C15-C16-C17
22	A	819	CLA	C1A-C2A-CAA-CBA
22	7	614	CLA	C1A-C2A-CAA-CBA
22	5	621	CLA	C1A-C2A-CAA-CBA
31	7	606	CHL	C1A-C2A-CAA-CBA
22	92	603	CLA	C4C-C3C-CAC-CBC
22	B	809	CLA	C6-C7-C8-C10
22	4	611	CLA	C6-C7-C8-C10
22	5	610	CLA	C2-C3-C5-C6
22	B2	828	CLA	C12-C13-C15-C16
22	92	613	CLA	C2-C3-C5-C6
31	8	601	CHL	C11-C12-C13-C15
24	B	851	LHG	C23-C24-C25-C26
22	4	612	CLA	CAA-CBA-CGA-O1A
31	Z	606	CHL	CAA-CBA-CGA-O2A
24	A	846	LHG	C11-C12-C13-C14
22	B	803	CLA	C8-C10-C11-C12
30	B	850	DGD	C9B-CAB-CBB-CCB

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Mol	Chain	Res	Type	Atoms
24	4	622	LHG	C5-C4-O6-P
24	3	623	LHG	C28-C29-C30-C31
22	1	612	CLA	CAA-CBA-CGA-O1A
22	B2	839	CLA	CAA-CBA-CGA-O2A
22	A	810	CLA	C5-C6-C7-C8
22	92	611	CLA	C8-C10-C11-C12
22	A	824	CLA	CAA-CBA-CGA-O2A
22	B	804	CLA	CAA-CBA-CGA-O2A
22	L2	204	CLA	CAA-CBA-CGA-O1A
22	B	810	CLA	C4-C3-C5-C6
22	4	603	CLA	C4-C3-C5-C6
22	4	611	CLA	C4-C3-C5-C6
22	5	603	CLA	C4-C3-C5-C6
22	5	612	CLA	CAA-CBA-CGA-O1A
22	L2	203	CLA	CAA-CBA-CGA-O2A
25	A	852	BCR	C11-C10-C9-C8
25	A	852	BCR	C16-C17-C18-C19
25	B	845	BCR	C11-C10-C9-C8
25	B	845	BCR	C20-C21-C22-C23
25	L	201	BCR	C11-C10-C9-C8
25	B2	845	BCR	C11-C10-C9-C8
25	B2	845	BCR	C20-C21-C22-C23
25	L2	201	BCR	C11-C10-C9-C8
29	F	305	LUT	C12-C13-C14-C15
33	5	625	NEX	C28-C29-C30-C31
33	6	625	NEX	C28-C29-C30-C31
24	9	622	LHG	O7-C5-C6-O8
30	B	850	DGD	O1G-C1G-C2G-O2G
22	3	609	CLA	C4C-C3C-CAC-CBC
31	3	608	CHL	C13-C15-C16-C17
27	Z	622	LMU	C3'-C4'-O1B-C1B
22	K	206	CLA	CAA-CBA-CGA-O2A
22	L2	204	CLA	CAA-CBA-CGA-O2A
28	8	629	LMG	C21-C22-C23-C24
28	4	624	LMG	O6-C1-O1-C7
22	A	824	CLA	CAA-CBA-CGA-O1A
22	4	612	CLA	CAA-CBA-CGA-O2A
31	7	606	CHL	CAA-CBA-CGA-O1A
31	8	606	CHL	C4-C3-C5-C6
31	Z	601	CHL	C4-C3-C5-C6
28	7	626	LMG	C14-C15-C16-C17
22	A	829	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
22	7	610	CLA	C2-C1-O2A-CGA
22	Z	609	CLA	C2-C1-O2A-CGA
31	8	607	CHL	C2-C1-O2A-CGA
22	B	810	CLA	C2-C3-C5-C6
22	B	834	CLA	C2-C3-C5-C6
22	3	607	CLA	C2-C3-C5-C6
22	5	613	CLA	C2-C3-C5-C6
22	6	603	CLA	C2-C3-C5-C6
22	6	604	CLA	C2-C3-C5-C6
22	7	610	CLA	O1A-CGA-O2A-C1
22	6	612	CLA	CAA-CBA-CGA-O2A
31	Z	606	CHL	CAA-CBA-CGA-O1A
27	K	208	LMU	C5-C6-C7-C8
22	4	613	CLA	CAA-CBA-CGA-O2A
31	92	607	CHL	CAA-CBA-CGA-O2A
22	5	612	CLA	CAA-CBA-CGA-O2A
25	L	205	BCR	C23-C24-C25-C26
25	L2	205	BCR	C23-C24-C25-C30
22	B	834	CLA	C8-C10-C11-C12
24	B	851	LHG	C4-C5-C6-O8
33	6	625	NEX	C9-C10-C11-C12
22	F	301	CLA	C4-C3-C5-C6
22	Z	604	CLA	C4-C3-C5-C6
22	5	609	CLA	C4-C3-C5-C6
31	5	607	CHL	C4-C3-C5-C6
27	1	621	LMU	C3'-C4'-O1B-C1B
27	6	631	LMU	C3-C4-C5-C6
22	A	821	CLA	C2-C3-C5-C6
22	3	613	CLA	C2-C3-C5-C6
22	B2	812	CLA	C2-C3-C5-C6
31	8	601	CHL	C2-C3-C5-C6
22	92	602	CLA	CAA-CBA-CGA-O2A
22	A	829	CLA	C10-C11-C12-C13
22	9	614	CLA	CAA-CBA-CGA-O2A
24	7	625	LHG	O6-C4-C5-O7
22	9	614	CLA	CAA-CBA-CGA-O1A
22	B	823	CLA	C4-C3-C5-C6
22	B	836	CLA	C4-C3-C5-C6
22	B	841	CLA	C4-C3-C5-C6
22	8	613	CLA	C4-C3-C5-C6
22	5	604	CLA	C4-C3-C5-C6
22	1	613	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
28	J	103	LMG	C22-C23-C24-C25
33	6	625	NEX	C33-C34-C35-C15
22	B	817	CLA	CAA-CBA-CGA-O2A
22	A	825	CLA	C2C-C3C-CAC-CBC
24	1	620	LHG	O7-C5-C6-O8
24	4	623	LHG	O7-C5-C6-O8
28	9	620	LMG	O1-C7-C8-O7
24	8	620	LHG	C12-C13-C14-C15
22	A	807	CLA	CAA-CBA-CGA-O2A
22	5	616	CLA	CAA-CBA-CGA-O2A
22	B2	813	CLA	CAA-CBA-CGA-O2A
24	6	619	LHG	O7-C7-C8-C9
22	Z	612	CLA	CAA-CBA-CGA-O2A
22	1	603	CLA	CAA-CBA-CGA-O2A
24	A	846	LHG	O8-C23-C24-C25
22	3	617	CLA	C2C-C3C-CAC-CBC
22	A	814	CLA	C4-C3-C5-C6
22	A	825	CLA	C4-C3-C5-C6
22	3	615	CLA	C4-C3-C5-C6
22	8	614	CLA	C4-C3-C5-C6
22	5	616	CLA	C4-C3-C5-C6
22	6	611	CLA	C4-C3-C5-C6
22	B2	814	CLA	C4-C3-C5-C6
22	B2	804	CLA	CAA-CBA-CGA-O1A
22	8	613	CLA	C2-C3-C5-C6
31	4	601	CHL	C2-C3-C5-C6
22	B	811	CLA	CAA-CBA-CGA-O2A
22	A	806	CLA	C14-C13-C15-C16
22	B	832	CLA	C11-C12-C13-C14
31	6	607	CHL	C14-C13-C15-C16
28	1	624	LMG	C31-C32-C33-C34
22	F	304	CLA	C3A-C2A-CAA-CBA
28	J	104	LMG	O7-C10-C11-C12
28	9	620	LMG	O7-C10-C11-C12
22	A	807	CLA	CAD-CBD-CGD-O2D
22	A	815	CLA	CAD-CBD-CGD-O2D
22	A	834	CLA	CAD-CBD-CGD-O2D
22	B	820	CLA	CAD-CBD-CGD-O2D
22	B	824	CLA	CAD-CBD-CGD-O2D
22	B	836	CLA	CAD-CBD-CGD-O2D
22	3	609	CLA	CAD-CBD-CGD-O2D
22	7	603	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
22	5	621	CLA	CAD-CBD-CGD-O2D
22	9	604	CLA	CAD-CBD-CGD-O2D
22	B2	811	CLA	CAD-CBD-CGD-O2D
31	8	601	CHL	CAD-CBD-CGD-O2D
22	4	609	CLA	C2-C1-O2A-CGA
22	5	616	CLA	C2-C1-O2A-CGA
22	92	609	CLA	CAA-CBA-CGA-O2A
22	92	612	CLA	C4C-C3C-CAC-CBC
28	8	626	LMG	O8-C28-C29-C30
28	A	859	LMG	C13-C14-C15-C16
22	B	811	CLA	C4-C3-C5-C6
22	3	604	CLA	C3-C5-C6-C7
22	B	811	CLA	C2-C3-C5-C6
22	4	603	CLA	C2-C3-C5-C6
22	4	611	CLA	C2-C3-C5-C6
22	5	603	CLA	C2-C3-C5-C6
31	5	607	CHL	C2-C3-C5-C6
22	5	604	CLA	CAA-CBA-CGA-O2A
24	4	622	LHG	O8-C23-C24-C25
28	1	624	LMG	O7-C10-C11-C12
22	92	614	CLA	CAA-CBA-CGA-O2A
22	B	821	CLA	O2A-C1-C2-C3
22	1	611	CLA	O2A-C1-C2-C3
31	6	607	CHL	O2A-C1-C2-C3
22	6	603	CLA	C13-C15-C16-C17
22	B	814	CLA	CAA-CBA-CGA-O2A
22	8	604	CLA	CAA-CBA-CGA-O2A
22	92	609	CLA	CAA-CBA-CGA-O1A
27	1	621	LMU	C5'-C4'-O1B-C1B
28	B	852	LMG	C12-C13-C14-C15
22	A	804	CLA	CHA-CBD-CGD-O2D
22	A	814	CLA	CHA-CBD-CGD-O1D
22	A	820	CLA	CHA-CBD-CGD-O1D
22	A	820	CLA	CHA-CBD-CGD-O2D
22	A	832	CLA	CHA-CBD-CGD-O2D
22	B	805	CLA	CHA-CBD-CGD-O2D
22	B	821	CLA	CHA-CBD-CGD-O2D
22	B	822	CLA	CHA-CBD-CGD-O1D
22	B	822	CLA	CHA-CBD-CGD-O2D
22	B	828	CLA	CHA-CBD-CGD-O1D
22	B	828	CLA	CHA-CBD-CGD-O2D
22	B	841	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
22	K	204	CLA	CHA-CBD-CGD-O1D
22	1	602	CLA	CHA-CBD-CGD-O2D
22	1	603	CLA	CHA-CBD-CGD-O2D
22	1	616	CLA	CHA-CBD-CGD-O1D
22	1	616	CLA	CHA-CBD-CGD-O2D
22	3	602	CLA	CHA-CBD-CGD-O2D
22	7	620	CLA	CHA-CBD-CGD-O2D
22	8	602	CLA	CHA-CBD-CGD-O2D
22	8	603	CLA	CHA-CBD-CGD-O1D
22	8	603	CLA	CHA-CBD-CGD-O2D
22	8	612	CLA	CHA-CBD-CGD-O1D
22	8	612	CLA	CHA-CBD-CGD-O2D
22	8	614	CLA	CHA-CBD-CGD-O1D
22	8	614	CLA	CHA-CBD-CGD-O2D
22	Z	602	CLA	CHA-CBD-CGD-O1D
22	Z	602	CLA	CHA-CBD-CGD-O2D
22	Z	603	CLA	CHA-CBD-CGD-O1D
22	Z	612	CLA	CHA-CBD-CGD-O2D
22	Z	613	CLA	CHA-CBD-CGD-O2D
22	4	612	CLA	CHA-CBD-CGD-O1D
22	4	612	CLA	CHA-CBD-CGD-O2D
22	5	613	CLA	CHA-CBD-CGD-O2D
22	6	602	CLA	CHA-CBD-CGD-O1D
22	6	602	CLA	CHA-CBD-CGD-O2D
22	6	604	CLA	CHA-CBD-CGD-O1D
22	6	604	CLA	CHA-CBD-CGD-O2D
22	6	610	CLA	CHA-CBD-CGD-O1D
22	6	610	CLA	CHA-CBD-CGD-O2D
22	6	622	CLA	CHA-CBD-CGD-O1D
22	6	622	CLA	CHA-CBD-CGD-O2D
22	9	602	CLA	CHA-CBD-CGD-O1D
22	9	602	CLA	CHA-CBD-CGD-O2D
22	9	603	CLA	CHA-CBD-CGD-O2D
22	9	612	CLA	CHA-CBD-CGD-O1D
22	9	612	CLA	CHA-CBD-CGD-O2D
22	92	612	CLA	CHA-CBD-CGD-O2D
31	1	607	CHL	CHA-CBD-CGD-O2D
31	7	601	CHL	CHA-CBD-CGD-O1D
31	Z	601	CHL	CHA-CBD-CGD-O1D
31	4	601	CHL	CHA-CBD-CGD-O1D
31	4	618	CHL	CHA-CBD-CGD-O1D
31	6	601	CHL	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
31	6	607	CHL	CHA-CBD-CGD-O2D
31	6	618	CHL	CHA-CBD-CGD-O1D
31	6	618	CHL	CHA-CBD-CGD-O2D
22	5	614	CLA	CAA-CBA-CGA-O2A
22	6	609	CLA	C4-C3-C5-C6
22	6	611	CLA	C2-C3-C5-C6
24	7	625	LHG	O6-C4-C5-C6
22	92	614	CLA	CAA-CBA-CGA-O1A
22	G	204	CLA	CAA-CBA-CGA-O2A
22	8	614	CLA	CAA-CBA-CGA-O2A
22	B2	820	CLA	CAA-CBA-CGA-O2A
24	3	721	LHG	O7-C7-C8-C9
28	A	860	LMG	O1-C7-C8-O7
28	1	624	LMG	O1-C7-C8-O7
22	B	827	CLA	C8-C10-C11-C12
27	1	625	LMU	C2-C3-C4-C5
22	B	809	CLA	CAA-CBA-CGA-O2A
22	7	603	CLA	CAA-CBA-CGA-O2A
22	5	603	CLA	CAA-CBA-CGA-O2A
27	A	865	LMU	C5-C6-C7-C8
24	B	851	LHG	C25-C26-C27-C28
28	7	626	LMG	O10-C28-C29-C30
22	A	814	CLA	C2-C3-C5-C6
22	8	614	CLA	C2-C3-C5-C6
22	F	304	CLA	CAA-CBA-CGA-O2A
22	4	614	CLA	CAA-CBA-CGA-O2A
24	92	622	LHG	O7-C7-C8-C9
22	A	816	CLA	C14-C13-C15-C16
22	B	837	CLA	C11-C12-C13-C14
22	B2	828	CLA	C14-C13-C15-C16
31	8	601	CHL	C11-C10-C8-C9
24	1	620	LHG	C11-C10-C9-C8
22	A	826	CLA	CAA-CBA-CGA-O2A
22	B	834	CLA	CAA-CBA-CGA-O2A
22	8	603	CLA	CAA-CBA-CGA-O2A
28	J	104	LMG	O8-C28-C29-C30
22	B	835	CLA	CAA-CBA-CGA-O2A
22	B2	804	CLA	CAA-CBA-CGA-O2A
22	B2	811	CLA	CAA-CBA-CGA-O2A
22	A	807	CLA	CAA-CBA-CGA-O1A
22	B	811	CLA	CAA-CBA-CGA-O1A
24	A	846	LHG	O10-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
24	6	619	LHG	O9-C7-C8-C9
31	3	608	CHL	C4-C3-C5-C6
22	B	836	CLA	C2-C3-C5-C6
22	F	304	CLA	CAA-CBA-CGA-O1A
22	5	604	CLA	CAA-CBA-CGA-O1A
21	A	801	CL0	C5-C6-C7-C8
22	A	836	CLA	C1A-C2A-CAA-CBA
22	3	615	CLA	C1A-C2A-CAA-CBA
22	8	614	CLA	C1A-C2A-CAA-CBA
22	Z	611	CLA	C1A-C2A-CAA-CBA
22	4	613	CLA	C1A-C2A-CAA-CBA
22	5	603	CLA	C1A-C2A-CAA-CBA
31	8	607	CHL	C1A-C2A-CAA-CBA
31	6	601	CHL	C1A-C2A-CAA-CBA
22	1	603	CLA	CAA-CBA-CGA-O1A
22	4	614	CLA	CAA-CBA-CGA-O1A
24	3	721	LHG	O9-C7-C8-C9
24	4	622	LHG	O10-C23-C24-C25
28	J	104	LMG	O9-C10-C11-C12
22	A	825	CLA	C4C-C3C-CAC-CBC
22	3	617	CLA	C4C-C3C-CAC-CBC
22	B	811	CLA	C2-C1-O2A-CGA
28	J	104	LMG	O10-C28-C29-C30
28	3	722	LMG	O1-C7-C8-C9
22	A	818	CLA	C2A-CAA-CBA-CGA
22	92	602	CLA	C2A-CAA-CBA-CGA
24	9	622	LHG	C4-O6-P-O3
22	A	826	CLA	CAA-CBA-CGA-O1A
22	8	614	CLA	CAA-CBA-CGA-O1A
22	B2	813	CLA	CAA-CBA-CGA-O1A
27	8	627	LMU	C4-C5-C6-C7
22	Z	603	CLA	CAA-CBA-CGA-O2A
22	4	603	CLA	CAA-CBA-CGA-O2A
22	5	621	CLA	CAA-CBA-CGA-O2A
22	8	604	CLA	CAA-CBA-CGA-O1A
22	5	616	CLA	CAA-CBA-CGA-O1A
28	9	620	LMG	O9-C10-C11-C12
22	A	810	CLA	C8-C10-C11-C12
24	A	847	LHG	C3-O3-P-O5
24	A	847	LHG	C4-O6-P-O5
24	1	620	LHG	C3-O3-P-O5
24	7	625	LHG	C4-O6-P-O5

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Mol	Chain	Res	Type	Atoms
24	6	619	LHG	C4-O6-P-O5
27	1	621	LMU	C2B-C1B-O1B-C4'
28	A	859	LMG	C29-C30-C31-C32
24	7	625	LHG	C10-C11-C12-C13
25	G	205	BCR	C5-C6-C7-C8
25	L	205	BCR	C23-C24-C25-C30
25	5	622	BCR	C1-C6-C7-C8
25	L2	205	BCR	C23-C24-C25-C26
29	4	619	LUT	C5-C6-C7-C8
24	92	622	LHG	O9-C7-C8-C9
28	1	624	LMG	O9-C10-C11-C12
24	B	851	LHG	O8-C23-C24-C25
24	7	625	LHG	O8-C23-C24-C25
28	B2	852	LMG	O7-C10-C11-C12
22	L	204	CLA	CAA-CBA-CGA-O2A
22	B2	813	CLA	C2A-CAA-CBA-CGA
22	B	814	CLA	CAA-CBA-CGA-O1A
24	6	619	LHG	C9-C10-C11-C12
22	3	613	CLA	C10-C11-C12-C13
28	3	722	LMG	O10-C28-C29-C30
22	A	803	CLA	C4-C3-C5-C6
22	B	824	CLA	C4-C3-C5-C6
28	A	859	LMG	C30-C31-C32-C33
22	5	604	CLA	C2-C3-C5-C6
22	A	828	CLA	CAD-CBD-CGD-O1D
22	B	813	CLA	CAD-CBD-CGD-O1D
22	G	203	CLA	CAD-CBD-CGD-O1D
22	5	613	CLA	CAD-CBD-CGD-O1D
22	6	610	CLA	CAD-CBD-CGD-O1D
22	B2	805	CLA	CAD-CBD-CGD-O1D
22	B2	813	CLA	CAD-CBD-CGD-O1D
28	9	620	LMG	C7-C8-O7-C10
30	B	850	DGD	C3G-C2G-O2G-C1B
31	Z	606	CHL	CAD-CBD-CGD-O1D
31	6	607	CHL	CAD-CBD-CGD-O1D
22	B	809	CLA	CAA-CBA-CGA-O1A
22	B2	812	CLA	C2C-C3C-CAC-CBC
22	A	823	CLA	C6-C7-C8-C9
22	4	611	CLA	C6-C7-C8-C9
22	9	612	CLA	C11-C12-C13-C14
31	7	601	CHL	C11-C10-C8-C9
31	8	606	CHL	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
31	8	606	CHL	C14-C13-C15-C16
22	B	835	CLA	CAA-CBA-CGA-O1A
22	5	614	CLA	CAA-CBA-CGA-O1A
22	Z	603	CLA	CAA-CBA-CGA-O1A
22	A	813	CLA	CAA-CBA-CGA-O2A
22	B	806	CLA	CAA-CBA-CGA-O2A
22	B	823	CLA	CAA-CBA-CGA-O2A
28	1	628	LMG	O8-C28-C29-C30
28	B2	855	LMG	O7-C10-C11-C12
24	9	622	LHG	C29-C30-C31-C32
22	8	603	CLA	CAA-CBA-CGA-O1A
22	3	609	CLA	C2C-C3C-CAC-CBC
22	92	612	CLA	C2C-C3C-CAC-CBC
22	A	837	CLA	CAA-CBA-CGA-O2A
22	6	603	CLA	CAA-CBA-CGA-O2A
24	7	625	LHG	O7-C7-C8-C9
24	5	623	LHG	O8-C23-C24-C25
28	A	860	LMG	O8-C28-C29-C30
28	8	629	LMG	O8-C28-C29-C30
22	7	603	CLA	CAA-CBA-CGA-O1A
22	B2	811	CLA	CAA-CBA-CGA-O1A
22	B2	820	CLA	CAA-CBA-CGA-O1A
22	A	836	CLA	C3A-C2A-CAA-CBA
22	A	843	CLA	C11-C10-C8-C7
22	B	822	CLA	C6-C7-C8-C10
22	3	615	CLA	C3A-C2A-CAA-CBA
22	8	614	CLA	C3A-C2A-CAA-CBA
22	4	613	CLA	C3A-C2A-CAA-CBA
22	4	614	CLA	C3A-C2A-CAA-CBA
22	5	603	CLA	C12-C13-C15-C16
22	5	604	CLA	C3A-C2A-CAA-CBA
22	5	616	CLA	C2-C3-C5-C6
22	9	611	CLA	C3A-C2A-CAA-CBA
23	A	844	PQN	C21-C22-C23-C25
23	B	842	PQN	C16-C17-C18-C20
31	1	601	CHL	C11-C10-C8-C7
31	Z	601	CHL	C2-C3-C5-C6
22	G	204	CLA	CAA-CBA-CGA-O1A
22	5	621	CLA	CAA-CBA-CGA-O1A
24	9	622	LHG	C26-C27-C28-C29
22	A	814	CLA	CAA-CBA-CGA-O2A
22	8	612	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
24	8	620	LHG	O7-C7-C8-C9
28	3	722	LMG	O7-C10-C11-C12
31	6	601	CHL	CAA-CBA-CGA-O2A
30	B	850	DGD	C7B-C8B-C9B-CAB
24	1	620	LHG	C23-C24-C25-C26
22	A	837	CLA	CAA-CBA-CGA-O1A
22	5	603	CLA	CAA-CBA-CGA-O1A
24	7	625	LHG	O9-C7-C8-C9
24	7	625	LHG	O10-C23-C24-C25
24	8	620	LHG	O9-C7-C8-C9
24	Z	620	LHG	C5-C6-O8-C23
31	6	601	CHL	CAA-CBA-CGA-O1A
22	F	303	CLA	CAA-CBA-CGA-O2A
22	L	204	CLA	CAA-CBA-CGA-O1A
27	A	861	LMU	C2-C1-O1'-C1'
22	1	613	CLA	CAA-CBA-CGA-O2A
22	7	613	CLA	CAA-CBA-CGA-O2A
28	B	852	LMG	O7-C10-C11-C12
22	8	612	CLA	CAA-CBA-CGA-O1A
22	B	809	CLA	C8-C10-C11-C12
22	A	816	CLA	CAA-CBA-CGA-O2A
22	B	816	CLA	CAA-CBA-CGA-O2A
22	K	203	CLA	CAA-CBA-CGA-O2A
22	3	611	CLA	CAA-CBA-CGA-O2A
22	7	612	CLA	CAA-CBA-CGA-O2A
22	9	603	CLA	CAA-CBA-CGA-O2A
24	3	623	LHG	C24-C25-C26-C27
22	B	802	CLA	C8-C10-C11-C12
22	4	610	CLA	C5-C6-C7-C8
22	A	813	CLA	CAA-CBA-CGA-O1A
22	4	603	CLA	CAA-CBA-CGA-O1A
28	A	860	LMG	O10-C28-C29-C30
28	B2	852	LMG	O9-C10-C11-C12
22	F	304	CLA	C15-C16-C17-C18
22	Z	611	CLA	C4C-C3C-CAC-CBC
22	B	806	CLA	CAA-CBA-CGA-O1A
24	B	851	LHG	O10-C23-C24-C25
22	1	602	CLA	CAA-CBA-CGA-O2A

All (1) ring outliers are listed below:

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Mol	Chain	Res	Type	Atoms
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Mol	Chain	Res	Type	Atoms
33	5	625	NEX	C1-C2-C3-C4-C5-C6

222 monomers are involved in 324 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	8	604	CLA	4	0
32	4	620	XAT	1	0
22	92	602	CLA	3	0
22	B	837	CLA	3	0
22	8	611	CLA	1	0
22	4	611	CLA	1	0
25	B	845	BCR	3	0
31	6	601	CHL	3	0
29	5	626	LUT	1	0
25	3	620	BCR	1	0
22	Z	610	CLA	1	0
22	B	833	CLA	2	0
25	3	718	BCR	1	0
22	B	830	CLA	1	0
25	B2	844	BCR	4	0
28	3	722	LMG	1	0
22	A	840	CLA	4	0
29	7	621	LUT	1	0
22	B	808	CLA	3	0
29	Z	617	LUT	1	0
22	6	614	CLA	3	0
22	7	610	CLA	4	0
22	A	812	CLA	1	0
22	A	803	CLA	2	0
28	A	860	LMG	1	0
22	A	809	CLA	2	0
32	5	624	XAT	1	0
29	4	619	LUT	2	0
22	A	825	CLA	1	0
22	B	817	CLA	2	0
29	1	617	LUT	3	0
25	B	843	BCR	2	0
27	A	858	LMU	2	0
25	3	719	BCR	5	0
22	K	201	CLA	1	0
22	1	614	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	9	616	LUT	2	0
31	4	601	CHL	1	0
25	L	201	BCR	1	0
25	L2	205	BCR	3	0
27	8	625	LMU	1	0
24	7	625	LHG	1	0
25	B2	845	BCR	2	0
31	6	608	CHL	3	0
31	1	601	CHL	1	0
25	I	172	BCR	1	0
22	4	612	CLA	2	0
22	Z	602	CLA	2	0
22	6	609	CLA	1	0
22	Z	609	CLA	1	0
22	F	304	CLA	1	0
22	5	603	CLA	1	0
25	L	205	BCR	4	0
22	3	602	CLA	2	0
29	92	616	LUT	1	0
24	1	620	LHG	1	0
24	4	623	LHG	1	0
22	A	820	CLA	2	0
22	B	821	CLA	1	0
22	6	617	CLA	1	0
32	7	622	XAT	1	0
22	92	611	CLA	1	0
22	3	610	CLA	4	0
22	Z	613	CLA	1	0
22	B	835	CLA	3	0
25	8	619	BCR	2	0
22	92	609	CLA	2	0
31	Z	601	CHL	2	0
33	6	625	NEX	1	0
22	Z	616	CLA	3	0
22	K	204	CLA	1	0
25	A	851	BCR	3	0
22	8	610	CLA	1	0
22	9	612	CLA	1	0
27	6	628	LMU	1	0
32	Z	618	XAT	1	0
22	1	602	CLA	2	0
22	7	620	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	4	606	CHL	4	0
29	F	305	LUT	4	0
25	J	102	BCR	1	0
22	92	603	CLA	1	0
22	4	603	CLA	1	0
24	92	622	LHG	1	0
27	B	853	LMU	3	0
25	9	623	BCR	2	0
22	9	614	CLA	1	0
22	92	613	CLA	2	0
25	A	848	BCR	3	0
22	A	811	CLA	2	0
22	B	841	CLA	5	0
22	A	817	CLA	2	0
22	3	609	CLA	1	0
22	1	603	CLA	4	0
22	A	854	CLA	5	0
22	3	615	CLA	5	0
22	A	829	CLA	3	0
29	92	617	LUT	1	0
22	A	843	CLA	3	0
28	B	854	LMG	1	0
22	A	833	CLA	3	0
22	1	613	CLA	2	0
25	K	202	BCR	3	0
29	1	619	LUT	1	0
22	B	839	CLA	2	0
31	4	608	CHL	1	0
24	6	619	LHG	1	0
22	A	813	CLA	2	0
22	8	614	CLA	1	0
22	92	610	CLA	2	0
32	1	618	XAT	2	0
22	B	829	CLA	6	0
22	3	607	CLA	3	0
24	5	623	LHG	1	0
22	A	826	CLA	3	0
22	5	616	CLA	3	0
31	8	606	CHL	3	0
31	8	601	CHL	2	0
22	B	819	CLA	1	0
22	6	613	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	B	847	BCR	1	0
22	A	810	CLA	2	0
22	B	834	CLA	3	0
22	1	608	CLA	2	0
22	B	832	CLA	2	0
31	5	606	CHL	1	0
25	A	850	BCR	1	0
29	3	621	LUT	2	0
31	3	608	CHL	1	0
27	9	624	LMU	1	0
29	9	617	LUT	3	0
22	A	806	CLA	1	0
28	J	103	LMG	1	0
22	1	604	CLA	2	0
22	6	610	CLA	2	0
22	L	203	CLA	2	0
22	B	824	CLA	1	0
22	3	603	CLA	3	0
22	4	614	CLA	1	0
22	4	609	CLA	2	0
22	6	602	CLA	2	0
22	3	606	CLA	2	0
27	A	862	LMU	1	0
21	A	801	CL0	1	0
22	B	806	CLA	2	0
22	4	602	CLA	2	0
22	8	613	CLA	1	0
27	8	627	LMU	1	0
27	A	857	LMU	1	0
22	6	603	CLA	1	0
22	B	836	CLA	2	0
27	Z	622	LMU	1	0
25	A	849	BCR	2	0
25	B	801	BCR	2	0
22	Z	603	CLA	3	0
22	B	813	CLA	2	0
31	Z	606	CHL	2	0
25	92	623	BCR	3	0
22	B2	828	CLA	4	0
30	B	850	DGD	1	0
22	5	617	CLA	2	0
25	K	207	BCR	3	0

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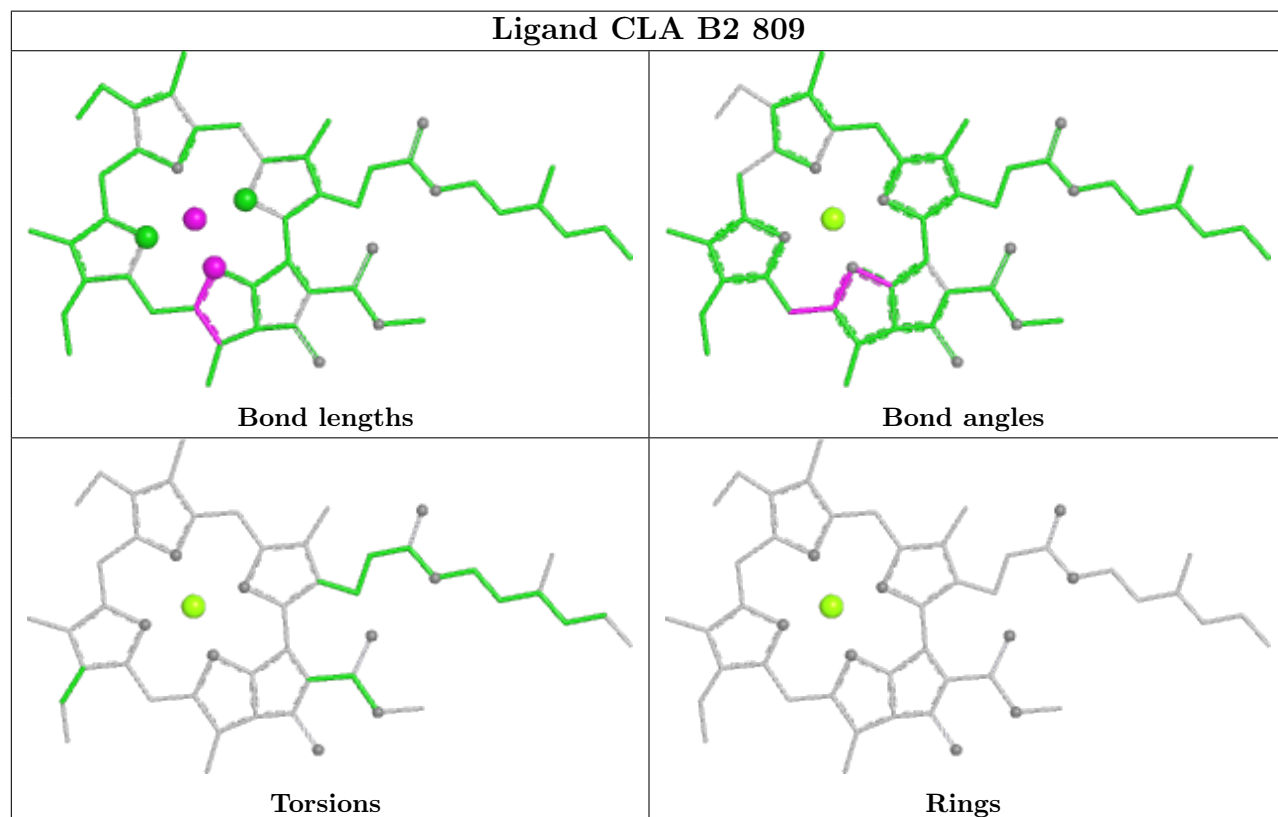
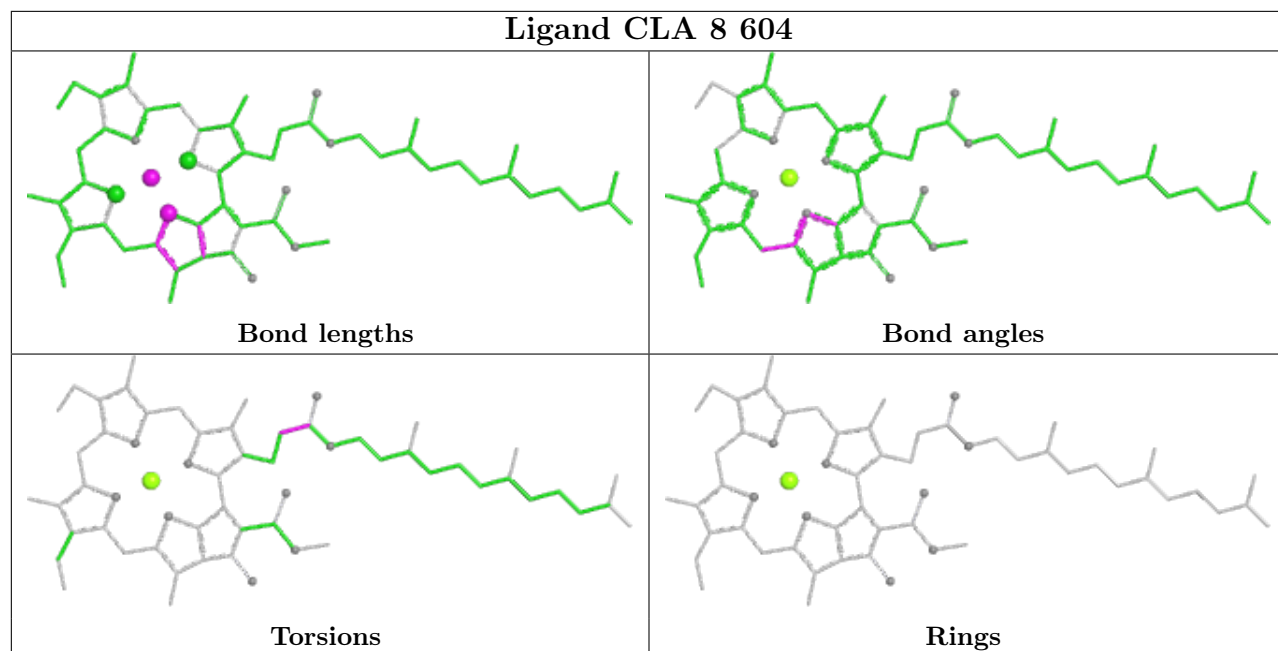
Mol	Chain	Res	Type	Clashes	Symm-Clashes
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22	8	602	CLA	3	0
22	3	612	CLA	1	0
28	9	620	LMG	2	0
22	5	621	CLA	3	0
22	B	827	CLA	1	0
31	6	606	CHL	2	0
22	A	838	CLA	1	0
22	Z	608	CLA	1	0
31	6	607	CHL	1	0
22	8	603	CLA	1	0
25	6	623	BCR	3	0
22	4	610	CLA	2	0
22	4	613	CLA	2	0
31	5	608	CHL	1	0
22	7	608	CLA	1	0
22	A	823	CLA	1	0
22	Z	604	CLA	1	0
29	5	620	LUT	3	0
25	A	852	BCR	4	0
22	B	811	CLA	1	0
22	5	602	CLA	3	0
22	A	804	CLA	1	0
28	J	104	LMG	1	0
22	A	802	CLA	4	0
22	B	838	CLA	1	0
22	9	602	CLA	1	0
22	A	831	CLA	1	0
22	A	839	CLA	1	0
29	7	624	LUT	4	0
32	8	618	XAT	1	0
32	6	624	XAT	1	0
22	1	610	CLA	1	0
22	B	823	CLA	2	0
22	9	609	CLA	1	0
22	8	612	CLA	1	0
22	B	840	CLA	2	0
27	92	624	LMU	2	0
23	B	842	PQN	1	0
29	A	856	LUT	1	0
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24	3	623	LHG	1	0

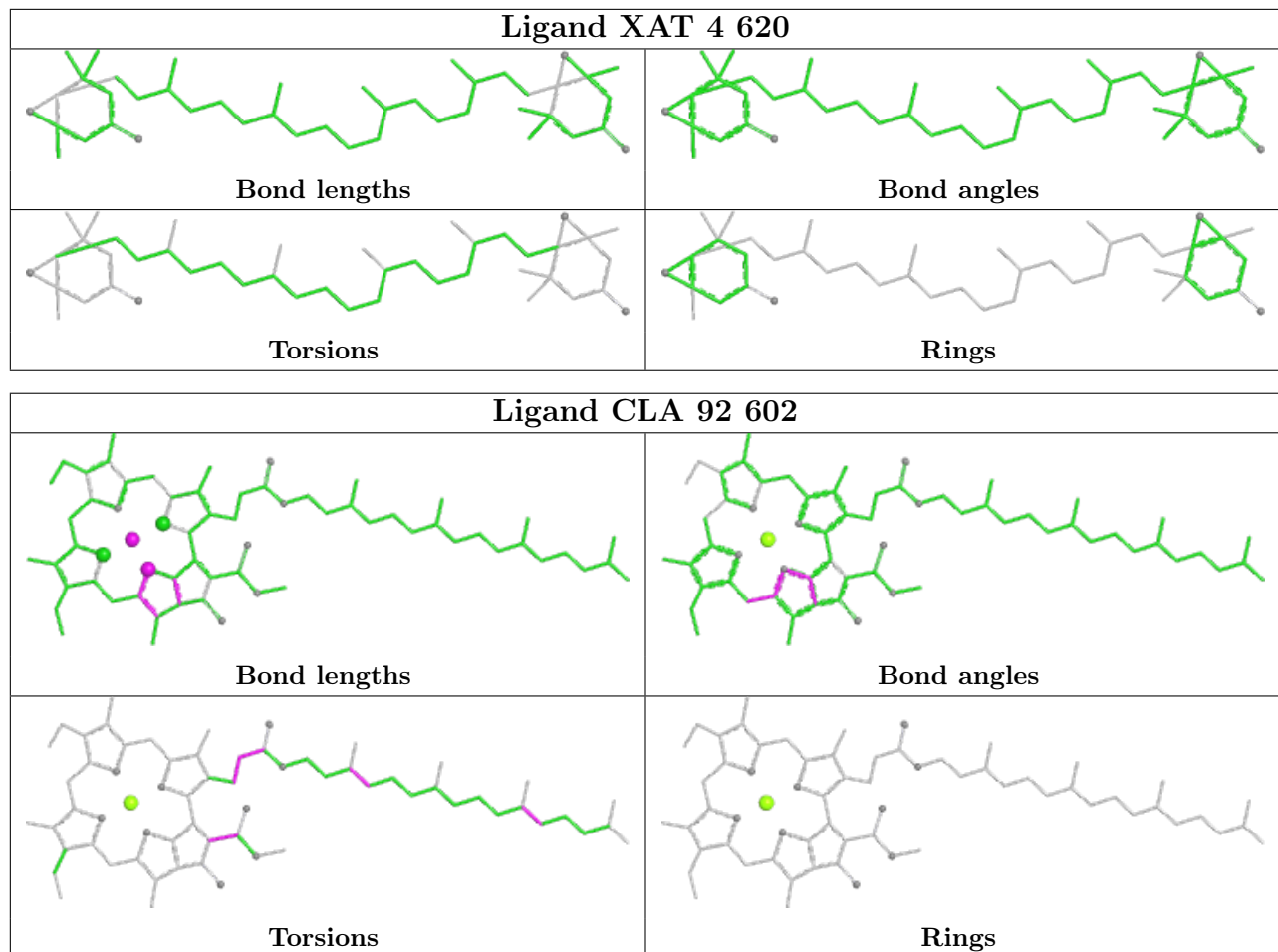
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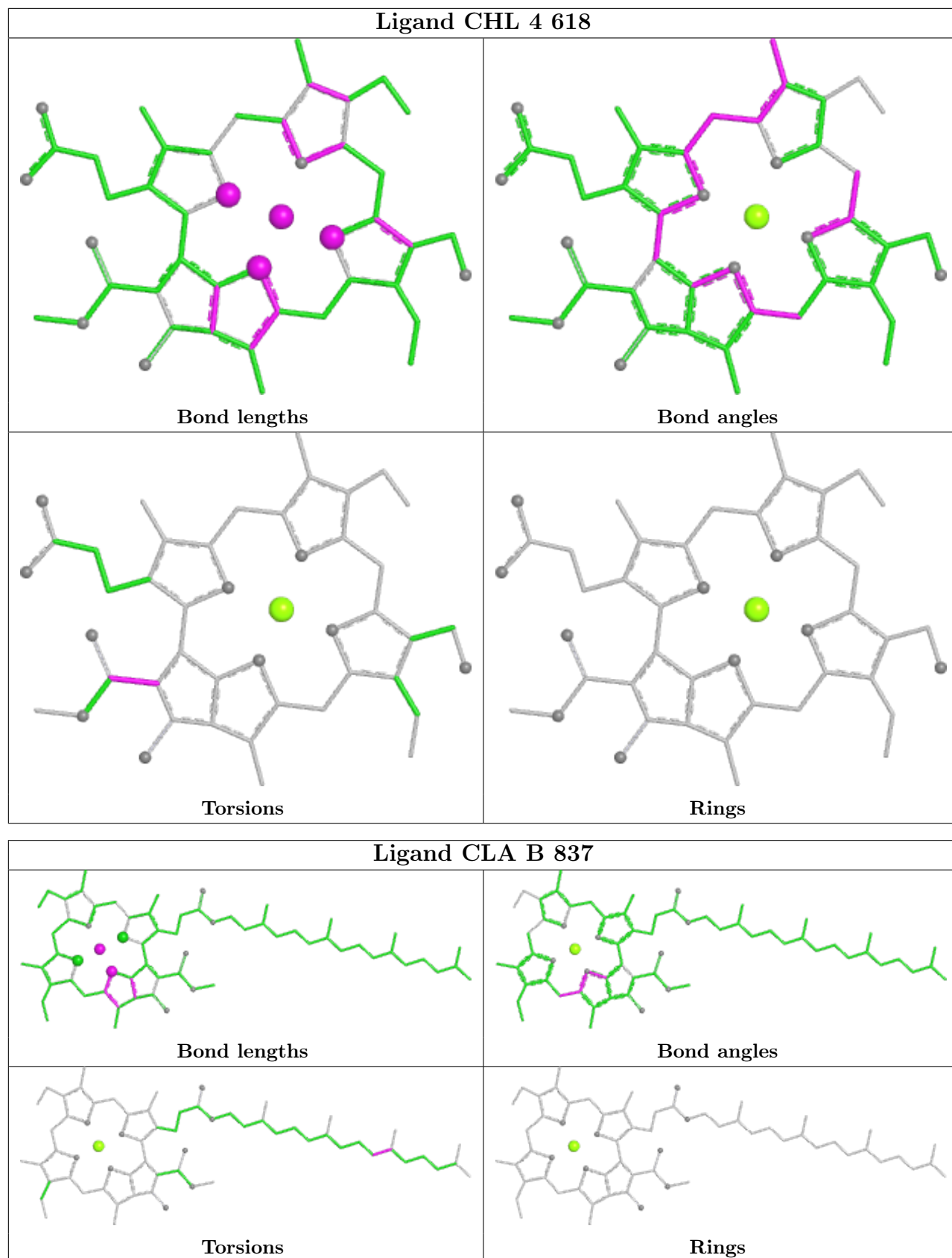
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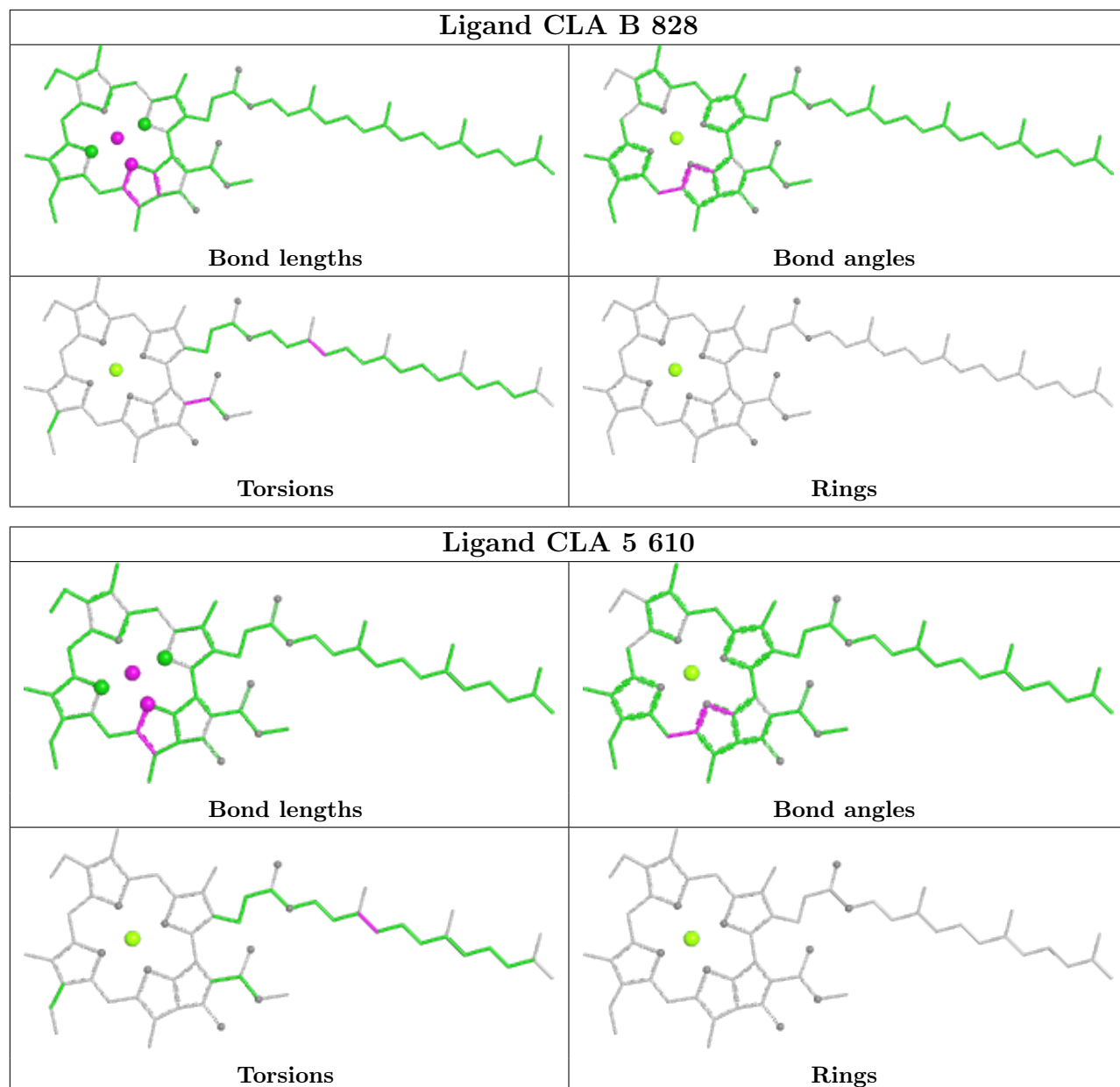
Mol	Chain	Res	Type	Clashes	Symm-Clashes
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22	3	611	CLA	1	0
31	7	601	CHL	3	0
22	A	822	CLA	2	0
27	A	863	LMU	1	0
22	B	802	CLA	4	0
27	7	628	LMU	1	0
29	6	621	LUT	2	0
22	92	604	CLA	1	0
25	B	848	BCR	1	0
22	B	816	CLA	2	0
22	7	602	CLA	1	0
22	7	609	CLA	1	0
22	B2	829	CLA	1	0
22	A	830	CLA	1	0
25	B	844	BCR	3	0
22	9	610	CLA	3	0
22	1	609	CLA	1	0

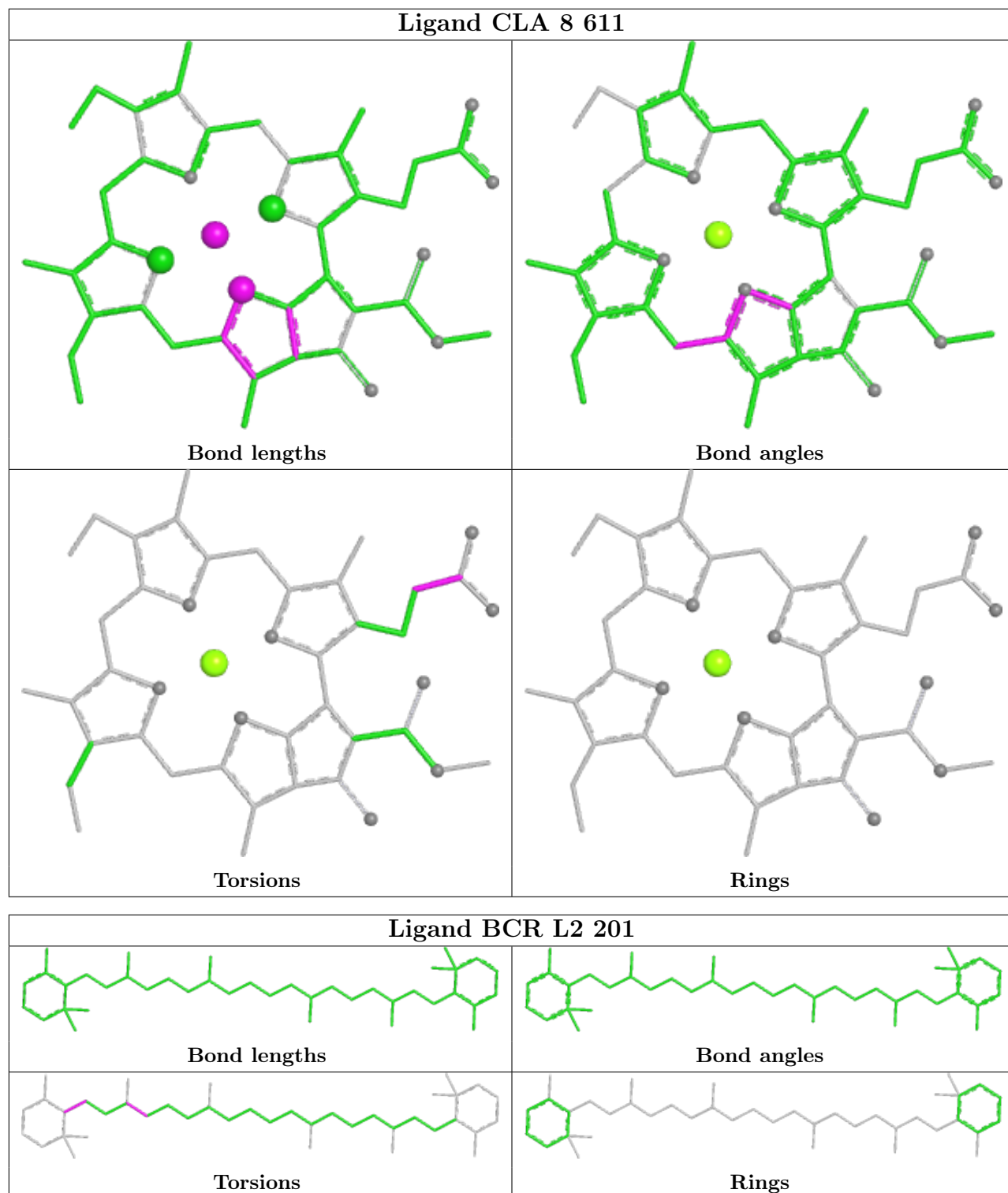
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

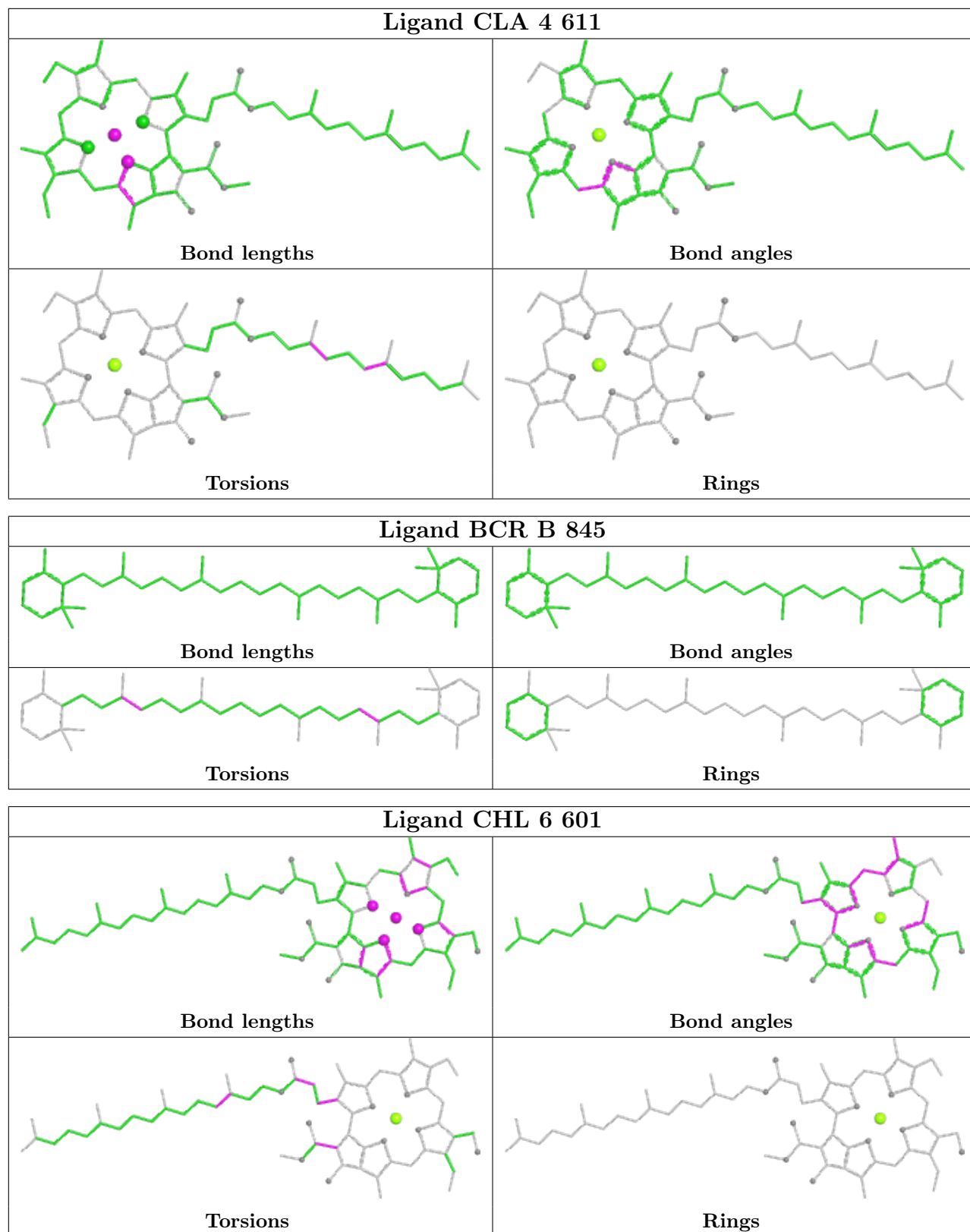


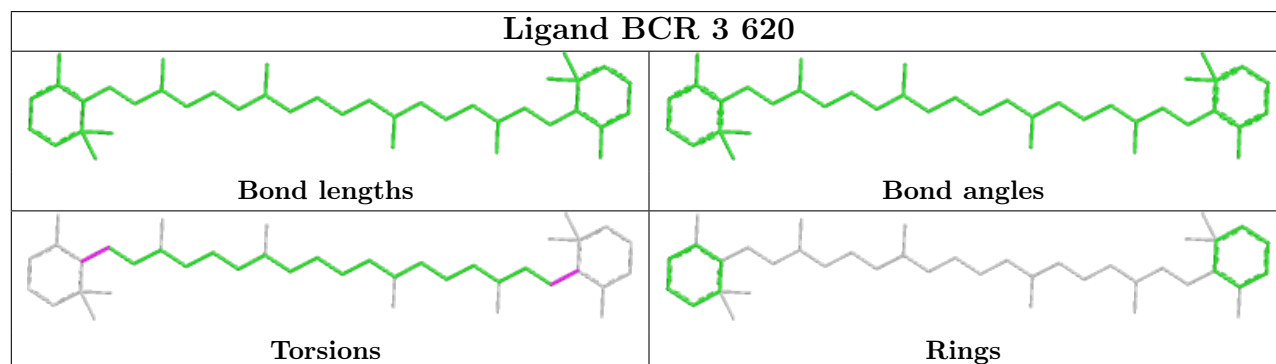
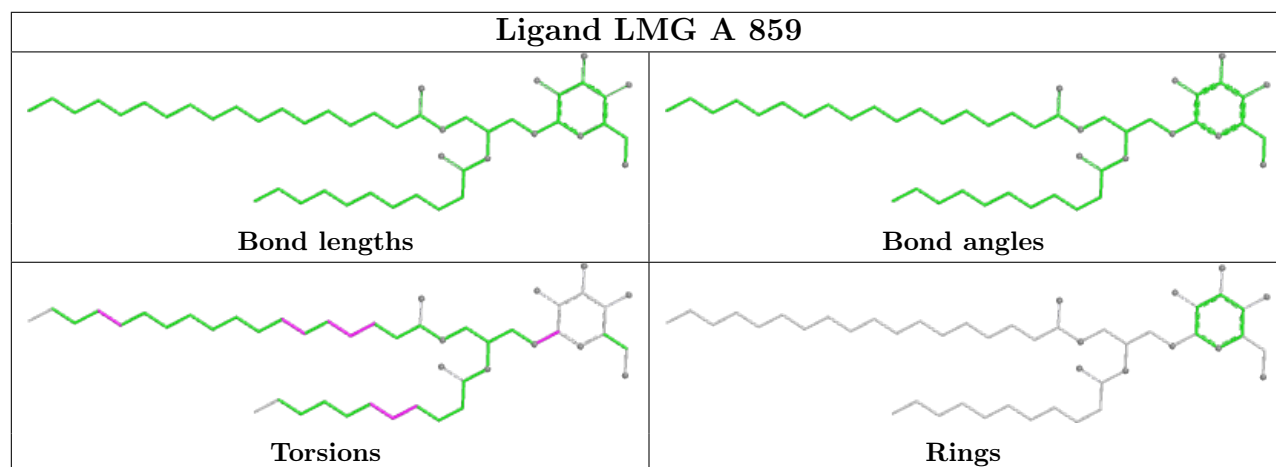
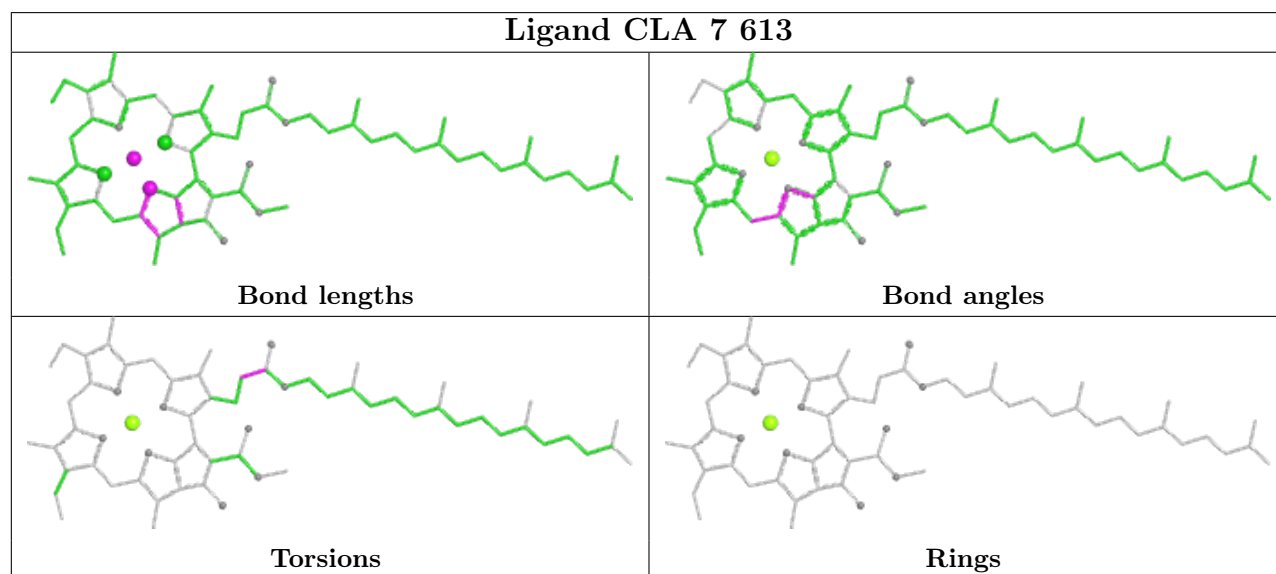
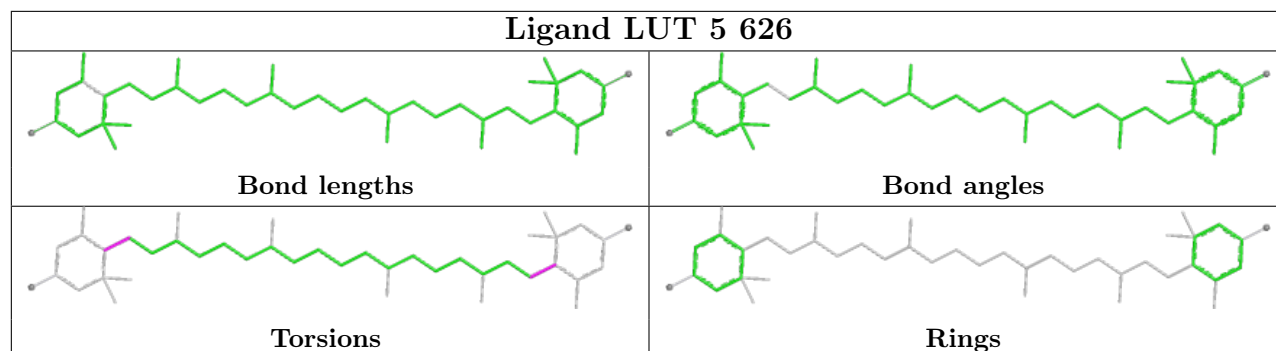


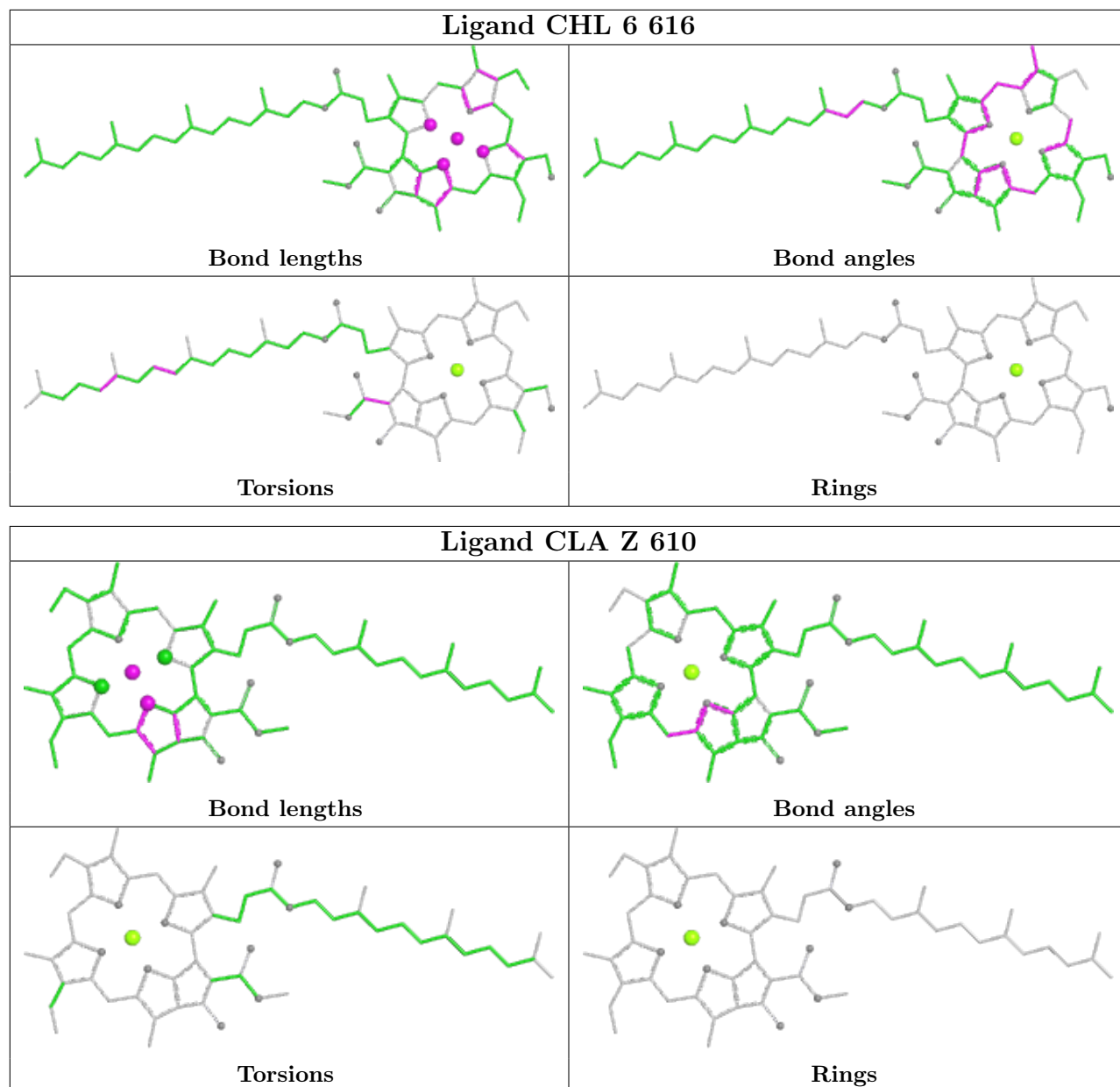


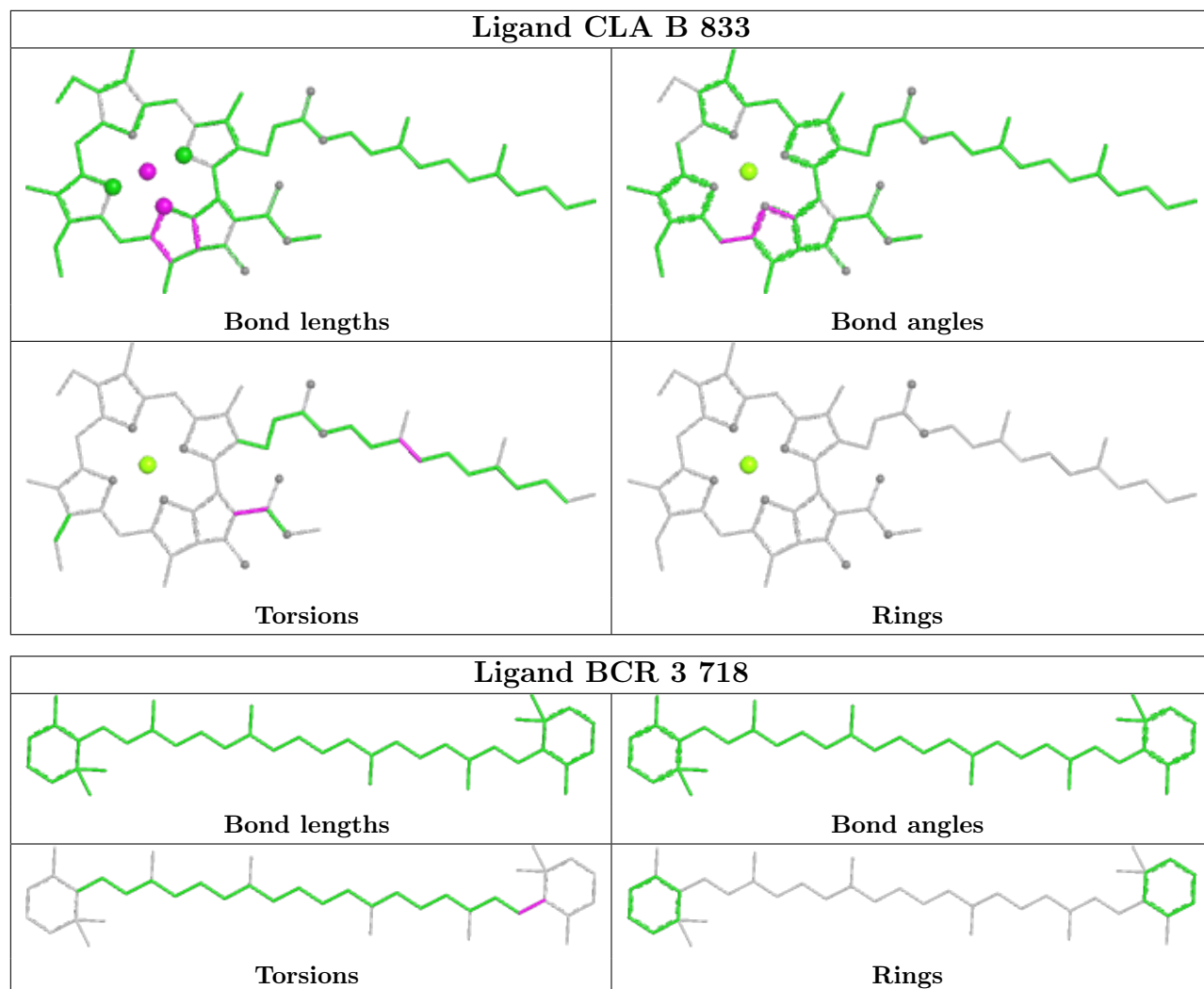


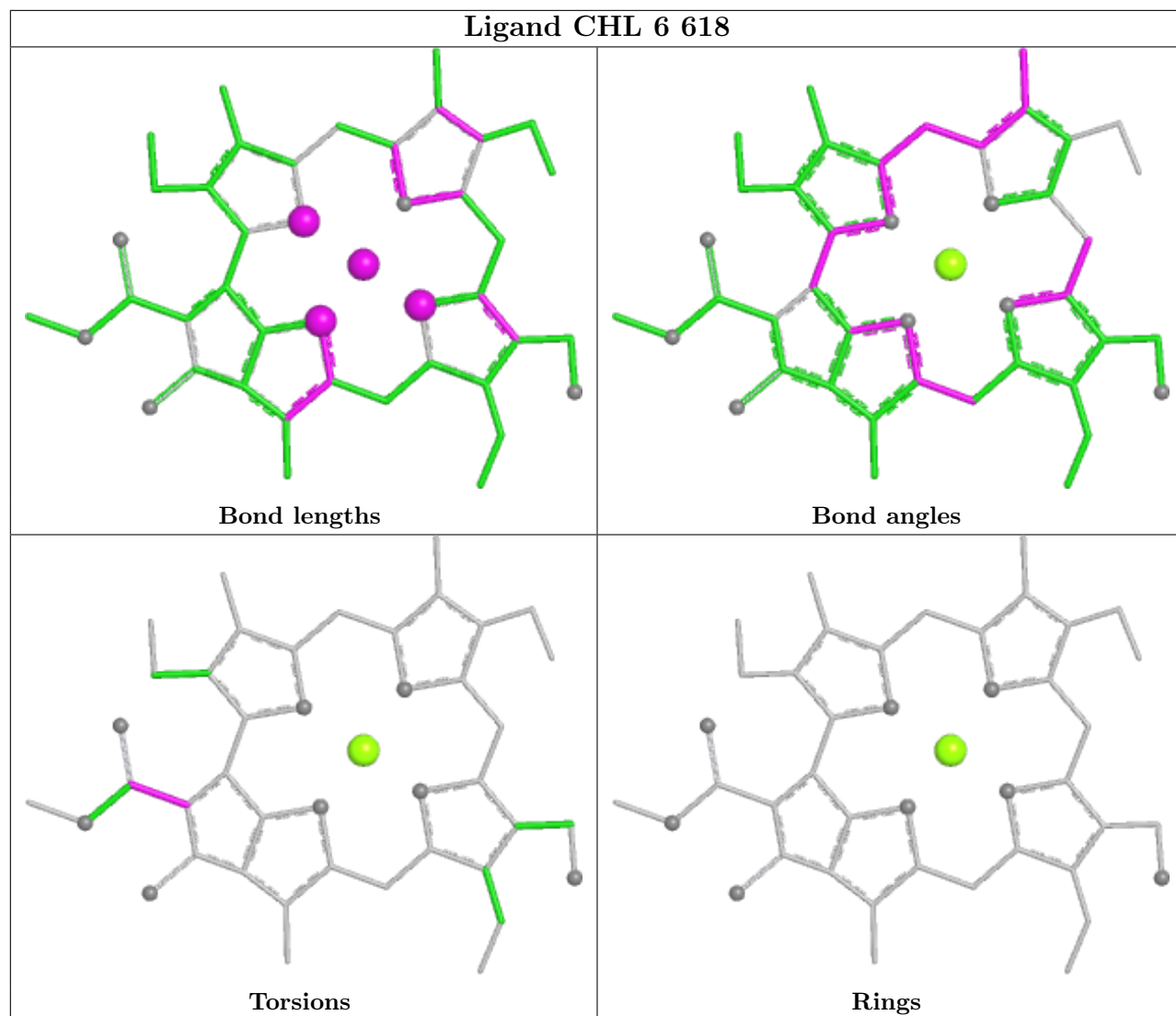


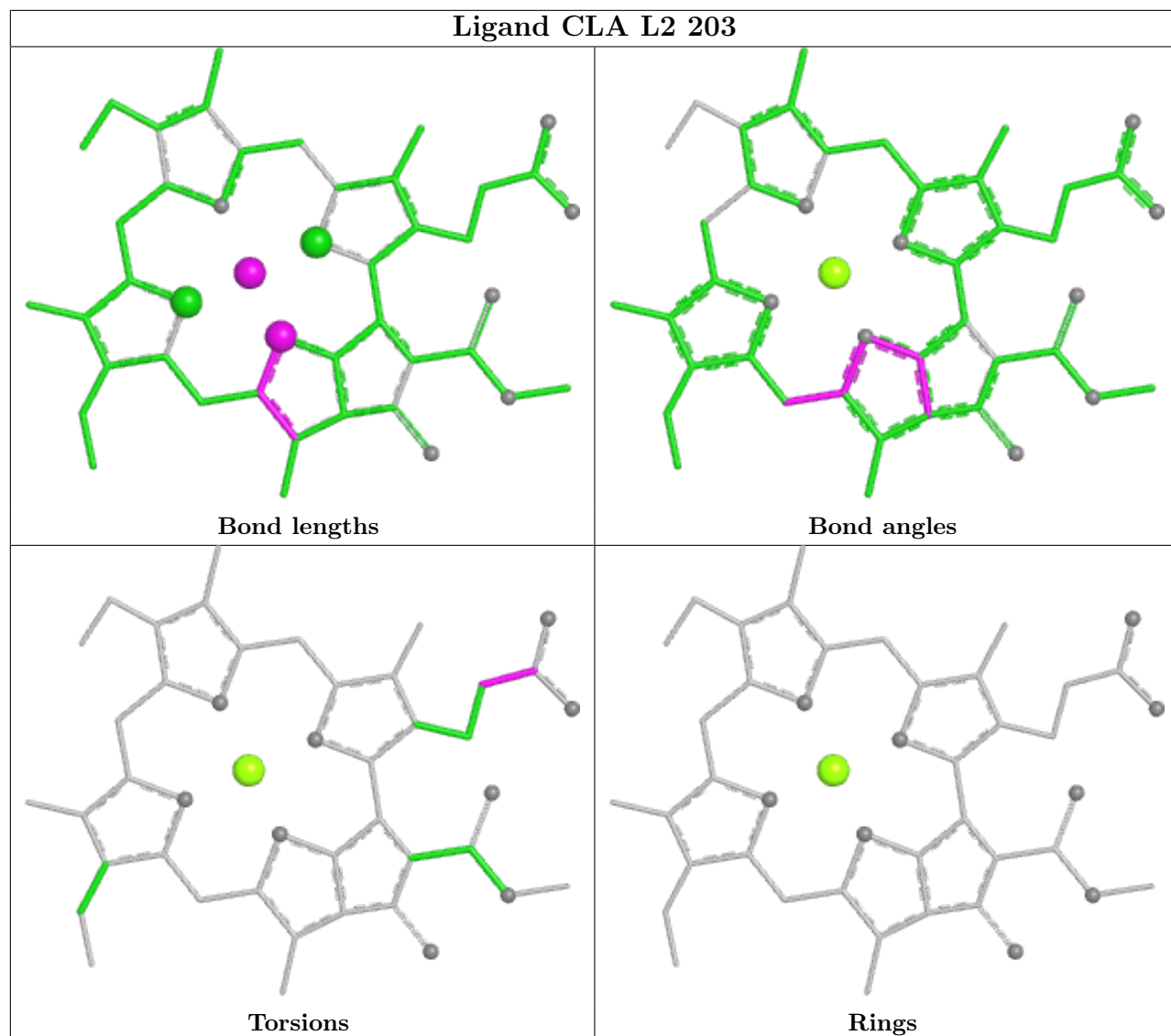


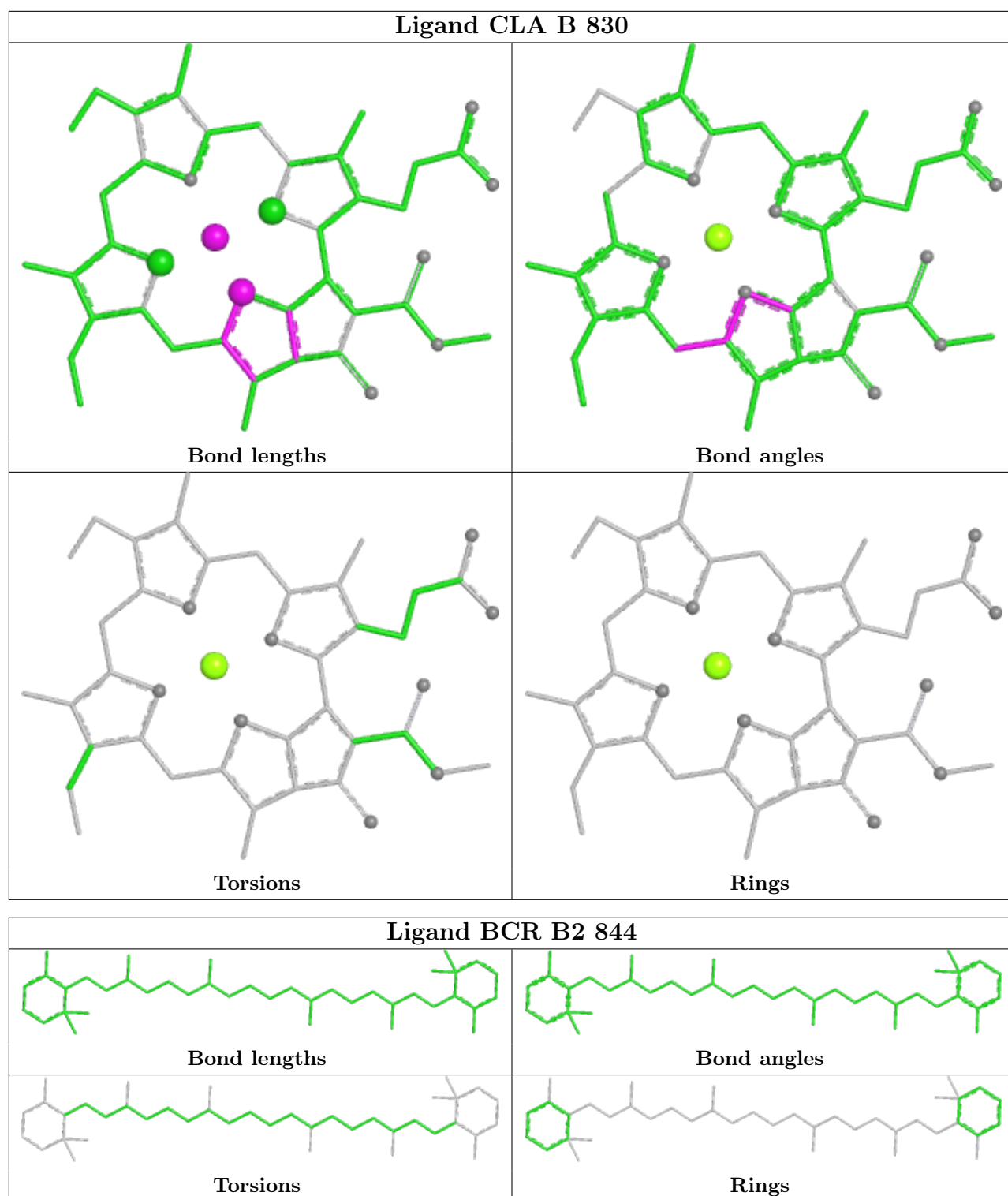


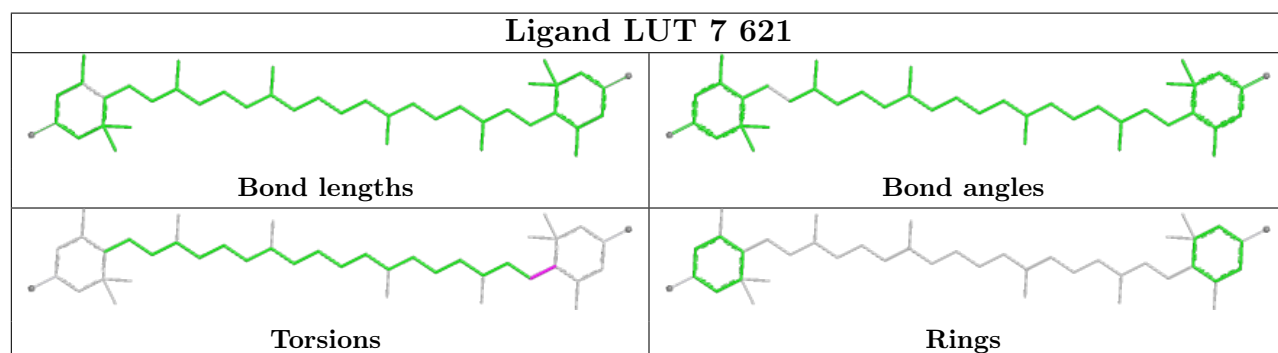
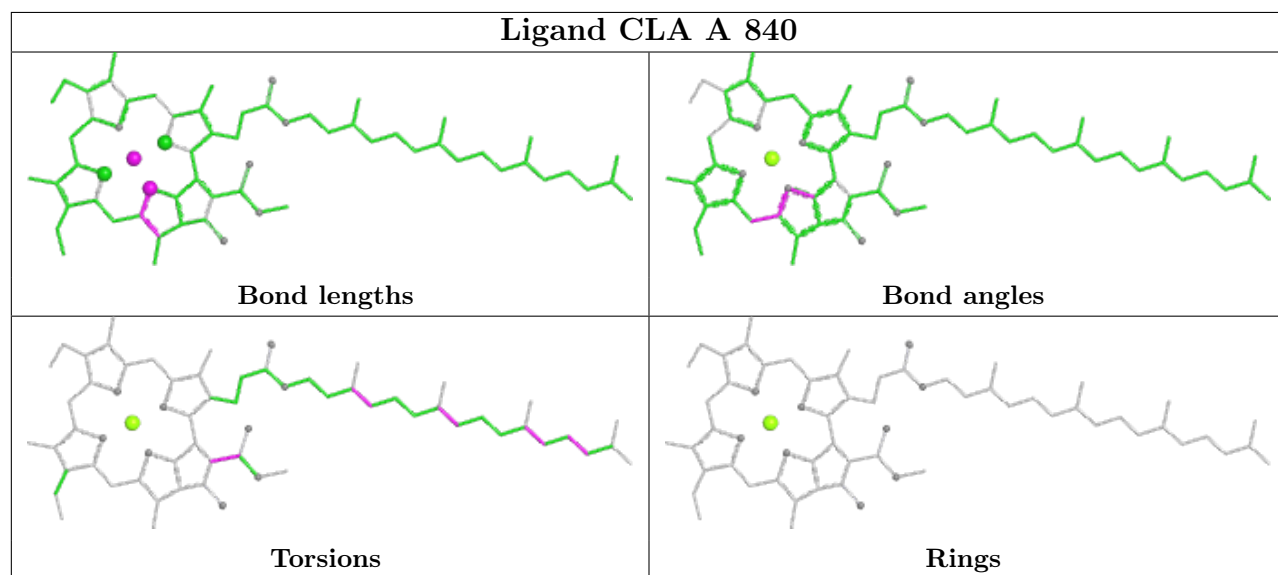
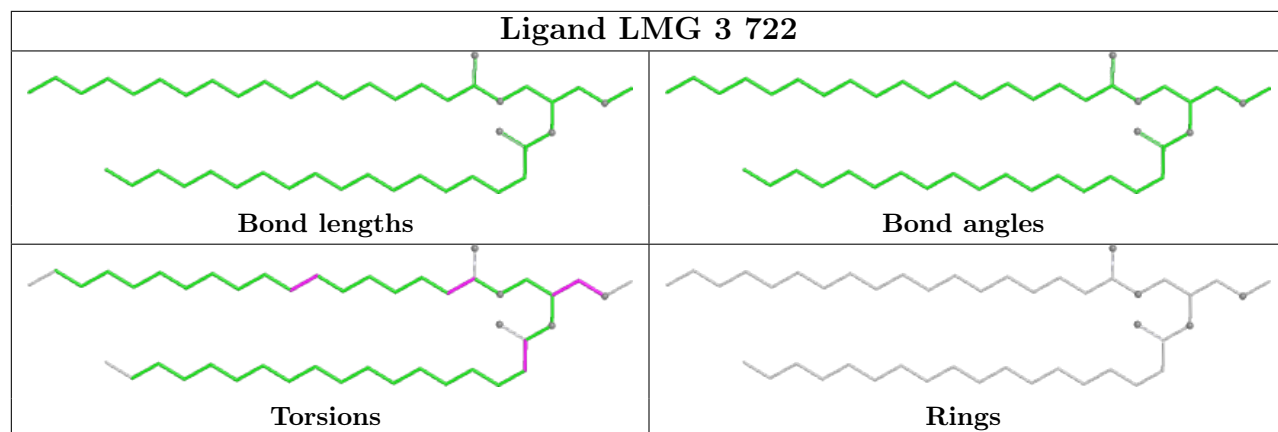


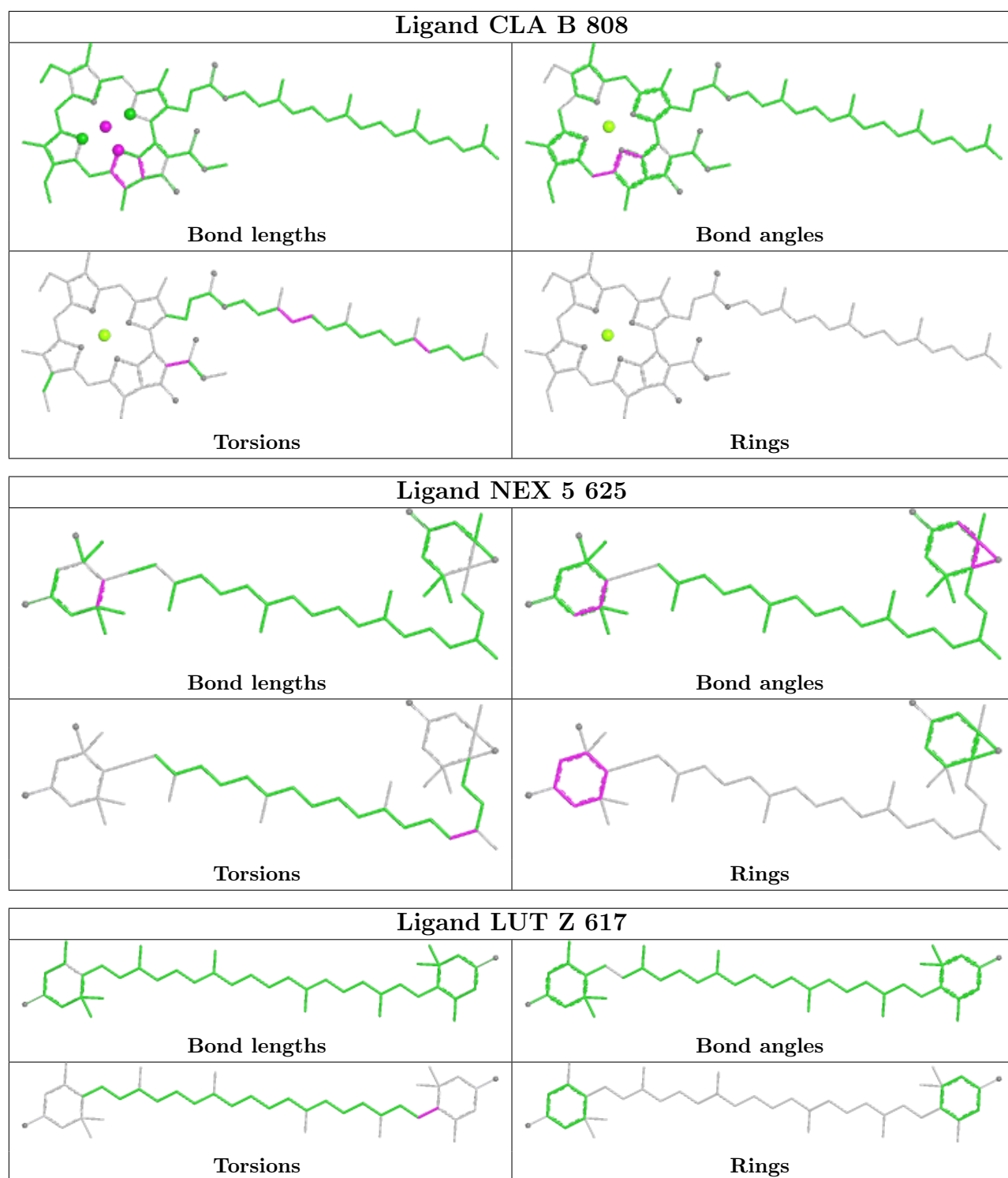


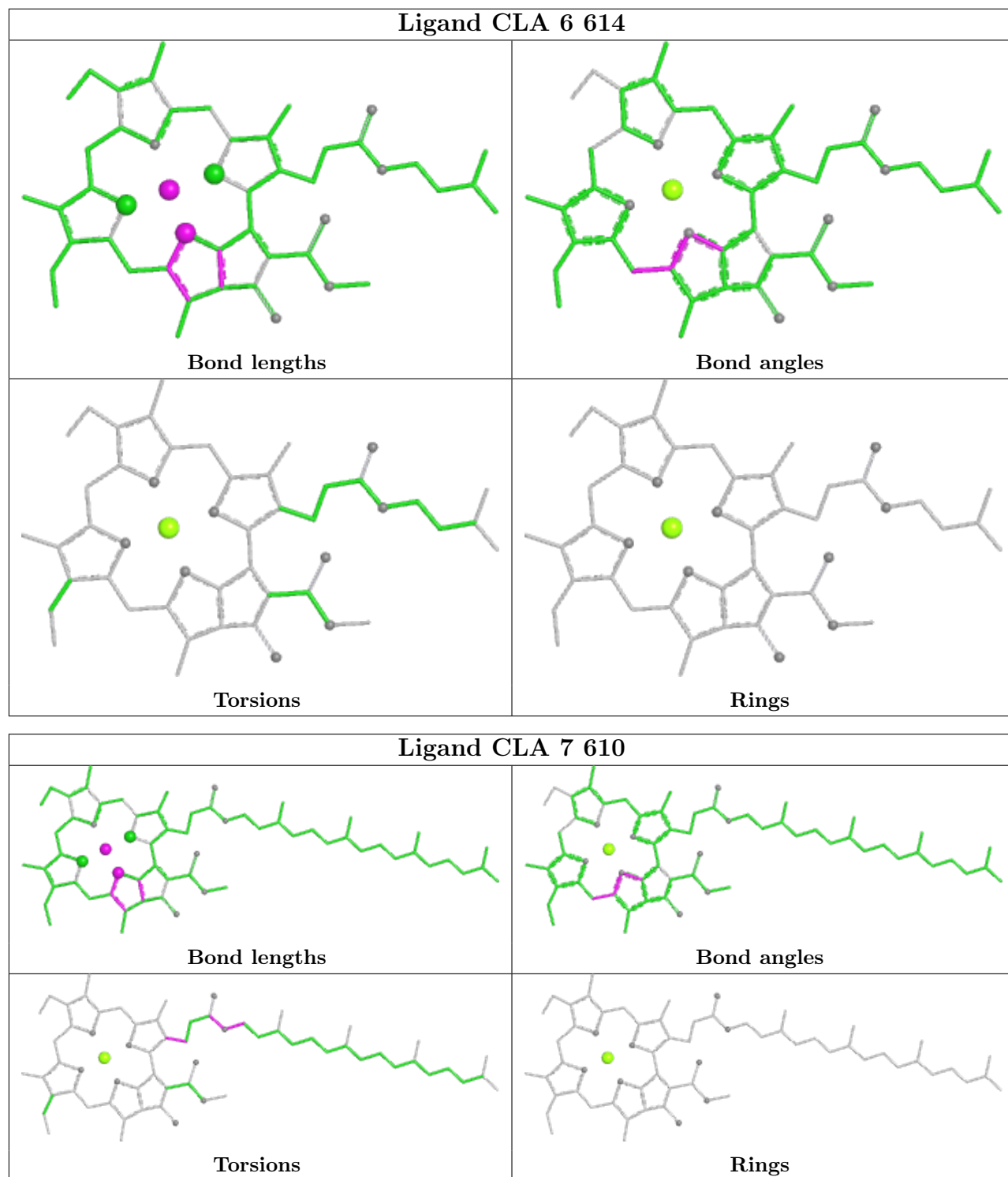


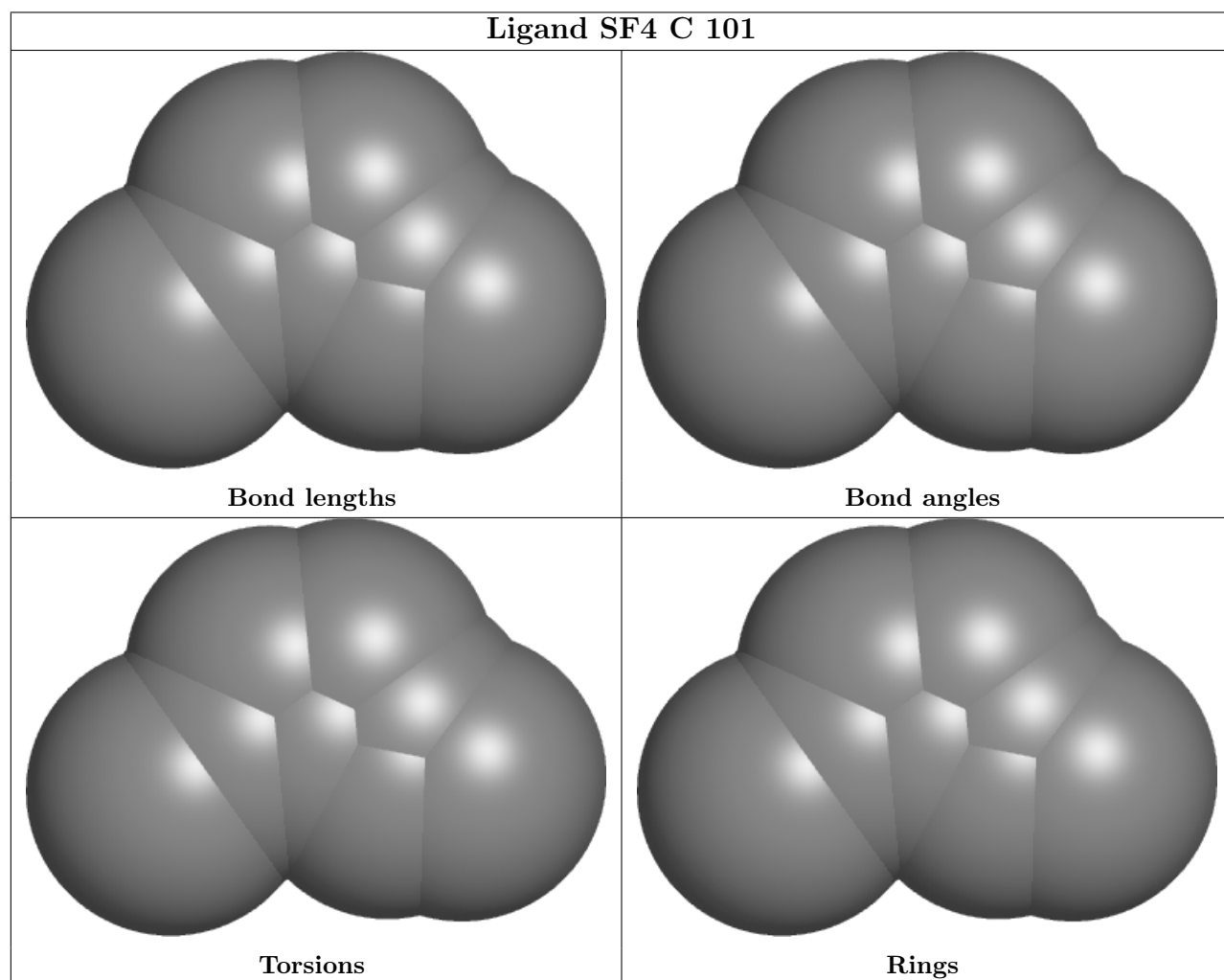
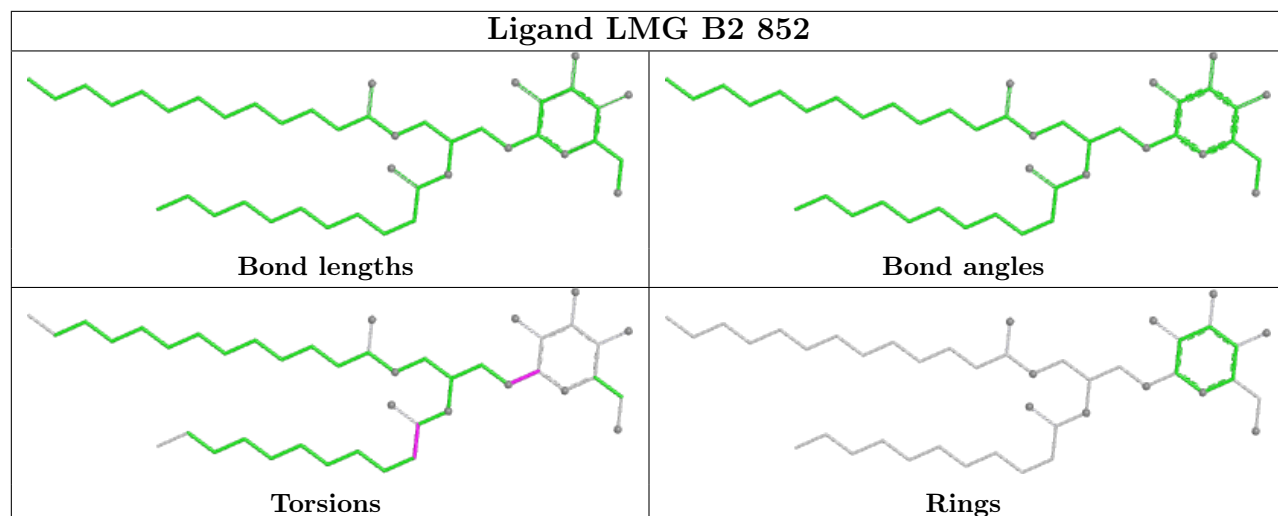


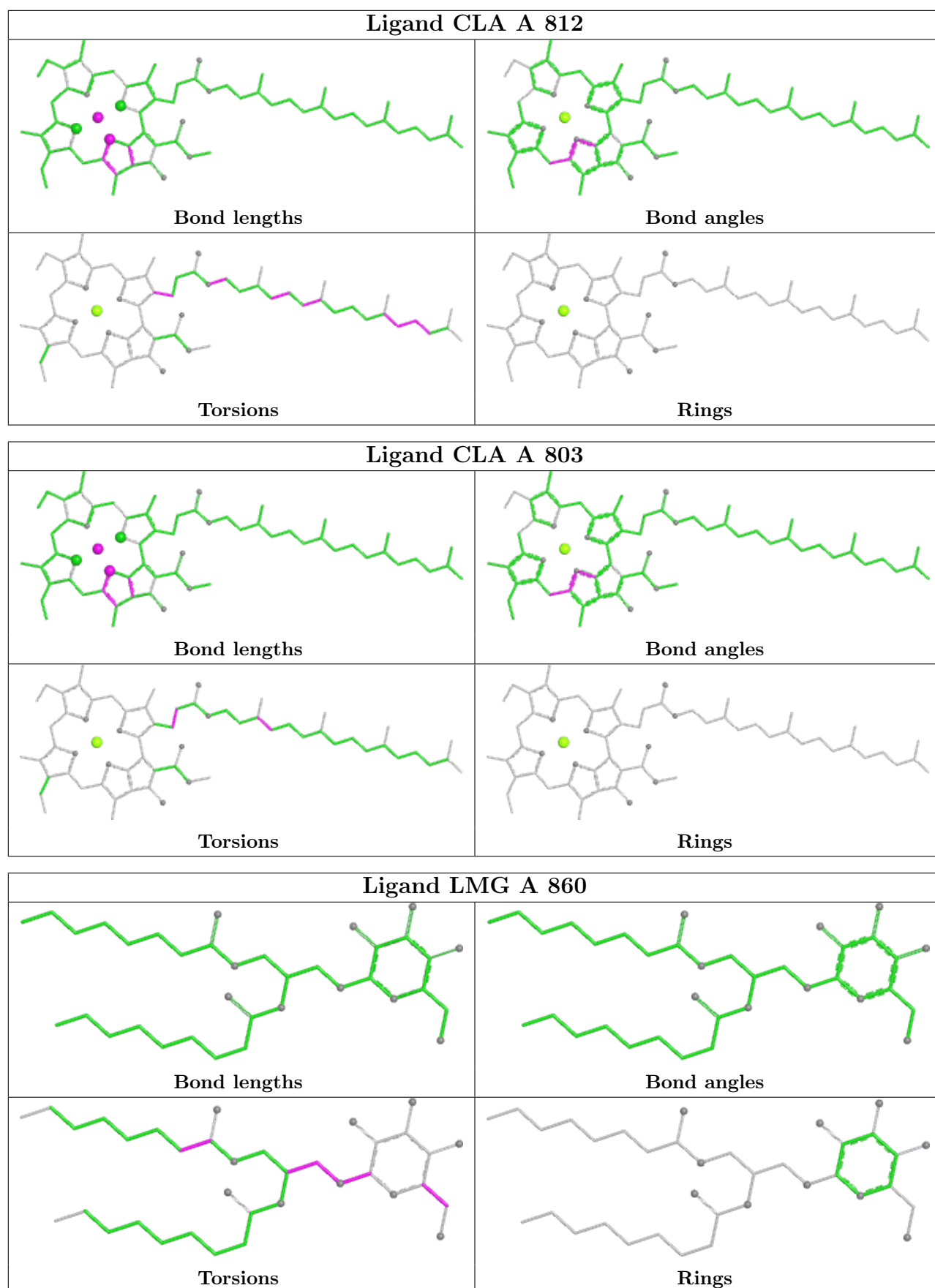


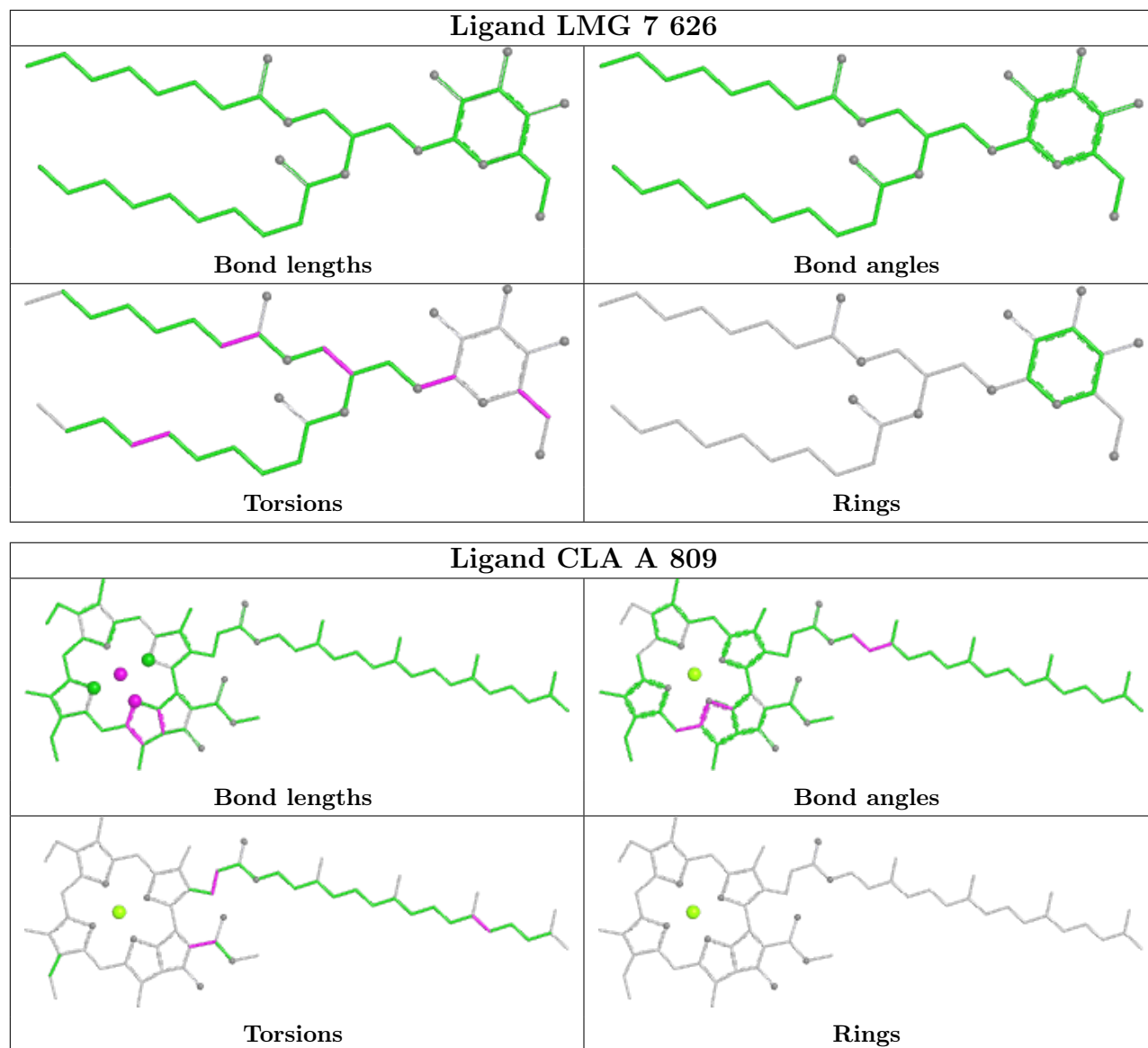


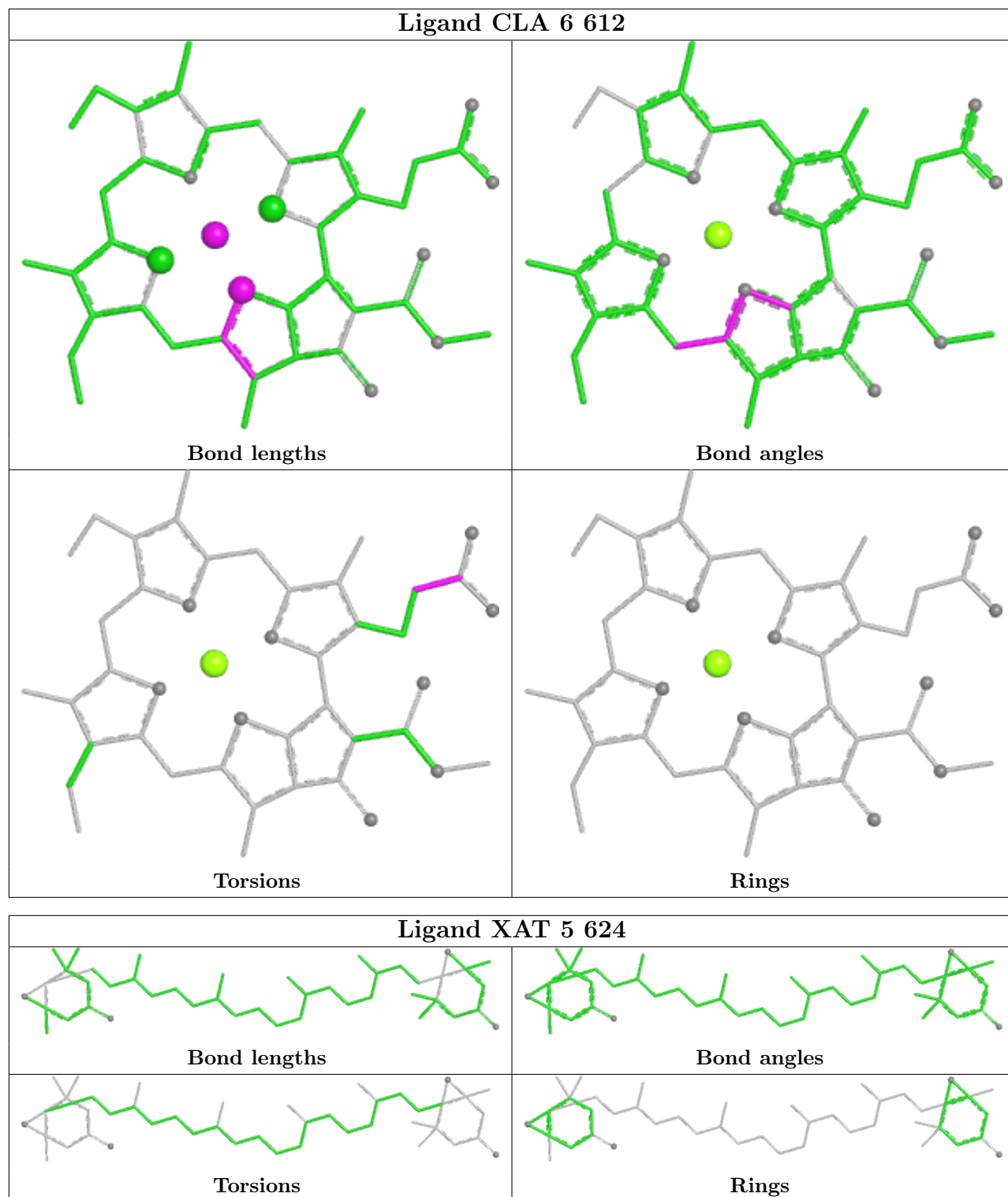


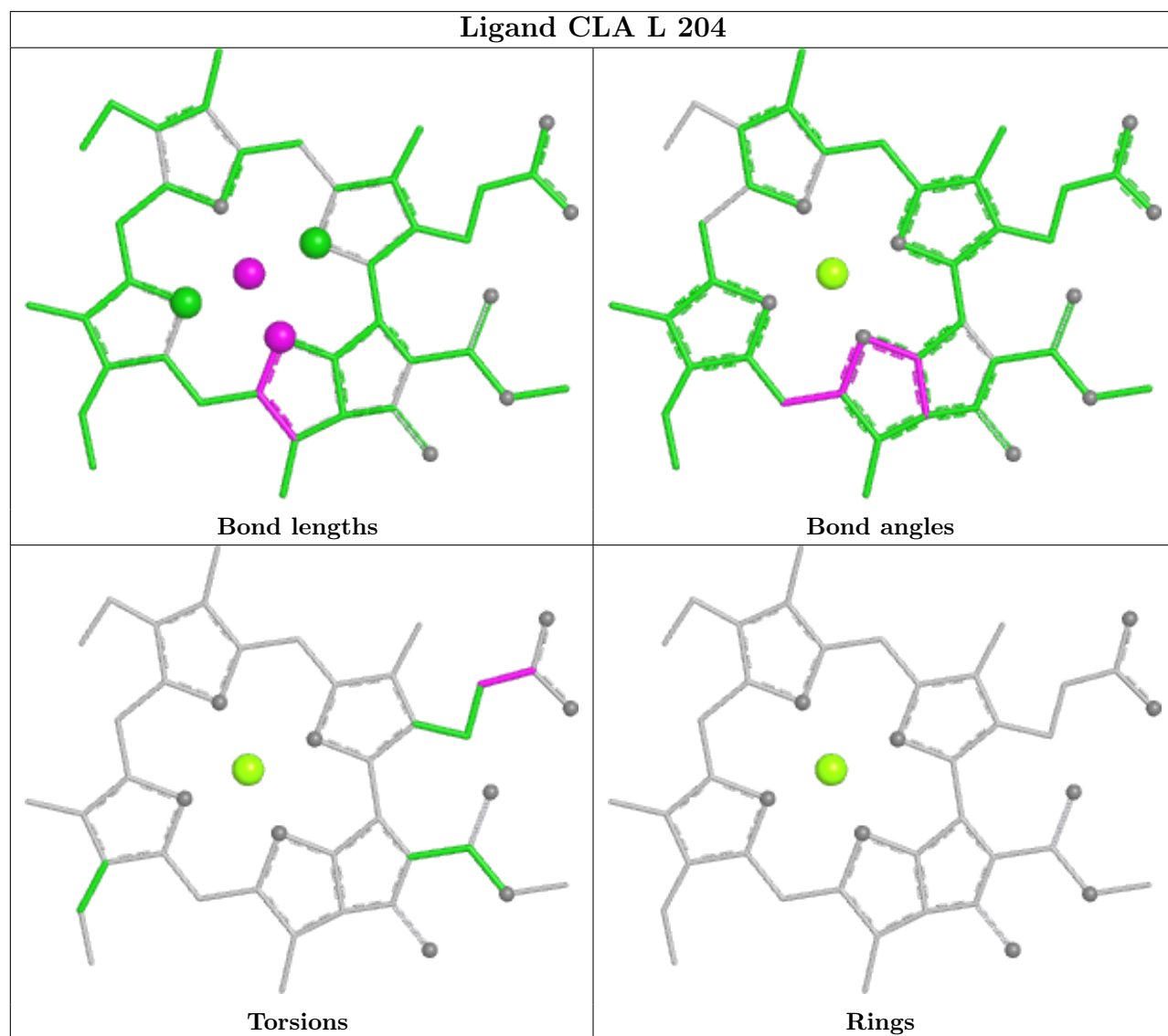
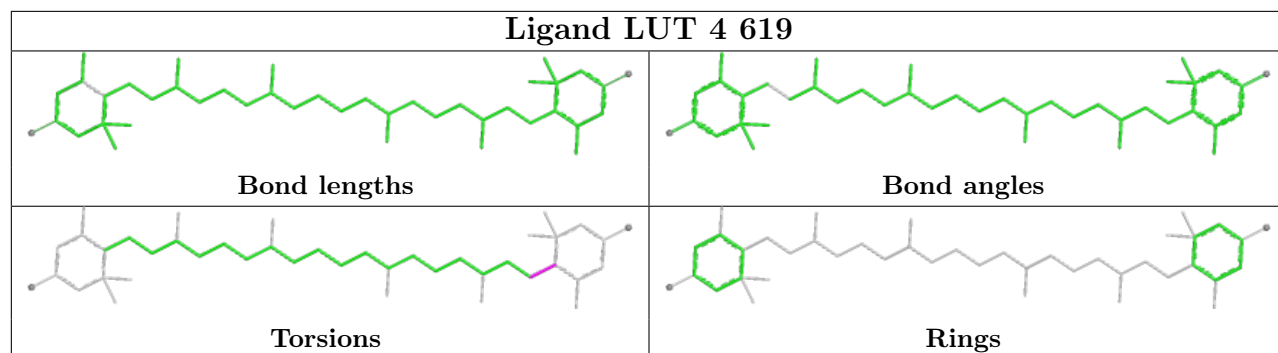


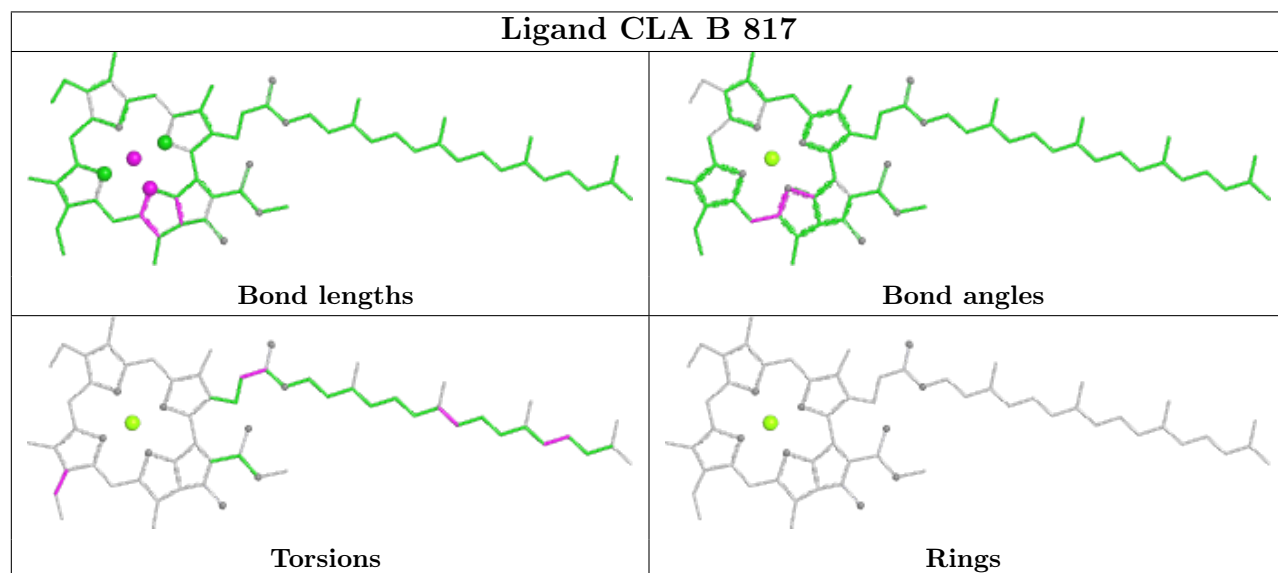
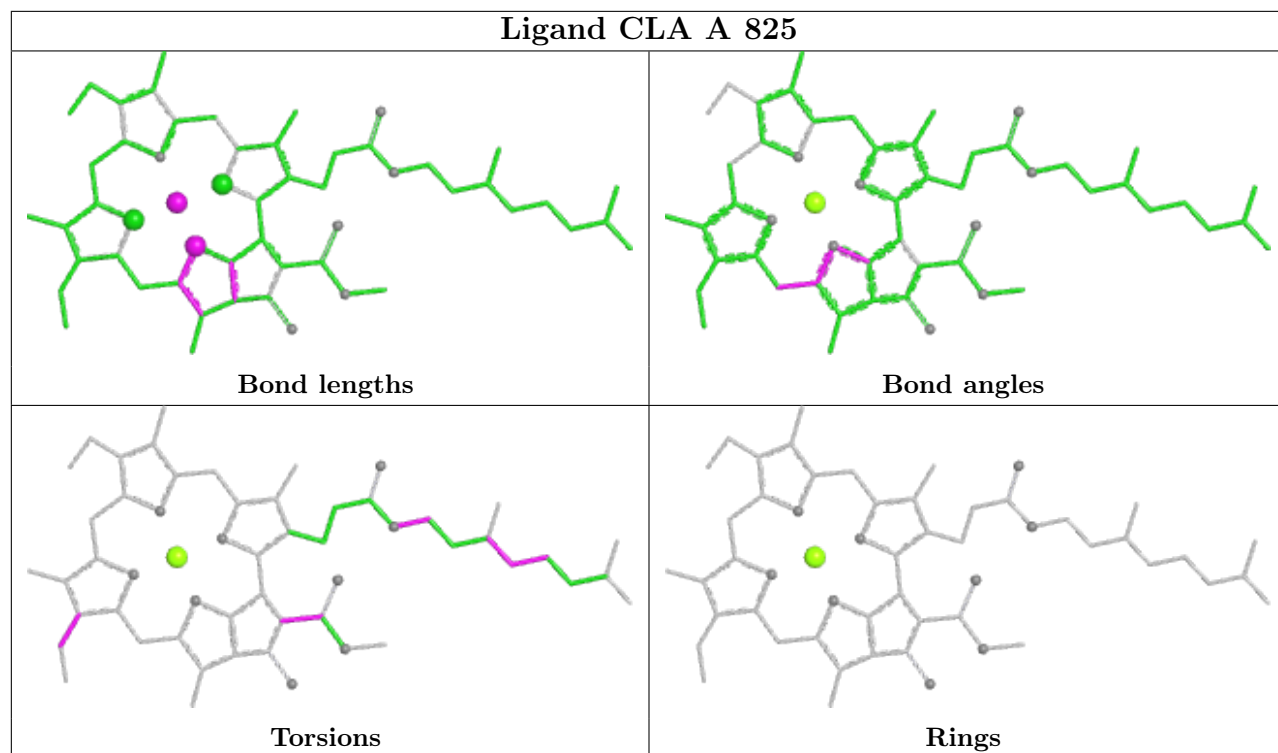


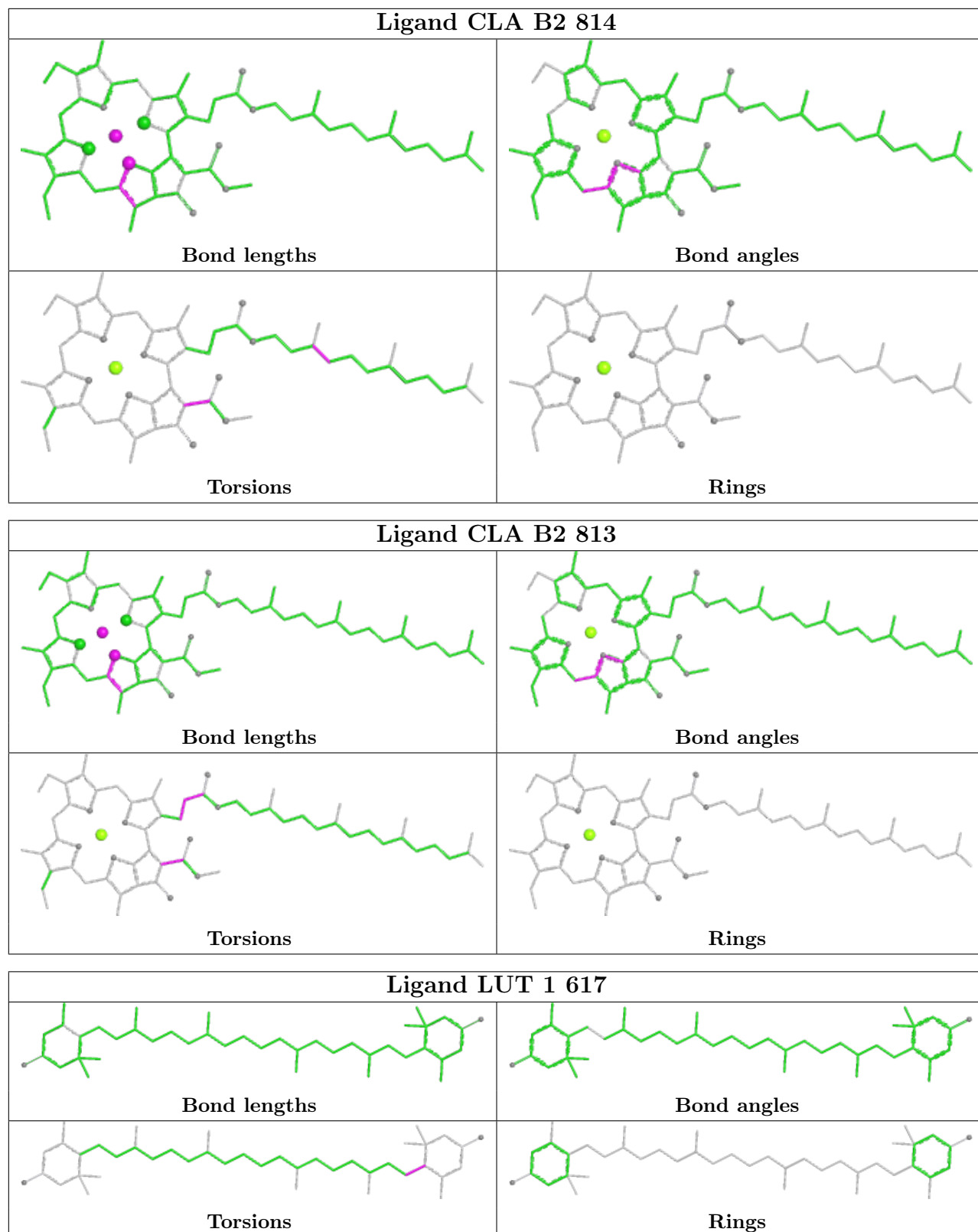


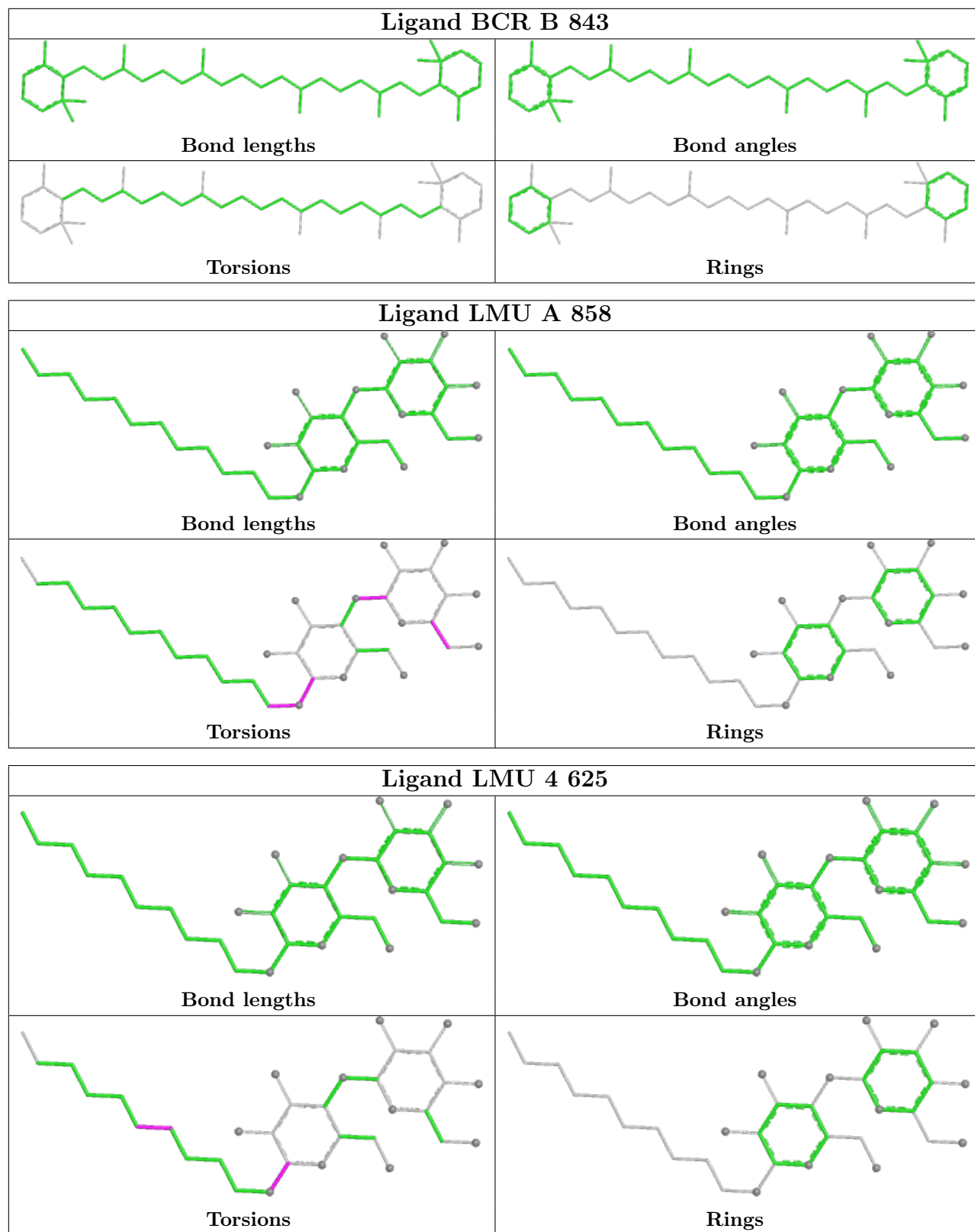


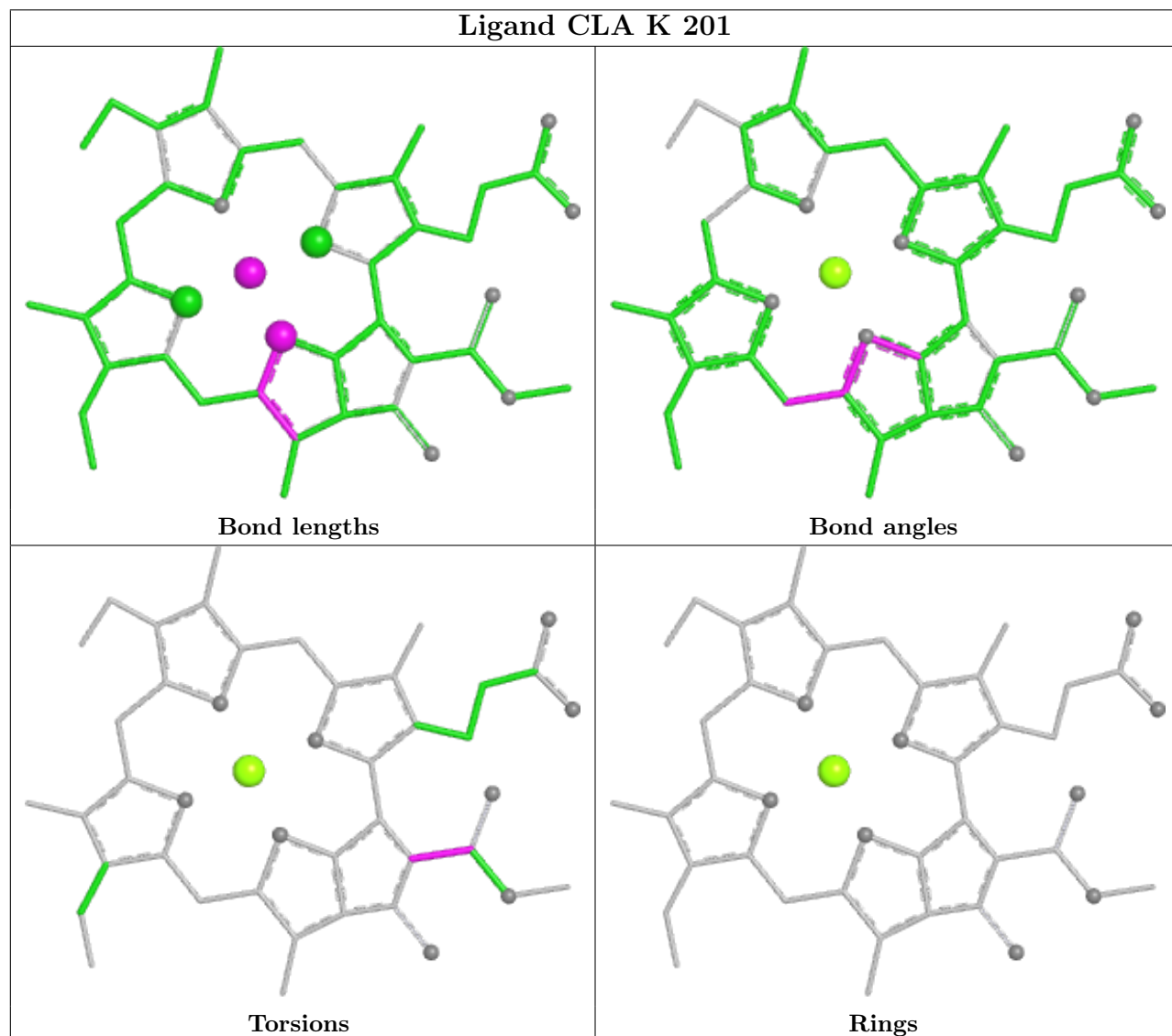
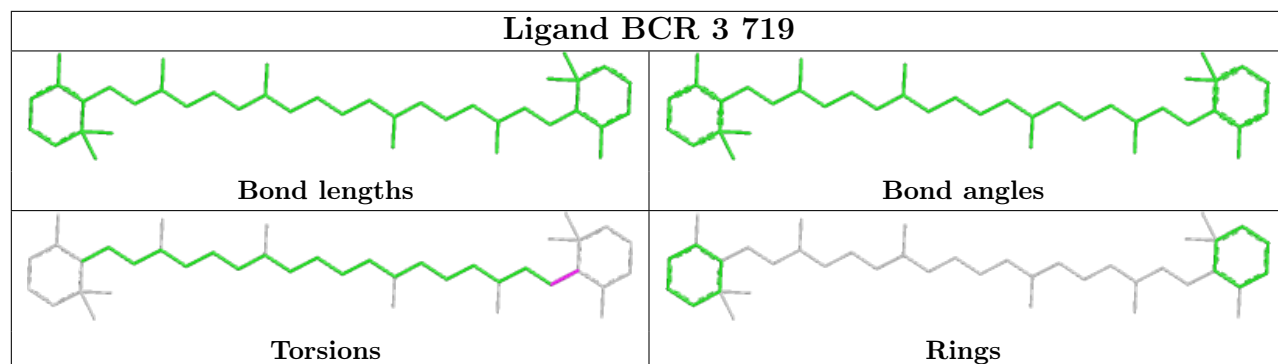


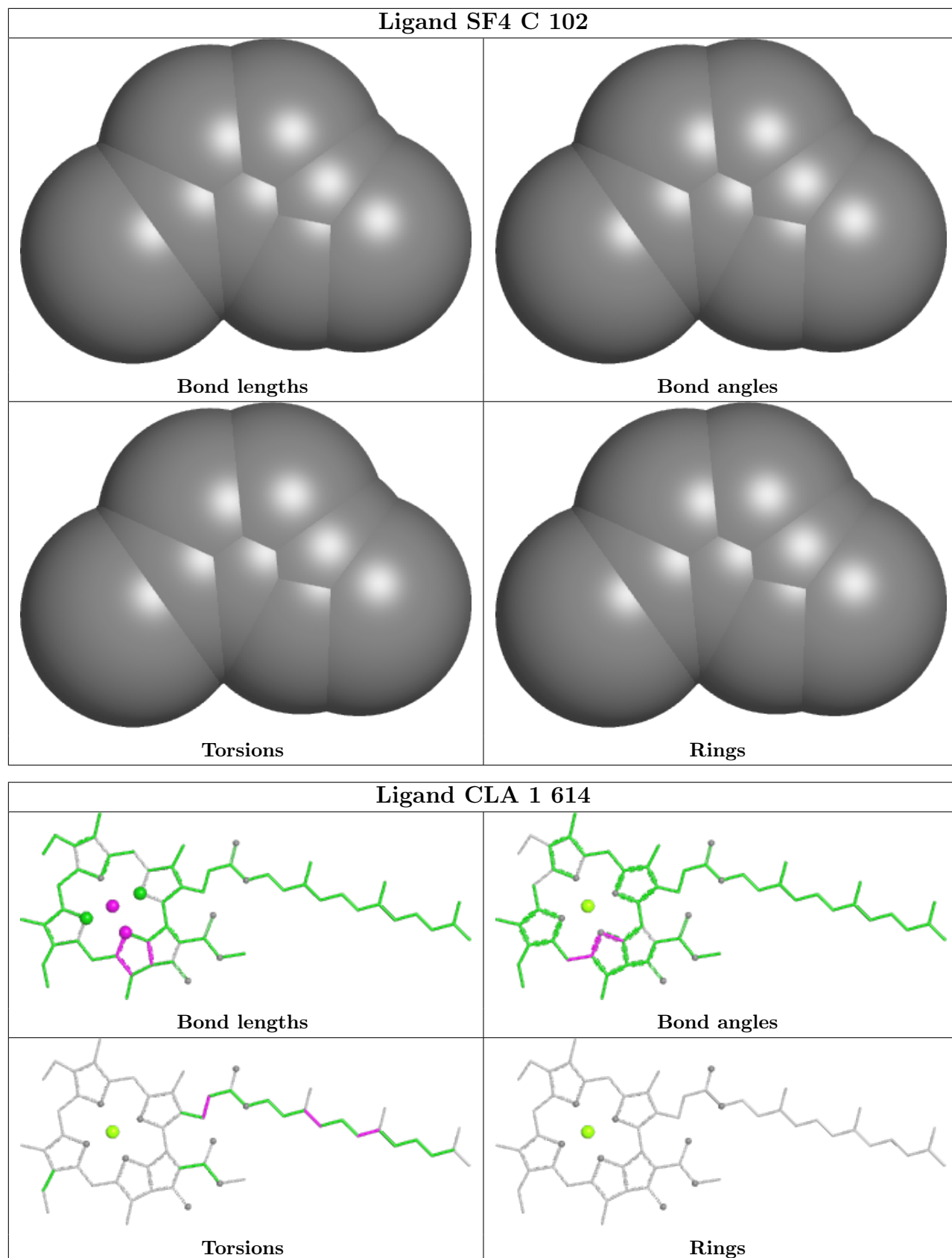


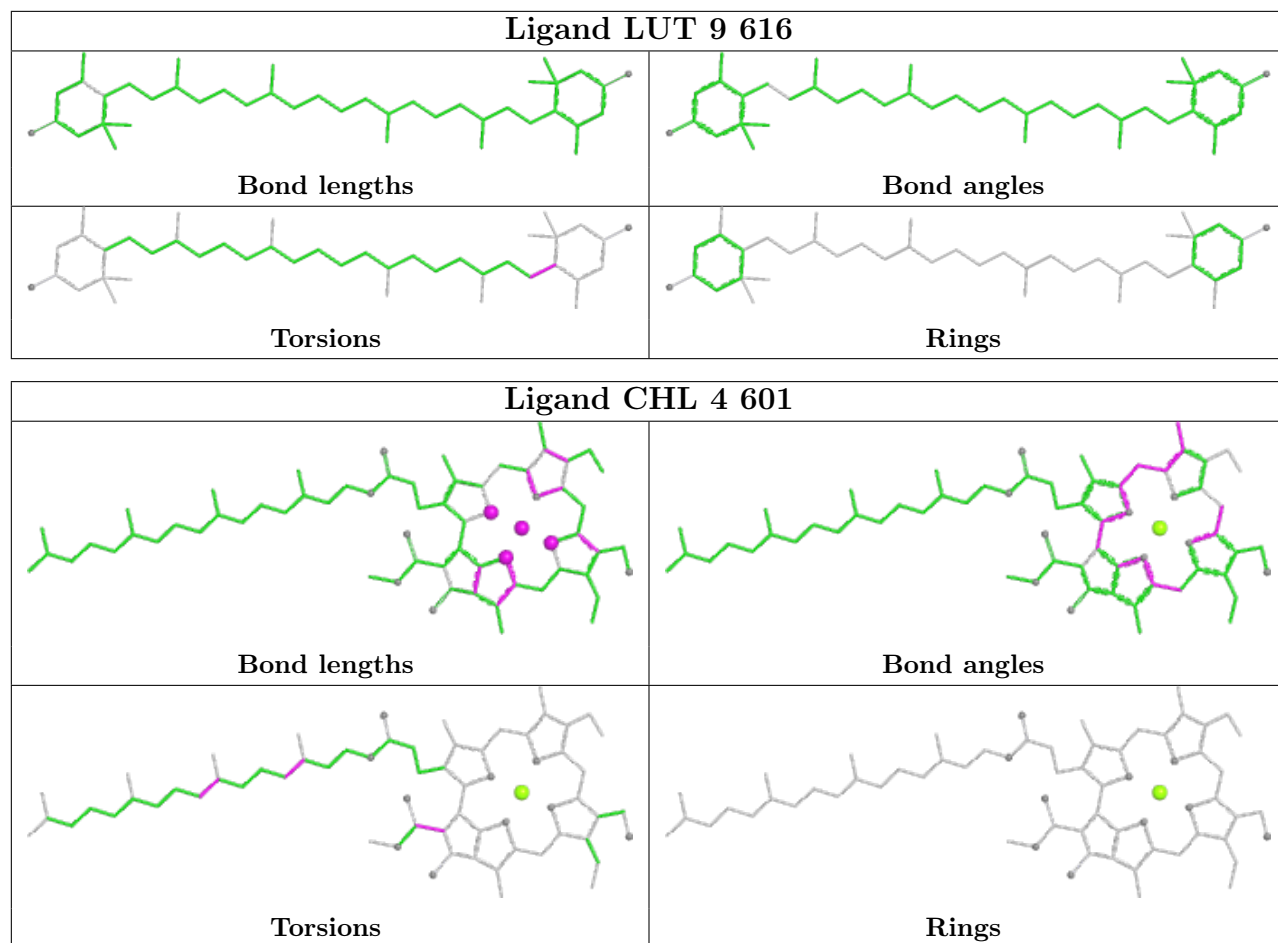


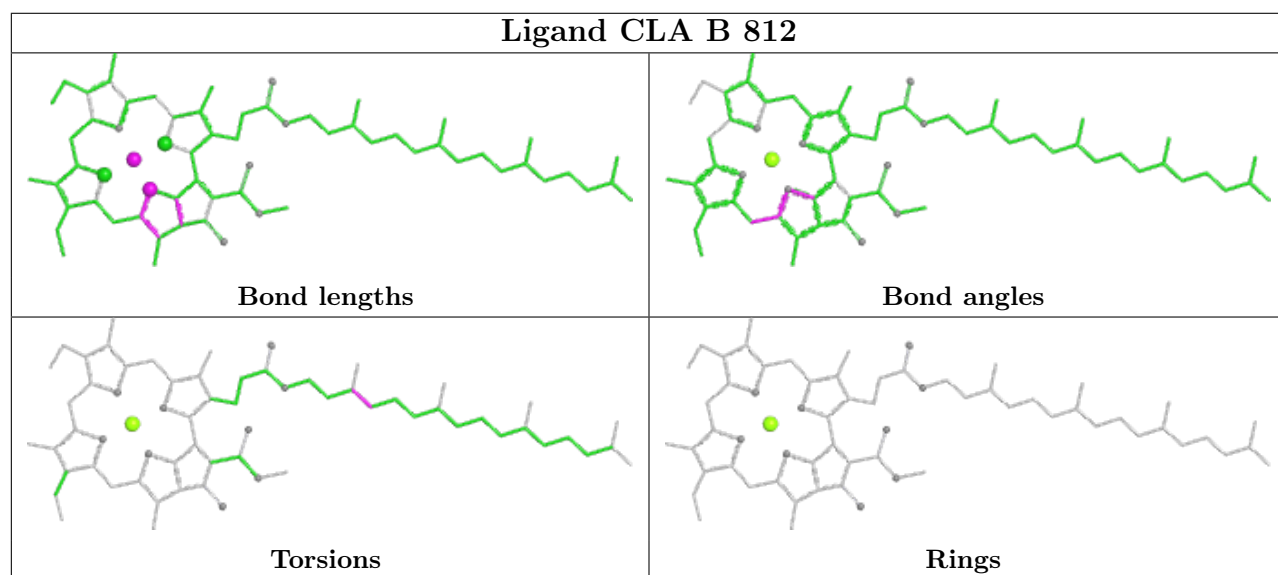
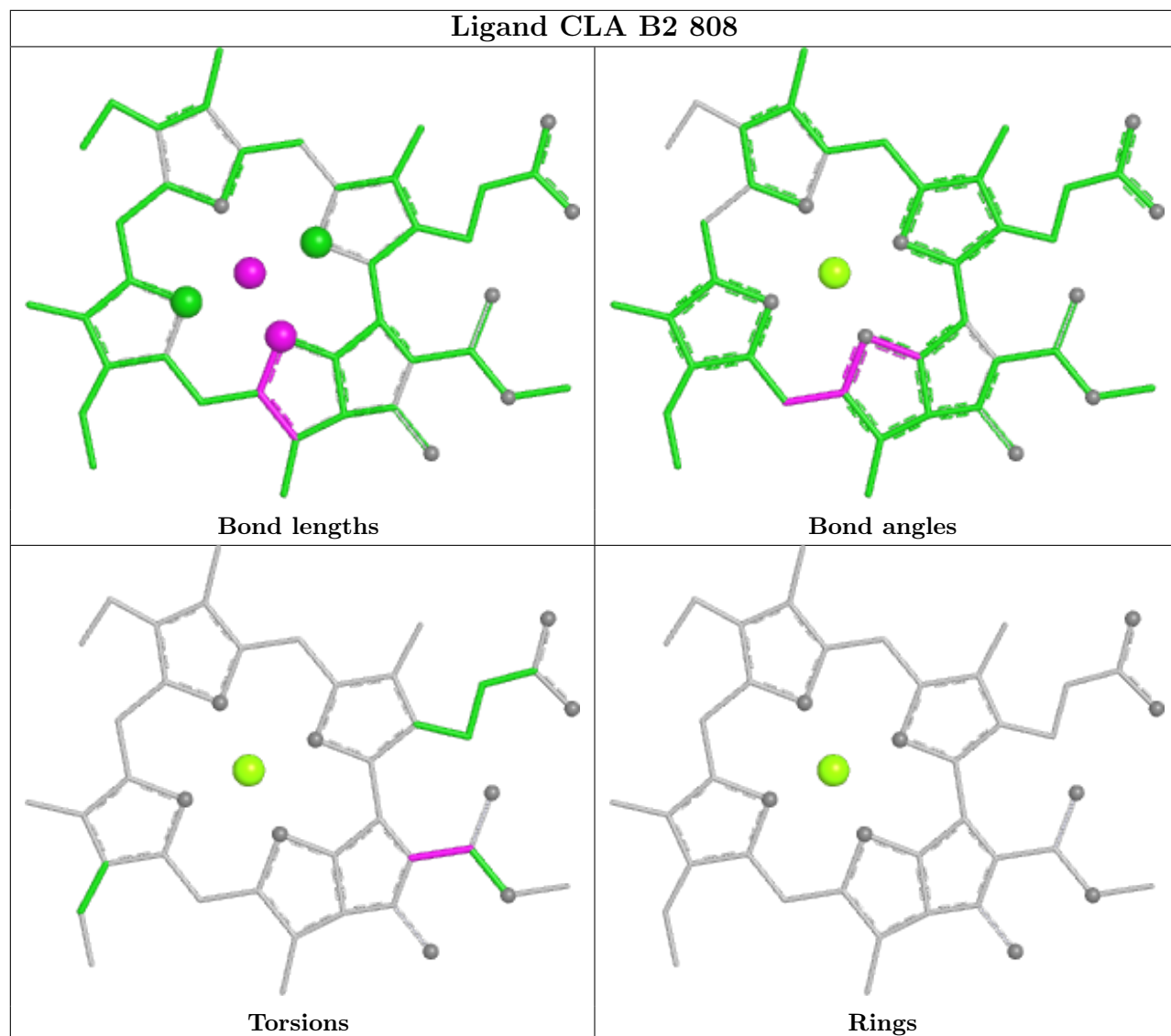


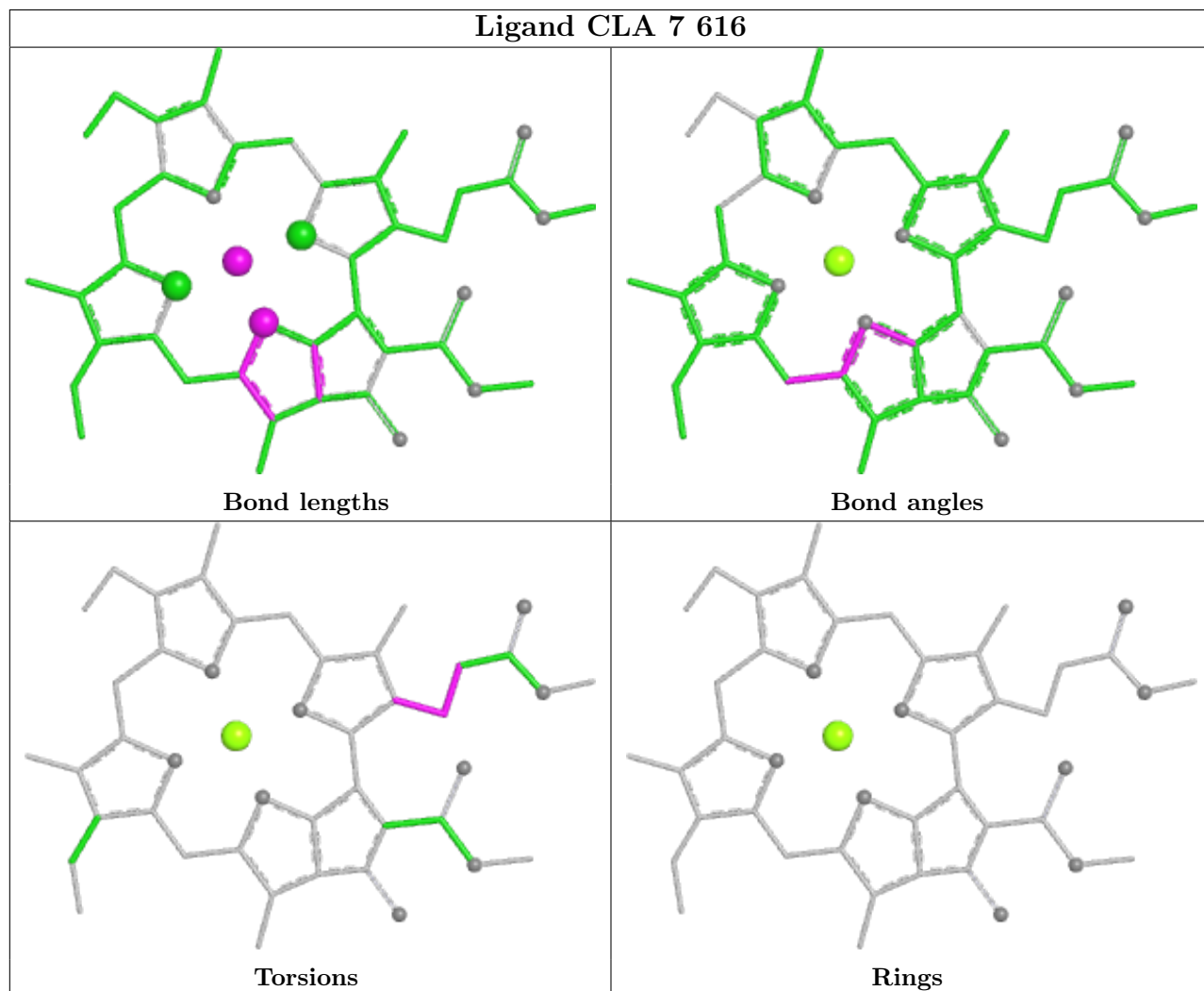
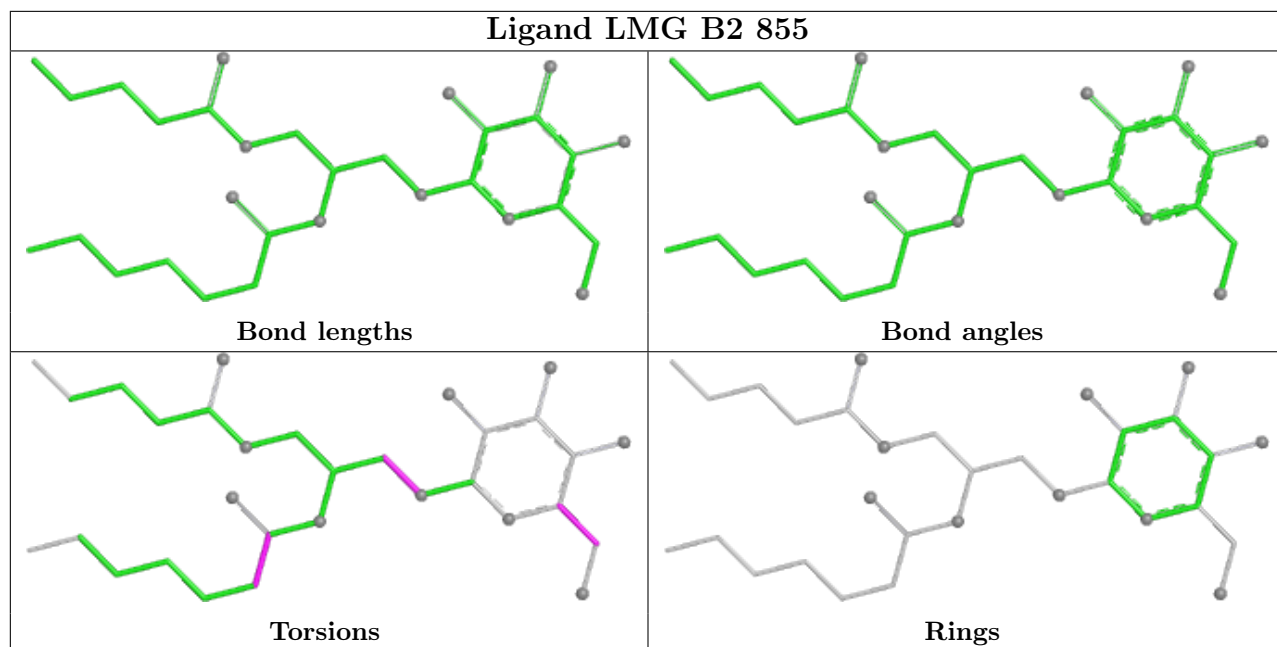


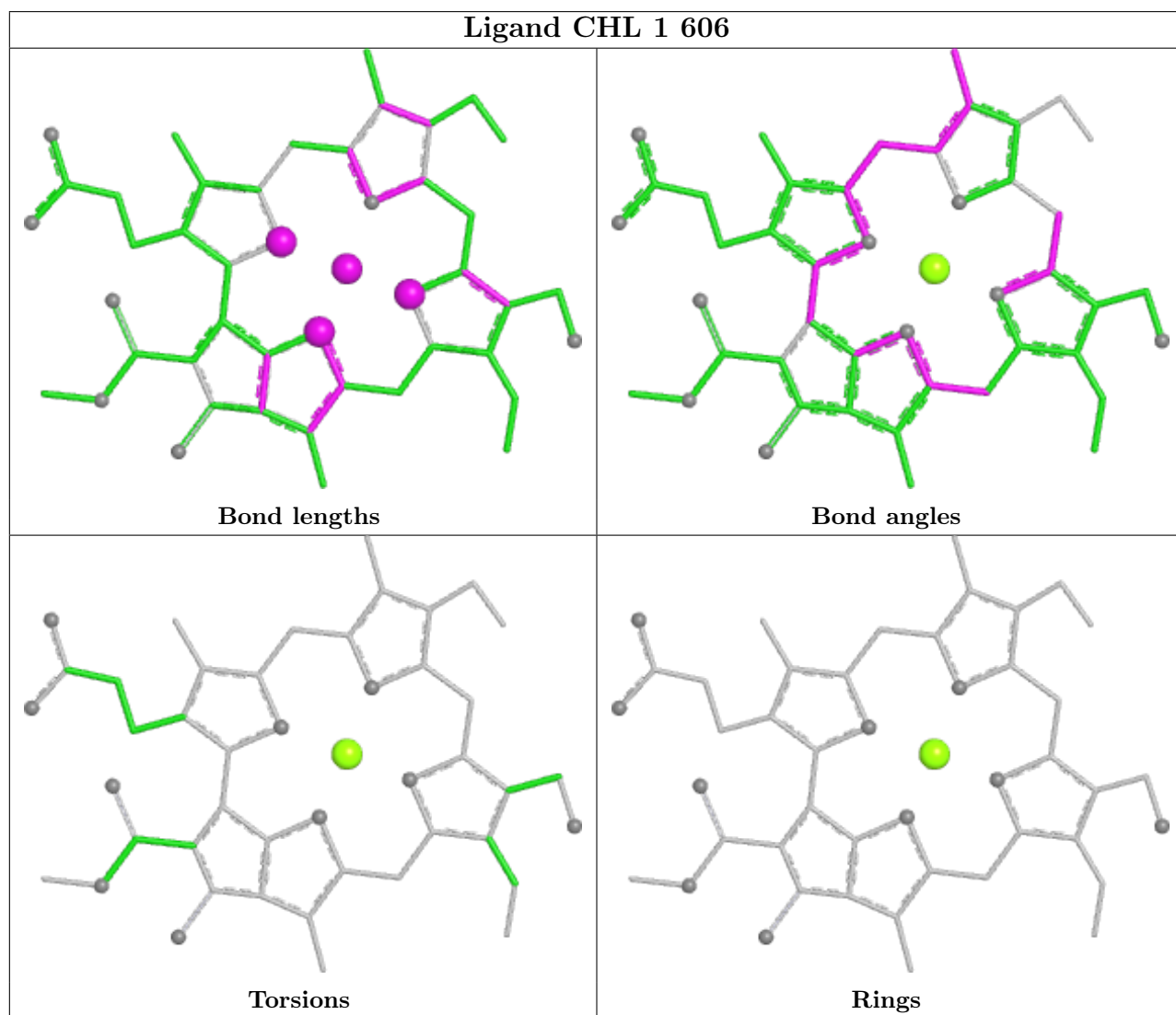
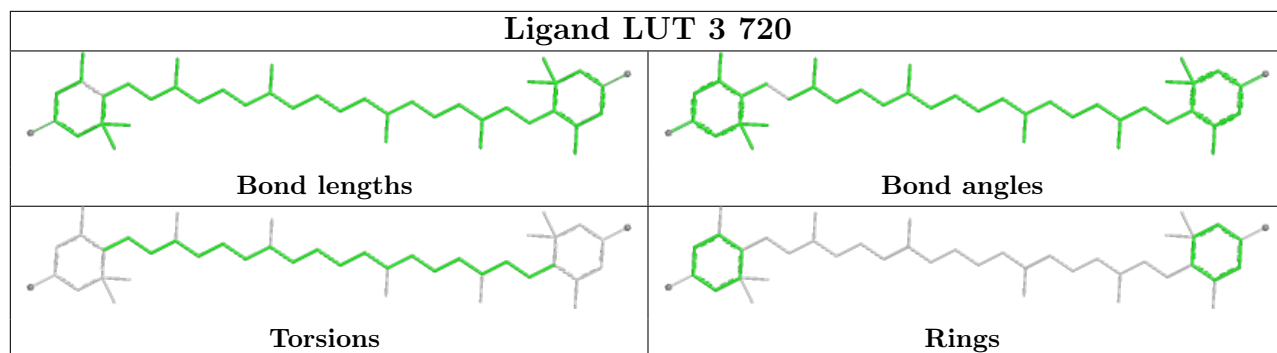


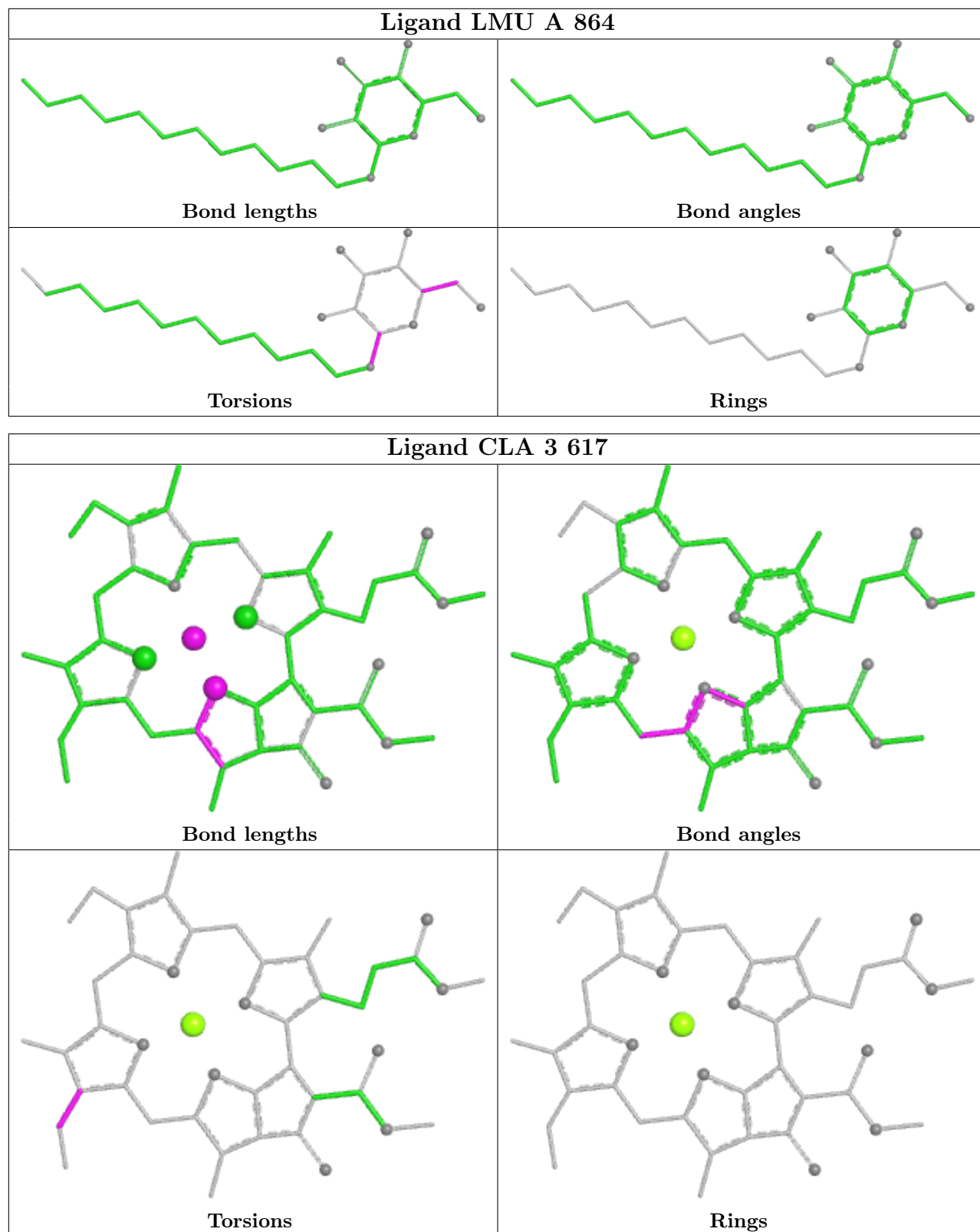


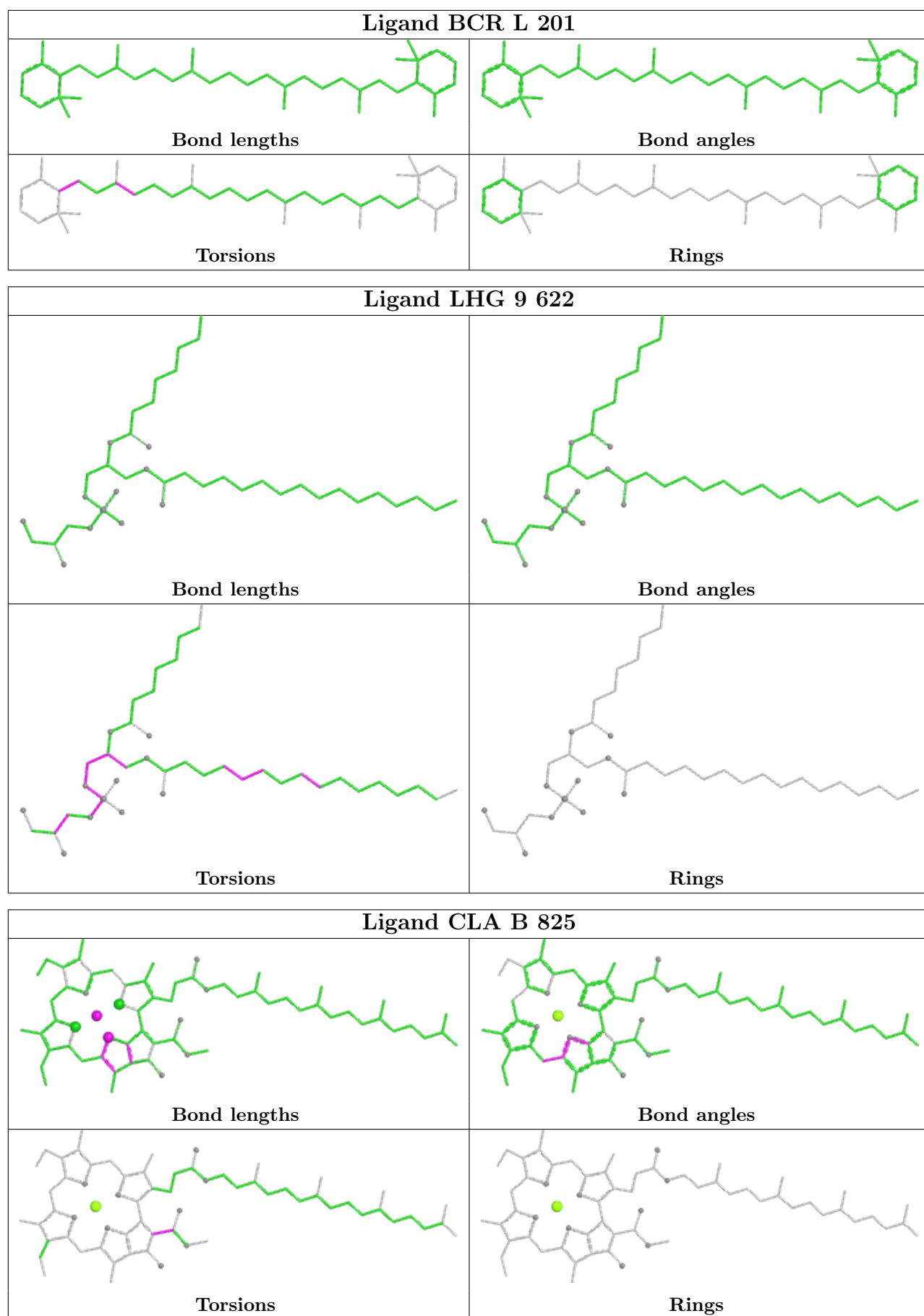


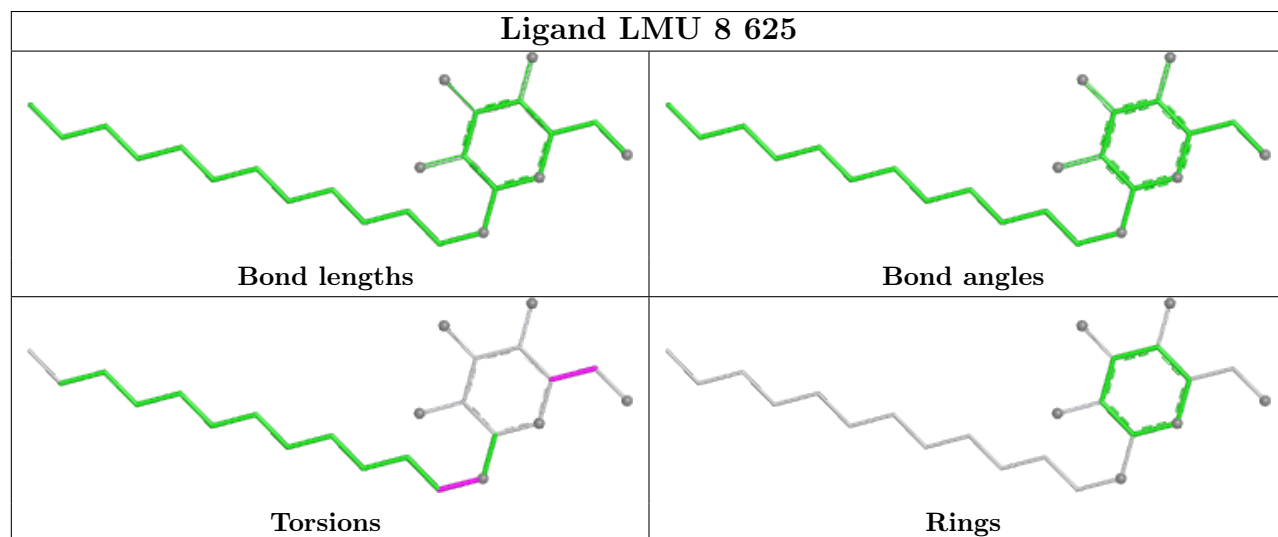
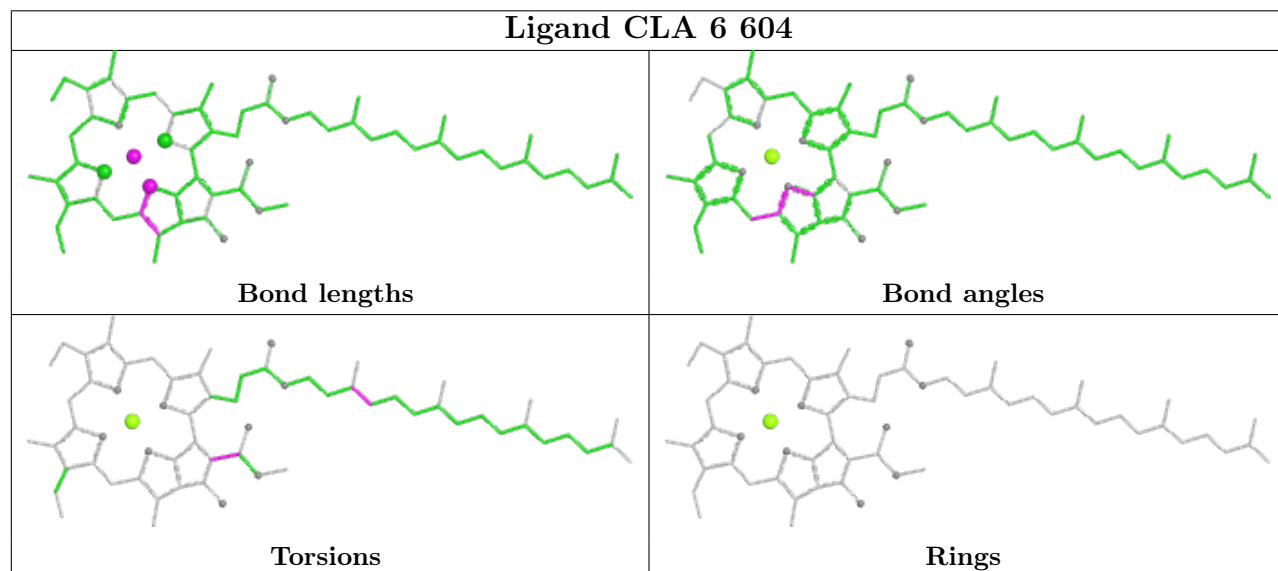
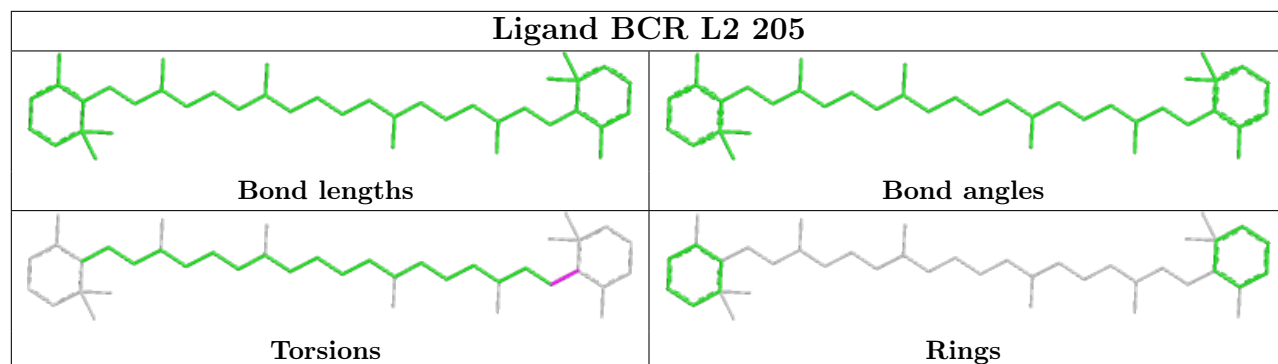


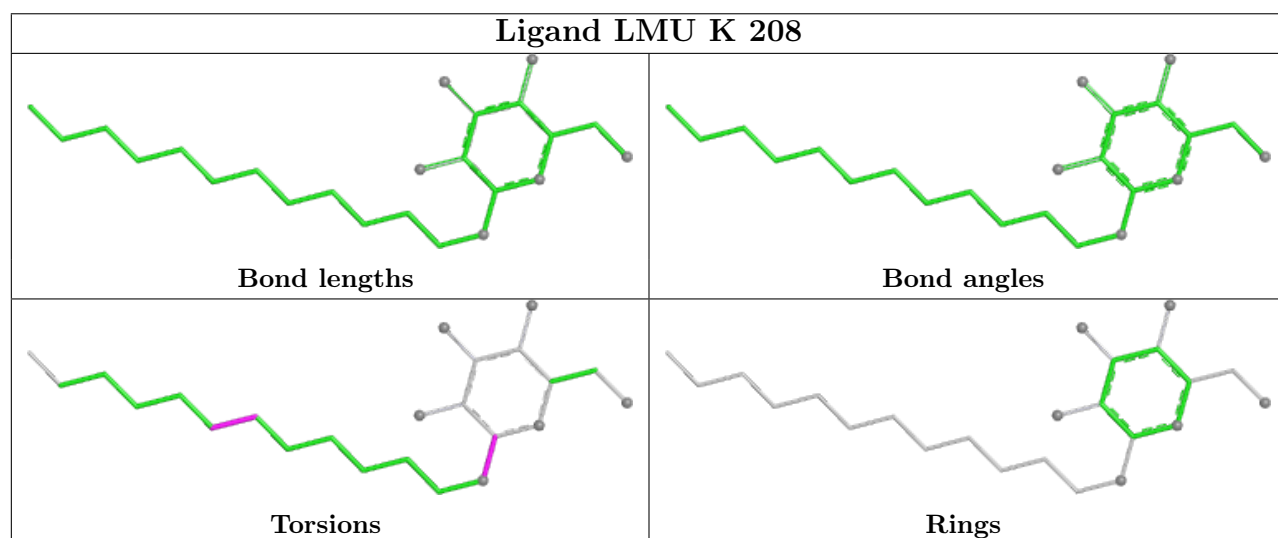
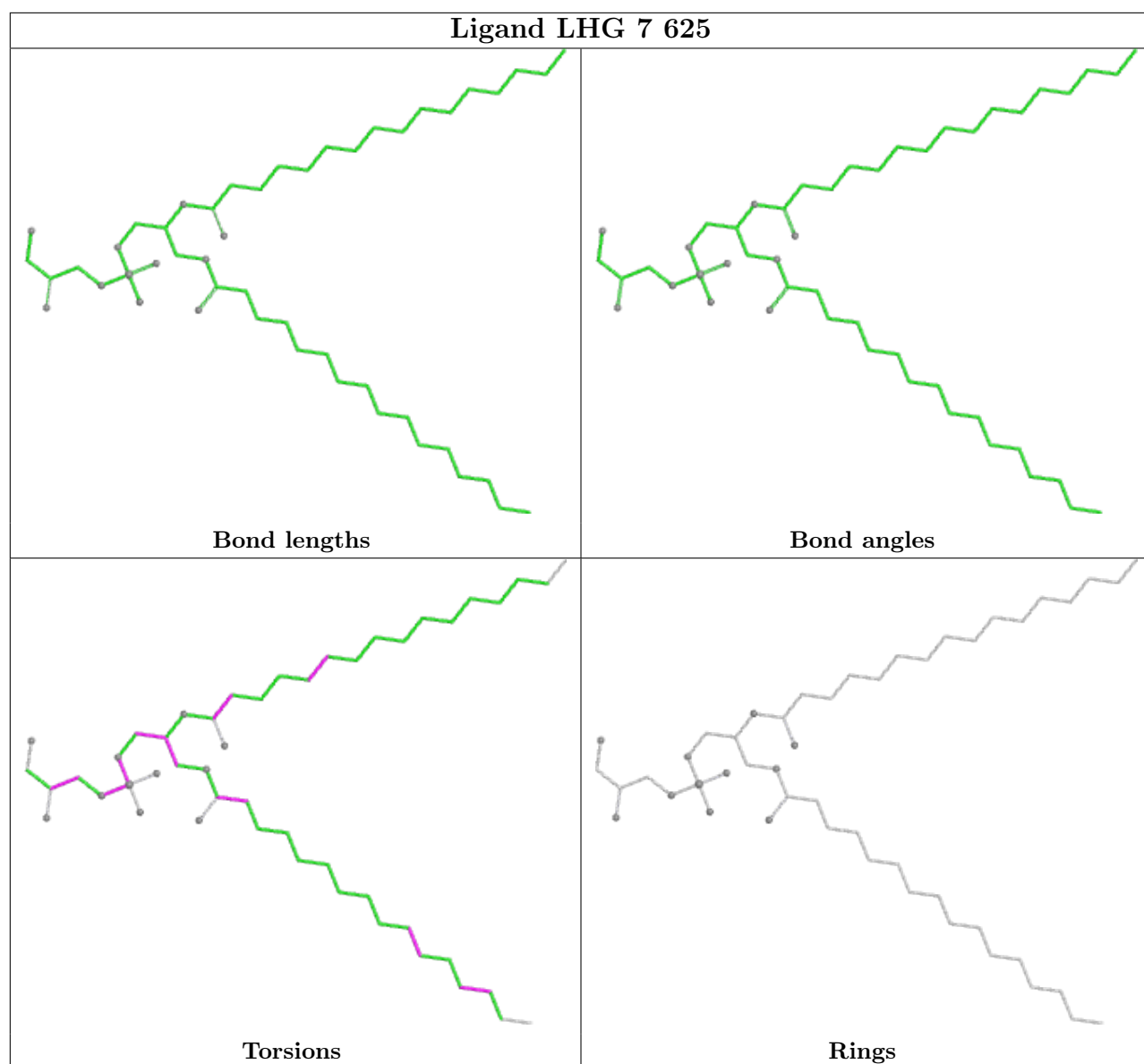


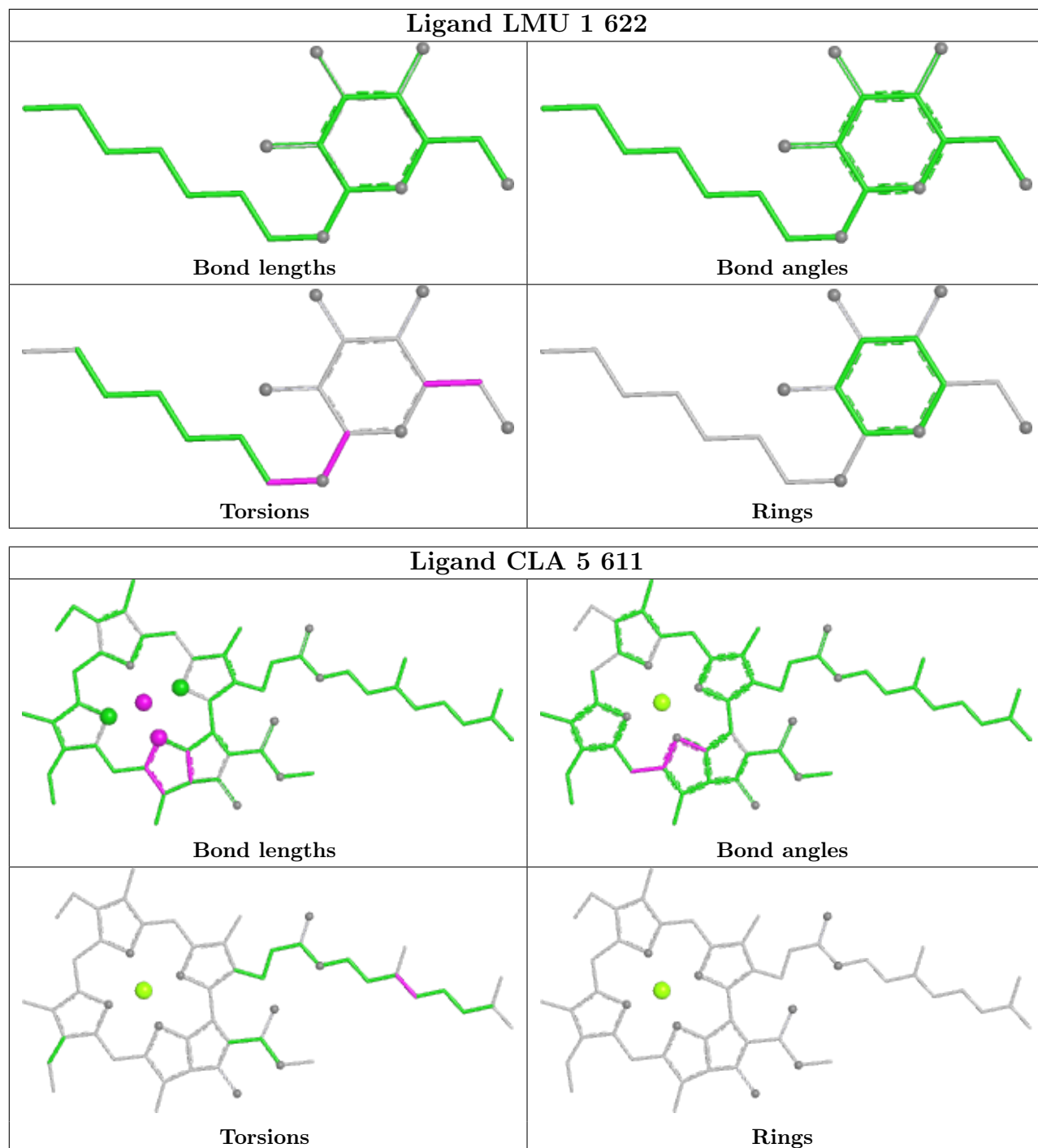


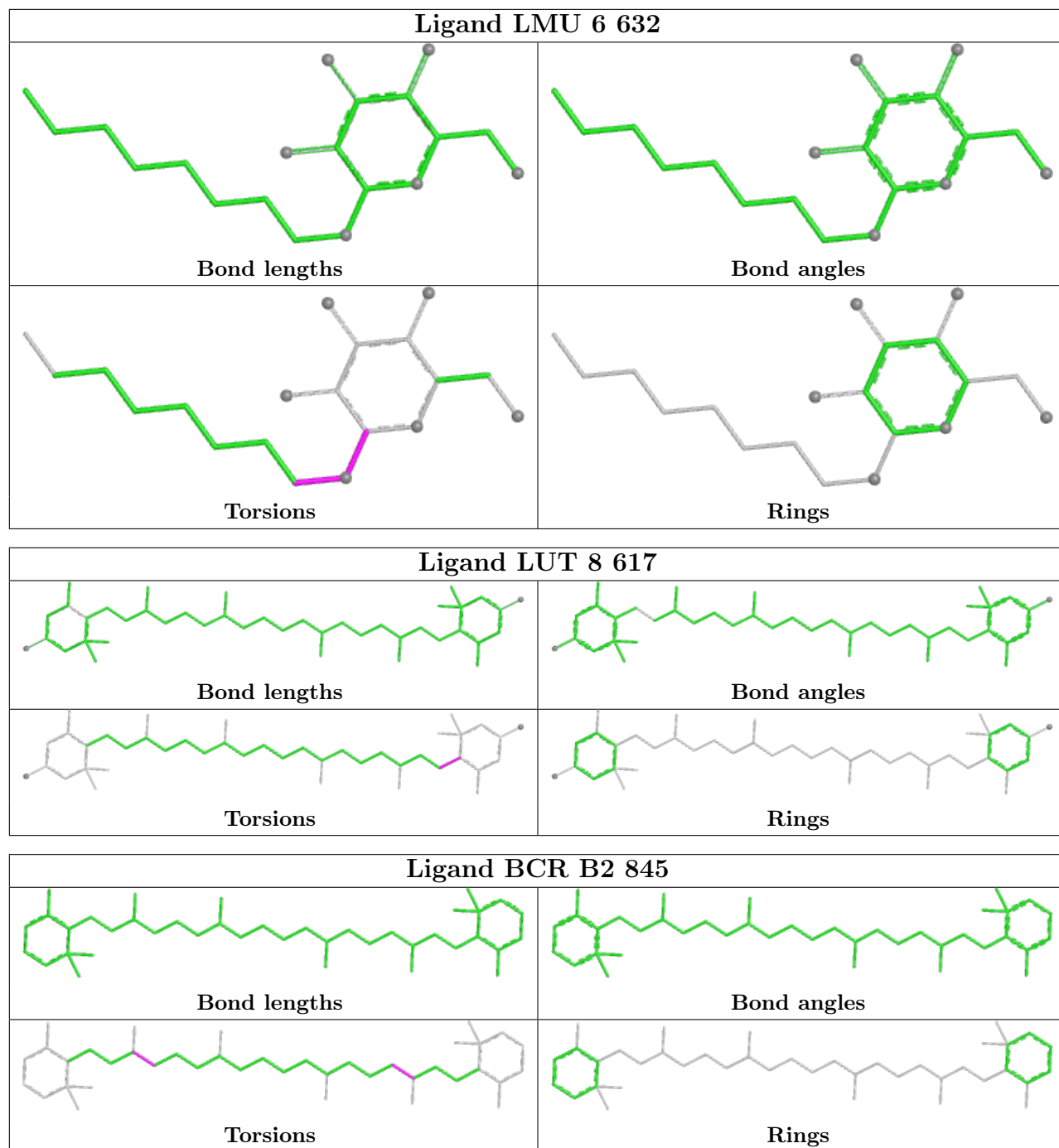


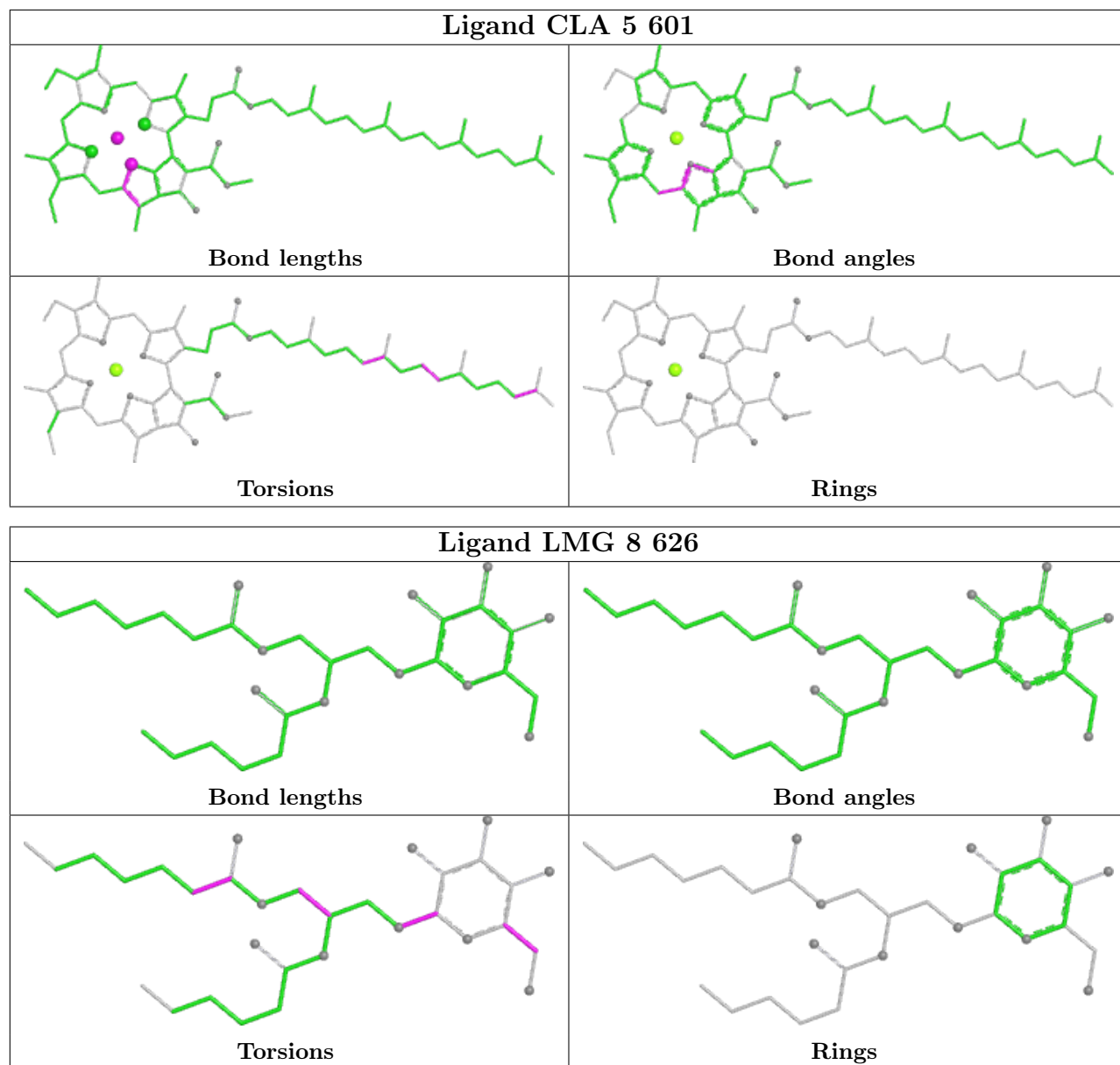


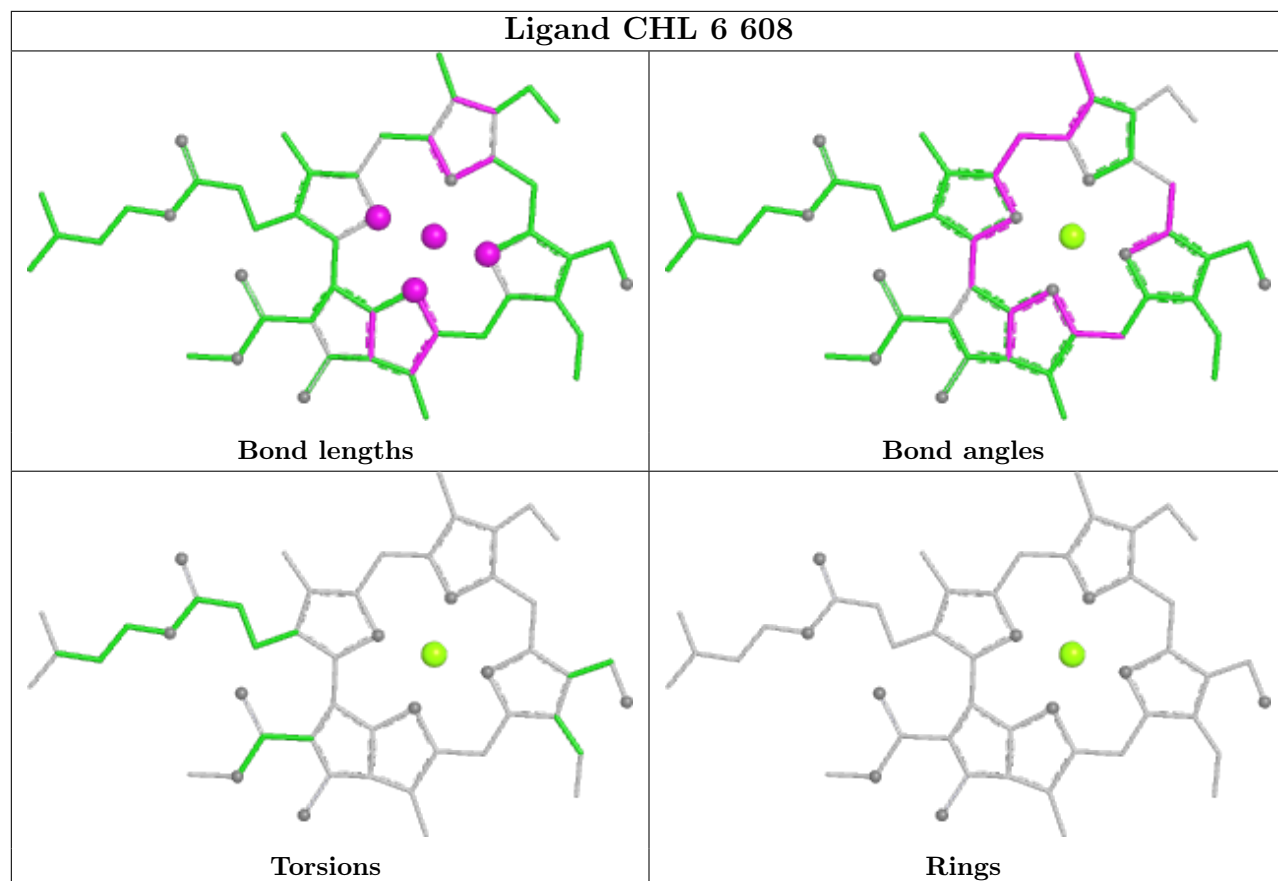


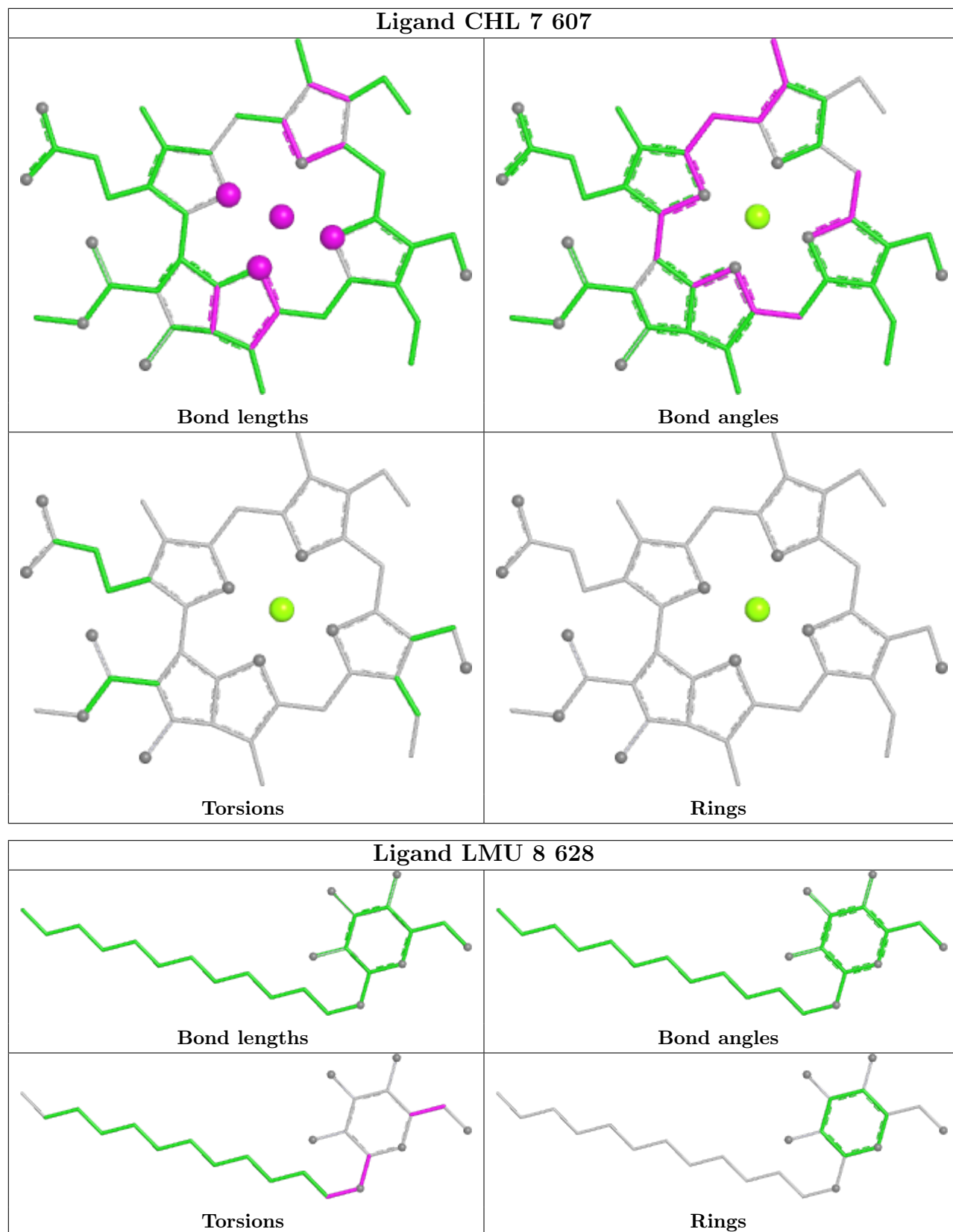


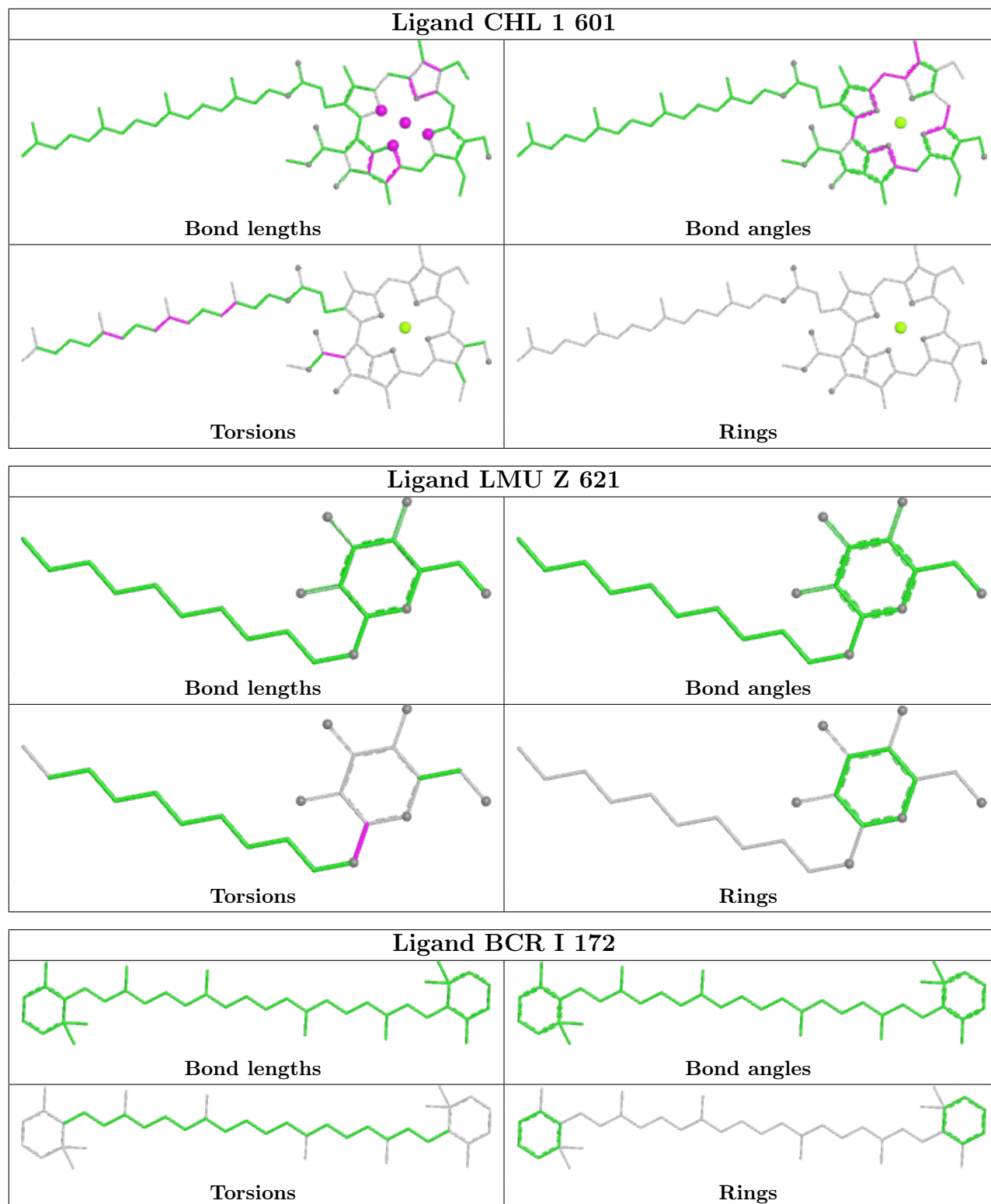




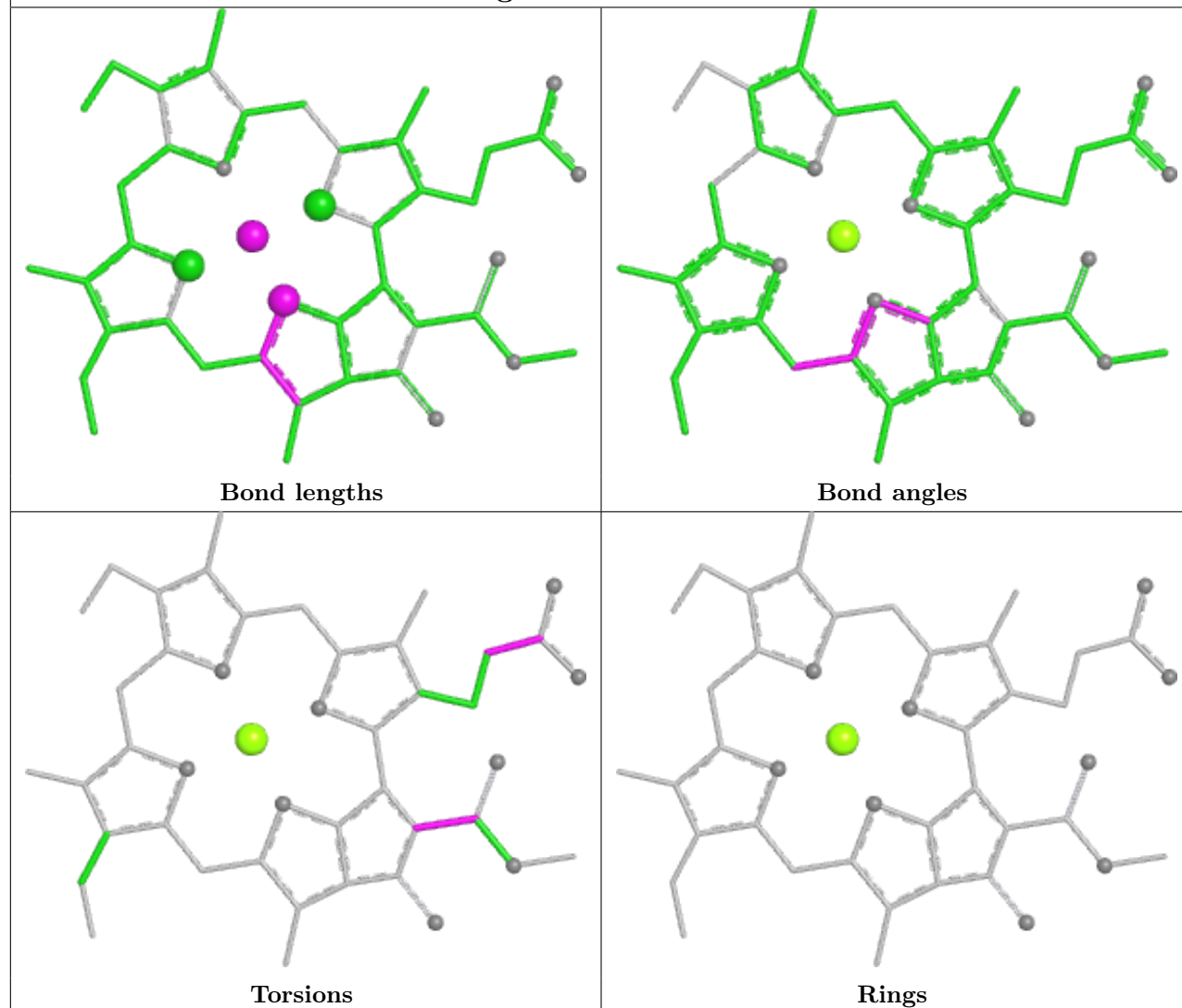




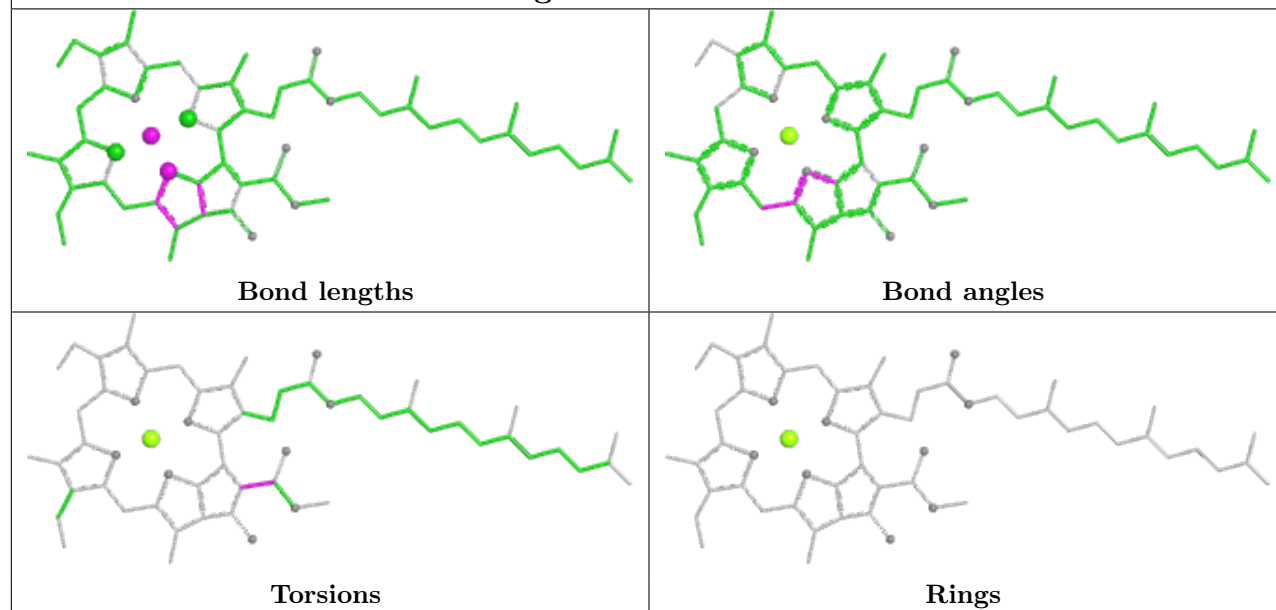


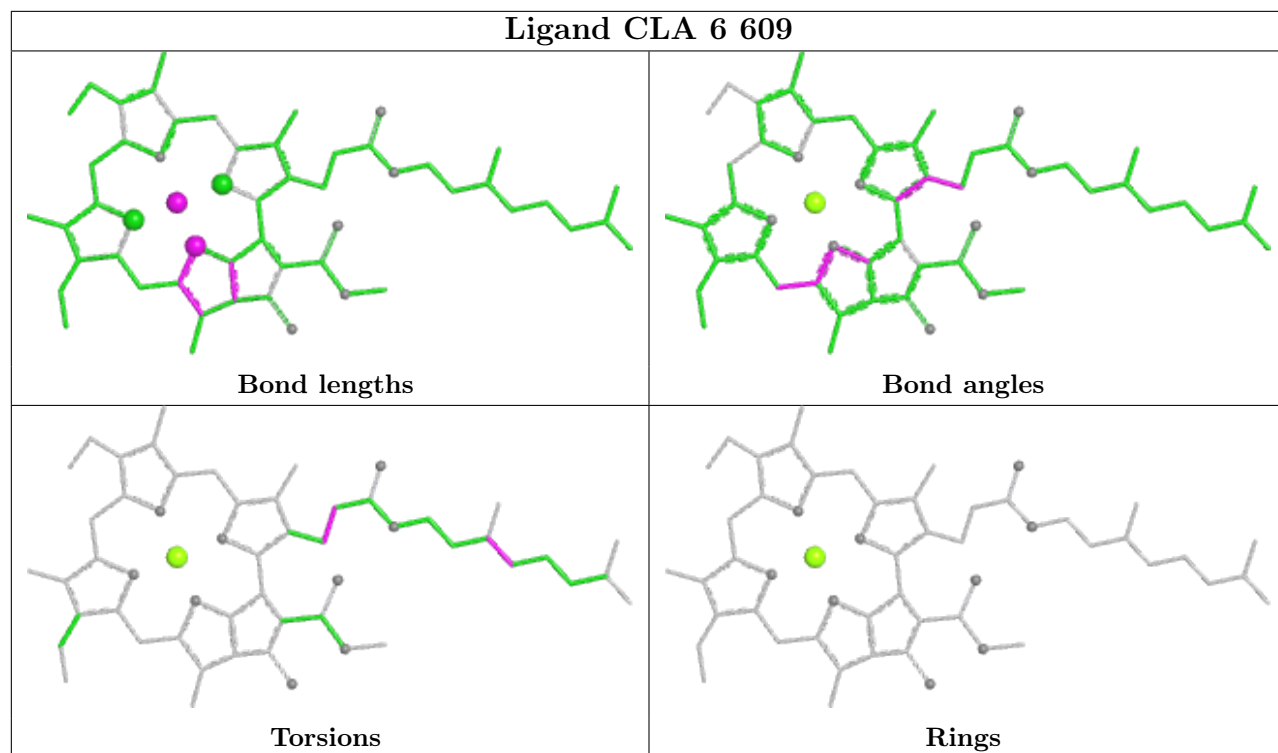


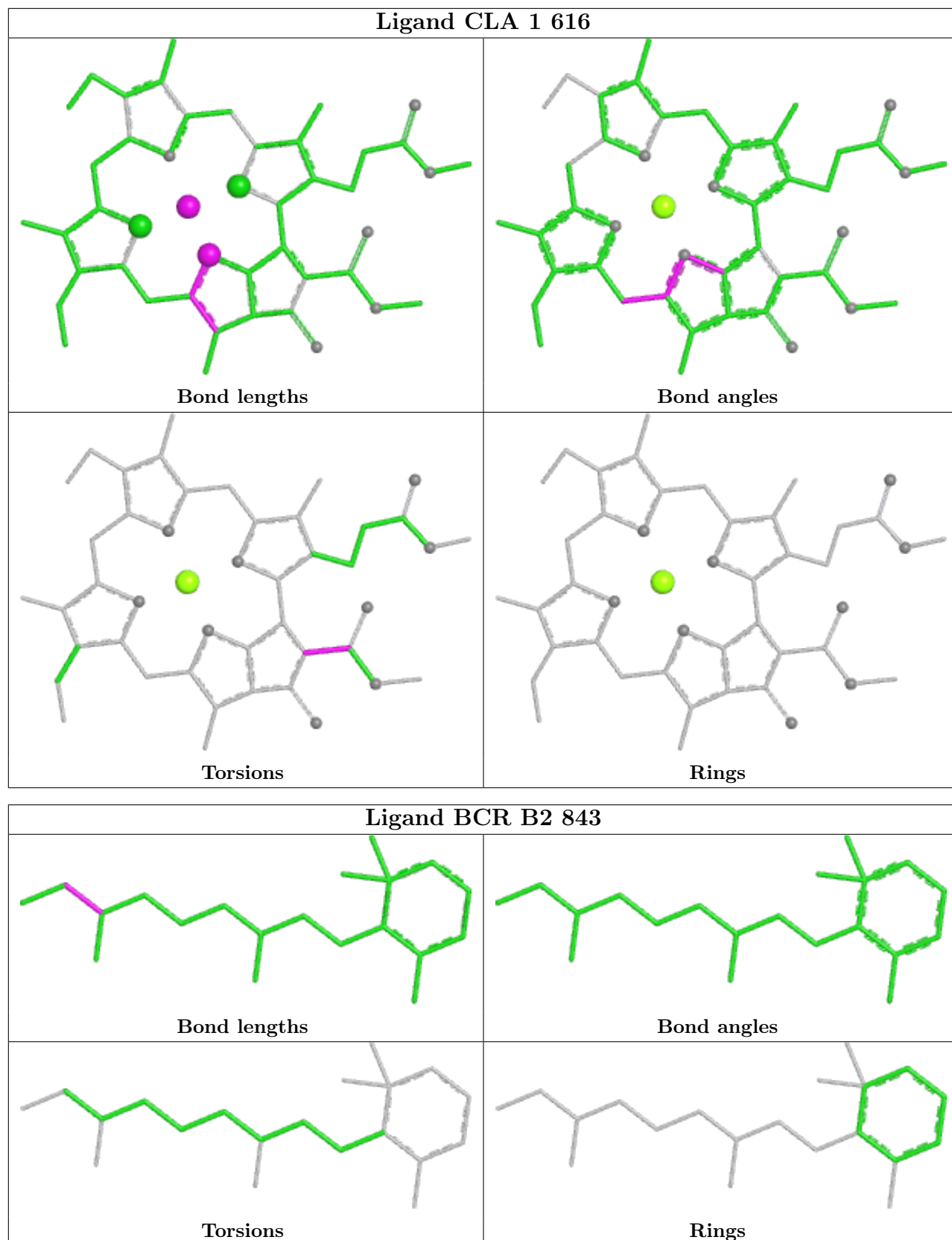
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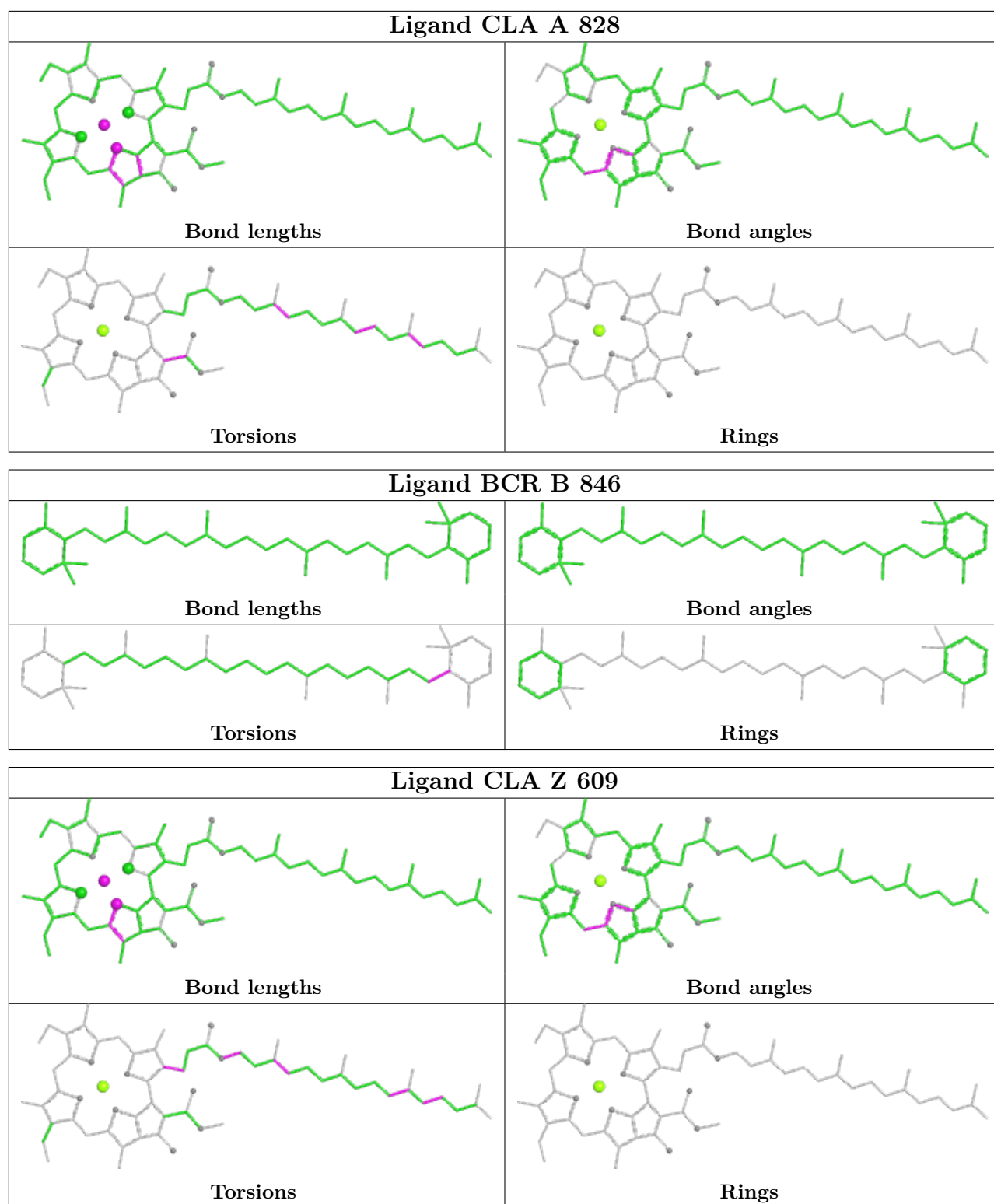


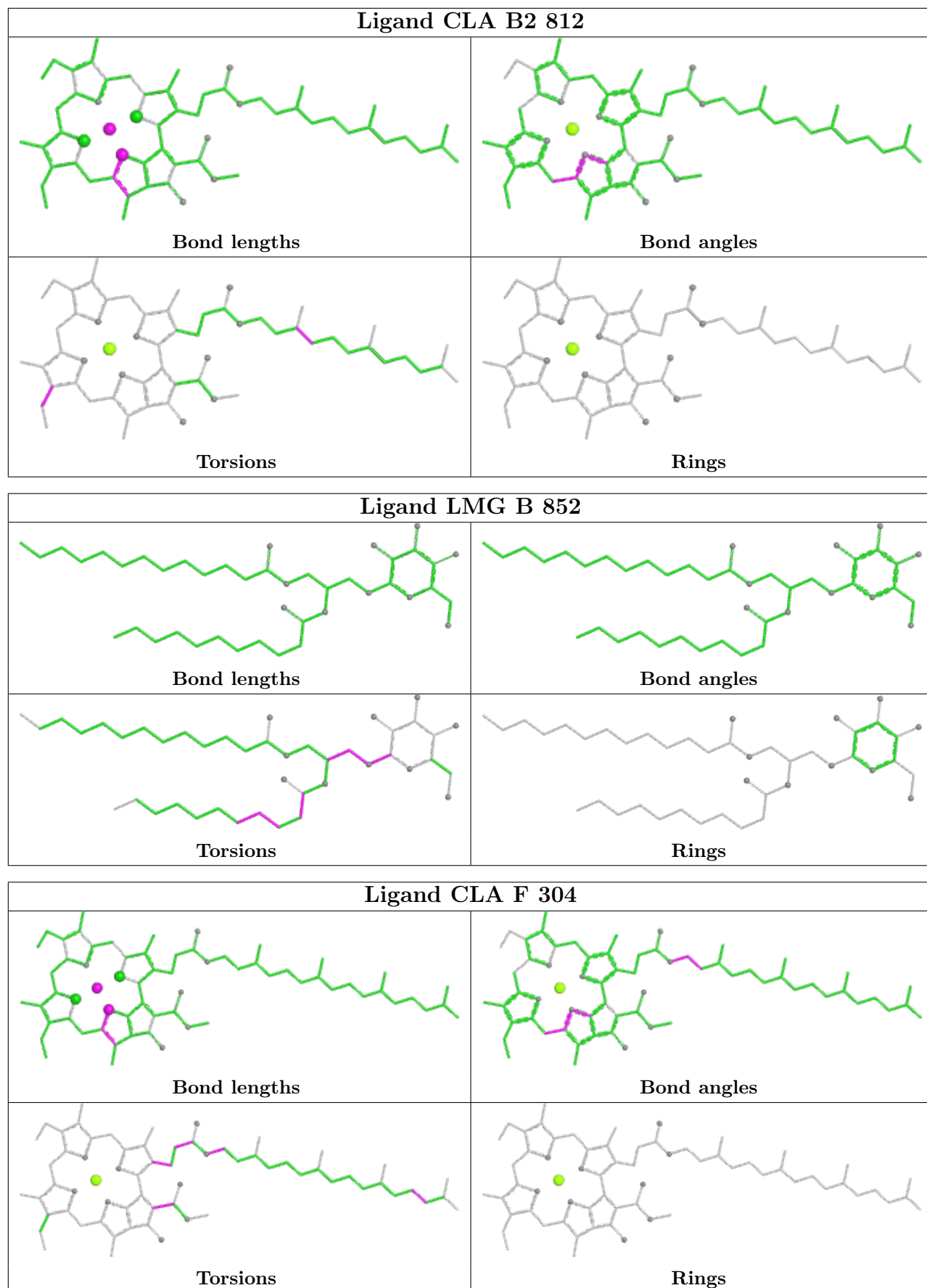
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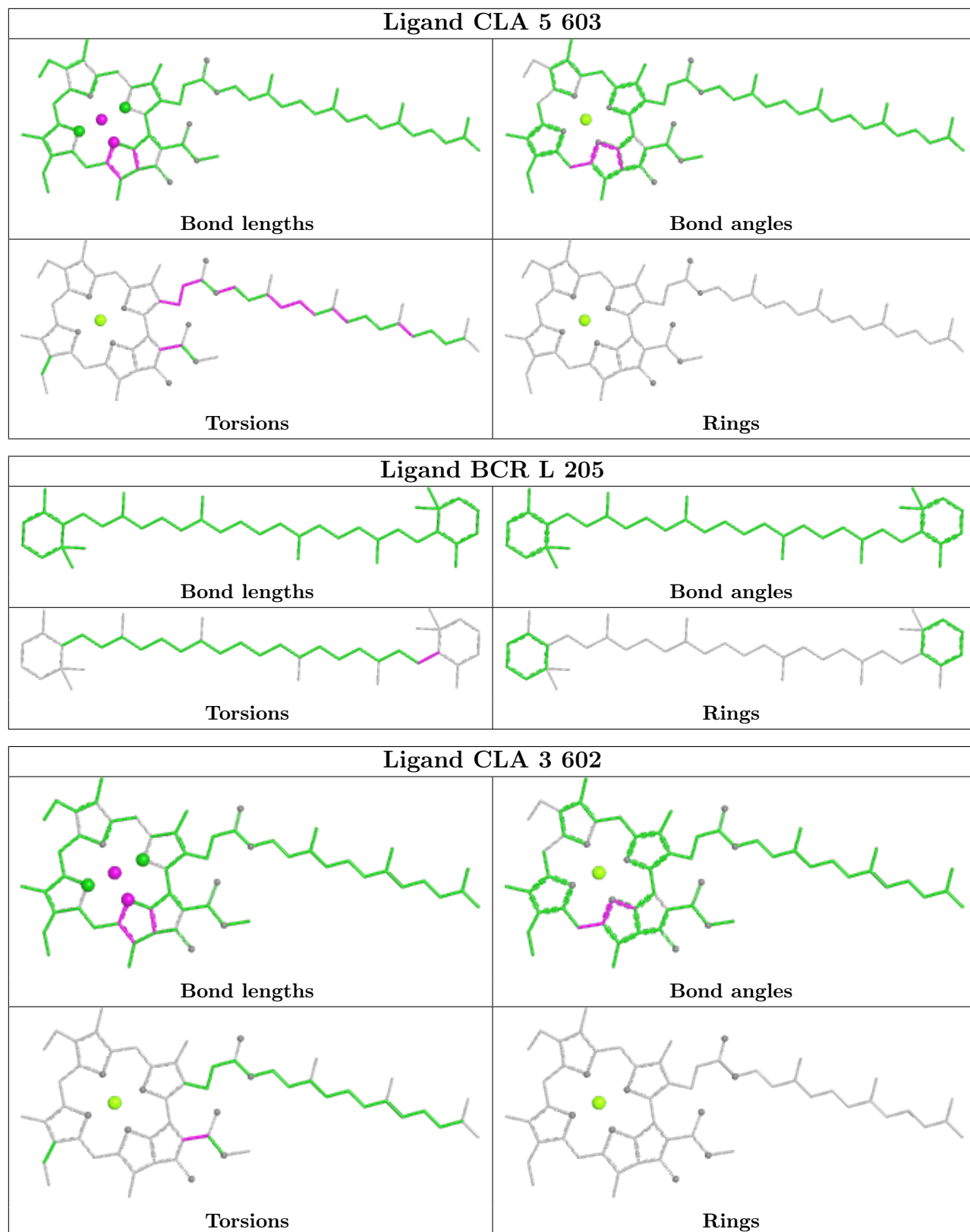


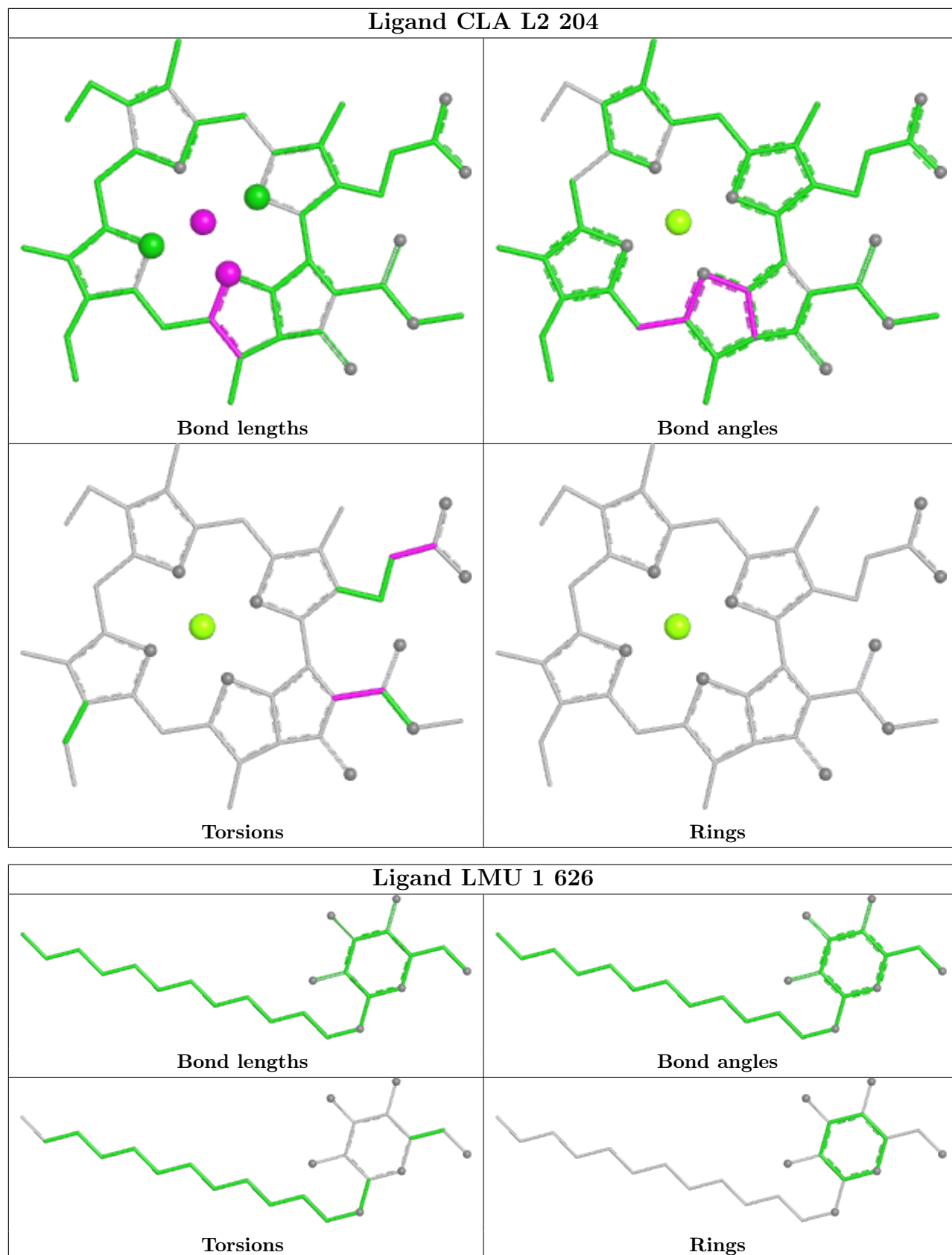


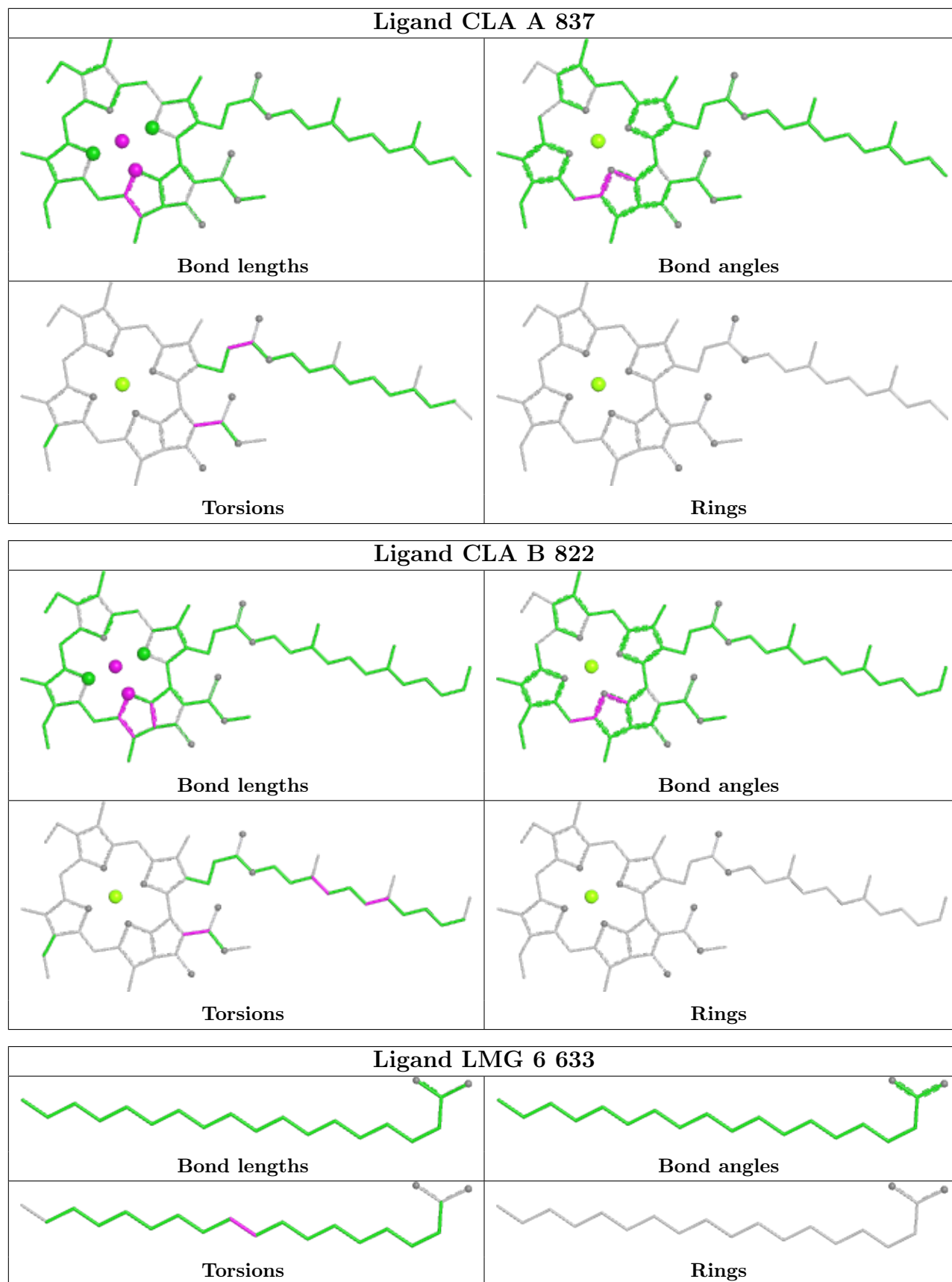


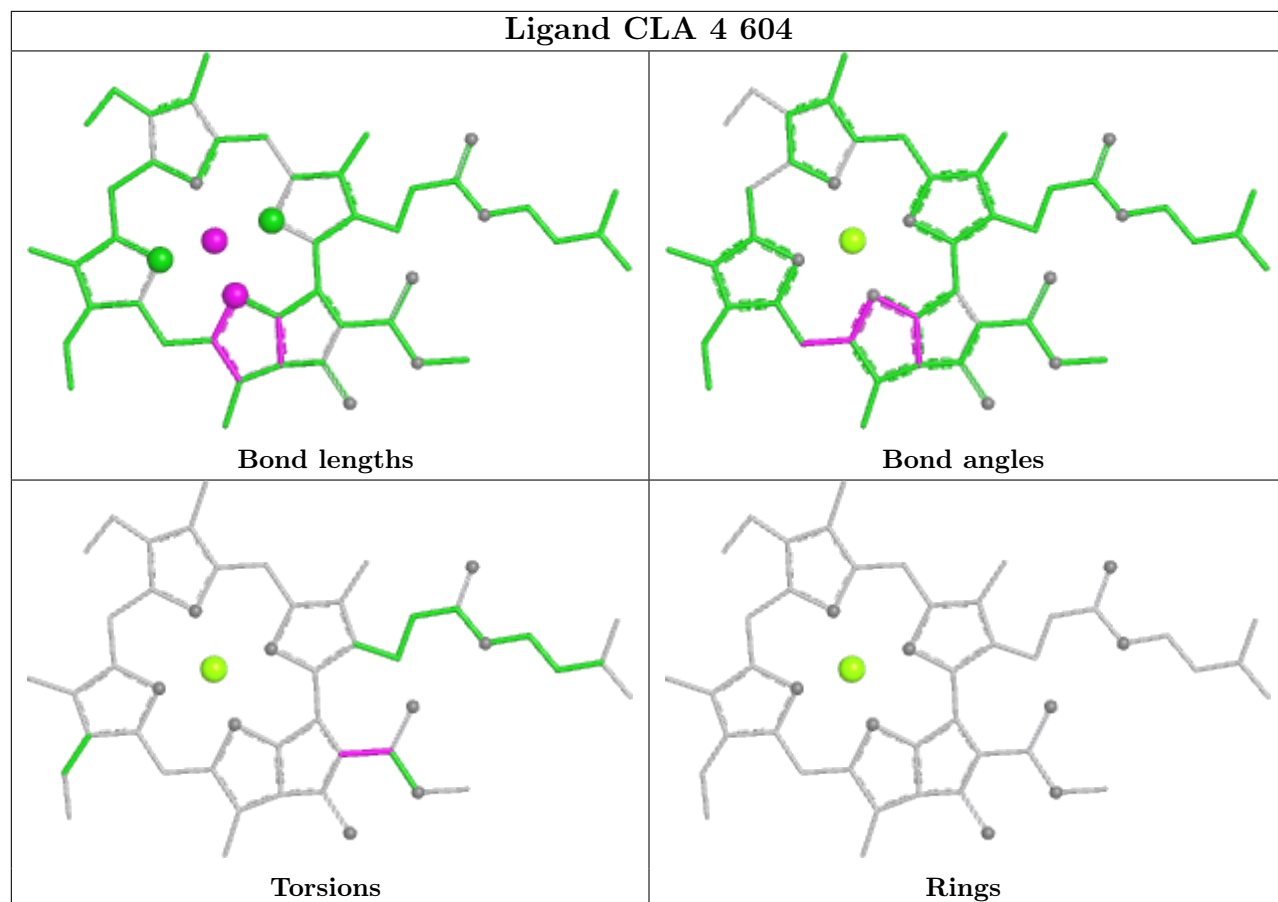


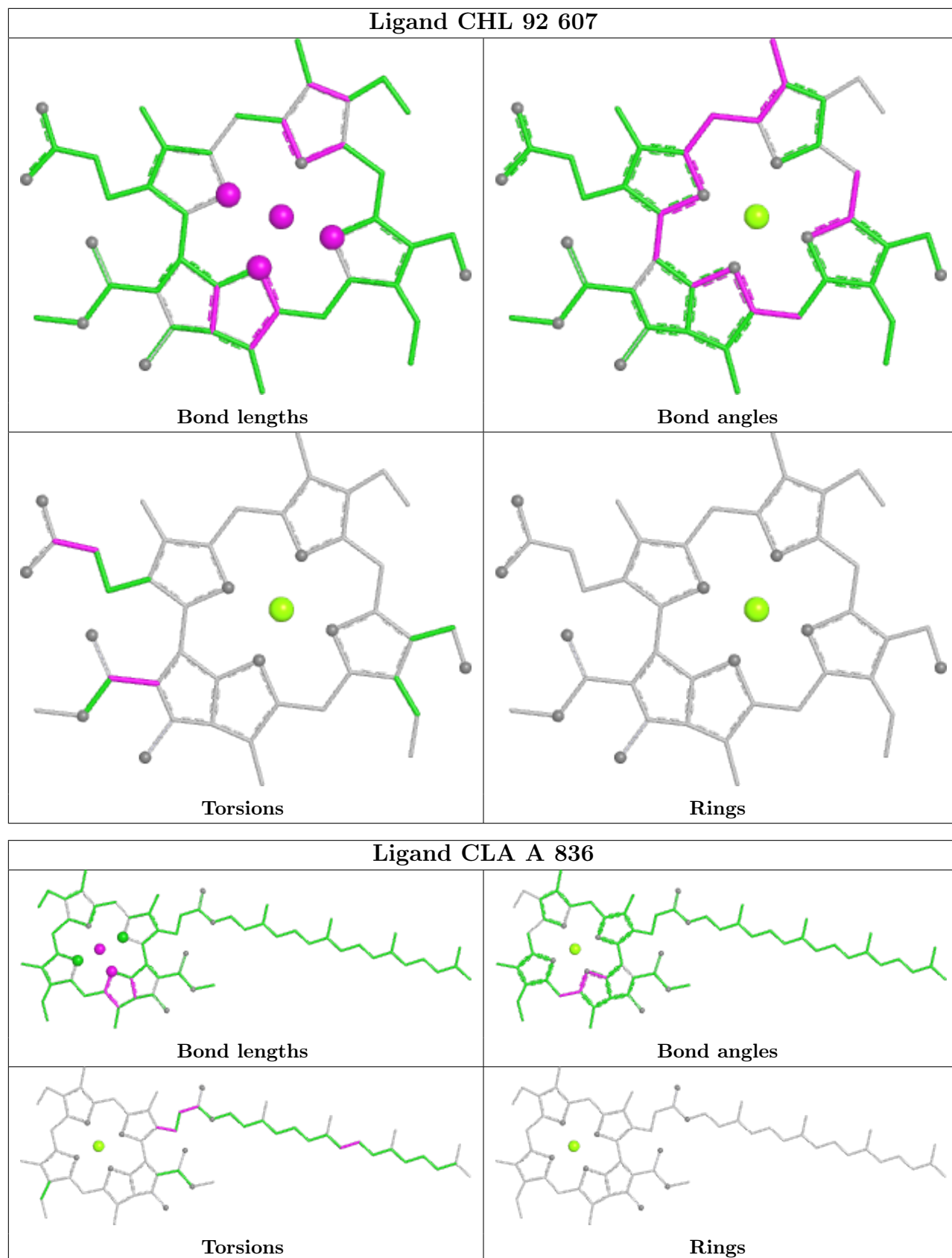


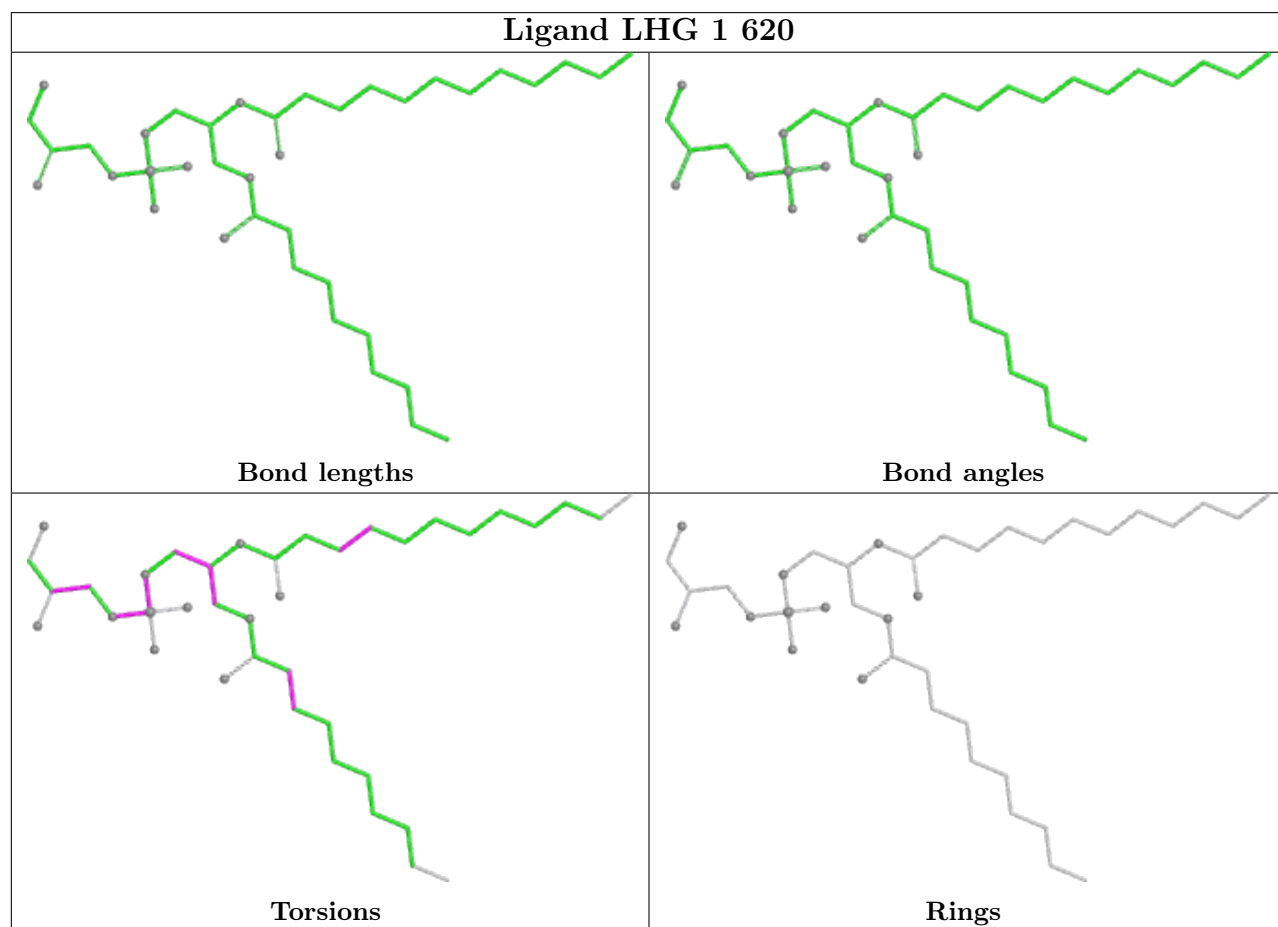
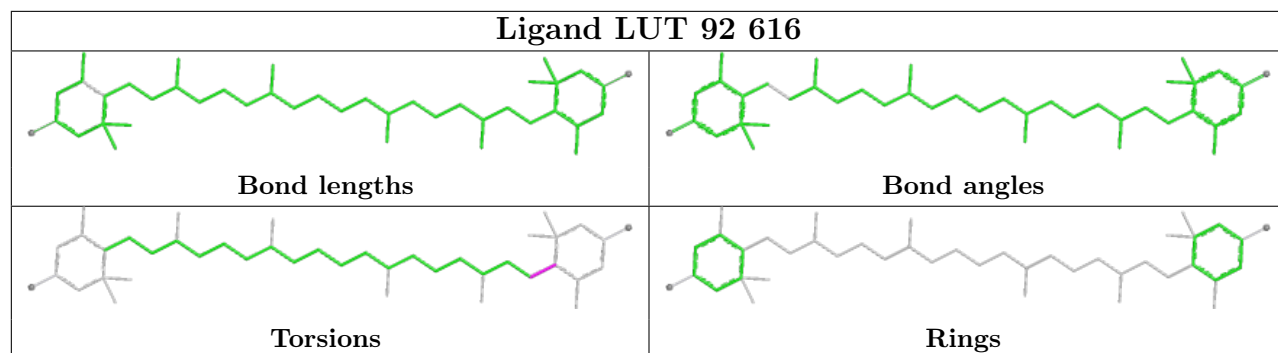


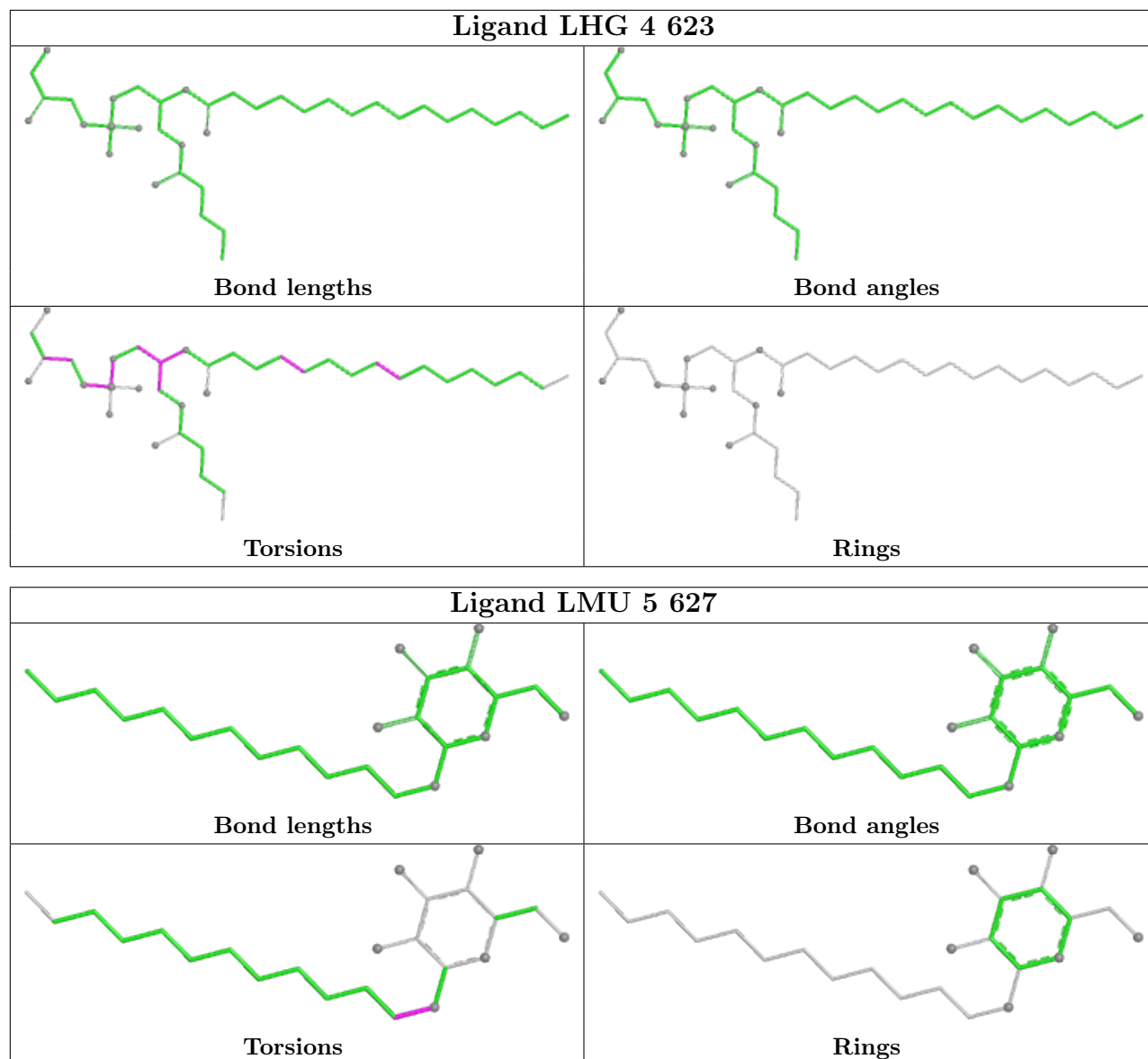


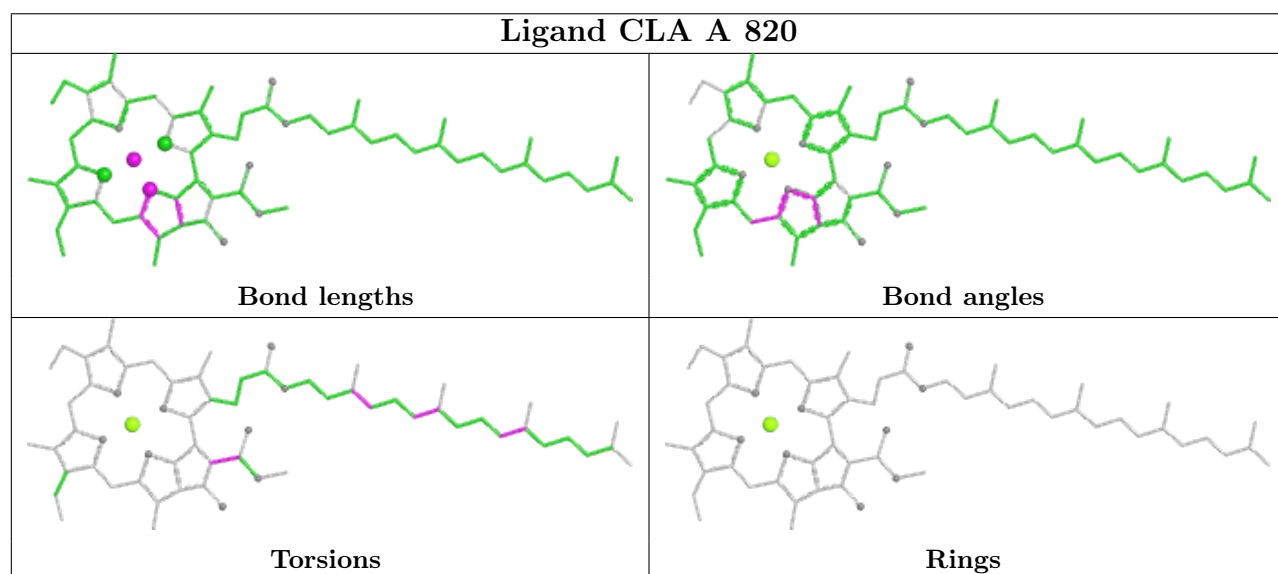
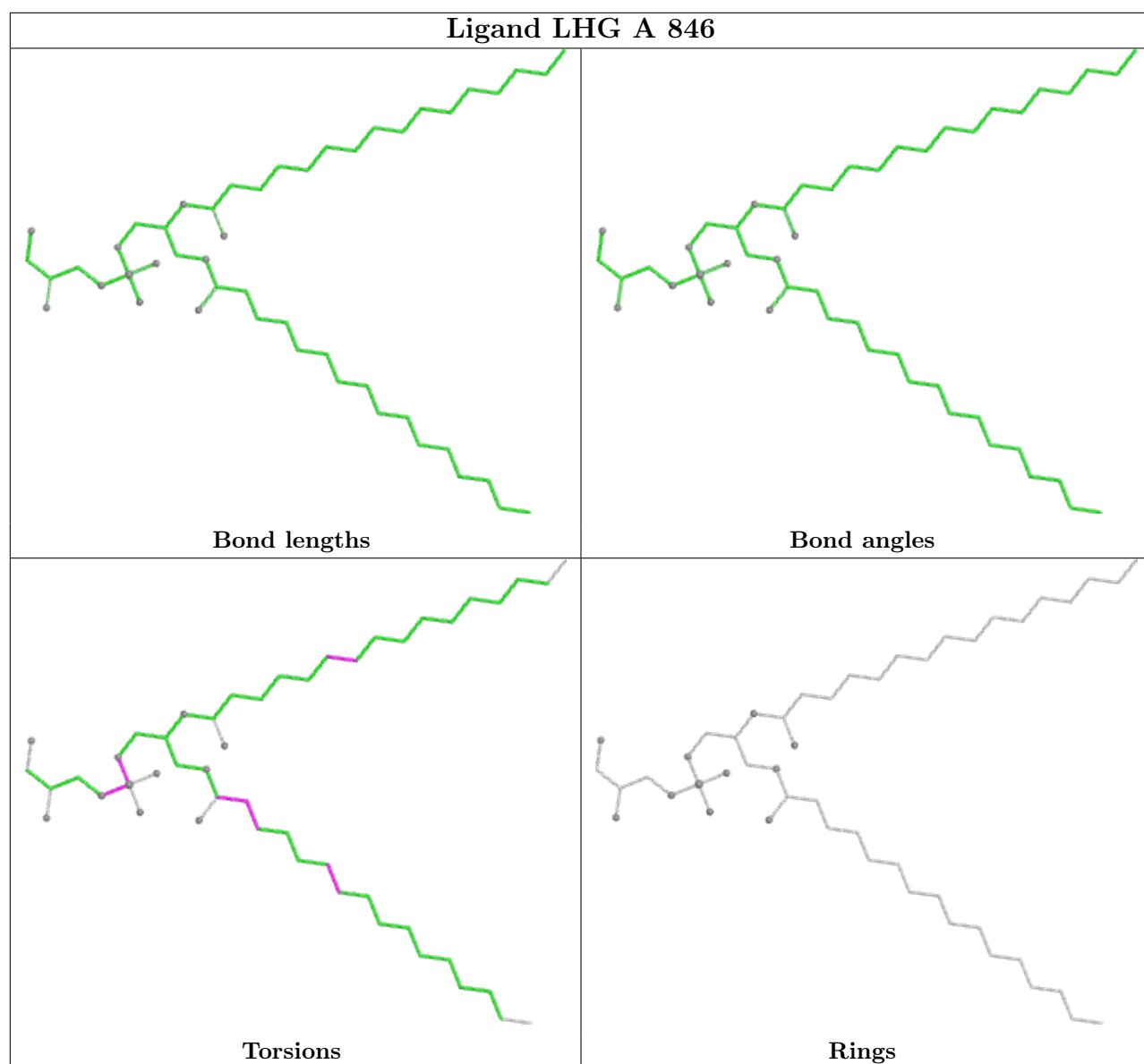


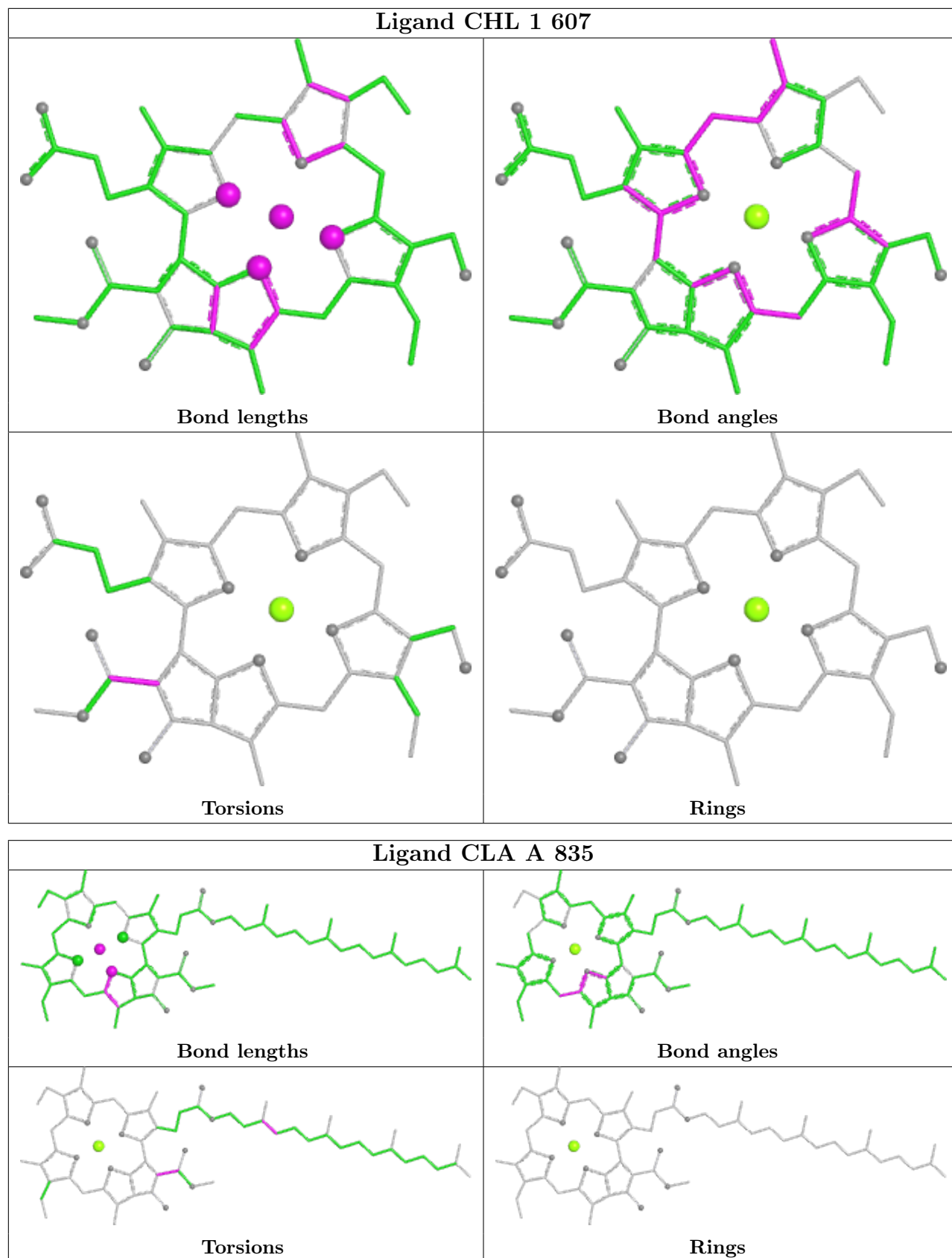


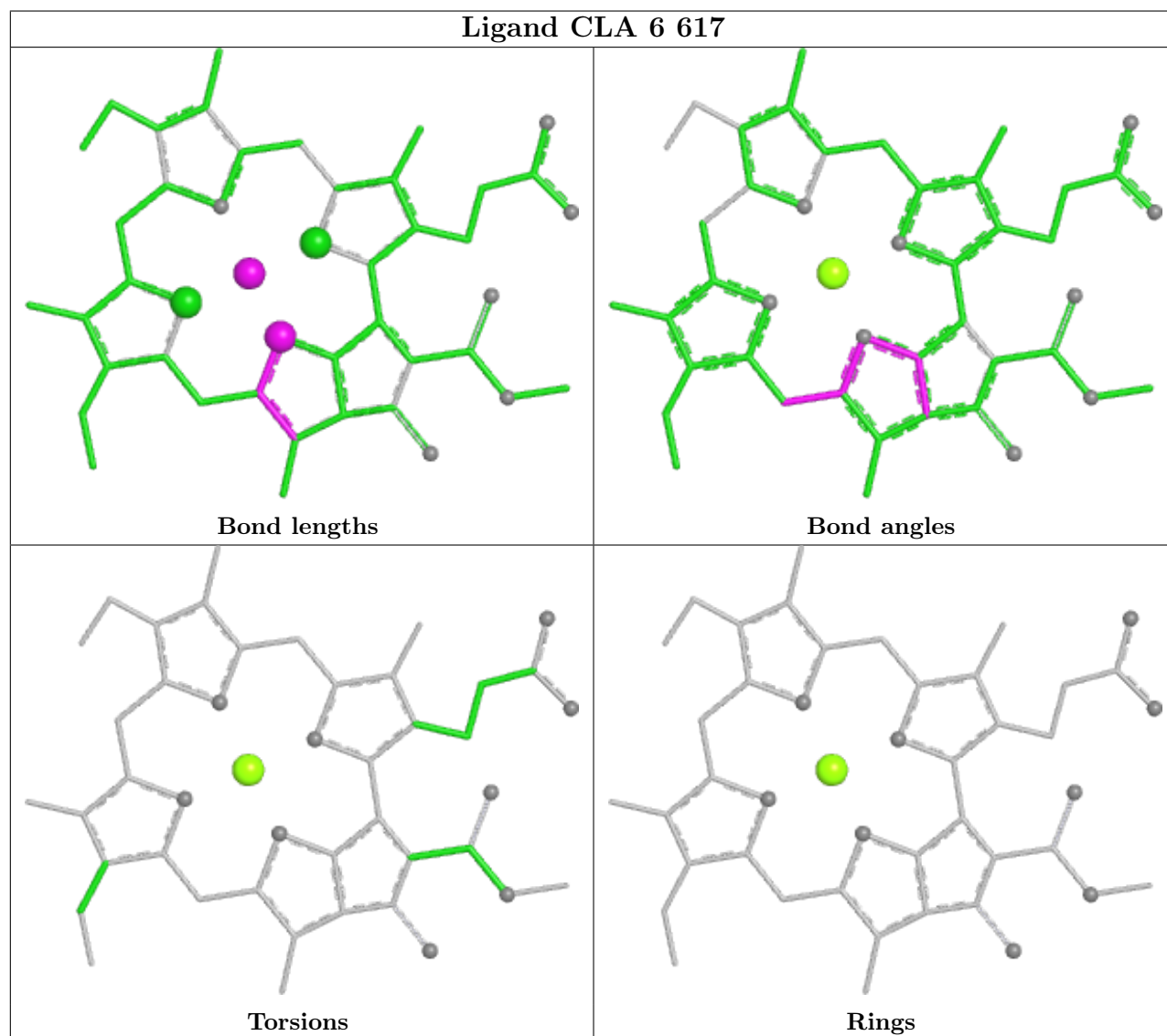
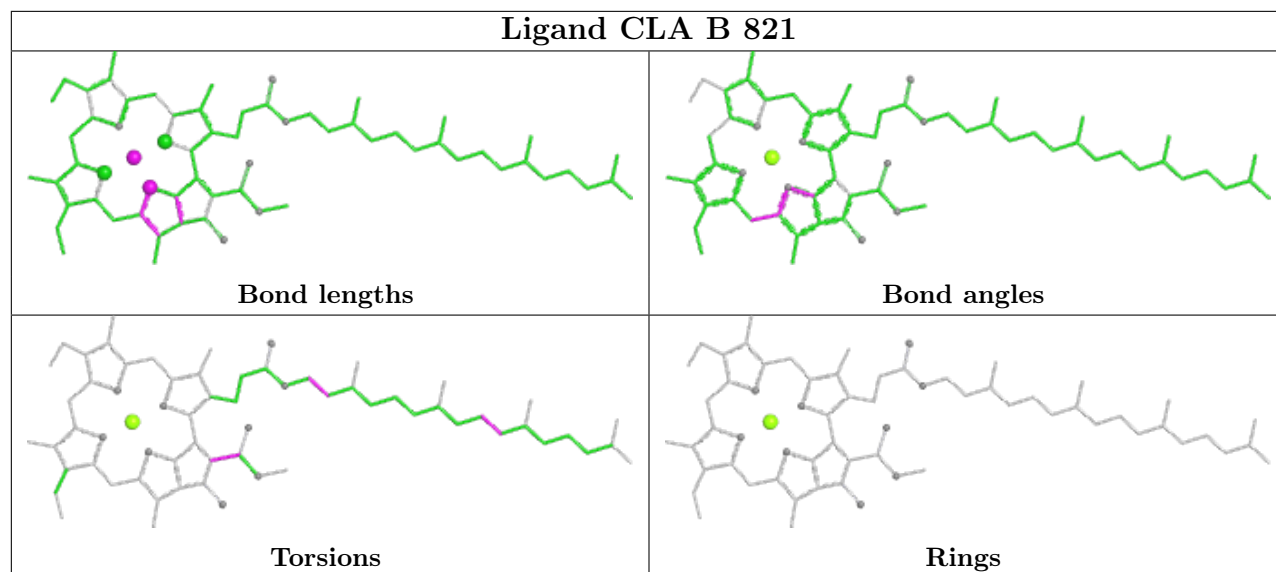


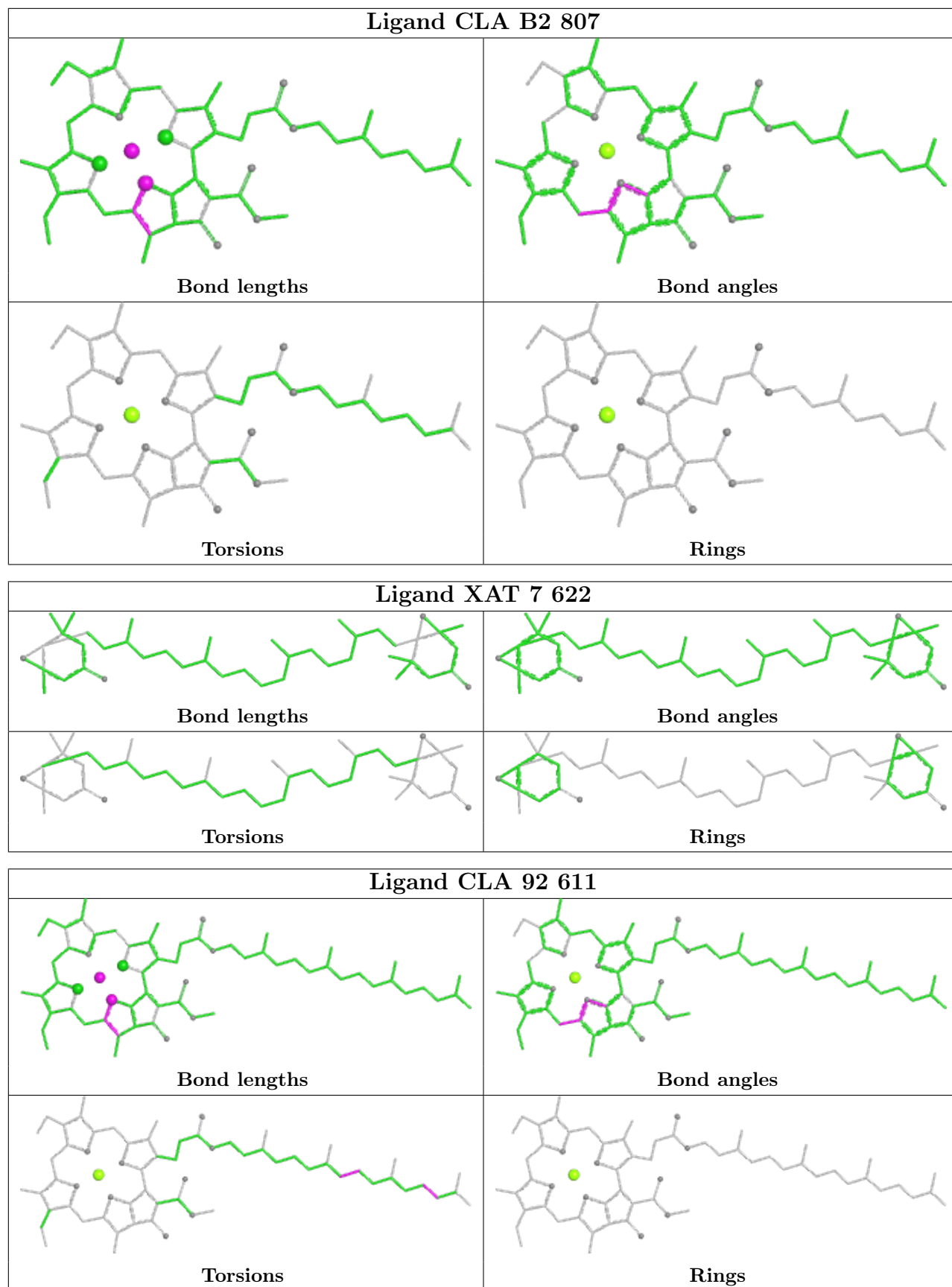


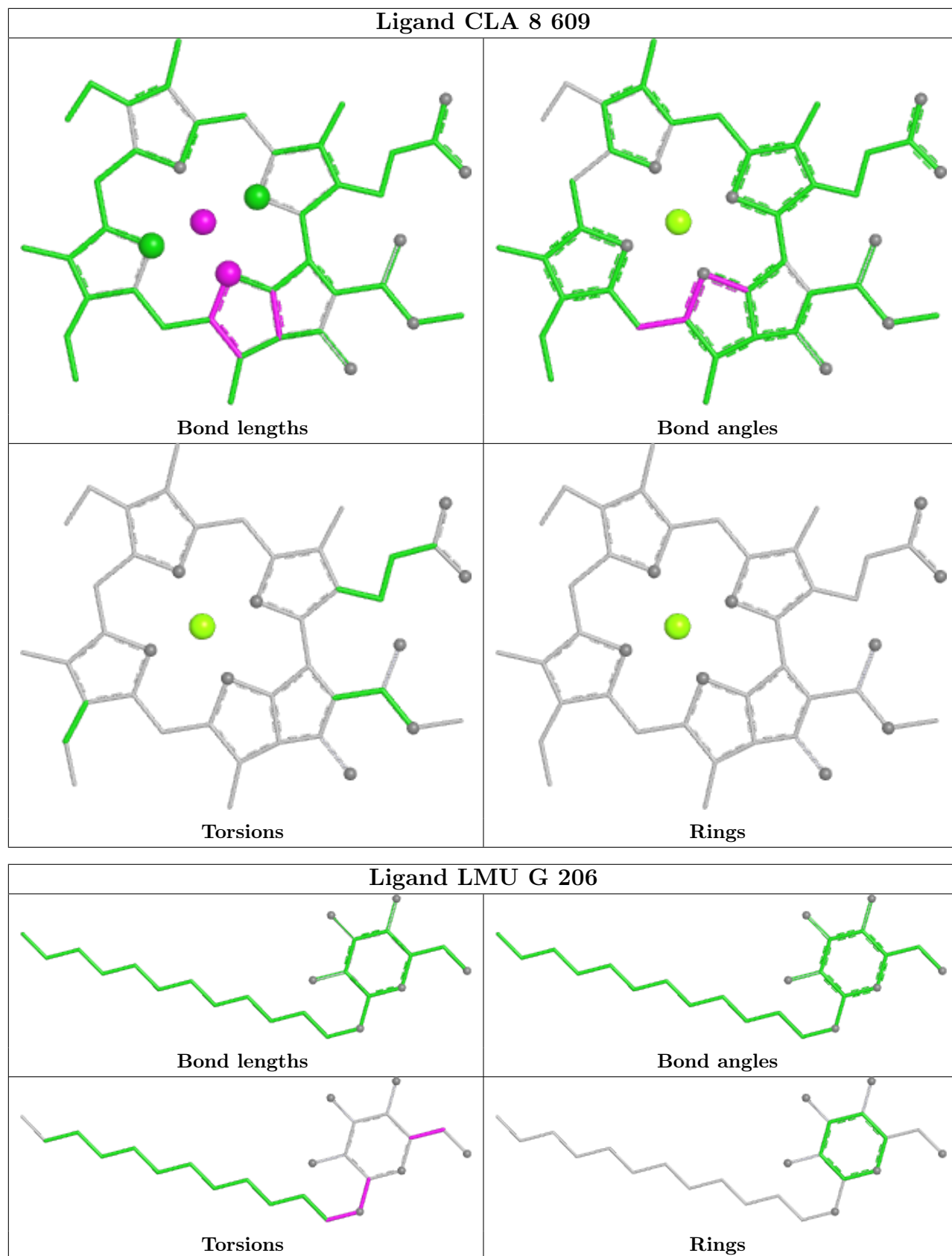


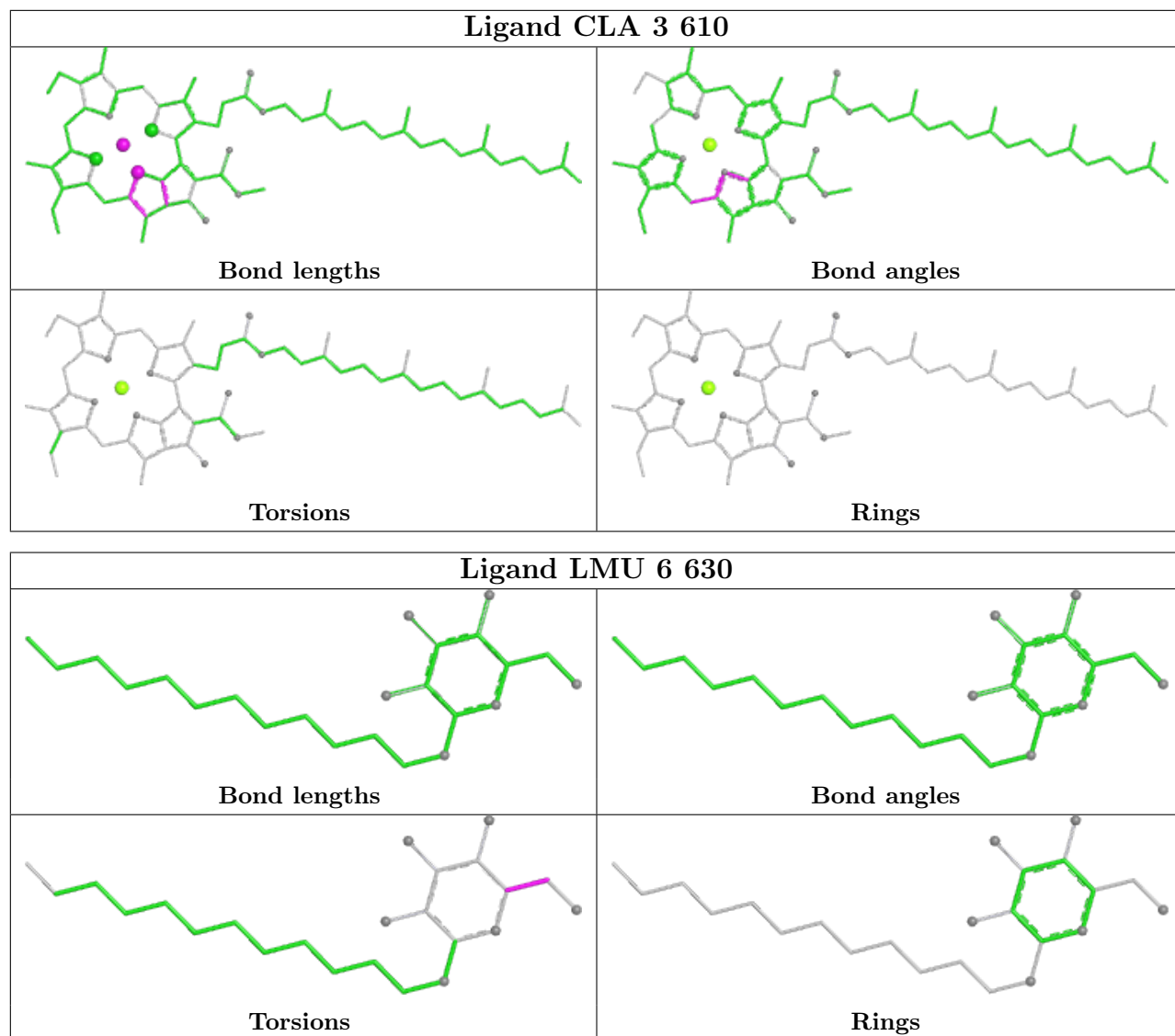


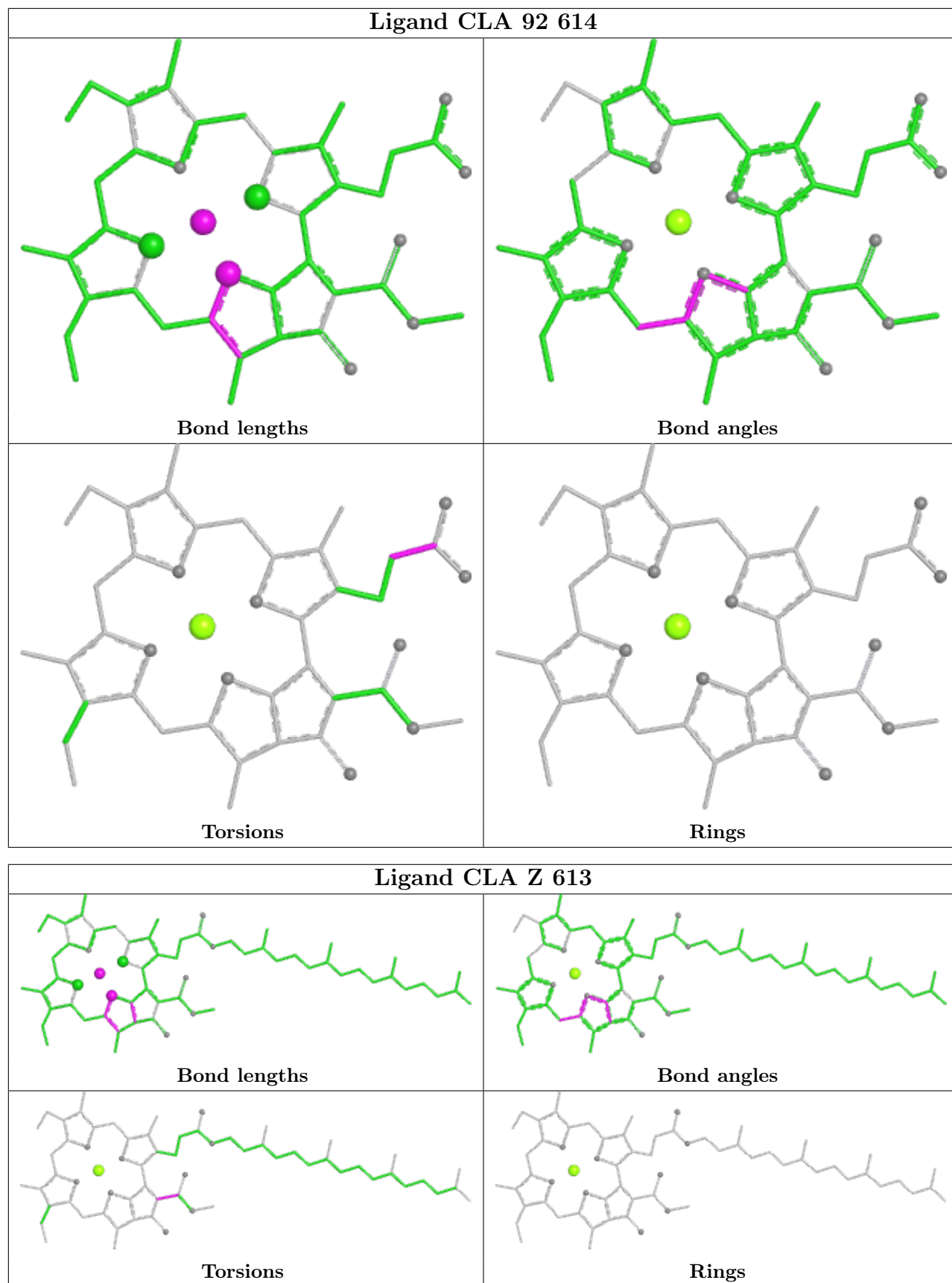


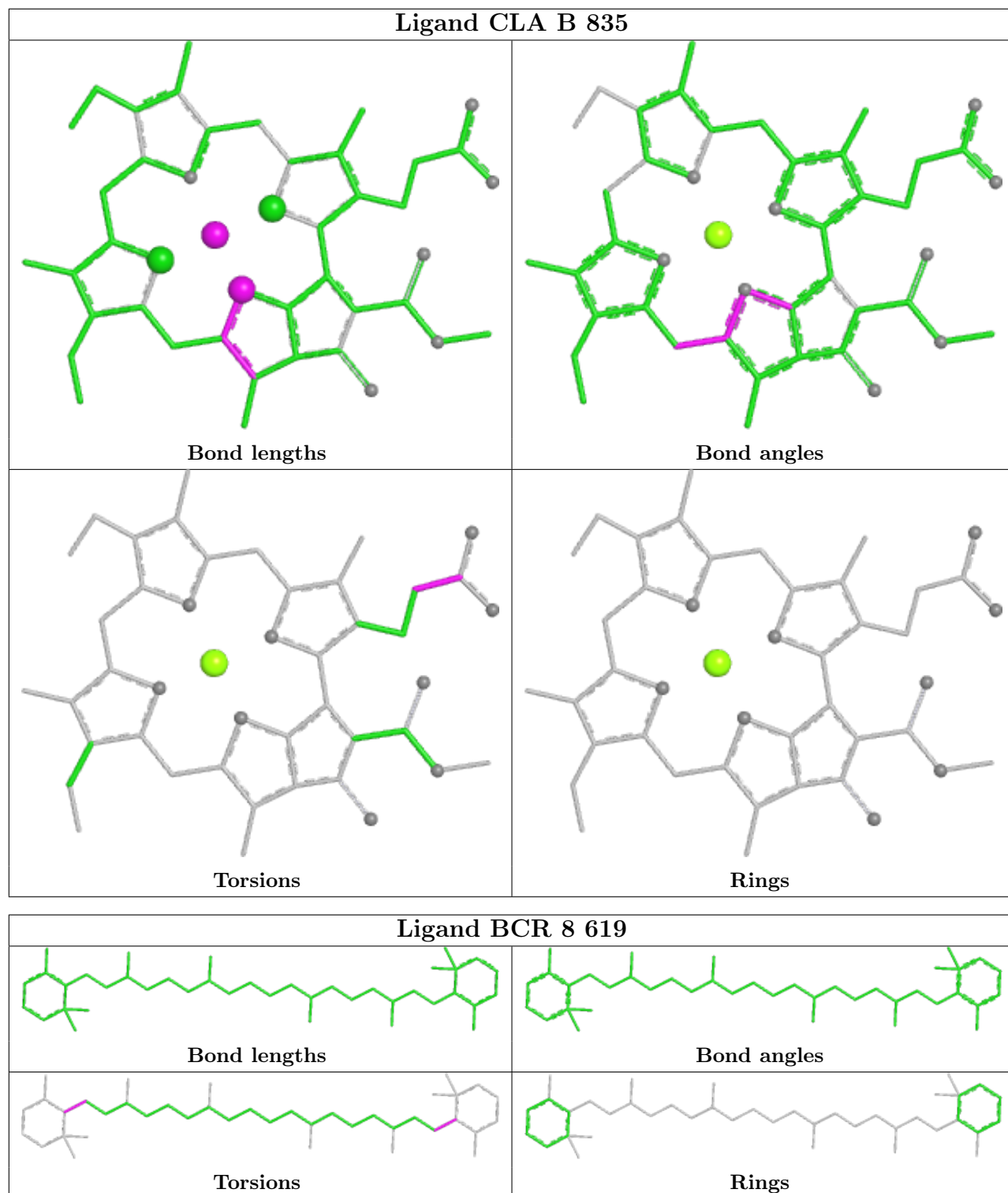


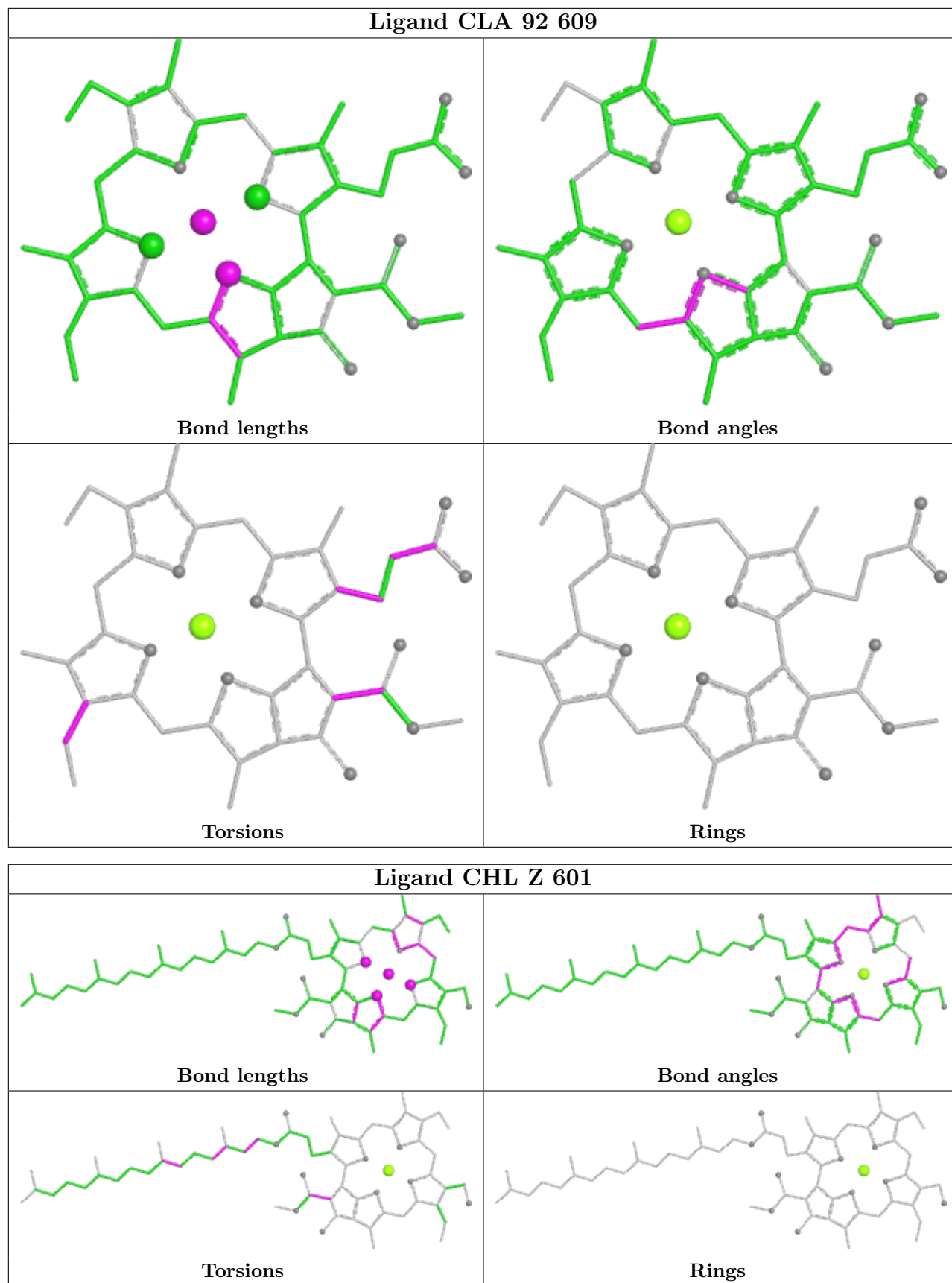


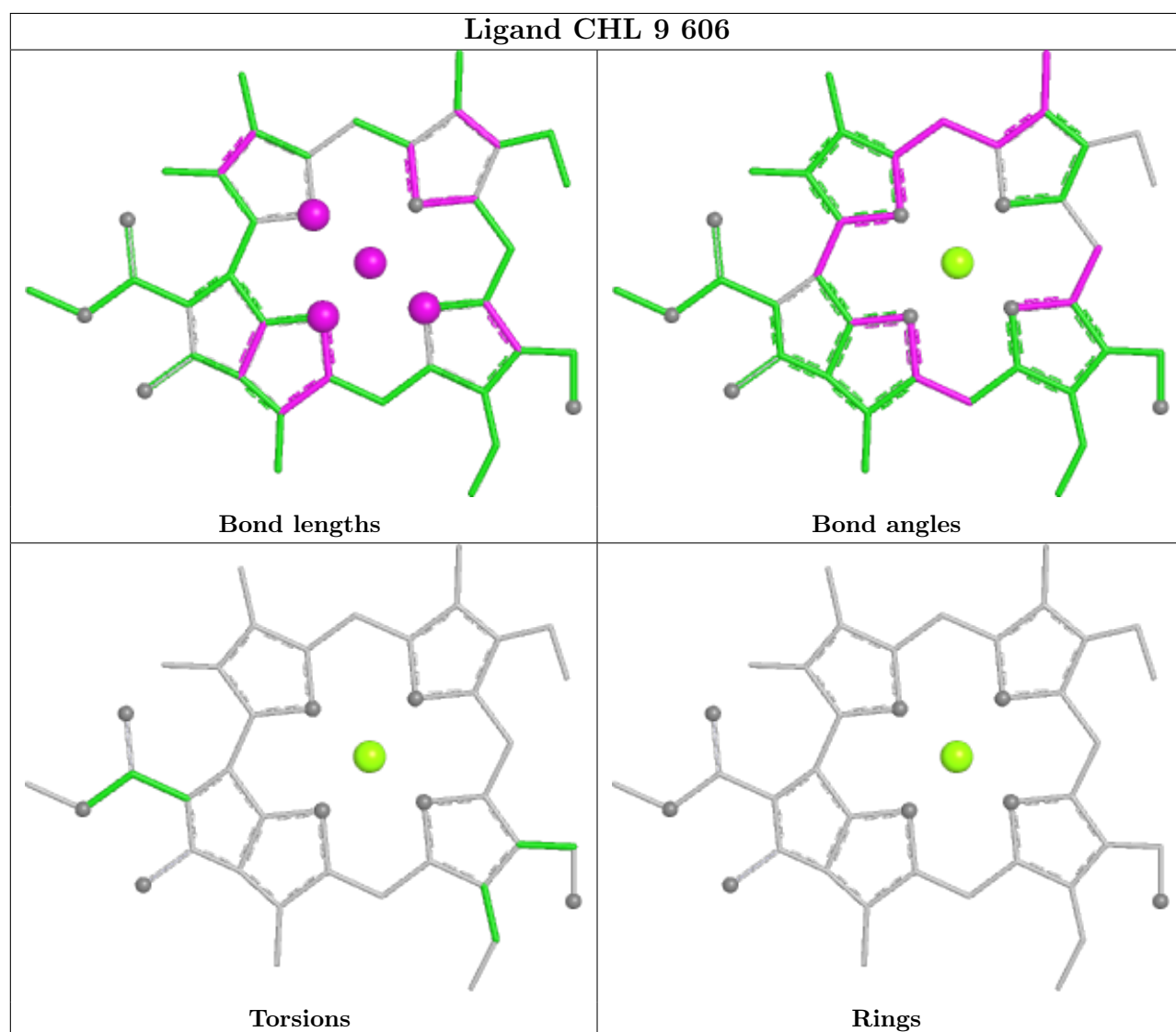
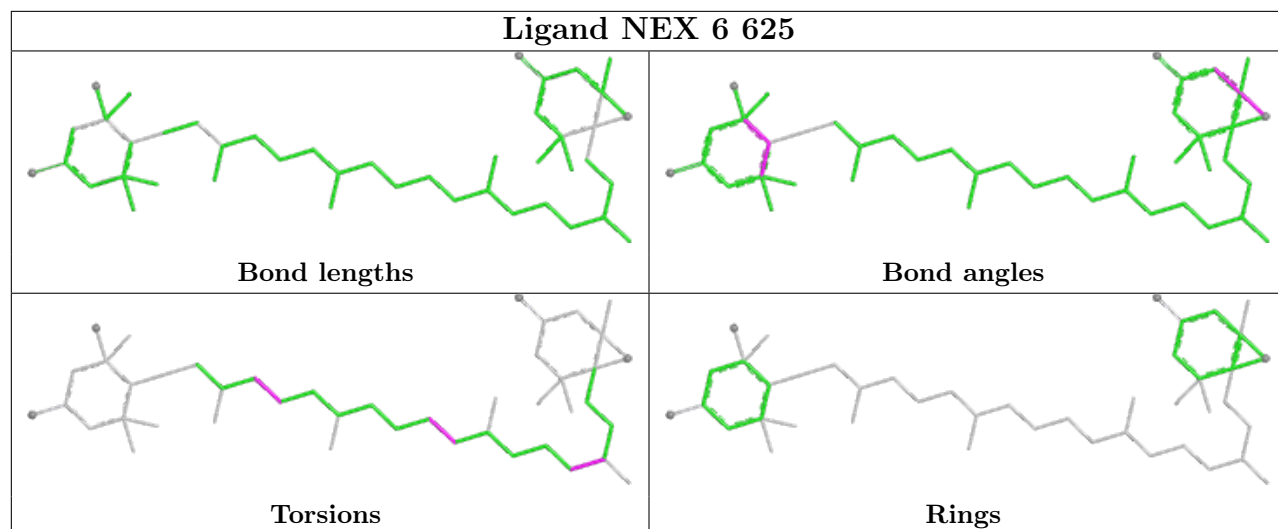


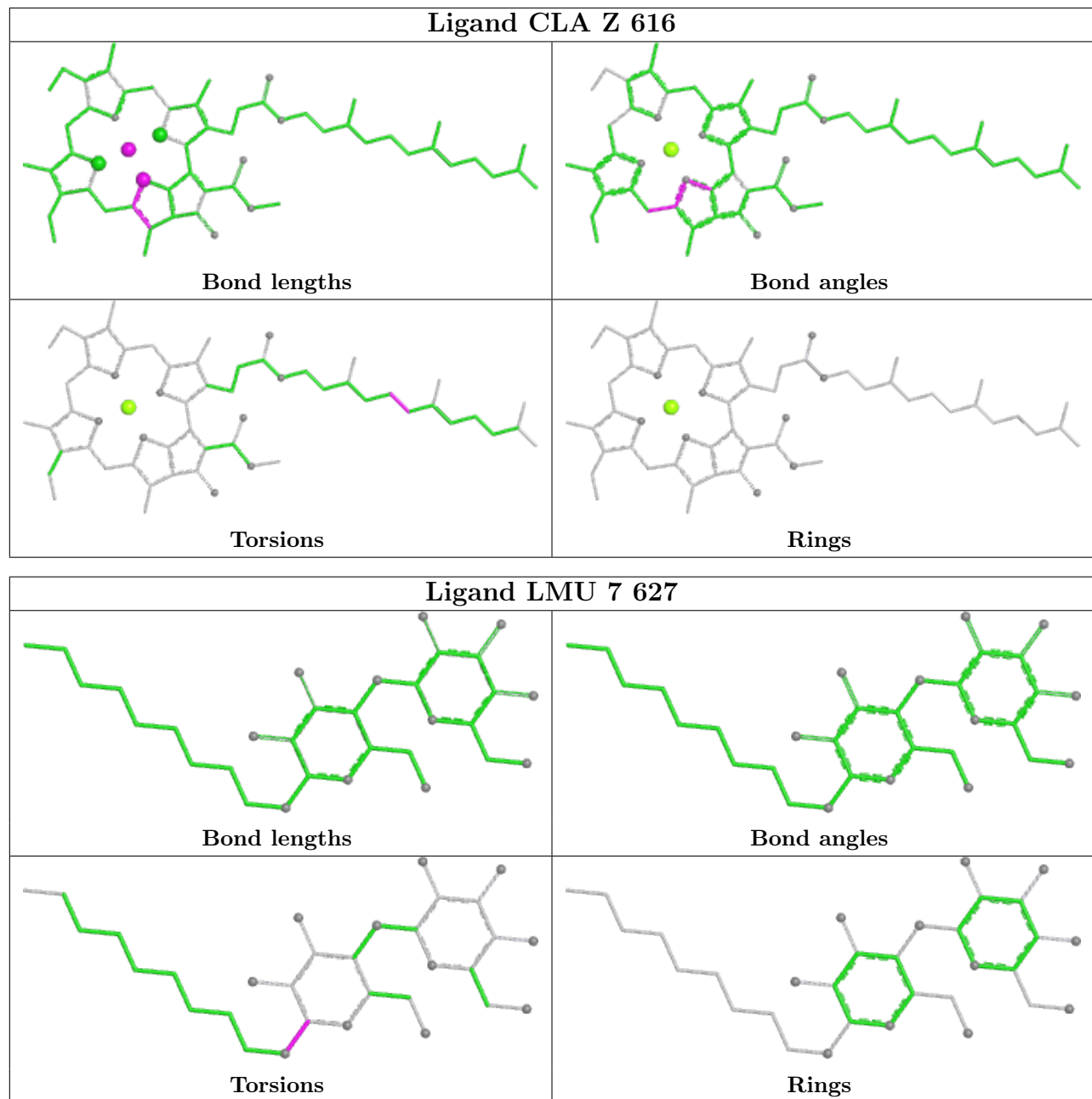


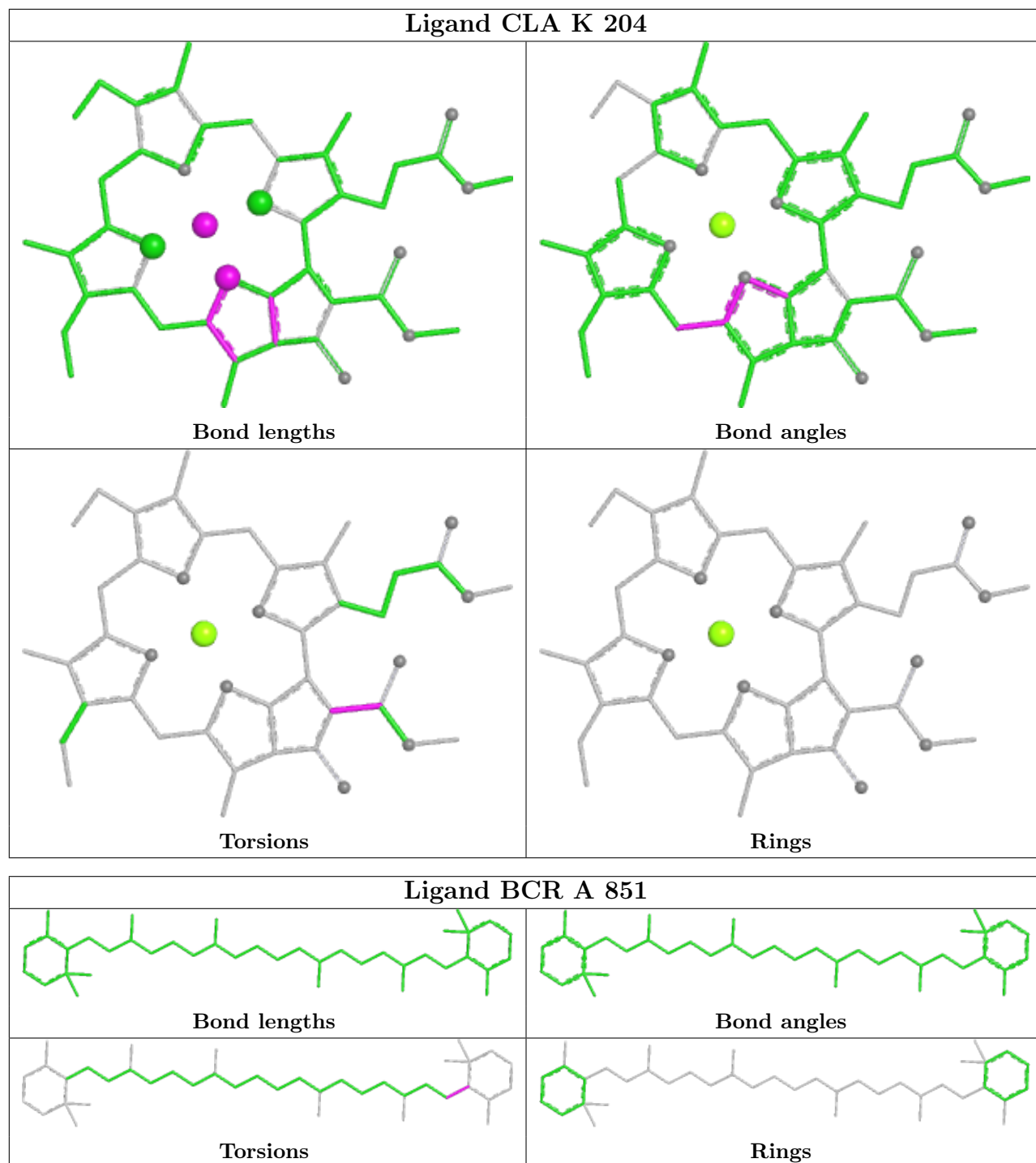


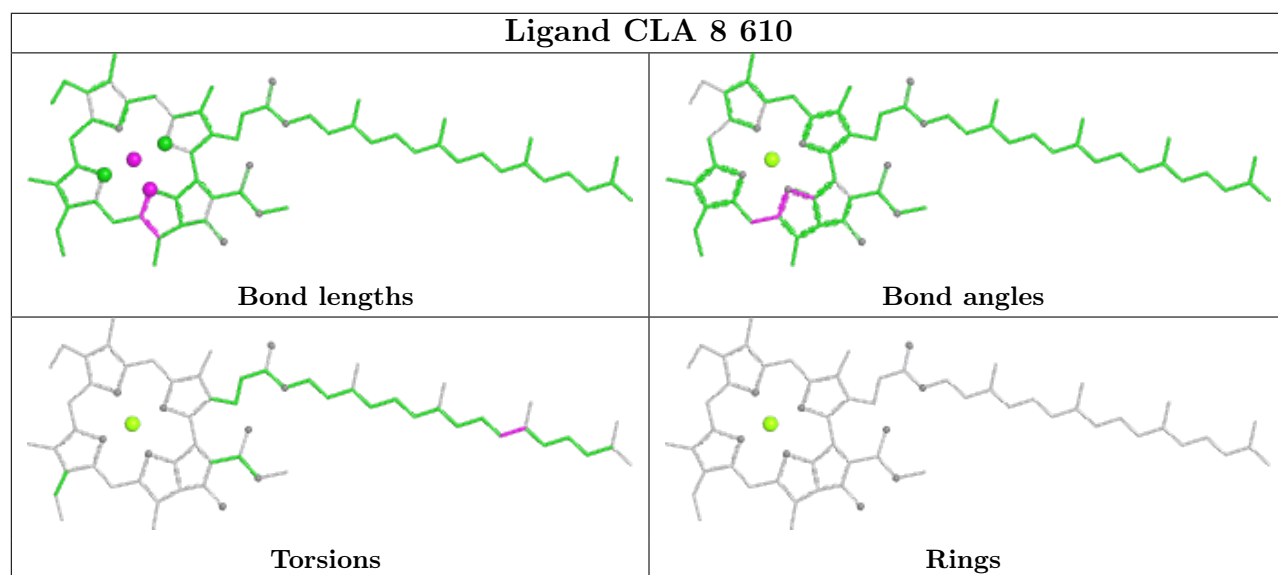
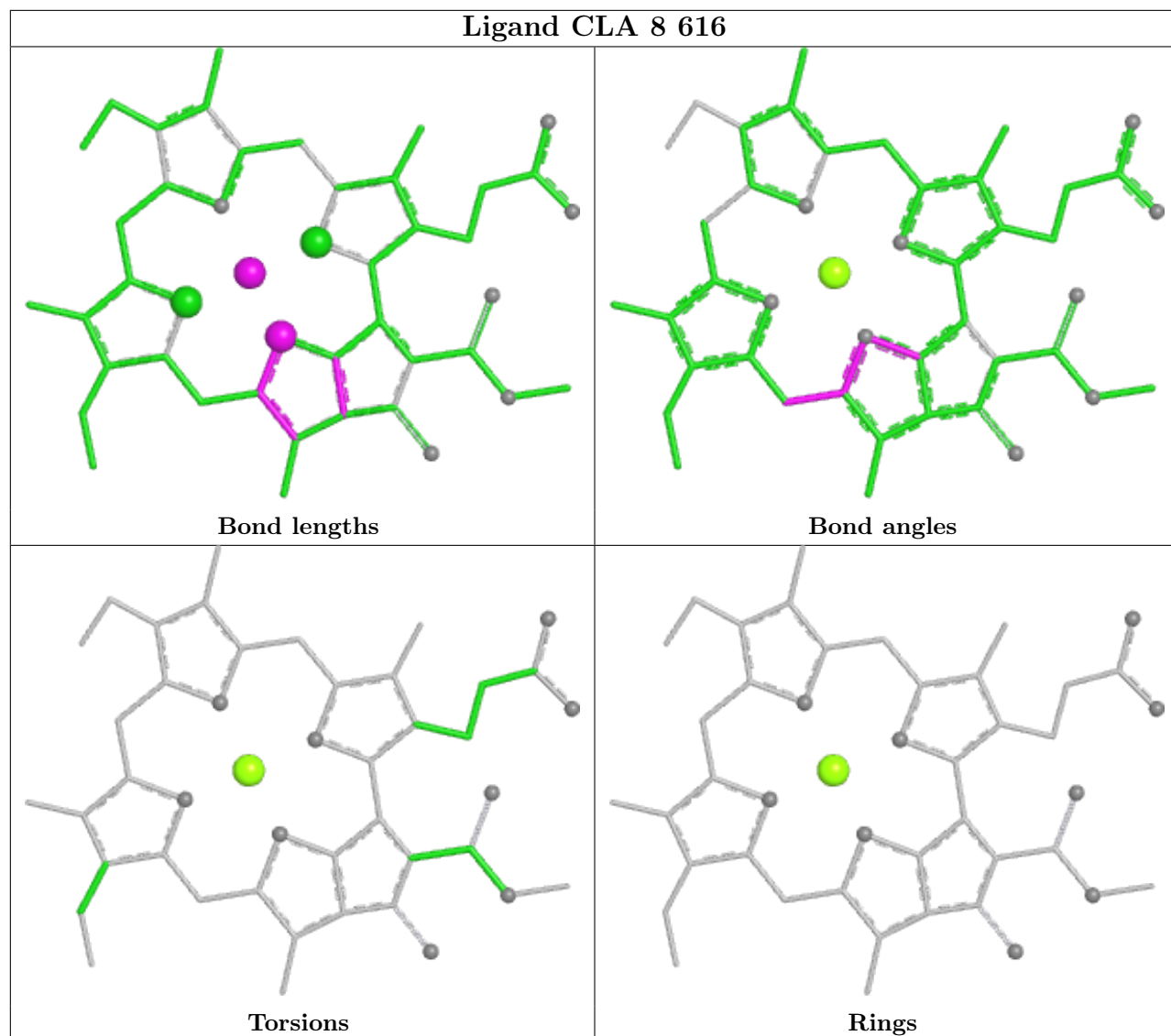


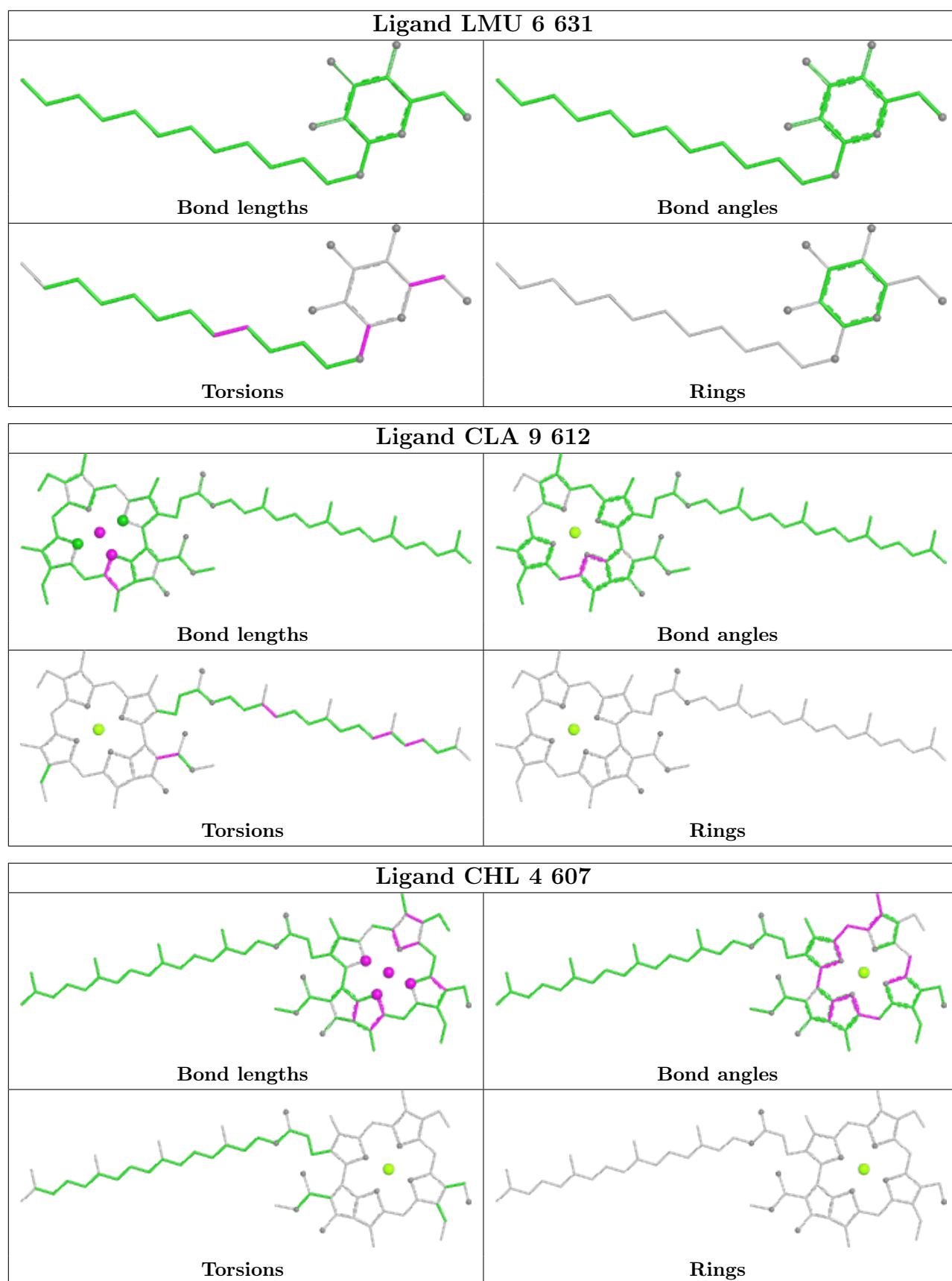


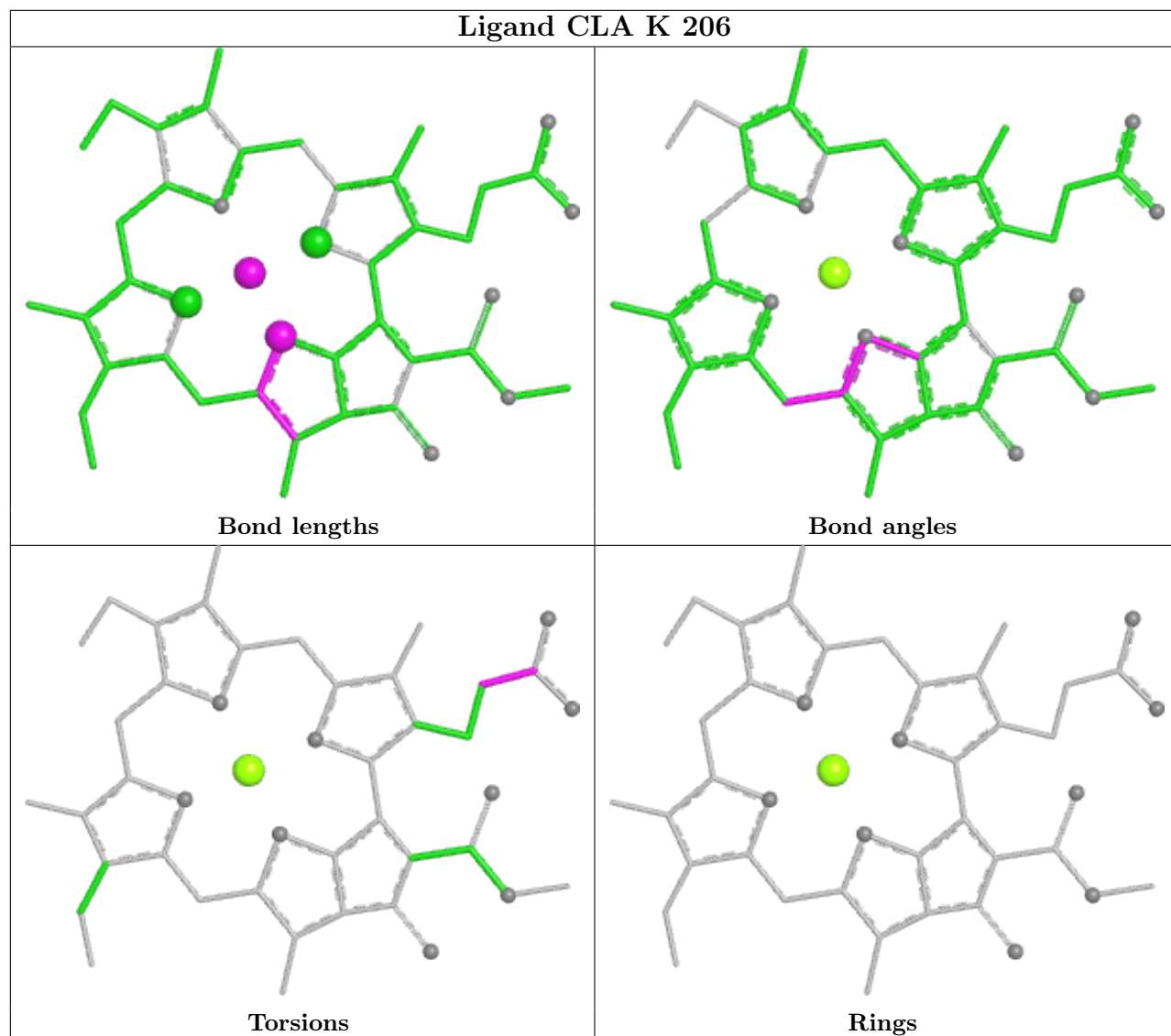


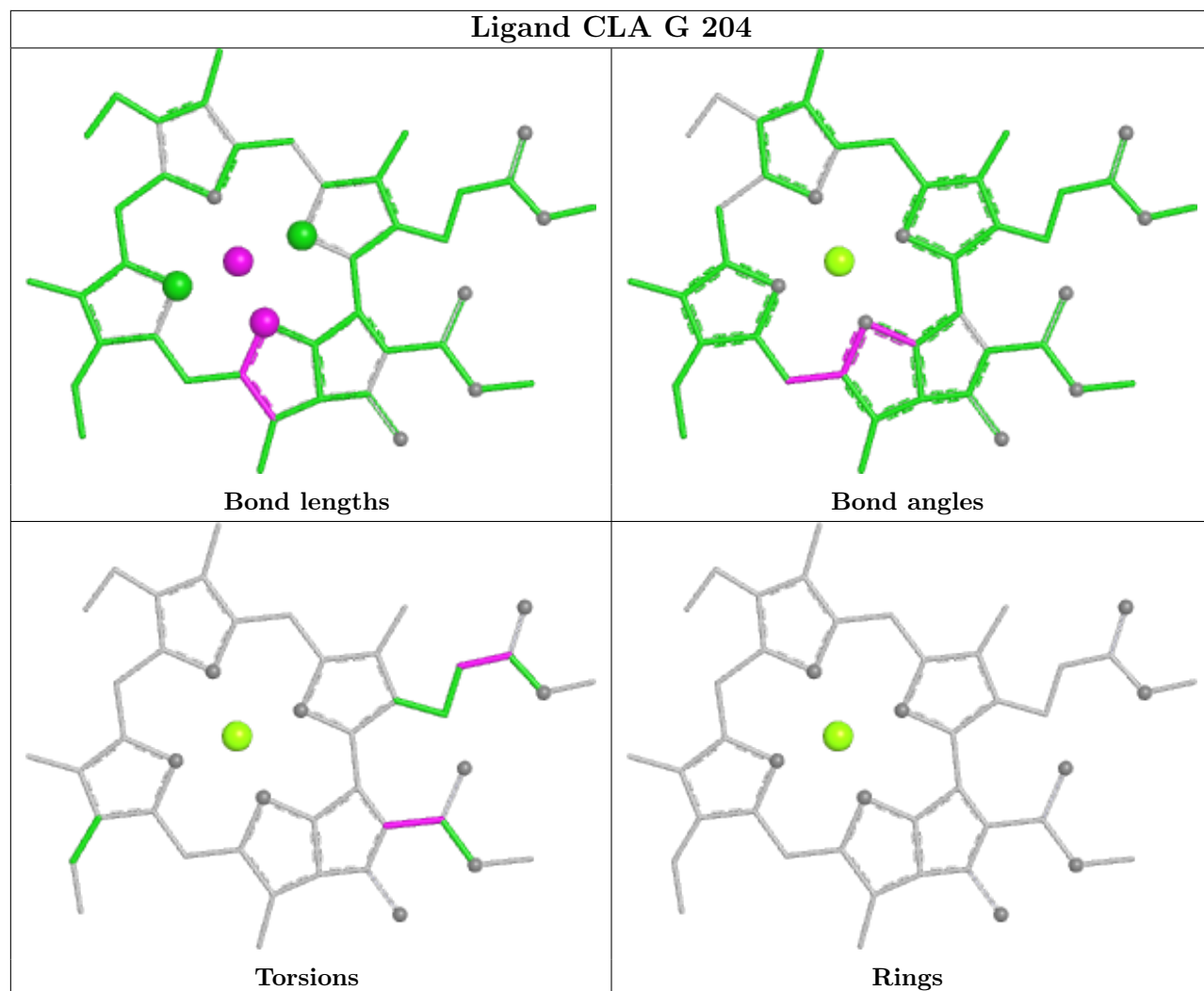


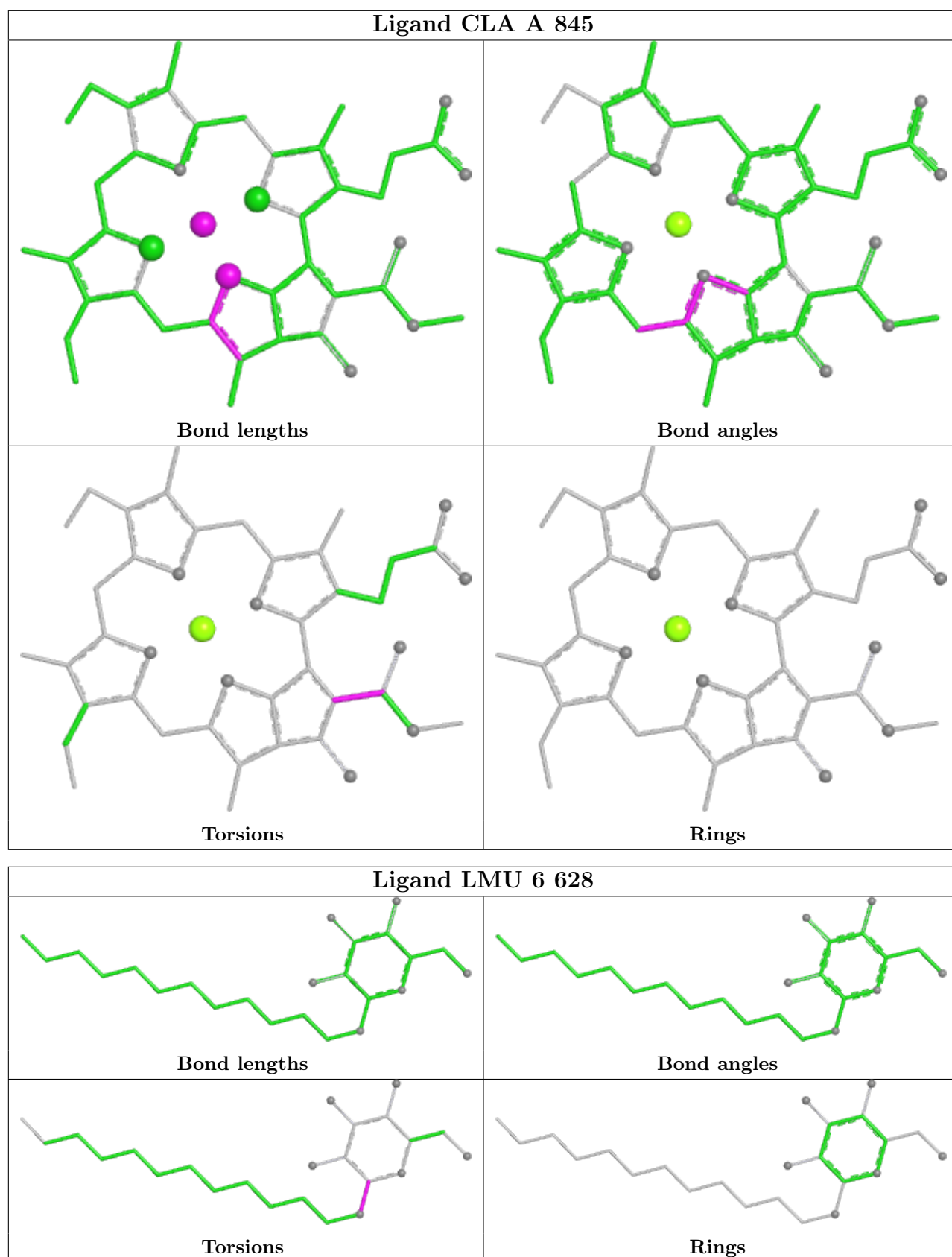


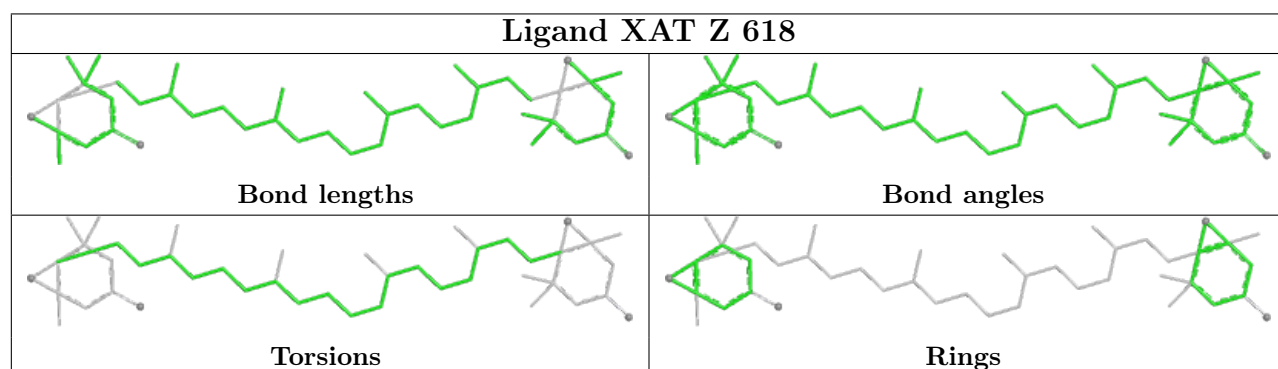
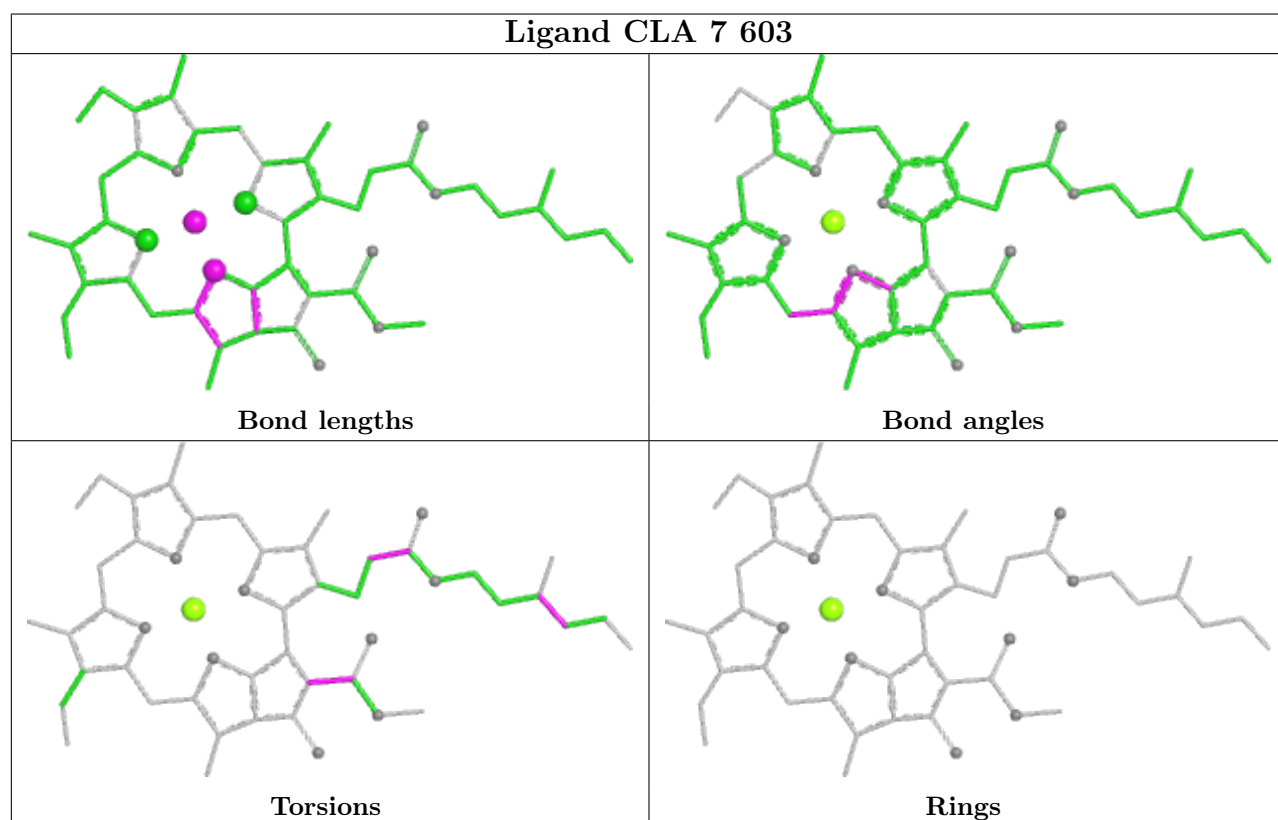
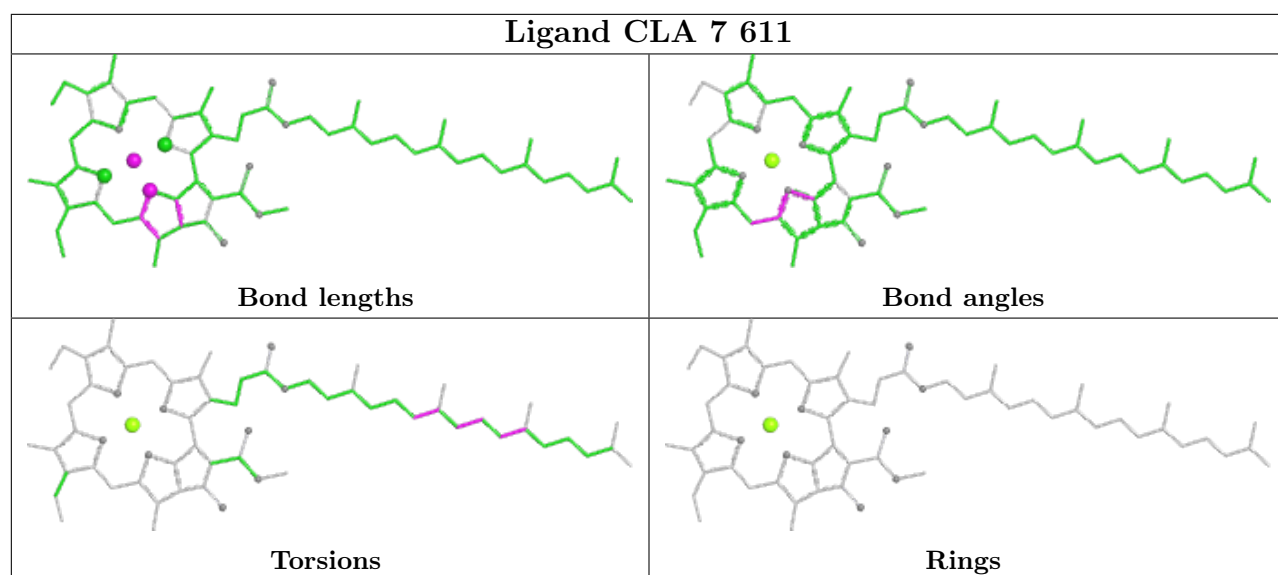


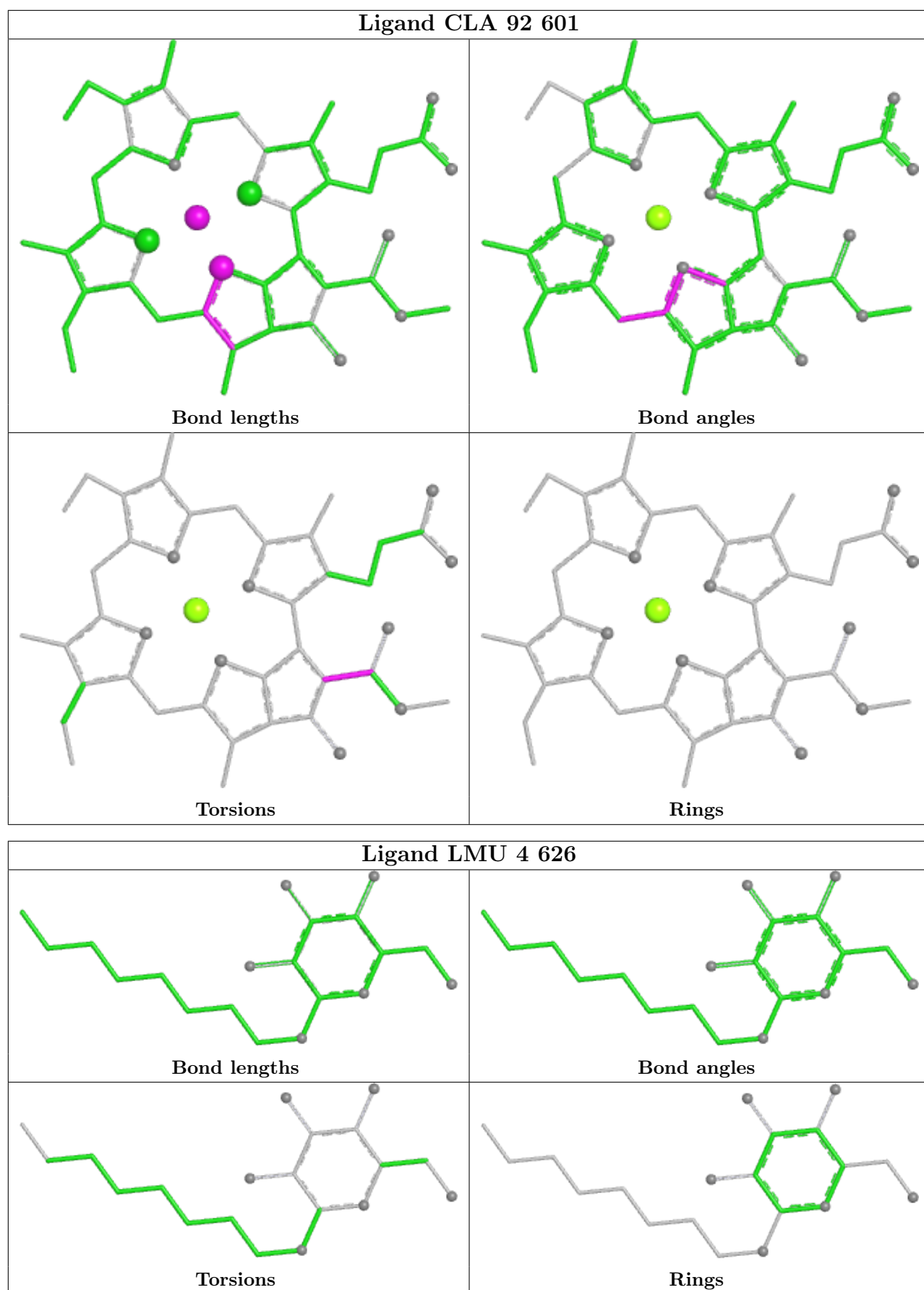


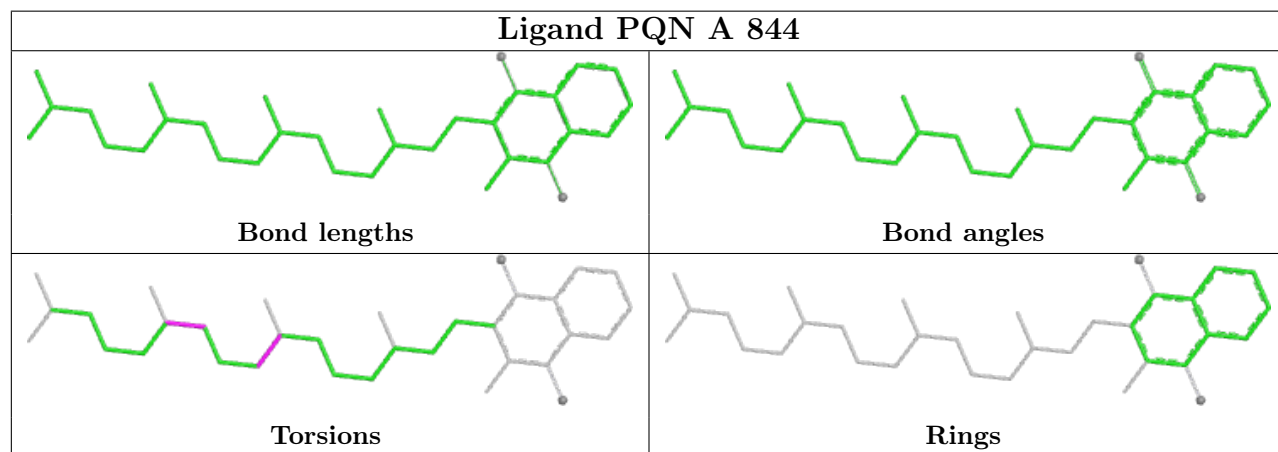
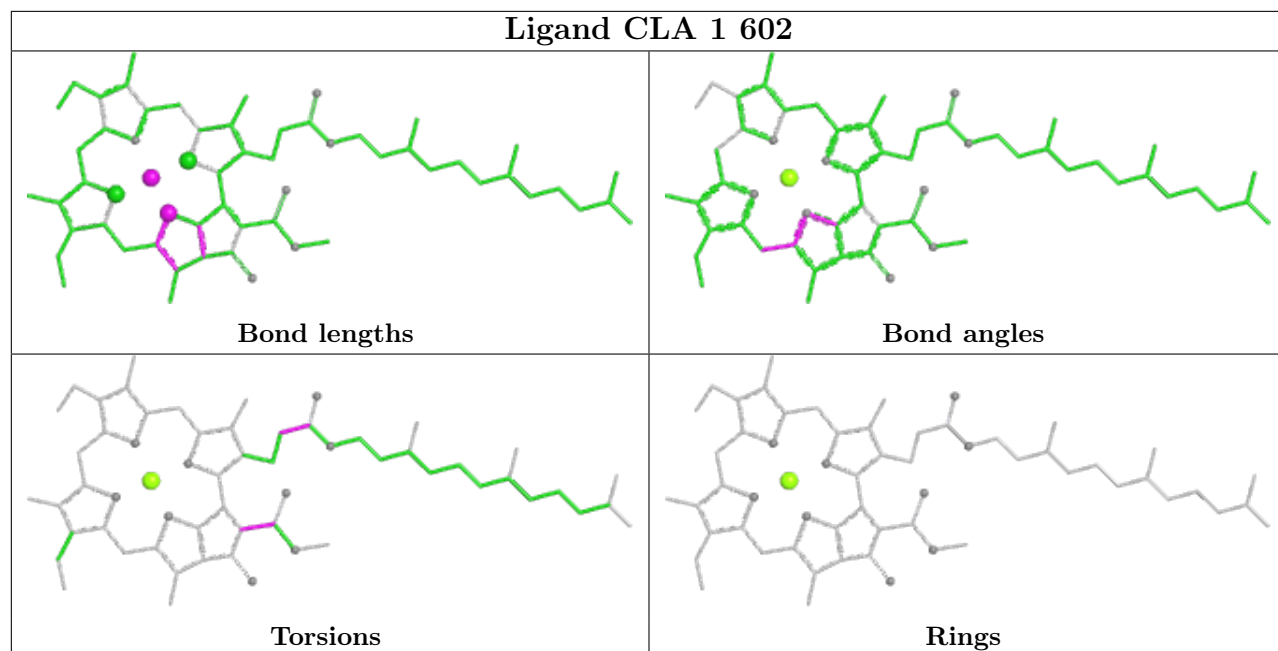


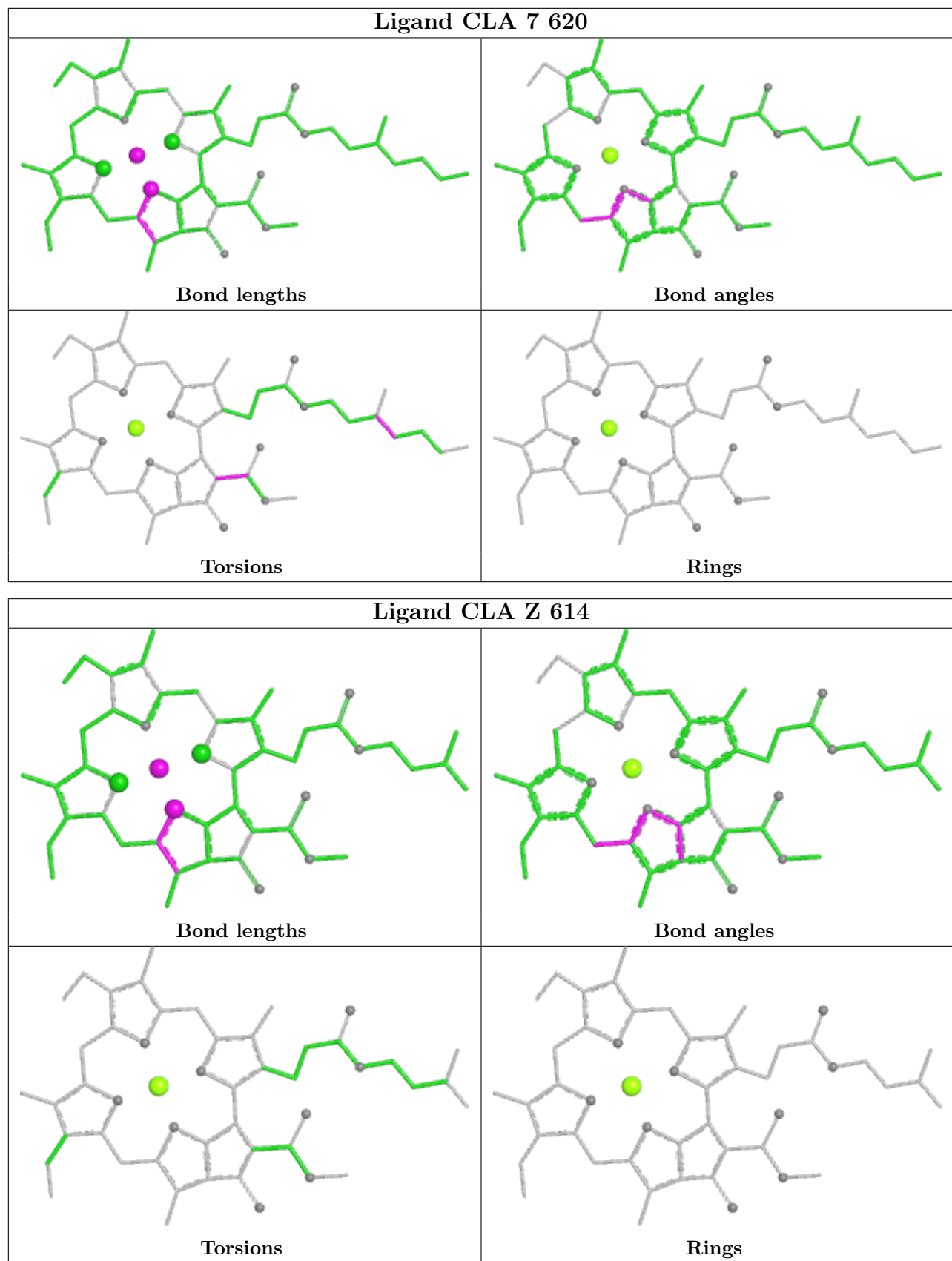


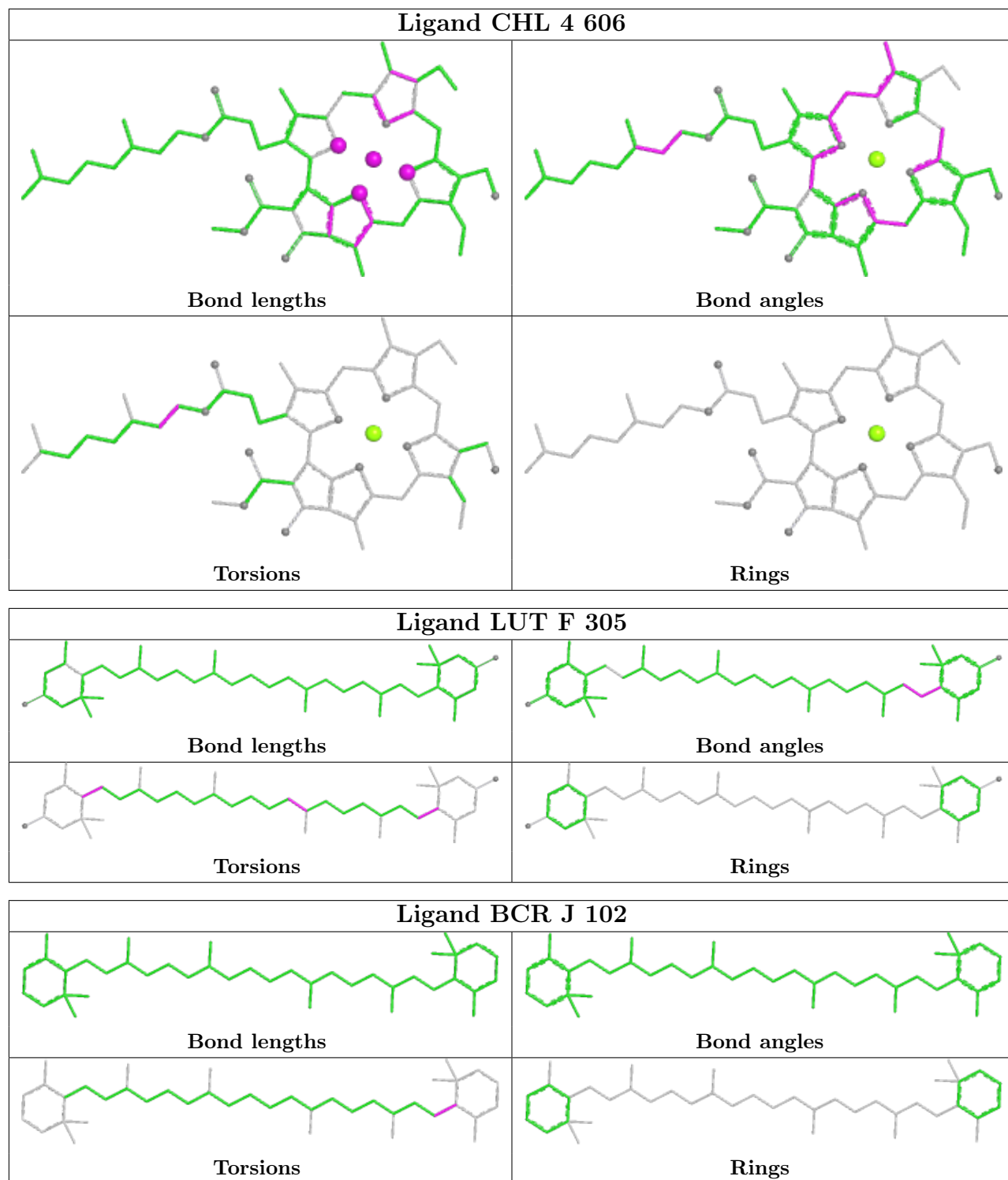


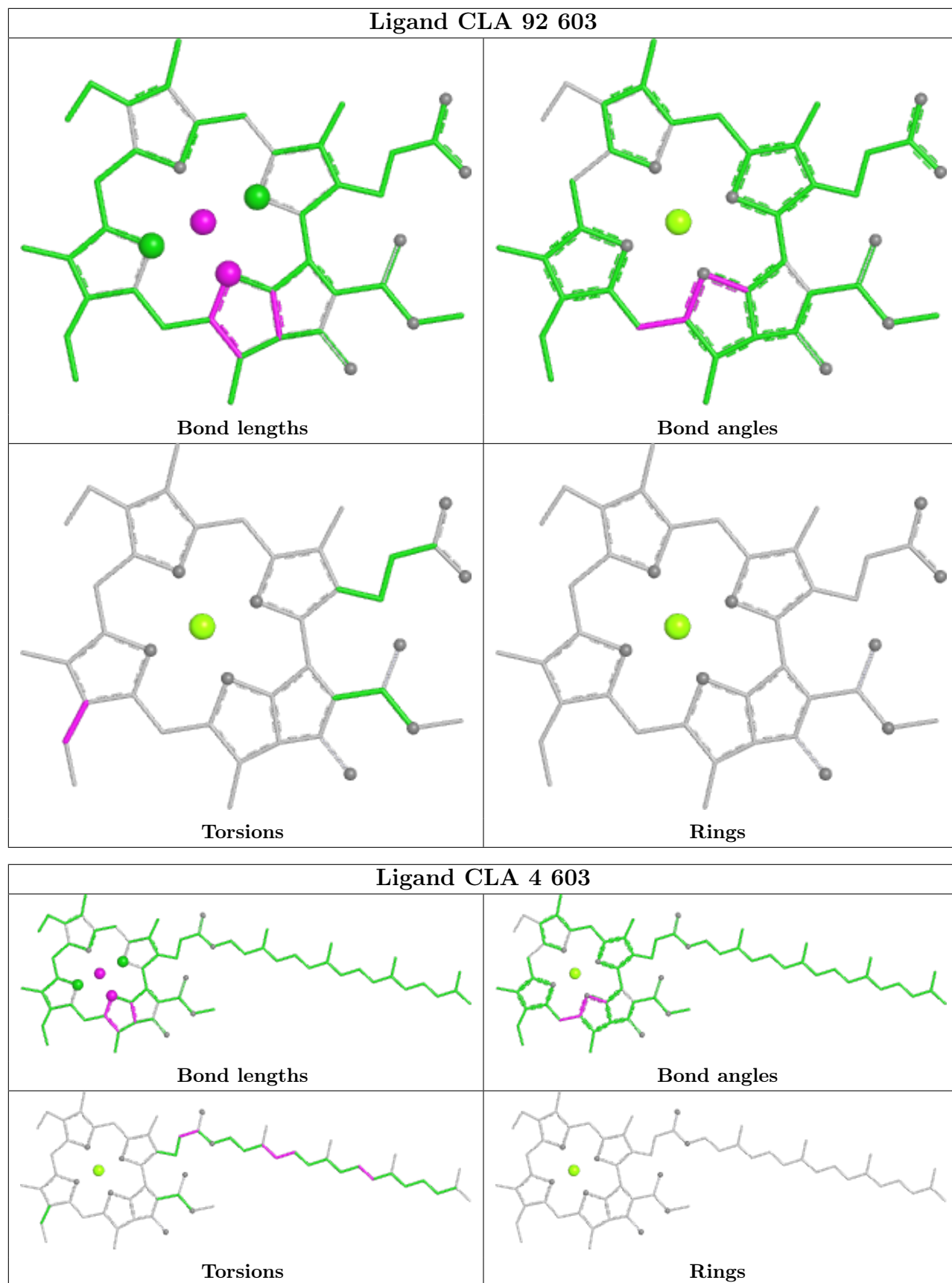


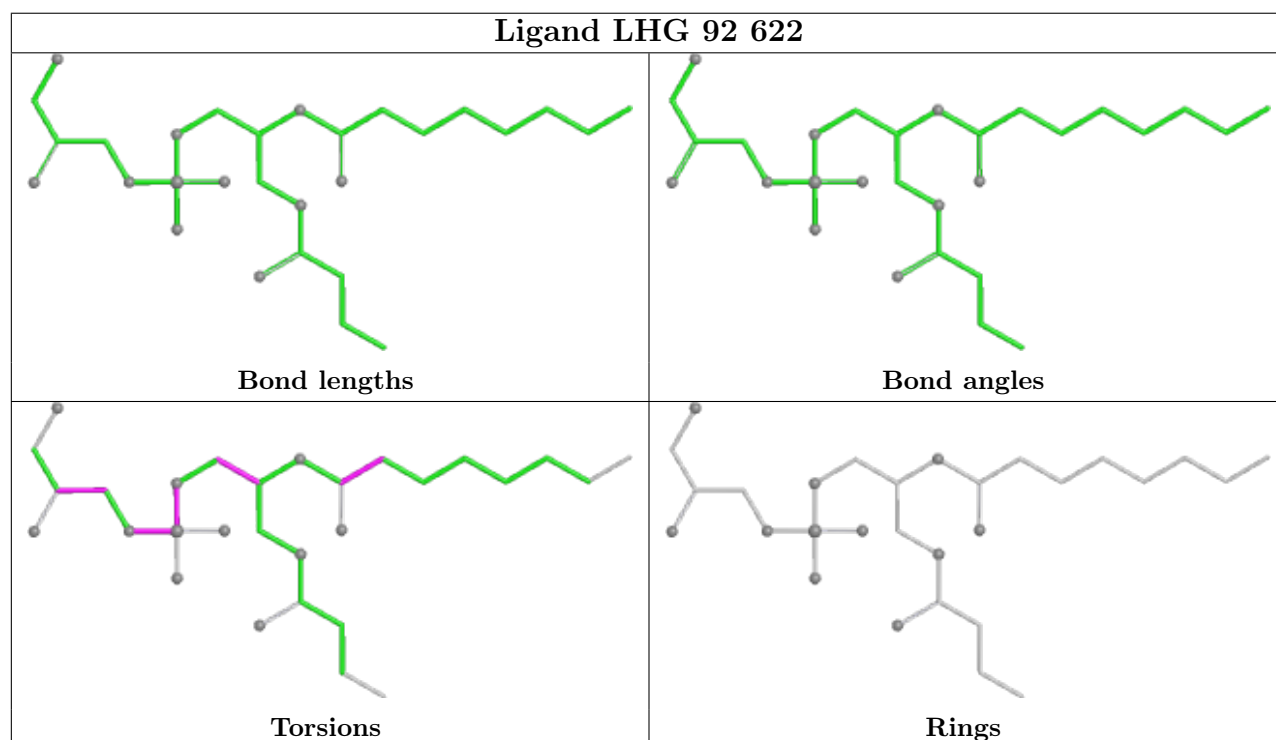
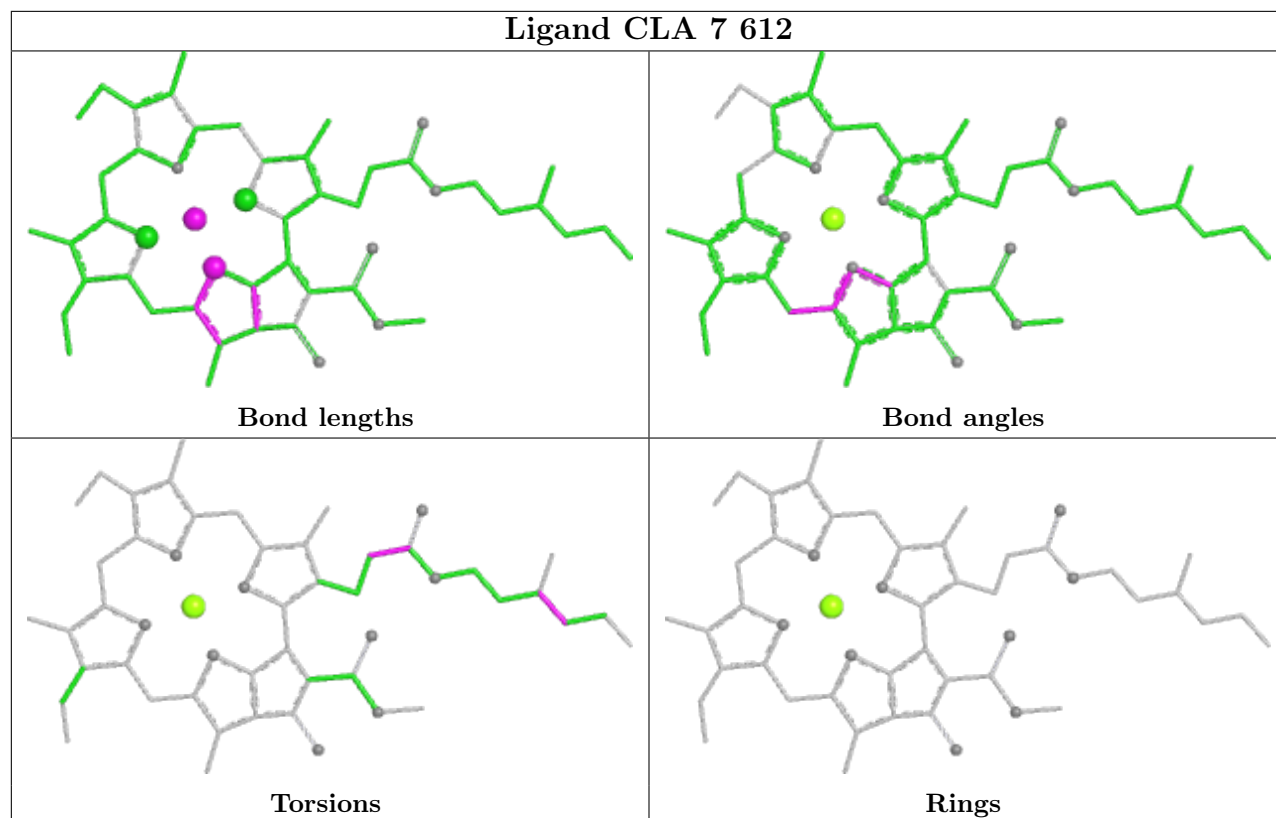


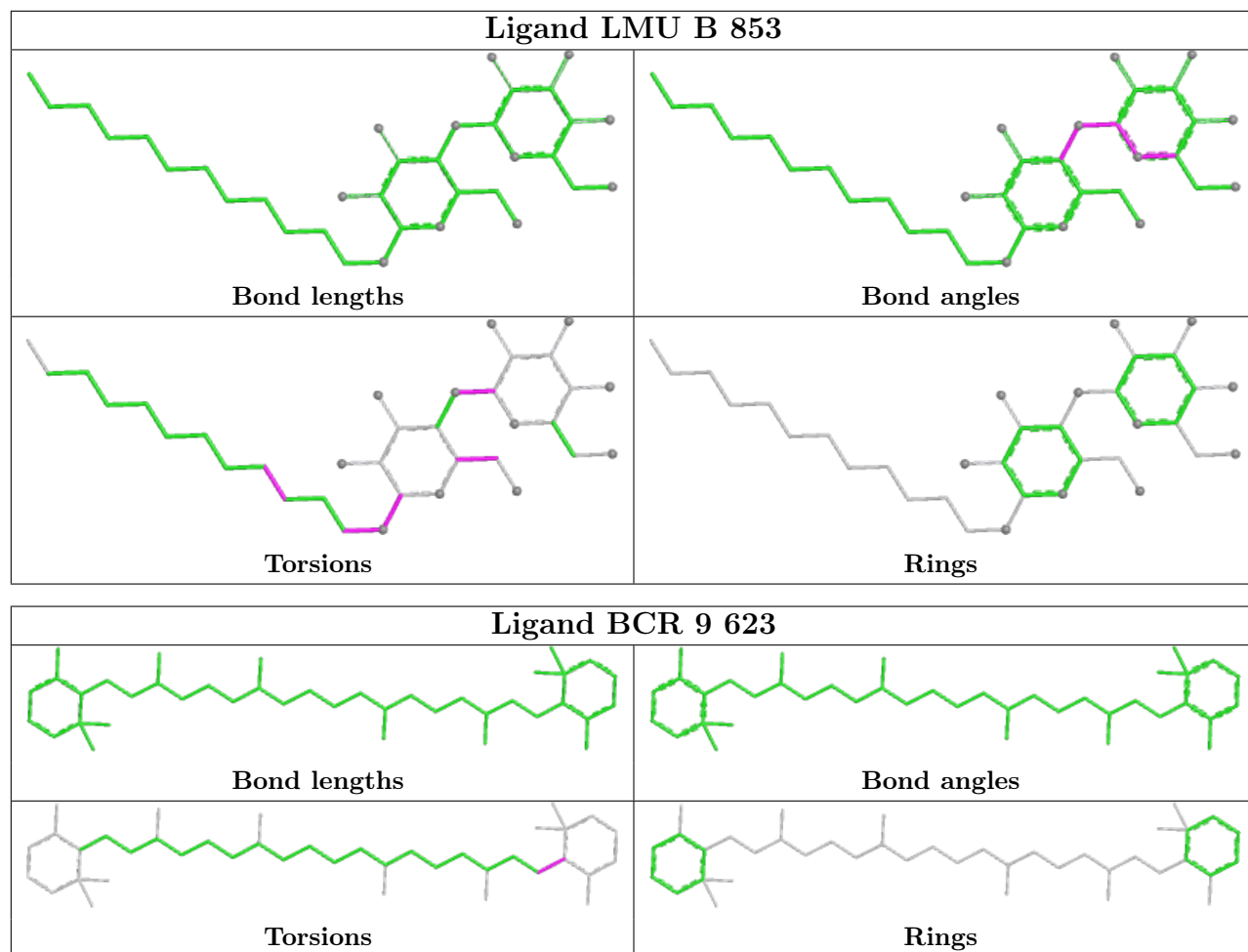


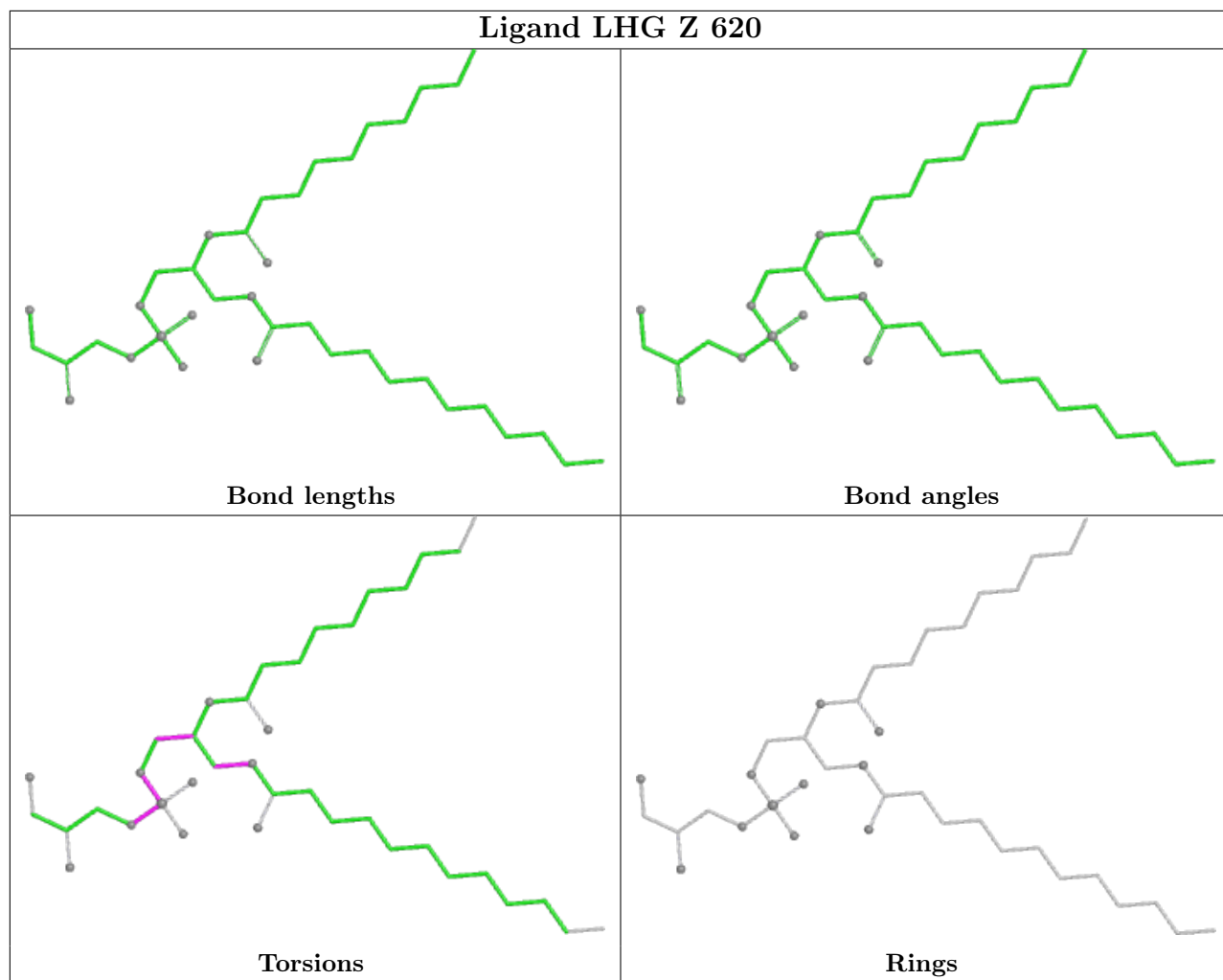


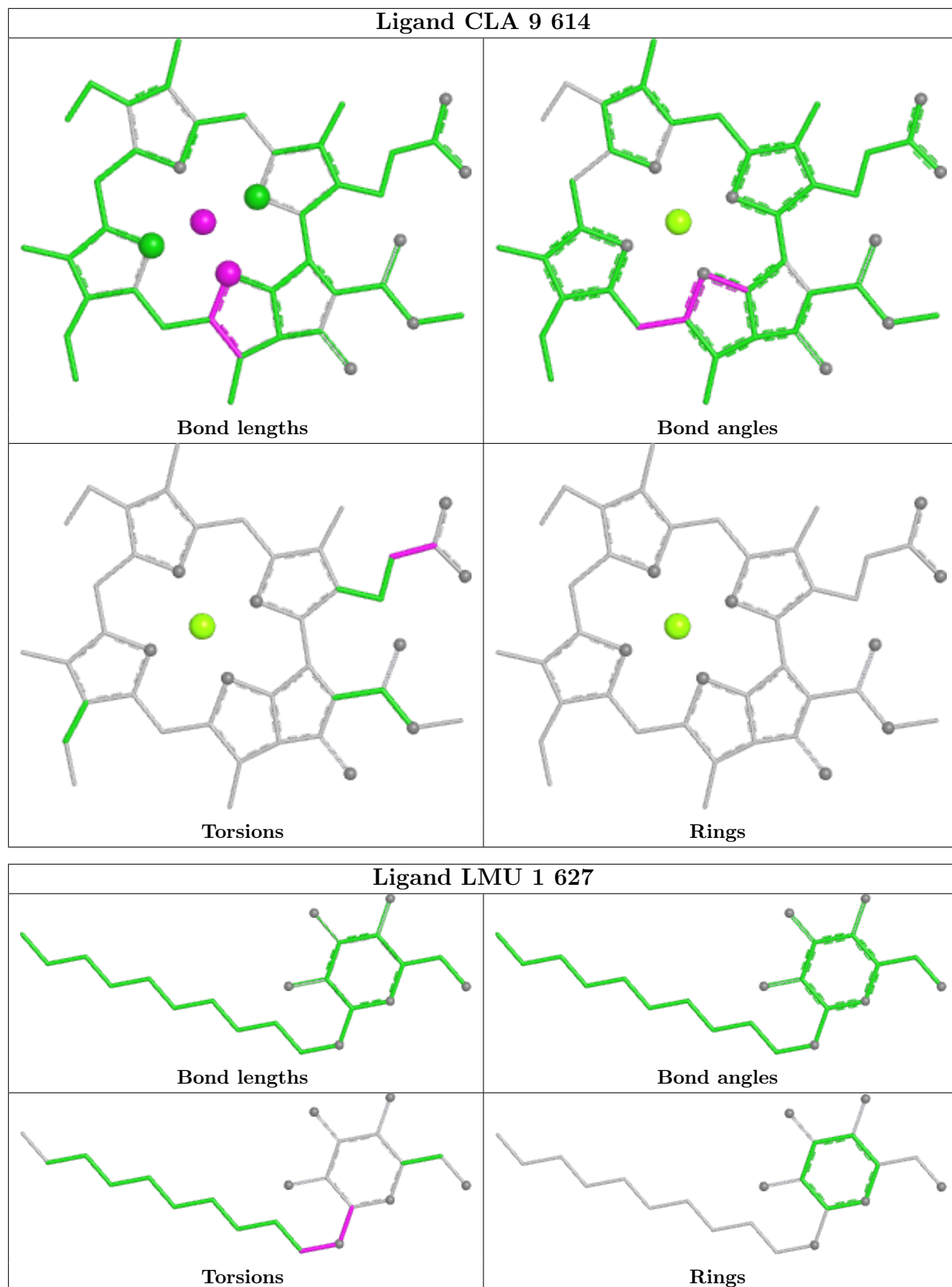


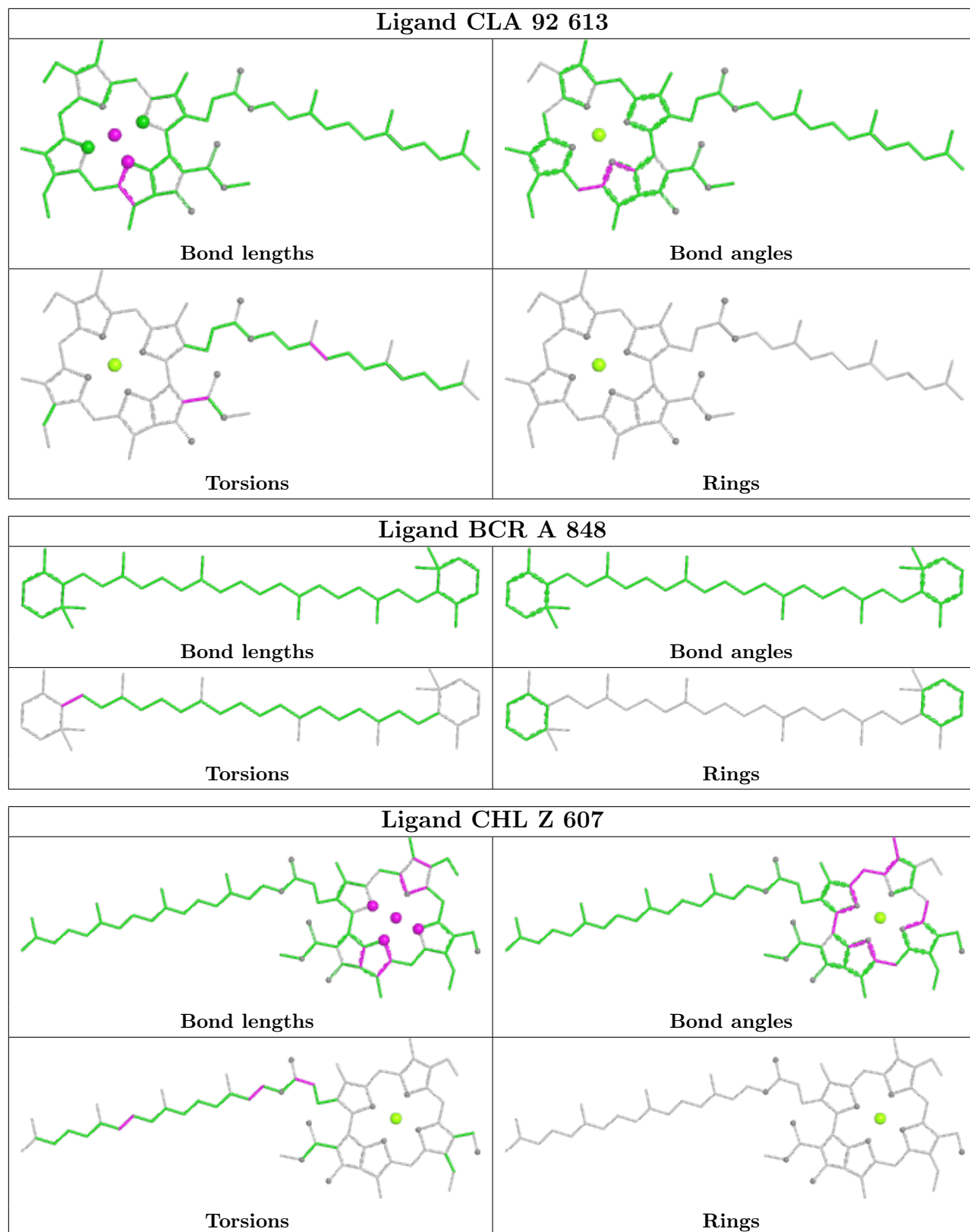


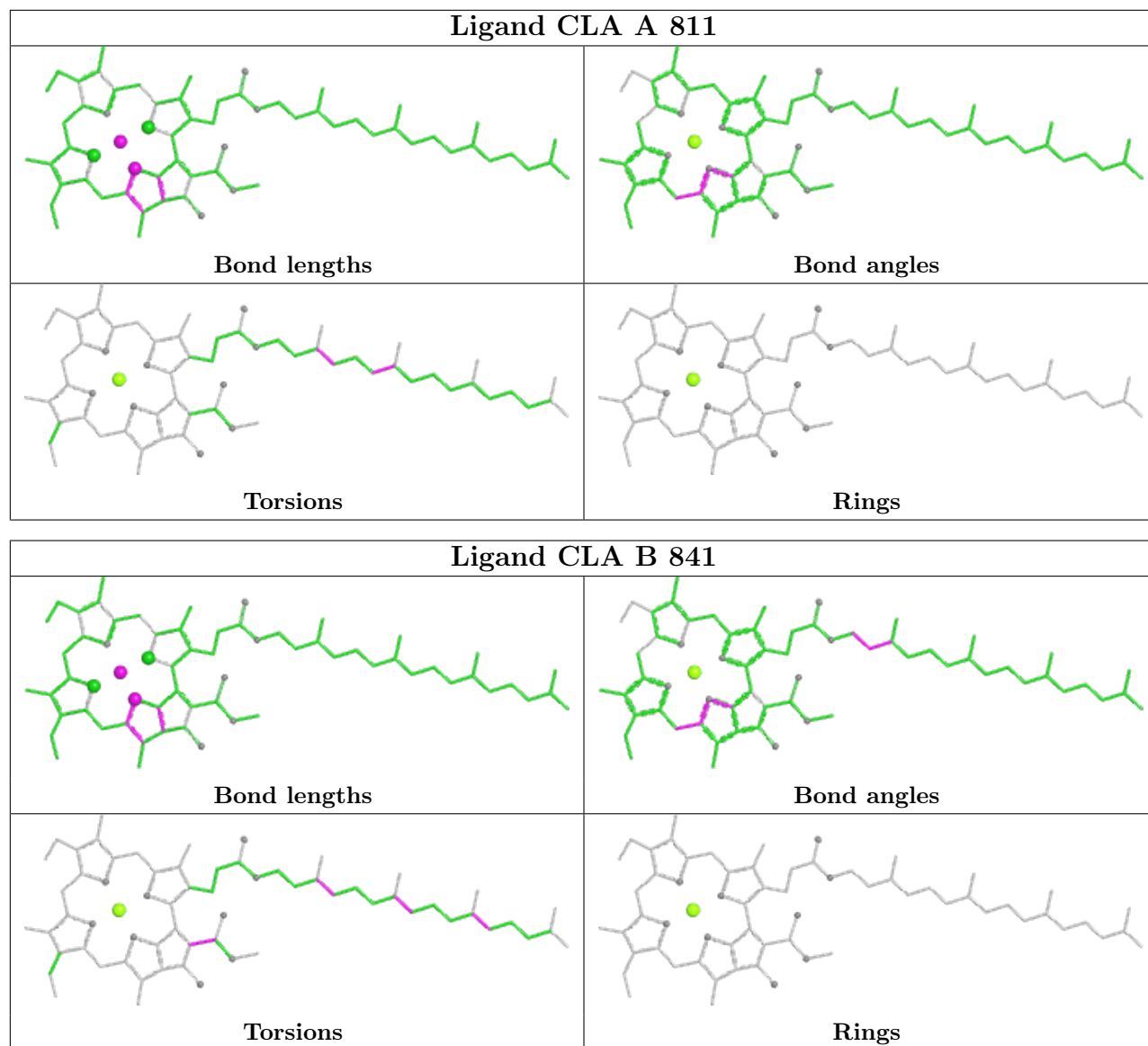


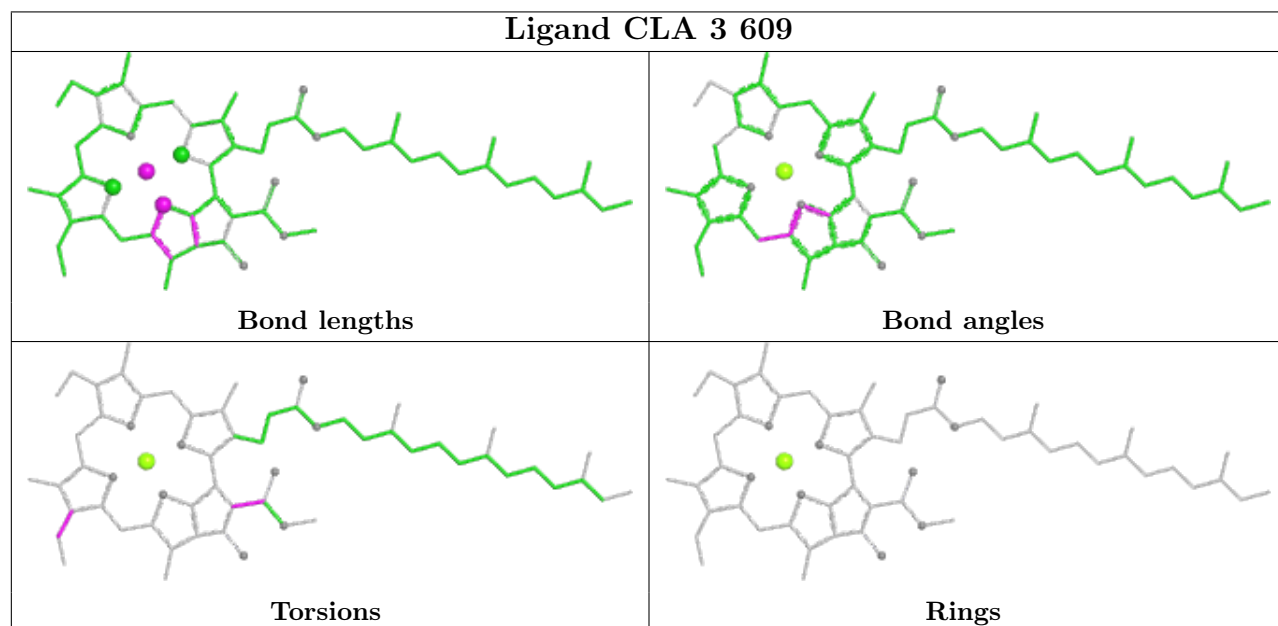
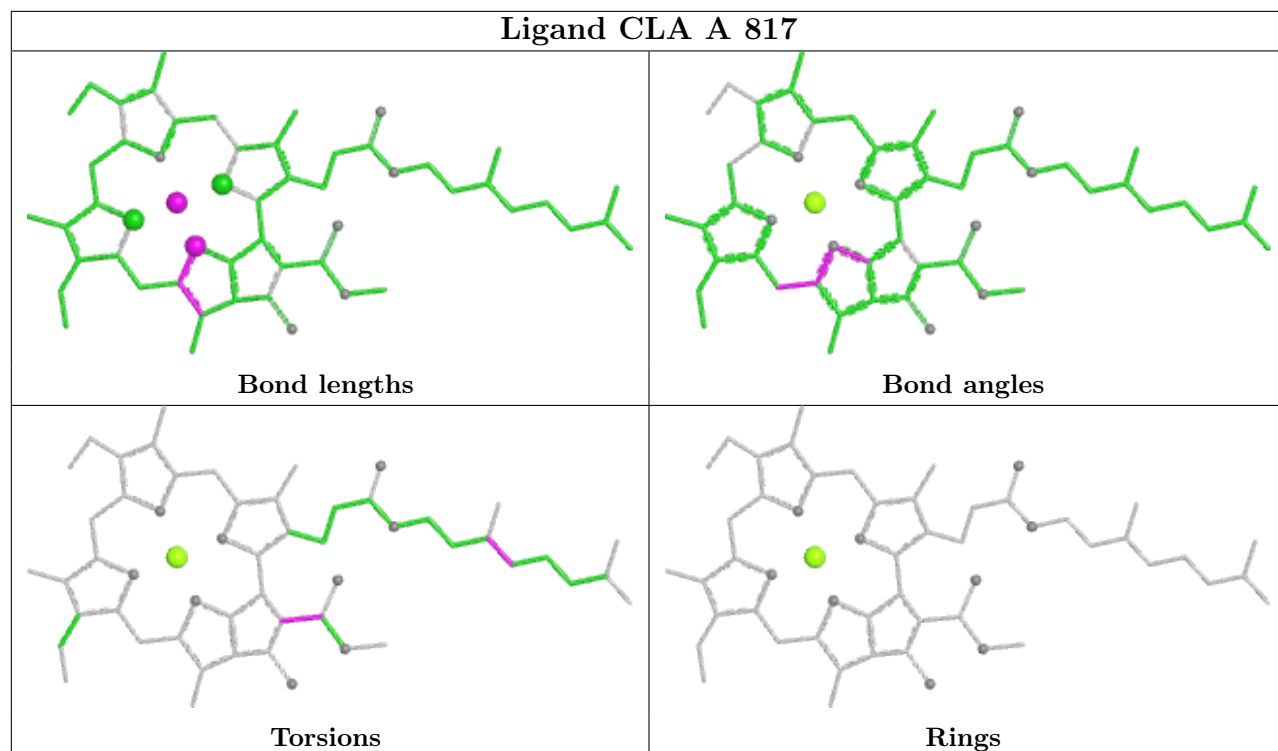


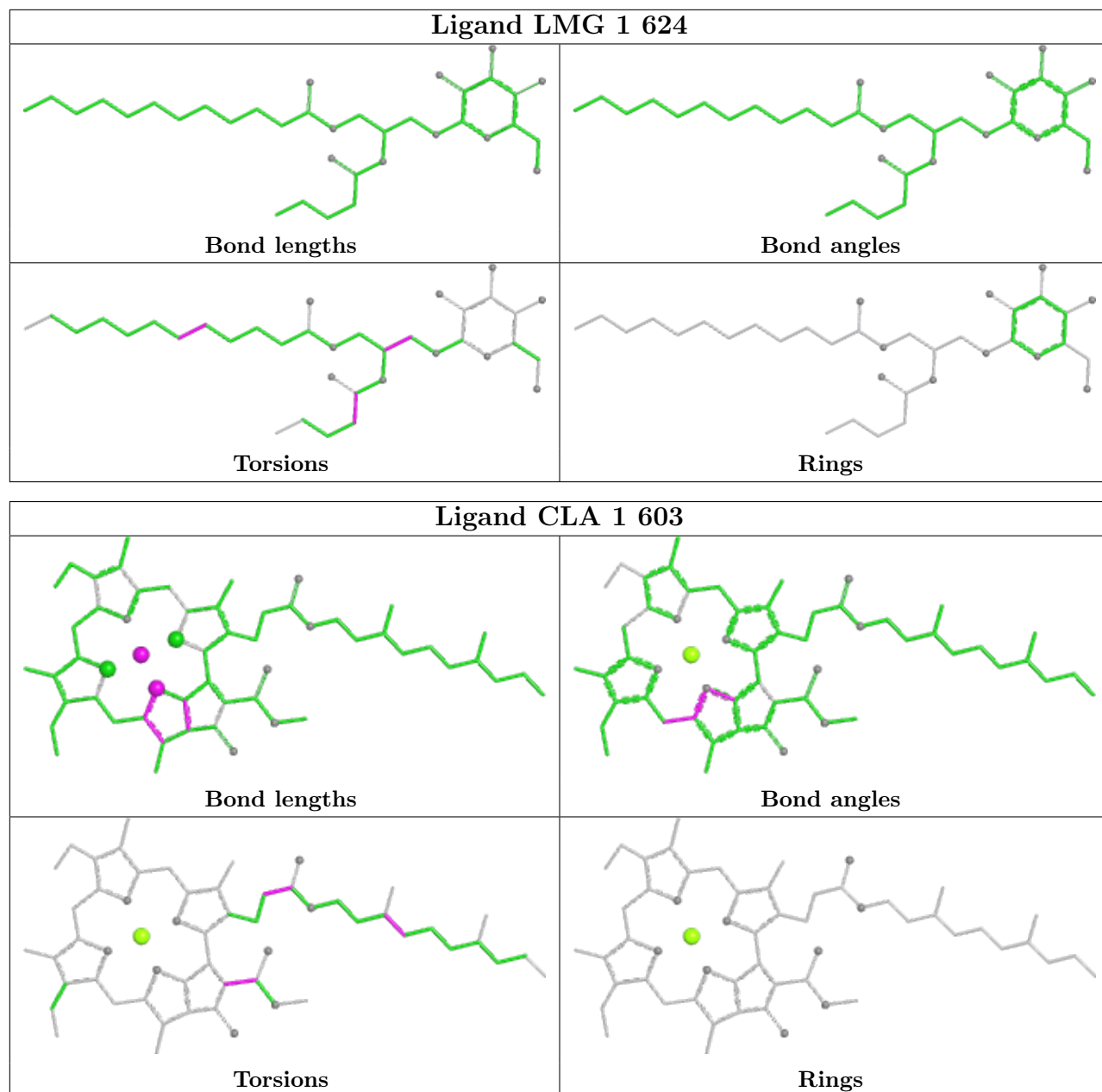


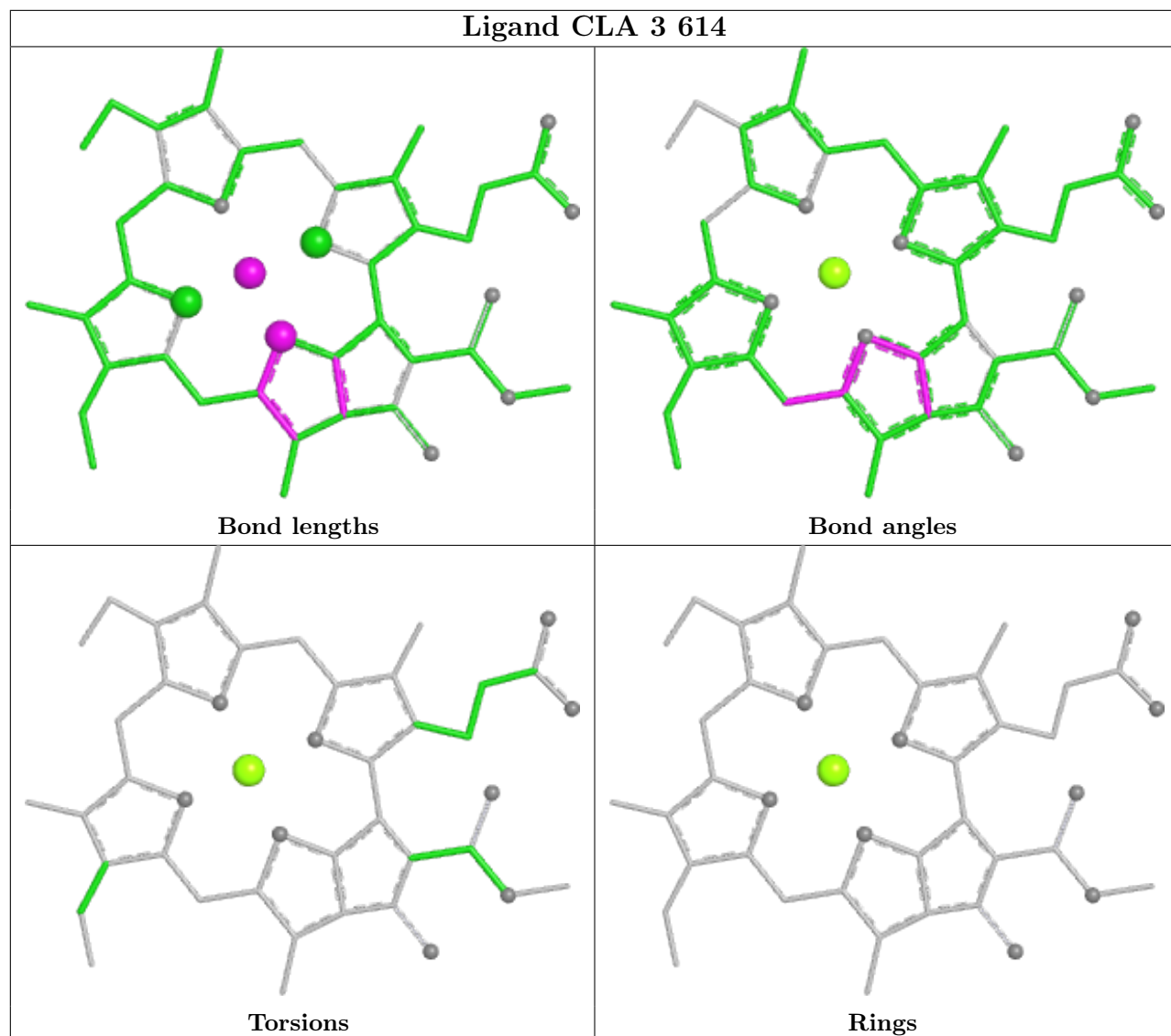


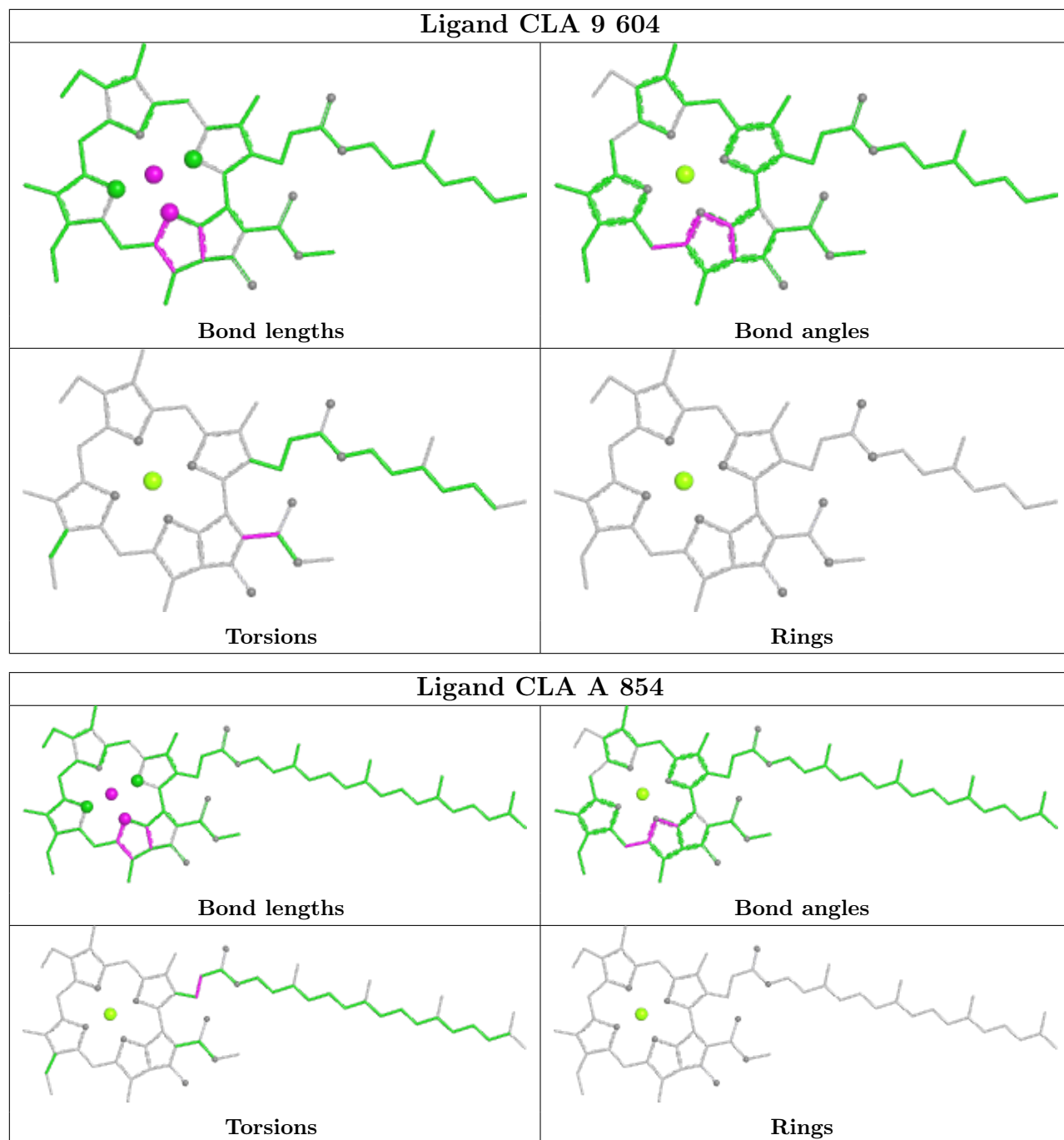


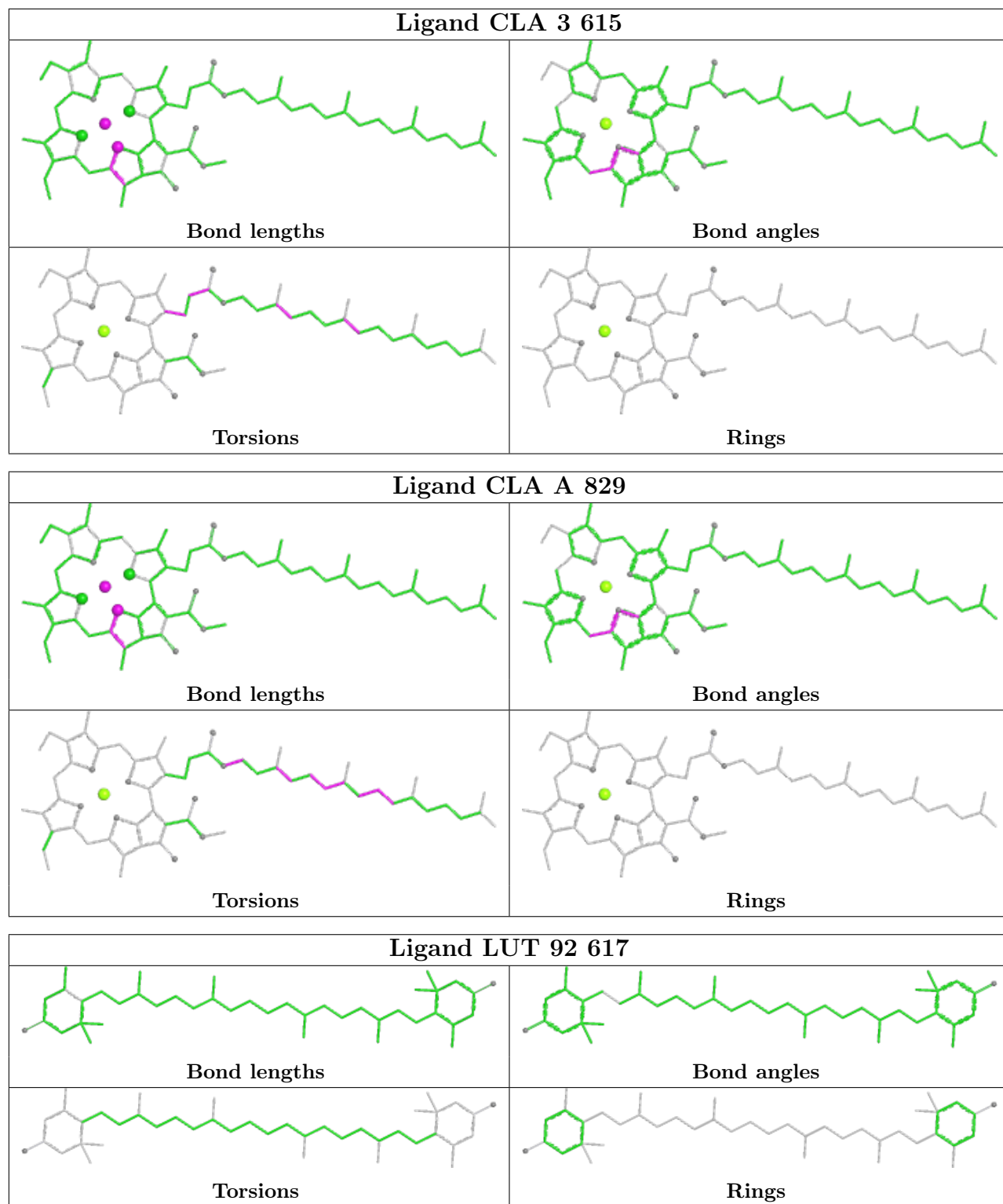


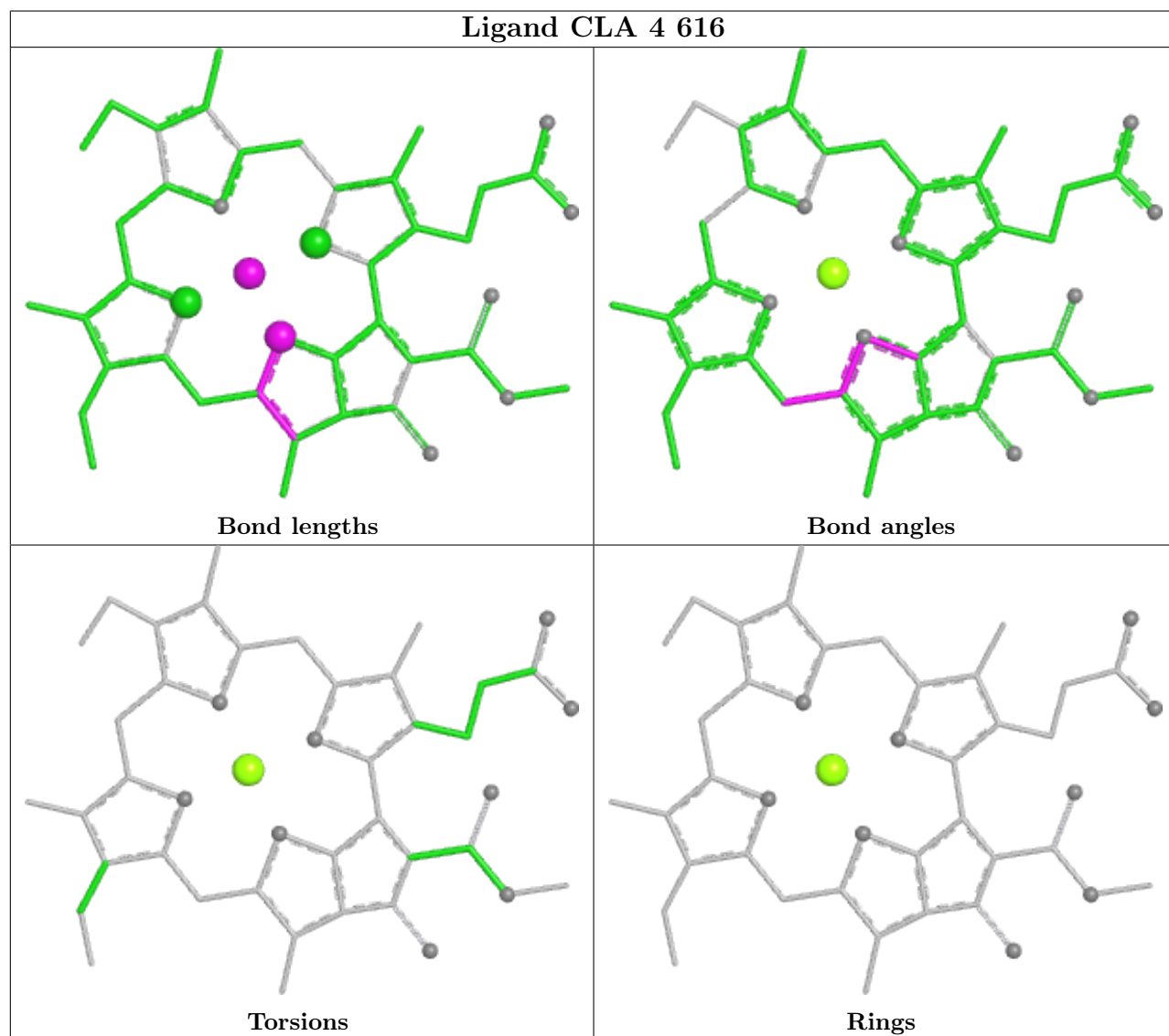
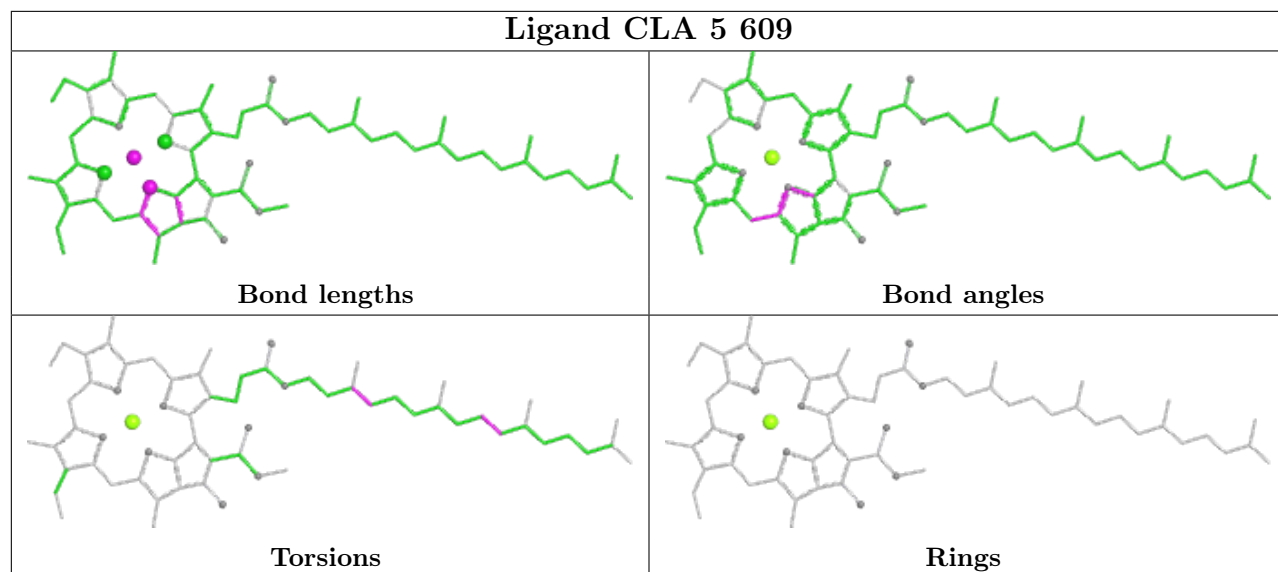


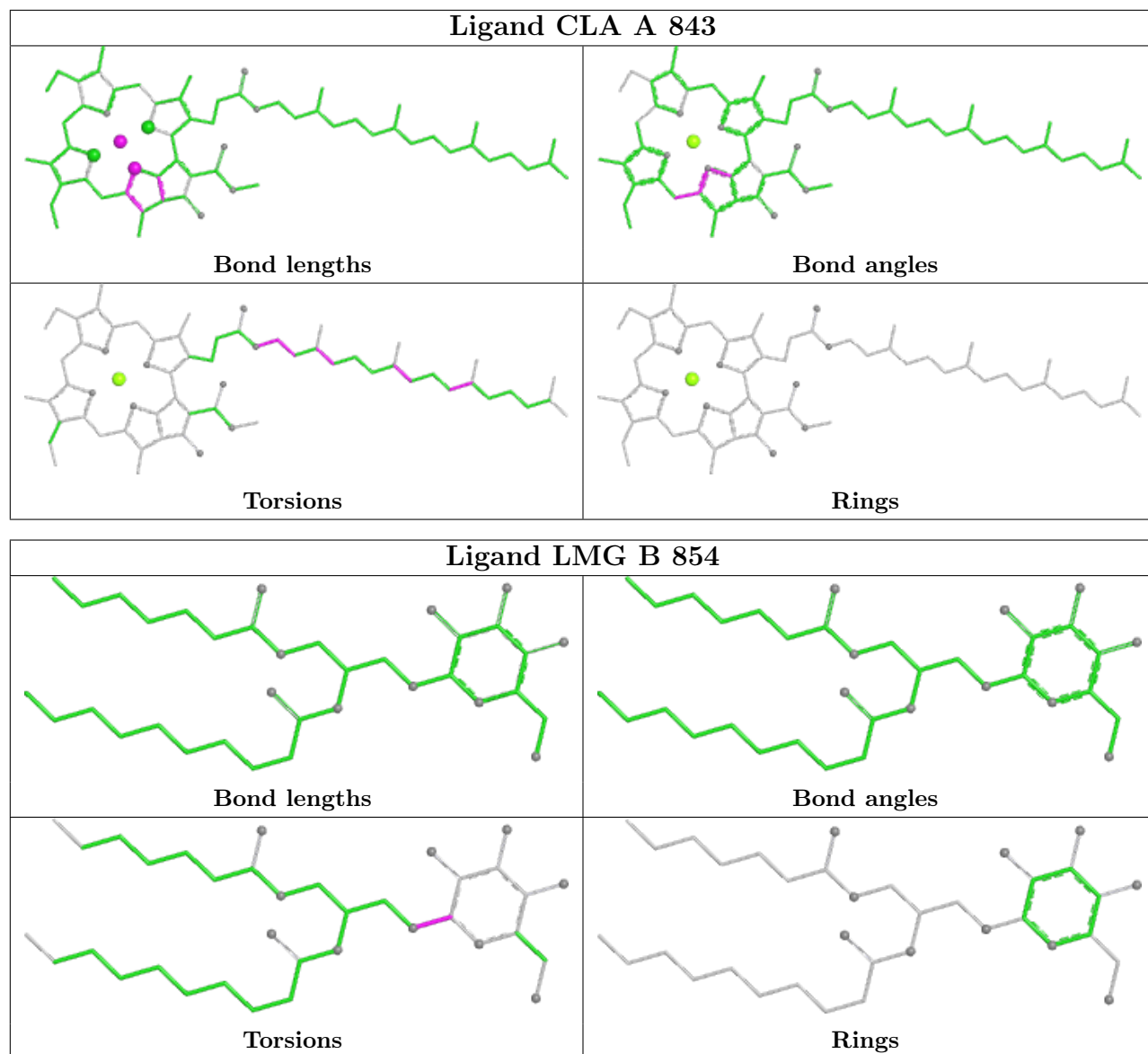


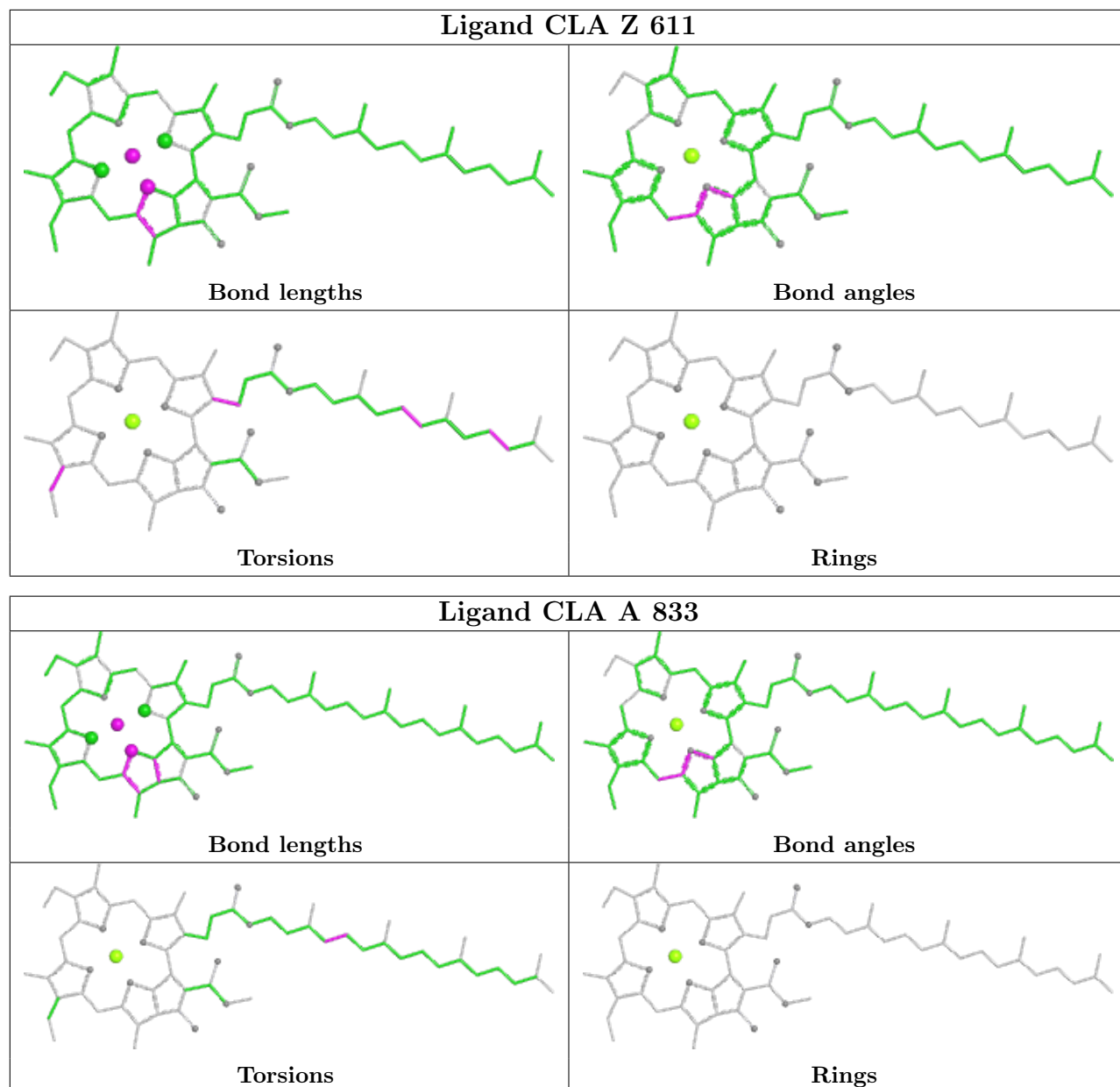


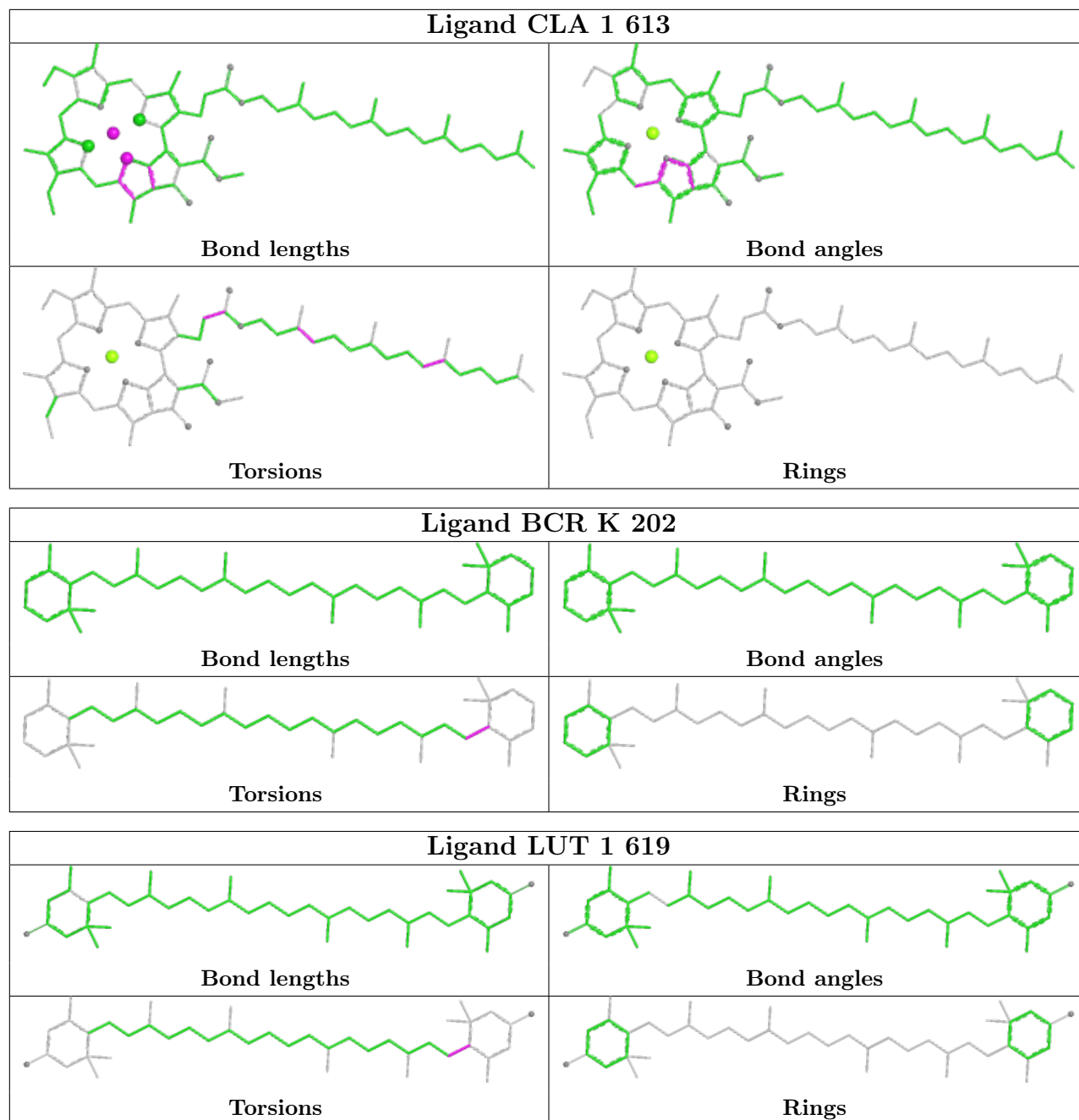


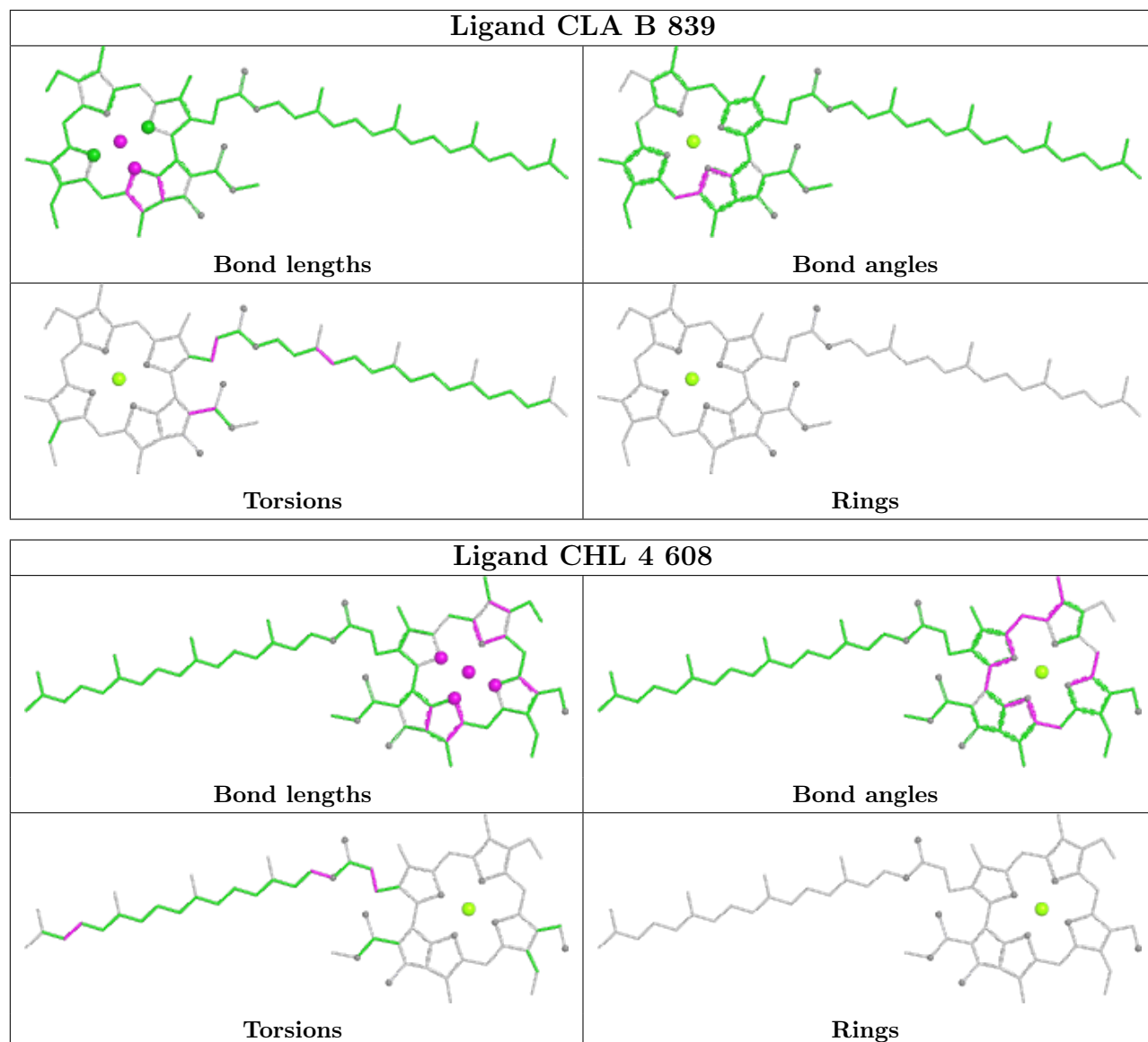


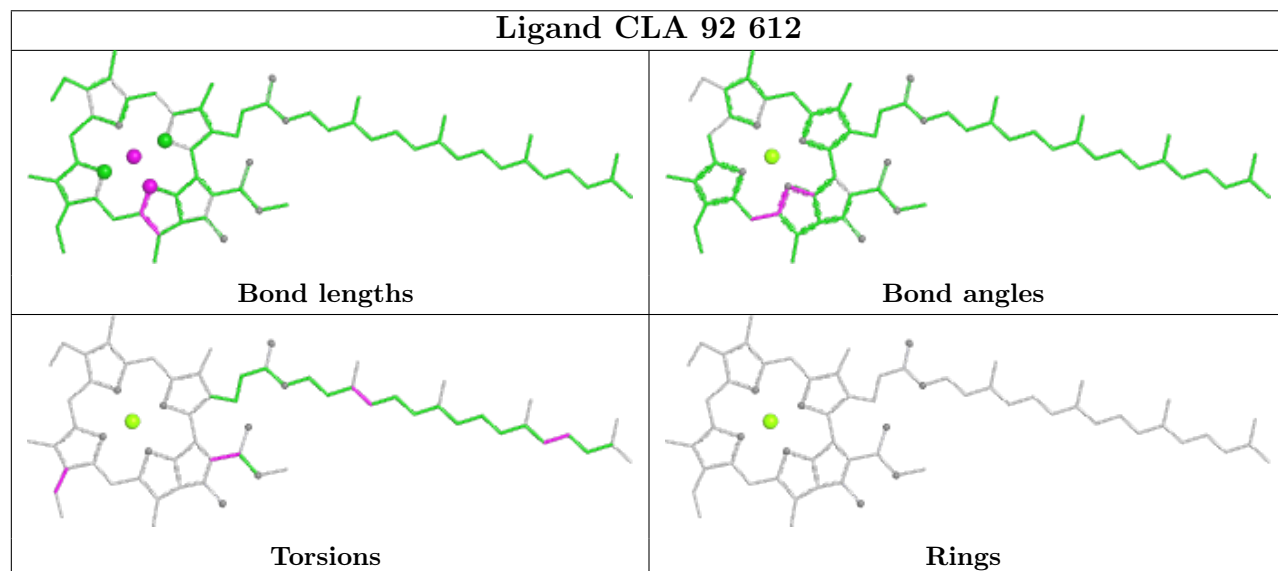
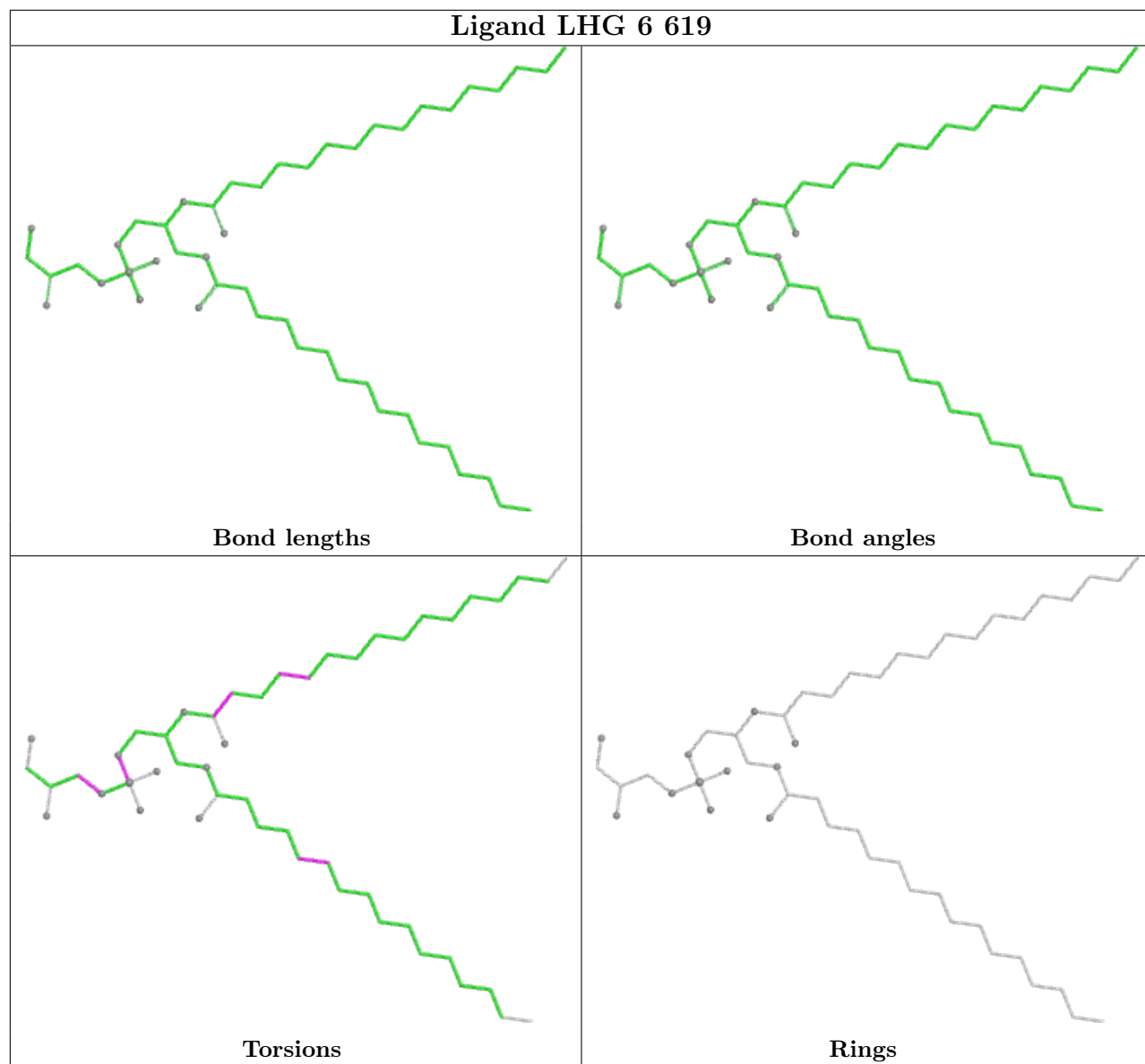


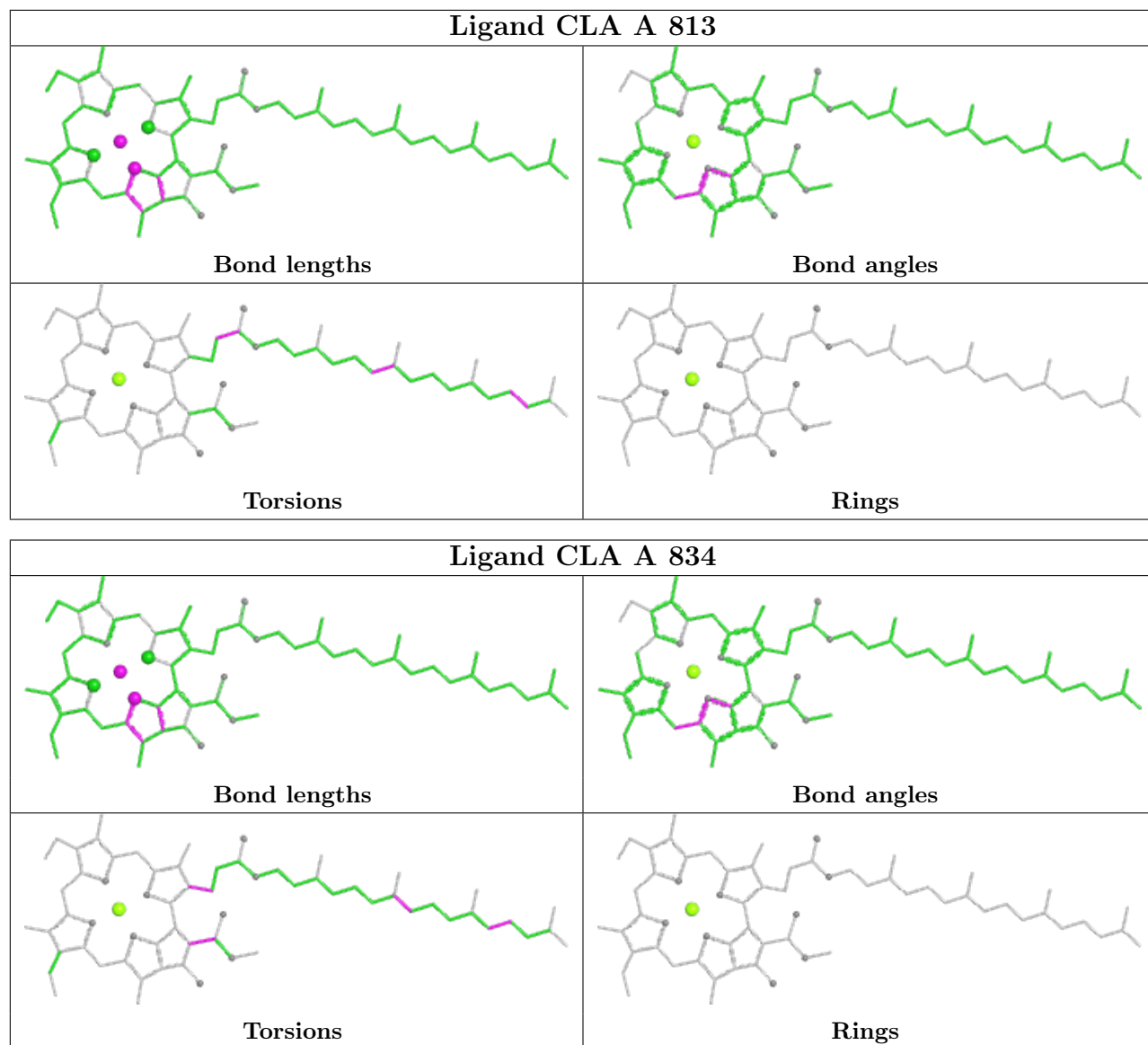


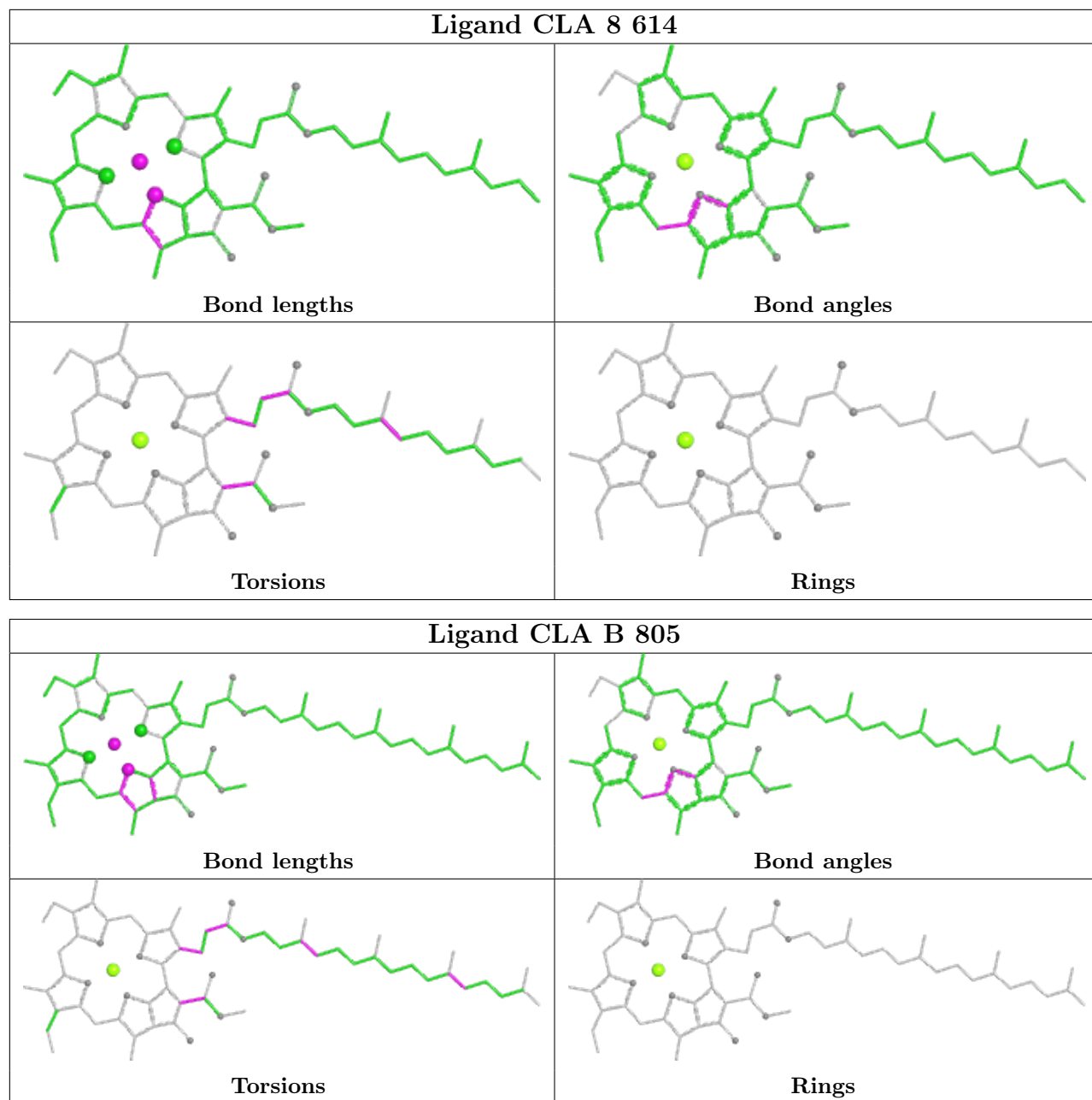


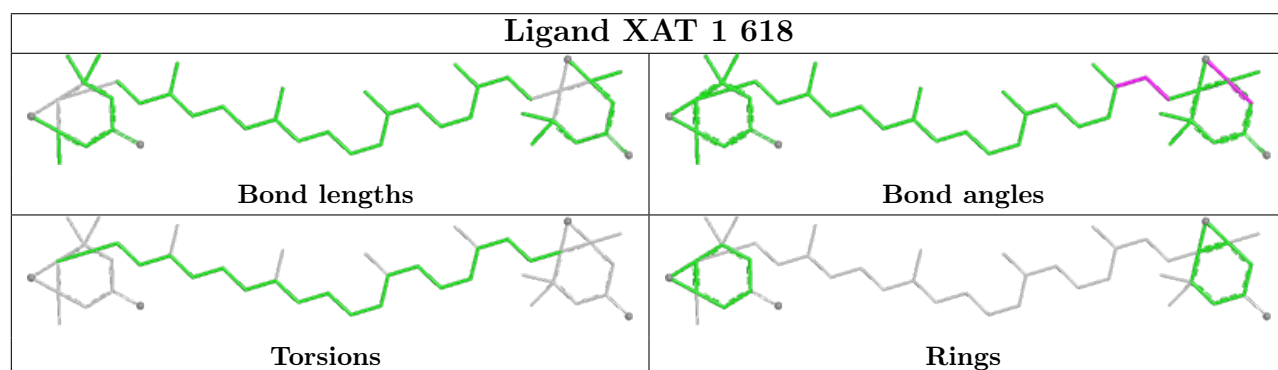
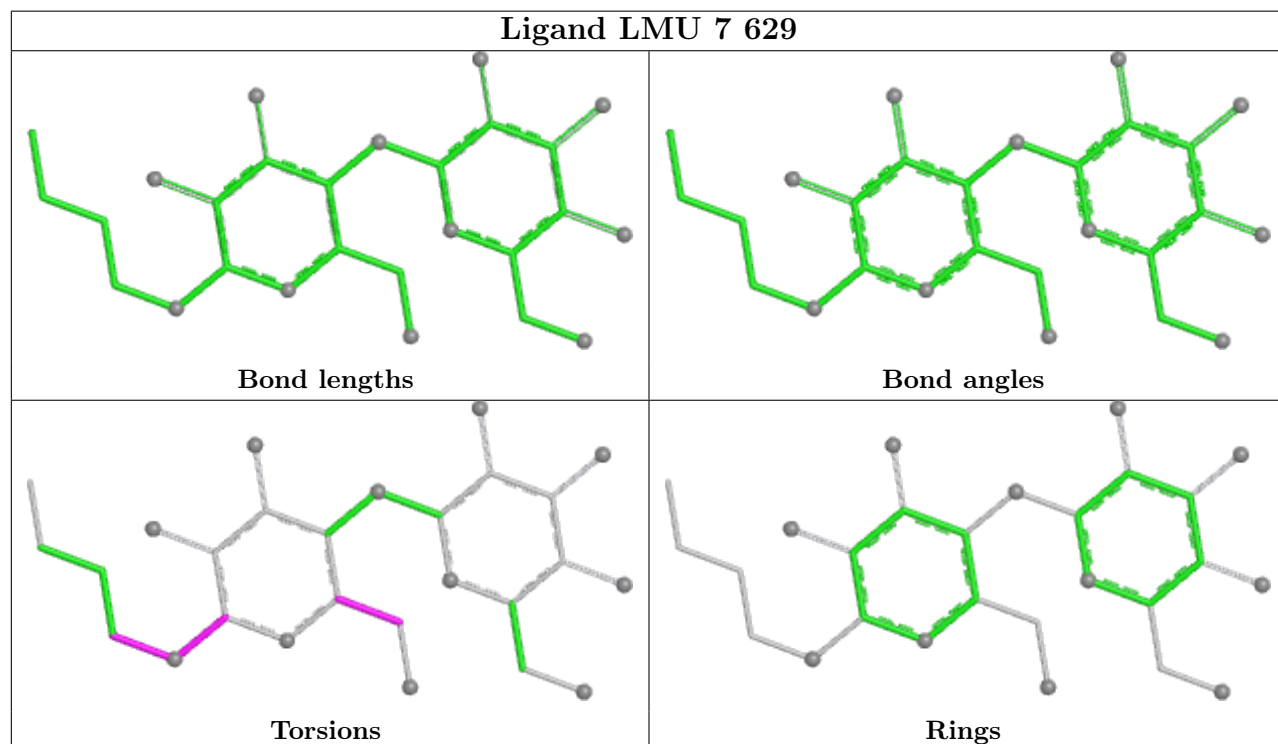
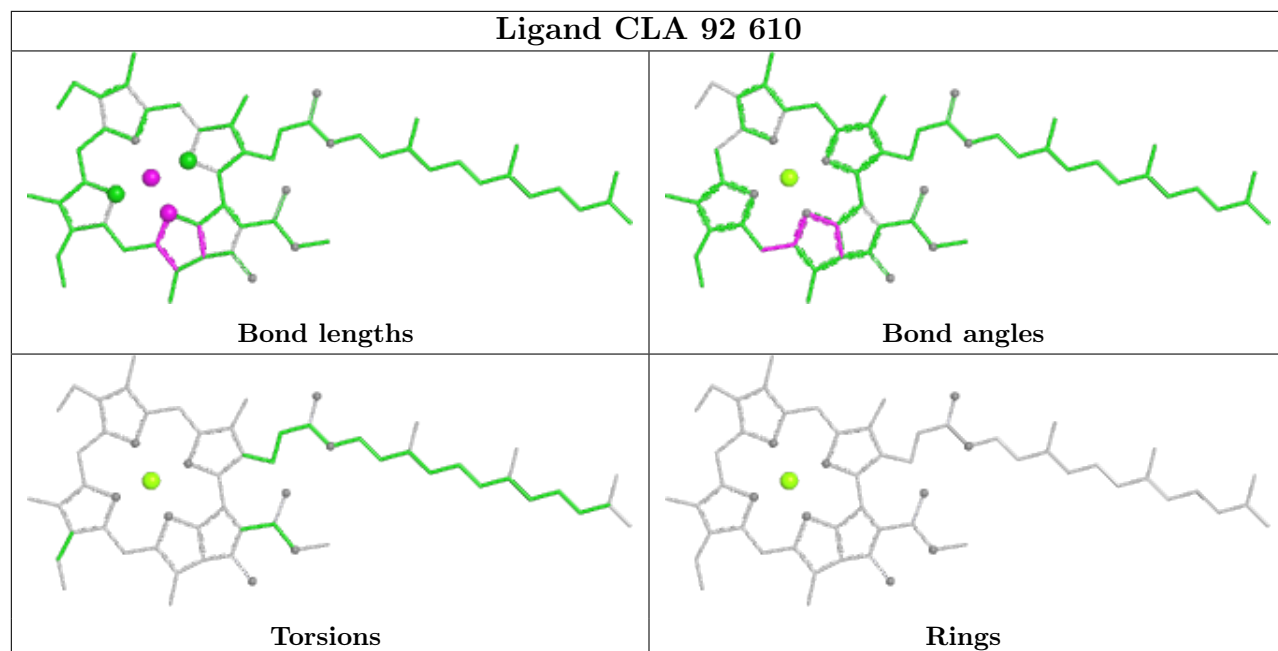


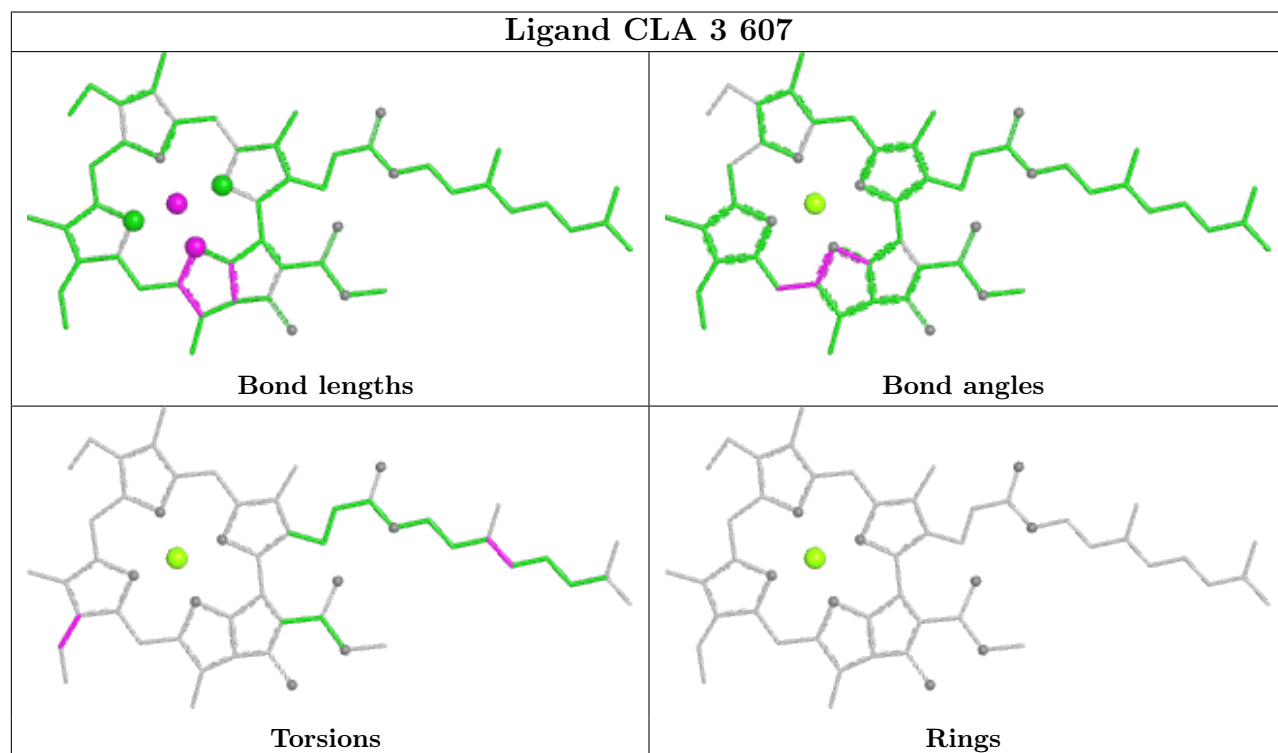
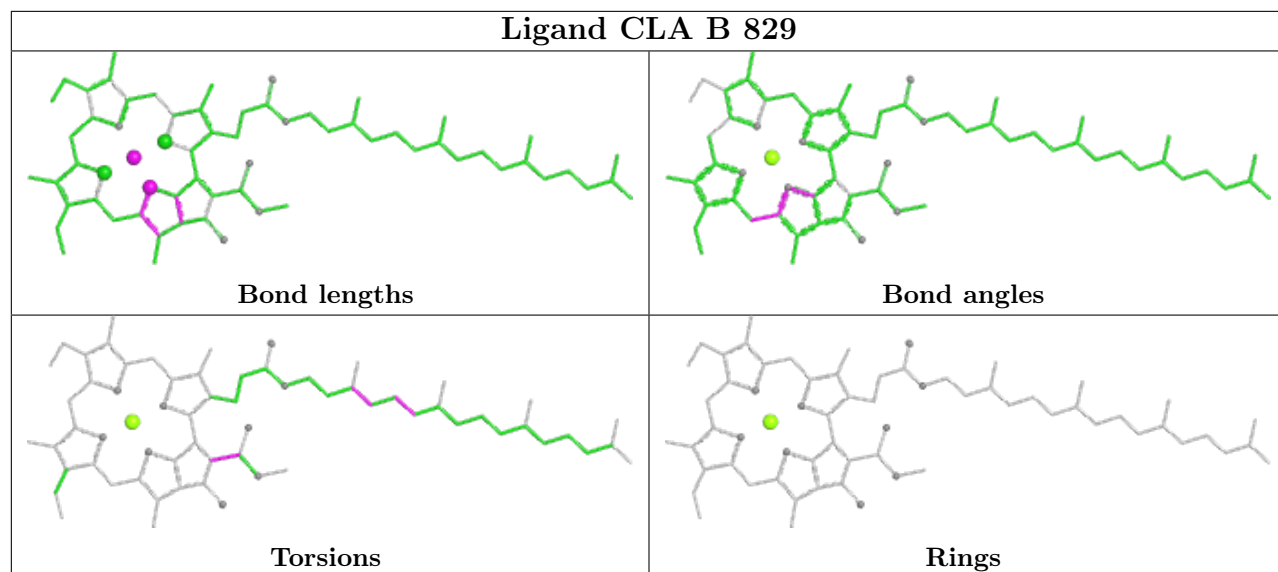


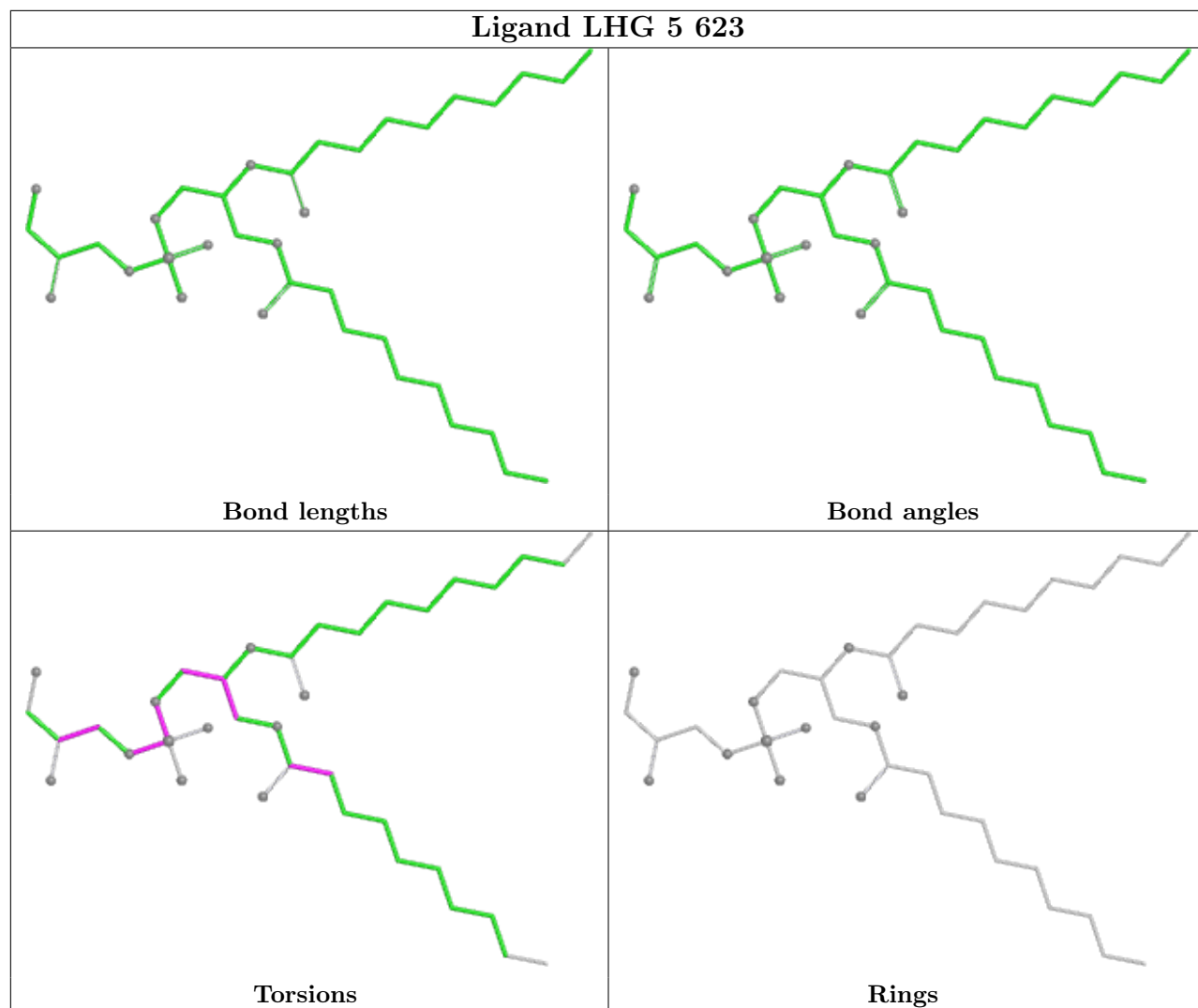


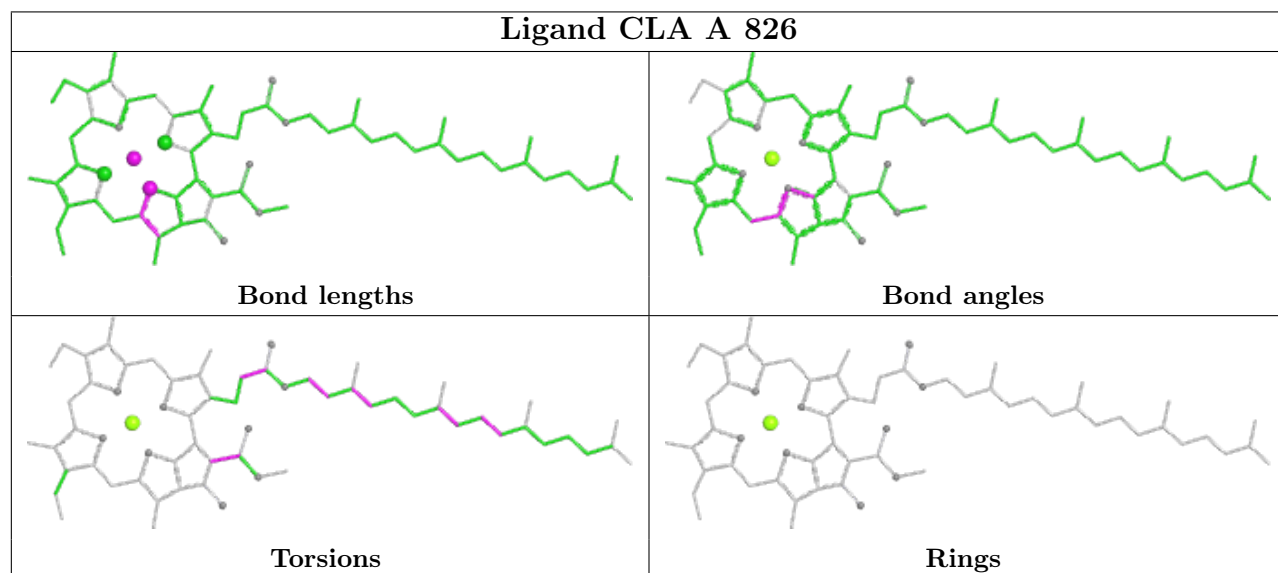
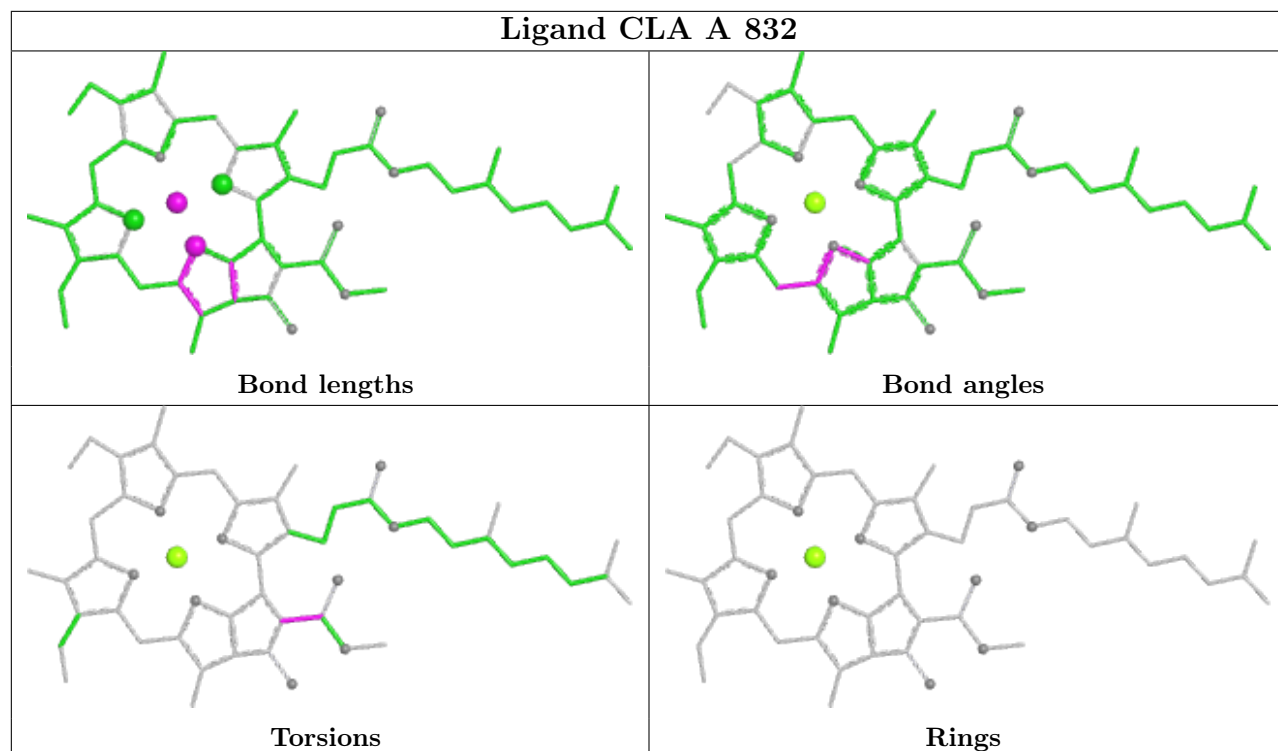


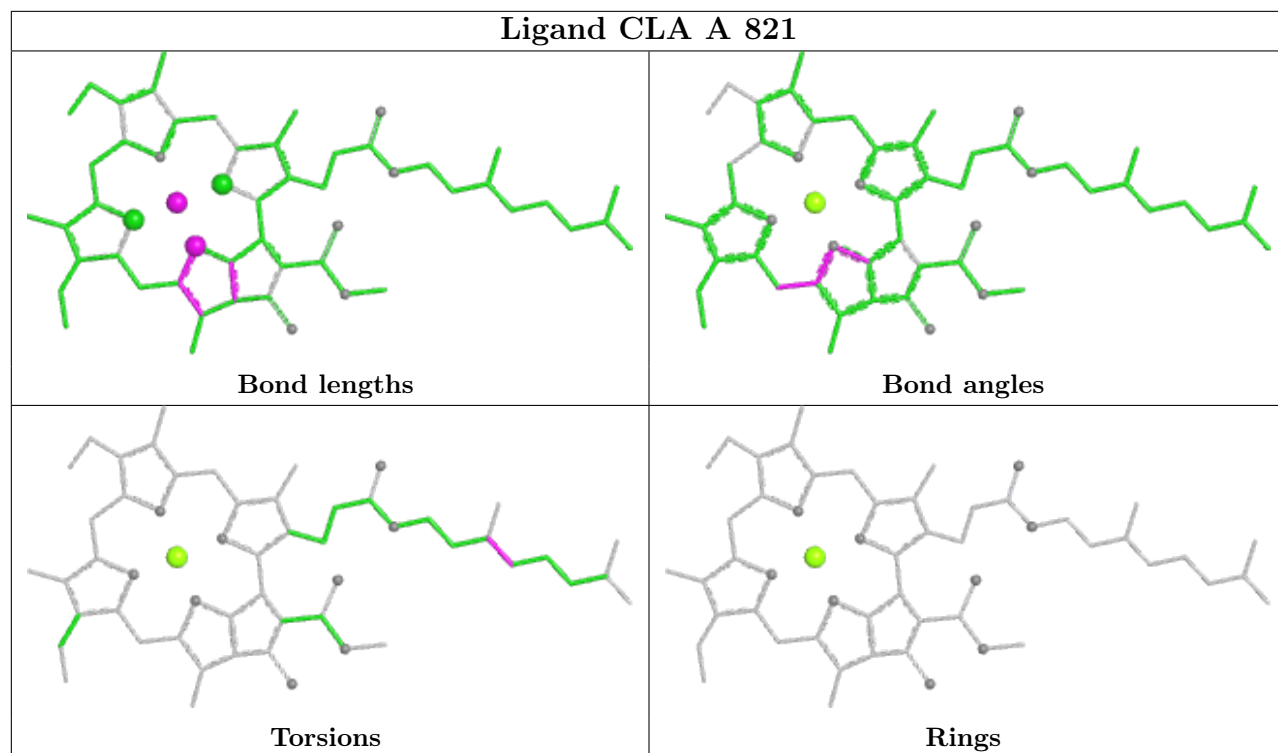


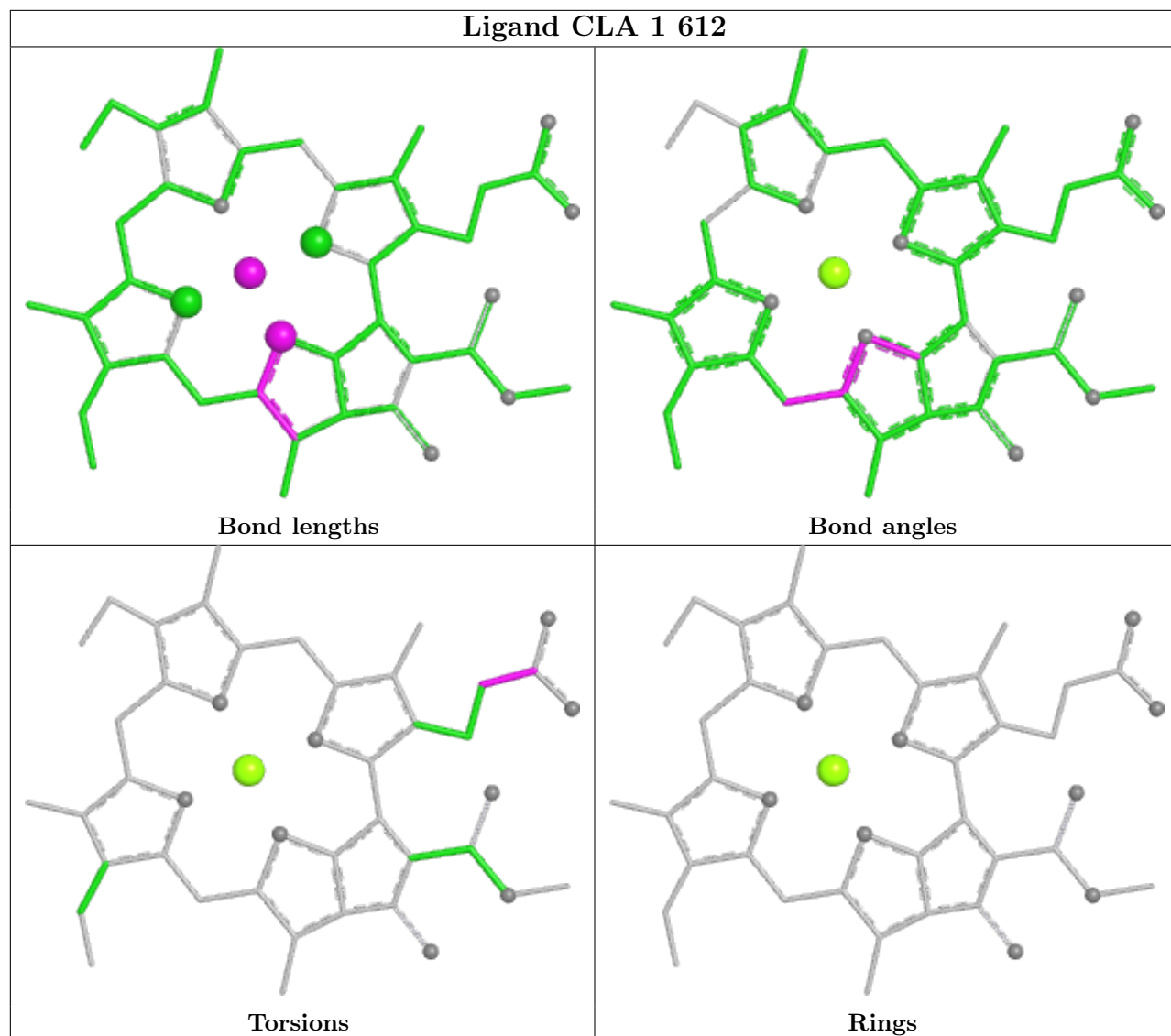


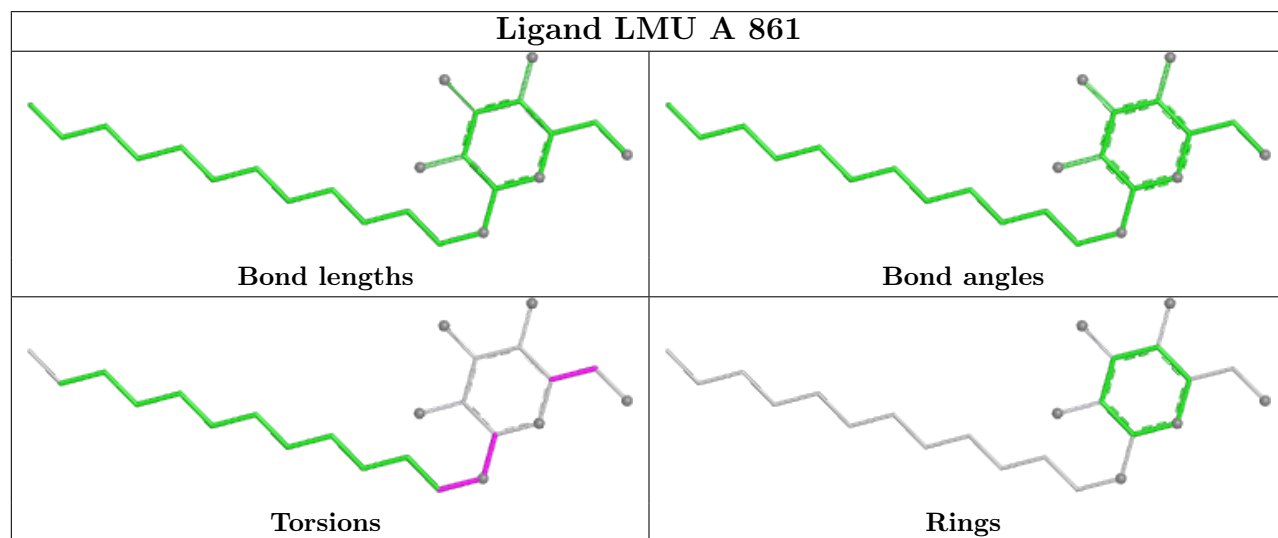
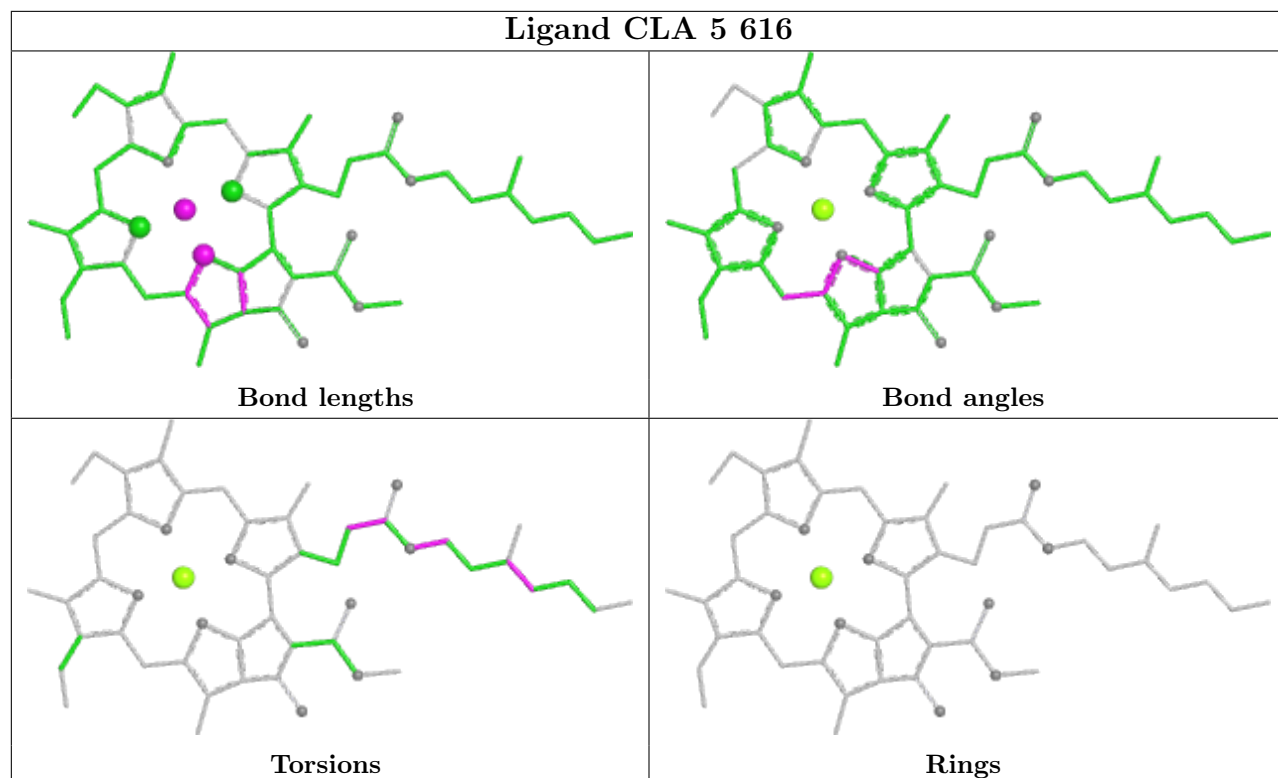


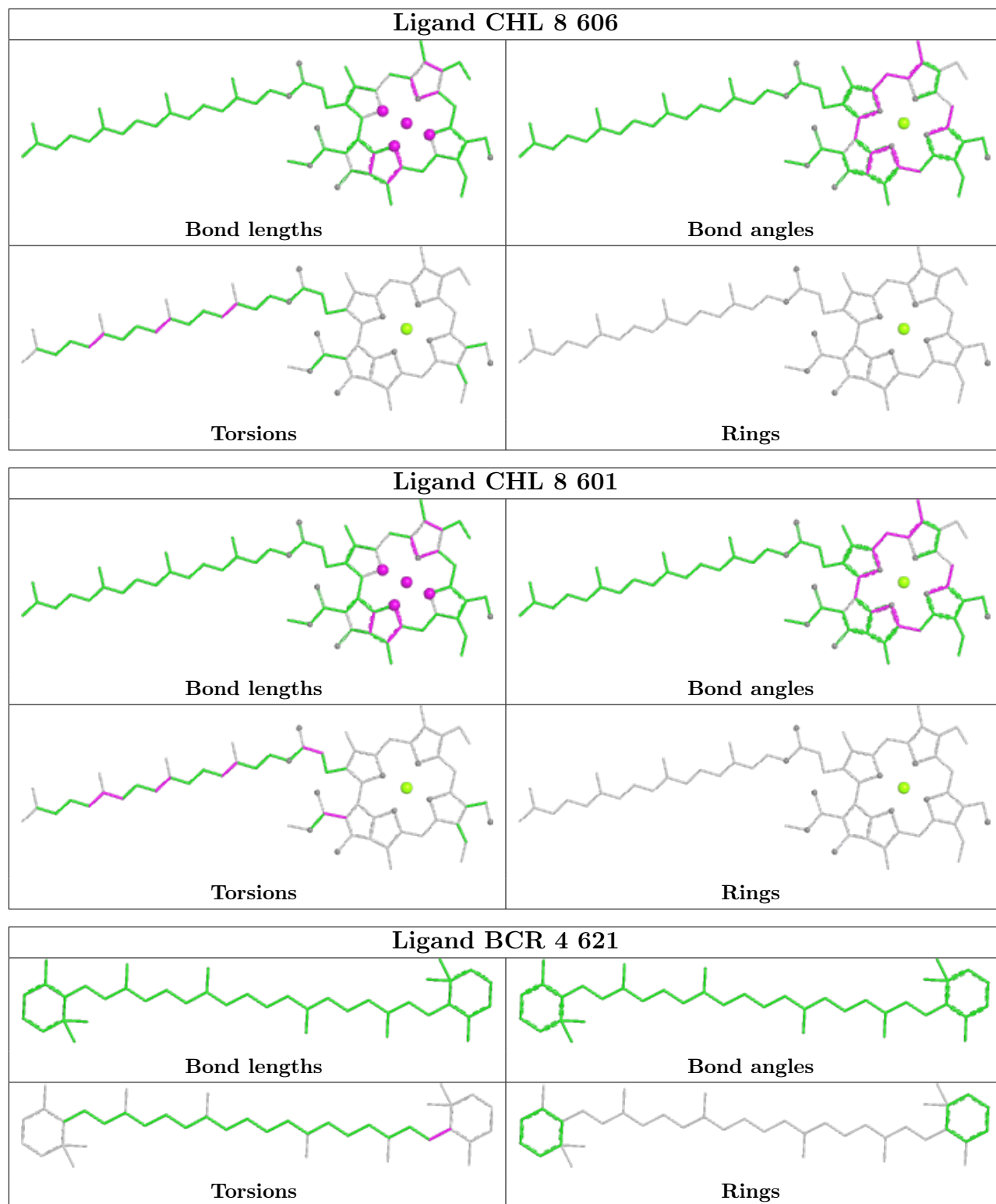


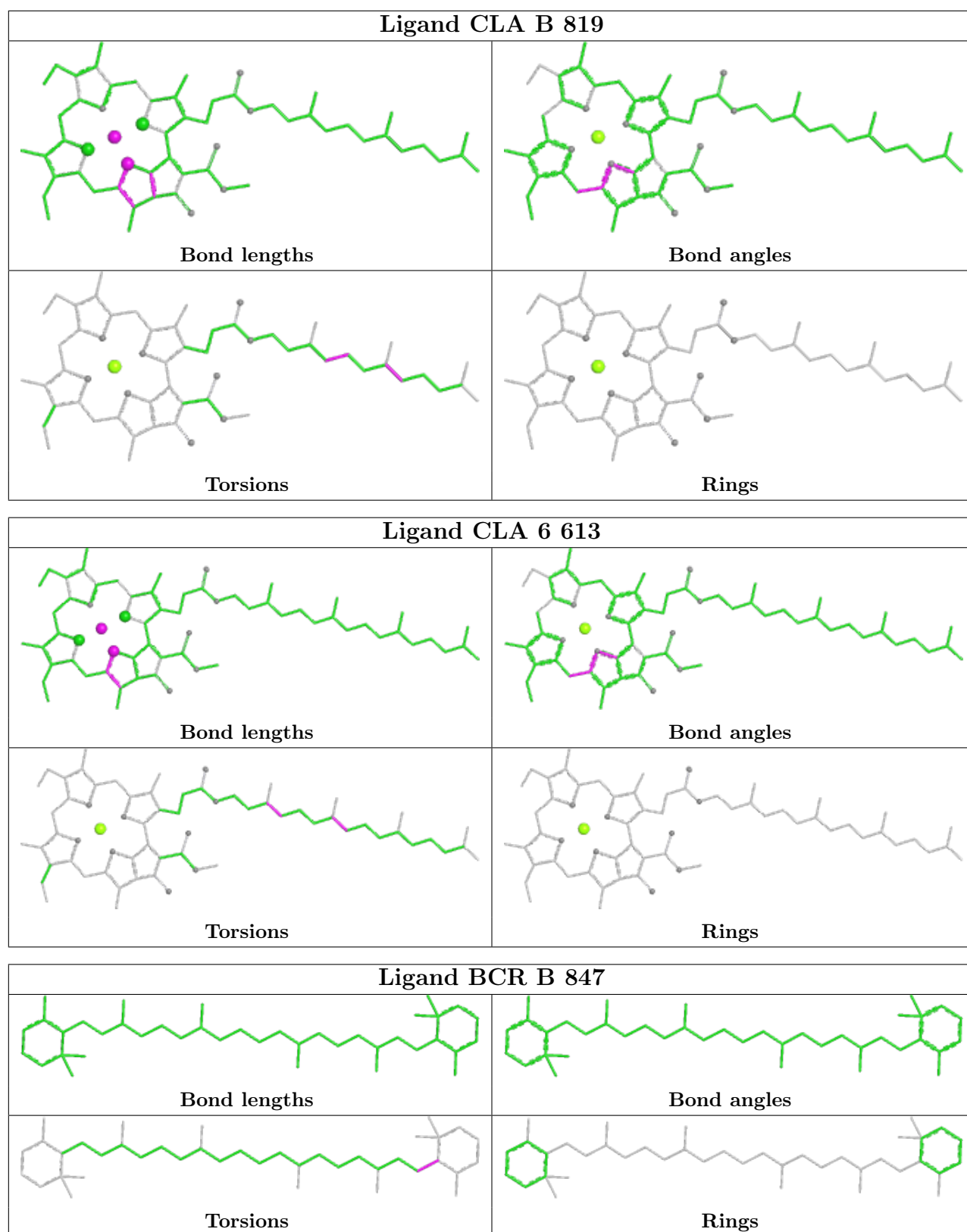


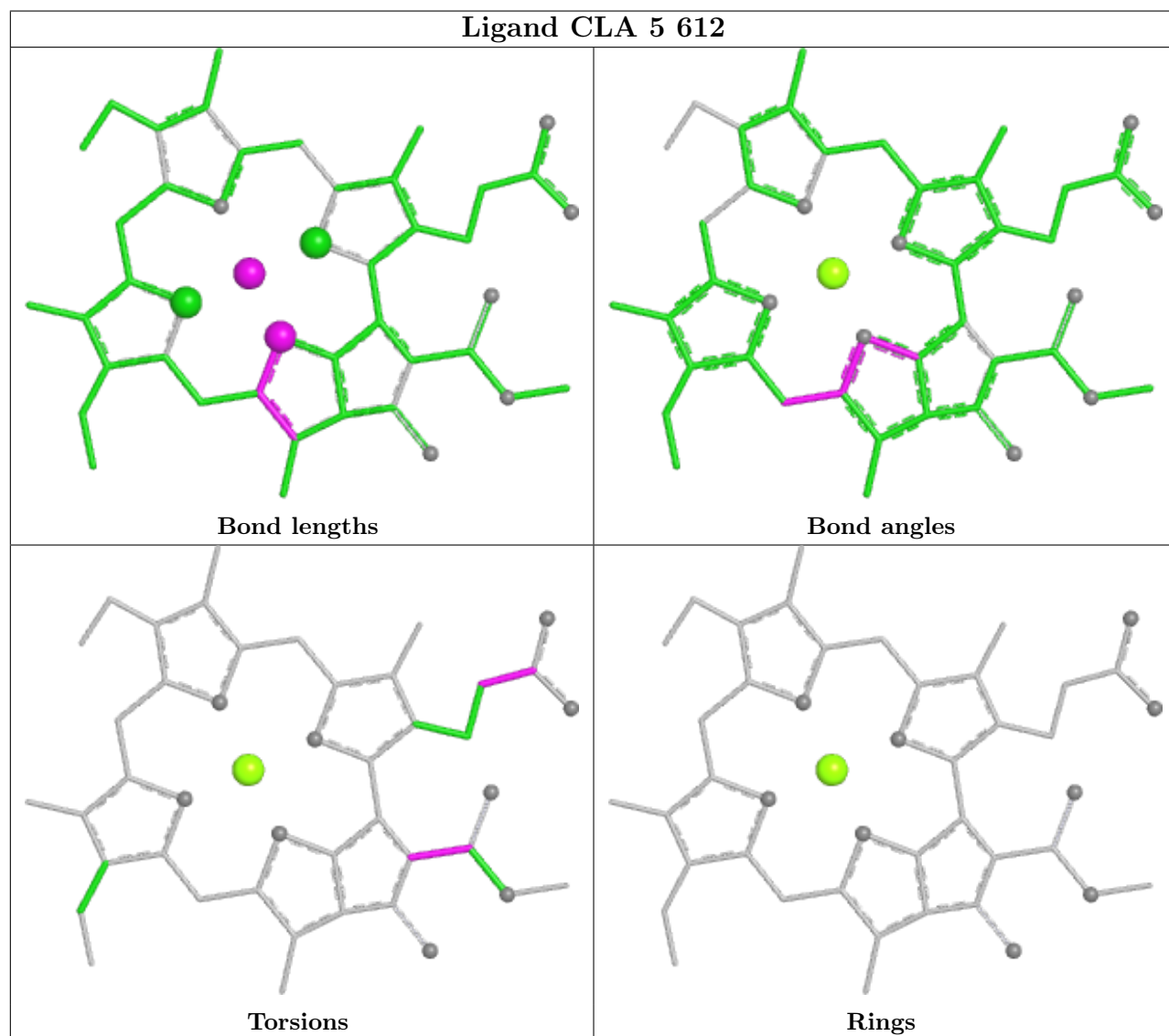
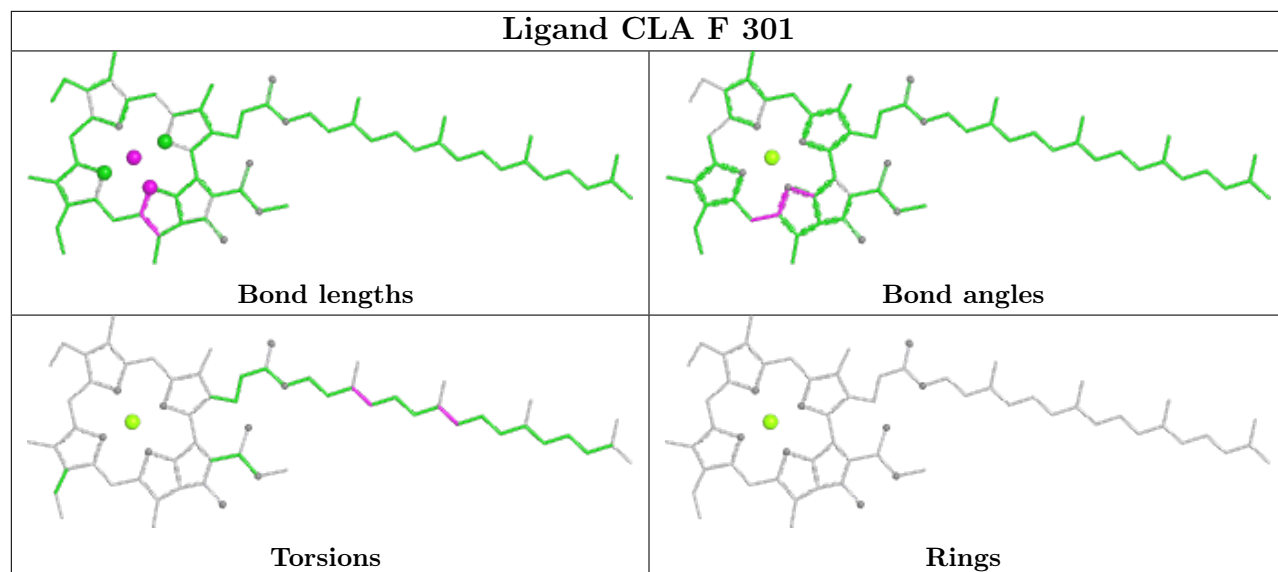


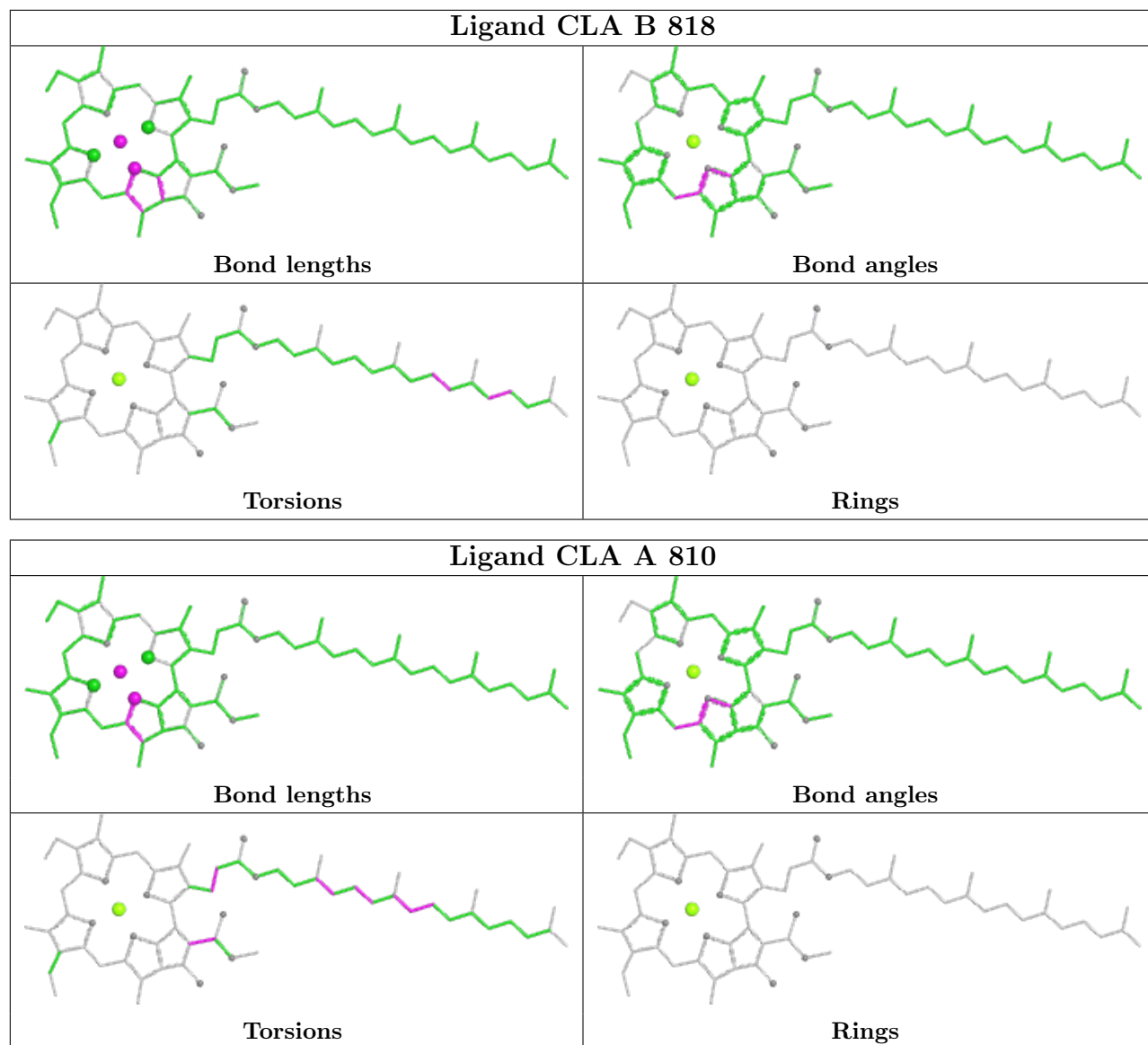


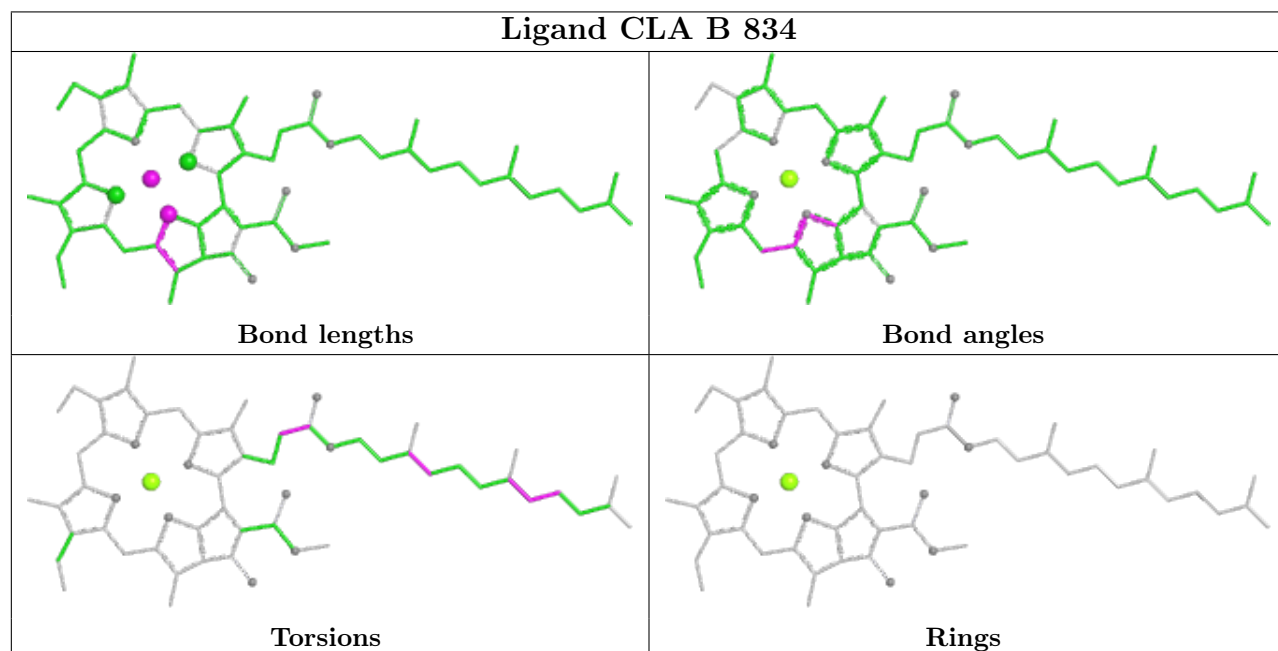
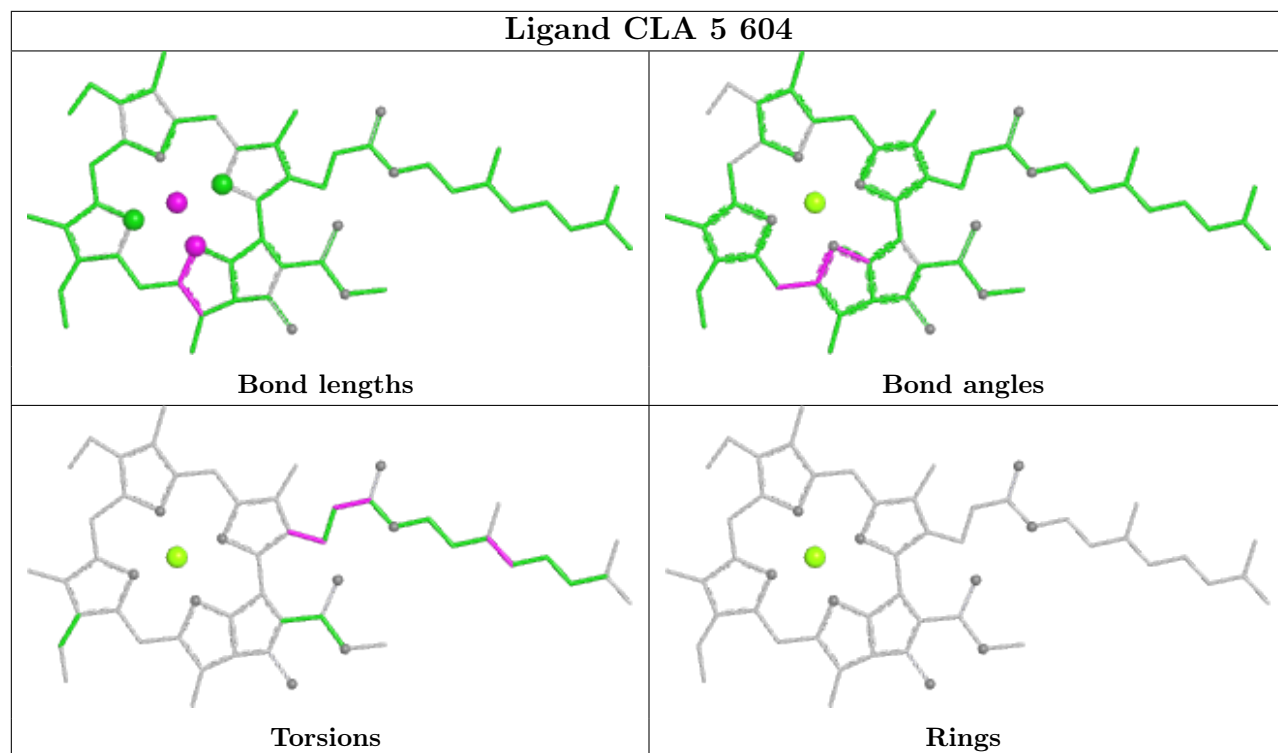


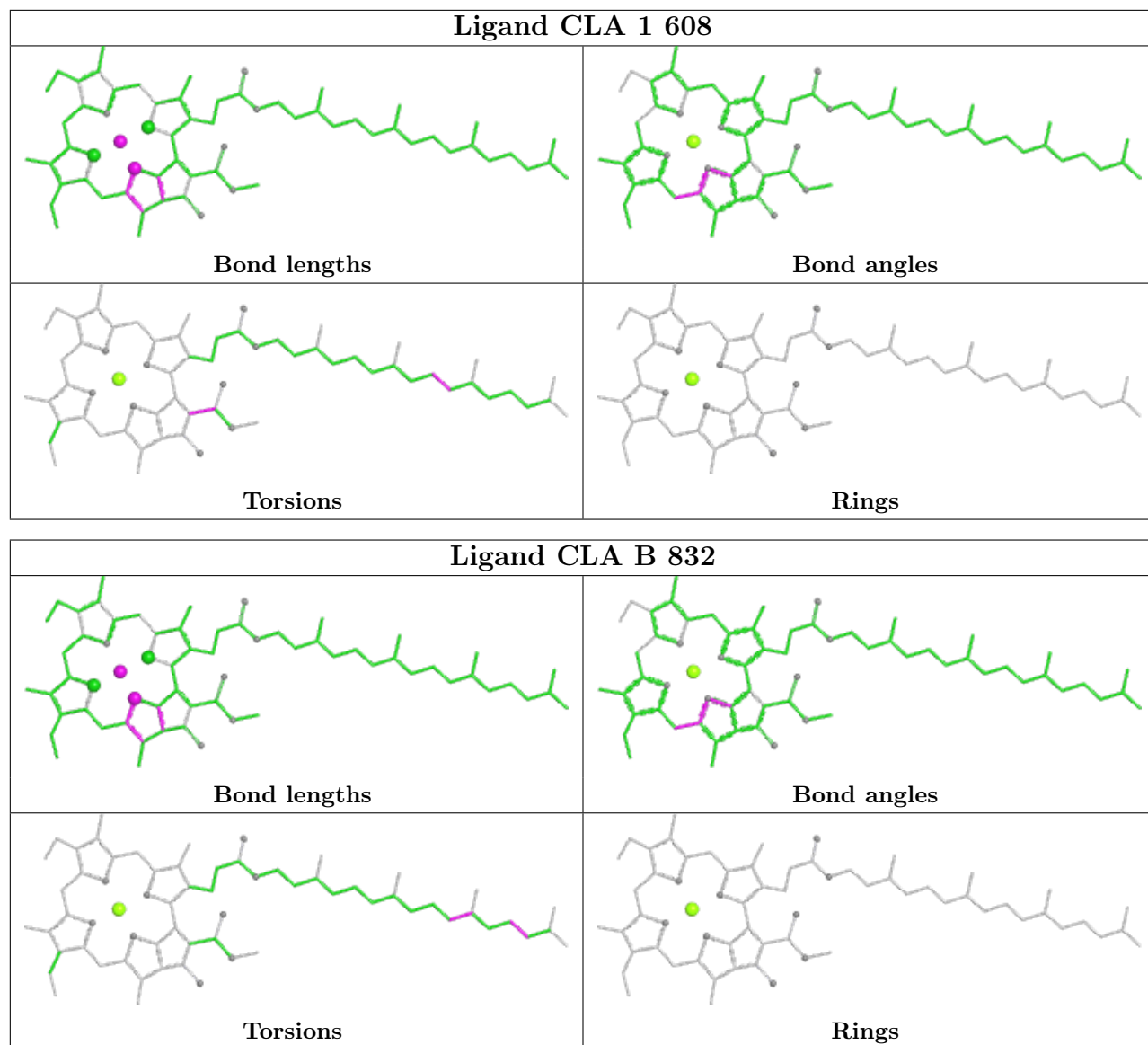


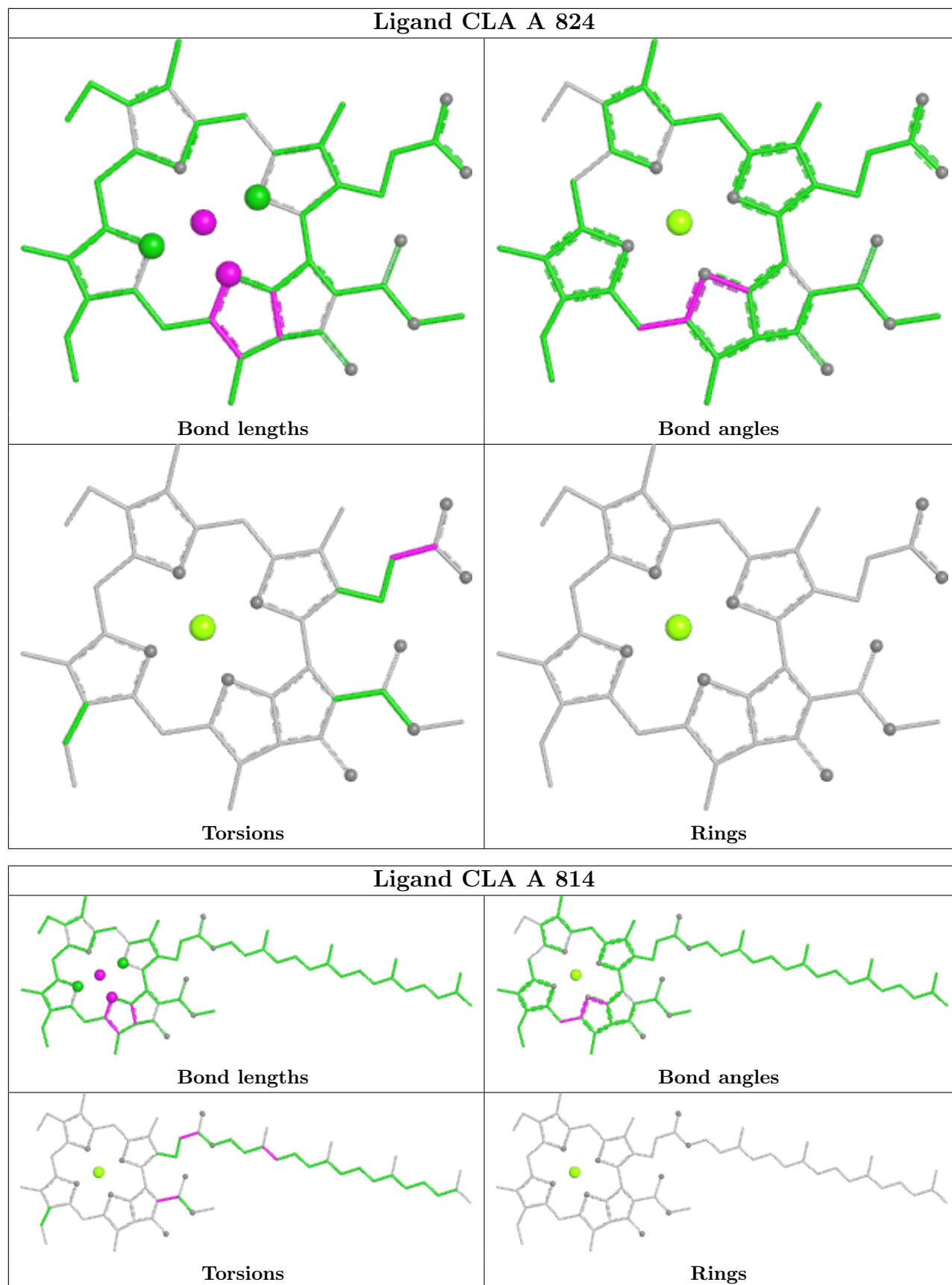


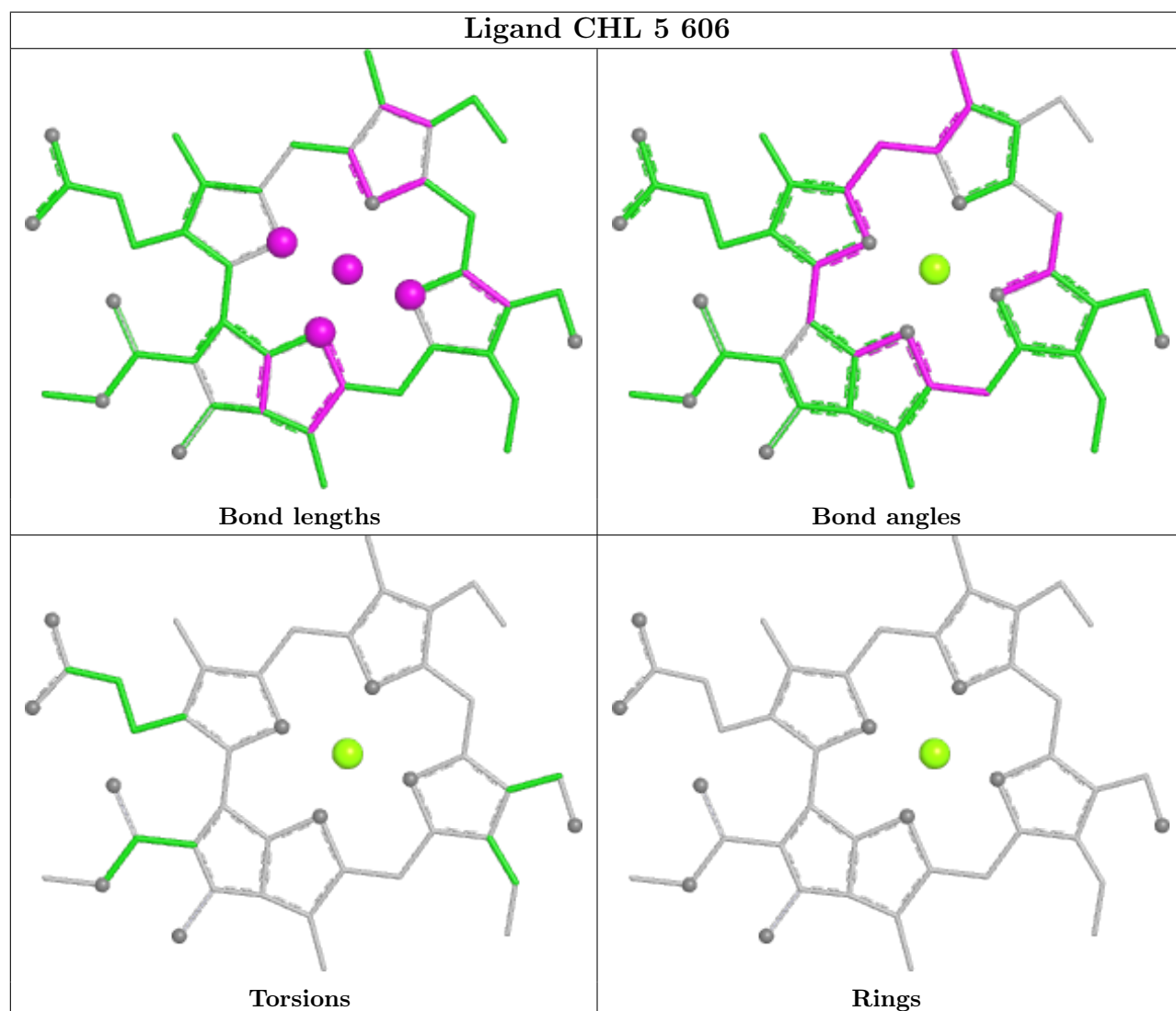
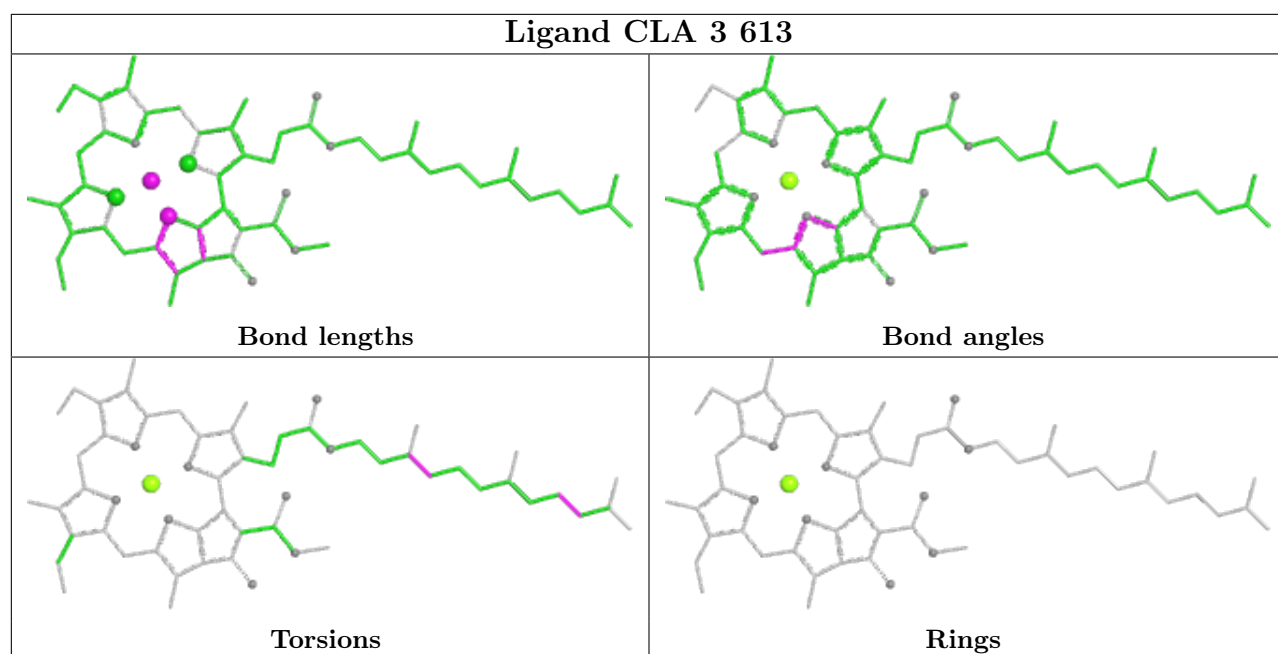


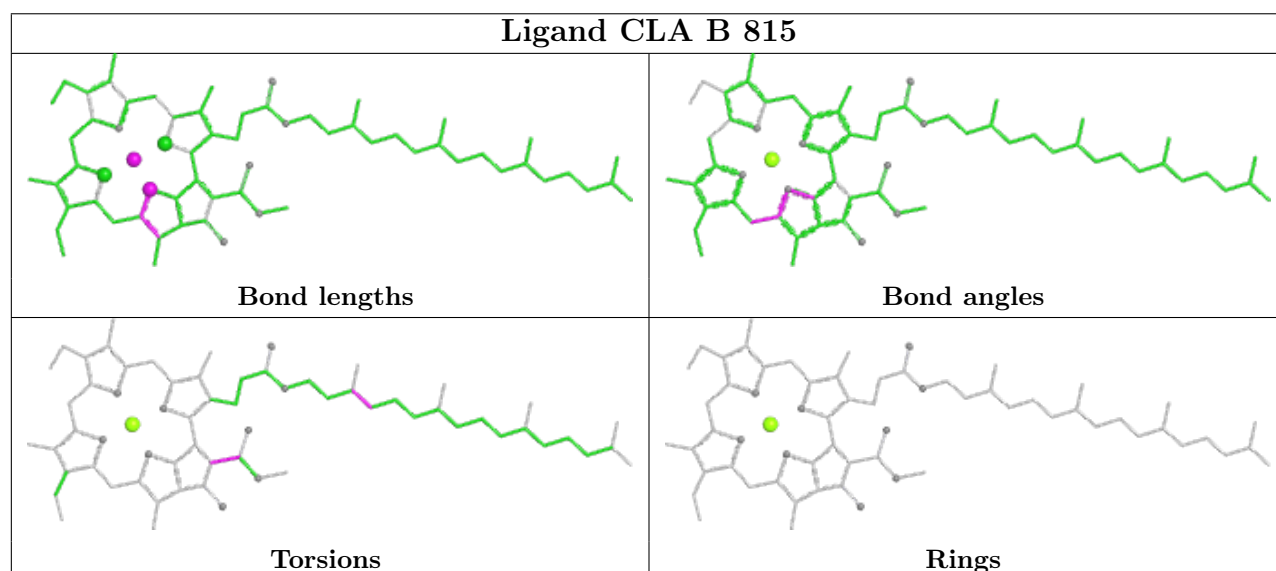
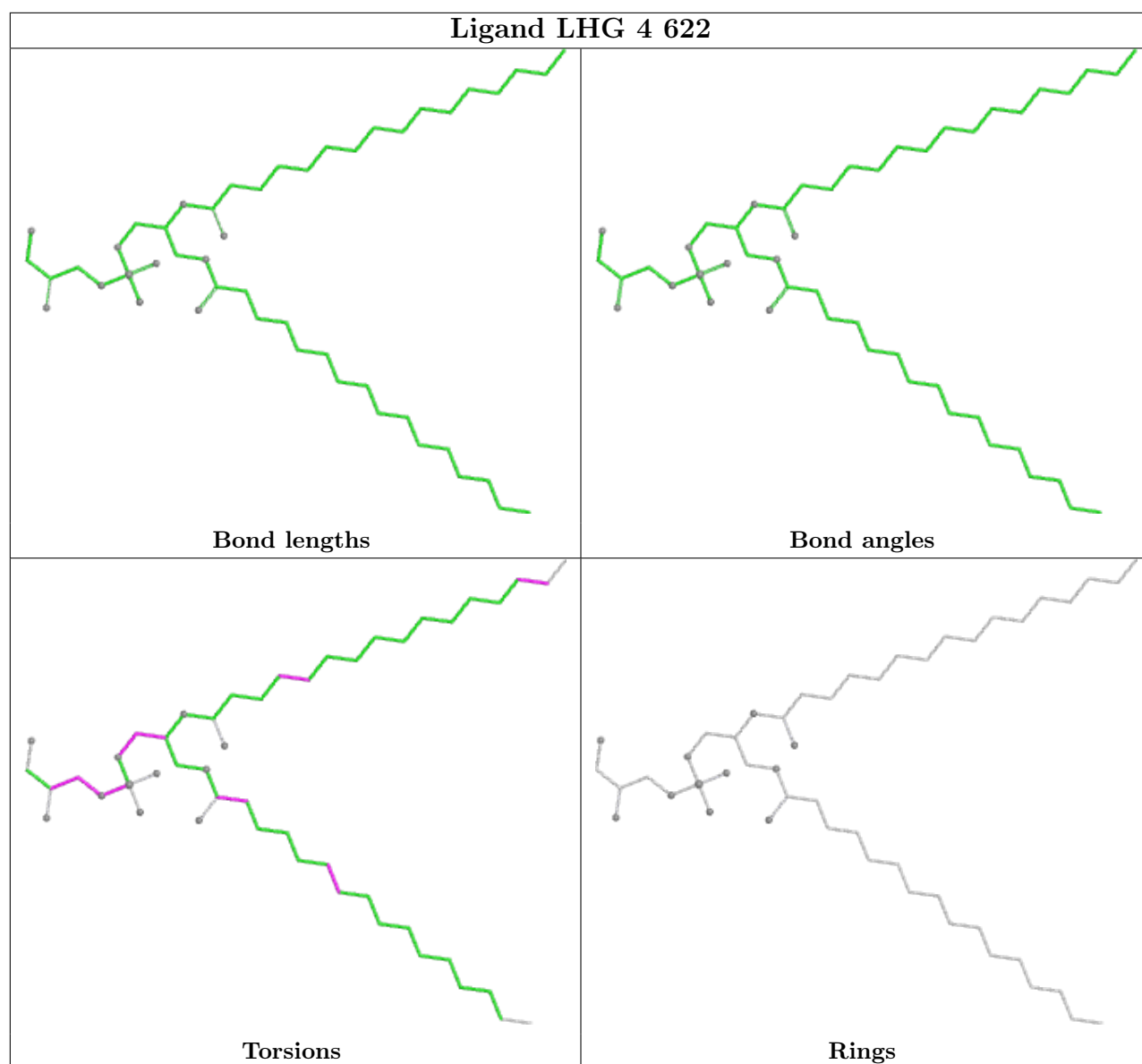


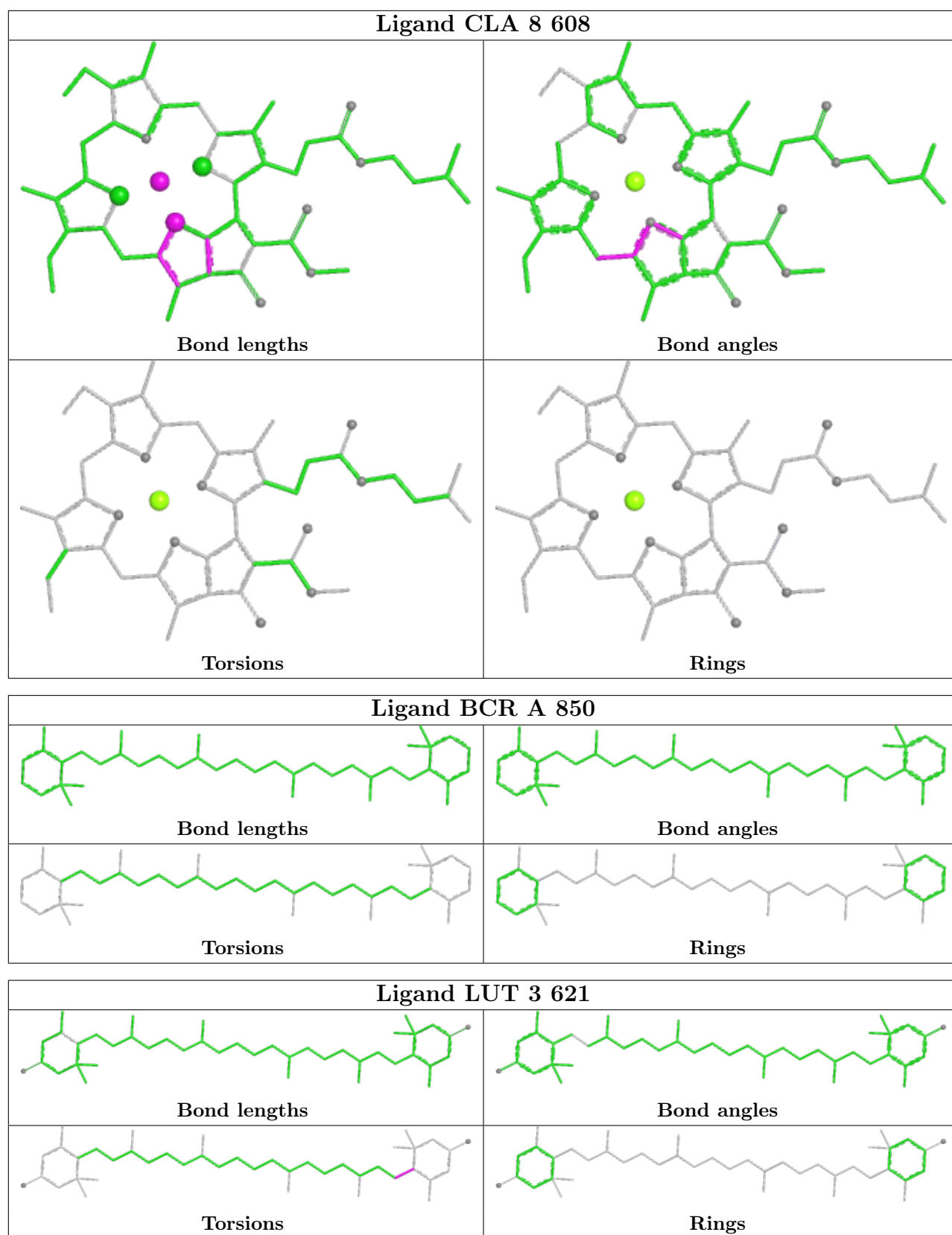


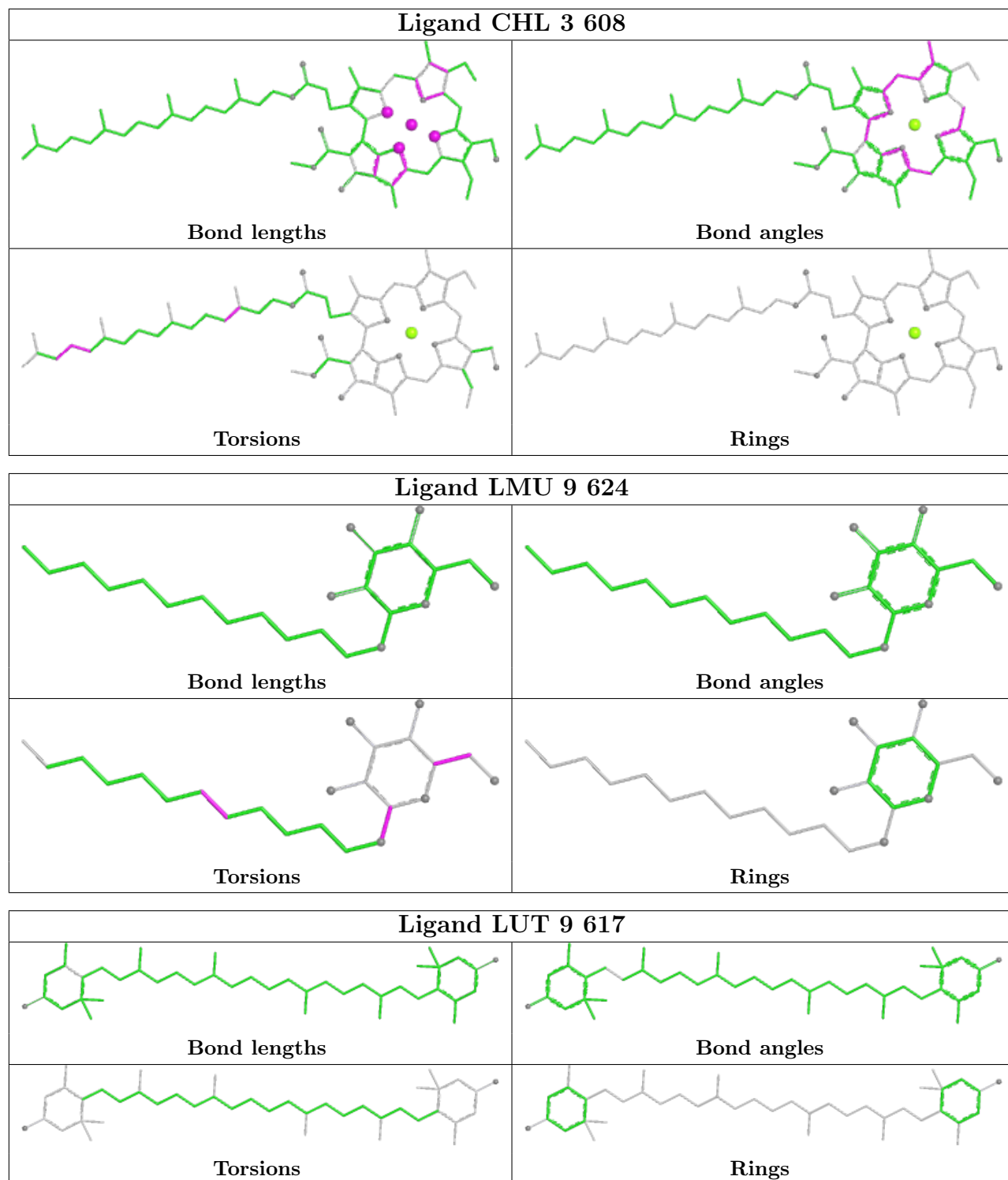


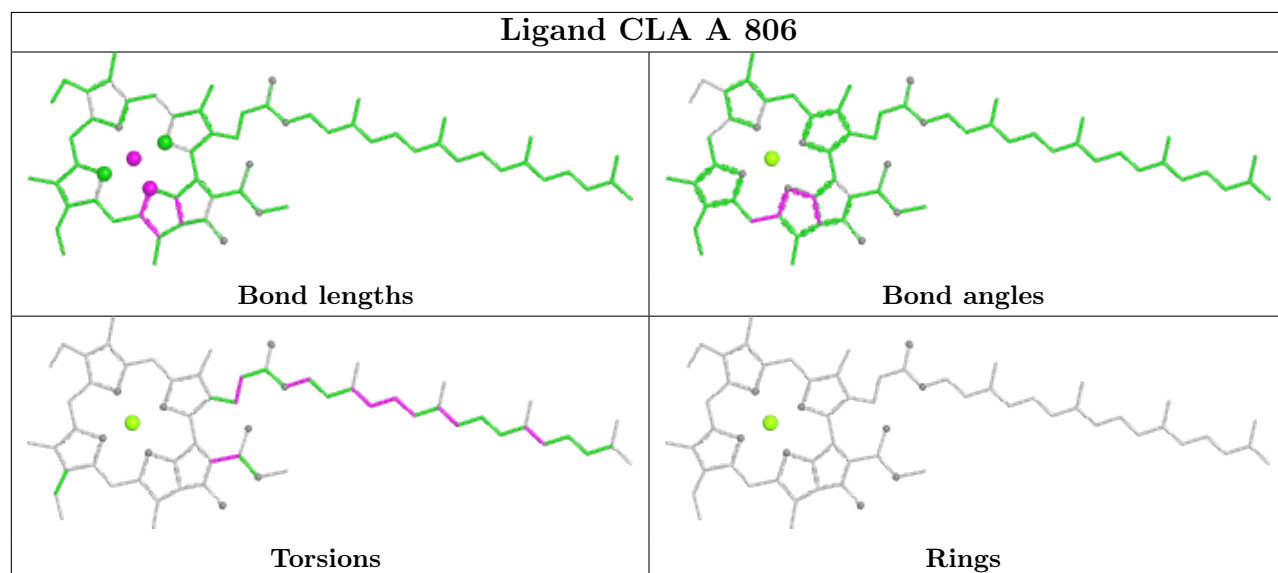
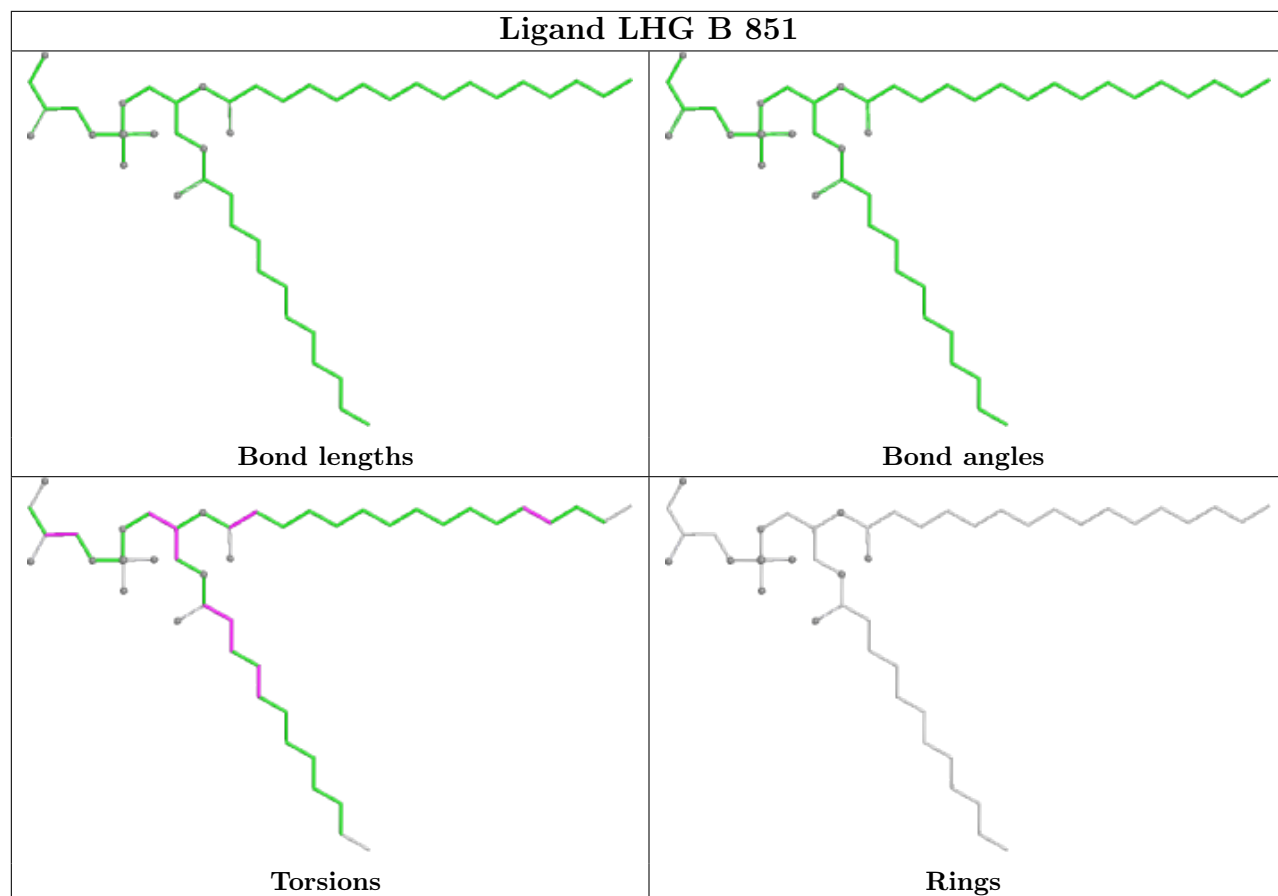


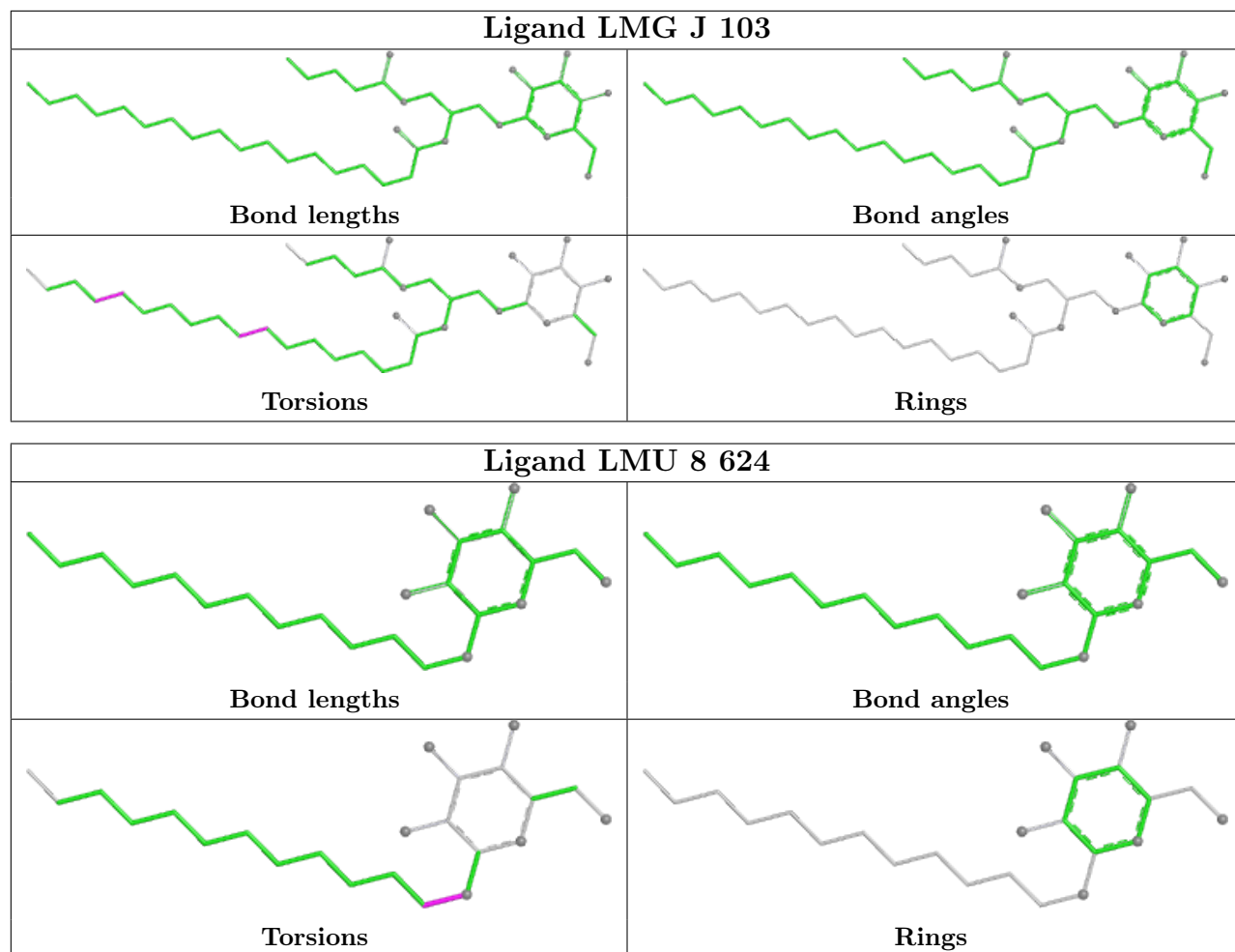


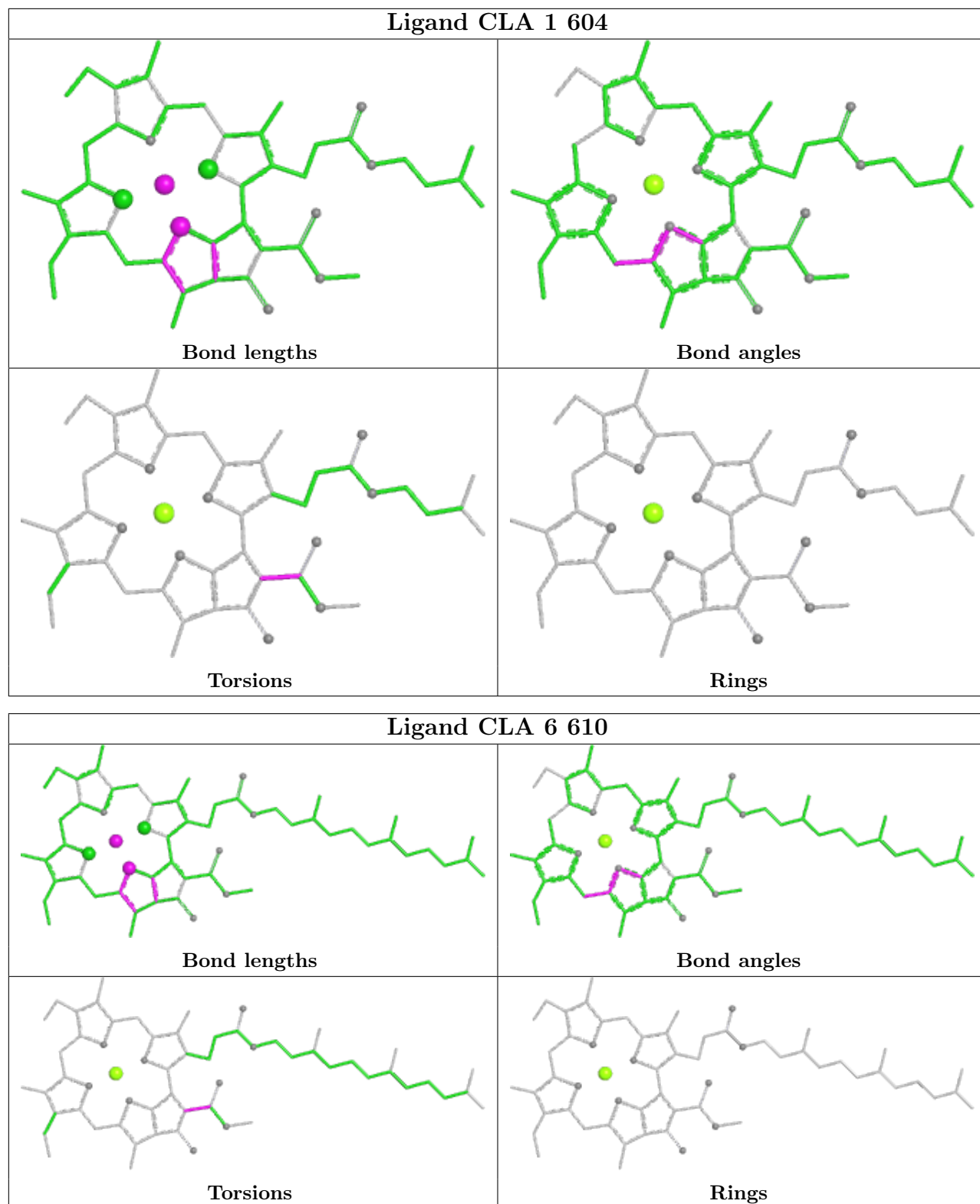


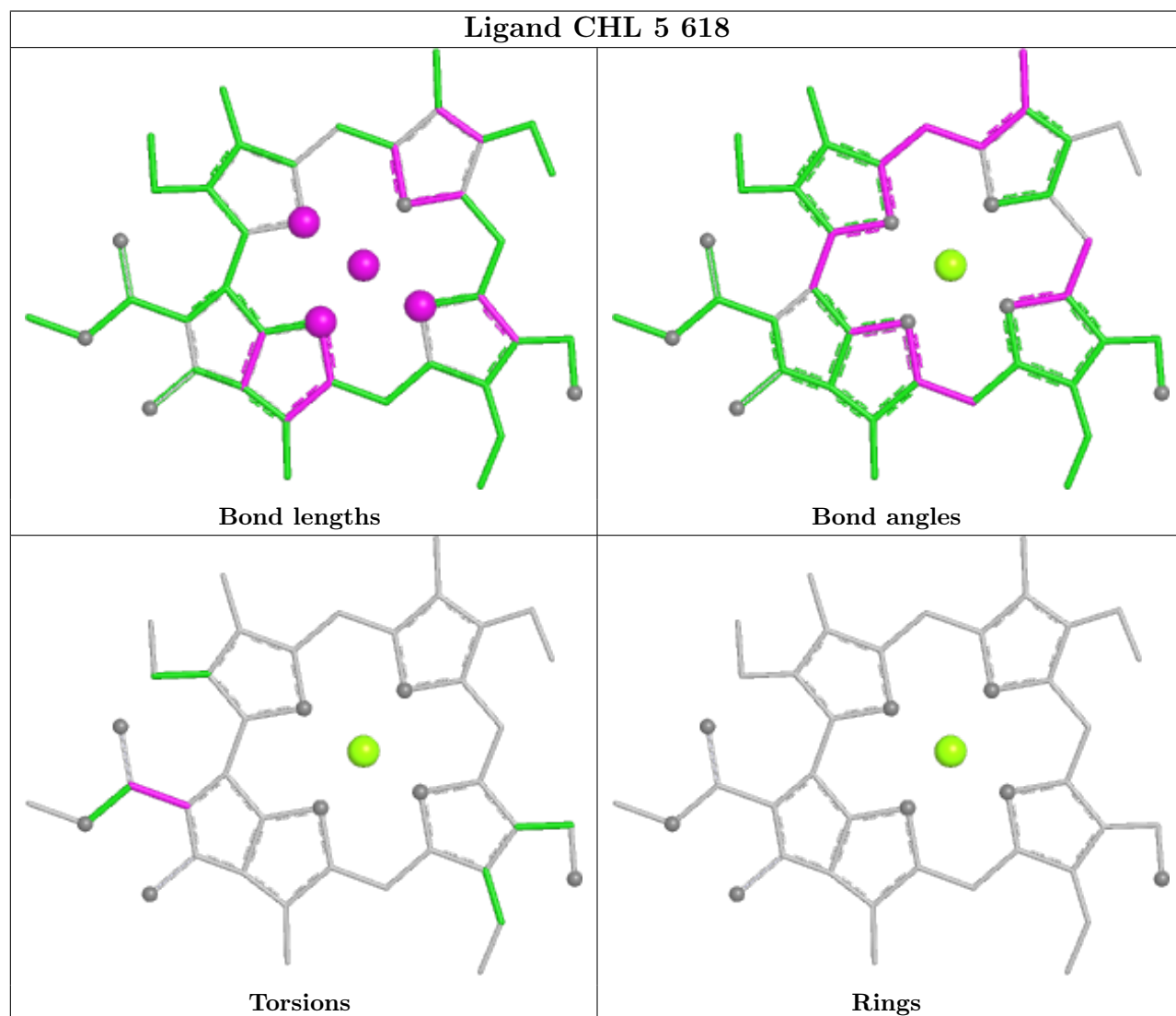
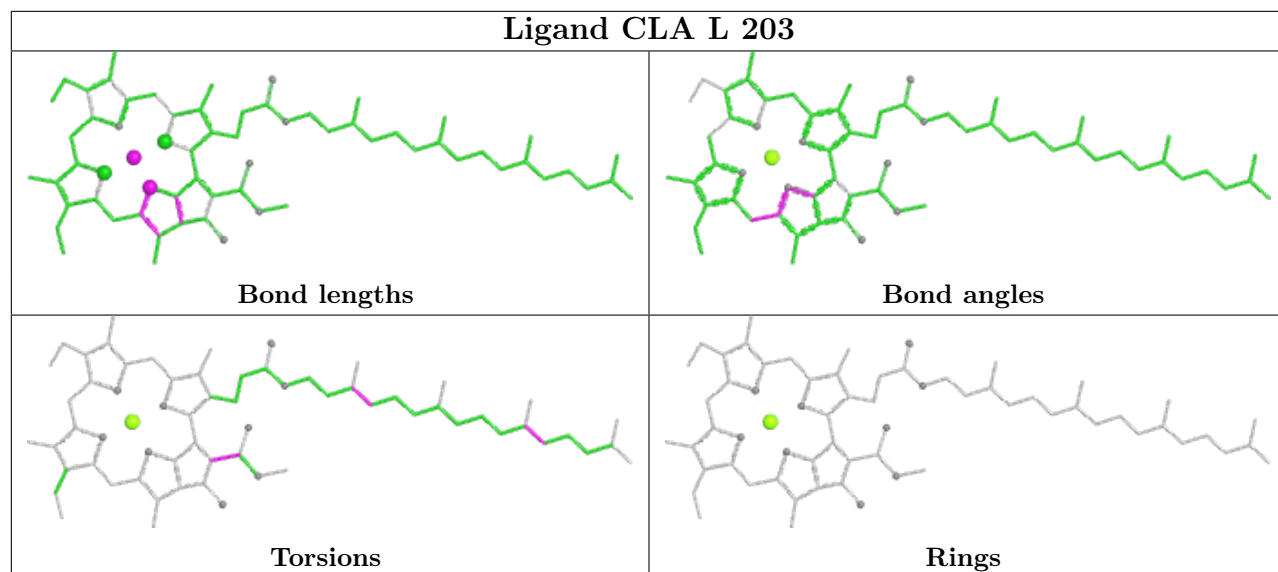


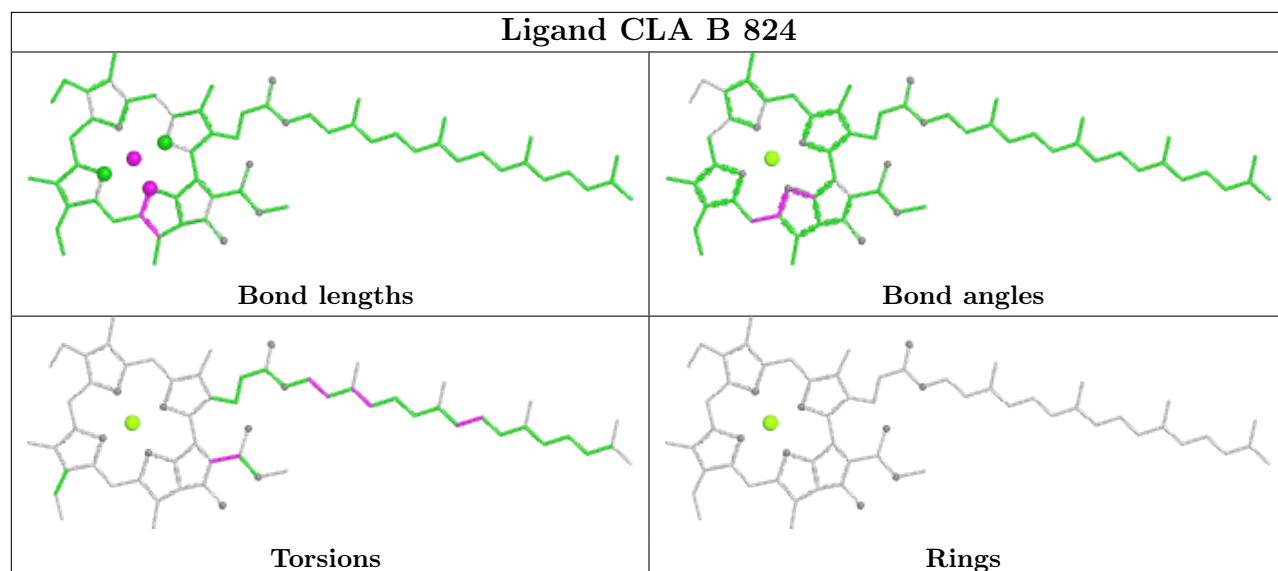
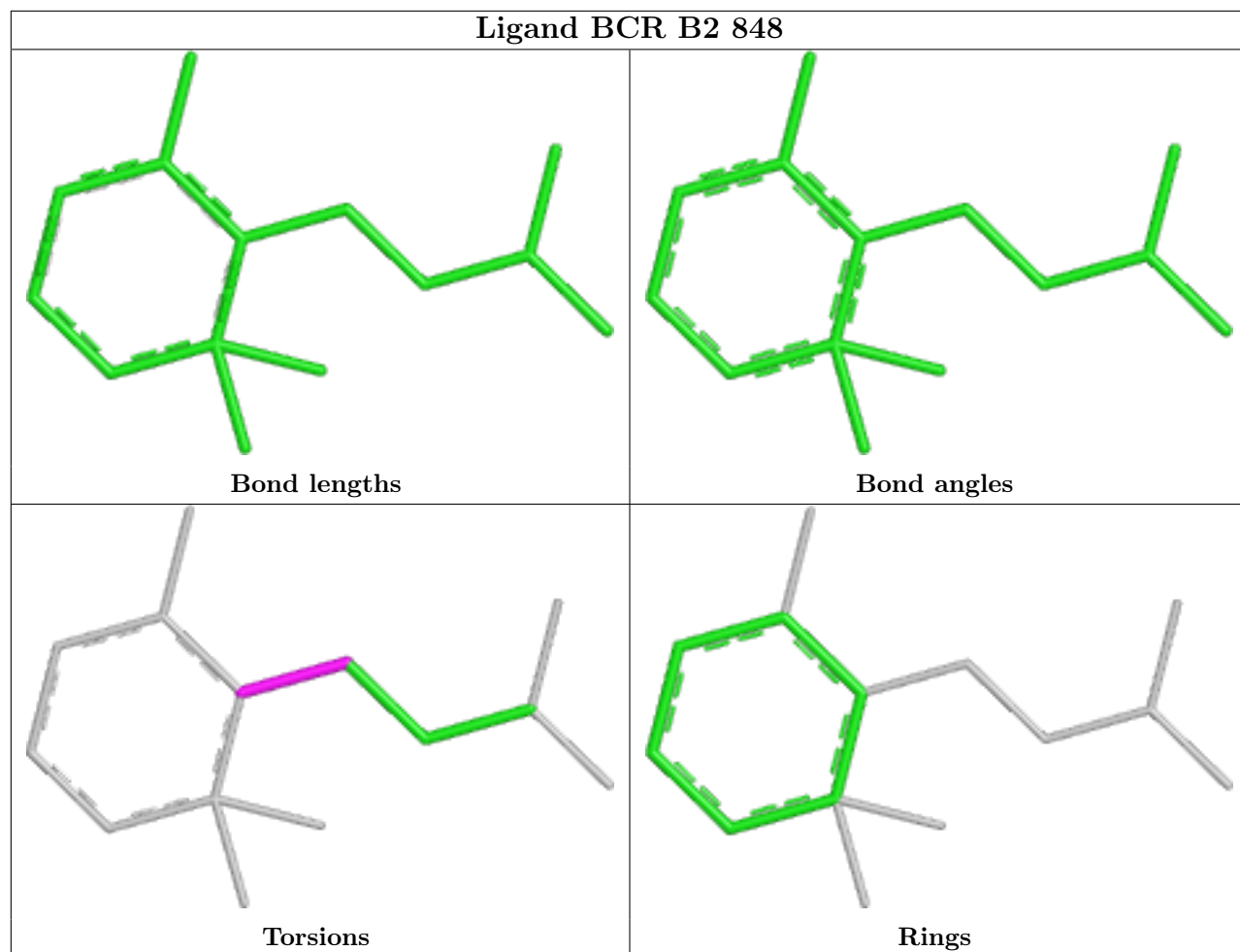


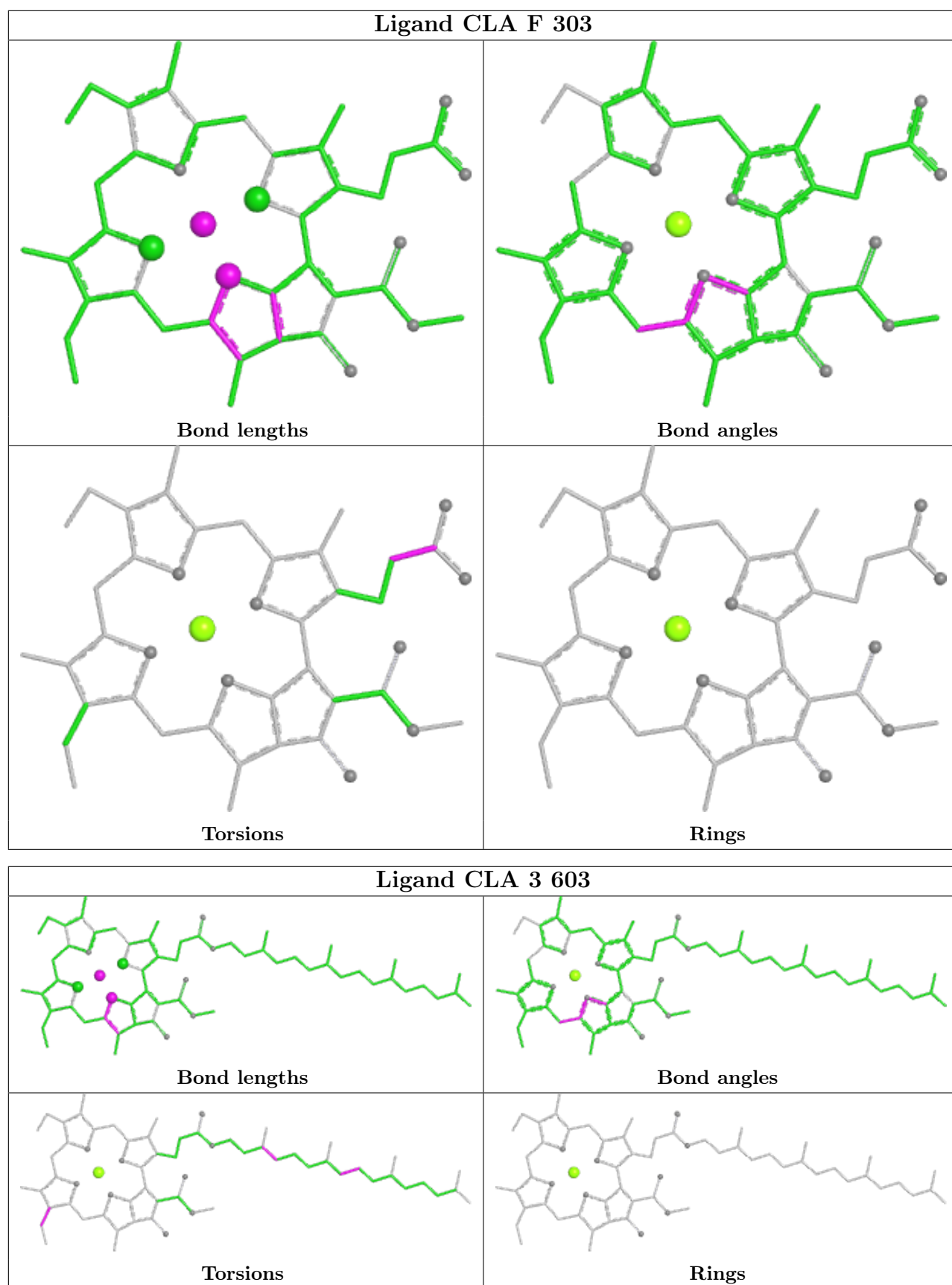


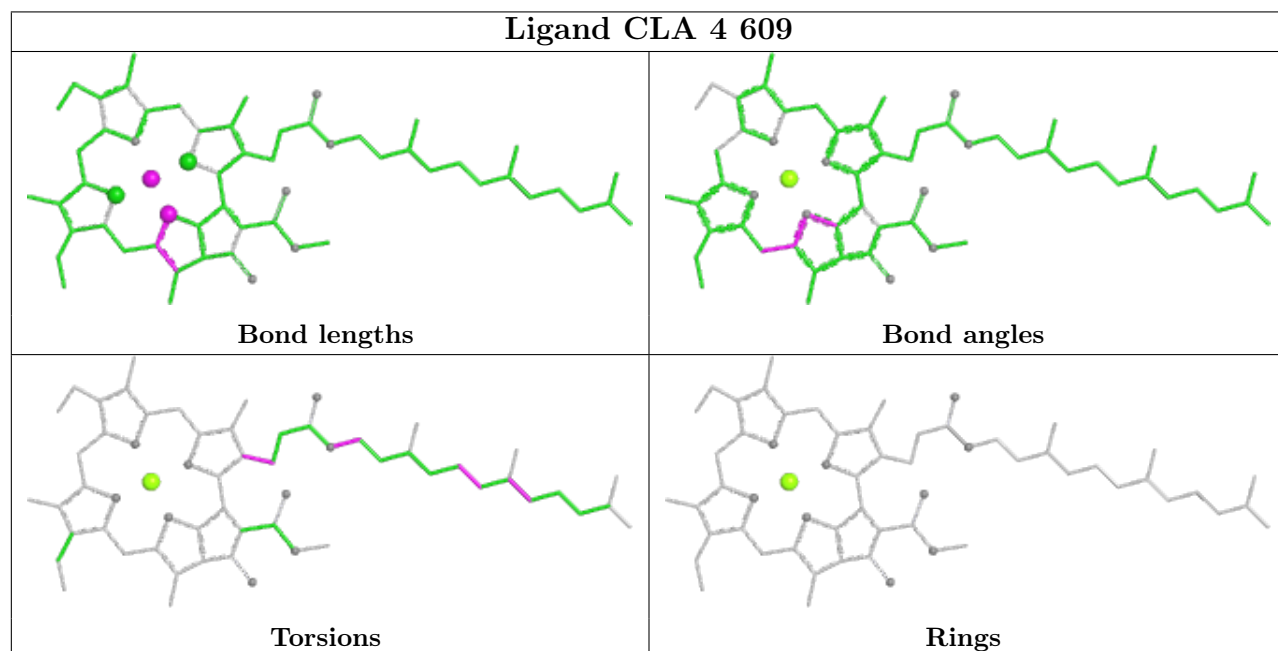
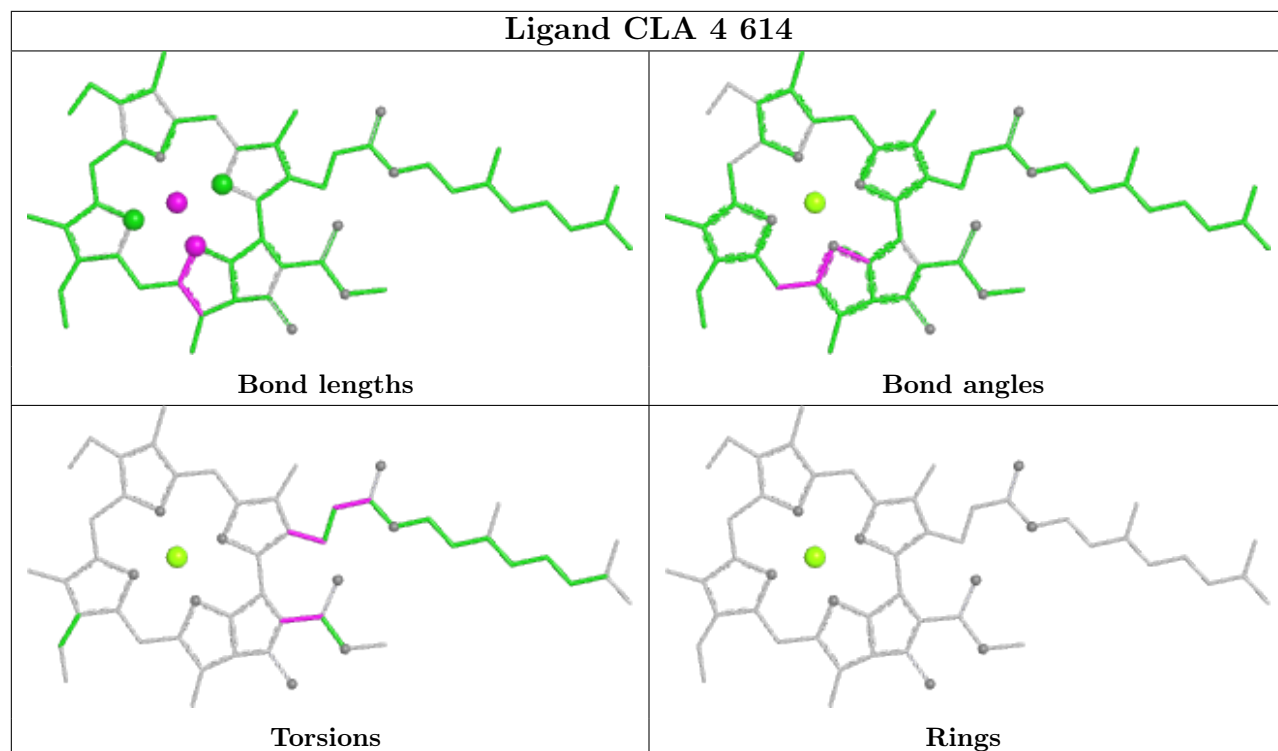


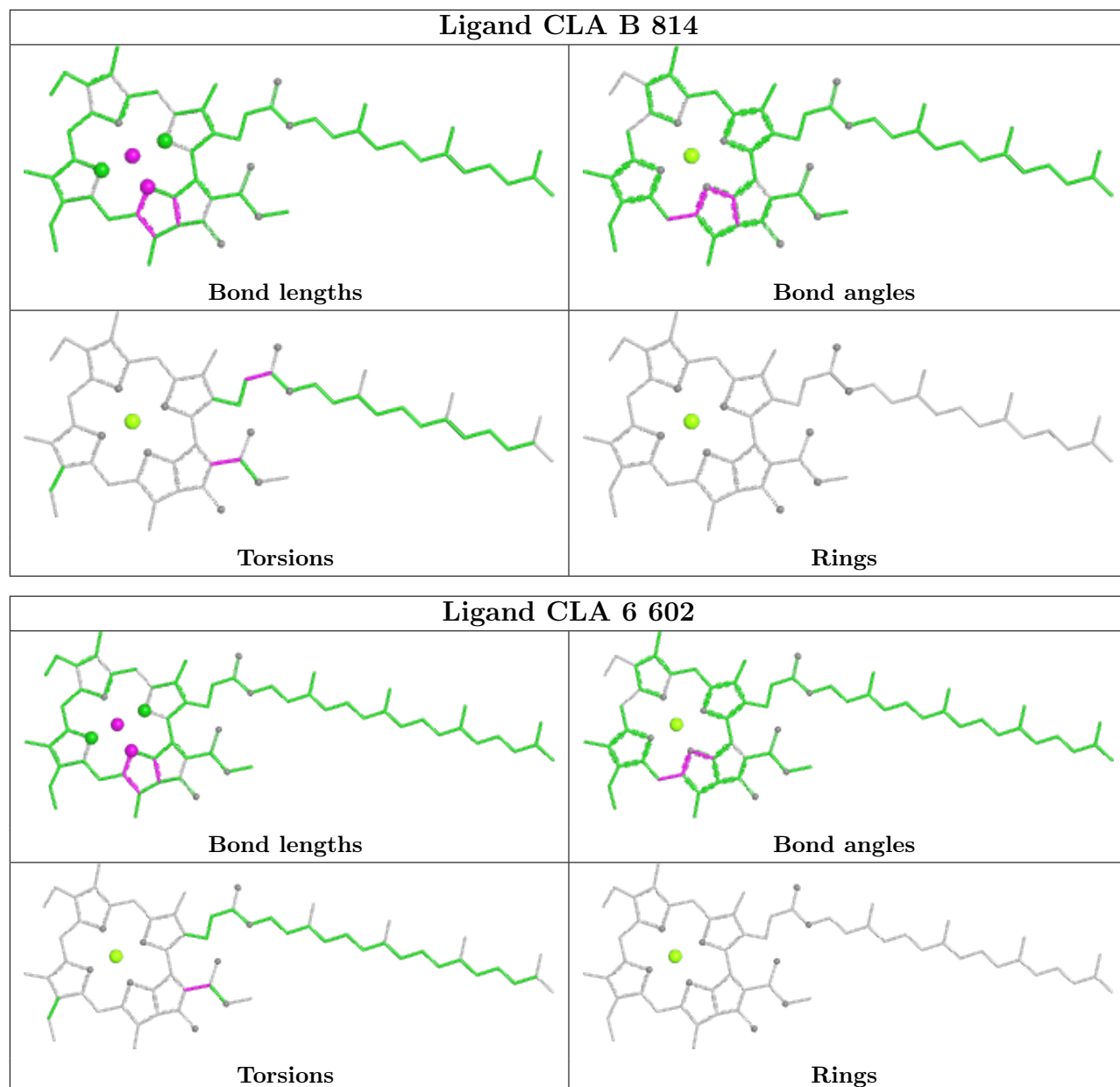


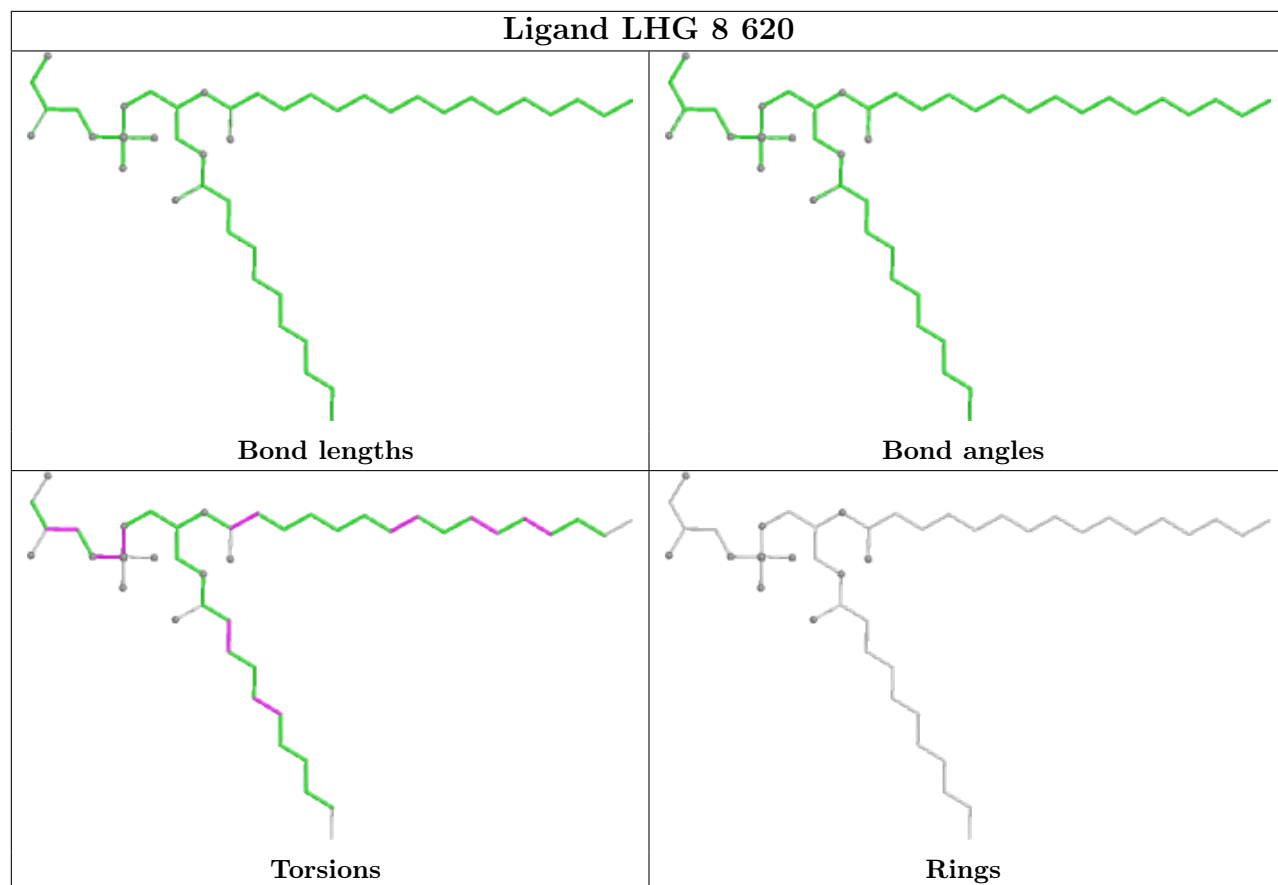


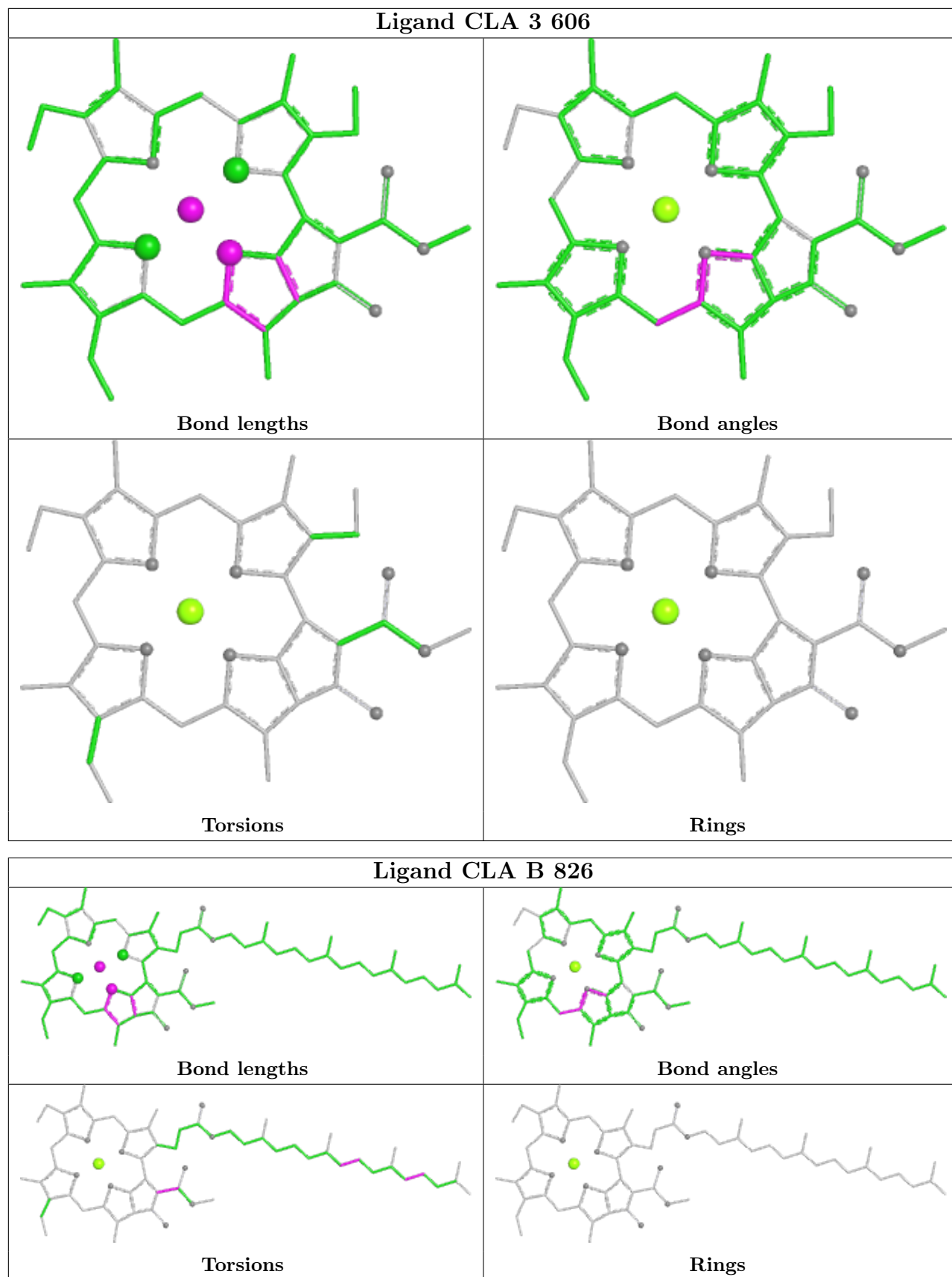


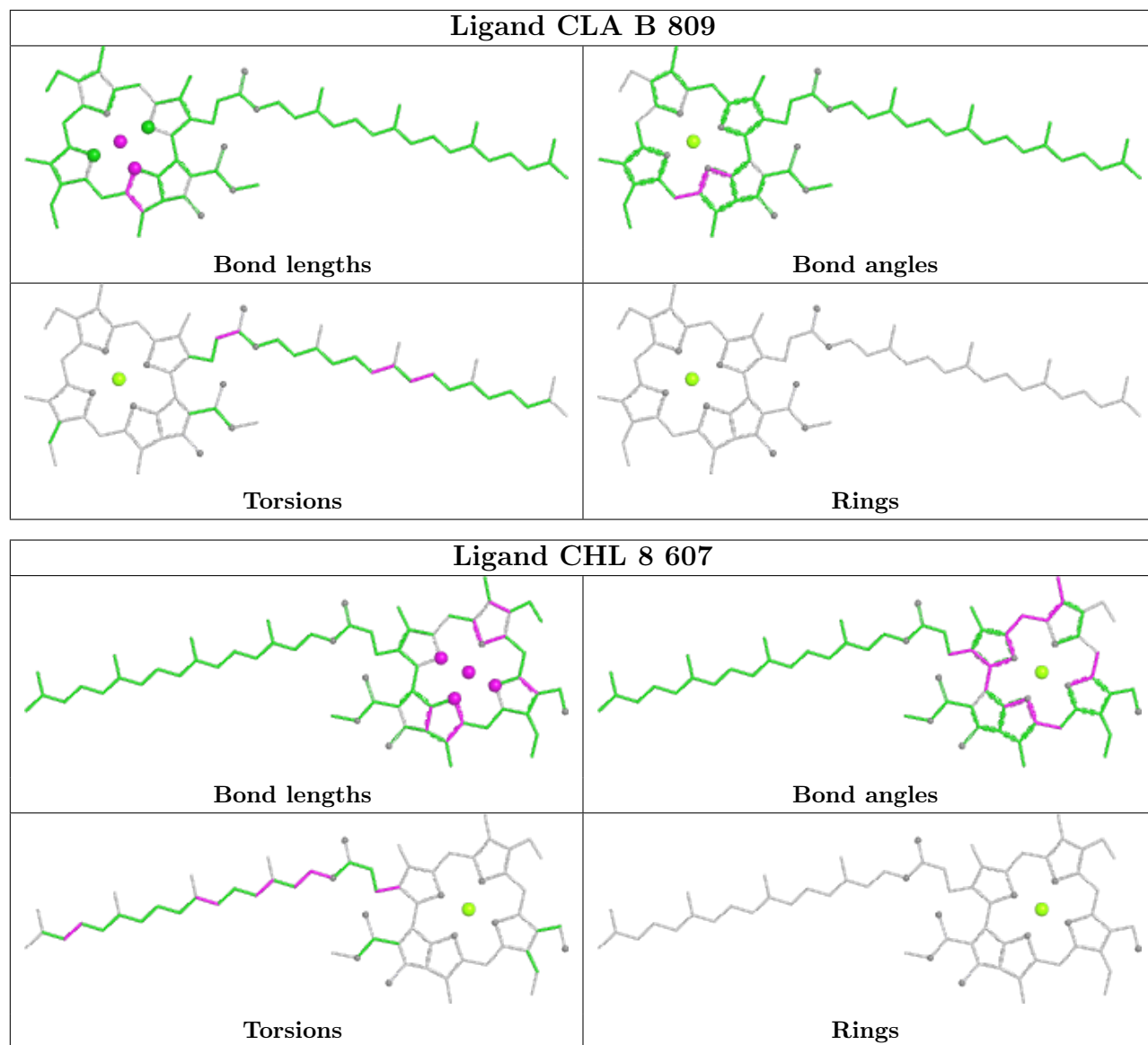


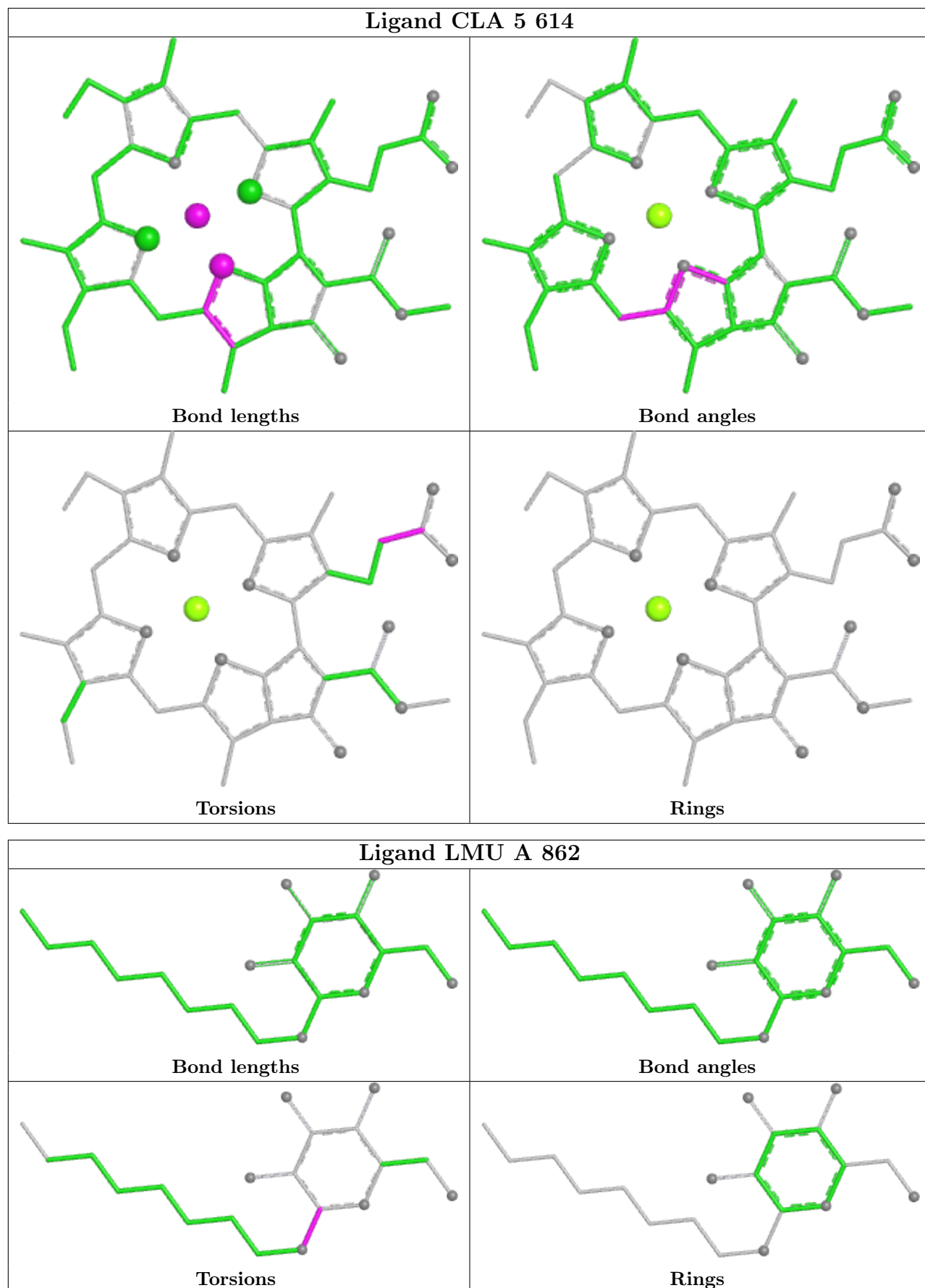


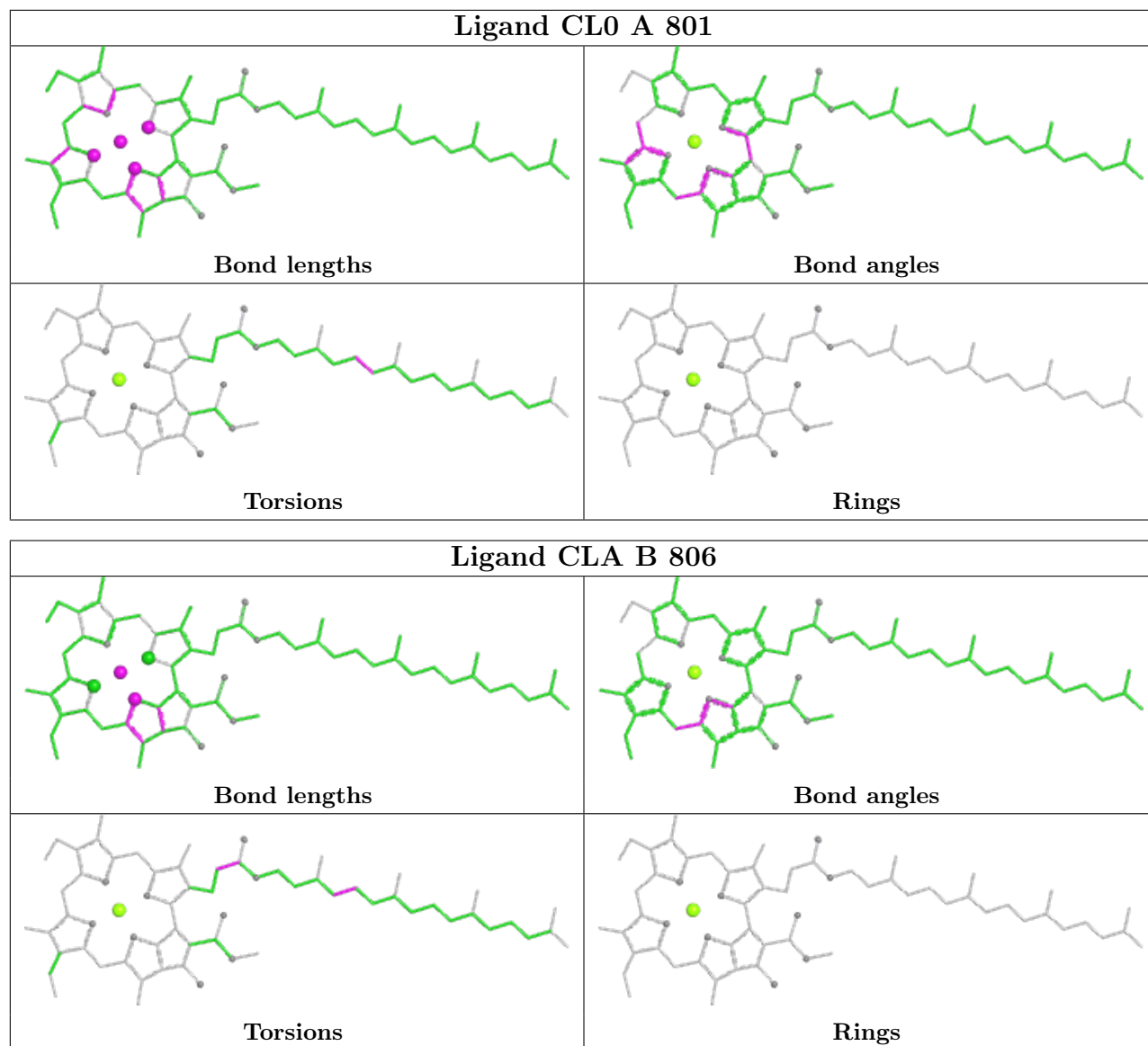


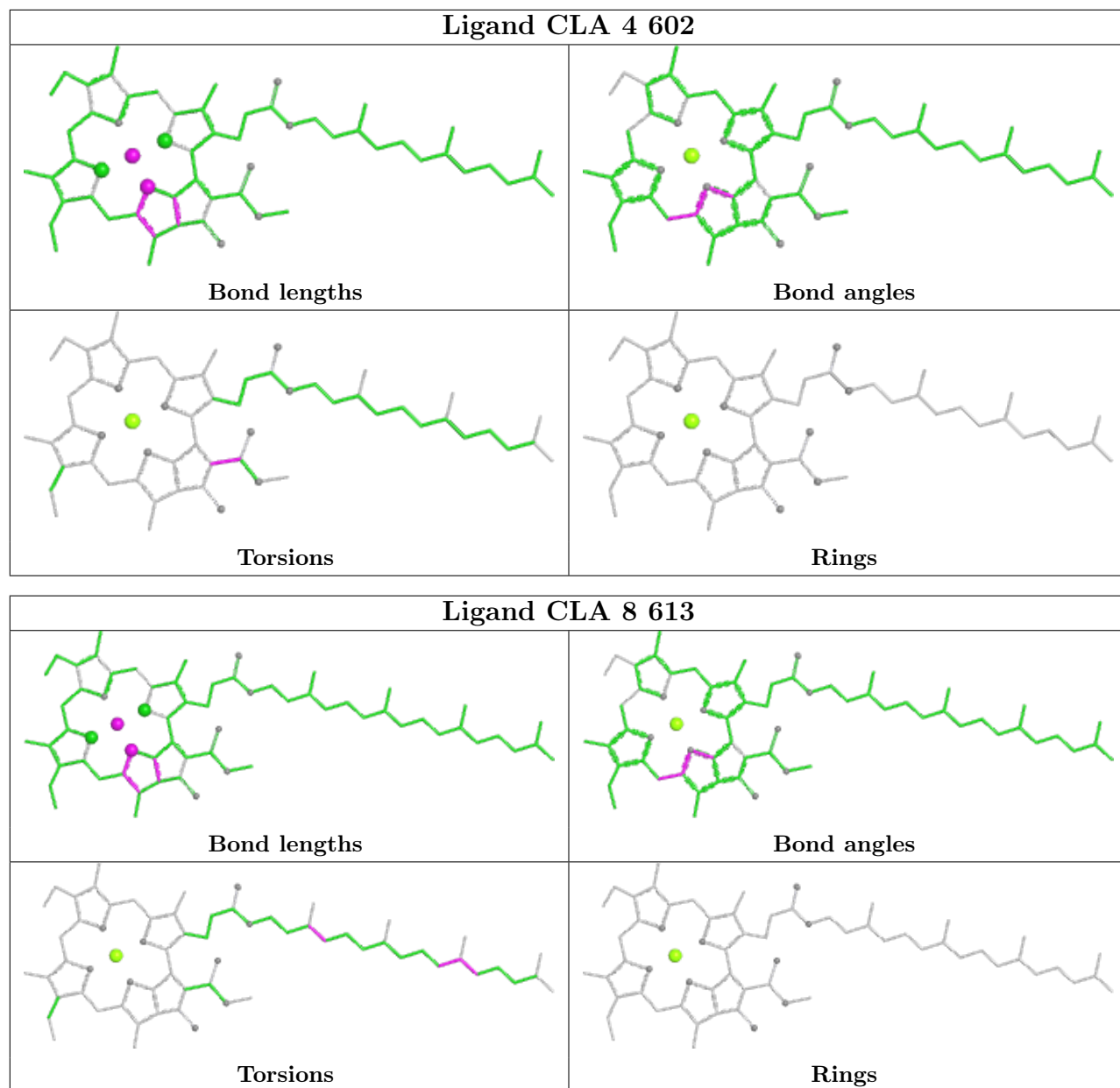


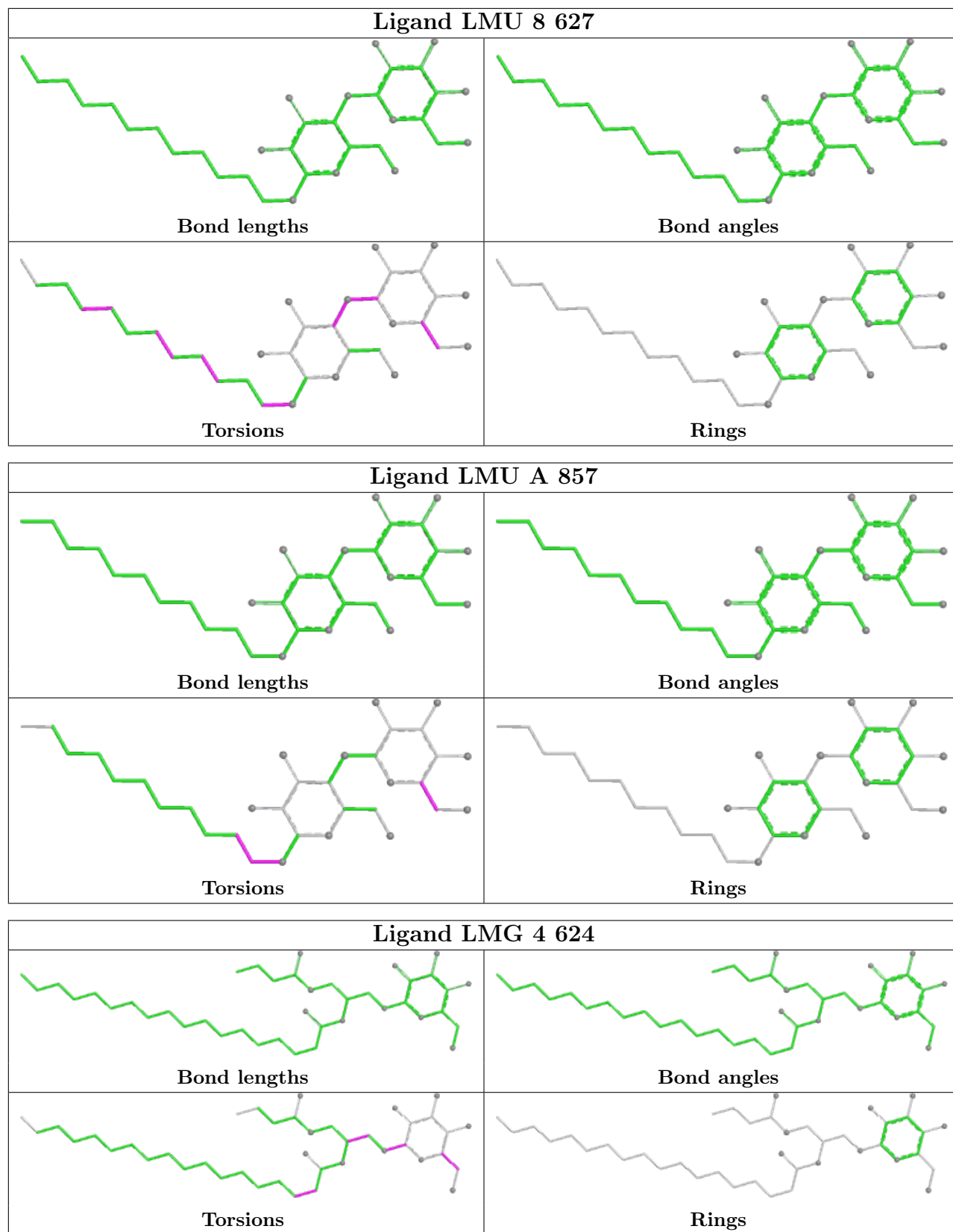


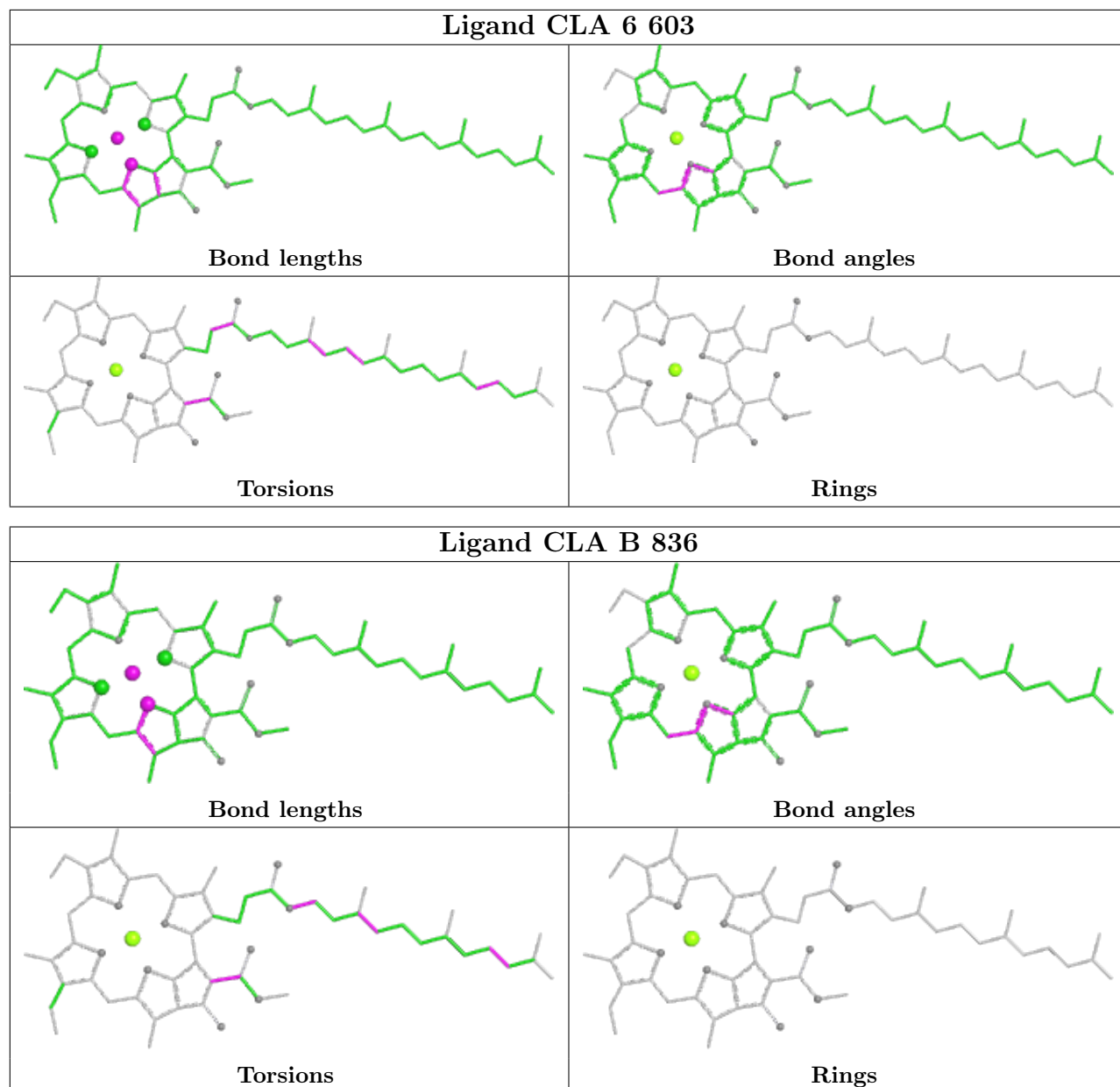


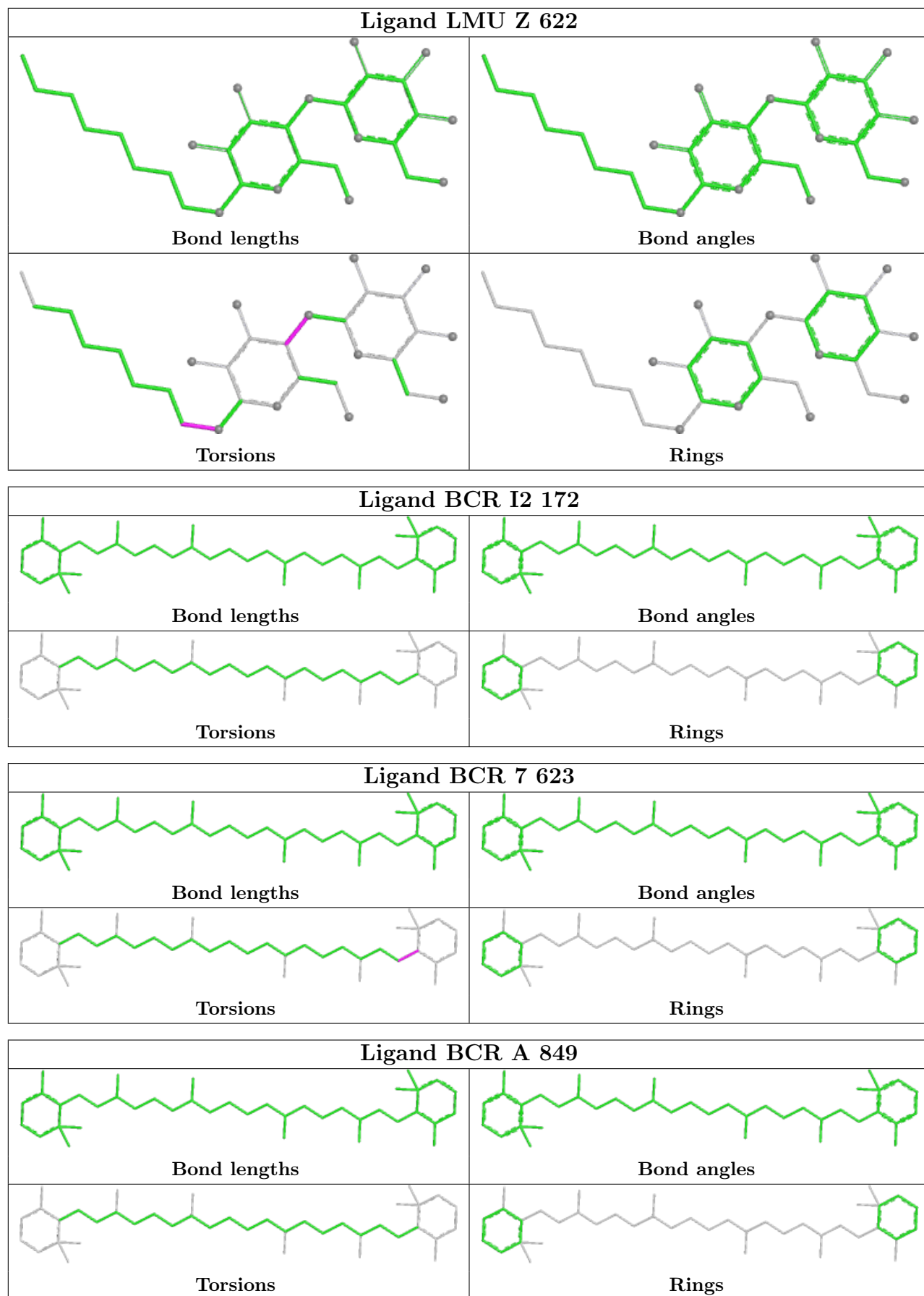


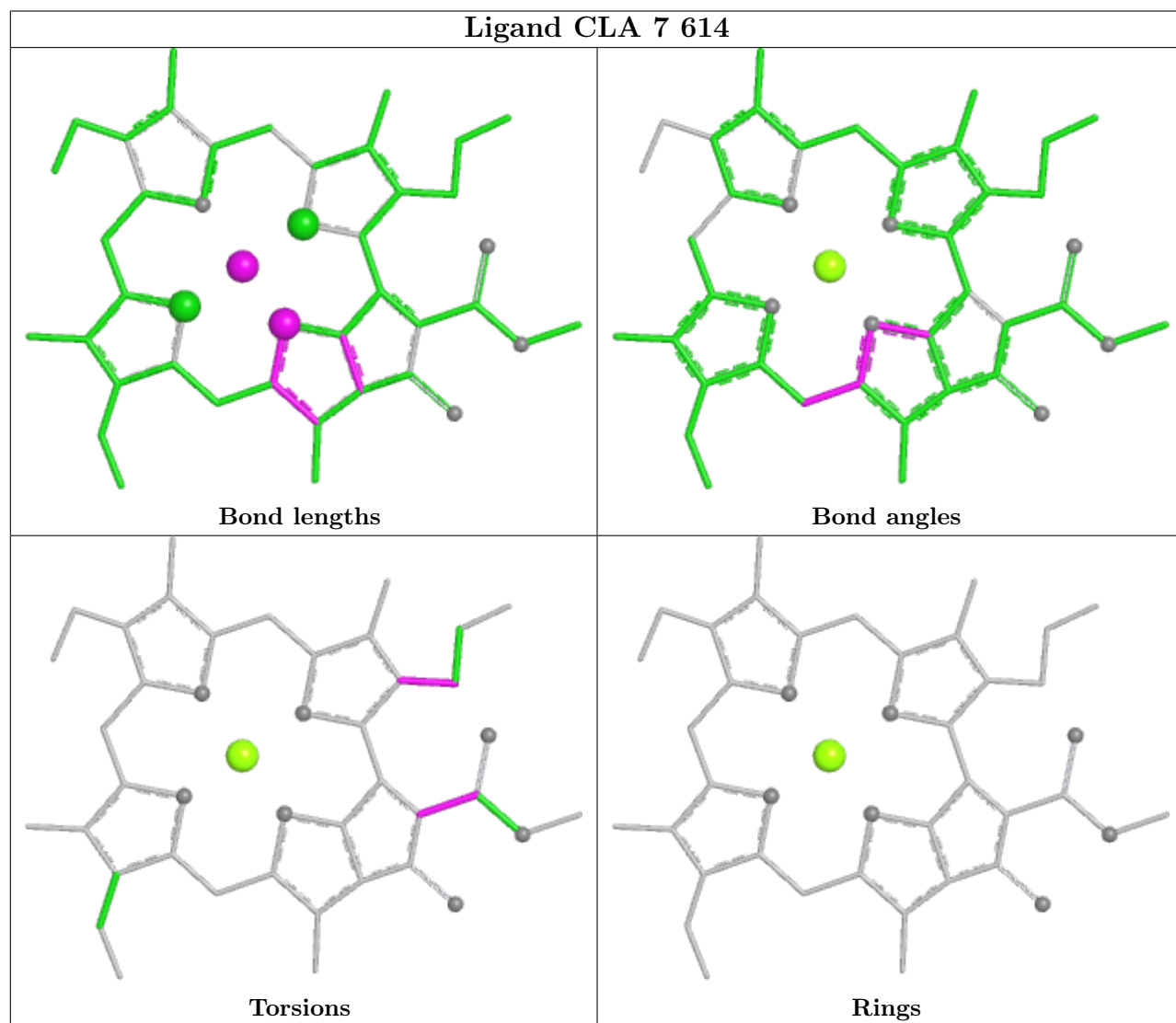
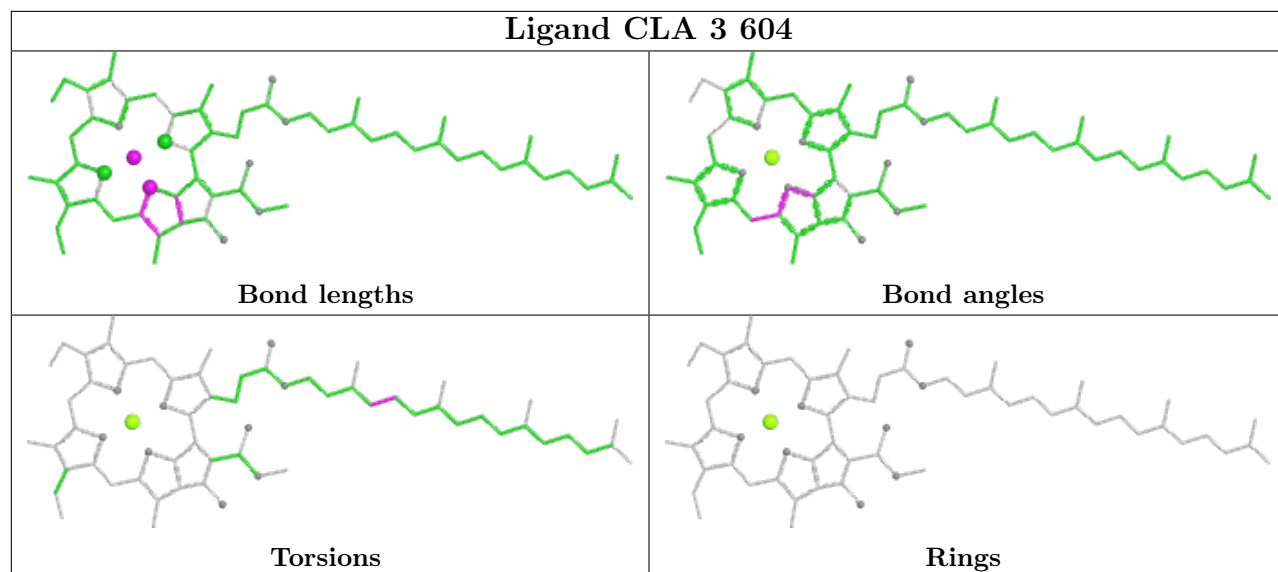


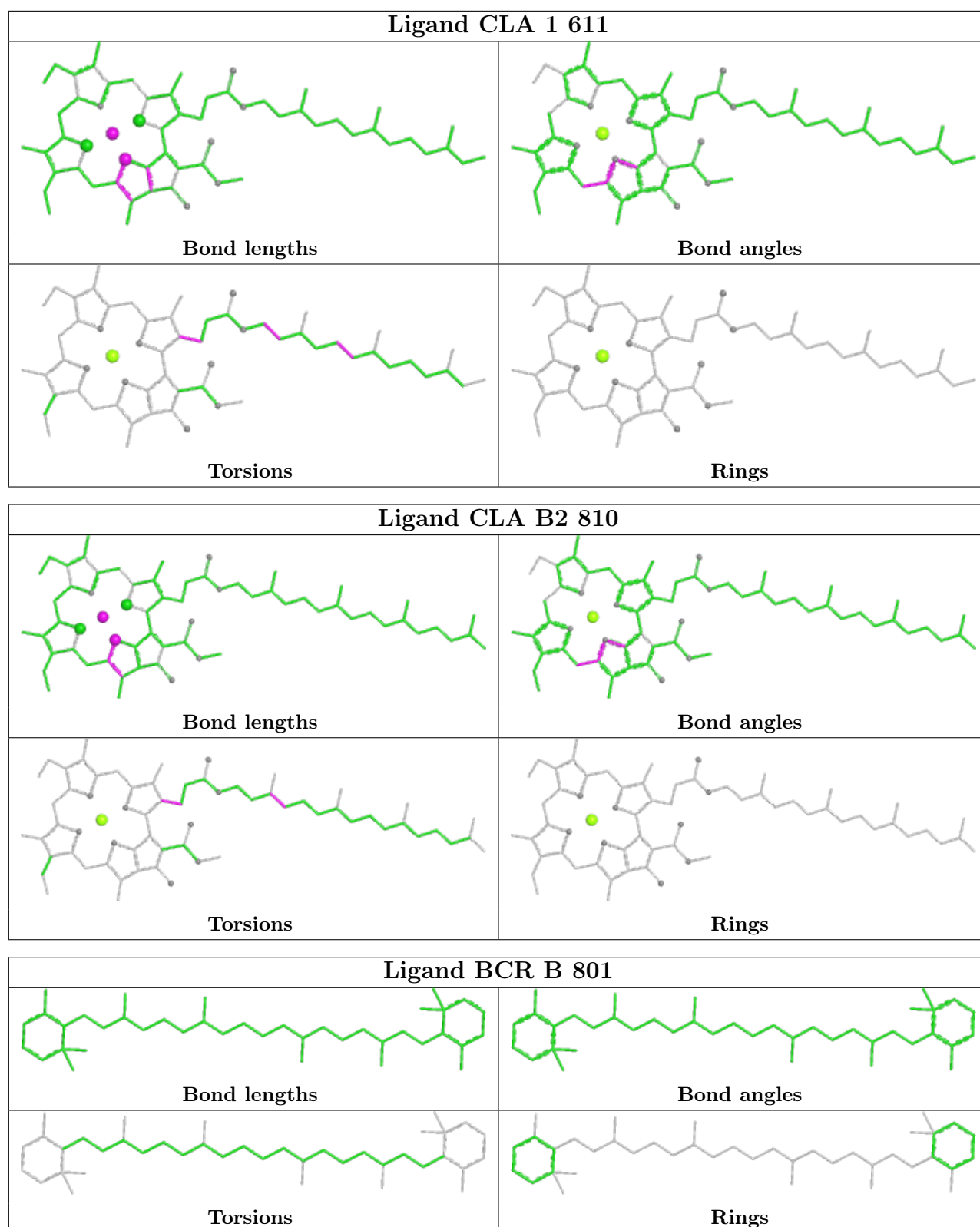


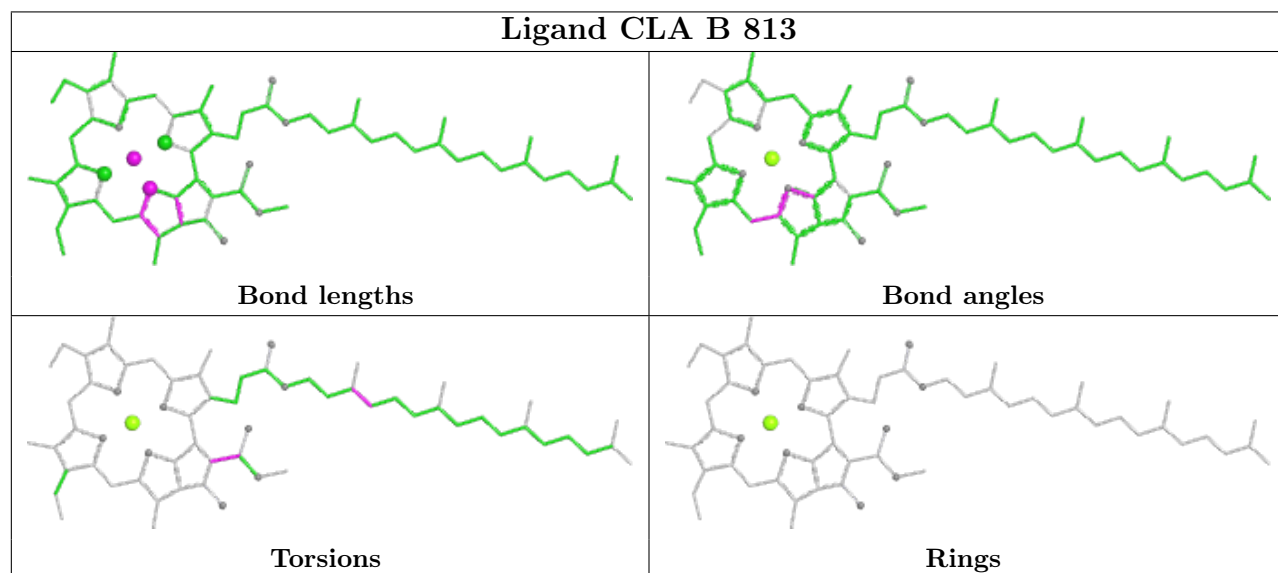
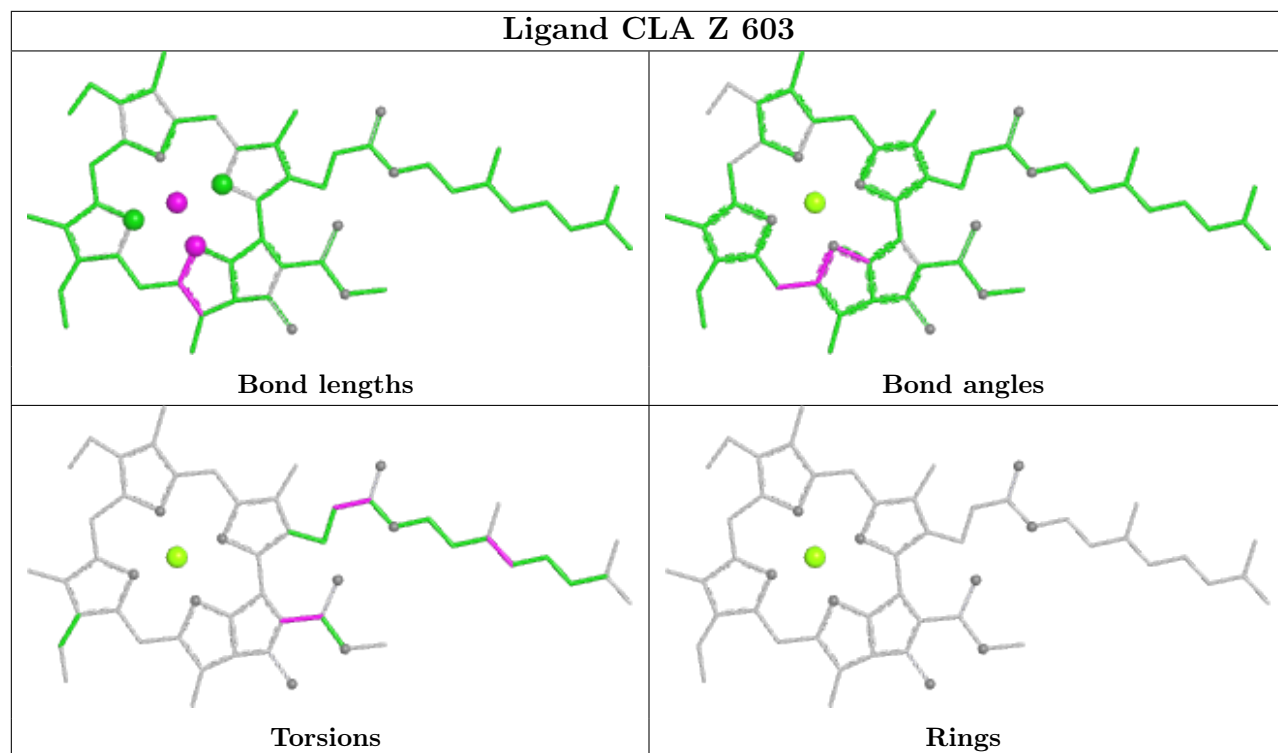


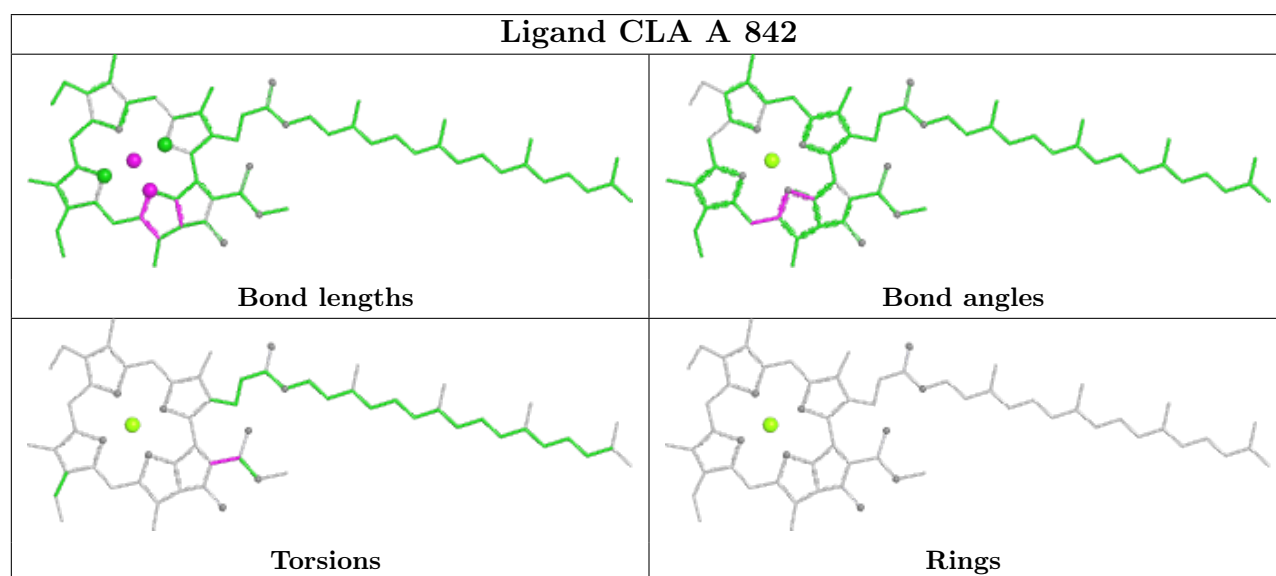
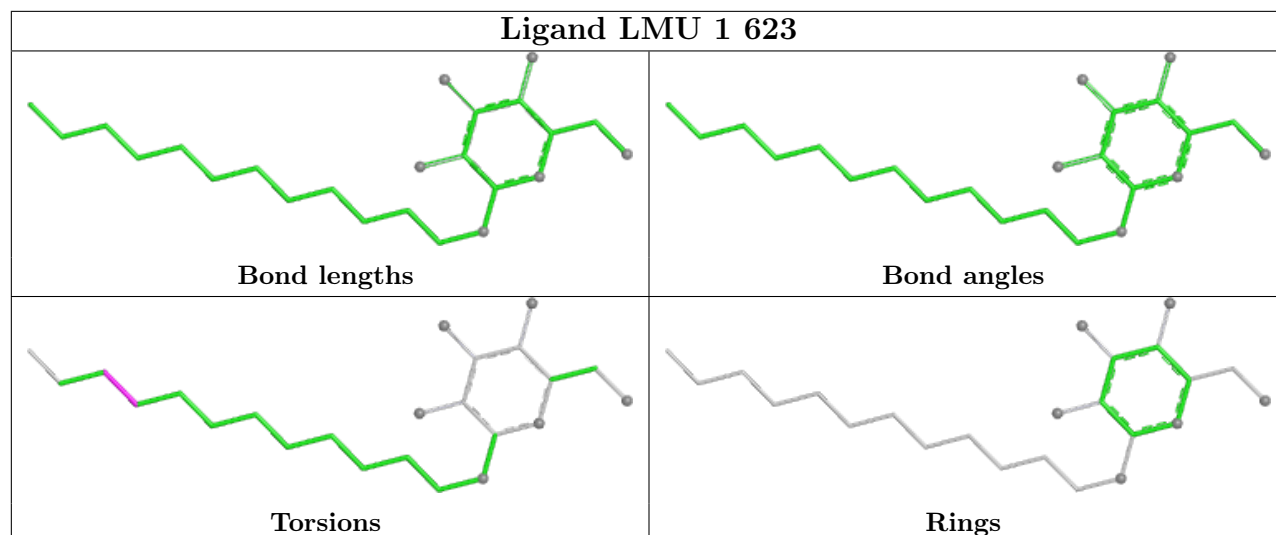


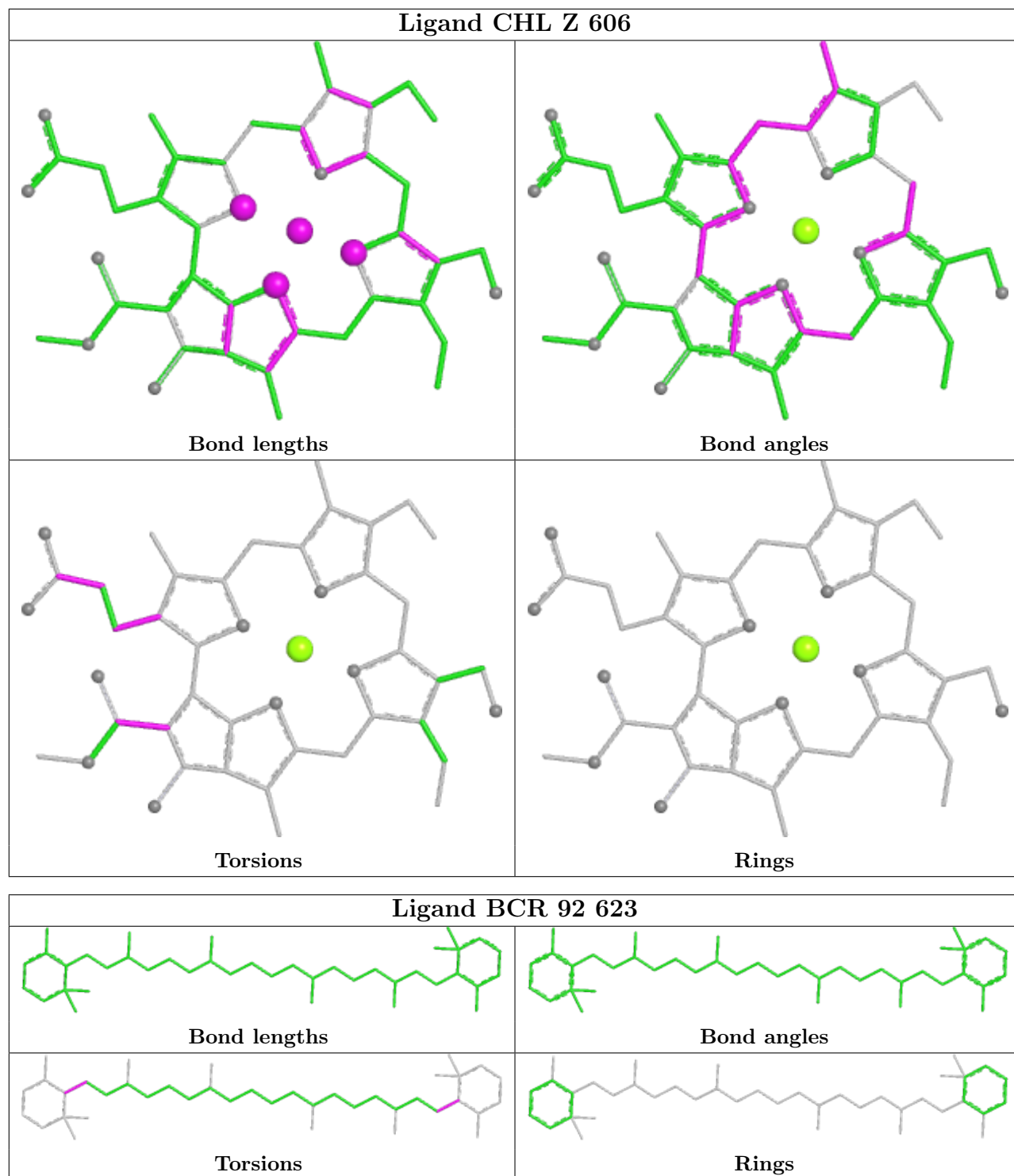


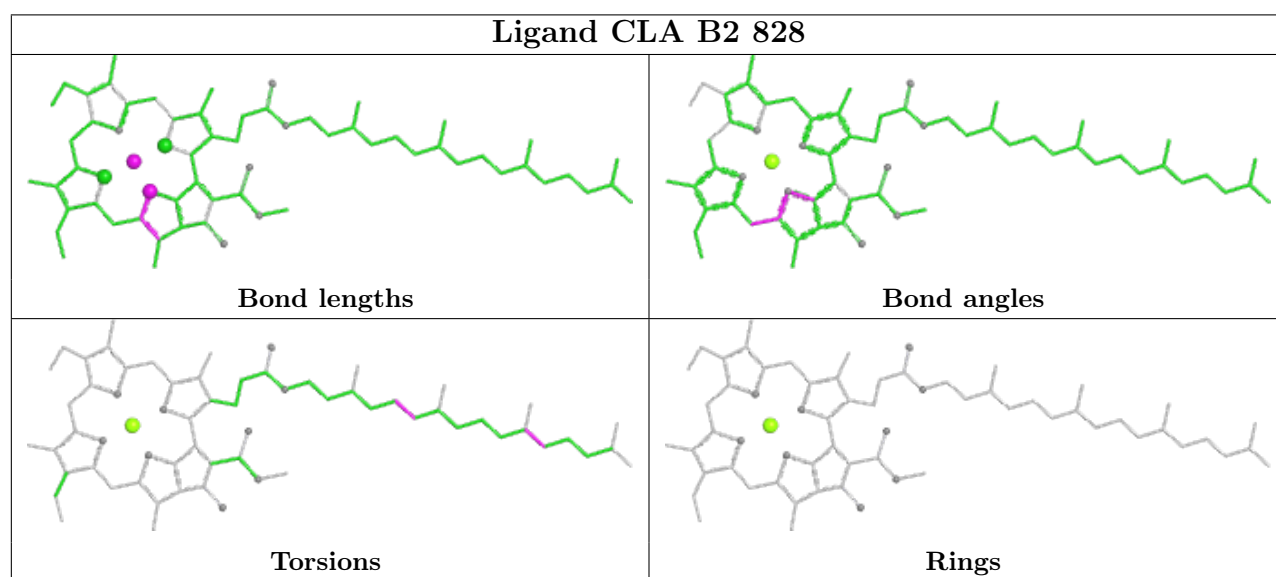
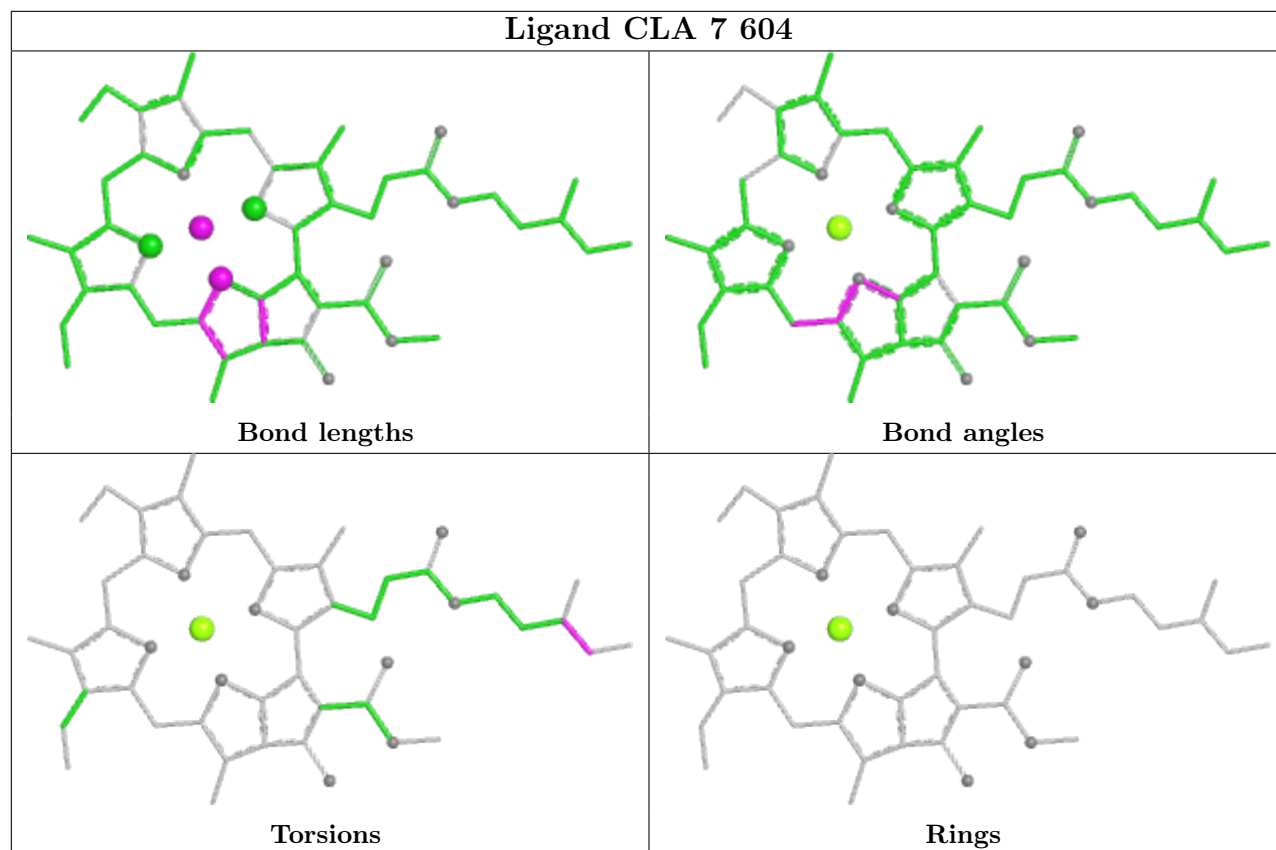


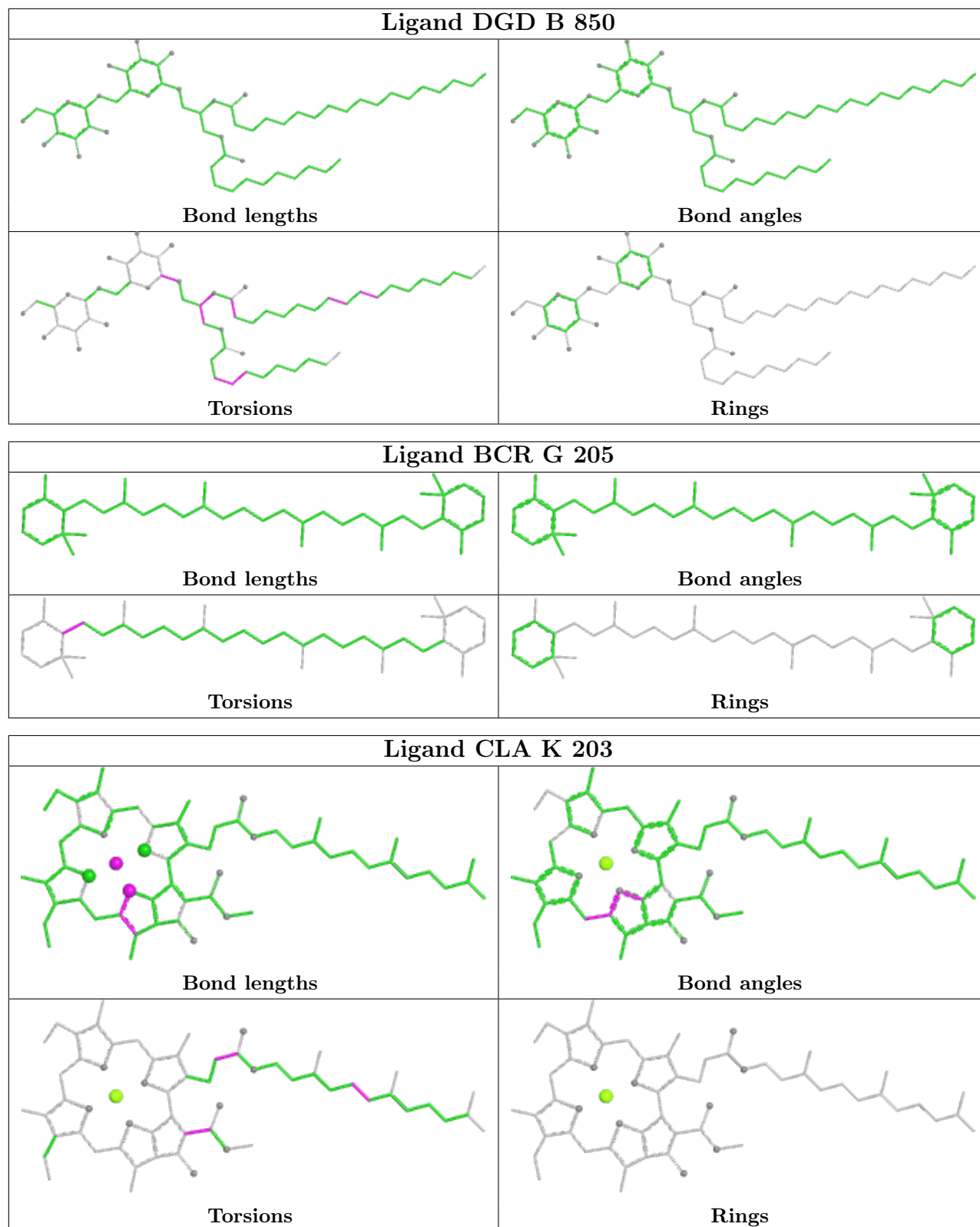


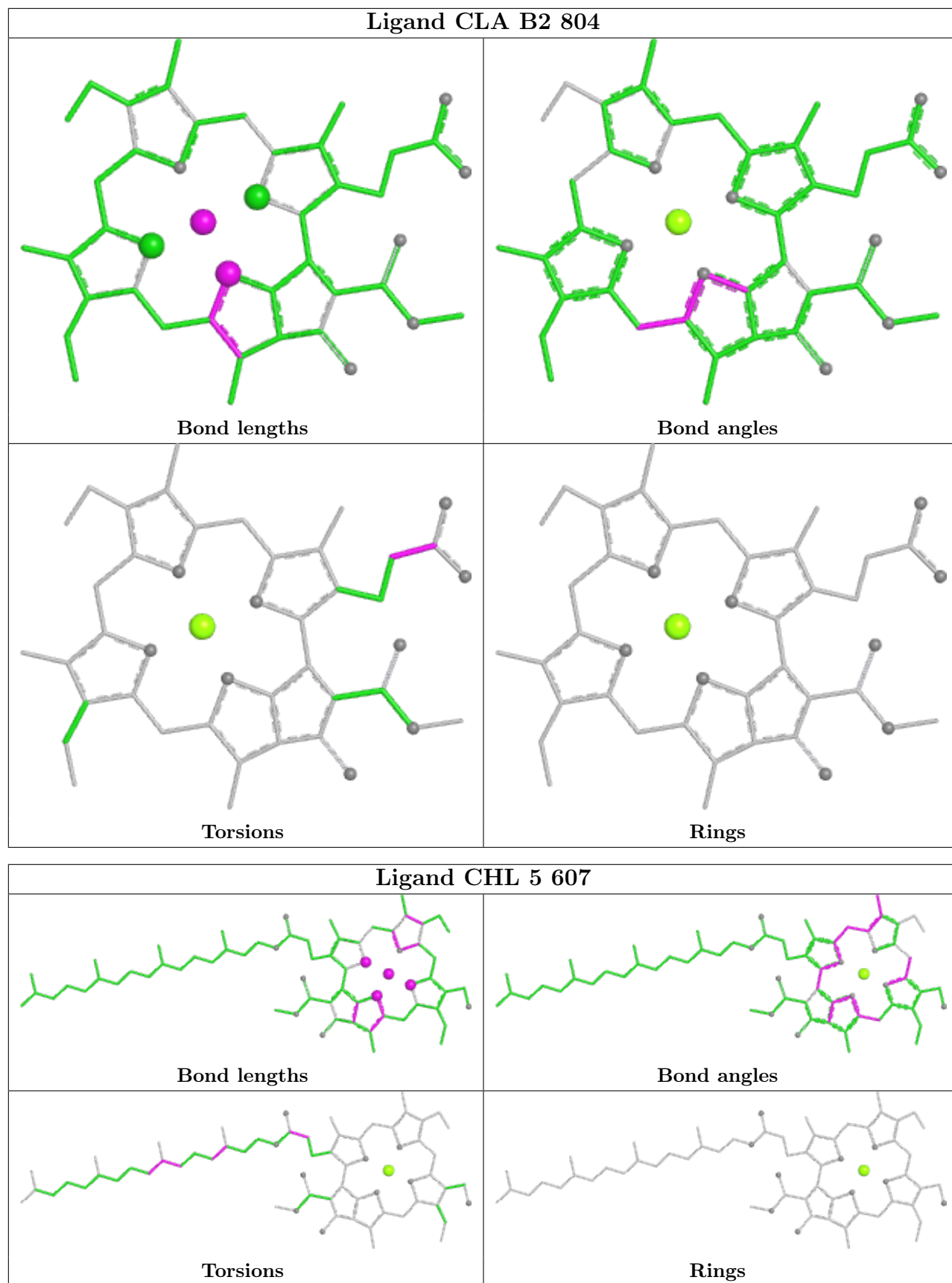


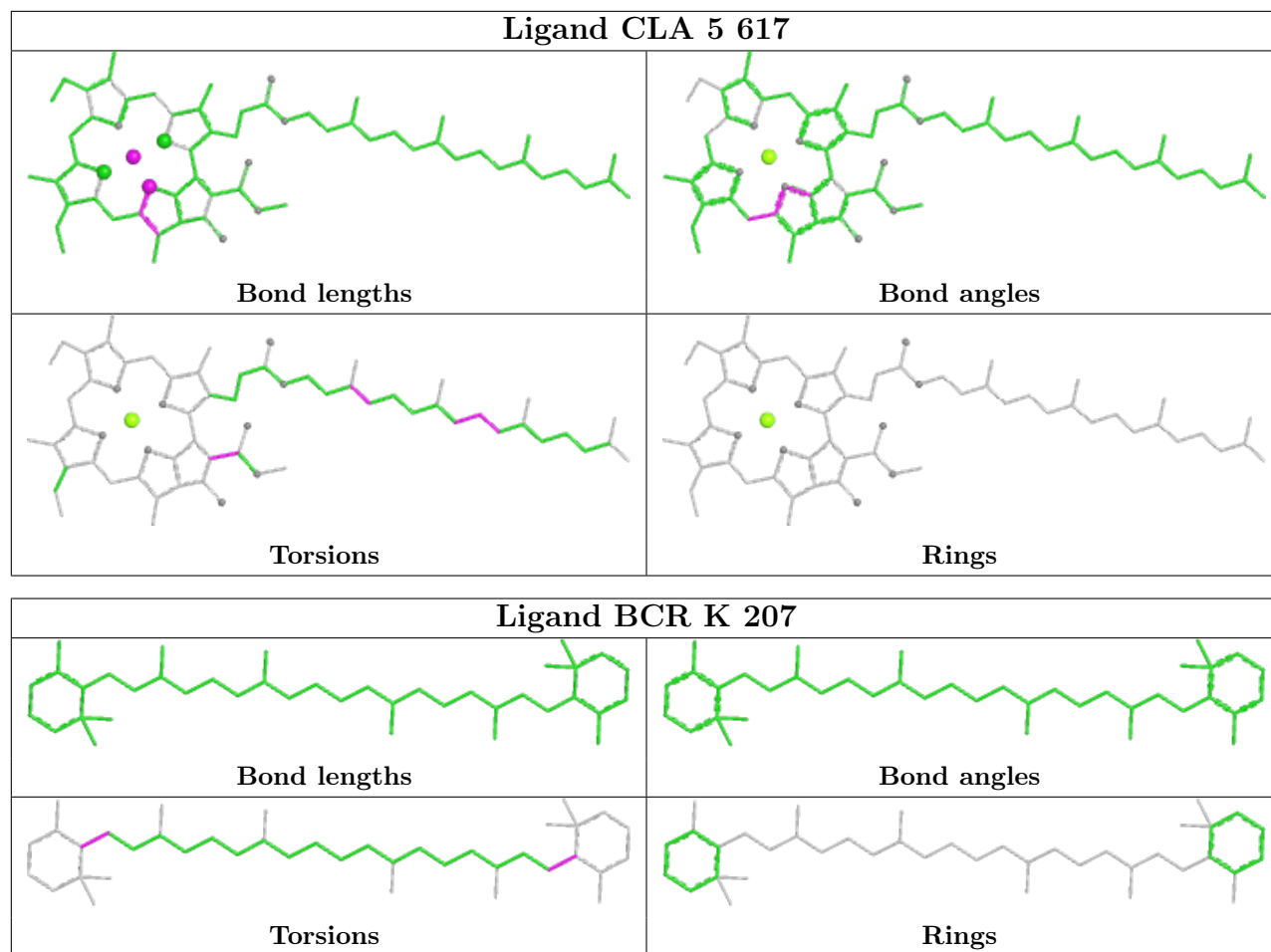


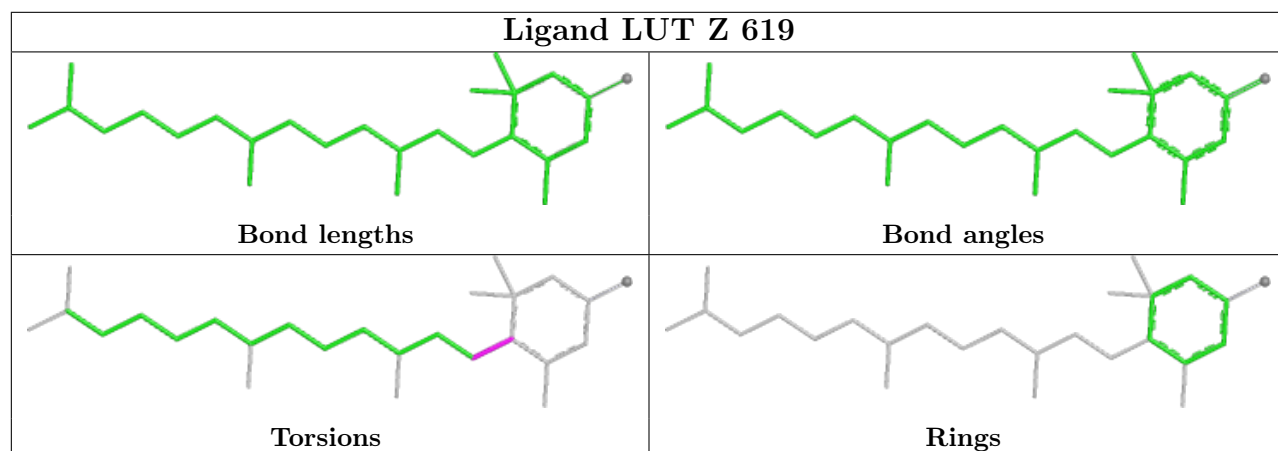
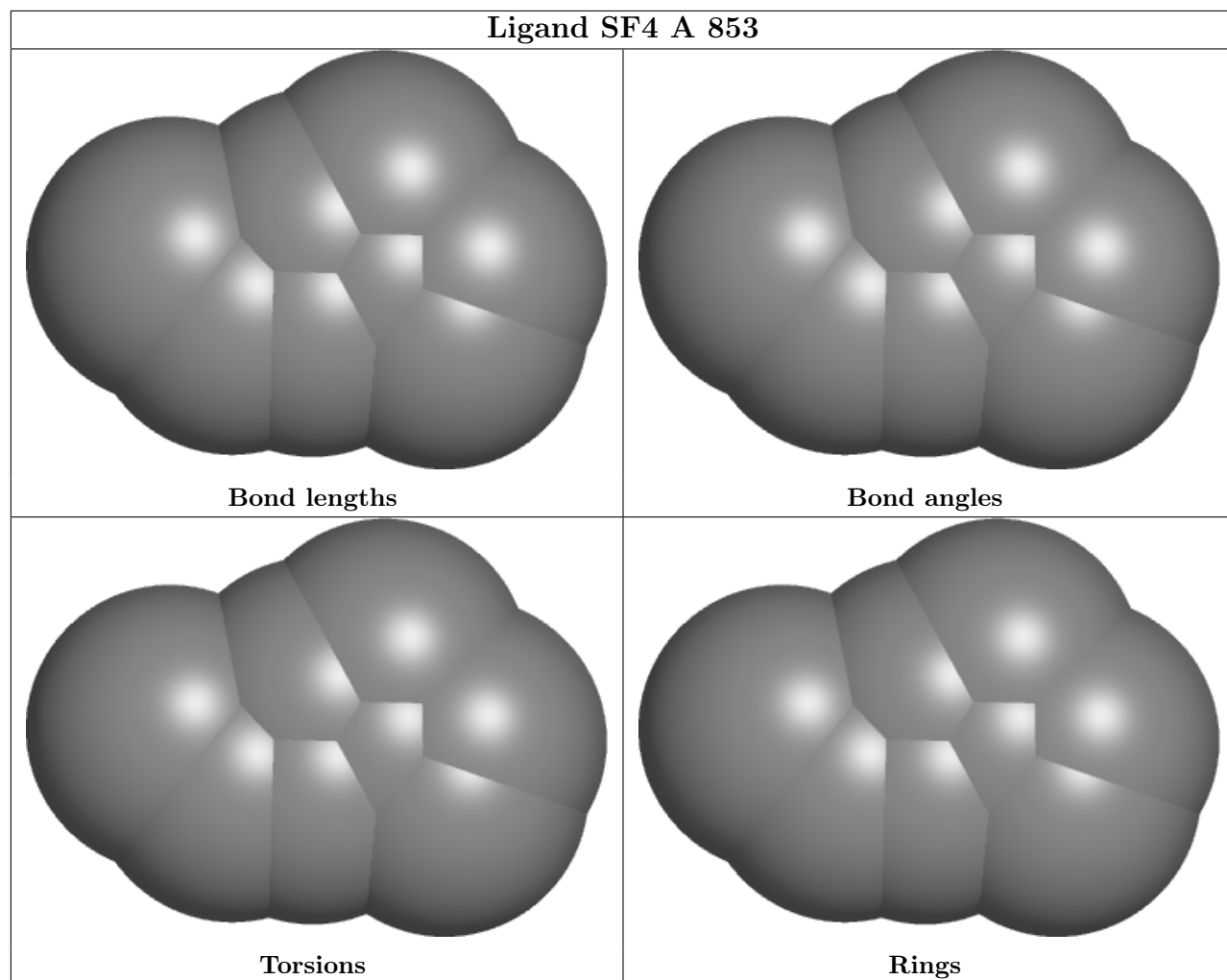


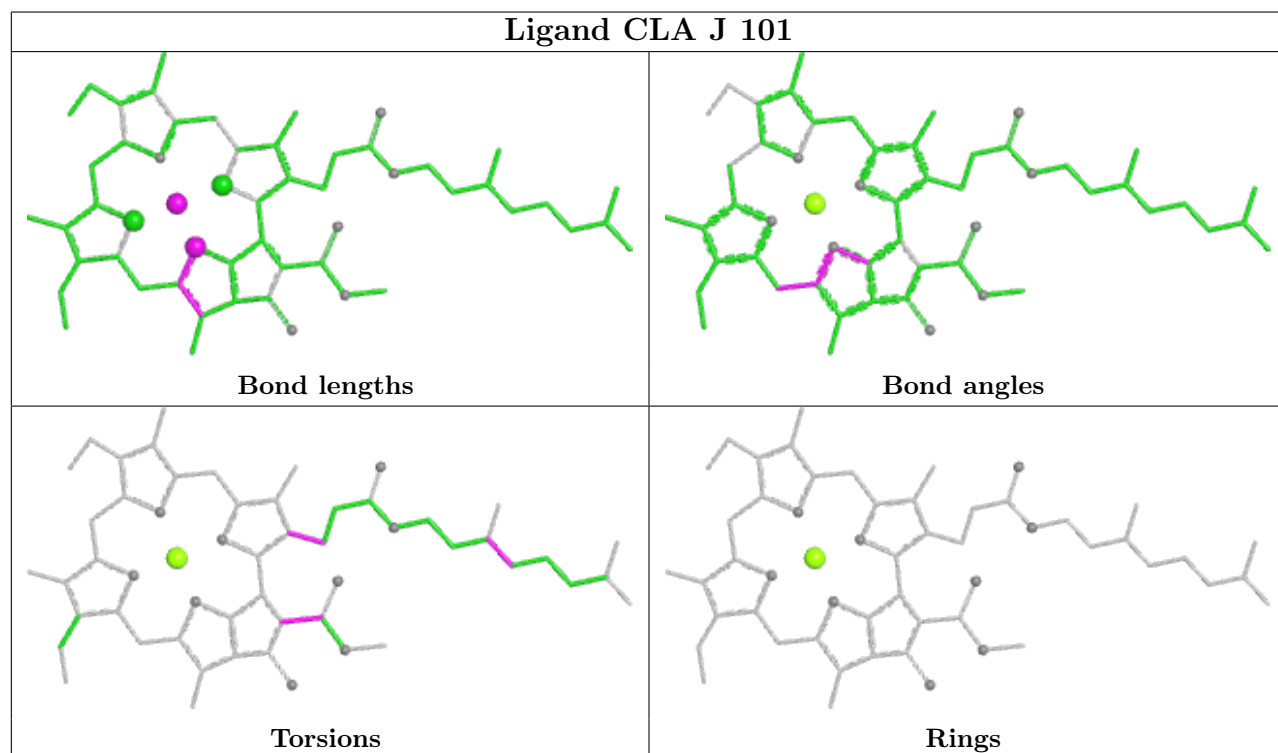
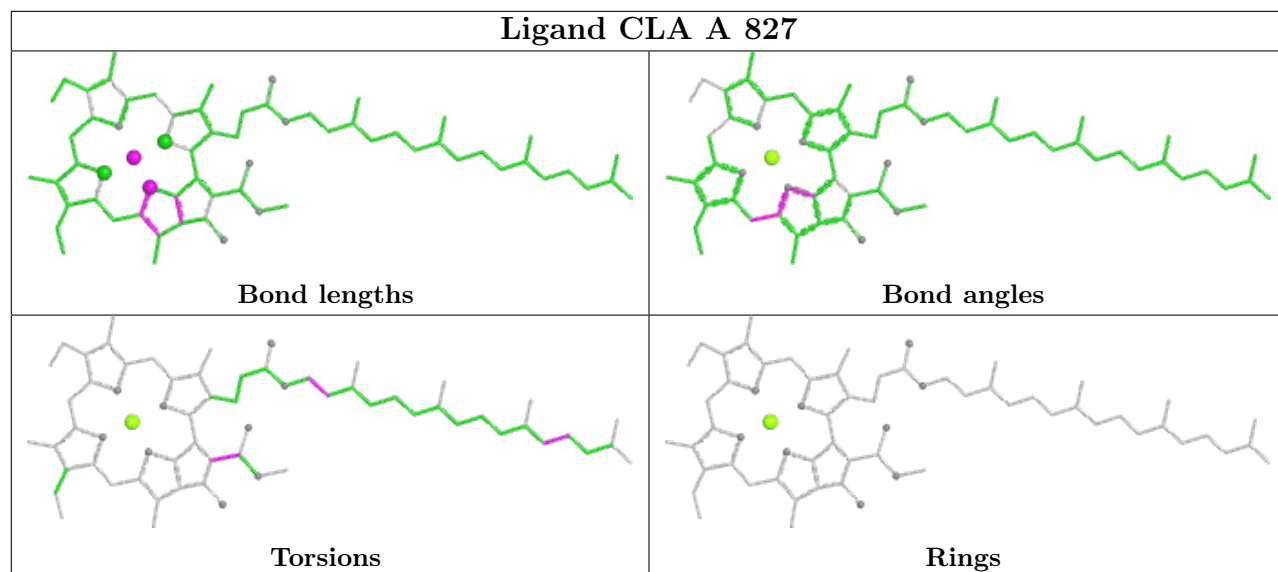


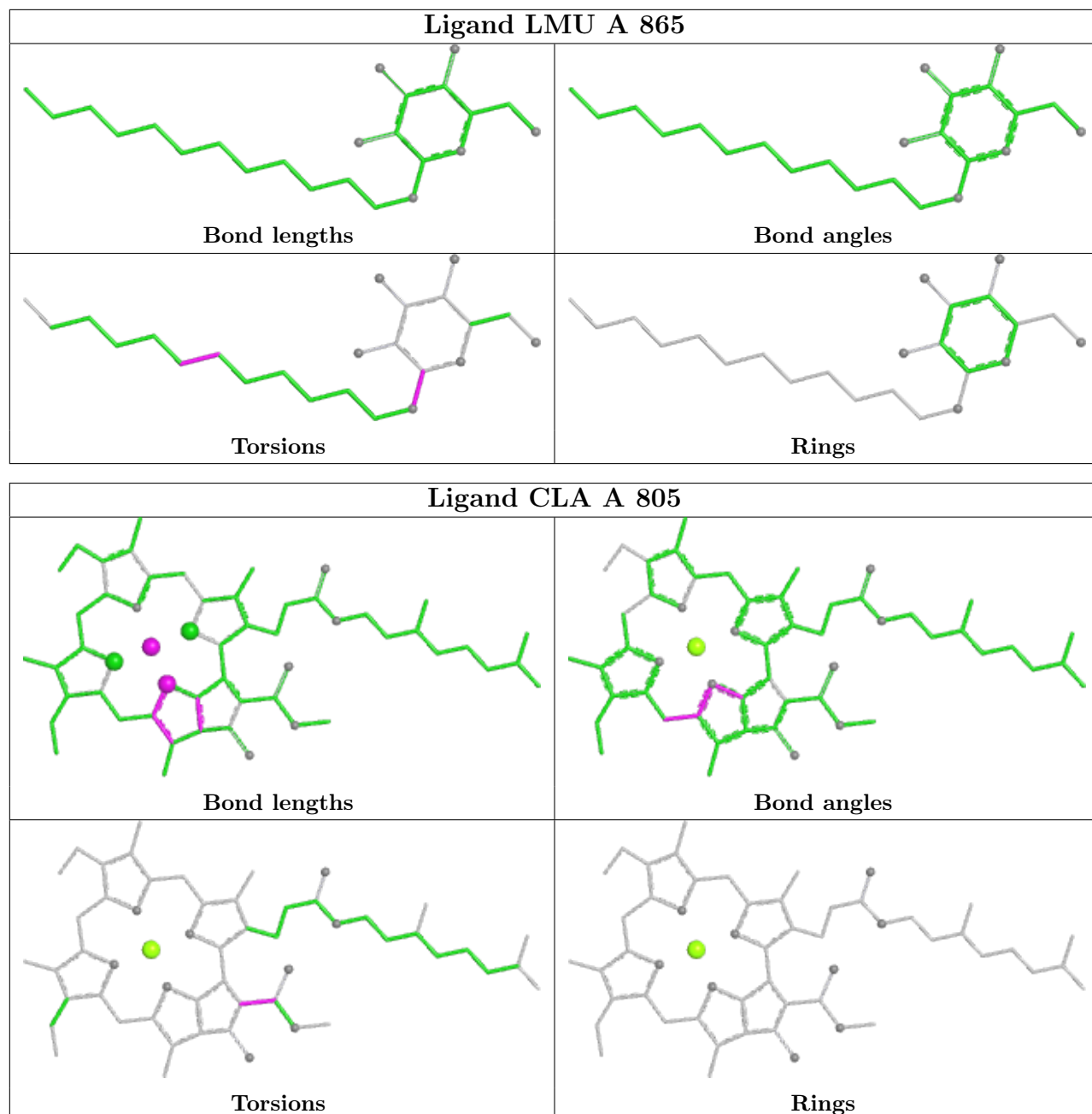


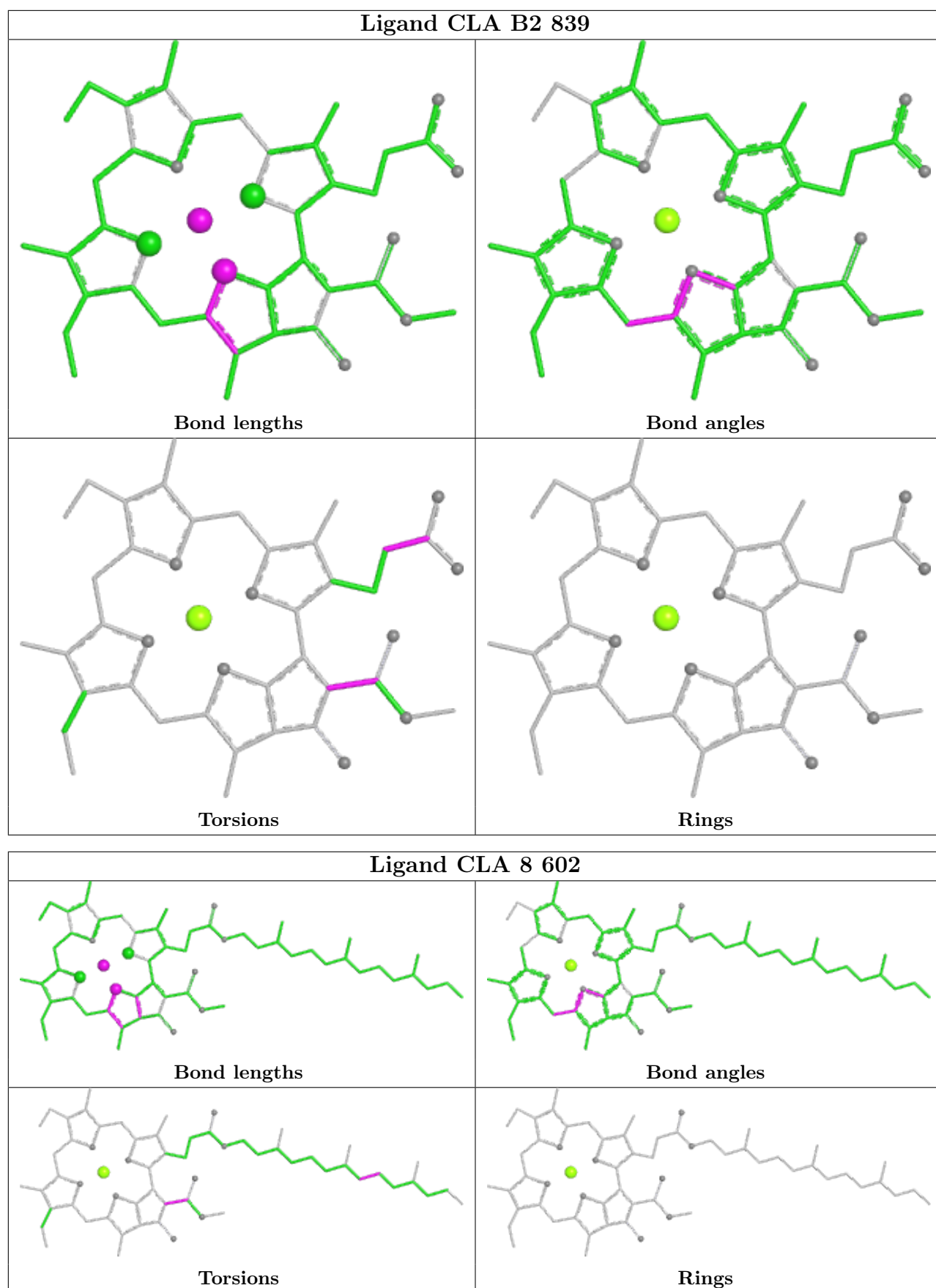


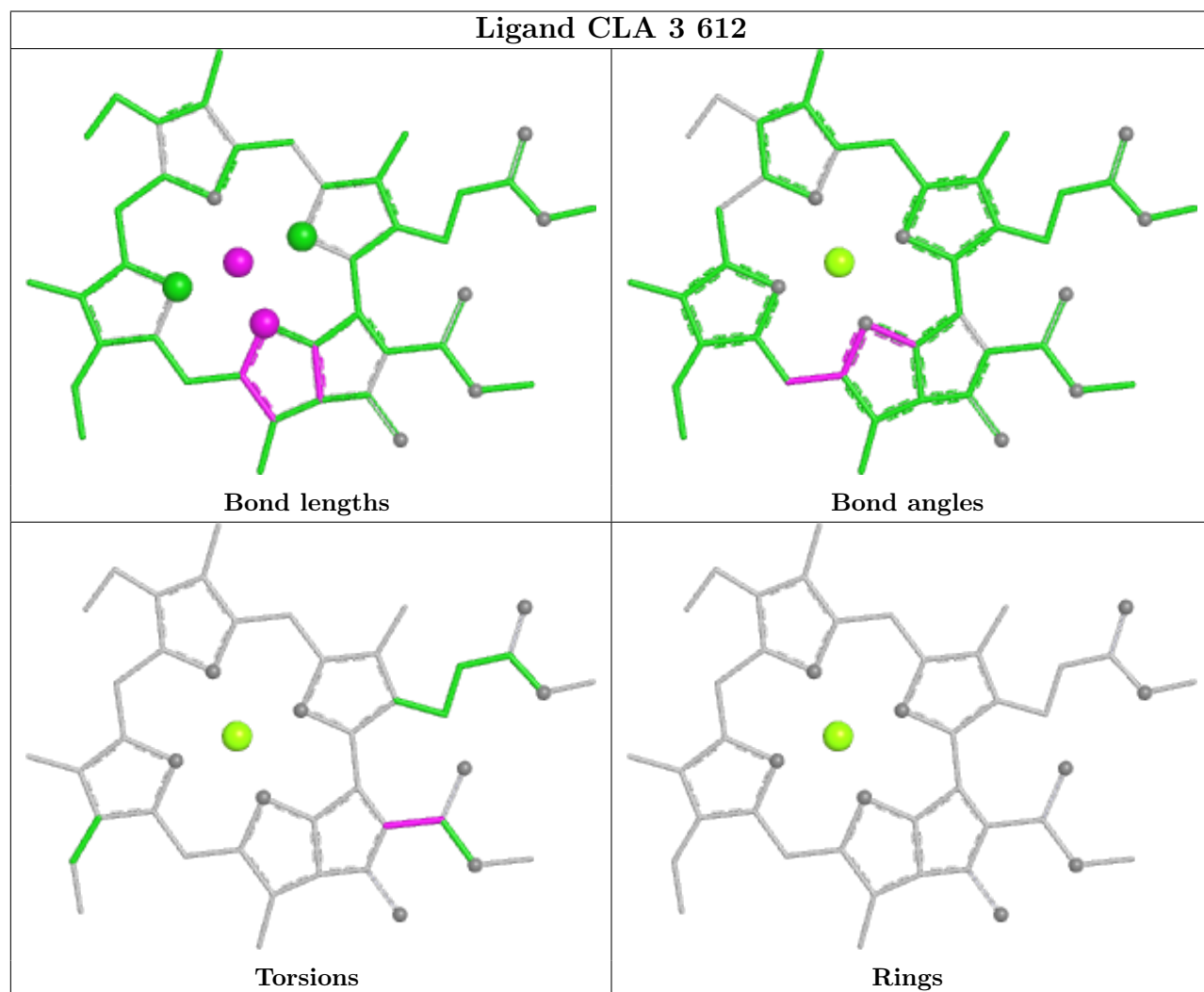
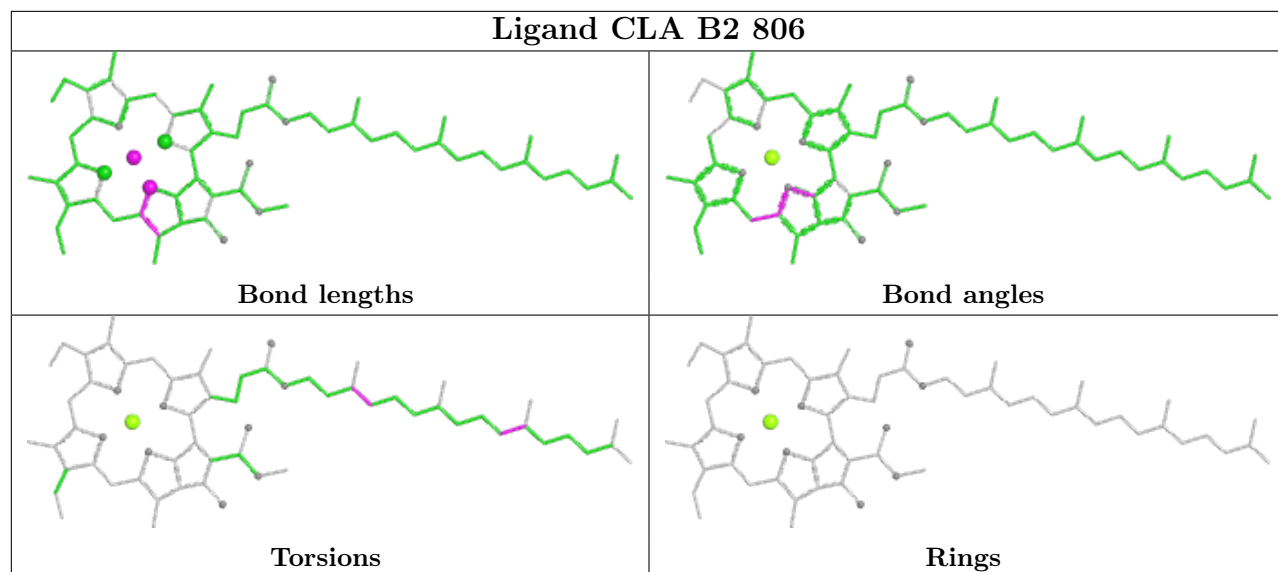


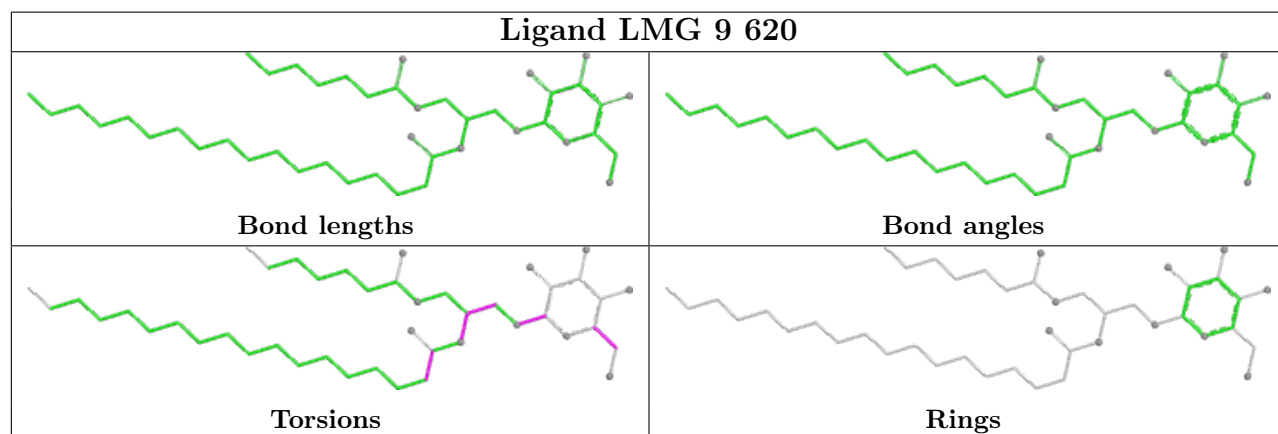
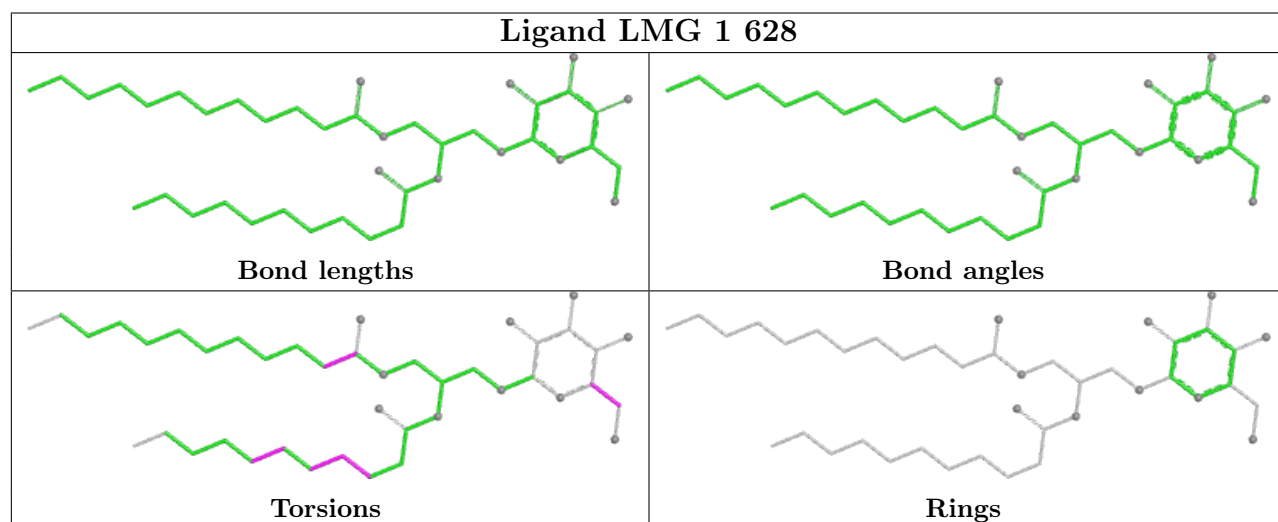
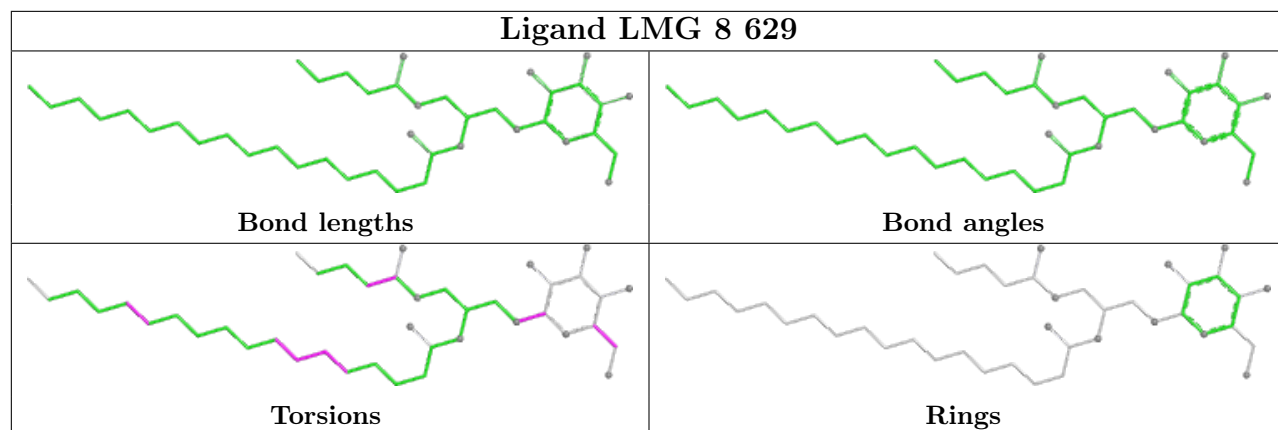


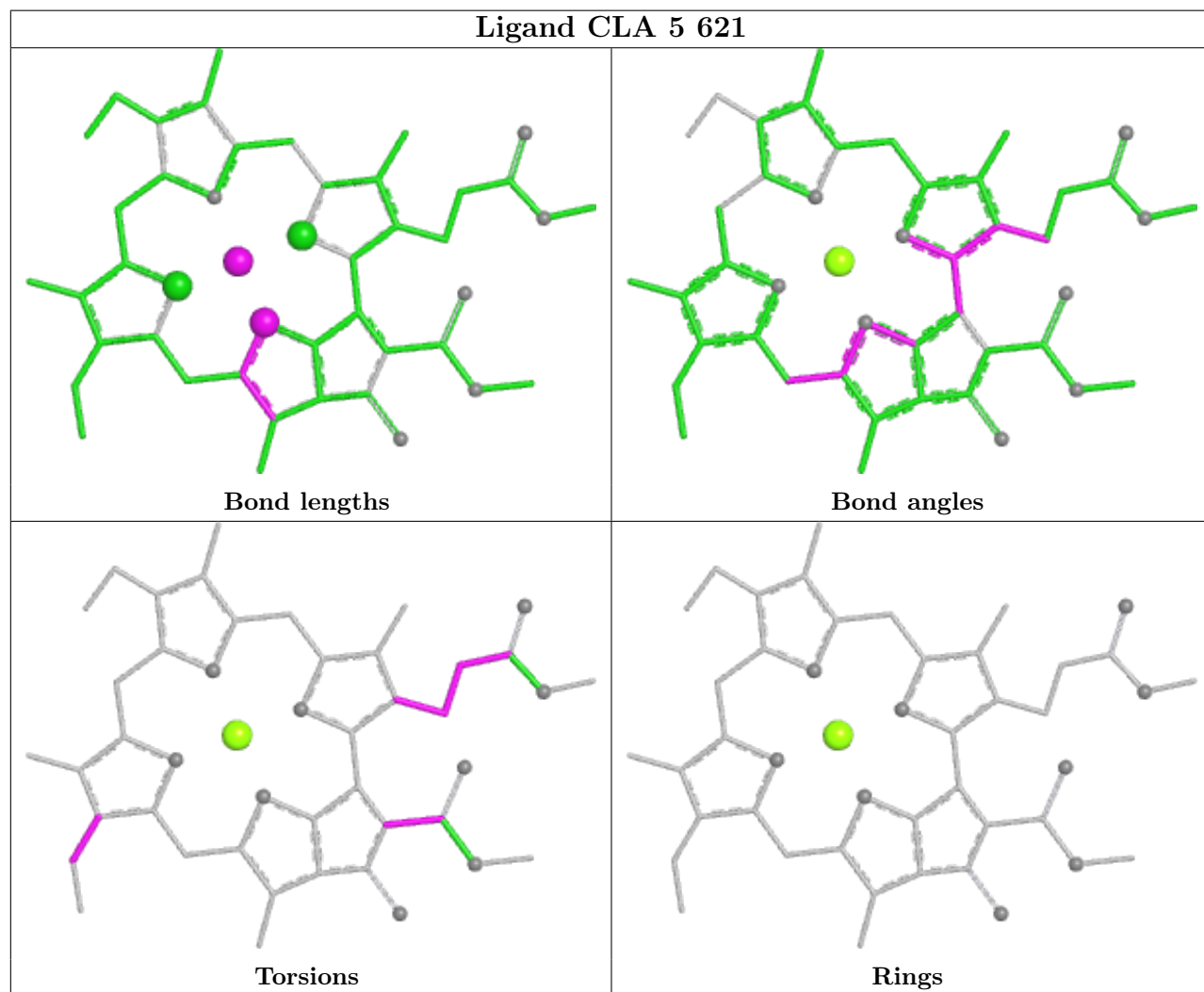
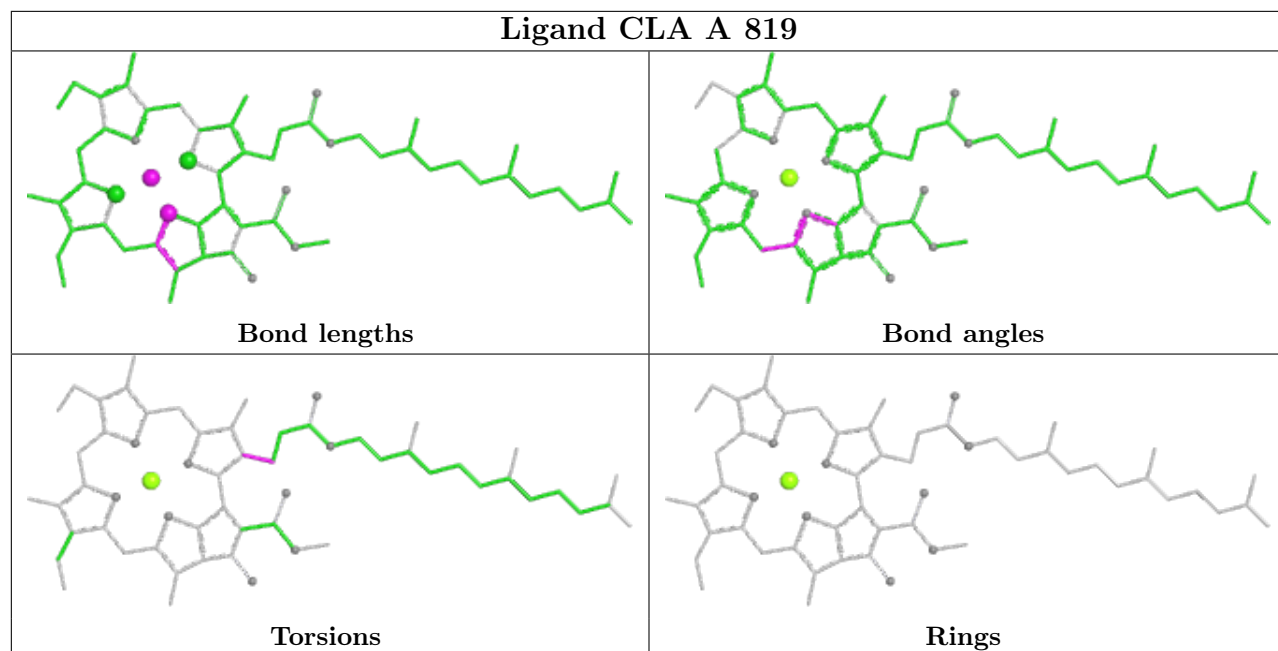


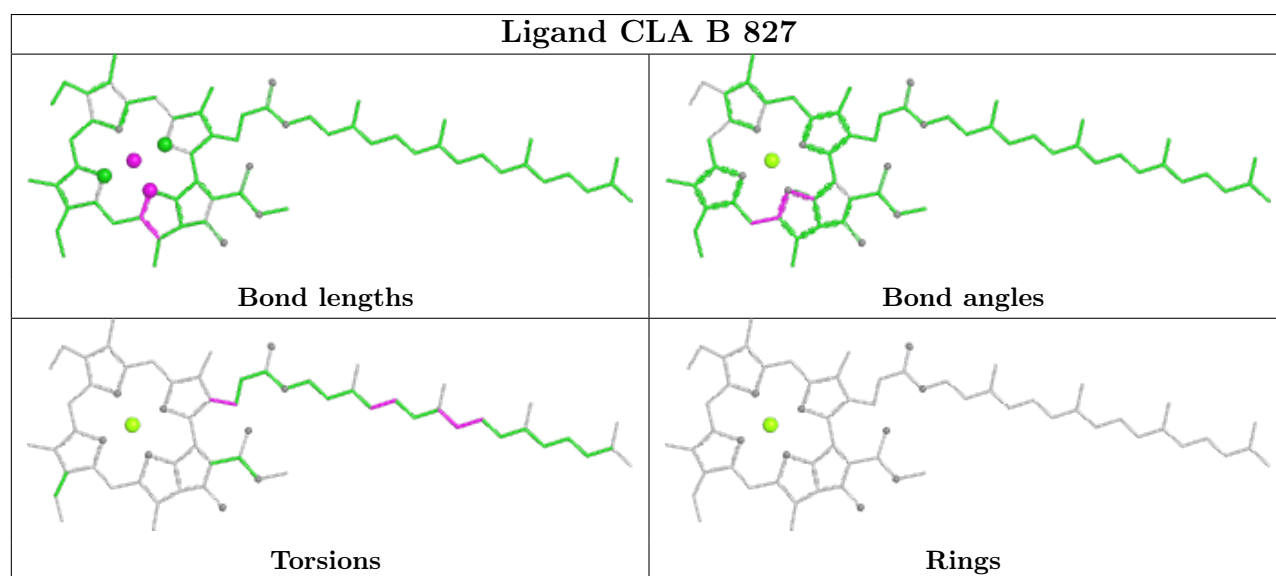
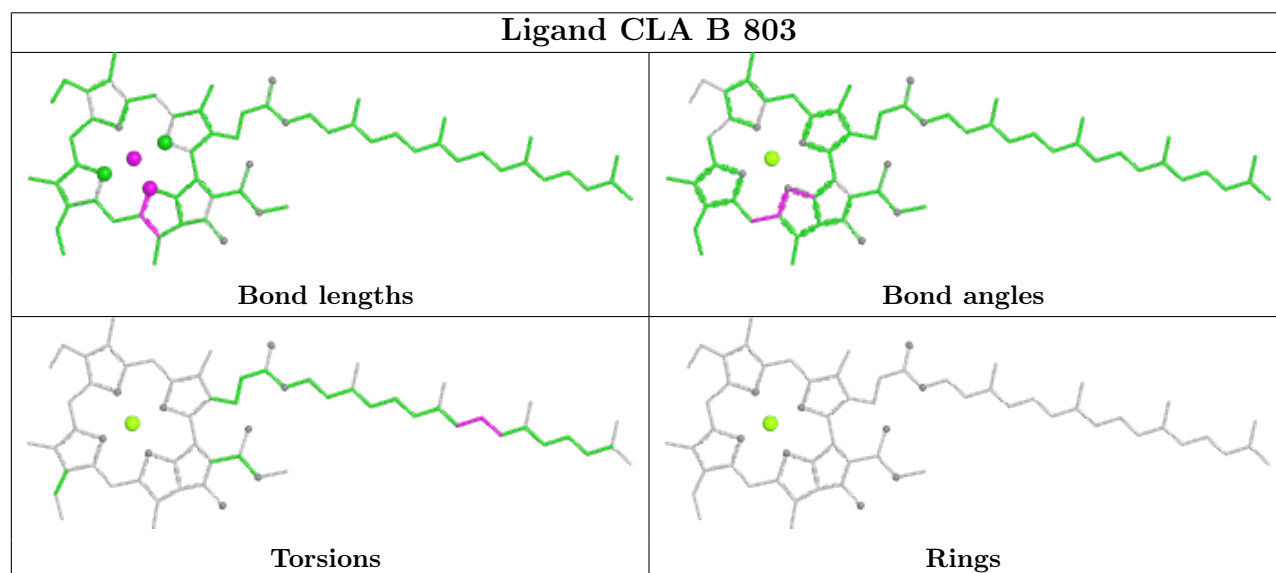
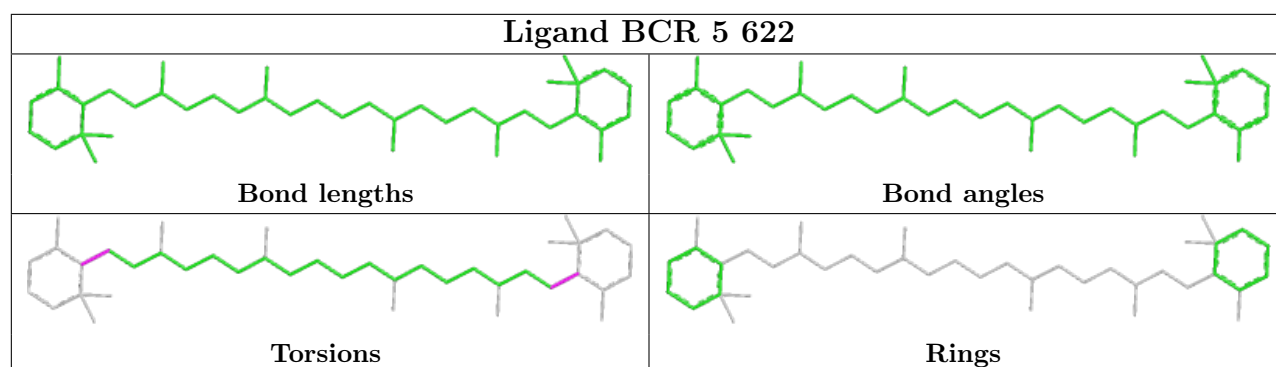


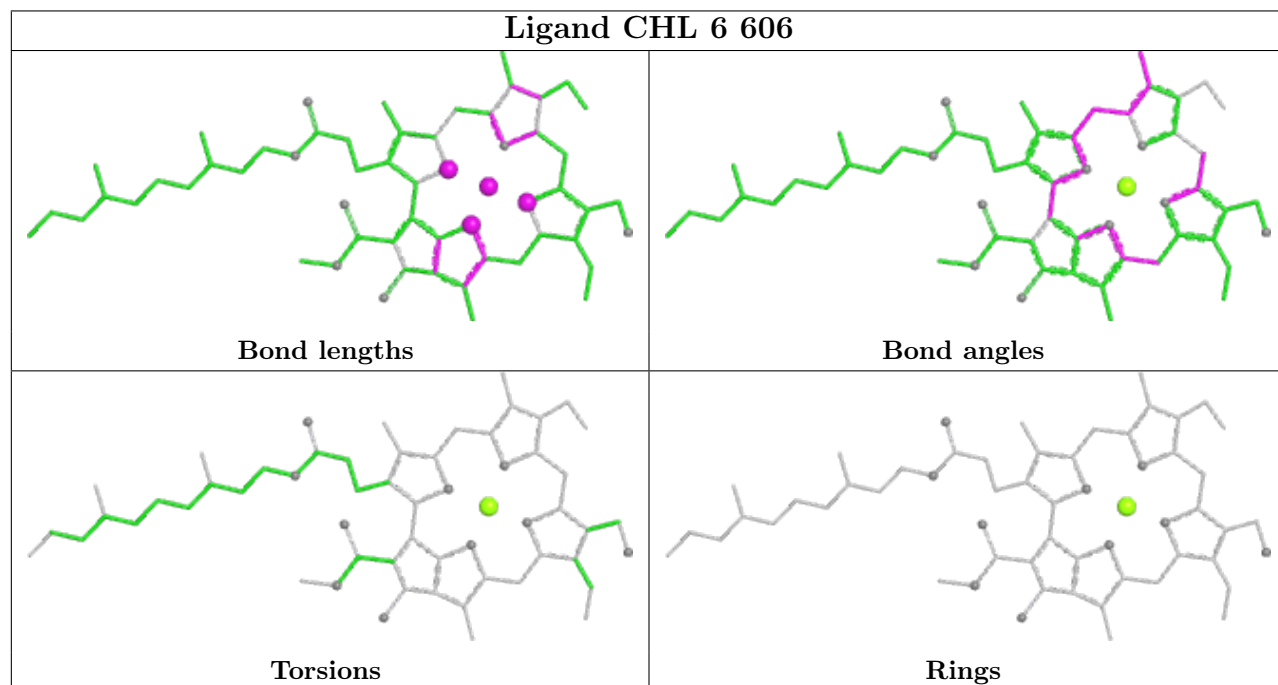
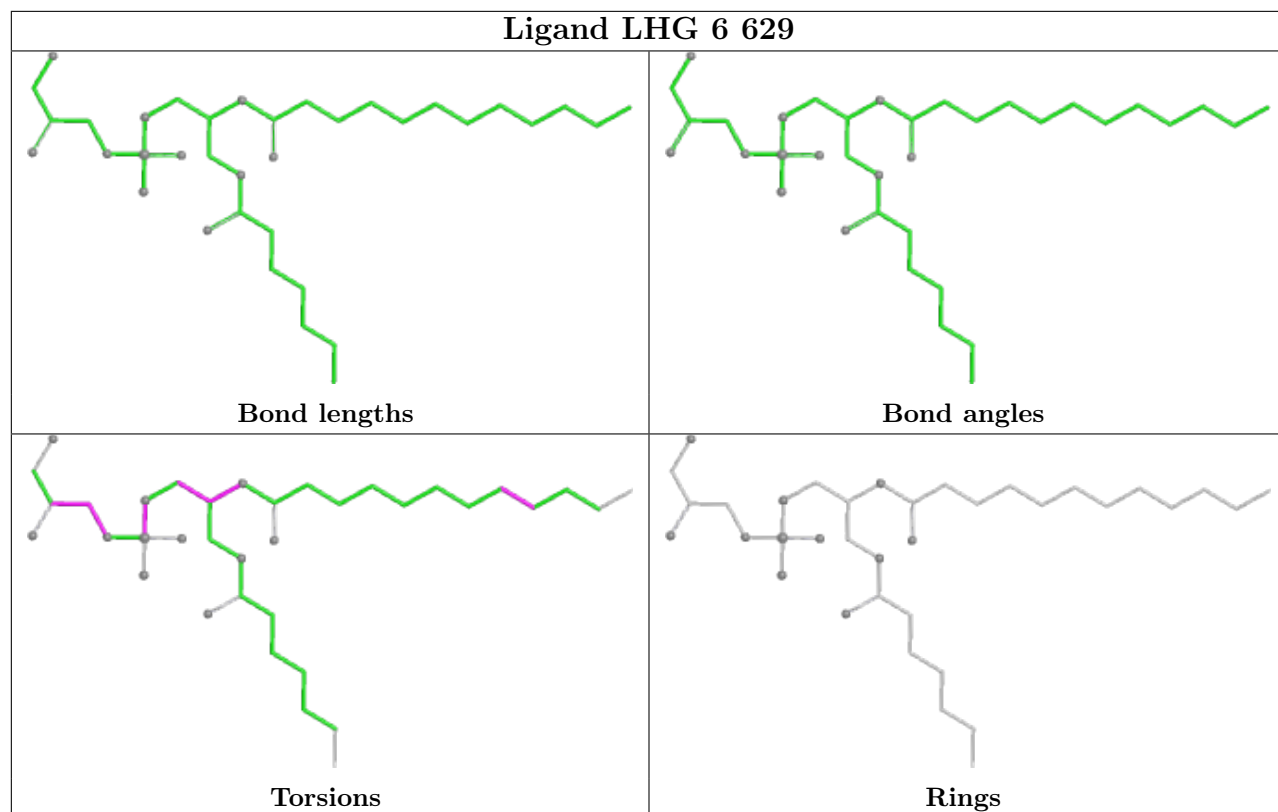


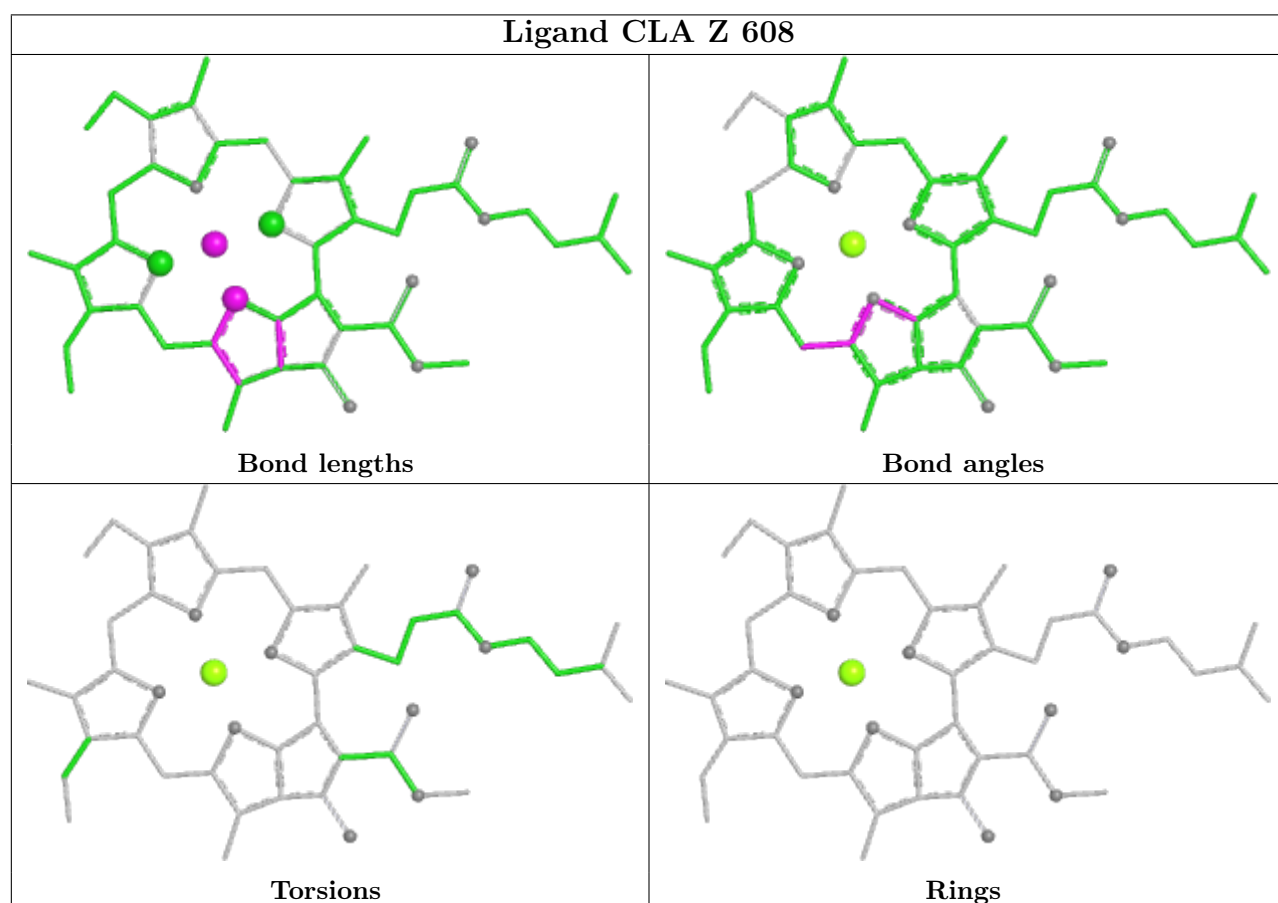
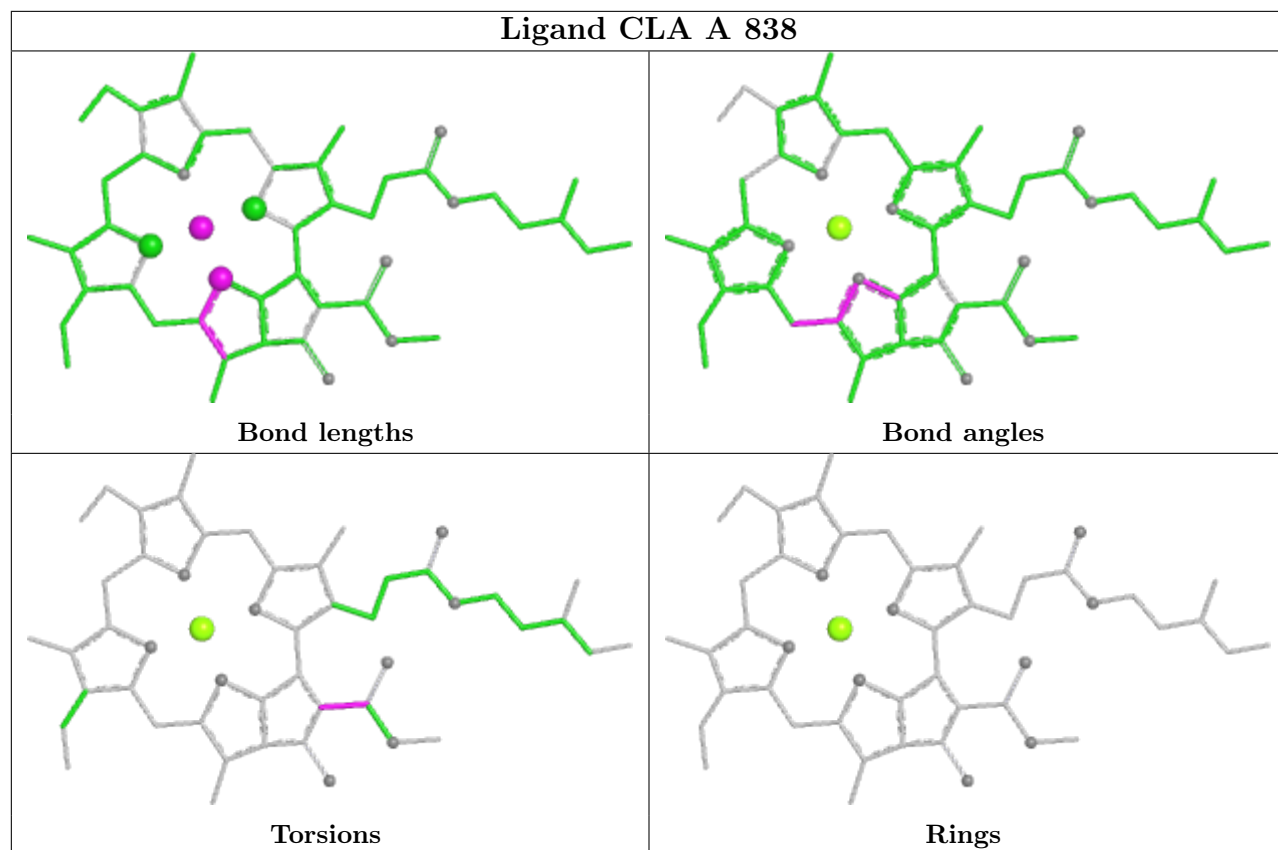


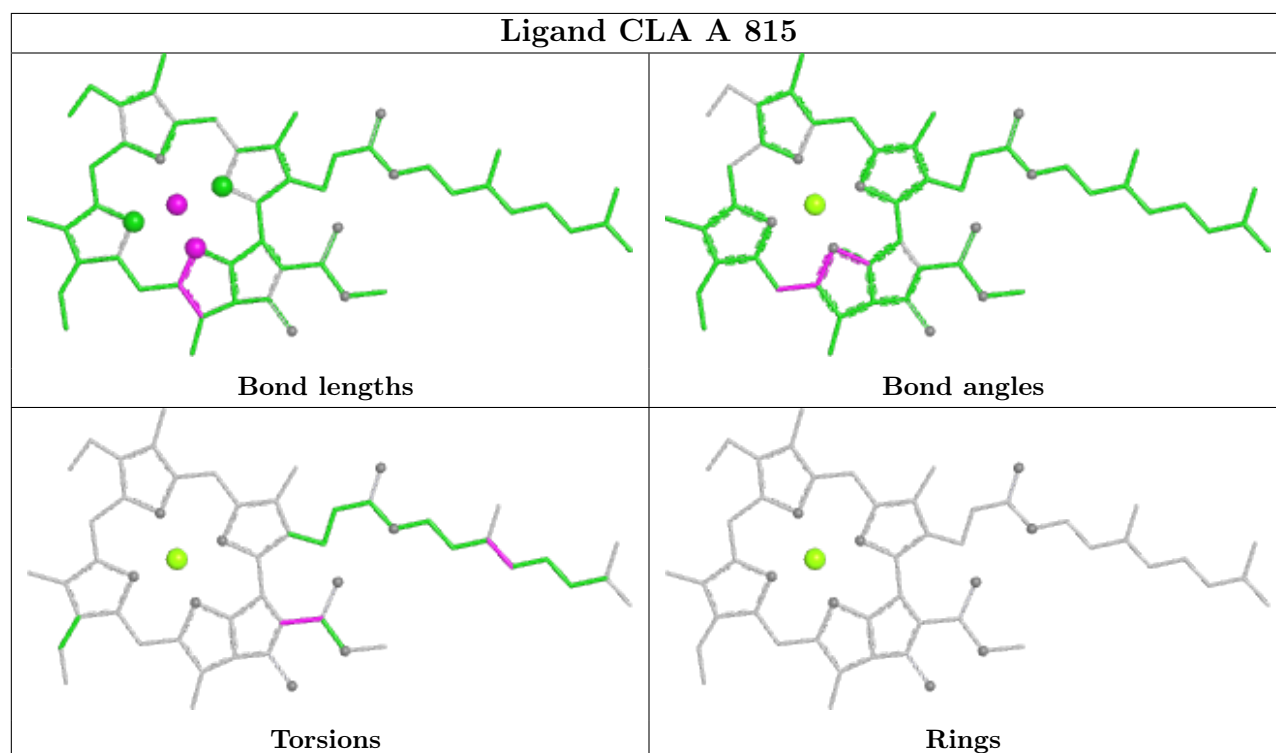
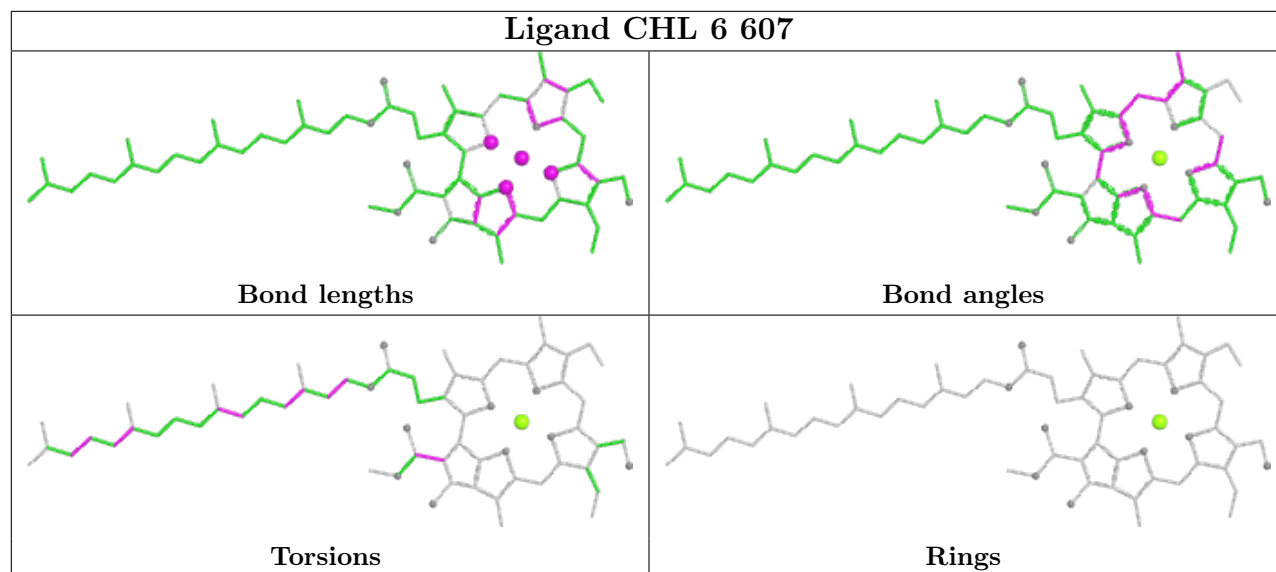


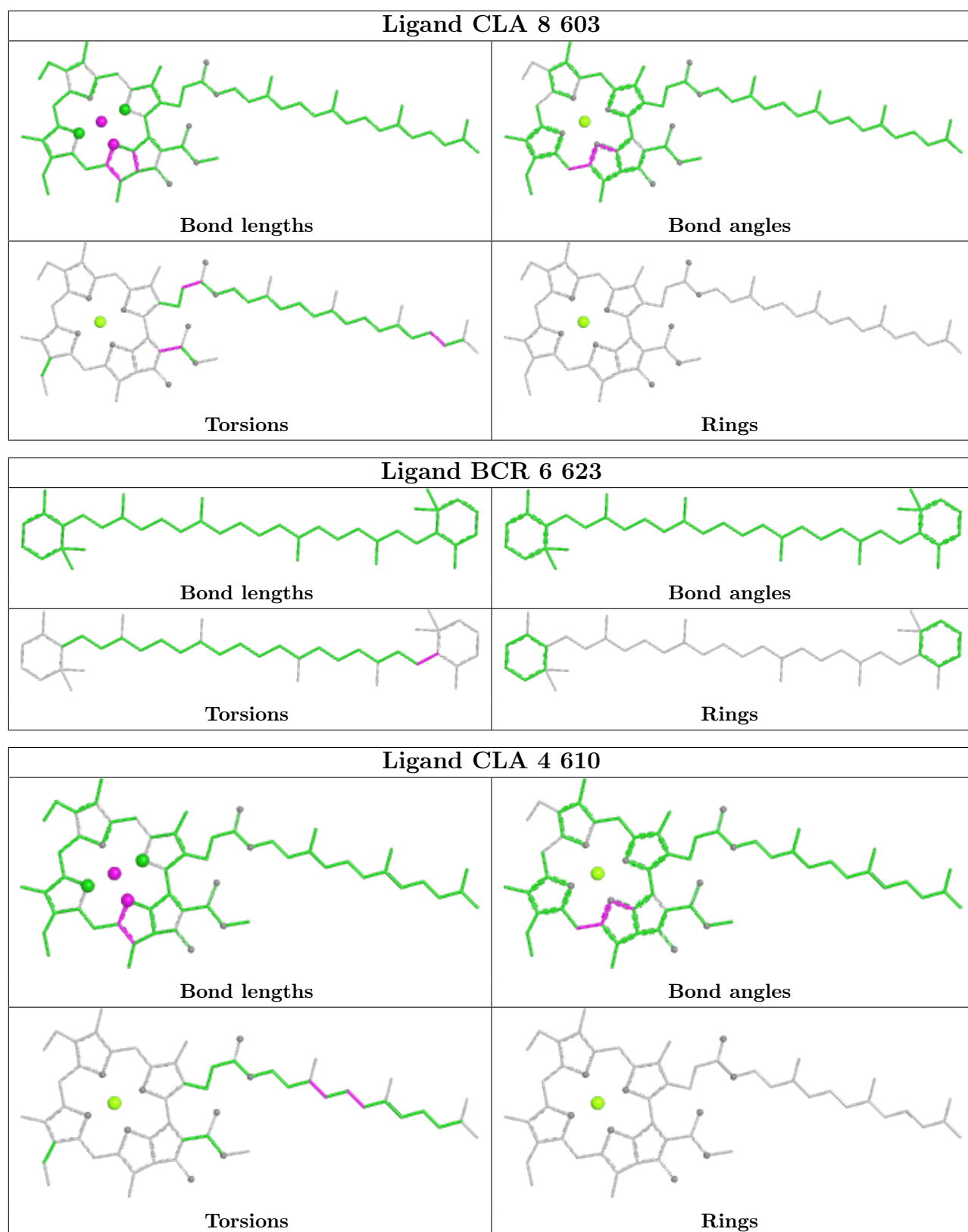


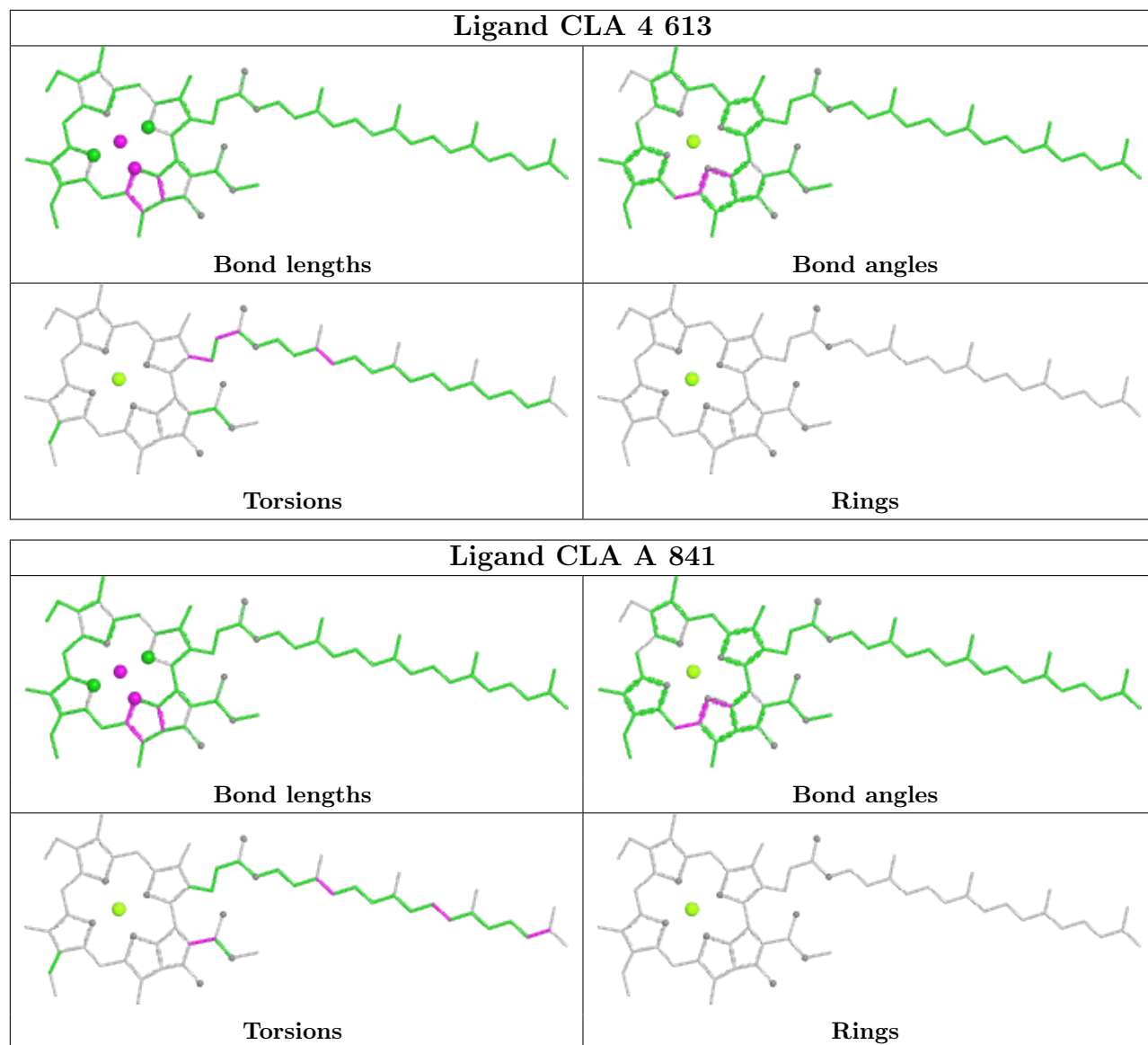


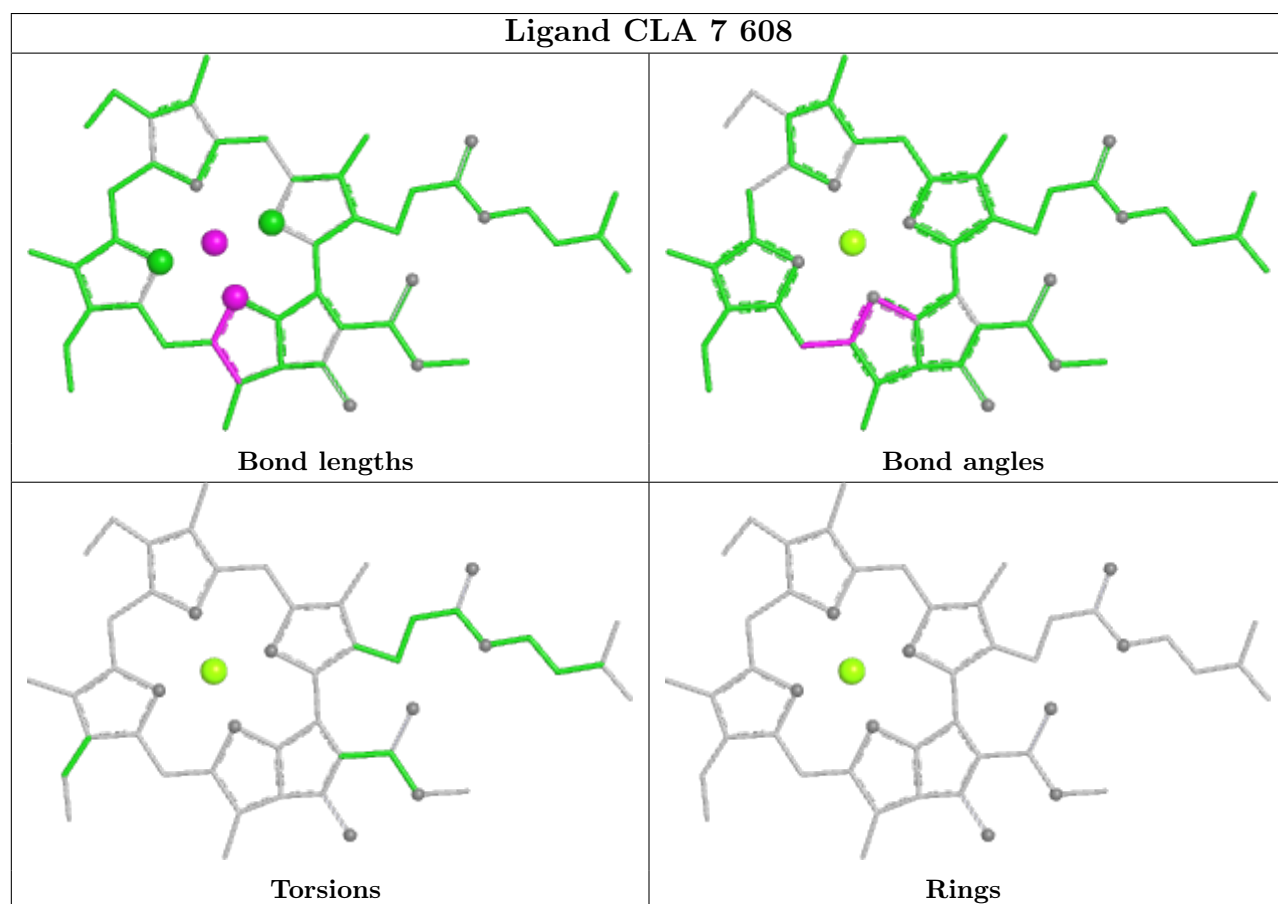
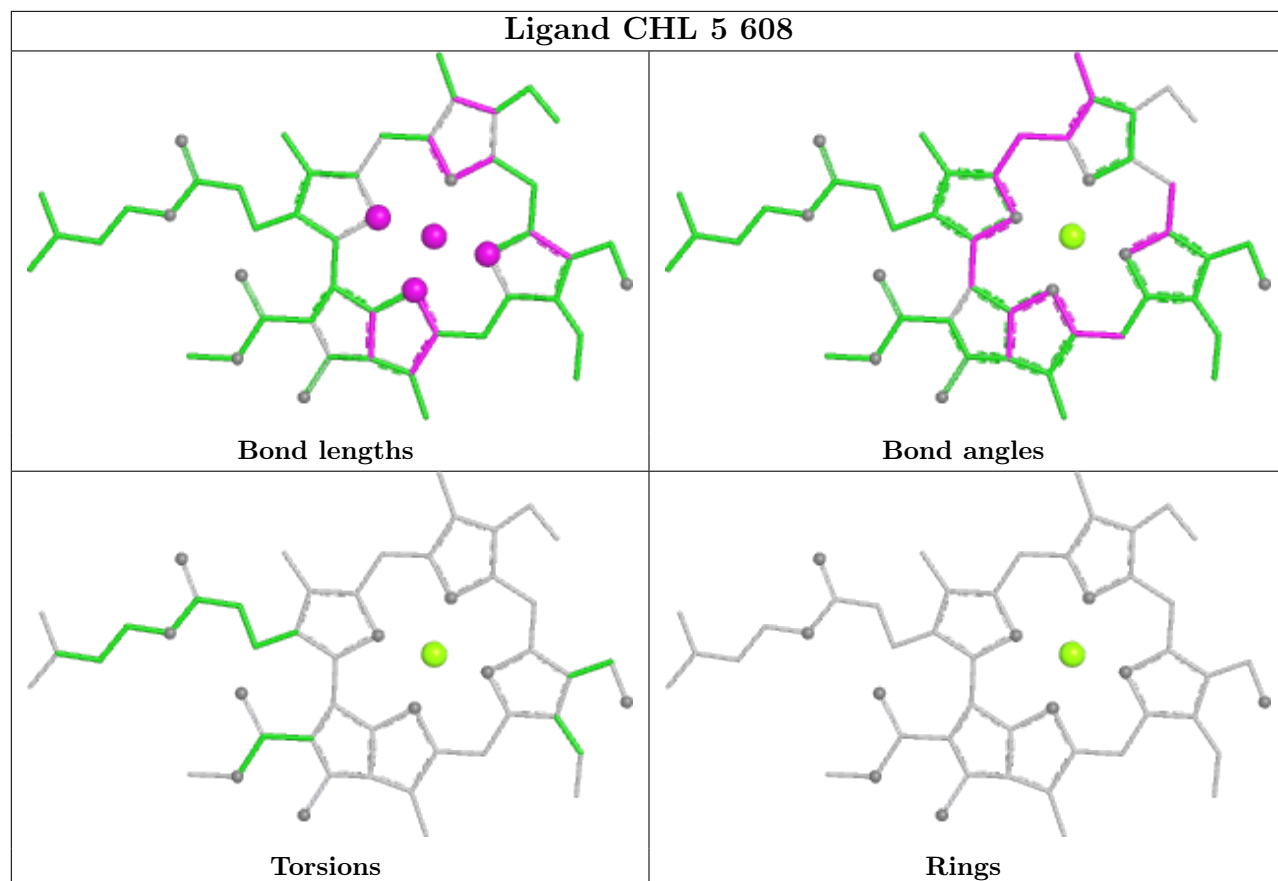


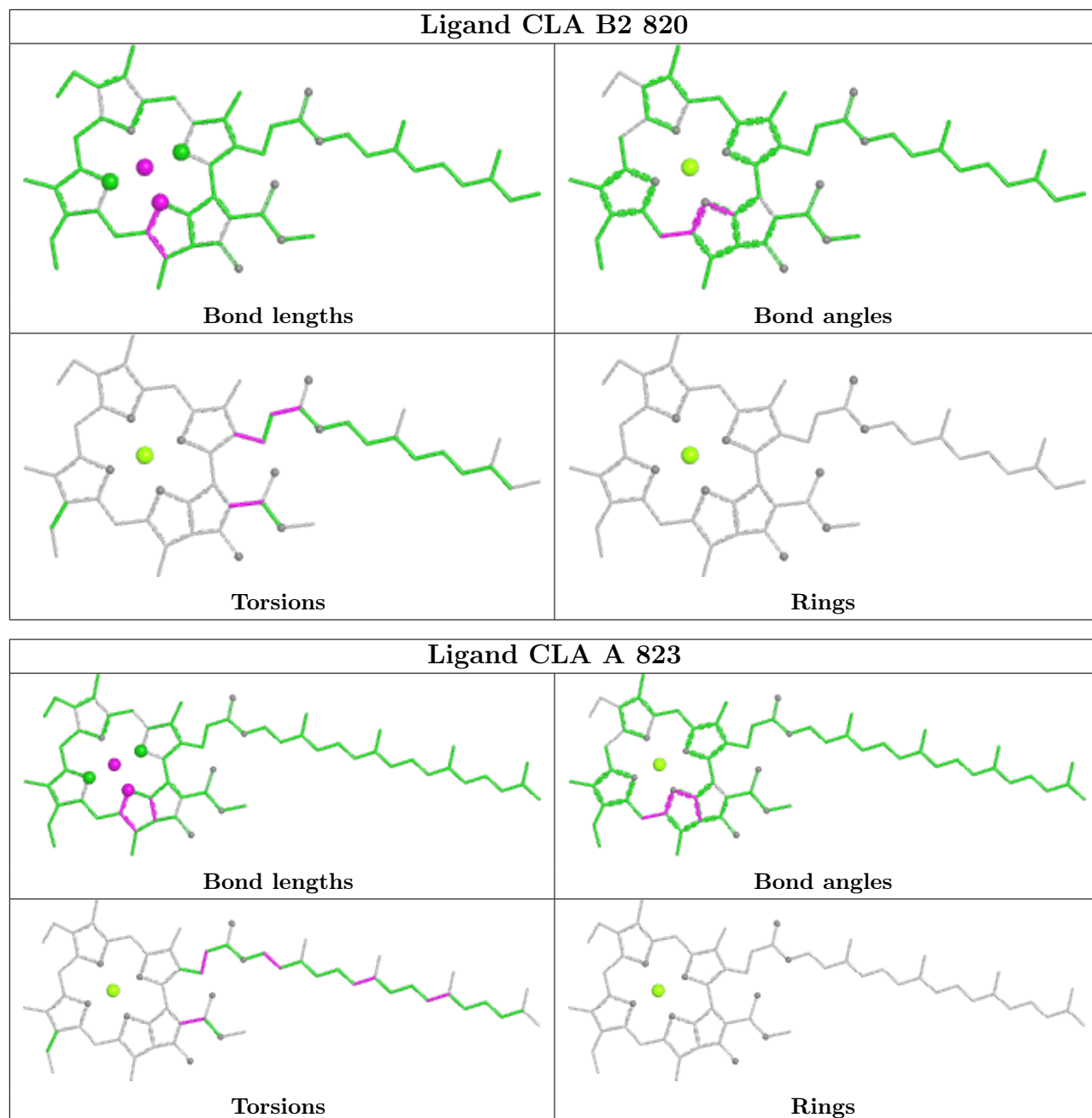


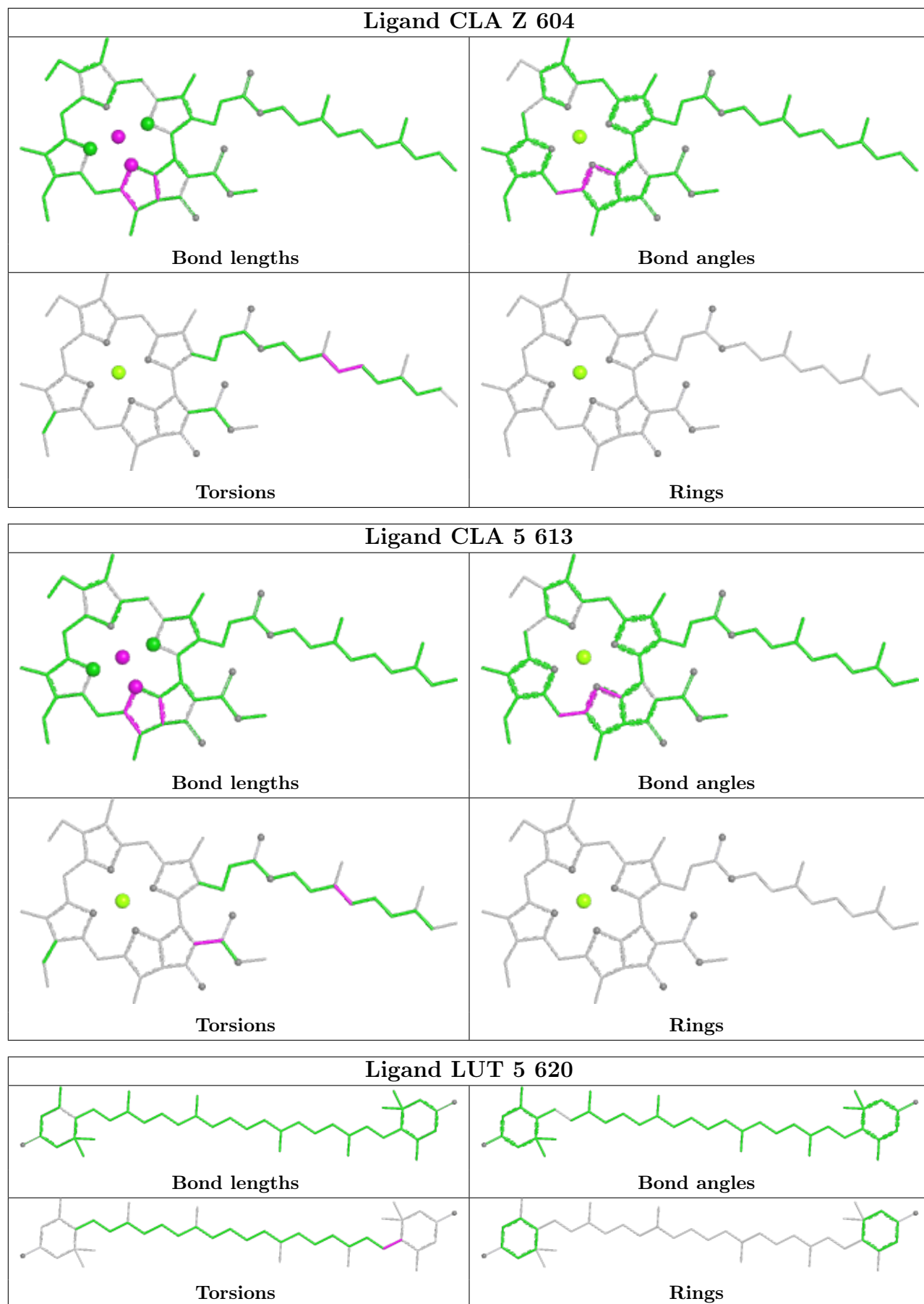


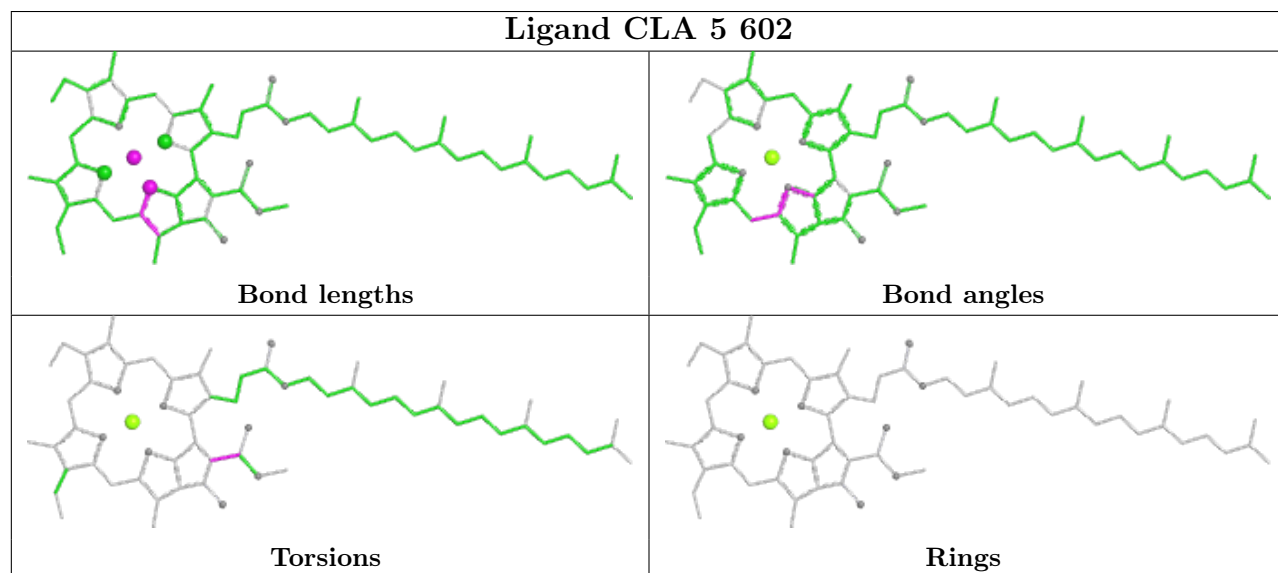
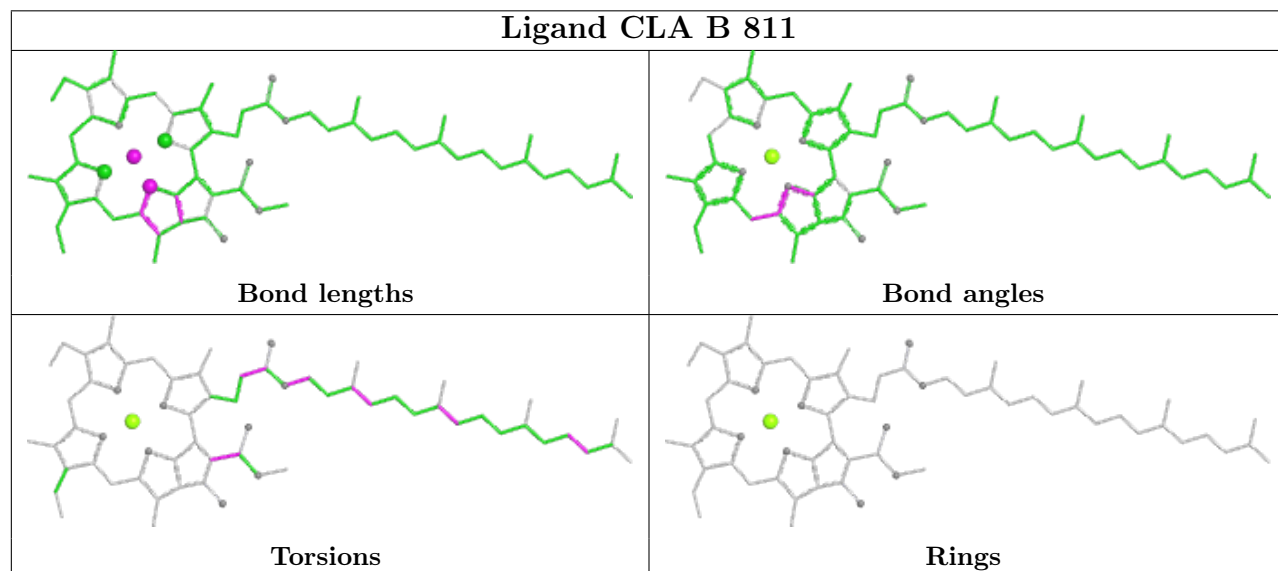
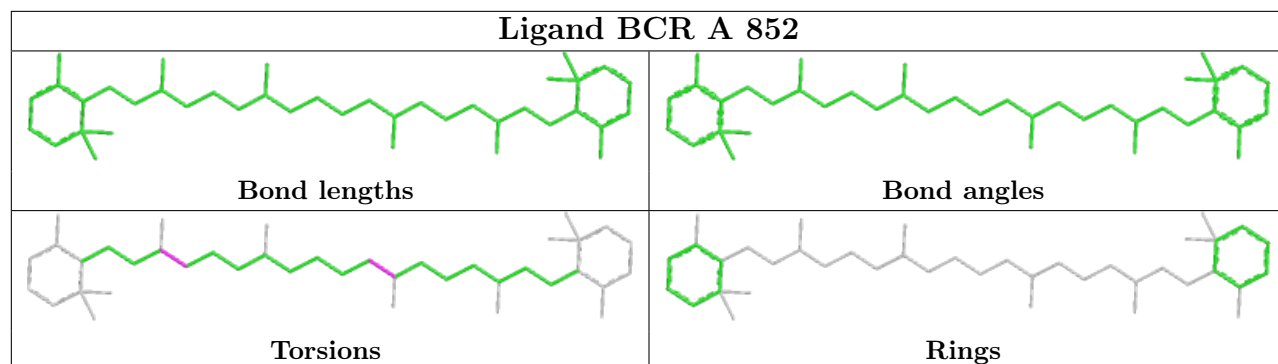


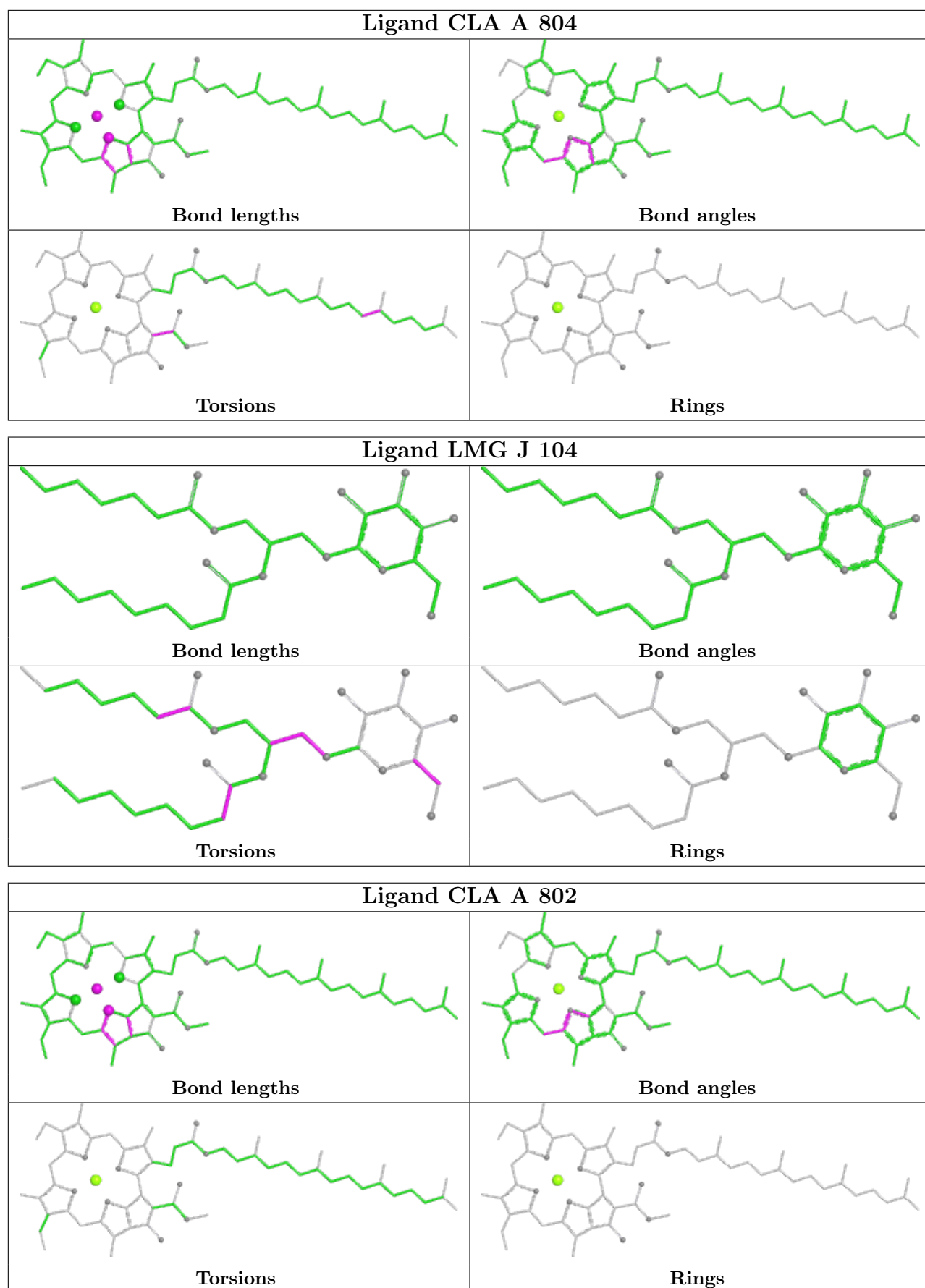


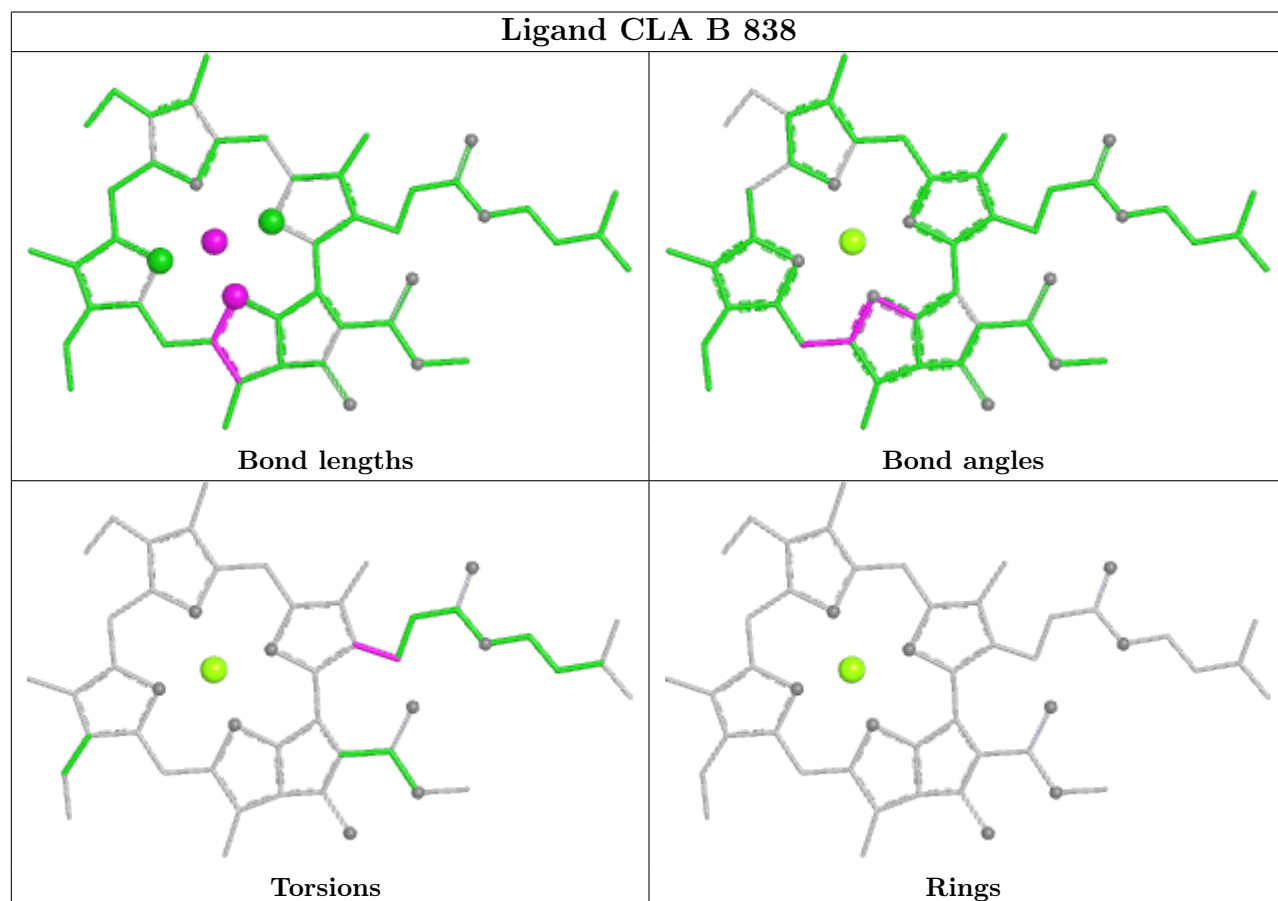
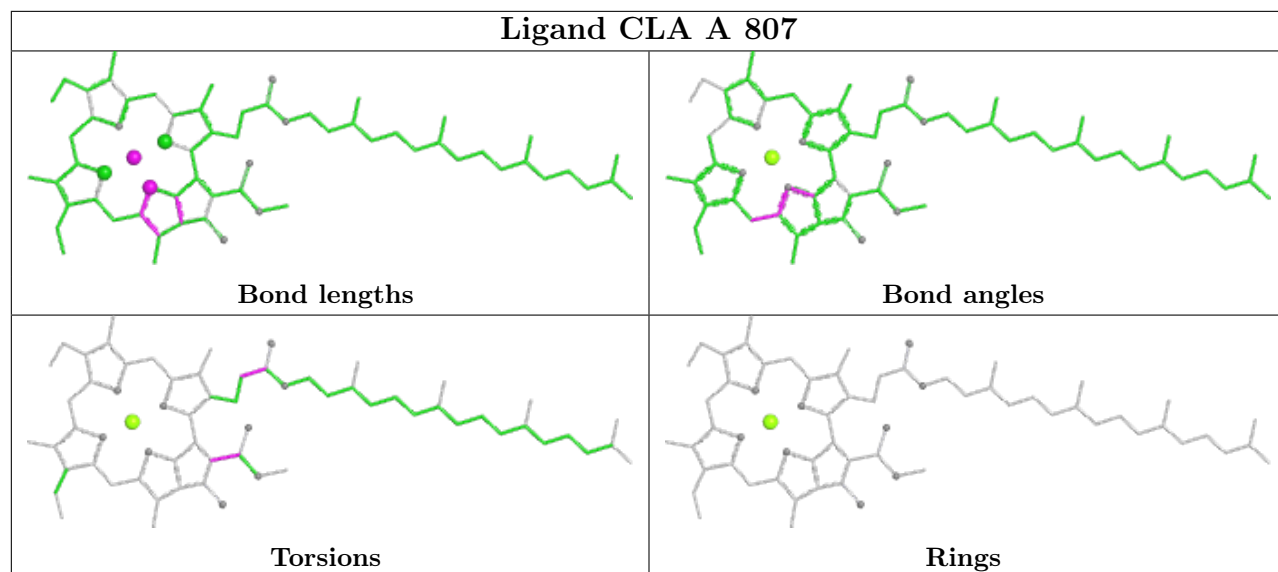


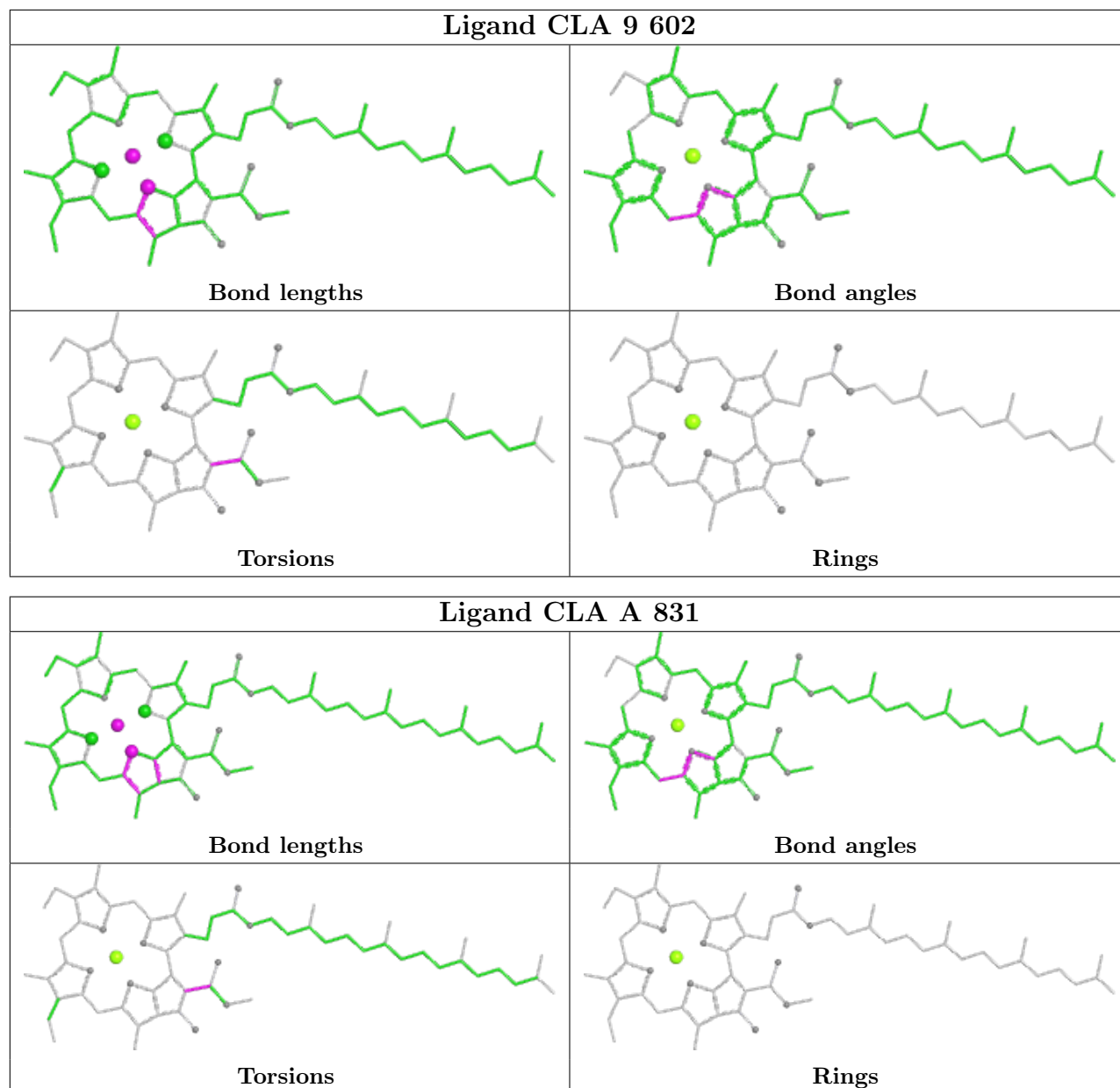


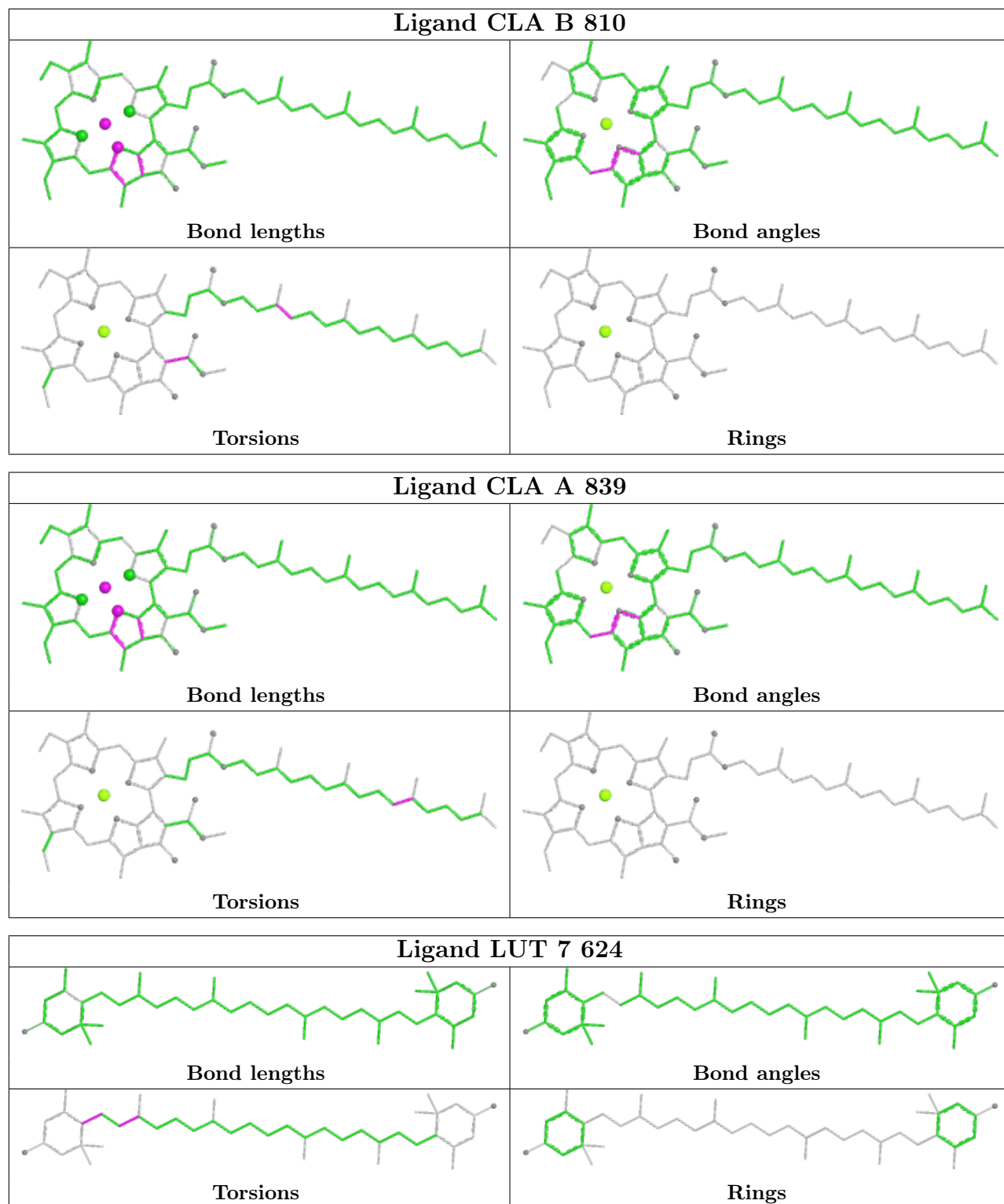


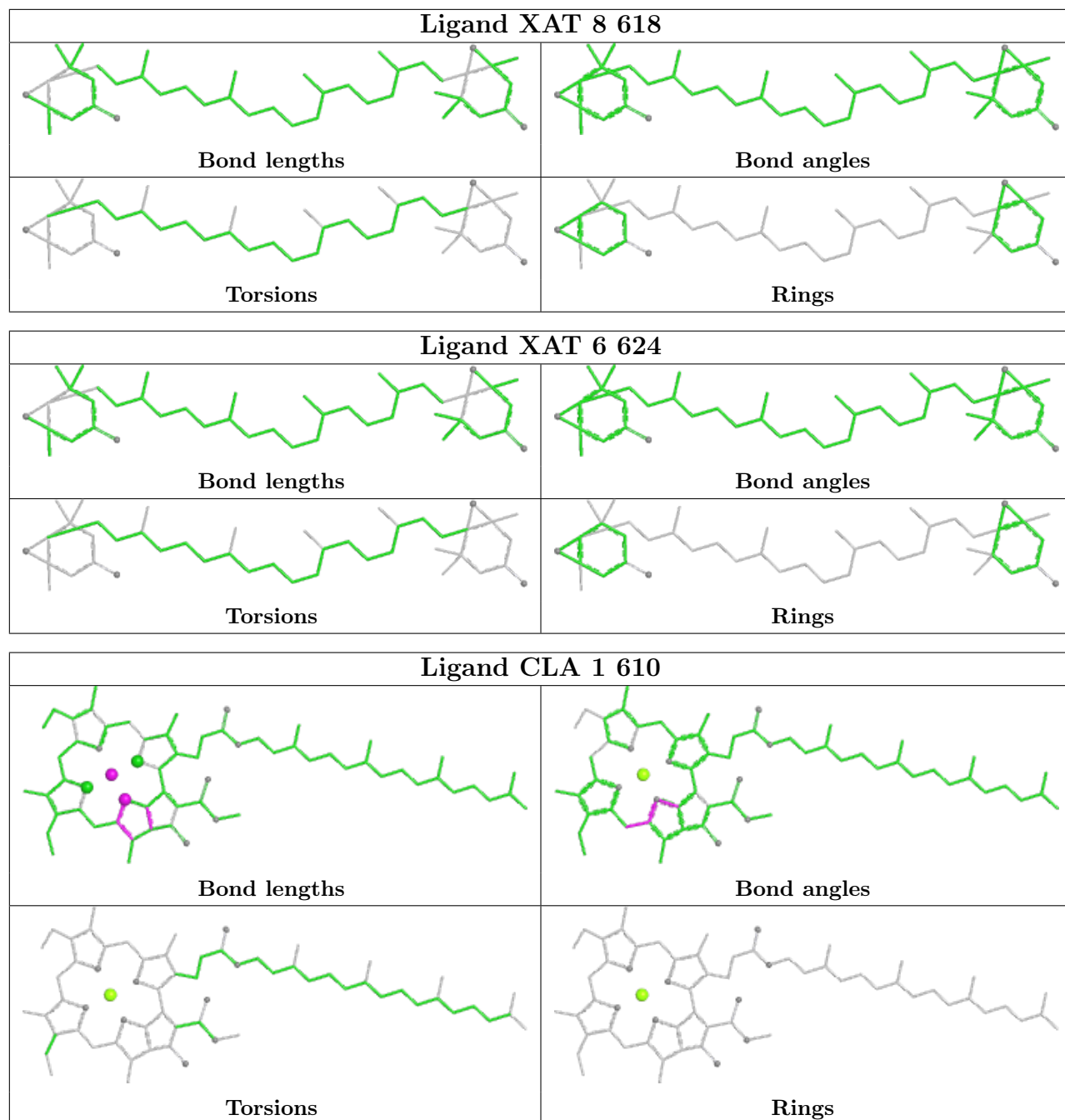


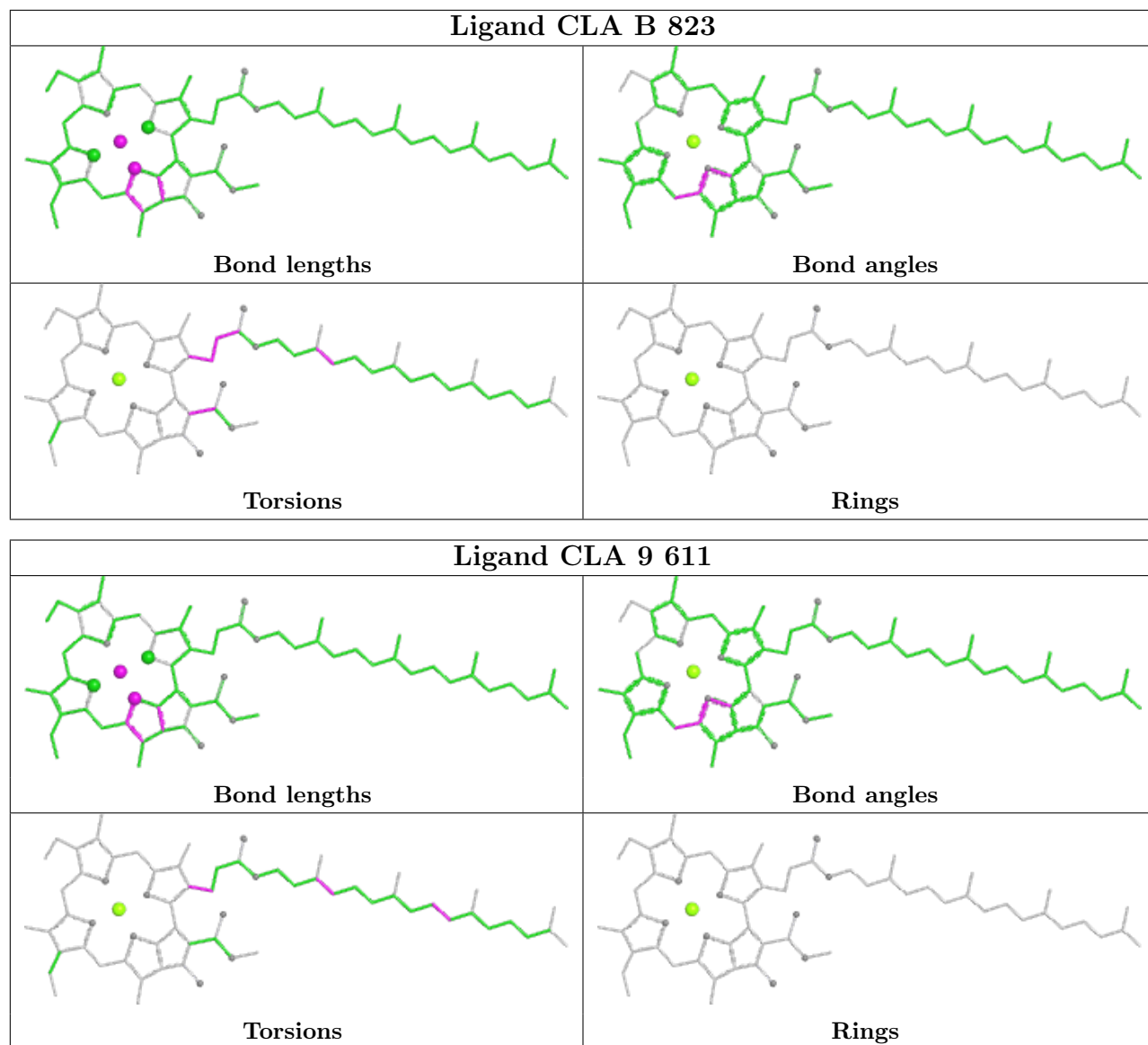


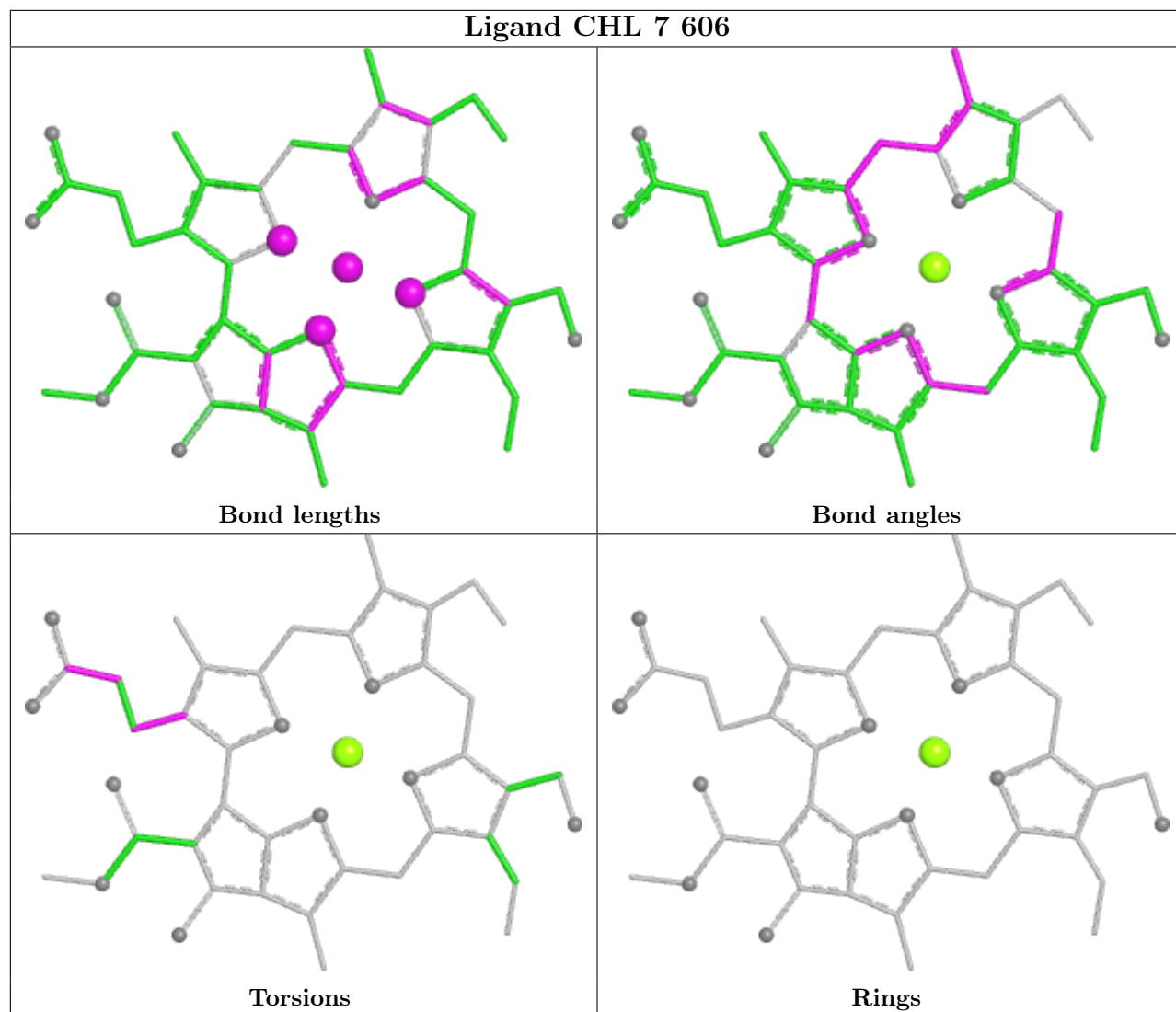


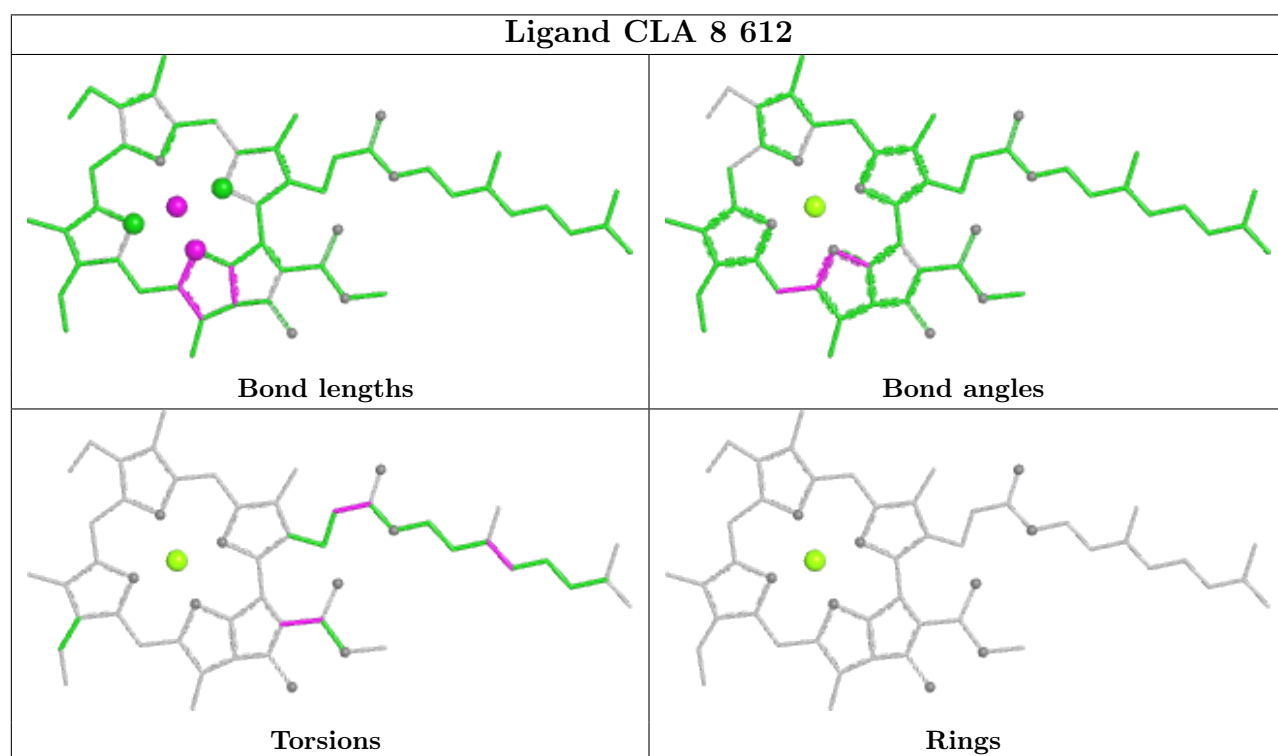
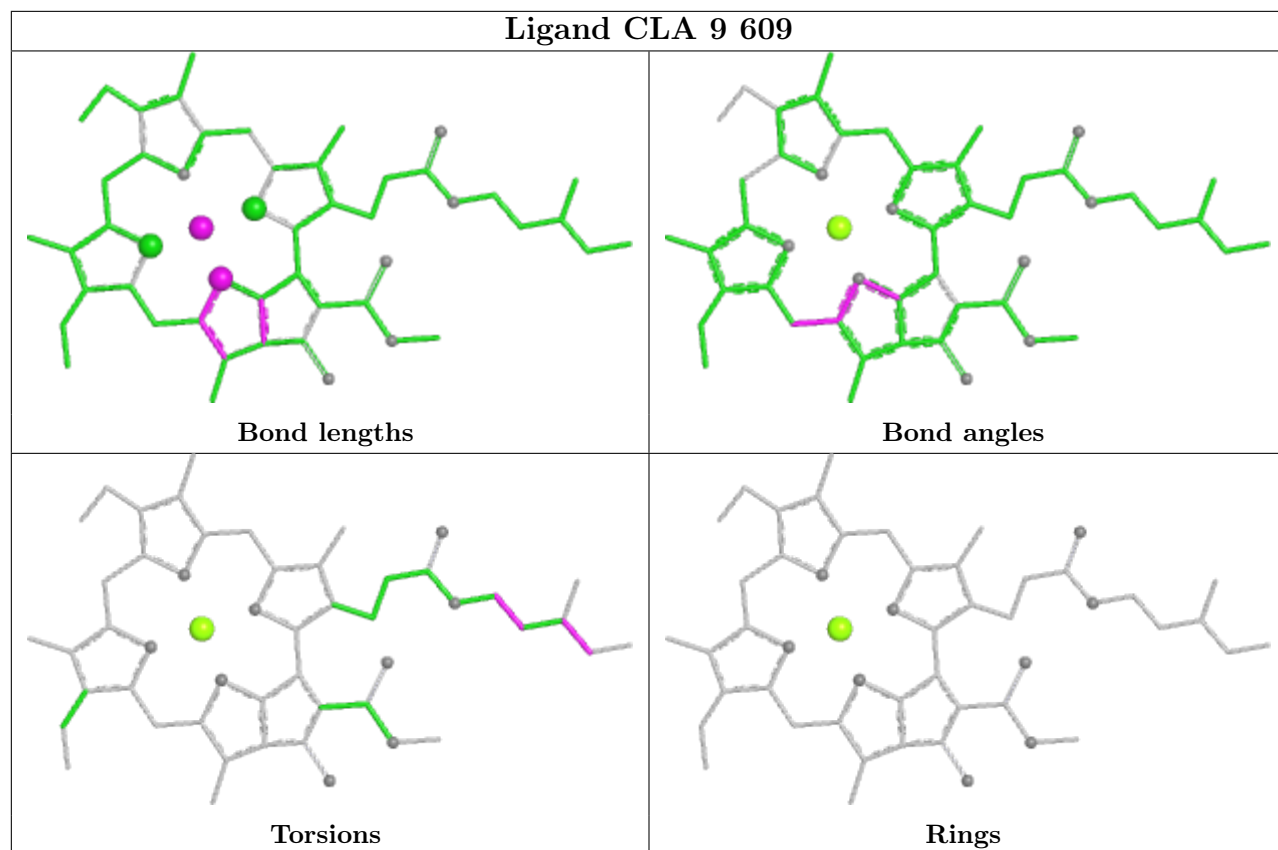


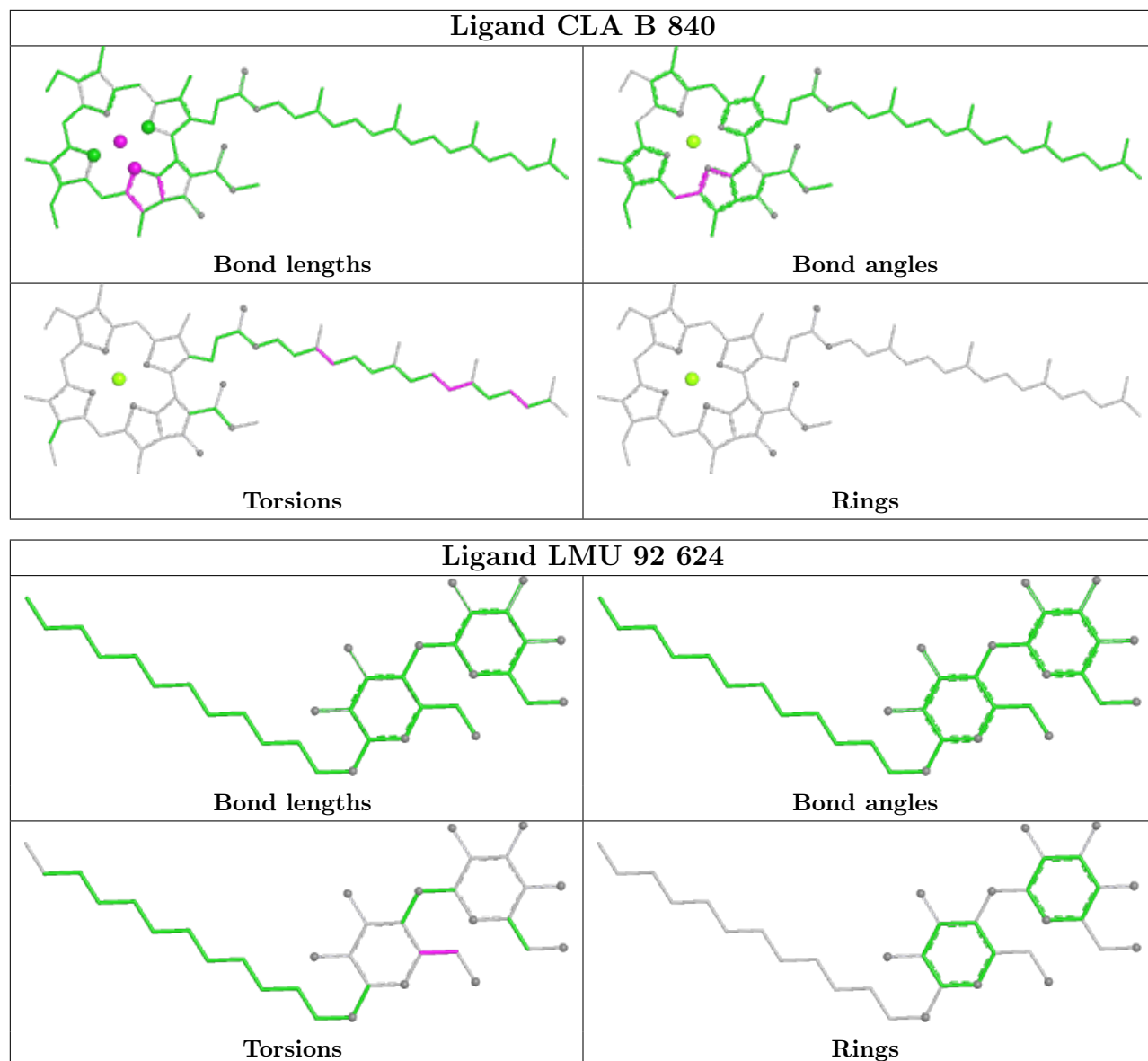


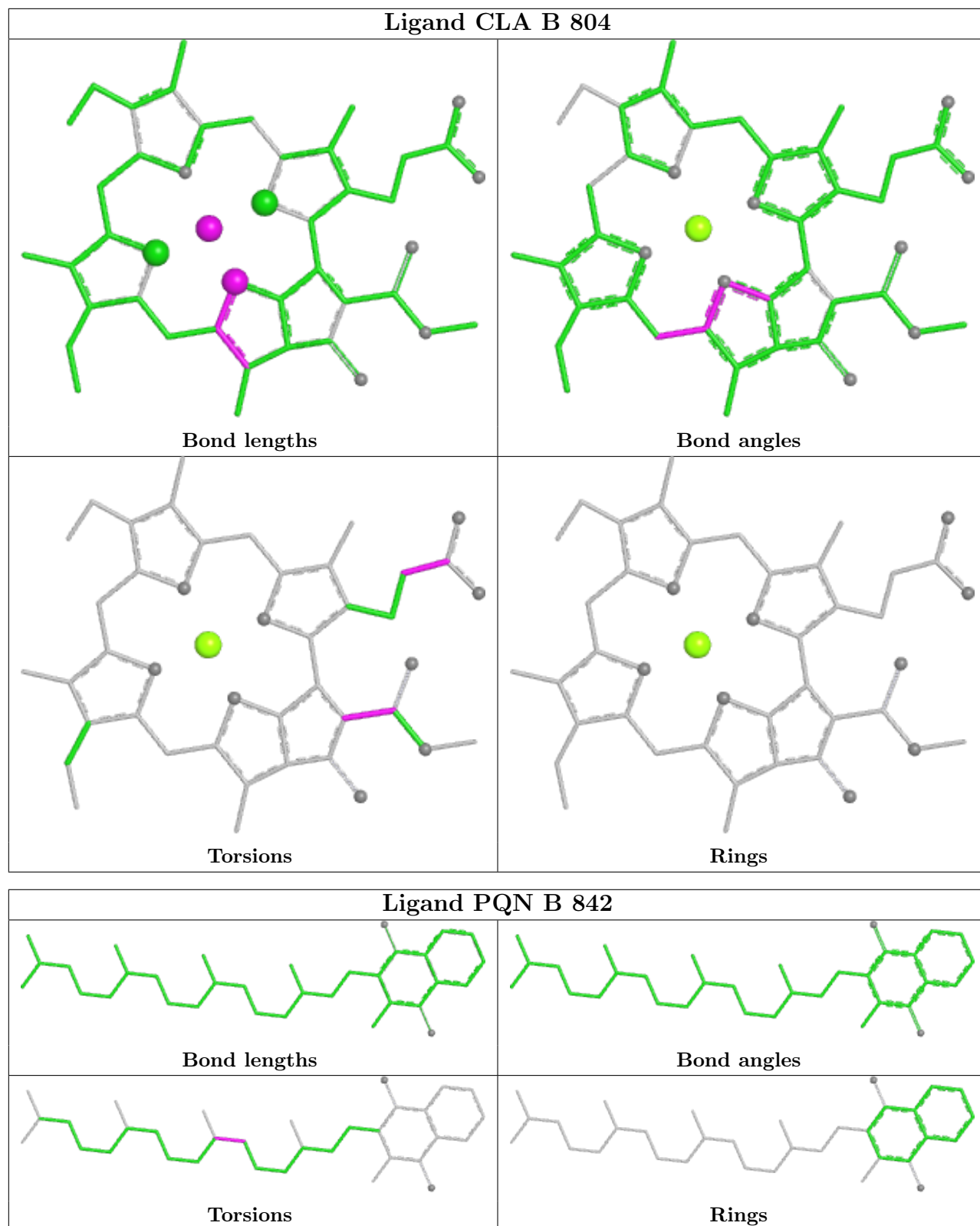


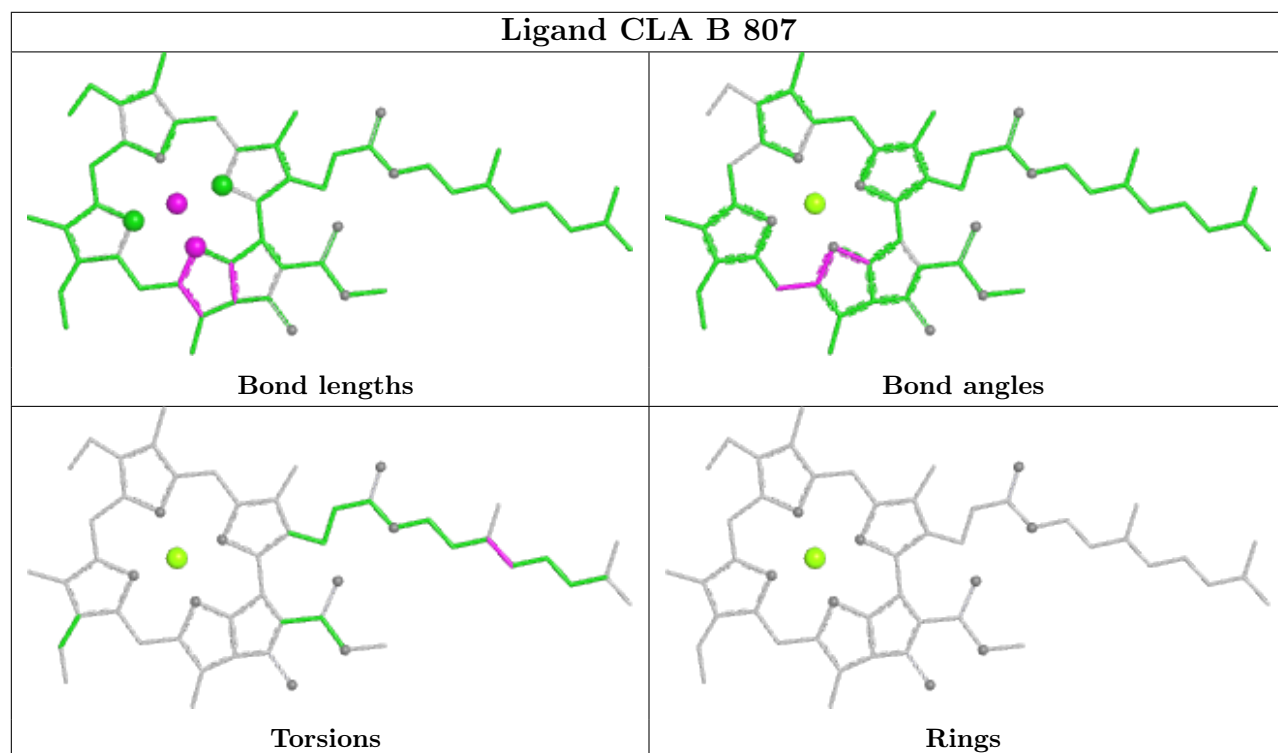
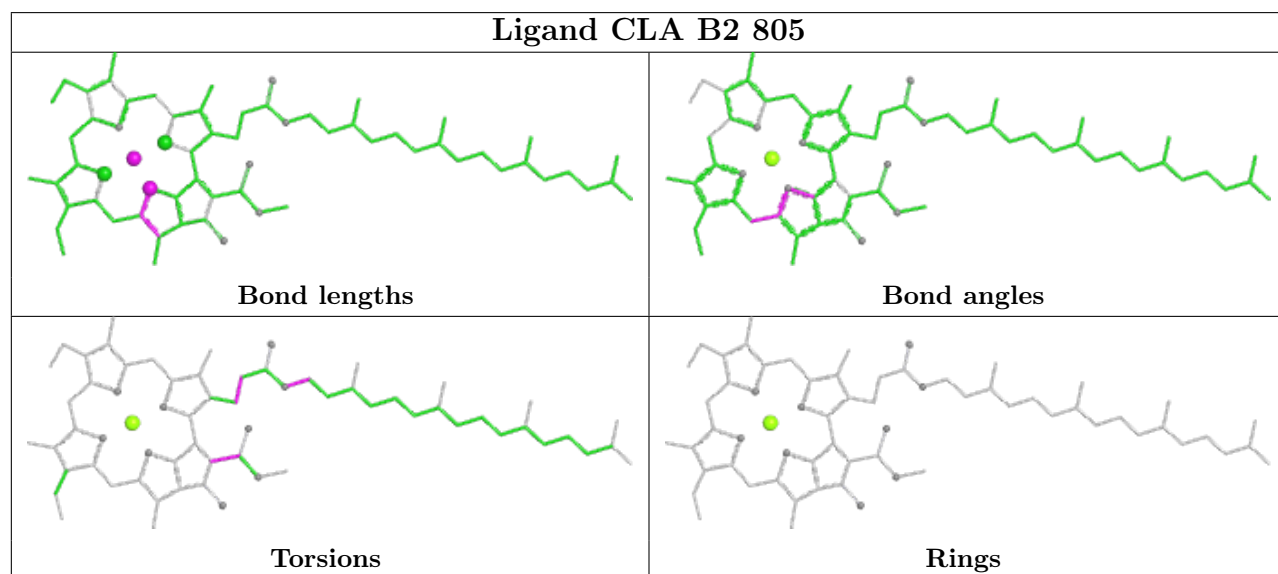
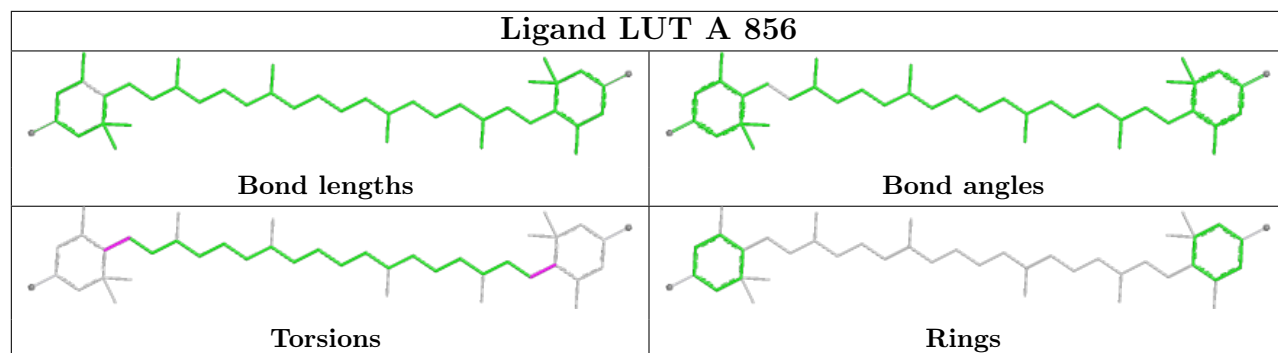


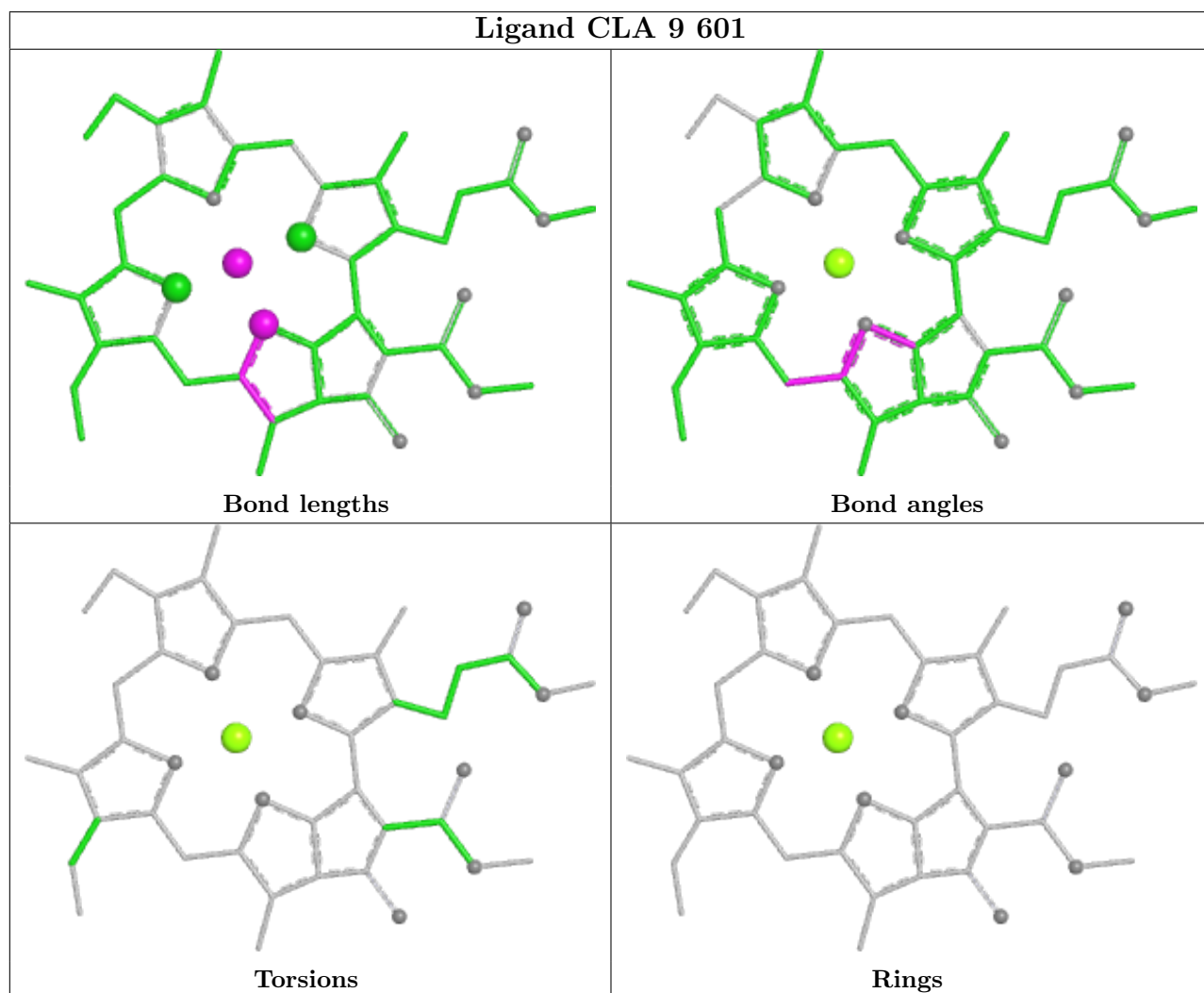
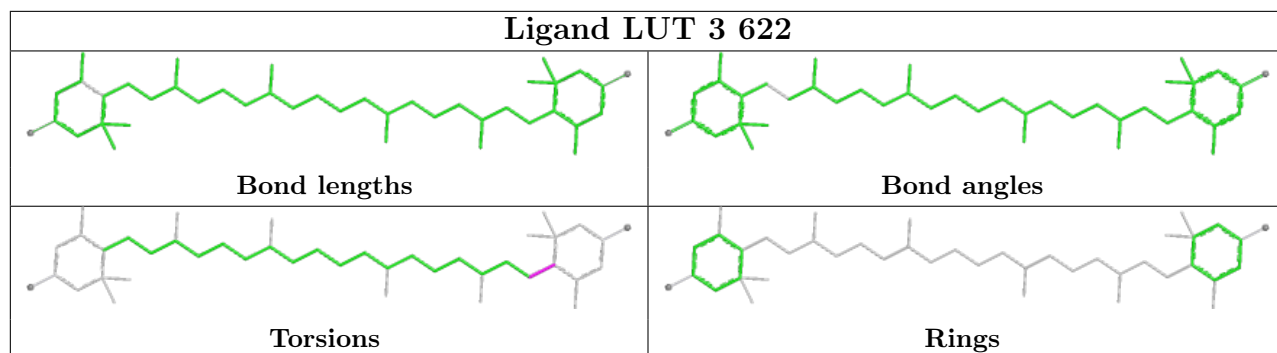


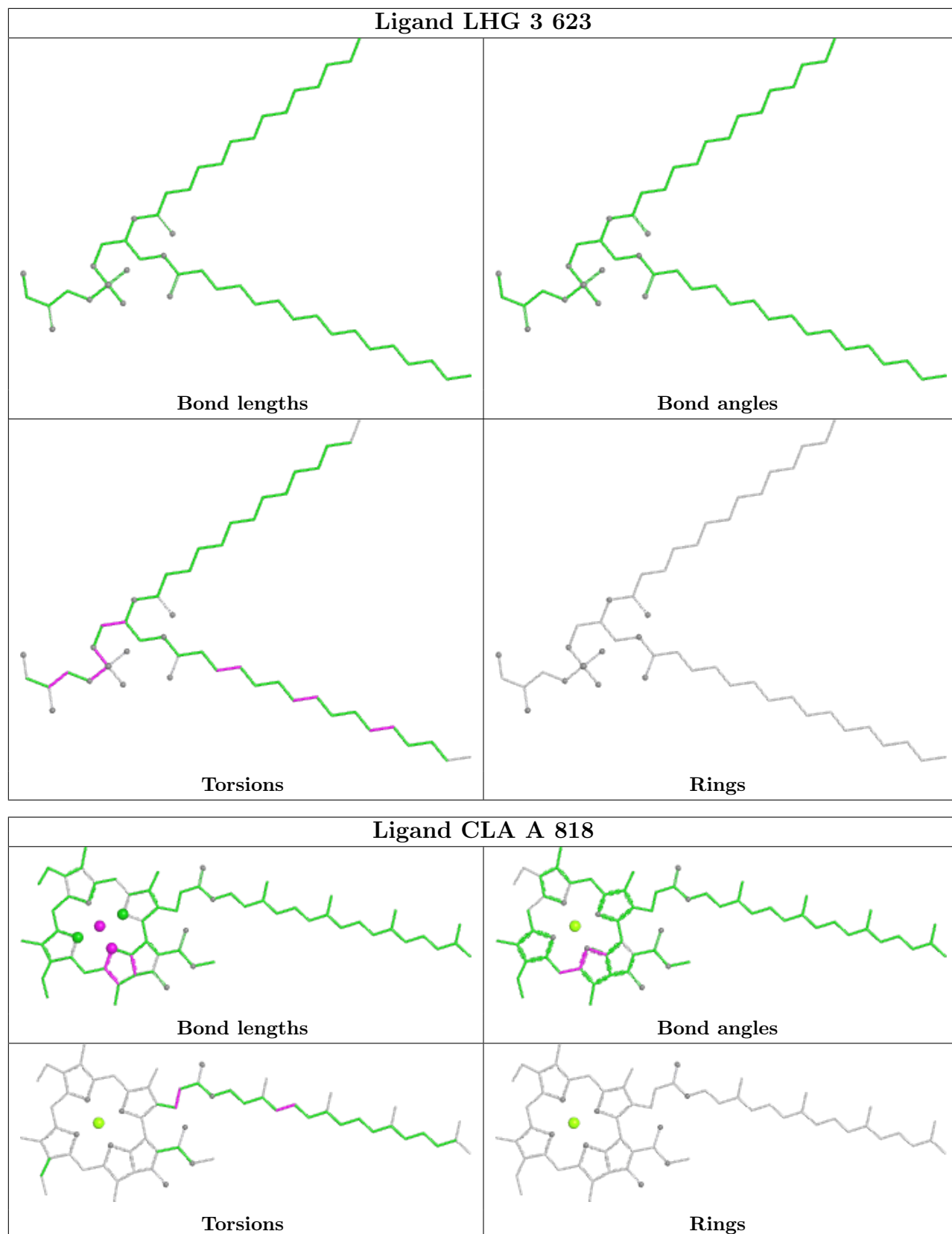


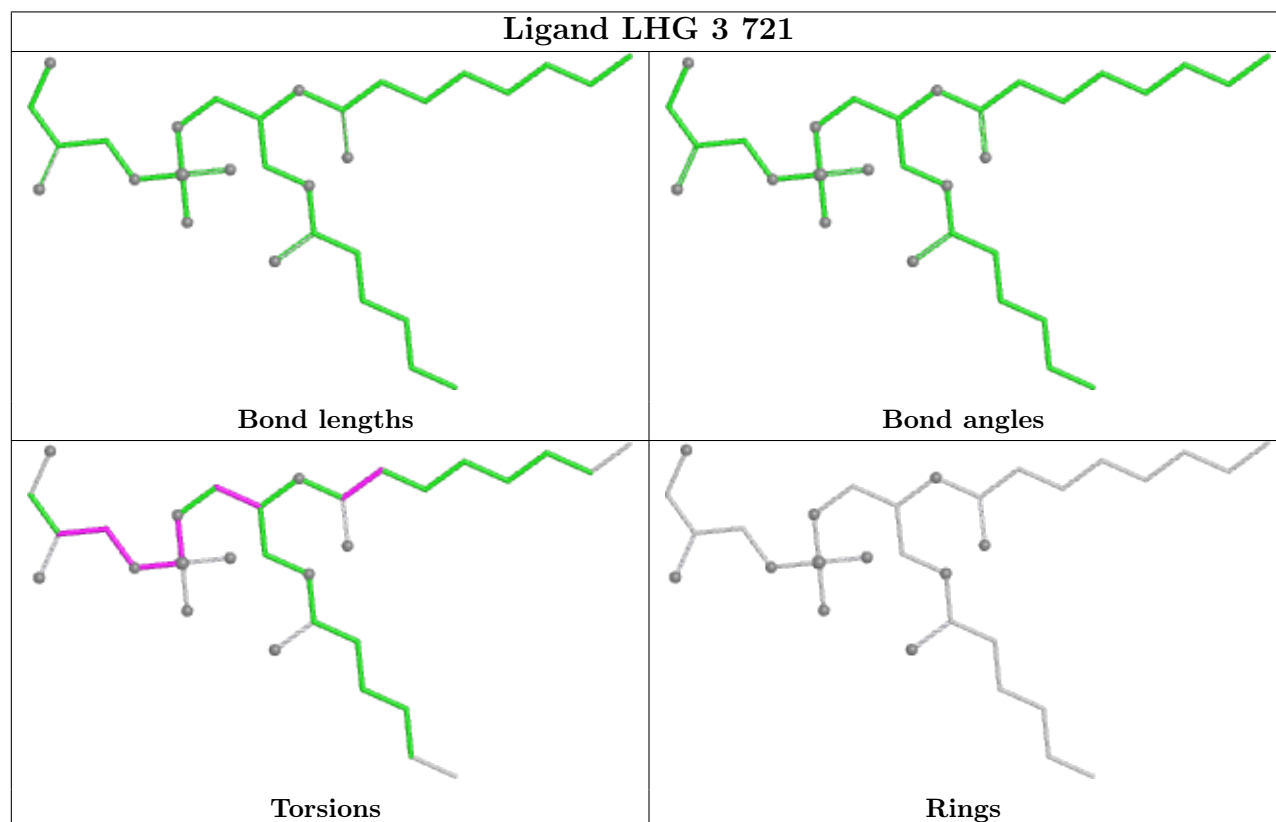
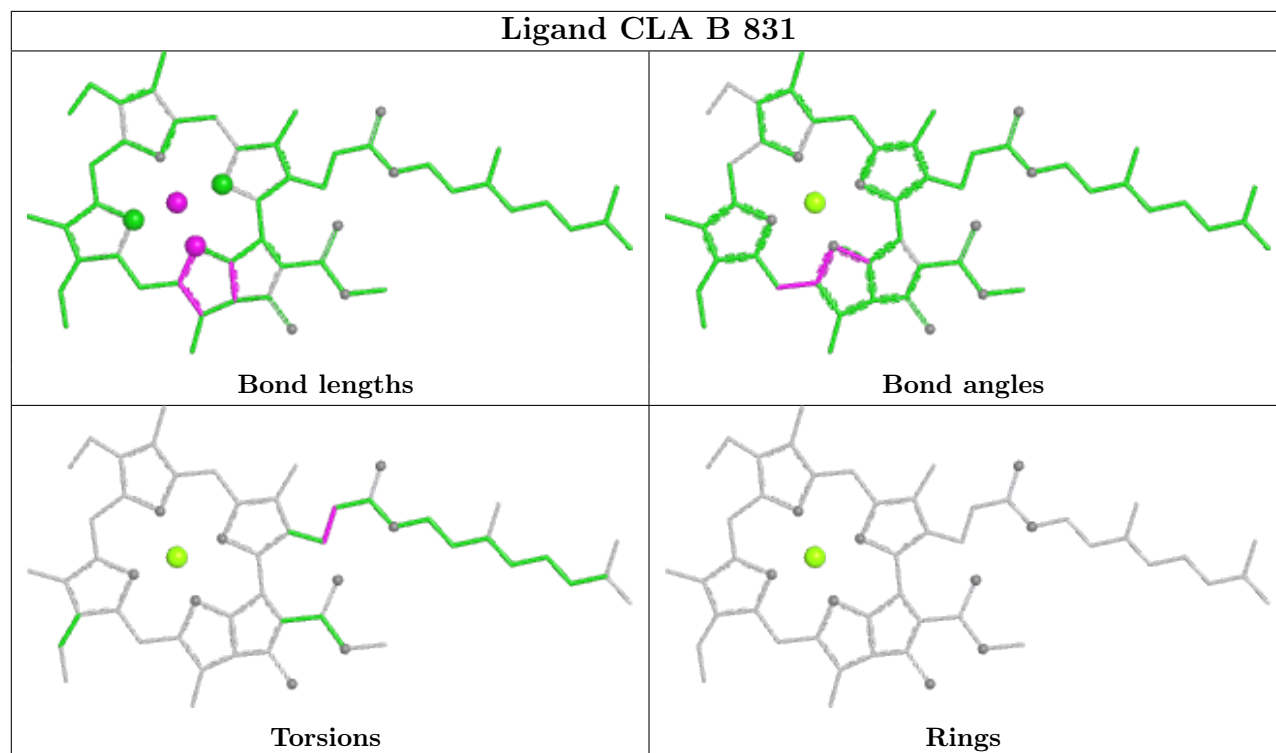


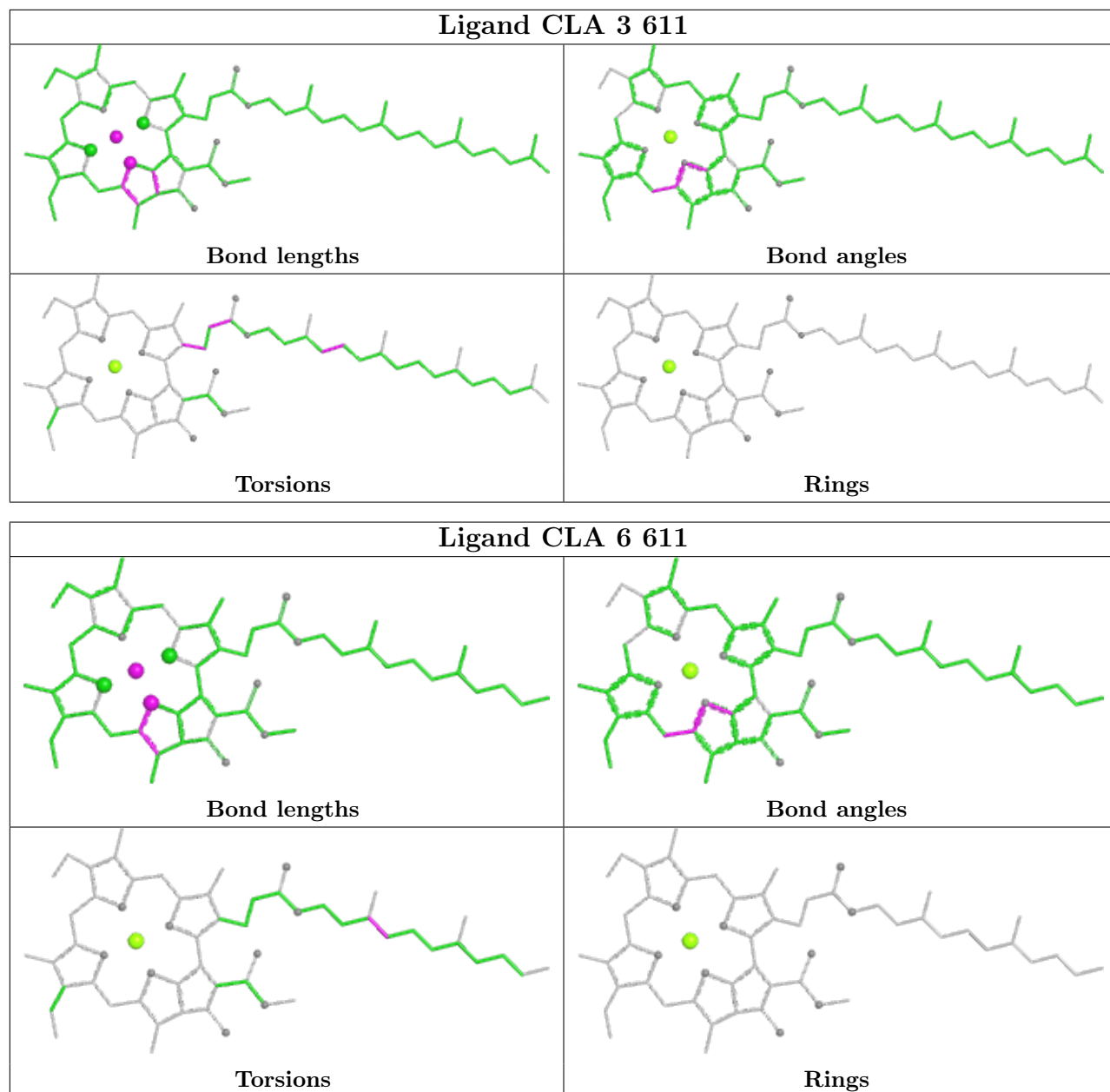


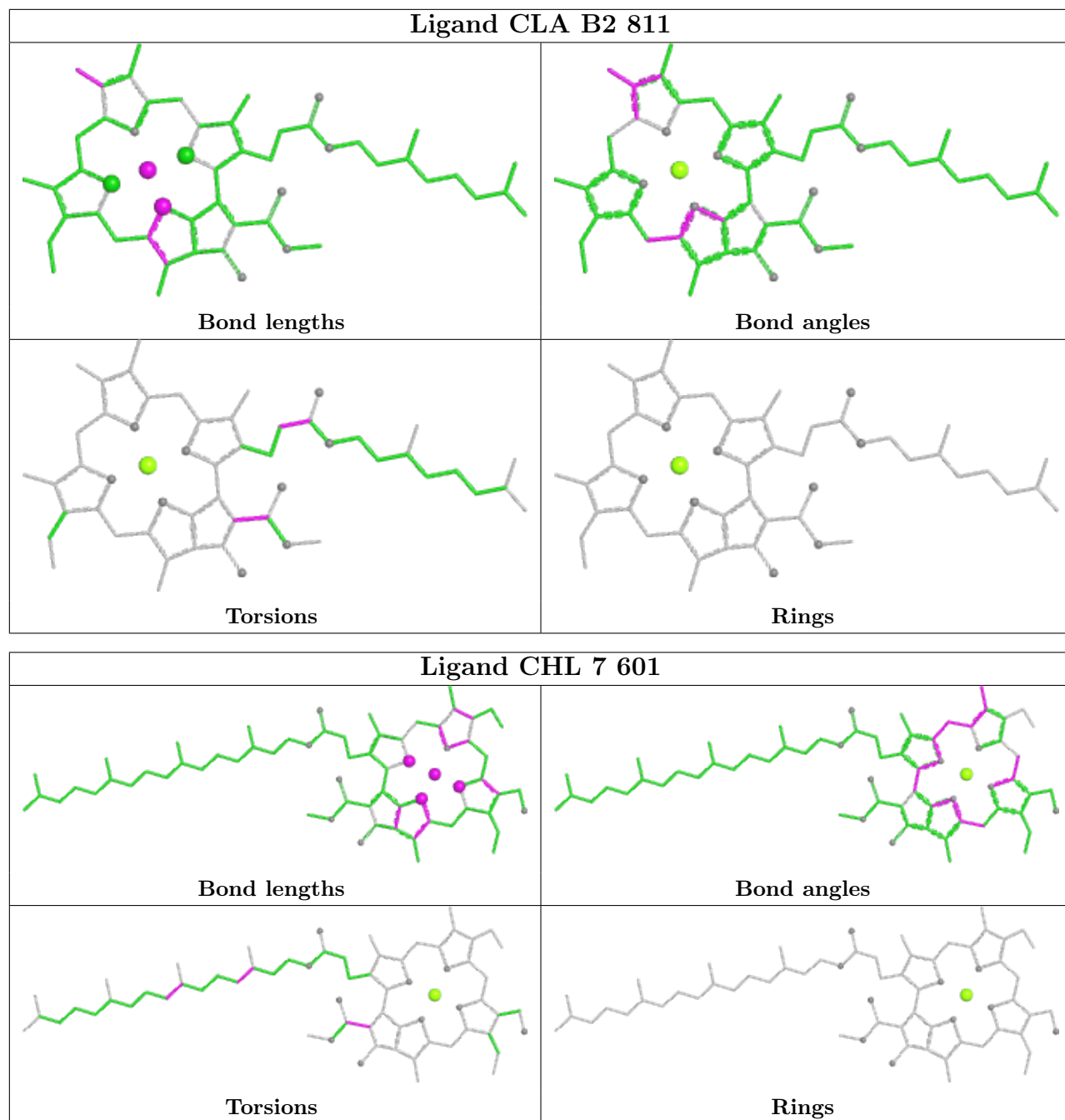


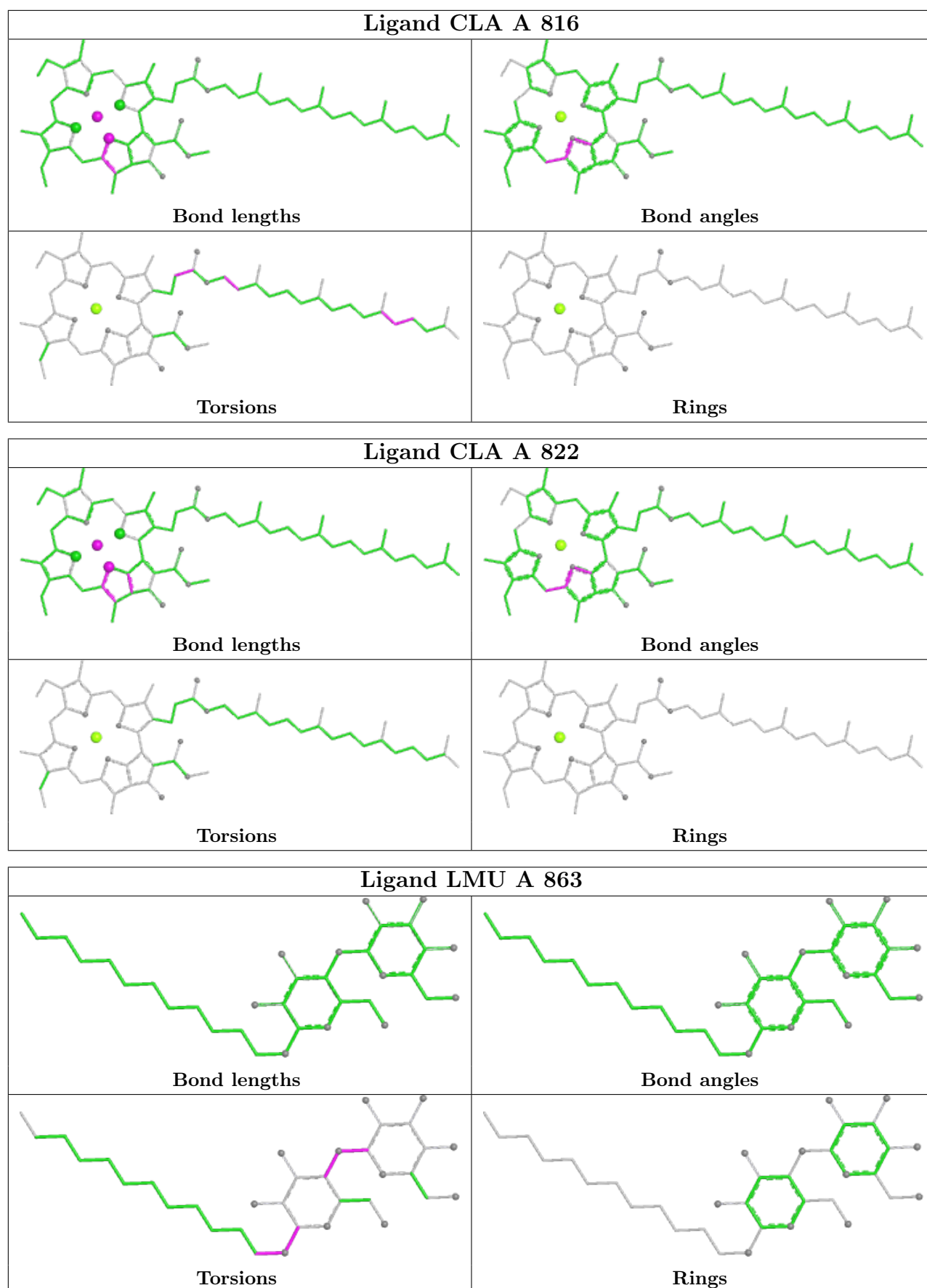


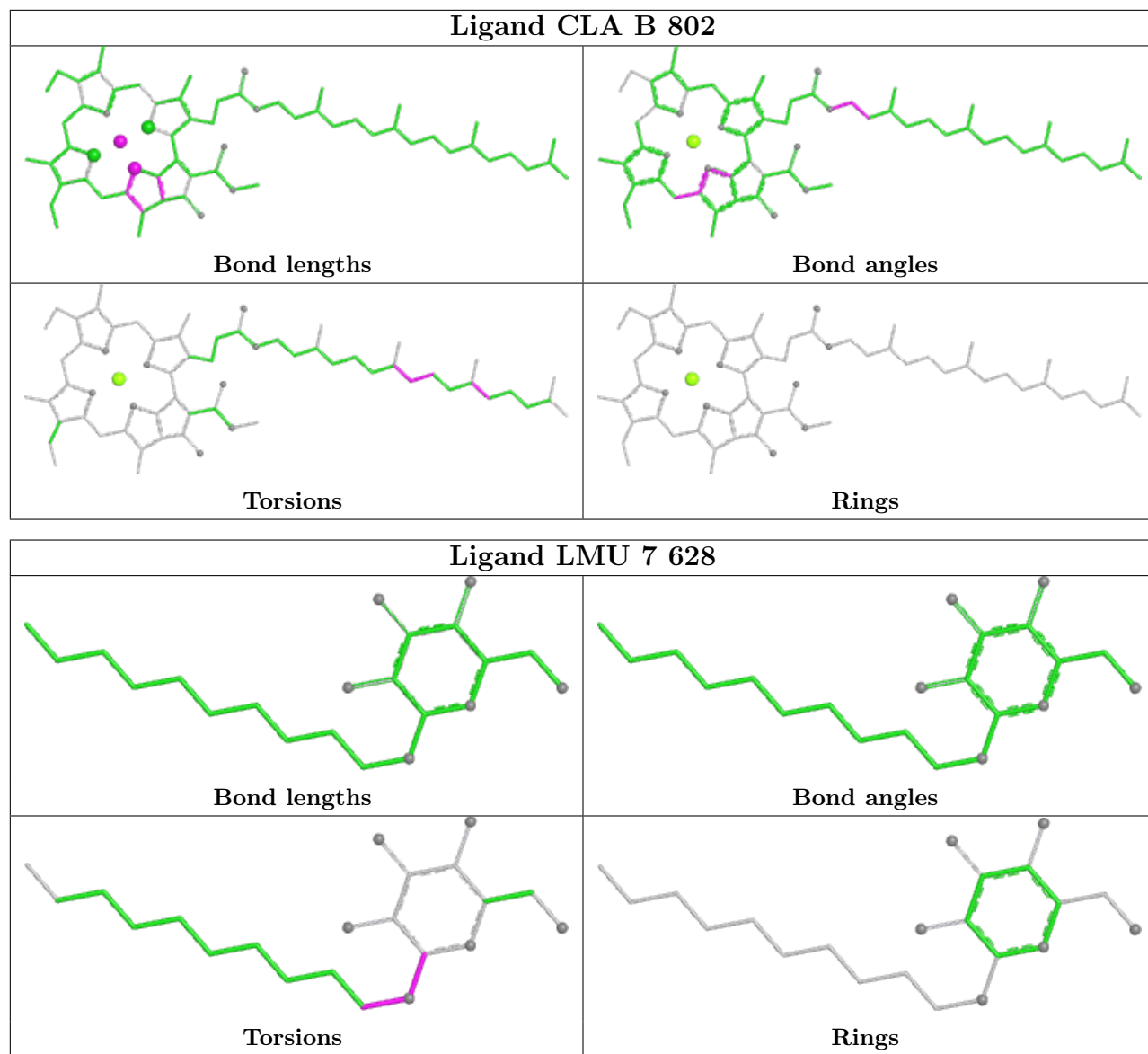


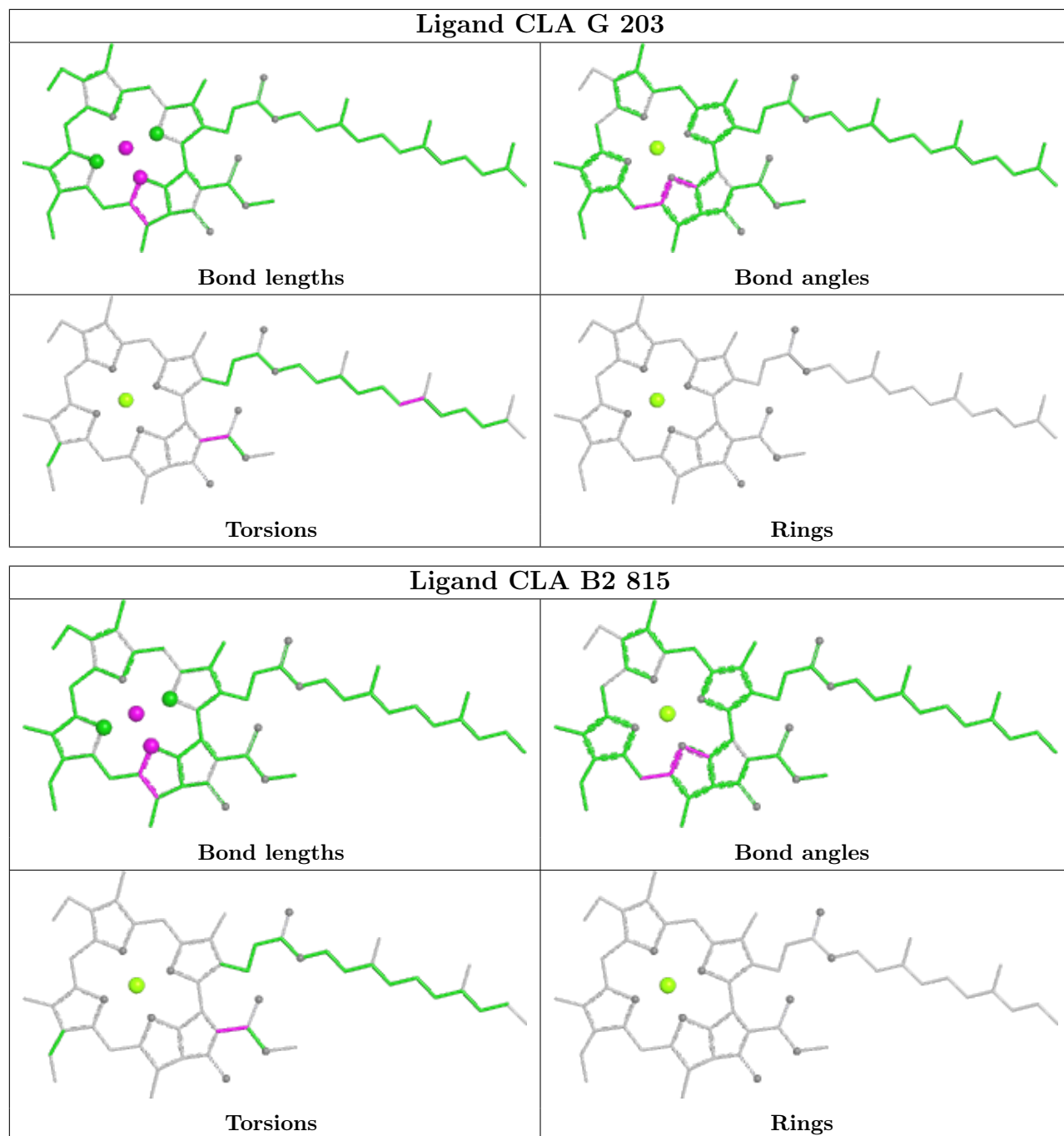


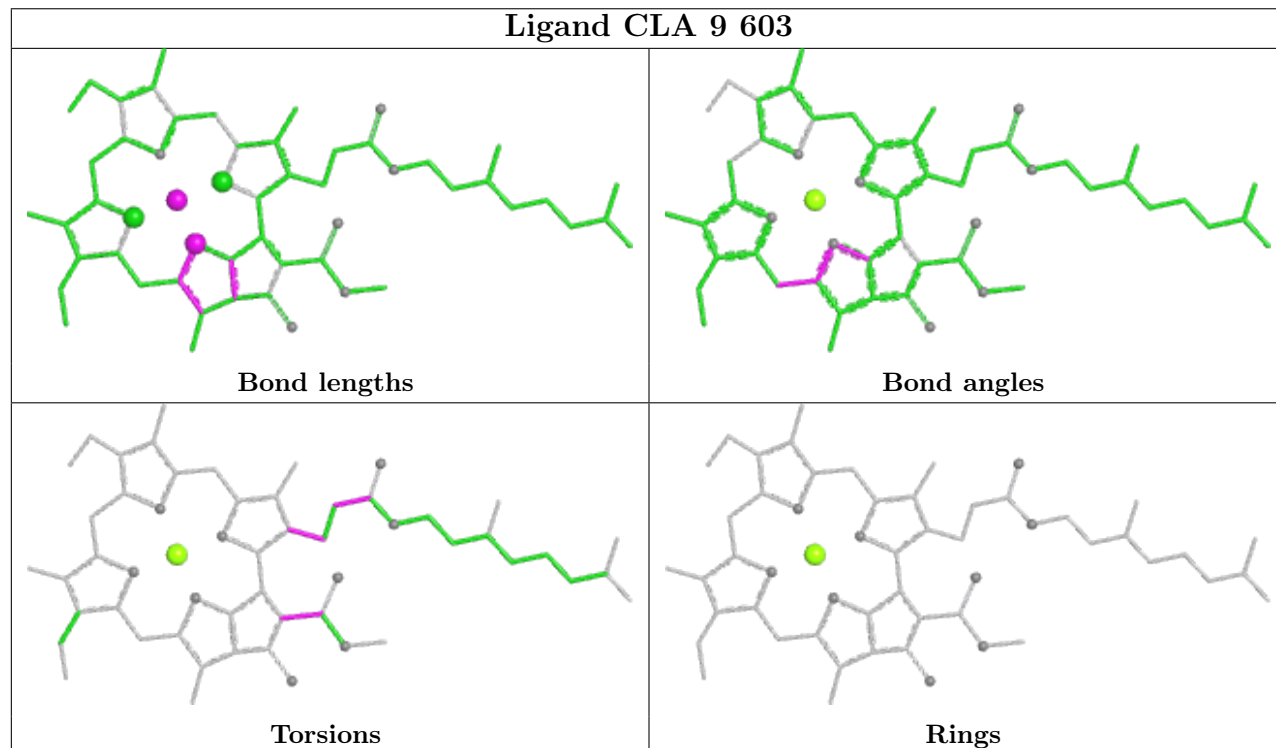
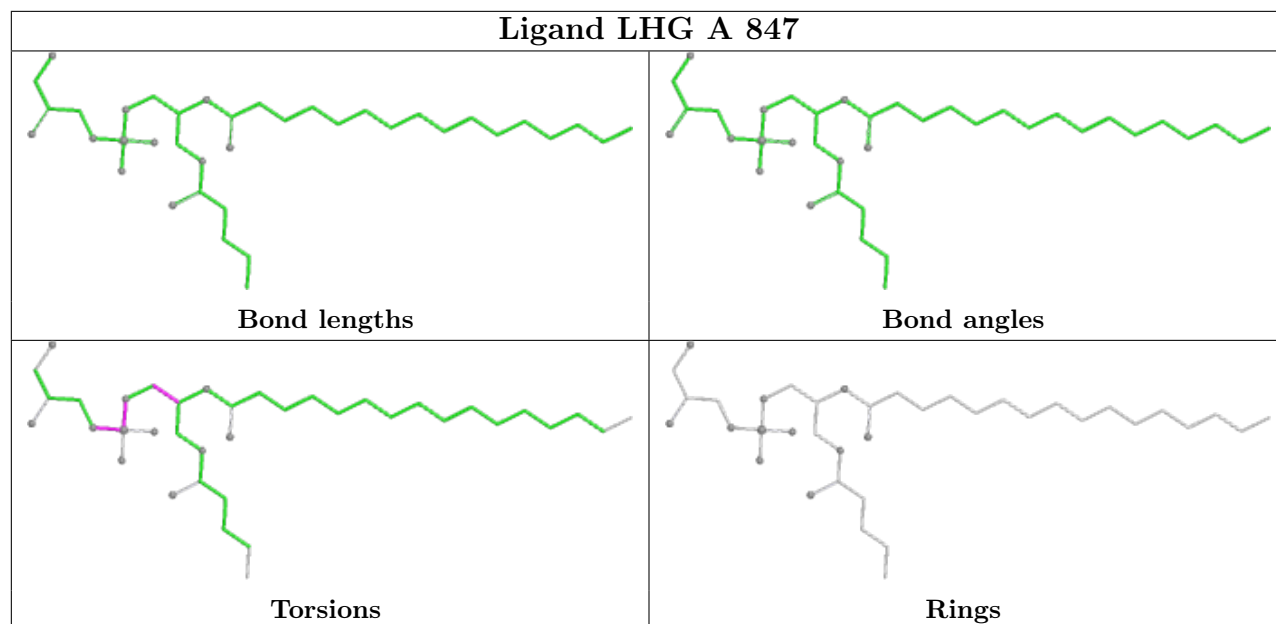


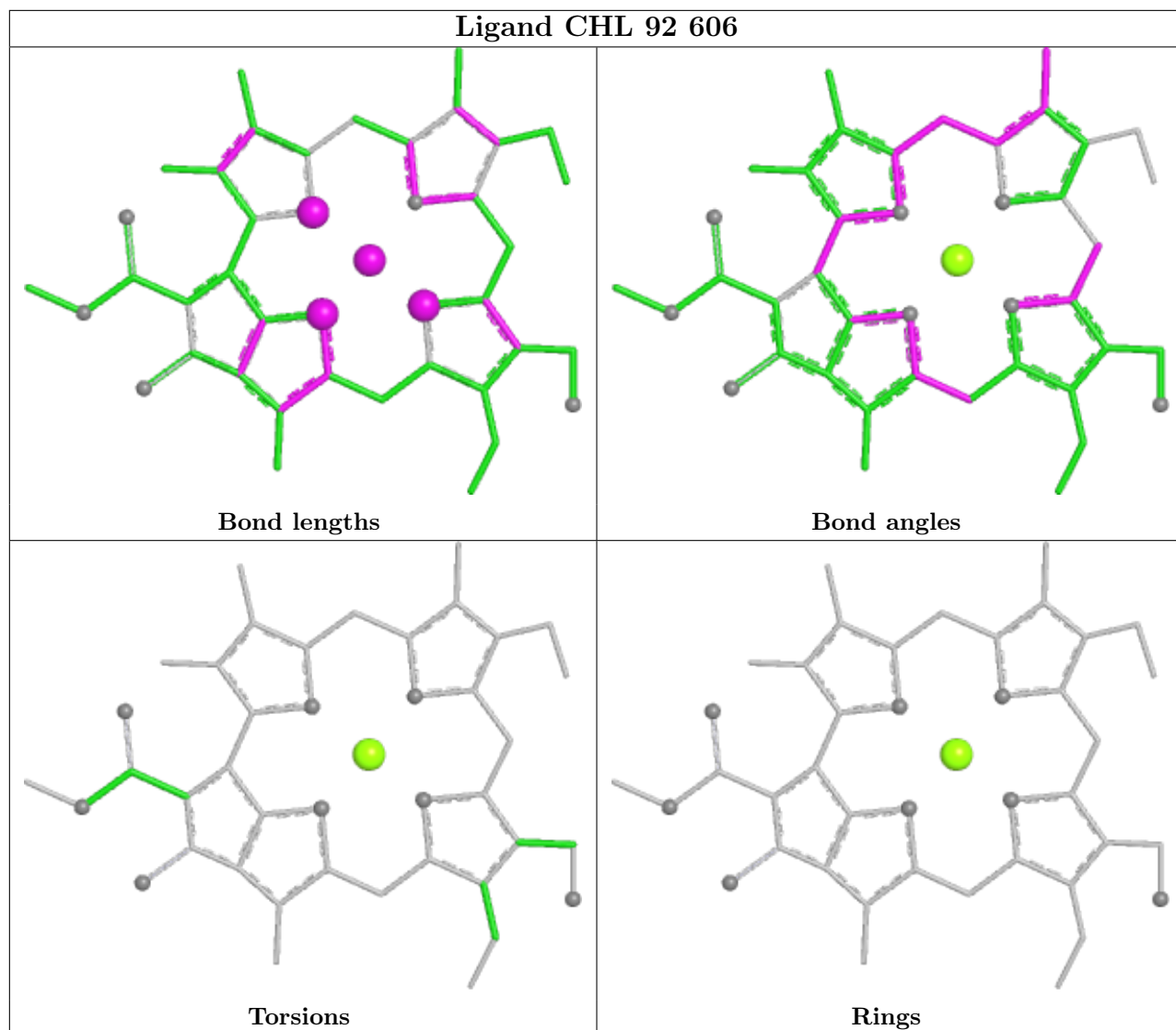


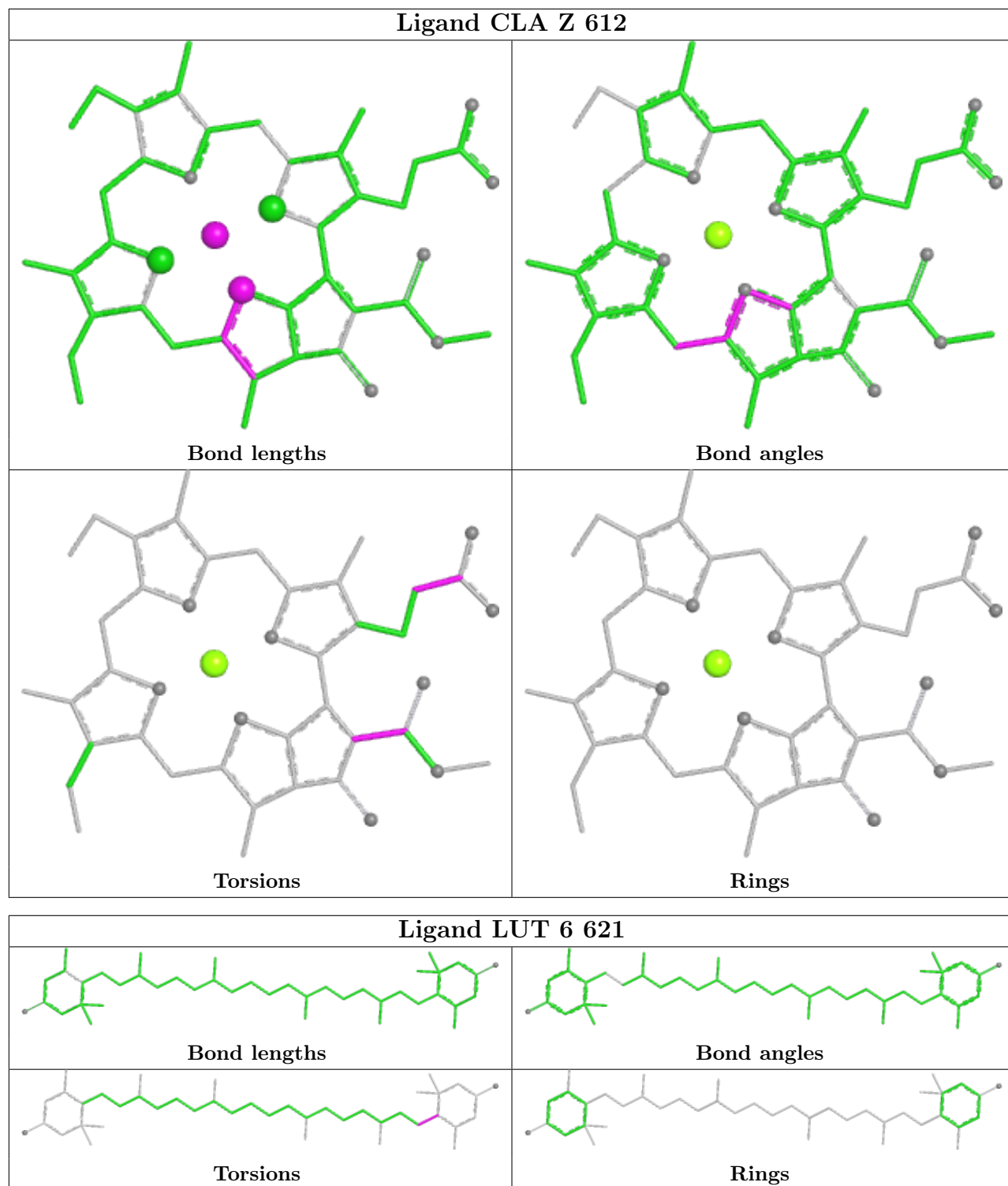


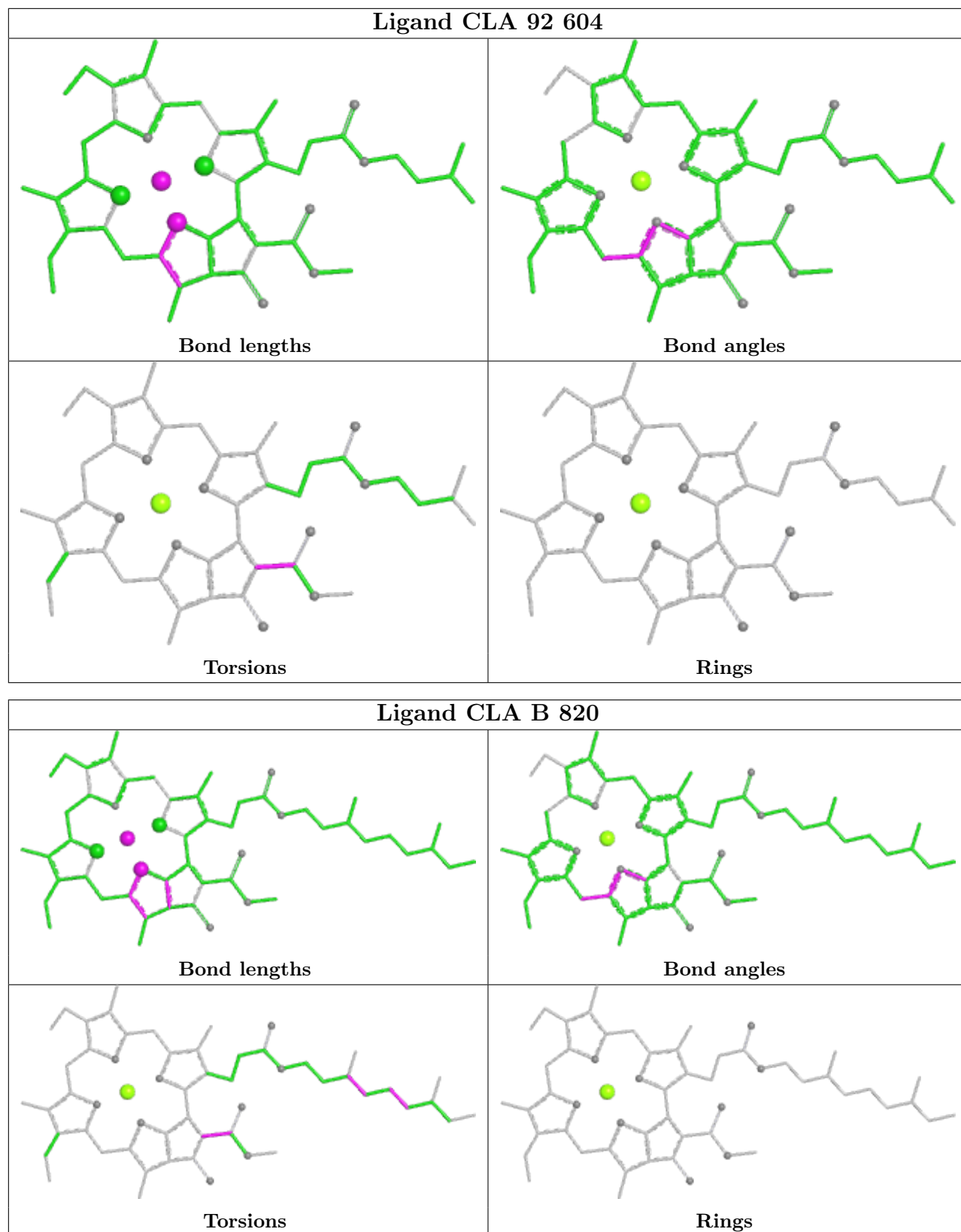


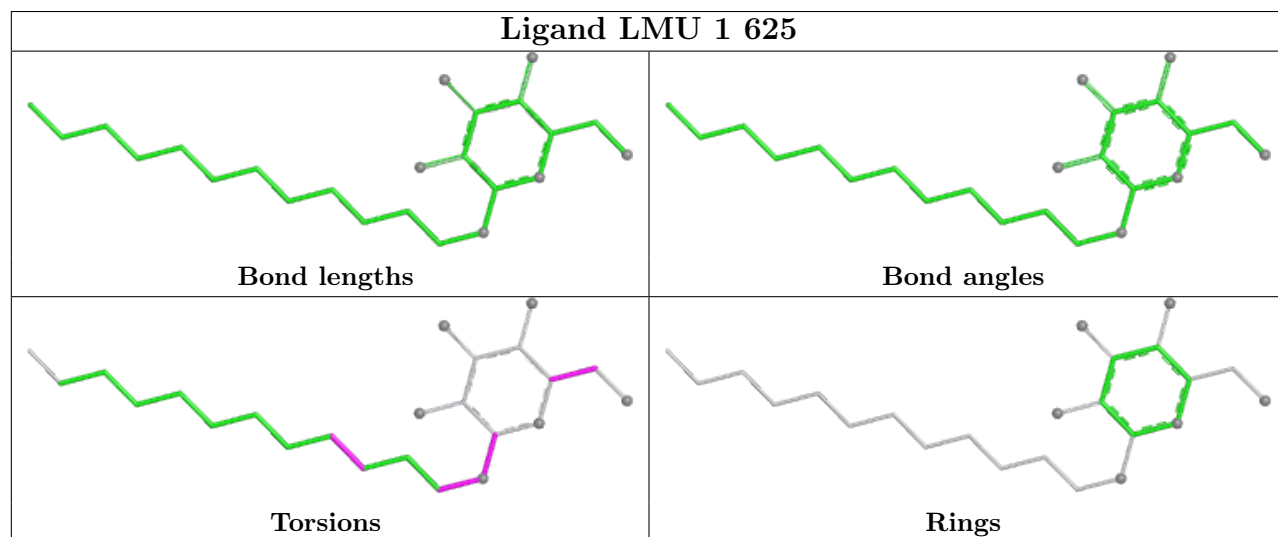
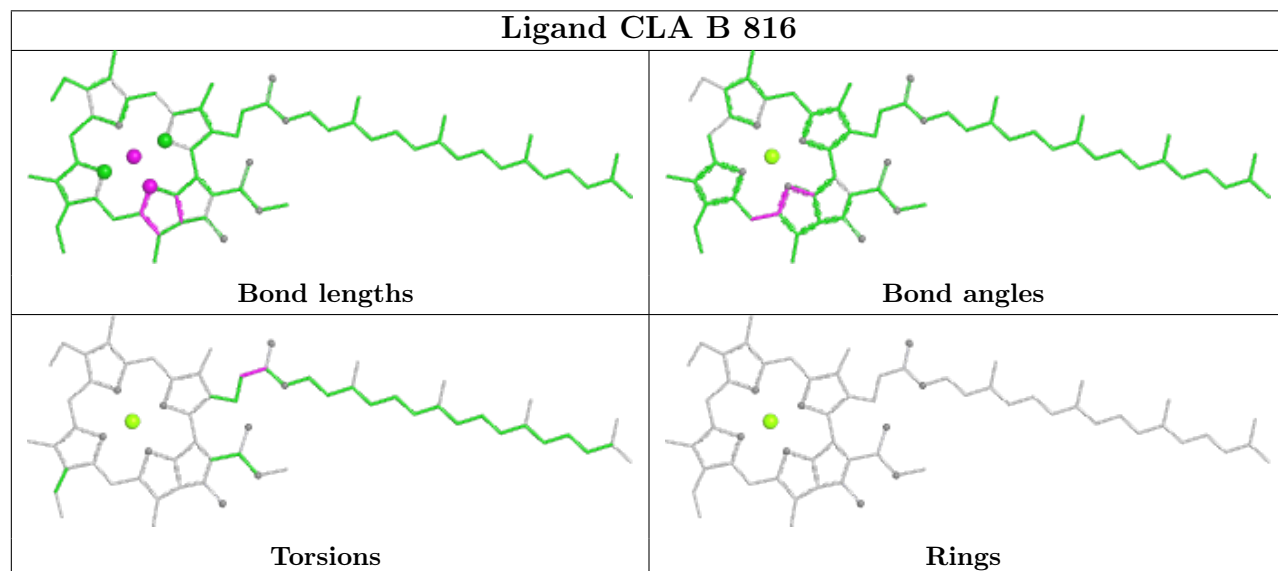
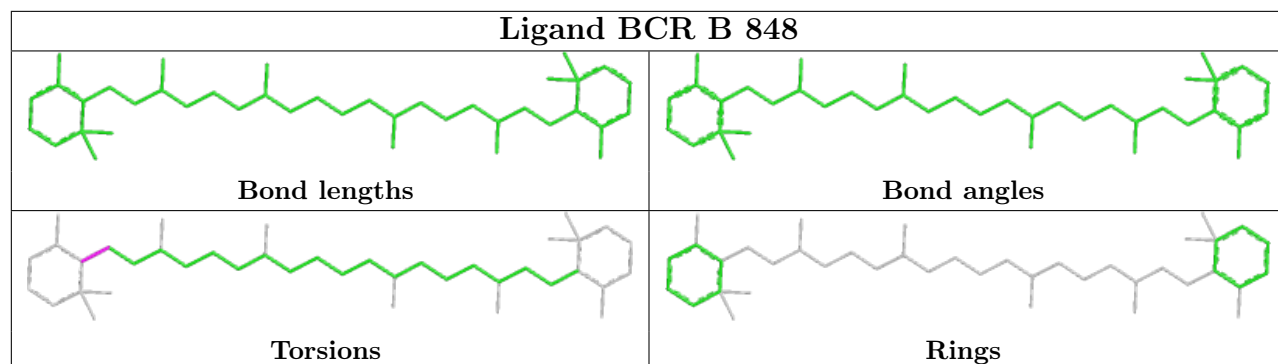


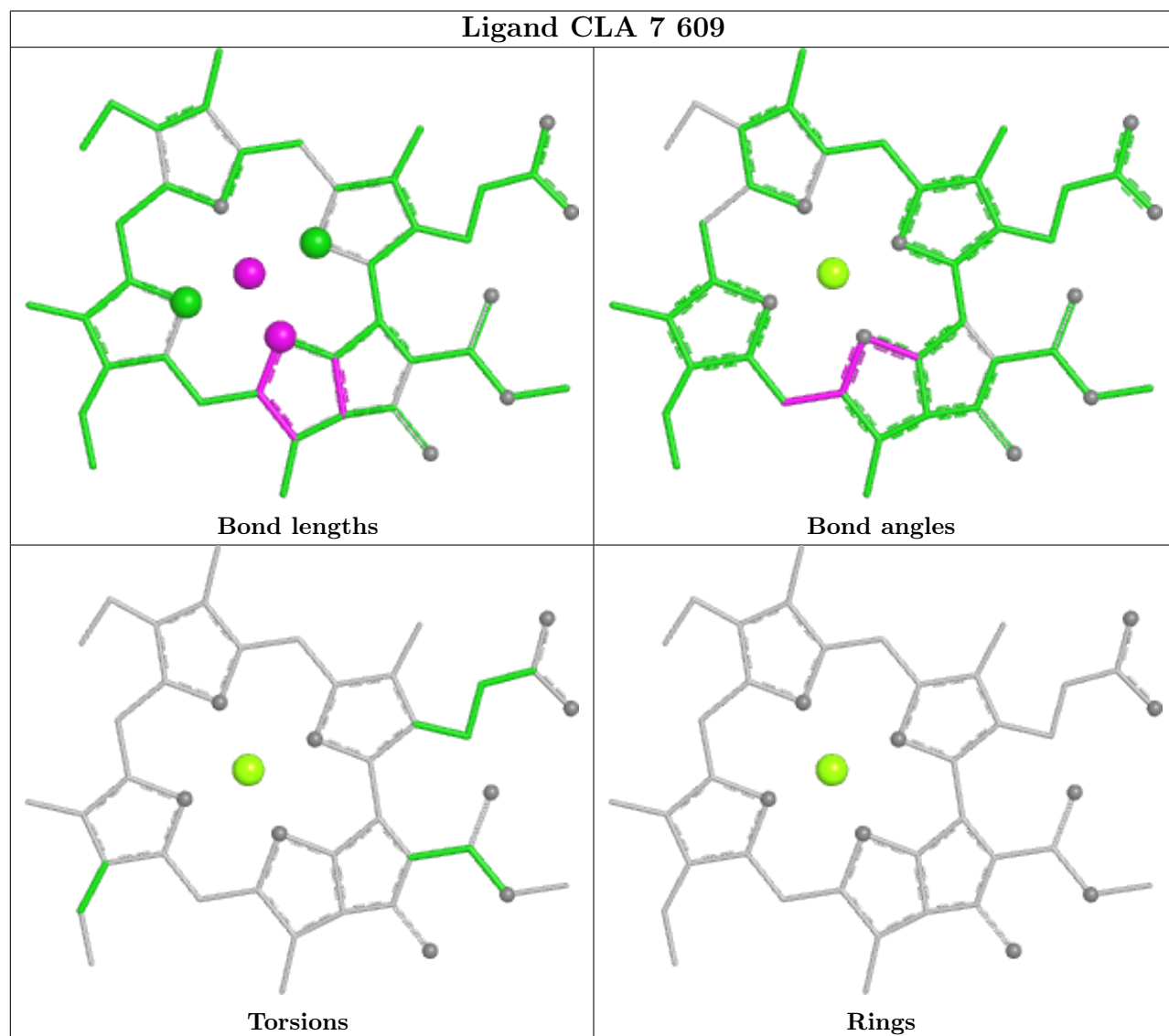
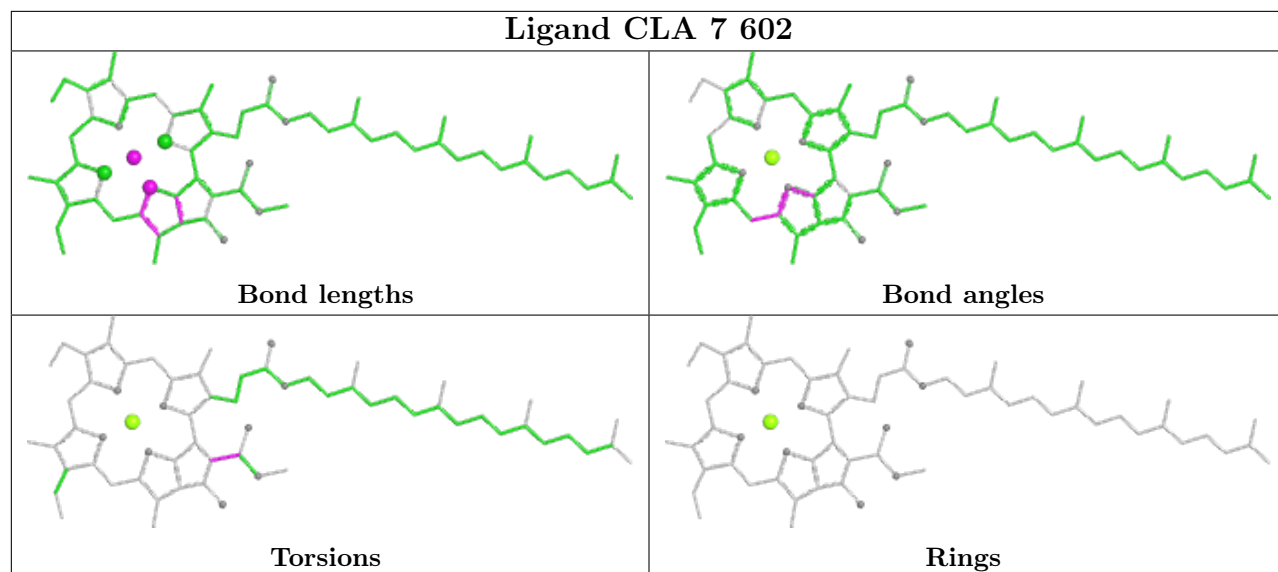


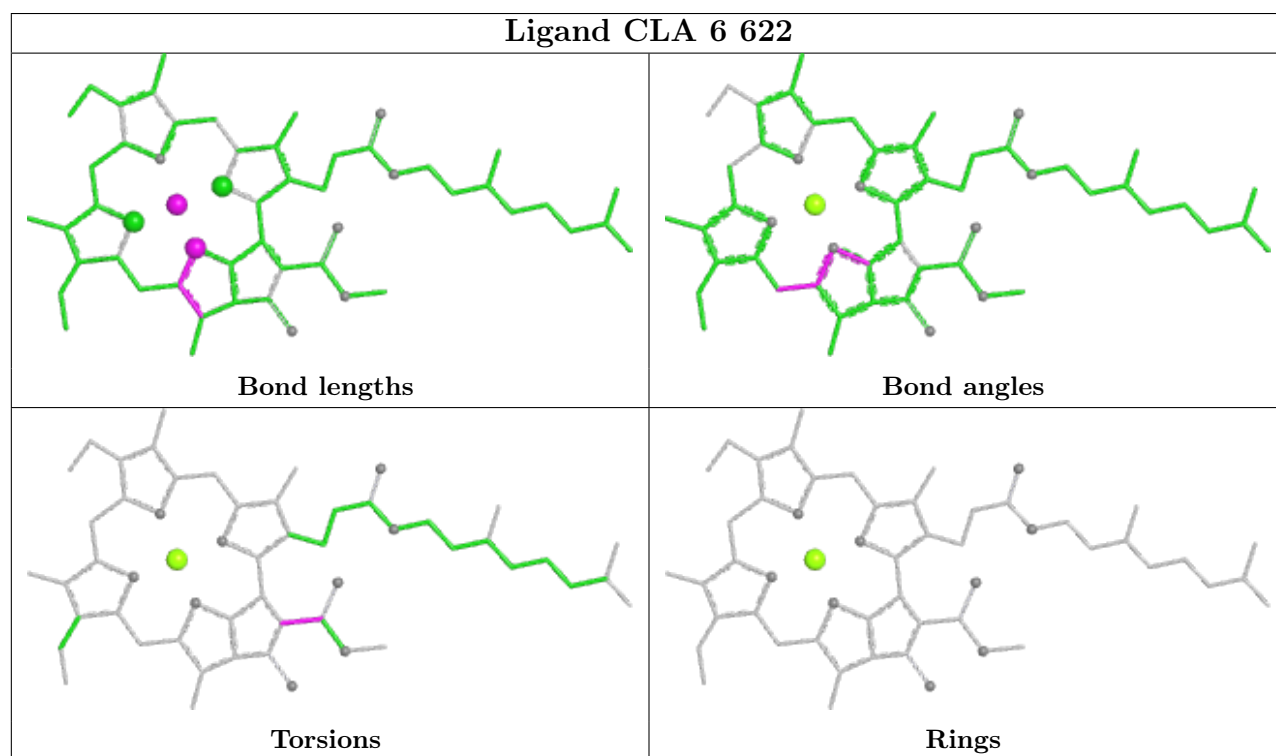
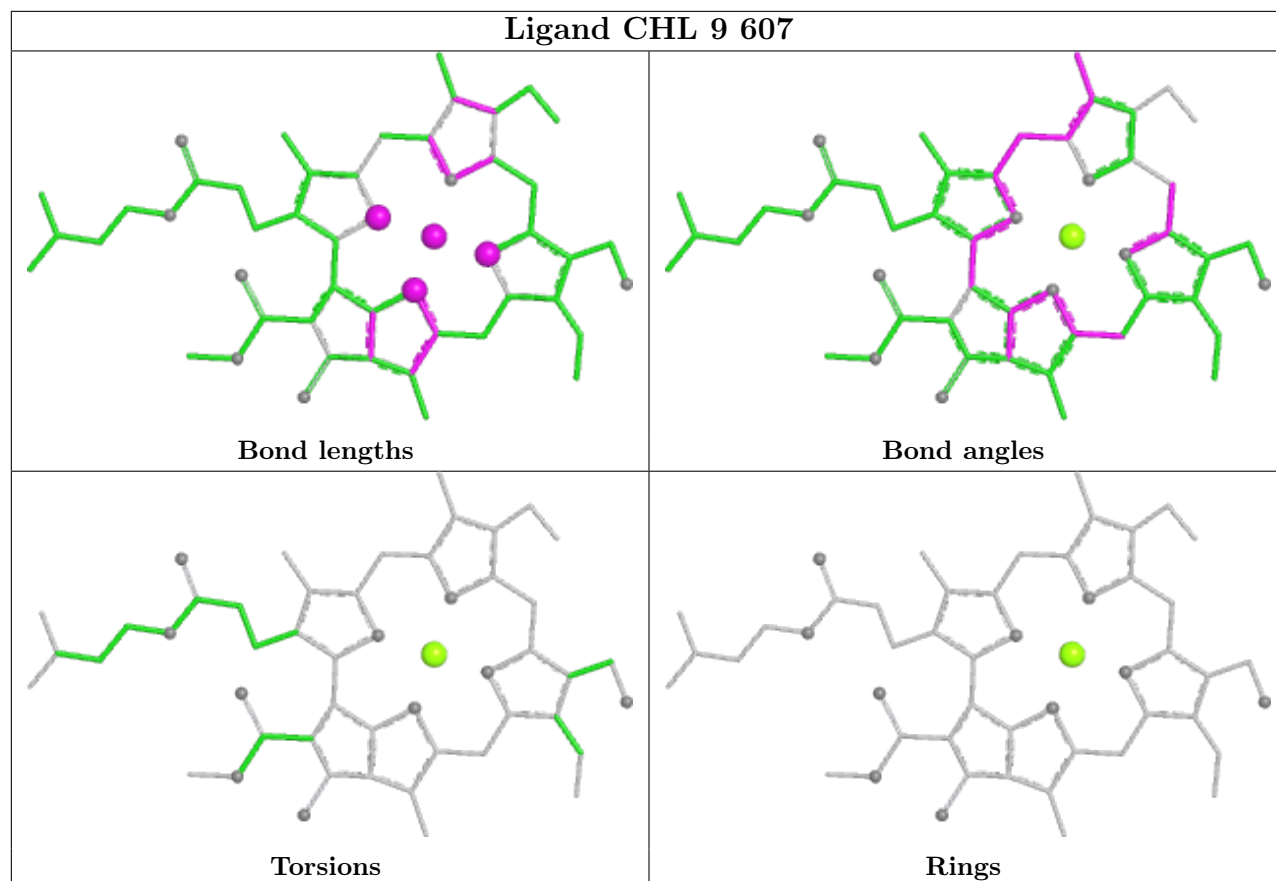


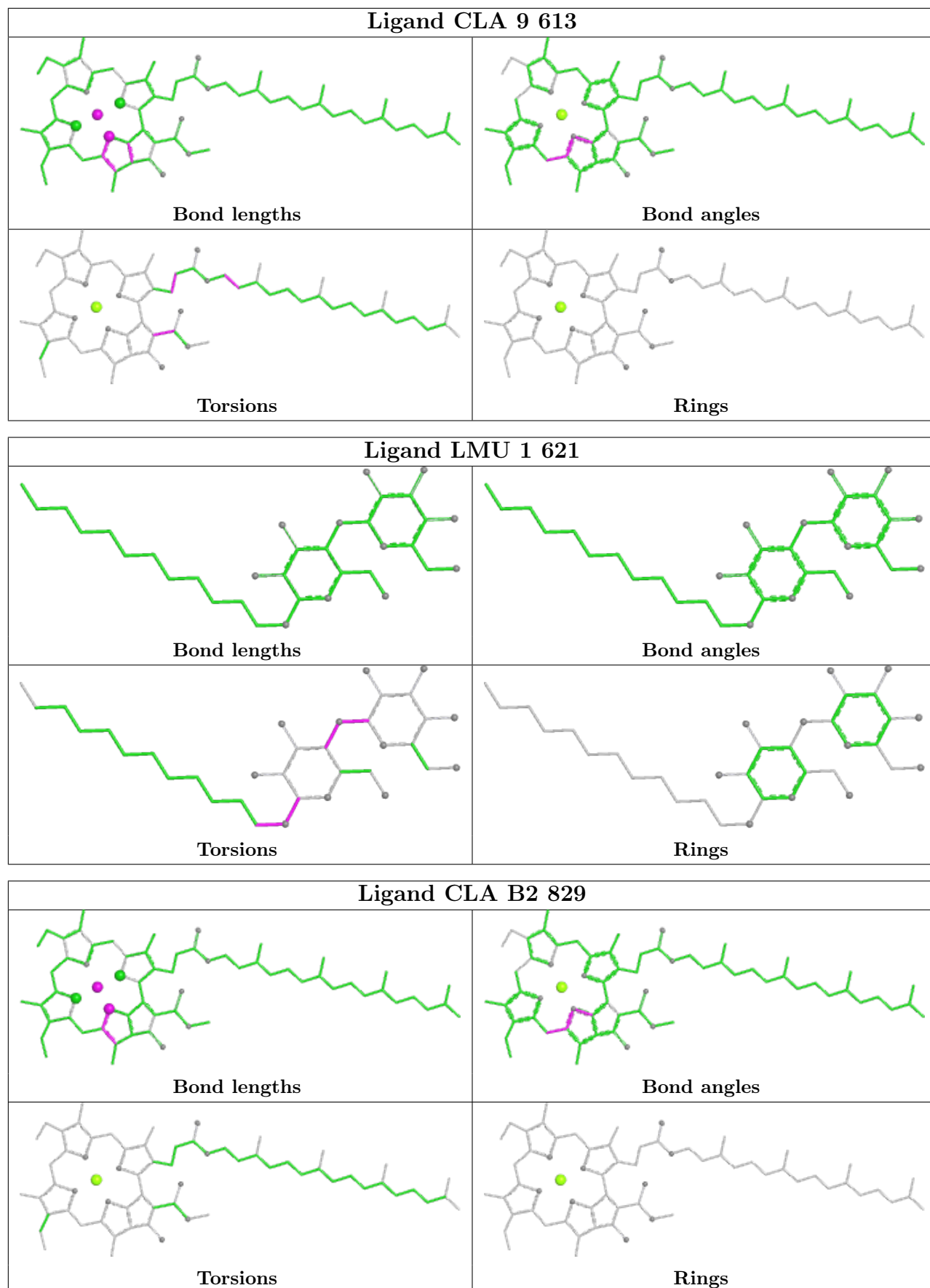


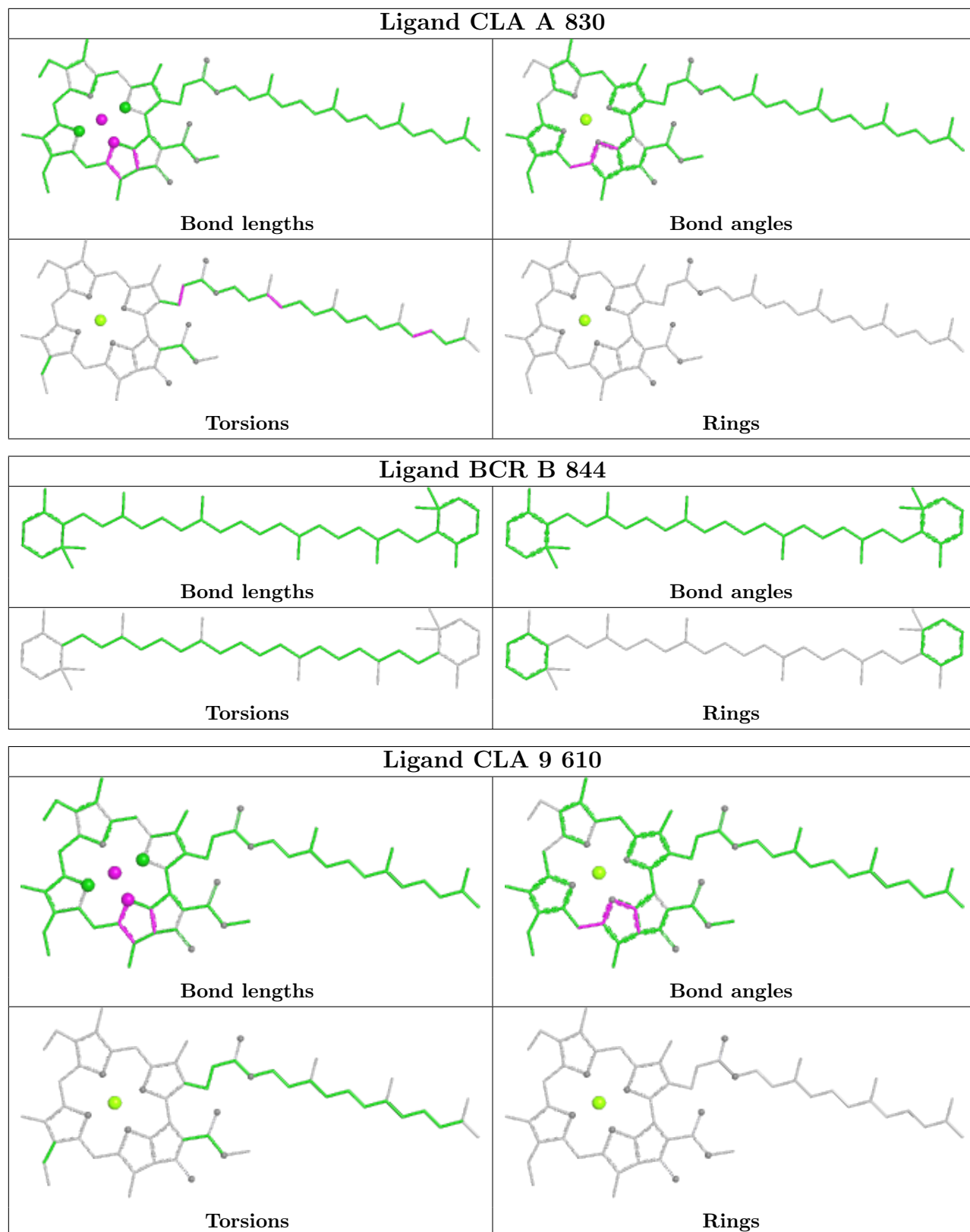


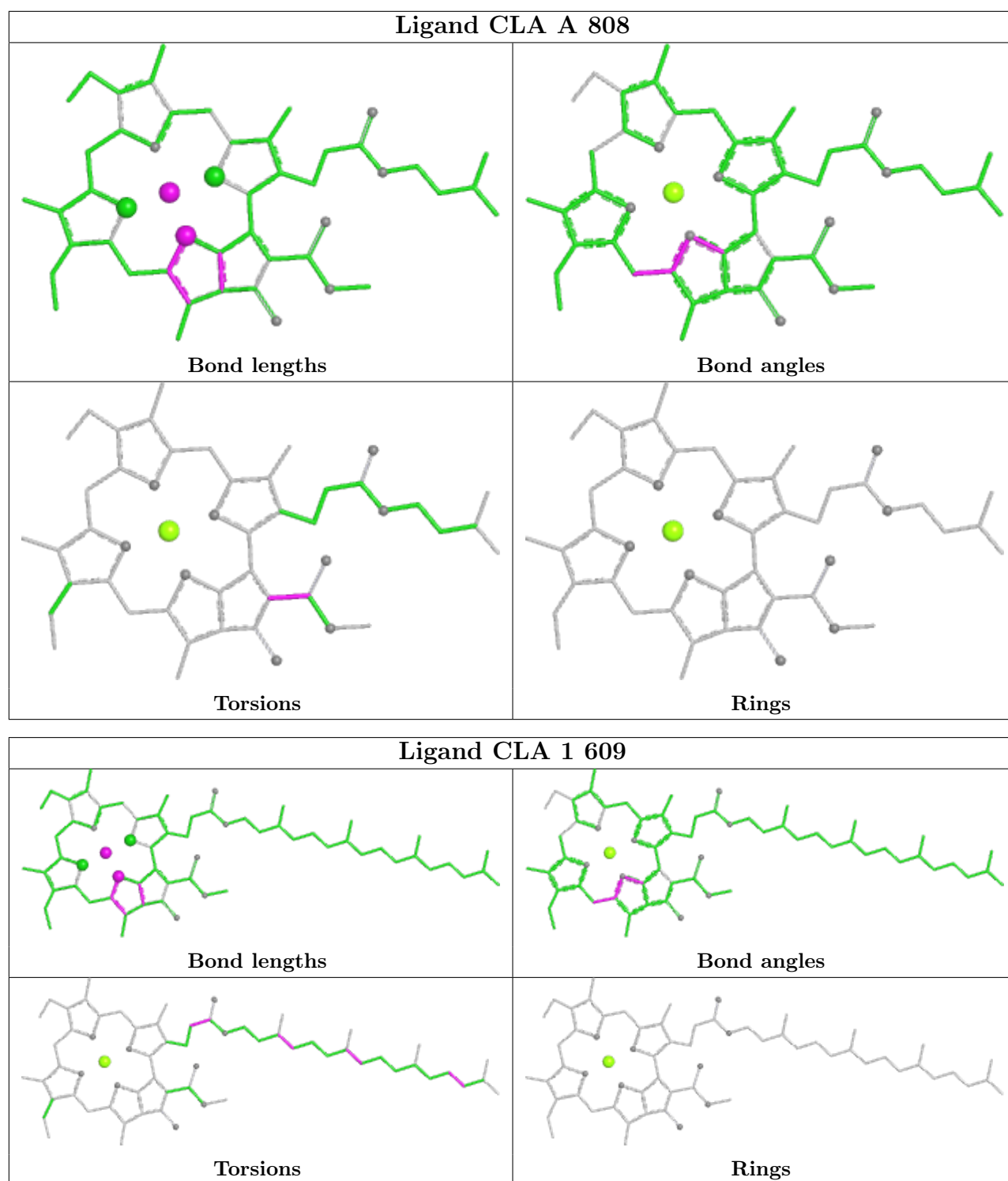












5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
20	B2	6

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B2	218:PRO	C	683:HIS	N	78.76
1	B2	169:PHE	C	191:TRP	N	27.65
1	B2	115:ASN	C	128:ILE	N	22.89
1	B2	77:GLN	C	88:ILE	N	9.86
1	B2	107:ARG	C	112:GLY	N	7.45
1	B2	201:PRO	C	207:HIS	N	6.93

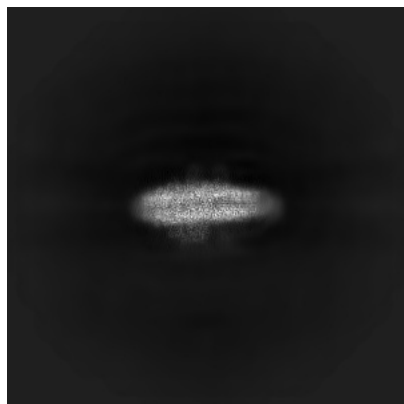
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14867. These allow visual inspection of the internal detail of the map and identification of artifacts.

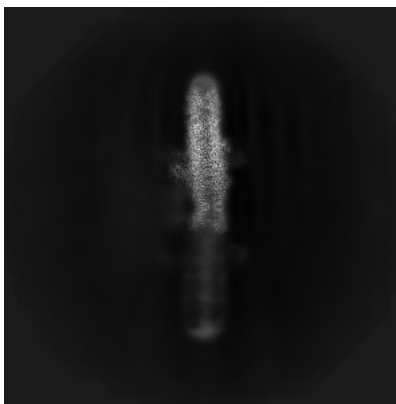
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

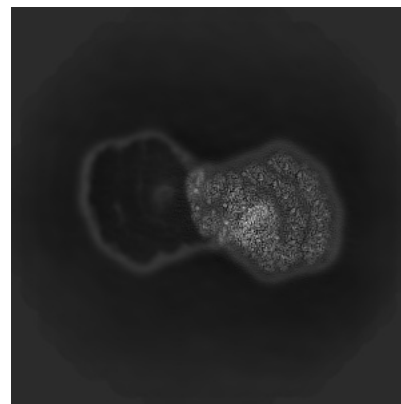
6.1.1 Primary map



X

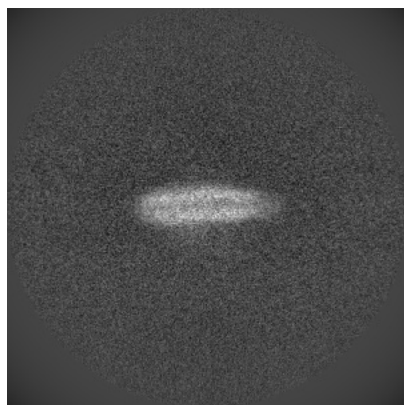


Y

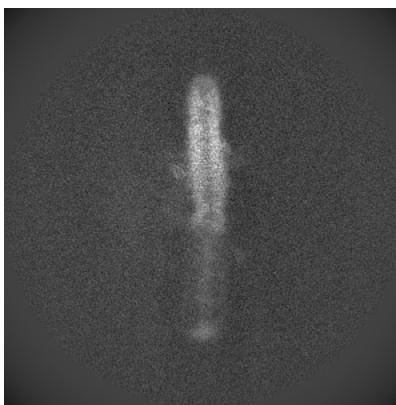


Z

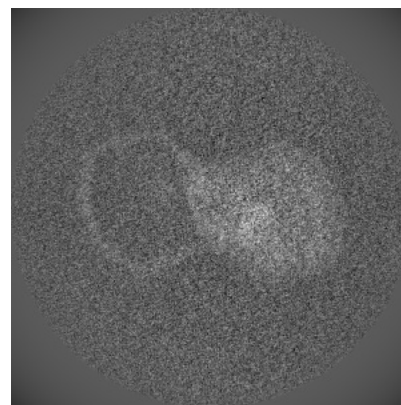
6.1.2 Raw map



X



Y



Z

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

6.2 Central slices [i](#)

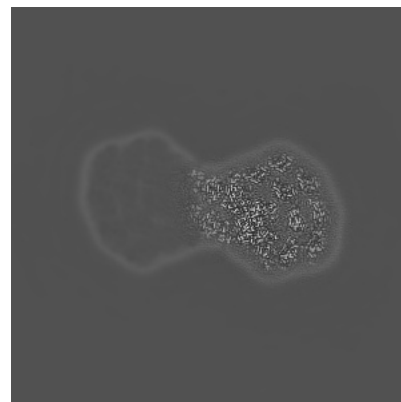
6.2.1 Primary map



X Index: 350

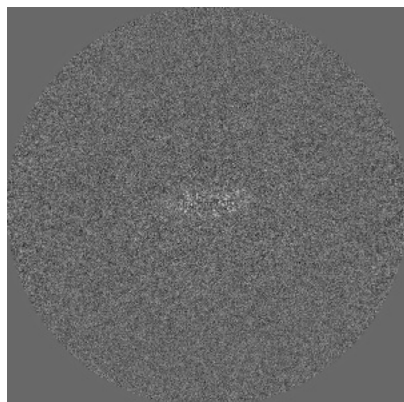


Y Index: 350

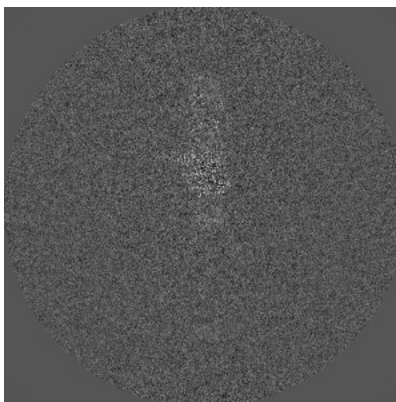


Z Index: 350

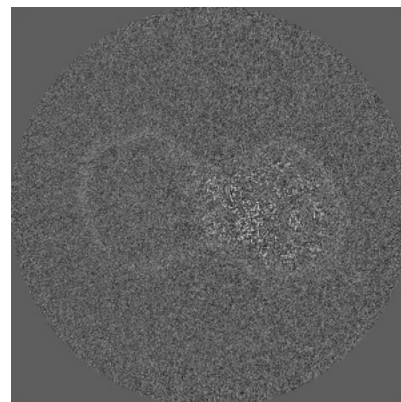
6.2.2 Raw map



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](#)

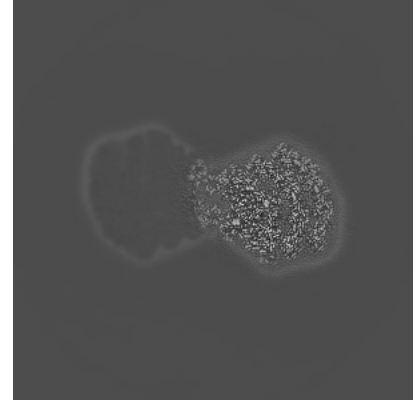
6.3.1 Primary map



X Index: 416

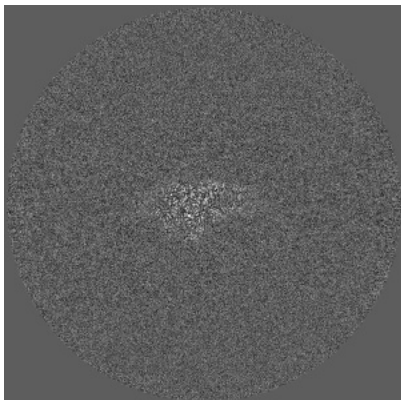


Y Index: 323

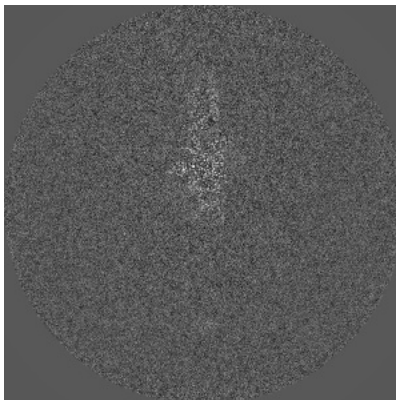


Z Index: 340

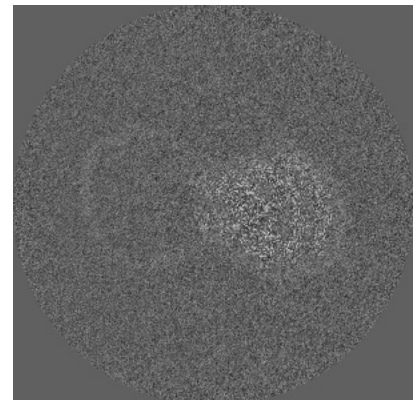
6.3.2 Raw map



X Index: 415



Y Index: 323

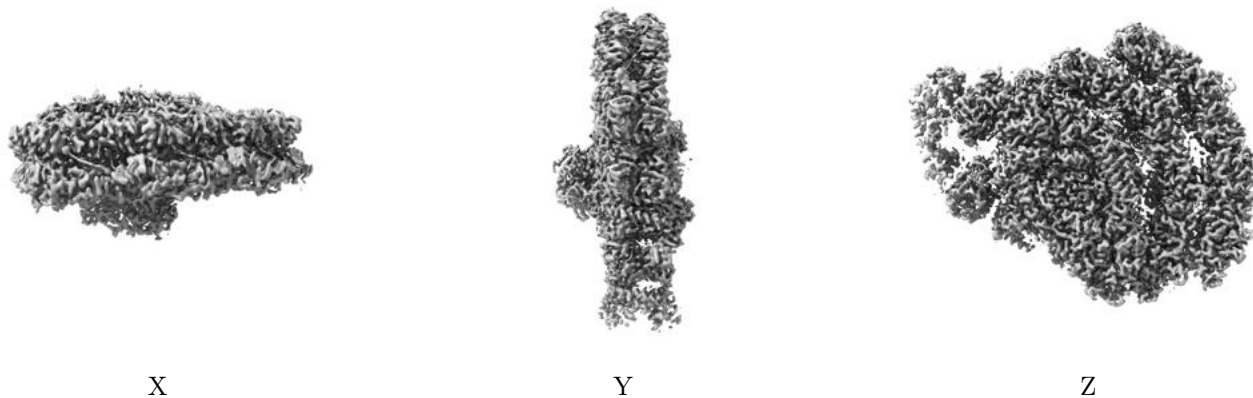


Z Index: 340

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

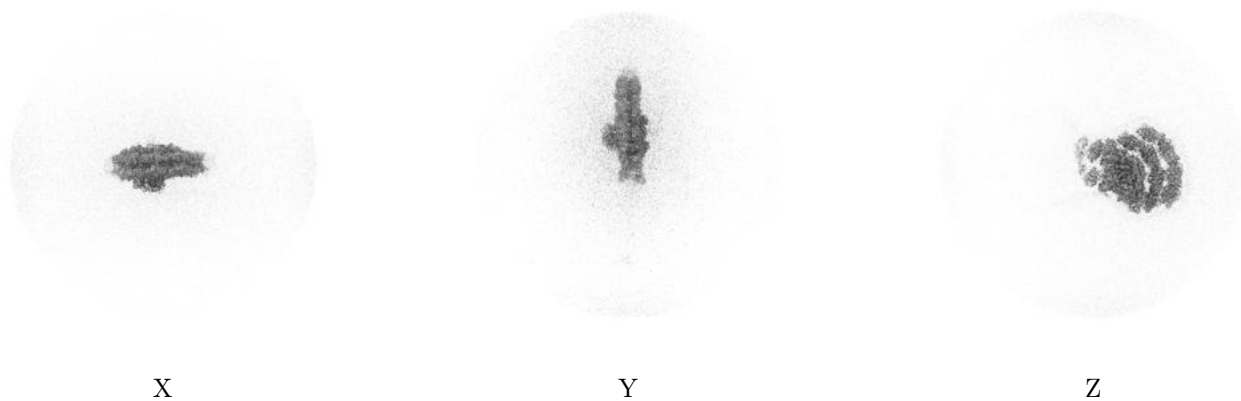
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.031. 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.

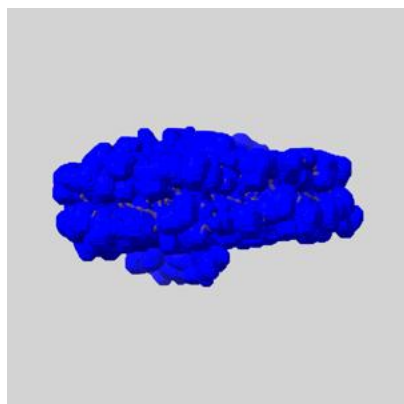
6.5 Mask visualisation [i](#)

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

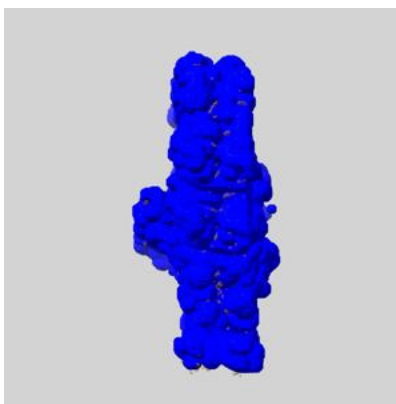
A mask typically either:

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

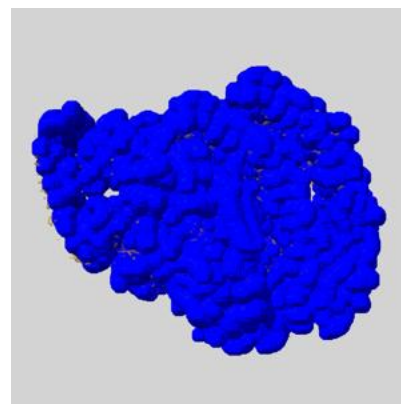
6.5.1 emd_14867_msk_1.map [i](#)



X



Y

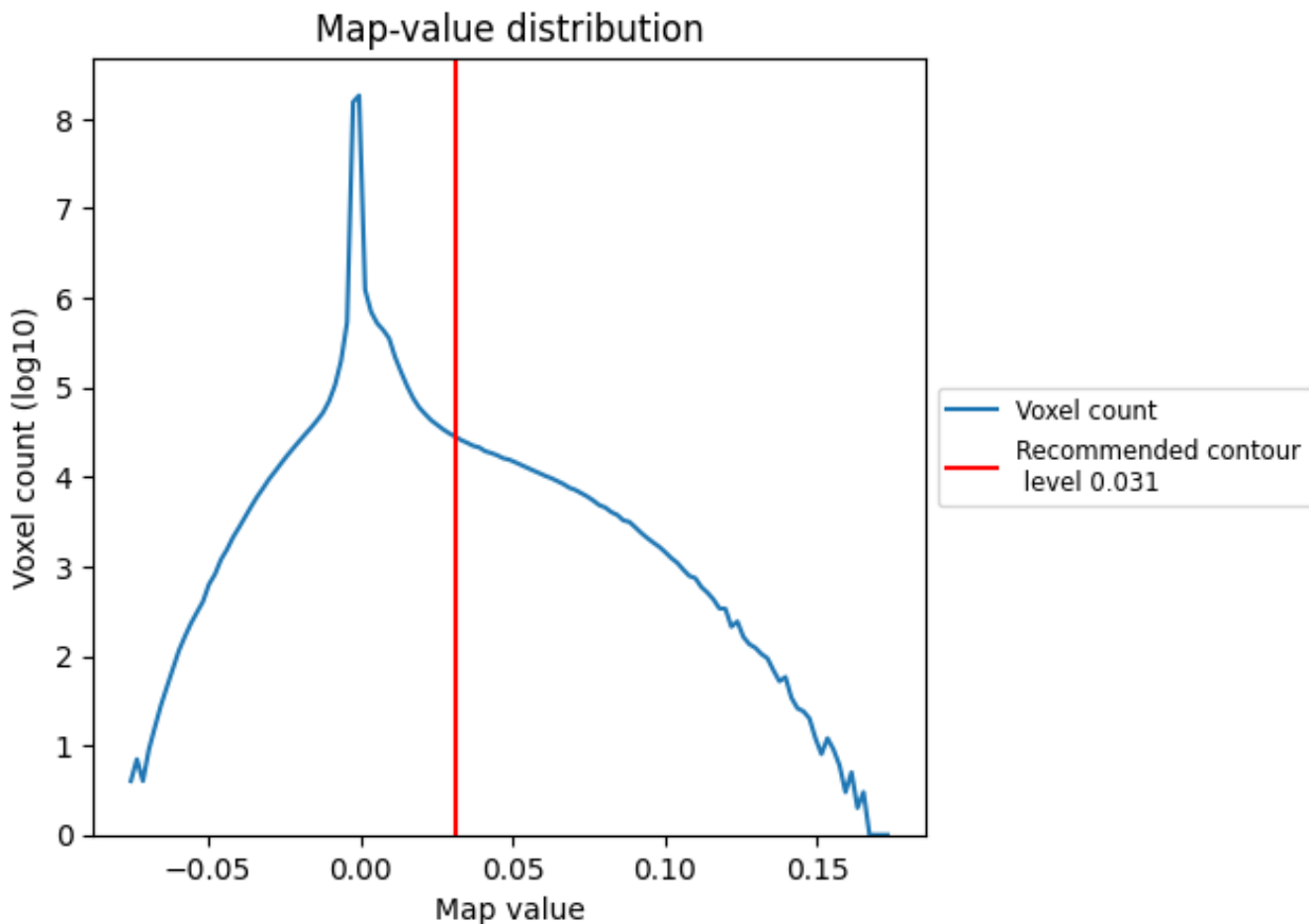


Z

7 Map analysis [i](#)

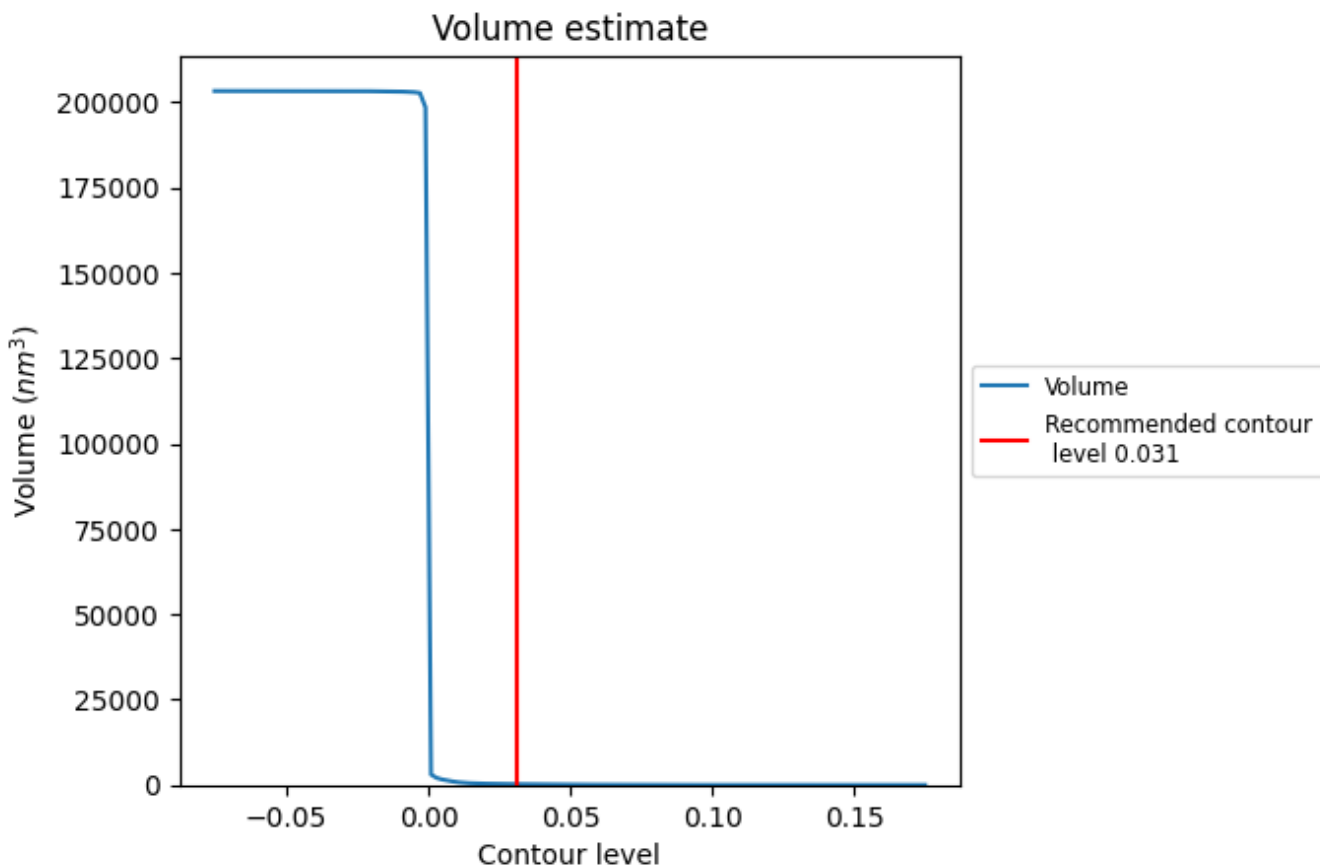
This section contains the results of statistical analysis of the map.

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.

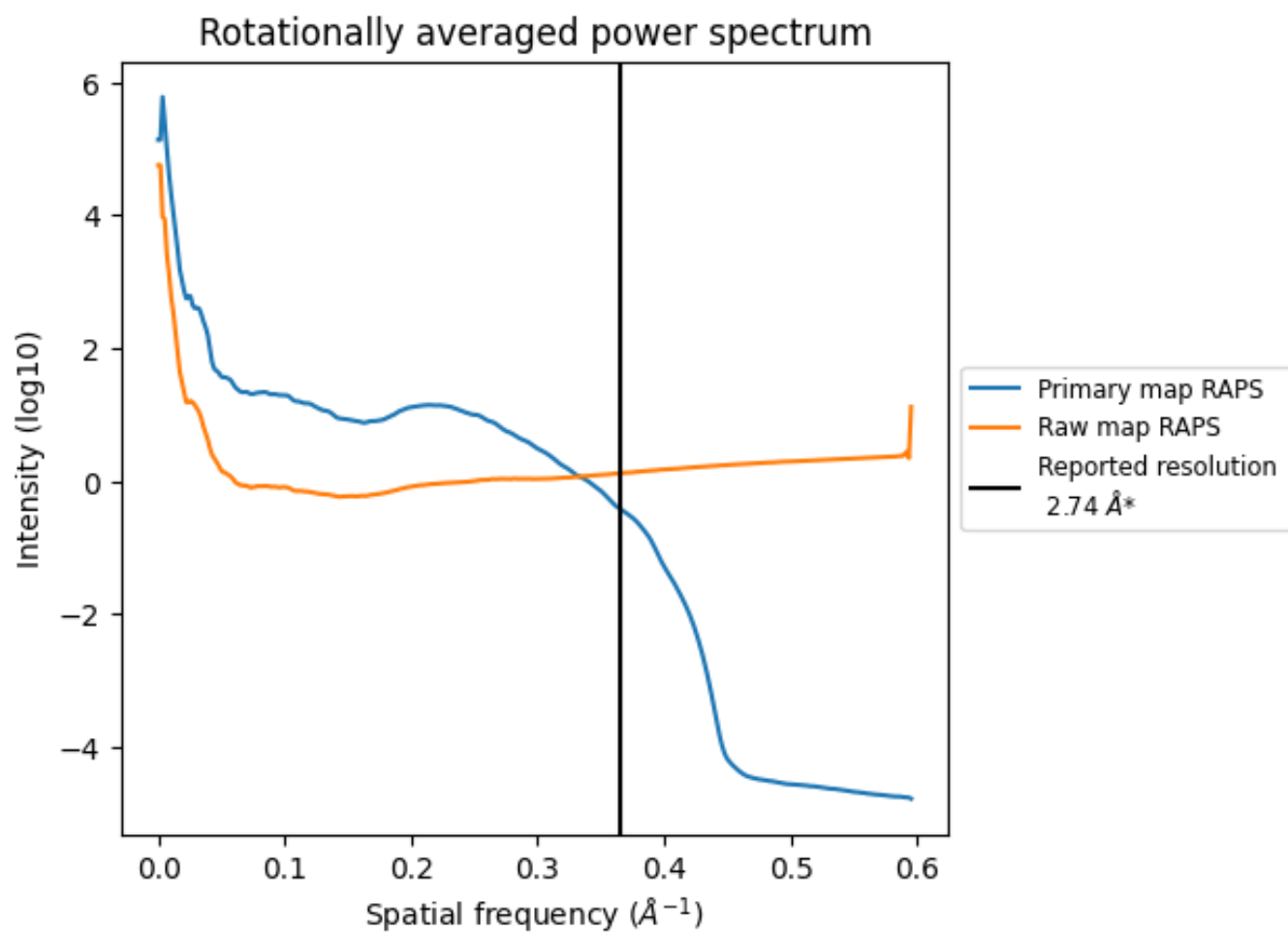
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 231 nm^3 ; this corresponds to an approximate mass of 209 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

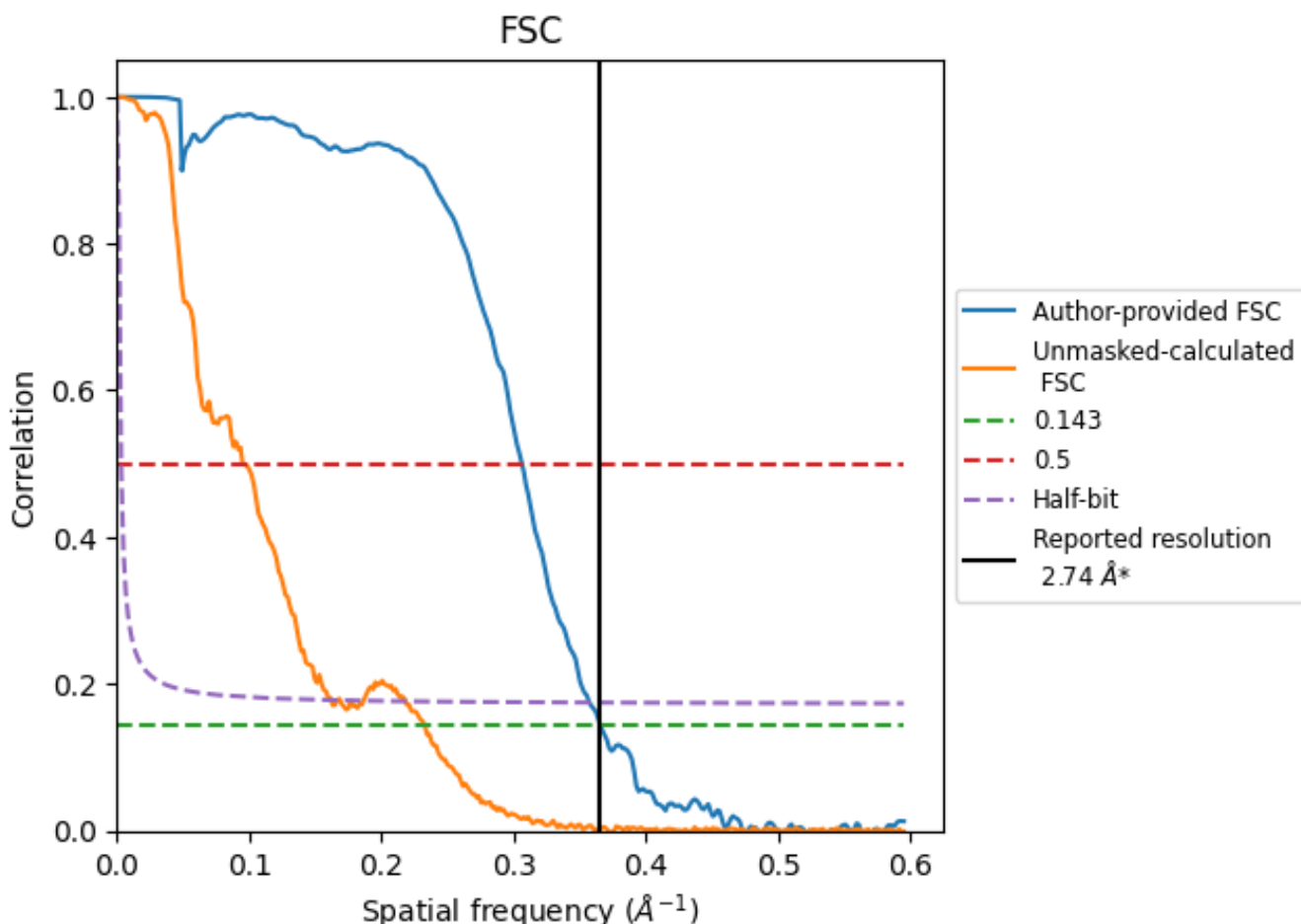


*Reported resolution corresponds to spatial frequency of 0.365 \AA^{-1}

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 0.365 Å⁻¹

8.2 Resolution estimates [i](#)

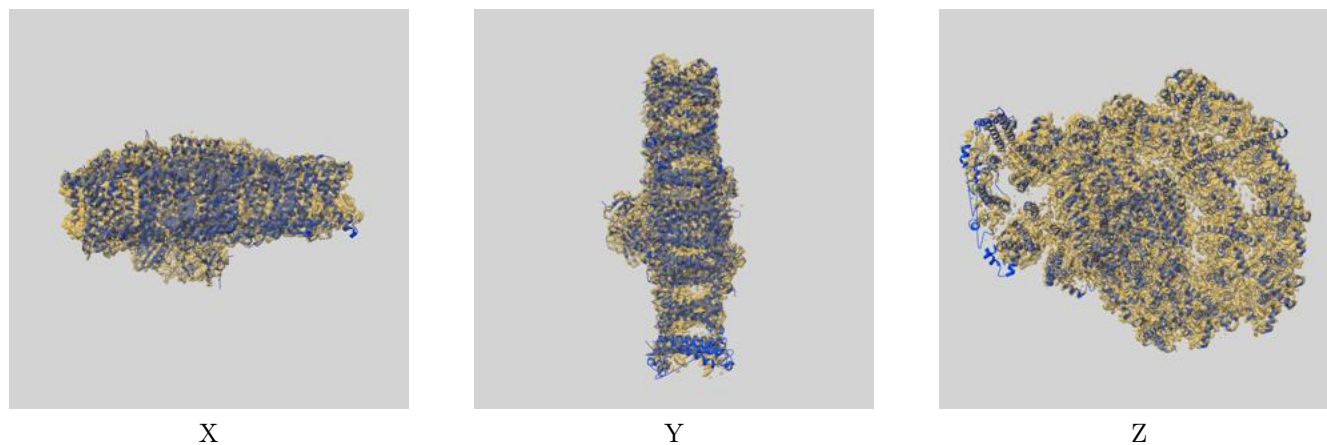
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.74	-	-
Author-provided FSC curve	2.73	3.26	2.80
Unmasked-calculated*	4.30	10.50	6.17

*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 4.30 differs from the reported value 2.74 by more than 10 %

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-14867 and PDB model 7ZQ9. Per-residue inclusion information can be found in section 3 on page 40.

9.1 Map-model overlay [i](#)

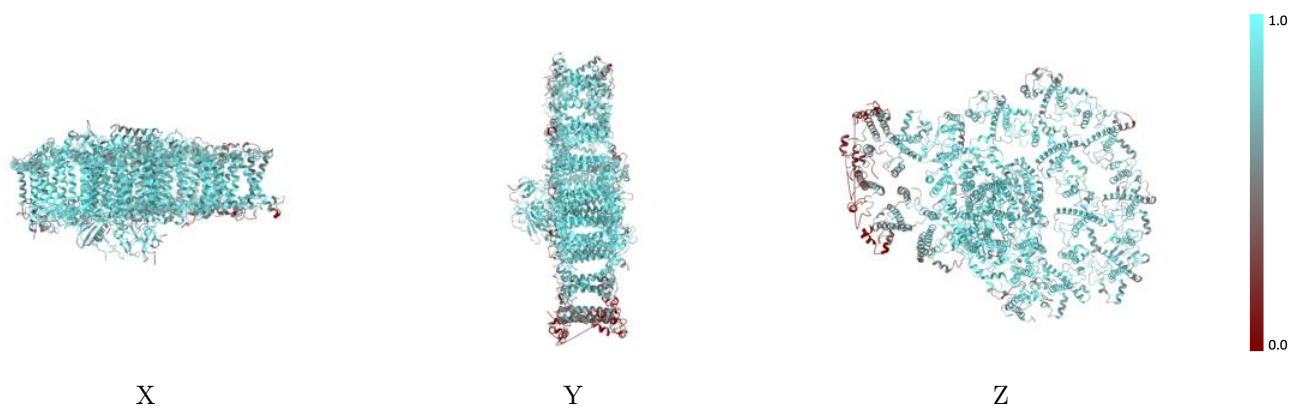


The images above show the 3D surface view of the map at the recommended contour level 0.031 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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

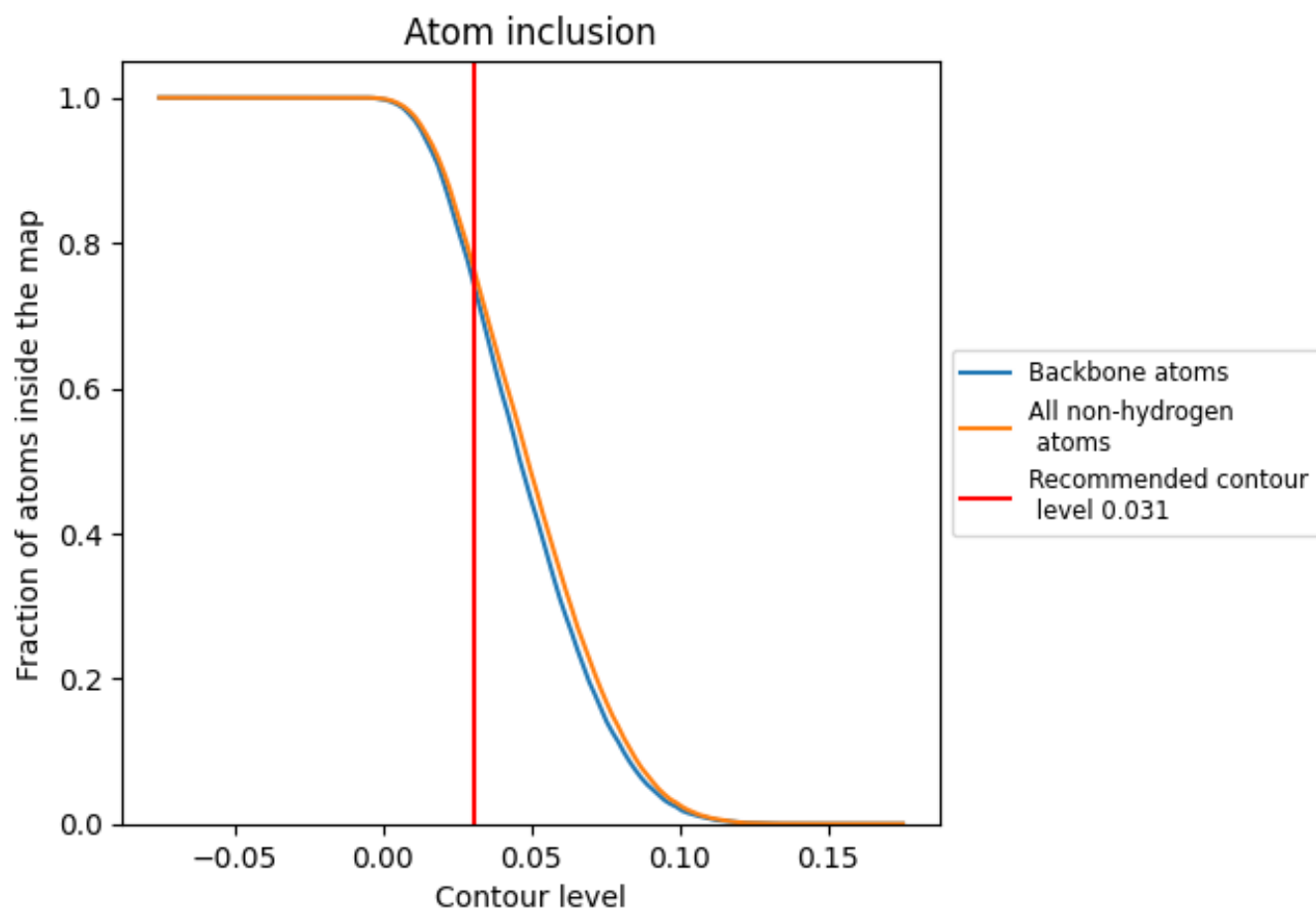
This section was not generated.

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 (0.031).


























9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 76% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.031) and Q-score for the entire model and for each chain.

Chain	Atom inclusion
All	 0.7582
1	 0.7688
3	 0.7890
4	 0.6764
5	 0.7357
6	 0.6907
7	 0.8217
8	 0.8331
9	 0.7149
92	 0.5280
A	 0.8970
B	 0.9099
B2	 0.2377
C	 0.9071
D	 0.7903
E	 0.7728
F	 0.8130
G	 0.7113
I	 0.8025
I2	 0.3950
J	 0.8415
K	 0.6185
L	 0.6654
L2	 0.3427
Z	 0.6755

