



Full wwPDB EM Validation Report ⓘ

Jun 10, 2026 – 02:46 PM EDT

PDB ID : 9YGV / pdb_00009ygv
EMDB ID : EMD-72770
Title : Photosystem I FCP Supercomplex from *Macrocystis pyrifera*
Authors : Maturana, P.; Maldonado, M.
Deposited on : 2025-09-29
Resolution : 2.47 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

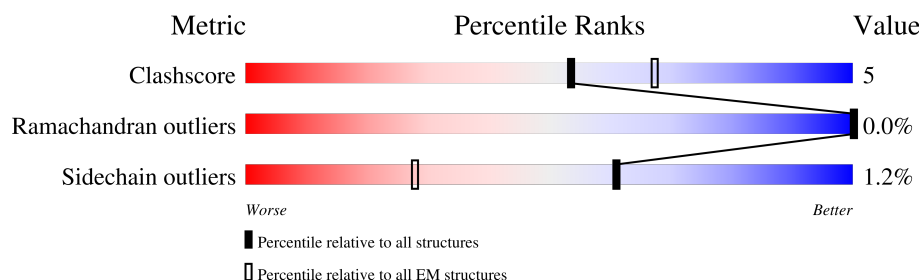
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.47 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	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

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	1	230	<div> <div>55%</div> <div> <div>73%</div> <div>23%</div> </div> </div>
2	3	191	<div> <div>61%</div> <div> <div>77%</div> <div>6%</div> <div>16%</div> </div> </div>
3	5	222	<div> <div>46%</div> <div> <div>71%</div> <div>7%</div> <div>21%</div> </div> </div>
4	7	169	<div> <div>61%</div> <div> <div>90%</div> <div>10%</div> </div> </div>
5	8	215	<div> <div>55%</div> <div> <div>75%</div> <div>7%</div> <div>18%</div> </div> </div>
6	A	749	<div> <div>61%</div> <div> <div>93%</div> <div>5%</div> </div> </div>
7	B	734	<div> <div>61%</div> <div> <div>92%</div> <div>7%</div> </div> </div>
8	C	81	<div> <div>65%</div> <div> <div>95%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
9	D	132	
10	E	61	
11	F	202	
12	I	36	
13	J	42	
14	M	30	
15	R	132	
16	b	141	
17	10	212	
17	6	212	
18	11	213	
19	13	216	
19	9	216	
20	15	155	
21	16	163	
22	17	218	
23	19	150	
24	2	104	
25	4	237	
26	L	145	
27	a	151	

2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 52767 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called FCP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	178	Total	C	N	O	S	0	0
			1336	860	218	250	8		

- Molecule 2 is a protein called FCP3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	3	161	Total	C	N	O	S	0	0
			1236	782	211	235	8		

- Molecule 3 is a protein called FCP5.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	5	175	Total	C	N	O	S	0	0
			1299	828	219	240	12		

- Molecule 4 is a protein called FCP7.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	7	169	Total	C	N	O	S	0	0
			1288	832	215	229	12		

- Molecule 5 is a protein called FCP8.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	8	176	Total	C	N	O	S	0	0
			1328	855	222	242	9		

- Molecule 6 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A	742	Total	C	N	O	S	0	0
			5834	3824	989	997	24		

- Molecule 7 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	B	730	Total	C	N	O	S	0	0
			5834	3839	980	997	18		

- Molecule 8 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	C	80	Total	C	N	O	S	0	0
			596	364	103	118	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	D	125	Total	C	N	O	S	0	0
			1002	649	170	179	4		

- Molecule 10 is a protein called Photosystem I reaction center subunit IV.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	E	60	Total	C	N	O	0	0
			482	311	82	89		

- Molecule 11 is a protein called Photosystem I reaction center subunit III.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	F	161	Total	C	N	O	S	0	0
			1271	817	212	237	5		

- Molecule 12 is a protein called Photosystem I reaction center subunit VIII.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	I	34	Total	C	N	O	S	0	0
			264	184	36	43	1		

- Molecule 13 is a protein called Photosystem I reaction center subunit IX.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	J	41	Total	C	N	O	S	0	0
			333	227	48	56	2		

- Molecule 14 is a protein called Photosystem I reaction center subunit XII.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	M	30	Total	C	N	O	S	0	0
			228	152	36	39	1		

- Molecule 15 is a protein called PsaR.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	R	85	Total	C	N	O	S	0	0
			627	410	102	113	2		

- Molecule 16 is a protein called FCPB.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	b	141	Total	C	N	O	S	0	0
			706	423	141	142			

- Molecule 17 is a protein called FCP6 and FCP10.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	6	173	Total	C	N	O	S	0	0
			1275	818	210	236	11		
17	10	172	Total	C	N	O	S	0	0
			1270	815	209	235	11		

- Molecule 18 is a protein called FCP11.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	11	167	Total	C	N	O	S	0	0
			1283	833	208	235	7		

- Molecule 19 is a protein called FCP9 and FCP13.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	13	141	Total	C	N	O	S	0	0
			1107	719	184	196	8		
19	9	136	Total	C	N	O	S	0	0
			1060	685	178	189	8		

- Molecule 20 is a protein called FCP15.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	15	155	Total	C	N	O	S	0	0
			775	465	155	155			

- Molecule 21 is a protein called FCP16.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	16	163	Total	C	N	O	0	0
			815	489	163	163		

- Molecule 22 is a protein called FCP17.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	17	146	Total	C	N	O	S	0	0
			1107	702	195	204	6		

- Molecule 23 is a protein called FCP19.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	19	150	Total	C	N	O	0	0
			750	450	150	150		

- Molecule 24 is a protein called FCP2.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	2	104	Total	C	N	O	0	0
			520	312	104	104		

- Molecule 25 is a protein called FCP4.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	4	180	Total	C	N	O	S	0	0
			1337	853	223	250	11		

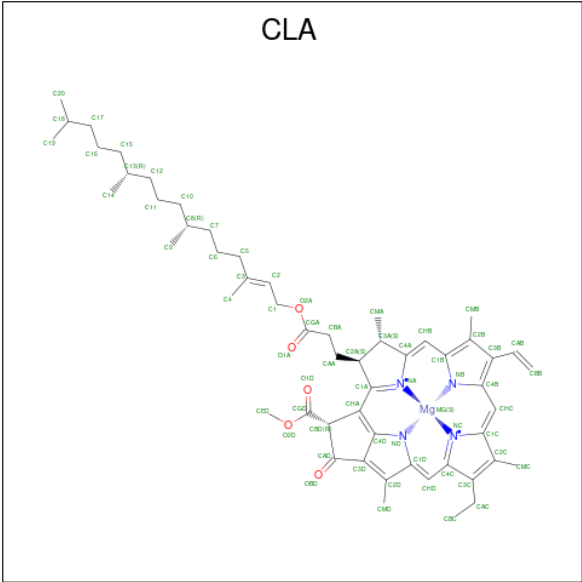
- Molecule 26 is a protein called Photosystem I reaction center subunit XI.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	L	134	Total	C	N	O	S	0	0
			1015	670	161	181	3		

- Molecule 27 is a protein called FCPA.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	a	151	Total	C	N	O	0	0
			755	453	151	151		

- Molecule 28 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					AltConf
28	1	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
28	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	1	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
28	1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
28	1	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
28	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
28	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
28	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	5	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
28	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	5	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
28	5	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
28	5	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
28	5	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
28	5	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
28	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	7	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
28	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	7	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
28	7	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
28	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	8	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	8	1	Total	C	Mg	N	O	0
			56	46	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
28	8	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
28	8	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
28	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	8	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
28	8	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
28	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
28	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
28	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	A	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
28	A	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
28	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
28	A	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
28	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
28	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	A	1	Total	C	Mg	N	O	0
			56	46	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
28	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	A	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
28	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
28	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
28	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	A	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
28	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
28	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
28	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
28	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
28	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
28	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	A	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
28	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			59	49	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
28	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
28	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	F	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	F	1	Total 43	C 35	Mg 1	N 4	O 3	0
28	J	1	Total 58	C 48	Mg 1	N 4	O 5	0
28	J	1	Total 42	C 34	Mg 1	N 4	O 3	0
28	R	1	Total 55	C 45	Mg 1	N 4	O 5	0
28	R	1	Total 51	C 41	Mg 1	N 4	O 5	0
28	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	6	1	Total 53	C 43	Mg 1	N 4	O 5	0
28	6	1	Total 55	C 45	Mg 1	N 4	O 5	0
28	6	1	Total 42	C 34	Mg 1	N 4	O 3	0
28	6	1	Total 58	C 48	Mg 1	N 4	O 5	0
28	6	1	Total 55	C 45	Mg 1	N 4	O 5	0
28	6	1	Total 51	C 41	Mg 1	N 4	O 5	0
28	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	10	1	Total 55	C 45	Mg 1	N 4	O 5	0
28	10	1	Total 46	C 36	Mg 1	N 4	O 5	0
28	10	1	Total 55	C 45	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
28	10	1	Total 46	C 36	Mg 1	N 4	O 5	0
28	10	1	Total 56	C 46	Mg 1	N 4	O 5	0
28	10	1	Total 57	C 47	Mg 1	N 4	O 5	0
28	10	1	Total 47	C 37	Mg 1	N 4	O 5	0
28	10	1	Total 43	C 35	Mg 1	N 4	O 3	0
28	10	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	11	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	11	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	11	1	Total 57	C 47	Mg 1	N 4	O 5	0
28	11	1	Total 60	C 50	Mg 1	N 4	O 5	0
28	11	1	Total 45	C 35	Mg 1	N 4	O 5	0
28	11	1	Total 45	C 35	Mg 1	N 4	O 5	0
28	11	1	Total 43	C 35	Mg 1	N 4	O 3	0
28	11	1	Total 50	C 40	Mg 1	N 4	O 5	0
28	11	1	Total 43	C 35	Mg 1	N 4	O 3	0
28	11	1	Total 43	C 35	Mg 1	N 4	O 3	0
28	13	1	Total 56	C 46	Mg 1	N 4	O 5	0
28	13	1	Total 45	C 35	Mg 1	N 4	O 5	0
28	13	1	Total 45	C 35	Mg 1	N 4	O 5	0
28	13	1	Total 46	C 36	Mg 1	N 4	O 5	0
28	13	1	Total 42	C 34	Mg 1	N 4	O 3	0

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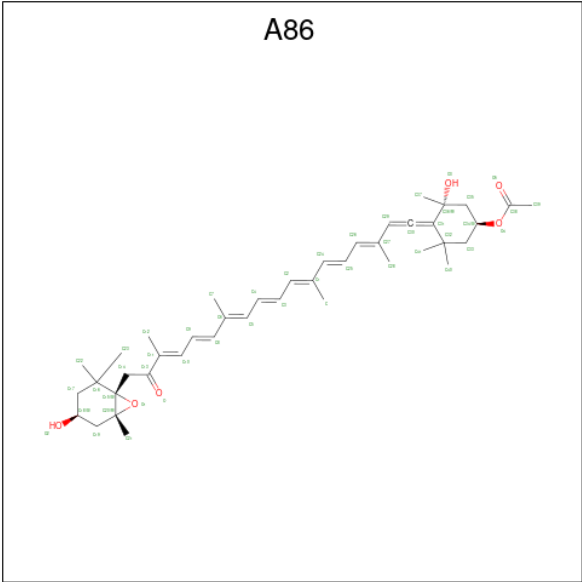
Mol	Chain	Residues	Atoms					AltConf
28	13	1	Total 45	C 35	Mg 1	N 4	O 5	0
28	15	1	Total 46	C 36	Mg 1	N 4	O 5	0
28	16	1	Total 45	C 35	Mg 1	N 4	O 5	0
28	16	1	Total 42	C 34	Mg 1	N 4	O 3	0
28	16	1	Total 47	C 37	Mg 1	N 4	O 5	0
28	16	1	Total 41	C 33	Mg 1	N 4	O 3	0
28	16	1	Total 43	C 35	Mg 1	N 4	O 3	0
28	17	1	Total 50	C 40	Mg 1	N 4	O 5	0
28	17	1	Total 43	C 35	Mg 1	N 4	O 3	0
28	17	1	Total 48	C 38	Mg 1	N 4	O 5	0
28	17	1	Total 49	C 39	Mg 1	N 4	O 5	0
28	17	1	Total 50	C 40	Mg 1	N 4	O 5	0
28	17	1	Total 47	C 37	Mg 1	N 4	O 5	0
28	17	1	Total 46	C 36	Mg 1	N 4	O 5	0
28	19	1	Total 46	C 36	Mg 1	N 4	O 5	0
28	19	1	Total 43	C 35	Mg 1	N 4	O 3	0
28	4	1	Total 55	C 45	Mg 1	N 4	O 5	0
28	4	1	Total 51	C 41	Mg 1	N 4	O 5	0
28	4	1	Total 42	C 34	Mg 1	N 4	O 3	0
28	4	1	Total 55	C 45	Mg 1	N 4	O 5	0
28	4	1	Total 60	C 50	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
28	4	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
28	4	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
28	9	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
28	9	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
28	9	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
28	9	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
28	9	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
28	9	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	9	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	L	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
28	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	a	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
28	a	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
28	a	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
28	a	1	Total	C	Mg	N	O	0
			42	34	1	4	3	

- Molecule 29 is (3S,3'S,5R,5'R,6S,6'R,8'R)-3,5'-dihydroxy-8-oxo-6',7'-didehydro-5,5',6,6',7,8-hexahydro-5,6-epoxy-beta,beta-caroten-3'-yl acetate (CCD ID: A86) (formula: C₄₂H₅₈O₆).



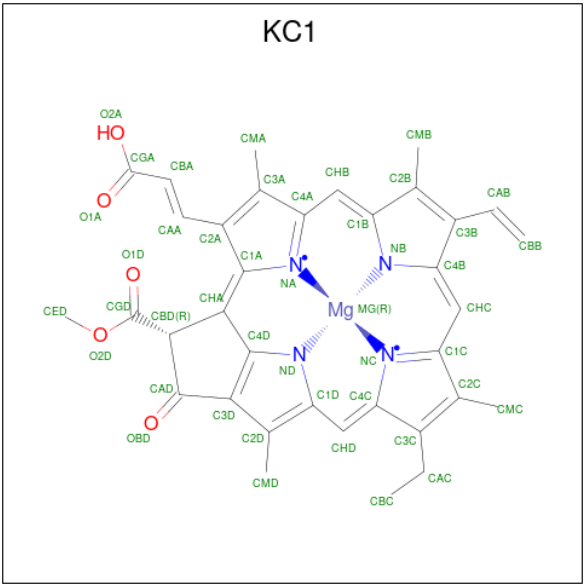
Mol	Chain	Residues	Atoms			AltConf
29	1	1	Total	C	O	0
			48	42	6	
29	1	1	Total	C	O	0
			48	42	6	
29	3	1	Total	C	O	0
			48	42	6	
29	3	1	Total	C	O	0
			48	42	6	
29	3	1	Total	C	O	0
			48	42	6	
29	5	1	Total	C	O	0
			48	42	6	
29	8	1	Total	C	O	0
			48	42	6	
29	J	1	Total	C	O	0
			48	42	6	
29	R	1	Total	C	O	0
			48	42	6	
29	R	1	Total	C	O	0
			48	42	6	
29	6	1	Total	C	O	0
			48	42	6	
29	10	1	Total	C	O	0
			48	42	6	
29	10	1	Total	C	O	0
			48	42	6	
29	11	1	Total	C	O	0
			48	42	6	

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Mol	Chain	Residues	Atoms			AltConf
29	17	1	Total	C	O	0
			48	42	6	
29	4	1	Total	C	O	0
			48	42	6	
29	4	1	Total	C	O	0
			48	42	6	
29	9	1	Total	C	O	0
			48	42	6	

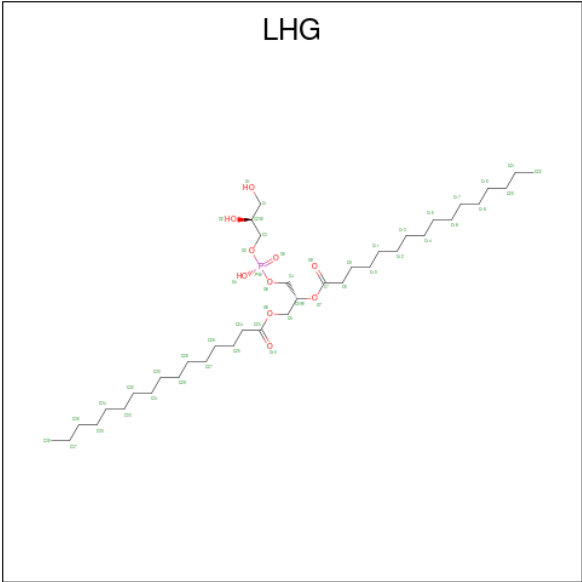
- Molecule 30 is Chlorophyll c1 (CCD ID: KC1) (formula: $C_{35}H_{30}MgN_4O_5$).



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Mol	Chain	Residues	Atoms					AltConf
30	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	10	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	10	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	10	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	11	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	13	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	17	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	17	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	9	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	9	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	a	1	Total 45	C 35	Mg 1	N 4	O 5	0

- Molecule 31 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



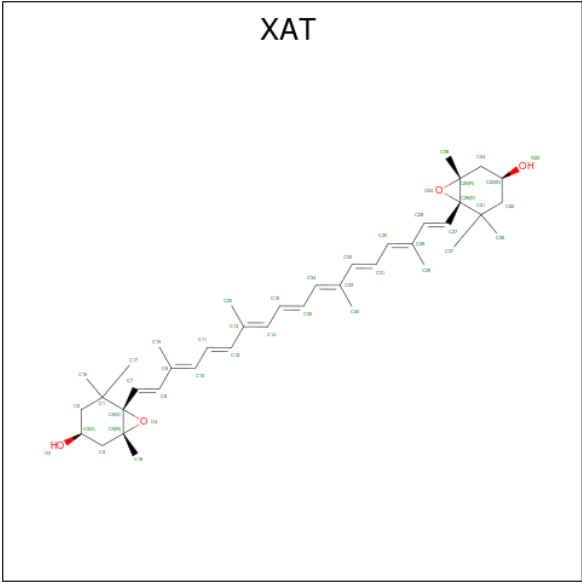
Mol	Chain	Residues	Atoms				AltConf
31	1	1	Total	C	O	P	0
			44	33	10	1	
31	5	1	Total	C	O	P	0
			24	13	10	1	
31	5	1	Total	C	O	P	0
			27	16	10	1	
31	7	1	Total	C	O	P	0
			27	16	10	1	
31	A	1	Total	C	O	P	0
			48	37	10	1	
31	A	1	Total	C	O	P	0
			27	16	10	1	
31	A	1	Total	C	O	P	0
			27	16	10	1	
31	B	1	Total	C	O	P	0
			27	16	10	1	
31	B	1	Total	C	O	P	0
			49	38	10	1	
31	I	1	Total	C	O	P	0
			49	38	10	1	
31	11	1	Total	C	O	P	0
			37	26	10	1	
31	4	1	Total	C	O	P	0
			25	14	10	1	
31	9	1	Total	C	O	P	0
			28	17	10	1	
31	9	1	Total	C	O	P	0
			30	19	10	1	

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Mol	Chain	Residues	Atoms				AltConf
31	9	1	Total	C	O	P	0
			33	22	10	1	

- 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 (CCD ID: XAT) (formula: C₄₀H₅₆O₄).



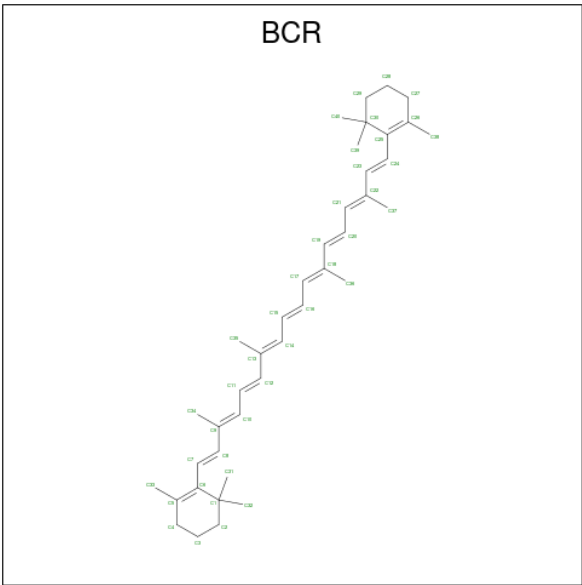
Mol	Chain	Residues	Atoms			AltConf
32	1	1	Total	C	O	0
			44	40	4	
32	3	1	Total	C	O	0
			44	40	4	
32	5	1	Total	C	O	0
			44	40	4	
32	5	1	Total	C	O	0
			44	40	4	
32	5	1	Total	C	O	0
			44	40	4	
32	5	1	Total	C	O	0
			44	40	4	
32	7	1	Total	C	O	0
			44	40	4	
32	7	1	Total	C	O	0
			44	40	4	
32	7	1	Total	C	O	0
			44	40	4	
32	7	1	Total	C	O	0
			44	40	4	

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Mol	Chain	Residues	Atoms			AltConf
32	7	1	Total	C	O	0
			44	40	4	
32	8	1	Total	C	O	0
			44	40	4	
32	8	1	Total	C	O	0
			44	40	4	
32	J	1	Total	C	O	0
			44	40	4	
32	6	1	Total	C	O	0
			44	40	4	
32	6	1	Total	C	O	0
			44	40	4	
32	6	1	Total	C	O	0
			44	40	4	
32	10	1	Total	C	O	0
			44	40	4	
32	10	1	Total	C	O	0
			44	40	4	
32	10	1	Total	C	O	0
			44	40	4	
32	11	1	Total	C	O	0
			44	40	4	
32	13	1	Total	C	O	0
			44	40	4	
32	13	1	Total	C	O	0
			44	40	4	
32	17	1	Total	C	O	0
			44	40	4	
32	4	1	Total	C	O	0
			44	40	4	
32	4	1	Total	C	O	0
			44	40	4	
32	9	1	Total	C	O	0
			43	39	4	

- Molecule 33 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



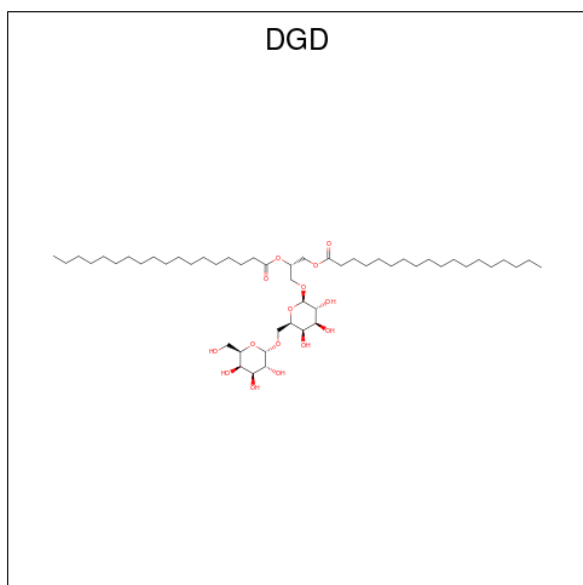
Mol	Chain	Residues	Atoms	AltConf
33	1	1	Total C 40 40	0
33	8	1	Total C 40 40	0
33	A	1	Total C 40 40	0
33	A	1	Total C 40 40	0
33	A	1	Total C 40 40	0
33	A	1	Total C 40 40	0
33	A	1	Total C 40 40	0
33	B	1	Total C 40 40	0
33	B	1	Total C 40 40	0
33	B	1	Total C 40 40	0
33	B	1	Total C 40 40	0
33	B	1	Total C 40 40	0
33	B	1	Total C 40 40	0
33	B	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
33	B	1	Total C 40 40	0
33	F	1	Total C 40 40	0
33	F	1	Total C 40 40	0
33	I	1	Total C 40 40	0
33	J	1	Total C 40 40	0
33	M	1	Total C 40 40	0
33	17	1	Total C 40 40	0
33	L	1	Total C 40 40	0
33	L	1	Total C 40 40	0

- Molecule 34 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



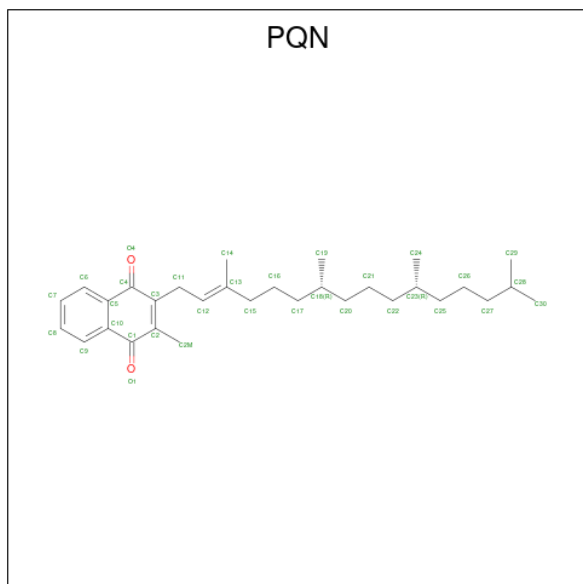
Mol	Chain	Residues	Atoms	AltConf
34	8	1	Total C O 31 17 14	0
34	4	1	Total C O 39 24 15	0

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Mol	Chain	Residues	Atoms			AltConf
34	4	1	Total	C	O	0
			29	17	12	

- Molecule 35 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



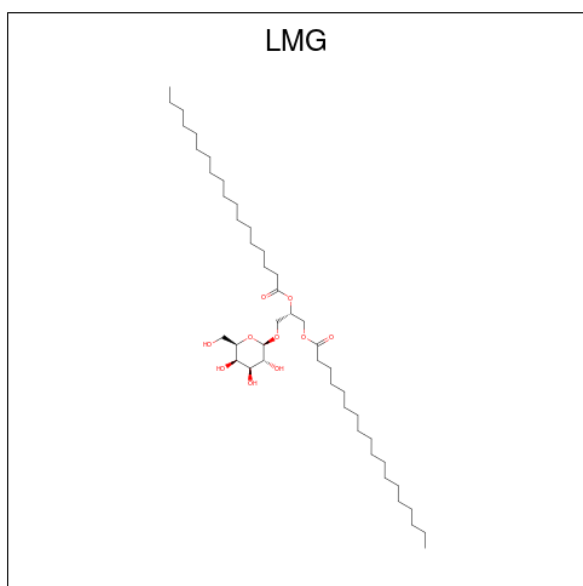
Mol	Chain	Residues	Atoms			AltConf
35	A	1	Total	C	O	0
			33	31	2	
35	B	1	Total	C	O	0
			33	31	2	

- Molecule 36 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



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

- Molecule 37 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).

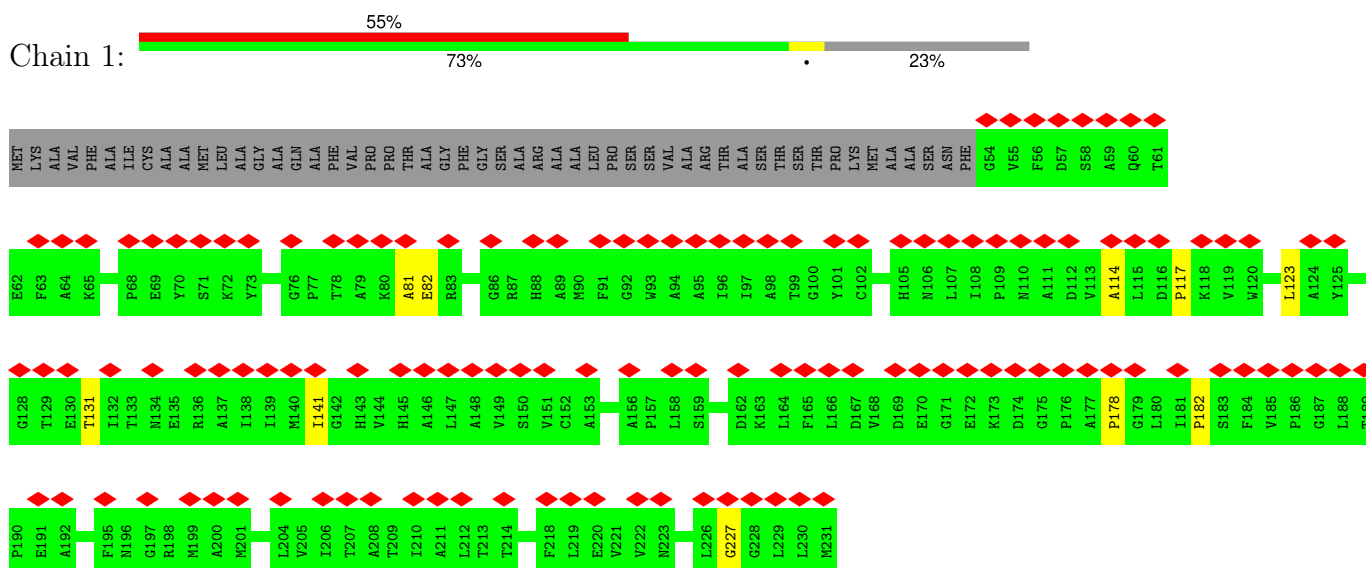


Mol	Chain	Residues	Atoms			AltConf
37	F	1	Total	C	O	0
			41	31	10	

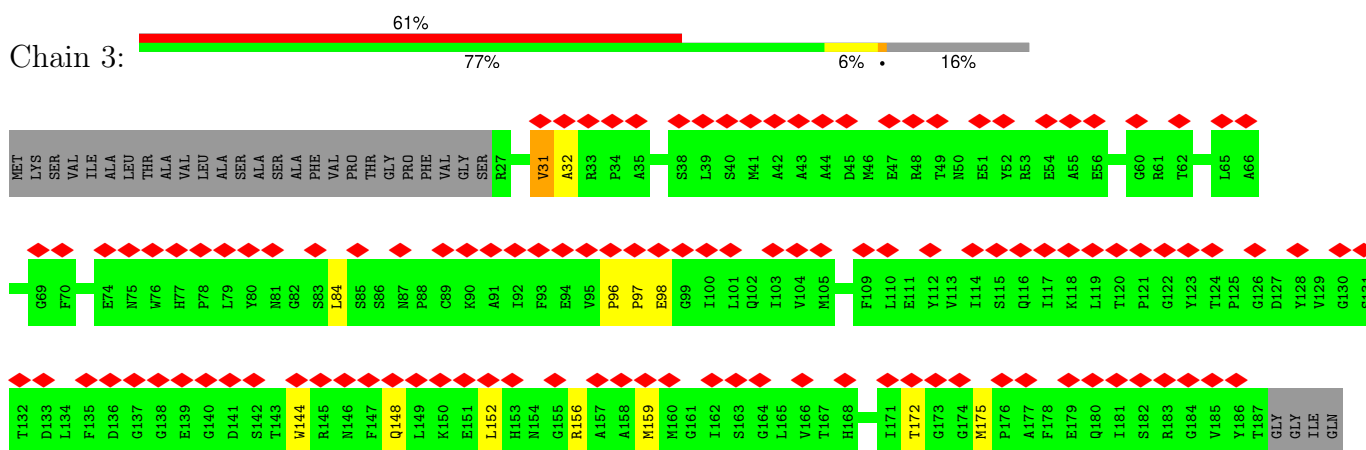
3 Residue-property plots [i](#)

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: FCP1

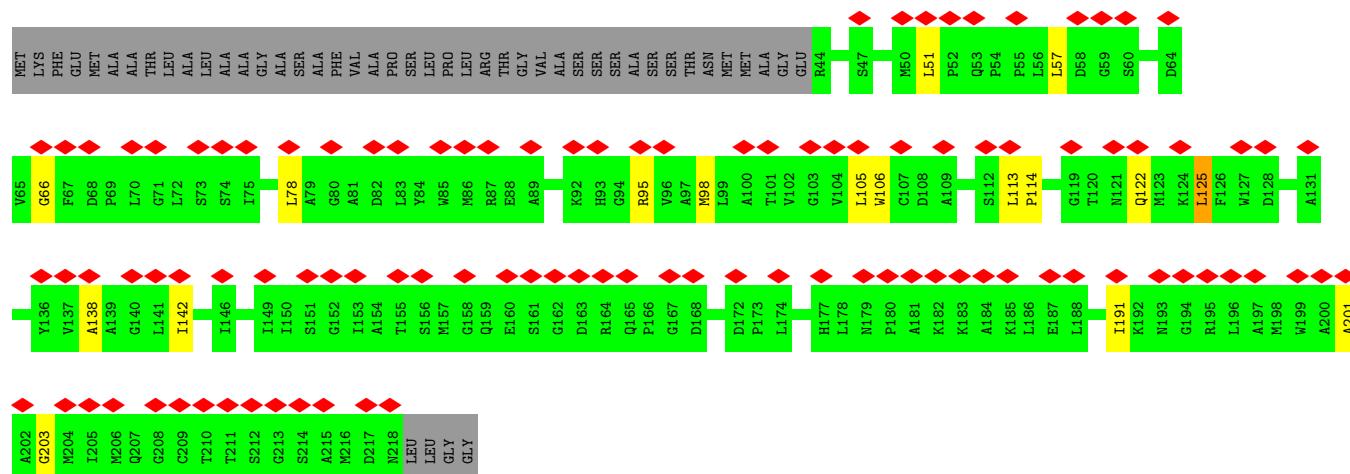


• Molecule 2: FCP3

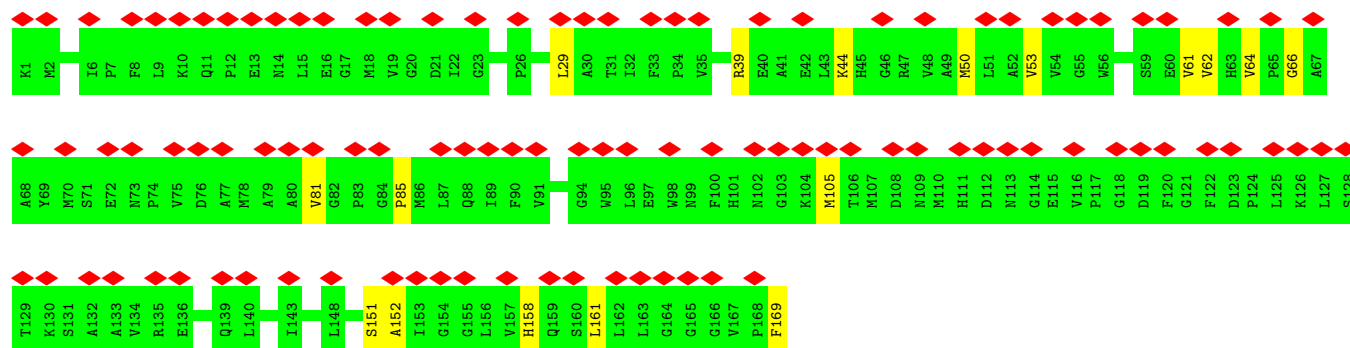
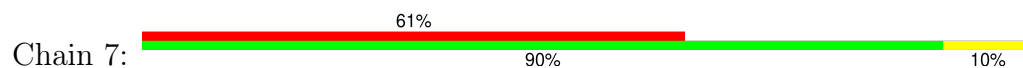


• Molecule 3: FCP5

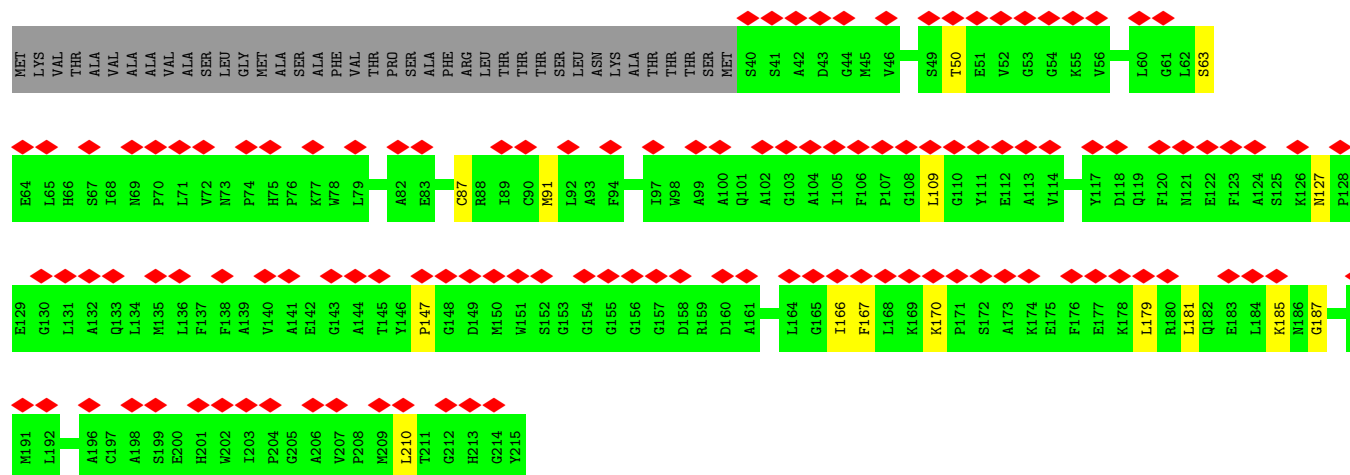
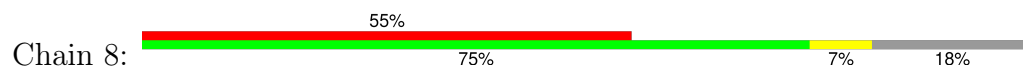




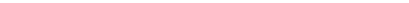
- Molecule 4: FCP7

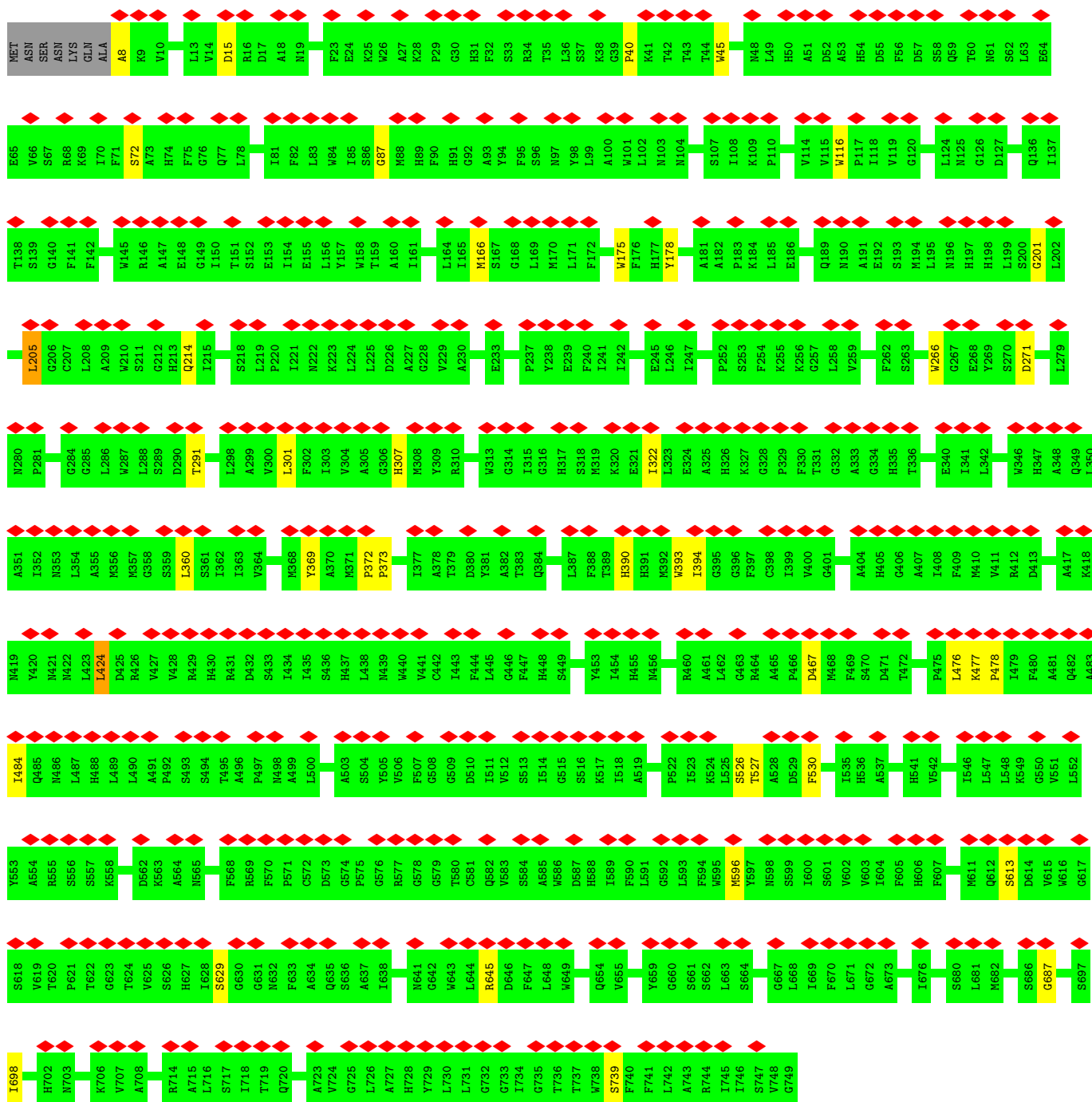


- Molecule 5: FCP8




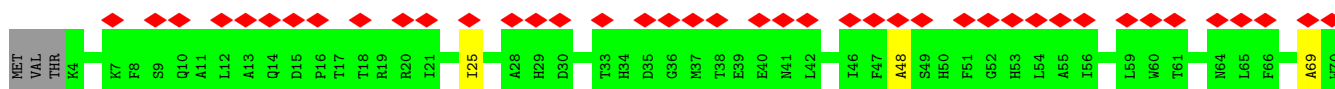
- Molecule 6: Photosystem I P700 chlorophyll a apoprotein A1

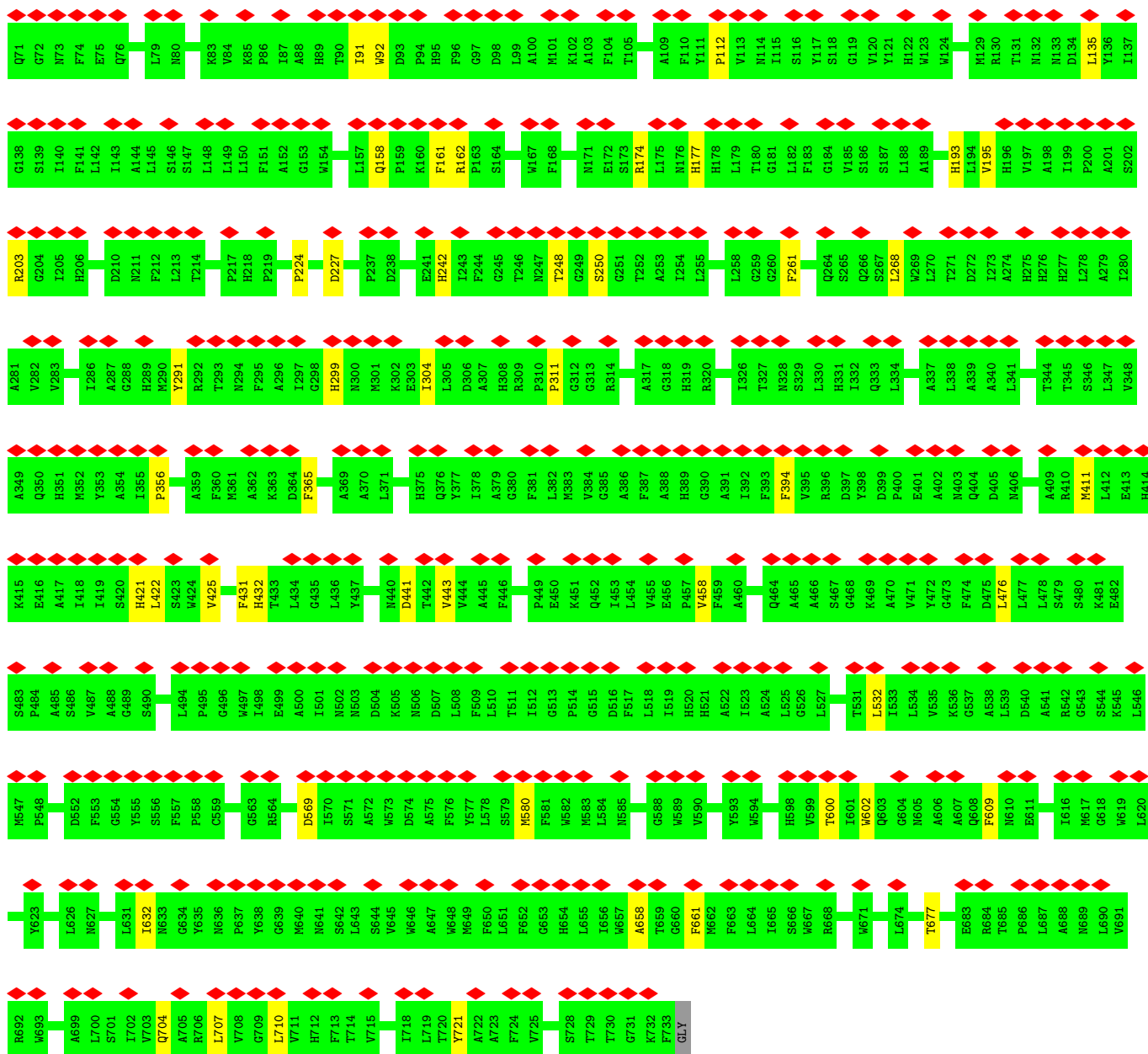
Chain A: 



- Molecule 7: Photosystem I P700 chlorophyll a apoprotein A2

Chain B:  61% 92% 7%



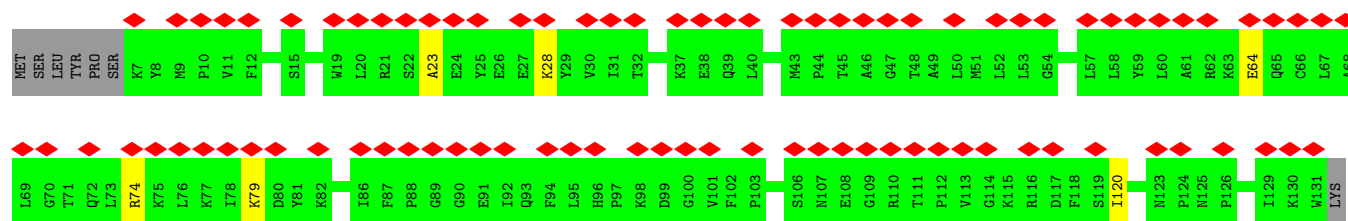


• Molecule 8: Photosystem I iron-sulfur center

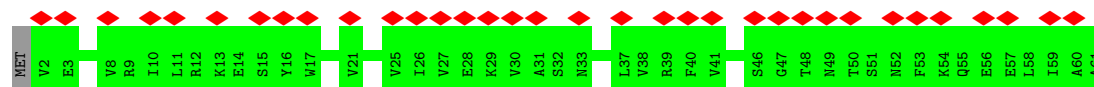


• Molecule 9: Photosystem I reaction center subunit II

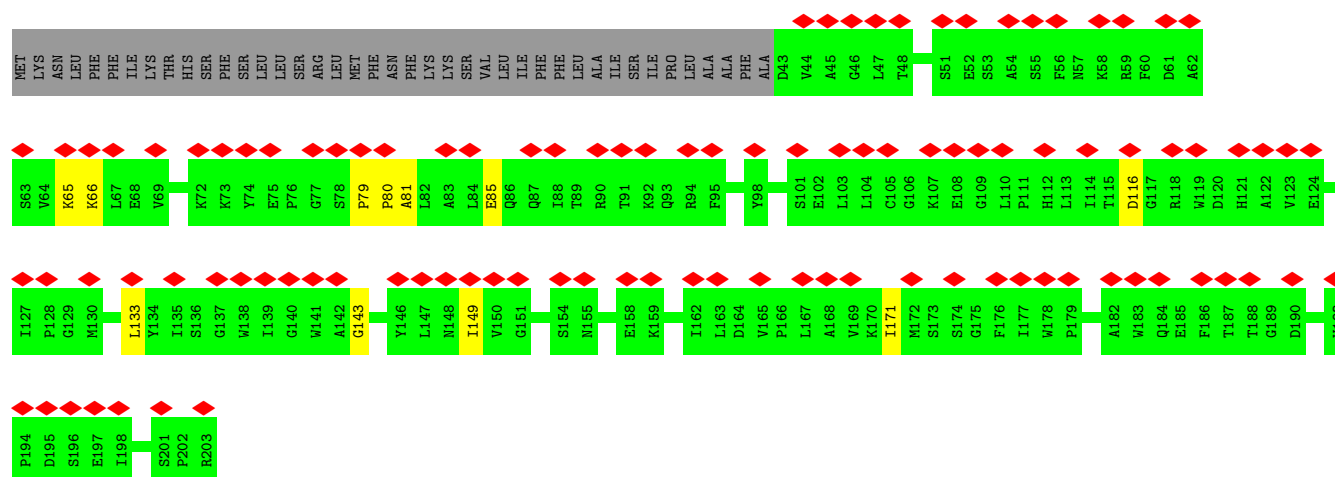




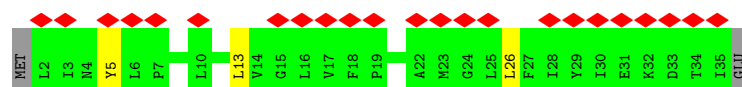
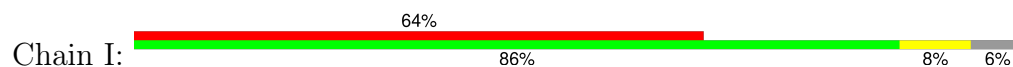
• Molecule 10: Photosystem I reaction center subunit IV



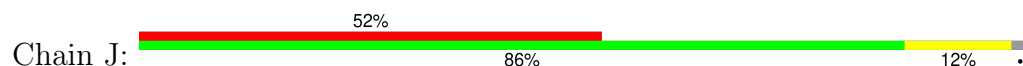
• Molecule 11: Photosystem I reaction center subunit III



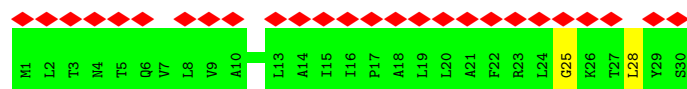
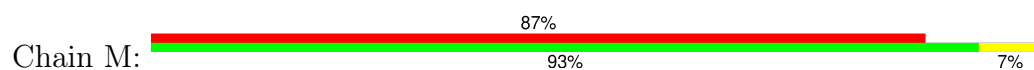
• Molecule 12: Photosystem I reaction center subunit VIII



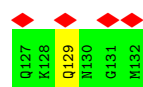
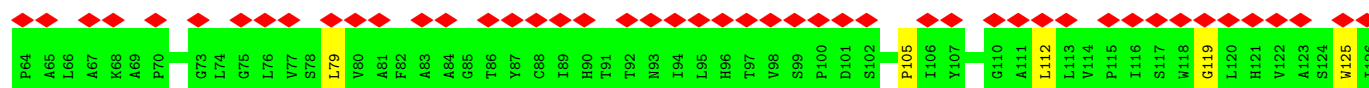
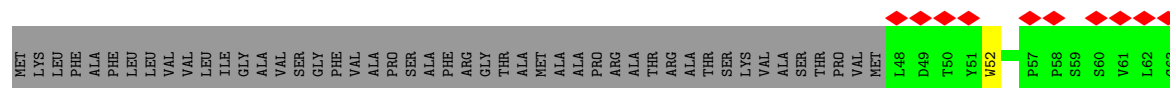
• Molecule 13: Photosystem I reaction center subunit IX



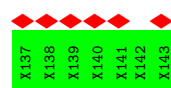
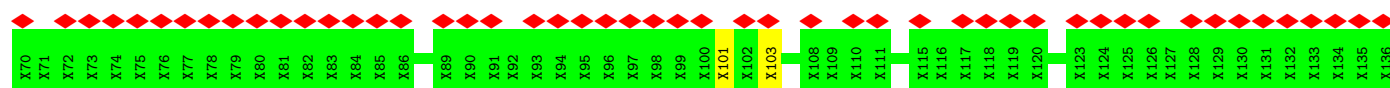
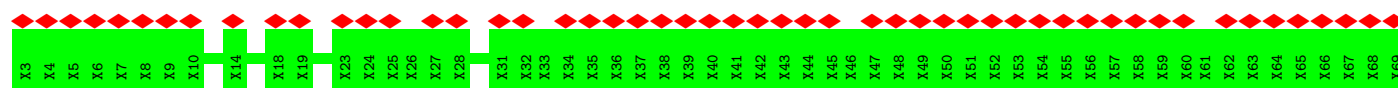
• Molecule 14: Photosystem I reaction center subunit XII



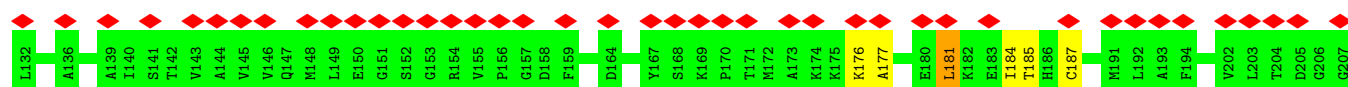
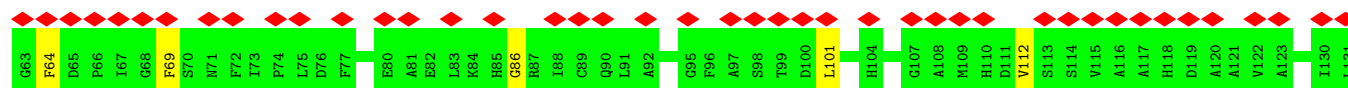
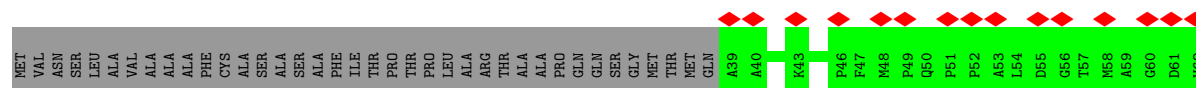
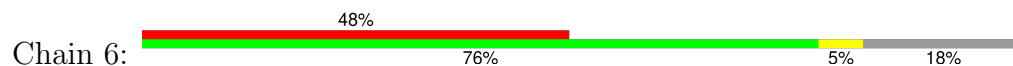
• Molecule 15: PsaR



• Molecule 16: FCPB

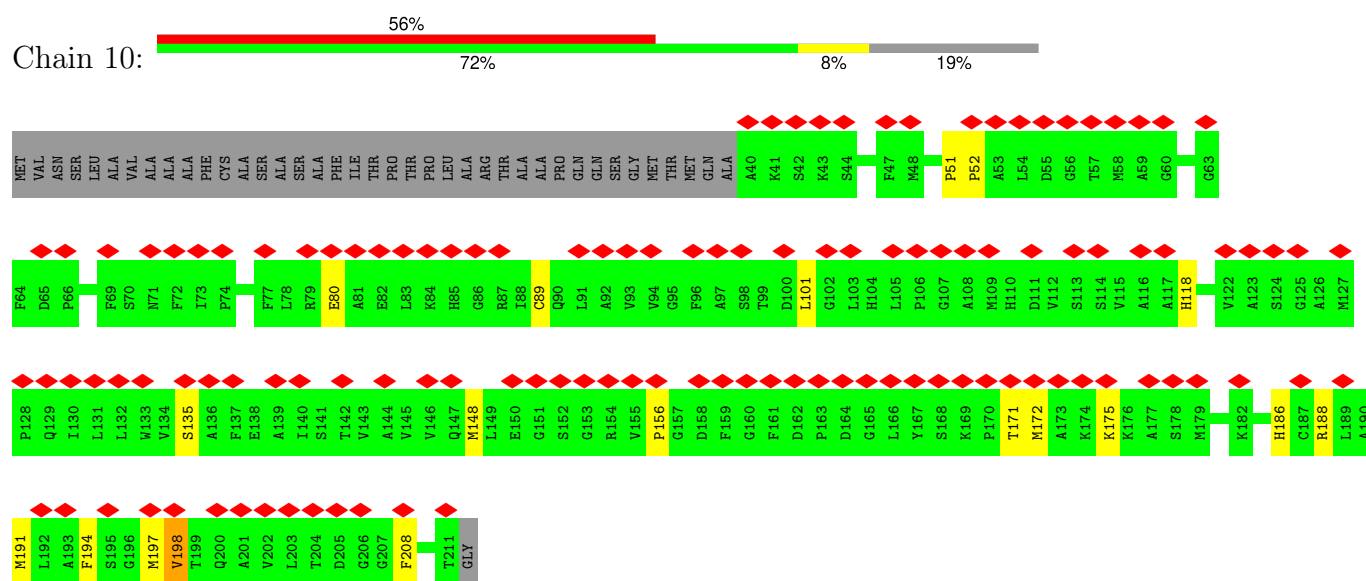


• Molecule 17: FCP6 and FCP10





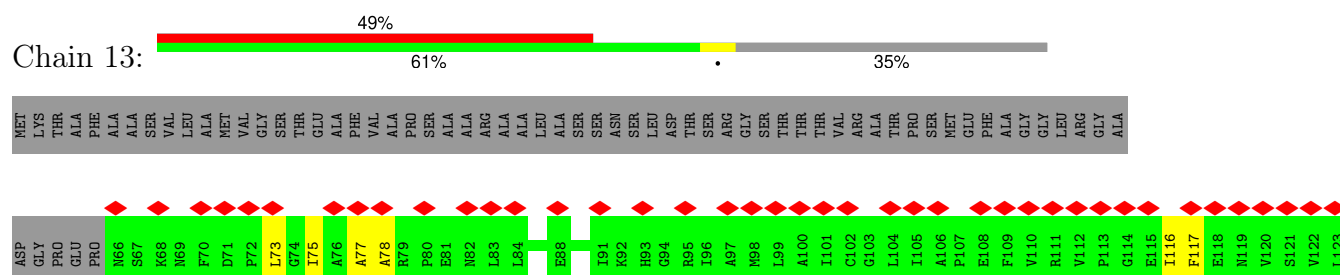
- Molecule 17: FCP6 and FCP10

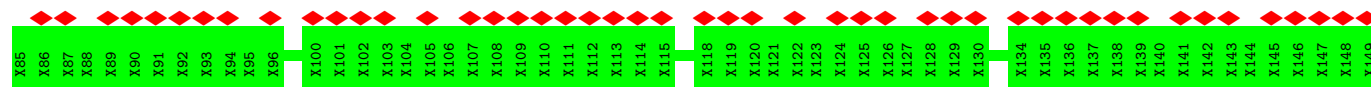


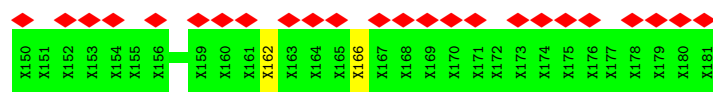
- Molecule 18: FCP11



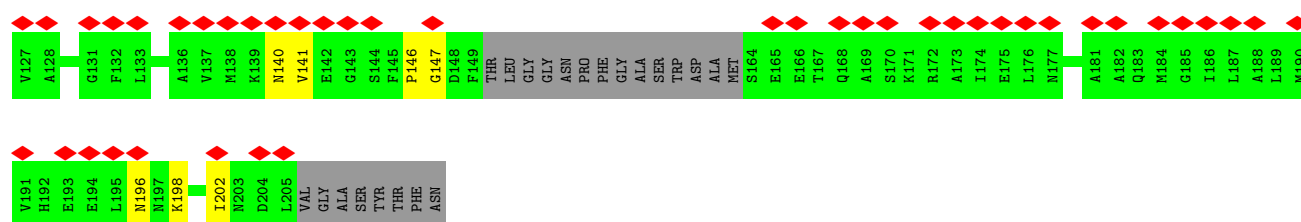
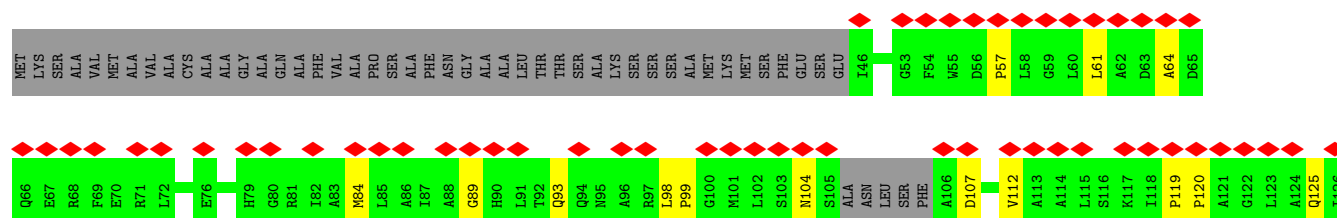
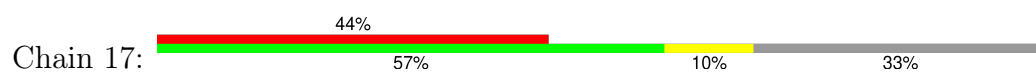
- Molecule 19: FCP9 and FCP13



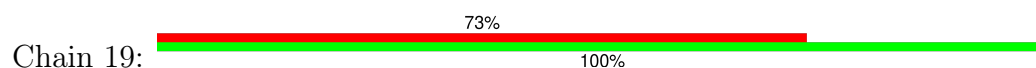




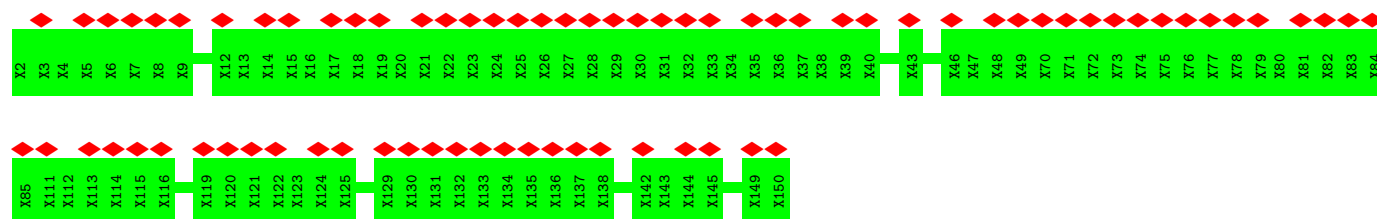
• Molecule 22: FCP17



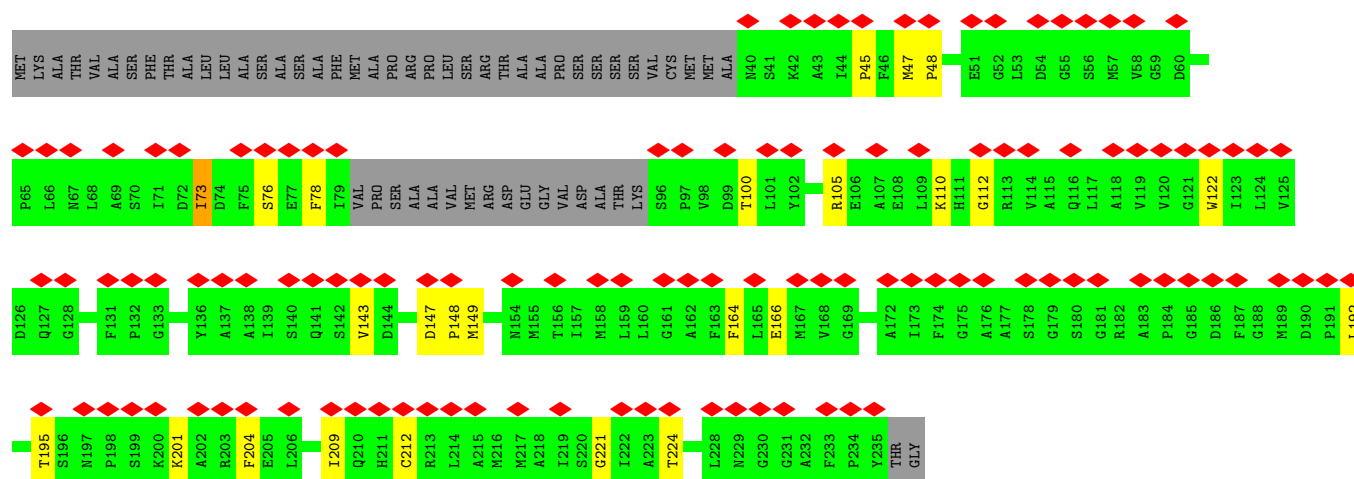
• Molecule 23: FCP19



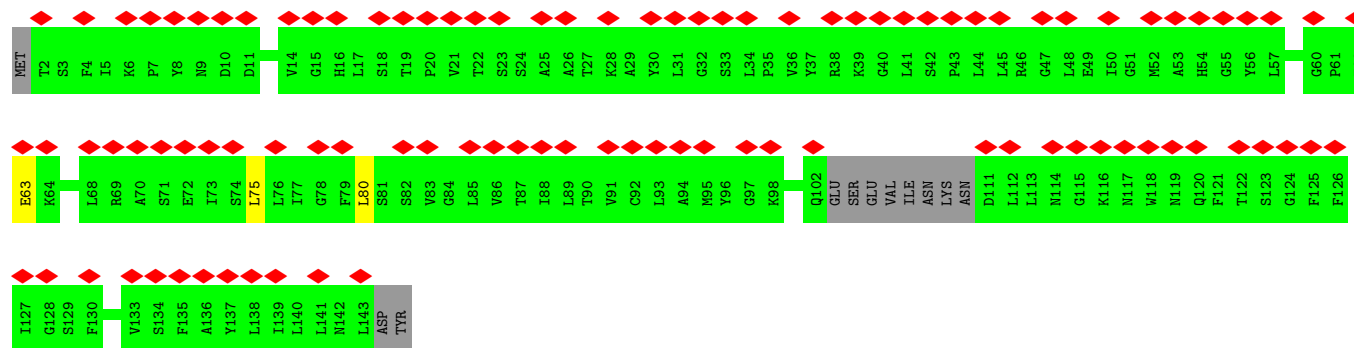
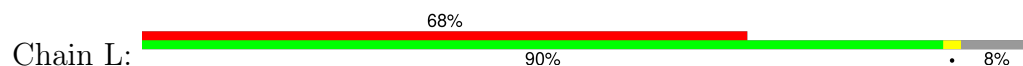
• Molecule 24: FCP2



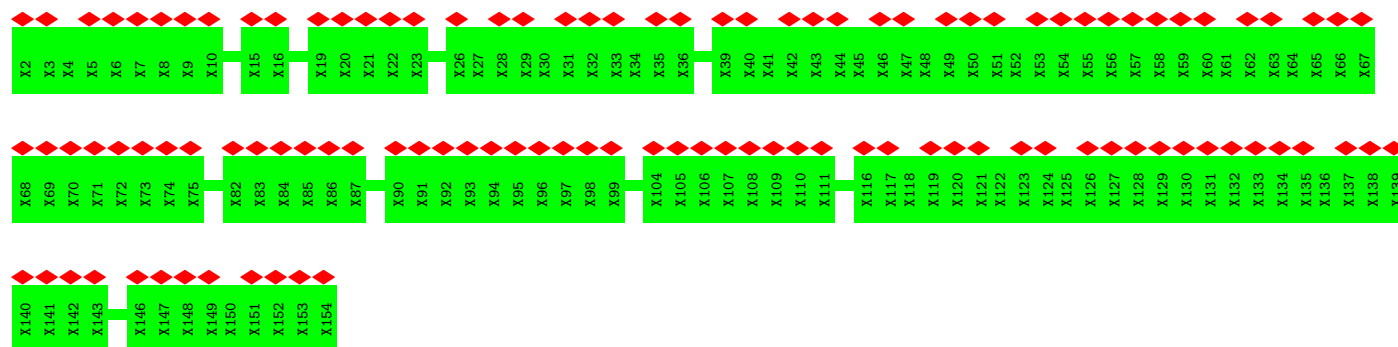
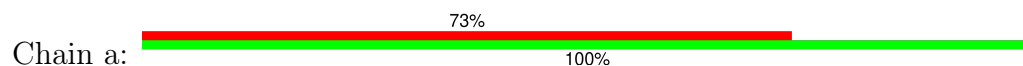
• Molecule 25: FCP4



• Molecule 26: Photosystem I reaction center subunit XI



• Molecule 27: FCPA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	133000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	7.047	Depositor
Minimum map value	-4.430	Depositor
Average map value	0.081	Depositor
Map value standard deviation	0.467	Depositor
Recommended contour level	0.45	Depositor
Map size (Å)	119.266, 233.664, 260.438	wwPDB
Map dimensions	214, 192, 98	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.217, 1.217, 1.2169999	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DGD, LHG, KC1, SF4, LMG, CLA, BCR, A86, PQN, XAT

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	1	0.13	0/1370	0.24	0/1868
2	3	0.15	0/1264	0.31	0/1713
3	5	0.13	0/1329	0.28	0/1799
4	7	0.15	0/1322	0.27	0/1786
5	8	0.10	0/1366	0.22	0/1850
6	A	0.18	0/6027	0.34	0/8202
7	B	0.18	0/6045	0.33	0/8254
8	C	0.16	0/606	0.38	0/823
9	D	0.12	0/1028	0.28	0/1386
10	E	0.14	0/490	0.26	0/663
11	F	0.15	0/1304	0.31	0/1769
12	I	0.15	0/270	0.29	0/370
13	J	0.18	0/345	0.40	0/471
14	M	0.13	0/230	0.25	0/312
15	R	0.13	0/646	0.27	0/888
17	10	0.10	0/1301	0.25	0/1764
17	6	0.15	0/1306	0.28	0/1771
18	11	0.11	0/1314	0.24	0/1781
19	13	0.12	0/1131	0.28	0/1526
19	9	0.12	0/1082	0.31	0/1461
22	17	0.11	0/1126	0.30	0/1522
25	4	0.14	0/1367	0.31	1/1851 (0.1%)
26	L	0.15	0/1039	0.30	0/1409
All	All	0.15	0/33308	0.30	1/45239 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	4	76	SER	CB-CA-C	-5.34	110.43	116.63

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	1	1336	0	1313	8	0
2	3	1236	0	1208	8	0
3	5	1299	0	1294	14	0
4	7	1288	0	1281	14	0
5	8	1328	0	1291	9	0
6	A	5834	0	5736	26	0
7	B	5834	0	5639	38	0
8	C	596	0	568	2	0
9	D	1002	0	1013	3	0
10	E	482	0	494	0	0
11	F	1271	0	1262	7	0
12	I	264	0	290	3	0
13	J	333	0	327	4	0
14	M	228	0	260	2	0
15	R	627	0	635	4	0
16	b	706	0	154	1	0
17	10	1270	0	1265	14	0
17	6	1275	0	1270	7	0
18	11	1283	0	1293	11	0
19	13	1107	0	1122	7	0
19	9	1060	0	1082	11	0
20	15	775	0	160	0	0
21	16	815	0	169	1	0
22	17	1107	0	1113	14	0
23	19	750	0	157	0	0
24	2	520	0	111	0	0
25	4	1337	0	1309	18	0
26	L	1015	0	1044	2	0
27	a	755	0	159	0	0
28	1	445	0	416	12	0
28	10	470	0	407	16	0
28	11	516	0	460	10	0
28	13	279	0	214	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	15	46	0	33	0	0
28	16	218	0	161	1	0
28	17	333	0	254	8	0
28	19	89	0	66	1	0
28	3	430	0	452	9	0
28	4	379	0	339	16	0
28	5	436	0	400	14	0
28	6	444	0	416	18	0
28	7	574	0	570	19	0
28	8	378	0	344	16	0
28	9	333	0	251	9	0
28	A	2540	0	2542	74	0
28	B	2474	0	2597	60	0
28	F	108	0	104	4	0
28	J	100	0	86	2	0
28	L	245	0	255	4	0
28	R	106	0	90	1	0
28	a	173	0	128	1	0
29	1	96	0	0	0	0
29	10	96	0	0	0	0
29	11	48	0	0	0	0
29	17	48	0	0	0	0
29	3	144	0	0	1	0
29	4	96	0	0	0	0
29	5	48	0	0	0	0
29	6	48	0	0	0	0
29	8	48	0	0	0	0
29	9	48	0	0	0	0
29	J	48	0	0	0	0
29	R	96	0	0	0	0
30	1	45	0	0	0	0
30	10	135	0	0	0	0
30	11	45	0	0	0	0
30	13	45	0	0	0	0
30	17	90	0	0	1	0
30	3	135	0	0	0	0
30	4	180	0	0	0	0
30	5	45	0	0	1	0
30	6	180	0	0	0	0
30	7	90	0	0	0	0
30	8	90	0	0	0	0
30	9	90	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	a	45	0	0	0	0
31	1	44	0	61	1	0
31	11	37	0	44	1	0
31	4	25	0	20	0	0
31	5	51	0	42	1	0
31	7	27	0	24	0	0
31	9	91	0	92	2	0
31	A	102	0	117	1	0
31	B	76	0	96	9	0
31	I	49	0	74	1	0
32	1	44	0	56	1	0
32	10	132	0	168	11	0
32	11	44	0	56	7	0
32	13	88	0	112	6	0
32	17	44	0	56	3	0
32	3	44	0	56	1	0
32	4	88	0	112	10	0
32	5	176	0	224	15	0
32	6	132	0	168	14	0
32	7	220	0	280	17	0
32	8	88	0	112	6	0
32	9	43	0	53	5	0
32	J	44	0	56	2	0
33	1	40	0	56	1	0
33	17	40	0	56	1	0
33	8	40	0	56	1	0
33	A	200	0	280	11	0
33	B	320	0	448	16	0
33	F	80	0	112	7	0
33	I	40	0	56	2	0
33	J	40	0	56	4	0
33	L	80	0	112	5	0
33	M	40	0	56	0	0
34	4	68	0	58	2	0
34	8	31	0	26	0	0
35	A	33	0	46	0	0
35	B	33	0	46	0	0
36	A	8	0	0	0	0
36	C	16	0	0	0	0
37	F	41	0	52	1	0
All	All	52767	0	47199	523	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 5.

All (523) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:9:303:CLA:HHC	32:9:313:XAT:H28	1.59	0.85
28:3:301:CLA:HBB	28:3:301:CLA:H2	1.63	0.81
7:B:704:GLN:HG3	31:B:844:LHG:H252	1.62	0.80
17:10:101:LEU:HD21	17:10:208:PHE:HB2	1.71	0.72
32:7:315:XAT:H30	32:7:315:XAT:H402	1.71	0.72
7:B:92:TRP:H	28:B:809:CLA:HED1	1.54	0.72
18:11:196:ILE:HD13	32:11:313:XAT:H10	1.71	0.72
28:1:304:CLA:HED1	28:1:305:CLA:HHD	1.71	0.71
28:6:302:CLA:HBB2	32:6:312:XAT:H15	1.71	0.70
6:A:530:PHE:HA	28:A:834:CLA:HED1	1.73	0.69
22:17:125:GLN:OE1	28:17:309:CLA:C4C	2.41	0.69
4:7:50:MET:HE1	28:7:305:CLA:HHC	1.75	0.68
5:8:147:PRO:HG3	28:8:304:CLA:HED2	1.77	0.67
19:9:204:GLN:HE22	28:9:310:CLA:HED2	1.59	0.67
28:B:819:CLA:HHC	28:B:835:CLA:HED1	1.76	0.67
32:17:311:XAT:H381	32:17:311:XAT:H393	1.77	0.66
28:A:802:CLA:H171	28:A:836:CLA:HAB	1.76	0.66
28:B:820:CLA:H42	28:B:821:CLA:H122	1.78	0.66
18:11:91:GLY:HA3	18:11:189:SER:HB2	1.78	0.65
18:11:112:ASP:HA	18:11:115:GLN:HE22	1.60	0.65
32:4:318:XAT:H192	32:4:318:XAT:H171	1.77	0.64
31:5:315:LHG:HC41	32:5:316:XAT:H361	1.80	0.64
32:8:312:XAT:H30	32:8:312:XAT:H402	1.78	0.64
28:A:817:CLA:HAB	28:A:817:CLA:H8	1.79	0.63
28:B:817:CLA:H2	28:B:820:CLA:H12	1.80	0.63
32:5:310:XAT:H381	32:5:310:XAT:H28	1.80	0.63
28:B:818:CLA:H3A	28:B:819:CLA:H2	1.80	0.63
28:B:801:CLA:H143	26:L:80:LEU:HG	1.81	0.63
2:3:31:VAL:HG13	2:3:32:ALA:H	1.64	0.62
28:A:831:CLA:HMD2	28:A:832:CLA:HAB	1.81	0.62
4:7:105:MET:HE1	28:7:304:CLA:HMB3	1.82	0.62
17:10:197:MET:HE3	32:10:314:XAT:H162	1.81	0.62
19:9:123:LEU:HD21	19:9:205:MET:HG2	1.81	0.62
25:4:149:MET:HG3	28:4:305:CLA:HMA2	1.80	0.62
7:B:422:LEU:HG	28:B:832:CLA:HBB1	1.81	0.62
28:10:306:CLA:H43	32:10:314:XAT:H28	1.81	0.62
33:B:850:BCR:H23C	33:B:850:BCR:H403	1.82	0.61
28:1:314:CLA:HED1	12:I:5:TYR:HB3	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:B:807:CLA:H201	31:I:102:LHG:H352	1.83	0.61
19:9:112:VAL:HG12	19:9:114:GLY:H	1.65	0.61
19:9:63:PRO:HB3	28:9:303:CLA:HAC2	1.82	0.60
7:B:721:TYR:HB2	28:B:803:CLA:HED2	1.84	0.60
28:L:206:CLA:H151	28:L:206:CLA:HMA3	1.84	0.60
3:5:78:LEU:HD22	6:A:8:ALA:HB2	1.84	0.60
9:D:23:ALA:HB1	9:D:28:LYS:HG3	1.84	0.59
6:A:393:TRP:CD1	28:A:826:CLA:HAB	2.37	0.59
28:A:837:CLA:HBA1	28:A:837:CLA:HBD	1.83	0.59
25:4:45:PRO:HG2	28:4:316:CLA:HMB3	1.84	0.59
6:A:322:ILE:HA	28:A:821:CLA:HED1	1.84	0.59
1:1:227:GLY:HA3	28:1:301:CLA:HAA1	1.84	0.59
28:6:301:CLA:H43	32:6:315:XAT:H362	1.84	0.59
28:A:824:CLA:HED3	28:A:824:CLA:CHA	2.31	0.59
28:6:302:CLA:HBB1	28:6:302:CLA:HMB1	1.84	0.59
4:7:64:VAL:HG12	4:7:66:GLY:H	1.67	0.59
32:6:312:XAT:H22	28:6:313:CLA:HED1	1.84	0.58
6:A:698:ILE:HA	28:A:852:CLA:HED1	1.86	0.58
28:B:847:CLA:H2	14:M:25:GLY:HA3	1.86	0.58
26:L:63:GLU:HG3	26:L:75:LEU:HD12	1.86	0.57
19:13:129:MET:HE3	19:13:134:PRO:HD2	1.86	0.57
28:5:313:CLA:HAA2	28:5:313:CLA:HBD	1.86	0.57
28:A:852:CLA:HBA1	28:A:852:CLA:HBD	1.87	0.57
19:13:75:ILE:HG12	19:13:77:ALA:H	1.70	0.57
28:10:301:CLA:HAB	32:10:315:XAT:H403	1.87	0.56
33:A:844:BCR:H403	33:A:844:BCR:H23C	1.86	0.56
25:4:73:ILE:HD11	25:4:100:THR:HG23	1.86	0.56
28:7:305:CLA:HAB	32:7:313:XAT:H203	1.87	0.56
28:7:304:CLA:HBB1	28:7:304:CLA:HMB1	1.85	0.56
7:B:25:ILE:HD11	33:B:850:BCR:H312	1.87	0.56
2:3:84:LEU:HB2	28:3:303:CLA:HED3	1.87	0.56
28:A:808:CLA:H143	28:A:810:CLA:H151	1.86	0.56
32:5:307:XAT:H30	32:5:307:XAT:C40	2.35	0.56
32:5:307:XAT:H8	32:5:307:XAT:H181	1.88	0.56
28:A:828:CLA:HBB1	28:A:828:CLA:HMB1	1.88	0.56
28:B:831:CLA:HBC2	33:B:846:BCR:H393	1.87	0.56
32:6:312:XAT:H181	32:6:312:XAT:H193	1.88	0.56
17:10:80:GLU:HG3	17:10:148:MET:HE1	1.88	0.56
28:10:301:CLA:H12	32:10:315:XAT:H363	1.88	0.55
28:13:301:CLA:HAB	32:13:308:XAT:H10	1.88	0.55
3:5:57:LEU:HD23	3:5:66:GLY:HA2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:A:841:BCR:H383	33:A:850:BCR:H21C	1.89	0.55
28:A:834:CLA:HBD	28:A:834:CLA:HBA1	1.87	0.55
19:13:129:MET:HG2	28:13:303:CLA:HMA2	1.88	0.55
25:4:195:THR:HA	25:4:201:LYS:HD2	1.89	0.55
22:17:93:GLN:HE22	28:17:302:CLA:CAD	2.21	0.54
3:5:113:LEU:HD13	3:5:114:PRO:HD2	1.89	0.54
28:A:804:CLA:H71	28:A:812:CLA:H2	1.90	0.54
17:10:118:HIS:NE2	28:10:316:CLA:C4D	2.70	0.54
28:10:316:CLA:HAA2	28:10:316:CLA:CGD	2.38	0.54
33:L:202:BCR:H361	33:L:202:BCR:H21C	1.89	0.54
32:5:311:XAT:H401	32:5:311:XAT:H15	1.89	0.54
28:11:304:CLA:H102	28:11:312:CLA:HMD1	1.90	0.54
1:1:117:PRO:HG3	1:1:131:THR:HG21	1.89	0.54
7:B:432:HIS:CG	33:B:846:BCR:H402	2.42	0.53
25:4:166:GLU:HG2	28:4:306:CLA:NB	2.22	0.53
7:B:69:ALA:HB2	7:B:135:LEU:HB2	1.90	0.53
19:13:75:ILE:HG23	19:13:78:ALA:H	1.74	0.53
32:4:318:XAT:H381	32:4:318:XAT:H393	1.91	0.53
32:9:313:XAT:H35	32:9:313:XAT:H201	1.91	0.53
28:7:303:CLA:HBA1	28:7:303:CLA:HBD	1.91	0.53
33:B:850:BCR:H323	12:I:26:LEU:HD22	1.90	0.53
3:5:113:LEU:HD21	32:5:311:XAT:H193	1.89	0.52
19:13:195:MET:HE3	32:13:308:XAT:H14	1.91	0.52
32:8:312:XAT:H193	32:8:312:XAT:H161	1.90	0.52
22:17:140:ASN:HD21	22:17:147:GLY:H	1.56	0.52
25:4:110:LYS:HG2	28:4:306:CLA:HMD3	1.92	0.52
32:8:312:XAT:H30	32:8:312:XAT:C40	2.40	0.52
28:A:817:CLA:H142	28:A:819:CLA:HAB	1.92	0.52
28:B:818:CLA:C4D	33:B:837:BCR:HC22	2.40	0.52
28:F:802:CLA:CAD	28:F:802:CLA:HED2	2.39	0.52
7:B:422:LEU:HD13	7:B:532:LEU:HA	1.91	0.52
18:11:138:ALA:HA	28:11:303:CLA:HAB	1.91	0.52
28:B:831:CLA:HMC1	33:B:846:BCR:H393	1.91	0.51
28:B:822:CLA:H43	28:B:828:CLA:HBB2	1.92	0.51
11:F:149:ILE:HD12	11:F:171:ILE:HD11	1.92	0.51
3:5:201:ALA:HB1	32:5:307:XAT:H191	1.93	0.51
6:A:87:GLY:HA3	28:A:806:CLA:HHC	1.92	0.51
33:B:850:BCR:H321	33:B:850:BCR:HC8	1.91	0.51
1:1:81:ALA:HA	28:1:307:CLA:HED3	1.92	0.51
28:A:803:CLA:HMB1	28:A:803:CLA:HBB1	1.92	0.51
17:6:86:GLY:HA3	17:6:187:CYS:HB3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:13:302:CLA:HHC	32:13:308:XAT:C35	2.41	0.51
4:7:53:VAL:HG11	32:7:313:XAT:H391	1.94	0.50
5:8:91:MET:SD	28:8:305:CLA:HHC	2.51	0.50
4:7:161:LEU:HD13	28:7:312:CLA:HAA1	1.92	0.50
28:7:305:CLA:H72	32:7:313:XAT:H191	1.93	0.50
28:B:806:CLA:H2	28:B:806:CLA:HED2	1.93	0.50
1:1:123:LEU:HD22	28:1:314:CLA:HMA1	1.93	0.50
7:B:411:MET:HE1	28:B:827:CLA:C3C	2.40	0.50
22:17:89:GLY:O	22:17:93:GLN:HG2	2.11	0.50
4:7:152:ALA:HB1	32:7:313:XAT:H393	1.92	0.50
7:B:91:ILE:HB	7:B:112:PRO:HB2	1.93	0.50
28:A:824:CLA:CHA	28:A:824:CLA:CED	2.89	0.50
7:B:299:HIS:HB3	7:B:304:ILE:HD11	1.92	0.50
6:A:613:SER:HA	6:A:629:SER:HB2	1.93	0.50
28:A:819:CLA:CGA	28:A:823:CLA:HBB1	2.42	0.50
28:A:802:CLA:HED1	33:F:801:BCR:H291	1.92	0.50
28:A:811:CLA:HBB1	28:A:818:CLA:C4C	2.41	0.50
32:6:315:XAT:H381	32:6:315:XAT:H393	1.94	0.50
7:B:600:THR:HG21	7:B:609:PHE:HB2	1.94	0.49
7:B:707:LEU:HD23	31:B:844:LHG:H242	1.94	0.49
33:A:841:BCR:H403	33:A:841:BCR:H23C	1.93	0.49
22:17:202:ILE:HG21	33:17:310:BCR:H291	1.94	0.49
22:17:61:LEU:HD12	22:17:64:ALA:HB3	1.94	0.49
19:9:126:HIS:NE2	28:9:311:CLA:C4C	2.73	0.49
3:5:113:LEU:HD11	32:5:311:XAT:H193	1.94	0.49
6:A:307:HIS:CD2	33:A:850:BCR:H12C	2.48	0.49
7:B:268:LEU:HD13	28:B:815:CLA:HMA2	1.95	0.49
32:10:315:XAT:H371	32:10:315:XAT:H393	1.95	0.49
32:7:317:XAT:H162	32:7:317:XAT:H193	1.95	0.49
28:10:307:CLA:CHA	28:10:307:CLA:HED3	2.43	0.49
28:8:310:CLA:HMD2	32:8:312:XAT:H12	1.94	0.48
28:A:822:CLA:H41	28:A:822:CLA:H61	1.53	0.48
28:B:817:CLA:H52	28:B:823:CLA:H101	1.95	0.48
28:A:847:CLA:H51	28:L:203:CLA:H43	1.94	0.48
28:10:307:CLA:HED2	28:10:307:CLA:CAD	2.43	0.48
28:3:306:CLA:H41	28:3:306:CLA:H61	1.57	0.48
28:A:824:CLA:HMB3	28:A:824:CLA:HBB1	1.94	0.48
19:9:126:HIS:HA	19:9:135:MET:HE1	1.95	0.48
33:L:202:BCR:H24C	33:L:202:BCR:H371	1.64	0.48
7:B:421:HIS:O	7:B:425:VAL:HG23	2.14	0.48
11:F:81:ALA:O	11:F:85:GLU:HG2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:4:147:ASP:HB2	25:4:148:PRO:HD3	1.95	0.48
18:11:180:ARG:HH22	28:11:312:CLA:HAA2	1.78	0.48
19:13:73:LEU:HD21	32:13:308:XAT:H172	1.94	0.48
32:17:311:XAT:H32	30:17:312:KC1:CAB	2.44	0.48
7:B:203:ARG:HD3	7:B:250:SER:HB2	1.95	0.48
28:10:303:CLA:H51	28:10:303:CLA:C4C	2.44	0.48
25:4:224:THR:HG21	28:4:310:CLA:HBC3	1.95	0.48
32:5:316:XAT:H241	17:6:185:THR:HG23	1.95	0.48
28:8:304:CLA:H3A	28:8:304:CLA:HBA2	1.63	0.48
28:A:835:CLA:H101	33:A:844:BCR:H373	1.95	0.48
28:B:824:CLA:H192	31:B:844:LHG:H362	1.96	0.48
28:3:306:CLA:HAB	29:3:310:A86:C24	2.44	0.47
32:7:317:XAT:H30	32:7:317:XAT:C40	2.44	0.47
17:10:194:PHE:CE2	32:10:315:XAT:H10	2.49	0.47
22:17:57:PRO:HG3	32:17:311:XAT:H241	1.95	0.47
6:A:214:GLN:NE2	28:A:817:CLA:HED1	2.29	0.47
28:A:819:CLA:H202	33:A:843:BCR:H272	1.96	0.47
33:A:841:BCR:H331	28:A:846:CLA:HHB	1.96	0.47
19:9:200:GLY:HA3	28:9:310:CLA:CHC	2.44	0.47
28:5:304:CLA:HHC	32:5:310:XAT:H201	1.96	0.47
28:8:303:CLA:H62	28:8:303:CLA:H41	1.62	0.47
6:A:266:TRP:CH2	28:A:815:CLA:HBB1	2.49	0.47
28:B:843:CLA:H111	28:B:843:CLA:H152	1.49	0.47
28:11:301:CLA:HHC	32:11:313:XAT:C30	2.45	0.47
28:5:306:CLA:HAC1	25:4:164:PHE:CE1	2.49	0.47
5:8:109:LEU:HD21	5:8:127:ASN:HD22	1.79	0.47
28:A:829:CLA:C4D	31:A:840:LHG:HC92	2.44	0.47
28:8:301:CLA:H122	32:8:311:XAT:H371	1.97	0.47
34:4:301:DGD:HB21	34:4:301:DGD:HG2	1.29	0.47
7:B:311:PRO:HD2	31:B:842:LHG:O4	2.14	0.47
28:10:306:CLA:H72	28:10:306:CLA:H41	1.97	0.47
28:10:308:CLA:HED2	28:10:308:CLA:HBD	1.65	0.47
28:11:314:CLA:HED2	28:11:314:CLA:HBD	1.63	0.47
32:7:316:XAT:H10	32:7:316:XAT:C20	2.45	0.47
33:A:843:BCR:H381	33:A:844:BCR:HC42	1.95	0.47
18:11:97:ALA:HB1	32:11:313:XAT:H8	1.97	0.47
2:3:98:GLU:HB2	28:3:304:CLA:HED1	1.97	0.47
28:5:303:CLA:H162	28:5:303:CLA:H122	1.66	0.47
4:7:39:ARG:HH22	28:7:301:CLA:HED1	1.79	0.47
28:A:806:CLA:H3A	28:A:806:CLA:HBA2	1.54	0.47
28:16:203:CLA:HED2	28:16:203:CLA:HBD	1.65	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:9:126:HIS:HD2	32:9:313:XAT:H163	1.79	0.47
28:1:303:CLA:H11	28:1:303:CLA:HBA1	1.55	0.47
31:1:309:LHG:H171	31:1:309:LHG:H132	1.96	0.47
2:3:159:MET:HE3	28:3:301:CLA:HMC3	1.97	0.47
7:B:177:HIS:CG	28:B:812:CLA:HMC2	2.50	0.47
7:B:242:HIS:HA	7:B:248:THR:O	2.15	0.47
32:5:311:XAT:H401	32:5:311:XAT:C15	2.45	0.46
28:7:311:CLA:C3D	32:7:316:XAT:H202	2.45	0.46
32:7:317:XAT:H30	32:7:317:XAT:H402	1.96	0.46
31:B:842:LHG:HC62	31:B:842:LHG:H242	1.40	0.46
18:11:108:HIS:CD2	18:11:115:GLN:HA	2.50	0.46
22:17:89:GLY:HA3	28:17:302:CLA:HHC	1.97	0.46
28:A:817:CLA:H61	28:A:817:CLA:H41	1.66	0.46
28:B:845:CLA:H61	28:B:845:CLA:H41	1.65	0.46
30:5:308:KC1:CAD	28:5:309:CLA:HMA3	2.46	0.46
6:A:72:SER:OG	6:A:178:TYR:HB2	2.16	0.46
28:A:809:CLA:H3A	28:A:809:CLA:HBA2	1.67	0.46
32:13:309:XAT:H381	32:13:309:XAT:H393	1.98	0.46
28:A:814:CLA:H3A	28:A:814:CLA:HBA2	1.50	0.46
28:A:852:CLA:H172	11:F:143:GLY:HA2	1.98	0.46
6:A:645:ARG:HG3	7:B:632:ILE:HD12	1.97	0.46
7:B:161:PHE:HA	28:B:810:CLA:HED3	1.98	0.46
28:6:302:CLA:H41	28:6:302:CLA:H61	1.65	0.46
28:11:305:CLA:HBD	28:11:312:CLA:HMA3	1.97	0.46
22:17:140:ASN:ND2	22:17:147:GLY:H	2.13	0.46
28:5:302:CLA:H11	28:5:302:CLA:HBA1	1.41	0.46
5:8:63:SER:OG	28:8:301:CLA:HBA1	2.14	0.46
31:B:842:LHG:H251	31:B:842:LHG:HC91	1.96	0.46
28:6:301:CLA:H141	32:6:312:XAT:H403	1.98	0.46
28:A:826:CLA:H142	28:A:828:CLA:H171	1.98	0.46
21:16:162:UNK:HA	21:16:166:UNK:HA	1.97	0.46
32:4:318:XAT:H10	32:4:318:XAT:C20	2.46	0.46
28:6:306:CLA:H3A	28:6:306:CLA:HBA2	1.75	0.46
32:9:313:XAT:H201	32:9:313:XAT:C35	2.45	0.46
28:L:204:CLA:HBA1	28:L:204:CLA:H12	1.41	0.46
1:1:141:ILE:HG13	32:1:311:XAT:H171	1.98	0.46
28:6:301:CLA:H3A	28:6:301:CLA:HBA2	1.60	0.46
28:9:311:CLA:HMC3	32:9:313:XAT:H161	1.97	0.46
28:B:811:CLA:H3A	28:B:811:CLA:HBA2	1.77	0.45
28:4:307:CLA:H12	28:4:307:CLA:HBA2	1.52	0.45
31:9:301:LHG:HC82	31:9:301:LHG:HC5	1.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:A:818:CLA:H3A	28:A:818:CLA:HBA2	1.52	0.45
28:B:815:CLA:H12	28:B:815:CLA:HBA2	1.50	0.45
25:4:105:ARG:HH21	25:4:209:ILE:HG13	1.82	0.45
28:8:303:CLA:HBA2	28:8:303:CLA:H12	1.52	0.45
33:A:841:BCR:H362	33:A:842:BCR:H21C	1.98	0.45
28:B:808:CLA:H62	28:B:808:CLA:H41	1.50	0.45
28:B:826:CLA:H62	28:B:826:CLA:H41	1.50	0.45
33:F:801:BCR:C10	28:F:802:CLA:HBB1	2.47	0.45
28:19:201:CLA:HBA2	28:19:201:CLA:HBD	1.99	0.45
28:1:310:CLA:HBC2	28:1:314:CLA:HMD2	1.98	0.45
28:A:830:CLA:HAA1	33:L:202:BCR:H14C	1.98	0.45
28:B:817:CLA:H111	28:B:817:CLA:H71	1.78	0.45
28:B:843:CLA:HBA1	28:B:843:CLA:H11	1.65	0.45
28:1:307:CLA:H62	28:1:307:CLA:H41	1.59	0.45
28:3:303:CLA:H143	28:3:303:CLA:H111	1.85	0.45
28:8:301:CLA:HBA2	28:8:301:CLA:H3A	1.52	0.45
6:A:201:GLY:O	6:A:205:LEU:HB2	2.17	0.45
7:B:580:MET:HG3	7:B:710:LEU:HD21	1.97	0.45
31:B:844:LHG:H242	31:B:844:LHG:HC61	1.29	0.45
28:4:304:CLA:HED2	28:4:304:CLA:HBD	1.66	0.45
3:5:106:TRP:HZ2	32:5:311:XAT:H171	1.81	0.45
28:A:803:CLA:HHC	28:A:810:CLA:H142	1.98	0.45
28:B:843:CLA:H41	15:R:105:PRO:HD3	1.99	0.45
28:A:829:CLA:HBA1	28:A:829:CLA:H3A	1.73	0.45
7:B:311:PRO:HG3	15:R:52:TRP:HH2	1.82	0.45
5:8:87:CYS:HB3	5:8:187:GLY:HA3	1.99	0.45
28:6:306:CLA:HBA2	28:6:306:CLA:H12	1.81	0.45
18:11:115:GLN:O	18:11:115:GLN:HG2	2.16	0.45
19:13:117:PHE:CE1	19:13:129:MET:HE1	2.52	0.45
6:A:291:THR:HG23	28:A:817:CLA:HMA3	1.98	0.45
28:A:808:CLA:CBB	33:J:104:BCR:H392	2.47	0.45
32:6:315:XAT:H10	32:6:315:XAT:C20	2.48	0.45
28:13:301:CLA:H61	28:13:301:CLA:H41	1.63	0.45
28:13:301:CLA:HAA1	28:13:301:CLA:HED2	1.98	0.45
28:5:303:CLA:HBA1	28:5:303:CLA:H3A	1.83	0.44
4:7:50:MET:HA	32:7:313:XAT:H401	2.00	0.44
28:7:303:CLA:H61	28:7:303:CLA:H41	1.74	0.44
7:B:193:HIS:HB2	28:B:813:CLA:CHC	2.47	0.44
28:B:828:CLA:C4C	28:B:829:CLA:HBB1	2.47	0.44
3:5:122:GLN:HA	3:5:125:LEU:HB2	1.99	0.44
6:A:687:GLY:HA3	7:B:569:ASP:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:A:815:CLA:HBD	28:A:815:CLA:HBA1	1.99	0.44
7:B:224:PRO:HA	7:B:227:ASP:OD1	2.17	0.44
28:B:806:CLA:H52	28:B:826:CLA:H51	2.00	0.44
28:B:811:CLA:C3D	28:B:812:CLA:HMC3	2.48	0.44
28:1:314:CLA:H41	28:1:314:CLA:H62	1.66	0.44
28:B:826:CLA:H142	31:B:844:LHG:H361	1.98	0.44
28:4:310:CLA:H62	28:4:310:CLA:H41	1.76	0.44
34:4:317:DGD:HG32	34:4:317:DGD:HD2	1.41	0.44
28:A:802:CLA:H203	28:A:849:CLA:H201	2.00	0.44
28:A:802:CLA:HED2	33:F:801:BCR:H401	1.99	0.44
28:B:845:CLA:H11	28:B:845:CLA:HBA2	1.41	0.44
25:4:47:MET:HG2	25:4:48:PRO:HD2	1.98	0.44
32:4:318:XAT:C8	32:4:318:XAT:H161	2.47	0.44
28:a:202:CLA:HED2	28:a:202:CLA:HBD	1.65	0.44
28:3:305:CLA:H3A	28:3:305:CLA:HBA2	1.66	0.44
28:B:847:CLA:H201	12:I:13:LEU:HB3	1.99	0.44
28:6:302:CLA:HBB2	32:6:312:XAT:C15	2.43	0.44
3:5:98:MET:HE1	28:5:305:CLA:HHC	1.98	0.44
4:7:61:VAL:HG23	4:7:62:VAL:HG23	2.00	0.44
28:A:820:CLA:HBA2	28:A:820:CLA:H11	1.54	0.44
28:B:806:CLA:H11	28:B:806:CLA:HBA1	1.28	0.44
33:B:846:BCR:H24C	33:B:846:BCR:H371	1.87	0.44
8:C:62:PHE:HD2	9:D:120:ILE:HG21	1.82	0.44
32:7:315:XAT:H30	32:7:315:XAT:C40	2.44	0.44
28:B:811:CLA:H12	18:11:74:LEU:HD21	1.99	0.44
33:B:837:BCR:H20C	33:B:837:BCR:H361	1.88	0.44
28:6:306:CLA:H12	28:6:306:CLA:HHB	2.00	0.44
28:7:303:CLA:H152	28:7:303:CLA:H203	2.00	0.44
28:8:301:CLA:H41	28:8:301:CLA:H62	1.76	0.44
7:B:658:ALA:HB3	28:B:804:CLA:HBB2	2.00	0.44
28:6:301:CLA:H52	28:6:302:CLA:H3A	2.00	0.44
31:11:311:LHG:HC61	31:11:311:LHG:H241	1.29	0.44
25:4:112:GLY:HA3	25:4:212:CYS:HB3	1.99	0.44
28:A:837:CLA:H41	28:A:837:CLA:H62	1.77	0.44
28:17:301:CLA:HED2	28:17:301:CLA:HBD	1.64	0.44
28:3:301:CLA:HHC	32:3:313:XAT:C30	2.48	0.43
28:A:836:CLA:H62	28:A:836:CLA:H41	1.75	0.43
28:17:307:CLA:HED2	28:17:307:CLA:HBD	1.62	0.43
3:5:203:GLY:HA2	28:5:313:CLA:CHC	2.48	0.43
28:5:313:CLA:HMA3	28:5:313:CLA:H42	1.99	0.43
28:A:815:CLA:HBA1	28:A:815:CLA:H11	1.55	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:A:830:CLA:HAA1	33:L:202:BCR:C14	2.48	0.43
33:A:850:BCR:H11C	33:A:850:BCR:H341	1.87	0.43
7:B:365:PHE:HB3	7:B:602:TRP:CZ3	2.53	0.43
7:B:458:VAL:HG21	11:F:116:ASP:HB3	2.00	0.43
28:B:849:CLA:H202	11:F:133:LEU:HB2	2.00	0.43
28:A:817:CLA:CAD	28:A:827:CLA:H41	2.49	0.43
28:13:305:CLA:HBA2	28:13:305:CLA:H3A	1.62	0.43
28:5:309:CLA:HED2	28:5:309:CLA:HBD	1.67	0.43
4:7:81:VAL:HB	4:7:85:PRO:HG2	2.01	0.43
28:6:306:CLA:H62	28:6:306:CLA:H41	1.65	0.43
17:10:80:GLU:HG2	17:10:156:PRO:HB3	2.01	0.43
28:10:306:CLA:H42	28:10:306:CLA:C2B	2.49	0.43
28:10:316:CLA:HED3	28:10:316:CLA:O1A	2.19	0.43
22:17:98:LEU:N	22:17:99:PRO:HD3	2.33	0.43
25:4:204:PHE:HB3	28:4:307:CLA:HMA1	1.99	0.43
6:A:424:LEU:HD23	6:A:424:LEU:HA	1.87	0.43
28:A:808:CLA:HBB2	33:J:104:BCR:H392	2.00	0.43
28:A:830:CLA:H72	28:A:830:CLA:H112	1.45	0.43
33:A:841:BCR:H20C	33:A:841:BCR:H361	1.84	0.43
13:J:16:VAL:HG21	32:J:105:XAT:H383	2.00	0.43
28:6:311:CLA:HHC	32:6:315:XAT:C16	2.49	0.43
28:4:303:CLA:H41	28:4:303:CLA:H61	1.41	0.43
17:10:135:SER:HA	28:10:305:CLA:HAB	2.00	0.43
28:A:808:CLA:H61	28:A:808:CLA:H41	1.81	0.43
1:1:114:ALA:HB1	1:1:131:THR:OG1	2.19	0.43
28:7:301:CLA:HBA2	28:7:301:CLA:H3A	1.50	0.43
7:B:299:HIS:CE1	28:B:818:CLA:NA	2.85	0.43
33:B:837:BCR:H24C	33:B:837:BCR:H371	1.84	0.43
25:4:122:TRP:HE3	32:4:318:XAT:H162	1.83	0.43
28:5:313:CLA:H102	28:5:313:CLA:H61	1.66	0.43
6:A:40:PRO:HB3	6:A:45:TRP:CE3	2.54	0.43
6:A:390:HIS:O	6:A:394:ILE:HG12	2.19	0.43
28:A:808:CLA:HBB1	33:J:104:BCR:H23C	2.00	0.43
8:C:51:CYS:SG	8:C:53:ARG:HD3	2.58	0.43
33:I:101:BCR:H20C	33:I:101:BCR:H361	1.90	0.43
17:6:181:LEU:HD22	28:6:307:CLA:HED1	2.00	0.43
28:17:303:CLA:H12	28:17:303:CLA:HBA1	1.74	0.43
1:1:178:PRO:HB3	1:1:182:PRO:HB3	2.01	0.43
28:1:310:CLA:H102	28:1:314:CLA:HBC1	2.00	0.43
4:7:158:HIS:ND1	28:7:308:CLA:HBC3	2.34	0.43
33:F:801:BCR:H24C	33:F:801:BCR:H371	1.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:b:101:UNK:C	16:b:103:UNK:H	2.32	0.43
32:6:315:XAT:H30	32:6:315:XAT:C40	2.49	0.43
28:5:306:CLA:HAC1	25:4:164:PHE:HE1	1.84	0.42
28:7:301:CLA:H61	28:7:301:CLA:H41	1.89	0.42
28:A:805:CLA:HBB2	28:A:827:CLA:HMC2	2.01	0.42
28:A:813:CLA:H3A	28:A:813:CLA:HBA2	1.63	0.42
28:B:809:CLA:H151	28:B:809:CLA:H111	1.56	0.42
17:10:194:PHE:O	17:10:198:VAL:HG12	2.19	0.42
28:13:302:CLA:HHC	32:13:308:XAT:H35	2.00	0.42
28:17:303:CLA:H3A	28:17:303:CLA:HBA2	1.79	0.42
28:9:304:CLA:HBA1	28:9:304:CLA:H3A	1.71	0.42
31:9:314:LHG:HC82	31:9:314:LHG:HC5	1.31	0.42
4:7:29:LEU:HD12	28:7:301:CLA:H12	2.01	0.42
28:A:802:CLA:HBA2	28:A:802:CLA:H12	1.44	0.42
28:A:805:CLA:HED2	28:A:805:CLA:H2	2.00	0.42
11:F:79:PRO:N	11:F:80:PRO:HD2	2.34	0.42
17:6:64:PHE:CE2	32:6:315:XAT:H373	2.54	0.42
17:10:89:CYS:SG	17:10:191:MET:HA	2.59	0.42
25:4:73:ILE:HD13	25:4:78:PHE:CG	2.54	0.42
6:A:484:ILE:HD13	28:A:831:CLA:HHC	2.02	0.42
28:A:831:CLA:H3A	28:A:831:CLA:HBA2	1.73	0.42
17:10:188:ARG:HA	17:10:191:MET:HE3	2.01	0.42
17:10:197:MET:HB2	32:10:314:XAT:H163	2.00	0.42
28:7:312:CLA:H11	28:7:312:CLA:HBA2	1.34	0.42
6:A:477:LYS:HA	6:A:478:PRO:HD3	1.92	0.42
28:A:817:CLA:CHB	28:A:817:CLA:H2	2.50	0.42
7:B:158:GLN:O	7:B:162:ARG:HG3	2.19	0.42
28:B:816:CLA:H3A	28:B:816:CLA:HBA2	1.75	0.42
2:3:152:LEU:O	2:3:156:ARG:HG3	2.18	0.42
28:A:846:CLA:HAA1	28:A:846:CLA:HBD	2.01	0.42
28:4:310:CLA:HBA2	28:4:310:CLA:H11	1.27	0.42
3:5:138:ALA:O	3:5:142:ILE:HG12	2.20	0.42
6:A:467:ASP:HB3	28:L:201:CLA:HED3	2.02	0.42
33:B:846:BCR:H403	33:B:846:BCR:H23C	2.02	0.42
33:I:101:BCR:H24C	33:I:101:BCR:H371	1.86	0.42
33:J:104:BCR:H20C	33:J:104:BCR:H361	1.91	0.42
1:1:82:GLU:HB2	28:1:303:CLA:C1B	2.50	0.42
6:A:476:LEU:HB2	6:A:527:THR:HG23	2.01	0.42
7:B:261:PHE:CE1	7:B:356:PRO:HD2	2.55	0.42
28:B:831:CLA:H41	28:B:831:CLA:H62	1.67	0.42
33:B:851:BCR:H24C	33:B:851:BCR:H371	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:F:801:BCR:HC32	28:J:102:CLA:H12	2.01	0.42
32:4:318:XAT:H31	32:4:318:XAT:H391	1.94	0.42
32:5:311:XAT:H30	32:5:311:XAT:C40	2.49	0.42
33:B:841:BCR:H20C	33:B:841:BCR:H361	1.87	0.42
33:F:804:BCR:H24C	33:F:804:BCR:H371	1.83	0.42
28:J:102:CLA:H12	28:J:102:CLA:HBA2	1.55	0.42
25:4:221:GLY:HA3	28:4:310:CLA:HHC	2.01	0.42
2:3:172:THR:HG23	2:3:175:MET:H	1.84	0.42
4:7:151:SER:HB3	32:7:315:XAT:H403	2.02	0.42
28:7:306:CLA:H61	28:7:306:CLA:H41	1.62	0.42
28:A:853:CLA:H122	13:J:18:TRP:HE3	1.84	0.42
28:B:822:CLA:C4	28:B:828:CLA:HBB2	2.50	0.42
28:10:306:CLA:HBA2	28:10:306:CLA:H3A	1.51	0.42
22:17:119:PRO:HA	22:17:120:PRO:HD3	1.95	0.42
28:4:306:CLA:H3A	28:4:306:CLA:HBA2	1.74	0.42
32:7:316:XAT:H35	32:7:316:XAT:H401	1.91	0.42
28:B:807:CLA:H112	28:B:807:CLA:H152	1.50	0.42
17:6:69:PHE:CD2	28:6:301:CLA:H12	2.54	0.42
28:9:307:CLA:H11	28:9:307:CLA:HBA2	1.48	0.42
32:5:307:XAT:H15	32:5:307:XAT:H201	1.85	0.41
28:8:301:CLA:H62	28:8:301:CLA:H102	1.87	0.41
28:A:852:CLA:HMB2	28:B:848:CLA:H52	2.02	0.41
33:B:841:BCR:H24C	33:B:841:BCR:H371	1.85	0.41
32:6:315:XAT:H10	32:6:315:XAT:H203	2.02	0.41
28:11:304:CLA:HBA2	28:11:304:CLA:H3A	1.67	0.41
28:11:304:CLA:H71	28:11:312:CLA:HMD1	2.03	0.41
28:11:310:CLA:CHA	28:11:310:CLA:HBA1	2.49	0.41
28:13:301:CLA:HED2	28:13:301:CLA:HBD	1.66	0.41
28:17:301:CLA:HBA1	28:17:301:CLA:HMA2	2.02	0.41
3:5:105:LEU:HD23	3:5:105:LEU:HA	1.89	0.41
32:7:313:XAT:H161	32:7:313:XAT:H192	2.01	0.41
28:A:834:CLA:H61	28:A:834:CLA:H41	1.87	0.41
28:R:202:CLA:H61	28:R:202:CLA:H41	1.82	0.41
28:1:308:CLA:HBC3	28:1:308:CLA:HHD	2.01	0.41
3:5:191:ILE:HD12	3:5:191:ILE:HA	1.94	0.41
5:8:181:LEU:HD22	5:8:185:LYS:NZ	2.36	0.41
33:8:309:BCR:H361	33:8:309:BCR:H20C	1.78	0.41
28:A:802:CLA:H2	7:B:431:PHE:CE1	2.55	0.41
28:A:823:CLA:H11	28:A:823:CLA:HBA1	1.25	0.41
17:10:172:MET:HB3	17:10:175:LYS:HB2	2.01	0.41
17:10:186:HIS:HD2	32:10:314:XAT:H201	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:5:307:XAT:H30	32:5:307:XAT:H403	2.02	0.41
32:7:317:XAT:H373	32:7:317:XAT:H392	2.01	0.41
5:8:167:PHE:HE2	5:8:170:LYS:HG2	1.85	0.41
6:A:116:TRP:CD2	28:A:808:CLA:HED3	2.54	0.41
7:B:291:TYR:HE1	28:B:817:CLA:HED1	1.84	0.41
7:B:304:ILE:HA	28:B:819:CLA:HED1	2.03	0.41
32:10:315:XAT:H31	32:10:315:XAT:H391	1.88	0.41
32:4:315:XAT:H30	32:4:315:XAT:C40	2.49	0.41
28:8:302:CLA:H61	28:8:302:CLA:H41	1.86	0.41
28:F:802:CLA:H61	28:F:802:CLA:H41	1.79	0.41
17:10:51:PRO:HA	17:10:52:PRO:HD3	1.96	0.41
32:10:314:XAT:C12	32:10:314:XAT:H191	2.50	0.41
33:L:205:BCR:H24C	33:L:205:BCR:H371	1.83	0.41
6:A:175:TRP:HD1	28:A:810:CLA:CHC	2.33	0.41
7:B:658:ALA:O	7:B:661:PHE:HB2	2.21	0.41
28:B:819:CLA:H43	15:R:119:GLY:HA3	2.02	0.41
9:D:74:ARG:HE	9:D:79:LYS:HE2	1.84	0.41
22:17:104:ASN:OD1	22:17:107:ASP:HA	2.20	0.41
28:4:303:CLA:H42	28:4:304:CLA:HBA1	2.03	0.41
6:A:372:PRO:HA	6:A:373:PRO:HD3	1.83	0.41
33:F:804:BCR:H20C	33:F:804:BCR:H361	1.87	0.41
13:J:22:THR:HA	13:J:25:PHE:CE2	2.56	0.41
28:6:303:CLA:H12	32:6:316:XAT:H14	2.02	0.41
32:10:315:XAT:H393	32:10:315:XAT:H361	2.02	0.41
5:8:179:LEU:HB3	28:8:305:CLA:HMA1	2.02	0.41
28:8:304:CLA:H62	28:8:304:CLA:H102	1.71	0.41
28:8:313:CLA:H62	28:8:313:CLA:H41	1.77	0.41
28:B:824:CLA:HED1	28:B:825:CLA:H3A	2.03	0.41
37:F:805:LMG:H221	13:J:13:VAL:HG13	2.03	0.41
32:6:312:XAT:H162	28:6:313:CLA:HED1	2.02	0.41
28:7:304:CLA:H3A	28:7:304:CLA:HBA2	1.59	0.41
28:8:303:CLA:H101	32:8:312:XAT:H403	2.01	0.41
7:B:174:ARG:HD2	28:B:821:CLA:OBD	2.20	0.41
28:B:816:CLA:O1A	28:B:825:CLA:HMD1	2.21	0.41
28:F:802:CLA:HED3	28:F:802:CLA:CHA	2.51	0.41
17:6:176:LYS:HG3	17:6:177:ALA:N	2.36	0.41
28:4:303:CLA:HAB	32:4:318:XAT:H391	2.02	0.41
32:4:315:XAT:H401	32:4:315:XAT:H15	2.02	0.41
19:9:99:LEU:HB3	28:9:305:CLA:HBB2	2.02	0.41
19:9:123:LEU:H	19:9:123:LEU:HD22	1.86	0.41
3:5:95:ARG:HD3	28:5:305:CLA:C4C	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:B:827:CLA:H3A	28:B:827:CLA:HBA2	1.60	0.41
28:B:832:CLA:H8	33:B:840:BCR:H342	2.03	0.41
32:J:105:XAT:H11	32:J:105:XAT:H191	1.96	0.41
15:R:125:TRP:O	15:R:129:GLN:HG2	2.21	0.41
22:17:140:ASN:HD21	22:17:146:PRO:HA	1.86	0.41
5:8:167:PHE:CE2	5:8:170:LYS:HG2	2.56	0.40
6:A:360:LEU:HD12	6:A:360:LEU:HA	1.89	0.40
28:B:826:CLA:H141	28:B:826:CLA:H162	1.95	0.40
32:7:314:XAT:H171	32:7:317:XAT:H7	2.03	0.40
28:A:801:CLA:HED2	28:A:801:CLA:HBD	1.66	0.40
18:11:90:HIS:HD2	32:11:313:XAT:H201	1.87	0.40
2:3:144:TRP:O	2:3:148:GLN:HG3	2.22	0.40
4:7:44:LYS:HD2	28:7:304:CLA:C3D	2.51	0.40
7:B:48:ALA:HB3	14:M:28:LEU:HD21	2.03	0.40
31:B:842:LHG:HC5	31:B:842:LHG:HC81	1.44	0.40
28:11:301:CLA:H121	32:11:313:XAT:H371	2.04	0.40
32:11:313:XAT:H8	32:11:313:XAT:H161	2.03	0.40
2:3:96:PRO:HA	2:3:97:PRO:HD3	1.97	0.40
28:A:825:CLA:HBB1	28:A:825:CLA:HMB1	2.02	0.40
28:A:837:CLA:H121	28:A:837:CLA:H8	1.97	0.40
28:A:837:CLA:H61	28:A:837:CLA:H92	1.86	0.40
28:B:810:CLA:H62	28:B:810:CLA:H41	1.78	0.40
17:6:184:ILE:HD12	17:6:184:ILE:HA	1.89	0.40
28:10:316:CLA:H142	28:10:316:CLA:H111	1.81	0.40
19:9:84:LEU:H	19:9:84:LEU:HD22	1.87	0.40
33:1:312:BCR:H20C	33:1:312:BCR:H361	1.92	0.40
28:B:816:CLA:H202	28:B:817:CLA:H141	2.03	0.40
28:B:828:CLA:HMD2	28:B:829:CLA:CHC	2.51	0.40
11:F:66:LYS:HB3	11:F:66:LYS:HE2	1.78	0.40
28:10:301:CLA:H3A	28:10:301:CLA:HBA2	1.72	0.40
18:11:101:PHE:HB2	32:11:313:XAT:H163	2.02	0.40
22:17:196:ASN:O	22:17:198:LYS:HG2	2.21	0.40
25:4:122:TRP:CE3	32:4:318:XAT:H162	2.56	0.40
28:4:307:CLA:H52	28:4:307:CLA:HBB1	2.04	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	1	176/230 (76%)	172 (98%)	4 (2%)	0	100	100
2	3	159/191 (83%)	154 (97%)	4 (2%)	1 (1%)	21	35
3	5	173/222 (78%)	169 (98%)	4 (2%)	0	100	100
4	7	167/169 (99%)	163 (98%)	4 (2%)	0	100	100
5	8	174/215 (81%)	168 (97%)	6 (3%)	0	100	100
6	A	740/749 (99%)	725 (98%)	15 (2%)	0	100	100
7	B	728/734 (99%)	707 (97%)	21 (3%)	0	100	100
8	C	78/81 (96%)	74 (95%)	4 (5%)	0	100	100
9	D	123/132 (93%)	123 (100%)	0	0	100	100
10	E	58/61 (95%)	57 (98%)	1 (2%)	0	100	100
11	F	159/202 (79%)	157 (99%)	2 (1%)	0	100	100
12	I	32/36 (89%)	31 (97%)	1 (3%)	0	100	100
13	J	39/42 (93%)	39 (100%)	0	0	100	100
14	M	28/30 (93%)	28 (100%)	0	0	100	100
15	R	83/132 (63%)	83 (100%)	0	0	100	100
17	10	170/212 (80%)	163 (96%)	7 (4%)	0	100	100
17	6	171/212 (81%)	166 (97%)	5 (3%)	0	100	100
18	11	165/213 (78%)	164 (99%)	1 (1%)	0	100	100
19	13	135/216 (62%)	126 (93%)	9 (7%)	0	100	100
19	9	130/216 (60%)	125 (96%)	4 (3%)	1 (1%)	16	28
22	17	142/218 (65%)	133 (94%)	9 (6%)	0	100	100
25	4	176/237 (74%)	170 (97%)	6 (3%)	0	100	100
26	L	130/145 (90%)	129 (99%)	1 (1%)	0	100	100
All	All	4136/4895 (84%)	4026 (97%)	108 (3%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	3	31	VAL
19	9	109	PHE

5.3.2 Protein sidechains ⓘ

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	1	136/170 (80%)	136 (100%)	0	100	100
2	3	132/153 (86%)	132 (100%)	0	100	100
3	5	133/164 (81%)	131 (98%)	2 (2%)	57	78
4	7	135/135 (100%)	134 (99%)	1 (1%)	76	88
5	8	133/163 (82%)	130 (98%)	3 (2%)	44	69
6	A	607/613 (99%)	597 (98%)	10 (2%)	55	77
7	B	600/603 (100%)	594 (99%)	6 (1%)	68	84
8	C	67/68 (98%)	67 (100%)	0	100	100
9	D	106/113 (94%)	105 (99%)	1 (1%)	70	86
10	E	53/54 (98%)	53 (100%)	0	100	100
11	F	140/177 (79%)	139 (99%)	1 (1%)	76	88
12	I	30/32 (94%)	30 (100%)	0	100	100
13	J	35/36 (97%)	35 (100%)	0	100	100
14	M	25/25 (100%)	25 (100%)	0	100	100
15	R	67/101 (66%)	65 (97%)	2 (3%)	36	61
17	10	134/161 (83%)	132 (98%)	2 (2%)	57	78
17	6	134/161 (83%)	131 (98%)	3 (2%)	45	70
18	11	139/172 (81%)	139 (100%)	0	100	100
19	13	117/170 (69%)	116 (99%)	1 (1%)	70	86
19	9	112/170 (66%)	108 (96%)	4 (4%)	31	55
22	17	113/162 (70%)	110 (97%)	3 (3%)	39	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
25	4	138/180 (77%)	135 (98%)	3 (2%)	45	70
26	L	111/122 (91%)	111 (100%)	0	100	100
All	All	3397/3905 (87%)	3355 (99%)	42 (1%)	61	81

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	5	51	LEU
3	5	125	LEU
4	7	169	PHE
5	8	50	THR
5	8	166	ILE
5	8	210	LEU
6	A	15	ASP
6	A	166	MET
6	A	205	LEU
6	A	271	ASP
6	A	301	LEU
6	A	369	TYR
6	A	424	LEU
6	A	526	SER
6	A	596	MET
6	A	739	SER
7	B	195	VAL
7	B	394	PHE
7	B	441	ASP
7	B	443	VAL
7	B	476	LEU
7	B	677	THR
9	D	64	GLU
11	F	65	LYS
15	R	79	LEU
15	R	112	LEU
17	6	101	LEU
17	6	112	VAL
17	6	181	LEU
17	10	171	THR
17	10	198	VAL
19	13	116	ILE
22	17	84	MET
22	17	112	VAL

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Mol	Chain	Res	Type
22	17	141	VAL
25	4	73	ILE
25	4	143	VAL
25	4	192	LEU
19	9	92	LYS
19	9	99	LEU
19	9	104	LEU
19	9	187	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	103	GLN
1	1	223	ASN
2	3	180	GLN
4	7	73	ASN
5	8	73	ASN
5	8	80	GLN
6	A	222	ASN
6	A	366	HIS
6	A	390	HIS
6	A	627	HIS
6	A	692	GLN
6	A	712	GLN
7	B	158	GLN
7	B	247	ASN
7	B	276	HIS
7	B	368	GLN
7	B	439	HIS
7	B	603	GLN
7	B	614	ASN
7	B	627	ASN
9	D	96	HIS
9	D	123	ASN
11	F	86	GLN
11	F	148	ASN
13	J	30	ASN
18	11	207	HIS
22	17	49	GLN
22	17	79	HIS
22	17	94	GLN
22	17	183	GLN

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Mol	Chain	Res	Type
25	4	229	ASN
19	9	69	ASN
19	9	204	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

318 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
28	CLA	B	823	7	69,73,73	0.97	4 (5%)	82,113,113	1.10	3 (3%)
36	SF4	C	102	8	0,12,12	-	-	-		
28	CLA	B	807	7	69,73,73	0.86	4 (5%)	82,113,113	1.08	5 (6%)
28	CLA	J	102	-	62,66,73	0.89	4 (6%)	73,104,113	1.20	4 (5%)
31	LHG	1	309	-	43,43,48	0.31	0	46,49,54	0.30	0
28	CLA	B	805	7	69,73,73	0.93	4 (5%)	82,113,113	1.06	6 (7%)
31	LHG	A	851	-	26,26,48	0.38	0	29,32,54	0.34	0
28	CLA	11	312	18	47,51,73	1.03	3 (6%)	55,86,113	1.62	8 (14%)
36	SF4	A	848	7,6	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	CLA	15	201	-	50,54,73	0.95	4 (8%)	59,90,113	1.33	8 (13%)
28	CLA	A	845	-	69,73,73	0.99	4 (5%)	82,113,113	1.04	5 (6%)
28	CLA	1	305	1	56,60,73	0.82	3 (5%)	65,97,113	1.27	9 (13%)
32	XAT	10	313	-	41,47,47	0.65	2 (4%)	54,74,74	0.67	2 (3%)
28	CLA	A	831	6	54,58,73	0.99	4 (7%)	64,95,113	1.13	3 (4%)
28	CLA	9	311	19	49,53,73	0.95	4 (8%)	58,89,113	1.46	7 (12%)
30	KC1	7	307	4	49,53,53	1.30	3 (6%)	61,89,89	1.42	13 (21%)
28	CLA	A	828	6	69,73,73	0.92	4 (5%)	82,113,113	1.02	5 (6%)
28	CLA	9	305	-	54,58,73	0.87	4 (7%)	64,95,113	1.30	9 (14%)
32	XAT	9	313	-	42,46,47	0.66	2 (4%)	52,71,74	0.82	2 (3%)
33	BCR	A	842	-	41,41,41	0.14	0	56,56,56	0.22	0
29	A86	R	203	-	47,50,50	0.44	1 (2%)	51,76,76	0.60	0
28	CLA	7	305	4	69,73,73	0.85	4 (5%)	82,113,113	1.05	6 (7%)
28	CLA	A	812	6	56,60,73	1.06	4 (7%)	65,97,113	1.15	5 (7%)
28	CLA	5	309	3	54,58,73	1.02	4 (7%)	64,95,113	1.46	9 (14%)
30	KC1	7	309	4	49,53,53	1.18	4 (8%)	61,89,89	1.43	10 (16%)
28	CLA	16	204	-	45,49,73	0.85	3 (6%)	54,84,113	1.51	9 (16%)
33	BCR	8	309	-	41,41,41	0.17	0	56,56,56	1.20	5 (8%)
31	LHG	5	314	-	23,23,48	0.41	0	26,29,54	0.36	0
32	XAT	3	313	-	41,47,47	0.67	2 (4%)	54,74,74	0.70	1 (1%)
32	XAT	5	307	-	41,47,47	0.42	0	54,74,74	1.54	7 (12%)
31	LHG	9	301	-	27,27,48	0.39	0	30,33,54	0.35	0
29	A86	4	314	-	47,50,50	0.43	1 (2%)	51,76,76	0.62	0
28	CLA	B	806	7	69,73,73	0.96	4 (5%)	82,113,113	1.01	3 (3%)
32	XAT	J	105	-	41,47,47	0.47	1 (2%)	54,74,74	1.23	5 (9%)
33	BCR	A	850	-	41,41,41	0.24	0	56,56,56	1.20	7 (12%)
28	CLA	10	305	17	50,54,73	0.94	4 (8%)	59,90,113	1.32	4 (6%)
29	A86	4	313	-	47,50,50	0.41	1 (2%)	51,76,76	0.53	0
28	CLA	11	304	18	64,68,73	0.81	4 (6%)	76,107,113	1.31	8 (10%)
28	CLA	B	813	-	64,68,73	0.94	4 (6%)	76,107,113	1.32	6 (7%)
28	CLA	A	849	6	69,73,73	0.83	4 (5%)	82,113,113	1.15	6 (7%)
28	CLA	6	301	17	69,73,73	0.83	4 (5%)	82,113,113	1.10	6 (7%)
32	XAT	7	316	-	41,47,47	0.62	2 (4%)	54,74,74	1.35	6 (11%)
28	CLA	16	201	-	49,53,73	0.82	3 (6%)	58,89,113	1.40	9 (15%)
30	KC1	17	306	-	49,53,53	1.11	4 (8%)	61,89,89	1.67	11 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	KC1	3	309	2	49,53,53	1.15	4 (8%)	61,89,89	1.60	8 (13%)
28	CLA	19	201	-	50,54,73	0.73	2 (4%)	59,90,113	1.42	10 (16%)
28	CLA	4	305	-	46,50,73	0.85	3 (6%)	53,85,113	1.43	7 (13%)
32	XAT	6	312	-	41,47,47	0.47	1 (2%)	54,74,74	1.26	3 (5%)
34	DGD	4	301	-	40,40,67	0.19	0	54,54,81	0.23	0
28	CLA	6	304	17	46,50,73	0.99	3 (6%)	53,85,113	1.56	6 (11%)
30	KC1	3	308	2	49,53,53	1.20	3 (6%)	61,89,89	1.54	10 (16%)
32	XAT	7	317	-	41,47,47	0.40	1 (2%)	54,74,74	1.44	7 (12%)
34	DGD	8	314	-	32,32,67	0.22	0	45,45,81	0.50	0
30	KC1	4	312	-	49,53,53	1.11	4 (8%)	61,89,89	1.34	9 (14%)
28	CLA	3	301	2	69,73,73	0.85	4 (5%)	82,113,113	1.13	4 (4%)
33	BCR	L	205	-	41,41,41	0.13	0	56,56,56	0.24	0
29	A86	J	101	-	47,50,50	0.47	1 (2%)	51,76,76	0.71	0
28	CLA	6	313	-	69,73,73	0.85	4 (5%)	82,113,113	1.21	7 (8%)
32	XAT	7	313	-	41,47,47	0.44	1 (2%)	54,74,74	1.19	4 (7%)
28	CLA	B	833	-	65,69,73	0.94	4 (6%)	77,108,113	1.09	3 (3%)
29	A86	1	313	28	47,50,50	0.40	1 (2%)	51,76,76	0.61	1 (1%)
28	CLA	A	830	6	69,73,73	0.93	4 (5%)	82,113,113	1.12	4 (4%)
28	CLA	A	803	6	59,63,73	0.88	4 (6%)	70,101,113	1.11	5 (7%)
32	XAT	6	315	-	41,47,47	0.47	0	54,74,74	1.00	5 (9%)
28	CLA	a	201	-	47,51,73	0.82	3 (6%)	55,86,113	1.56	6 (10%)
30	KC1	6	305	17	49,53,53	1.23	4 (8%)	61,89,89	1.47	9 (14%)
28	CLA	10	301	17	59,63,73	0.82	3 (5%)	70,101,113	1.23	7 (10%)
28	CLA	A	852	6	69,73,73	0.98	4 (5%)	82,113,113	1.08	5 (6%)
29	A86	8	308	-	47,50,50	0.49	1 (2%)	51,76,76	0.65	0
28	CLA	10	307	-	61,65,73	0.80	3 (4%)	72,103,113	1.27	7 (9%)
28	CLA	A	827	6	69,73,73	1.00	4 (5%)	82,113,113	1.26	6 (7%)
28	CLA	a	203	-	50,54,73	0.81	3 (6%)	59,90,113	1.61	8 (13%)
32	XAT	6	316	-	41,47,47	0.62	2 (4%)	54,74,74	0.78	1 (1%)
28	CLA	11	305	-	49,53,73	0.96	3 (6%)	58,89,113	1.46	8 (13%)
28	CLA	5	305	3	60,64,73	0.84	4 (6%)	71,102,113	1.12	5 (7%)
30	KC1	17	312	22	49,53,53	1.19	4 (8%)	61,89,89	1.56	6 (9%)
28	CLA	1	301	1	54,58,73	0.79	2 (3%)	64,95,113	1.51	11 (17%)
28	CLA	11	309	18	47,51,73	1.02	4 (8%)	55,86,113	1.37	4 (7%)
28	CLA	A	807	6	69,73,73	1.00	4 (5%)	82,113,113	1.04	4 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	LHG	4	302	-	24,24,48	0.40	0	27,30,54	0.35	0
28	CLA	A	847	6	69,73,73	0.79	4 (5%)	82,113,113	1.28	7 (8%)
29	A86	3	310	-	47,50,50	0.42	1 (2%)	51,76,76	0.73	2 (3%)
28	CLA	B	831	7	69,73,73	0.86	4 (5%)	82,113,113	1.04	6 (7%)
33	BCR	F	804	-	41,41,41	0.13	0	56,56,56	0.27	0
28	CLA	A	820	6	53,57,73	1.06	4 (7%)	61,93,113	1.14	3 (4%)
28	CLA	17	305	-	54,58,73	0.92	3 (5%)	64,95,113	1.50	8 (12%)
28	CLA	17	302	22	47,51,73	1.06	3 (6%)	55,86,113	1.33	7 (12%)
28	CLA	6	307	-	59,63,73	0.91	3 (5%)	70,101,113	1.22	4 (5%)
31	LHG	A	839	-	47,47,48	0.31	0	50,53,54	0.35	0
28	CLA	17	309	22	50,54,73	0.76	2 (4%)	59,90,113	1.62	11 (18%)
28	CLA	8	304	5	61,65,73	0.83	4 (6%)	72,103,113	1.31	7 (9%)
28	CLA	B	815	-	63,67,73	0.83	3 (4%)	74,105,113	1.21	4 (5%)
28	CLA	a	204	-	46,50,73	0.98	4 (8%)	53,85,113	1.64	7 (13%)
29	A86	R	201	-	47,50,50	0.42	1 (2%)	51,76,76	0.51	0
28	CLA	7	318	-	49,53,73	0.96	4 (8%)	58,89,113	1.54	9 (15%)
28	CLA	B	802	-	69,73,73	1.04	4 (5%)	82,113,113	1.07	4 (4%)
28	CLA	11	306	18	49,53,73	0.94	4 (8%)	58,89,113	1.25	6 (10%)
28	CLA	7	303	-	69,73,73	0.80	4 (5%)	82,113,113	1.15	8 (9%)
31	LHG	11	311	-	36,36,48	0.34	0	39,42,54	0.35	0
28	CLA	A	809	6	60,64,73	0.90	4 (6%)	71,102,113	1.23	5 (7%)
29	A86	10	317	-	47,50,50	0.53	1 (2%)	51,76,76	0.67	1 (1%)
31	LHG	A	840	28	26,26,48	0.41	0	29,32,54	0.31	0
31	LHG	I	102	-	48,48,48	0.29	0	51,54,54	0.29	0
28	CLA	L	201	-	69,73,73	0.81	4 (5%)	82,113,113	1.18	4 (4%)
30	KC1	8	307	5	49,53,53	1.25	4 (8%)	61,89,89	1.39	12 (19%)
30	KC1	4	311	25	49,53,53	1.03	3 (6%)	61,89,89	1.47	9 (14%)
28	CLA	B	804	-	69,73,73	0.78	3 (4%)	82,113,113	1.23	5 (6%)
28	CLA	L	204	-	54,58,73	0.94	4 (7%)	64,95,113	1.34	7 (10%)
28	CLA	9	304	19	54,58,73	0.97	4 (7%)	64,95,113	1.24	8 (12%)
32	XAT	10	314	-	41,47,47	0.60	2 (4%)	54,74,74	0.85	1 (1%)
28	CLA	B	821	-	69,73,73	0.91	4 (5%)	82,113,113	1.08	4 (4%)
28	CLA	7	312	4	69,73,73	0.78	3 (4%)	82,113,113	1.35	5 (6%)
28	CLA	F	803	11	47,51,73	1.13	4 (8%)	55,86,113	1.27	5 (9%)
28	CLA	B	814	7	63,67,73	1.00	4 (6%)	74,105,113	1.18	5 (6%)
28	CLA	A	805	6	69,73,73	1.07	4 (5%)	82,113,113	1.08	8 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	CLA	8	313	-	60,64,73	0.80	4 (6%)	71,102,113	1.21	7 (9%)
28	CLA	8	302	5	60,64,73	0.93	4 (6%)	71,102,113	1.29	8 (11%)
30	KC1	10	311	-	49,53,53	1.26	3 (6%)	61,89,89	1.27	9 (14%)
28	CLA	A	808	6	69,73,73	1.02	4 (5%)	82,113,113	1.12	5 (6%)
28	CLA	1	307	1	59,63,73	0.95	4 (6%)	70,101,113	1.14	6 (8%)
28	CLA	8	301	5	69,73,73	0.83	4 (5%)	82,113,113	1.12	8 (9%)
28	CLA	A	836	6	69,73,73	0.87	4 (5%)	82,113,113	1.21	9 (10%)
28	CLA	B	818	7	50,54,73	1.13	4 (8%)	59,90,113	1.33	4 (6%)
32	XAT	8	311	-	41,47,47	0.62	2 (4%)	54,74,74	0.85	2 (3%)
32	XAT	5	311	-	41,47,47	0.60	2 (4%)	54,74,74	0.83	2 (3%)
28	CLA	A	824	-	69,73,73	1.02	4 (5%)	82,113,113	1.15	5 (6%)
28	CLA	5	306	3	45,49,73	0.93	3 (6%)	54,84,113	1.46	9 (16%)
28	CLA	B	826	7	69,73,73	0.90	4 (5%)	82,113,113	1.15	5 (6%)
34	DGD	4	317	30	30,30,67	0.20	0	42,42,81	0.36	0
28	CLA	B	825	7	69,73,73	0.96	4 (5%)	82,113,113	1.02	5 (6%)
28	CLA	19	202	-	47,51,73	0.99	4 (8%)	55,86,113	1.52	8 (14%)
28	CLA	5	302	3	59,63,73	0.89	4 (6%)	70,101,113	1.16	6 (8%)
28	CLA	4	303	-	59,63,73	0.80	3 (5%)	70,101,113	1.31	7 (10%)
28	CLA	B	834	7	69,73,73	0.94	4 (5%)	82,113,113	1.14	6 (7%)
32	XAT	5	310	-	41,47,47	0.53	1 (2%)	54,74,74	0.92	2 (3%)
28	CLA	3	305	2	64,68,73	0.88	4 (6%)	76,107,113	1.19	7 (9%)
28	CLA	5	301	3	69,73,73	0.81	4 (5%)	82,113,113	1.06	5 (6%)
28	CLA	9	307	19	54,58,73	0.84	3 (5%)	64,95,113	1.41	7 (10%)
28	CLA	A	813	6	54,58,73	1.09	4 (7%)	64,95,113	1.18	5 (7%)
28	CLA	A	832	6	49,53,73	1.02	4 (8%)	58,89,113	1.39	5 (8%)
28	CLA	A	815	6	69,73,73	0.91	4 (5%)	82,113,113	1.02	6 (7%)
31	LHG	B	842	28	25,25,48	0.42	0	28,31,54	0.46	0
28	CLA	L	206	26	69,73,73	0.84	3 (4%)	82,113,113	1.35	7 (8%)
28	CLA	B	829	-	49,53,73	1.17	4 (8%)	58,89,113	1.33	7 (12%)
30	KC1	1	306	1	49,53,53	1.15	4 (8%)	61,89,89	1.46	9 (14%)
28	CLA	A	822	6	59,63,73	0.97	4 (6%)	70,101,113	1.05	5 (7%)
28	CLA	13	302	19	49,53,73	0.99	4 (8%)	58,89,113	1.42	8 (13%)
29	A86	3	312	-	47,50,50	0.52	1 (2%)	51,76,76	0.59	1 (1%)
28	CLA	B	801	7	69,73,73	0.85	4 (5%)	82,113,113	1.17	6 (7%)
32	XAT	7	314	-	41,47,47	0.62	2 (4%)	54,74,74	0.66	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	KC1	5	308	-	49,53,53	1.14	3 (6%)	61,89,89	1.20	8 (13%)
28	CLA	17	303	22	52,56,73	0.88	3 (5%)	61,92,113	1.41	6 (9%)
32	XAT	11	313	-	41,47,47	0.58	2 (4%)	54,74,74	0.71	2 (3%)
28	CLA	10	302	17	50,54,73	0.97	4 (8%)	59,90,113	1.30	7 (11%)
32	XAT	13	309	-	41,47,47	0.67	2 (4%)	54,74,74	0.71	2 (3%)
28	CLA	J	103	13	46,50,73	0.99	4 (8%)	53,85,113	1.56	5 (9%)
33	BCR	B	841	-	41,41,41	0.18	0	56,56,56	0.34	0
28	CLA	13	301	19	60,64,73	0.91	4 (6%)	71,102,113	1.40	10 (14%)
28	CLA	3	306	2	69,73,73	0.89	4 (5%)	82,113,113	0.99	5 (6%)
28	CLA	B	810	7	58,62,73	0.96	4 (6%)	71,100,113	1.17	4 (5%)
28	CLA	1	304	1	49,53,73	0.89	4 (8%)	58,89,113	1.29	8 (13%)
28	CLA	4	306	25	59,63,73	1.05	4 (6%)	70,101,113	1.13	5 (7%)
28	CLA	13	307	19	49,53,73	0.79	3 (6%)	58,89,113	1.52	8 (13%)
28	CLA	13	303	-	49,53,73	0.80	3 (6%)	58,89,113	1.55	7 (12%)
28	CLA	B	811	7	59,63,73	1.06	4 (6%)	70,101,113	1.24	5 (7%)
28	CLA	5	303	-	69,73,73	0.91	4 (5%)	82,113,113	1.17	5 (6%)
28	CLA	8	303	-	61,65,73	0.95	4 (6%)	72,103,113	1.18	4 (5%)
28	CLA	B	819	7	59,63,73	0.93	4 (6%)	70,101,113	1.13	5 (7%)
28	CLA	B	843	7	69,73,73	0.95	4 (5%)	82,113,113	1.04	3 (3%)
28	CLA	L	203	26	69,73,73	0.93	4 (5%)	82,113,113	1.09	3 (3%)
28	CLA	B	817	-	69,73,73	0.88	4 (5%)	82,113,113	1.05	5 (6%)
28	CLA	10	306	17	60,64,73	0.87	4 (6%)	71,102,113	1.21	5 (7%)
33	BCR	B	846	-	41,41,41	0.21	0	56,56,56	0.56	0
33	BCR	1	312	-	41,41,41	0.12	0	56,56,56	0.35	0
28	CLA	A	846	6	51,55,73	1.02	4 (7%)	60,91,113	1.42	4 (6%)
29	A86	6	314	-	47,50,50	0.45	1 (2%)	51,76,76	0.83	2 (3%)
28	CLA	B	845	7	69,73,73	0.91	4 (5%)	82,113,113	1.04	3 (3%)
28	CLA	11	314	-	47,51,73	0.92	4 (8%)	55,86,113	1.44	5 (9%)
28	CLA	4	304	25	55,59,73	0.91	4 (7%)	64,96,113	1.41	7 (10%)
28	CLA	B	816	7	69,73,73	0.98	4 (5%)	82,113,113	1.04	3 (3%)
28	CLA	7	306	31	69,73,73	0.83	4 (5%)	82,113,113	1.22	7 (8%)
28	CLA	10	308	17	51,55,73	0.94	4 (7%)	60,91,113	1.26	5 (8%)
28	CLA	6	303	-	59,63,73	0.88	4 (6%)	70,101,113	1.27	7 (10%)
28	CLA	7	302	4	54,58,73	1.10	4 (7%)	64,95,113	1.29	5 (7%)
28	CLA	B	812	7	69,73,73	1.06	4 (5%)	82,113,113	0.96	4 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	CLA	A	853	-	69,73,73	1.06	4 (5%)	82,113,113	1.10	5 (6%)
31	LHG	9	314	-	32,32,48	0.35	0	35,38,54	0.33	0
36	SF4	C	101	8	0,12,12	-	-	-		
28	CLA	9	310	-	49,53,73	1.06	4 (8%)	58,89,113	1.42	7 (12%)
30	KC1	9	306	19	49,53,53	1.15	3 (6%)	61,89,89	1.47	11 (18%)
28	CLA	4	316	25	65,69,73	0.65	3 (4%)	77,108,113	1.19	9 (11%)
28	CLA	A	833	6	55,59,73	1.13	3 (5%)	64,96,113	1.36	5 (7%)
32	XAT	17	311	-	41,47,47	0.48	1 (2%)	54,74,74	0.96	6 (11%)
28	CLA	A	835	6	69,73,73	0.99	4 (5%)	82,113,113	1.15	7 (8%)
31	LHG	B	844	-	48,48,48	0.30	0	51,54,54	0.30	0
32	XAT	4	315	-	41,47,47	0.50	1 (2%)	54,74,74	0.95	3 (5%)
28	CLA	7	304	4	69,73,73	0.84	4 (5%)	82,113,113	1.01	2 (2%)
28	CLA	B	827	7	54,58,73	1.05	4 (7%)	64,95,113	1.24	6 (9%)
28	CLA	R	202	15	59,63,73	0.91	4 (6%)	70,101,113	1.25	5 (7%)
28	CLA	B	849	7	69,73,73	0.93	4 (5%)	82,113,113	0.91	5 (6%)
32	XAT	13	308	-	41,47,47	0.70	2 (4%)	54,74,74	0.53	0
29	A86	10	312	-	47,50,50	0.51	1 (2%)	51,76,76	1.03	5 (9%)
28	CLA	B	824	-	69,73,73	0.76	3 (4%)	82,113,113	1.18	8 (9%)
30	KC1	11	307	18	49,53,53	1.23	4 (8%)	61,89,89	1.51	10 (16%)
33	BCR	B	839	-	41,41,41	0.20	0	56,56,56	1.22	6 (10%)
28	CLA	A	806	6	59,63,73	1.02	4 (6%)	70,101,113	1.30	5 (7%)
28	CLA	3	314	31	69,73,73	0.85	4 (5%)	82,113,113	1.18	5 (6%)
28	CLA	8	305	5	49,53,73	1.04	4 (8%)	58,89,113	1.21	3 (5%)
30	KC1	13	304	19	49,53,53	1.02	3 (6%)	61,89,89	1.37	10 (16%)
28	CLA	1	314	-	69,73,73	0.82	4 (5%)	82,113,113	1.20	6 (7%)
31	LHG	7	310	28	26,26,48	0.40	0	29,32,54	0.37	0
28	CLA	11	303	18	61,65,73	0.84	4 (6%)	72,103,113	1.31	6 (8%)
33	BCR	J	104	-	41,41,41	0.23	0	56,56,56	0.29	0
28	CLA	6	311	17	51,57,73	1.67	4 (7%)	55,88,113	2.63	7 (12%)
28	CLA	16	205	-	47,51,73	0.86	3 (6%)	55,86,113	1.42	8 (14%)
33	BCR	17	310	-	41,41,41	0.12	0	56,56,56	0.61	1 (1%)
29	A86	1	302	-	47,50,50	0.54	1 (2%)	51,76,76	0.80	2 (3%)
30	KC1	6	308	17	49,53,53	1.08	4 (8%)	61,89,89	1.46	8 (13%)
28	CLA	A	804	6	69,73,73	0.82	4 (5%)	82,113,113	1.00	6 (7%)
28	CLA	4	310	-	59,63,73	0.99	4 (6%)	70,101,113	1.29	5 (7%)
33	BCR	B	840	-	41,41,41	0.26	0	56,56,56	0.50	1 (1%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	BCR	B	850	-	41,41,41	0.27	0	56,56,56	0.50	0
28	CLA	A	837	-	69,73,73	0.83	4 (5%)	82,113,113	1.02	7 (8%)
33	BCR	I	101	-	41,41,41	0.16	0	56,56,56	0.28	0
28	CLA	3	304	2	49,53,73	1.06	4 (8%)	58,89,113	1.20	4 (6%)
28	CLA	16	203	-	51,55,73	1.04	4 (7%)	60,91,113	1.44	7 (11%)
28	CLA	8	310	5	46,50,73	0.88	4 (8%)	53,85,113	1.29	4 (7%)
28	CLA	A	814	-	49,53,73	1.12	4 (8%)	58,89,113	1.33	4 (6%)
30	KC1	3	302	2	49,53,53	1.08	4 (8%)	61,89,89	1.45	10 (16%)
32	XAT	8	312	-	41,47,47	0.61	2 (4%)	54,74,74	0.75	1 (1%)
28	CLA	10	303	-	59,63,73	0.80	4 (6%)	70,101,113	1.24	7 (10%)
28	CLA	16	202	-	46,50,73	1.02	4 (8%)	53,85,113	1.53	8 (15%)
28	CLA	B	830	7	62,66,73	1.15	4 (6%)	73,104,113	1.13	2 (2%)
28	CLA	6	306	17	62,66,73	0.82	4 (6%)	73,104,113	1.27	6 (8%)
28	CLA	13	305	-	50,54,73	0.83	3 (6%)	59,90,113	1.49	6 (10%)
30	KC1	10	304	17	49,53,53	1.20	4 (8%)	61,89,89	1.35	9 (14%)
28	CLA	R	204	15	55,59,73	0.84	4 (7%)	64,96,113	1.21	6 (9%)
28	CLA	6	302	17	57,61,73	1.00	4 (7%)	67,98,113	1.05	4 (5%)
37	LMG	F	805	-	41,41,55	0.19	0	49,49,63	0.18	0
28	CLA	B	828	-	69,73,73	0.91	4 (5%)	82,113,113	1.07	5 (6%)
28	CLA	11	302	18	69,73,73	0.83	4 (5%)	82,113,113	1.06	7 (8%)
31	LHG	5	315	-	26,26,48	0.39	0	29,32,54	0.44	0
28	CLA	B	808	7	69,73,73	0.87	4 (5%)	82,113,113	1.03	6 (7%)
33	BCR	A	843	-	41,41,41	0.12	0	56,56,56	0.20	0
28	CLA	7	308	4	47,51,73	0.96	4 (8%)	55,86,113	1.15	3 (5%)
28	CLA	11	301	18	69,73,73	0.76	4 (5%)	82,113,113	1.03	5 (6%)
31	LHG	9	302	-	29,29,48	0.34	0	32,35,54	0.34	0
30	KC1	a	205	-	49,53,53	1.06	4 (8%)	61,89,89	1.34	10 (16%)
30	KC1	8	306	5	49,53,53	1.26	4 (8%)	61,89,89	1.43	10 (16%)
28	CLA	A	825	6	69,73,73	0.95	4 (5%)	82,113,113	1.17	6 (7%)
30	KC1	6	309	17	49,53,53	1.20	4 (8%)	61,89,89	1.31	8 (13%)
28	CLA	10	309	17	47,51,73	1.00	4 (8%)	55,86,113	1.47	5 (9%)
33	BCR	F	801	-	41,41,41	0.13	0	56,56,56	0.40	0
29	A86	17	308	-	47,50,50	0.40	1 (2%)	51,76,76	0.62	1 (1%)
33	BCR	B	838	-	41,41,41	0.18	0	56,56,56	0.34	0
30	KC1	4	308	34	49,53,53	1.12	4 (8%)	61,89,89	1.29	9 (14%)
28	CLA	1	308	1	52,56,73	1.08	4 (7%)	61,92,113	1.38	6 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	CLA	A	834	6	59,63,73	0.99	4 (6%)	70,101,113	1.28	4 (5%)
28	CLA	A	818	6	49,53,73	0.94	4 (8%)	58,89,113	1.33	4 (6%)
28	CLA	9	308	-	50,54,73	0.74	2 (4%)	59,90,113	1.47	10 (16%)
28	CLA	B	835	31	69,73,73	0.84	4 (5%)	82,113,113	1.08	4 (4%)
30	KC1	6	310	17	49,53,53	1.20	4 (8%)	61,89,89	1.42	10 (16%)
32	XAT	4	318	-	41,47,47	0.31	0	54,74,74	1.09	4 (7%)
28	CLA	B	847	7	69,73,73	0.93	4 (5%)	82,113,113	1.16	6 (7%)
28	CLA	F	802	-	69,73,73	1.08	4 (5%)	82,113,113	1.28	5 (6%)
33	BCR	B	851	-	41,41,41	0.16	0	56,56,56	0.32	0
28	CLA	A	821	6	55,59,73	1.02	4 (7%)	64,96,113	1.21	4 (6%)
28	CLA	A	829	6	54,58,73	0.98	4 (7%)	64,95,113	1.11	6 (9%)
28	CLA	13	306	19	46,50,73	0.93	3 (6%)	53,85,113	1.48	7 (13%)
33	BCR	A	844	-	41,41,41	0.18	0	56,56,56	0.36	0
32	XAT	1	311	-	41,47,47	0.57	2 (4%)	54,74,74	1.26	3 (5%)
28	CLA	1	310	29	69,73,73	0.94	4 (5%)	82,113,113	1.10	3 (3%)
28	CLA	A	801	6	69,73,73	0.84	4 (5%)	82,113,113	1.07	6 (7%)
30	KC1	10	310	17	49,53,53	1.08	4 (8%)	61,89,89	1.42	9 (14%)
28	CLA	A	826	-	66,70,73	0.84	4 (6%)	78,109,113	1.17	6 (7%)
28	CLA	B	832	7	69,73,73	0.91	4 (5%)	82,113,113	1.10	4 (4%)
28	CLA	B	848	7	69,73,73	1.00	4 (5%)	82,113,113	1.18	6 (7%)
32	XAT	7	315	-	41,47,47	0.36	0	54,74,74	1.06	6 (11%)
30	KC1	9	309	19	49,53,53	1.15	4 (8%)	61,89,89	1.50	8 (13%)
33	BCR	L	202	-	41,41,41	0.31	0	56,56,56	1.60	9 (16%)
28	CLA	5	304	3	51,55,73	0.94	4 (7%)	60,91,113	1.27	5 (8%)
33	BCR	A	841	-	41,41,41	0.23	0	56,56,56	0.38	0
28	CLA	B	822	-	68,72,73	0.85	4 (5%)	80,111,113	1.01	5 (6%)
28	CLA	A	810	6	66,70,73	0.95	4 (6%)	78,109,113	1.07	6 (7%)
28	CLA	11	310	-	54,58,73	1.01	4 (7%)	64,95,113	1.42	6 (9%)
28	CLA	17	304	22	53,57,73	0.79	3 (5%)	61,93,113	1.31	7 (11%)
29	A86	11	308	-	47,50,50	0.51	1 (2%)	51,76,76	0.58	0
33	BCR	M	101	-	41,41,41	0.15	0	56,56,56	0.22	0
28	CLA	3	307	-	69,73,73	0.93	4 (5%)	82,113,113	1.19	7 (8%)
32	XAT	5	316	-	41,47,47	0.57	2 (4%)	54,74,74	0.90	2 (3%)
28	CLA	4	307	25	64,68,73	0.83	3 (4%)	76,107,113	1.31	7 (9%)
35	PQN	B	836	-	34,34,34	0.27	0	43,45,45	0.44	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	CLA	3	303	2	69,73,73	0.80	4 (5%)	82,113,113	1.03	6 (7%)
29	A86	9	312	-	47,50,50	0.49	1 (2%)	51,76,76	0.64	0
28	CLA	A	811	6	58,62,73	1.06	4 (6%)	68,99,113	1.29	3 (4%)
28	CLA	B	809	7	69,73,73	0.89	4 (5%)	82,113,113	1.08	6 (7%)
28	CLA	A	819	-	69,73,73	0.87	4 (5%)	82,113,113	1.12	5 (6%)
28	CLA	7	311	4	50,54,73	0.81	2 (4%)	59,90,113	1.30	6 (10%)
28	CLA	A	817	6	69,73,73	0.92	4 (5%)	82,113,113	1.02	3 (3%)
33	BCR	B	837	-	41,41,41	0.24	0	56,56,56	0.37	0
28	CLA	B	803	7	69,73,73	0.89	4 (5%)	82,113,113	1.10	6 (7%)
28	CLA	A	802	-	69,73,73	0.89	4 (5%)	82,113,113	1.11	6 (7%)
35	PQN	A	838	-	34,34,34	0.26	0	43,45,45	0.44	1 (2%)
28	CLA	A	823	-	69,73,73	0.99	4 (5%)	82,113,113	1.08	6 (7%)
28	CLA	B	820	7	57,61,73	0.93	4 (7%)	67,98,113	1.10	3 (4%)
28	CLA	9	303	19	51,55,73	0.81	3 (5%)	60,91,113	1.49	9 (15%)
29	A86	5	312	-	47,50,50	0.55	1 (2%)	51,76,76	0.88	4 (7%)
28	CLA	7	301	4	69,73,73	0.83	4 (5%)	82,113,113	1.09	7 (8%)
32	XAT	10	315	-	41,47,47	0.48	1 (2%)	54,74,74	1.61	5 (9%)
29	A86	3	311	-	47,50,50	0.57	1 (2%)	51,76,76	1.15	3 (5%)
28	CLA	5	313	3	61,65,73	0.99	4 (6%)	72,103,113	1.24	4 (5%)
28	CLA	17	301	22	54,58,73	1.07	4 (7%)	64,95,113	1.49	10 (15%)
28	CLA	A	816	-	60,64,73	0.88	4 (6%)	71,102,113	1.36	5 (7%)
30	KC1	4	309	25	49,53,53	1.39	4 (8%)	61,89,89	1.27	9 (14%)
28	CLA	a	202	-	46,50,73	1.02	4 (8%)	53,85,113	1.52	7 (13%)
28	CLA	1	303	1	69,73,73	0.65	2 (2%)	82,113,113	1.23	8 (9%)
28	CLA	10	316	17	69,73,73	0.81	4 (5%)	82,113,113	1.16	7 (8%)
28	CLA	17	307	22	51,55,73	0.89	3 (5%)	60,91,113	1.44	6 (10%)

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
28	CLA	B	823	7	-	5/39/115/115	-
36	SF4	C	102	8	-	-	0/6/5/5
28	CLA	B	807	7	-	17/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	CLA	J	102	-	-	13/31/107/115	-
31	LHG	1	309	-	-	15/48/48/53	-
28	CLA	B	805	7	-	10/39/115/115	-
31	LHG	A	851	-	-	6/31/31/53	-
28	CLA	11	312	18	-	7/13/89/115	-
36	SF4	A	848	7,6	-	-	0/6/5/5
28	CLA	15	201	-	-	3/17/93/115	-
28	CLA	A	845	-	-	5/39/115/115	-
28	CLA	1	305	1	-	10/24/100/115	-
32	XAT	10	313	-	-	1/31/93/93	0/4/4/4
28	CLA	A	831	6	-	9/21/97/115	-
28	CLA	9	311	19	-	3/15/91/115	-
30	KC1	7	307	4	-	3/15/71/71	-
28	CLA	A	828	6	-	5/39/115/115	-
28	CLA	9	305	-	-	8/21/97/115	-
32	XAT	9	313	-	-	5/31/88/93	0/4/4/4
33	BCR	A	842	-	-	0/29/63/63	0/2/2/2
29	A86	R	203	-	-	4/34/90/90	0/3/3/3
28	CLA	7	305	4	-	12/39/115/115	-
28	CLA	A	812	6	-	7/24/100/115	-
28	CLA	5	309	3	-	7/21/97/115	-
30	KC1	7	309	4	-	7/15/71/71	-
28	CLA	16	204	-	-	4/10/86/115	-
33	BCR	8	309	-	-	11/29/63/63	0/2/2/2
31	LHG	5	314	-	-	3/28/28/53	-
32	XAT	3	313	-	-	0/31/93/93	0/4/4/4
32	XAT	5	307	-	-	5/31/93/93	0/4/4/4
31	LHG	9	301	-	-	10/32/32/53	-
29	A86	4	314	-	-	5/34/90/90	0/3/3/3
28	CLA	B	806	7	-	10/39/115/115	-
32	XAT	J	105	-	-	4/31/93/93	0/4/4/4
33	BCR	A	850	-	-	6/29/63/63	0/2/2/2
28	CLA	10	305	17	-	5/17/93/115	-
29	A86	4	313	-	-	7/34/90/90	0/3/3/3
28	CLA	11	304	18	-	15/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	CLA	B	813	-	-	9/33/109/115	-
28	CLA	A	849	6	-	12/39/115/115	-
28	CLA	6	301	17	-	15/39/115/115	-
32	XAT	7	316	-	-	4/31/93/93	0/4/4/4
28	CLA	16	201	-	-	3/15/91/115	-
30	KC1	17	306	-	-	5/15/71/71	-
30	KC1	3	309	2	-	6/15/71/71	-
28	CLA	19	201	-	-	5/17/93/115	-
28	CLA	4	305	-	-	5/12/88/115	-
32	XAT	6	312	-	-	9/31/93/93	0/4/4/4
34	DGD	4	301	-	-	12/28/68/95	0/2/2/2
28	CLA	6	304	17	-	3/12/88/115	-
30	KC1	3	308	2	-	3/15/71/71	-
32	XAT	7	317	-	-	7/31/93/93	0/4/4/4
34	DGD	8	314	-	-	8/17/57/95	0/2/2/2
30	KC1	4	312	-	-	7/15/71/71	-
28	CLA	3	301	2	-	10/39/115/115	-
33	BCR	L	205	-	-	2/29/63/63	0/2/2/2
29	A86	J	101	-	-	15/34/90/90	0/3/3/3
28	CLA	6	313	-	-	16/39/115/115	-
32	XAT	7	313	-	-	4/31/93/93	0/4/4/4
28	CLA	B	833	-	-	5/35/111/115	-
29	A86	1	313	28	-	5/34/90/90	0/3/3/3
28	CLA	A	830	6	-	16/39/115/115	-
28	CLA	A	803	6	-	7/27/103/115	-
32	XAT	6	315	-	-	5/31/93/93	0/4/4/4
28	CLA	a	201	-	-	3/13/89/115	-
30	KC1	6	305	17	-	7/15/71/71	-
28	CLA	10	301	17	-	8/27/103/115	-
28	CLA	A	852	6	-	9/39/115/115	-
29	A86	8	308	-	-	4/34/90/90	0/3/3/3
28	CLA	10	307	-	-	15/30/106/115	-
28	CLA	A	827	6	-	8/39/115/115	-
28	CLA	a	203	-	-	5/17/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	XAT	6	316	-	-	4/31/93/93	0/4/4/4
28	CLA	11	305	-	-	2/15/91/115	-
28	CLA	5	305	3	-	11/29/105/115	-
30	KC1	17	312	22	-	3/15/71/71	-
28	CLA	1	301	1	-	5/21/97/115	-
28	CLA	11	309	18	-	5/13/89/115	-
28	CLA	A	807	6	-	13/39/115/115	-
31	LHG	4	302	-	-	11/29/29/53	-
28	CLA	A	847	6	-	15/39/115/115	-
29	A86	3	310	-	-	5/34/90/90	0/3/3/3
28	CLA	B	831	7	-	10/39/115/115	-
33	BCR	F	804	-	-	2/29/63/63	0/2/2/2
28	CLA	A	820	6	-	8/20/96/115	-
28	CLA	17	305	-	-	7/21/97/115	-
28	CLA	17	302	22	-	4/13/89/115	-
28	CLA	6	307	-	-	9/27/103/115	-
31	LHG	A	839	-	-	7/52/52/53	-
28	CLA	17	309	22	-	6/17/93/115	-
28	CLA	8	304	5	-	14/30/106/115	-
28	CLA	B	815	-	-	13/32/108/115	-
28	CLA	a	204	-	-	2/12/88/115	-
29	A86	R	201	-	-	4/34/90/90	0/3/3/3
28	CLA	7	318	-	-	9/15/91/115	-
28	CLA	B	802	-	-	2/39/115/115	-
28	CLA	11	306	18	-	2/15/91/115	-
28	CLA	7	303	-	-	21/39/115/115	-
31	LHG	11	311	-	-	13/41/41/53	-
28	CLA	A	809	6	-	9/29/105/115	-
29	A86	10	317	-	-	11/34/90/90	0/3/3/3
31	LHG	A	840	28	-	6/31/31/53	-
31	LHG	I	102	-	-	23/53/53/53	-
28	CLA	L	201	-	-	7/39/115/115	-
30	KC1	8	307	5	-	2/15/71/71	-
30	KC1	4	311	25	-	5/15/71/71	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	CLA	B	804	-	-	11/39/115/115	-
28	CLA	L	204	-	-	6/21/97/115	-
28	CLA	9	304	19	-	10/21/97/115	-
32	XAT	10	314	-	-	4/31/93/93	0/4/4/4
28	CLA	B	821	-	-	9/39/115/115	-
28	CLA	7	312	4	-	16/39/115/115	-
28	CLA	F	803	11	-	5/13/89/115	-
28	CLA	B	814	7	-	9/32/108/115	-
28	CLA	A	805	6	-	12/39/115/115	-
28	CLA	8	313	-	-	7/29/105/115	-
28	CLA	8	302	5	-	8/29/105/115	-
30	KC1	10	311	-	-	5/15/71/71	-
28	CLA	A	808	6	-	15/39/115/115	-
28	CLA	1	307	1	-	10/27/103/115	-
28	CLA	8	301	5	-	15/39/115/115	-
28	CLA	A	836	6	-	14/39/115/115	-
28	CLA	B	818	7	-	3/17/93/115	-
32	XAT	8	311	-	-	2/31/93/93	0/4/4/4
32	XAT	5	311	-	-	7/31/93/93	0/4/4/4
28	CLA	A	824	-	-	8/39/115/115	-
28	CLA	5	306	3	-	2/10/86/115	-
28	CLA	B	826	7	-	6/39/115/115	-
34	DGD	4	317	30	-	7/16/52/95	0/2/2/2
28	CLA	B	825	7	-	2/39/115/115	-
28	CLA	19	202	-	-	3/13/89/115	-
28	CLA	5	302	3	-	10/27/103/115	-
28	CLA	4	303	-	-	13/27/103/115	-
28	CLA	B	834	7	-	16/39/115/115	-
32	XAT	5	310	-	-	4/31/93/93	0/4/4/4
28	CLA	3	305	2	-	13/33/109/115	-
28	CLA	5	301	3	-	13/39/115/115	-
28	CLA	9	307	19	-	7/21/97/115	-
28	CLA	A	813	6	-	5/21/97/115	-
28	CLA	A	832	6	-	2/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	CLA	A	815	6	-	20/39/115/115	-
31	LHG	B	842	28	-	10/30/30/53	-
28	CLA	L	206	26	-	15/39/115/115	-
28	CLA	B	829	-	-	4/15/91/115	-
30	KC1	1	306	1	-	6/15/71/71	-
28	CLA	A	822	6	-	12/27/103/115	-
28	CLA	13	302	19	-	4/15/91/115	-
29	A86	3	312	-	-	5/34/90/90	1/3/3/3
28	CLA	B	801	7	-	9/39/115/115	-
32	XAT	7	314	-	-	0/31/93/93	0/4/4/4
30	KC1	5	308	-	-	7/15/71/71	-
28	CLA	17	303	22	-	7/19/95/115	-
32	XAT	11	313	-	-	4/31/93/93	0/4/4/4
28	CLA	10	302	17	-	6/17/93/115	-
32	XAT	13	309	-	-	7/31/93/93	0/4/4/4
28	CLA	J	103	13	-	1/12/88/115	-
33	BCR	B	841	-	-	0/29/63/63	0/2/2/2
28	CLA	13	301	19	-	14/29/105/115	-
28	CLA	3	306	2	-	8/39/115/115	-
28	CLA	B	810	7	-	10/25/101/115	-
28	CLA	1	304	1	-	6/15/91/115	-
28	CLA	4	306	25	-	14/27/103/115	-
28	CLA	13	307	19	-	4/15/91/115	-
28	CLA	13	303	-	-	6/15/91/115	-
28	CLA	B	811	7	-	13/27/103/115	-
28	CLA	5	303	-	-	11/39/115/115	-
28	CLA	8	303	-	-	14/30/106/115	-
28	CLA	B	819	7	-	5/27/103/115	-
28	CLA	B	843	7	-	14/39/115/115	-
28	CLA	L	203	26	-	5/39/115/115	-
28	CLA	B	817	-	-	17/39/115/115	-
28	CLA	10	306	17	-	11/29/105/115	-
33	BCR	B	846	-	-	2/29/63/63	0/2/2/2
33	BCR	1	312	-	-	4/29/63/63	0/2/2/2
28	CLA	A	846	6	-	5/18/94/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	A86	6	314	-	-	8/34/90/90	0/3/3/3
28	CLA	B	845	7	-	18/39/115/115	-
28	CLA	11	314	-	-	6/13/89/115	-
28	CLA	4	304	25	-	5/23/99/115	-
28	CLA	B	816	7	-	11/39/115/115	-
28	CLA	7	306	31	-	11/39/115/115	-
28	CLA	10	308	17	-	4/18/94/115	-
28	CLA	6	303	-	-	6/27/103/115	-
28	CLA	7	302	4	-	5/21/97/115	-
28	CLA	B	812	7	-	10/39/115/115	-
28	CLA	A	853	-	-	6/39/115/115	-
31	LHG	9	314	-	-	10/37/37/53	-
36	SF4	C	101	8	-	-	0/6/5/5
28	CLA	9	310	-	-	7/15/91/115	-
30	KC1	9	306	19	-	7/15/71/71	-
28	CLA	4	316	25	-	13/35/111/115	-
28	CLA	A	833	6	-	7/23/99/115	-
32	XAT	17	311	-	-	5/31/93/93	0/4/4/4
28	CLA	A	835	6	-	5/39/115/115	-
31	LHG	B	844	-	-	10/53/53/53	-
32	XAT	4	315	-	-	10/31/93/93	0/4/4/4
28	CLA	7	304	4	-	12/39/115/115	-
28	CLA	B	827	7	-	5/21/97/115	-
28	CLA	R	202	15	-	9/27/103/115	-
28	CLA	B	849	7	-	7/39/115/115	-
32	XAT	13	308	-	-	1/31/93/93	0/4/4/4
29	A86	10	312	-	-	12/34/90/90	0/3/3/3
28	CLA	B	824	-	-	9/39/115/115	-
30	KC1	11	307	18	-	5/15/71/71	-
33	BCR	B	839	-	-	1/29/63/63	0/2/2/2
28	CLA	A	806	6	-	12/27/103/115	-
28	CLA	3	314	31	-	9/39/115/115	-
28	CLA	8	305	5	-	7/15/91/115	-
30	KC1	13	304	19	-	7/15/71/71	-
28	CLA	1	314	-	-	12/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	LHG	7	310	28	-	8/31/31/53	-
28	CLA	11	303	18	-	11/30/106/115	-
33	BCR	J	104	-	-	1/29/63/63	0/2/2/2
28	CLA	6	311	17	-	14/30/92/115	-
28	CLA	16	205	-	-	7/13/89/115	-
33	BCR	17	310	-	-	7/29/63/63	0/2/2/2
29	A86	1	302	-	-	10/34/90/90	0/3/3/3
30	KC1	6	308	17	-	4/15/71/71	-
28	CLA	A	804	6	-	9/39/115/115	-
28	CLA	4	310	-	-	11/27/103/115	-
33	BCR	B	840	-	-	4/29/63/63	0/2/2/2
33	BCR	B	850	-	-	2/29/63/63	0/2/2/2
28	CLA	A	837	-	-	20/39/115/115	-
33	BCR	I	101	-	-	0/29/63/63	0/2/2/2
28	CLA	3	304	2	-	6/15/91/115	-
28	CLA	16	203	-	-	9/18/94/115	-
28	CLA	8	310	5	-	4/12/88/115	-
28	CLA	A	814	-	-	7/15/91/115	-
30	KC1	3	302	2	-	2/15/71/71	-
32	XAT	8	312	-	-	6/31/93/93	0/4/4/4
28	CLA	10	303	-	-	13/27/103/115	-
28	CLA	16	202	-	-	3/12/88/115	-
28	CLA	B	830	7	-	5/31/107/115	-
28	CLA	6	306	17	-	10/31/107/115	-
28	CLA	13	305	-	-	7/17/93/115	-
30	KC1	10	304	17	-	5/15/71/71	-
28	CLA	R	204	15	-	7/23/99/115	-
28	CLA	6	302	17	-	7/25/101/115	-
37	LMG	F	805	-	-	3/36/56/70	0/1/1/1
28	CLA	B	828	-	-	10/39/115/115	-
28	CLA	11	302	18	-	17/39/115/115	-
31	LHG	5	315	-	-	11/31/31/53	-
28	CLA	B	808	7	-	17/39/115/115	-
33	BCR	A	843	-	-	0/29/63/63	0/2/2/2
28	CLA	7	308	4	-	8/13/89/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	CLA	11	301	18	-	14/39/115/115	-
31	LHG	9	302	-	-	8/33/33/53	-
30	KC1	a	205	-	-	2/15/71/71	-
30	KC1	8	306	5	-	2/15/71/71	-
28	CLA	A	825	6	-	7/39/115/115	-
30	KC1	6	309	17	-	7/15/71/71	-
28	CLA	10	309	17	-	5/13/89/115	-
33	BCR	F	801	-	-	0/29/63/63	0/2/2/2
29	A86	17	308	-	-	2/34/90/90	0/3/3/3
33	BCR	B	838	-	-	0/29/63/63	0/2/2/2
30	KC1	4	308	34	-	6/15/71/71	-
28	CLA	1	308	1	-	5/19/95/115	-
28	CLA	A	834	6	-	10/27/103/115	-
28	CLA	A	818	6	-	5/15/91/115	-
28	CLA	9	308	-	-	2/17/93/115	-
28	CLA	B	835	31	-	8/39/115/115	-
30	KC1	6	310	17	-	7/15/71/71	-
32	XAT	4	318	-	-	5/31/93/93	0/4/4/4
28	CLA	B	847	7	-	12/39/115/115	-
28	CLA	F	802	-	-	12/39/115/115	-
33	BCR	B	851	-	-	3/29/63/63	0/2/2/2
28	CLA	A	821	6	-	7/23/99/115	-
28	CLA	A	829	6	-	8/21/97/115	-
28	CLA	13	306	19	-	6/12/88/115	-
33	BCR	A	844	-	-	3/29/63/63	0/2/2/2
32	XAT	1	311	-	-	2/31/93/93	0/4/4/4
28	CLA	1	310	29	-	11/39/115/115	-
28	CLA	A	801	6	-	3/39/115/115	-
30	KC1	10	310	17	-	5/15/71/71	-
28	CLA	A	826	-	-	7/36/112/115	-
28	CLA	B	832	7	-	15/39/115/115	-
28	CLA	B	848	7	-	5/39/115/115	-
32	XAT	7	315	-	-	8/31/93/93	0/4/4/4
30	KC1	9	309	19	-	4/15/71/71	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	BCR	L	202	-	-	6/29/63/63	0/2/2/2
28	CLA	5	304	3	-	7/18/94/115	-
33	BCR	A	841	-	-	4/29/63/63	0/2/2/2
28	CLA	B	822	-	-	9/38/114/115	-
28	CLA	A	810	6	-	12/36/112/115	-
28	CLA	11	310	-	-	10/21/97/115	-
28	CLA	17	304	22	-	6/20/96/115	-
29	A86	11	308	-	-	4/34/90/90	0/3/3/3
33	BCR	M	101	-	-	0/29/63/63	0/2/2/2
28	CLA	3	307	-	-	15/39/115/115	-
32	XAT	5	316	-	-	0/31/93/93	0/4/4/4
28	CLA	4	307	25	-	13/33/109/115	-
35	PQN	B	836	-	-	5/23/43/43	0/2/2/2
28	CLA	3	303	2	-	16/39/115/115	-
29	A86	9	312	-	-	13/34/90/90	0/3/3/3
28	CLA	A	811	6	-	7/26/102/115	-
28	CLA	B	809	7	-	7/39/115/115	-
28	CLA	A	819	-	-	4/39/115/115	-
28	CLA	7	311	4	-	7/17/93/115	-
28	CLA	A	817	6	-	15/39/115/115	-
33	BCR	B	837	-	-	3/29/63/63	0/2/2/2
28	CLA	B	803	7	-	13/39/115/115	-
28	CLA	A	802	-	-	12/39/115/115	-
35	PQN	A	838	-	-	3/23/43/43	0/2/2/2
28	CLA	A	823	-	-	16/39/115/115	-
28	CLA	B	820	7	-	10/25/101/115	-
28	CLA	9	303	19	-	5/18/94/115	-
29	A86	5	312	-	-	7/34/90/90	0/3/3/3
28	CLA	7	301	4	-	13/39/115/115	-
32	XAT	10	315	-	-	4/31/93/93	0/4/4/4
29	A86	3	311	-	-	11/34/90/90	0/3/3/3
28	CLA	5	313	3	-	13/30/106/115	-
28	CLA	17	301	22	-	5/21/97/115	-
28	CLA	A	816	-	-	9/29/105/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	KC1	4	309	25	-	7/15/71/71	-
28	CLA	a	202	-	-	6/12/88/115	-
28	CLA	1	303	1	-	16/39/115/115	-
28	CLA	10	316	17	-	12/39/115/115	-
28	CLA	17	307	22	-	5/18/94/115	-

All (907) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	6	311	CLA	C2D-C1D	-9.74	1.37	1.50
30	4	309	KC1	MG-NA	6.51	2.21	2.06
30	8	306	KC1	MG-NA	6.05	2.20	2.06
30	10	311	KC1	MG-NA	6.00	2.20	2.06
30	7	307	KC1	MG-NA	5.80	2.20	2.06
28	F	802	CLA	MG-NA	5.76	2.19	2.06
30	8	307	KC1	MG-NA	5.71	2.19	2.06
28	B	802	CLA	MG-NA	5.71	2.19	2.06
28	B	812	CLA	MG-NA	5.69	2.19	2.06
30	10	304	KC1	MG-NA	5.65	2.19	2.06
28	A	853	CLA	MG-NA	5.65	2.19	2.06
30	6	309	KC1	MG-NA	5.63	2.19	2.06
30	17	312	KC1	MG-NA	5.58	2.19	2.06
28	A	835	CLA	MG-NA	5.57	2.19	2.06
30	11	307	KC1	MG-NA	5.53	2.19	2.06
30	6	310	KC1	MG-NA	5.53	2.19	2.06
30	6	305	KC1	MG-NA	5.47	2.19	2.06
28	A	805	CLA	MG-NA	5.45	2.19	2.06
30	3	308	KC1	MG-NA	5.39	2.19	2.06
30	7	309	KC1	MG-NA	5.29	2.18	2.06
28	A	852	CLA	MG-NA	5.18	2.18	2.06
30	4	308	KC1	MG-NA	5.16	2.18	2.06
28	B	814	CLA	MG-NA	5.06	2.18	2.06
28	B	830	CLA	MG-NA	5.06	2.18	2.06
28	A	812	CLA	MG-NA	5.05	2.18	2.06
30	1	306	KC1	MG-NA	5.04	2.18	2.06
30	9	306	KC1	MG-NA	5.03	2.18	2.06
28	A	807	CLA	MG-NA	5.01	2.18	2.06
30	5	308	KC1	MG-NA	5.00	2.18	2.06
28	A	833	CLA	MG-NA	4.99	2.18	2.06
28	A	845	CLA	MG-NA	4.98	2.18	2.06
28	B	830	CLA	MG-NC	4.93	2.18	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	A	806	CLA	MG-NC	4.90	2.17	2.06
28	B	848	CLA	MG-NA	4.89	2.17	2.06
28	A	834	CLA	MG-NA	4.89	2.17	2.06
28	A	808	CLA	MG-NC	4.86	2.17	2.06
28	A	824	CLA	MG-NA	4.79	2.17	2.06
30	9	309	KC1	MG-NA	4.76	2.17	2.06
28	B	806	CLA	MG-NC	4.75	2.17	2.06
28	A	827	CLA	MG-NA	4.74	2.17	2.06
28	B	805	CLA	MG-NC	4.72	2.17	2.06
28	B	823	CLA	MG-NA	4.71	2.17	2.06
28	A	823	CLA	MG-NC	4.69	2.17	2.06
28	6	311	CLA	MG-NC	4.69	2.17	2.06
28	B	813	CLA	MG-NA	4.69	2.17	2.06
28	1	310	CLA	MG-NA	4.68	2.17	2.06
28	A	833	CLA	MG-NC	4.68	2.17	2.06
30	4	312	KC1	MG-NA	4.67	2.17	2.06
28	A	825	CLA	MG-NA	4.64	2.17	2.06
28	B	816	CLA	MG-NC	4.61	2.17	2.06
28	A	814	CLA	MG-NA	4.61	2.17	2.06
28	A	808	CLA	MG-NA	4.60	2.17	2.06
28	A	811	CLA	MG-NC	4.60	2.17	2.06
28	B	811	CLA	MG-NC	4.59	2.17	2.06
28	9	310	CLA	MG-NA	4.57	2.17	2.06
30	7	307	KC1	MG-NC	4.57	2.17	2.06
28	B	826	CLA	MG-NA	4.56	2.17	2.06
28	4	306	CLA	C1D-C2D	-4.56	1.36	1.45
28	A	824	CLA	MG-NC	4.56	2.17	2.06
28	A	817	CLA	MG-NA	4.56	2.17	2.06
28	A	801	CLA	MG-NA	4.53	2.17	2.06
28	A	813	CLA	MG-NC	4.52	2.17	2.06
28	A	810	CLA	MG-NA	4.52	2.17	2.06
30	3	309	KC1	MG-NA	4.47	2.16	2.06
28	B	818	CLA	MG-NC	4.46	2.16	2.06
28	7	305	CLA	MG-NC	4.43	2.16	2.06
28	17	302	CLA	MG-NC	4.42	2.16	2.06
28	B	825	CLA	MG-NA	4.41	2.16	2.06
28	B	803	CLA	MG-NC	4.41	2.16	2.06
28	A	802	CLA	MG-NA	4.40	2.16	2.06
28	17	301	CLA	MG-NA	4.39	2.16	2.06
28	3	304	CLA	MG-NC	4.37	2.16	2.06
28	9	304	CLA	MG-NC	4.37	2.16	2.06
28	B	821	CLA	MG-NA	4.36	2.16	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	B	804	CLA	MG-NA	4.36	2.16	2.06
28	A	832	CLA	MG-NA	4.35	2.16	2.06
28	A	805	CLA	MG-NC	4.35	2.16	2.06
28	A	846	CLA	MG-NA	4.34	2.16	2.06
28	B	829	CLA	MG-NA	4.33	2.16	2.06
28	1	308	CLA	MG-NC	4.33	2.16	2.06
28	11	312	CLA	C1D-C2D	-4.31	1.36	1.45
28	L	206	CLA	MG-NA	4.31	2.16	2.06
30	10	311	KC1	MG-NC	4.30	2.16	2.06
28	A	828	CLA	MG-NA	4.29	2.16	2.06
28	A	822	CLA	MG-NC	4.29	2.16	2.06
28	A	827	CLA	MG-NC	4.28	2.16	2.06
28	B	847	CLA	MG-NA	4.27	2.16	2.06
28	6	307	CLA	MG-NA	4.27	2.16	2.06
28	B	847	CLA	MG-NC	4.26	2.16	2.06
28	7	302	CLA	MG-NA	4.26	2.16	2.06
28	6	304	CLA	MG-NA	4.25	2.16	2.06
28	B	833	CLA	MG-NA	4.25	2.16	2.06
28	3	307	CLA	MG-NC	4.24	2.16	2.06
30	4	309	KC1	MG-NC	4.24	2.16	2.06
28	B	832	CLA	MG-NC	4.24	2.16	2.06
28	A	820	CLA	MG-NC	4.24	2.16	2.06
28	F	803	CLA	MG-NC	4.22	2.16	2.06
28	B	834	CLA	MG-NA	4.20	2.16	2.06
30	13	304	KC1	MG-NA	4.20	2.16	2.06
28	B	849	CLA	MG-NC	4.19	2.16	2.06
28	8	301	CLA	MG-NA	4.18	2.16	2.06
28	11	310	CLA	MG-NC	4.18	2.16	2.06
28	3	307	CLA	MG-NA	4.17	2.16	2.06
28	F	802	CLA	MG-NC	4.17	2.16	2.06
28	B	811	CLA	MG-NA	4.16	2.16	2.06
28	5	303	CLA	MG-NC	4.16	2.16	2.06
28	8	303	CLA	MG-NA	4.15	2.16	2.06
28	B	843	CLA	MG-NC	4.14	2.16	2.06
28	A	815	CLA	MG-NA	4.14	2.16	2.06
28	A	845	CLA	MG-NC	4.14	2.16	2.06
28	A	823	CLA	MG-NA	4.12	2.16	2.06
28	1	308	CLA	MG-NA	4.11	2.16	2.06
28	11	309	CLA	MG-NC	4.11	2.16	2.06
28	L	203	CLA	MG-NA	4.10	2.16	2.06
28	B	823	CLA	MG-NC	4.10	2.16	2.06
28	A	830	CLA	MG-NC	4.10	2.16	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	A	836	CLA	MG-NC	4.08	2.16	2.06
28	B	828	CLA	MG-NC	4.08	2.16	2.06
28	B	829	CLA	MG-NC	4.07	2.15	2.06
28	B	845	CLA	MG-NA	4.06	2.15	2.06
28	3	306	CLA	MG-NC	4.06	2.15	2.06
28	J	102	CLA	MG-NA	4.05	2.15	2.06
28	B	831	CLA	MG-NA	4.05	2.15	2.06
28	B	802	CLA	MG-NC	4.05	2.15	2.06
28	A	807	CLA	MG-NC	4.04	2.15	2.06
28	B	849	CLA	MG-NA	4.03	2.15	2.06
28	B	817	CLA	MG-NA	4.03	2.15	2.06
28	13	301	CLA	MG-NC	4.02	2.15	2.06
28	A	810	CLA	MG-NC	4.02	2.15	2.06
28	A	803	CLA	MG-NA	4.01	2.15	2.06
28	6	302	CLA	MG-NC	4.00	2.15	2.06
30	10	310	KC1	MG-NA	3.98	2.15	2.06
28	16	203	CLA	MG-NA	3.97	2.15	2.06
28	A	821	CLA	MG-NC	3.96	2.15	2.06
30	8	307	KC1	MG-NC	3.95	2.15	2.06
28	5	313	CLA	MG-NC	3.94	2.15	2.06
28	B	809	CLA	MG-NA	3.94	2.15	2.06
28	4	306	CLA	MG-NC	3.91	2.15	2.06
30	3	302	KC1	MG-NA	3.88	2.15	2.06
28	B	816	CLA	MG-NA	3.88	2.15	2.06
28	B	827	CLA	MG-NC	3.85	2.15	2.06
28	3	305	CLA	MG-NA	3.84	2.15	2.06
30	5	308	KC1	MG-NC	3.84	2.15	2.06
28	17	305	CLA	MG-NA	3.84	2.15	2.06
28	A	811	CLA	MG-NA	3.84	2.15	2.06
28	8	302	CLA	MG-NA	3.84	2.15	2.06
28	A	819	CLA	MG-NC	3.84	2.15	2.06
30	3	308	KC1	MG-NC	3.83	2.15	2.06
28	B	824	CLA	MG-NA	3.82	2.15	2.06
28	B	801	CLA	MG-NA	3.81	2.15	2.06
30	a	205	KC1	MG-NA	3.80	2.15	2.06
28	5	304	CLA	MG-NA	3.80	2.15	2.06
28	10	309	CLA	MG-NA	3.78	2.15	2.06
28	a	202	CLA	MG-NA	3.78	2.15	2.06
28	5	309	CLA	MG-NA	3.78	2.15	2.06
28	A	829	CLA	MG-NC	3.77	2.15	2.06
28	6	313	CLA	MG-NA	3.77	2.15	2.06
28	A	825	CLA	MG-NC	3.77	2.15	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	4	310	CLA	MG-NC	3.77	2.15	2.06
30	6	308	KC1	C1B-C2B	-3.75	1.37	1.45
28	B	843	CLA	MG-NA	3.75	2.15	2.06
28	5	313	CLA	MG-NA	3.75	2.15	2.06
30	10	304	KC1	MG-NC	3.74	2.15	2.06
28	17	301	CLA	C1D-C2D	-3.74	1.37	1.45
28	B	827	CLA	MG-NA	3.74	2.15	2.06
28	B	818	CLA	MG-NA	3.74	2.15	2.06
30	4	311	KC1	MG-NA	3.74	2.15	2.06
28	7	302	CLA	MG-NC	3.74	2.15	2.06
28	A	819	CLA	MG-NA	3.73	2.15	2.06
28	8	305	CLA	MG-NA	3.73	2.15	2.06
28	7	303	CLA	MG-NC	3.72	2.15	2.06
28	A	849	CLA	MG-NC	3.71	2.15	2.06
28	4	307	CLA	MG-NA	3.70	2.15	2.06
28	B	848	CLA	MG-NC	3.70	2.15	2.06
28	A	853	CLA	C1C-NC	3.70	1.43	1.37
30	11	307	KC1	MG-NC	3.69	2.15	2.06
28	B	814	CLA	MG-NC	3.69	2.15	2.06
28	5	301	CLA	MG-NA	3.68	2.15	2.06
30	17	306	KC1	C4C-NC	3.68	1.43	1.37
28	5	309	CLA	MG-NC	3.67	2.15	2.06
28	17	302	CLA	C1D-C2D	-3.67	1.38	1.45
28	B	825	CLA	MG-NC	3.67	2.15	2.06
28	F	803	CLA	MG-NA	3.67	2.15	2.06
28	3	301	CLA	MG-NA	3.67	2.15	2.06
28	17	301	CLA	MG-NC	3.67	2.15	2.06
28	B	828	CLA	MG-NA	3.66	2.15	2.06
28	11	303	CLA	MG-NA	3.66	2.15	2.06
28	B	832	CLA	MG-NA	3.65	2.14	2.06
28	a	204	CLA	MG-NA	3.64	2.14	2.06
28	17	303	CLA	MG-NA	3.64	2.14	2.06
28	A	830	CLA	MG-NA	3.64	2.14	2.06
30	6	308	KC1	MG-NA	3.63	2.14	2.06
28	7	312	CLA	MG-NA	3.63	2.14	2.06
28	B	820	CLA	MG-NA	3.63	2.14	2.06
28	B	809	CLA	MG-NC	3.62	2.14	2.06
28	A	813	CLA	MG-NA	3.62	2.14	2.06
28	6	303	CLA	MG-NC	3.61	2.14	2.06
28	1	310	CLA	MG-NC	3.61	2.14	2.06
28	A	809	CLA	MG-NA	3.61	2.14	2.06
28	7	306	CLA	MG-NA	3.60	2.14	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	13	302	CLA	MG-NA	3.59	2.14	2.06
28	B	819	CLA	MG-NA	3.59	2.14	2.06
28	10	302	CLA	MG-NA	3.59	2.14	2.06
28	B	806	CLA	MG-NA	3.58	2.14	2.06
28	3	314	CLA	MG-NA	3.58	2.14	2.06
28	11	306	CLA	MG-NC	3.57	2.14	2.06
28	A	816	CLA	MG-NA	3.57	2.14	2.06
28	7	311	CLA	C1D-C2D	-3.57	1.38	1.45
28	7	301	CLA	MG-NA	3.57	2.14	2.06
28	11	305	CLA	MG-NC	3.57	2.14	2.06
28	10	305	CLA	MG-NA	3.56	2.14	2.06
28	B	812	CLA	MG-NC	3.56	2.14	2.06
28	B	808	CLA	C1D-C2D	-3.56	1.38	1.45
28	B	807	CLA	MG-NA	3.56	2.14	2.06
28	A	818	CLA	MG-NA	3.54	2.14	2.06
28	4	304	CLA	MG-NA	3.53	2.14	2.06
28	A	837	CLA	MG-NA	3.52	2.14	2.06
28	L	203	CLA	MG-NC	3.52	2.14	2.06
28	L	204	CLA	MG-NC	3.52	2.14	2.06
28	1	307	CLA	MG-NA	3.51	2.14	2.06
28	A	820	CLA	MG-NA	3.51	2.14	2.06
28	7	318	CLA	MG-NA	3.50	2.14	2.06
28	L	201	CLA	MG-NA	3.50	2.14	2.06
30	17	312	KC1	C1B-C2B	-3.50	1.38	1.45
28	A	806	CLA	MG-NA	3.50	2.14	2.06
28	6	301	CLA	MG-NA	3.50	2.14	2.06
28	A	831	CLA	MG-NC	3.49	2.14	2.06
28	3	303	CLA	C1C-NC	3.49	1.43	1.37
29	3	311	A86	C32-C31	-3.48	1.48	1.54
28	A	826	CLA	MG-NA	3.47	2.14	2.06
28	A	829	CLA	MG-NA	3.46	2.14	2.06
30	8	306	KC1	MG-NC	3.46	2.14	2.06
28	16	203	CLA	C1D-C2D	-3.45	1.38	1.45
28	4	310	CLA	C1C-NC	3.45	1.43	1.37
28	B	833	CLA	MG-NC	3.45	2.14	2.06
30	17	306	KC1	MG-NA	3.45	2.14	2.06
28	5	306	CLA	MG-NA	3.44	2.14	2.06
30	4	311	KC1	C1B-C2B	-3.43	1.38	1.45
28	15	201	CLA	C1D-C2D	-3.43	1.38	1.45
28	B	826	CLA	MG-NC	3.43	2.14	2.06
28	5	303	CLA	MG-NA	3.43	2.14	2.06
28	A	847	CLA	MG-NA	3.43	2.14	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	11	302	CLA	MG-NC	3.42	2.14	2.06
28	B	801	CLA	MG-NC	3.42	2.14	2.06
29	1	302	A86	C32-C31	-3.42	1.48	1.54
28	16	202	CLA	MG-NA	3.41	2.14	2.06
30	9	309	KC1	C4C-NC	3.41	1.43	1.37
28	B	834	CLA	C1C-NC	3.41	1.43	1.37
28	10	308	CLA	MG-NA	3.41	2.14	2.06
28	B	808	CLA	MG-NC	3.41	2.14	2.06
30	9	306	KC1	MG-NC	3.41	2.14	2.06
28	B	830	CLA	C1C-NC	3.40	1.43	1.37
28	7	302	CLA	C1D-C2D	-3.40	1.38	1.45
30	10	310	KC1	C1B-C2B	-3.40	1.38	1.45
28	A	827	CLA	C1D-C2D	-3.40	1.38	1.45
28	A	852	CLA	C1C-NC	3.39	1.43	1.37
30	3	309	KC1	MG-NC	3.39	2.14	2.06
28	A	846	CLA	C1C-NC	3.39	1.43	1.37
28	4	310	CLA	MG-NA	3.39	2.14	2.06
28	6	313	CLA	MG-NC	3.39	2.14	2.06
28	A	805	CLA	C1D-C2D	-3.38	1.38	1.45
28	A	835	CLA	MG-NC	3.38	2.14	2.06
32	13	308	XAT	C26-C27	-3.38	1.44	1.50
28	1	314	CLA	MG-NA	3.38	2.14	2.06
28	13	302	CLA	MG-NC	3.37	2.14	2.06
28	B	815	CLA	MG-NA	3.37	2.14	2.06
28	8	305	CLA	C1C-NC	3.37	1.43	1.37
29	10	317	A86	C32-C31	-3.37	1.48	1.54
28	B	807	CLA	MG-NC	3.37	2.14	2.06
29	3	312	A86	C32-C31	-3.37	1.48	1.54
28	5	313	CLA	C1C-NC	3.36	1.43	1.37
30	3	302	KC1	C1B-C2B	-3.35	1.38	1.45
30	6	309	KC1	MG-NC	3.35	2.14	2.06
28	19	202	CLA	MG-NC	3.35	2.14	2.06
28	8	302	CLA	MG-NC	3.34	2.14	2.06
28	11	312	CLA	MG-NA	3.34	2.14	2.06
28	A	804	CLA	MG-NC	3.33	2.14	2.06
28	13	306	CLA	MG-NC	3.33	2.14	2.06
28	B	812	CLA	C1C-NC	3.33	1.43	1.37
29	5	312	A86	C32-C31	-3.33	1.49	1.54
28	16	202	CLA	MG-NC	3.33	2.14	2.06
28	10	301	CLA	MG-NA	3.33	2.14	2.06
30	3	308	KC1	C1B-C2B	-3.33	1.38	1.45
28	9	307	CLA	MG-NA	3.32	2.14	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	11	305	CLA	MG-NA	3.31	2.14	2.06
28	4	306	CLA	MG-NA	3.30	2.14	2.06
30	6	310	KC1	C1B-C2B	-3.29	1.38	1.45
28	6	307	CLA	C1C-NC	3.29	1.43	1.37
28	A	817	CLA	MG-NC	3.29	2.14	2.06
28	A	828	CLA	C1D-C2D	-3.29	1.38	1.45
30	4	309	KC1	C1B-C2B	-3.29	1.38	1.45
28	B	829	CLA	C1C-NC	3.28	1.43	1.37
28	A	835	CLA	C1D-C2D	-3.28	1.38	1.45
28	A	821	CLA	C1C-NC	3.28	1.43	1.37
28	B	808	CLA	MG-NA	3.27	2.14	2.06
28	B	819	CLA	C1C-NC	3.27	1.43	1.37
28	10	316	CLA	C1C-NC	3.27	1.43	1.37
28	3	304	CLA	C1C-NC	3.27	1.43	1.37
28	L	204	CLA	MG-NA	3.27	2.14	2.06
28	16	203	CLA	C1C-NC	3.26	1.43	1.37
30	6	305	KC1	C1B-C2B	-3.26	1.38	1.45
28	A	831	CLA	MG-NA	3.26	2.14	2.06
28	A	849	CLA	MG-NA	3.26	2.14	2.06
28	1	307	CLA	C1C-NC	3.25	1.43	1.37
28	13	305	CLA	MG-NA	3.25	2.14	2.06
28	3	307	CLA	C1D-C2D	-3.25	1.38	1.45
28	7	304	CLA	MG-NC	3.25	2.14	2.06
28	B	831	CLA	MG-NC	3.25	2.14	2.06
28	A	814	CLA	MG-NC	3.24	2.14	2.06
30	3	309	KC1	C4C-NC	3.24	1.43	1.37
30	17	306	KC1	MG-NC	3.24	2.14	2.06
30	3	302	KC1	MG-NC	3.24	2.14	2.06
28	B	822	CLA	MG-NA	3.24	2.14	2.06
28	11	310	CLA	MG-NA	3.24	2.14	2.06
29	10	312	A86	C32-C31	-3.24	1.49	1.54
28	F	802	CLA	C1D-C2D	-3.23	1.38	1.45
28	B	821	CLA	MG-NC	3.23	2.14	2.06
28	8	304	CLA	MG-NA	3.23	2.13	2.06
28	B	835	CLA	C1C-NC	3.23	1.43	1.37
28	R	204	CLA	MG-NA	3.23	2.13	2.06
28	9	303	CLA	MG-NA	3.23	2.13	2.06
28	A	823	CLA	C1C-NC	3.22	1.43	1.37
28	B	815	CLA	C1C-NC	3.22	1.43	1.37
28	B	821	CLA	C1C-NC	3.22	1.43	1.37
28	10	306	CLA	MG-NA	3.22	2.13	2.06
28	A	802	CLA	C1C-NC	3.22	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	3	313	XAT	C26-C27	-3.22	1.45	1.50
29	11	308	A86	C32-C31	-3.21	1.49	1.54
28	A	812	CLA	MG-NC	3.21	2.13	2.06
30	6	308	KC1	C4C-NC	3.21	1.43	1.37
30	6	305	KC1	MG-NC	3.21	2.13	2.06
28	A	831	CLA	C1C-NC	3.21	1.43	1.37
30	4	309	KC1	C4C-NC	3.21	1.43	1.37
28	A	815	CLA	MG-NC	3.21	2.13	2.06
28	6	301	CLA	MG-NC	3.20	2.13	2.06
28	A	828	CLA	MG-NC	3.20	2.13	2.06
28	5	302	CLA	MG-NA	3.20	2.13	2.06
28	A	834	CLA	MG-NC	3.19	2.13	2.06
28	B	845	CLA	C1C-NC	3.19	1.43	1.37
28	B	812	CLA	C1D-C2D	-3.19	1.39	1.45
28	9	311	CLA	C1C-NC	3.19	1.43	1.37
30	10	310	KC1	C4C-NC	3.18	1.43	1.37
28	19	202	CLA	C1C-NC	3.18	1.43	1.37
28	6	302	CLA	MG-NA	3.18	2.13	2.06
28	A	804	CLA	MG-NA	3.18	2.13	2.06
30	4	312	KC1	MG-NC	3.18	2.13	2.06
29	9	312	A86	C32-C31	-3.18	1.49	1.54
30	17	306	KC1	C1B-C2B	-3.18	1.39	1.45
28	B	834	CLA	MG-NC	3.18	2.13	2.06
28	B	835	CLA	MG-NC	3.18	2.13	2.06
30	7	307	KC1	C1B-C2B	-3.17	1.39	1.45
28	8	303	CLA	C1C-NC	3.17	1.43	1.37
28	a	202	CLA	MG-NC	3.17	2.13	2.06
28	7	306	CLA	MG-NC	3.17	2.13	2.06
28	A	821	CLA	MG-NA	3.17	2.13	2.06
28	B	813	CLA	MG-NC	3.17	2.13	2.06
28	B	835	CLA	MG-NA	3.16	2.13	2.06
28	10	307	CLA	MG-NA	3.16	2.13	2.06
28	6	306	CLA	MG-NC	3.15	2.13	2.06
28	16	202	CLA	C1C-NC	3.15	1.43	1.37
28	J	103	CLA	MG-NA	3.15	2.13	2.06
28	B	819	CLA	MG-NC	3.15	2.13	2.06
28	R	202	CLA	MG-NA	3.14	2.13	2.06
28	A	836	CLA	MG-NA	3.14	2.13	2.06
28	A	837	CLA	MG-NC	3.14	2.13	2.06
28	a	202	CLA	C1D-C2D	-3.14	1.39	1.45
28	B	825	CLA	C1C-NC	3.14	1.43	1.37
28	R	202	CLA	MG-NC	3.14	2.13	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	A	853	CLA	MG-NC	3.14	2.13	2.06
28	15	201	CLA	C1C-NC	3.13	1.42	1.37
28	10	308	CLA	C1D-C2D	-3.13	1.39	1.45
28	A	853	CLA	C1D-C2D	-3.13	1.39	1.45
28	16	201	CLA	C1C-NC	3.13	1.42	1.37
28	1	307	CLA	MG-NC	3.13	2.13	2.06
30	9	309	KC1	MG-NC	3.12	2.13	2.06
28	17	309	CLA	C1C-NC	3.12	1.42	1.37
28	17	307	CLA	MG-NC	3.12	2.13	2.06
32	13	309	XAT	C6-C7	-3.12	1.45	1.50
30	6	305	KC1	C4C-NC	3.12	1.42	1.37
28	9	311	CLA	MG-NC	3.12	2.13	2.06
28	B	845	CLA	MG-NC	3.12	2.13	2.06
30	9	306	KC1	C1B-C2B	-3.12	1.39	1.45
28	11	304	CLA	MG-NC	3.12	2.13	2.06
28	8	303	CLA	MG-NC	3.11	2.13	2.06
30	4	312	KC1	C1B-C2B	-3.11	1.39	1.45
30	7	309	KC1	C1B-C2B	-3.10	1.39	1.45
28	B	848	CLA	C1C-NC	3.09	1.42	1.37
28	B	805	CLA	MG-NA	3.09	2.13	2.06
28	A	820	CLA	C1C-NC	3.09	1.42	1.37
28	13	301	CLA	C1D-C2D	-3.09	1.39	1.45
28	11	314	CLA	MG-NA	3.09	2.13	2.06
28	10	316	CLA	MG-NA	3.08	2.13	2.06
28	3	314	CLA	C1C-NC	3.08	1.42	1.37
28	A	809	CLA	MG-NC	3.08	2.13	2.06
28	5	302	CLA	MG-NC	3.08	2.13	2.06
28	7	302	CLA	C1C-NC	3.08	1.42	1.37
28	A	826	CLA	C1C-NC	3.07	1.42	1.37
28	1	314	CLA	MG-NC	3.07	2.13	2.06
30	13	304	KC1	C1B-C2B	-3.07	1.39	1.45
28	B	810	CLA	MG-NC	3.07	2.13	2.06
28	4	303	CLA	C1C-NC	3.06	1.42	1.37
30	8	307	KC1	C1B-C2B	-3.06	1.39	1.45
28	B	810	CLA	MG-NA	3.06	2.13	2.06
28	F	803	CLA	C1C-NC	3.06	1.42	1.37
28	B	810	CLA	C1C-NC	3.06	1.42	1.37
28	A	811	CLA	C1D-C2D	-3.06	1.39	1.45
28	9	310	CLA	MG-NC	3.06	2.13	2.06
28	B	805	CLA	C1D-C2D	-3.05	1.39	1.45
30	1	306	KC1	MG-NC	3.05	2.13	2.06
28	B	818	CLA	C1C-NC	3.05	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	8	304	CLA	MG-NC	3.05	2.13	2.06
28	A	807	CLA	C1C-NC	3.05	1.42	1.37
30	a	205	KC1	MG-NC	3.05	2.13	2.06
30	4	311	KC1	C4C-NC	3.05	1.42	1.37
28	6	303	CLA	MG-NA	3.05	2.13	2.06
30	a	205	KC1	C1B-C2B	-3.05	1.39	1.45
30	3	309	KC1	C1B-C2B	-3.04	1.39	1.45
30	11	307	KC1	C1B-C2B	-3.04	1.39	1.45
29	8	308	A86	C32-C31	-3.03	1.49	1.54
28	B	820	CLA	C1C-NC	3.03	1.42	1.37
28	B	843	CLA	C1D-C2D	-3.03	1.39	1.45
28	L	201	CLA	C1C-NC	3.03	1.42	1.37
28	10	316	CLA	C1D-C2D	-3.03	1.39	1.45
30	4	308	KC1	C1B-C2B	-3.02	1.39	1.45
28	7	308	CLA	MG-NA	3.02	2.13	2.06
28	A	811	CLA	C1C-NC	3.02	1.42	1.37
28	L	203	CLA	C1C-NC	3.02	1.42	1.37
28	L	206	CLA	C1D-C2D	-3.01	1.39	1.45
28	13	306	CLA	MG-NA	3.01	2.13	2.06
28	A	814	CLA	C1C-NC	3.01	1.42	1.37
28	5	305	CLA	MG-NA	3.01	2.13	2.06
28	B	816	CLA	C1C-NC	3.00	1.42	1.37
28	11	309	CLA	C1D-C2D	-3.00	1.39	1.45
28	B	809	CLA	C1C-NC	3.00	1.42	1.37
32	10	313	XAT	C26-C27	-2.99	1.45	1.50
28	9	304	CLA	MG-NA	2.99	2.13	2.06
28	A	812	CLA	C1C-NC	2.99	1.42	1.37
28	a	204	CLA	MG-NC	2.99	2.13	2.06
28	A	852	CLA	C1D-C2D	-2.99	1.39	1.45
28	3	314	CLA	MG-NC	2.99	2.13	2.06
28	13	303	CLA	MG-NA	2.99	2.13	2.06
28	11	304	CLA	MG-NA	2.99	2.13	2.06
28	B	822	CLA	MG-NC	2.98	2.13	2.06
28	B	822	CLA	C1C-NC	2.98	1.42	1.37
28	1	304	CLA	MG-NC	2.98	2.13	2.06
28	B	832	CLA	C1C-NC	2.98	1.42	1.37
28	B	803	CLA	MG-NA	2.98	2.13	2.06
28	3	301	CLA	MG-NC	2.97	2.13	2.06
28	8	313	CLA	C1D-C2D	-2.97	1.39	1.45
28	B	817	CLA	MG-NC	2.97	2.13	2.06
28	7	304	CLA	MG-NA	2.97	2.13	2.06
28	6	306	CLA	MG-NA	2.97	2.13	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	A	815	CLA	C1C-NC	2.97	1.42	1.37
30	1	306	KC1	C1B-C2B	-2.96	1.39	1.45
28	6	304	CLA	C1D-C2D	-2.96	1.39	1.45
28	A	809	CLA	C1D-C2D	-2.96	1.39	1.45
28	J	103	CLA	MG-NC	2.96	2.13	2.06
28	A	830	CLA	C1C-NC	2.96	1.42	1.37
28	B	843	CLA	C1C-NC	2.95	1.42	1.37
28	19	201	CLA	C1D-C2D	-2.95	1.39	1.45
28	4	307	CLA	MG-NC	2.94	2.13	2.06
30	6	309	KC1	C1B-C2B	-2.94	1.39	1.45
28	B	828	CLA	C1C-NC	2.94	1.42	1.37
28	A	847	CLA	MG-NC	2.93	2.13	2.06
28	7	304	CLA	C1C-NC	2.93	1.42	1.37
28	16	204	CLA	MG-NC	2.93	2.13	2.06
28	8	305	CLA	MG-NC	2.93	2.13	2.06
28	16	205	CLA	C1C-NC	2.93	1.42	1.37
28	A	817	CLA	C1C-NC	2.93	1.42	1.37
28	3	305	CLA	C1C-NC	2.93	1.42	1.37
28	B	827	CLA	C1C-NC	2.92	1.42	1.37
30	7	309	KC1	C4C-NC	2.92	1.42	1.37
28	7	308	CLA	C1D-C2D	-2.92	1.39	1.45
32	13	308	XAT	C6-C7	-2.92	1.45	1.50
28	B	806	CLA	C1C-NC	2.92	1.42	1.37
28	7	312	CLA	C1D-C2D	-2.92	1.39	1.45
28	A	822	CLA	MG-NA	2.92	2.13	2.06
32	7	314	XAT	C26-C27	-2.92	1.45	1.50
32	13	309	XAT	C26-C27	-2.92	1.45	1.50
28	A	845	CLA	C1D-C2D	-2.91	1.39	1.45
29	J	101	A86	C32-C31	-2.91	1.49	1.54
28	3	306	CLA	C1C-NC	2.91	1.42	1.37
28	6	302	CLA	C1D-C2D	-2.91	1.39	1.45
32	8	311	XAT	C26-C27	-2.91	1.45	1.50
28	B	829	CLA	C1D-C2D	-2.91	1.39	1.45
28	A	813	CLA	C1D-C2D	-2.90	1.39	1.45
28	B	834	CLA	C1D-C2D	-2.90	1.39	1.45
28	13	301	CLA	MG-NA	2.90	2.13	2.06
28	1	310	CLA	C1C-NC	2.90	1.42	1.37
32	6	316	XAT	C6-C7	-2.90	1.45	1.50
28	A	830	CLA	C1D-C2D	-2.90	1.39	1.45
28	B	818	CLA	C1D-C2D	-2.90	1.39	1.45
28	B	807	CLA	C1C-NC	2.90	1.42	1.37
28	17	305	CLA	MG-NC	2.90	2.13	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	6	302	CLA	C1C-NC	2.90	1.42	1.37
28	10	307	CLA	C1C-NC	2.90	1.42	1.37
28	8	310	CLA	MG-NC	2.89	2.13	2.06
28	11	310	CLA	C1C-NC	2.89	1.42	1.37
28	1	305	CLA	MG-NA	2.89	2.13	2.06
28	B	802	CLA	C1D-C2D	-2.88	1.39	1.45
28	F	802	CLA	C1C-NC	2.88	1.42	1.37
30	6	310	KC1	MG-NC	2.88	2.13	2.06
28	10	305	CLA	C1C-NC	2.88	1.42	1.37
30	7	309	KC1	MG-NC	2.87	2.13	2.06
28	B	849	CLA	C1C-NC	2.87	1.42	1.37
28	A	816	CLA	C1C-NC	2.87	1.42	1.37
28	1	307	CLA	C1D-C2D	-2.86	1.39	1.45
28	17	303	CLA	C1D-C2D	-2.86	1.39	1.45
28	7	308	CLA	C1C-NC	2.86	1.42	1.37
28	A	821	CLA	C1D-C2D	-2.86	1.39	1.45
28	5	305	CLA	C1C-NC	2.86	1.42	1.37
28	4	304	CLA	MG-NC	2.86	2.13	2.06
28	17	307	CLA	MG-NA	2.86	2.13	2.06
28	5	309	CLA	C1D-C2D	-2.85	1.39	1.45
28	A	813	CLA	C1C-NC	2.85	1.42	1.37
28	B	811	CLA	C1C-NC	2.85	1.42	1.37
30	1	306	KC1	C4C-NC	2.85	1.42	1.37
32	5	310	XAT	C6-C7	-2.85	1.45	1.50
28	B	827	CLA	C1D-C2D	-2.85	1.39	1.45
30	8	306	KC1	C1B-C2B	-2.85	1.39	1.45
28	11	302	CLA	MG-NA	2.84	2.13	2.06
30	a	205	KC1	C4C-NC	2.84	1.42	1.37
28	11	301	CLA	C1D-C2D	-2.84	1.39	1.45
28	7	318	CLA	MG-NC	2.84	2.13	2.06
28	1	301	CLA	C1D-C2D	-2.84	1.39	1.45
28	10	305	CLA	C1D-C2D	-2.84	1.39	1.45
32	11	313	XAT	C26-C27	-2.84	1.45	1.50
30	9	309	KC1	C1B-C2B	-2.84	1.39	1.45
28	15	201	CLA	MG-NA	2.84	2.13	2.06
28	A	808	CLA	C1C-NC	2.83	1.42	1.37
28	B	845	CLA	C1D-C2D	-2.83	1.39	1.45
28	3	306	CLA	MG-NA	2.83	2.13	2.06
28	5	303	CLA	C1C-NC	2.83	1.42	1.37
28	R	202	CLA	C1C-NC	2.83	1.42	1.37
28	10	306	CLA	C1C-NC	2.83	1.42	1.37
28	5	304	CLA	C1D-C2D	-2.82	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	10	313	XAT	C6-C7	-2.82	1.45	1.50
28	A	816	CLA	MG-NC	2.82	2.13	2.06
28	5	303	CLA	C1D-C2D	-2.82	1.39	1.45
28	A	806	CLA	C1D-C2D	-2.82	1.39	1.45
28	B	810	CLA	C1D-C2D	-2.82	1.39	1.45
28	A	822	CLA	C1C-NC	2.81	1.42	1.37
28	A	815	CLA	C1D-C2D	-2.81	1.39	1.45
28	5	306	CLA	C1C-NC	2.80	1.42	1.37
28	a	203	CLA	MG-NA	2.80	2.12	2.06
28	A	805	CLA	C1C-NC	2.80	1.42	1.37
30	5	308	KC1	C1B-C2B	-2.80	1.39	1.45
28	B	820	CLA	MG-NC	2.79	2.12	2.06
28	A	814	CLA	C1D-C2D	-2.79	1.39	1.45
30	8	306	KC1	C4C-NC	2.79	1.42	1.37
28	10	306	CLA	C1D-C2D	-2.79	1.39	1.45
28	A	804	CLA	C1D-C2D	-2.79	1.39	1.45
28	10	302	CLA	MG-NC	2.79	2.12	2.06
28	A	822	CLA	C1D-C2D	-2.79	1.39	1.45
28	19	202	CLA	MG-NA	2.78	2.12	2.06
28	B	807	CLA	C1D-C2D	-2.78	1.39	1.45
28	A	820	CLA	C1D-C2D	-2.78	1.39	1.45
28	1	301	CLA	MG-NA	2.78	2.12	2.06
28	5	304	CLA	C1C-NC	2.78	1.42	1.37
28	A	829	CLA	C1D-C2D	-2.78	1.39	1.45
28	9	305	CLA	C1D-C2D	-2.77	1.39	1.45
28	5	302	CLA	C1D-C2D	-2.77	1.39	1.45
28	11	301	CLA	MG-NA	2.77	2.12	2.06
28	16	203	CLA	MG-NC	2.77	2.12	2.06
28	10	309	CLA	C1D-C2D	-2.77	1.39	1.45
30	17	312	KC1	C4C-NC	2.77	1.42	1.37
28	5	301	CLA	C1D-C2D	-2.77	1.39	1.45
28	A	801	CLA	C1D-C2D	-2.77	1.39	1.45
28	6	313	CLA	C1D-C2D	-2.77	1.39	1.45
28	3	314	CLA	C1D-C2D	-2.76	1.39	1.45
28	B	816	CLA	C1D-C2D	-2.76	1.39	1.45
28	3	301	CLA	C1C-NC	2.76	1.42	1.37
28	3	301	CLA	C1D-C2D	-2.76	1.39	1.45
32	10	314	XAT	C6-C7	-2.76	1.45	1.50
28	J	102	CLA	MG-NC	2.76	2.12	2.06
28	A	833	CLA	C1D-C2D	-2.75	1.39	1.45
28	A	824	CLA	C1D-C2D	-2.75	1.39	1.45
32	9	313	XAT	C26-C27	-2.75	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	7	316	XAT	C26-C27	-2.75	1.45	1.50
28	A	852	CLA	MG-NC	2.75	2.12	2.06
30	13	304	KC1	C4C-NC	2.74	1.42	1.37
28	3	305	CLA	MG-NC	2.74	2.12	2.06
28	7	304	CLA	C1D-C2D	-2.74	1.39	1.45
32	3	313	XAT	C6-C7	-2.74	1.45	1.50
30	10	311	KC1	C1B-C2B	-2.74	1.39	1.45
28	B	802	CLA	C1C-NC	2.73	1.42	1.37
28	B	830	CLA	C1D-C2D	-2.73	1.39	1.45
28	6	311	CLA	MG-NA	2.72	2.12	2.06
28	A	808	CLA	C1D-C2D	-2.72	1.40	1.45
28	7	301	CLA	MG-NC	2.72	2.12	2.06
28	5	306	CLA	C1D-C2D	-2.72	1.40	1.45
28	L	201	CLA	MG-NC	2.72	2.12	2.06
28	3	306	CLA	C1D-C2D	-2.72	1.40	1.45
28	1	305	CLA	C1C-NC	2.71	1.42	1.37
28	A	803	CLA	C1C-NC	2.71	1.42	1.37
28	A	818	CLA	MG-NC	2.71	2.12	2.06
28	A	837	CLA	C1D-C2D	-2.71	1.40	1.45
28	A	824	CLA	C1C-NC	2.71	1.42	1.37
28	9	305	CLA	C1C-NC	2.71	1.42	1.37
28	B	848	CLA	C1D-C2D	-2.71	1.40	1.45
32	7	316	XAT	C6-C7	-2.71	1.46	1.50
28	7	305	CLA	C1D-C2D	-2.70	1.40	1.45
28	A	846	CLA	C1D-C2D	-2.70	1.40	1.45
28	B	806	CLA	C1D-C2D	-2.70	1.40	1.45
28	A	845	CLA	C1C-NC	2.70	1.42	1.37
28	11	314	CLA	C1D-C2D	-2.70	1.40	1.45
28	17	305	CLA	C1D-C2D	-2.70	1.40	1.45
28	1	308	CLA	C1D-C2D	-2.69	1.40	1.45
29	4	314	A86	C32-C31	-2.69	1.50	1.54
28	4	306	CLA	C1C-NC	2.69	1.42	1.37
28	J	103	CLA	C1C-NC	2.69	1.42	1.37
28	10	303	CLA	MG-NA	2.69	2.12	2.06
28	11	310	CLA	C1D-C2D	-2.68	1.40	1.45
28	B	825	CLA	C1D-C2D	-2.68	1.40	1.45
32	10	315	XAT	C6-C7	-2.68	1.46	1.50
28	A	832	CLA	C1C-NC	2.68	1.42	1.37
28	8	301	CLA	C1D-C2D	-2.68	1.40	1.45
28	R	202	CLA	C1D-C2D	-2.68	1.40	1.45
28	10	302	CLA	C1C-NC	2.68	1.42	1.37
28	11	302	CLA	C1C-NC	2.67	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	10	304	KC1	C1B-C2B	-2.67	1.40	1.45
28	17	304	CLA	C1D-C2D	-2.66	1.40	1.45
28	7	301	CLA	C1D-C2D	-2.66	1.40	1.45
28	16	205	CLA	MG-NC	2.66	2.12	2.06
28	17	304	CLA	MG-NA	2.66	2.12	2.06
28	11	303	CLA	C1D-C2D	-2.66	1.40	1.45
28	11	302	CLA	C1D-C2D	-2.66	1.40	1.45
28	5	302	CLA	C1C-NC	2.66	1.42	1.37
29	R	201	A86	C32-C31	-2.66	1.50	1.54
32	8	312	XAT	C6-C7	-2.65	1.46	1.50
28	7	303	CLA	MG-NA	2.65	2.12	2.06
32	1	311	XAT	C6-C7	-2.65	1.46	1.50
28	A	828	CLA	C1C-NC	2.65	1.42	1.37
28	A	832	CLA	C1D-C2D	-2.65	1.40	1.45
28	A	826	CLA	MG-NC	2.65	2.12	2.06
28	B	817	CLA	C1C-NC	2.65	1.42	1.37
28	B	833	CLA	C1C-NC	2.65	1.42	1.37
28	5	305	CLA	MG-NC	2.65	2.12	2.06
28	11	309	CLA	MG-NA	2.64	2.12	2.06
28	F	803	CLA	C1D-C2D	-2.64	1.40	1.45
28	A	831	CLA	C1D-C2D	-2.64	1.40	1.45
28	10	302	CLA	C1D-C2D	-2.63	1.40	1.45
28	A	825	CLA	C1C-NC	2.63	1.42	1.37
29	R	203	A86	C32-C31	-2.63	1.50	1.54
28	a	201	CLA	C1D-C2D	-2.63	1.40	1.45
28	1	304	CLA	MG-NA	2.63	2.12	2.06
28	8	313	CLA	C1C-NC	2.63	1.42	1.37
28	4	305	CLA	C1C-NC	2.63	1.42	1.37
28	17	307	CLA	C1D-C2D	-2.63	1.40	1.45
28	5	309	CLA	C1C-NC	2.62	1.42	1.37
28	10	306	CLA	MG-NC	2.62	2.12	2.06
32	5	316	XAT	C6-C7	-2.62	1.46	1.50
32	5	311	XAT	C6-C7	-2.62	1.46	1.50
28	7	306	CLA	C1D-C2D	-2.62	1.40	1.45
28	10	309	CLA	MG-NC	2.62	2.12	2.06
28	8	302	CLA	C1C-NC	2.62	1.42	1.37
30	6	310	KC1	C4C-NC	2.62	1.42	1.37
28	10	308	CLA	C1C-NC	2.62	1.42	1.37
28	A	807	CLA	C1D-C2D	-2.62	1.40	1.45
28	17	302	CLA	C1C-NC	2.61	1.42	1.37
28	8	305	CLA	C1D-C2D	-2.61	1.40	1.45
28	11	304	CLA	C1D-C2D	-2.61	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	9	313	XAT	C6-C5	2.61	1.50	1.47
28	5	301	CLA	C1C-NC	2.61	1.42	1.37
28	J	102	CLA	C1D-C2D	-2.61	1.40	1.45
28	A	834	CLA	C1C-NC	2.61	1.42	1.37
28	B	833	CLA	C1D-C2D	-2.60	1.40	1.45
28	B	831	CLA	C1C-NC	2.60	1.42	1.37
30	10	310	KC1	MG-NC	2.60	2.12	2.06
28	10	303	CLA	MG-NC	2.60	2.12	2.06
28	B	803	CLA	C1D-C2D	-2.59	1.40	1.45
32	8	311	XAT	C6-C7	-2.59	1.46	1.50
32	8	312	XAT	C26-C27	-2.59	1.46	1.50
32	7	314	XAT	C6-C7	-2.59	1.46	1.50
28	L	203	CLA	C1D-C2D	-2.59	1.40	1.45
29	4	313	A86	C32-C31	-2.58	1.50	1.54
28	B	823	CLA	C1C-NC	2.58	1.42	1.37
28	19	202	CLA	C1D-C2D	-2.58	1.40	1.45
28	A	829	CLA	C1C-NC	2.58	1.42	1.37
32	17	311	XAT	C6-C7	-2.58	1.46	1.50
28	A	818	CLA	C1C-NC	2.58	1.42	1.37
28	7	305	CLA	MG-NA	2.58	2.12	2.06
28	4	310	CLA	C1D-C2D	-2.58	1.40	1.45
28	R	204	CLA	MG-NC	2.57	2.12	2.06
28	B	803	CLA	C1C-NC	2.57	1.42	1.37
28	8	310	CLA	C1D-C2D	-2.57	1.40	1.45
28	A	802	CLA	MG-NC	2.57	2.12	2.06
28	5	305	CLA	C1D-C2D	-2.57	1.40	1.45
28	A	836	CLA	C1D-C2D	-2.57	1.40	1.45
28	9	311	CLA	MG-NA	2.57	2.12	2.06
28	J	103	CLA	C1D-C2D	-2.56	1.40	1.45
28	A	827	CLA	C1C-NC	2.56	1.42	1.37
32	5	311	XAT	C26-C27	-2.56	1.46	1.50
28	B	828	CLA	C1D-C2D	-2.56	1.40	1.45
28	11	306	CLA	MG-NA	2.56	2.12	2.06
28	a	201	CLA	MG-NA	2.56	2.12	2.06
30	3	302	KC1	C4C-NC	2.56	1.42	1.37
28	A	802	CLA	C1D-C2D	-2.56	1.40	1.45
28	A	817	CLA	C1D-C2D	-2.56	1.40	1.45
30	6	308	KC1	MG-NC	2.56	2.12	2.06
28	13	302	CLA	C1C-NC	2.56	1.42	1.37
28	1	303	CLA	C1C-NC	2.56	1.42	1.37
28	8	313	CLA	MG-NC	2.55	2.12	2.06
28	11	314	CLA	C1C-NC	2.55	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	9	310	CLA	C1C-NC	2.55	1.42	1.37
28	15	201	CLA	MG-NC	2.55	2.12	2.06
28	16	204	CLA	C1D-C2D	-2.55	1.40	1.45
28	13	305	CLA	C1D-C2D	-2.55	1.40	1.45
28	5	313	CLA	C1D-C2D	-2.55	1.40	1.45
28	8	303	CLA	C1D-C2D	-2.55	1.40	1.45
28	9	305	CLA	MG-NA	2.55	2.12	2.06
28	10	308	CLA	MG-NC	2.54	2.12	2.06
28	7	318	CLA	C1D-C2D	-2.54	1.40	1.45
28	9	311	CLA	C1D-C2D	-2.54	1.40	1.45
28	B	823	CLA	C1D-C2D	-2.54	1.40	1.45
28	1	314	CLA	C1D-C2D	-2.54	1.40	1.45
28	9	307	CLA	C1D-C2D	-2.53	1.40	1.45
28	A	826	CLA	C1D-C2D	-2.53	1.40	1.45
32	7	313	XAT	C6-C7	-2.53	1.46	1.50
30	11	307	KC1	C4C-NC	2.53	1.42	1.37
28	4	304	CLA	C1D-C2D	-2.53	1.40	1.45
28	3	304	CLA	C1D-C2D	-2.53	1.40	1.45
28	11	306	CLA	C1D-C2D	-2.53	1.40	1.45
32	10	314	XAT	C26-C27	-2.53	1.46	1.50
28	1	310	CLA	C1D-C2D	-2.53	1.40	1.45
28	4	303	CLA	C1D-C2D	-2.53	1.40	1.45
28	10	307	CLA	C1D-C2D	-2.52	1.40	1.45
28	A	837	CLA	C1C-NC	2.52	1.42	1.37
28	11	301	CLA	C1C-NC	2.52	1.42	1.37
28	B	821	CLA	C1D-C2D	-2.52	1.40	1.45
28	4	307	CLA	C1D-C2D	-2.52	1.40	1.45
28	A	823	CLA	C1D-C2D	-2.51	1.40	1.45
32	6	316	XAT	C26-C27	-2.51	1.46	1.50
28	7	318	CLA	C1C-NC	2.51	1.42	1.37
28	17	309	CLA	C1D-C2D	-2.51	1.40	1.45
28	B	809	CLA	C1D-C2D	-2.51	1.40	1.45
28	B	826	CLA	C1D-C2D	-2.51	1.40	1.45
28	6	303	CLA	C1D-C2D	-2.50	1.40	1.45
28	11	303	CLA	MG-NC	2.50	2.12	2.06
28	3	303	CLA	MG-NA	2.50	2.12	2.06
28	B	813	CLA	C1C-NC	2.49	1.41	1.37
28	13	302	CLA	C1D-C2D	-2.49	1.40	1.45
29	6	314	A86	C32-C31	-2.49	1.50	1.54
28	B	808	CLA	C1C-NC	2.49	1.41	1.37
28	A	819	CLA	C1C-NC	2.48	1.41	1.37
28	B	817	CLA	C1D-C2D	-2.48	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	6	301	CLA	C1D-C2D	-2.48	1.40	1.45
28	11	312	CLA	MG-NC	2.48	2.12	2.06
28	B	822	CLA	C1D-C2D	-2.48	1.40	1.45
28	a	203	CLA	C1C-NC	2.48	1.41	1.37
28	10	301	CLA	C1D-C2D	-2.48	1.40	1.45
28	B	835	CLA	C1D-C2D	-2.47	1.40	1.45
28	7	301	CLA	C1C-NC	2.47	1.41	1.37
32	6	312	XAT	C26-C27	-2.47	1.46	1.50
28	10	309	CLA	C1C-NC	2.47	1.41	1.37
28	8	302	CLA	C1D-C2D	-2.46	1.40	1.45
28	11	305	CLA	C1D-C2D	-2.46	1.40	1.45
28	4	303	CLA	MG-NA	2.46	2.12	2.06
28	10	316	CLA	MG-NC	2.46	2.12	2.06
29	3	310	A86	C32-C31	-2.46	1.50	1.54
32	4	315	XAT	C26-C27	-2.46	1.46	1.50
28	B	824	CLA	C1D-C2D	-2.46	1.40	1.45
28	B	814	CLA	C1C-NC	2.45	1.41	1.37
28	B	815	CLA	C1D-C2D	-2.45	1.40	1.45
28	11	314	CLA	MG-NC	2.45	2.12	2.06
28	B	849	CLA	C1D-C2D	-2.44	1.40	1.45
28	6	307	CLA	C1D-C2D	-2.44	1.40	1.45
30	4	308	KC1	C4C-NC	2.44	1.41	1.37
28	4	305	CLA	C1D-C2D	-2.44	1.40	1.45
28	9	308	CLA	C1D-C2D	-2.43	1.40	1.45
28	9	310	CLA	C1D-C2D	-2.43	1.40	1.45
28	B	847	CLA	C1D-C2D	-2.43	1.40	1.45
28	9	305	CLA	MG-NC	2.42	2.12	2.06
28	6	304	CLA	C1C-NC	2.42	1.41	1.37
28	B	832	CLA	C1D-C2D	-2.42	1.40	1.45
28	3	304	CLA	MG-NA	2.42	2.12	2.06
28	A	810	CLA	C1D-C2D	-2.42	1.40	1.45
32	5	316	XAT	C26-C27	-2.41	1.46	1.50
28	7	308	CLA	MG-NC	2.41	2.12	2.06
28	9	304	CLA	C1D-C2D	-2.41	1.40	1.45
28	16	201	CLA	C1D-C2D	-2.41	1.40	1.45
30	6	309	KC1	C4C-NC	2.41	1.41	1.37
28	6	306	CLA	C1D-C2D	-2.40	1.40	1.45
28	L	204	CLA	C1C-NC	2.40	1.41	1.37
28	10	301	CLA	C1C-NC	2.40	1.41	1.37
28	9	303	CLA	C1D-C2D	-2.40	1.40	1.45
28	A	834	CLA	C1D-C2D	-2.40	1.40	1.45
28	B	805	CLA	C1C-NC	2.39	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	8	307	KC1	C4C-NC	2.39	1.41	1.37
28	6	301	CLA	C1C-NC	2.39	1.41	1.37
28	8	301	CLA	C1C-NC	2.38	1.41	1.37
28	8	304	CLA	C1D-C2D	-2.38	1.40	1.45
28	1	314	CLA	C1C-NC	2.38	1.41	1.37
28	16	205	CLA	C1D-C2D	-2.38	1.40	1.45
28	9	304	CLA	C1C-NC	2.38	1.41	1.37
28	B	819	CLA	C1D-C2D	-2.38	1.40	1.45
28	B	813	CLA	C1D-C2D	-2.38	1.40	1.45
28	A	825	CLA	C1D-C2D	-2.38	1.40	1.45
28	13	303	CLA	C1D-C2D	-2.37	1.40	1.45
32	1	311	XAT	C26-C27	-2.37	1.46	1.50
28	B	814	CLA	C1D-C2D	-2.37	1.40	1.45
28	16	202	CLA	C1D-C2D	-2.36	1.40	1.45
29	17	308	A86	C32-C31	-2.36	1.50	1.54
28	B	801	CLA	C1D-C2D	-2.36	1.40	1.45
28	10	303	CLA	C1D-C2D	-2.36	1.40	1.45
28	a	204	CLA	C1D-C2D	-2.36	1.40	1.45
28	4	304	CLA	C1C-NC	2.36	1.41	1.37
28	7	306	CLA	C1C-NC	2.36	1.41	1.37
28	6	303	CLA	C1C-NC	2.35	1.41	1.37
29	1	313	A86	C32-C31	-2.34	1.50	1.54
28	a	203	CLA	C1D-C2D	-2.34	1.40	1.45
28	17	304	CLA	C1C-NC	2.34	1.41	1.37
28	A	801	CLA	C1C-NC	2.34	1.41	1.37
28	R	204	CLA	C1D-C2D	-2.34	1.40	1.45
28	4	316	CLA	C1D-C2D	-2.34	1.40	1.45
28	A	847	CLA	C1C-NC	2.34	1.41	1.37
28	A	847	CLA	C1D-C2D	-2.33	1.40	1.45
28	L	204	CLA	C1D-C2D	-2.33	1.40	1.45
28	3	305	CLA	C1D-C2D	-2.33	1.40	1.45
28	A	849	CLA	C1D-C2D	-2.33	1.40	1.45
28	7	303	CLA	C1C-NC	2.32	1.41	1.37
28	1	303	CLA	C1D-C2D	-2.32	1.40	1.45
28	9	308	CLA	MG-NA	2.32	2.11	2.06
28	8	301	CLA	MG-NC	2.32	2.11	2.06
28	A	832	CLA	MG-NC	2.32	2.11	2.06
28	11	306	CLA	C1C-NC	2.31	1.41	1.37
28	L	206	CLA	C1C-NC	2.31	1.41	1.37
28	B	811	CLA	C1D-C2D	-2.31	1.40	1.45
28	7	303	CLA	C1D-C2D	-2.31	1.40	1.45
28	B	824	CLA	C1C-NC	2.31	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	R	204	CLA	C1C-NC	2.30	1.41	1.37
32	11	313	XAT	C6-C7	-2.30	1.46	1.50
28	4	305	CLA	MG-NA	2.30	2.11	2.06
28	A	819	CLA	C1D-C2D	-2.29	1.40	1.45
28	1	305	CLA	C1D-C2D	-2.29	1.40	1.45
28	3	303	CLA	C1D-C2D	-2.29	1.40	1.45
28	9	307	CLA	C1C-NC	2.29	1.41	1.37
28	B	801	CLA	C1C-NC	2.29	1.41	1.37
28	8	310	CLA	C1C-NC	2.28	1.41	1.37
28	8	304	CLA	C1C-NC	2.28	1.41	1.37
28	1	304	CLA	C1C-NC	2.27	1.41	1.37
28	A	812	CLA	C1D-C2D	-2.26	1.40	1.45
28	L	201	CLA	C1D-C2D	-2.26	1.40	1.45
28	13	306	CLA	C1D-C2D	-2.25	1.40	1.45
28	13	307	CLA	C1D-C2D	-2.25	1.40	1.45
30	4	308	KC1	MG-NC	2.24	2.11	2.06
28	5	301	CLA	MG-NC	2.24	2.11	2.06
28	A	835	CLA	C1C-NC	2.23	1.41	1.37
28	J	102	CLA	C1C-NC	2.23	1.41	1.37
28	16	204	CLA	C1C-NC	2.23	1.41	1.37
28	B	820	CLA	C1D-C2D	-2.22	1.40	1.45
28	8	313	CLA	MG-NA	2.22	2.11	2.06
28	A	810	CLA	C1C-NC	2.21	1.41	1.37
28	4	316	CLA	C1C-NC	2.21	1.41	1.37
28	11	301	CLA	MG-NC	2.21	2.11	2.06
28	B	804	CLA	C1D-C2D	-2.21	1.41	1.45
28	4	316	CLA	MG-NA	2.21	2.11	2.06
28	11	303	CLA	C1C-NC	2.20	1.41	1.37
28	1	304	CLA	C1D-C2D	-2.20	1.41	1.45
28	B	826	CLA	C1C-NC	2.19	1.41	1.37
28	3	307	CLA	C1C-NC	2.19	1.41	1.37
28	13	301	CLA	C1C-NC	2.19	1.41	1.37
28	10	303	CLA	C1C-NC	2.19	1.41	1.37
32	J	105	XAT	C6-C7	-2.18	1.46	1.50
28	B	831	CLA	C1D-C2D	-2.18	1.41	1.45
28	A	809	CLA	C1C-NC	2.18	1.41	1.37
28	17	301	CLA	C1C-NC	2.18	1.41	1.37
28	a	202	CLA	C1C-NC	2.17	1.41	1.37
32	7	317	XAT	C26-C27	-2.16	1.46	1.50
28	A	806	CLA	C1C-NC	2.16	1.41	1.37
28	11	309	CLA	C1C-NC	2.16	1.41	1.37
28	A	818	CLA	C1D-C2D	-2.15	1.41	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	4	312	KC1	C4C-NC	2.15	1.41	1.37
28	A	849	CLA	C1C-NC	2.15	1.41	1.37
28	A	816	CLA	C1D-C2D	-2.15	1.41	1.45
28	16	201	CLA	MG-NC	2.14	2.11	2.06
28	6	311	CLA	C1C-NC	2.14	1.41	1.37
28	3	303	CLA	MG-NC	2.13	2.11	2.06
28	7	312	CLA	C1C-NC	2.13	1.41	1.37
28	A	803	CLA	C1D-C2D	-2.12	1.41	1.45
28	A	801	CLA	MG-NC	2.12	2.11	2.06
28	B	847	CLA	C1C-NC	2.11	1.41	1.37
28	6	313	CLA	C1C-NC	2.11	1.41	1.37
28	10	305	CLA	MG-NC	2.11	2.11	2.06
30	17	312	KC1	MG-NC	2.11	2.11	2.06
28	13	307	CLA	C4D-CHA	-2.10	1.31	1.38
28	9	303	CLA	C1C-NC	2.09	1.41	1.37
28	A	804	CLA	C1C-NC	2.08	1.41	1.37
28	a	201	CLA	C1C-NC	2.08	1.41	1.37
28	a	204	CLA	C1C-NC	2.08	1.41	1.37
28	7	311	CLA	C1C-NC	2.07	1.41	1.37
28	1	308	CLA	C1C-NC	2.07	1.41	1.37
28	A	836	CLA	C1C-NC	2.07	1.41	1.37
28	6	306	CLA	C1C-NC	2.06	1.41	1.37
28	19	201	CLA	MG-NA	2.06	2.11	2.06
28	5	304	CLA	MG-NC	2.06	2.11	2.06
28	17	303	CLA	MG-NC	2.05	2.11	2.06
28	13	305	CLA	C1C-NC	2.05	1.41	1.37
28	8	310	CLA	MG-NA	2.04	2.11	2.06
28	A	846	CLA	MG-NC	2.04	2.11	2.06
28	B	804	CLA	C1C-NC	2.04	1.41	1.37
28	A	803	CLA	MG-NC	2.03	2.11	2.06
30	10	304	KC1	C4C-NC	2.02	1.41	1.37
28	13	307	CLA	C1C-NC	2.02	1.41	1.37
28	13	303	CLA	C1C-NC	2.02	1.41	1.37
28	11	304	CLA	C1C-NC	2.01	1.41	1.37
28	7	305	CLA	C1C-NC	2.00	1.41	1.37

All (1566) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	6	311	CLA	C2D-C1D-ND	-15.97	109.53	120.88
28	7	312	CLA	C4A-NA-C1A	8.72	110.66	106.68
28	6	311	CLA	CMD-C2D-C1D	8.23	126.54	113.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	a	203	CLA	C4A-NA-C1A	7.92	110.29	106.68
28	17	301	CLA	C4A-NA-C1A	7.66	110.17	106.68
28	1	301	CLA	C4A-NA-C1A	7.62	110.16	106.68
28	11	310	CLA	C4A-NA-C1A	7.58	110.14	106.68
28	17	305	CLA	C4A-NA-C1A	7.56	110.13	106.68
28	a	204	CLA	C4A-NA-C1A	7.55	110.12	106.68
28	13	301	CLA	C4A-NA-C1A	7.52	110.11	106.68
28	B	804	CLA	C4A-NA-C1A	7.47	110.09	106.68
28	9	303	CLA	C4A-NA-C1A	7.37	110.04	106.68
28	4	310	CLA	C4A-NA-C1A	7.35	110.03	106.68
28	a	201	CLA	C4A-NA-C1A	7.31	110.02	106.68
28	11	312	CLA	C4A-NA-C1A	7.28	110.00	106.68
28	6	304	CLA	C4A-NA-C1A	7.26	109.99	106.68
28	13	303	CLA	C4A-NA-C1A	7.26	109.99	106.68
28	17	307	CLA	C4A-NA-C1A	7.26	109.99	106.68
28	B	818	CLA	C4A-NA-C1A	7.18	109.95	106.68
28	17	309	CLA	C1D-ND-C4D	-7.17	101.28	106.31
28	A	811	CLA	C4A-NA-C1A	7.13	109.93	106.68
30	3	309	KC1	C1D-ND-C4D	-7.12	101.32	106.31
28	19	202	CLA	C4A-NA-C1A	7.05	109.90	106.68
28	F	802	CLA	C4A-NA-C1A	7.02	109.88	106.68
28	5	303	CLA	C4A-NA-C1A	7.01	109.88	106.68
28	A	833	CLA	C4A-NA-C1A	6.96	109.86	106.68
28	9	311	CLA	C4A-NA-C1A	6.96	109.86	106.68
28	9	308	CLA	C4A-NA-C1A	6.96	109.85	106.68
28	A	809	CLA	C4A-NA-C1A	6.95	109.85	106.68
28	13	305	CLA	C4A-NA-C1A	6.94	109.85	106.68
32	J	105	XAT	C7-C8-C9	6.92	136.27	125.53
28	7	318	CLA	C4A-NA-C1A	6.90	109.83	106.68
28	5	313	CLA	C4A-NA-C1A	6.90	109.83	106.68
28	16	204	CLA	C4A-NA-C1A	6.88	109.82	106.68
32	1	311	XAT	C27-C28-C29	6.84	136.15	125.53
28	A	846	CLA	C4A-NA-C1A	6.83	109.80	106.68
28	4	307	CLA	C4A-NA-C1A	6.81	109.78	106.68
28	a	202	CLA	C4A-NA-C1A	6.72	109.75	106.68
28	A	827	CLA	C4A-NA-C1A	6.69	109.73	106.68
28	5	309	CLA	C4A-NA-C1A	6.66	109.72	106.68
28	B	813	CLA	C4A-NA-C1A	6.66	109.72	106.68
28	A	847	CLA	C4A-NA-C1A	6.65	109.72	106.68
28	11	305	CLA	C4A-NA-C1A	6.58	109.68	106.68
28	A	806	CLA	C4A-NA-C1A	6.58	109.68	106.68
28	A	830	CLA	C4A-NA-C1A	6.53	109.66	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	4	304	CLA	C1D-ND-C4D	-6.49	101.76	106.31
28	13	307	CLA	C4A-NA-C1A	6.48	109.63	106.68
28	13	302	CLA	C4A-NA-C1A	6.47	109.63	106.68
28	A	832	CLA	C4A-NA-C1A	6.46	109.62	106.68
28	J	103	CLA	C4A-NA-C1A	6.46	109.62	106.68
28	11	314	CLA	C4A-NA-C1A	6.45	109.62	106.68
28	11	303	CLA	C4A-NA-C1A	6.44	109.62	106.68
28	6	313	CLA	C4A-NA-C1A	6.43	109.61	106.68
28	16	203	CLA	C4A-NA-C1A	6.40	109.60	106.68
28	L	201	CLA	C4A-NA-C1A	6.35	109.58	106.68
28	B	802	CLA	C4A-NA-C1A	6.34	109.57	106.68
28	A	834	CLA	C4A-NA-C1A	6.33	109.57	106.68
30	9	309	KC1	C1A-NA-C4A	6.32	109.56	106.68
28	17	303	CLA	C4A-NA-C1A	6.31	109.56	106.68
28	3	314	CLA	C4A-NA-C1A	6.30	109.56	106.68
28	A	824	CLA	C4A-NA-C1A	6.30	109.55	106.68
28	16	205	CLA	C4A-NA-C1A	6.30	109.55	106.68
28	B	829	CLA	C4A-NA-C1A	6.29	109.55	106.68
28	11	309	CLA	C4A-NA-C1A	6.28	109.54	106.68
28	L	206	CLA	C4A-NA-C1A	6.26	109.54	106.68
28	B	828	CLA	C4A-NA-C1A	6.26	109.54	106.68
28	10	309	CLA	C4A-NA-C1A	6.26	109.53	106.68
28	9	310	CLA	C4A-NA-C1A	6.24	109.53	106.68
28	1	310	CLA	C4A-NA-C1A	6.23	109.52	106.68
28	A	814	CLA	C4A-NA-C1A	6.22	109.52	106.68
28	8	302	CLA	C4A-NA-C1A	6.22	109.52	106.68
33	L	202	BCR	C15-C16-C17	6.20	136.21	123.52
28	3	305	CLA	C4A-NA-C1A	6.19	109.50	106.68
28	A	802	CLA	C4A-NA-C1A	6.19	109.50	106.68
28	11	304	CLA	C4A-NA-C1A	6.18	109.50	106.68
28	A	808	CLA	C4A-NA-C1A	6.17	109.49	106.68
28	16	201	CLA	C4A-NA-C1A	6.15	109.49	106.68
28	9	307	CLA	C4A-NA-C1A	6.10	109.46	106.68
28	B	811	CLA	C4A-NA-C1A	6.10	109.46	106.68
28	B	816	CLA	C4A-NA-C1A	6.09	109.46	106.68
28	B	847	CLA	C4A-NA-C1A	6.09	109.46	106.68
28	F	803	CLA	C4A-NA-C1A	6.09	109.46	106.68
28	7	302	CLA	C4A-NA-C1A	6.08	109.45	106.68
32	10	315	XAT	C15-C35-C34	6.08	135.95	123.52
28	B	834	CLA	C4A-NA-C1A	6.04	109.43	106.68
28	3	307	CLA	C4A-NA-C1A	6.03	109.43	106.68
28	B	830	CLA	C4A-NA-C1A	6.03	109.43	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	L	204	CLA	C4A-NA-C1A	6.02	109.42	106.68
28	8	303	CLA	C4A-NA-C1A	6.01	109.42	106.68
28	1	308	CLA	C4A-NA-C1A	6.01	109.42	106.68
28	B	835	CLA	C4A-NA-C1A	5.99	109.41	106.68
28	8	304	CLA	C4A-NA-C1A	5.99	109.41	106.68
28	B	823	CLA	C4A-NA-C1A	5.99	109.41	106.68
30	3	308	KC1	CHB-C4A-C3A	-5.98	115.58	125.03
28	3	301	CLA	C4A-NA-C1A	5.98	109.41	106.68
28	B	826	CLA	C4A-NA-C1A	5.98	109.41	106.68
28	A	835	CLA	C4A-NA-C1A	5.96	109.40	106.68
28	B	814	CLA	C4A-NA-C1A	5.94	109.39	106.68
28	B	833	CLA	C4A-NA-C1A	5.94	109.39	106.68
28	7	306	CLA	C4A-NA-C1A	5.93	109.38	106.68
30	17	306	KC1	C1D-ND-C4D	-5.91	102.16	106.31
28	B	824	CLA	C4A-NA-C1A	5.90	109.37	106.68
28	B	801	CLA	C4A-NA-C1A	5.90	109.37	106.68
28	1	314	CLA	C4A-NA-C1A	5.88	109.36	106.68
28	A	816	CLA	C4A-NA-C1A	5.87	109.36	106.68
28	A	813	CLA	C4A-NA-C1A	5.85	109.35	106.68
28	A	825	CLA	C4A-NA-C1A	5.83	109.34	106.68
28	A	816	CLA	C1D-ND-C4D	-5.79	102.25	106.31
30	17	312	KC1	C1A-C2A-C3A	-5.77	101.97	107.28
28	B	848	CLA	C4A-NA-C1A	5.76	109.31	106.68
28	7	311	CLA	C4A-NA-C1A	5.76	109.31	106.68
28	B	843	CLA	C4A-NA-C1A	5.76	109.31	106.68
28	L	203	CLA	C4A-NA-C1A	5.74	109.30	106.68
28	B	815	CLA	C4A-NA-C1A	5.70	109.28	106.68
28	A	821	CLA	C4A-NA-C1A	5.68	109.27	106.68
28	A	836	CLA	C4A-NA-C1A	5.67	109.27	106.68
28	A	849	CLA	C4A-NA-C1A	5.67	109.27	106.68
28	A	819	CLA	C4A-NA-C1A	5.62	109.24	106.68
28	17	302	CLA	C4A-NA-C1A	5.61	109.24	106.68
28	A	852	CLA	C4A-NA-C1A	5.60	109.23	106.68
28	A	853	CLA	C4A-NA-C1A	5.60	109.23	106.68
28	A	820	CLA	C4A-NA-C1A	5.60	109.23	106.68
28	13	306	CLA	C4A-NA-C1A	5.59	109.23	106.68
28	B	832	CLA	C4A-NA-C1A	5.59	109.23	106.68
28	6	307	CLA	C4A-NA-C1A	5.59	109.23	106.68
28	10	306	CLA	C4A-NA-C1A	5.59	109.23	106.68
28	B	806	CLA	C4A-NA-C1A	5.58	109.22	106.68
32	7	316	XAT	C27-C28-C29	-5.56	116.90	125.53
28	10	302	CLA	C4A-NA-C1A	5.55	109.21	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	A	845	CLA	C4A-NA-C1A	5.54	109.21	106.68
28	6	306	CLA	C4A-NA-C1A	5.54	109.20	106.68
28	7	305	CLA	C4A-NA-C1A	5.53	109.20	106.68
28	B	845	CLA	C4A-NA-C1A	5.52	109.20	106.68
28	B	827	CLA	C4A-NA-C1A	5.52	109.20	106.68
28	B	809	CLA	C4A-NA-C1A	5.49	109.18	106.68
28	3	304	CLA	C4A-NA-C1A	5.48	109.18	106.68
28	A	812	CLA	C4A-NA-C1A	5.48	109.18	106.68
28	4	316	CLA	C4A-NA-C1A	5.47	109.17	106.68
28	B	807	CLA	C4A-NA-C1A	5.41	109.14	106.68
28	11	306	CLA	C4A-NA-C1A	5.41	109.14	106.68
32	5	307	XAT	C35-C15-C14	5.40	134.57	123.52
28	16	202	CLA	C4A-NA-C1A	5.40	109.14	106.68
28	5	306	CLA	C4A-NA-C1A	5.34	109.11	106.68
28	6	303	CLA	C4A-NA-C1A	5.32	109.11	106.68
28	J	102	CLA	C4A-NA-C1A	5.32	109.11	106.68
28	A	823	CLA	C4A-NA-C1A	5.30	109.10	106.68
28	10	305	CLA	C4A-NA-C1A	5.30	109.10	106.68
28	8	310	CLA	C4A-NA-C1A	5.29	109.09	106.68
28	5	304	CLA	C4A-NA-C1A	5.29	109.09	106.68
32	5	307	XAT	C15-C35-C34	5.27	134.31	123.52
28	A	831	CLA	C4A-NA-C1A	5.24	109.07	106.68
28	B	821	CLA	C4A-NA-C1A	5.23	109.06	106.68
28	1	303	CLA	C4A-NA-C1A	5.22	109.06	106.68
28	7	304	CLA	C4A-NA-C1A	5.21	109.06	106.68
28	B	813	CLA	C1D-ND-C4D	-5.20	102.66	106.31
28	17	304	CLA	C4A-NA-C1A	5.20	109.05	106.68
28	A	826	CLA	C4A-NA-C1A	5.17	109.04	106.68
28	5	302	CLA	C4A-NA-C1A	5.15	109.03	106.68
28	B	817	CLA	C4A-NA-C1A	5.14	109.02	106.68
28	A	818	CLA	C4A-NA-C1A	5.13	109.02	106.68
32	7	317	XAT	C27-C28-C29	5.10	133.44	125.53
28	B	803	CLA	C4A-NA-C1A	5.09	109.00	106.68
28	A	810	CLA	C4A-NA-C1A	5.09	109.00	106.68
32	10	315	XAT	C35-C15-C14	5.07	133.90	123.52
32	7	317	XAT	C7-C8-C9	5.07	133.40	125.53
28	L	206	CLA	CHA-C4D-ND	-5.06	122.10	132.55
28	A	807	CLA	C4A-NA-C1A	5.06	108.99	106.68
28	16	202	CLA	C1D-ND-C4D	-5.05	102.77	106.31
28	A	801	CLA	C4A-NA-C1A	5.03	108.98	106.68
30	8	306	KC1	C1D-ND-C4D	-5.03	102.78	106.31
30	11	307	KC1	C1D-ND-C4D	-5.02	102.79	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	6	312	XAT	C35-C15-C14	5.02	133.79	123.52
28	19	201	CLA	C4A-NA-C1A	5.02	108.97	106.68
28	11	304	CLA	C1D-ND-C4D	-5.01	102.80	106.31
28	13	307	CLA	C1D-ND-C4D	-5.01	102.80	106.31
28	A	817	CLA	C4A-NA-C1A	5.01	108.97	106.68
28	4	303	CLA	C4A-NA-C1A	5.00	108.96	106.68
28	J	103	CLA	C1D-ND-C4D	-4.99	102.81	106.31
28	8	301	CLA	C4A-NA-C1A	4.95	108.94	106.68
28	L	201	CLA	C1D-ND-C4D	-4.95	102.84	106.31
30	6	305	KC1	C1A-C2A-C3A	-4.93	102.75	107.28
30	1	306	KC1	C1D-ND-C4D	-4.91	102.86	106.31
28	10	308	CLA	C4A-NA-C1A	4.89	108.91	106.68
28	10	301	CLA	C4A-NA-C1A	4.86	108.90	106.68
28	8	305	CLA	C4A-NA-C1A	4.86	108.90	106.68
30	3	302	KC1	C1A-C2A-C3A	-4.86	102.82	107.28
30	6	308	KC1	C1A-NA-C4A	-4.85	104.47	106.68
32	6	312	XAT	C15-C35-C34	4.83	133.40	123.52
32	7	313	XAT	C7-C8-C9	-4.83	118.04	125.53
28	R	204	CLA	C4A-NA-C1A	4.80	108.87	106.68
33	8	309	BCR	C16-C15-C14	4.79	133.33	123.52
28	5	301	CLA	C4A-NA-C1A	4.78	108.86	106.68
30	4	311	KC1	C1A-NA-C4A	-4.77	104.50	106.68
33	8	309	BCR	C15-C16-C17	4.76	133.26	123.52
28	11	301	CLA	C4A-NA-C1A	4.75	108.85	106.68
32	5	316	XAT	C27-C28-C29	4.75	132.90	125.53
28	15	201	CLA	C4A-NA-C1A	4.73	108.83	106.68
28	B	805	CLA	C4A-NA-C1A	4.70	108.82	106.68
28	8	304	CLA	C1D-ND-C4D	-4.66	103.04	106.31
28	A	804	CLA	C4A-NA-C1A	4.65	108.80	106.68
28	B	825	CLA	C4A-NA-C1A	4.63	108.79	106.68
28	7	303	CLA	C4A-NA-C1A	4.62	108.79	106.68
30	6	310	KC1	CHC-C1C-C2C	-4.60	117.77	125.03
28	6	306	CLA	C1D-ND-C4D	-4.59	103.09	106.31
28	R	202	CLA	C1D-ND-C4D	-4.58	103.10	106.31
28	A	849	CLA	C1D-ND-C4D	-4.57	103.11	106.31
28	4	305	CLA	C4A-NA-C1A	4.56	108.76	106.68
28	5	305	CLA	C4A-NA-C1A	4.55	108.75	106.68
28	1	304	CLA	C4A-NA-C1A	4.55	108.75	106.68
32	5	310	XAT	C27-C28-C29	4.54	132.58	125.53
30	17	306	KC1	C1A-C2A-C3A	-4.54	103.10	107.28
28	11	303	CLA	C1D-ND-C4D	-4.52	103.14	106.31
28	R	202	CLA	C1-C2-C3	-4.52	118.80	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	a	205	KC1	C1D-ND-C4D	-4.51	103.15	106.31
28	A	829	CLA	C4A-NA-C1A	4.49	108.73	106.68
33	L	202	BCR	C16-C15-C14	-4.49	114.33	123.52
28	B	810	CLA	C4A-NA-C1A	4.48	108.72	106.68
32	8	311	XAT	C7-C8-C9	4.48	132.49	125.53
28	19	201	CLA	CHA-C4D-ND	-4.48	123.30	132.55
28	9	304	CLA	C4A-NA-C1A	4.46	108.72	106.68
30	17	306	KC1	C2A-C3A-C4A	-4.46	103.06	106.41
28	3	306	CLA	C4A-NA-C1A	4.46	108.71	106.68
28	A	803	CLA	C4A-NA-C1A	4.45	108.71	106.68
28	17	303	CLA	C1D-ND-C4D	-4.44	103.20	106.31
28	10	309	CLA	C1D-ND-C4D	-4.44	103.20	106.31
28	A	819	CLA	C1D-ND-C4D	-4.43	103.20	106.31
28	a	202	CLA	CHA-C4D-ND	-4.43	123.40	132.55
28	8	313	CLA	C4A-NA-C1A	4.42	108.70	106.68
28	7	301	CLA	C4A-NA-C1A	4.42	108.70	106.68
28	4	305	CLA	C1D-ND-C4D	-4.42	103.21	106.31
28	16	203	CLA	CHA-C4D-ND	-4.41	123.45	132.55
28	A	846	CLA	C1D-ND-C4D	-4.40	103.23	106.31
30	1	306	KC1	C1A-C2A-C3A	-4.39	103.24	107.28
33	B	839	BCR	C15-C16-C17	4.39	132.51	123.52
28	10	303	CLA	C4A-NA-C1A	4.39	108.68	106.68
28	7	308	CLA	C4A-NA-C1A	4.38	108.68	106.68
28	10	316	CLA	CHA-C4D-ND	-4.36	123.56	132.55
28	6	303	CLA	C1D-ND-C4D	-4.36	103.25	106.31
28	13	305	CLA	C1D-ND-C4D	-4.34	103.27	106.31
28	10	307	CLA	CGD-CBD-CAD	4.34	124.88	110.85
33	L	202	BCR	C21-C20-C19	4.33	135.75	123.20
28	11	302	CLA	C4A-NA-C1A	4.32	108.65	106.68
28	A	828	CLA	C4A-NA-C1A	4.29	108.64	106.68
30	17	312	KC1	C1A-NA-C4A	-4.29	104.72	106.68
30	6	308	KC1	C1D-ND-C4D	-4.29	103.30	106.31
28	A	806	CLA	C1-C2-C3	-4.28	119.18	126.20
30	6	309	KC1	CAD-C3D-C2D	-4.28	135.24	144.26
30	4	308	KC1	C1A-NA-C4A	-4.28	104.73	106.68
28	1	307	CLA	C4A-NA-C1A	4.28	108.63	106.68
30	17	312	KC1	C2A-C3A-C4A	-4.27	103.21	106.41
28	A	827	CLA	C1D-ND-C4D	-4.27	103.32	106.31
28	B	812	CLA	C4A-NA-C1A	4.25	108.62	106.68
28	A	825	CLA	C1D-ND-C4D	-4.25	103.33	106.31
28	17	309	CLA	C4A-NA-C1A	4.24	108.61	106.68
29	3	311	A86	C3-C4-C5	4.22	132.16	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	J	102	CLA	C1D-ND-C4D	-4.22	103.35	106.31
28	8	302	CLA	C1D-ND-C4D	-4.21	103.36	106.31
28	10	308	CLA	CHA-C4D-ND	-4.20	123.88	132.55
28	6	301	CLA	C1D-ND-C4D	-4.20	103.37	106.31
28	4	304	CLA	C4A-NA-C1A	4.19	108.59	106.68
30	10	310	KC1	C1A-NA-C4A	-4.19	104.77	106.68
28	7	303	CLA	C1D-ND-C4D	-4.18	103.38	106.31
30	3	302	KC1	C1D-ND-C4D	-4.17	103.39	106.31
28	A	847	CLA	C1D-ND-C4D	-4.16	103.40	106.31
28	11	312	CLA	CHA-C4D-ND	-4.14	124.00	132.55
30	9	306	KC1	C1A-NA-C4A	-4.13	104.79	106.68
32	5	307	XAT	C7-C8-C9	4.13	131.94	125.53
28	A	815	CLA	C4A-NA-C1A	4.12	108.56	106.68
28	10	307	CLA	C4A-NA-C1A	4.11	108.56	106.68
30	7	309	KC1	CHB-C4A-C3A	-4.11	118.54	125.03
28	4	306	CLA	C4A-NA-C1A	4.11	108.55	106.68
28	1	303	CLA	C1D-ND-C4D	-4.10	103.43	106.31
28	10	316	CLA	C4A-NA-C1A	4.10	108.55	106.68
28	a	203	CLA	C1D-ND-C4D	-4.09	103.44	106.31
28	B	826	CLA	C1D-ND-C4D	-4.06	103.46	106.31
28	A	805	CLA	C1D-ND-C4D	-4.06	103.46	106.31
32	10	314	XAT	C27-C28-C29	4.02	131.77	125.53
33	A	850	BCR	C10-C11-C12	4.00	134.80	123.20
29	3	311	A86	C4-C3-C2	4.00	131.70	123.52
30	8	306	KC1	CHB-C4A-C3A	-4.00	118.72	125.03
28	13	306	CLA	C1D-ND-C4D	-3.96	103.53	106.31
28	6	302	CLA	C4A-NA-C1A	3.94	108.48	106.68
28	15	201	CLA	CHA-C4D-ND	-3.93	124.43	132.55
28	B	848	CLA	C1D-ND-C4D	-3.93	103.56	106.31
28	9	307	CLA	C1D-ND-C4D	-3.92	103.56	106.31
30	10	310	KC1	C1D-ND-C4D	-3.91	103.57	106.31
30	7	309	KC1	C1A-NA-C4A	-3.91	104.89	106.68
28	B	815	CLA	C1D-ND-C4D	-3.91	103.57	106.31
28	A	832	CLA	C1D-ND-C4D	-3.91	103.57	106.31
28	A	818	CLA	C1D-ND-C4D	-3.90	103.58	106.31
30	11	307	KC1	CHB-C4A-C3A	-3.89	118.89	125.03
28	A	805	CLA	C4A-NA-C1A	3.88	108.45	106.68
28	B	808	CLA	CHA-C4D-ND	-3.88	124.55	132.55
28	4	303	CLA	C3B-C4B-NB	-3.85	107.09	110.53
28	10	316	CLA	C2A-C1A-CHA	3.84	130.53	123.87
28	9	310	CLA	C1D-ND-C4D	-3.82	103.63	106.31
28	B	822	CLA	C4A-NA-C1A	3.81	108.42	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	11	307	KC1	CHC-C1C-C2C	-3.80	119.02	125.03
28	R	202	CLA	C4A-NA-C1A	3.80	108.41	106.68
30	6	310	KC1	C1A-C2A-C3A	-3.80	103.79	107.28
30	3	309	KC1	CHB-C4A-C3A	-3.80	119.04	125.03
30	3	309	KC1	CHC-C1C-C2C	-3.79	119.04	125.03
28	B	823	CLA	C3B-C4B-NB	-3.79	107.15	110.53
30	1	306	KC1	CHC-C1C-C2C	-3.76	119.09	125.03
28	B	819	CLA	C4A-NA-C1A	3.75	108.39	106.68
30	7	307	KC1	C1B-CHB-C4A	-3.74	118.08	126.02
32	4	318	XAT	C6-C7-C8	3.73	133.88	125.99
30	10	311	KC1	CAD-C3D-C2D	-3.73	136.41	144.26
28	A	822	CLA	C4A-NA-C1A	3.73	108.38	106.68
28	11	312	CLA	C1D-CHD-C4C	-3.72	118.11	126.02
30	6	309	KC1	CHB-C4A-C3A	-3.72	119.16	125.03
28	B	820	CLA	C4A-NA-C1A	3.72	108.38	106.68
28	B	810	CLA	C1-C2-C3	-3.72	120.11	126.20
32	7	313	XAT	C27-C28-C29	3.71	131.29	125.53
30	17	306	KC1	C1A-NA-C4A	-3.71	104.99	106.68
28	B	808	CLA	C4A-NA-C1A	3.71	108.37	106.68
28	13	303	CLA	C1D-ND-C4D	-3.71	103.71	106.31
30	6	309	KC1	CHC-C1C-C2C	-3.71	119.17	125.03
30	17	312	KC1	CAD-C3D-C2D	-3.70	136.47	144.26
28	1	314	CLA	C1D-ND-C4D	-3.70	103.72	106.31
28	6	313	CLA	C1D-ND-C4D	-3.70	103.72	106.31
28	A	828	CLA	CHA-C4D-ND	-3.69	124.94	132.55
28	3	314	CLA	C1D-ND-C4D	-3.68	103.73	106.31
28	8	305	CLA	C1D-ND-C4D	-3.67	103.73	106.31
30	10	304	KC1	CAD-C3D-C2D	-3.67	136.53	144.26
28	a	204	CLA	C1D-ND-C4D	-3.67	103.74	106.31
30	9	309	KC1	C1D-ND-C4D	-3.67	103.74	106.31
28	B	810	CLA	C1D-ND-C4D	-3.65	103.75	106.31
28	10	303	CLA	C1D-ND-C4D	-3.64	103.76	106.31
30	10	304	KC1	CHB-C4A-C3A	-3.64	119.28	125.03
32	6	316	XAT	C7-C8-C9	3.63	131.16	125.53
28	3	307	CLA	CHA-C4D-ND	-3.63	125.05	132.55
28	B	801	CLA	C3B-C4B-NB	-3.62	107.29	110.53
28	B	811	CLA	C1-C2-C3	-3.62	120.26	126.20
28	8	313	CLA	C3B-C4B-NB	-3.61	107.31	110.53
30	6	308	KC1	CHC-C1C-C2C	-3.60	119.34	125.03
30	10	304	KC1	C1A-C2A-C3A	-3.60	103.97	107.28
30	4	311	KC1	CAD-C3D-C2D	-3.60	136.69	144.26
30	7	309	KC1	CHC-C1C-C2C	-3.59	119.35	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	7	317	XAT	C6-C7-C8	3.59	133.58	125.99
30	8	307	KC1	C4D-C3D-C2D	-3.59	102.59	107.42
33	B	839	BCR	C24-C23-C22	3.56	131.51	126.23
28	5	304	CLA	C1D-ND-C4D	-3.56	103.81	106.31
28	A	853	CLA	CHA-C4D-ND	-3.56	125.20	132.55
30	13	304	KC1	C1A-NA-C4A	-3.55	105.06	106.68
28	1	314	CLA	C1D-CHD-C4C	-3.55	118.48	126.02
28	10	301	CLA	C1D-ND-C4D	-3.54	103.83	106.31
28	17	301	CLA	CHA-C4D-ND	-3.54	125.23	132.55
28	A	816	CLA	CHD-C4C-C3C	-3.54	119.61	124.77
28	10	305	CLA	C1D-ND-C4D	-3.54	103.83	106.31
30	4	312	KC1	CAD-C3D-C2D	-3.54	136.80	144.26
28	4	307	CLA	C1D-ND-C4D	-3.54	103.83	106.31
28	1	308	CLA	C1D-CHD-C4C	-3.53	118.51	126.02
28	5	309	CLA	C1D-ND-C4D	-3.52	103.84	106.31
28	A	826	CLA	C1D-ND-C4D	-3.52	103.84	106.31
28	B	820	CLA	C1D-ND-C4D	-3.52	103.84	106.31
30	9	306	KC1	C1A-C2A-C3A	-3.52	104.05	107.28
30	4	311	KC1	C4D-C3D-C2D	-3.51	102.70	107.42
28	7	306	CLA	C3B-C4B-NB	-3.50	107.41	110.53
28	F	802	CLA	CGD-CBD-CAD	3.49	122.15	110.85
28	B	801	CLA	C1D-ND-C4D	-3.49	103.86	106.31
28	6	301	CLA	C4A-NA-C1A	3.49	108.27	106.68
28	7	301	CLA	C1D-ND-C4D	-3.48	103.87	106.31
28	6	304	CLA	C3B-C4B-NB	-3.48	107.43	110.53
28	B	831	CLA	C3B-C4B-NB	-3.47	107.44	110.53
33	B	839	BCR	C16-C15-C14	-3.46	116.44	123.52
30	6	305	KC1	CHC-C1C-C2C	-3.46	119.57	125.03
28	17	302	CLA	C1D-CHD-C4C	-3.45	118.69	126.02
28	9	307	CLA	C3B-C4B-NB	-3.44	107.45	110.53
28	L	206	CLA	C3B-C4B-NB	-3.44	107.46	110.53
28	7	302	CLA	CHA-C4D-ND	-3.44	125.45	132.55
30	7	309	KC1	C1A-C2A-C3A	-3.43	104.12	107.28
28	6	307	CLA	C3B-C4B-NB	-3.43	107.47	110.53
28	a	201	CLA	C3B-C4B-NB	-3.43	107.47	110.53
30	4	309	KC1	C1D-ND-C4D	-3.43	103.91	106.31
30	6	308	KC1	C1A-C2A-C3A	-3.43	104.13	107.28
28	1	303	CLA	C3B-C4B-NB	-3.43	107.47	110.53
28	6	304	CLA	CHA-C4D-ND	-3.43	125.48	132.55
28	17	305	CLA	C1D-ND-C4D	-3.42	103.91	106.31
28	L	206	CLA	C1D-ND-C4D	3.42	108.71	106.31
28	9	305	CLA	C1D-ND-C4D	-3.42	103.92	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	10	304	KC1	CHC-C1C-C2C	-3.41	119.64	125.03
30	7	307	KC1	C1A-NA-C4A	3.40	108.23	106.68
30	9	306	KC1	CHC-C1C-C2C	-3.40	119.65	125.03
32	7	315	XAT	C15-C35-C34	3.40	130.48	123.52
28	1	305	CLA	C4A-NA-C1A	3.40	108.23	106.68
30	10	310	KC1	CHC-C1C-C2C	-3.39	119.68	125.03
30	6	305	KC1	C1D-ND-C4D	-3.38	103.94	106.31
30	13	304	KC1	C1A-C2A-C3A	-3.38	104.17	107.28
28	a	203	CLA	C3B-C4B-NB	-3.38	107.51	110.53
32	6	315	XAT	C26-C27-C28	3.38	133.14	125.99
28	5	309	CLA	C1D-CHD-C4C	-3.38	118.84	126.02
28	1	305	CLA	C3B-C4B-NB	-3.38	107.52	110.53
30	11	307	KC1	C1A-C2A-C3A	-3.37	104.18	107.28
28	A	808	CLA	C3B-C4B-NB	-3.36	107.53	110.53
28	B	814	CLA	C3B-C4B-NB	-3.36	107.53	110.53
30	3	308	KC1	CHC-C1C-C2C	-3.36	119.73	125.03
28	10	307	CLA	C3B-C4B-NB	-3.35	107.54	110.53
28	9	305	CLA	C1-C2-C3	-3.35	121.35	126.76
30	3	302	KC1	CHB-C4A-C3A	-3.34	119.75	125.03
28	7	312	CLA	C1D-CHD-C4C	-3.34	118.92	126.02
30	3	308	KC1	CAA-CBA-CGA	3.34	144.01	127.05
30	17	306	KC1	CHC-C1C-C2C	-3.33	119.76	125.03
28	8	310	CLA	C1D-CHD-C4C	-3.33	118.93	126.02
28	10	305	CLA	C3B-C4B-NB	-3.33	107.56	110.53
28	R	204	CLA	C3B-C4B-NB	-3.32	107.56	110.53
28	3	301	CLA	C1D-CHD-C4C	-3.32	118.97	126.02
28	11	303	CLA	C3B-C4B-NB	-3.32	107.57	110.53
28	B	847	CLA	C1D-ND-C4D	-3.32	103.99	106.31
33	L	202	BCR	C16-C17-C18	3.31	131.93	127.28
28	A	836	CLA	C1D-ND-C4D	-3.31	103.99	106.31
33	17	310	BCR	C24-C23-C22	3.31	131.13	126.23
28	9	303	CLA	C3B-C4B-NB	-3.31	107.58	110.53
28	L	203	CLA	C1D-ND-C4D	-3.31	103.99	106.31
30	6	305	KC1	C2A-C3A-C4A	-3.30	103.93	106.41
28	8	301	CLA	C3B-C4B-NB	-3.30	107.58	110.53
28	7	306	CLA	C1D-ND-C4D	-3.30	104.00	106.31
28	10	309	CLA	C3B-C4B-NB	-3.30	107.58	110.53
28	9	303	CLA	C1D-ND-C4D	-3.30	104.00	106.31
28	13	303	CLA	C3B-C4B-NB	-3.30	107.59	110.53
32	11	313	XAT	C7-C8-C9	3.29	130.64	125.53
30	3	309	KC1	C1A-C2A-C3A	-3.29	104.25	107.28
28	4	307	CLA	C1D-CHD-C4C	-3.27	119.07	126.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	11	310	CLA	C1D-ND-C4D	-3.27	104.02	106.31
30	9	309	KC1	CAD-C3D-C2D	-3.27	137.38	144.26
28	3	303	CLA	C1D-ND-C4D	-3.27	104.02	106.31
28	10	301	CLA	C3B-C4B-NB	-3.27	107.61	110.53
28	B	821	CLA	C3B-C4B-NB	-3.26	107.62	110.53
28	B	805	CLA	C1-C2-C3	-3.26	120.86	126.20
28	4	303	CLA	C1D-ND-C4D	-3.25	104.03	106.31
30	4	311	KC1	C1D-ND-C4D	-3.25	104.03	106.31
29	1	302	A86	C3-C4-C5	3.25	130.17	123.52
28	B	803	CLA	C1D-ND-C4D	-3.25	104.03	106.31
28	B	848	CLA	C3B-C4B-NB	-3.25	107.63	110.53
28	13	306	CLA	C1D-CHD-C4C	-3.24	119.13	126.02
28	17	304	CLA	C3B-C4B-NB	-3.24	107.64	110.53
28	11	306	CLA	C1D-CHD-C4C	-3.24	119.14	126.02
28	11	301	CLA	C3B-C4B-NB	-3.23	107.65	110.53
28	A	837	CLA	C3B-C4B-NB	-3.23	107.65	110.53
28	1	305	CLA	C1D-ND-C4D	-3.22	104.05	106.31
30	4	308	KC1	C1A-C2A-C3A	-3.22	104.32	107.28
28	B	812	CLA	C3B-C4B-NB	-3.22	107.66	110.53
30	9	306	KC1	CAD-C3D-C2D	-3.22	137.48	144.26
28	B	834	CLA	C1D-ND-C4D	-3.22	104.06	106.31
28	A	835	CLA	CHA-C4D-ND	-3.22	125.91	132.55
30	4	312	KC1	CGD-CBD-CAD	3.21	121.25	110.85
28	J	102	CLA	C3B-C4B-NB	-3.21	107.66	110.53
28	11	309	CLA	C1D-CHD-C4C	-3.21	119.19	126.02
30	3	308	KC1	C1A-C2A-C3A	-3.21	104.33	107.28
28	L	204	CLA	C1D-ND-C4D	-3.21	104.06	106.31
28	B	822	CLA	C1D-ND-C4D	-3.21	104.06	106.31
30	10	310	KC1	C1A-C2A-C3A	-3.21	104.33	107.28
28	17	309	CLA	CHC-C4B-NB	-3.20	119.25	124.05
28	3	314	CLA	C1D-CHD-C4C	-3.20	119.22	126.02
33	A	850	BCR	C8-C7-C6	3.20	135.55	127.00
30	4	311	KC1	C1A-C2A-C3A	-3.20	104.34	107.28
30	8	307	KC1	C1A-C2A-C3A	-3.19	104.34	107.28
32	7	316	XAT	C26-C27-C28	3.19	132.74	125.99
28	A	830	CLA	C1-C2-C3	-3.19	120.97	126.20
28	10	306	CLA	C1D-ND-C4D	-3.19	104.07	106.31
28	11	305	CLA	C1D-ND-C4D	-3.19	104.08	106.31
28	11	314	CLA	C3B-C4B-NB	-3.18	107.69	110.53
28	17	302	CLA	CHA-C4D-ND	-3.18	125.98	132.55
28	6	301	CLA	C3B-C4B-NB	-3.17	107.70	110.53
30	6	305	KC1	CAD-C3D-C2D	-3.17	137.58	144.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	A	826	CLA	C1-C2-C3	-3.17	121.00	126.20
32	3	313	XAT	C7-C8-C9	3.17	130.45	125.53
28	B	815	CLA	C3B-C4B-NB	-3.17	107.70	110.53
28	7	318	CLA	C1D-CHD-C4C	-3.17	119.29	126.02
28	6	313	CLA	C1D-CHD-C4C	-3.16	119.30	126.02
28	A	822	CLA	C1-C2-C3	-3.16	121.02	126.20
32	10	315	XAT	C30-C31-C32	3.16	132.35	123.20
28	3	301	CLA	C3B-C4B-NB	-3.16	107.71	110.53
28	L	204	CLA	C1D-CHD-C4C	-3.16	119.31	126.02
28	3	305	CLA	C1D-ND-C4D	-3.16	104.10	106.31
32	6	312	XAT	C6-C7-C8	3.15	132.66	125.99
28	A	829	CLA	C3B-C4B-NB	-3.15	107.72	110.53
29	10	312	A86	C26-C25-C24	3.15	132.31	123.20
28	A	835	CLA	C3B-C4B-NB	-3.14	107.73	110.53
33	A	850	BCR	C16-C15-C14	3.13	129.93	123.52
30	4	312	KC1	CHC-C1C-C2C	-3.13	120.08	125.03
28	A	836	CLA	C1D-CHD-C4C	-3.13	119.36	126.02
28	10	316	CLA	CHA-C1A-NA	-3.13	119.30	126.39
32	7	315	XAT	C35-C15-C14	3.13	129.92	123.52
30	5	308	KC1	C1A-C2A-C3A	-3.13	104.40	107.28
28	7	311	CLA	C3B-C4B-NB	-3.13	107.74	110.53
28	B	826	CLA	C1D-CHD-C4C	-3.13	119.38	126.02
30	a	205	KC1	C1A-C2A-C3A	-3.12	104.41	107.28
28	B	835	CLA	C1D-ND-C4D	-3.12	104.13	106.31
28	A	827	CLA	C1-C2-C3	-3.12	121.09	126.20
30	7	307	KC1	C4D-C3D-C2D	-3.11	103.23	107.42
28	7	311	CLA	CHA-C4D-ND	-3.11	126.13	132.55
28	9	304	CLA	C1D-CHD-C4C	-3.11	119.41	126.02
28	B	804	CLA	C3B-C4B-NB	-3.11	107.75	110.53
29	1	313	A86	C33-C32-C31	3.11	112.23	109.21
28	4	316	CLA	C3B-C4B-NB	-3.11	107.76	110.53
28	5	306	CLA	C3B-C4B-NB	-3.10	107.76	110.53
28	B	824	CLA	C3B-C4B-NB	-3.10	107.76	110.53
28	A	810	CLA	C1D-CHD-C4C	-3.09	119.44	126.02
30	9	306	KC1	CHB-C4A-C3A	-3.09	120.14	125.03
28	A	807	CLA	CHA-C4D-ND	-3.09	126.17	132.55
30	8	307	KC1	C1B-CHB-C4A	-3.09	119.45	126.02
28	A	823	CLA	C1-C2-C3	-3.09	121.14	126.20
32	10	315	XAT	C26-C27-C28	3.08	132.51	125.99
30	1	306	KC1	C4D-C3D-C2D	-3.08	103.27	107.42
28	7	306	CLA	C1-C2-C3	-3.08	121.14	126.20
28	4	306	CLA	C1D-ND-C4D	-3.08	104.15	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	5	301	CLA	C1-C2-C3	-3.08	121.16	126.20
28	10	301	CLA	C1-C2-C3	-3.07	121.16	126.20
28	A	833	CLA	C1D-ND-C4D	-3.06	104.16	106.31
30	3	309	KC1	C4D-C3D-C2D	-3.06	103.31	107.42
32	17	311	XAT	C30-C31-C32	3.06	132.05	123.20
28	B	831	CLA	C1-C2-C3	-3.05	121.19	126.20
28	16	202	CLA	C3B-C4B-NB	-3.05	107.81	110.53
30	6	310	KC1	CAD-C3D-C2D	-3.05	137.83	144.26
28	A	846	CLA	C3B-C4B-NB	-3.05	107.81	110.53
30	a	205	KC1	CHC-C1C-C2C	-3.04	120.23	125.03
28	A	832	CLA	C3B-C4B-NB	-3.04	107.82	110.53
28	11	304	CLA	C1D-CHD-C4C	-3.04	119.57	126.02
28	16	203	CLA	C3B-C4B-NB	-3.03	107.82	110.53
28	A	816	CLA	C3B-C4B-NB	-3.03	107.83	110.53
28	10	316	CLA	C3B-C4B-NB	-3.03	107.83	110.53
28	B	845	CLA	C1D-ND-C4D	-3.02	104.19	106.31
28	5	301	CLA	C3B-C4B-NB	-3.02	107.84	110.53
28	9	311	CLA	CHC-C4B-NB	-3.01	119.53	124.05
28	A	834	CLA	C3B-C4B-NB	-3.01	107.84	110.53
28	7	312	CLA	C3B-C4B-NB	-3.01	107.85	110.53
30	11	307	KC1	C4D-C3D-C2D	-3.01	103.37	107.42
28	9	308	CLA	C3B-C4B-NB	-3.00	107.85	110.53
30	9	306	KC1	C4D-C3D-C2D	-3.00	103.38	107.42
28	9	305	CLA	C4A-NA-C1A	2.99	108.05	106.68
28	A	836	CLA	C1-C2-C3	-2.99	121.29	126.20
28	11	314	CLA	C1D-CHD-C4C	-2.99	119.66	126.02
30	5	308	KC1	CHC-C1C-C2C	-2.99	120.31	125.03
28	F	802	CLA	CHA-C4D-ND	-2.99	126.38	132.55
30	17	306	KC1	CAA-CBA-CGA	2.99	142.25	127.05
28	1	304	CLA	C1D-CHD-C4C	-2.99	119.67	126.02
28	6	301	CLA	C1-C2-C3	-2.99	121.30	126.20
28	A	852	CLA	C1-C2-C3	-2.99	121.31	126.20
28	8	313	CLA	C1D-CHD-C4C	-2.98	119.68	126.02
28	B	847	CLA	C3B-C4B-NB	-2.98	107.87	110.53
32	10	315	XAT	C27-C28-C29	-2.98	120.91	125.53
28	L	203	CLA	C3B-C4B-NB	-2.98	107.87	110.53
28	13	307	CLA	C1D-CHD-C4C	-2.98	119.70	126.02
30	13	304	KC1	CHD-C4C-C3C	2.97	130.71	125.23
28	6	306	CLA	C1D-CHD-C4C	-2.97	119.70	126.02
30	8	307	KC1	CAD-C3D-C2D	-2.97	138.00	144.26
28	A	837	CLA	C1D-ND-C4D	-2.97	104.23	106.31
30	6	310	KC1	C1D-ND-C4D	-2.97	104.23	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	10	303	CLA	C1D-CHD-C4C	-2.97	119.71	126.02
30	13	304	KC1	C4D-C3D-C2D	-2.97	103.43	107.42
28	A	812	CLA	C3B-C4B-NB	-2.97	107.88	110.53
30	10	311	KC1	CHB-C4A-C3A	-2.97	120.34	125.03
30	1	306	KC1	CAD-C3D-C2D	-2.96	138.02	144.26
28	B	847	CLA	C1D-CHD-C4C	-2.96	119.73	126.02
28	A	852	CLA	C3B-C4B-NB	-2.96	107.89	110.53
28	19	202	CLA	CHC-C4B-NB	-2.95	119.62	124.05
28	17	309	CLA	C1D-CHD-C4C	-2.95	119.75	126.02
28	11	302	CLA	C1-C2-C3	-2.94	121.38	126.20
30	4	309	KC1	CHB-C4A-C3A	-2.94	120.38	125.03
28	13	305	CLA	C3B-C4B-NB	-2.94	107.91	110.53
28	5	304	CLA	C3B-C4B-NB	-2.94	107.91	110.53
28	A	805	CLA	C3B-C4B-NB	-2.93	107.91	110.53
28	13	301	CLA	C1D-CHD-C4C	-2.93	119.79	126.02
28	11	305	CLA	C1D-CHD-C4C	-2.93	119.79	126.02
28	17	307	CLA	C1D-CHD-C4C	-2.93	119.80	126.02
28	B	828	CLA	C3B-C4B-NB	-2.92	107.92	110.53
28	B	802	CLA	C3B-C4B-NB	-2.92	107.92	110.53
30	10	311	KC1	C4B-CHC-C1C	-2.92	119.82	126.02
28	11	309	CLA	C3B-C4B-NB	-2.91	107.93	110.53
28	A	803	CLA	C3B-C4B-NB	-2.91	107.93	110.53
30	10	310	KC1	CAD-C3D-C2D	-2.91	138.13	144.26
30	11	307	KC1	CAD-C3D-C2D	-2.91	138.13	144.26
28	1	301	CLA	C1D-CHD-C4C	-2.91	119.84	126.02
28	B	805	CLA	C1D-CHD-C4C	-2.91	119.84	126.02
28	A	807	CLA	C1-C2-C3	-2.91	121.44	126.20
30	6	305	KC1	C4D-C3D-C2D	-2.90	103.51	107.42
28	A	833	CLA	C1D-CHD-C4C	-2.90	119.85	126.02
30	8	306	KC1	C1A-C2A-C3A	-2.90	104.62	107.28
32	7	315	XAT	C26-C27-C28	2.90	132.12	125.99
28	11	312	CLA	C2A-C1A-CHA	2.89	128.89	123.87
28	7	318	CLA	C3B-C4B-NB	-2.89	107.95	110.53
28	11	303	CLA	C1D-CHD-C4C	-2.89	119.89	126.02
28	B	827	CLA	C3B-C4B-NB	-2.88	107.96	110.53
28	19	201	CLA	C3B-C4B-NB	-2.88	107.96	110.53
28	8	304	CLA	C1D-CHD-C4C	-2.88	119.90	126.02
30	8	306	KC1	CHC-C1C-C2C	-2.88	120.48	125.03
28	17	301	CLA	C1D-CHD-C4C	-2.87	119.91	126.02
30	4	309	KC1	C1B-CHB-C4A	-2.87	119.91	126.02
28	B	849	CLA	C4A-NA-C1A	2.87	107.99	106.68
30	11	307	KC1	C1A-NA-C4A	-2.87	105.37	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	A	833	CLA	C3B-C4B-NB	-2.87	107.97	110.53
30	5	308	KC1	C1A-NA-C4A	-2.86	105.37	106.68
28	15	201	CLA	C3B-C4B-NB	-2.86	107.98	110.53
28	A	845	CLA	CHA-C4D-ND	-2.86	126.64	132.55
30	6	310	KC1	CHB-C4A-C3A	-2.86	120.51	125.03
32	6	315	XAT	C30-C31-C32	2.86	131.48	123.20
28	A	814	CLA	C1D-ND-C4D	-2.86	104.31	106.31
28	B	811	CLA	C3B-C4B-NB	-2.85	107.98	110.53
28	A	847	CLA	C1-C2-C3	-2.85	121.52	126.20
28	A	827	CLA	C3B-C4B-NB	-2.85	107.98	110.53
30	4	311	KC1	CHD-C4C-C3C	2.85	130.48	125.23
28	B	807	CLA	C3B-C4B-NB	-2.85	107.98	110.53
30	6	305	KC1	C1B-CHB-C4A	-2.85	119.97	126.02
28	B	827	CLA	C1-C2-C3	-2.84	122.16	126.76
28	B	822	CLA	C1-C2-C3	-2.84	121.54	126.20
28	9	310	CLA	C1D-CHD-C4C	-2.84	119.98	126.02
33	B	839	BCR	C21-C20-C19	-2.84	114.98	123.20
28	3	303	CLA	C3B-C4B-NB	-2.84	108.00	110.53
28	17	303	CLA	C1D-CHD-C4C	-2.83	119.99	126.02
30	3	302	KC1	C4D-C3D-C2D	-2.83	103.61	107.42
28	3	307	CLA	C3B-C4B-NB	-2.83	108.00	110.53
28	17	309	CLA	C3D-C4D-ND	-2.83	105.38	109.99
28	B	849	CLA	C3B-C4B-NB	-2.83	108.00	110.53
29	5	312	A86	C10-C9-C8	2.83	131.39	123.20
32	13	309	XAT	C27-C28-C29	2.82	129.91	125.53
28	J	103	CLA	C1D-CHD-C4C	-2.82	120.02	126.02
28	a	202	CLA	C1D-CHD-C4C	-2.82	120.02	126.02
30	3	302	KC1	CHC-C1C-C2C	-2.82	120.57	125.03
28	A	809	CLA	C3B-C4B-NB	-2.82	108.01	110.53
28	B	816	CLA	C3B-C4B-NB	-2.82	108.01	110.53
28	17	305	CLA	C1D-CHD-C4C	-2.81	120.04	126.02
28	17	301	CLA	C3B-C4B-NB	-2.81	108.02	110.53
28	1	310	CLA	C3B-C4B-NB	-2.81	108.02	110.53
28	a	202	CLA	C3B-C4B-NB	-2.81	108.02	110.53
28	13	305	CLA	C1D-CHD-C4C	-2.81	120.04	126.02
28	7	303	CLA	C1D-CHD-C4C	-2.81	120.05	126.02
28	5	305	CLA	C3B-C4B-NB	-2.81	108.03	110.53
28	A	853	CLA	C3B-C4B-NB	-2.81	108.03	110.53
28	B	828	CLA	C1-C2-C3	-2.81	121.60	126.20
28	19	201	CLA	C1D-ND-C4D	2.80	108.28	106.31
33	L	202	BCR	C20-C19-C18	2.80	134.04	126.36
28	B	813	CLA	C3B-C4B-NB	-2.80	108.03	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	B	825	CLA	C3B-C4B-NB	-2.80	108.03	110.53
28	B	805	CLA	C1D-ND-C4D	2.79	108.27	106.31
28	17	305	CLA	C3B-C4B-NB	-2.79	108.04	110.53
28	7	318	CLA	CHC-C4B-NB	-2.79	119.86	124.05
28	B	802	CLA	CHA-C4D-ND	-2.79	126.79	132.55
32	5	307	XAT	C10-C11-C12	2.79	131.28	123.20
28	A	836	CLA	C3B-C4B-NB	-2.79	108.04	110.53
32	7	313	XAT	C26-C27-C28	2.78	131.88	125.99
28	5	303	CLA	C1D-CHD-C4C	-2.78	120.11	126.02
28	6	304	CLA	C1D-CHD-C4C	-2.78	120.11	126.02
28	a	204	CLA	C3B-C4B-NB	-2.78	108.05	110.53
28	8	301	CLA	C1D-CHD-C4C	-2.78	120.11	126.02
28	A	828	CLA	C3B-C4B-NB	-2.78	108.05	110.53
28	L	204	CLA	C3B-C4B-NB	-2.77	108.05	110.53
28	B	830	CLA	C3B-C4B-NB	-2.77	108.06	110.53
32	6	315	XAT	C10-C11-C12	2.77	131.22	123.20
28	3	304	CLA	C3B-C4B-NB	-2.77	108.06	110.53
32	4	315	XAT	C30-C31-C32	2.76	131.21	123.20
28	B	811	CLA	C1D-CHD-C4C	-2.76	120.15	126.02
28	1	304	CLA	C3B-C4B-NB	-2.76	108.07	110.53
28	L	206	CLA	CHD-C4C-NC	-2.76	119.95	124.23
28	11	305	CLA	C3B-C4B-NB	-2.76	108.07	110.53
28	A	829	CLA	C1-C2-C3	-2.76	122.30	126.76
30	4	312	KC1	C1B-CHB-C4A	-2.76	120.16	126.02
30	6	308	KC1	C4D-C3D-C2D	-2.75	103.71	107.42
28	A	845	CLA	C3B-C4B-NB	-2.75	108.07	110.53
28	A	801	CLA	CHA-C4D-ND	-2.75	126.87	132.55
28	A	811	CLA	C1-C2-C3	-2.75	121.69	126.20
28	7	303	CLA	C3B-C4B-NB	-2.75	108.08	110.53
28	9	310	CLA	C3B-C4B-NB	-2.75	108.08	110.53
30	13	304	KC1	CHB-C4A-C3A	-2.75	120.69	125.03
28	17	307	CLA	C3B-C4B-NB	-2.75	108.08	110.53
28	1	301	CLA	C3B-C4B-NB	-2.74	108.08	110.53
28	A	817	CLA	C3B-C4B-NB	-2.74	108.08	110.53
28	13	306	CLA	C3B-C4B-NB	-2.74	108.08	110.53
28	11	304	CLA	C1-C2-C3	-2.74	121.71	126.20
28	A	802	CLA	C3B-C4B-NB	-2.74	108.08	110.53
28	3	306	CLA	C3B-C4B-NB	-2.74	108.09	110.53
30	6	305	KC1	C1A-NA-C4A	-2.74	105.43	106.68
28	B	831	CLA	C4A-NA-C1A	2.74	107.93	106.68
28	7	308	CLA	C3B-C4B-NB	-2.73	108.09	110.53
28	A	837	CLA	C2A-C3A-C4A	-2.73	97.45	101.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	A	810	CLA	C3B-C4B-NB	-2.73	108.09	110.53
28	8	303	CLA	C1D-ND-C4D	-2.73	104.40	106.31
30	7	309	KC1	CAD-C3D-C2D	-2.73	138.51	144.26
28	J	102	CLA	C1D-CHD-C4C	-2.73	120.22	126.02
28	A	825	CLA	CHD-C4C-C3C	-2.73	120.80	124.77
28	A	802	CLA	C1D-ND-C4D	-2.73	104.40	106.31
28	B	803	CLA	C3B-C4B-NB	-2.73	108.09	110.53
30	7	307	KC1	CHC-C1C-C2C	-2.72	120.73	125.03
28	B	815	CLA	C1-C2-C3	-2.72	121.74	126.20
28	6	306	CLA	C3B-C4B-NB	-2.72	108.10	110.53
28	B	817	CLA	C3B-C4B-NB	-2.72	108.10	110.53
28	9	304	CLA	C3B-C4B-NB	-2.72	108.11	110.53
28	19	202	CLA	C1D-CHD-C4C	-2.72	120.25	126.02
28	L	206	CLA	C1D-CHD-C4C	-2.72	120.25	126.02
33	L	202	BCR	C23-C24-C25	2.72	134.25	127.00
33	A	850	BCR	C7-C8-C9	-2.71	122.22	126.23
32	5	311	XAT	C30-C31-C32	2.71	131.06	123.20
32	4	315	XAT	C15-C35-C34	2.71	129.06	123.52
28	A	818	CLA	C3B-C4B-NB	-2.71	108.11	110.53
28	16	205	CLA	C1D-ND-C4D	-2.71	104.41	106.31
28	13	301	CLA	C3B-C4B-NB	-2.71	108.11	110.53
30	1	306	KC1	C1B-CHB-C4A	-2.71	120.27	126.02
30	3	308	KC1	CAD-C3D-C2D	-2.70	138.56	144.26
28	B	813	CLA	C1D-CHD-C4C	-2.70	120.27	126.02
30	8	306	KC1	C4D-C3D-C2D	-2.70	103.78	107.42
28	7	304	CLA	C1-C2-C3	-2.70	121.77	126.20
30	9	309	KC1	C1B-CHB-C4A	-2.70	120.28	126.02
28	A	822	CLA	C3B-C4B-NB	-2.70	108.12	110.53
28	A	819	CLA	C3B-C4B-NB	-2.70	108.12	110.53
30	4	309	KC1	CAD-C3D-C2D	-2.69	138.59	144.26
28	3	305	CLA	C3B-C4B-NB	-2.69	108.13	110.53
28	A	801	CLA	C3B-C4B-NB	-2.69	108.13	110.53
28	A	831	CLA	C1-C2-C3	-2.69	122.41	126.76
28	4	305	CLA	C3B-C4B-NB	-2.69	108.13	110.53
30	8	307	KC1	C1D-ND-C4D	-2.69	104.43	106.31
30	6	310	KC1	C4D-C3D-C2D	-2.68	103.81	107.42
28	10	303	CLA	C3B-C4B-NB	-2.68	108.14	110.53
28	1	308	CLA	CHA-C4D-ND	-2.68	127.02	132.55
28	B	803	CLA	C1D-CHD-C4C	-2.68	120.32	126.02
28	B	808	CLA	C3B-C4B-NB	-2.68	108.14	110.53
28	16	205	CLA	C3B-C4B-NB	-2.68	108.14	110.53
32	1	311	XAT	C7-C8-C9	2.68	129.69	125.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	7	301	CLA	C3B-C4B-NB	-2.68	108.14	110.53
28	B	806	CLA	C3B-C4B-NB	-2.68	108.14	110.53
28	F	803	CLA	C3B-C4B-NB	-2.67	108.14	110.53
28	a	204	CLA	C1D-CHD-C4C	-2.67	120.35	126.02
28	17	305	CLA	C1-C2-C3	-2.67	122.45	126.76
28	F	802	CLA	C3B-C4B-NB	-2.66	108.15	110.53
32	7	316	XAT	C30-C31-C32	2.66	130.91	123.20
28	A	835	CLA	C1-C2-C3	-2.66	121.84	126.20
28	7	308	CLA	C1D-CHD-C4C	-2.66	120.37	126.02
28	4	307	CLA	C3B-C4B-NB	-2.66	108.16	110.53
28	A	824	CLA	C3B-C4B-NB	-2.65	108.16	110.53
28	11	301	CLA	C1D-CHD-C4C	-2.65	120.38	126.02
32	7	316	XAT	C15-C35-C34	2.65	128.95	123.52
28	A	836	CLA	C3D-C4D-ND	-2.65	105.67	109.99
33	B	839	BCR	C23-C24-C25	-2.65	119.92	127.00
28	B	829	CLA	C3B-C4B-NB	-2.64	108.17	110.53
28	5	303	CLA	C3B-C4B-NB	-2.64	108.17	110.53
28	B	805	CLA	CHA-C4D-ND	-2.64	127.10	132.55
28	3	303	CLA	C1-C2-C3	-2.64	121.87	126.20
28	7	301	CLA	C1-C2-C3	-2.64	121.87	126.20
28	8	302	CLA	C3B-C4B-NB	-2.64	108.17	110.53
28	13	302	CLA	C3B-C4B-NB	-2.64	108.17	110.53
29	5	312	A86	C3-C4-C5	2.64	128.92	123.52
28	A	836	CLA	CHA-C4D-ND	-2.64	127.10	132.55
28	6	311	CLA	C4A-NA-C1A	2.64	107.88	106.68
28	A	809	CLA	C1D-CHD-C4C	-2.64	120.41	126.02
28	7	318	CLA	C1D-ND-C4D	-2.64	104.46	106.31
30	7	307	KC1	C4B-CHC-C1C	-2.64	120.42	126.02
30	4	312	KC1	CHD-C1D-ND	-2.64	120.10	124.05
28	A	847	CLA	C1D-CHD-C4C	-2.63	120.43	126.02
30	5	308	KC1	C4B-CHC-C1C	-2.63	120.43	126.02
28	10	302	CLA	C3B-C4B-NB	-2.63	108.18	110.53
28	9	304	CLA	C3D-C4D-ND	-2.63	105.71	109.99
28	A	825	CLA	C3B-C4B-NB	-2.63	108.19	110.53
28	B	804	CLA	C1D-ND-C4D	-2.63	104.47	106.31
30	3	308	KC1	CHD-C4C-C3C	2.63	130.07	125.23
30	4	308	KC1	CHD-C4C-C3C	2.62	130.07	125.23
28	11	310	CLA	C1D-CHD-C4C	-2.62	120.44	126.02
29	1	302	A86	C4-C3-C2	2.62	128.89	123.52
28	10	308	CLA	C1D-ND-C4D	2.62	108.15	106.31
30	17	306	KC1	CHD-C1D-ND	-2.62	120.11	124.05
28	9	305	CLA	C3D-C2D-C1D	-2.62	102.26	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	A	811	CLA	C3B-C4B-NB	-2.62	108.19	110.53
28	B	848	CLA	C1D-CHD-C4C	-2.62	120.46	126.02
28	5	306	CLA	C1D-CHD-C4C	-2.62	120.46	126.02
28	A	813	CLA	C1-C2-C3	-2.62	122.53	126.76
30	4	312	KC1	CHD-C4C-C3C	2.61	130.05	125.23
28	9	305	CLA	C3B-C4B-NB	-2.61	108.20	110.53
32	9	313	XAT	C7-C8-C9	2.61	129.59	125.53
28	B	819	CLA	C3B-C4B-NB	-2.61	108.20	110.53
28	16	204	CLA	C3B-C4B-NB	-2.61	108.20	110.53
28	16	205	CLA	C1D-CHD-C4C	-2.61	120.47	126.02
32	4	318	XAT	C10-C11-C12	2.61	130.76	123.20
28	11	310	CLA	C3B-C4B-NB	-2.61	108.20	110.53
28	13	302	CLA	CHC-C4B-NB	-2.61	120.14	124.05
28	10	303	CLA	C1-C2-C3	-2.60	121.93	126.20
28	13	301	CLA	CHC-C4B-NB	-2.60	120.15	124.05
30	4	308	KC1	CHC-C1C-C2C	-2.60	120.92	125.03
28	11	306	CLA	C3B-C4B-NB	-2.60	108.21	110.53
28	4	310	CLA	C1D-ND-C4D	-2.60	104.49	106.31
30	a	205	KC1	C4D-C3D-C2D	-2.59	103.93	107.42
32	10	313	XAT	C27-C28-C29	2.59	129.55	125.53
30	4	312	KC1	C1A-C2A-C3A	-2.59	104.90	107.28
28	4	304	CLA	C1D-CHD-C4C	-2.59	120.52	126.02
28	3	314	CLA	C3B-C4B-NB	-2.59	108.22	110.53
28	17	302	CLA	C3B-C4B-NB	-2.59	108.22	110.53
30	4	311	KC1	CHD-C1D-ND	-2.59	120.17	124.05
28	A	823	CLA	CHD-C4C-C3C	-2.58	121.01	124.77
28	15	201	CLA	CHC-C4B-NB	-2.58	120.18	124.05
30	3	309	KC1	CHD-C1D-ND	-2.58	120.18	124.05
28	1	304	CLA	CHA-C4D-ND	-2.58	127.23	132.55
28	10	316	CLA	C1D-CHD-C4C	-2.57	120.55	126.02
28	6	303	CLA	C1D-CHD-C4C	-2.57	120.55	126.02
28	B	845	CLA	C3B-C4B-NB	-2.57	108.23	110.53
28	3	306	CLA	C1-C2-C3	-2.57	121.98	126.20
28	17	303	CLA	C3B-C4B-NB	-2.57	108.24	110.53
30	13	304	KC1	CHD-C1D-ND	-2.57	120.20	124.05
33	A	850	BCR	C15-C14-C13	2.56	130.87	127.28
28	A	826	CLA	C3B-C4B-NB	-2.56	108.25	110.53
28	7	305	CLA	C3B-C4B-NB	-2.56	108.25	110.53
28	4	305	CLA	C1D-CHD-C4C	-2.56	120.58	126.02
28	16	201	CLA	C1D-CHD-C4C	-2.56	120.59	126.02
32	7	315	XAT	O24-C25-C26	-2.55	56.90	58.93
28	1	308	CLA	C3B-C4B-NB	-2.55	108.25	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	4	304	CLA	C3D-C4D-ND	-2.55	105.84	109.99
28	F	802	CLA	C1D-ND-C4D	2.55	108.10	106.31
32	5	311	XAT	C15-C35-C34	2.55	128.74	123.52
28	6	313	CLA	C3D-C4D-ND	-2.55	105.84	109.99
30	8	306	KC1	CHD-C4C-C3C	2.55	129.93	125.23
28	J	103	CLA	C3B-C4B-NB	-2.55	108.25	110.53
33	A	850	BCR	C11-C12-C13	2.55	133.35	126.36
32	7	313	XAT	C6-C7-C8	2.54	131.37	125.99
28	9	305	CLA	C2A-C3A-C4A	-2.54	97.76	101.87
28	16	202	CLA	CHC-C4B-NB	-2.54	120.23	124.05
28	5	309	CLA	C3B-C4B-NB	-2.54	108.26	110.53
30	3	302	KC1	CAD-C3D-C2D	-2.54	138.91	144.26
30	6	310	KC1	C2A-C3A-C4A	-2.54	104.50	106.41
28	7	318	CLA	C3D-C4D-ND	-2.53	105.87	109.99
28	19	202	CLA	C3B-C4B-NB	-2.53	108.27	110.53
28	A	806	CLA	C1D-CHD-C4C	-2.53	120.64	126.02
30	4	311	KC1	C4B-CHC-C1C	-2.53	120.64	126.02
28	7	311	CLA	C1D-CHD-C4C	-2.53	120.64	126.02
30	6	308	KC1	CAD-C3D-C2D	-2.53	138.94	144.26
28	A	805	CLA	CHA-C1A-NA	-2.52	120.67	126.39
28	9	305	CLA	CHA-C4D-ND	-2.52	127.34	132.55
28	1	301	CLA	CHD-C4C-NC	-2.52	120.32	124.23
32	9	313	XAT	C4-C3-C2	2.52	114.48	111.03
28	8	302	CLA	C1D-CHD-C4C	-2.52	120.66	126.02
30	6	309	KC1	C1A-C2A-C3A	-2.52	104.97	107.28
28	A	815	CLA	C1D-ND-C4D	-2.52	104.55	106.31
28	B	821	CLA	C3D-C4D-ND	-2.52	105.89	109.99
28	4	303	CLA	CHC-C4B-NB	-2.52	120.28	124.05
28	11	304	CLA	C3D-C4D-ND	-2.52	105.90	109.99
28	B	820	CLA	C3B-C4B-NB	-2.51	108.29	110.53
28	11	302	CLA	C1D-ND-C4D	-2.51	104.55	106.31
30	9	306	KC1	C4B-CHC-C1C	-2.51	120.68	126.02
28	B	803	CLA	C3D-C4D-ND	-2.51	105.91	109.99
30	4	308	KC1	CAA-C2A-C1A	2.51	135.63	124.64
28	A	849	CLA	C1-C2-C3	-2.51	122.09	126.20
28	13	307	CLA	C3B-C4B-NB	-2.51	108.29	110.53
30	8	307	KC1	C4B-CHC-C1C	-2.51	120.69	126.02
30	17	312	KC1	CHD-C4C-C3C	2.50	129.84	125.23
28	A	807	CLA	C3B-C4B-NB	-2.50	108.30	110.53
28	8	304	CLA	C3B-C4B-NB	-2.50	108.30	110.53
28	1	301	CLA	CHA-C1A-NA	-2.50	120.74	126.39
28	3	303	CLA	C2A-C3A-C4A	-2.49	97.84	101.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	16	201	CLA	CHC-C4B-NB	-2.49	120.31	124.05
28	10	308	CLA	C3B-C4B-NB	-2.49	108.30	110.53
28	B	807	CLA	C1-C2-C3	-2.49	122.11	126.20
28	B	805	CLA	C3B-C4B-NB	-2.49	108.31	110.53
28	10	301	CLA	C1D-CHD-C4C	-2.49	120.73	126.02
28	B	824	CLA	C3D-C4D-ND	-2.49	105.94	109.99
28	6	303	CLA	C3B-C4B-NB	-2.49	108.31	110.53
28	A	837	CLA	C4A-NA-C1A	2.49	107.81	106.68
28	9	307	CLA	C1-C2-C3	-2.49	122.74	126.76
30	10	311	KC1	C4D-C3D-C2D	-2.48	104.08	107.42
30	7	309	KC1	C2A-C3A-C4A	-2.48	104.55	106.41
32	8	312	XAT	C10-C11-C12	2.48	130.38	123.20
28	B	821	CLA	C1D-CHD-C4C	-2.48	120.75	126.02
28	9	307	CLA	C3D-C4D-ND	-2.48	105.96	109.99
28	8	303	CLA	C3B-C4B-NB	-2.47	108.32	110.53
30	7	307	KC1	CAA-C2A-C1A	2.47	135.48	124.64
28	B	819	CLA	C2A-C3A-C4A	-2.47	97.87	101.87
28	6	313	CLA	C3B-C4B-NB	-2.47	108.32	110.53
28	11	301	CLA	C1-C2-C3	-2.47	122.15	126.20
28	B	833	CLA	C3B-C4B-NB	-2.47	108.33	110.53
28	B	809	CLA	C3B-C4B-NB	-2.47	108.33	110.53
28	R	204	CLA	C1D-CHD-C4C	-2.47	120.77	126.02
28	10	308	CLA	C1D-CHD-C4C	-2.47	120.78	126.02
28	10	307	CLA	C1D-ND-C4D	-2.47	104.58	106.31
28	9	308	CLA	CHC-C4B-NB	-2.46	120.35	124.05
28	A	801	CLA	CHA-C1A-NA	-2.46	120.82	126.39
28	3	307	CLA	C1D-CHD-C4C	-2.46	120.80	126.02
28	A	810	CLA	C1D-ND-C4D	-2.46	104.59	106.31
28	A	815	CLA	C3B-C4B-NB	-2.46	108.34	110.53
32	17	311	XAT	C26-C27-C28	2.45	131.18	125.99
28	17	304	CLA	CHA-C4D-ND	-2.45	127.48	132.55
28	13	302	CLA	C1D-ND-C4D	-2.45	104.59	106.31
28	9	308	CLA	C3D-C4D-ND	-2.45	106.00	109.99
30	a	205	KC1	CHD-C4C-C3C	2.45	129.75	125.23
28	7	302	CLA	C3B-C4B-NB	-2.45	108.34	110.53
28	6	303	CLA	C1-C2-C3	-2.45	122.18	126.20
28	B	827	CLA	C1D-CHD-C4C	-2.45	120.81	126.02
33	L	202	BCR	C24-C23-C22	-2.45	122.61	126.23
28	A	823	CLA	C3B-C4B-NB	-2.45	108.34	110.53
32	7	316	XAT	C10-C11-C12	2.45	130.29	123.20
30	3	308	KC1	CHD-C1D-ND	-2.45	120.38	124.05
28	B	809	CLA	C3D-C4D-ND	-2.45	106.01	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	B	808	CLA	C1D-CHD-C4C	-2.45	120.82	126.02
28	A	813	CLA	C3B-C4B-NB	-2.45	108.35	110.53
28	B	813	CLA	C1-C2-C3	-2.45	122.19	126.20
30	a	205	KC1	C1A-NA-C4A	-2.45	105.56	106.68
28	A	821	CLA	C3B-C4B-NB	-2.45	108.35	110.53
28	5	306	CLA	C1D-ND-C4D	-2.44	104.60	106.31
28	A	833	CLA	C3D-C4D-ND	-2.44	106.02	109.99
28	A	831	CLA	C3B-C4B-NB	-2.44	108.35	110.53
28	11	310	CLA	C1-C2-C3	-2.44	122.82	126.76
30	a	205	KC1	CHD-C1D-ND	-2.44	120.39	124.05
28	A	824	CLA	C3D-C4D-ND	-2.44	106.03	109.99
28	1	307	CLA	C3B-C4B-NB	-2.44	108.36	110.53
30	7	309	KC1	C4D-C3D-C2D	-2.43	104.14	107.42
28	A	803	CLA	C1D-ND-C4D	-2.43	104.60	106.31
28	B	826	CLA	C3B-C4B-NB	-2.43	108.36	110.53
28	19	201	CLA	C1D-CHD-C4C	-2.43	120.85	126.02
28	3	305	CLA	C1-C2-C3	-2.43	122.21	126.20
28	10	309	CLA	C1D-CHD-C4C	-2.43	120.85	126.02
30	8	307	KC1	CHD-C4C-C3C	2.43	129.71	125.23
28	16	203	CLA	C1D-CHD-C4C	-2.43	120.86	126.02
30	3	302	KC1	CHD-C4C-C3C	2.43	129.71	125.23
28	11	312	CLA	C3B-C4B-NB	-2.43	108.36	110.53
28	4	310	CLA	C3B-C4B-NB	-2.43	108.36	110.53
28	4	306	CLA	CHA-C4D-ND	-2.43	127.54	132.55
28	1	307	CLA	C3D-C4D-ND	-2.43	106.04	109.99
28	1	305	CLA	C2A-C3A-C4A	-2.42	97.96	101.87
28	A	816	CLA	C1-C2-C3	-2.42	122.23	126.20
28	6	311	CLA	C3B-C4B-NB	-2.42	108.37	110.53
28	16	201	CLA	C3B-C4B-NB	-2.42	108.37	110.53
28	A	812	CLA	C1D-ND-C4D	-2.42	104.62	106.31
30	6	309	KC1	CHD-C4C-C3C	2.41	129.68	125.23
28	17	301	CLA	CHC-C4B-NB	-2.41	120.43	124.05
28	A	806	CLA	C3B-C4B-NB	-2.41	108.38	110.53
30	5	308	KC1	C1B-CHB-C4A	-2.41	120.89	126.02
28	B	807	CLA	C1D-CHD-C4C	-2.41	120.89	126.02
28	1	314	CLA	C3D-C4D-ND	-2.41	106.07	109.99
28	A	814	CLA	C3B-C4B-NB	-2.41	108.38	110.53
28	A	825	CLA	C1D-CHD-C4C	-2.41	120.90	126.02
28	B	818	CLA	C3B-C4B-NB	-2.41	108.38	110.53
28	9	304	CLA	C1-C2-C3	-2.41	122.87	126.76
28	16	204	CLA	CHC-C4B-NB	-2.40	120.44	124.05
28	5	302	CLA	C3B-C4B-NB	-2.40	108.38	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	B	822	CLA	C3B-C4B-NB	-2.40	108.38	110.53
28	10	302	CLA	C1D-ND-C4D	-2.40	104.63	106.31
28	16	204	CLA	C1D-ND-C4D	-2.40	104.63	106.31
30	3	308	KC1	CBA-CAA-C2A	2.40	135.10	125.45
28	B	811	CLA	C1D-ND-C4D	-2.40	104.63	106.31
28	8	313	CLA	CHD-C4C-NC	-2.40	120.51	124.23
28	B	825	CLA	CHA-C4D-ND	-2.40	127.60	132.55
28	B	819	CLA	C1D-ND-C4D	-2.40	104.63	106.31
28	A	818	CLA	CHD-C4C-C3C	-2.40	121.28	124.77
28	L	204	CLA	C1-C2-C3	-2.40	122.89	126.76
28	R	202	CLA	C3B-C4B-NB	-2.40	108.39	110.53
30	9	306	KC1	CHD-C4C-C3C	2.39	129.64	125.23
28	11	305	CLA	C3D-C4D-ND	-2.39	106.09	109.99
28	1	307	CLA	C1D-ND-C4D	-2.39	104.63	106.31
28	A	827	CLA	C1D-CHD-C4C	-2.39	120.93	126.02
28	9	305	CLA	CMD-C2D-C1D	2.39	128.94	124.73
30	8	307	KC1	C1A-NA-C4A	2.39	107.77	106.68
28	B	829	CLA	CHD-C4C-C3C	-2.39	121.29	124.77
28	17	303	CLA	C3D-C4D-ND	-2.38	106.11	109.99
28	B	801	CLA	C1D-CHD-C4C	-2.38	120.95	126.02
28	11	302	CLA	C3D-C4D-ND	-2.38	106.11	109.99
29	6	314	A86	C3-C4-C5	2.38	128.39	123.52
29	3	311	A86	C10-C9-C8	2.38	130.10	123.20
32	7	317	XAT	C30-C31-C32	2.38	130.10	123.20
30	10	304	KC1	CHD-C4C-C3C	2.38	129.62	125.23
28	11	302	CLA	CHD-C4C-C3C	-2.38	121.30	124.77
28	A	849	CLA	C1D-CHD-C4C	-2.38	120.96	126.02
30	3	308	KC1	C4B-CHC-C1C	-2.38	120.96	126.02
32	7	314	XAT	C27-C28-C29	2.38	129.22	125.53
30	4	312	KC1	C4B-CHC-C1C	-2.38	120.97	126.02
28	A	849	CLA	C3B-C4B-NB	-2.38	108.41	110.53
28	6	302	CLA	C3B-C4B-NB	-2.38	108.41	110.53
28	7	303	CLA	C3D-C4D-ND	-2.38	106.12	109.99
29	10	312	A86	C3-C4-C5	2.38	128.38	123.52
28	9	303	CLA	C3D-C4D-ND	-2.38	106.12	109.99
28	7	303	CLA	C1-C2-C3	-2.37	122.31	126.20
32	7	317	XAT	C35-C15-C14	2.37	128.38	123.52
28	6	306	CLA	C4D-C3D-CAD	-2.37	105.53	108.11
32	7	317	XAT	C26-C27-C28	2.37	131.01	125.99
30	10	311	KC1	CHD-C4C-C3C	2.37	129.60	125.23
28	A	852	CLA	CHA-C1A-NA	-2.37	121.02	126.39
30	8	306	KC1	CAD-C3D-C2D	-2.37	139.26	144.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	8	307	KC1	CHD-C1D-ND	-2.37	120.49	124.05
30	4	309	KC1	C4B-CHC-C1C	-2.37	120.98	126.02
28	19	201	CLA	CHB-C1B-NB	-2.37	120.50	124.05
28	1	303	CLA	C1D-CHD-C4C	-2.37	120.99	126.02
30	7	307	KC1	CGD-CBD-CAD	-2.37	103.18	110.85
28	7	302	CLA	CHA-C1A-NA	-2.36	121.04	126.39
29	6	314	A86	C33-C32-C31	2.36	111.51	109.21
33	B	839	BCR	C16-C17-C18	2.36	130.59	127.28
28	B	832	CLA	C3B-C4B-NB	-2.36	108.42	110.53
29	10	312	A86	C33-C32-C31	2.36	111.51	109.21
28	a	201	CLA	C1D-CHD-C4C	-2.36	121.00	126.02
28	1	314	CLA	C3B-C4B-NB	-2.36	108.42	110.53
28	B	834	CLA	C3B-C4B-NB	-2.36	108.42	110.53
28	B	812	CLA	CHA-C4D-ND	-2.36	127.68	132.55
28	16	203	CLA	CHC-C4B-NB	-2.36	120.51	124.05
28	8	310	CLA	C3B-C4B-NB	-2.36	108.42	110.53
28	B	843	CLA	C3B-C4B-NB	-2.36	108.42	110.53
28	17	307	CLA	C1D-ND-C4D	-2.36	104.66	106.31
28	A	830	CLA	C3B-C4B-NB	-2.36	108.43	110.53
28	B	825	CLA	CHD-C4C-C3C	-2.35	121.34	124.77
28	7	301	CLA	CHD-C4C-C3C	-2.35	121.34	124.77
28	A	834	CLA	C1-C2-C3	-2.35	122.35	126.20
28	16	202	CLA	C3D-C4D-ND	-2.35	106.17	109.99
28	4	310	CLA	C1D-CHD-C4C	-2.35	121.03	126.02
28	1	305	CLA	CMD-C2D-C1D	2.35	128.86	124.73
30	9	306	KC1	CHD-C1D-ND	-2.35	120.53	124.05
30	5	308	KC1	CHD-C4C-C3C	2.34	129.55	125.23
30	17	306	KC1	CHD-C4C-C3C	2.34	129.55	125.23
32	7	317	XAT	O4-C5-C6	-2.34	57.07	58.93
28	4	306	CLA	C3B-C4B-NB	-2.34	108.44	110.53
28	8	313	CLA	C4D-C3D-CAD	-2.34	105.56	108.11
28	8	305	CLA	C3B-C4B-NB	-2.34	108.44	110.53
28	a	204	CLA	CHC-C4B-NB	-2.34	120.54	124.05
28	9	310	CLA	C3D-C4D-ND	-2.34	106.18	109.99
28	13	301	CLA	C1-C2-C3	-2.34	122.37	126.20
28	B	807	CLA	C3D-C4D-ND	-2.34	106.19	109.99
28	B	843	CLA	CHD-C4C-C3C	-2.34	121.37	124.77
32	7	315	XAT	C7-C8-C9	2.33	129.15	125.53
30	13	304	KC1	C2A-C3A-C4A	-2.33	104.66	106.41
28	17	309	CLA	C4B-CHC-C1C	-2.33	120.76	126.25
30	10	311	KC1	CHD-C1D-ND	-2.33	120.55	124.05
28	10	306	CLA	C1-C2-C3	-2.33	122.38	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	7	307	KC1	CHB-C4A-C3A	-2.33	121.35	125.03
28	A	804	CLA	CHA-C4D-ND	-2.33	127.74	132.55
28	A	853	CLA	CHA-C1A-NA	-2.33	121.12	126.39
28	B	824	CLA	C1-C2-C3	-2.33	122.38	126.20
28	A	820	CLA	C3B-C4B-NB	-2.33	108.45	110.53
30	17	306	KC1	C4D-C3D-C2D	-2.32	104.29	107.42
28	A	808	CLA	C1-C2-C3	-2.32	122.39	126.20
30	a	205	KC1	CAD-C3D-C2D	-2.32	139.37	144.26
30	4	309	KC1	C1A-C2A-C3A	-2.32	105.15	107.28
28	a	203	CLA	CHC-C4B-NB	-2.32	120.57	124.05
28	11	303	CLA	C3D-C4D-ND	-2.32	106.21	109.99
30	10	311	KC1	C1A-C2A-C3A	-2.32	105.15	107.28
30	10	310	KC1	C4D-C3D-C2D	-2.32	104.30	107.42
28	7	318	CLA	CHB-C1B-NB	-2.32	120.58	124.05
30	9	309	KC1	C1A-C2A-C3A	-2.31	105.15	107.28
28	17	309	CLA	C3B-C4B-NB	-2.31	108.47	110.53
28	B	817	CLA	C1D-CHD-C4C	-2.31	121.11	126.02
28	6	302	CLA	C1-C2-C3	-2.31	122.41	126.20
32	10	313	XAT	C7-C8-C9	2.31	129.11	125.53
30	9	309	KC1	C4B-CHC-C1C	-2.31	121.12	126.02
28	8	303	CLA	C3D-C4D-ND	-2.31	106.24	109.99
30	7	307	KC1	C1D-ND-C4D	-2.30	104.69	106.31
28	B	848	CLA	CHD-C4C-C3C	-2.30	121.41	124.77
30	8	306	KC1	C4B-CHC-C1C	-2.30	121.12	126.02
28	A	815	CLA	C1-C2-C3	-2.30	122.43	126.20
28	A	821	CLA	C1-C2-C3	-2.30	122.43	126.20
28	5	301	CLA	C1D-CHD-C4C	-2.30	121.13	126.02
28	A	813	CLA	CHD-C4C-C3C	-2.30	121.42	124.77
28	3	301	CLA	C1-C2-C3	-2.30	122.43	126.20
28	3	304	CLA	C1D-CHD-C4C	-2.30	121.14	126.02
28	13	303	CLA	CHC-C4B-NB	-2.29	120.61	124.05
28	15	201	CLA	CHB-C1B-NB	-2.29	120.61	124.05
28	8	304	CLA	C3D-C4D-ND	-2.29	106.26	109.99
28	1	304	CLA	C3D-C4D-ND	-2.29	106.26	109.99
28	17	304	CLA	C1D-CHD-C4C	-2.29	121.15	126.02
28	A	822	CLA	C2A-C3A-C4A	-2.29	98.17	101.87
32	J	105	XAT	C38-C25-C26	2.29	126.07	122.30
30	8	306	KC1	CHD-C1D-ND	-2.29	120.61	124.05
28	10	306	CLA	C3B-C4B-NB	-2.29	108.49	110.53
28	9	303	CLA	CHA-C4D-ND	-2.29	127.83	132.55
28	8	301	CLA	CHA-C4D-ND	-2.29	127.83	132.55
30	9	309	KC1	CHD-C1D-ND	-2.28	120.62	124.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	A	823	CLA	C3D-C4D-ND	-2.28	106.27	109.99
28	A	821	CLA	CHD-C4C-C3C	-2.28	121.44	124.77
28	17	307	CLA	CHB-C1B-NB	-2.28	120.62	124.05
28	17	304	CLA	C1D-ND-C4D	-2.28	104.71	106.31
30	4	309	KC1	CHD-C4C-C3C	2.28	129.43	125.23
28	B	817	CLA	CHA-C4D-ND	-2.28	127.84	132.55
32	5	310	XAT	O24-C25-C26	-2.28	57.12	58.93
28	3	303	CLA	C4A-NA-C1A	2.28	107.72	106.68
28	7	306	CLA	CHD-C4C-C3C	-2.28	121.45	124.77
28	R	204	CLA	C1-C2-C3	-2.28	122.46	126.20
28	16	202	CLA	CHB-C1B-NB	-2.28	120.63	124.05
30	13	304	KC1	CAD-C3D-C2D	-2.28	139.47	144.26
29	3	310	A86	C26-C25-C24	2.28	129.80	123.20
29	3	310	A86	C36-C31-C32	-2.28	117.44	119.70
28	B	814	CLA	CMD-C2D-C1D	2.28	128.74	124.73
28	4	307	CLA	C3D-C4D-ND	-2.28	106.29	109.99
28	4	303	CLA	CHB-C1B-NB	-2.27	120.64	124.05
28	a	202	CLA	CHC-C4B-NB	-2.27	120.64	124.05
28	A	819	CLA	C1D-CHD-C4C	-2.27	121.19	126.02
28	A	847	CLA	C3B-C4B-NB	-2.27	108.50	110.53
28	B	832	CLA	CHA-C1A-NA	-2.27	121.24	126.39
30	6	310	KC1	C1A-NA-C4A	-2.27	105.64	106.68
28	3	306	CLA	C1D-ND-C4D	-2.27	104.72	106.31
28	B	801	CLA	C3D-C4D-ND	-2.27	106.30	109.99
30	6	308	KC1	CHD-C4C-C3C	2.27	129.41	125.23
28	9	311	CLA	CHB-C1B-NB	-2.27	120.65	124.05
28	B	823	CLA	C1-C2-C3	-2.27	122.49	126.20
28	7	306	CLA	C3D-C4D-ND	-2.26	106.30	109.99
30	10	304	KC1	CHD-C1D-ND	-2.26	120.65	124.05
28	9	308	CLA	C1D-CHD-C4C	-2.26	121.21	126.02
28	5	304	CLA	C3D-C4D-ND	-2.26	106.31	109.99
28	a	203	CLA	C3D-C4D-ND	-2.26	106.31	109.99
30	8	307	KC1	CAA-C2A-C1A	2.26	134.56	124.64
28	13	305	CLA	CHC-C1C-NC	-2.26	120.90	124.31
28	A	835	CLA	CHA-C1A-NA	-2.26	121.27	126.39
28	B	835	CLA	C3B-C4B-NB	-2.26	108.51	110.53
28	A	810	CLA	C3D-C4D-ND	-2.26	106.31	109.99
32	7	316	XAT	C35-C15-C14	-2.26	118.90	123.52
28	17	305	CLA	CHC-C4B-NB	-2.26	120.66	124.05
30	10	311	KC1	CHC-C1C-C2C	-2.26	121.47	125.03
30	5	308	KC1	CHD-C1D-ND	-2.26	120.66	124.05
28	13	303	CLA	CHB-C1B-NB	-2.26	120.67	124.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	6	304	CLA	CHD-C4C-NC	-2.25	120.74	124.23
32	13	309	XAT	C7-C8-C9	2.25	129.03	125.53
28	4	303	CLA	C4B-C3B-C2B	-2.25	104.50	107.30
28	11	304	CLA	C3B-C4B-NB	-2.25	108.52	110.53
28	1	303	CLA	C1-C2-C3	-2.25	122.51	126.20
33	L	202	BCR	C19-C18-C17	-2.25	115.47	119.01
28	16	201	CLA	CHA-C1A-NA	-2.25	121.31	126.39
30	10	310	KC1	CHD-C4C-C3C	2.24	129.37	125.23
28	A	853	CLA	C1-C2-C3	-2.24	122.52	126.20
33	A	850	BCR	C15-C16-C17	-2.24	118.93	123.52
28	11	302	CLA	C3B-C4B-NB	-2.24	108.53	110.53
28	B	831	CLA	CHA-C4D-ND	-2.24	127.92	132.55
28	5	302	CLA	C3D-C4D-ND	-2.24	106.34	109.99
28	a	201	CLA	CHC-C4B-NB	-2.24	120.69	124.05
28	15	201	CLA	C1D-CHD-C4C	-2.24	121.26	126.02
28	5	302	CLA	CHD-C4C-C3C	-2.24	121.51	124.77
32	17	311	XAT	C7-C8-C9	2.24	129.00	125.53
28	6	311	CLA	CHD-C4C-NC	-2.24	120.77	124.23
28	1	301	CLA	C1-C2-C3	-2.24	123.14	126.76
28	9	305	CLA	C1D-CHD-C4C	-2.24	121.27	126.02
28	17	303	CLA	CHC-C1C-NC	-2.24	120.94	124.31
28	9	311	CLA	C3B-C4B-NB	-2.23	108.53	110.53
28	13	302	CLA	C1D-CHD-C4C	-2.23	121.27	126.02
28	1	308	CLA	CHC-C1C-NC	-2.23	120.95	124.31
28	10	302	CLA	C3D-C4D-ND	-2.23	106.36	109.99
28	5	309	CLA	C1-C2-C3	-2.23	123.15	126.76
28	A	803	CLA	C1D-CHD-C4C	-2.23	121.28	126.02
28	11	312	CLA	CHC-C1C-NC	-2.23	120.95	124.31
30	6	308	KC1	C2A-C3A-C4A	-2.23	104.74	106.41
28	5	309	CLA	CHC-C1C-NC	-2.23	120.95	124.31
28	a	203	CLA	CHB-C1B-NB	-2.23	120.71	124.05
30	6	309	KC1	C1B-CHB-C4A	-2.23	121.29	126.02
28	7	318	CLA	CHC-C1C-NC	-2.22	120.96	124.31
30	1	306	KC1	CHD-C4C-C3C	2.22	129.33	125.23
28	L	201	CLA	C3B-C4B-NB	-2.22	108.55	110.53
28	17	309	CLA	CHC-C1C-NC	-2.22	120.96	124.31
28	B	813	CLA	C3D-C4D-ND	-2.22	106.37	109.99
28	B	834	CLA	C3D-C4D-ND	-2.22	106.38	109.99
30	5	308	KC1	CAD-C3D-C2D	-2.22	139.58	144.26
28	9	308	CLA	C1D-ND-C4D	-2.22	104.75	106.31
30	3	309	KC1	CHD-C4C-C3C	2.22	129.32	125.23
28	B	847	CLA	C1-C2-C3	-2.22	122.56	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	13	306	CLA	C3D-C4D-ND	-2.22	106.38	109.99
32	7	314	XAT	C7-C8-C9	2.22	128.97	125.53
30	4	308	KC1	C2A-C3A-C4A	-2.22	104.75	106.41
28	7	302	CLA	CHD-C4C-C3C	-2.22	121.54	124.77
28	J	103	CLA	C3D-C4D-ND	-2.22	106.38	109.99
30	9	306	KC1	CAA-C2A-C1A	2.21	134.35	124.64
30	7	309	KC1	CHD-C4C-C3C	2.21	129.31	125.23
28	8	310	CLA	CHC-C1C-NC	-2.21	120.98	124.31
28	B	802	CLA	CHA-C1A-NA	-2.21	121.38	126.39
30	10	304	KC1	C1A-NA-C4A	-2.21	105.67	106.68
28	A	846	CLA	C3D-C4D-ND	-2.21	106.39	109.99
28	B	814	CLA	CHD-C4C-C3C	-2.21	121.55	124.77
28	L	201	CLA	C1D-CHD-C4C	-2.21	121.31	126.02
30	7	307	KC1	CHD-C4C-C3C	2.21	129.31	125.23
28	5	313	CLA	C3B-C4B-NB	-2.21	108.56	110.53
28	10	301	CLA	CHD-C4C-NC	-2.21	120.81	124.23
28	B	818	CLA	C1D-ND-C4D	-2.21	104.76	106.31
28	13	301	CLA	CHC-C1C-NC	-2.21	120.98	124.31
28	4	304	CLA	C3B-C4B-NB	-2.21	108.56	110.53
28	A	817	CLA	C1D-ND-C4D	-2.21	104.76	106.31
28	A	824	CLA	CED-O2D-CGD	2.21	120.92	115.92
28	11	312	CLA	CHA-C1A-NA	-2.21	121.39	126.39
28	B	825	CLA	C3D-C4D-ND	-2.21	106.40	109.99
28	6	301	CLA	C1D-CHD-C4C	-2.21	121.33	126.02
29	10	317	A86	C26-C25-C24	2.21	129.59	123.20
28	7	303	CLA	CHA-C4D-ND	-2.20	128.00	132.55
28	A	829	CLA	CHA-C4D-ND	-2.20	128.00	132.55
28	17	305	CLA	CHC-C1C-NC	-2.20	120.99	124.31
32	17	311	XAT	O24-C25-C26	-2.20	57.18	58.93
28	17	307	CLA	CHC-C1C-NC	-2.20	120.99	124.31
28	19	202	CLA	CHC-C1C-NC	-2.20	120.99	124.31
28	6	303	CLA	CHD-C4C-C3C	-2.20	121.56	124.77
29	10	312	A86	C4-C3-C2	-2.20	119.01	123.52
28	5	301	CLA	CHD-C4C-C3C	-2.20	121.56	124.77
28	9	307	CLA	C1D-CHD-C4C	-2.20	121.34	126.02
28	A	852	CLA	CHD-C4C-C3C	-2.20	121.57	124.77
28	5	305	CLA	CHA-C4D-ND	-2.20	128.01	132.55
28	11	314	CLA	CHB-C1B-NB	-2.20	120.75	124.05
28	A	805	CLA	CHA-C4D-ND	-2.20	128.02	132.55
28	9	308	CLA	CHA-C4D-ND	-2.19	128.02	132.55
28	15	201	CLA	C1D-ND-C4D	-2.19	104.77	106.31
28	B	826	CLA	C1-C2-C3	-2.19	122.60	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	3	309	KC1	CAD-C3D-C2D	-2.19	139.65	144.26
28	10	302	CLA	CHD-C4C-C3C	-2.19	121.58	124.77
28	B	808	CLA	C1-C2-C3	-2.19	122.61	126.20
28	9	311	CLA	C1D-CHD-C4C	-2.19	121.36	126.02
30	4	308	KC1	C4B-CHC-C1C	-2.19	121.36	126.02
28	A	845	CLA	CHA-C1A-NA	-2.19	121.43	126.39
28	16	204	CLA	CHA-C1A-NA	-2.19	121.43	126.39
28	A	804	CLA	C3B-C4B-NB	-2.19	108.58	110.53
28	A	837	CLA	C3D-C4D-ND	-2.19	106.43	109.99
28	B	833	CLA	C1D-ND-C4D	-2.19	104.78	106.31
28	6	311	CLA	C2A-C3A-C4A	-2.19	98.34	101.87
28	1	304	CLA	CMD-C2D-C1D	2.19	128.58	124.73
28	1	308	CLA	CHB-C1B-NB	-2.19	120.77	124.05
28	17	301	CLA	C1-C2-C3	-2.19	123.23	126.76
28	A	837	CLA	C1D-CHD-C4C	-2.19	121.37	126.02
28	11	306	CLA	CHC-C1C-NC	-2.18	121.02	124.31
28	4	316	CLA	CHA-C4D-ND	-2.18	128.05	132.55
28	16	204	CLA	CHC-C1C-NC	-2.18	121.03	124.31
32	J	105	XAT	C26-C27-C28	2.18	130.60	125.99
32	6	315	XAT	O24-C25-C26	-2.18	57.20	58.93
30	11	307	KC1	CHD-C4C-C3C	2.18	129.24	125.23
28	13	301	CLA	CHB-C1B-NB	-2.18	120.78	124.05
28	4	307	CLA	CHC-C1C-NC	-2.18	121.03	124.31
28	A	809	CLA	C1-C2-C3	-2.17	122.63	126.20
28	B	849	CLA	CHD-C4C-C3C	-2.17	121.60	124.77
28	16	203	CLA	CHB-C1B-NB	-2.17	120.79	124.05
28	11	305	CLA	CHC-C1C-NC	-2.17	121.04	124.31
28	B	829	CLA	CMD-C2D-C1D	2.17	128.56	124.73
28	B	831	CLA	C2A-C3A-C4A	-2.17	98.36	101.87
30	3	308	KC1	C1D-ND-C4D	2.17	107.83	106.31
33	L	202	BCR	C15-C14-C13	2.17	130.32	127.28
28	A	812	CLA	C1-C2-C3	-2.17	122.64	126.20
28	8	313	CLA	C3D-C4D-ND	-2.17	106.46	109.99
30	13	304	KC1	C3C-C4C-NC	-2.17	107.58	109.90
28	11	305	CLA	CHA-C4D-ND	-2.17	128.07	132.55
28	1	301	CLA	CMD-C2D-C1D	2.17	128.55	124.73
28	8	301	CLA	CMD-C2D-C1D	2.17	128.54	124.73
28	A	835	CLA	C1D-CHD-C4C	-2.17	121.41	126.02
28	B	824	CLA	C1D-CHD-C4C	-2.17	121.41	126.02
30	17	306	KC1	CBA-CAA-C2A	2.17	134.15	125.45
28	7	301	CLA	CHA-C4D-ND	-2.16	128.08	132.55
28	A	808	CLA	C3D-C4D-ND	-2.16	106.47	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	4	309	KC1	CHC-C1C-C2C	-2.16	121.61	125.03
28	A	823	CLA	C1D-ND-C4D	-2.16	104.79	106.31
28	3	305	CLA	C1D-CHD-C4C	-2.16	121.42	126.02
28	8	301	CLA	C1-C2-C3	-2.16	122.66	126.20
28	B	806	CLA	C4D-C3D-CAD	-2.16	105.76	108.11
28	4	305	CLA	CHA-C4D-ND	-2.16	128.09	132.55
28	a	204	CLA	CHB-C1B-NB	-2.16	120.81	124.05
28	a	204	CLA	CHC-C1C-NC	-2.16	121.06	124.31
28	3	314	CLA	C3D-C4D-ND	-2.16	106.47	109.99
28	4	303	CLA	C3D-C4D-ND	-2.16	106.48	109.99
30	4	308	KC1	C3C-C4C-NC	-2.16	107.59	109.90
28	a	202	CLA	CHB-C1B-NB	-2.16	120.81	124.05
28	5	303	CLA	C4D-C3D-CAD	-2.16	105.77	108.11
28	B	828	CLA	C1D-CHD-C4C	-2.16	121.44	126.02
28	1	301	CLA	C1D-ND-C4D	-2.15	104.80	106.31
28	B	814	CLA	C3D-C4D-ND	-2.15	106.48	109.99
28	B	832	CLA	C3D-C4D-ND	-2.15	106.48	109.99
28	1	301	CLA	CHC-C1C-NC	-2.15	121.07	124.31
28	5	302	CLA	C1D-ND-C4D	-2.15	104.80	106.31
28	16	201	CLA	C1D-ND-C4D	-2.15	104.80	106.31
28	4	316	CLA	C1D-CHD-C4C	-2.15	121.44	126.02
28	a	201	CLA	CHB-C1B-NB	-2.15	120.82	124.05
28	19	201	CLA	CHC-C1C-NC	-2.15	121.07	124.31
33	B	840	BCR	C24-C23-C22	2.15	129.41	126.23
30	11	307	KC1	C2A-C3A-C4A	-2.15	104.80	106.41
30	10	310	KC1	C4B-CHC-C1C	-2.15	121.45	126.02
28	13	307	CLA	C4D-C3D-CAD	-2.15	105.77	108.11
32	5	307	XAT	C6-C7-C8	2.15	130.53	125.99
28	13	301	CLA	C3D-C2D-C1D	-2.15	102.90	105.83
28	A	825	CLA	C3D-C4D-ND	-2.15	106.50	109.99
32	1	311	XAT	C26-C27-C28	-2.14	121.46	125.99
28	4	304	CLA	CHD-C4C-C3C	-2.14	121.65	124.77
28	3	307	CLA	CHC-C1C-NC	-2.14	121.08	124.31
28	13	306	CLA	CHC-C1C-NC	-2.14	121.08	124.31
28	8	304	CLA	C1-C2-C3	-2.14	122.69	126.20
30	4	312	KC1	CHB-C4A-C3A	-2.14	121.65	125.03
28	3	305	CLA	CHA-C4D-ND	-2.14	128.13	132.55
28	B	810	CLA	C3D-C4D-ND	-2.14	106.51	109.99
28	13	301	CLA	CMD-C2D-C1D	2.14	128.50	124.73
28	4	316	CLA	CHC-C4B-NB	-2.14	120.84	124.05
28	3	306	CLA	C1D-CHD-C4C	-2.14	121.48	126.02
28	B	834	CLA	CHD-C4C-C3C	-2.14	121.66	124.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	17	306	KC1	C1B-CHB-C4A	-2.14	121.48	126.02
28	A	815	CLA	C4D-C3D-CAD	-2.14	105.79	108.11
28	19	202	CLA	C1D-ND-C4D	-2.13	104.81	106.31
28	A	803	CLA	CMD-C2D-C1D	2.13	128.49	124.73
28	10	303	CLA	CHA-C4D-ND	-2.13	128.15	132.55
28	A	829	CLA	C1D-ND-C4D	2.13	107.81	106.31
30	17	312	KC1	C4B-CHC-C1C	-2.13	121.49	126.02
30	3	302	KC1	C1B-CHB-C4A	-2.13	121.49	126.02
30	4	311	KC1	C3C-C4C-NC	-2.13	107.62	109.90
28	A	804	CLA	C1D-CHD-C4C	-2.13	121.50	126.02
28	13	302	CLA	CHB-C1B-NB	-2.13	120.86	124.05
28	A	826	CLA	C3D-C4D-ND	-2.13	106.53	109.99
28	5	306	CLA	C3D-C2D-C1D	-2.13	102.93	105.83
28	7	301	CLA	C3D-C4D-ND	-2.13	106.53	109.99
28	7	305	CLA	C1-C2-C3	-2.13	122.71	126.20
28	9	303	CLA	CHC-C1C-NC	-2.13	121.11	124.31
30	9	309	KC1	CHD-C4C-C3C	2.12	129.15	125.23
33	8	309	BCR	C8-C7-C6	2.12	132.67	127.00
28	9	308	CLA	CHB-C1B-NB	-2.12	120.86	124.05
28	A	847	CLA	C3D-C4D-ND	-2.12	106.53	109.99
30	4	308	KC1	C1D-ND-C4D	2.12	107.80	106.31
30	3	302	KC1	C3C-C4C-NC	-2.12	107.63	109.90
28	5	306	CLA	CHA-C4D-ND	-2.12	128.17	132.55
28	4	310	CLA	C1-C2-C3	-2.12	122.72	126.20
28	11	309	CLA	CHC-C1C-NC	-2.12	121.12	124.31
28	17	301	CLA	C2A-C1A-CHA	2.12	127.55	123.87
28	16	203	CLA	CHC-C1C-NC	-2.12	121.12	124.31
28	3	305	CLA	C3D-C4D-ND	-2.12	106.54	109.99
28	A	805	CLA	CHD-C4C-C3C	-2.12	121.69	124.77
28	17	301	CLA	CHA-C1A-NA	-2.12	121.59	126.39
28	B	849	CLA	C1-C2-C3	-2.12	122.73	126.20
28	9	304	CLA	C1D-ND-C4D	-2.12	104.83	106.31
28	13	302	CLA	CHC-C1C-NC	-2.12	121.12	124.31
28	7	305	CLA	CHC-C1C-NC	-2.12	121.12	124.31
28	1	314	CLA	CMD-C2D-C1D	2.12	128.46	124.73
32	J	105	XAT	O4-C5-C6	-2.12	57.25	58.93
30	4	309	KC1	C1A-NA-C4A	2.12	107.64	106.68
33	8	309	BCR	C24-C23-C22	2.12	129.36	126.23
28	B	829	CLA	C3D-C4D-ND	-2.11	106.55	109.99
28	1	305	CLA	C3D-C2D-C1D	-2.11	102.95	105.83
28	6	306	CLA	CHC-C1C-NC	-2.11	121.13	124.31
28	9	311	CLA	CHC-C1C-NC	-2.11	121.13	124.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	A	837	CLA	C1-C2-C3	-2.11	122.73	126.20
28	A	834	CLA	C3D-C4D-ND	-2.11	106.55	109.99
29	5	312	A86	C4-C5-C6	2.11	130.24	127.28
28	8	301	CLA	C3D-C2D-C1D	-2.11	102.95	105.83
28	a	202	CLA	CHC-C1C-NC	-2.11	121.13	124.31
28	16	205	CLA	CHC-C4B-NB	-2.11	120.88	124.05
28	4	316	CLA	C3D-C4D-ND	-2.11	106.56	109.99
28	4	316	CLA	CHC-C1C-NC	-2.11	121.13	124.31
28	B	808	CLA	C2A-C3A-C4A	-2.11	98.46	101.87
28	5	309	CLA	CHA-C1A-NA	-2.11	121.62	126.39
28	6	307	CLA	C4D-C3D-CAD	-2.11	105.82	108.11
28	a	201	CLA	CHC-C1C-NC	-2.11	121.14	124.31
28	17	301	CLA	CHC-C1C-NC	-2.11	121.14	124.31
28	11	302	CLA	C1D-CHD-C4C	-2.10	121.55	126.02
28	5	306	CLA	CMD-C2D-C1D	2.10	128.43	124.73
28	1	304	CLA	CHC-C1C-NC	-2.10	121.15	124.31
28	11	314	CLA	CHC-C1C-NC	-2.10	121.15	124.31
32	7	314	XAT	O24-C25-C26	-2.10	57.26	58.93
28	19	201	CLA	CHD-C4C-NC	-2.10	120.98	124.23
28	A	809	CLA	CHC-C1C-NC	-2.10	121.15	124.31
28	1	307	CLA	CMD-C2D-C1D	2.10	128.43	124.73
32	4	318	XAT	C15-C35-C34	2.10	127.81	123.52
28	13	305	CLA	C3D-C4D-ND	-2.10	106.58	109.99
28	13	306	CLA	CHA-C4D-ND	-2.10	128.22	132.55
28	1	301	CLA	C3D-C4D-ND	-2.10	106.58	109.99
28	1	305	CLA	C1D-CHD-C4C	-2.10	121.57	126.02
30	a	205	KC1	C4B-CHC-C1C	-2.09	121.57	126.02
28	B	827	CLA	C3D-C4D-ND	-2.09	106.58	109.99
28	A	801	CLA	C2A-C1A-CHA	2.09	127.50	123.87
29	5	312	A86	C9-C8-C6	2.09	132.10	126.36
32	7	315	XAT	O4-C5-C6	-2.09	57.27	58.93
28	A	801	CLA	C4D-CHA-C1A	-2.09	118.75	121.24
28	5	302	CLA	C1D-CHD-C4C	-2.09	121.58	126.02
28	A	824	CLA	O2D-CGD-CBD	2.09	114.88	111.23
32	5	316	XAT	C7-C8-C9	2.09	128.77	125.53
30	8	306	KC1	C3C-C4C-NC	-2.09	107.67	109.90
28	1	303	CLA	C3D-C4D-ND	-2.09	106.59	109.99
28	9	303	CLA	CMD-C2D-C1D	2.09	128.40	124.73
28	9	304	CLA	CHC-C1C-NC	-2.09	121.17	124.31
32	5	307	XAT	C30-C31-C32	2.09	129.24	123.20
28	8	313	CLA	CHC-C1C-NC	-2.08	121.17	124.31
28	1	301	CLA	C3D-C2D-C1D	-2.08	102.99	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	B	847	CLA	C3D-C4D-ND	-2.08	106.60	109.99
28	A	832	CLA	C1D-CHD-C4C	-2.08	121.59	126.02
28	13	307	CLA	CHC-C1C-NC	-2.08	121.17	124.31
28	B	818	CLA	C3D-C4D-ND	-2.08	106.60	109.99
32	5	307	XAT	O24-C25-C26	-2.08	57.28	58.93
33	8	309	BCR	C21-C20-C19	2.08	129.23	123.20
28	6	307	CLA	C1D-CHD-C4C	-2.08	121.59	126.02
30	10	304	KC1	C2A-C3A-C4A	-2.08	104.85	106.41
28	9	307	CLA	CHC-C1C-NC	-2.08	121.18	124.31
28	8	302	CLA	C3D-C4D-ND	-2.08	106.60	109.99
28	19	202	CLA	C3D-C4D-ND	-2.08	106.60	109.99
28	4	305	CLA	CHB-C1B-NB	-2.08	120.93	124.05
28	9	303	CLA	CHB-C1B-NB	-2.08	120.93	124.05
28	10	305	CLA	C3D-C4D-ND	-2.08	106.60	109.99
28	A	819	CLA	C1-C2-C3	-2.08	122.79	126.20
30	7	309	KC1	CHD-C1D-ND	-2.08	120.93	124.05
28	16	204	CLA	C3D-C4D-ND	-2.08	106.61	109.99
28	17	309	CLA	C2A-C1A-CHA	2.08	127.48	123.87
30	7	307	KC1	CAD-C3D-C2D	-2.08	139.88	144.26
28	13	307	CLA	CHA-C1A-NA	-2.08	121.68	126.39
28	16	201	CLA	CHC-C1C-NC	-2.08	121.18	124.31
28	11	304	CLA	CMD-C2D-C1D	2.08	128.39	124.73
28	16	202	CLA	CHC-C1C-NC	-2.08	121.18	124.31
28	7	312	CLA	CHC-C1C-NC	-2.08	121.18	124.31
28	13	303	CLA	C3D-C4D-ND	-2.08	106.61	109.99
28	4	305	CLA	C3D-C4D-ND	-2.08	106.61	109.99
28	11	301	CLA	CHC-C1C-NC	-2.08	121.18	124.31
30	10	304	KC1	C4B-CHC-C1C	-2.08	121.61	126.02
30	6	309	KC1	CHD-C1D-ND	-2.08	120.93	124.05
28	8	302	CLA	CHC-C1C-NC	-2.08	121.18	124.31
28	B	831	CLA	CMD-C2D-C1D	2.08	128.38	124.73
28	9	308	CLA	CMD-C2D-C1D	2.08	128.38	124.73
28	B	801	CLA	C1-C2-C3	-2.08	122.80	126.20
28	B	829	CLA	C3D-C2D-C1D	-2.08	103.00	105.83
28	A	814	CLA	CHD-C4C-C3C	-2.08	121.75	124.77
28	19	202	CLA	CHB-C1B-NB	-2.08	120.94	124.05
28	3	303	CLA	CHA-C4D-ND	-2.07	128.27	132.55
28	10	309	CLA	C4D-C3D-CAD	-2.07	105.85	108.11
35	A	838	PQN	C11-C3-C4	-2.07	116.39	118.58
28	A	815	CLA	CHA-C1A-NA	-2.07	121.69	126.39
28	B	824	CLA	CHA-C1A-NA	-2.07	121.69	126.39
28	F	803	CLA	C1D-CHD-C4C	-2.07	121.61	126.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	1	306	KC1	CHD-C1D-ND	-2.07	120.94	124.05
28	5	309	CLA	CHD-C4C-NC	-2.07	121.02	124.23
28	15	201	CLA	CHC-C1C-NC	-2.07	121.19	124.31
28	A	830	CLA	C3D-C4D-ND	-2.07	106.62	109.99
30	7	309	KC1	C1D-ND-C4D	-2.07	104.86	106.31
28	A	802	CLA	CMD-C2D-C1D	2.07	128.37	124.73
32	17	311	XAT	C31-C32-C33	2.07	132.04	126.36
28	6	311	CLA	CHC-C1C-NC	-2.07	121.19	124.31
28	4	306	CLA	CHC-C1C-NC	-2.07	121.19	124.31
28	9	308	CLA	CHC-C1C-NC	-2.07	121.20	124.31
28	L	204	CLA	CHC-C1C-NC	-2.07	121.20	124.31
28	10	307	CLA	CHC-C1C-NC	-2.07	121.20	124.31
28	a	203	CLA	CHC-C1C-NC	-2.07	121.20	124.31
28	A	828	CLA	C2C-C1C-NC	-2.07	107.81	109.98
28	8	304	CLA	CHC-C1C-NC	-2.07	121.20	124.31
30	6	310	KC1	C1B-CHB-C4A	-2.07	121.63	126.02
28	B	848	CLA	C3D-C4D-ND	-2.06	106.63	109.99
30	9	306	KC1	CHC-C1C-NC	-2.06	121.03	124.23
29	10	312	A86	C25-C24-C1	2.06	132.02	126.36
28	9	303	CLA	C1D-CHD-C4C	-2.06	121.64	126.02
28	16	201	CLA	C3D-C4D-ND	-2.06	106.63	109.99
30	13	304	KC1	CAA-C2A-C1A	2.06	133.68	124.64
28	11	303	CLA	CHC-C1C-NC	-2.06	121.21	124.31
28	11	310	CLA	CHC-C1C-NC	-2.06	121.21	124.31
28	10	307	CLA	C1D-CHD-C4C	-2.06	121.64	126.02
28	17	305	CLA	C3D-C4D-ND	-2.06	106.64	109.99
30	8	307	KC1	CHB-C4A-C3A	-2.06	121.78	125.03
28	8	302	CLA	CHC-C4B-NB	-2.06	120.96	124.05
28	1	304	CLA	C3D-C2D-C1D	-2.06	103.02	105.83
30	6	309	KC1	C4B-CHC-C1C	-2.06	121.64	126.02
28	16	205	CLA	C3D-C4D-ND	-2.06	106.64	109.99
28	11	312	CLA	CHD-C4C-NC	-2.06	121.04	124.23
28	A	804	CLA	C1-C2-C3	-2.06	122.83	126.20
28	B	812	CLA	CHA-C1A-NA	-2.06	121.73	126.39
28	16	205	CLA	CHC-C1C-NC	-2.06	121.21	124.31
28	17	304	CLA	CHC-C1C-NC	-2.06	121.21	124.31
28	A	805	CLA	CMD-C2D-C1D	2.06	128.35	124.73
28	B	816	CLA	C3D-C4D-ND	-2.06	106.64	109.99
28	B	835	CLA	C3D-C4D-ND	-2.06	106.64	109.99
28	10	306	CLA	CHA-C4D-ND	-2.06	128.31	132.55
28	5	313	CLA	C3D-C4D-ND	-2.06	106.64	109.99
28	B	809	CLA	CMD-C2D-C1D	2.06	128.35	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	A	804	CLA	CHC-C1C-NC	-2.06	121.22	124.31
28	R	204	CLA	CHC-C1C-NC	-2.06	121.22	124.31
28	9	310	CLA	CHB-C1B-NB	-2.06	120.97	124.05
28	11	306	CLA	CMD-C2D-C1D	2.06	128.35	124.73
32	17	311	XAT	C27-C28-C29	-2.05	122.34	125.53
28	7	305	CLA	CHD-C4C-C3C	-2.05	121.78	124.77
28	4	304	CLA	CHD-C4C-NC	-2.05	121.05	124.23
28	16	205	CLA	CHA-C1A-NA	-2.05	121.74	126.39
28	1	303	CLA	CHC-C1C-NC	-2.05	121.22	124.31
28	A	826	CLA	CHA-C1A-NA	-2.05	121.74	126.39
28	A	845	CLA	C1D-CHD-C4C	-2.05	121.66	126.02
28	3	307	CLA	CHC-C4B-NB	-2.05	120.97	124.05
28	3	304	CLA	CHC-C1C-NC	-2.05	121.22	124.31
35	B	836	PQN	C11-C3-C4	-2.05	116.42	118.58
28	8	301	CLA	C3D-C4D-ND	-2.05	106.65	109.99
28	a	203	CLA	C1D-CHD-C4C	-2.05	121.66	126.02
28	17	302	CLA	C1D-ND-C4D	-2.05	104.87	106.31
28	6	304	CLA	CHC-C1C-NC	-2.05	121.23	124.31
28	B	824	CLA	CBA-CAA-C2A	2.05	119.89	113.79
28	16	201	CLA	CHB-C1B-NB	-2.05	120.98	124.05
28	16	204	CLA	CHD-C4C-C3C	-2.05	121.79	124.77
28	F	803	CLA	C2C-C1C-NC	-2.05	107.83	109.98
28	9	311	CLA	C3D-C4D-ND	-2.05	106.66	109.99
30	10	310	KC1	C2A-C3A-C4A	-2.05	104.88	106.41
28	7	311	CLA	CHC-C1C-NC	-2.05	121.23	124.31
28	6	303	CLA	CHC-C1C-NC	-2.05	121.23	124.31
28	B	809	CLA	C1-C2-C3	-2.05	122.85	126.20
28	B	829	CLA	C1D-ND-C4D	-2.05	104.88	106.31
28	13	301	CLA	C4D-C3D-CAD	-2.04	105.89	108.11
28	13	302	CLA	C3D-C4D-ND	-2.04	106.66	109.99
28	5	304	CLA	C1D-CHD-C4C	-2.04	121.67	126.02
28	A	813	CLA	C1D-CHD-C4C	-2.04	121.68	126.02
28	A	828	CLA	C1D-CHD-C4C	-2.04	121.68	126.02
30	6	310	KC1	CHD-C4C-C3C	2.04	128.99	125.23
28	B	827	CLA	C1D-ND-C4D	-2.04	104.88	106.31
28	1	303	CLA	CHB-C1B-NB	-2.04	120.99	124.05
28	17	304	CLA	CHD-C4C-NC	-2.04	121.07	124.23
28	R	204	CLA	C3D-C4D-ND	-2.04	106.67	109.99
28	17	309	CLA	CHA-C1A-NA	-2.04	121.77	126.39
30	7	307	KC1	C2A-C3A-C4A	2.04	107.94	106.41
28	5	306	CLA	CHC-C4B-NB	-2.04	120.99	124.05
30	6	305	KC1	CHD-C4C-C3C	2.04	128.99	125.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	R	202	CLA	CHA-C1A-NA	-2.04	121.78	126.39
28	7	303	CLA	CHC-C1C-NC	-2.04	121.24	124.31
28	A	829	CLA	CHC-C1C-NC	-2.04	121.24	124.31
28	B	824	CLA	C1D-ND-C4D	-2.04	104.88	106.31
28	10	316	CLA	C2C-C1C-NC	-2.04	107.84	109.98
28	4	316	CLA	C1-C2-C3	-2.04	122.86	126.20
28	9	304	CLA	CMD-C2D-C1D	2.04	128.31	124.73
28	5	303	CLA	CHC-C1C-NC	-2.03	121.25	124.31
28	A	812	CLA	C3D-C4D-ND	-2.03	106.68	109.99
28	10	301	CLA	CHC-C1C-NC	-2.03	121.25	124.31
28	3	307	CLA	CHB-C1B-NB	-2.03	121.00	124.05
32	J	105	XAT	C6-C7-C8	-2.03	121.70	125.99
28	B	828	CLA	C3D-C4D-ND	-2.03	106.68	109.99
32	8	311	XAT	O24-C25-C26	-2.03	57.32	58.93
28	13	303	CLA	CHC-C1C-NC	-2.03	121.25	124.31
32	11	313	XAT	O24-C25-C26	-2.03	57.32	58.93
28	19	201	CLA	CHA-C1A-NA	-2.03	121.80	126.39
28	A	805	CLA	C1-C2-C3	-2.03	122.88	126.20
30	8	307	KC1	CHC-C1C-C2C	-2.03	121.83	125.03
28	6	313	CLA	CHA-C4D-ND	-2.03	128.37	132.55
28	B	804	CLA	CHC-C1C-NC	-2.03	121.26	124.31
28	B	803	CLA	CHC-C1C-NC	-2.02	121.26	124.31
28	6	313	CLA	CHC-C1C-NC	-2.02	121.26	124.31
28	B	819	CLA	C3D-C4D-ND	-2.02	106.70	109.99
28	1	305	CLA	C1-C2-C3	-2.02	122.88	126.20
28	16	202	CLA	C1D-CHD-C4C	-2.02	121.72	126.02
28	A	802	CLA	C3D-C2D-C1D	-2.02	103.07	105.83
28	A	806	CLA	CHC-C1C-NC	-2.02	121.26	124.31
28	11	305	CLA	CHC-C4B-NB	-2.02	121.02	124.05
28	9	310	CLA	CHC-C1C-NC	-2.02	121.27	124.31
29	3	312	A86	C19-C18-C17	2.02	114.57	110.79
28	B	804	CLA	C1D-CHD-C4C	-2.02	121.72	126.02
30	10	311	KC1	C1D-ND-C4D	-2.02	104.89	106.31
28	A	836	CLA	CHC-C1C-NC	-2.02	121.27	124.31
28	B	834	CLA	CMD-C2D-C1D	2.02	128.28	124.73
28	7	311	CLA	CHB-C1B-NB	-2.02	121.02	124.05
28	17	301	CLA	CHB-C1B-NB	-2.02	121.02	124.05
30	11	307	KC1	CHD-C1D-ND	-2.02	121.02	124.05
28	A	849	CLA	CHC-C1C-NC	-2.02	121.27	124.31
28	19	201	CLA	C2A-C1A-CHA	2.02	127.37	123.87
28	17	309	CLA	CMD-C2D-C1D	2.02	128.28	124.73
28	B	822	CLA	C2C-C1C-NC	-2.02	107.86	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	1	305	CLA	CHC-C1C-NC	-2.02	121.27	124.31
28	A	810	CLA	CMD-C2D-C1D	2.02	128.28	124.73
28	B	849	CLA	C1D-ND-C4D	-2.02	104.90	106.31
30	3	302	KC1	CAA-C2A-C1A	2.01	133.47	124.64
28	5	309	CLA	CHB-C1B-NB	-2.01	121.03	124.05
32	4	318	XAT	O24-C25-C26	-2.01	57.33	58.93
28	A	827	CLA	CHA-C1A-NA	-2.01	121.83	126.39
30	1	306	KC1	C2A-C3A-C4A	-2.01	104.90	106.41
32	4	315	XAT	C31-C32-C33	2.01	131.88	126.36
28	B	817	CLA	C4D-C3D-CAD	-2.01	105.92	108.11
28	A	832	CLA	CHC-C1C-NC	-2.01	121.28	124.31
28	13	307	CLA	CHA-C4D-ND	-2.01	128.40	132.55
28	F	803	CLA	CHD-C4C-C3C	-2.01	121.84	124.77
28	10	303	CLA	CHC-C1C-NC	-2.01	121.28	124.31
28	7	305	CLA	C1D-CHD-C4C	-2.01	121.75	126.02
28	A	802	CLA	C4D-C3D-CAD	-2.01	105.92	108.11
30	7	307	KC1	C1A-C2A-C3A	-2.01	105.43	107.28
28	B	809	CLA	CHA-C1A-NA	-2.01	121.84	126.39
28	5	306	CLA	C3D-C4D-ND	-2.01	106.72	109.99
28	L	206	CLA	C2C-C1C-NC	-2.01	107.87	109.98
28	4	307	CLA	CHC-C4B-NB	-2.01	121.03	124.05
28	17	302	CLA	CHC-C1C-NC	-2.01	121.28	124.31
28	1	307	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
28	5	313	CLA	C1D-CHD-C4C	-2.01	121.75	126.02
28	10	302	CLA	CHC-C1C-NC	-2.01	121.28	124.31
30	a	205	KC1	C3C-C4C-NC	-2.01	107.75	109.90
28	A	822	CLA	C3D-C4D-ND	-2.01	106.72	109.99
28	1	310	CLA	C1-C2-C3	-2.01	122.91	126.20
28	7	306	CLA	C1D-CHD-C4C	-2.01	121.75	126.02
28	L	204	CLA	C4D-C3D-CAD	-2.01	105.93	108.11
28	A	835	CLA	CHC-C1C-NC	-2.01	121.29	124.31
28	A	808	CLA	CHA-C1A-NA	-2.01	121.85	126.39
28	A	847	CLA	CMD-C2D-C1D	2.01	128.26	124.73
28	10	307	CLA	C1-C2-C3	-2.01	122.91	126.20
29	17	308	A86	C33-C32-C31	2.01	111.16	109.21
32	6	315	XAT	O4-C5-C6	-2.00	57.34	58.93
28	17	302	CLA	CHA-C1A-NA	-2.00	121.85	126.39
28	7	318	CLA	CMD-C2D-C1D	2.00	128.26	124.73
28	6	302	CLA	CHD-C4C-C3C	-2.00	121.85	124.77
28	A	820	CLA	C3D-C4D-ND	-2.00	106.73	109.99
28	8	302	CLA	C1-C2-C3	-2.00	122.92	126.20
28	11	304	CLA	CHC-C1C-NC	-2.00	121.29	124.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	11	306	CLA	C4D-C3D-CAD	-2.00	105.93	108.11
28	10	302	CLA	CHC-C4B-NB	-2.00	121.05	124.05
28	5	305	CLA	CMD-C2D-C1D	2.00	128.25	124.73
28	A	836	CLA	CMD-C2D-C1D	2.00	128.25	124.73
28	7	312	CLA	CHD-C4C-NC	-2.00	121.13	124.23
28	6	301	CLA	C4D-C3D-CAD	-2.00	105.93	108.11
28	16	204	CLA	CMD-C2D-C1D	2.00	128.25	124.73
28	4	316	CLA	C1D-ND-C4D	-2.00	104.91	106.31
28	5	305	CLA	C3D-C4D-ND	-2.00	106.73	109.99

There are no chirality outliers.

All (2406) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
28	1	301	CLA	C1-C2-C3-C4
28	1	301	CLA	C1-C2-C3-C5
28	1	303	CLA	CBA-CGA-O2A-C1
28	1	303	CLA	O1A-CGA-O2A-C1
28	1	303	CLA	CBD-CGD-O2D-CED
28	1	303	CLA	O1D-CGD-O2D-CED
28	1	303	CLA	C1-C2-C3-C4
28	1	303	CLA	C1-C2-C3-C5
28	1	303	CLA	C11-C10-C8-C9
28	1	304	CLA	C1A-C2A-CAA-CBA
28	1	304	CLA	C3A-C2A-CAA-CBA
28	1	305	CLA	CHA-CBD-CGD-O1D
28	1	305	CLA	CHA-CBD-CGD-O2D
28	1	305	CLA	C1-C2-C3-C4
28	1	307	CLA	C1A-C2A-CAA-CBA
28	1	307	CLA	CHA-CBD-CGD-O1D
28	1	307	CLA	CHA-CBD-CGD-O2D
28	1	308	CLA	CBD-CGD-O2D-CED
28	1	308	CLA	O1D-CGD-O2D-CED
28	1	310	CLA	C4B-C3B-CAB-CBB
28	1	310	CLA	C1-C2-C3-C4
28	1	314	CLA	CAD-CBD-CGD-O1D
28	1	314	CLA	CAD-CBD-CGD-O2D
28	1	314	CLA	C1-C2-C3-C4
28	1	314	CLA	C1-C2-C3-C5
28	3	301	CLA	C4B-C3B-CAB-CBB
28	3	301	CLA	C1-C2-C3-C4
28	3	303	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
28	3	303	CLA	CAD-CBD-CGD-O1D
28	3	303	CLA	CAD-CBD-CGD-O2D
28	3	304	CLA	C2B-C3B-CAB-CBB
28	3	304	CLA	C4B-C3B-CAB-CBB
28	3	304	CLA	CAD-CBD-CGD-O1D
28	3	304	CLA	CAD-CBD-CGD-O2D
28	3	305	CLA	C1A-C2A-CAA-CBA
28	3	305	CLA	C3A-C2A-CAA-CBA
28	3	305	CLA	CBA-CGA-O2A-C1
28	3	305	CLA	O1A-CGA-O2A-C1
28	3	305	CLA	C2B-C3B-CAB-CBB
28	3	305	CLA	C4B-C3B-CAB-CBB
28	3	305	CLA	C1-C2-C3-C4
28	3	305	CLA	C1-C2-C3-C5
28	3	306	CLA	C1A-C2A-CAA-CBA
28	3	306	CLA	C2-C3-C5-C6
28	3	306	CLA	C4-C3-C5-C6
28	3	307	CLA	C1A-C2A-CAA-CBA
28	3	307	CLA	C1-C2-C3-C4
28	3	307	CLA	C1-C2-C3-C5
28	5	301	CLA	C14-C13-C15-C16
28	5	302	CLA	CBA-CGA-O2A-C1
28	5	302	CLA	O1A-CGA-O2A-C1
28	5	302	CLA	C1-C2-C3-C5
28	5	303	CLA	C1A-C2A-CAA-CBA
28	5	303	CLA	C3A-C2A-CAA-CBA
28	5	303	CLA	C4B-C3B-CAB-CBB
28	5	304	CLA	C1A-C2A-CAA-CBA
28	5	304	CLA	C4B-C3B-CAB-CBB
28	5	304	CLA	CHA-CBD-CGD-O1D
28	5	304	CLA	CHA-CBD-CGD-O2D
28	5	305	CLA	C1A-C2A-CAA-CBA
28	5	305	CLA	C3A-C2A-CAA-CBA
28	5	305	CLA	CHA-CBD-CGD-O1D
28	5	305	CLA	CHA-CBD-CGD-O2D
28	5	305	CLA	C1-C2-C3-C4
28	5	305	CLA	C1-C2-C3-C5
28	5	309	CLA	CBD-CGD-O2D-CED
28	5	309	CLA	O1D-CGD-O2D-CED
28	5	313	CLA	C1-C2-C3-C4
28	5	313	CLA	C1-C2-C3-C5
28	7	301	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
28	7	301	CLA	C1-C2-C3-C5
28	7	302	CLA	C4B-C3B-CAB-CBB
28	7	303	CLA	C2B-C3B-CAB-CBB
28	7	303	CLA	C4B-C3B-CAB-CBB
28	7	303	CLA	C1-C2-C3-C5
28	7	303	CLA	C6-C7-C8-C9
28	7	303	CLA	C14-C13-C15-C16
28	7	304	CLA	C1A-C2A-CAA-CBA
28	7	304	CLA	C3A-C2A-CAA-CBA
28	7	304	CLA	C1-C2-C3-C4
28	7	304	CLA	C1-C2-C3-C5
28	7	305	CLA	C1-C2-C3-C5
28	7	306	CLA	C1A-C2A-CAA-CBA
28	7	306	CLA	C3A-C2A-CAA-CBA
28	7	306	CLA	CHA-CBD-CGD-O1D
28	7	306	CLA	CHA-CBD-CGD-O2D
28	7	308	CLA	CAD-CBD-CGD-O1D
28	7	308	CLA	CAD-CBD-CGD-O2D
28	7	311	CLA	C1A-C2A-CAA-CBA
28	7	311	CLA	C2B-C3B-CAB-CBB
28	7	311	CLA	C4B-C3B-CAB-CBB
28	7	312	CLA	CBA-CGA-O2A-C1
28	7	312	CLA	O1A-CGA-O2A-C1
28	7	318	CLA	C1A-C2A-CAA-CBA
28	7	318	CLA	C4B-C3B-CAB-CBB
28	7	318	CLA	CBD-CGD-O2D-CED
28	7	318	CLA	O1D-CGD-O2D-CED
28	8	301	CLA	C3A-C2A-CAA-CBA
28	8	301	CLA	C1-C2-C3-C5
28	8	303	CLA	CBA-CGA-O2A-C1
28	8	303	CLA	O1A-CGA-O2A-C1
28	8	303	CLA	C1-C2-C3-C4
28	8	303	CLA	C1-C2-C3-C5
28	8	304	CLA	C1A-C2A-CAA-CBA
28	8	304	CLA	C3A-C2A-CAA-CBA
28	8	304	CLA	CHA-CBD-CGD-O2D
28	8	305	CLA	CHA-CBD-CGD-O1D
28	8	305	CLA	CHA-CBD-CGD-O2D
28	A	801	CLA	CBD-CGD-O2D-CED
28	A	801	CLA	O1D-CGD-O2D-CED
28	A	802	CLA	CBA-CGA-O2A-C1
28	A	802	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
28	A	802	CLA	C1-C2-C3-C4
28	A	802	CLA	C1-C2-C3-C5
28	A	803	CLA	C1-C2-C3-C5
28	A	804	CLA	CAD-CBD-CGD-O1D
28	A	804	CLA	CAD-CBD-CGD-O2D
28	A	805	CLA	C2B-C3B-CAB-CBB
28	A	805	CLA	C4B-C3B-CAB-CBB
28	A	806	CLA	C3A-C2A-CAA-CBA
28	A	806	CLA	C1-C2-C3-C4
28	A	806	CLA	C1-C2-C3-C5
28	A	807	CLA	C3A-C2A-CAA-CBA
28	A	807	CLA	CHA-CBD-CGD-O2D
28	A	807	CLA	C1-C2-C3-C5
28	A	809	CLA	C1A-C2A-CAA-CBA
28	A	809	CLA	C3A-C2A-CAA-CBA
28	A	809	CLA	C1-C2-C3-C4
28	A	810	CLA	CHA-CBD-CGD-O1D
28	A	810	CLA	CHA-CBD-CGD-O2D
28	A	810	CLA	C1-C2-C3-C4
28	A	810	CLA	C1-C2-C3-C5
28	A	810	CLA	C11-C10-C8-C9
28	A	811	CLA	C1A-C2A-CAA-CBA
28	A	811	CLA	C2B-C3B-CAB-CBB
28	A	811	CLA	C4B-C3B-CAB-CBB
28	A	812	CLA	CBA-CGA-O2A-C1
28	A	812	CLA	O1A-CGA-O2A-C1
28	A	812	CLA	C1-C2-C3-C5
28	A	813	CLA	C1A-C2A-CAA-CBA
28	A	813	CLA	C3A-C2A-CAA-CBA
28	A	813	CLA	C1-C2-C3-C4
28	A	813	CLA	C1-C2-C3-C5
28	A	814	CLA	C1A-C2A-CAA-CBA
28	A	814	CLA	C3A-C2A-CAA-CBA
28	A	814	CLA	C4B-C3B-CAB-CBB
28	A	815	CLA	CBA-CGA-O2A-C1
28	A	815	CLA	O1A-CGA-O2A-C1
28	A	815	CLA	CHA-CBD-CGD-O1D
28	A	815	CLA	CHA-CBD-CGD-O2D
28	A	815	CLA	C1-C2-C3-C5
28	A	815	CLA	C11-C12-C13-C14
28	A	816	CLA	C1A-C2A-CAA-CBA
28	A	816	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
28	A	817	CLA	C1A-C2A-CAA-CBA
28	A	817	CLA	C1-C2-C3-C5
28	A	818	CLA	C3A-C2A-CAA-CBA
28	A	820	CLA	CBA-CGA-O2A-C1
28	A	820	CLA	O1A-CGA-O2A-C1
28	A	821	CLA	C1A-C2A-CAA-CBA
28	A	821	CLA	C1-C2-C3-C4
28	A	822	CLA	C2B-C3B-CAB-CBB
28	A	822	CLA	C4B-C3B-CAB-CBB
28	A	822	CLA	C1-C2-C3-C5
28	A	823	CLA	CBA-CGA-O2A-C1
28	A	823	CLA	O1A-CGA-O2A-C1
28	A	823	CLA	C11-C12-C13-C14
28	A	824	CLA	CBD-CGD-O2D-CED
28	A	824	CLA	O1D-CGD-O2D-CED
28	A	828	CLA	C1A-C2A-CAA-CBA
28	A	828	CLA	CHA-CBD-CGD-O1D
28	A	828	CLA	CHA-CBD-CGD-O2D
28	A	829	CLA	C1A-C2A-CAA-CBA
28	A	829	CLA	C3A-C2A-CAA-CBA
28	A	830	CLA	CHA-CBD-CGD-O1D
28	A	830	CLA	CHA-CBD-CGD-O2D
28	A	831	CLA	C1A-C2A-CAA-CBA
28	A	831	CLA	C3A-C2A-CAA-CBA
28	A	831	CLA	C1-C2-C3-C4
28	A	831	CLA	C1-C2-C3-C5
28	A	834	CLA	C1A-C2A-CAA-CBA
28	A	834	CLA	C1-C2-C3-C4
28	A	834	CLA	C1-C2-C3-C5
28	A	836	CLA	C2B-C3B-CAB-CBB
28	A	836	CLA	C4B-C3B-CAB-CBB
28	A	836	CLA	CAD-CBD-CGD-O1D
28	A	836	CLA	CAD-CBD-CGD-O2D
28	A	836	CLA	C1-C2-C3-C5
28	A	837	CLA	C2B-C3B-CAB-CBB
28	A	837	CLA	C4B-C3B-CAB-CBB
28	A	846	CLA	C1A-C2A-CAA-CBA
28	A	847	CLA	C1A-C2A-CAA-CBA
28	A	847	CLA	C3A-C2A-CAA-CBA
28	A	847	CLA	CHA-CBD-CGD-O1D
28	A	847	CLA	CHA-CBD-CGD-O2D
28	A	852	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
28	A	853	CLA	CHA-CBD-CGD-O1D
28	A	853	CLA	CHA-CBD-CGD-O2D
28	B	804	CLA	C3A-C2A-CAA-CBA
28	B	806	CLA	CBA-CGA-O2A-C1
28	B	806	CLA	O1A-CGA-O2A-C1
28	B	806	CLA	C6-C7-C8-C9
28	B	807	CLA	C1A-C2A-CAA-CBA
28	B	807	CLA	C1-C2-C3-C4
28	B	807	CLA	C1-C2-C3-C5
28	B	808	CLA	C1A-C2A-CAA-CBA
28	B	808	CLA	C2B-C3B-CAB-CBB
28	B	808	CLA	C4B-C3B-CAB-CBB
28	B	808	CLA	CHA-CBD-CGD-O1D
28	B	808	CLA	CHA-CBD-CGD-O2D
28	B	808	CLA	C1-C2-C3-C4
28	B	808	CLA	C1-C2-C3-C5
28	B	810	CLA	C1A-C2A-CAA-CBA
28	B	810	CLA	C3A-C2A-CAA-CBA
28	B	810	CLA	CHA-CBD-CGD-O1D
28	B	810	CLA	CHA-CBD-CGD-O2D
28	B	811	CLA	C1A-C2A-CAA-CBA
28	B	811	CLA	C3A-C2A-CAA-CBA
28	B	811	CLA	C1-C2-C3-C5
28	B	812	CLA	C1-C2-C3-C5
28	B	814	CLA	C4B-C3B-CAB-CBB
28	B	814	CLA	CHA-CBD-CGD-O1D
28	B	814	CLA	CHA-CBD-CGD-O2D
28	B	815	CLA	C1A-C2A-CAA-CBA
28	B	815	CLA	C3A-C2A-CAA-CBA
28	B	815	CLA	CBA-CGA-O2A-C1
28	B	815	CLA	O1A-CGA-O2A-C1
28	B	815	CLA	C2B-C3B-CAB-CBB
28	B	815	CLA	C4B-C3B-CAB-CBB
28	B	815	CLA	C1-C2-C3-C4
28	B	815	CLA	C1-C2-C3-C5
28	B	816	CLA	C3A-C2A-CAA-CBA
28	B	816	CLA	C1-C2-C3-C4
28	B	816	CLA	C1-C2-C3-C5
28	B	817	CLA	C1A-C2A-CAA-CBA
28	B	817	CLA	C4B-C3B-CAB-CBB
28	B	817	CLA	C1-C2-C3-C4
28	B	817	CLA	C1-C2-C3-C5

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Mol	Chain	Res	Type	Atoms
28	B	817	CLA	C14-C13-C15-C16
28	B	819	CLA	C1A-C2A-CAA-CBA
28	B	820	CLA	C1A-C2A-CAA-CBA
28	B	820	CLA	C3A-C2A-CAA-CBA
28	B	820	CLA	C1-C2-C3-C5
28	B	822	CLA	CHA-CBD-CGD-O1D
28	B	822	CLA	CHA-CBD-CGD-O2D
28	B	822	CLA	C1-C2-C3-C5
28	B	823	CLA	C1A-C2A-CAA-CBA
28	B	824	CLA	C1A-C2A-CAA-CBA
28	B	824	CLA	C1-C2-C3-C4
28	B	824	CLA	C1-C2-C3-C5
28	B	827	CLA	C3A-C2A-CAA-CBA
28	B	828	CLA	C1-C2-C3-C5
28	B	829	CLA	CHA-CBD-CGD-O1D
28	B	829	CLA	CHA-CBD-CGD-O2D
28	B	831	CLA	C1A-C2A-CAA-CBA
28	B	831	CLA	C1-C2-C3-C4
28	B	831	CLA	C1-C2-C3-C5
28	B	831	CLA	C4-C3-C5-C6
28	B	832	CLA	CBA-CGA-O2A-C1
28	B	832	CLA	O1A-CGA-O2A-C1
28	B	832	CLA	C4B-C3B-CAB-CBB
28	B	832	CLA	O2A-C1-C2-C3
28	B	832	CLA	C1-C2-C3-C4
28	B	833	CLA	C2B-C3B-CAB-CBB
28	B	833	CLA	C4B-C3B-CAB-CBB
28	B	834	CLA	C1A-C2A-CAA-CBA
28	B	834	CLA	C3A-C2A-CAA-CBA
28	B	834	CLA	CAD-CBD-CGD-O1D
28	B	834	CLA	CAD-CBD-CGD-O2D
28	B	835	CLA	C11-C10-C8-C9
28	B	843	CLA	CBA-CGA-O2A-C1
28	B	843	CLA	O1A-CGA-O2A-C1
28	B	845	CLA	CBA-CGA-O2A-C1
28	B	845	CLA	O1A-CGA-O2A-C1
28	B	845	CLA	C1-C2-C3-C5
28	B	847	CLA	C2-C3-C5-C6
28	B	847	CLA	C4-C3-C5-C6
28	B	848	CLA	C1A-C2A-CAA-CBA
28	B	848	CLA	C3A-C2A-CAA-CBA
28	B	848	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
28	B	848	CLA	CAD-CBD-CGD-O2D
28	F	802	CLA	CBD-CGD-O2D-CED
28	F	802	CLA	O1D-CGD-O2D-CED
28	F	802	CLA	C4-C3-C5-C6
28	F	802	CLA	C11-C12-C13-C14
28	F	803	CLA	CHA-CBD-CGD-O1D
28	F	803	CLA	CHA-CBD-CGD-O2D
28	J	102	CLA	CBA-CGA-O2A-C1
28	J	102	CLA	O1A-CGA-O2A-C1
28	J	102	CLA	CHA-CBD-CGD-O1D
28	J	102	CLA	CHA-CBD-CGD-O2D
28	J	102	CLA	C1-C2-C3-C4
28	J	103	CLA	C3A-C2A-CAA-CBA
28	R	204	CLA	C2B-C3B-CAB-CBB
28	R	204	CLA	C4B-C3B-CAB-CBB
28	R	204	CLA	C2-C3-C5-C6
28	6	301	CLA	C3A-C2A-CAA-CBA
28	6	302	CLA	C4-C3-C5-C6
28	6	306	CLA	C1A-C2A-CAA-CBA
28	6	306	CLA	C3A-C2A-CAA-CBA
28	6	306	CLA	CBA-CGA-O2A-C1
28	6	306	CLA	O1A-CGA-O2A-C1
28	6	306	CLA	C4-C3-C5-C6
28	6	307	CLA	C2B-C3B-CAB-CBB
28	6	307	CLA	C4B-C3B-CAB-CBB
28	6	307	CLA	C1-C2-C3-C5
28	6	311	CLA	C2B-C3B-CAB-CBB
28	6	311	CLA	C4B-C3B-CAB-CBB
28	6	311	CLA	CHD-C1D-C2D-CMD
28	6	311	CLA	ND-C1D-C2D-CMD
28	6	311	CLA	C1-C2-C3-C4
28	6	311	CLA	C1-C2-C3-C5
28	6	313	CLA	C1-C2-C3-C4
28	6	313	CLA	C1-C2-C3-C5
28	10	301	CLA	C1A-C2A-CAA-CBA
28	10	301	CLA	C3A-C2A-CAA-CBA
28	10	301	CLA	C1-C2-C3-C5
28	10	303	CLA	C1A-C2A-CAA-CBA
28	10	303	CLA	C2B-C3B-CAB-CBB
28	10	303	CLA	C4B-C3B-CAB-CBB
28	10	305	CLA	C2B-C3B-CAB-CBB
28	10	305	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
28	10	305	CLA	CHA-CBD-CGD-O1D
28	10	305	CLA	CHA-CBD-CGD-O2D
28	10	306	CLA	C3A-C2A-CAA-CBA
28	10	306	CLA	CHA-CBD-CGD-O1D
28	10	306	CLA	CHA-CBD-CGD-O2D
28	10	306	CLA	C1-C2-C3-C5
28	10	307	CLA	CBD-CGD-O2D-CED
28	10	307	CLA	O1D-CGD-O2D-CED
28	10	307	CLA	C1-C2-C3-C5
28	10	308	CLA	CBD-CGD-O2D-CED
28	10	308	CLA	O1D-CGD-O2D-CED
28	10	309	CLA	C2B-C3B-CAB-CBB
28	10	309	CLA	C4B-C3B-CAB-CBB
28	10	316	CLA	C2B-C3B-CAB-CBB
28	10	316	CLA	C4B-C3B-CAB-CBB
28	11	301	CLA	C3A-C2A-CAA-CBA
28	11	301	CLA	CHA-CBD-CGD-O1D
28	11	301	CLA	CHA-CBD-CGD-O2D
28	11	302	CLA	CHA-CBD-CGD-O1D
28	11	302	CLA	CHA-CBD-CGD-O2D
28	11	302	CLA	C1-C2-C3-C5
28	11	303	CLA	C1A-C2A-CAA-CBA
28	11	303	CLA	C3A-C2A-CAA-CBA
28	11	303	CLA	C2B-C3B-CAB-CBB
28	11	303	CLA	C4B-C3B-CAB-CBB
28	11	303	CLA	CHA-CBD-CGD-O1D
28	11	303	CLA	CHA-CBD-CGD-O2D
28	11	304	CLA	C1A-C2A-CAA-CBA
28	11	304	CLA	C3A-C2A-CAA-CBA
28	11	304	CLA	CBA-CGA-O2A-C1
28	11	304	CLA	O1A-CGA-O2A-C1
28	11	306	CLA	C2B-C3B-CAB-CBB
28	11	306	CLA	C4B-C3B-CAB-CBB
28	11	309	CLA	C2A-CAA-CBA-CGA
28	11	309	CLA	C2B-C3B-CAB-CBB
28	11	309	CLA	C4B-C3B-CAB-CBB
28	11	310	CLA	CBA-CGA-O2A-C1
28	11	310	CLA	O1A-CGA-O2A-C1
28	11	310	CLA	C2B-C3B-CAB-CBB
28	11	310	CLA	C4B-C3B-CAB-CBB
28	11	310	CLA	C1-C2-C3-C4
28	11	310	CLA	C1-C2-C3-C5

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Mol	Chain	Res	Type	Atoms
28	11	312	CLA	CHA-CBD-CGD-O1D
28	11	312	CLA	CHA-CBD-CGD-O2D
28	11	314	CLA	C1A-C2A-CAA-CBA
28	11	314	CLA	CBD-CGD-O2D-CED
28	11	314	CLA	O1D-CGD-O2D-CED
28	13	301	CLA	C4B-C3B-CAB-CBB
28	13	301	CLA	CBD-CGD-O2D-CED
28	13	301	CLA	O1D-CGD-O2D-CED
28	13	301	CLA	C6-C7-C8-C9
28	13	303	CLA	C1A-C2A-CAA-CBA
28	13	305	CLA	C1A-C2A-CAA-CBA
28	13	306	CLA	C1A-C2A-CAA-CBA
28	16	201	CLA	C1A-C2A-CAA-CBA
28	16	201	CLA	C3A-C2A-CAA-CBA
28	16	202	CLA	C1A-C2A-CAA-CBA
28	16	202	CLA	CHA-CBD-CGD-O1D
28	16	202	CLA	CHA-CBD-CGD-O2D
28	16	203	CLA	C1A-C2A-CAA-CBA
28	16	203	CLA	C3A-C2A-CAA-CBA
28	16	203	CLA	CBA-CGA-O2A-C1
28	16	203	CLA	O1A-CGA-O2A-C1
28	16	203	CLA	CBD-CGD-O2D-CED
28	16	203	CLA	O1D-CGD-O2D-CED
28	16	204	CLA	CBD-CGD-O2D-CED
28	16	204	CLA	O1D-CGD-O2D-CED
28	16	205	CLA	C2A-CAA-CBA-CGA
28	16	205	CLA	C4B-C3B-CAB-CBB
28	17	301	CLA	CBA-CGA-O2A-C1
28	17	301	CLA	O1A-CGA-O2A-C1
28	17	301	CLA	CBD-CGD-O2D-CED
28	17	301	CLA	O1D-CGD-O2D-CED
28	17	302	CLA	C2B-C3B-CAB-CBB
28	17	302	CLA	C4B-C3B-CAB-CBB
28	17	303	CLA	C1A-C2A-CAA-CBA
28	17	303	CLA	C3A-C2A-CAA-CBA
28	17	303	CLA	CBA-CGA-O2A-C1
28	17	303	CLA	O1A-CGA-O2A-C1
28	17	303	CLA	C2B-C3B-CAB-CBB
28	17	303	CLA	C4B-C3B-CAB-CBB
28	17	304	CLA	C1A-C2A-CAA-CBA
28	17	304	CLA	CHA-CBD-CGD-O1D
28	17	304	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
28	17	304	CLA	C1-C2-C3-C4
28	17	305	CLA	C1A-C2A-CAA-CBA
28	17	305	CLA	C2B-C3B-CAB-CBB
28	17	305	CLA	C4B-C3B-CAB-CBB
28	17	305	CLA	C1-C2-C3-C4
28	17	305	CLA	C1-C2-C3-C5
28	17	307	CLA	CBD-CGD-O2D-CED
28	17	307	CLA	O1D-CGD-O2D-CED
28	17	309	CLA	C2B-C3B-CAB-CBB
28	17	309	CLA	C4B-C3B-CAB-CBB
28	4	303	CLA	CBA-CGA-O2A-C1
28	4	303	CLA	O1A-CGA-O2A-C1
28	4	303	CLA	C1-C2-C3-C4
28	4	303	CLA	C1-C2-C3-C5
28	4	304	CLA	CBD-CGD-O2D-CED
28	4	304	CLA	O1D-CGD-O2D-CED
28	4	304	CLA	C1-C2-C3-C4
28	4	305	CLA	C1A-C2A-CAA-CBA
28	4	306	CLA	C1A-C2A-CAA-CBA
28	4	306	CLA	C3A-C2A-CAA-CBA
28	4	307	CLA	C1A-C2A-CAA-CBA
28	4	307	CLA	C3A-C2A-CAA-CBA
28	4	307	CLA	CBA-CGA-O2A-C1
28	4	307	CLA	O1A-CGA-O2A-C1
28	4	307	CLA	CHA-CBD-CGD-O1D
28	4	307	CLA	CHA-CBD-CGD-O2D
28	4	310	CLA	CBA-CGA-O2A-C1
28	4	310	CLA	O1A-CGA-O2A-C1
28	4	310	CLA	C2B-C3B-CAB-CBB
28	4	310	CLA	C4B-C3B-CAB-CBB
28	4	310	CLA	C1-C2-C3-C5
28	4	316	CLA	C1-C2-C3-C5
28	9	303	CLA	CHA-CBD-CGD-O1D
28	9	303	CLA	CHA-CBD-CGD-O2D
28	9	304	CLA	C1A-C2A-CAA-CBA
28	9	304	CLA	C3A-C2A-CAA-CBA
28	9	304	CLA	CBA-CGA-O2A-C1
28	9	304	CLA	O1A-CGA-O2A-C1
28	9	304	CLA	CHA-CBD-CGD-O2D
28	9	304	CLA	C1-C2-C3-C4
28	9	304	CLA	C1-C2-C3-C5
28	9	305	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
28	9	305	CLA	CHA-CBD-CGD-O2D
28	9	307	CLA	CBA-CGA-O2A-C1
28	9	307	CLA	O1A-CGA-O2A-C1
28	9	307	CLA	C2B-C3B-CAB-CBB
28	9	307	CLA	C4B-C3B-CAB-CBB
28	9	307	CLA	C1-C2-C3-C4
28	9	307	CLA	C1-C2-C3-C5
28	9	310	CLA	CAD-CBD-CGD-O1D
28	9	310	CLA	CAD-CBD-CGD-O2D
28	9	311	CLA	C4B-C3B-CAB-CBB
28	L	201	CLA	CHA-CBD-CGD-O1D
28	L	201	CLA	CHA-CBD-CGD-O2D
28	L	204	CLA	CBA-CGA-O2A-C1
28	L	204	CLA	O1A-CGA-O2A-C1
28	L	206	CLA	C1A-C2A-CAA-CBA
28	L	206	CLA	C3A-C2A-CAA-CBA
28	L	206	CLA	CAD-CBD-CGD-O1D
28	L	206	CLA	CAD-CBD-CGD-O2D
28	L	206	CLA	O2A-C1-C2-C3
28	L	206	CLA	C1-C2-C3-C4
28	L	206	CLA	C1-C2-C3-C5
28	a	202	CLA	C3A-C2A-CAA-CBA
28	a	202	CLA	CBD-CGD-O2D-CED
28	a	202	CLA	O1D-CGD-O2D-CED
28	a	203	CLA	C2B-C3B-CAB-CBB
28	a	203	CLA	C4B-C3B-CAB-CBB
28	a	203	CLA	CBD-CGD-O2D-CED
28	a	203	CLA	O1D-CGD-O2D-CED
29	1	302	A86	C10-C11-C13-O
29	1	302	A86	C12-C11-C13-O
29	1	302	A86	C3-C4-C5-C6
29	1	302	A86	C5-C6-C8-C9
29	1	313	A86	C26-C27-C29-C30
29	1	313	A86	C28-C27-C29-C30
29	3	311	A86	C2-C1-C24-C25
29	3	311	A86	O-C13-C14-C15
29	3	311	A86	C28-C27-C29-C30
29	3	311	A86	C5-C6-C8-C9
29	3	312	A86	C10-C11-C13-O
29	3	312	A86	C12-C11-C13-O
29	3	312	A86	C26-C27-C29-C30
29	3	312	A86	C28-C27-C29-C30

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Mol	Chain	Res	Type	Atoms
29	5	312	A86	C9-C10-C11-C12
29	5	312	A86	C9-C10-C11-C13
29	8	308	A86	C13-C14-C15-O1
29	J	101	A86	O-C13-C14-C15
29	J	101	A86	C13-C14-C15-C16
29	J	101	A86	C13-C14-C15-O1
29	J	101	A86	C26-C27-C29-C30
29	J	101	A86	C28-C27-C29-C30
29	R	201	A86	O-C13-C14-C15
29	R	201	A86	C11-C13-C14-C15
29	6	314	A86	C11-C10-C9-C8
29	6	314	A86	C13-C14-C15-O1
29	10	312	A86	C9-C10-C11-C12
29	10	312	A86	C9-C10-C11-C13
29	10	312	A86	C11-C10-C9-C8
29	10	312	A86	C13-C14-C15-O1
29	10	312	A86	C7-C6-C8-C9
29	10	317	A86	C9-C10-C11-C12
29	10	317	A86	C9-C10-C11-C13
29	10	317	A86	C26-C27-C29-C30
29	10	317	A86	C28-C27-C29-C30
29	11	308	A86	C5-C6-C8-C9
29	11	308	A86	C7-C6-C8-C9
29	4	313	A86	C10-C11-C13-O
29	4	313	A86	C12-C11-C13-O
29	4	313	A86	C26-C27-C29-C30
29	4	313	A86	C28-C27-C29-C30
29	9	312	A86	C-C1-C24-C25
29	9	312	A86	C2-C1-C24-C25
29	9	312	A86	C10-C11-C13-O
29	9	312	A86	C12-C11-C13-O
30	1	306	KC1	CHA-CBD-CGD-O1D
30	1	306	KC1	CHA-CBD-CGD-O2D
30	3	309	KC1	CAD-CBD-CGD-O1D
30	3	309	KC1	CAD-CBD-CGD-O2D
30	5	308	KC1	C3A-C2A-CAA-CBA
30	5	308	KC1	C2B-C3B-CAB-CBB
30	5	308	KC1	C4B-C3B-CAB-CBB
30	5	308	KC1	CHA-CBD-CGD-O1D
30	5	308	KC1	CHA-CBD-CGD-O2D
30	7	309	KC1	C3A-C2A-CAA-CBA
30	7	309	KC1	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
30	7	309	KC1	C4B-C3B-CAB-CBB
30	7	309	KC1	CHA-CBD-CGD-O1D
30	7	309	KC1	CHA-CBD-CGD-O2D
30	6	305	KC1	C1A-C2A-CAA-CBA
30	6	305	KC1	C3A-C2A-CAA-CBA
30	6	305	KC1	CHA-CBD-CGD-O1D
30	6	305	KC1	CHA-CBD-CGD-O2D
30	6	308	KC1	CHA-CBD-CGD-O1D
30	6	308	KC1	CHA-CBD-CGD-O2D
30	6	309	KC1	C3A-C2A-CAA-CBA
30	6	309	KC1	CBD-CGD-O2D-CED
30	6	309	KC1	O1D-CGD-O2D-CED
30	6	310	KC1	C3A-C2A-CAA-CBA
30	6	310	KC1	CHA-CBD-CGD-O1D
30	6	310	KC1	CHA-CBD-CGD-O2D
30	10	304	KC1	C2B-C3B-CAB-CBB
30	10	304	KC1	C4B-C3B-CAB-CBB
30	10	304	KC1	CHA-CBD-CGD-O1D
30	10	304	KC1	CHA-CBD-CGD-O2D
30	10	310	KC1	C3A-C2A-CAA-CBA
30	10	311	KC1	C3A-C2A-CAA-CBA
30	11	307	KC1	C3A-C2A-CAA-CBA
30	11	307	KC1	C2B-C3B-CAB-CBB
30	11	307	KC1	C4B-C3B-CAB-CBB
30	13	304	KC1	C3A-C2A-CAA-CBA
30	13	304	KC1	CHA-CBD-CGD-O1D
30	13	304	KC1	CHA-CBD-CGD-O2D
30	17	312	KC1	C3A-C2A-CAA-CBA
30	4	308	KC1	C1A-C2A-CAA-CBA
30	4	308	KC1	C3A-C2A-CAA-CBA
30	4	308	KC1	CHA-CBD-CGD-O1D
30	4	308	KC1	CHA-CBD-CGD-O2D
30	4	309	KC1	C3A-C2A-CAA-CBA
30	4	309	KC1	C2B-C3B-CAB-CBB
30	4	309	KC1	CBD-CGD-O2D-CED
30	4	309	KC1	O1D-CGD-O2D-CED
30	4	311	KC1	C2B-C3B-CAB-CBB
30	4	311	KC1	CBD-CGD-O2D-CED
30	4	311	KC1	O1D-CGD-O2D-CED
30	4	312	KC1	C1A-C2A-CAA-CBA
30	4	312	KC1	CBD-CGD-O2D-CED
30	4	312	KC1	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
30	9	306	KC1	C3A-C2A-CAA-CBA
30	9	309	KC1	C3A-C2A-CAA-CBA
30	a	205	KC1	C2B-C3B-CAB-CBB
30	a	205	KC1	C4B-C3B-CAB-CBB
31	1	309	LHG	C3-O3-P-O6
31	1	309	LHG	C4-O6-P-O3
31	1	309	LHG	O10-C23-O8-C6
31	1	309	LHG	C24-C23-O8-C6
31	5	315	LHG	C1-C2-C3-O3
31	5	315	LHG	C3-O3-P-O4
31	5	315	LHG	C3-O3-P-O5
31	5	315	LHG	C3-O3-P-O6
31	5	315	LHG	C4-O6-P-O5
31	5	315	LHG	O10-C23-O8-C6
31	5	315	LHG	C24-C23-O8-C6
31	7	310	LHG	C3-O3-P-O6
31	7	310	LHG	C4-O6-P-O5
31	A	839	LHG	C3-O3-P-O5
31	A	840	LHG	C3-O3-P-O4
31	A	840	LHG	C3-O3-P-O6
31	A	840	LHG	O7-C5-C6-O8
31	A	851	LHG	C4-O6-P-O3
31	A	851	LHG	C4-O6-P-O4
31	B	842	LHG	C4-O6-P-O5
31	B	842	LHG	O7-C5-C6-O8
31	B	842	LHG	O9-C7-O7-C5
31	B	842	LHG	C8-C7-O7-C5
31	B	842	LHG	O10-C23-O8-C6
31	B	842	LHG	C24-C23-O8-C6
31	B	844	LHG	C3-O3-P-O4
31	B	844	LHG	C3-O3-P-O6
31	B	844	LHG	C4-O6-P-O3
31	B	844	LHG	C4-O6-P-O4
31	B	844	LHG	O10-C23-O8-C6
31	B	844	LHG	C24-C23-O8-C6
31	I	102	LHG	C1-C2-C3-O3
31	I	102	LHG	C3-O3-P-O4
31	I	102	LHG	C3-O3-P-O5
31	I	102	LHG	C3-O3-P-O6
31	I	102	LHG	C4-O6-P-O5
31	I	102	LHG	C5-C4-O6-P
31	11	311	LHG	C2-C3-O3-P

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Mol	Chain	Res	Type	Atoms
31	11	311	LHG	C3-O3-P-O4
31	11	311	LHG	C3-O3-P-O5
31	11	311	LHG	C3-O3-P-O6
31	11	311	LHG	C4-O6-P-O5
31	11	311	LHG	O10-C23-O8-C6
31	11	311	LHG	C24-C23-O8-C6
31	4	302	LHG	C4-O6-P-O3
31	4	302	LHG	C4-O6-P-O5
31	9	301	LHG	C4-O6-P-O5
31	9	301	LHG	O9-C7-O7-C5
31	9	301	LHG	C8-C7-O7-C5
31	9	301	LHG	O10-C23-O8-C6
31	9	301	LHG	C24-C23-O8-C6
31	9	302	LHG	C2-C3-O3-P
31	9	302	LHG	C3-O3-P-O6
31	9	302	LHG	C4-O6-P-O3
31	9	302	LHG	C4-O6-P-O4
31	9	314	LHG	C3-O3-P-O5
31	9	314	LHG	C3-O3-P-O6
31	9	314	LHG	C4-O6-P-O3
31	9	314	LHG	O9-C7-O7-C5
31	9	314	LHG	C8-C7-O7-C5
32	5	307	XAT	C5-C6-C7-C8
32	5	307	XAT	C6-C7-C8-C9
32	5	307	XAT	C9-C10-C11-C12
32	5	307	XAT	C26-C27-C28-C29
32	5	310	XAT	C6-C7-C8-C9
32	5	310	XAT	C26-C27-C28-C29
32	5	311	XAT	O4-C6-C7-C8
32	5	311	XAT	C6-C7-C8-C9
32	5	311	XAT	C7-C8-C9-C10
32	5	311	XAT	C26-C27-C28-C29
32	7	313	XAT	C6-C7-C8-C9
32	7	313	XAT	O24-C26-C27-C28
32	7	313	XAT	C26-C27-C28-C29
32	7	315	XAT	C6-C7-C8-C9
32	7	315	XAT	C9-C10-C11-C12
32	7	315	XAT	C25-C26-C27-C28
32	7	315	XAT	O24-C26-C27-C28
32	7	315	XAT	C31-C32-C33-C34
32	7	316	XAT	C6-C7-C8-C9
32	7	316	XAT	O24-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
32	7	316	XAT	C26-C27-C28-C29
32	7	317	XAT	C5-C6-C7-C8
32	7	317	XAT	C6-C7-C8-C9
32	7	317	XAT	C26-C27-C28-C29
32	7	317	XAT	C27-C28-C29-C30
32	8	312	XAT	C6-C7-C8-C9
32	8	312	XAT	C11-C12-C13-C14
32	J	105	XAT	C25-C26-C27-C28
32	6	312	XAT	C6-C7-C8-C9
32	6	312	XAT	C26-C27-C28-C29
32	6	315	XAT	C26-C27-C28-C29
32	6	316	XAT	O4-C6-C7-C8
32	6	316	XAT	C6-C7-C8-C9
32	6	316	XAT	C7-C8-C9-C10
32	6	316	XAT	C7-C8-C9-C19
32	10	313	XAT	C6-C7-C8-C9
32	10	314	XAT	O4-C6-C7-C8
32	10	314	XAT	C26-C27-C28-C29
32	10	315	XAT	O24-C26-C27-C28
32	10	315	XAT	C26-C27-C28-C29
32	11	313	XAT	O4-C6-C7-C8
32	11	313	XAT	C6-C7-C8-C9
32	11	313	XAT	C7-C8-C9-C10
32	11	313	XAT	C7-C8-C9-C19
32	13	308	XAT	C6-C7-C8-C9
32	13	309	XAT	C6-C7-C8-C9
32	13	309	XAT	O24-C26-C27-C28
32	13	309	XAT	C26-C27-C28-C29
32	13	309	XAT	C27-C28-C29-C30
32	17	311	XAT	C25-C26-C27-C28
32	17	311	XAT	C26-C27-C28-C29
32	4	315	XAT	C6-C7-C8-C9
32	4	315	XAT	O24-C26-C27-C28
32	4	315	XAT	C26-C27-C28-C29
32	4	315	XAT	C27-C28-C29-C30
32	4	318	XAT	C1-C6-C7-C8
32	4	318	XAT	C6-C7-C8-C9
32	4	318	XAT	C26-C27-C28-C29
32	9	313	XAT	C5-C6-C7-C8
32	9	313	XAT	O24-C26-C27-C28
32	9	313	XAT	C26-C27-C28-C29
33	8	309	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
33	8	309	BCR	C5-C6-C7-C8
33	A	841	BCR	C23-C24-C25-C26
33	A	841	BCR	C23-C24-C25-C30
33	A	850	BCR	C1-C6-C7-C8
33	A	850	BCR	C5-C6-C7-C8
33	A	850	BCR	C13-C14-C15-C16
33	B	846	BCR	C23-C24-C25-C26
33	B	846	BCR	C23-C24-C25-C30
33	B	850	BCR	C1-C6-C7-C8
33	B	850	BCR	C5-C6-C7-C8
33	B	851	BCR	C1-C6-C7-C8
33	B	851	BCR	C5-C6-C7-C8
34	8	314	DGD	O1G-C1G-C2G-O2G
34	4	301	DGD	C2B-C1B-O2G-C2G
34	4	301	DGD	O1B-C1B-O2G-C2G
34	4	301	DGD	O1G-C1G-C2G-O2G
34	4	301	DGD	C2E-C1E-O5D-C6D
34	4	317	DGD	C2D-C1D-O3G-C3G
34	4	317	DGD	O6D-C1D-O3G-C3G
28	7	311	CLA	O1A-CGA-O2A-C1
28	13	305	CLA	O1A-CGA-O2A-C1
28	17	309	CLA	O1A-CGA-O2A-C1
28	7	311	CLA	CBA-CGA-O2A-C1
28	13	305	CLA	CBA-CGA-O2A-C1
28	17	309	CLA	CBA-CGA-O2A-C1
28	10	307	CLA	C3-C5-C6-C7
28	4	306	CLA	C3-C5-C6-C7
28	5	313	CLA	C4-C3-C5-C6
28	7	303	CLA	C4-C3-C5-C6
28	8	303	CLA	C4-C3-C5-C6
28	8	313	CLA	C4-C3-C5-C6
28	A	810	CLA	C4-C3-C5-C6
28	A	817	CLA	C4-C3-C5-C6
28	A	834	CLA	C4-C3-C5-C6
28	A	836	CLA	C4-C3-C5-C6
28	A	845	CLA	C4-C3-C5-C6
28	A	847	CLA	C4-C3-C5-C6
28	B	808	CLA	C4-C3-C5-C6
28	B	826	CLA	C4-C3-C5-C6
28	B	830	CLA	C4-C3-C5-C6
28	B	835	CLA	C4-C3-C5-C6
28	11	304	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
28	13	301	CLA	C4-C3-C5-C6
28	4	306	CLA	C4-C3-C5-C6
28	4	310	CLA	C4-C3-C5-C6
28	4	316	CLA	C4-C3-C5-C6
28	L	206	CLA	C4-C3-C5-C6
28	8	303	CLA	C2-C3-C5-C6
28	8	313	CLA	C2-C3-C5-C6
28	A	810	CLA	C2-C3-C5-C6
28	A	834	CLA	C2-C3-C5-C6
28	A	836	CLA	C2-C3-C5-C6
28	A	845	CLA	C2-C3-C5-C6
28	B	808	CLA	C2-C3-C5-C6
28	B	826	CLA	C2-C3-C5-C6
28	B	831	CLA	C2-C3-C5-C6
28	B	835	CLA	C2-C3-C5-C6
28	F	802	CLA	C2-C3-C5-C6
28	6	302	CLA	C2-C3-C5-C6
28	6	306	CLA	C2-C3-C5-C6
28	13	301	CLA	C2-C3-C5-C6
28	L	206	CLA	C2-C3-C5-C6
28	7	318	CLA	C2A-CAA-CBA-CGA
28	8	303	CLA	C2A-CAA-CBA-CGA
28	A	806	CLA	C2A-CAA-CBA-CGA
28	A	820	CLA	C2A-CAA-CBA-CGA
28	4	306	CLA	C2A-CAA-CBA-CGA
28	4	307	CLA	C2A-CAA-CBA-CGA
28	A	806	CLA	C3-C5-C6-C7
29	6	314	A86	C3-C4-C5-C6
32	5	310	XAT	C33-C34-C35-C15
32	5	311	XAT	C13-C14-C15-C35
33	B	839	BCR	C15-C16-C17-C18
33	L	202	BCR	C15-C16-C17-C18
29	3	310	A86	C39-C38-O4-C34
29	J	101	A86	C39-C38-O4-C34
29	6	314	A86	C39-C38-O4-C34
29	10	317	A86	C39-C38-O4-C34
29	9	312	A86	C39-C38-O4-C34
28	13	301	CLA	C3-C5-C6-C7
28	4	303	CLA	C3-C5-C6-C7
31	5	315	LHG	O2-C2-C3-O3
31	I	102	LHG	O2-C2-C3-O3
31	11	311	LHG	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
29	3	310	A86	O5-C38-O4-C34
29	J	101	A86	O5-C38-O4-C34
29	6	314	A86	O5-C38-O4-C34
29	10	317	A86	O5-C38-O4-C34
29	9	312	A86	O5-C38-O4-C34
28	L	206	CLA	C2C-C3C-CAC-CBC
28	1	314	CLA	C4-C3-C5-C6
28	A	822	CLA	C4-C3-C5-C6
28	B	834	CLA	C4-C3-C5-C6
28	B	845	CLA	C4-C3-C5-C6
28	R	202	CLA	C4-C3-C5-C6
28	10	301	CLA	C4-C3-C5-C6
28	4	303	CLA	C4-C3-C5-C6
28	5	313	CLA	C2-C3-C5-C6
28	A	822	CLA	C2-C3-C5-C6
28	A	847	CLA	C2-C3-C5-C6
28	B	834	CLA	C2-C3-C5-C6
28	B	845	CLA	C2-C3-C5-C6
28	R	202	CLA	C2-C3-C5-C6
28	10	301	CLA	C2-C3-C5-C6
28	4	303	CLA	C2-C3-C5-C6
28	4	306	CLA	C2-C3-C5-C6
28	4	310	CLA	C2-C3-C5-C6
28	4	316	CLA	C2-C3-C5-C6
31	1	309	LHG	C2-C3-O3-P
31	5	315	LHG	C2-C3-O3-P
28	3	314	CLA	C2A-CAA-CBA-CGA
28	9	310	CLA	C2A-CAA-CBA-CGA
34	8	314	DGD	O6D-C1D-O3G-C3G
34	8	314	DGD	O6E-C1E-O5D-C6D
34	4	301	DGD	O6D-C1D-O3G-C3G
30	3	308	KC1	CAA-CBA-CGA-O1A
28	A	847	CLA	C3-C5-C6-C7
29	5	312	A86	C1-C2-C3-C4
29	8	308	A86	C3-C4-C5-C6
32	8	312	XAT	C9-C10-C11-C12
28	1	307	CLA	C4-C3-C5-C6
28	7	306	CLA	C4-C3-C5-C6
28	1	307	CLA	C2-C3-C5-C6
28	1	314	CLA	C2-C3-C5-C6
28	7	303	CLA	C2-C3-C5-C6
28	A	817	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
28	B	830	CLA	C2-C3-C5-C6
28	11	304	CLA	C2-C3-C5-C6
28	1	310	CLA	C6-C7-C8-C9
28	3	301	CLA	C6-C7-C8-C9
28	3	301	CLA	C11-C12-C13-C14
28	3	306	CLA	C14-C13-C15-C16
28	3	307	CLA	C11-C10-C8-C9
28	7	303	CLA	C11-C10-C8-C9
28	7	304	CLA	C11-C10-C8-C9
28	7	312	CLA	C6-C7-C8-C9
28	7	312	CLA	C11-C10-C8-C9
28	7	312	CLA	C14-C13-C15-C16
28	8	303	CLA	C6-C7-C8-C9
28	8	303	CLA	C11-C10-C8-C9
28	A	817	CLA	C11-C10-C8-C9
28	A	824	CLA	C11-C12-C13-C14
28	A	826	CLA	C6-C7-C8-C9
28	A	826	CLA	C14-C13-C15-C16
28	A	836	CLA	C11-C10-C8-C9
28	A	837	CLA	C11-C12-C13-C14
28	A	849	CLA	C6-C7-C8-C9
28	A	849	CLA	C11-C12-C13-C14
28	A	853	CLA	C14-C13-C15-C16
28	B	801	CLA	C11-C10-C8-C9
28	B	803	CLA	C11-C12-C13-C14
28	B	805	CLA	C14-C13-C15-C16
28	B	807	CLA	C11-C10-C8-C9
28	B	808	CLA	C14-C13-C15-C16
28	B	812	CLA	C6-C7-C8-C9
28	B	814	CLA	C11-C10-C8-C9
28	B	821	CLA	C11-C12-C13-C14
28	B	834	CLA	C11-C12-C13-C14
28	B	843	CLA	C11-C10-C8-C9
28	B	847	CLA	C11-C10-C8-C9
28	B	847	CLA	C14-C13-C15-C16
28	J	102	CLA	C11-C10-C8-C9
28	6	301	CLA	C11-C10-C8-C9
28	10	316	CLA	C11-C12-C13-C14
28	11	301	CLA	C14-C13-C15-C16
28	11	302	CLA	C11-C10-C8-C9
28	4	316	CLA	C6-C7-C8-C9
34	8	314	DGD	C2D-C1D-O3G-C3G

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Mol	Chain	Res	Type	Atoms
34	8	314	DGD	C2E-C1E-O5D-C6D
34	4	301	DGD	C2D-C1D-O3G-C3G
29	1	302	A86	C7-C6-C8-C9
29	J	101	A86	C7-C6-C8-C9
29	10	312	A86	C-C1-C24-C25
32	1	311	XAT	C27-C28-C29-C39
32	7	317	XAT	C27-C28-C29-C39
32	8	311	XAT	C7-C8-C9-C19
32	8	312	XAT	C11-C12-C13-C20
32	J	105	XAT	C7-C8-C9-C19
32	13	309	XAT	C27-C28-C29-C39
32	4	315	XAT	C11-C12-C13-C20
33	1	312	BCR	C7-C8-C9-C34
33	8	309	BCR	C37-C22-C23-C24
33	B	840	BCR	C37-C22-C23-C24
29	10	312	A86	C5-C6-C8-C9
32	1	311	XAT	C27-C28-C29-C30
32	8	311	XAT	C7-C8-C9-C10
32	J	105	XAT	C7-C8-C9-C10
32	4	315	XAT	C11-C12-C13-C14
33	1	312	BCR	C7-C8-C9-C10
33	8	309	BCR	C21-C22-C23-C24
33	B	840	BCR	C21-C22-C23-C24
33	17	310	BCR	C21-C22-C23-C24
28	6	306	CLA	C2A-CAA-CBA-CGA
28	13	305	CLA	C2A-CAA-CBA-CGA
28	19	201	CLA	C2A-CAA-CBA-CGA
28	9	311	CLA	C2A-CAA-CBA-CGA
30	3	308	KC1	CAA-CBA-CGA-O2A
28	1	314	CLA	C11-C12-C13-C15
28	7	305	CLA	C12-C13-C15-C16
28	7	306	CLA	C12-C13-C15-C16
28	8	301	CLA	C6-C7-C8-C10
28	8	304	CLA	C6-C7-C8-C10
28	A	805	CLA	C6-C7-C8-C10
28	A	825	CLA	C12-C13-C15-C16
28	A	830	CLA	C11-C10-C8-C7
28	B	807	CLA	C11-C12-C13-C15
28	B	812	CLA	C11-C12-C13-C15
28	B	813	CLA	C6-C7-C8-C10
28	B	822	CLA	C11-C12-C13-C15
28	B	843	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
28	6	313	CLA	C11-C10-C8-C7
35	A	838	PQN	C22-C23-C25-C26
28	6	301	CLA	C4-C3-C5-C6
29	J	101	A86	C3-C4-C5-C6
29	4	314	A86	C11-C10-C9-C8
29	17	308	A86	C33-C34-O4-C38
28	A	825	CLA	C13-C15-C16-C17
28	B	834	CLA	C8-C10-C11-C12
28	1	308	CLA	C2A-CAA-CBA-CGA
28	7	301	CLA	C2A-CAA-CBA-CGA
28	A	808	CLA	C2A-CAA-CBA-CGA
28	A	812	CLA	C2A-CAA-CBA-CGA
28	A	813	CLA	C2A-CAA-CBA-CGA
28	A	836	CLA	C2A-CAA-CBA-CGA
28	A	837	CLA	C2A-CAA-CBA-CGA
28	B	817	CLA	C2A-CAA-CBA-CGA
28	B	827	CLA	C2A-CAA-CBA-CGA
28	B	832	CLA	C2A-CAA-CBA-CGA
28	J	102	CLA	C2A-CAA-CBA-CGA
28	6	311	CLA	C2A-CAA-CBA-CGA
28	6	313	CLA	C2A-CAA-CBA-CGA
28	11	301	CLA	C2A-CAA-CBA-CGA
28	11	304	CLA	C2A-CAA-CBA-CGA
28	13	301	CLA	C2A-CAA-CBA-CGA
28	17	301	CLA	C2A-CAA-CBA-CGA
28	17	304	CLA	C2A-CAA-CBA-CGA
28	17	307	CLA	C2A-CAA-CBA-CGA
28	4	303	CLA	C2A-CAA-CBA-CGA
28	9	305	CLA	C2A-CAA-CBA-CGA
28	L	206	CLA	C2A-CAA-CBA-CGA
28	A	830	CLA	C5-C6-C7-C8
28	A	830	CLA	C8-C10-C11-C12
33	17	310	BCR	C22-C23-C24-C25
34	4	301	DGD	O6E-C1E-O5D-C6D
28	7	304	CLA	C13-C15-C16-C17
28	B	832	CLA	C13-C15-C16-C17
28	11	312	CLA	C2A-CAA-CBA-CGA
28	J	102	CLA	C5-C6-C7-C8
28	7	306	CLA	C2-C3-C5-C6
28	7	308	CLA	C2A-CAA-CBA-CGA
32	9	313	XAT	C33-C34-C35-C15
28	3	314	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
28	1	307	CLA	C2A-CAA-CBA-CGA
28	7	304	CLA	C2A-CAA-CBA-CGA
28	A	802	CLA	C2A-CAA-CBA-CGA
28	A	827	CLA	C2A-CAA-CBA-CGA
28	A	847	CLA	C2A-CAA-CBA-CGA
28	B	810	CLA	C2A-CAA-CBA-CGA
28	10	306	CLA	C2A-CAA-CBA-CGA
28	3	303	CLA	C10-C11-C12-C13
28	B	824	CLA	C5-C6-C7-C8
28	3	303	CLA	C5-C6-C7-C8
28	4	303	CLA	C5-C6-C7-C8
29	4	313	A86	C33-C34-O4-C38
28	L	203	CLA	C8-C10-C11-C12
28	7	302	CLA	C1-C2-C3-C5
28	A	829	CLA	C1-C2-C3-C4
28	A	829	CLA	C1-C2-C3-C5
28	9	305	CLA	C1-C2-C3-C5
28	B	808	CLA	C3-C5-C6-C7
28	3	314	CLA	C14-C13-C15-C16
28	B	834	CLA	C14-C13-C15-C16
28	10	316	CLA	C6-C7-C8-C9
34	4	317	DGD	C2E-C1E-O5D-C6D
30	17	306	KC1	CAA-CBA-CGA-O1A
30	17	306	KC1	CAA-CBA-CGA-O2A
32	4	315	XAT	C27-C28-C29-C39
33	17	310	BCR	C37-C22-C23-C24
29	4	313	A86	C35-C34-O4-C38
28	1	301	CLA	C2A-CAA-CBA-CGA
28	8	301	CLA	C2A-CAA-CBA-CGA
28	A	815	CLA	C2A-CAA-CBA-CGA
28	A	818	CLA	C2A-CAA-CBA-CGA
28	A	831	CLA	C2A-CAA-CBA-CGA
28	3	307	CLA	O2A-C1-C2-C3
28	B	804	CLA	O2A-C1-C2-C3
34	4	317	DGD	O6E-C1E-O5D-C6D
28	3	305	CLA	C11-C12-C13-C14
28	B	811	CLA	C6-C7-C8-C9
28	R	202	CLA	C6-C7-C8-C10
28	6	307	CLA	C6-C7-C8-C9
28	1	307	CLA	C3-C5-C6-C7
29	3	311	A86	C24-C1-C2-C3
29	3	311	A86	C4-C5-C6-C8

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Mol	Chain	Res	Type	Atoms
29	10	312	A86	C24-C1-C2-C3
29	10	312	A86	C4-C5-C6-C8
32	6	312	XAT	C12-C13-C14-C15
32	6	312	XAT	C32-C33-C34-C35
32	10	315	XAT	C32-C33-C34-C35
33	8	309	BCR	C12-C13-C14-C15
33	8	309	BCR	C16-C17-C18-C19
28	B	821	CLA	C13-C15-C16-C17
29	1	302	A86	C9-C10-C11-C13
28	3	305	CLA	C11-C12-C13-C15
28	6	307	CLA	C6-C7-C8-C10
28	11	304	CLA	C11-C12-C13-C14
28	4	303	CLA	C6-C7-C8-C9
28	4	316	CLA	C14-C13-C15-C16
34	4	301	DGD	O6D-C5D-C6D-O5D
28	1	301	CLA	C4B-C3B-CAB-CBB
28	1	303	CLA	C4B-C3B-CAB-CBB
28	1	304	CLA	C4B-C3B-CAB-CBB
28	5	301	CLA	C4B-C3B-CAB-CBB
28	5	302	CLA	C4B-C3B-CAB-CBB
28	7	308	CLA	C4B-C3B-CAB-CBB
28	8	301	CLA	C4B-C3B-CAB-CBB
28	8	303	CLA	C4B-C3B-CAB-CBB
28	8	305	CLA	C4B-C3B-CAB-CBB
28	A	806	CLA	C4B-C3B-CAB-CBB
28	A	808	CLA	C4B-C3B-CAB-CBB
28	A	815	CLA	C4B-C3B-CAB-CBB
28	A	829	CLA	C4B-C3B-CAB-CBB
28	A	832	CLA	C4B-C3B-CAB-CBB
28	A	834	CLA	C4B-C3B-CAB-CBB
28	A	847	CLA	C4B-C3B-CAB-CBB
28	B	803	CLA	C4B-C3B-CAB-CBB
28	B	807	CLA	C4B-C3B-CAB-CBB
28	B	809	CLA	C4B-C3B-CAB-CBB
28	B	818	CLA	C4B-C3B-CAB-CBB
28	B	819	CLA	C4B-C3B-CAB-CBB
28	B	820	CLA	C4B-C3B-CAB-CBB
28	B	827	CLA	C4B-C3B-CAB-CBB
28	B	828	CLA	C4B-C3B-CAB-CBB
28	B	829	CLA	C4B-C3B-CAB-CBB
28	R	202	CLA	C4B-C3B-CAB-CBB
28	6	303	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
28	10	302	CLA	C4B-C3B-CAB-CBB
28	10	307	CLA	C4B-C3B-CAB-CBB
28	11	314	CLA	C4B-C3B-CAB-CBB
28	13	306	CLA	C4B-C3B-CAB-CBB
28	16	203	CLA	C4B-C3B-CAB-CBB
28	16	204	CLA	C4B-C3B-CAB-CBB
28	4	305	CLA	C4B-C3B-CAB-CBB
28	4	307	CLA	C4B-C3B-CAB-CBB
28	9	303	CLA	C4B-C3B-CAB-CBB
28	L	204	CLA	C4B-C3B-CAB-CBB
28	a	202	CLA	C4B-C3B-CAB-CBB
28	5	302	CLA	C6-C7-C8-C9
28	5	302	CLA	C6-C7-C8-C10
28	A	803	CLA	C6-C7-C8-C9
28	B	811	CLA	C6-C7-C8-C10
28	B	806	CLA	C2A-CAA-CBA-CGA
28	10	316	CLA	C2A-CAA-CBA-CGA
28	B	821	CLA	C15-C16-C17-C18
28	5	313	CLA	C6-C7-C8-C10
28	B	809	CLA	C11-C12-C13-C15
28	B	845	CLA	C11-C12-C13-C15
28	3	307	CLA	C3A-C2A-CAA-CBA
28	5	304	CLA	C3A-C2A-CAA-CBA
28	5	309	CLA	C3A-C2A-CAA-CBA
28	7	312	CLA	C3A-C2A-CAA-CBA
28	7	318	CLA	C3A-C2A-CAA-CBA
28	A	811	CLA	C3A-C2A-CAA-CBA
28	A	817	CLA	C3A-C2A-CAA-CBA
28	A	828	CLA	C3A-C2A-CAA-CBA
28	A	834	CLA	C3A-C2A-CAA-CBA
28	A	852	CLA	C3A-C2A-CAA-CBA
28	B	807	CLA	C3A-C2A-CAA-CBA
28	B	808	CLA	C3A-C2A-CAA-CBA
28	B	823	CLA	C3A-C2A-CAA-CBA
28	B	824	CLA	C3A-C2A-CAA-CBA
28	B	831	CLA	C3A-C2A-CAA-CBA
28	6	311	CLA	C3A-C2A-CAA-CBA
28	11	309	CLA	C3A-C2A-CAA-CBA
28	11	314	CLA	C3A-C2A-CAA-CBA
28	13	302	CLA	C3A-C2A-CAA-CBA
28	13	303	CLA	C3A-C2A-CAA-CBA
28	13	305	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
28	16	205	CLA	C3A-C2A-CAA-CBA
28	17	305	CLA	C3A-C2A-CAA-CBA
28	6	301	CLA	C2-C3-C5-C6
28	L	206	CLA	C4C-C3C-CAC-CBC
28	A	803	CLA	C6-C7-C8-C10
31	I	102	LHG	C18-C19-C20-C21
28	A	802	CLA	C16-C17-C18-C20
28	A	806	CLA	C6-C7-C8-C10
28	A	834	CLA	C6-C7-C8-C10
28	4	303	CLA	C6-C7-C8-C10
28	1	301	CLA	C2B-C3B-CAB-CBB
28	1	310	CLA	C2B-C3B-CAB-CBB
28	3	301	CLA	C2B-C3B-CAB-CBB
28	5	303	CLA	C2B-C3B-CAB-CBB
28	5	304	CLA	C2B-C3B-CAB-CBB
28	7	302	CLA	C2B-C3B-CAB-CBB
28	7	318	CLA	C2B-C3B-CAB-CBB
28	A	814	CLA	C2B-C3B-CAB-CBB
28	B	814	CLA	C2B-C3B-CAB-CBB
28	B	817	CLA	C2B-C3B-CAB-CBB
28	B	829	CLA	C2B-C3B-CAB-CBB
28	B	832	CLA	C2B-C3B-CAB-CBB
28	F	803	CLA	C2B-C3B-CAB-CBB
28	10	307	CLA	C2B-C3B-CAB-CBB
28	13	301	CLA	C2B-C3B-CAB-CBB
28	16	204	CLA	C2B-C3B-CAB-CBB
28	16	205	CLA	C2B-C3B-CAB-CBB
28	4	305	CLA	C2B-C3B-CAB-CBB
28	9	305	CLA	C2B-C3B-CAB-CBB
28	9	311	CLA	C2B-C3B-CAB-CBB
33	8	309	BCR	C23-C24-C25-C30
33	A	844	BCR	C23-C24-C25-C26
33	A	844	BCR	C23-C24-C25-C30
33	B	837	BCR	C5-C6-C7-C8
33	17	310	BCR	C1-C6-C7-C8
33	17	310	BCR	C5-C6-C7-C8
33	17	310	BCR	C23-C24-C25-C26
33	17	310	BCR	C23-C24-C25-C30
31	9	314	LHG	C2-C3-O3-P
28	A	845	CLA	C2A-CAA-CBA-CGA
28	6	301	CLA	C2A-CAA-CBA-CGA
28	4	310	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
28	5	305	CLA	C11-C10-C8-C7
28	A	816	CLA	C11-C10-C8-C7
28	7	312	CLA	C11-C12-C13-C14
28	A	810	CLA	C14-C13-C15-C16
28	A	824	CLA	C6-C7-C8-C9
28	A	847	CLA	C6-C7-C8-C9
28	A	847	CLA	C11-C12-C13-C14
28	B	832	CLA	C11-C10-C8-C9
28	4	316	CLA	C11-C10-C8-C9
34	8	314	DGD	O1G-C1G-C2G-C3G
29	17	308	A86	C35-C34-O4-C38
29	5	312	A86	C3-C4-C5-C6
29	J	101	A86	C1-C2-C3-C4
29	R	203	A86	C1-C2-C3-C4
29	10	317	A86	C-C1-C24-C25
32	7	315	XAT	C31-C32-C33-C40
32	6	312	XAT	C31-C32-C33-C34
28	B	848	CLA	C2A-CAA-CBA-CGA
28	1	310	CLA	C4-C3-C5-C6
28	A	837	CLA	C4-C3-C5-C6
30	1	306	KC1	C2B-C3B-CAB-CBB
30	3	302	KC1	C2B-C3B-CAB-CBB
30	7	307	KC1	C2B-C3B-CAB-CBB
30	8	306	KC1	C2B-C3B-CAB-CBB
30	8	307	KC1	C2B-C3B-CAB-CBB
30	6	308	KC1	C2B-C3B-CAB-CBB
30	6	310	KC1	C2B-C3B-CAB-CBB
30	10	310	KC1	C2B-C3B-CAB-CBB
30	10	311	KC1	C2B-C3B-CAB-CBB
30	17	306	KC1	C2B-C3B-CAB-CBB
30	9	309	KC1	C2B-C3B-CAB-CBB
28	10	306	CLA	C3-C5-C6-C7
28	A	837	CLA	C5-C6-C7-C8
28	11	302	CLA	C10-C11-C12-C13
31	9	301	LHG	O6-C4-C5-O7
30	1	306	KC1	C2A-CAA-CBA-CGA
30	3	308	KC1	C2A-CAA-CBA-CGA
30	3	309	KC1	C2A-CAA-CBA-CGA
30	5	308	KC1	C2A-CAA-CBA-CGA
30	7	307	KC1	C4B-C3B-CAB-CBB
30	7	309	KC1	C2A-CAA-CBA-CGA
30	8	307	KC1	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
30	6	305	KC1	C2A-CAA-CBA-CGA
30	6	309	KC1	C2A-CAA-CBA-CGA
30	6	310	KC1	C2A-CAA-CBA-CGA
30	10	304	KC1	C2A-CAA-CBA-CGA
30	10	310	KC1	C2A-CAA-CBA-CGA
30	10	311	KC1	C2A-CAA-CBA-CGA
30	11	307	KC1	C2A-CAA-CBA-CGA
30	13	304	KC1	C2A-CAA-CBA-CGA
30	17	306	KC1	C2A-CAA-CBA-CGA
30	17	312	KC1	C2A-CAA-CBA-CGA
30	4	309	KC1	C4B-C3B-CAB-CBB
30	4	309	KC1	C2A-CAA-CBA-CGA
30	4	311	KC1	C4B-C3B-CAB-CBB
30	4	311	KC1	C2A-CAA-CBA-CGA
30	4	312	KC1	C2A-CAA-CBA-CGA
30	9	306	KC1	C2A-CAA-CBA-CGA
28	R	202	CLA	C6-C7-C8-C9
34	4	317	DGD	O6E-C5E-C6E-O5E
31	1	309	LHG	O7-C5-C6-O8
31	A	839	LHG	O7-C5-C6-O8
31	I	102	LHG	O7-C5-C6-O8
28	A	815	CLA	C5-C6-C7-C8
34	8	314	DGD	O6E-C5E-C6E-O5E
28	A	806	CLA	C2-C1-O2A-CGA
28	R	202	CLA	C2-C1-O2A-CGA
28	B	834	CLA	C5-C6-C7-C8
31	B	844	LHG	C2-C3-O3-P
28	B	813	CLA	C2-C3-C5-C6
28	1	305	CLA	C2A-CAA-CBA-CGA
28	5	313	CLA	C2A-CAA-CBA-CGA
28	A	809	CLA	C2A-CAA-CBA-CGA
28	A	814	CLA	C2A-CAA-CBA-CGA
28	A	821	CLA	C2A-CAA-CBA-CGA
28	B	802	CLA	C2A-CAA-CBA-CGA
28	B	811	CLA	C2A-CAA-CBA-CGA
28	13	307	CLA	C2A-CAA-CBA-CGA
28	17	309	CLA	C2A-CAA-CBA-CGA
28	4	316	CLA	C2A-CAA-CBA-CGA
28	B	807	CLA	C8-C10-C11-C12
37	F	805	LMG	O6-C5-C6-O5
28	17	302	CLA	C2A-CAA-CBA-CGA
28	3	305	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
28	5	309	CLA	C1A-C2A-CAA-CBA
28	7	301	CLA	C1A-C2A-CAA-CBA
28	7	312	CLA	C1A-C2A-CAA-CBA
28	8	301	CLA	C1A-C2A-CAA-CBA
28	8	303	CLA	C1A-C2A-CAA-CBA
28	A	806	CLA	C1A-C2A-CAA-CBA
28	A	807	CLA	C1A-C2A-CAA-CBA
28	A	808	CLA	C1A-C2A-CAA-CBA
28	A	810	CLA	C1A-C2A-CAA-CBA
28	A	818	CLA	C1A-C2A-CAA-CBA
28	B	804	CLA	C1A-C2A-CAA-CBA
28	B	816	CLA	C1A-C2A-CAA-CBA
28	B	827	CLA	C1A-C2A-CAA-CBA
28	B	845	CLA	C1A-C2A-CAA-CBA
28	6	301	CLA	C1A-C2A-CAA-CBA
28	6	311	CLA	C1A-C2A-CAA-CBA
28	10	306	CLA	C1A-C2A-CAA-CBA
28	11	301	CLA	C1A-C2A-CAA-CBA
28	11	309	CLA	C1A-C2A-CAA-CBA
28	11	310	CLA	C1A-C2A-CAA-CBA
28	11	312	CLA	C1A-C2A-CAA-CBA
28	13	302	CLA	C1A-C2A-CAA-CBA
28	16	205	CLA	C1A-C2A-CAA-CBA
28	3	314	CLA	C13-C15-C16-C17
28	10	316	CLA	C8-C10-C11-C12
29	1	302	A86	C9-C10-C11-C12
28	1	303	CLA	C6-C7-C8-C10
28	1	303	CLA	C11-C10-C8-C7
28	3	303	CLA	C12-C13-C15-C16
28	3	307	CLA	C11-C10-C8-C7
28	5	303	CLA	C12-C13-C15-C16
28	7	304	CLA	C11-C12-C13-C15
28	8	303	CLA	C11-C10-C8-C7
28	8	304	CLA	C11-C10-C8-C7
28	A	819	CLA	C6-C7-C8-C10
28	A	826	CLA	C12-C13-C15-C16
28	A	827	CLA	C12-C13-C15-C16
28	A	830	CLA	C6-C7-C8-C10
28	A	837	CLA	C11-C12-C13-C15
28	A	852	CLA	C11-C10-C8-C7
28	A	853	CLA	C12-C13-C15-C16
28	B	801	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
28	B	807	CLA	C11-C10-C8-C7
28	B	807	CLA	C12-C13-C15-C16
28	B	808	CLA	C11-C10-C8-C7
28	B	808	CLA	C12-C13-C15-C16
28	B	814	CLA	C6-C7-C8-C10
28	B	816	CLA	C11-C10-C8-C7
28	B	817	CLA	C12-C13-C15-C16
28	B	832	CLA	C12-C13-C15-C16
28	B	849	CLA	C11-C10-C8-C7
28	F	802	CLA	C11-C12-C13-C15
28	6	301	CLA	C12-C13-C15-C16
31	1	309	LHG	C16-C17-C18-C19
28	3	314	CLA	C15-C16-C17-C18
28	A	827	CLA	C4-C3-C5-C6
28	A	823	CLA	C2-C3-C5-C6
28	B	822	CLA	C2-C3-C5-C6
28	9	305	CLA	C1-C2-C3-C4
28	B	832	CLA	C3-C5-C6-C7
28	A	807	CLA	C2A-CAA-CBA-CGA
28	16	203	CLA	C2A-CAA-CBA-CGA
28	1	303	CLA	C6-C7-C8-C9
28	3	301	CLA	C14-C13-C15-C16
28	3	303	CLA	C14-C13-C15-C16
28	5	301	CLA	C6-C7-C8-C9
28	5	303	CLA	C11-C12-C13-C14
28	8	304	CLA	C11-C10-C8-C9
28	A	802	CLA	C14-C13-C15-C16
28	A	823	CLA	C11-C10-C8-C9
28	A	827	CLA	C14-C13-C15-C16
28	A	830	CLA	C6-C7-C8-C9
28	B	803	CLA	C6-C7-C8-C9
28	B	807	CLA	C6-C7-C8-C9
28	B	807	CLA	C11-C12-C13-C14
28	B	843	CLA	C14-C13-C15-C16
28	B	849	CLA	C11-C10-C8-C9
28	11	304	CLA	C6-C7-C8-C9
28	L	201	CLA	C14-C13-C15-C16
28	A	834	CLA	C6-C7-C8-C9
28	A	820	CLA	C1-C2-C3-C4
31	I	102	LHG	C15-C16-C17-C18
28	5	305	CLA	C11-C10-C8-C9
31	1	309	LHG	C4-C5-C6-O8

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Mol	Chain	Res	Type	Atoms
31	B	842	LHG	C4-C5-C6-O8
28	3	305	CLA	C8-C10-C11-C12
28	B	813	CLA	C4-C3-C5-C6
28	B	822	CLA	C4-C3-C5-C6
28	A	827	CLA	C2-C3-C5-C6
28	A	815	CLA	C10-C11-C12-C13
28	B	843	CLA	C5-C6-C7-C8
28	6	313	CLA	C5-C6-C7-C8
31	9	302	LHG	C9-C10-C11-C12
28	A	806	CLA	C6-C7-C8-C9
31	11	311	LHG	C23-C24-C25-C26
28	8	313	CLA	C5-C6-C7-C8
28	B	817	CLA	C8-C10-C11-C12
28	7	303	CLA	C2A-CAA-CBA-CGA
28	B	813	CLA	C2A-CAA-CBA-CGA
28	A	802	CLA	O2A-C1-C2-C3
28	A	803	CLA	O2A-C1-C2-C3
28	6	302	CLA	O2A-C1-C2-C3
28	1	303	CLA	C8-C10-C11-C12
32	5	311	XAT	C33-C34-C35-C15
32	4	315	XAT	C9-C10-C11-C12
28	11	304	CLA	C11-C12-C13-C15
29	1	302	A86	C4-C5-C6-C8
28	8	301	CLA	C4-C3-C5-C6
28	B	810	CLA	C4-C3-C5-C6
28	11	303	CLA	C4-C3-C5-C6
28	A	837	CLA	C2-C3-C5-C6
31	I	102	LHG	C11-C12-C13-C14
31	1	309	LHG	C29-C30-C31-C32
28	9	308	CLA	C2A-CAA-CBA-CGA
28	B	810	CLA	C6-C7-C8-C9
28	A	830	CLA	C15-C16-C17-C18
32	4	315	XAT	C33-C34-C35-C15
32	9	313	XAT	C13-C14-C15-C35
34	4	301	DGD	C4D-C5D-C6D-O5D
28	8	302	CLA	C4-C3-C5-C6
28	A	807	CLA	C4-C3-C5-C6
28	A	812	CLA	C4-C3-C5-C6
28	A	825	CLA	C4-C3-C5-C6
28	6	303	CLA	C4-C3-C5-C6
28	6	311	CLA	C4-C3-C5-C6
28	A	805	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
28	B	809	CLA	C8-C10-C11-C12
28	1	310	CLA	C11-C12-C13-C14
28	3	303	CLA	C6-C7-C8-C9
28	5	301	CLA	C11-C10-C8-C9
28	5	303	CLA	C11-C10-C8-C9
28	7	306	CLA	C11-C12-C13-C14
28	A	819	CLA	C6-C7-C8-C9
28	A	830	CLA	C11-C10-C8-C9
28	A	837	CLA	C6-C7-C8-C9
28	A	852	CLA	C11-C10-C8-C9
28	B	801	CLA	C14-C13-C15-C16
28	B	803	CLA	C11-C10-C8-C9
28	B	807	CLA	C14-C13-C15-C16
28	B	808	CLA	C11-C10-C8-C9
28	B	814	CLA	C6-C7-C8-C9
28	B	815	CLA	C11-C10-C8-C9
28	B	816	CLA	C11-C10-C8-C9
28	B	832	CLA	C14-C13-C15-C16
28	B	835	CLA	C11-C12-C13-C14
28	B	843	CLA	C11-C12-C13-C14
28	6	301	CLA	C14-C13-C15-C16
28	6	313	CLA	C11-C10-C8-C9
28	1	314	CLA	C4B-C3B-CAB-CBB
28	3	303	CLA	C4B-C3B-CAB-CBB
28	3	307	CLA	C4B-C3B-CAB-CBB
28	5	305	CLA	C4B-C3B-CAB-CBB
28	5	309	CLA	C4B-C3B-CAB-CBB
28	7	301	CLA	C4B-C3B-CAB-CBB
28	7	305	CLA	C4B-C3B-CAB-CBB
28	8	310	CLA	C4B-C3B-CAB-CBB
28	8	313	CLA	C4B-C3B-CAB-CBB
28	A	807	CLA	C4B-C3B-CAB-CBB
28	A	820	CLA	C4B-C3B-CAB-CBB
28	A	827	CLA	C4B-C3B-CAB-CBB
28	A	831	CLA	C4B-C3B-CAB-CBB
28	A	833	CLA	C4B-C3B-CAB-CBB
28	A	846	CLA	C4B-C3B-CAB-CBB
28	A	852	CLA	C4B-C3B-CAB-CBB
28	B	805	CLA	C4B-C3B-CAB-CBB
28	B	806	CLA	C4B-C3B-CAB-CBB
28	B	811	CLA	C4B-C3B-CAB-CBB
28	B	816	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
28	B	824	CLA	C4B-C3B-CAB-CBB
28	B	831	CLA	C4B-C3B-CAB-CBB
28	B	847	CLA	C4B-C3B-CAB-CBB
28	F	803	CLA	C4B-C3B-CAB-CBB
28	10	308	CLA	C4B-C3B-CAB-CBB
28	11	304	CLA	C4B-C3B-CAB-CBB
28	15	201	CLA	C4B-C3B-CAB-CBB
28	9	304	CLA	C4B-C3B-CAB-CBB
28	9	305	CLA	C4B-C3B-CAB-CBB
28	L	203	CLA	C4B-C3B-CAB-CBB
28	a	204	CLA	C4B-C3B-CAB-CBB
28	7	312	CLA	C15-C16-C17-C18
28	B	820	CLA	C2A-CAA-CBA-CGA
28	B	845	CLA	C2A-CAA-CBA-CGA
28	1	310	CLA	C11-C12-C13-C15
28	3	307	CLA	C12-C13-C15-C16
28	5	301	CLA	C6-C7-C8-C10
28	5	303	CLA	C11-C12-C13-C15
28	7	303	CLA	C12-C13-C15-C16
28	8	303	CLA	C6-C7-C8-C10
28	A	802	CLA	C12-C13-C15-C16
28	A	804	CLA	C12-C13-C15-C16
28	A	808	CLA	C6-C7-C8-C10
28	A	815	CLA	C6-C7-C8-C10
28	A	823	CLA	C11-C10-C8-C7
28	A	823	CLA	C11-C12-C13-C15
28	A	824	CLA	C11-C12-C13-C15
28	A	849	CLA	C11-C12-C13-C15
28	B	803	CLA	C6-C7-C8-C10
28	B	803	CLA	C11-C10-C8-C7
28	B	805	CLA	C11-C12-C13-C15
28	B	808	CLA	C6-C7-C8-C10
28	B	815	CLA	C11-C10-C8-C7
28	B	843	CLA	C11-C10-C8-C7
28	B	843	CLA	C12-C13-C15-C16
28	6	301	CLA	C11-C12-C13-C15
28	13	301	CLA	C6-C7-C8-C10
28	L	201	CLA	C12-C13-C15-C16
35	B	836	PQN	C16-C17-C18-C20
28	B	832	CLA	C10-C11-C12-C13
28	B	815	CLA	C11-C12-C13-C14
28	A	821	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
28	A	823	CLA	C4-C3-C5-C6
28	A	846	CLA	C3A-C2A-CAA-CBA
28	B	803	CLA	C4-C3-C5-C6
28	B	805	CLA	C4-C3-C5-C6
28	B	817	CLA	C3A-C2A-CAA-CBA
28	11	312	CLA	C3A-C2A-CAA-CBA
28	4	303	CLA	C3A-C2A-CAA-CBA
28	1	305	CLA	C2-C3-C5-C6
28	A	807	CLA	C2-C3-C5-C6
28	A	825	CLA	C2-C3-C5-C6
29	8	308	A86	C1-C2-C3-C4
29	R	203	A86	C3-C4-C5-C6
32	10	314	XAT	C9-C10-C11-C12
32	10	315	XAT	C33-C34-C35-C15
28	R	204	CLA	C4-C3-C5-C6
31	I	102	LHG	C26-C27-C28-C29
29	3	311	A86	C12-C11-C13-O
31	A	840	LHG	C4-C5-C6-O8
31	I	102	LHG	C4-C5-C6-O8
31	4	302	LHG	C4-C5-C6-O8
34	4	301	DGD	O1G-C1G-C2G-C3G
28	A	817	CLA	C10-C11-C12-C13
28	5	302	CLA	C1-C2-C3-C4
28	7	305	CLA	C1-C2-C3-C4
28	8	301	CLA	C1-C2-C3-C4
28	8	302	CLA	C1-C2-C3-C4
28	A	807	CLA	C1-C2-C3-C4
28	A	808	CLA	C1-C2-C3-C4
28	A	811	CLA	C1-C2-C3-C4
28	A	817	CLA	C1-C2-C3-C4
28	A	830	CLA	C1-C2-C3-C4
28	A	836	CLA	C1-C2-C3-C4
28	A	837	CLA	C1-C2-C3-C4
28	B	811	CLA	C1-C2-C3-C4
28	B	812	CLA	C1-C2-C3-C4
28	B	820	CLA	C1-C2-C3-C4
28	B	822	CLA	C1-C2-C3-C4
28	B	828	CLA	C1-C2-C3-C4
28	B	834	CLA	C1-C2-C3-C4
28	B	847	CLA	C1-C2-C3-C4
28	F	802	CLA	C1-C2-C3-C4
28	6	301	CLA	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
28	10	301	CLA	C1-C2-C3-C4
28	10	306	CLA	C1-C2-C3-C4
28	10	316	CLA	C1-C2-C3-C4
28	11	302	CLA	C1-C2-C3-C4
28	L	201	CLA	C1-C2-C3-C4
28	1	305	CLA	C4-C3-C5-C6
28	B	843	CLA	C4-C3-C5-C6
29	3	311	A86	C10-C11-C13-O
28	A	831	CLA	C2B-C3B-CAB-CBB
33	8	309	BCR	C23-C24-C25-C26
33	B	840	BCR	C1-C6-C7-C8
28	A	816	CLA	C2A-CAA-CBA-CGA
28	a	203	CLA	C2A-CAA-CBA-CGA
28	B	817	CLA	C13-C15-C16-C17
31	4	302	LHG	O7-C5-C6-O8
29	10	312	A86	C1-C24-C25-C26
28	B	803	CLA	C2-C3-C5-C6
28	6	303	CLA	C2-C3-C5-C6
28	6	311	CLA	C2-C3-C5-C6
28	5	301	CLA	C1-C2-C3-C5
28	8	302	CLA	C1-C2-C3-C5
28	8	304	CLA	C1-C2-C3-C5
28	A	808	CLA	C1-C2-C3-C5
28	A	811	CLA	C1-C2-C3-C5
28	A	821	CLA	C1-C2-C3-C5
28	A	825	CLA	C1-C2-C3-C5
28	A	830	CLA	C1-C2-C3-C5
28	A	833	CLA	C1-C2-C3-C5
28	A	837	CLA	C1-C2-C3-C5
28	A	849	CLA	C1-C2-C3-C5
28	B	804	CLA	C1-C2-C3-C5
28	B	813	CLA	C1-C2-C3-C5
28	B	814	CLA	C1-C2-C3-C5
28	B	819	CLA	C1-C2-C3-C5
28	B	830	CLA	C1-C2-C3-C5
28	B	834	CLA	C1-C2-C3-C5
28	B	847	CLA	C1-C2-C3-C5
28	6	302	CLA	C1-C2-C3-C5
28	10	316	CLA	C1-C2-C3-C5
28	11	301	CLA	C1-C2-C3-C5
28	11	303	CLA	C1-C2-C3-C5
28	13	301	CLA	C1-C2-C3-C5

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Mol	Chain	Res	Type	Atoms
28	4	304	CLA	C1-C2-C3-C5
28	A	802	CLA	C16-C17-C18-C19
28	7	302	CLA	C1-C2-C3-C4
28	3	307	CLA	C14-C13-C15-C16
28	A	804	CLA	C14-C13-C15-C16
28	A	837	CLA	C11-C10-C8-C9
28	B	804	CLA	C11-C12-C13-C14
28	B	808	CLA	C6-C7-C8-C9
28	B	817	CLA	C11-C12-C13-C14
28	6	301	CLA	C11-C12-C13-C14
28	6	313	CLA	C11-C12-C13-C14
28	11	304	CLA	C11-C10-C8-C9
35	B	836	PQN	C16-C17-C18-C19
32	6	312	XAT	C14-C15-C35-C34
31	I	102	LHG	C29-C30-C31-C32
28	6	304	CLA	C1A-C2A-CAA-CBA
28	A	811	CLA	C6-C7-C8-C9
28	A	822	CLA	C3-C5-C6-C7
31	I	102	LHG	O7-C7-C8-C9
31	I	102	LHG	C33-C34-C35-C36
28	7	306	CLA	C3-C5-C6-C7
28	A	816	CLA	CAA-CBA-CGA-O2A
28	A	836	CLA	C8-C10-C11-C12
28	1	310	CLA	C6-C7-C8-C10
28	3	301	CLA	C11-C12-C13-C15
28	3	306	CLA	C12-C13-C15-C16
28	5	313	CLA	C11-C10-C8-C7
28	7	301	CLA	C11-C12-C13-C15
28	7	303	CLA	C11-C12-C13-C15
28	7	304	CLA	C12-C13-C15-C16
28	7	312	CLA	C6-C7-C8-C10
28	A	810	CLA	C11-C12-C13-C15
28	A	817	CLA	C12-C13-C15-C16
28	A	835	CLA	C6-C7-C8-C10
28	A	836	CLA	C11-C10-C8-C7
28	A	836	CLA	C12-C13-C15-C16
28	B	804	CLA	C6-C7-C8-C10
28	B	804	CLA	C11-C12-C13-C15
28	B	806	CLA	C6-C7-C8-C10
28	B	821	CLA	C6-C7-C8-C10
28	B	845	CLA	C11-C10-C8-C7
28	B	847	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
28	B	847	CLA	C12-C13-C15-C16
28	10	307	CLA	C11-C10-C8-C7
28	10	316	CLA	C11-C12-C13-C15
28	11	301	CLA	C12-C13-C15-C16
28	4	316	CLA	C6-C7-C8-C10
35	A	838	PQN	C21-C22-C23-C25
35	B	836	PQN	C22-C23-C25-C26
32	7	315	XAT	C11-C12-C13-C14
32	6	312	XAT	C11-C12-C13-C14
32	6	315	XAT	C27-C28-C29-C30
33	B	837	BCR	C7-C8-C9-C10
34	4	301	DGD	C5D-C6D-O5D-C1E
31	A	839	LHG	C24-C25-C26-C27
28	A	816	CLA	C11-C10-C8-C9
28	6	301	CLA	C16-C17-C18-C20
28	B	821	CLA	C4-C3-C5-C6
28	10	303	CLA	C4-C3-C5-C6
28	B	805	CLA	C2-C3-C5-C6
28	B	843	CLA	C2-C3-C5-C6
30	3	309	KC1	C2B-C3B-CAB-CBB
30	6	305	KC1	C2B-C3B-CAB-CBB
30	6	309	KC1	C2B-C3B-CAB-CBB
30	13	304	KC1	C2B-C3B-CAB-CBB
30	4	308	KC1	C2B-C3B-CAB-CBB
30	4	312	KC1	C2B-C3B-CAB-CBB
30	9	306	KC1	C2B-C3B-CAB-CBB
28	A	830	CLA	C13-C15-C16-C17
28	10	316	CLA	C10-C11-C12-C13
28	A	837	CLA	O2A-C1-C2-C3
28	J	102	CLA	O2A-C1-C2-C3
28	10	307	CLA	O2A-C1-C2-C3
28	B	810	CLA	C6-C7-C8-C10
28	7	312	CLA	C13-C15-C16-C17
31	11	311	LHG	O6-C4-C5-O7
28	3	306	CLA	C13-C15-C16-C17
30	3	309	KC1	C4B-C3B-CAB-CBB
30	9	306	KC1	C4B-C3B-CAB-CBB
28	5	301	CLA	C4-C3-C5-C6
28	B	815	CLA	C2A-CAA-CBA-CGA
29	4	314	A86	C28-C27-C29-C30
28	A	815	CLA	C3-C5-C6-C7
31	5	314	LHG	O7-C5-C6-O8

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Mol	Chain	Res	Type	Atoms
28	7	304	CLA	C14-C13-C15-C16
28	8	301	CLA	C6-C7-C8-C9
28	8	304	CLA	C6-C7-C8-C9
28	A	805	CLA	C6-C7-C8-C9
28	A	835	CLA	C6-C7-C8-C9
28	A	836	CLA	C14-C13-C15-C16
28	B	803	CLA	C14-C13-C15-C16
28	B	804	CLA	C14-C13-C15-C16
28	B	805	CLA	C11-C12-C13-C14
28	B	834	CLA	C6-C7-C8-C9
28	10	307	CLA	C11-C10-C8-C9
28	11	302	CLA	C6-C7-C8-C9
28	L	206	CLA	C11-C12-C13-C14
28	4	307	CLA	C11-C12-C13-C15
29	1	302	A86	C13-C14-C15-O1
29	1	313	A86	C13-C14-C15-O1
29	R	203	A86	C13-C14-C15-O1
29	10	317	A86	C13-C14-C15-O1
29	9	312	A86	C13-C14-C15-O1
29	6	314	A86	C9-C10-C11-C13
28	B	824	CLA	C2-C1-O2A-CGA
28	A	822	CLA	C6-C7-C8-C10
28	11	302	CLA	C16-C17-C18-C20
28	6	307	CLA	C4-C3-C5-C6
28	8	301	CLA	C2-C3-C5-C6
28	10	303	CLA	C2-C3-C5-C6
31	9	302	LHG	C12-C13-C14-C15
28	5	302	CLA	C1A-C2A-CAA-CBA
28	5	313	CLA	C4B-C3B-CAB-CBB
28	A	816	CLA	C4B-C3B-CAB-CBB
28	B	801	CLA	C4B-C3B-CAB-CBB
28	B	823	CLA	C4B-C3B-CAB-CBB
28	R	202	CLA	C1A-C2A-CAA-CBA
28	11	312	CLA	C4B-C3B-CAB-CBB
28	13	305	CLA	C4B-C3B-CAB-CBB
28	13	307	CLA	C4B-C3B-CAB-CBB
28	19	201	CLA	C4B-C3B-CAB-CBB
28	9	308	CLA	C1A-C2A-CAA-CBA
28	9	310	CLA	C4B-C3B-CAB-CBB
28	L	206	CLA	C4B-C3B-CAB-CBB
29	1	302	A86	O-C13-C14-C15
28	3	303	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
28	1	310	CLA	C2-C3-C5-C6
29	6	314	A86	C9-C10-C11-C12
28	8	301	CLA	C11-C10-C8-C7
28	A	802	CLA	C6-C7-C8-C10
28	A	805	CLA	C11-C10-C8-C7
28	A	805	CLA	C12-C13-C15-C16
28	A	807	CLA	C6-C7-C8-C10
28	A	808	CLA	C12-C13-C15-C16
28	A	824	CLA	C12-C13-C15-C16
28	A	830	CLA	C12-C13-C15-C16
28	B	825	CLA	C6-C7-C8-C10
28	B	834	CLA	C11-C12-C13-C15
28	B	835	CLA	C12-C13-C15-C16
28	B	843	CLA	C6-C7-C8-C10
28	F	802	CLA	C6-C7-C8-C10
28	11	304	CLA	C11-C10-C8-C7
28	4	307	CLA	C11-C10-C8-C7
31	B	844	LHG	C25-C26-C27-C28
28	5	302	CLA	C3A-C2A-CAA-CBA
28	5	303	CLA	C4-C3-C5-C6
28	R	202	CLA	C3A-C2A-CAA-CBA
28	5	301	CLA	C2-C3-C5-C6
31	A	839	LHG	O6-C4-C5-O7
28	5	313	CLA	C11-C10-C8-C9
28	7	301	CLA	C11-C12-C13-C14
28	7	303	CLA	C11-C12-C13-C14
28	7	306	CLA	C14-C13-C15-C16
28	A	815	CLA	C6-C7-C8-C9
28	B	804	CLA	C6-C7-C8-C9
28	B	813	CLA	C6-C7-C8-C9
28	B	821	CLA	C6-C7-C8-C9
28	B	822	CLA	C11-C12-C13-C14
28	B	845	CLA	C11-C10-C8-C9
28	B	847	CLA	C6-C7-C8-C9
35	B	836	PQN	C24-C23-C25-C26
29	3	311	A86	C26-C27-C29-C30
29	10	312	A86	C26-C27-C29-C30
30	6	309	KC1	C1A-C2A-CAA-CBA
30	10	311	KC1	C1A-C2A-CAA-CBA
30	13	304	KC1	C1A-C2A-CAA-CBA
30	17	312	KC1	C1A-C2A-CAA-CBA
30	4	312	KC1	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
30	9	306	KC1	C1A-C2A-CAA-CBA
28	4	306	CLA	C6-C7-C8-C9
28	1	304	CLA	CAD-CBD-CGD-O2D
28	3	314	CLA	CAD-CBD-CGD-O2D
28	5	306	CLA	CAD-CBD-CGD-O2D
28	7	303	CLA	CAD-CBD-CGD-O2D
28	7	312	CLA	CAD-CBD-CGD-O2D
28	8	301	CLA	CAD-CBD-CGD-O2D
28	A	837	CLA	CAD-CBD-CGD-O2D
28	A	852	CLA	CAD-CBD-CGD-O2D
28	B	826	CLA	CAD-CBD-CGD-O2D
28	6	313	CLA	CAD-CBD-CGD-O2D
28	10	303	CLA	CAD-CBD-CGD-O2D
28	11	310	CLA	CAD-CBD-CGD-O2D
29	8	308	A86	C13-C14-C15-C20
29	6	314	A86	C13-C14-C15-C20
28	4	306	CLA	C6-C7-C8-C10
28	10	307	CLA	C2A-CAA-CBA-CGA
28	15	201	CLA	C2A-CAA-CBA-CGA
28	9	303	CLA	C2A-CAA-CBA-CGA
28	1	304	CLA	CAD-CBD-CGD-O1D
28	3	314	CLA	CAD-CBD-CGD-O1D
28	5	306	CLA	CAD-CBD-CGD-O1D
28	7	301	CLA	CHA-CBD-CGD-O2D
28	7	303	CLA	CAD-CBD-CGD-O1D
28	7	305	CLA	CHA-CBD-CGD-O1D
28	7	305	CLA	CHA-CBD-CGD-O2D
28	7	312	CLA	CAD-CBD-CGD-O1D
28	8	301	CLA	CAD-CBD-CGD-O1D
28	8	304	CLA	CHA-CBD-CGD-O1D
28	8	310	CLA	CHA-CBD-CGD-O1D
28	8	310	CLA	CHA-CBD-CGD-O2D
28	A	807	CLA	CHA-CBD-CGD-O1D
28	A	823	CLA	CHA-CBD-CGD-O1D
28	A	823	CLA	CHA-CBD-CGD-O2D
28	A	833	CLA	CHA-CBD-CGD-O1D
28	A	833	CLA	CHA-CBD-CGD-O2D
28	A	837	CLA	CAD-CBD-CGD-O1D
28	A	849	CLA	CHA-CBD-CGD-O1D
28	A	849	CLA	CHA-CBD-CGD-O2D
28	A	852	CLA	CAD-CBD-CGD-O1D
28	B	811	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
28	B	811	CLA	CHA-CBD-CGD-O2D
28	B	826	CLA	CAD-CBD-CGD-O1D
28	B	831	CLA	CAD-CBD-CGD-O1D
28	6	304	CLA	CHA-CBD-CGD-O1D
28	6	304	CLA	CHA-CBD-CGD-O2D
28	6	306	CLA	CHA-CBD-CGD-O1D
28	6	306	CLA	CHA-CBD-CGD-O2D
28	6	313	CLA	CAD-CBD-CGD-O1D
28	10	302	CLA	CHA-CBD-CGD-O1D
28	10	302	CLA	CHA-CBD-CGD-O2D
28	10	303	CLA	CAD-CBD-CGD-O1D
28	10	309	CLA	CHA-CBD-CGD-O1D
28	10	309	CLA	CHA-CBD-CGD-O2D
28	11	310	CLA	CAD-CBD-CGD-O1D
28	13	306	CLA	CHA-CBD-CGD-O1D
28	13	306	CLA	CHA-CBD-CGD-O2D
28	16	205	CLA	CHA-CBD-CGD-O1D
28	16	205	CLA	CHA-CBD-CGD-O2D
28	19	202	CLA	CHA-CBD-CGD-O1D
28	19	202	CLA	CHA-CBD-CGD-O2D
28	4	305	CLA	CHA-CBD-CGD-O1D
28	4	305	CLA	CHA-CBD-CGD-O2D
28	4	306	CLA	CHA-CBD-CGD-O1D
28	4	306	CLA	CHA-CBD-CGD-O2D
28	4	316	CLA	CHA-CBD-CGD-O1D
28	4	316	CLA	CHA-CBD-CGD-O2D
28	9	304	CLA	CHA-CBD-CGD-O1D
28	L	204	CLA	CAD-CBD-CGD-O1D
29	J	101	A86	C10-C11-C13-C14
30	9	306	KC1	CHA-CBD-CGD-O1D
30	9	306	KC1	CHA-CBD-CGD-O2D
31	1	309	LHG	C3-O3-P-O5
31	1	309	LHG	C4-O6-P-O5
31	5	314	LHG	C4-O6-P-O5
31	7	310	LHG	C3-O3-P-O5
31	7	310	LHG	C4-O6-P-O3
31	7	310	LHG	C4-O6-P-O4
31	I	102	LHG	C4-O6-P-O3
31	I	102	LHG	C4-O6-P-O4
31	4	302	LHG	C4-O6-P-O4
31	9	301	LHG	C4-O6-P-O3
31	9	301	LHG	C4-O6-P-O4

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Mol	Chain	Res	Type	Atoms
31	9	302	LHG	C3-O3-P-O5
31	9	314	LHG	C4-O6-P-O5
34	4	317	DGD	C3G-C2G-O2G-C1B
28	1	303	CLA	C2B-C3B-CAB-CBB
28	1	304	CLA	C2B-C3B-CAB-CBB
28	5	301	CLA	C2B-C3B-CAB-CBB
28	5	302	CLA	C2B-C3B-CAB-CBB
28	7	308	CLA	C2B-C3B-CAB-CBB
28	8	301	CLA	C2B-C3B-CAB-CBB
28	8	303	CLA	C2B-C3B-CAB-CBB
28	8	305	CLA	C2B-C3B-CAB-CBB
28	8	313	CLA	C2B-C3B-CAB-CBB
28	A	806	CLA	C2B-C3B-CAB-CBB
28	A	808	CLA	C2B-C3B-CAB-CBB
28	A	815	CLA	C2B-C3B-CAB-CBB
28	A	829	CLA	C2B-C3B-CAB-CBB
28	A	832	CLA	C2B-C3B-CAB-CBB
28	A	834	CLA	C2B-C3B-CAB-CBB
28	A	847	CLA	C2B-C3B-CAB-CBB
28	B	801	CLA	C2B-C3B-CAB-CBB
28	B	803	CLA	C2B-C3B-CAB-CBB
28	B	807	CLA	C2B-C3B-CAB-CBB
28	B	809	CLA	C2B-C3B-CAB-CBB
28	B	818	CLA	C2B-C3B-CAB-CBB
28	B	819	CLA	C2B-C3B-CAB-CBB
28	B	820	CLA	C2B-C3B-CAB-CBB
28	B	823	CLA	C2B-C3B-CAB-CBB
28	B	827	CLA	C2B-C3B-CAB-CBB
28	R	202	CLA	C2B-C3B-CAB-CBB
28	6	303	CLA	C2B-C3B-CAB-CBB
28	10	302	CLA	C2B-C3B-CAB-CBB
28	10	308	CLA	C2B-C3B-CAB-CBB
28	11	314	CLA	C2B-C3B-CAB-CBB
28	13	305	CLA	C2B-C3B-CAB-CBB
28	13	306	CLA	C2B-C3B-CAB-CBB
28	16	203	CLA	C2B-C3B-CAB-CBB
28	4	307	CLA	C2B-C3B-CAB-CBB
28	9	303	CLA	C2B-C3B-CAB-CBB
28	L	204	CLA	C2B-C3B-CAB-CBB
28	a	202	CLA	C2B-C3B-CAB-CBB
28	B	821	CLA	C2-C3-C5-C6
31	A	851	LHG	C2-C3-O3-P

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Mol	Chain	Res	Type	Atoms
31	I	102	LHG	C2-C3-O3-P
31	4	302	LHG	C5-C4-O6-P
31	9	301	LHG	C5-C4-O6-P
28	F	803	CLA	C2A-CAA-CBA-CGA
29	3	311	A86	C12-C11-C13-C14
29	3	312	A86	C12-C11-C13-C14
29	5	312	A86	C12-C11-C13-C14
29	J	101	A86	C12-C11-C13-C14
34	8	314	DGD	O2G-C2G-C3G-O3G
31	A	840	LHG	O1-C1-C2-C3
28	A	809	CLA	C11-C10-C8-C7
29	3	310	A86	C1-C24-C25-C26
29	5	312	A86	C6-C8-C9-C10
29	J	101	A86	C6-C8-C9-C10
29	10	317	A86	C1-C24-C25-C26
29	11	308	A86	C6-C8-C9-C10
29	9	312	A86	C1-C24-C25-C26
32	5	307	XAT	C30-C31-C32-C33
32	5	311	XAT	C30-C31-C32-C33
32	7	315	XAT	C30-C31-C32-C33
32	7	316	XAT	C10-C11-C12-C13
32	7	317	XAT	C30-C31-C32-C33
32	8	312	XAT	C10-C11-C12-C13
32	8	312	XAT	C30-C31-C32-C33
32	6	315	XAT	C10-C11-C12-C13
32	6	315	XAT	C30-C31-C32-C33
32	17	311	XAT	C30-C31-C32-C33
32	4	315	XAT	C30-C31-C32-C33
32	4	318	XAT	C10-C11-C12-C13
33	A	850	BCR	C10-C11-C12-C13
33	L	202	BCR	C18-C19-C20-C21
28	7	305	CLA	C16-C17-C18-C20
31	B	844	LHG	C13-C14-C15-C16
31	9	301	LHG	O6-C4-C5-C6
28	7	305	CLA	C14-C13-C15-C16
28	A	808	CLA	C6-C7-C8-C9
28	A	810	CLA	C11-C12-C13-C14
28	A	837	CLA	C14-C13-C15-C16
28	A	845	CLA	C11-C10-C8-C9
28	B	809	CLA	C14-C13-C15-C16
28	B	812	CLA	C11-C12-C13-C14
28	B	845	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
28	6	313	CLA	C14-C13-C15-C16
28	10	307	CLA	C6-C7-C8-C9
28	11	302	CLA	C11-C12-C13-C14
28	4	316	CLA	C11-C12-C13-C14
35	A	838	PQN	C21-C22-C23-C24
28	A	809	CLA	C11-C10-C8-C9
28	7	306	CLA	C11-C12-C13-C15
28	B	807	CLA	C6-C7-C8-C10
28	B	817	CLA	C11-C10-C8-C7
28	B	834	CLA	C6-C7-C8-C10
31	9	302	LHG	C1-C2-C3-O3
28	3	307	CLA	C15-C16-C17-C18
28	5	301	CLA	C15-C16-C17-C18
28	B	810	CLA	C2-C3-C5-C6
28	11	303	CLA	C2-C3-C5-C6
28	B	818	CLA	CAA-CBA-CGA-O2A
31	9	314	LHG	O8-C23-C24-C25
28	6	301	CLA	C16-C17-C18-C19
28	10	303	CLA	C6-C7-C8-C10
28	11	302	CLA	C8-C10-C11-C12
28	A	817	CLA	C2-C1-O2A-CGA
28	A	808	CLA	C4-C3-C5-C6
28	11	302	CLA	C4-C3-C5-C6
28	5	309	CLA	CAA-CBA-CGA-O2A
31	A	839	LHG	C4-C5-C6-O8
28	B	812	CLA	C8-C10-C11-C12
28	5	305	CLA	C2A-CAA-CBA-CGA
28	7	305	CLA	C2A-CAA-CBA-CGA
28	A	817	CLA	C2A-CAA-CBA-CGA
28	6	303	CLA	C2A-CAA-CBA-CGA
28	A	835	CLA	C4-C3-C5-C6
28	B	849	CLA	C4-C3-C5-C6
28	J	102	CLA	C4-C3-C5-C6
28	6	307	CLA	C2-C3-C5-C6
31	9	314	LHG	C13-C14-C15-C16
29	R	201	A86	C13-C14-C15-C16
28	1	303	CLA	C11-C12-C13-C14
28	A	804	CLA	C11-C12-C13-C14
28	B	816	CLA	C6-C7-C8-C9
28	B	817	CLA	C6-C7-C8-C9
28	3	306	CLA	C4B-C3B-CAB-CBB
28	A	826	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
28	B	830	CLA	C4B-C3B-CAB-CBB
28	11	301	CLA	C4B-C3B-CAB-CBB
28	11	302	CLA	C4B-C3B-CAB-CBB
28	13	303	CLA	C4B-C3B-CAB-CBB
35	B	836	PQN	C25-C26-C27-C28
28	10	302	CLA	C2A-CAA-CBA-CGA
28	8	302	CLA	C2-C3-C5-C6
30	1	306	KC1	C4B-C3B-CAB-CBB
30	3	302	KC1	C4B-C3B-CAB-CBB
30	8	306	KC1	C4B-C3B-CAB-CBB
30	6	305	KC1	C4B-C3B-CAB-CBB
30	6	308	KC1	C4B-C3B-CAB-CBB
30	6	310	KC1	C4B-C3B-CAB-CBB
30	10	310	KC1	C4B-C3B-CAB-CBB
30	10	311	KC1	C4B-C3B-CAB-CBB
30	17	306	KC1	C4B-C3B-CAB-CBB
30	9	309	KC1	C4B-C3B-CAB-CBB
28	B	849	CLA	C16-C17-C18-C20
28	A	804	CLA	C11-C12-C13-C15
28	A	837	CLA	C12-C13-C15-C16
28	B	801	CLA	C11-C10-C8-C7
28	B	812	CLA	C11-C10-C8-C7
28	B	815	CLA	C6-C7-C8-C10
28	B	823	CLA	C11-C12-C13-C15
28	6	313	CLA	C12-C13-C15-C16
28	11	302	CLA	C11-C12-C13-C15
33	8	309	BCR	C14-C15-C16-C17
28	A	822	CLA	C6-C7-C8-C9
28	4	307	CLA	C11-C12-C13-C14
31	1	309	LHG	C14-C15-C16-C17
28	1	303	CLA	C3A-C2A-CAA-CBA
28	1	307	CLA	C3A-C2A-CAA-CBA
28	7	303	CLA	C3A-C2A-CAA-CBA
28	A	815	CLA	C4-C3-C5-C6
28	A	849	CLA	C3A-C2A-CAA-CBA
28	B	812	CLA	C3A-C2A-CAA-CBA
28	B	828	CLA	C3A-C2A-CAA-CBA
28	6	313	CLA	C3A-C2A-CAA-CBA
28	10	303	CLA	C3A-C2A-CAA-CBA
28	11	302	CLA	C2-C3-C5-C6
29	3	310	A86	C25-C26-C27-C28
29	10	317	A86	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
29	9	312	A86	C-C1-C2-C3
29	9	312	A86	C25-C26-C27-C28
33	F	804	BCR	C35-C13-C14-C15
33	L	202	BCR	C11-C10-C9-C34
28	8	302	CLA	C11-C10-C8-C9
28	A	815	CLA	C8-C10-C11-C12
32	6	312	XAT	C13-C14-C15-C35
28	9	310	CLA	CAA-CBA-CGA-O1A
29	J	101	A86	C5-C6-C8-C9
32	13	309	XAT	C31-C32-C33-C34
28	B	820	CLA	C4-C3-C5-C6
28	3	303	CLA	C2-C3-C5-C6
28	5	303	CLA	C2-C3-C5-C6
31	11	311	LHG	C1-C2-C3-O3
28	B	805	CLA	C2A-CAA-CBA-CGA
29	R	201	A86	C12-C11-C13-O
31	5	314	LHG	C4-C5-C6-O8
28	A	830	CLA	C3-C5-C6-C7
28	11	305	CLA	CAA-CBA-CGA-O1A
28	7	305	CLA	C6-C7-C8-C9
28	8	301	CLA	C11-C10-C8-C9
28	A	802	CLA	C6-C7-C8-C9
28	A	819	CLA	C11-C10-C8-C9
28	A	835	CLA	C11-C10-C8-C9
28	A	852	CLA	C14-C13-C15-C16
28	B	825	CLA	C6-C7-C8-C9
28	B	828	CLA	C6-C7-C8-C9
28	B	828	CLA	C14-C13-C15-C16
28	11	302	CLA	C14-C13-C15-C16
28	11	303	CLA	C6-C7-C8-C9
28	L	203	CLA	C6-C7-C8-C9
28	6	303	CLA	C6-C7-C8-C10
31	1	309	LHG	C9-C10-C11-C12
28	5	301	CLA	C1-C2-C3-C4
28	7	301	CLA	C1-C2-C3-C4
28	7	303	CLA	C1-C2-C3-C4
28	8	304	CLA	C1-C2-C3-C4
28	A	803	CLA	C1-C2-C3-C4
28	A	812	CLA	C1-C2-C3-C4
28	A	815	CLA	C1-C2-C3-C4
28	A	822	CLA	C1-C2-C3-C4
28	A	825	CLA	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
28	A	833	CLA	C1-C2-C3-C4
28	A	849	CLA	C1-C2-C3-C4
28	B	804	CLA	C1-C2-C3-C4
28	B	813	CLA	C1-C2-C3-C4
28	B	814	CLA	C1-C2-C3-C4
28	B	819	CLA	C1-C2-C3-C4
28	B	845	CLA	C1-C2-C3-C4
28	6	302	CLA	C1-C2-C3-C4
28	6	307	CLA	C1-C2-C3-C4
28	10	307	CLA	C1-C2-C3-C4
28	11	301	CLA	C1-C2-C3-C4
28	11	303	CLA	C1-C2-C3-C4
28	4	310	CLA	C1-C2-C3-C4
28	4	316	CLA	C1-C2-C3-C4
28	9	310	CLA	CAA-CBA-CGA-O2A
28	6	311	CLA	CAA-CBA-CGA-O2A
31	A	840	LHG	O1-C1-C2-O2
28	1	310	CLA	C2A-CAA-CBA-CGA
28	1	314	CLA	C1A-C2A-CAA-CBA
28	7	308	CLA	C1A-C2A-CAA-CBA
28	A	823	CLA	C1A-C2A-CAA-CBA
28	A	849	CLA	C1A-C2A-CAA-CBA
28	A	853	CLA	C1A-C2A-CAA-CBA
28	B	812	CLA	C1A-C2A-CAA-CBA
28	6	313	CLA	C1A-C2A-CAA-CBA
28	10	305	CLA	C1A-C2A-CAA-CBA
28	17	302	CLA	C1A-C2A-CAA-CBA
28	19	201	CLA	C1A-C2A-CAA-CBA
28	4	303	CLA	C1A-C2A-CAA-CBA
29	3	310	A86	C25-C26-C27-C29
29	10	317	A86	C25-C26-C27-C29
29	4	314	A86	C10-C11-C13-O
29	9	312	A86	C24-C1-C2-C3
29	9	312	A86	C25-C26-C27-C29
33	F	804	BCR	C12-C13-C14-C15
33	L	202	BCR	C11-C10-C9-C8
28	13	303	CLA	CAA-CBA-CGA-O1A
31	4	302	LHG	O6-C4-C5-O7
28	A	808	CLA	C13-C15-C16-C17
28	1	305	CLA	C2B-C3B-CAB-CBB
28	3	303	CLA	C2B-C3B-CAB-CBB
28	3	306	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
28	3	314	CLA	C2B-C3B-CAB-CBB
28	5	305	CLA	C2B-C3B-CAB-CBB
28	5	313	CLA	C2B-C3B-CAB-CBB
28	7	301	CLA	C2B-C3B-CAB-CBB
28	8	310	CLA	C2B-C3B-CAB-CBB
28	A	804	CLA	C2B-C3B-CAB-CBB
28	A	816	CLA	C2B-C3B-CAB-CBB
28	A	820	CLA	C2B-C3B-CAB-CBB
28	A	827	CLA	C2B-C3B-CAB-CBB
28	A	852	CLA	C2B-C3B-CAB-CBB
28	B	805	CLA	C2B-C3B-CAB-CBB
28	B	811	CLA	C2B-C3B-CAB-CBB
28	B	824	CLA	C2B-C3B-CAB-CBB
28	B	828	CLA	C2B-C3B-CAB-CBB
28	B	830	CLA	C2B-C3B-CAB-CBB
28	B	831	CLA	C2B-C3B-CAB-CBB
28	B	847	CLA	C2B-C3B-CAB-CBB
28	F	802	CLA	C2B-C3B-CAB-CBB
28	11	312	CLA	C2B-C3B-CAB-CBB
28	13	303	CLA	C2B-C3B-CAB-CBB
28	13	307	CLA	C2B-C3B-CAB-CBB
28	15	201	CLA	C2B-C3B-CAB-CBB
28	19	201	CLA	C2B-C3B-CAB-CBB
28	4	306	CLA	C2B-C3B-CAB-CBB
28	9	310	CLA	C2B-C3B-CAB-CBB
28	L	206	CLA	C2B-C3B-CAB-CBB
33	1	312	BCR	C1-C6-C7-C8
33	A	841	BCR	C1-C6-C7-C8
33	A	850	BCR	C23-C24-C25-C30
33	B	837	BCR	C1-C6-C7-C8
33	B	840	BCR	C5-C6-C7-C8
33	J	104	BCR	C23-C24-C25-C30
33	L	202	BCR	C1-C6-C7-C8
33	L	202	BCR	C5-C6-C7-C8
28	7	318	CLA	CAA-CBA-CGA-O2A
31	7	310	LHG	C5-C4-O6-P
31	9	314	LHG	C5-C4-O6-P
28	7	304	CLA	C4-C3-C5-C6
28	A	849	CLA	C4-C3-C5-C6
28	B	806	CLA	C4-C3-C5-C6
31	4	302	LHG	O6-C4-C5-C6
28	B	820	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
28	J	102	CLA	C2-C3-C5-C6
28	A	814	CLA	CAA-CBA-CGA-O1A
28	1	303	CLA	C11-C12-C13-C15
28	A	805	CLA	C11-C12-C13-C15
28	A	823	CLA	C12-C13-C15-C16
28	A	828	CLA	C12-C13-C15-C16
28	A	837	CLA	C11-C10-C8-C7
28	A	847	CLA	C12-C13-C15-C16
28	B	803	CLA	C12-C13-C15-C16
28	B	805	CLA	C12-C13-C15-C16
28	B	816	CLA	C6-C7-C8-C10
28	B	816	CLA	C11-C12-C13-C15
28	B	817	CLA	C11-C12-C13-C15
28	B	821	CLA	C11-C12-C13-C15
28	11	301	CLA	C11-C10-C8-C7
28	3	301	CLA	C2A-CAA-CBA-CGA
28	7	311	CLA	C2A-CAA-CBA-CGA
28	8	305	CLA	C2A-CAA-CBA-CGA
28	10	303	CLA	C2A-CAA-CBA-CGA
28	13	306	CLA	C3A-C2A-CAA-CBA
28	A	817	CLA	CAA-CBA-CGA-O2A
28	7	305	CLA	C16-C17-C18-C19
31	1	309	LHG	C1-C2-C3-O3
37	F	805	LMG	C12-C13-C14-C15
28	4	316	CLA	C12-C13-C15-C16
32	6	315	XAT	C27-C28-C29-C39
28	13	302	CLA	CAA-CBA-CGA-O1A
28	3	307	CLA	C4-C3-C5-C6
28	10	303	CLA	CAA-CBA-CGA-O2A
28	A	812	CLA	C2-C3-C5-C6
28	A	835	CLA	C2-C3-C5-C6
28	A	849	CLA	C2-C3-C5-C6
28	1	305	CLA	C1-C2-C3-C5
28	1	310	CLA	C1-C2-C3-C5
28	3	301	CLA	C1-C2-C3-C5
28	A	809	CLA	C1-C2-C3-C5
28	B	809	CLA	C2-C1-O2A-CGA
28	B	832	CLA	C1-C2-C3-C5
28	F	802	CLA	C1-C2-C3-C5
28	J	102	CLA	C1-C2-C3-C5
28	6	301	CLA	C1-C2-C3-C5
28	9	307	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
28	L	201	CLA	C1-C2-C3-C5
28	A	808	CLA	C11-C12-C13-C14
28	B	826	CLA	C6-C7-C8-C9
28	B	833	CLA	C6-C7-C8-C9
28	3	307	CLA	C13-C15-C16-C17
28	7	318	CLA	CAA-CBA-CGA-O1A
28	11	301	CLA	C10-C11-C12-C13
28	7	301	CLA	C4-C3-C5-C6
28	A	805	CLA	C4-C3-C5-C6
28	A	809	CLA	C4-C3-C5-C6
28	B	812	CLA	C4-C3-C5-C6
28	B	832	CLA	C8-C10-C11-C12
31	A	851	LHG	C5-C4-O6-P
28	A	808	CLA	C2-C3-C5-C6
28	A	820	CLA	O2A-C1-C2-C3
28	A	817	CLA	C5-C6-C7-C8
28	11	305	CLA	CAA-CBA-CGA-O2A
28	13	302	CLA	CAA-CBA-CGA-O2A
28	13	303	CLA	CAA-CBA-CGA-O2A
28	a	202	CLA	C1A-C2A-CAA-CBA
28	8	304	CLA	C2A-CAA-CBA-CGA
31	B	842	LHG	O6-C4-C5-O7
28	B	811	CLA	C4-C3-C5-C6
28	6	313	CLA	C4-C3-C5-C6
28	10	307	CLA	C4-C3-C5-C6
28	B	828	CLA	CAA-CBA-CGA-O2A
28	B	845	CLA	C10-C11-C12-C13
28	1	305	CLA	C4B-C3B-CAB-CBB
28	1	308	CLA	C4B-C3B-CAB-CBB
28	3	314	CLA	C4B-C3B-CAB-CBB
28	A	804	CLA	C4B-C3B-CAB-CBB
28	F	802	CLA	C4B-C3B-CAB-CBB
28	4	306	CLA	C4B-C3B-CAB-CBB
28	a	201	CLA	C4B-C3B-CAB-CBB
28	A	814	CLA	CAA-CBA-CGA-O2A
31	A	839	LHG	C28-C29-C30-C31
28	B	843	CLA	C8-C10-C11-C12
31	7	310	LHG	O6-C4-C5-C6
31	B	842	LHG	O6-C4-C5-C6
28	A	849	CLA	C6-C7-C8-C10
34	4	317	DGD	O6D-C5D-C6D-O5D
28	R	204	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
28	A	826	CLA	C13-C15-C16-C17
28	A	818	CLA	CAA-CBA-CGA-O1A
28	A	818	CLA	CAA-CBA-CGA-O2A
28	3	303	CLA	C11-C12-C13-C14
28	A	817	CLA	C6-C7-C8-C9
28	A	825	CLA	C14-C13-C15-C16
28	B	801	CLA	C11-C12-C13-C14
28	F	802	CLA	C6-C7-C8-C9
28	10	316	CLA	C14-C13-C15-C16
28	4	307	CLA	C11-C10-C8-C9
28	B	801	CLA	C8-C10-C11-C12
37	F	805	LMG	C8-C7-O1-C1
28	B	835	CLA	C13-C15-C16-C17
28	R	204	CLA	C2A-CAA-CBA-CGA
28	A	810	CLA	C2-C1-O2A-CGA
28	A	819	CLA	C2-C1-O2A-CGA
28	B	806	CLA	C2-C1-O2A-CGA
28	10	301	CLA	C2-C1-O2A-CGA
28	11	304	CLA	C2-C1-O2A-CGA
28	B	849	CLA	C16-C17-C18-C19
28	1	314	CLA	C3A-C2A-CAA-CBA
28	7	311	CLA	C3A-C2A-CAA-CBA
28	A	823	CLA	C3A-C2A-CAA-CBA
28	B	817	CLA	C4-C3-C5-C6
28	17	304	CLA	C3A-C2A-CAA-CBA
31	4	302	LHG	O8-C23-C24-C25
28	B	845	CLA	O2A-C1-C2-C3
31	A	839	LHG	C16-C17-C18-C19
28	A	815	CLA	C2-C3-C5-C6
32	7	317	XAT	O4-C6-C7-C8
32	J	105	XAT	O24-C26-C27-C28
32	17	311	XAT	O4-C6-C7-C8
32	17	311	XAT	O24-C26-C27-C28
32	4	318	XAT	O24-C26-C27-C28
28	8	305	CLA	CAA-CBA-CGA-O2A
31	11	311	LHG	C5-C4-O6-P
30	6	309	KC1	C4B-C3B-CAB-CBB
30	13	304	KC1	C4B-C3B-CAB-CBB
30	4	308	KC1	C4B-C3B-CAB-CBB
30	4	312	KC1	C4B-C3B-CAB-CBB
28	4	310	CLA	C6-C7-C8-C10
28	3	303	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
28	A	822	CLA	C2A-CAA-CBA-CGA
28	A	821	CLA	CAA-CBA-CGA-O2A
32	6	312	XAT	C33-C34-C35-C15
28	10	307	CLA	C2C-C3C-CAC-CBC
34	4	301	DGD	O2G-C2G-C3G-O3G
28	A	807	CLA	C6-C7-C8-C9
28	A	815	CLA	C11-C10-C8-C9
28	A	830	CLA	C14-C13-C15-C16
28	B	804	CLA	C11-C10-C8-C9
28	B	824	CLA	C11-C10-C8-C9
28	B	835	CLA	C14-C13-C15-C16
28	A	830	CLA	C16-C17-C18-C20
28	A	805	CLA	CAA-CBA-CGA-O2A
31	5	315	LHG	O7-C7-C8-C9
28	3	307	CLA	C2C-C3C-CAC-CBC
31	I	102	LHG	O9-C7-C8-C9
33	8	309	BCR	C11-C12-C13-C14
29	11	308	A86	C13-C14-C15-O1
29	4	313	A86	C13-C14-C15-O1
29	4	314	A86	C13-C14-C15-O1
28	A	803	CLA	CAA-CBA-CGA-O2A
28	3	303	CLA	C11-C10-C8-C7
28	7	303	CLA	C11-C10-C8-C7
28	A	808	CLA	C11-C12-C13-C15
28	A	824	CLA	C6-C7-C8-C10
28	A	826	CLA	C6-C7-C8-C10
28	A	847	CLA	C6-C7-C8-C10
28	B	803	CLA	C11-C12-C13-C15
28	B	833	CLA	C6-C7-C8-C10
28	B	834	CLA	C12-C13-C15-C16
28	6	301	CLA	C11-C10-C8-C7
28	11	302	CLA	C11-C10-C8-C7
29	1	313	A86	C9-C10-C11-C13
28	1	308	CLA	C2B-C3B-CAB-CBB
28	1	314	CLA	C2B-C3B-CAB-CBB
28	3	307	CLA	C2B-C3B-CAB-CBB
28	5	309	CLA	C2B-C3B-CAB-CBB
28	7	305	CLA	C2B-C3B-CAB-CBB
28	A	807	CLA	C2B-C3B-CAB-CBB
28	A	823	CLA	C2B-C3B-CAB-CBB
28	A	826	CLA	C2B-C3B-CAB-CBB
28	A	833	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
28	A	846	CLA	C2B-C3B-CAB-CBB
28	B	806	CLA	C2B-C3B-CAB-CBB
28	B	816	CLA	C2B-C3B-CAB-CBB
28	6	306	CLA	C2B-C3B-CAB-CBB
28	10	306	CLA	C2B-C3B-CAB-CBB
28	11	301	CLA	C2B-C3B-CAB-CBB
28	11	302	CLA	C2B-C3B-CAB-CBB
28	11	304	CLA	C2B-C3B-CAB-CBB
28	17	307	CLA	C2B-C3B-CAB-CBB
28	9	304	CLA	C2B-C3B-CAB-CBB
28	L	203	CLA	C2B-C3B-CAB-CBB
28	a	201	CLA	C2B-C3B-CAB-CBB
28	a	204	CLA	C2B-C3B-CAB-CBB
33	1	312	BCR	C5-C6-C7-C8
33	A	841	BCR	C5-C6-C7-C8
33	A	844	BCR	C1-C6-C7-C8
33	A	850	BCR	C23-C24-C25-C26
33	L	205	BCR	C23-C24-C25-C26
33	L	205	BCR	C23-C24-C25-C30
28	1	314	CLA	C2-C1-O2A-CGA
28	A	820	CLA	C2-C1-O2A-CGA
28	A	845	CLA	C2-C1-O2A-CGA
28	B	810	CLA	C2-C1-O2A-CGA
28	B	820	CLA	C2-C1-O2A-CGA
28	R	204	CLA	C2-C1-O2A-CGA
28	A	829	CLA	CAA-CBA-CGA-O2A
28	6	302	CLA	CAA-CBA-CGA-O2A
28	13	301	CLA	CAA-CBA-CGA-O2A
28	17	305	CLA	CAA-CBA-CGA-O2A
28	B	802	CLA	C4-C3-C5-C6
28	5	313	CLA	CAA-CBA-CGA-O2A
28	8	305	CLA	CAA-CBA-CGA-O1A
28	7	312	CLA	C2A-CAA-CBA-CGA
28	A	823	CLA	C2A-CAA-CBA-CGA
28	6	307	CLA	C2A-CAA-CBA-CGA
28	10	301	CLA	C2A-CAA-CBA-CGA
28	8	313	CLA	CAA-CBA-CGA-O2A
28	4	306	CLA	CAA-CBA-CGA-O2A
28	7	303	CLA	C16-C17-C18-C20
31	4	302	LHG	O7-C7-C8-C9
28	8	302	CLA	C11-C10-C8-C7
28	B	833	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
28	8	304	CLA	C4-C3-C5-C6
28	10	316	CLA	C4-C3-C5-C6
28	7	304	CLA	C2-C3-C5-C6
28	B	849	CLA	C2-C3-C5-C6
28	3	304	CLA	CAA-CBA-CGA-O2A
28	A	816	CLA	CAA-CBA-CGA-O1A
28	A	805	CLA	C14-C13-C15-C16
28	A	827	CLA	C11-C10-C8-C9
28	B	822	CLA	C14-C13-C15-C16
28	B	843	CLA	C6-C7-C8-C9
28	6	313	CLA	C15-C16-C17-C18
31	B	844	LHG	C4-C5-C6-O8
31	11	311	LHG	C4-C5-C6-O8
28	3	301	CLA	C1A-C2A-CAA-CBA
28	5	313	CLA	C1A-C2A-CAA-CBA
28	8	302	CLA	C4B-C3B-CAB-CBB
28	8	304	CLA	C4B-C3B-CAB-CBB
28	A	801	CLA	C1A-C2A-CAA-CBA
28	B	828	CLA	C1A-C2A-CAA-CBA
28	10	306	CLA	C4B-C3B-CAB-CBB
28	13	307	CLA	C1A-C2A-CAA-CBA
28	17	307	CLA	C4B-C3B-CAB-CBB
28	17	309	CLA	C1A-C2A-CAA-CBA
29	R	203	A86	O-C13-C14-C15
29	10	312	A86	O-C13-C14-C15
28	7	308	CLA	C4C-C3C-CAC-CBC
28	11	301	CLA	C4-C3-C5-C6
28	B	807	CLA	C10-C11-C12-C13
28	10	309	CLA	C2A-CAA-CBA-CGA
28	3	304	CLA	CAA-CBA-CGA-O1A
32	13	309	XAT	C7-C8-C9-C10
28	1	307	CLA	CAA-CBA-CGA-O2A
31	A	851	LHG	O8-C23-C24-C25
28	B	821	CLA	C2A-CAA-CBA-CGA
28	B	845	CLA	CAA-CBA-CGA-O2A
28	B	845	CLA	C5-C6-C7-C8
28	7	303	CLA	C15-C16-C17-C18
28	7	312	CLA	C2-C1-O2A-CGA
28	8	304	CLA	C2-C1-O2A-CGA
28	6	311	CLA	C2-C1-O2A-CGA
28	9	305	CLA	C2-C1-O2A-CGA
28	5	301	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
28	7	312	CLA	C12-C13-C15-C16
28	A	817	CLA	C11-C10-C8-C7
28	B	801	CLA	C11-C12-C13-C15
28	B	809	CLA	C6-C7-C8-C10
28	B	828	CLA	C6-C7-C8-C10
28	B	835	CLA	C11-C10-C8-C7
28	L	201	CLA	C6-C7-C8-C10
28	L	203	CLA	C11-C10-C8-C7
28	B	806	CLA	C2-C3-C5-C6
31	I	102	LHG	C32-C33-C34-C35
28	a	201	CLA	C2A-CAA-CBA-CGA
28	7	308	CLA	C2C-C3C-CAC-CBC
28	6	311	CLA	CHA-CBD-CGD-O2D
28	11	310	CLA	C2A-CAA-CBA-CGA
28	B	803	CLA	C16-C17-C18-C20
28	A	837	CLA	C8-C10-C11-C12
28	1	305	CLA	C3A-C2A-CAA-CBA
28	A	815	CLA	C3A-C2A-CAA-CBA
28	A	822	CLA	C3A-C2A-CAA-CBA
28	A	837	CLA	C3A-C2A-CAA-CBA
28	A	853	CLA	C3A-C2A-CAA-CBA
28	B	845	CLA	C3A-C2A-CAA-CBA
28	J	102	CLA	C3A-C2A-CAA-CBA
28	19	201	CLA	C3A-C2A-CAA-CBA
28	A	829	CLA	CAA-CBA-CGA-O1A
31	7	310	LHG	O6-C4-C5-O7
28	8	302	CLA	CAA-CBA-CGA-O2A
28	17	303	CLA	CAA-CBA-CGA-O2A
28	5	313	CLA	CAA-CBA-CGA-O1A
28	4	306	CLA	CAA-CBA-CGA-O1A
31	4	302	LHG	O9-C7-C8-C9
31	1	309	LHG	C13-C14-C15-C16
28	5	301	CLA	C2A-CAA-CBA-CGA
28	5	303	CLA	C14-C13-C15-C16
28	A	808	CLA	C14-C13-C15-C16
28	A	824	CLA	C14-C13-C15-C16
28	B	805	CLA	C6-C7-C8-C9
28	A	831	CLA	CAA-CBA-CGA-O2A
28	6	313	CLA	C13-C15-C16-C17
33	8	309	BCR	C15-C16-C17-C18
28	A	806	CLA	C4-C3-C5-C6
28	B	807	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
28	6	302	CLA	CAA-CBA-CGA-O1A
28	13	301	CLA	CAA-CBA-CGA-O1A
29	4	314	A86	C26-C27-C29-C30
30	1	306	KC1	C1A-C2A-CAA-CBA
30	3	309	KC1	C1A-C2A-CAA-CBA
30	5	308	KC1	C1A-C2A-CAA-CBA
30	7	307	KC1	C1A-C2A-CAA-CBA
30	7	309	KC1	C1A-C2A-CAA-CBA
30	6	310	KC1	C1A-C2A-CAA-CBA
30	10	310	KC1	C1A-C2A-CAA-CBA
30	11	307	KC1	C1A-C2A-CAA-CBA
30	4	309	KC1	C1A-C2A-CAA-CBA
30	9	309	KC1	C1A-C2A-CAA-CBA
32	5	310	XAT	C21-C26-C27-C28
32	10	314	XAT	C21-C26-C27-C28
28	A	803	CLA	CAA-CBA-CGA-O1A
32	7	313	XAT	C31-C32-C33-C34
33	B	851	BCR	C7-C8-C9-C10
28	A	821	CLA	CAA-CBA-CGA-O1A
28	8	313	CLA	CAA-CBA-CGA-O1A
31	5	315	LHG	O9-C7-C8-C9
29	1	313	A86	C12-C11-C13-O
29	5	312	A86	C12-C11-C13-O
29	J	101	A86	C12-C11-C13-O
28	1	307	CLA	CAA-CBA-CGA-O1A
28	A	805	CLA	CAA-CBA-CGA-O1A
29	3	311	A86	C2-C3-C4-C5
28	3	305	CLA	CAA-CBA-CGA-O2A
28	A	822	CLA	CAA-CBA-CGA-O2A
28	10	307	CLA	CAA-CBA-CGA-O2A
28	4	304	CLA	CAA-CBA-CGA-O2A
28	A	809	CLA	C2-C3-C5-C6
31	I	102	LHG	C24-C25-C26-C27
28	7	301	CLA	CAD-CBD-CGD-O2D
28	A	833	CLA	CAD-CBD-CGD-O2D
28	A	846	CLA	CAD-CBD-CGD-O2D
28	B	813	CLA	CAD-CBD-CGD-O2D
28	B	817	CLA	CAD-CBD-CGD-O2D
28	B	831	CLA	CAD-CBD-CGD-O2D
28	B	847	CLA	CAD-CBD-CGD-O2D
28	10	302	CLA	CAD-CBD-CGD-O2D
28	16	201	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
28	19	202	CLA	CAD-CBD-CGD-O2D
28	L	204	CLA	CAD-CBD-CGD-O2D
29	9	312	A86	C13-C14-C15-C20
28	10	306	CLA	CAA-CBA-CGA-O2A
28	B	845	CLA	CAA-CBA-CGA-O1A
28	B	813	CLA	C2-C1-O2A-CGA
28	B	849	CLA	C2-C1-O2A-CGA
28	A	831	CLA	CAA-CBA-CGA-O1A
31	A	851	LHG	O10-C23-C24-C25
28	B	811	CLA	CAA-CBA-CGA-O2A
28	3	303	CLA	C1-C2-C3-C4
28	A	823	CLA	C1-C2-C3-C4
28	B	826	CLA	C1-C2-C3-C4
28	10	303	CLA	C1-C2-C3-C4
28	13	301	CLA	C1-C2-C3-C4
28	10	303	CLA	C6-C7-C8-C9
28	7	303	CLA	C6-C7-C8-C10
28	5	304	CLA	CAA-CBA-CGA-O2A
28	A	847	CLA	CAA-CBA-CGA-O2A
31	B	842	LHG	O7-C7-C8-C9
28	7	303	CLA	C16-C17-C18-C19
28	7	302	CLA	CAA-CBA-CGA-O2A
28	A	804	CLA	CAA-CBA-CGA-O2A
28	4	310	CLA	CAA-CBA-CGA-O2A
31	I	102	LHG	C23-C24-C25-C26
28	7	301	CLA	CAA-CBA-CGA-O1A

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
29	3	312	A86	C31-C32-C33-C34-C35-C36

222 monomers are involved in 418 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	B	823	CLA	1	0
28	B	807	CLA	2	0
28	J	102	CLA	2	0
31	1	309	LHG	1	0
28	11	312	CLA	4	0
28	1	305	CLA	1	0
28	A	831	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	9	311	CLA	2	0
28	A	828	CLA	2	0
28	9	305	CLA	1	0
32	9	313	XAT	5	0
33	A	842	BCR	1	0
28	7	305	CLA	3	0
28	A	812	CLA	1	0
28	5	309	CLA	2	0
33	8	309	BCR	1	0
32	3	313	XAT	1	0
32	5	307	XAT	5	0
31	9	301	LHG	1	0
28	B	806	CLA	3	0
32	J	105	XAT	2	0
33	A	850	BCR	3	0
28	10	305	CLA	1	0
28	11	304	CLA	3	0
28	B	813	CLA	1	0
28	A	849	CLA	1	0
28	6	301	CLA	5	0
32	7	316	XAT	3	0
28	19	201	CLA	1	0
28	4	305	CLA	1	0
32	6	312	XAT	6	0
34	4	301	DGD	1	0
32	7	317	XAT	5	0
28	3	301	CLA	3	0
33	L	205	BCR	1	0
28	6	313	CLA	2	0
32	7	313	XAT	6	0
28	A	830	CLA	3	0
28	A	803	CLA	2	0
32	6	315	XAT	7	0
28	10	301	CLA	3	0
28	A	852	CLA	4	0
28	10	307	CLA	2	0
28	A	827	CLA	2	0
32	6	316	XAT	1	0
28	11	305	CLA	1	0
28	5	305	CLA	2	0
30	17	312	KC1	1	0
28	1	301	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	A	847	CLA	1	0
29	3	310	A86	1	0
28	B	831	CLA	3	0
33	F	804	BCR	2	0
28	A	820	CLA	1	0
28	17	302	CLA	2	0
28	6	307	CLA	1	0
28	17	309	CLA	1	0
28	8	304	CLA	3	0
28	B	815	CLA	2	0
28	7	303	CLA	3	0
31	11	311	LHG	1	0
28	A	809	CLA	1	0
31	A	840	LHG	1	0
31	I	102	LHG	1	0
28	L	201	CLA	1	0
28	B	804	CLA	1	0
28	L	204	CLA	1	0
28	9	304	CLA	1	0
32	10	314	XAT	5	0
28	B	821	CLA	2	0
28	7	312	CLA	2	0
28	A	805	CLA	2	0
28	8	313	CLA	1	0
28	8	302	CLA	1	0
28	A	808	CLA	6	0
28	1	307	CLA	2	0
28	8	301	CLA	5	0
28	A	836	CLA	2	0
28	B	818	CLA	3	0
32	8	311	XAT	1	0
32	5	311	XAT	6	0
28	A	824	CLA	3	0
28	5	306	CLA	2	0
28	B	826	CLA	4	0
34	4	317	DGD	1	0
28	B	825	CLA	2	0
28	5	302	CLA	1	0
28	4	303	CLA	3	0
32	5	310	XAT	2	0
28	3	305	CLA	1	0
28	9	307	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	A	813	CLA	1	0
28	A	832	CLA	1	0
28	A	815	CLA	3	0
31	B	842	LHG	4	0
28	L	206	CLA	1	0
28	B	829	CLA	2	0
28	A	822	CLA	1	0
28	13	302	CLA	2	0
28	B	801	CLA	1	0
32	7	314	XAT	1	0
30	5	308	KC1	1	0
28	17	303	CLA	2	0
32	11	313	XAT	7	0
32	13	309	XAT	1	0
33	B	841	BCR	2	0
28	13	301	CLA	4	0
28	3	306	CLA	2	0
28	B	810	CLA	2	0
28	1	304	CLA	1	0
28	4	306	CLA	3	0
28	13	303	CLA	1	0
28	B	811	CLA	3	0
28	5	303	CLA	2	0
28	8	303	CLA	3	0
28	B	819	CLA	4	0
28	B	843	CLA	3	0
28	L	203	CLA	1	0
28	B	817	CLA	5	0
28	10	306	CLA	4	0
33	B	846	BCR	5	0
33	1	312	BCR	1	0
28	A	846	CLA	2	0
28	B	845	CLA	2	0
28	11	314	CLA	1	0
28	4	304	CLA	2	0
28	B	816	CLA	3	0
28	7	306	CLA	1	0
28	10	308	CLA	1	0
28	6	303	CLA	1	0
28	B	812	CLA	2	0
28	A	853	CLA	1	0
31	9	314	LHG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	9	310	CLA	2	0
28	4	316	CLA	1	0
32	17	311	XAT	3	0
28	A	835	CLA	1	0
31	B	844	LHG	5	0
32	4	315	XAT	2	0
28	7	304	CLA	4	0
28	B	827	CLA	2	0
28	R	202	CLA	1	0
28	B	849	CLA	1	0
32	13	308	XAT	5	0
28	B	824	CLA	2	0
28	A	806	CLA	2	0
28	8	305	CLA	2	0
28	1	314	CLA	5	0
28	11	303	CLA	1	0
33	J	104	BCR	4	0
28	6	311	CLA	1	0
33	17	310	BCR	1	0
28	A	804	CLA	1	0
28	4	310	CLA	4	0
33	B	840	BCR	1	0
33	B	850	BCR	4	0
28	A	837	CLA	4	0
33	I	101	BCR	2	0
28	3	304	CLA	1	0
28	16	203	CLA	1	0
28	8	310	CLA	1	0
28	A	814	CLA	1	0
32	8	312	XAT	5	0
28	10	303	CLA	1	0
28	6	306	CLA	4	0
28	13	305	CLA	1	0
28	6	302	CLA	5	0
37	F	805	LMG	1	0
28	B	828	CLA	4	0
31	5	315	LHG	1	0
28	B	808	CLA	1	0
33	A	843	BCR	2	0
28	7	308	CLA	1	0
28	11	301	CLA	2	0
28	A	825	CLA	1	0

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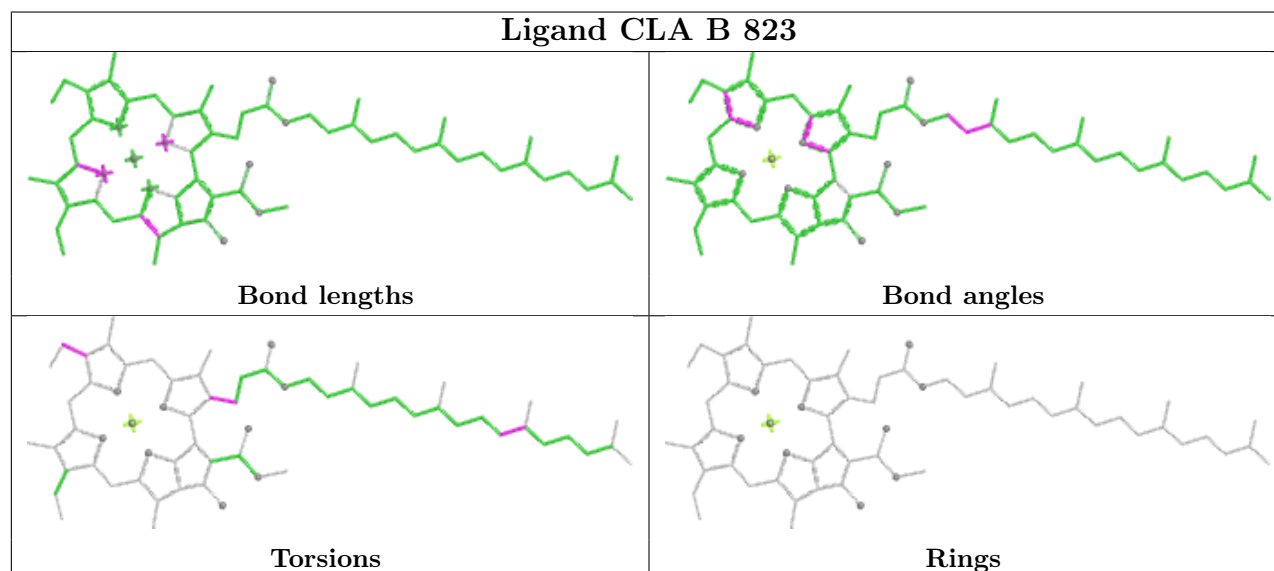
Mol	Chain	Res	Type	Clashes	Symm-Clashes
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28	1	308	CLA	1	0
28	A	834	CLA	3	0
28	A	818	CLA	2	0
28	B	835	CLA	1	0
32	4	318	XAT	8	0
28	B	847	CLA	2	0
28	F	802	CLA	4	0
33	B	851	BCR	1	0
28	A	821	CLA	1	0
28	A	829	CLA	2	0
33	A	844	BCR	3	0
32	1	311	XAT	1	0
28	1	310	CLA	2	0
28	A	801	CLA	1	0
28	A	826	CLA	2	0
28	B	832	CLA	2	0
28	B	848	CLA	1	0
32	7	315	XAT	3	0
33	L	202	BCR	4	0
28	5	304	CLA	1	0
33	A	841	BCR	5	0
28	B	822	CLA	2	0
28	A	810	CLA	3	0
28	11	310	CLA	1	0
32	5	316	XAT	2	0
28	4	307	CLA	3	0
28	3	303	CLA	2	0
28	A	811	CLA	1	0
28	B	809	CLA	2	0
28	A	819	CLA	3	0
28	7	311	CLA	1	0
28	A	817	CLA	7	0
33	B	837	BCR	3	0
28	B	803	CLA	1	0
28	A	802	CLA	6	0
28	A	823	CLA	2	0
28	B	820	CLA	2	0
28	9	303	CLA	2	0
28	7	301	CLA	4	0
32	10	315	XAT	6	0
28	5	313	CLA	4	0

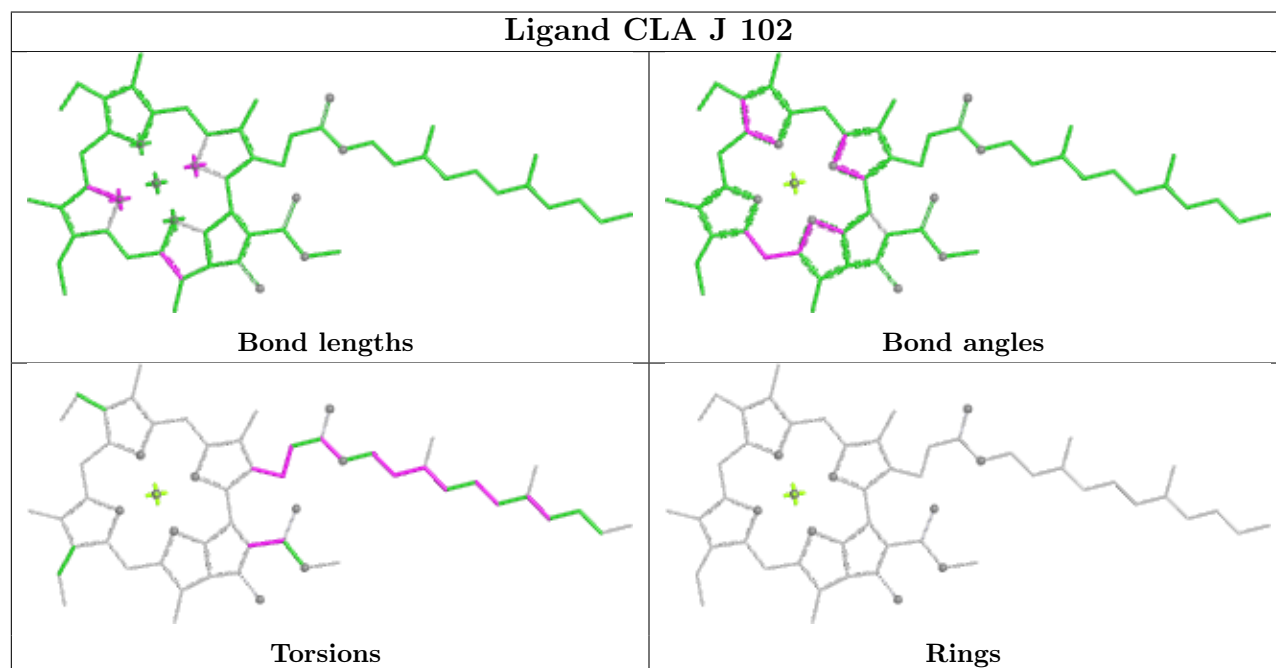
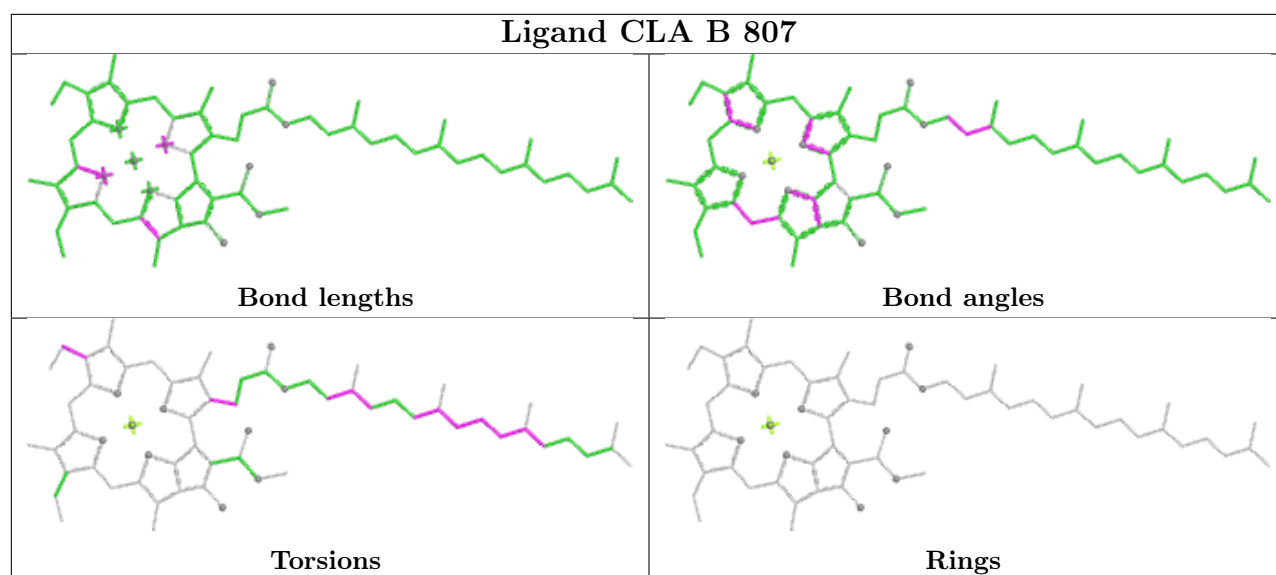
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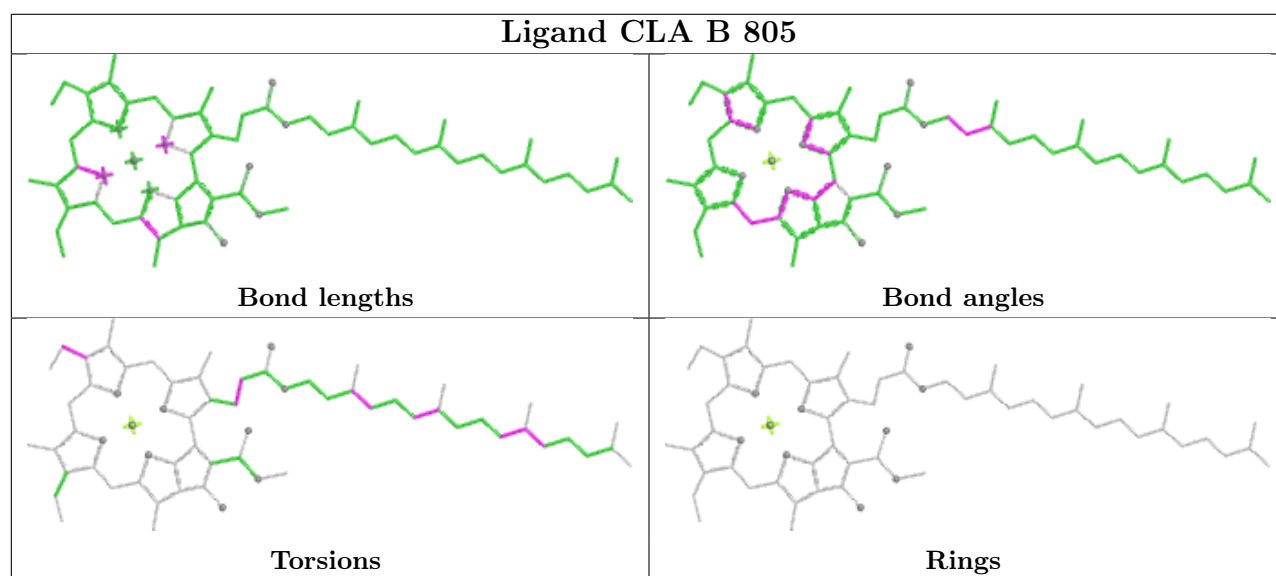
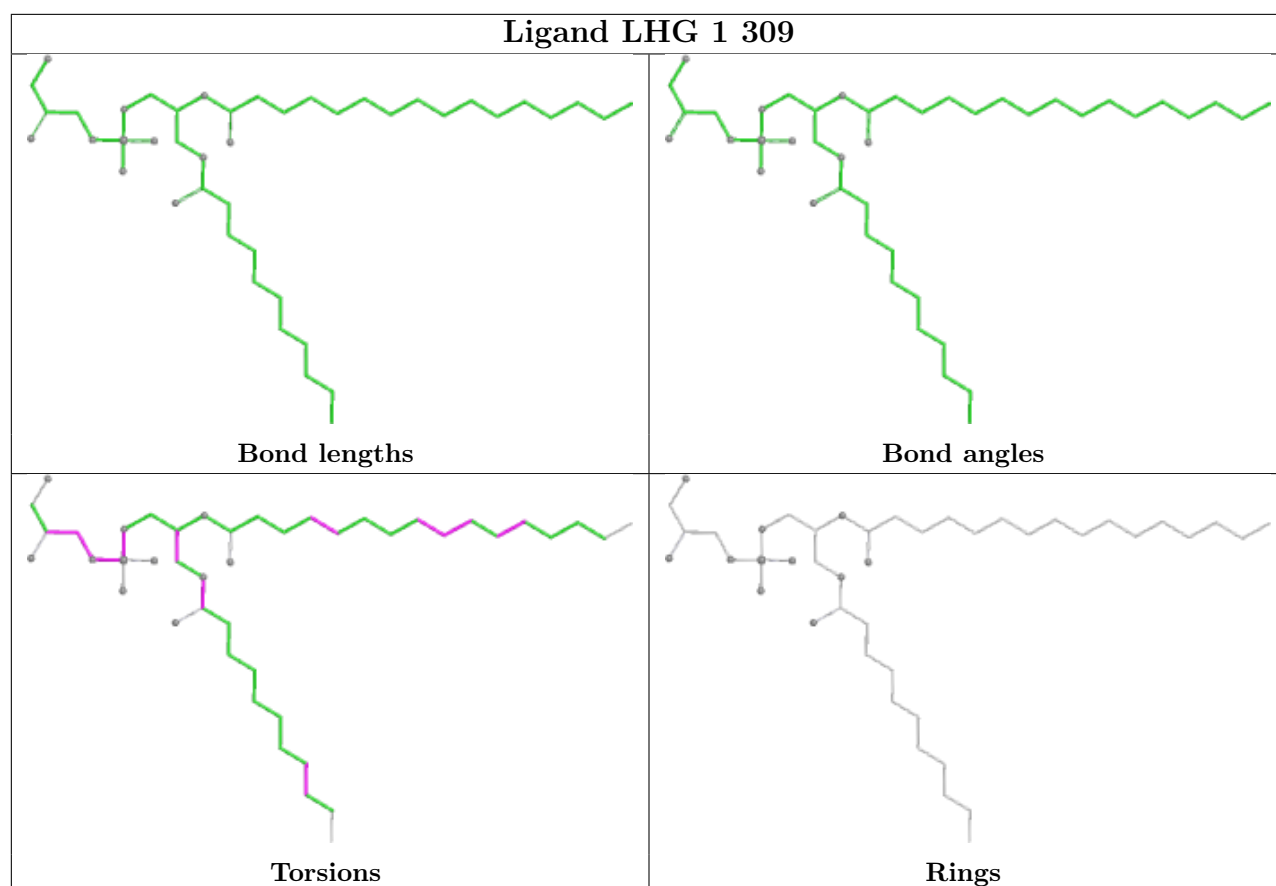
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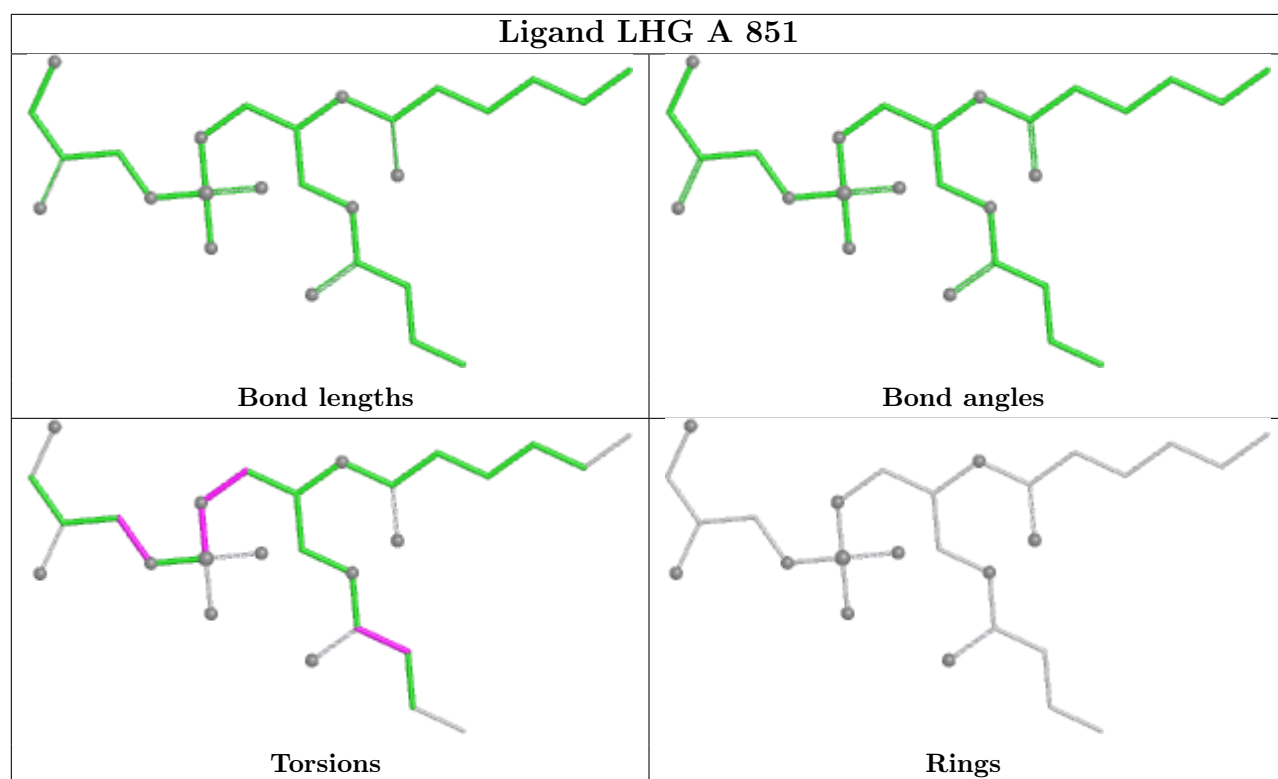
Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	17	301	CLA	2	0
28	a	202	CLA	1	0
28	1	303	CLA	2	0
28	10	316	CLA	4	0
28	17	307	CLA	1	0

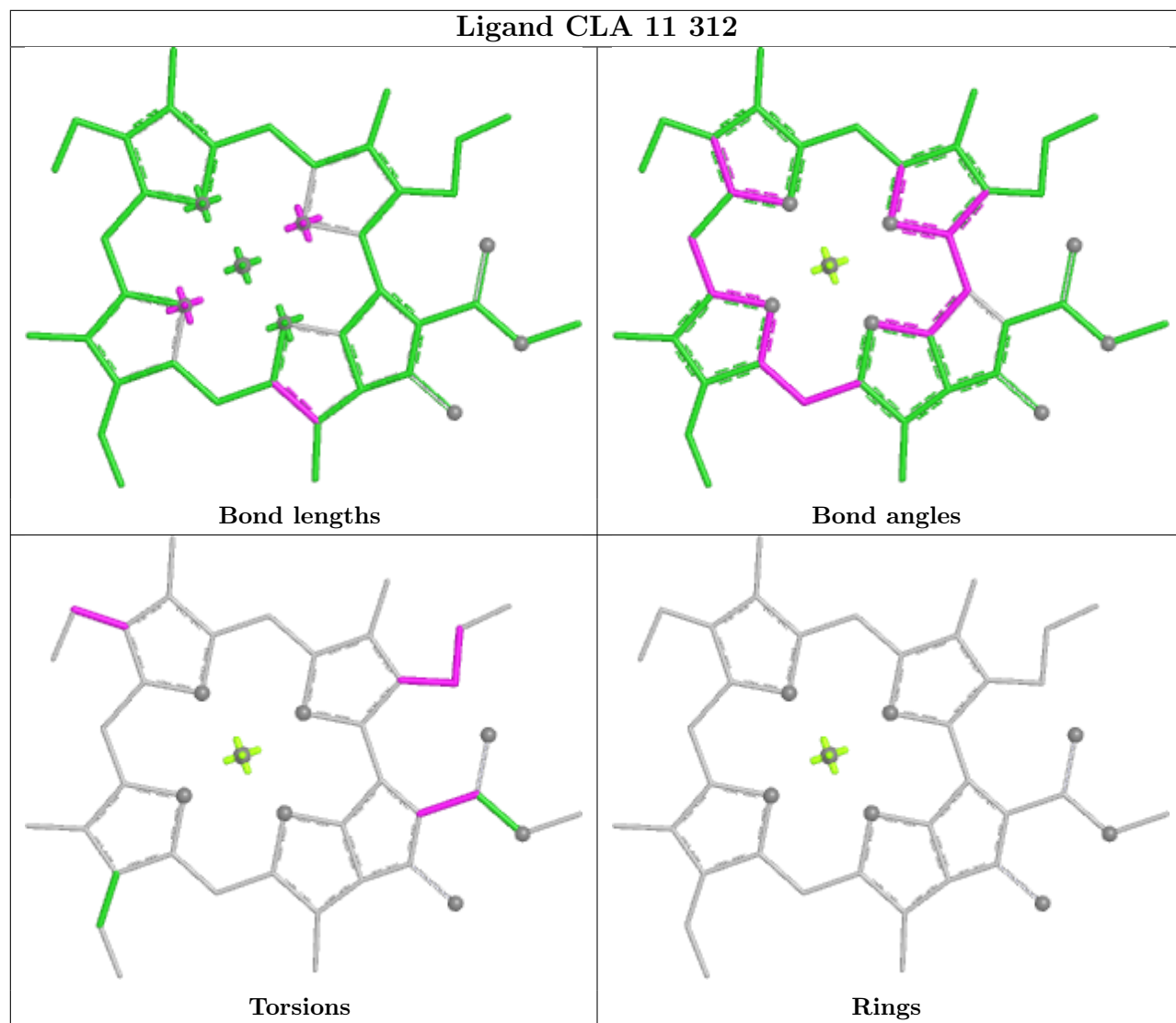
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

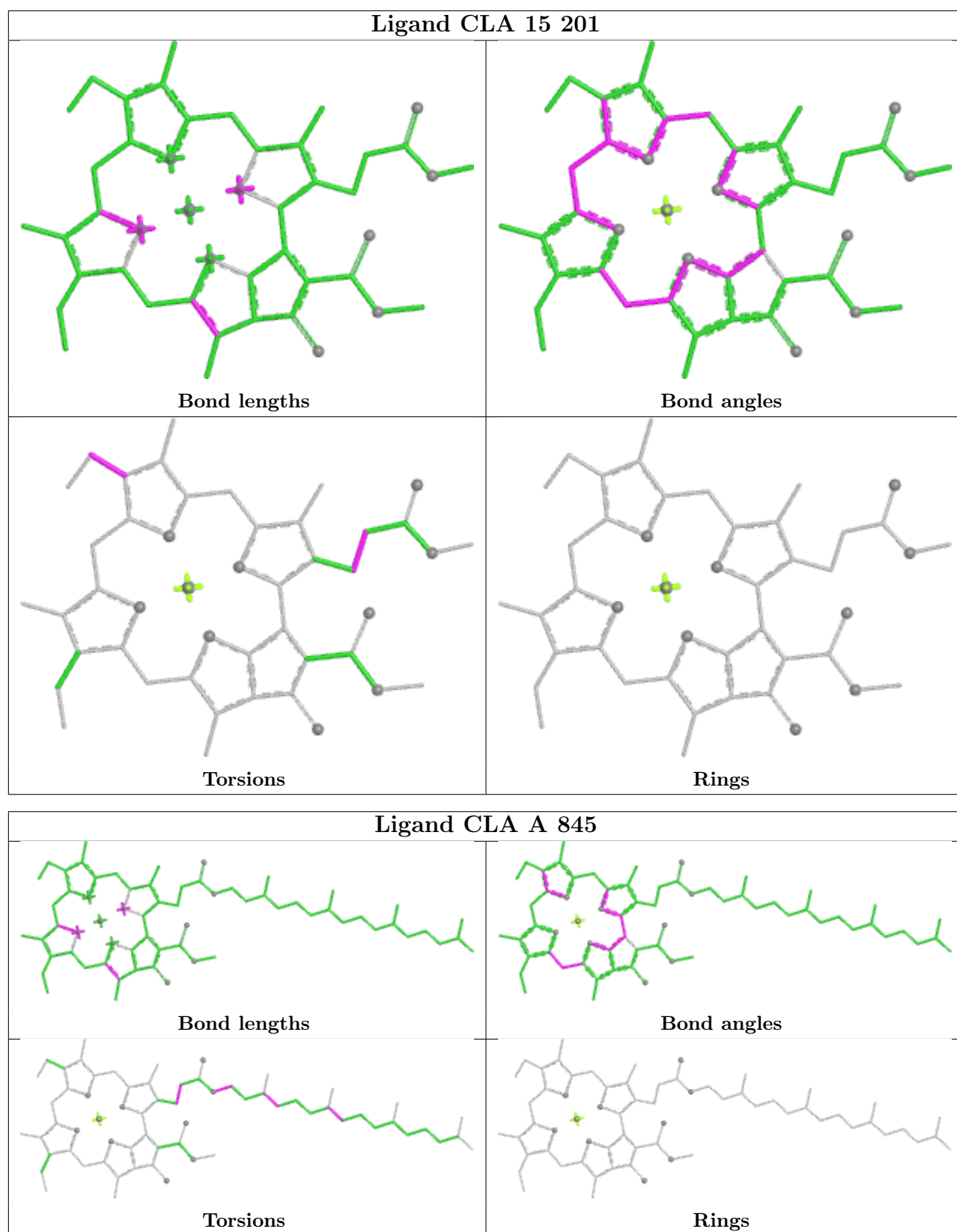


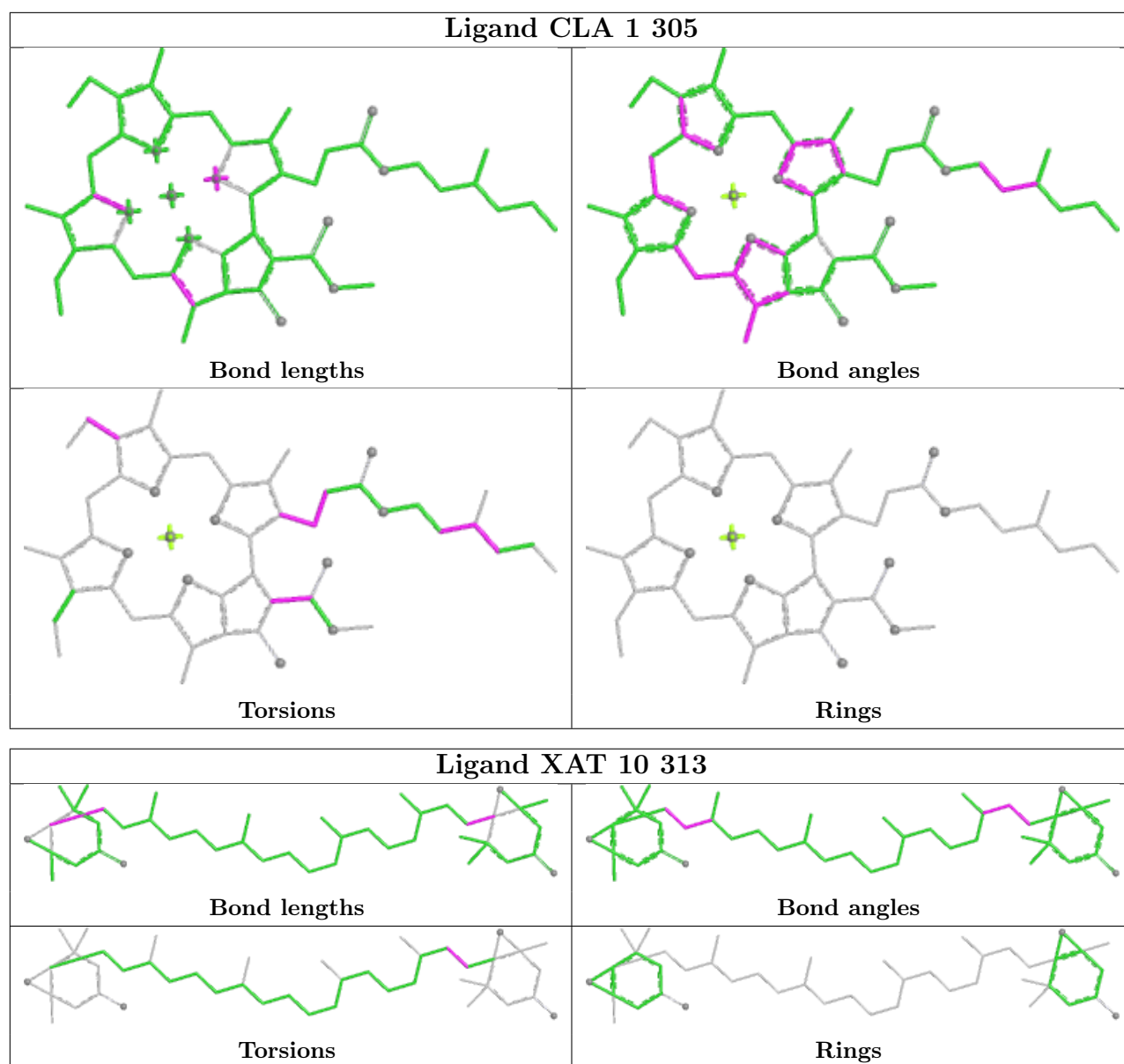


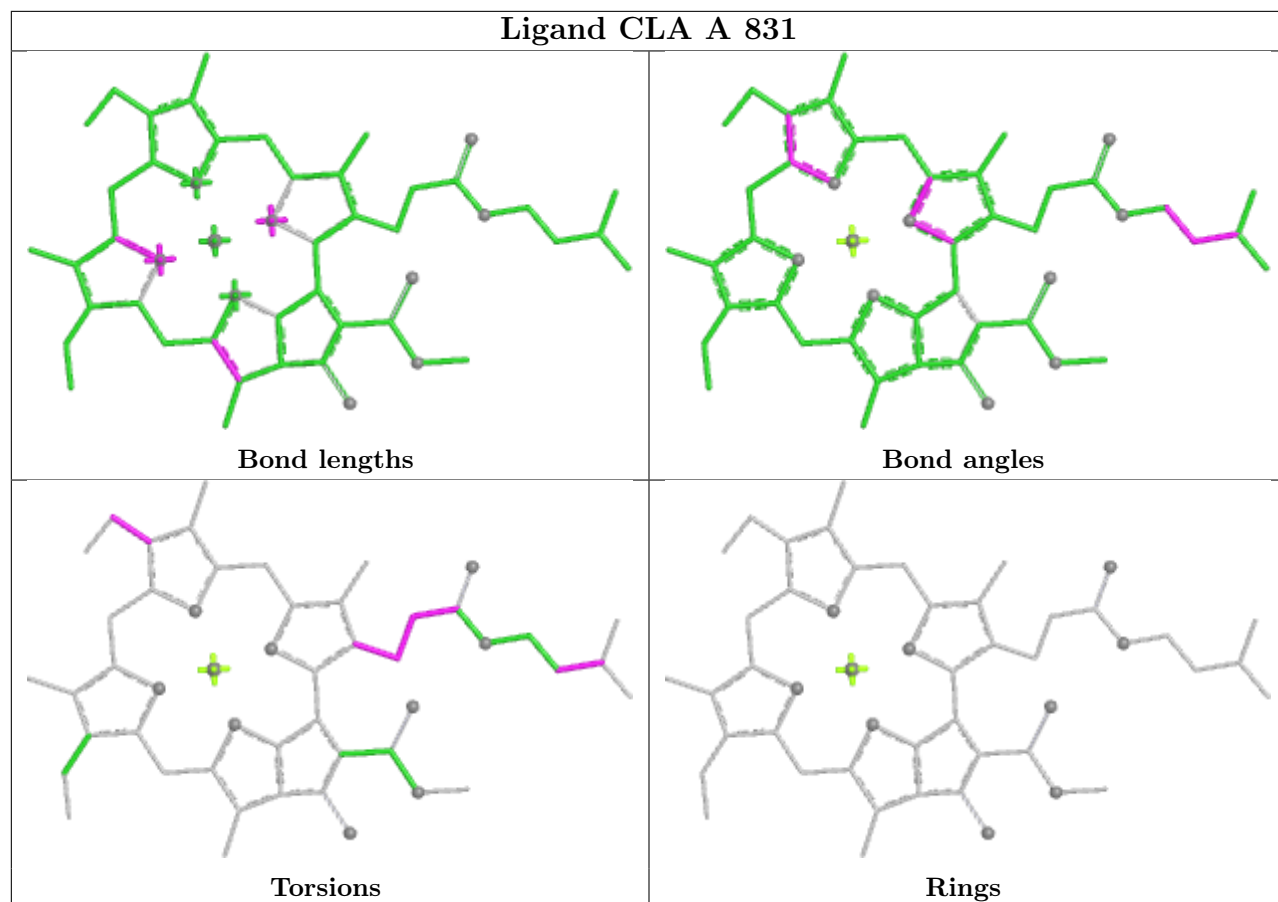




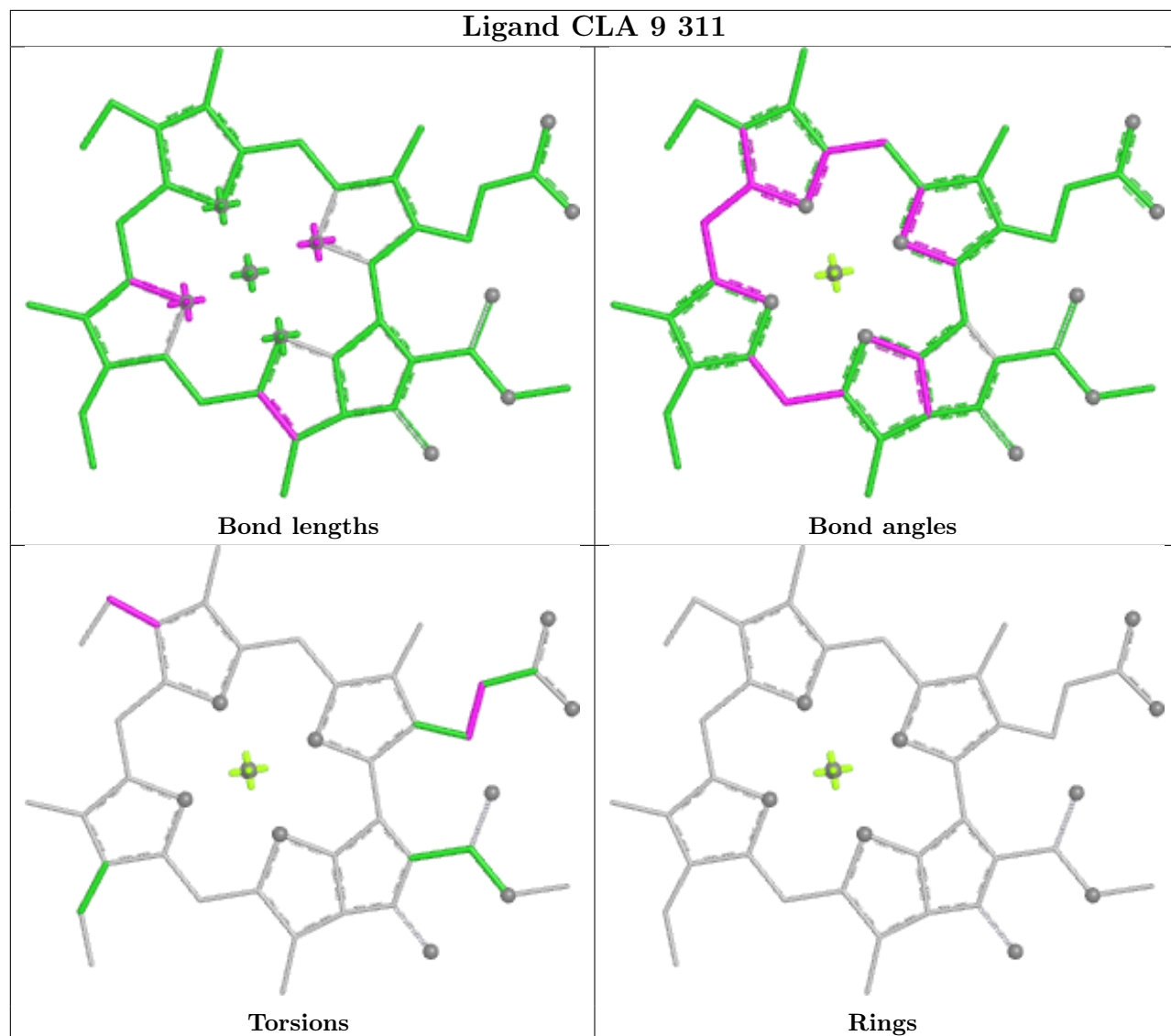




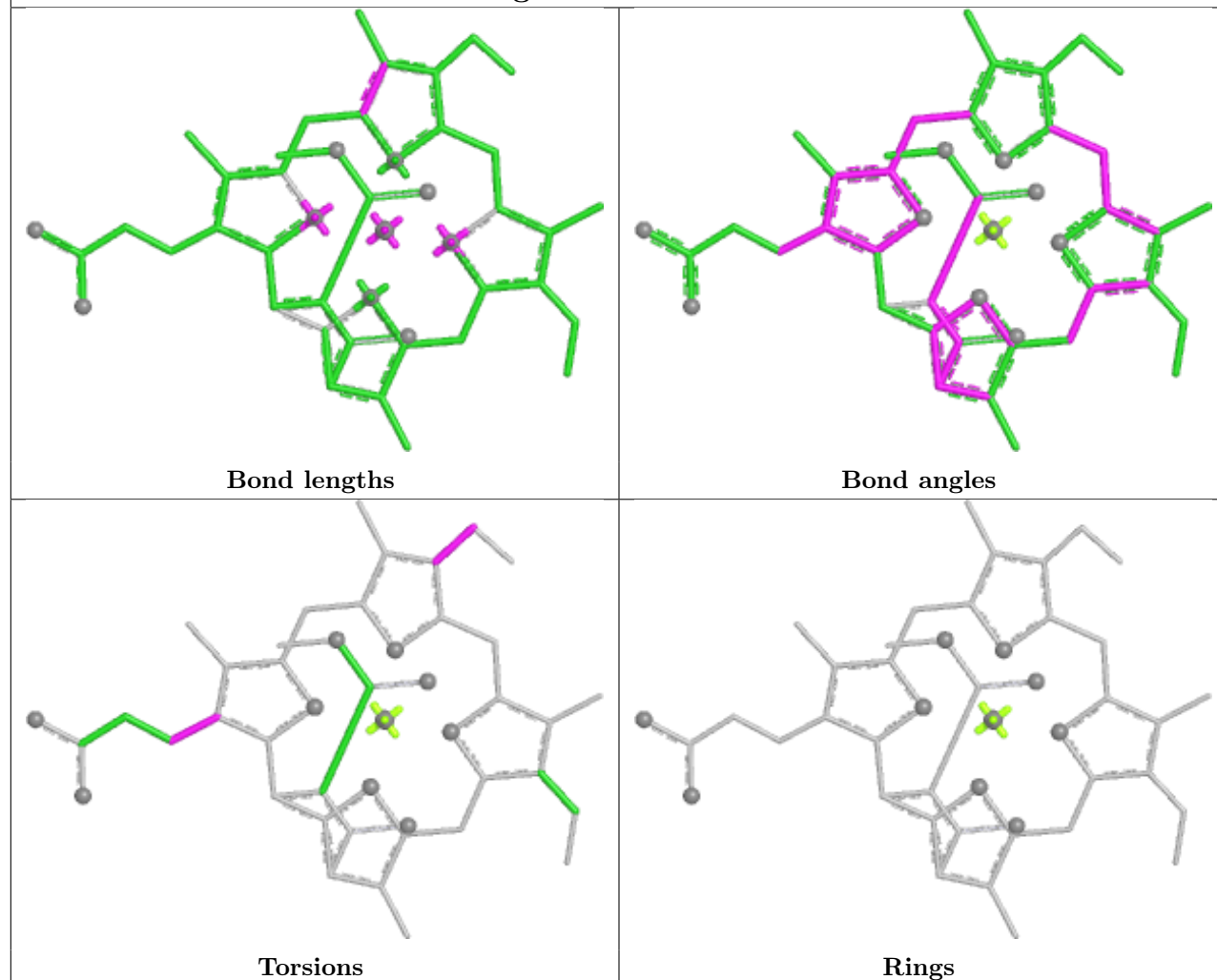




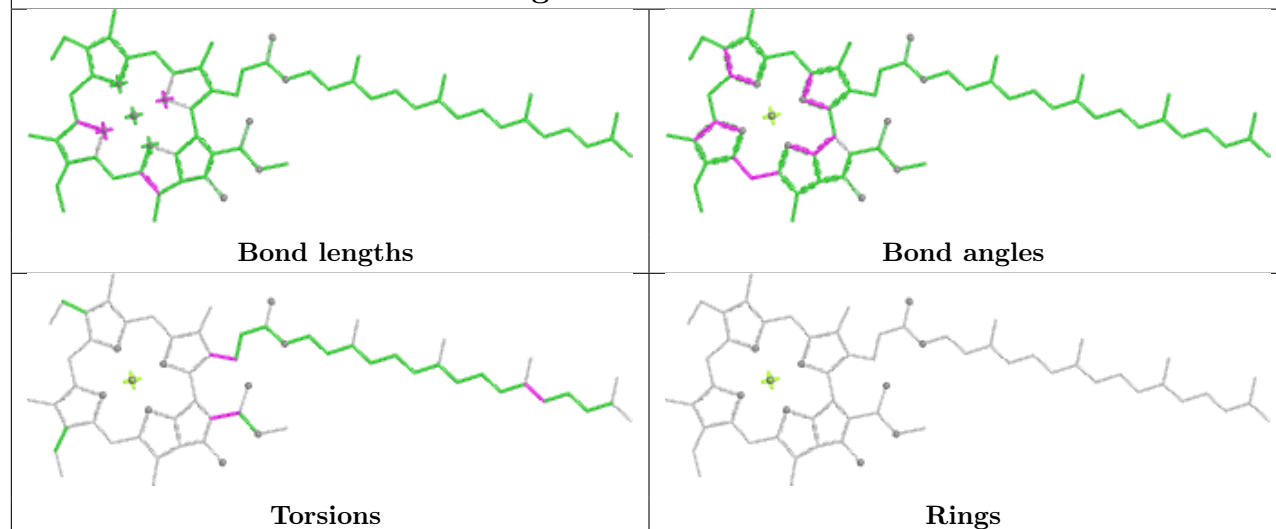
Ligand CLA 9 311



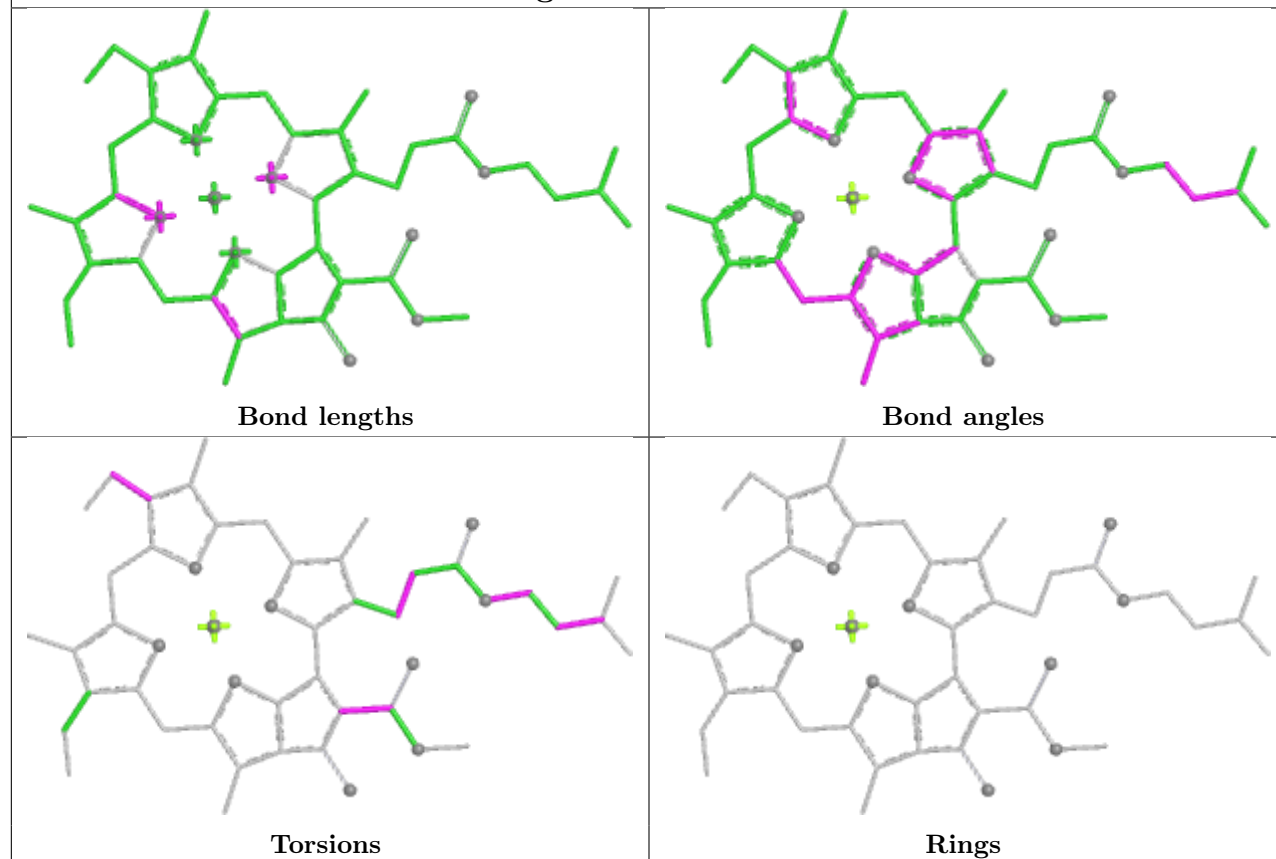
Ligand KC1 7 307



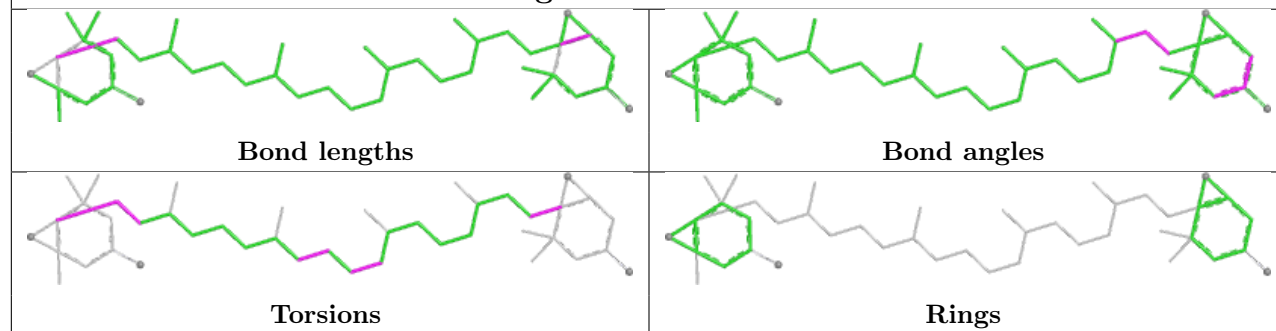
Ligand CLA A 828

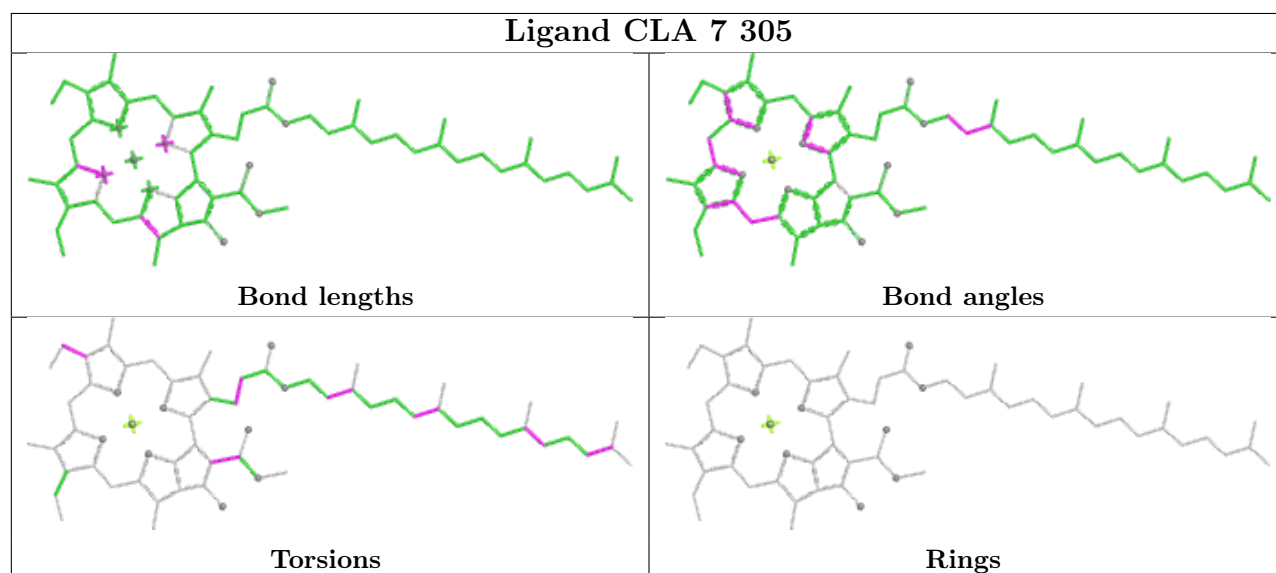
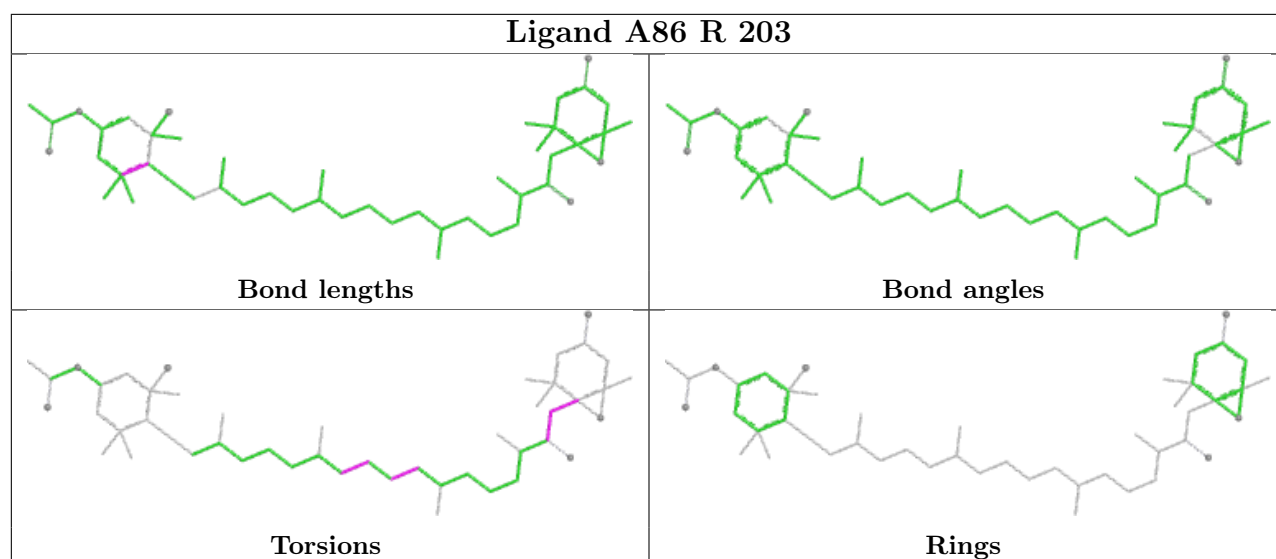


Ligand CLA 9 305

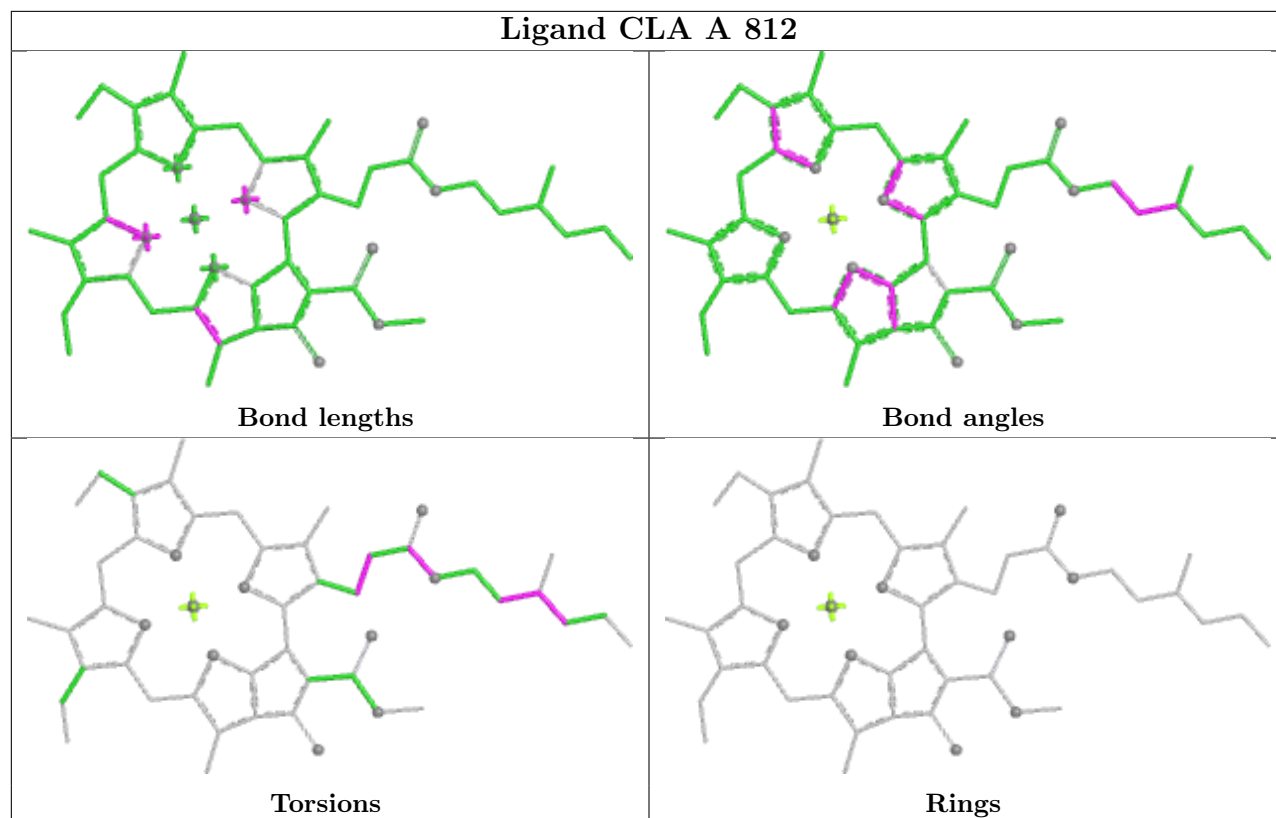


Ligand XAT 9 313

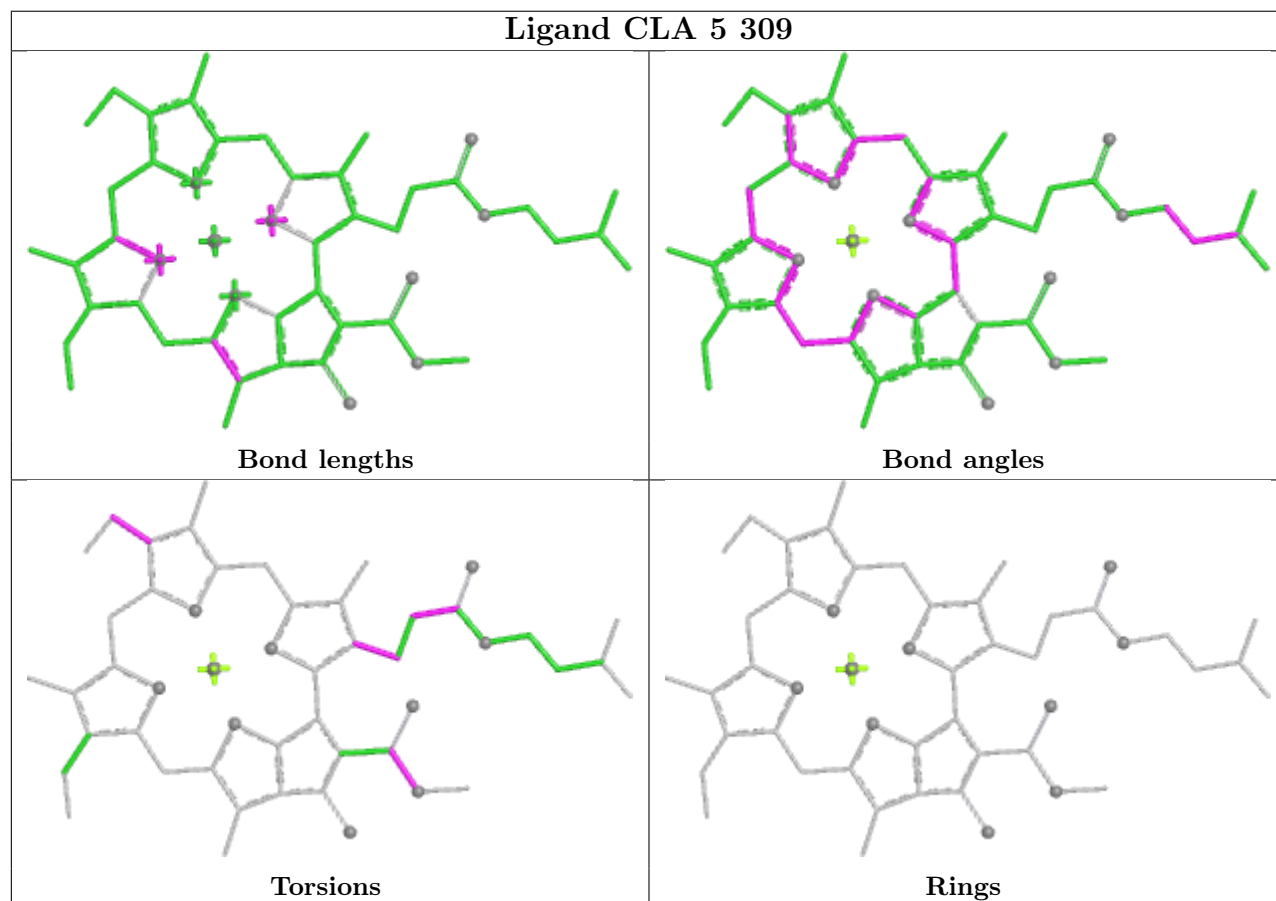




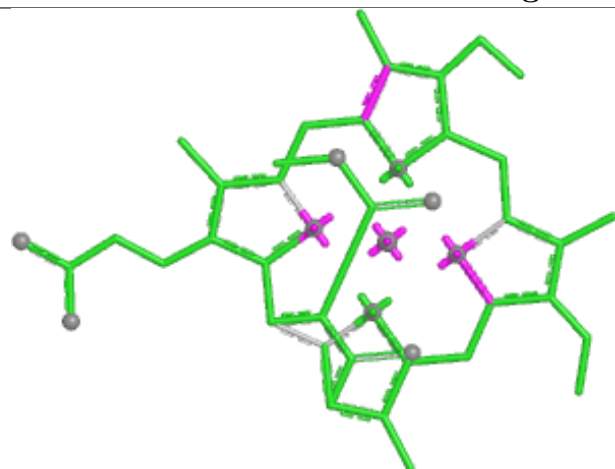
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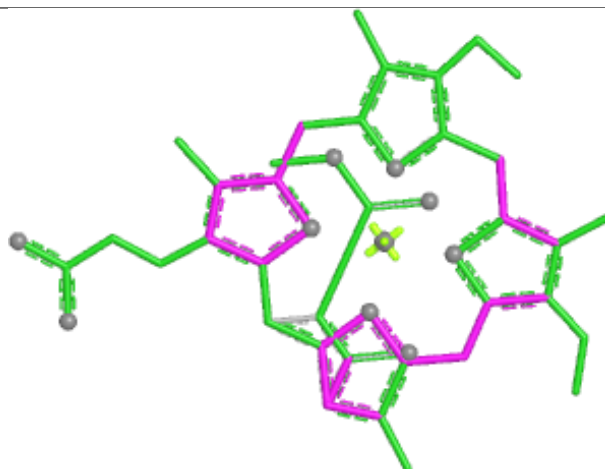
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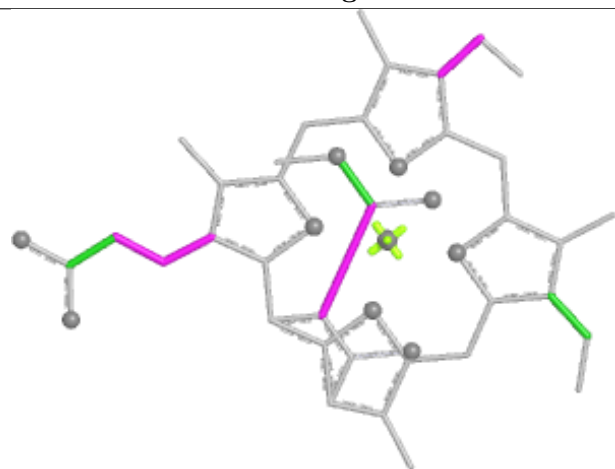
Ligand KC1 7 309



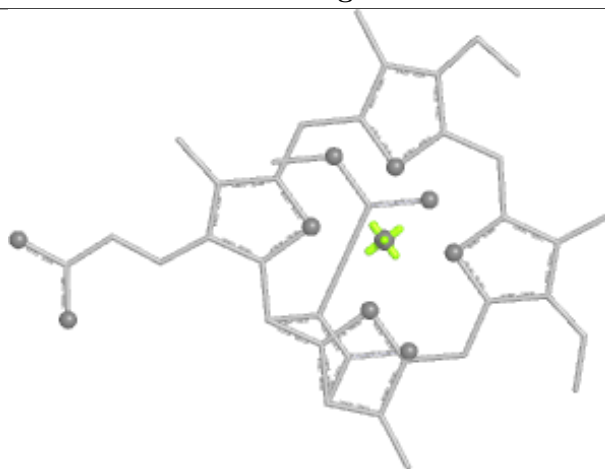
Bond lengths



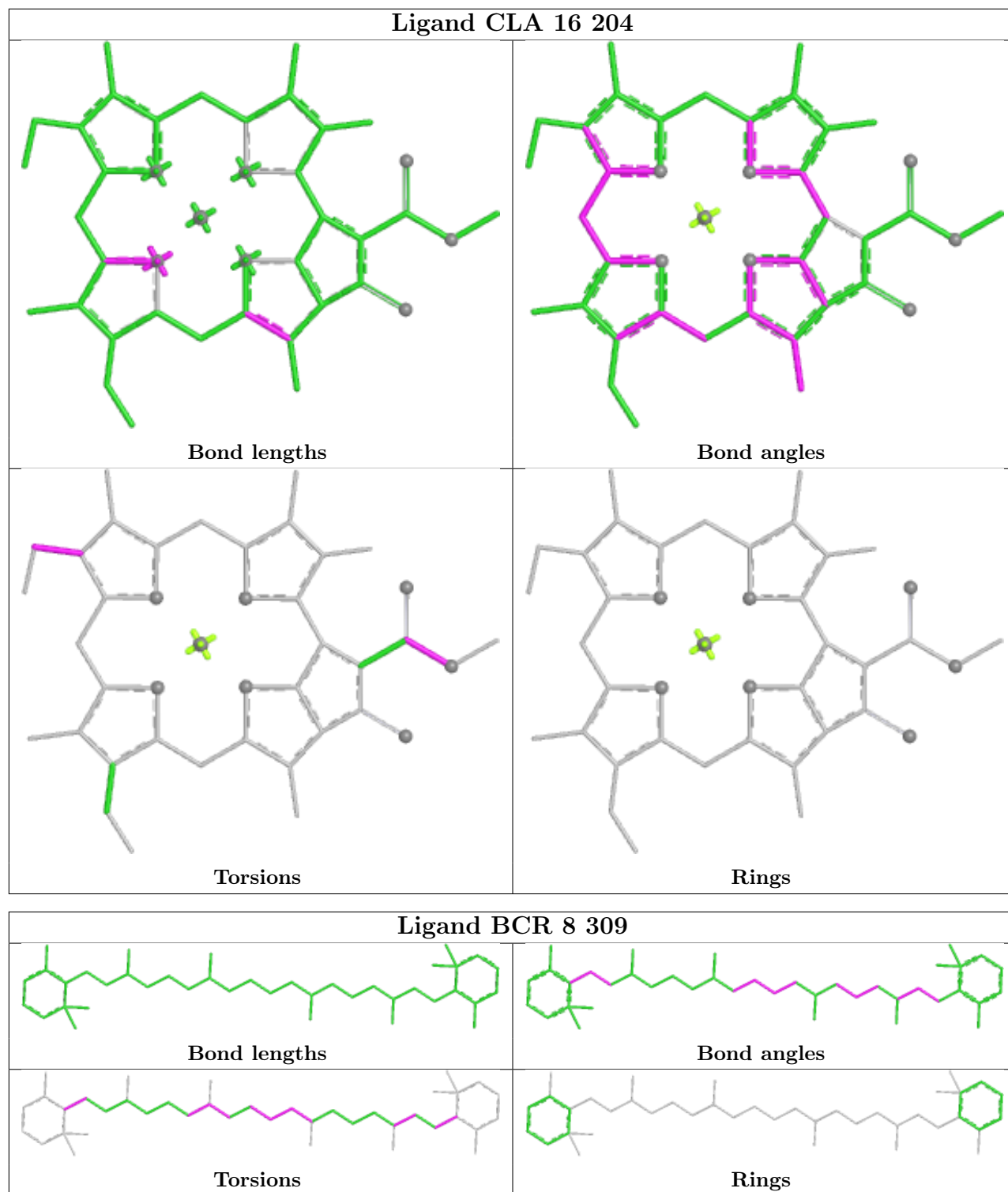
Bond angles

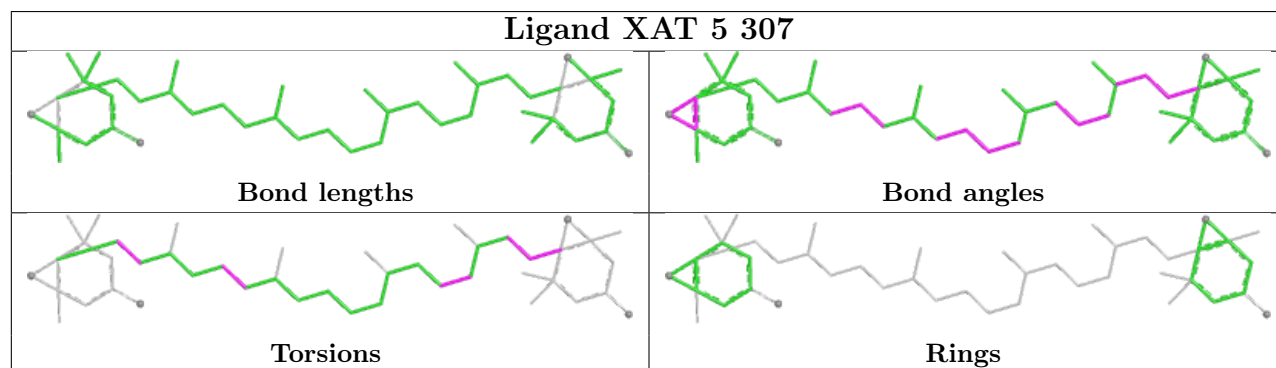
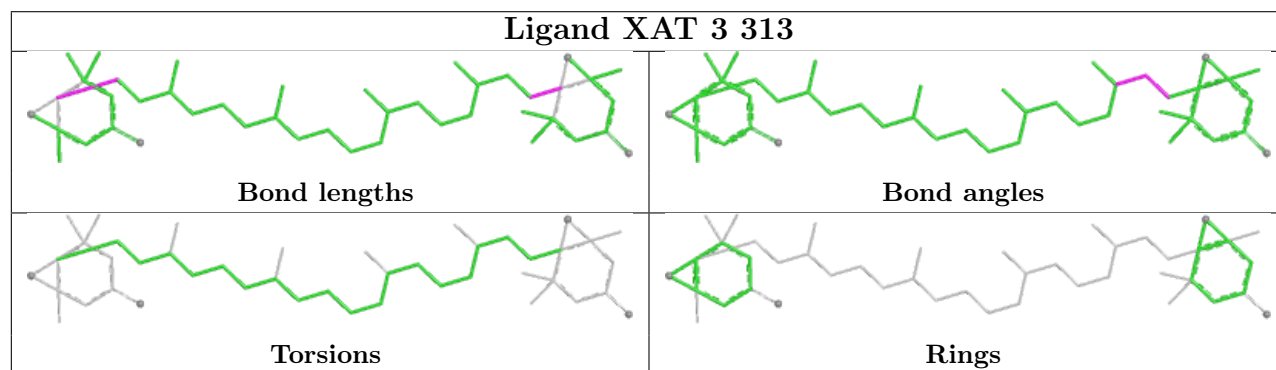
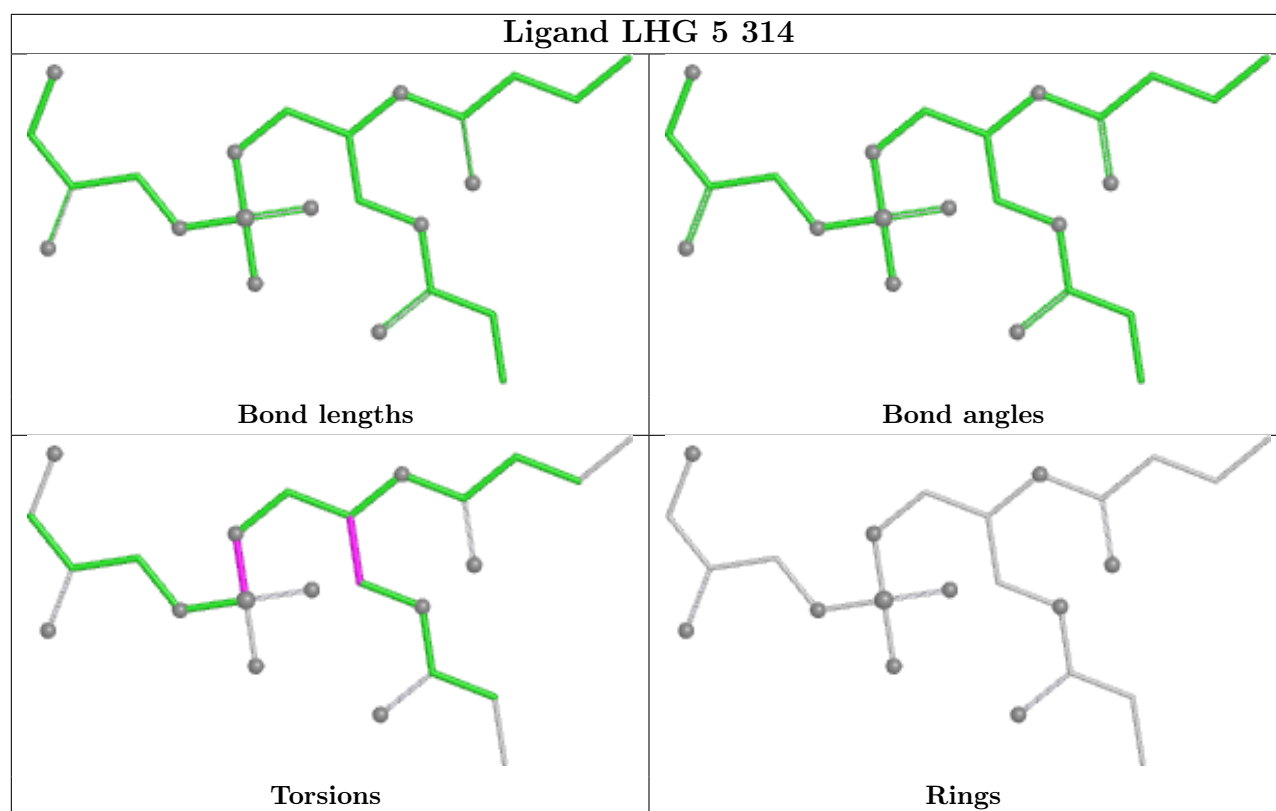


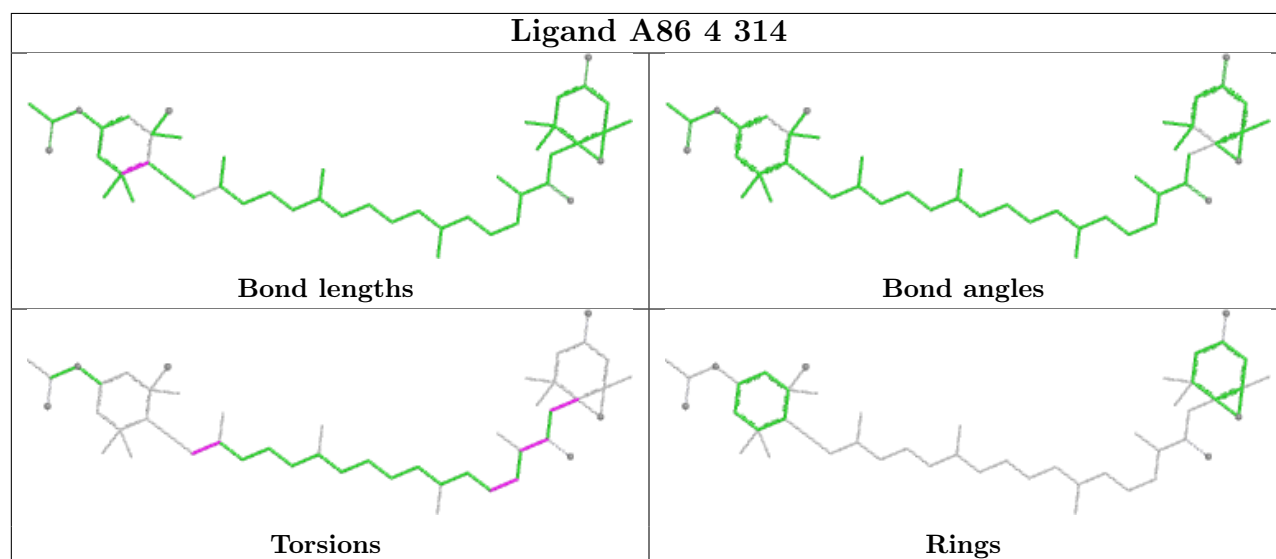
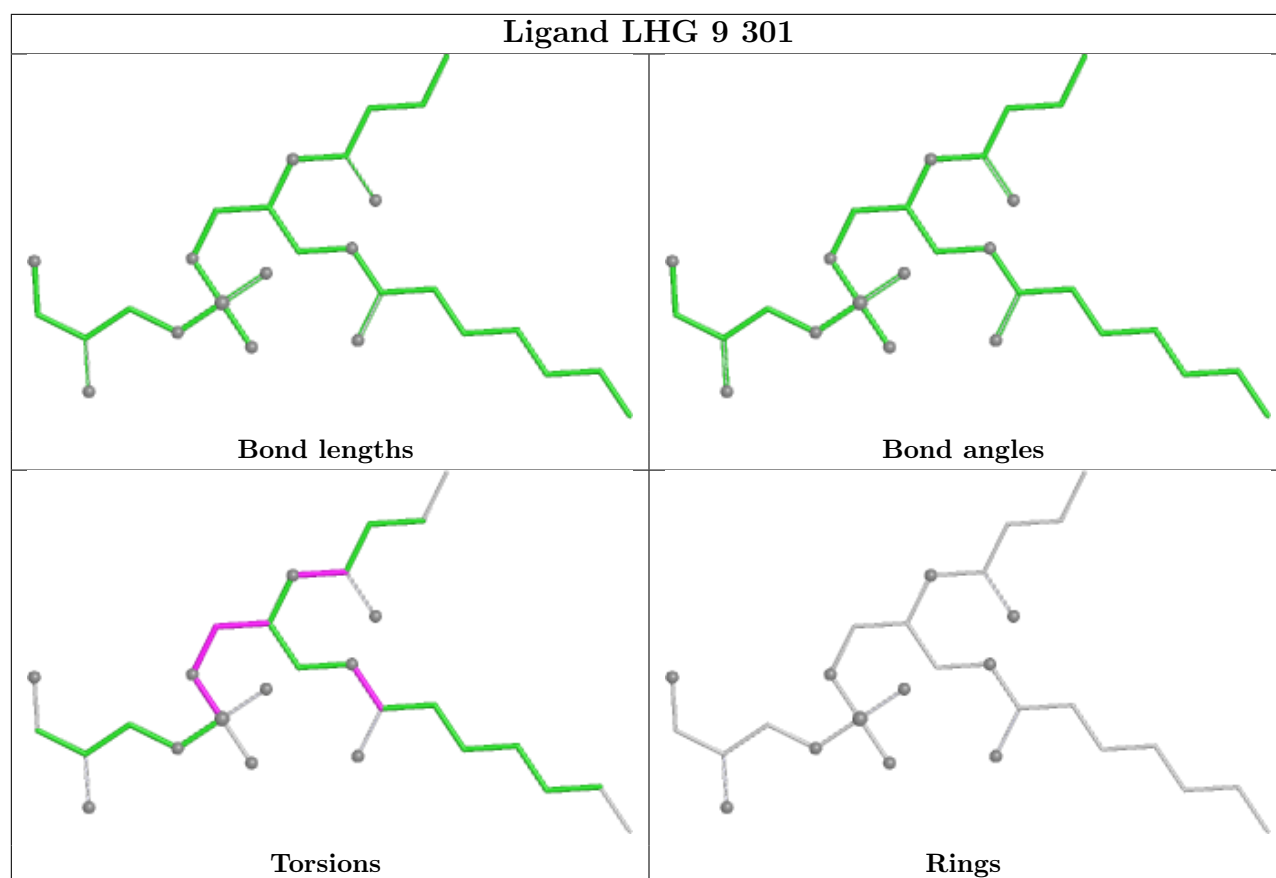
Torsions

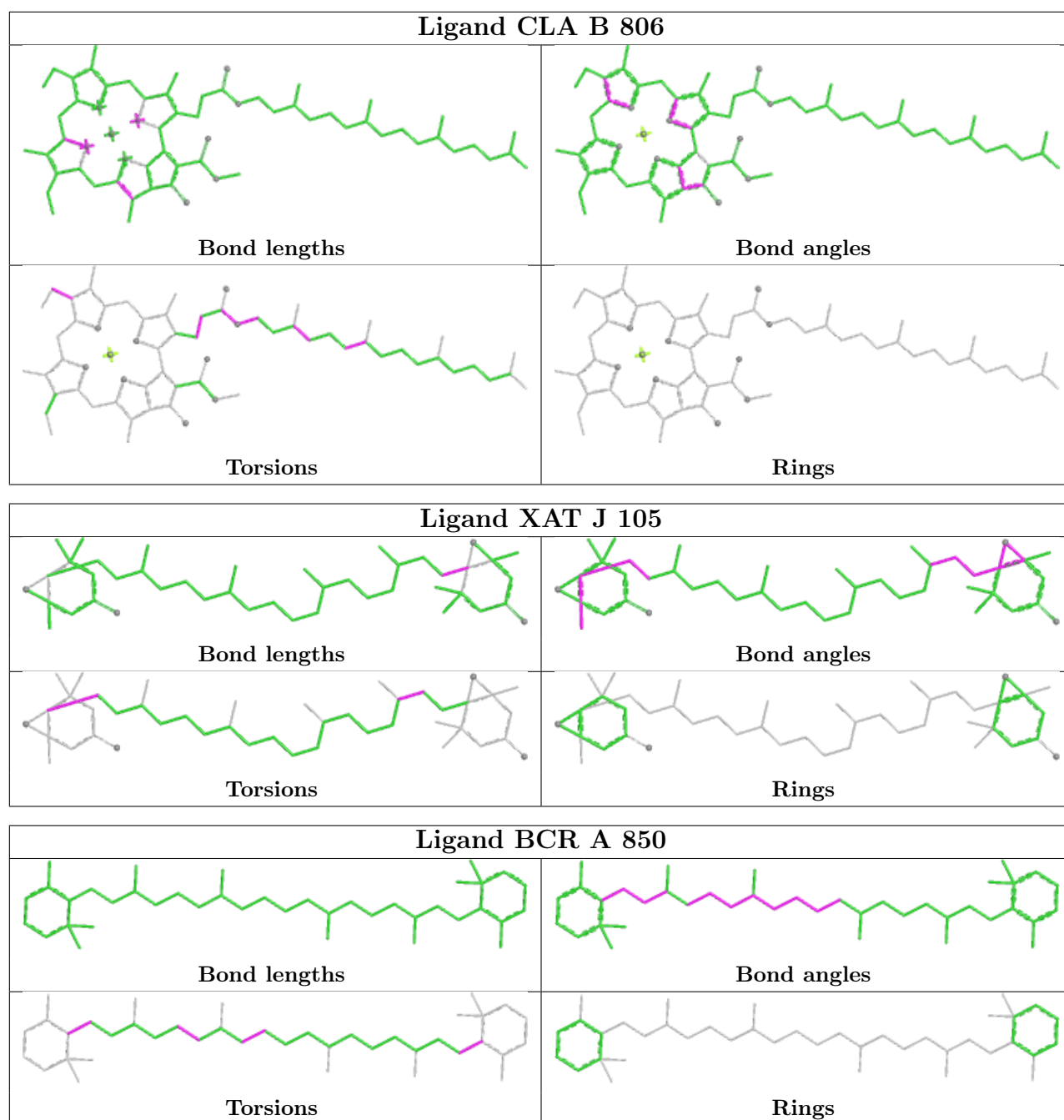


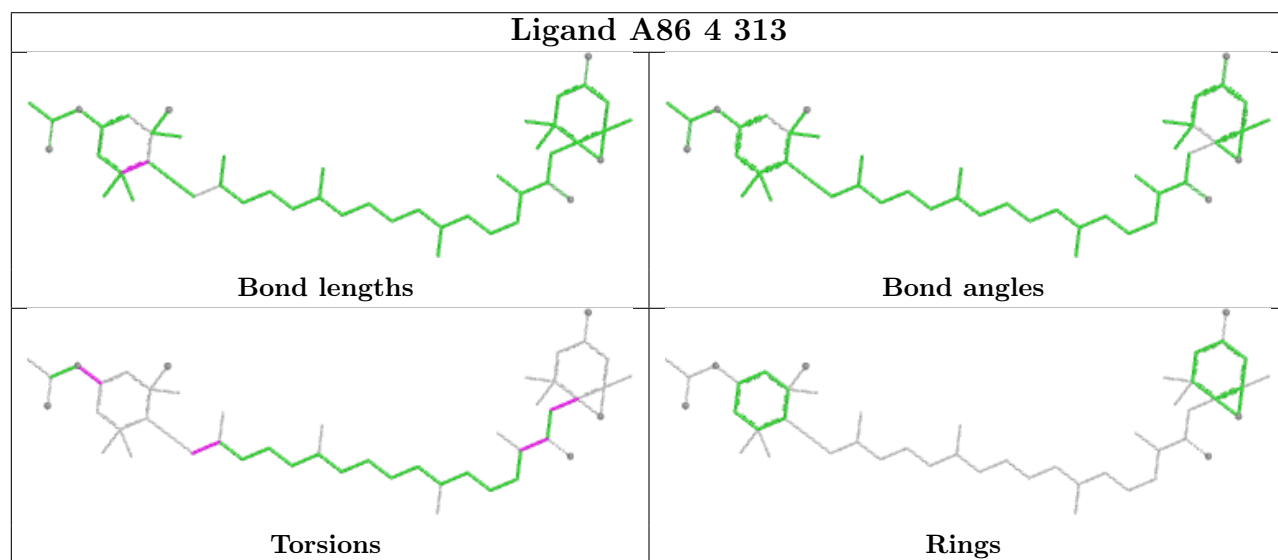
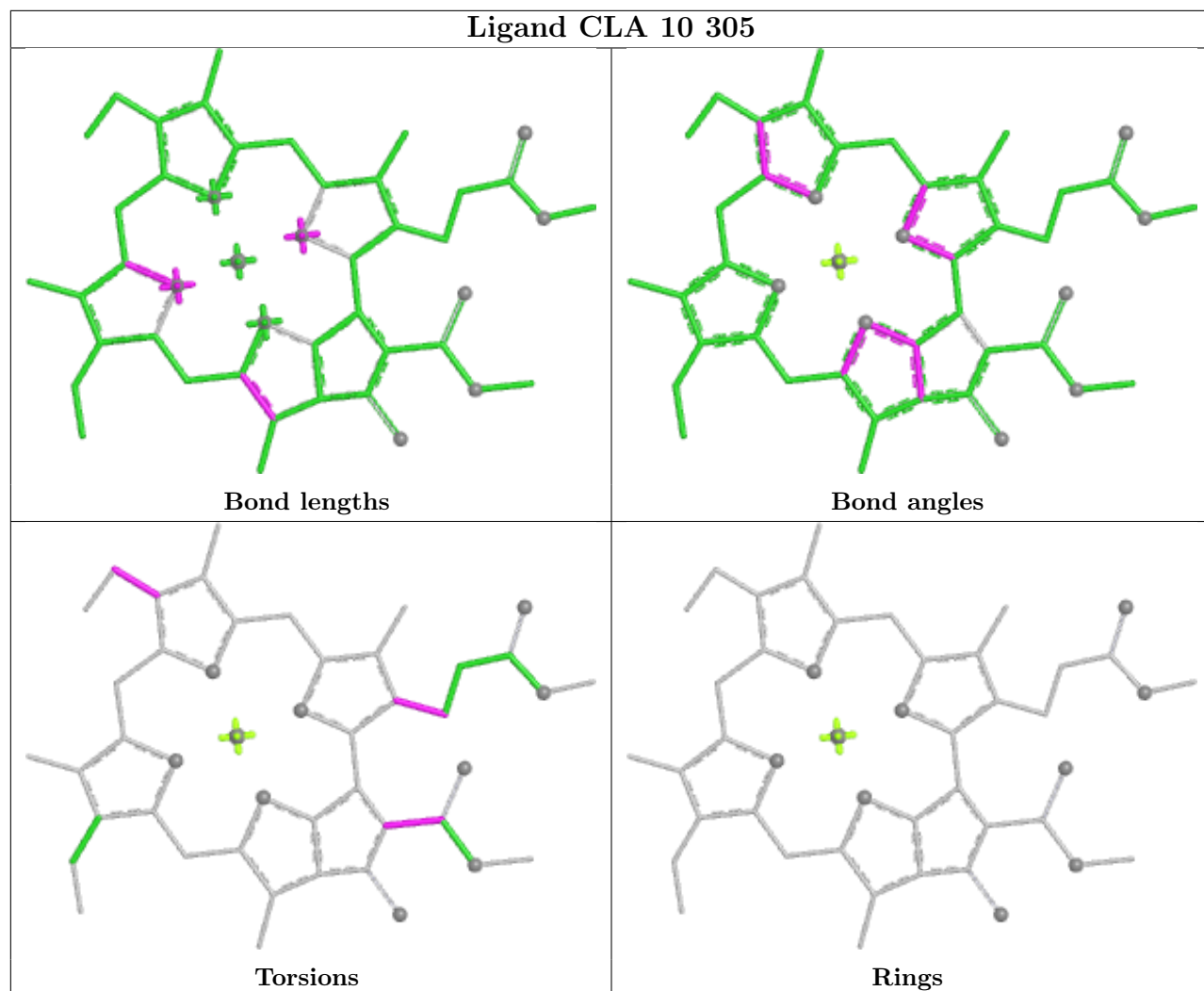
Rings

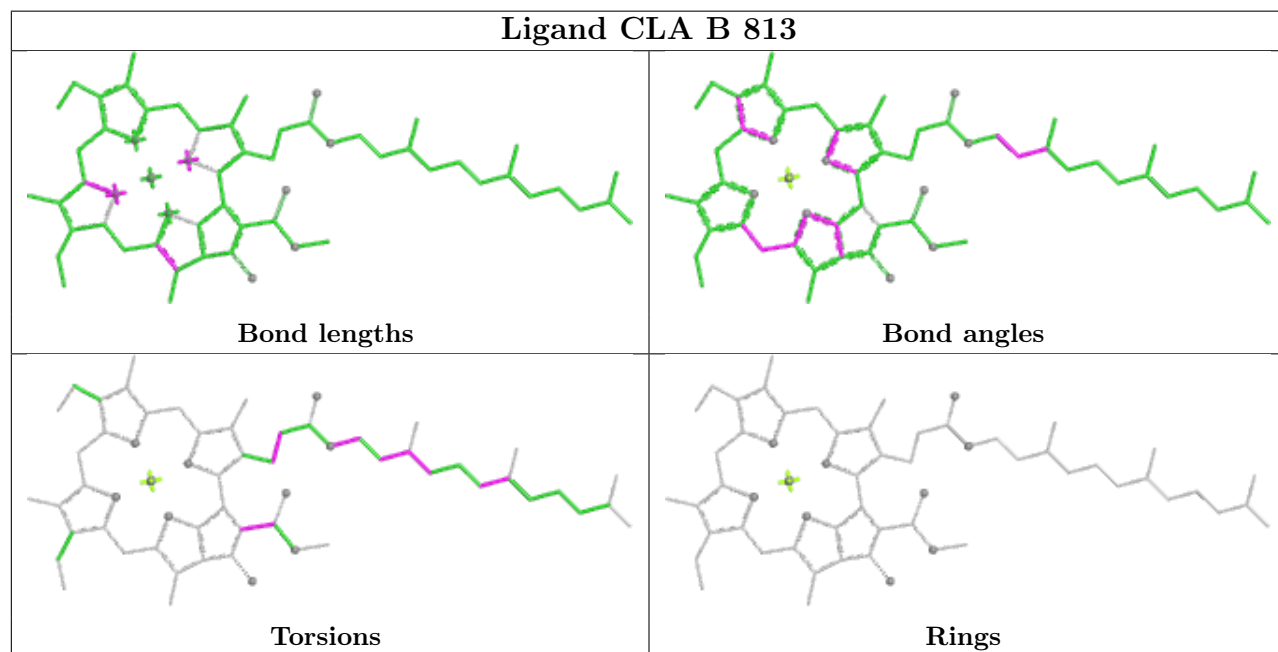
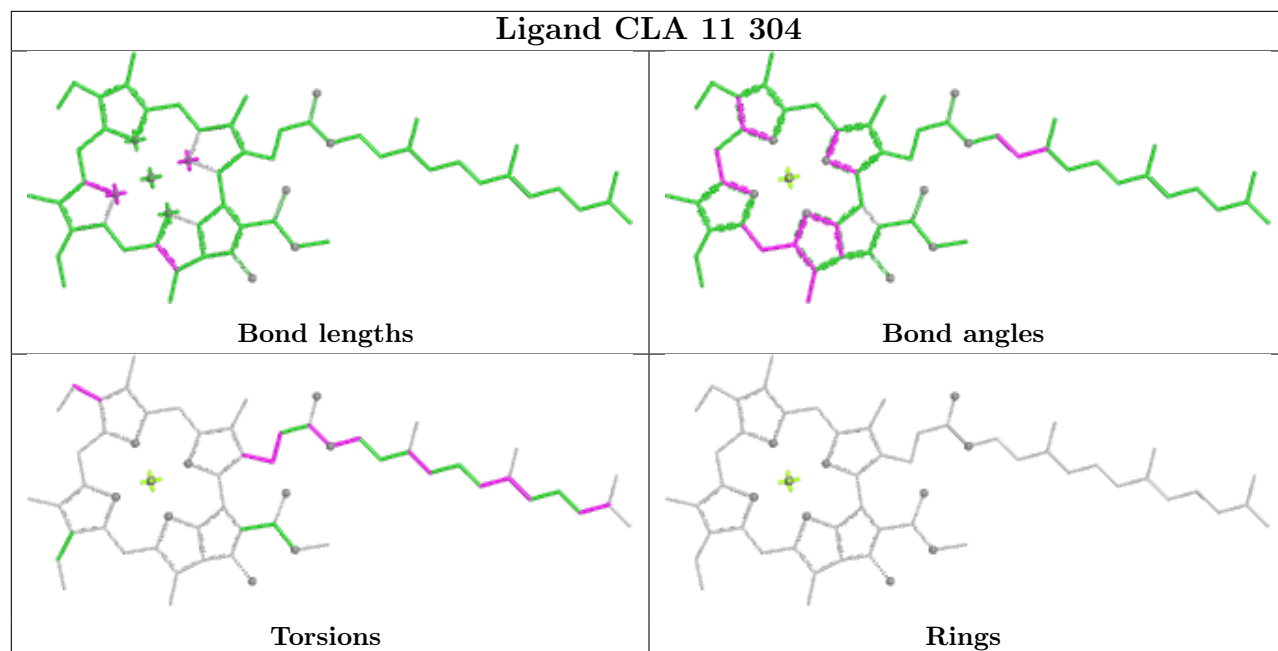


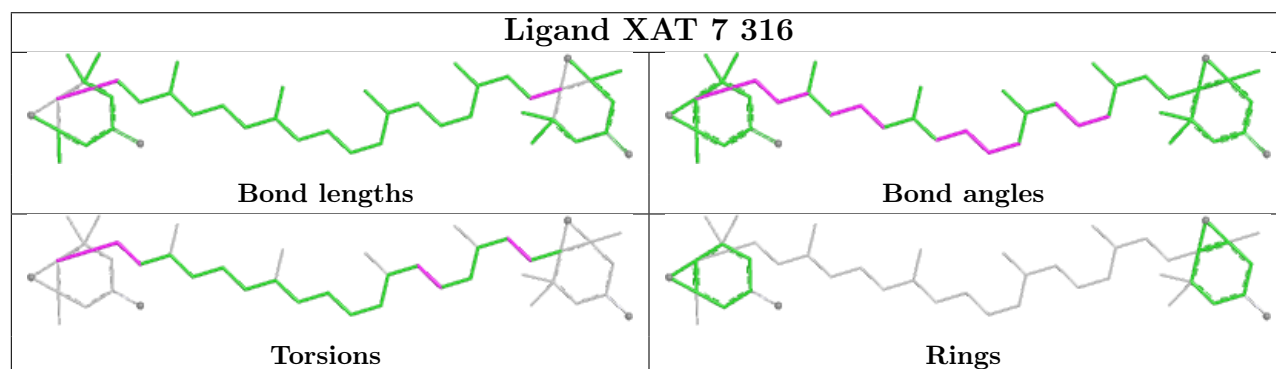
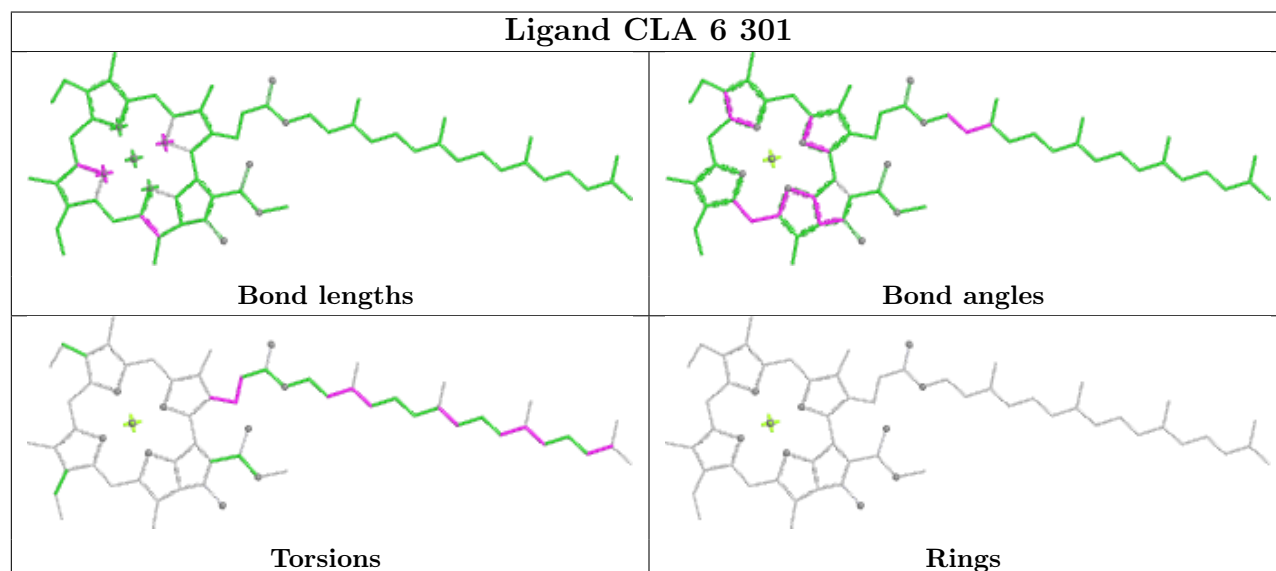
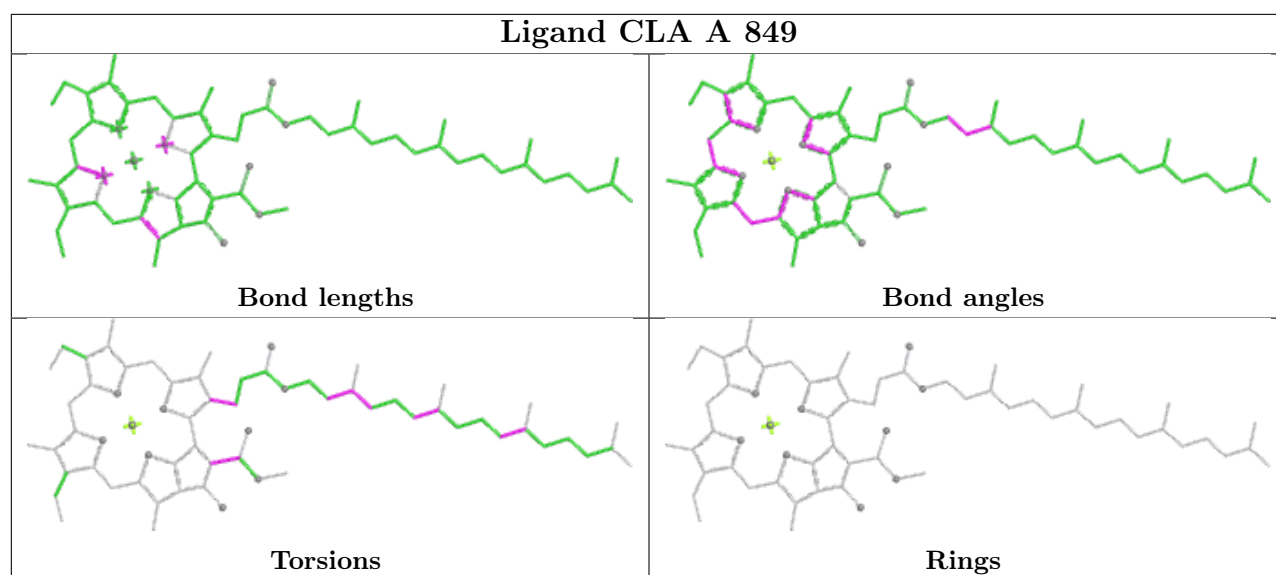


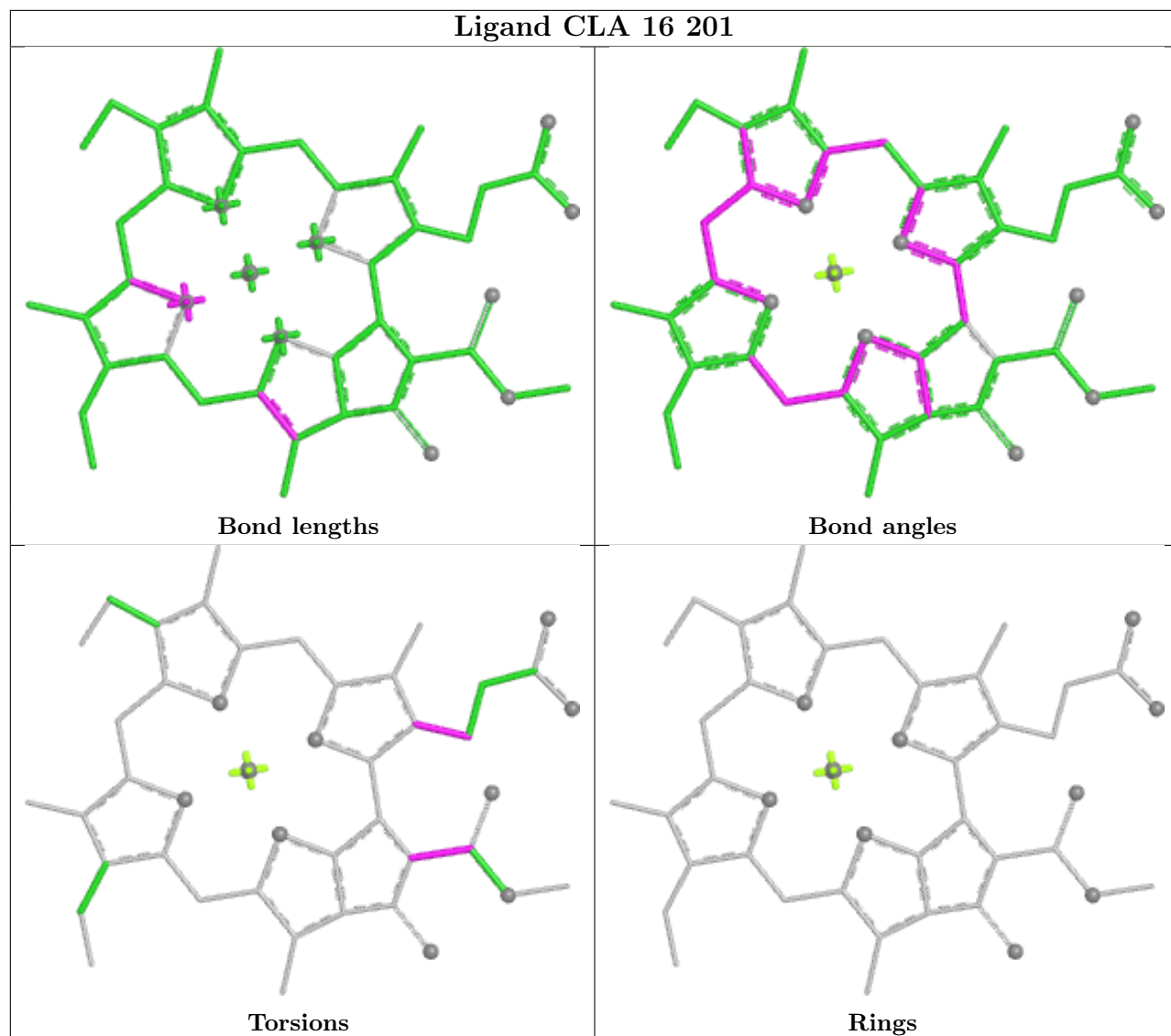


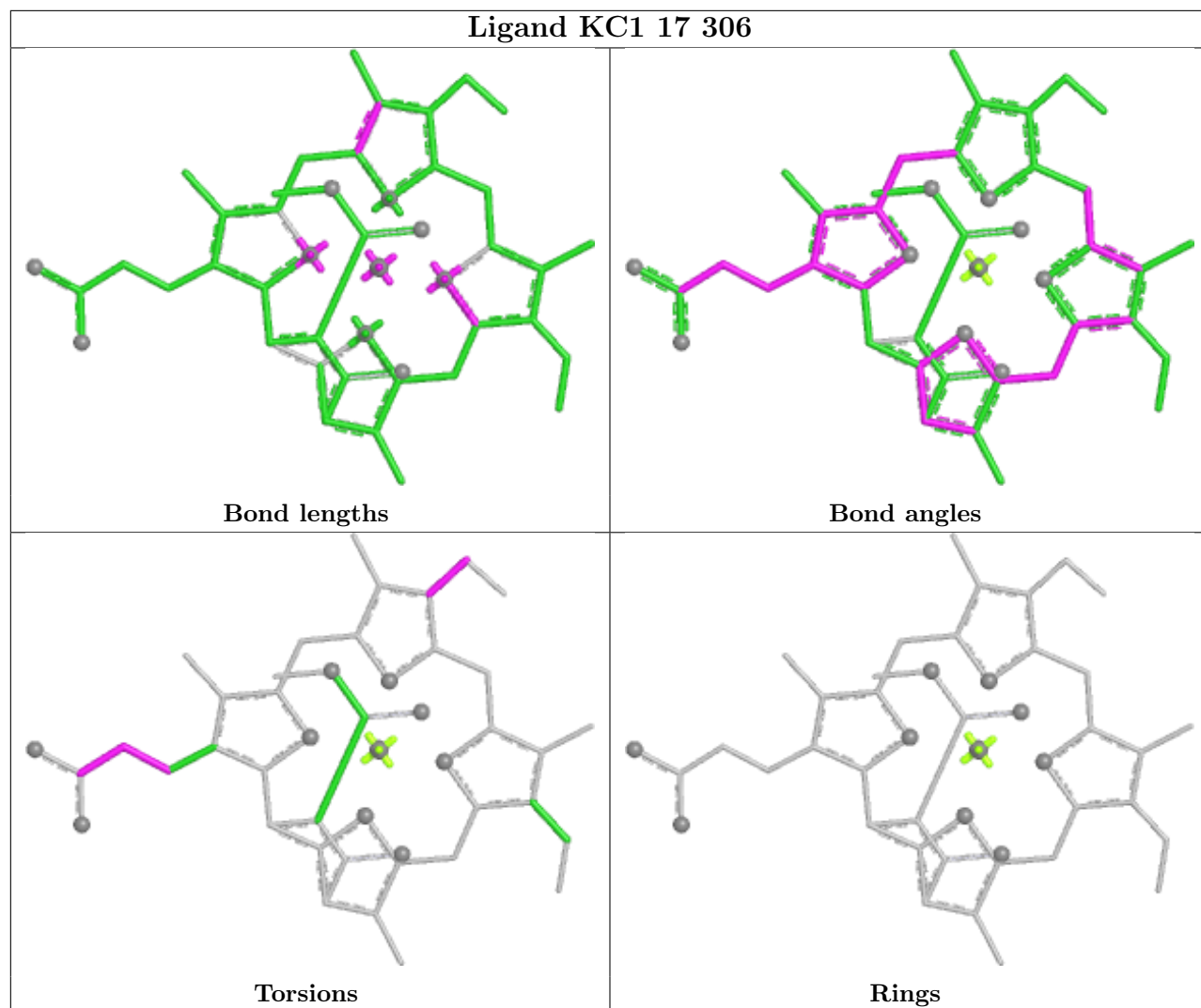




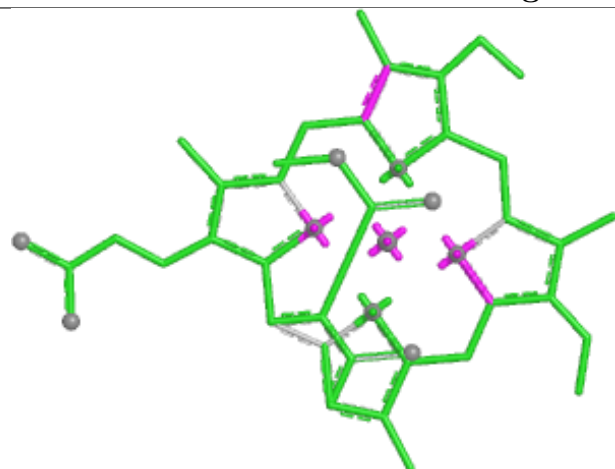




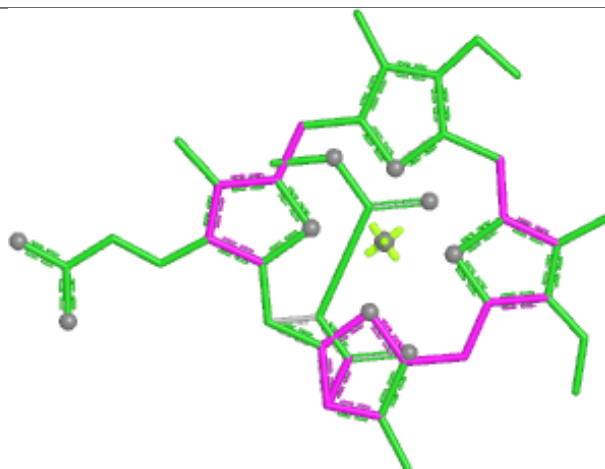




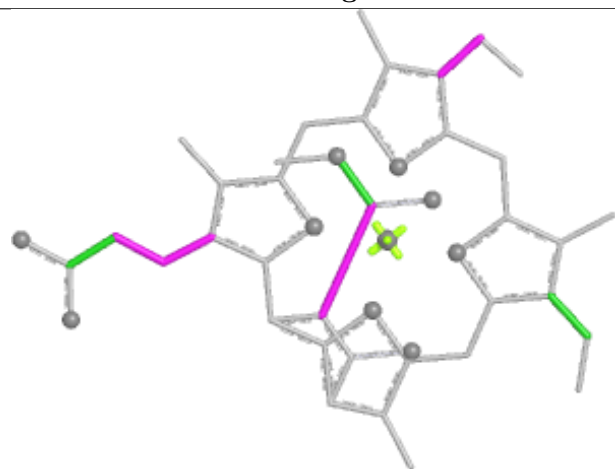
Ligand KC1 3 309



Bond lengths



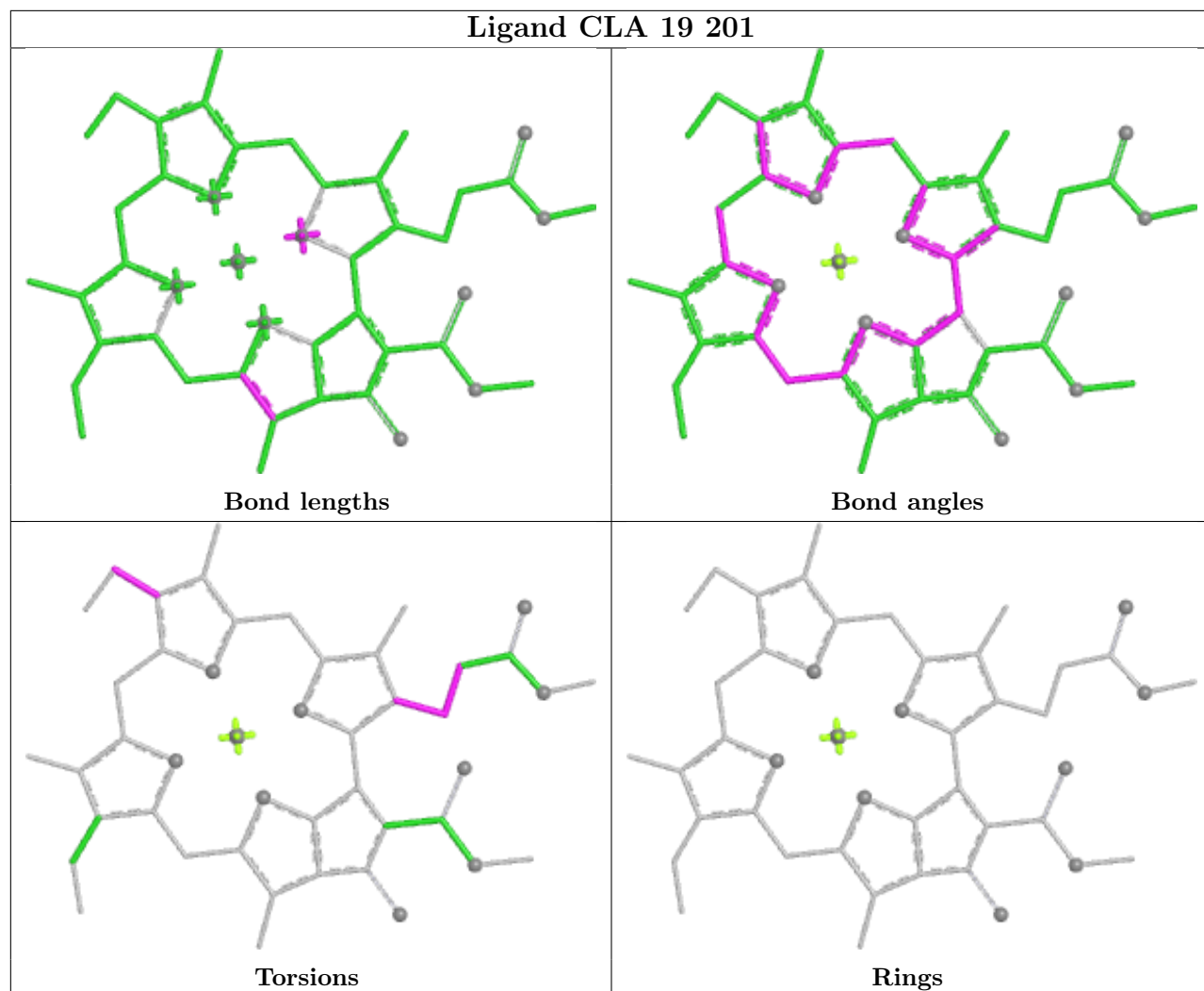
Bond angles



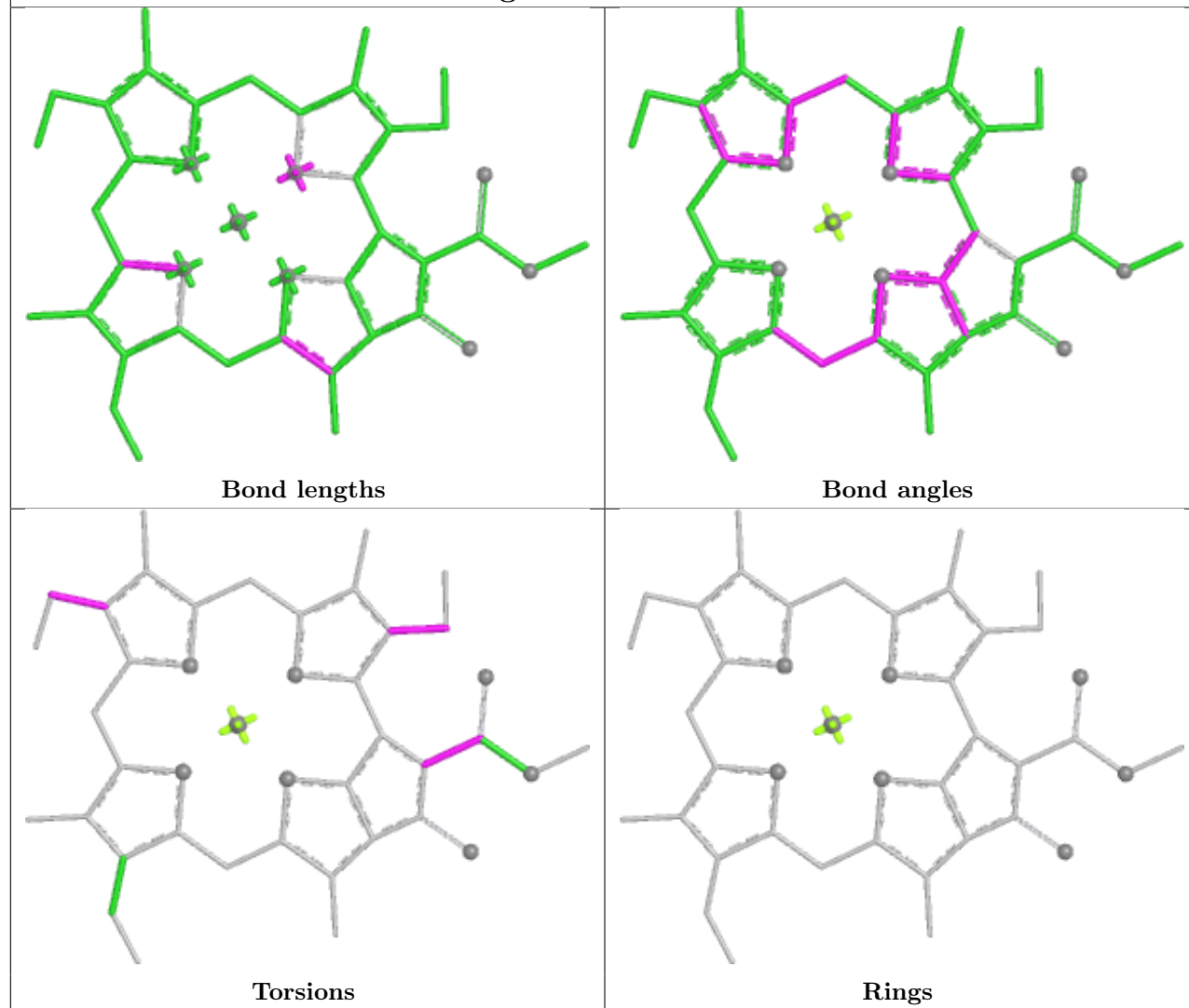
Torsions



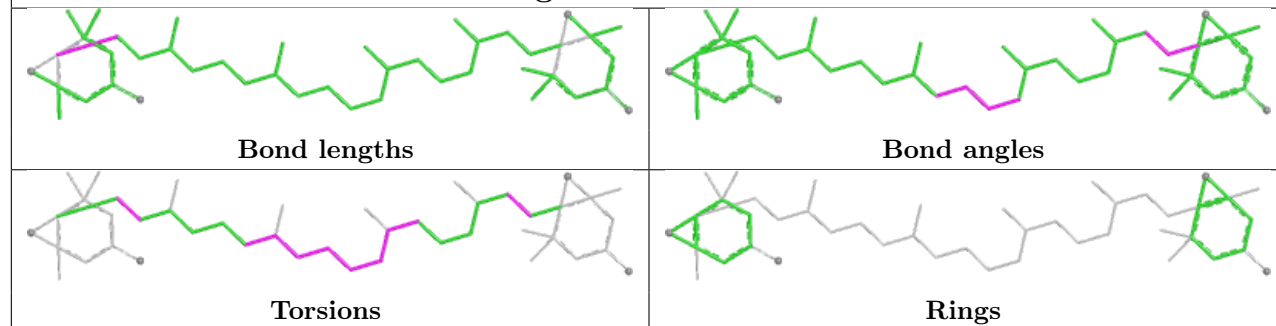
Rings

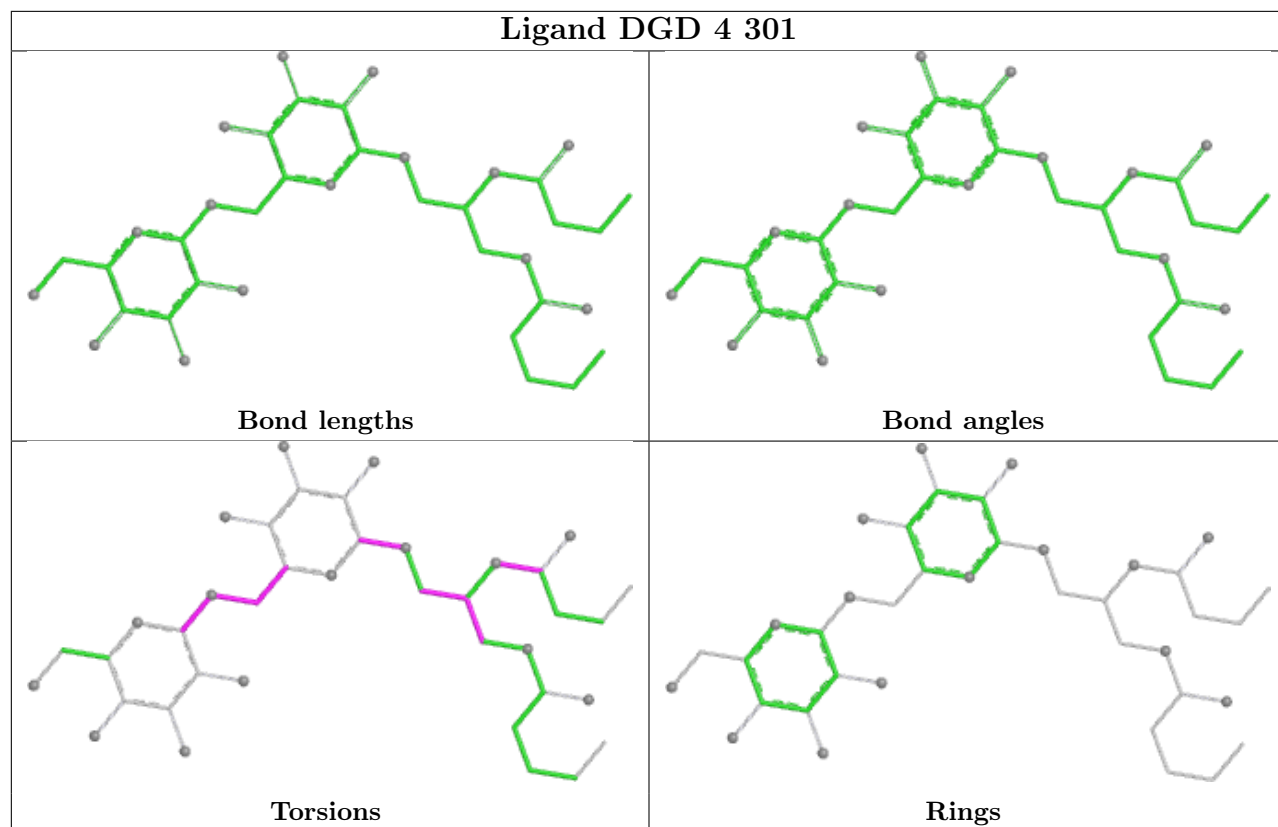


Ligand CLA 4 305

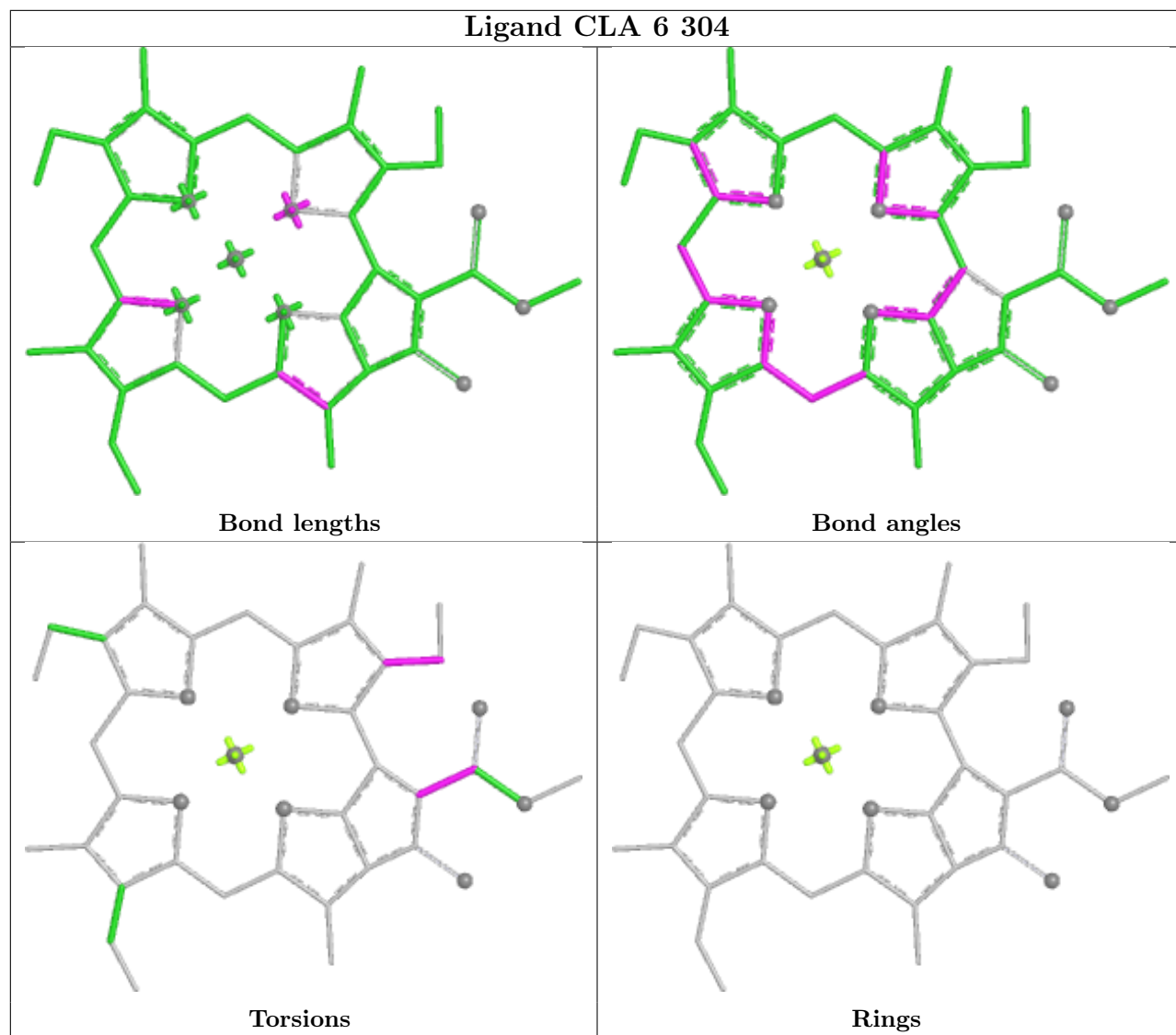


Ligand XAT 6 312

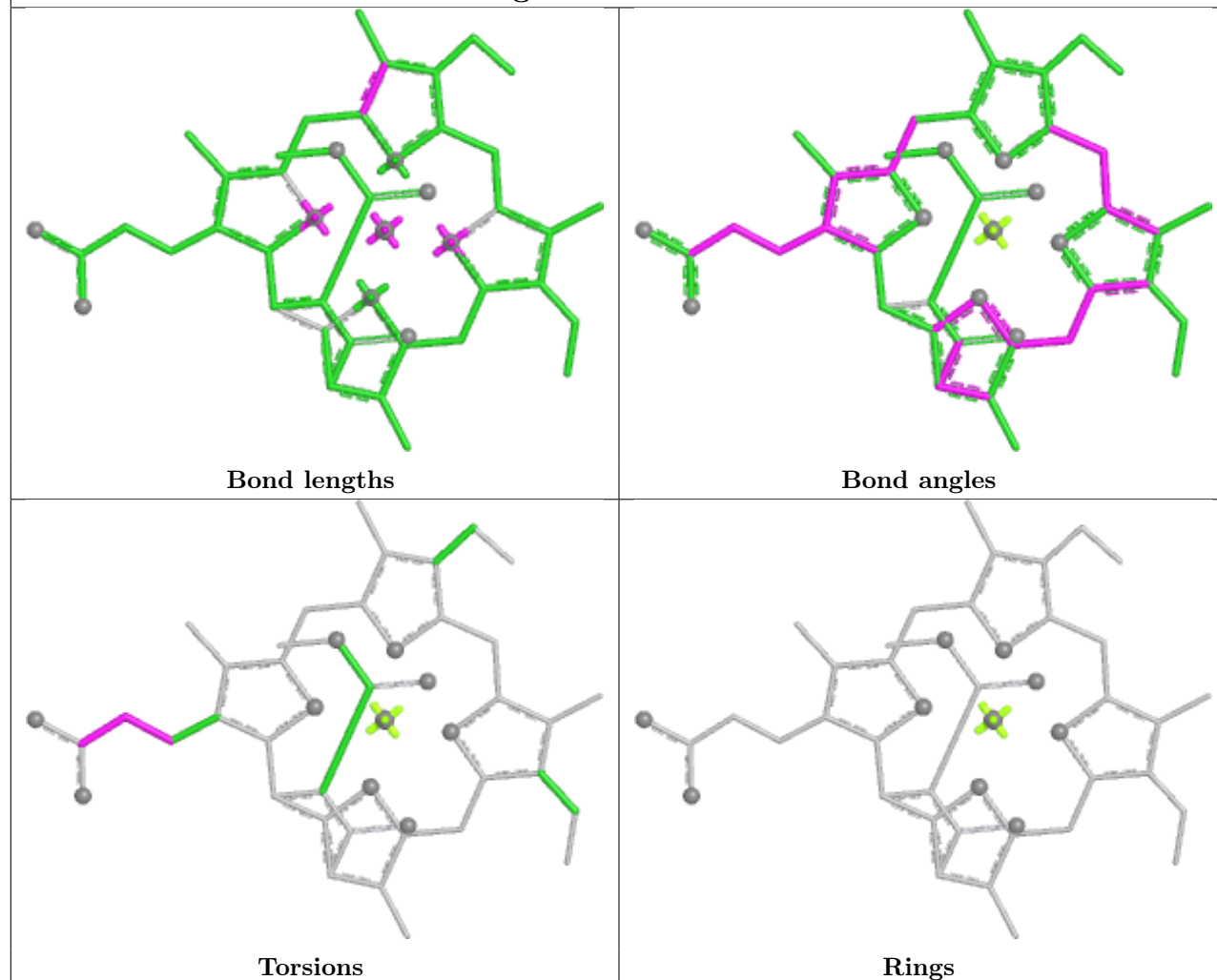




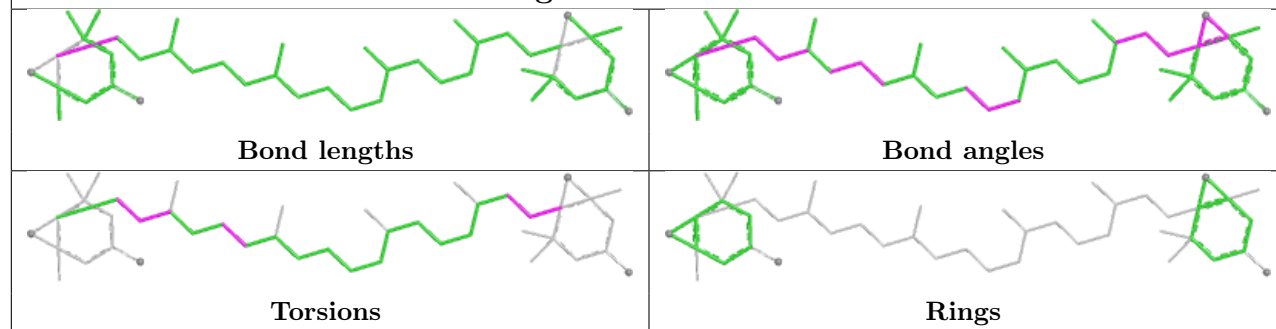
Ligand CLA 6 304

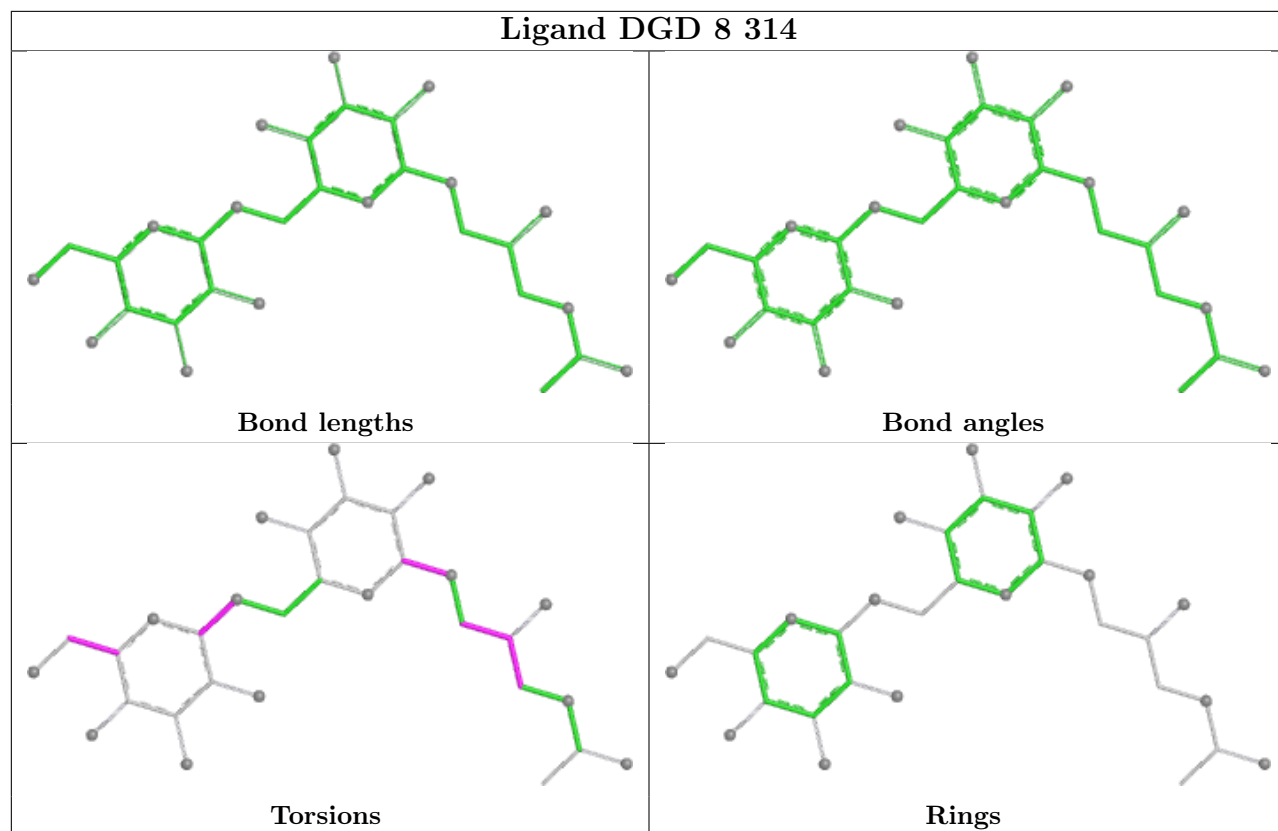


Ligand KC1 3 308

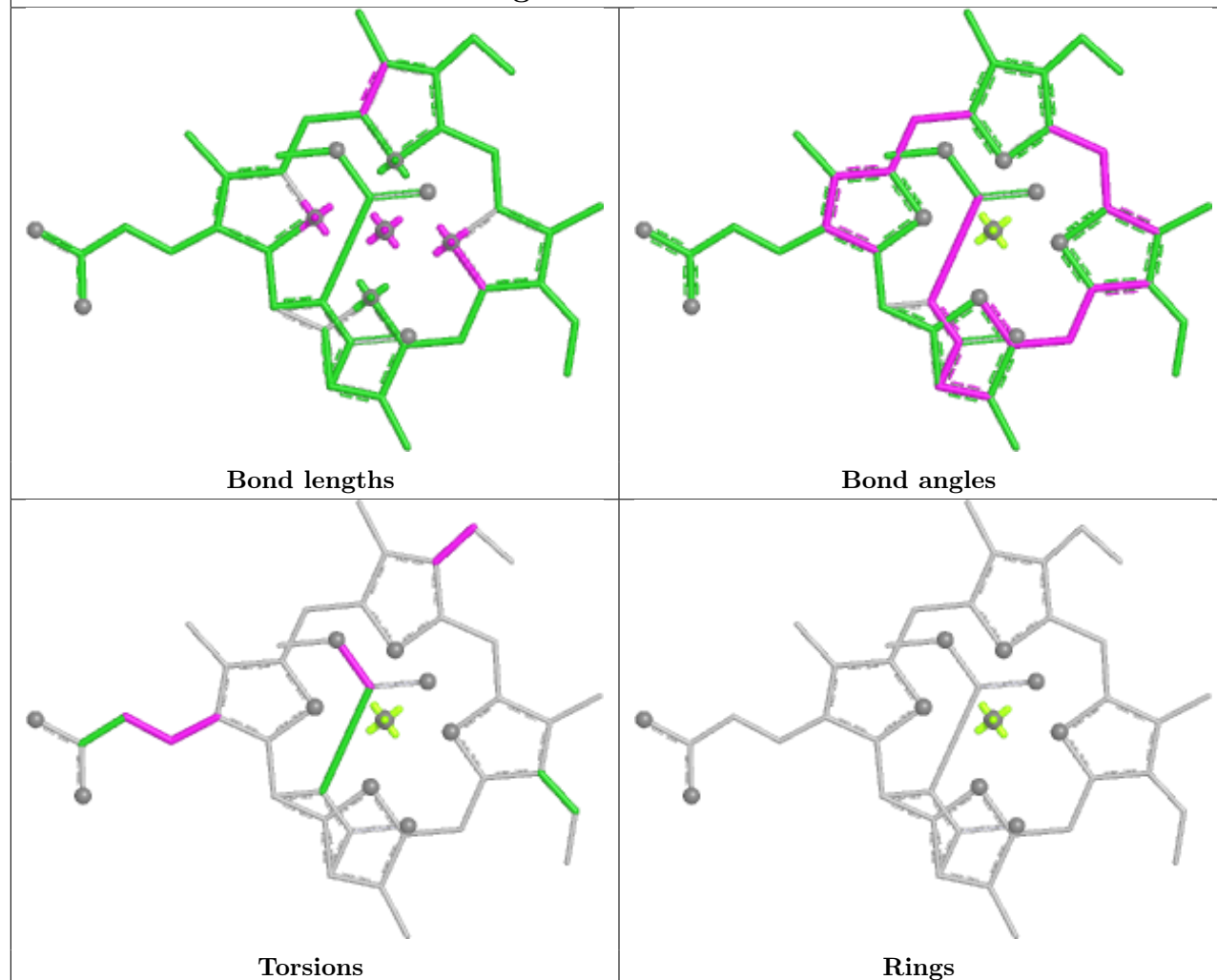


Ligand XAT 7 317

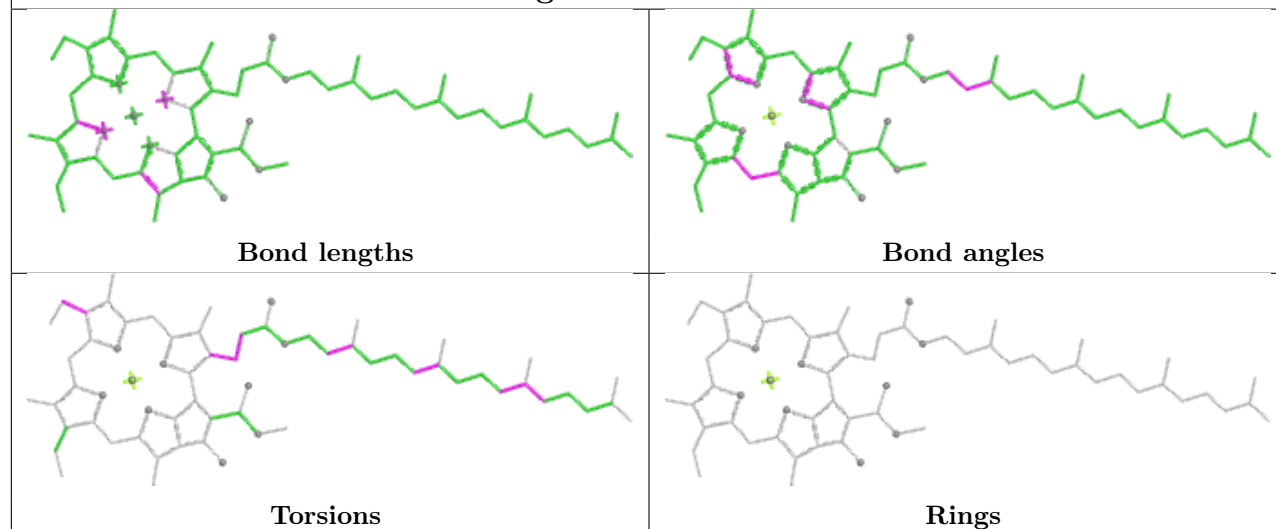


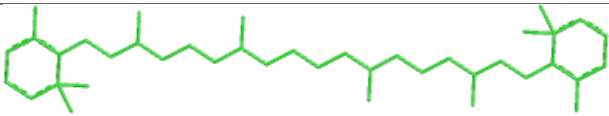
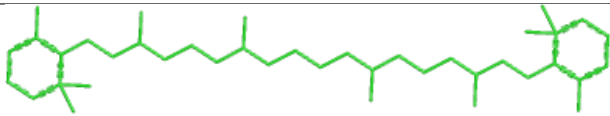
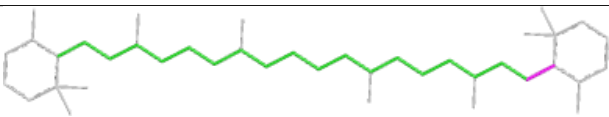
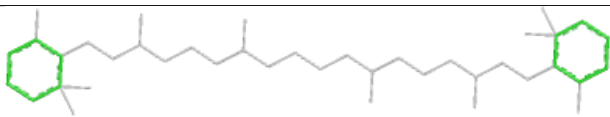




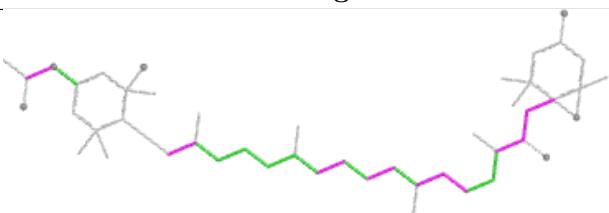
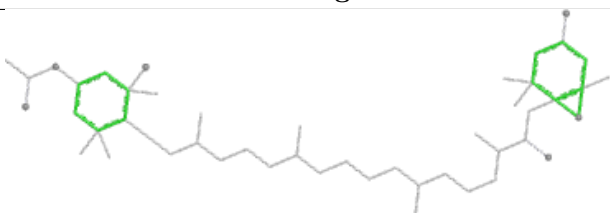
Ligand KC1 4 312

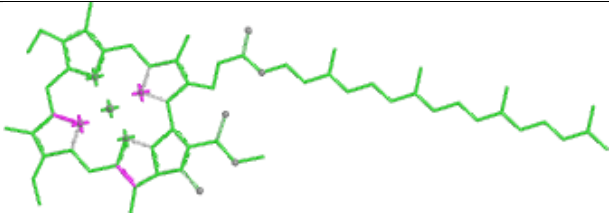
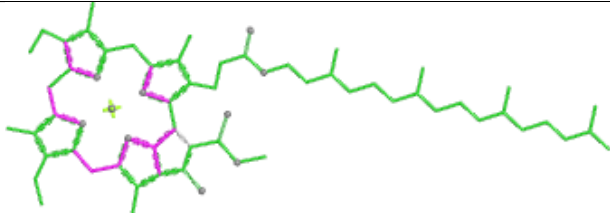
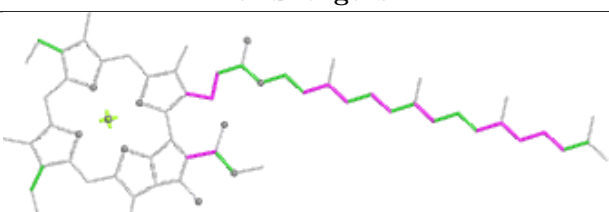
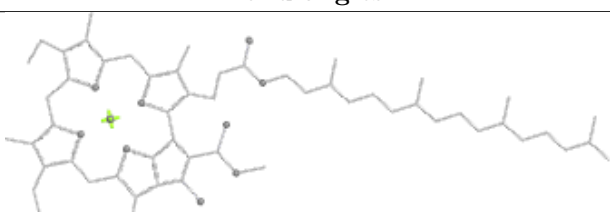


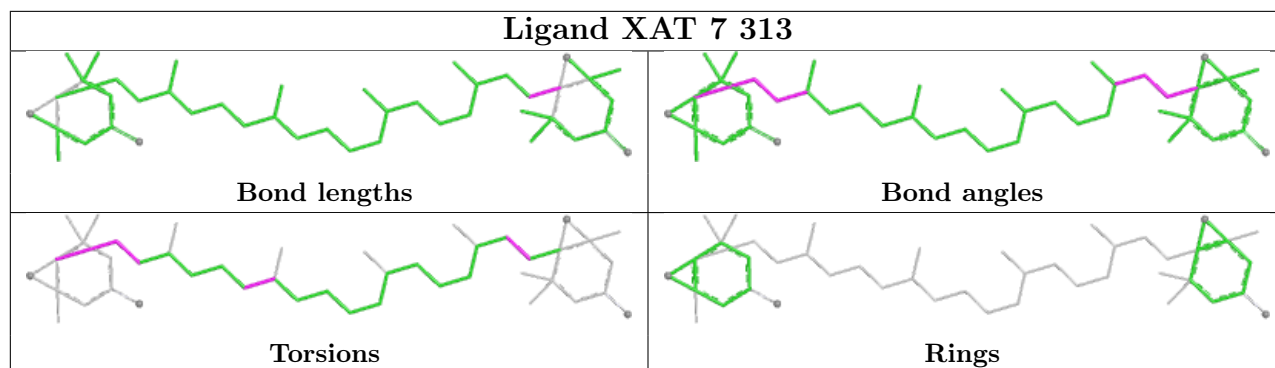
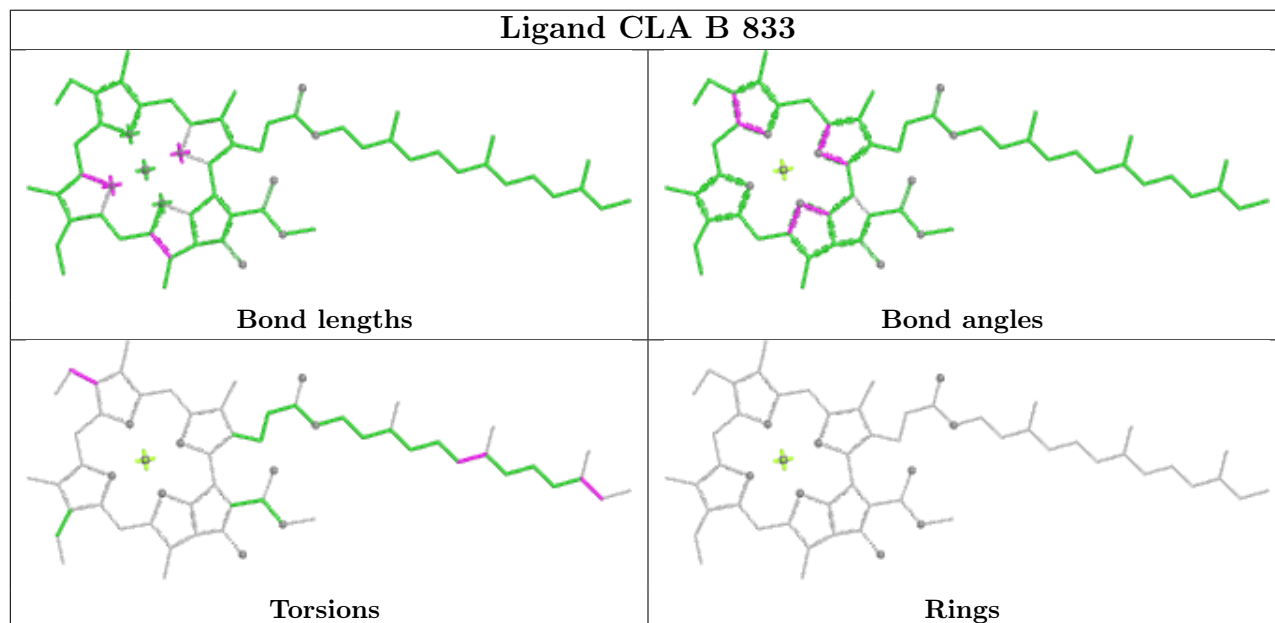
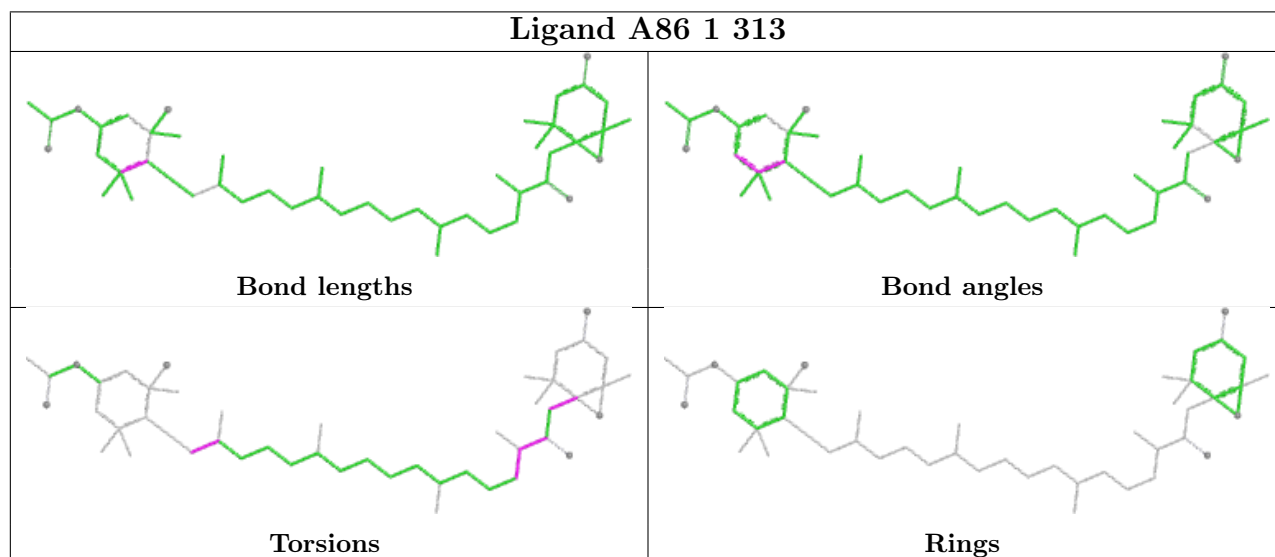
Ligand CLA 3 301

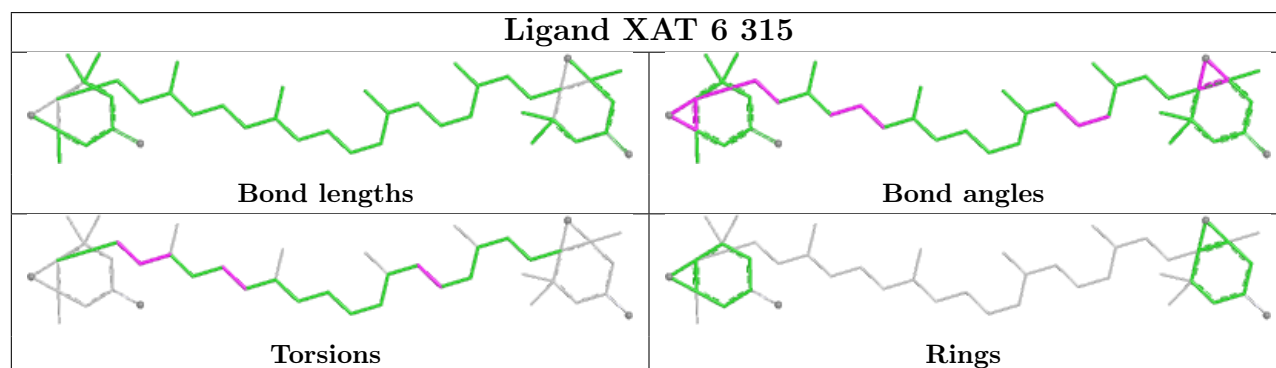
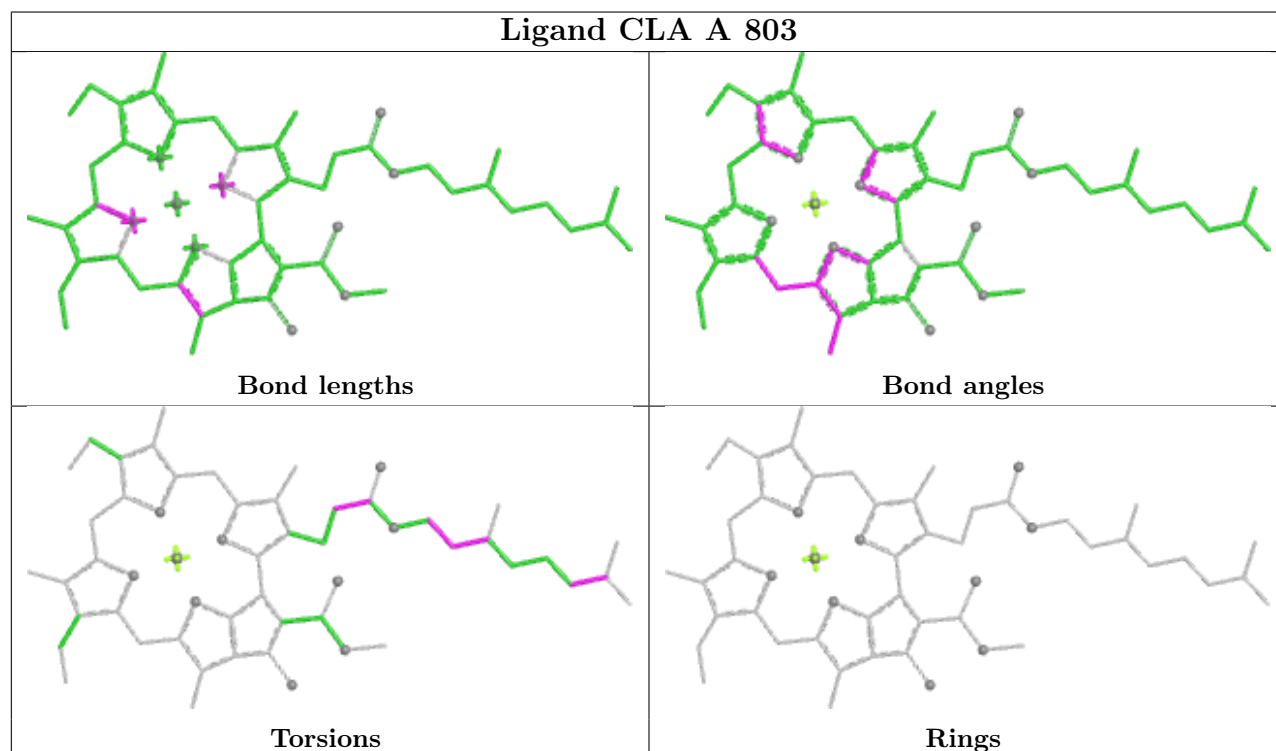
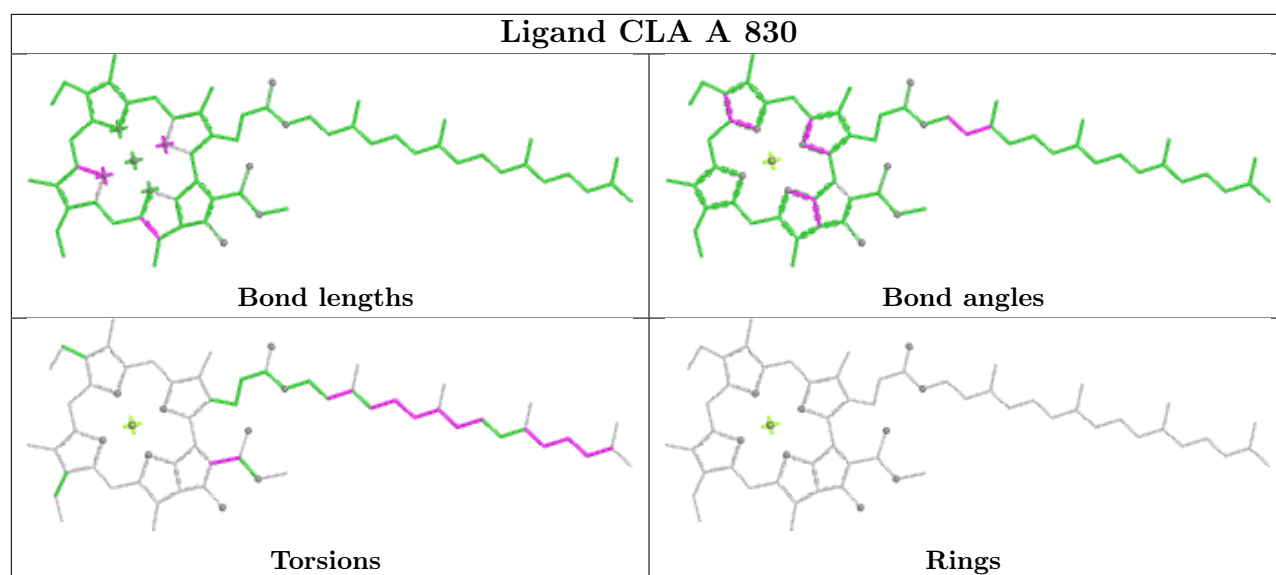


Ligand BCR L 205	
	
Bond lengths	Bond angles
	
Torsions	Rings

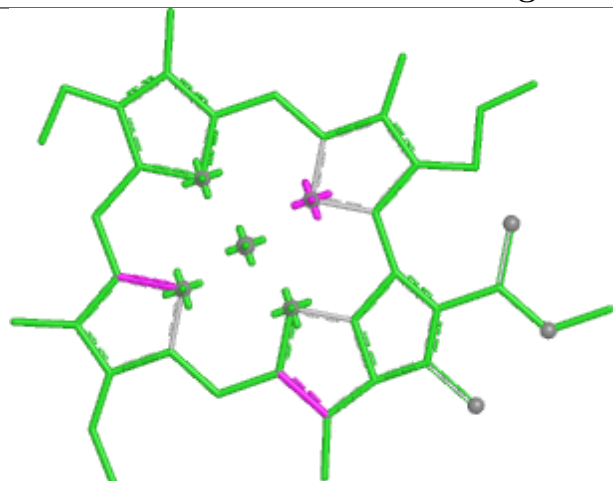
Ligand A86 J 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 6 313	
	
Bond lengths	Bond angles
	
Torsions	Rings

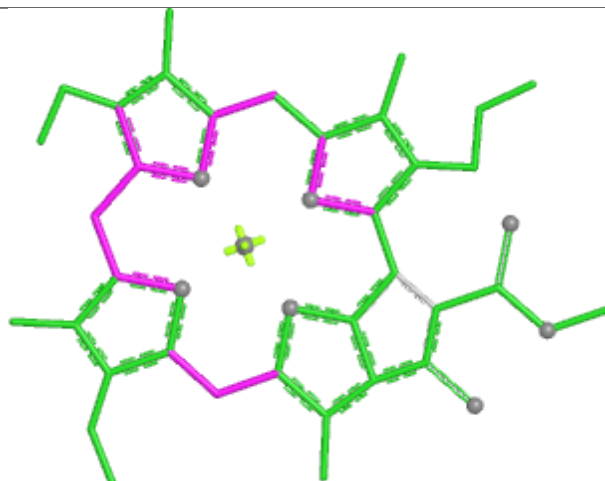
Ligand XAT 7 313**Ligand CLA B 833****Ligand A86 1 313**



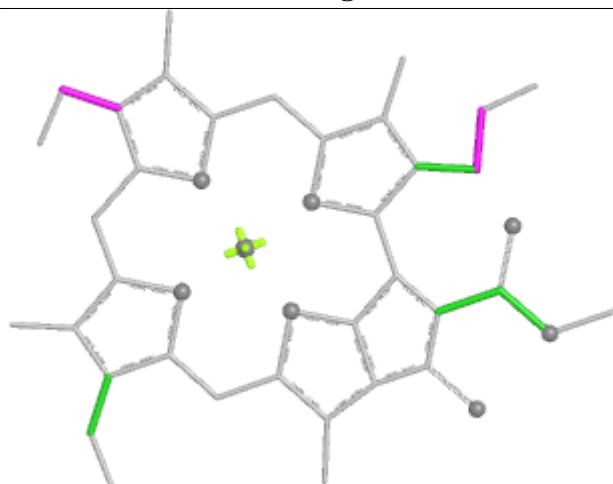
Ligand CLA a 201



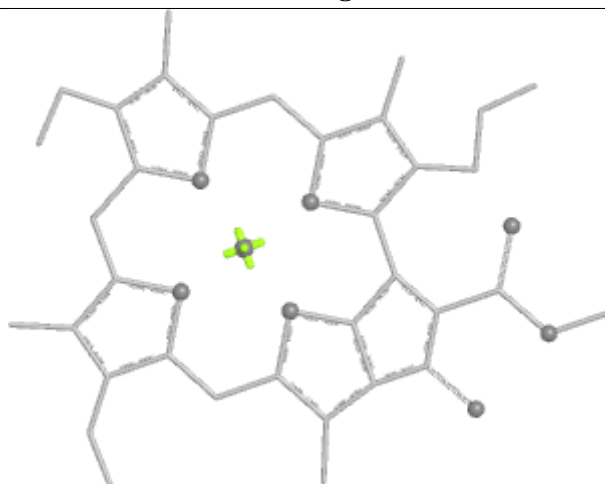
Bond lengths



Bond angles

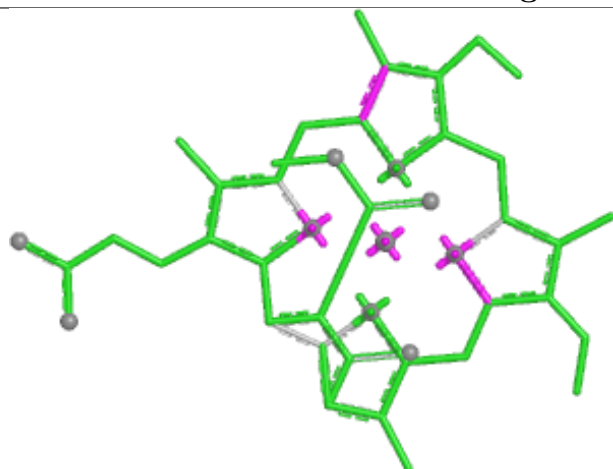


Torsions

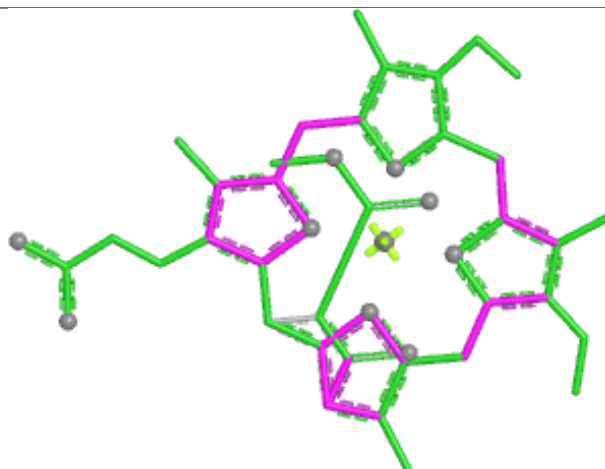


Rings

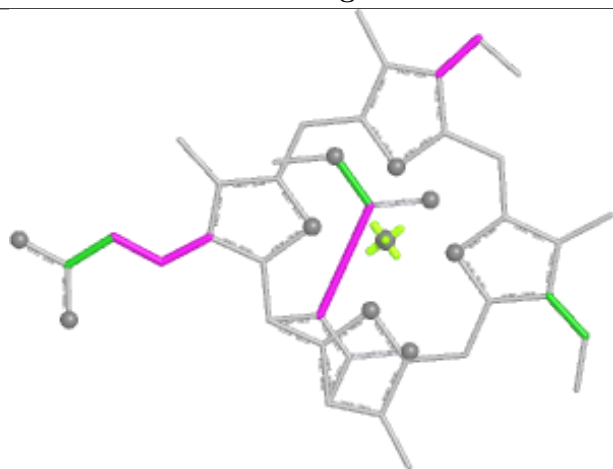
Ligand KC1 6 305



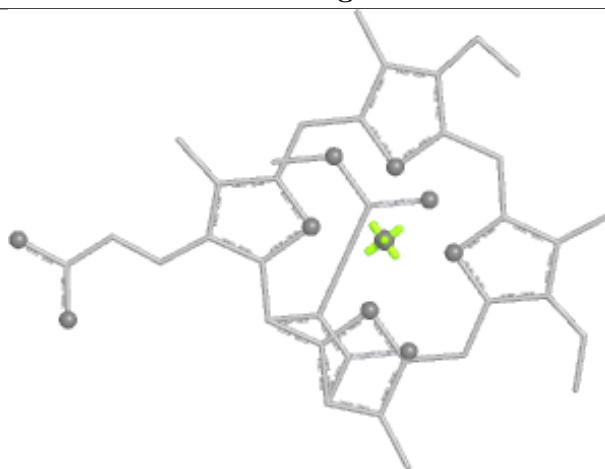
Bond lengths



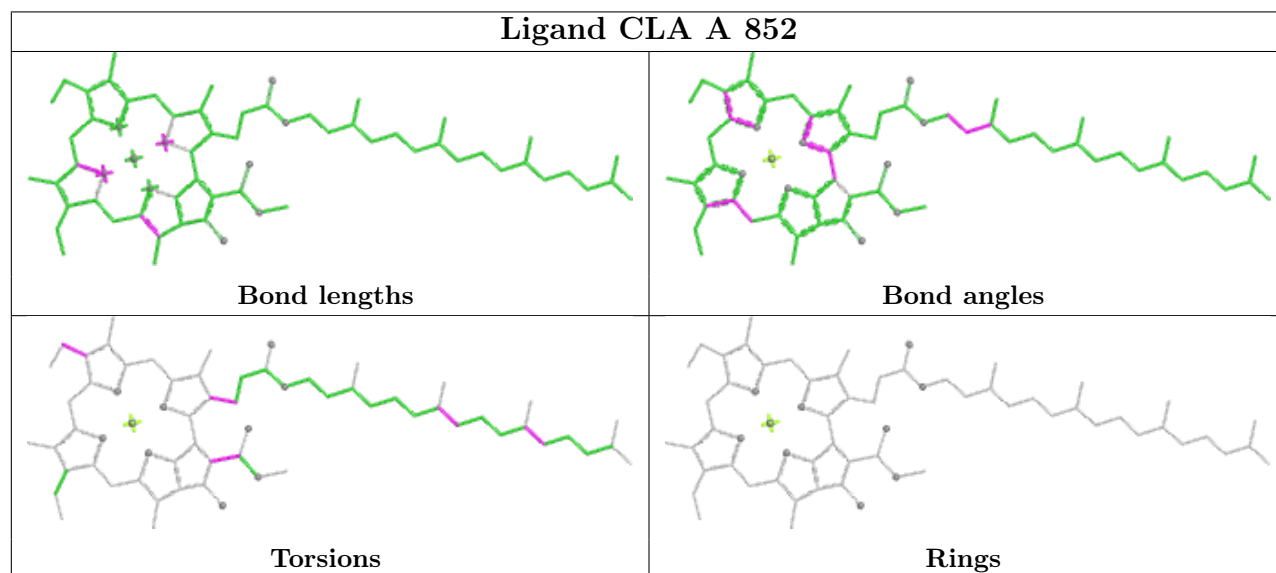
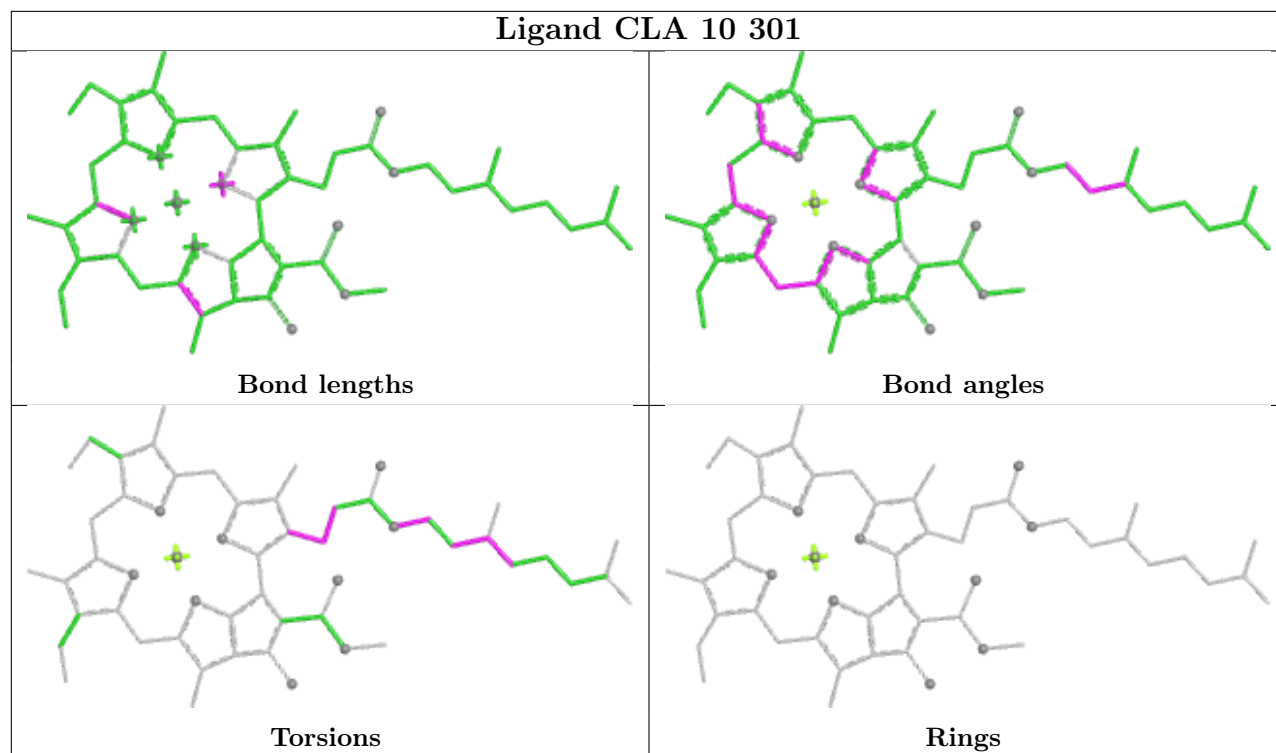
Bond angles

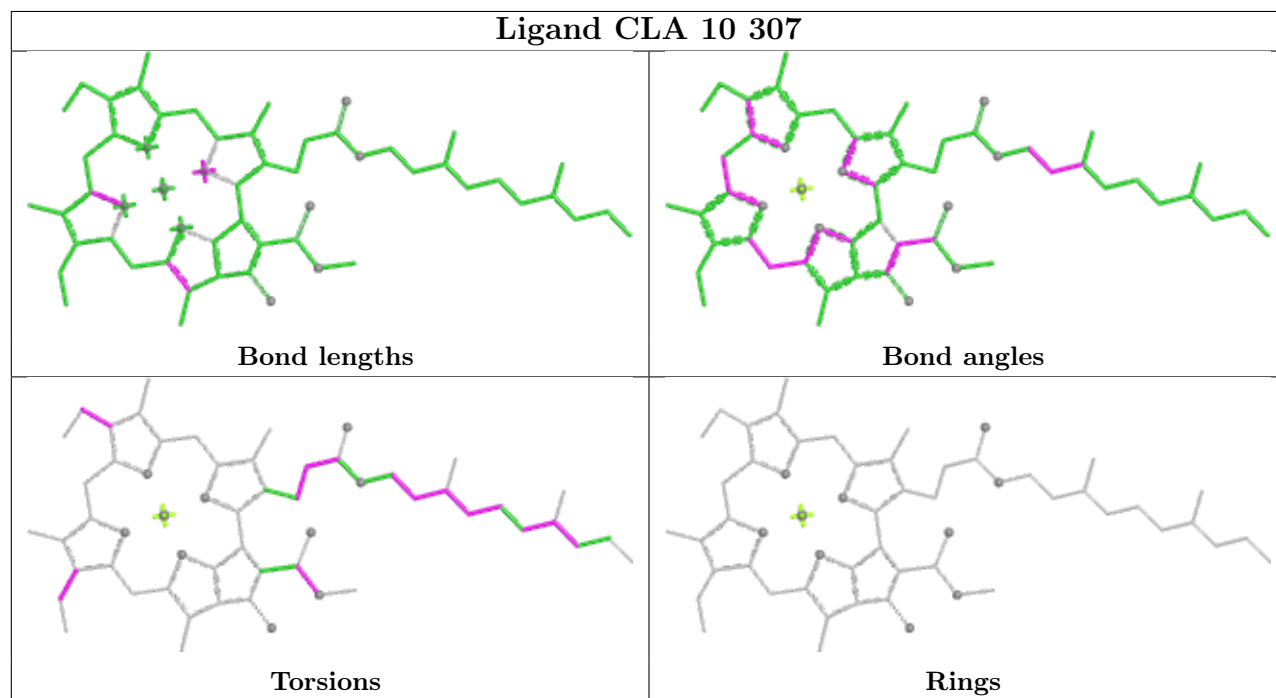
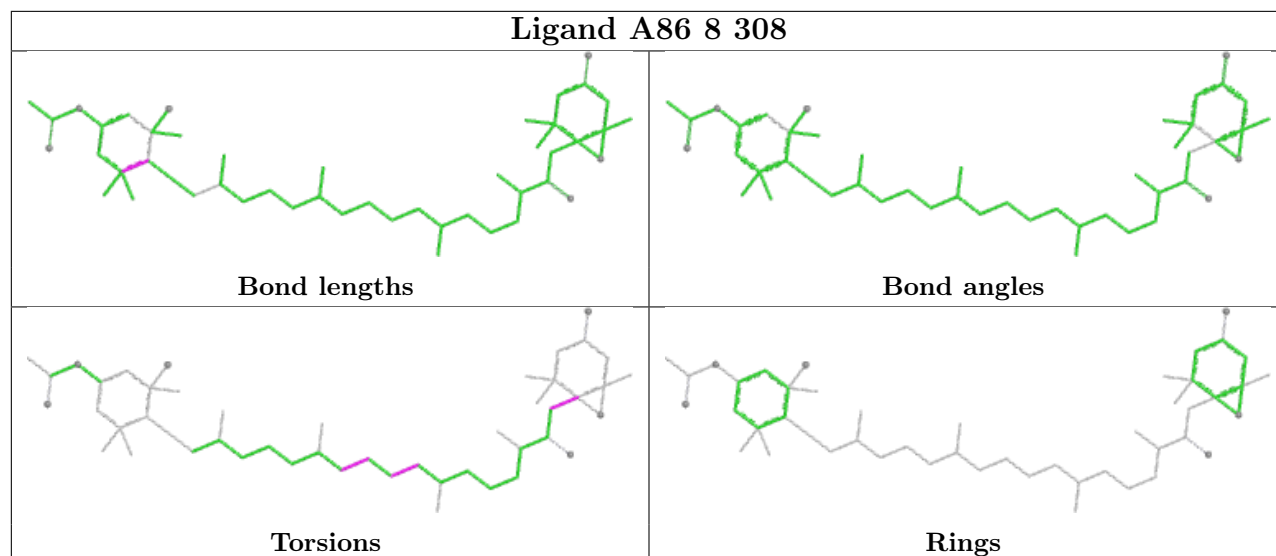


Torsions

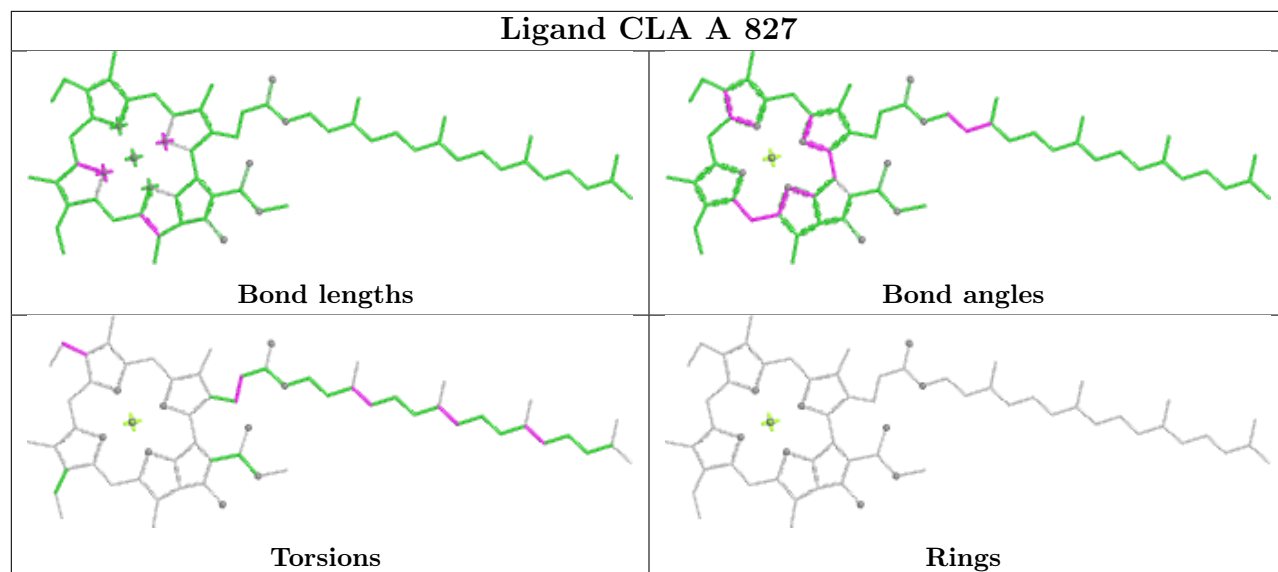


Rings

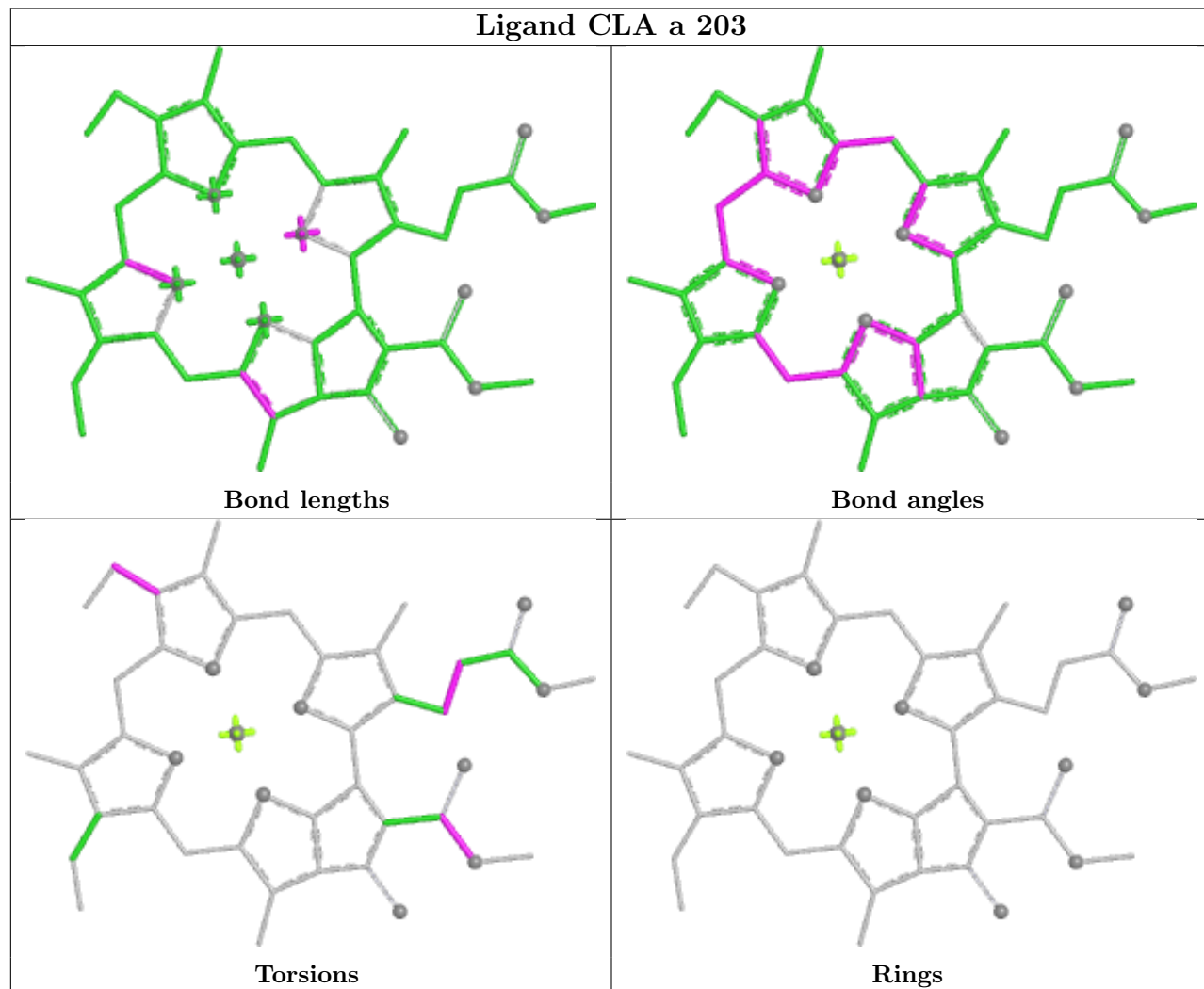




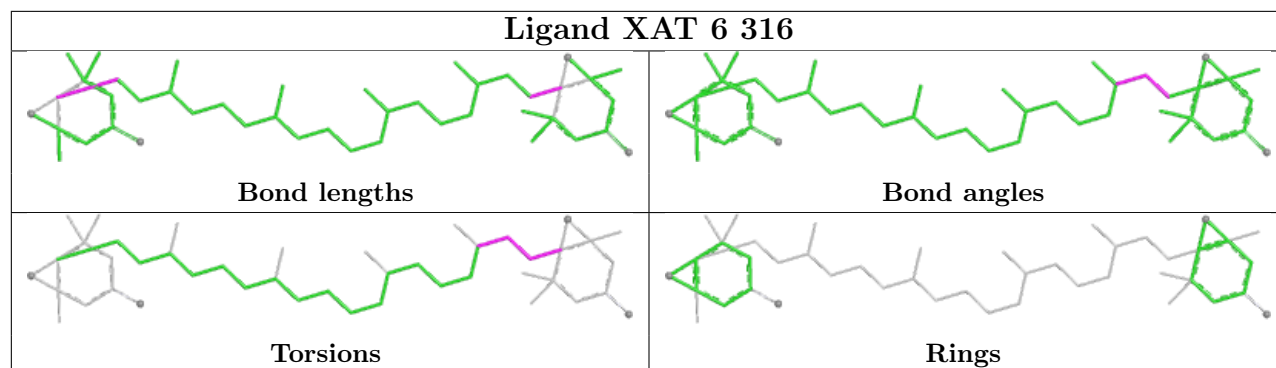
Ligand CLA A 827



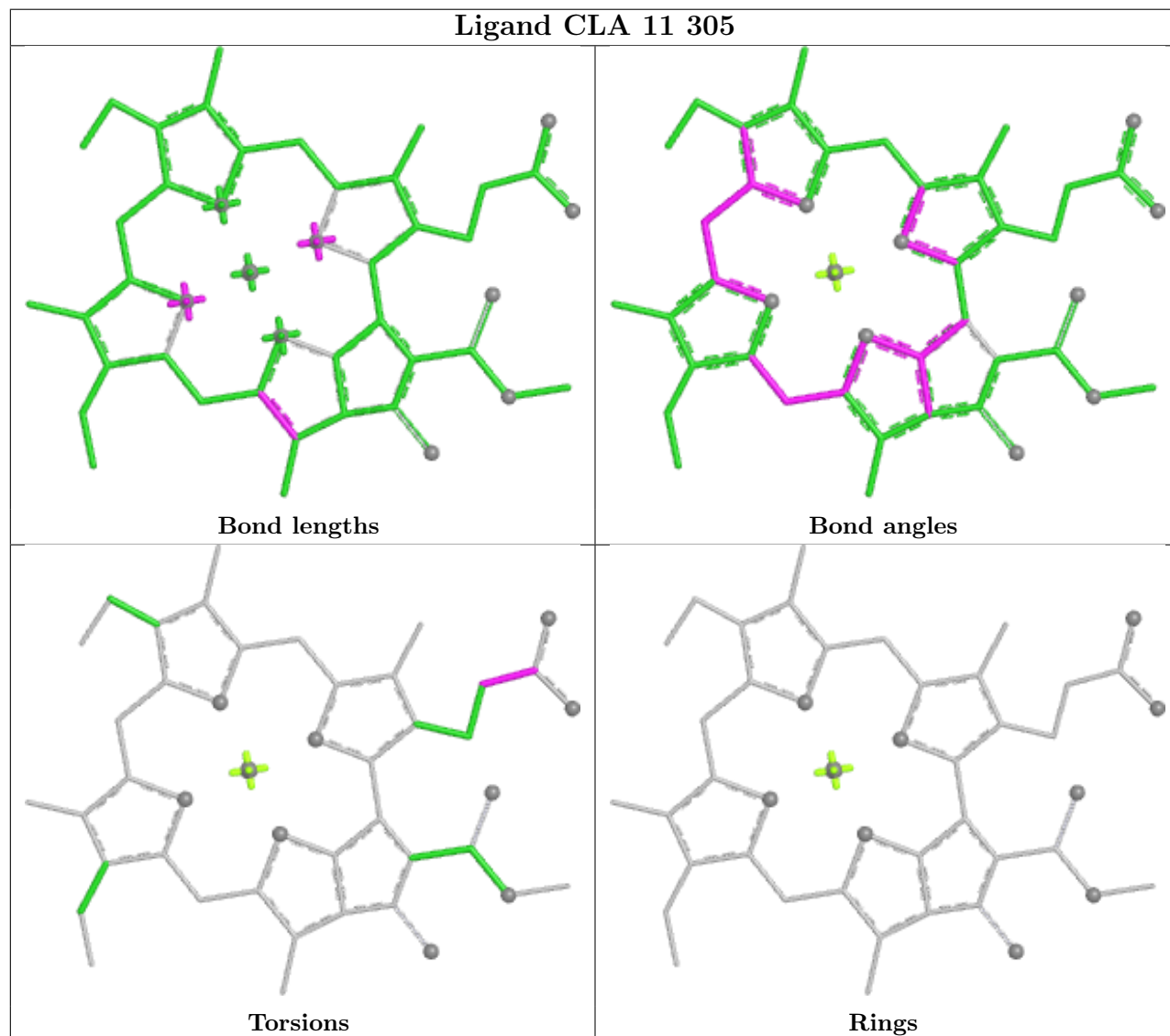
Ligand CLA a 203



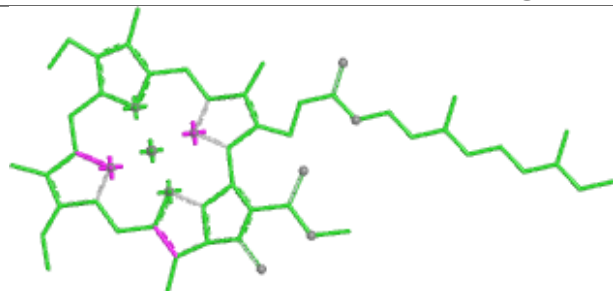
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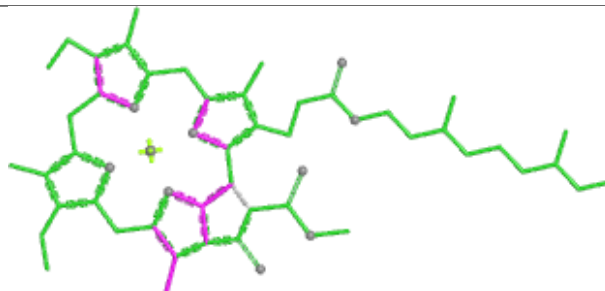
Ligand CLA 11 305



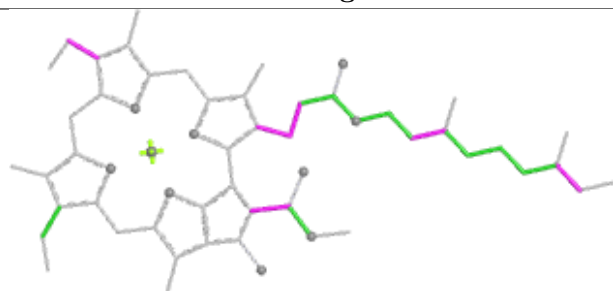
Ligand CLA 5 305



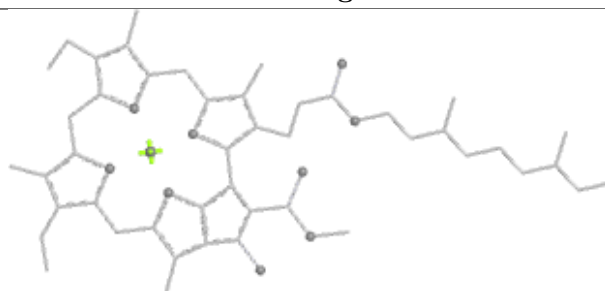
Bond lengths



Bond angles

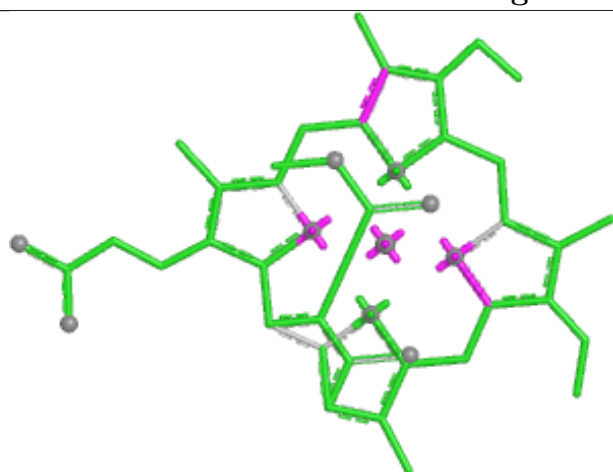


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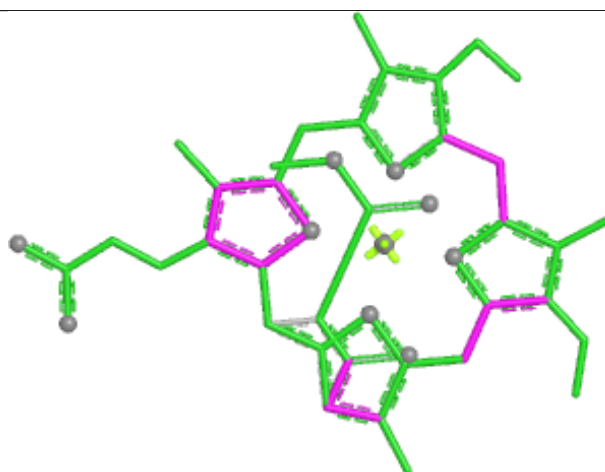


Rings

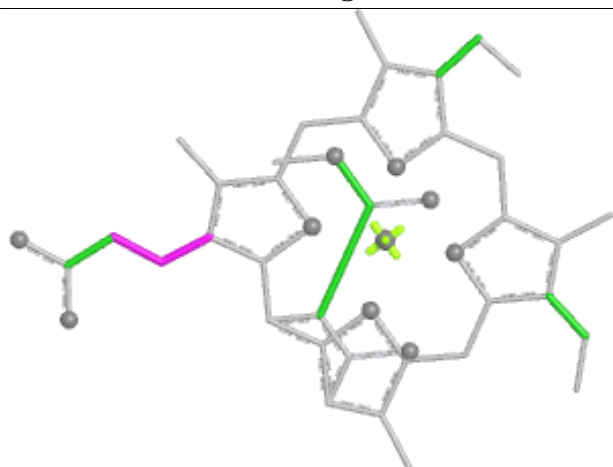
Ligand KC1 17 312



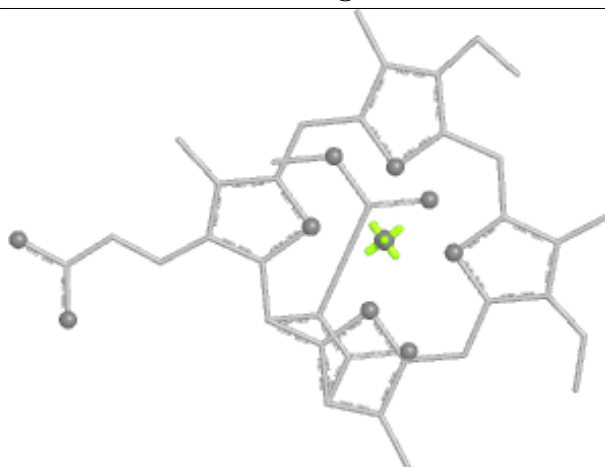
Bond lengths



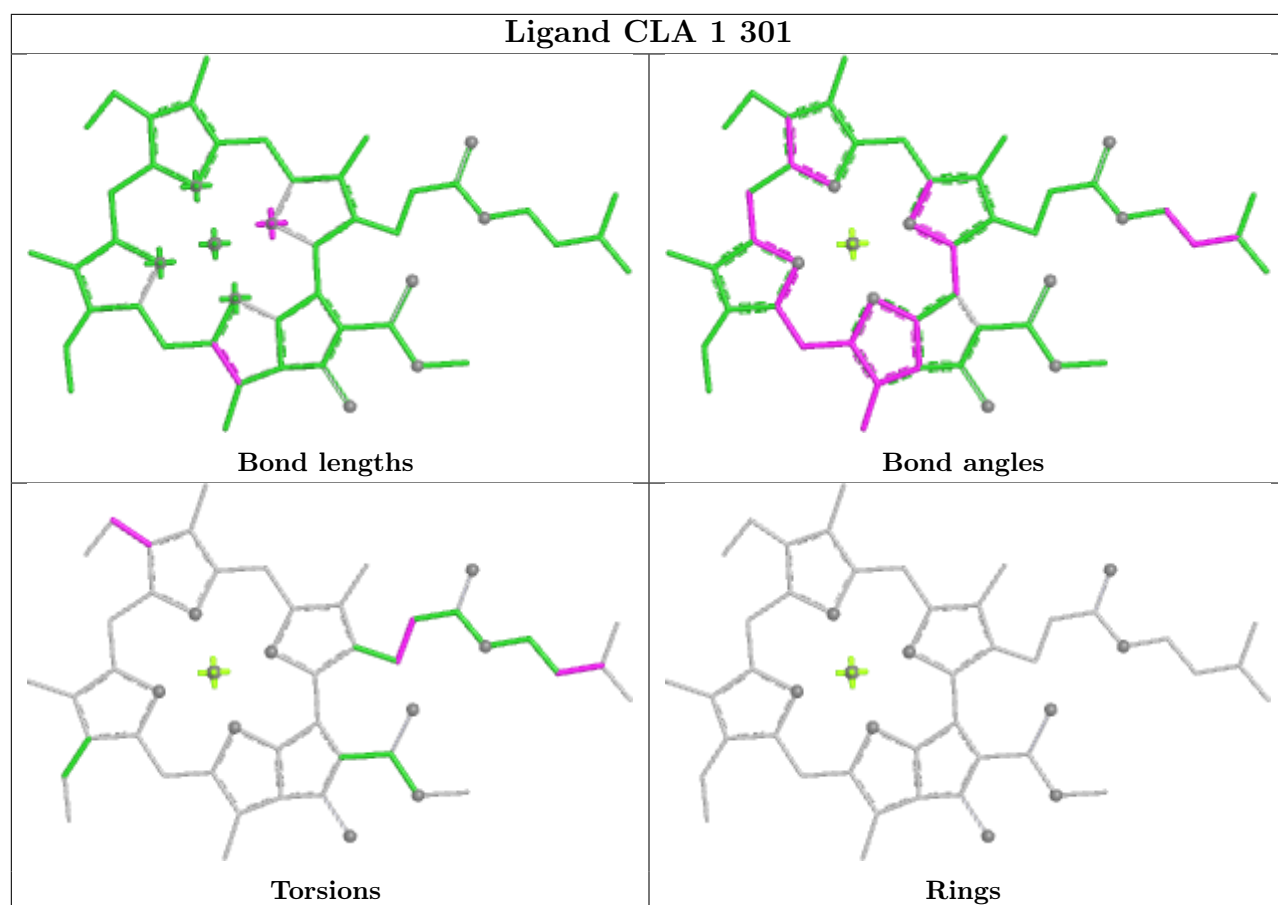
Bond angles

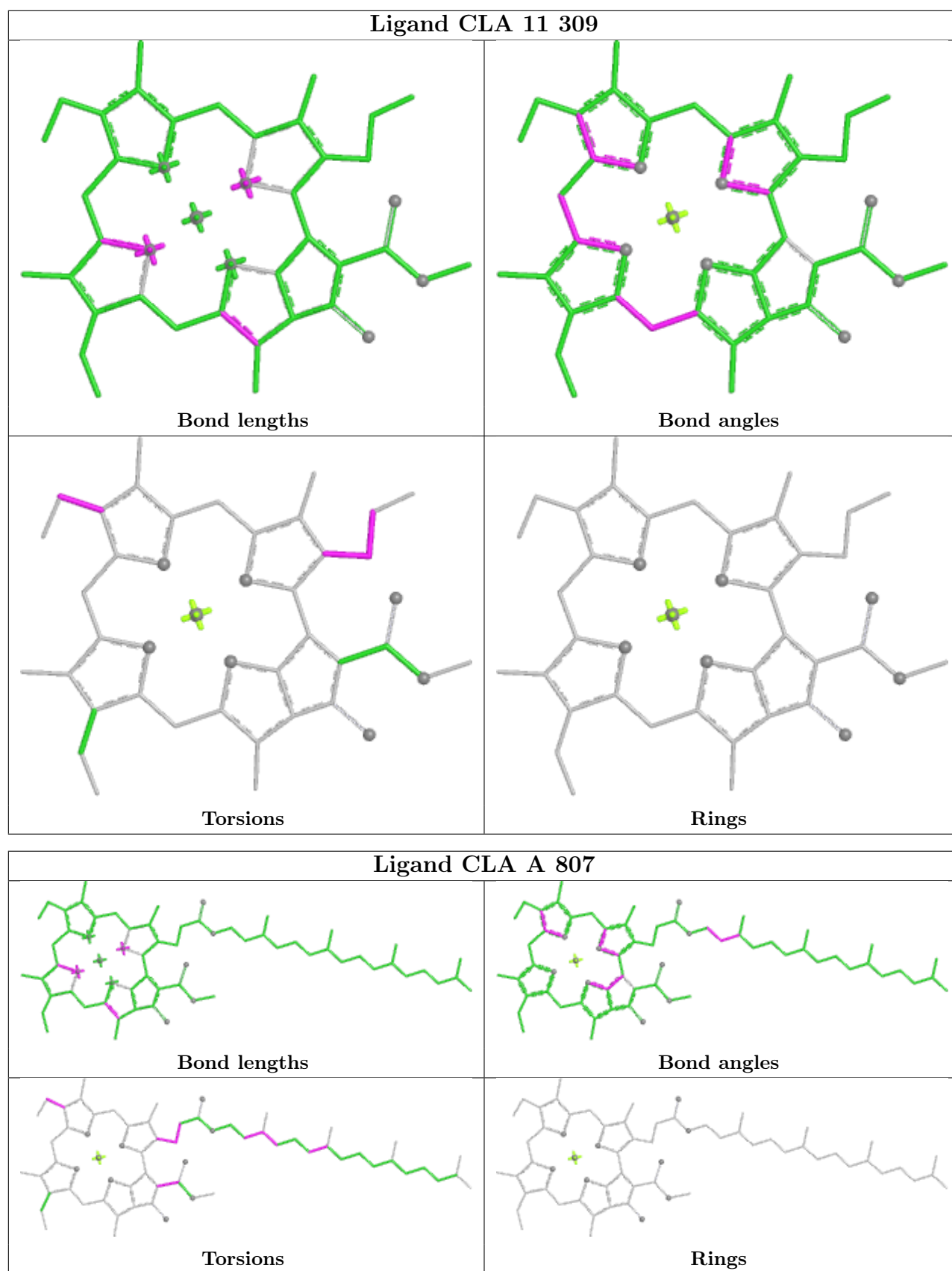


Torsions

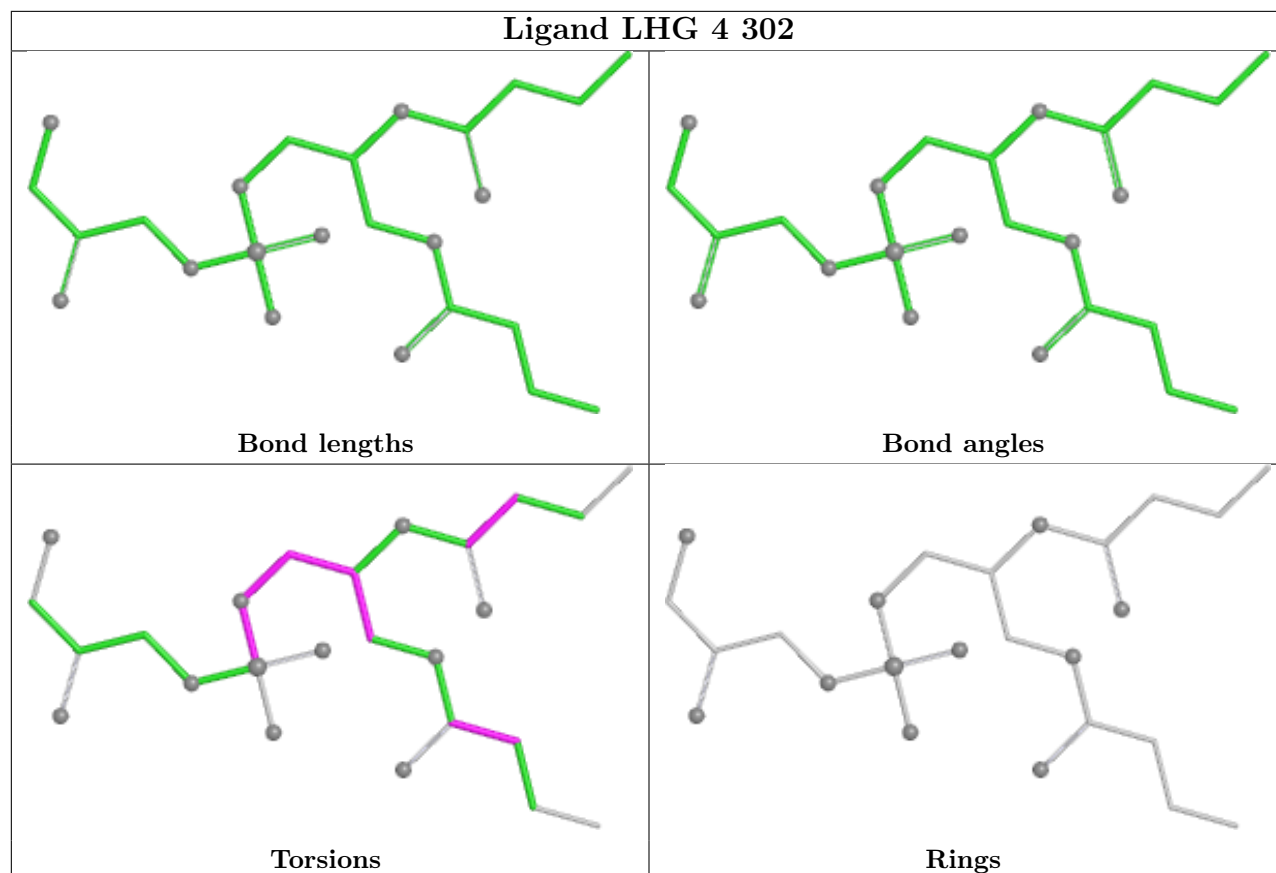


Rings

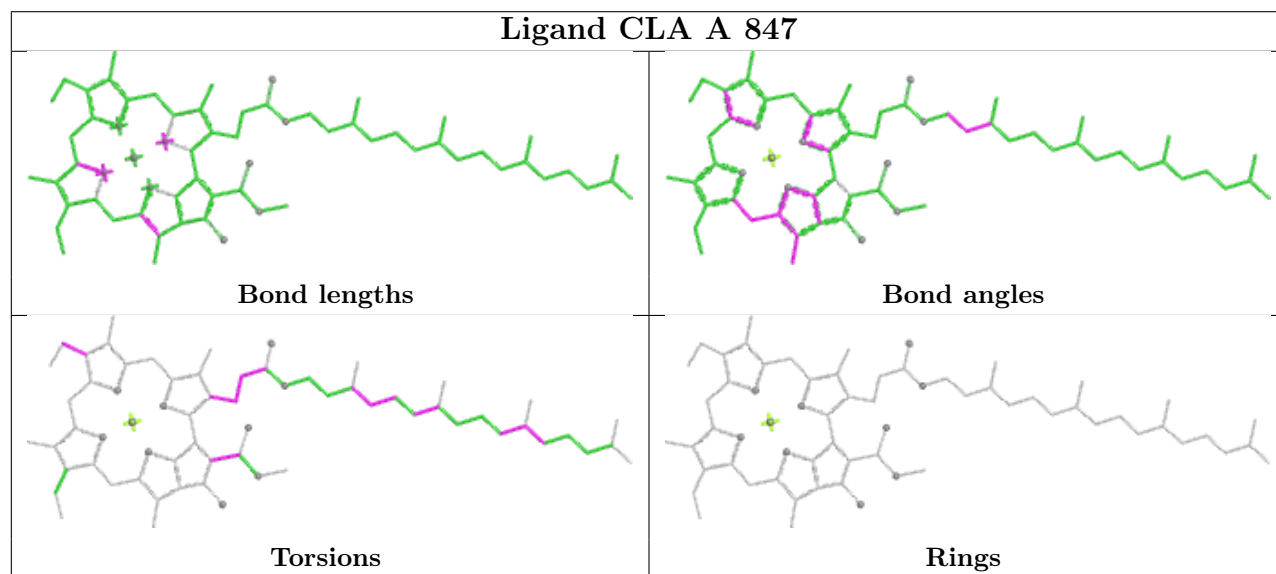


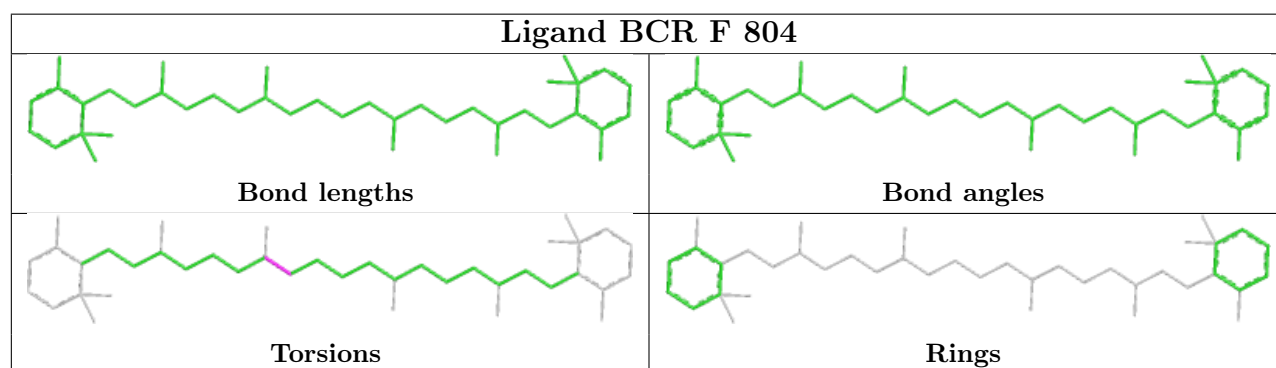
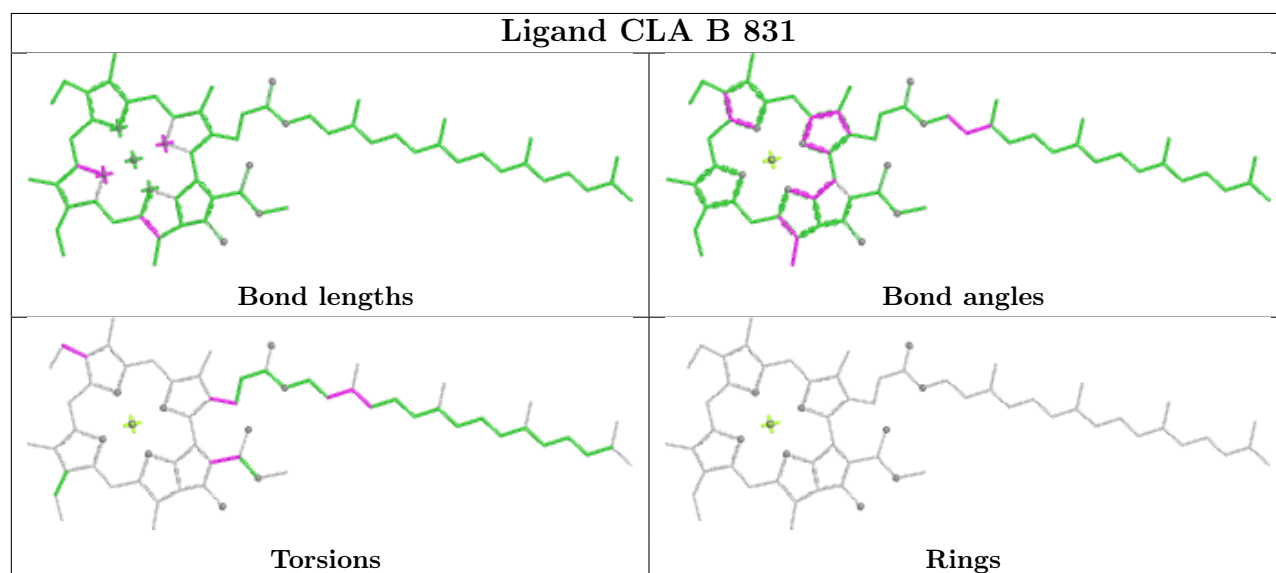
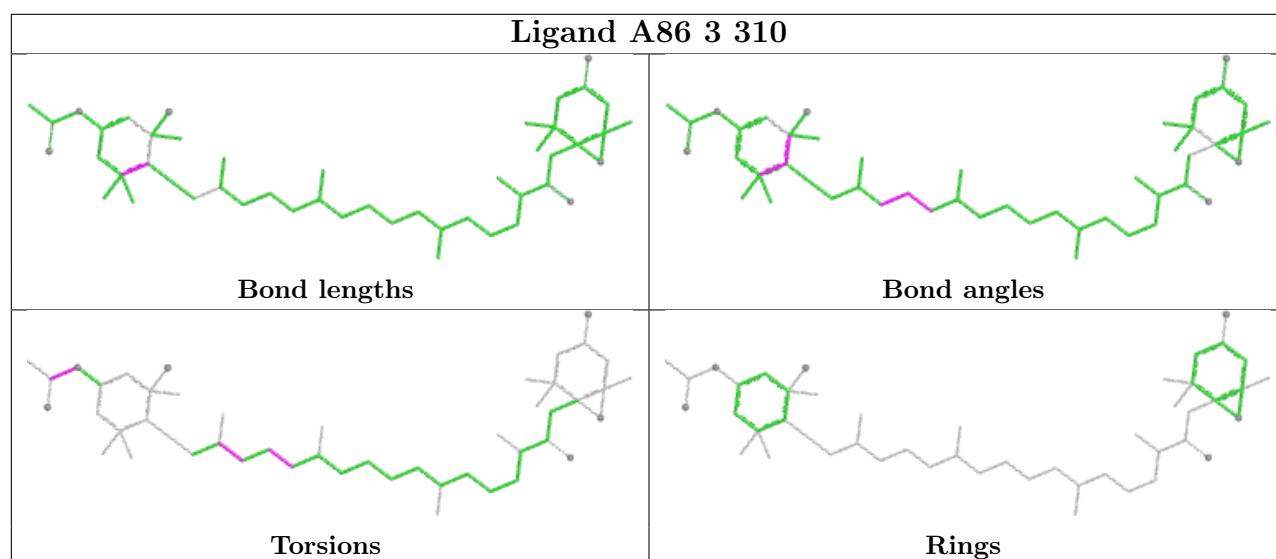


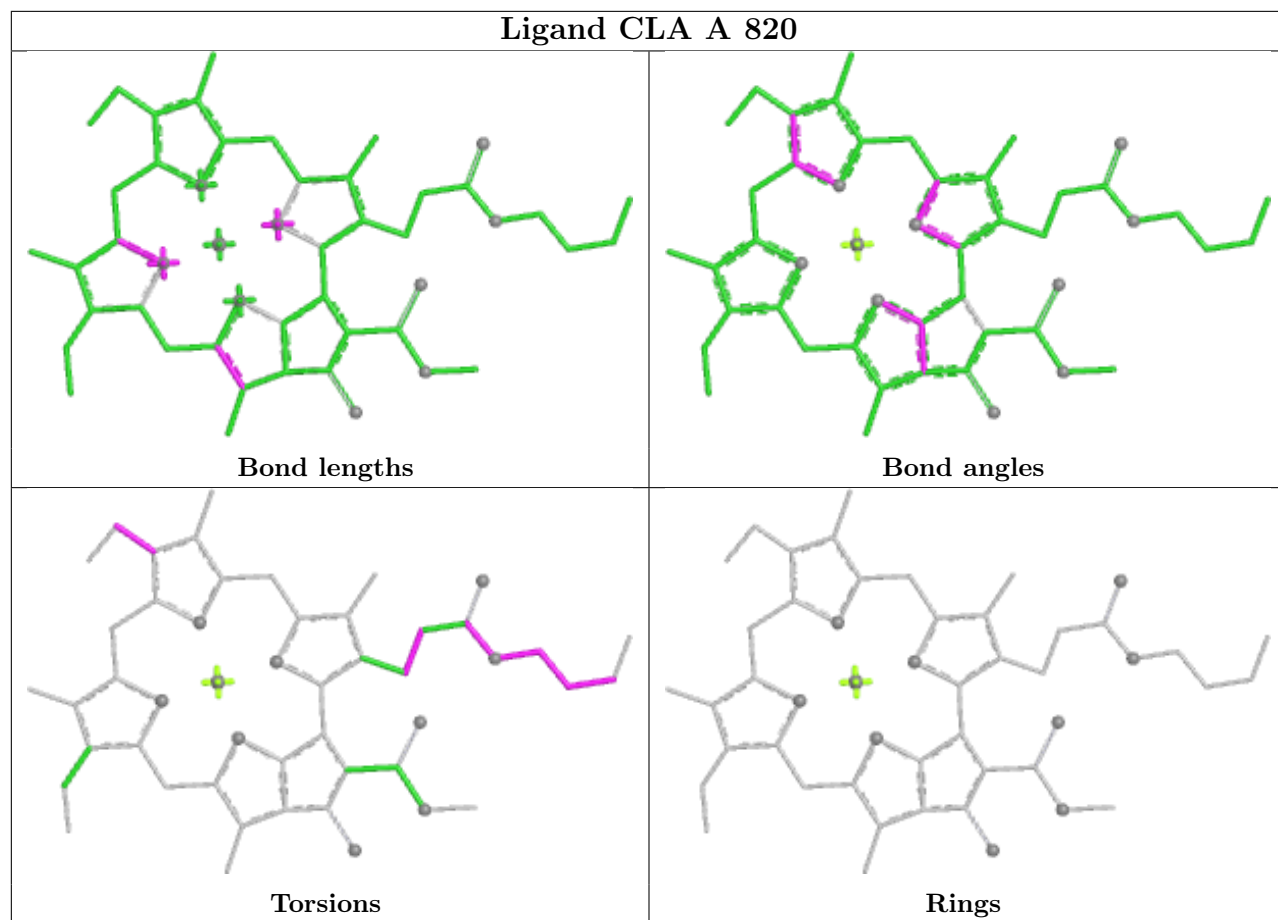
Ligand LHG 4 302

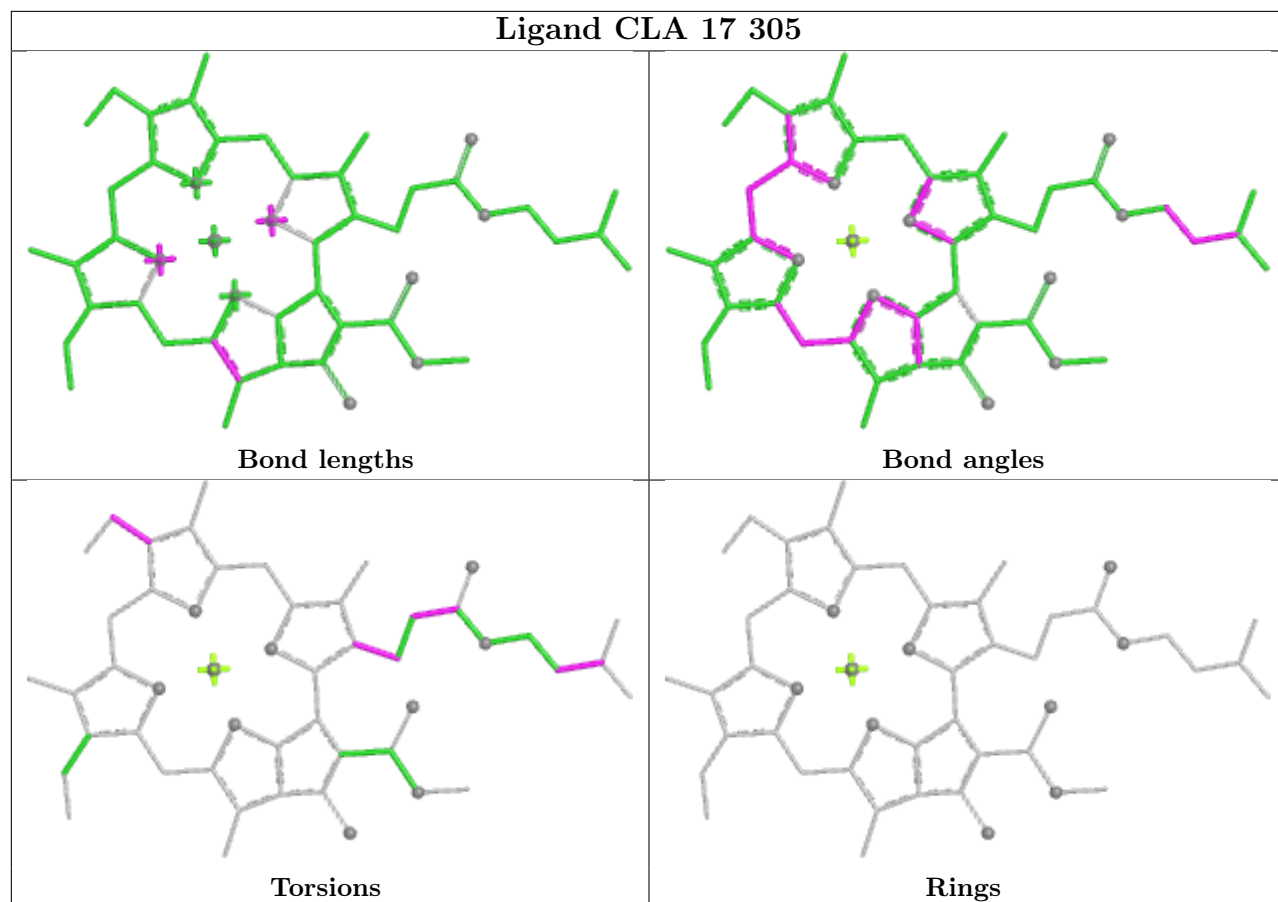


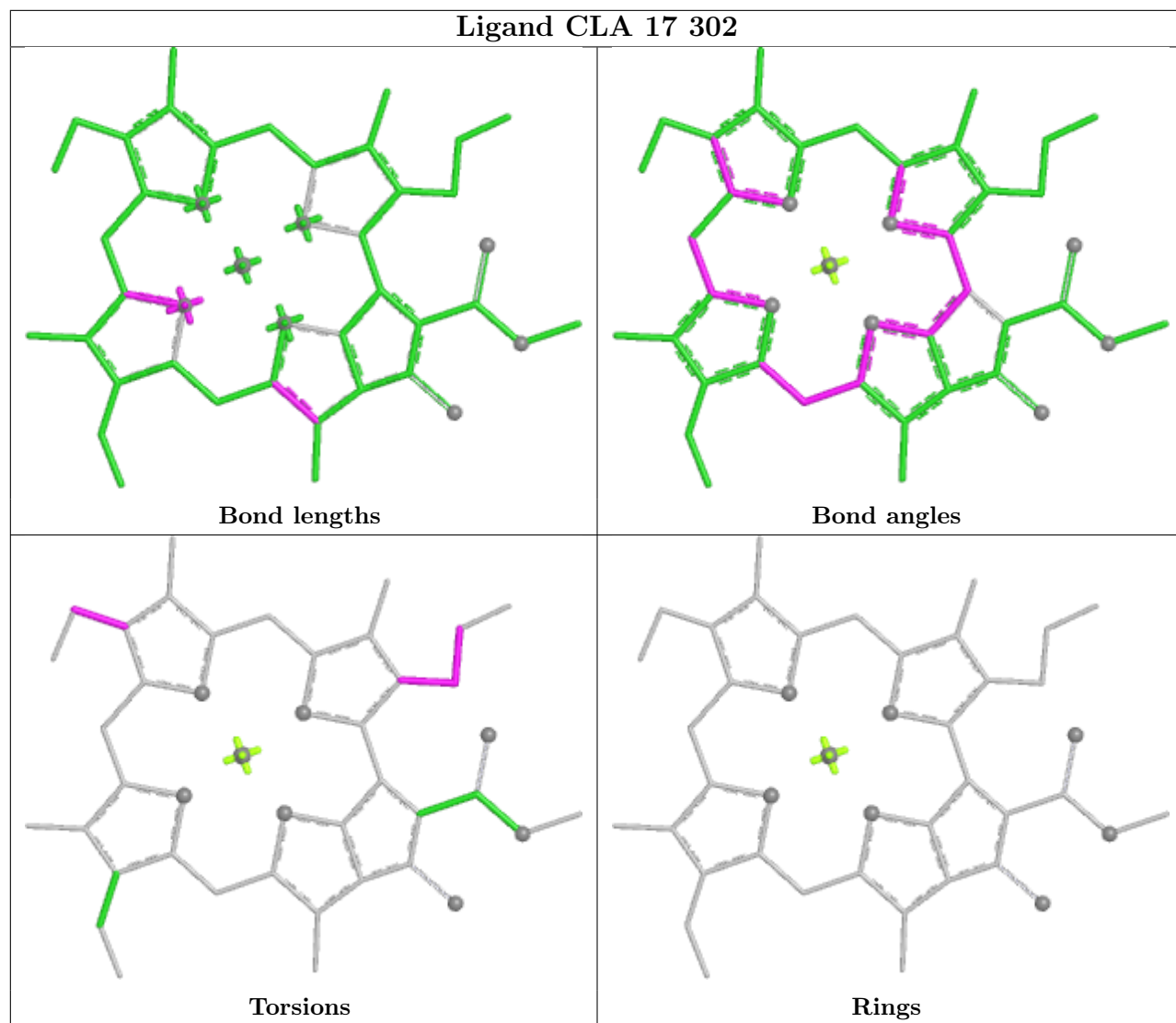
Ligand CLA A 847

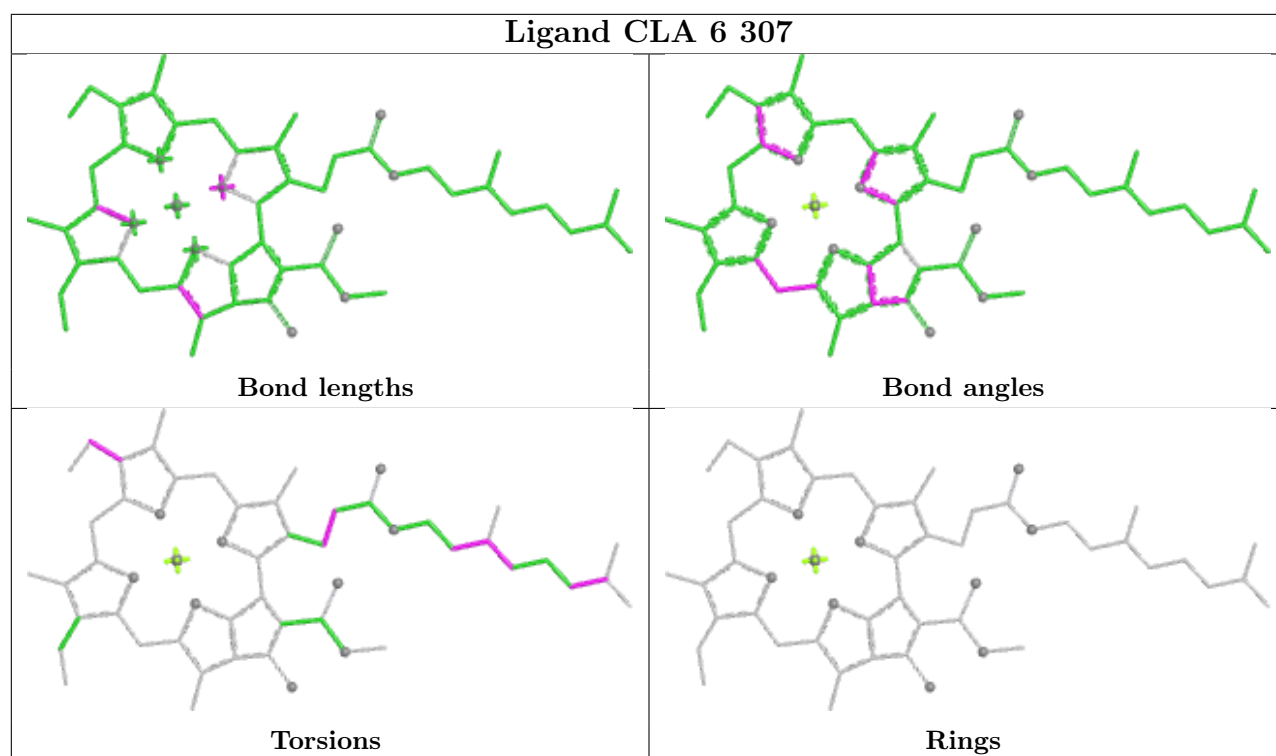


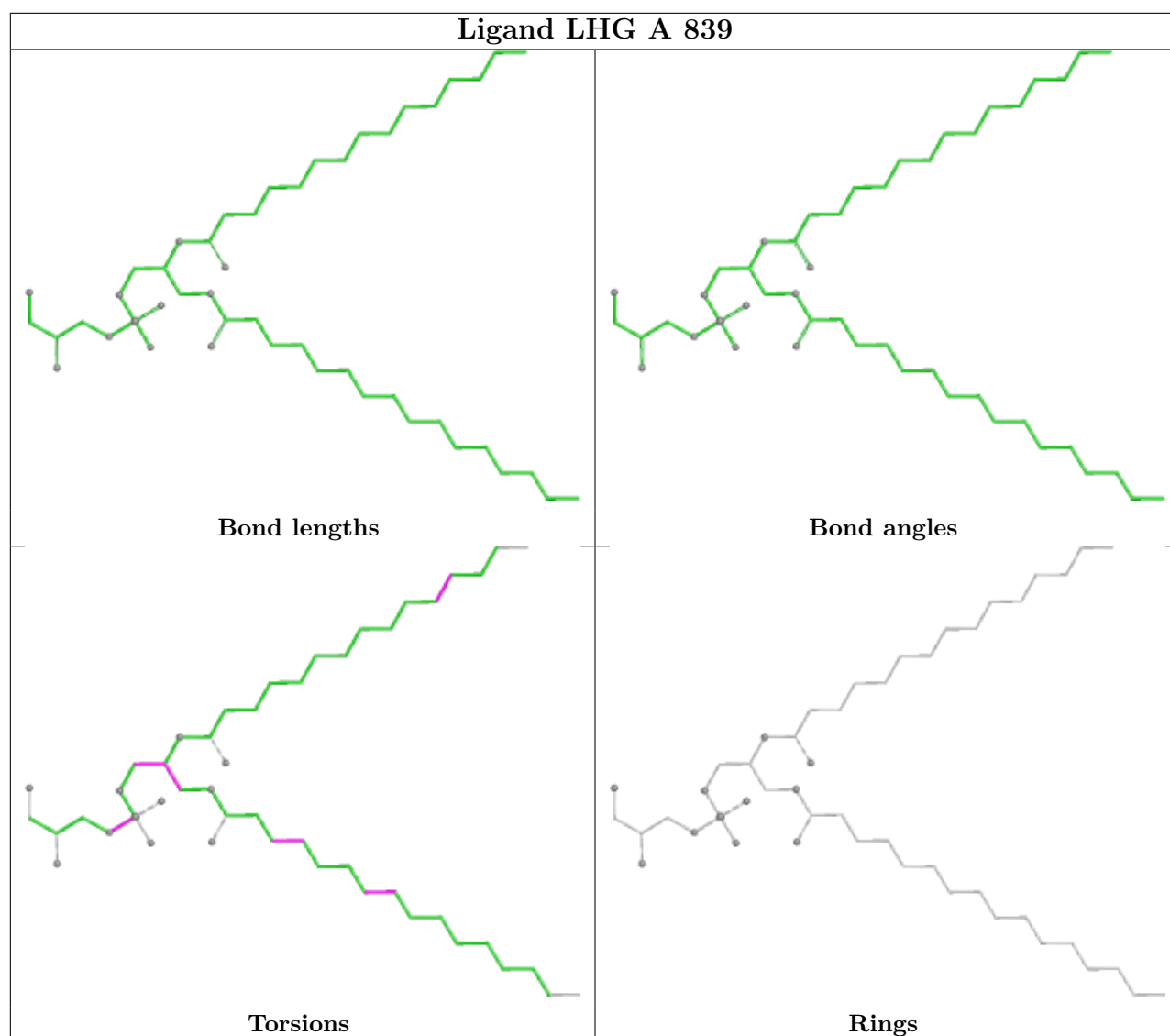


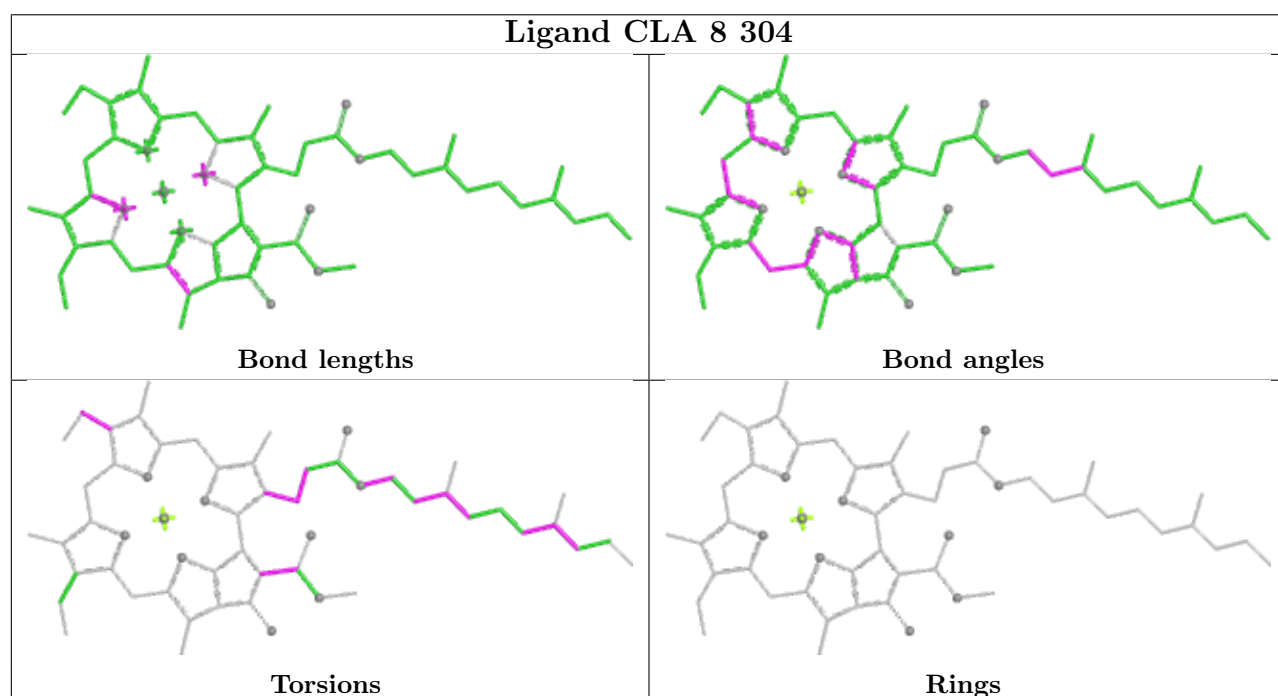
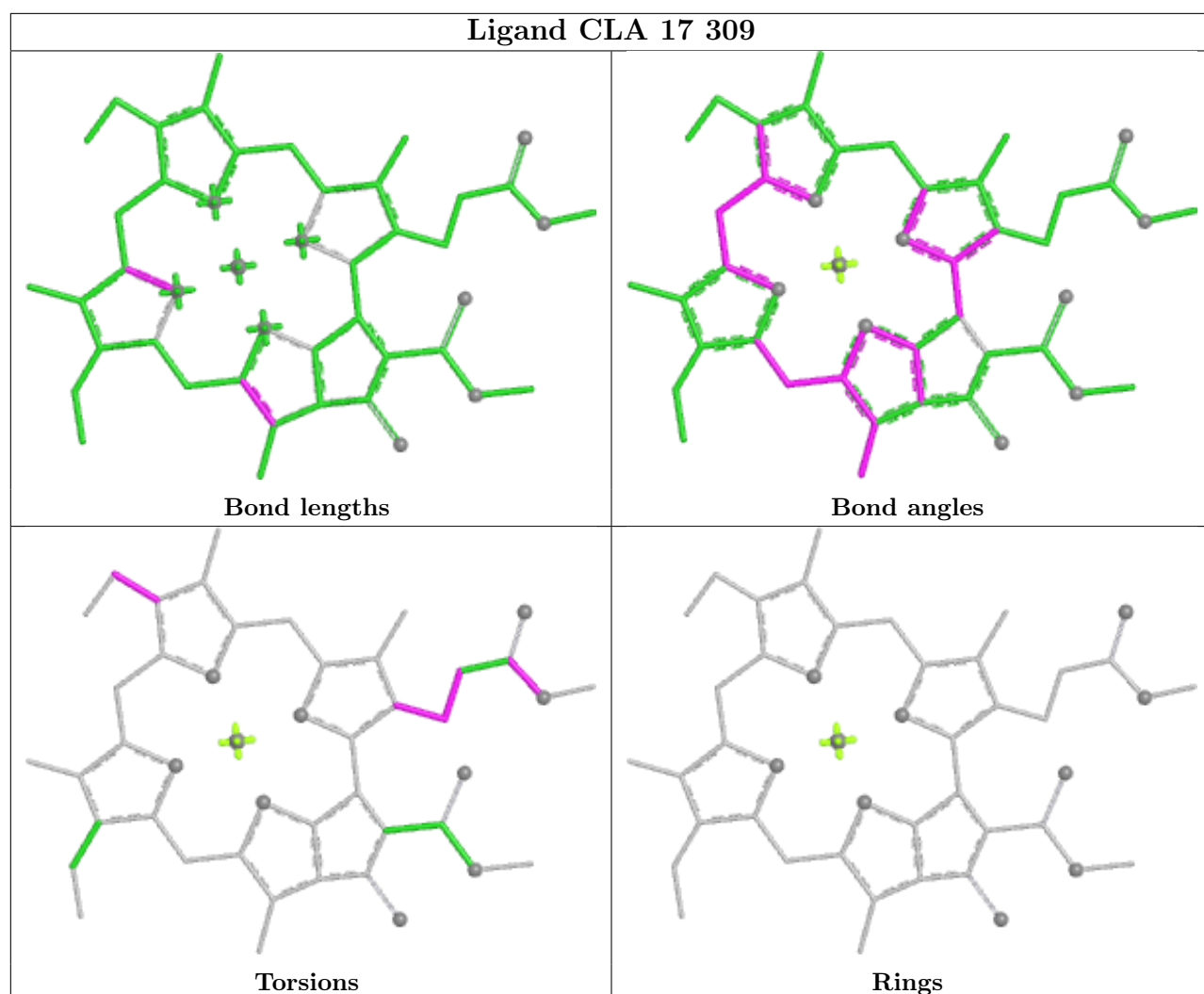




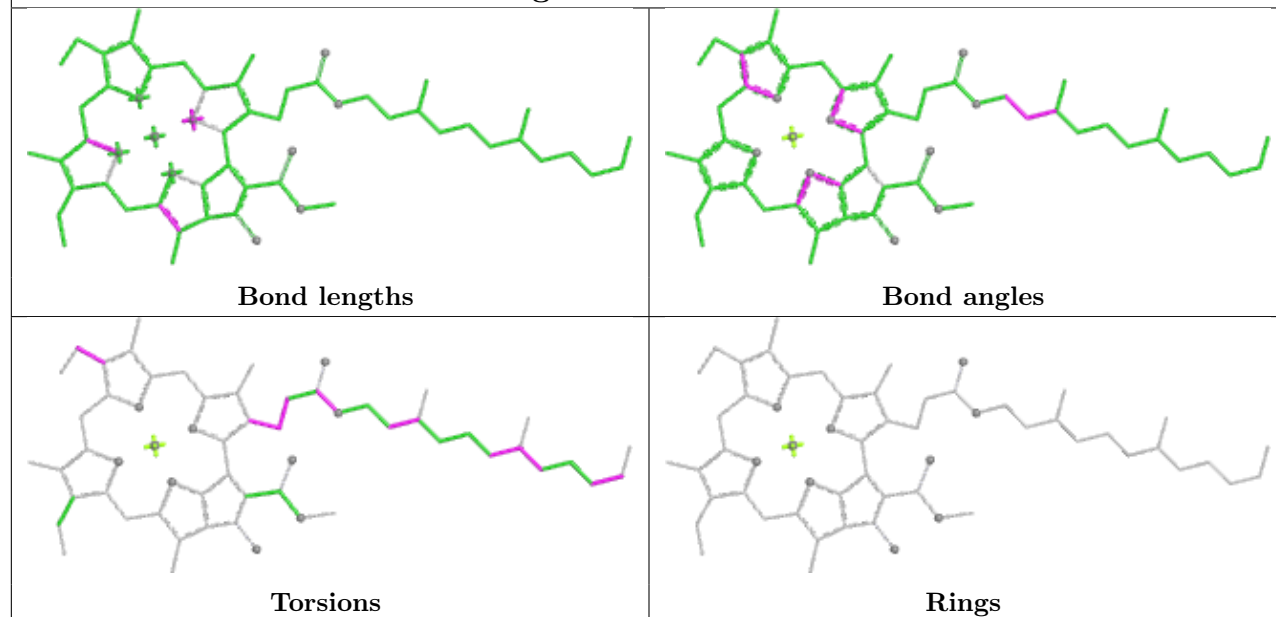




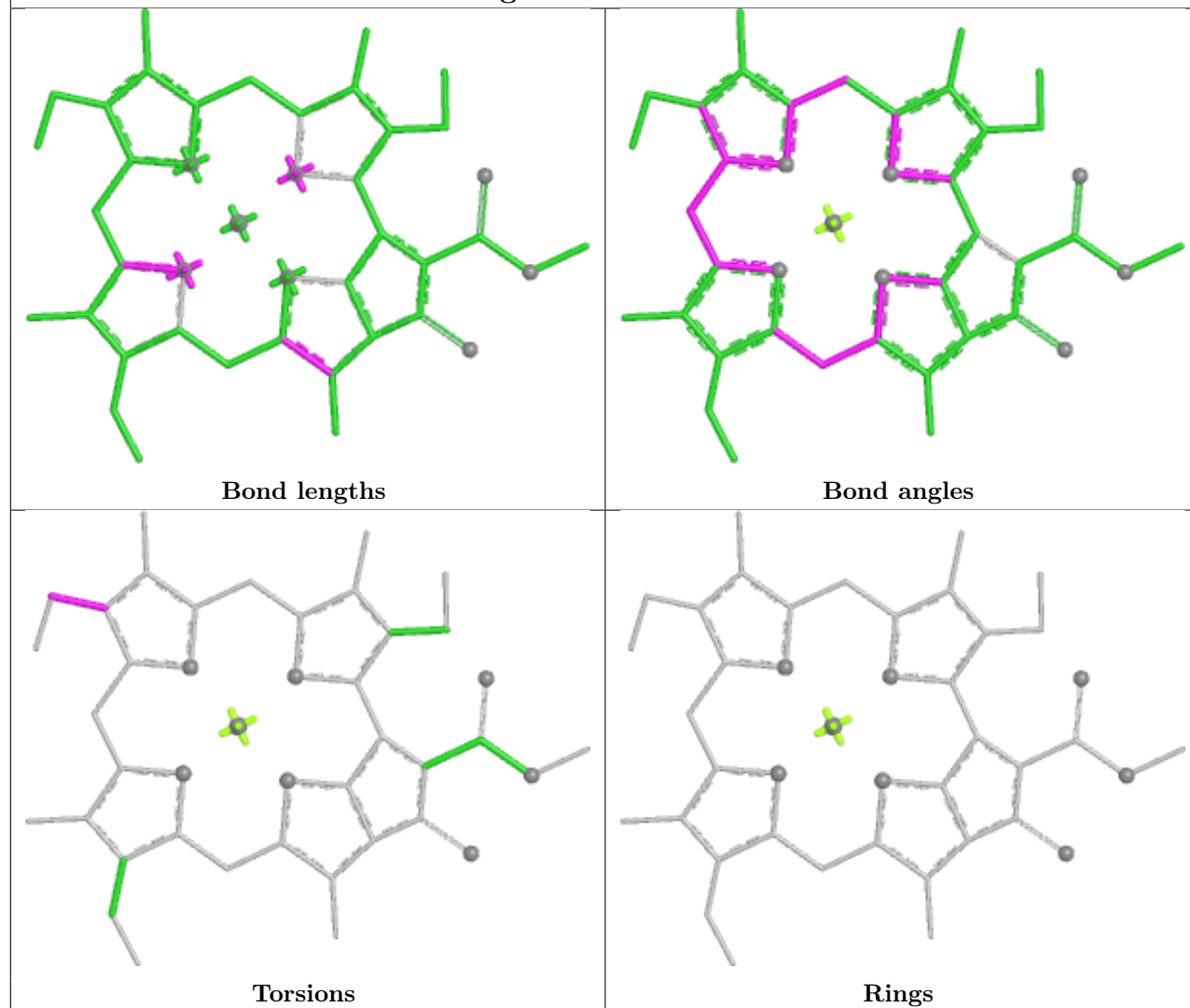




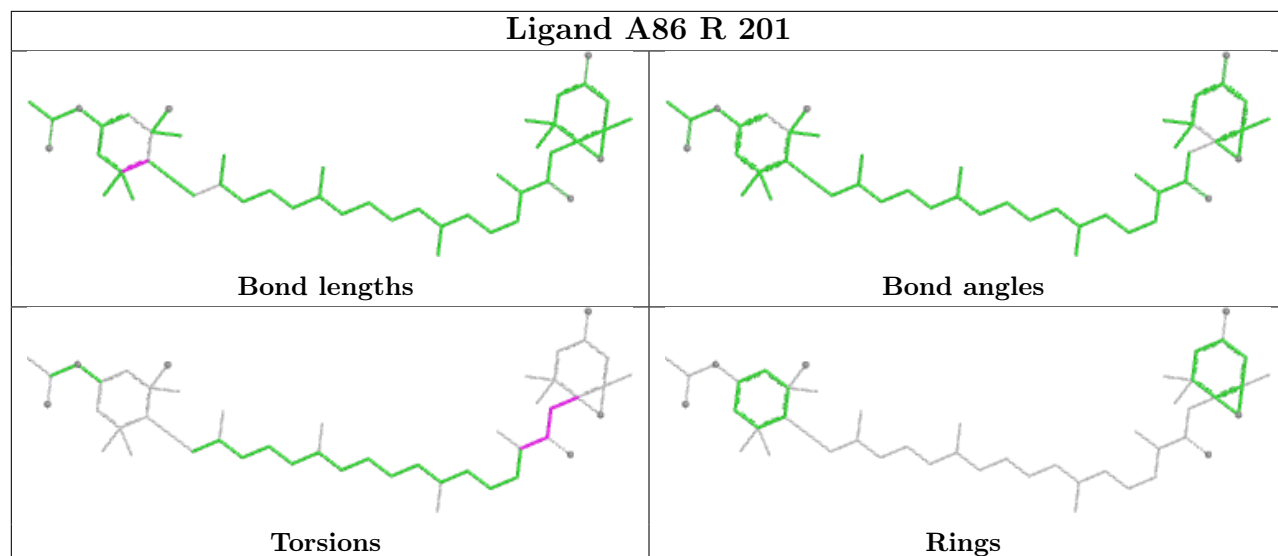
Ligand CLA B 815



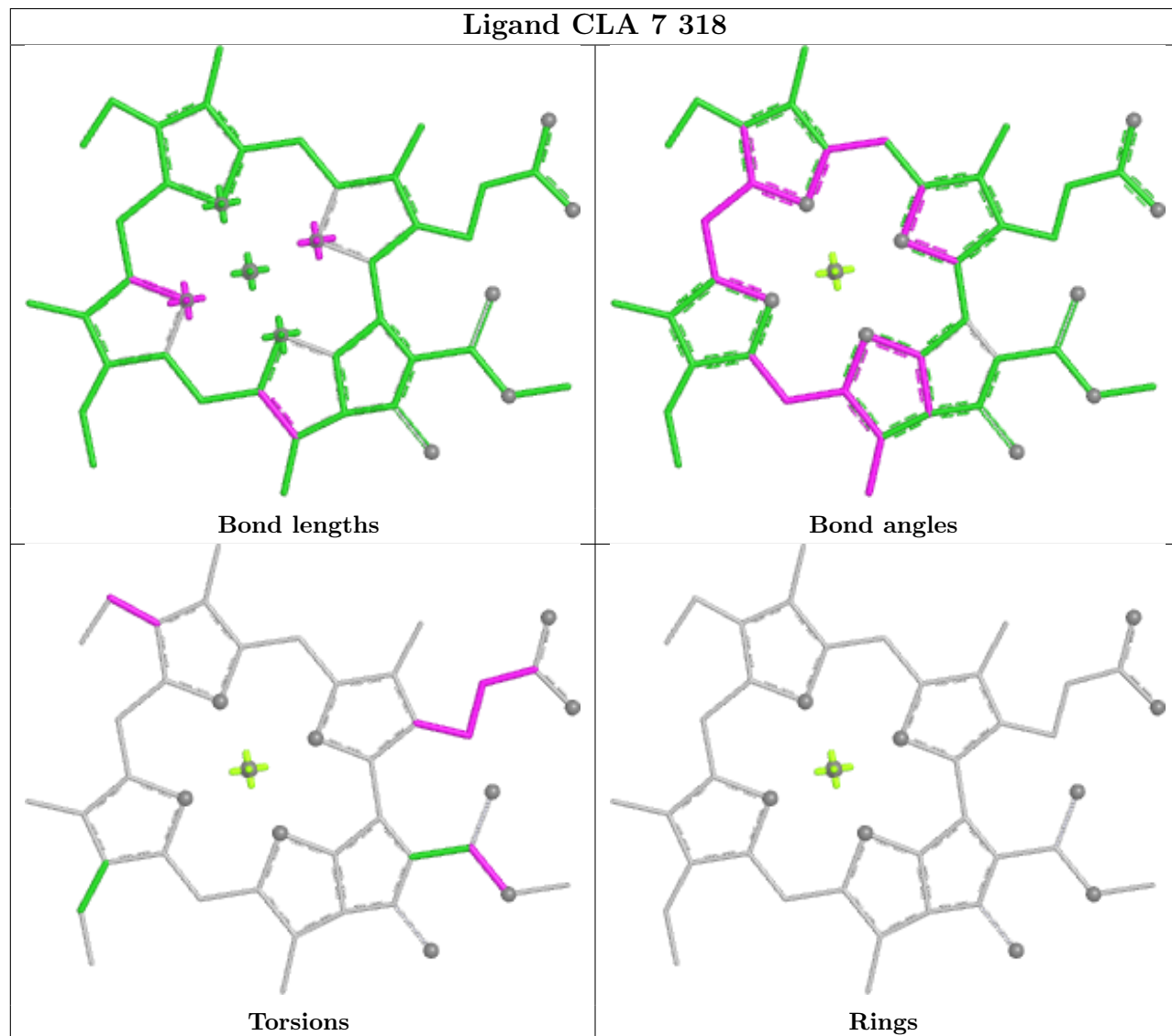
Ligand CLA a 204

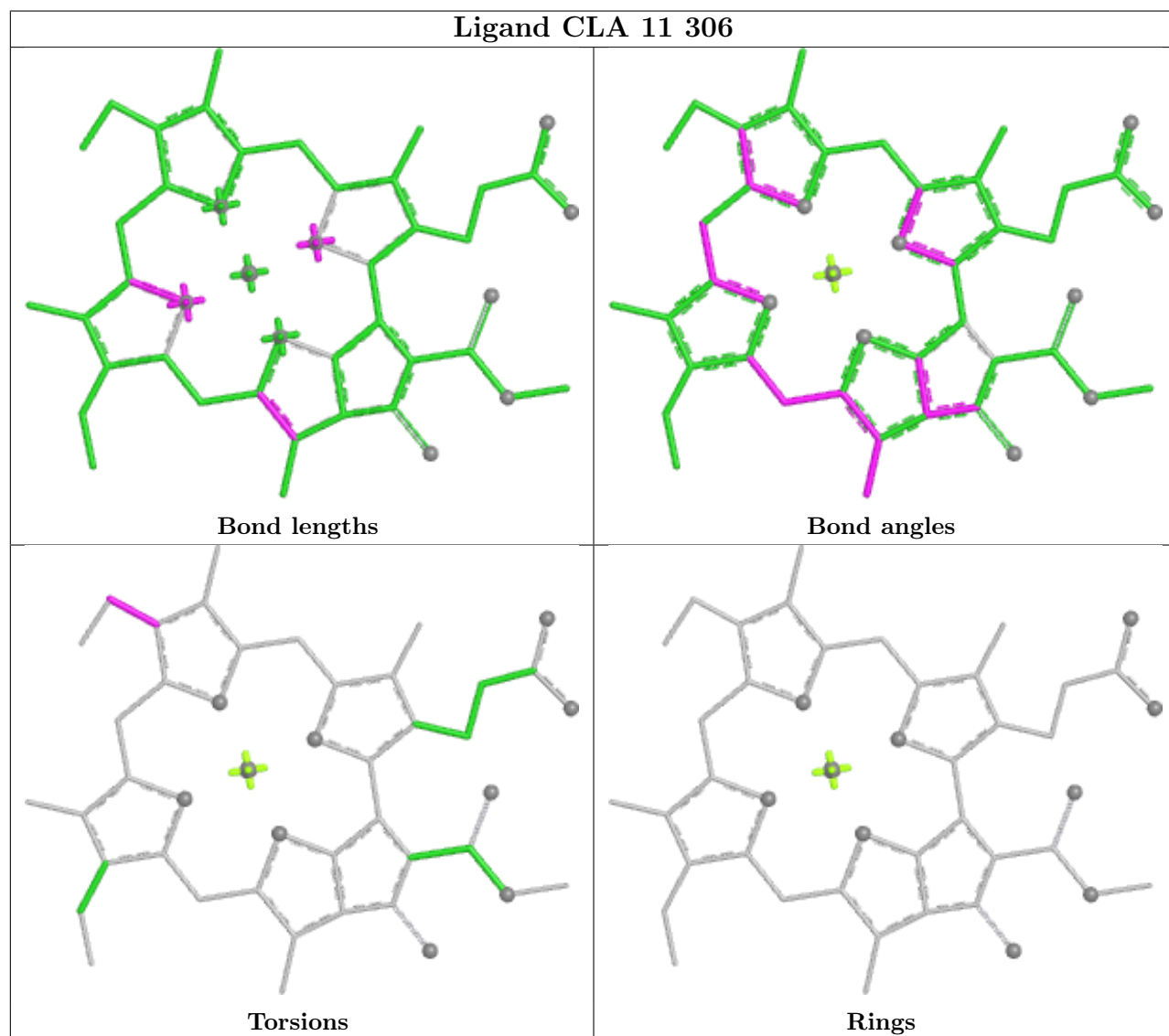
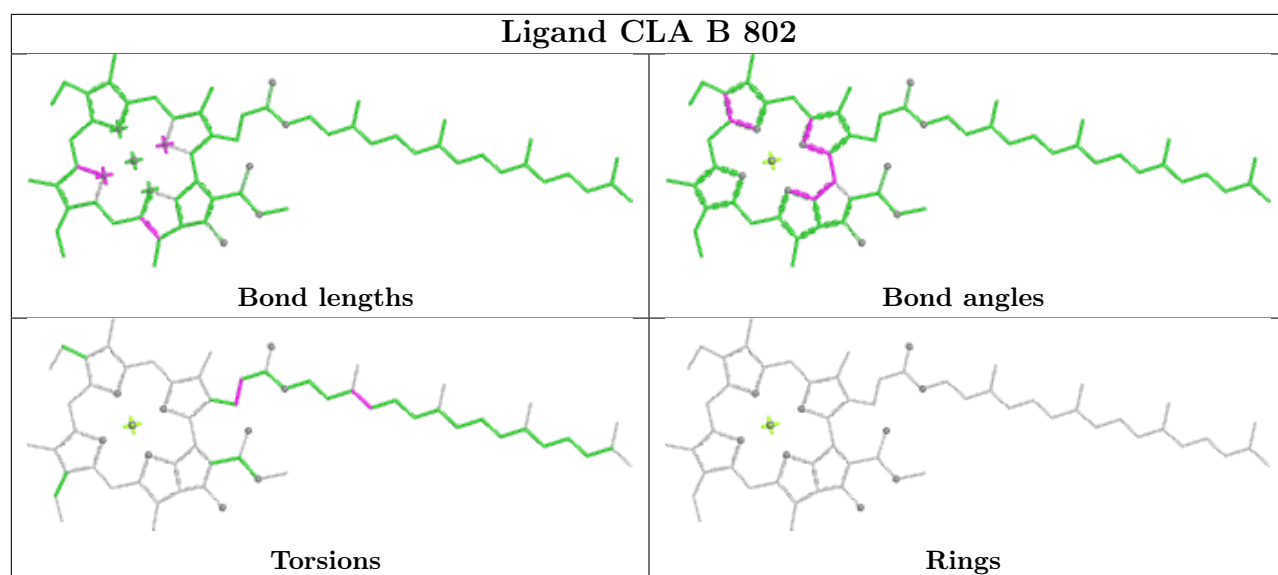


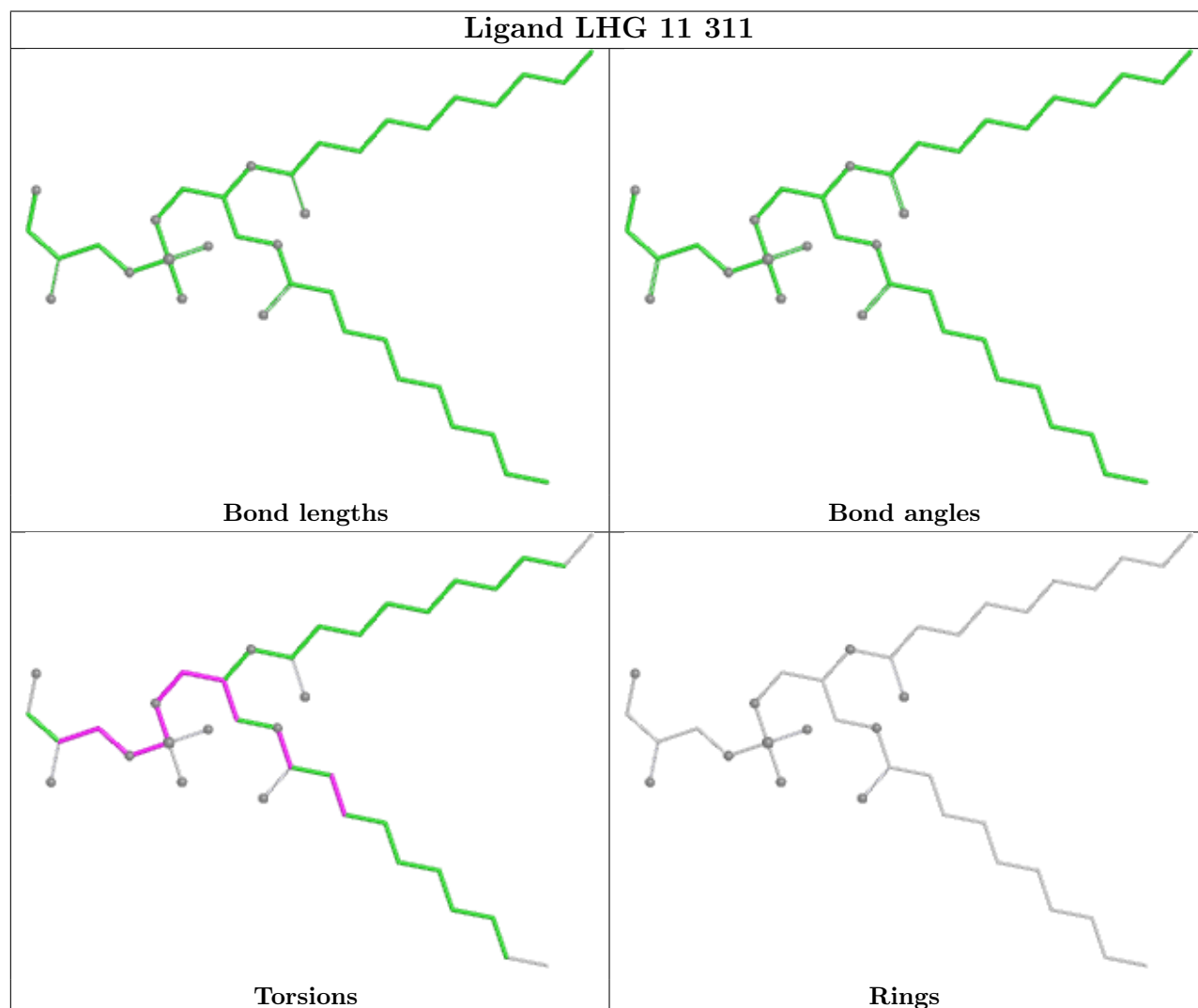
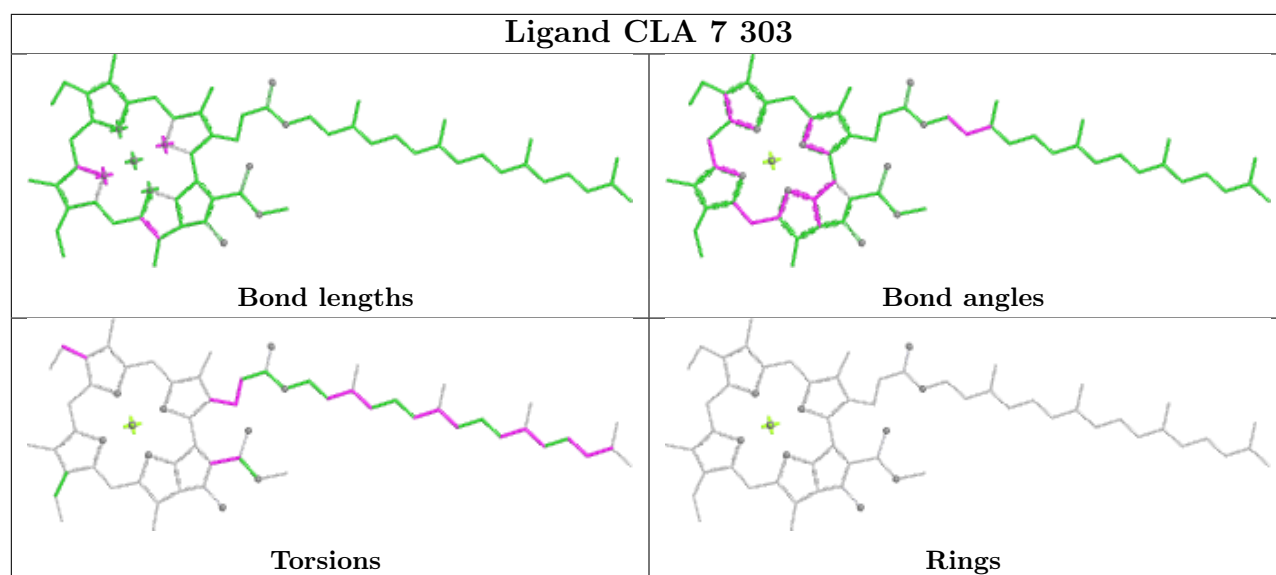
Ligand A86 R 201

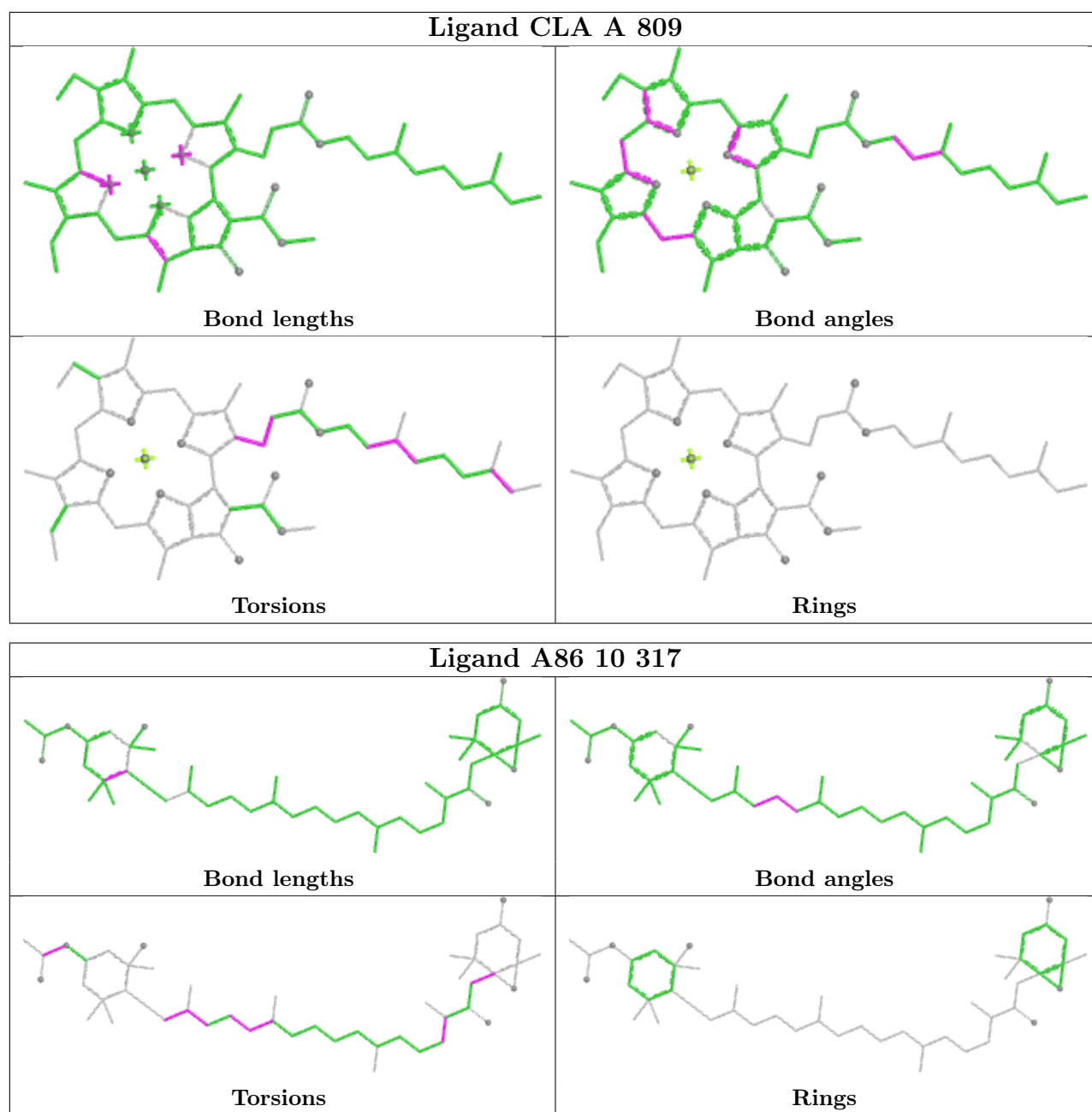


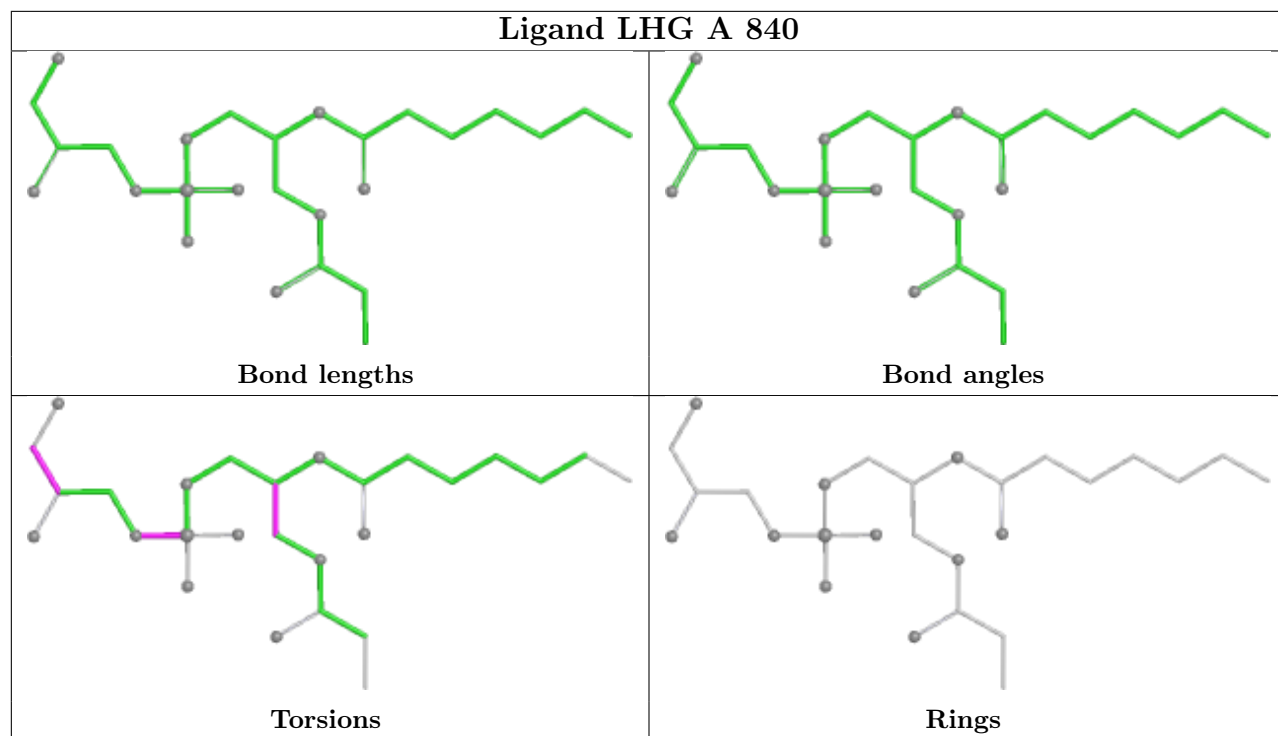
Ligand CLA 7 318

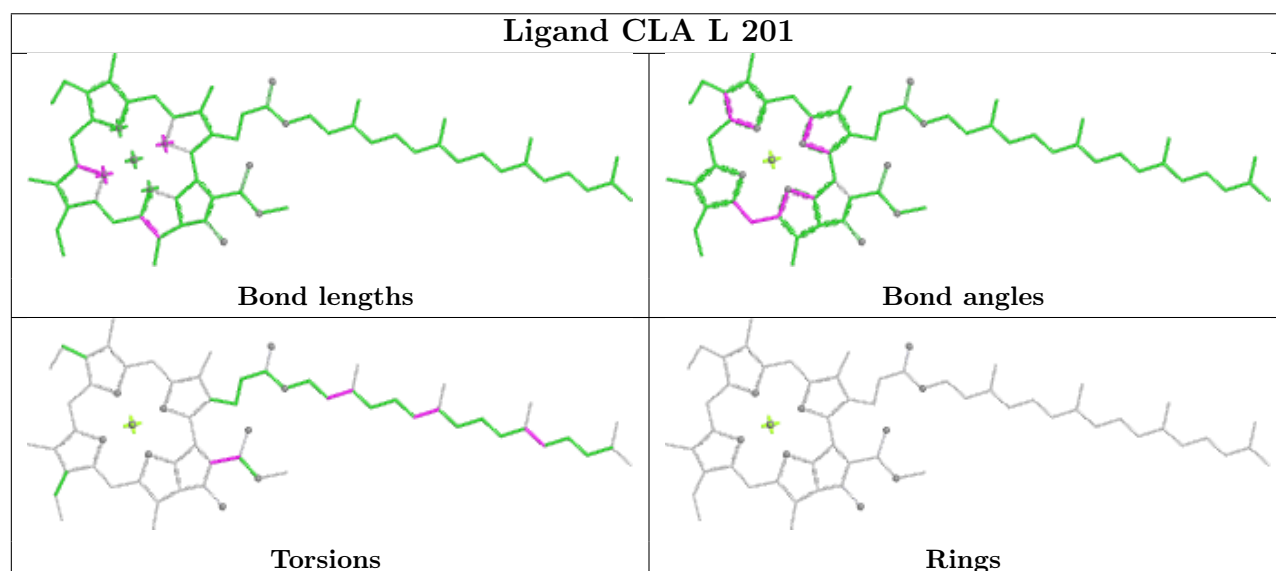
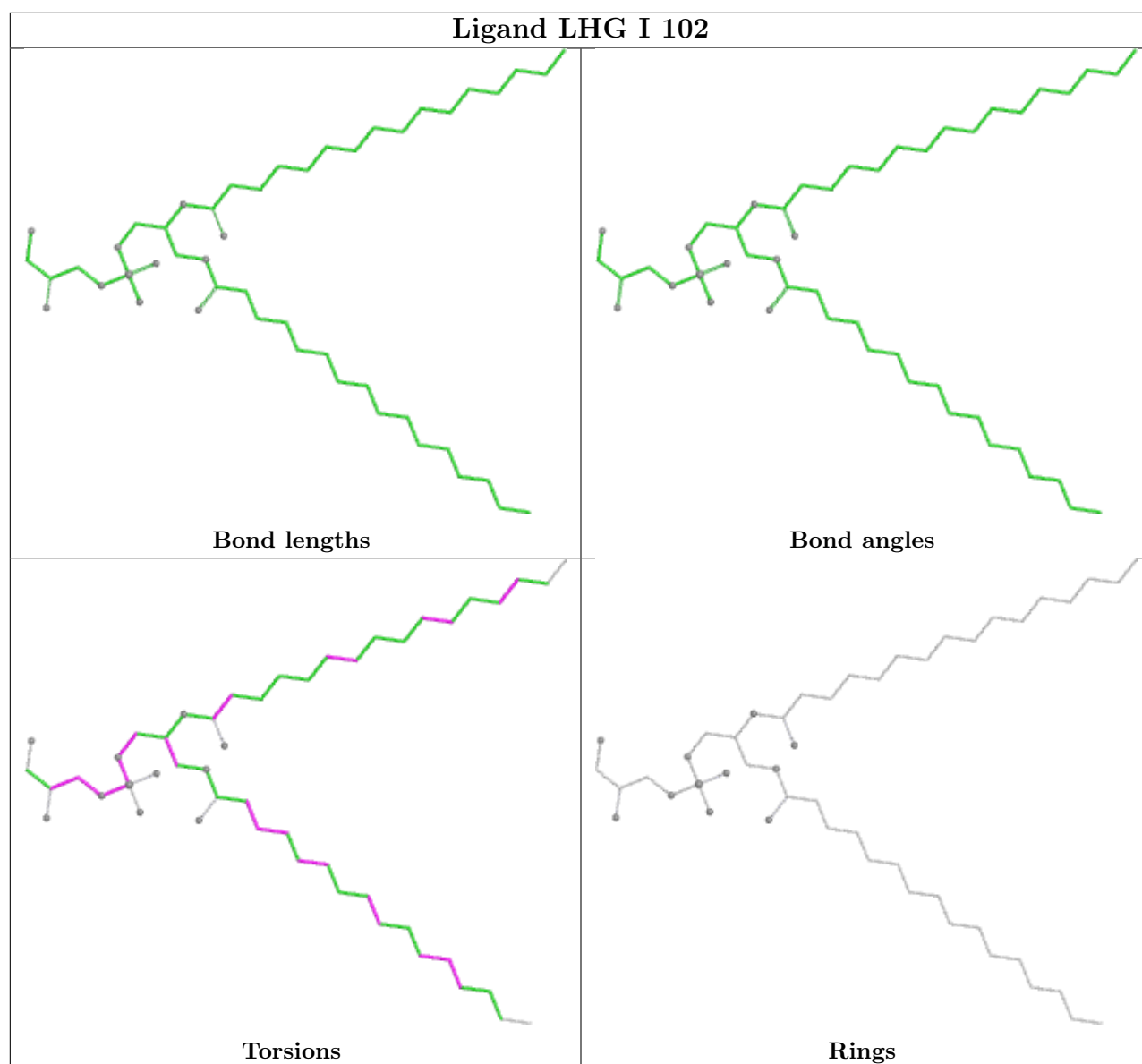




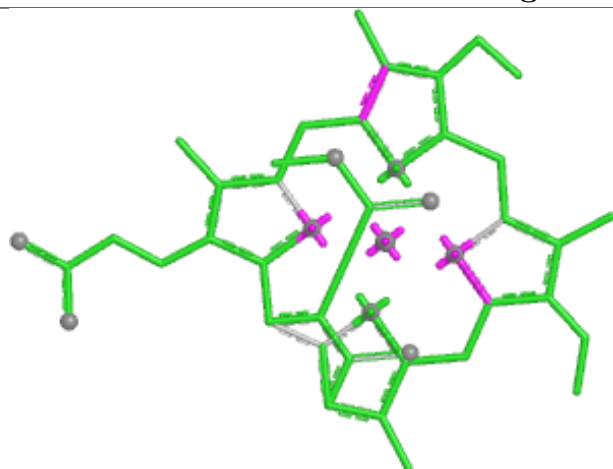




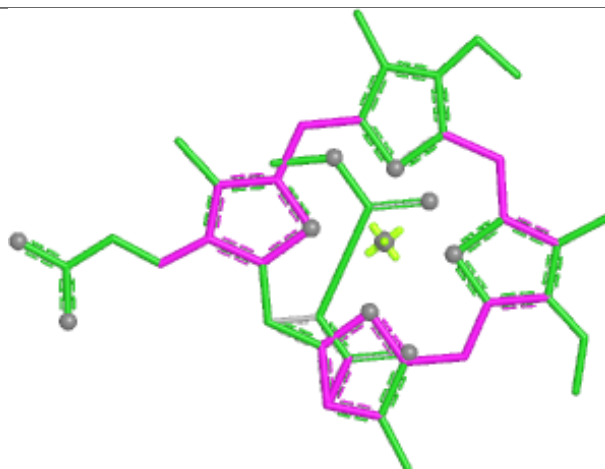




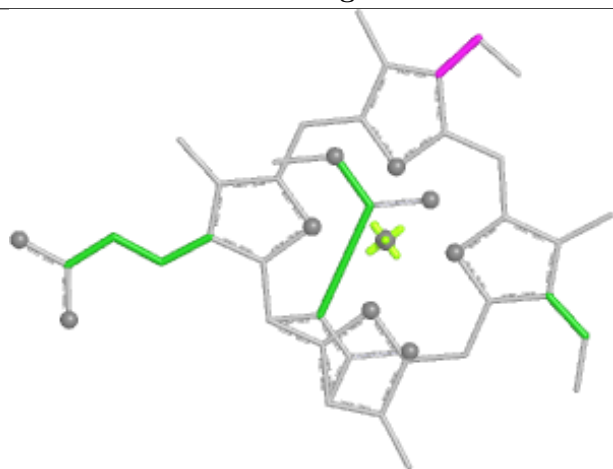
Ligand KC1 8 307



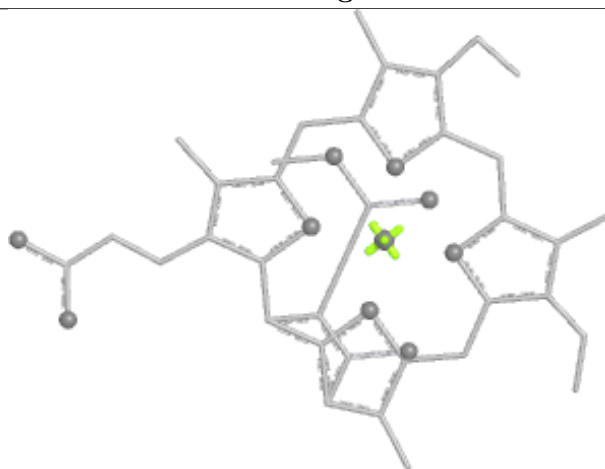
Bond lengths



Bond angles

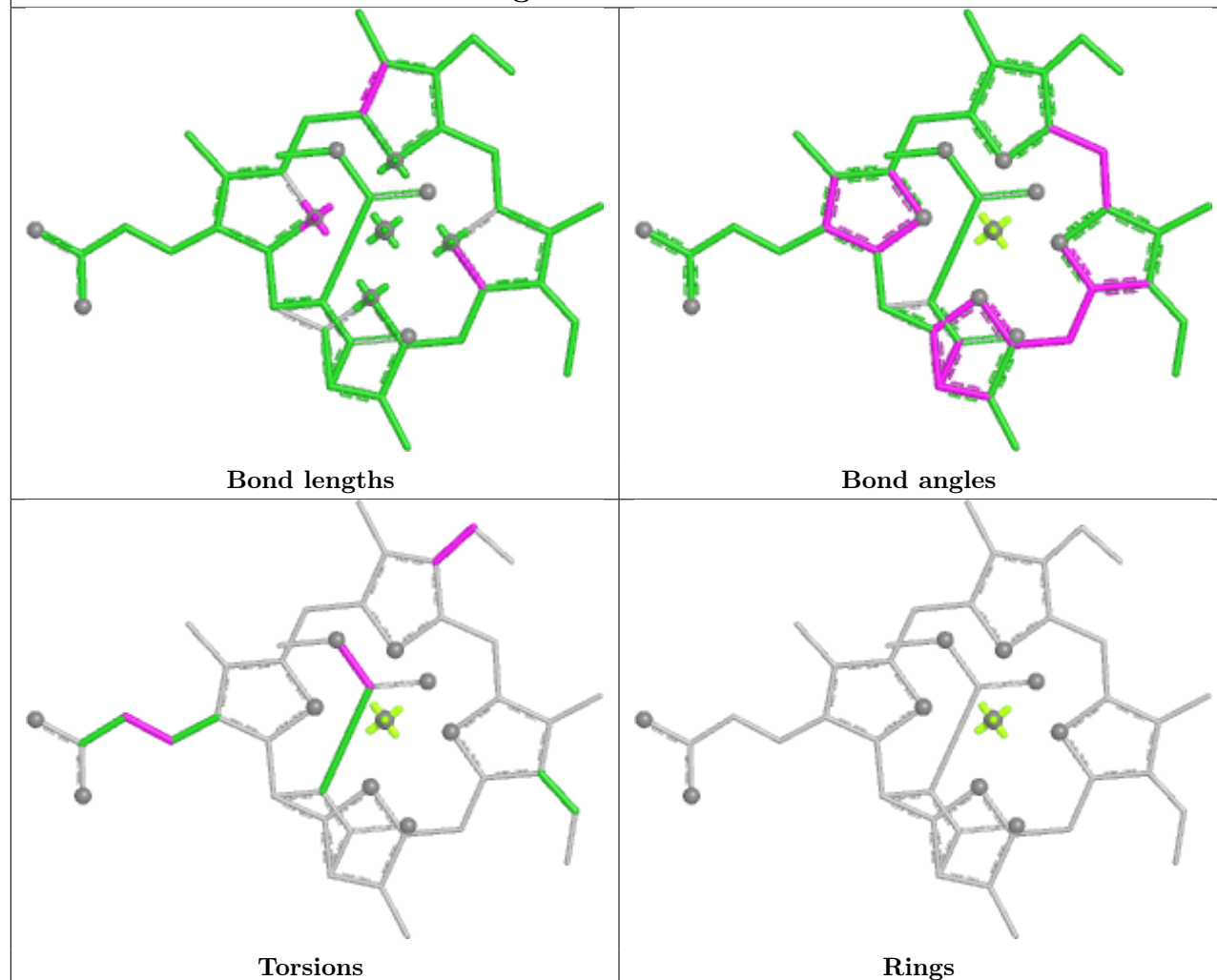


Torsions

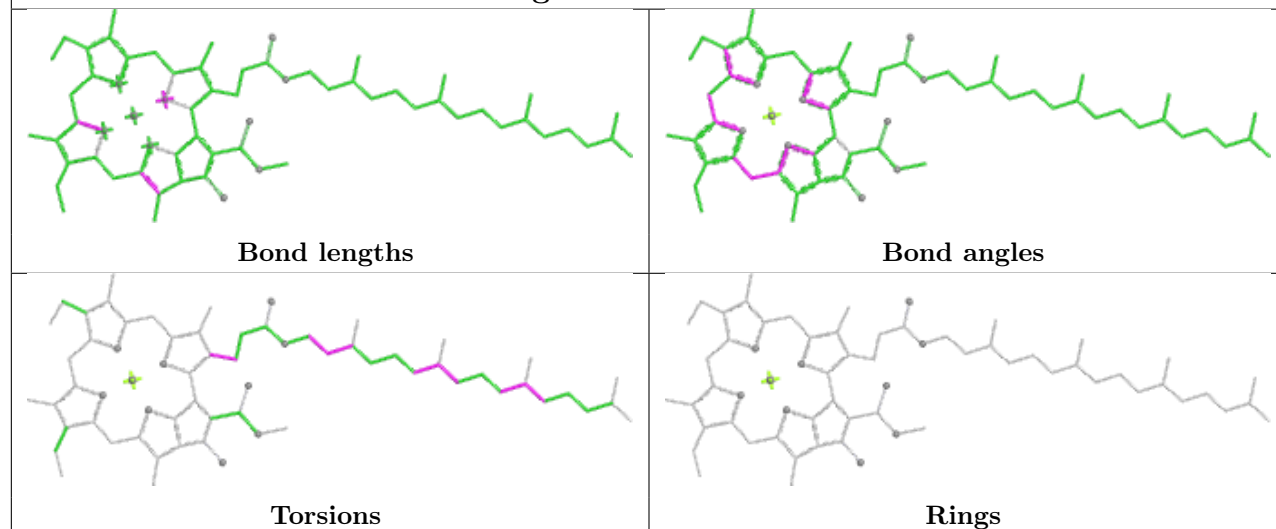


Rings

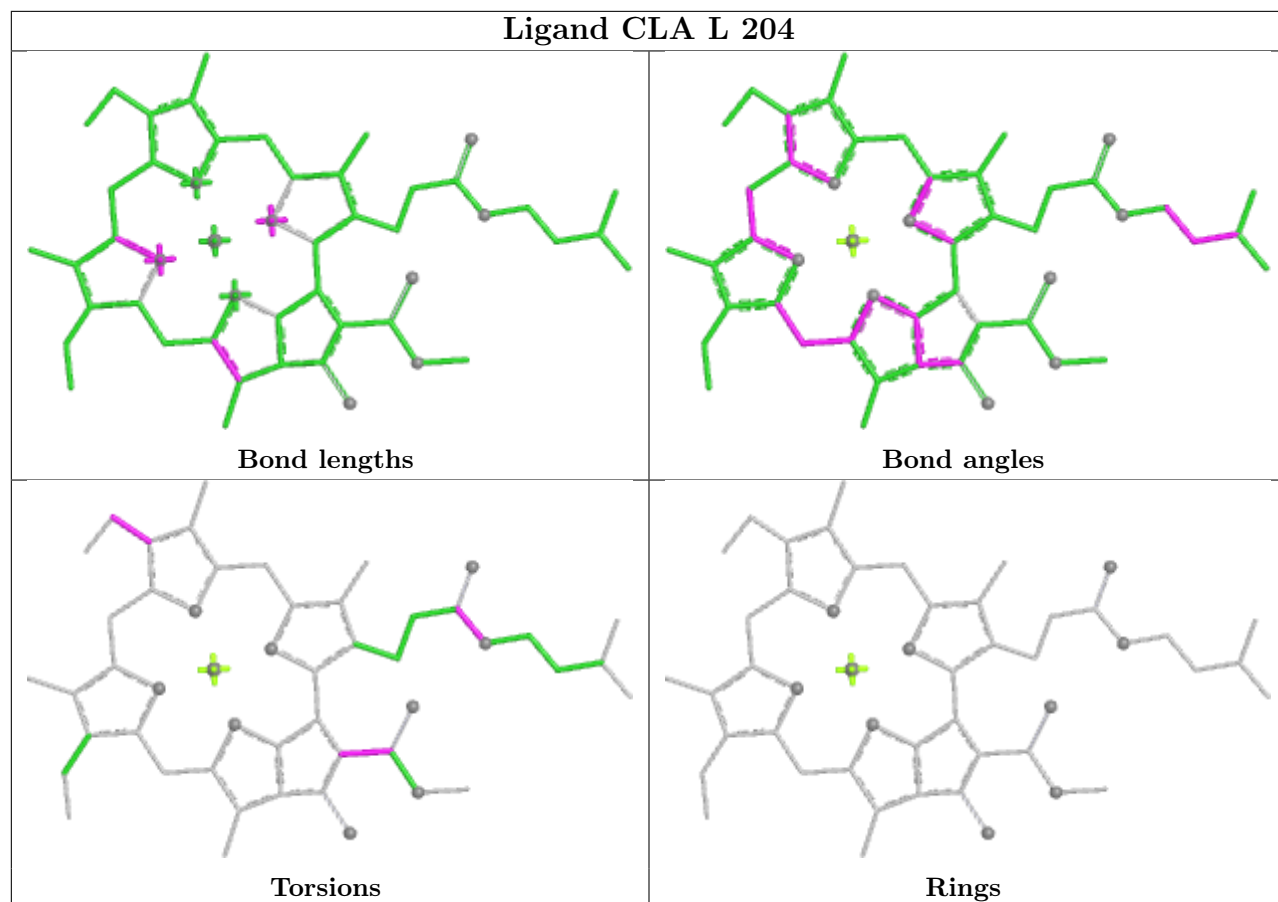
Ligand KC1 4 311



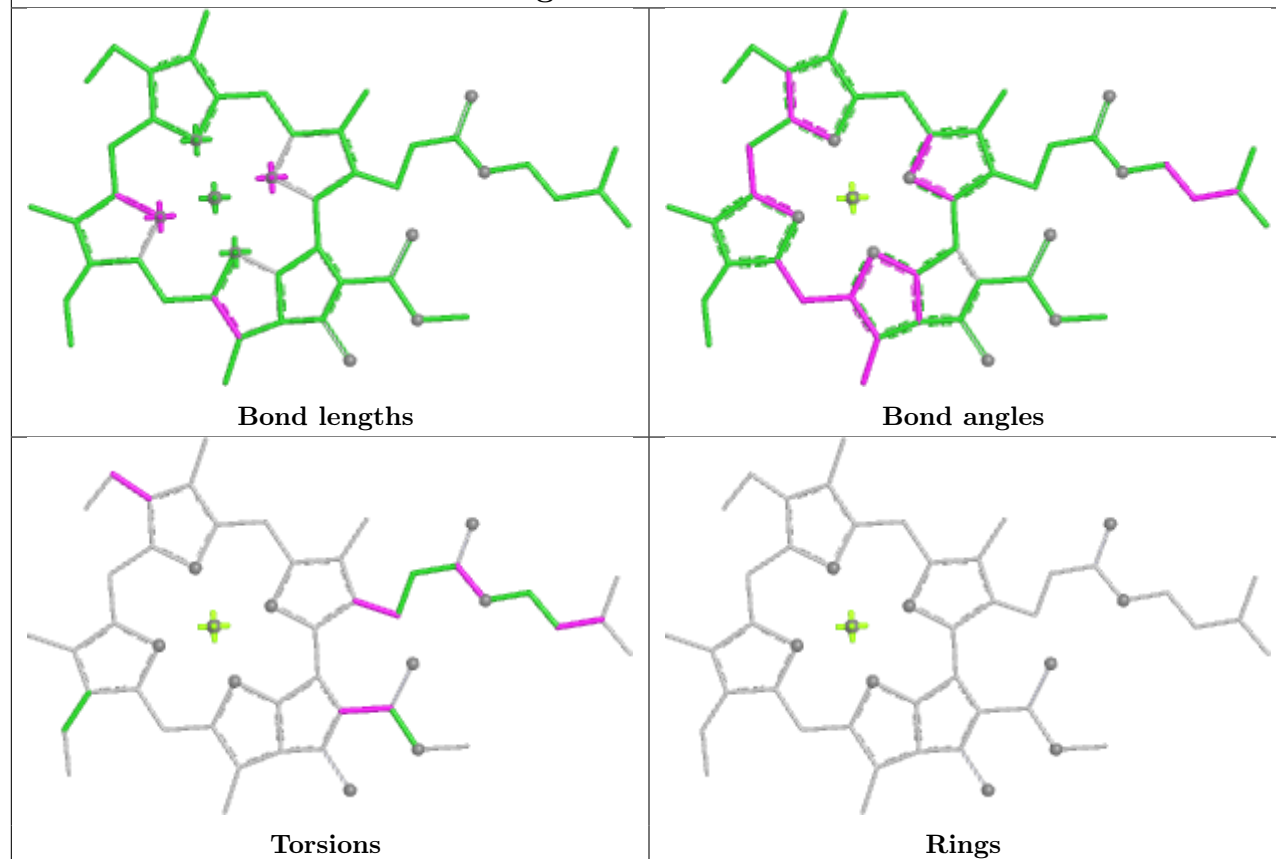
Ligand CLA B 804



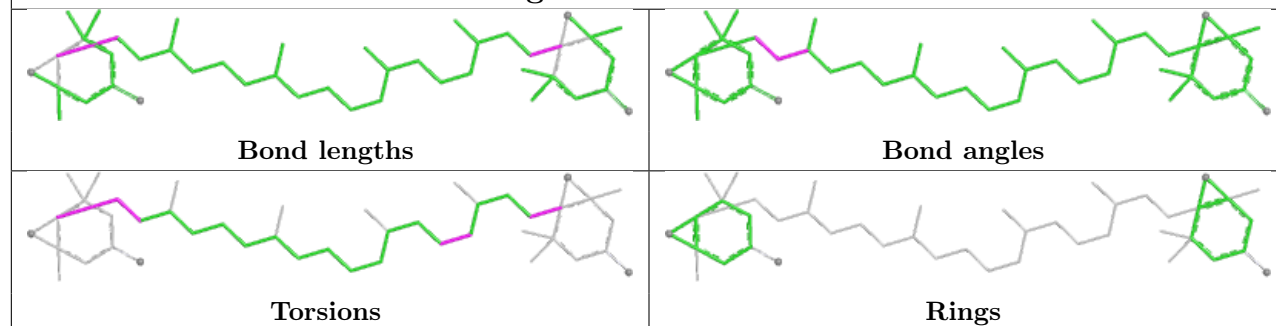
Ligand CLA L 204

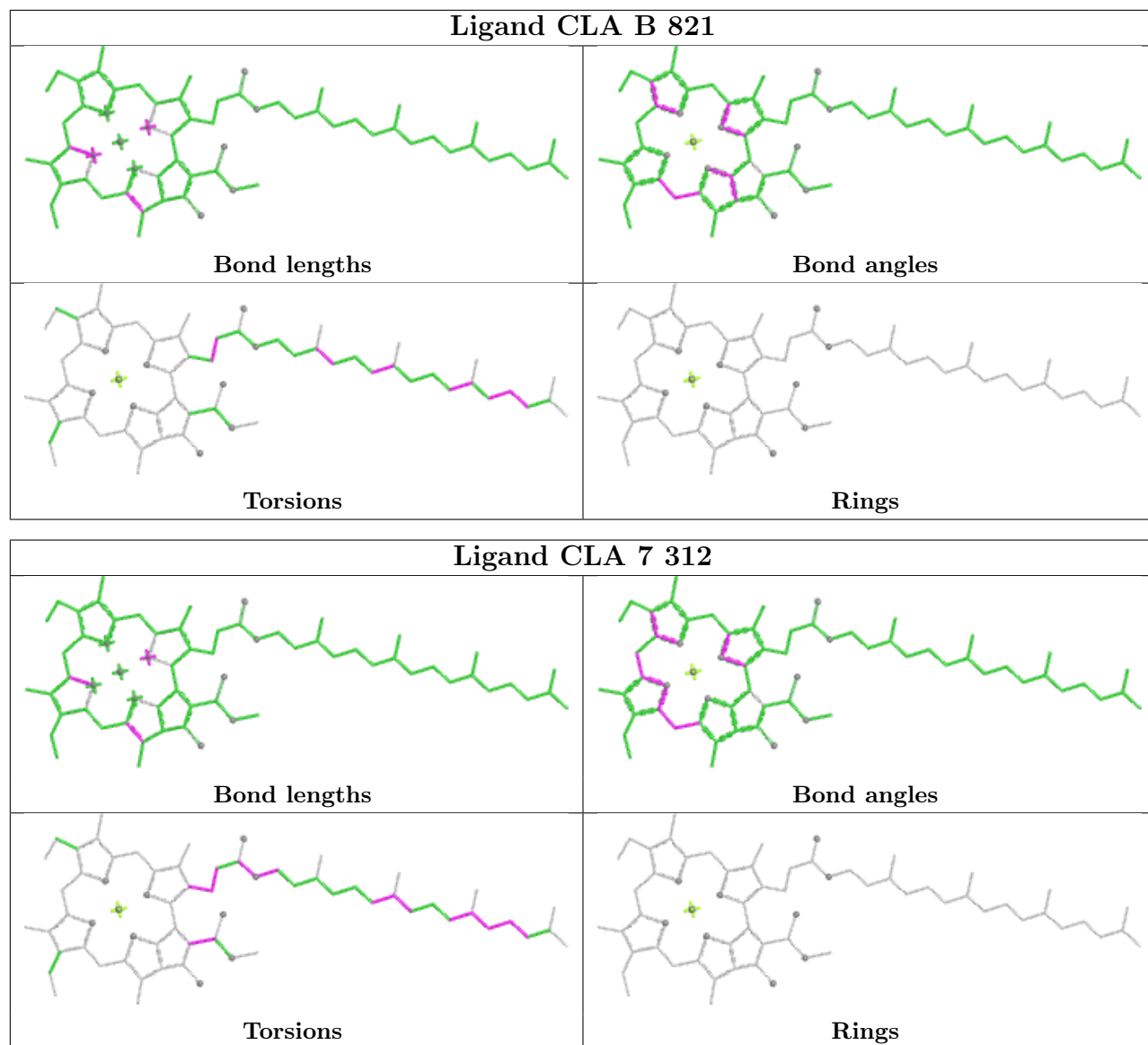


Ligand CLA 9 304

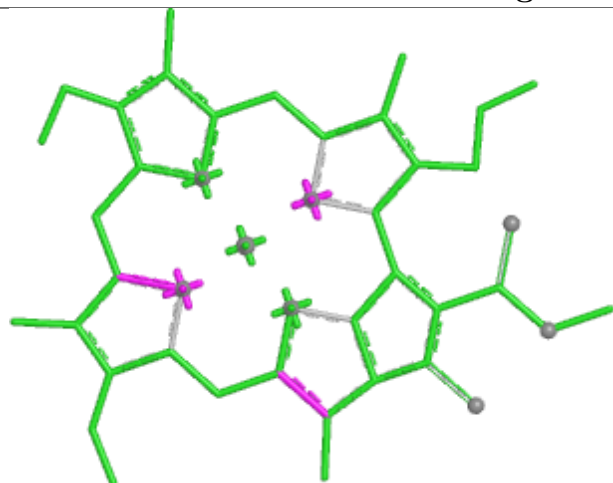


Ligand XAT 10 314

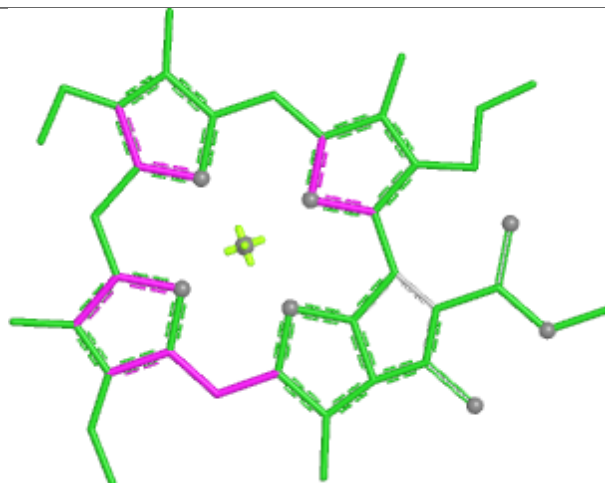




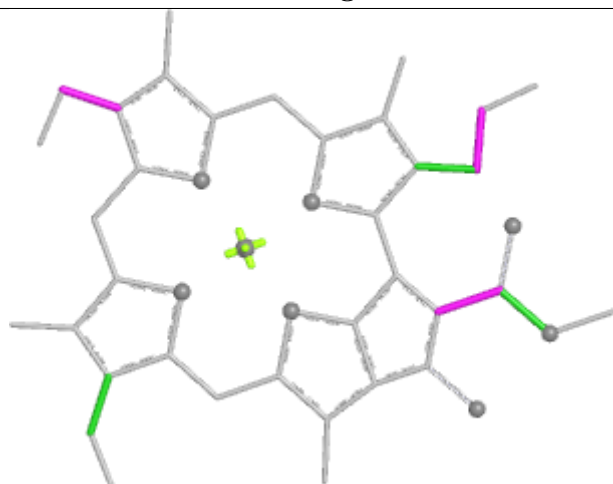
Ligand CLA F 803



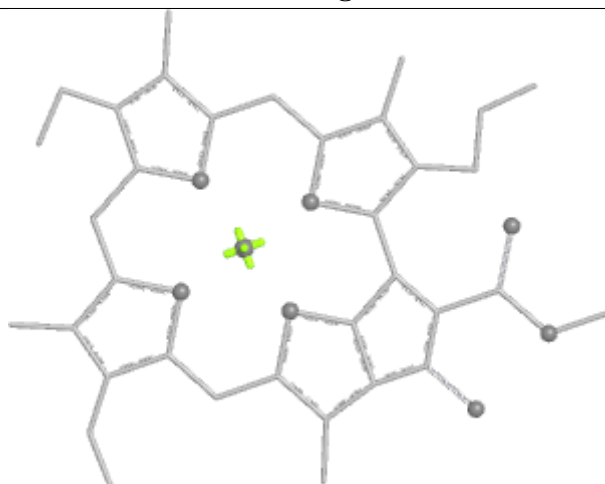
Bond lengths



Bond angles

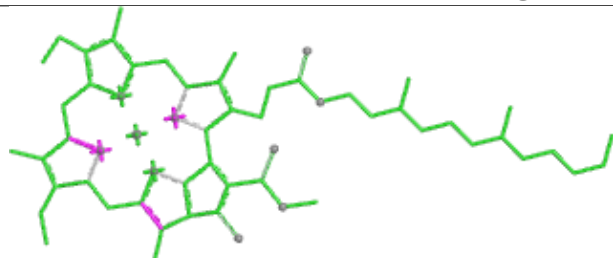


Torsions

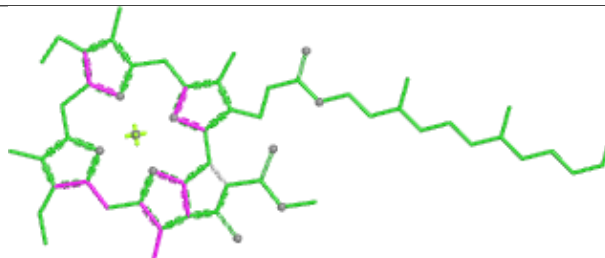


Rings

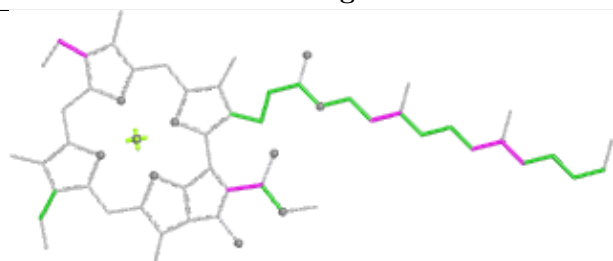
Ligand CLA B 814



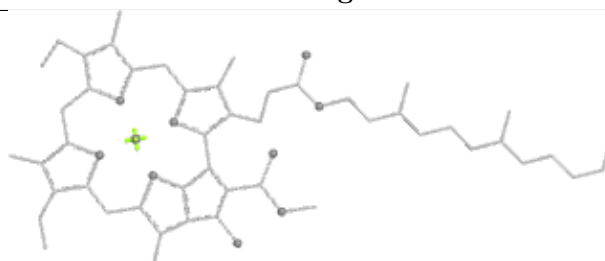
Bond lengths



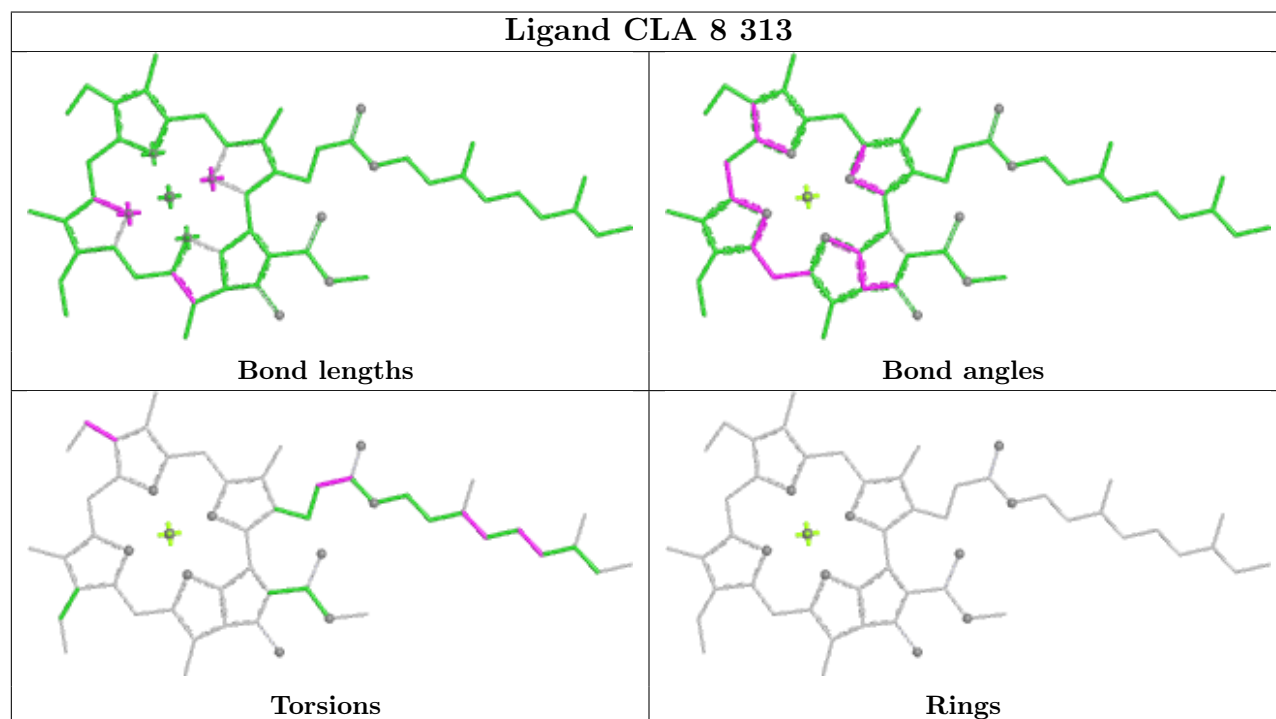
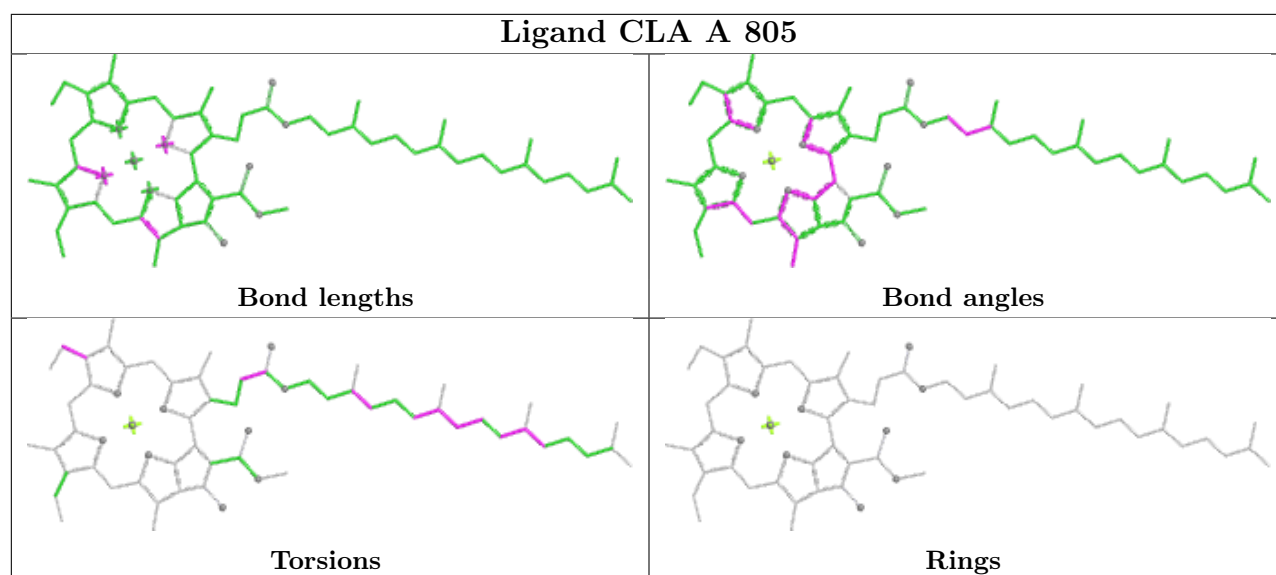
Bond angles



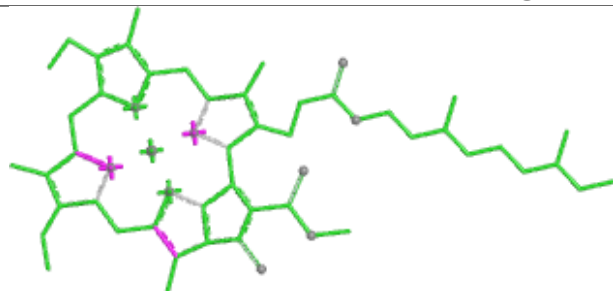
Torsions



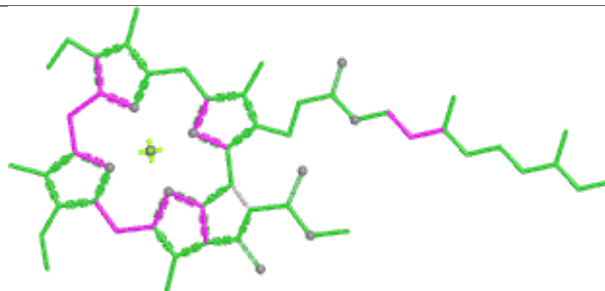
Rings



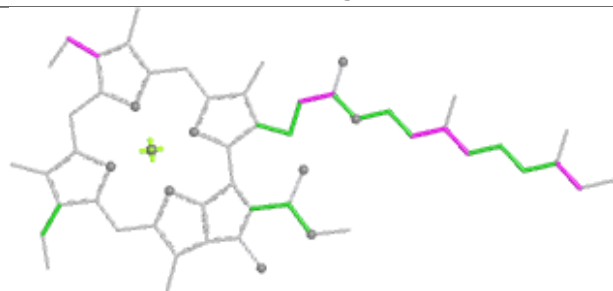
Ligand CLA 8 302



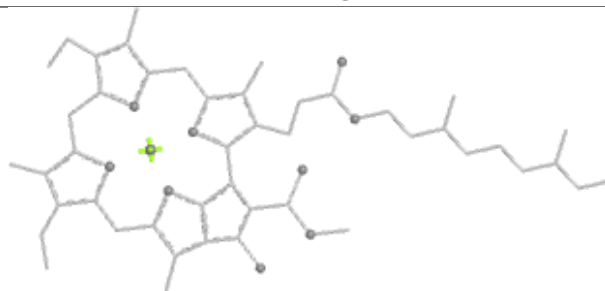
Bond lengths



Bond angles

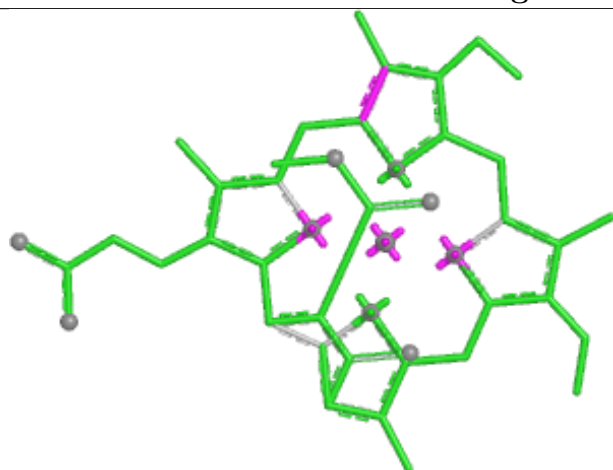


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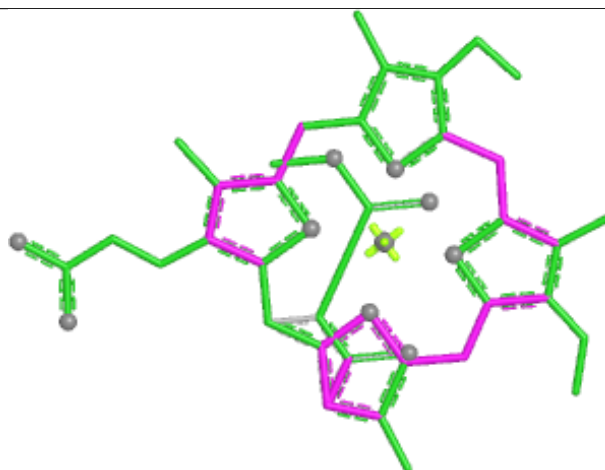


Rings

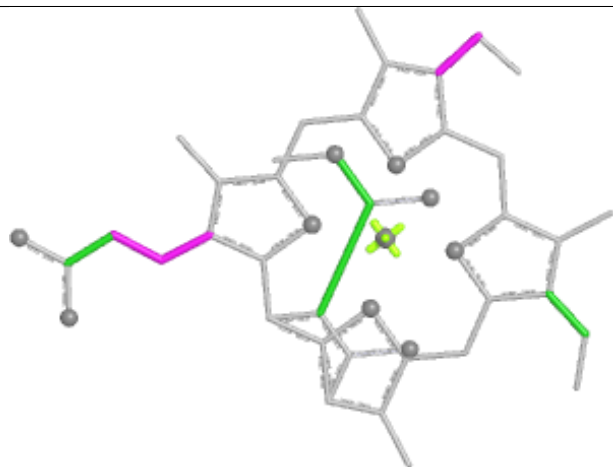
Ligand KC1 10 311



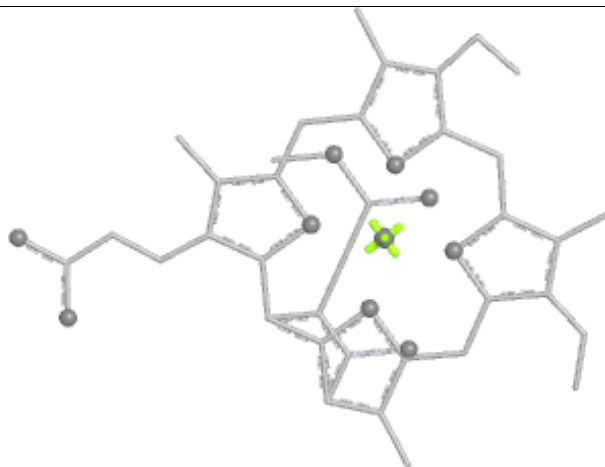
Bond lengths



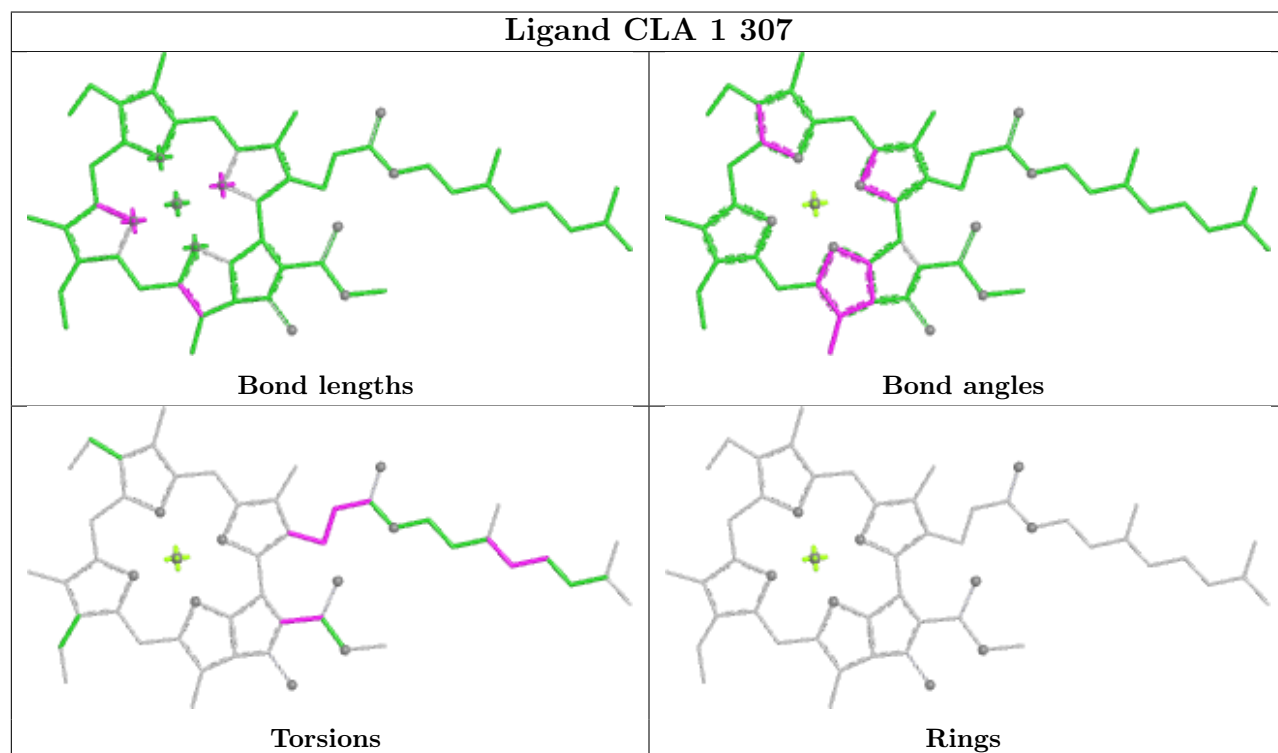
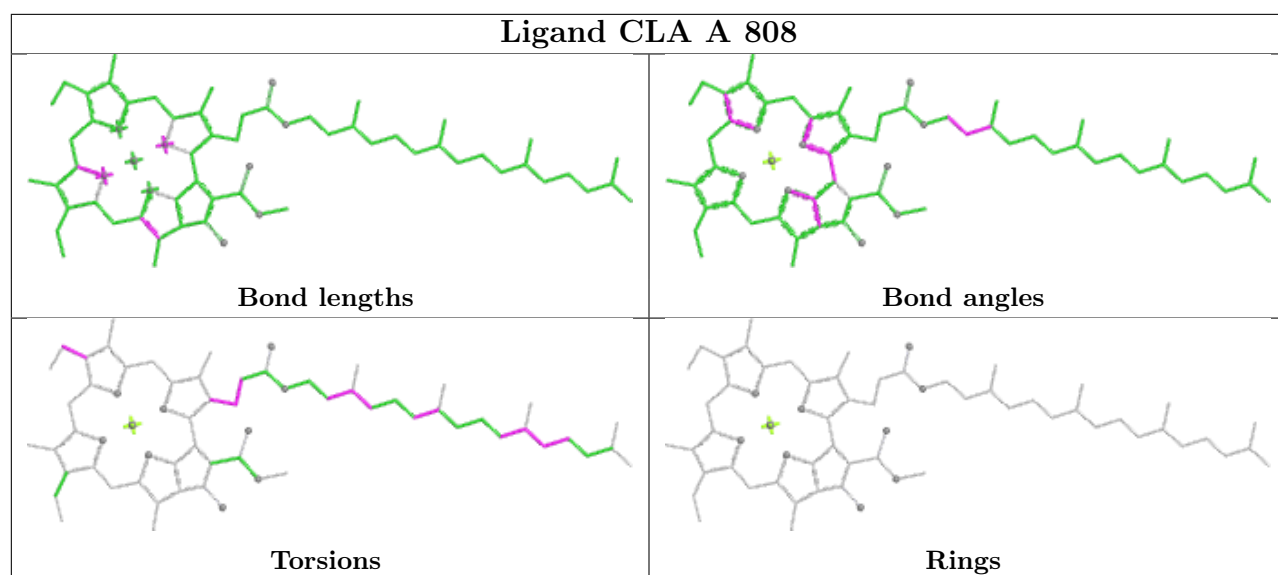
Bond angles

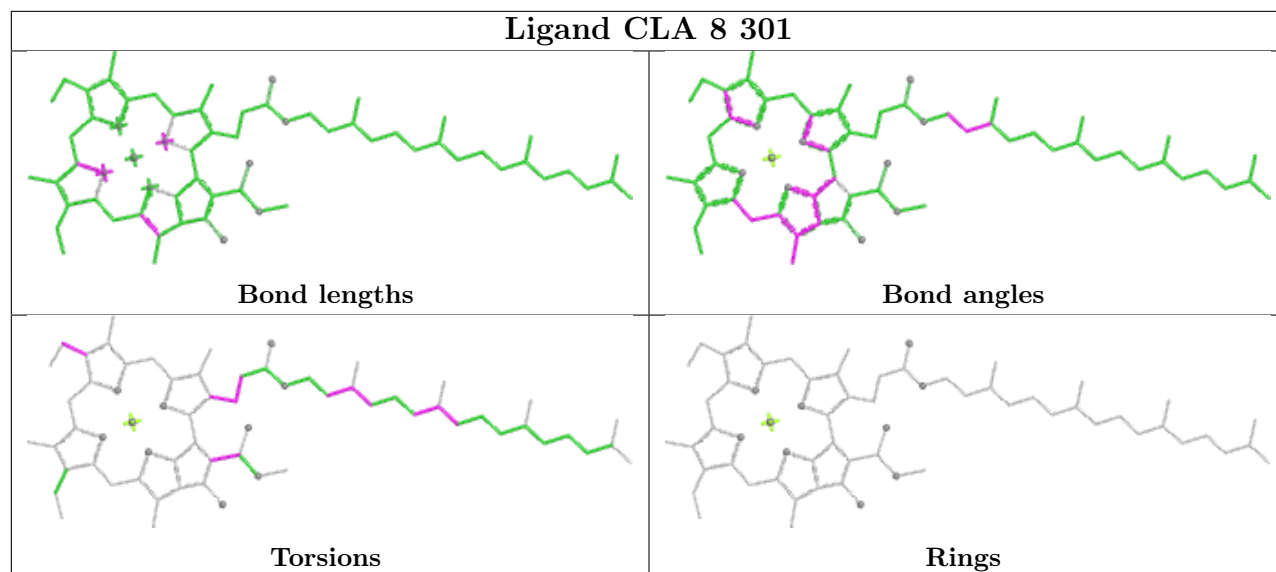
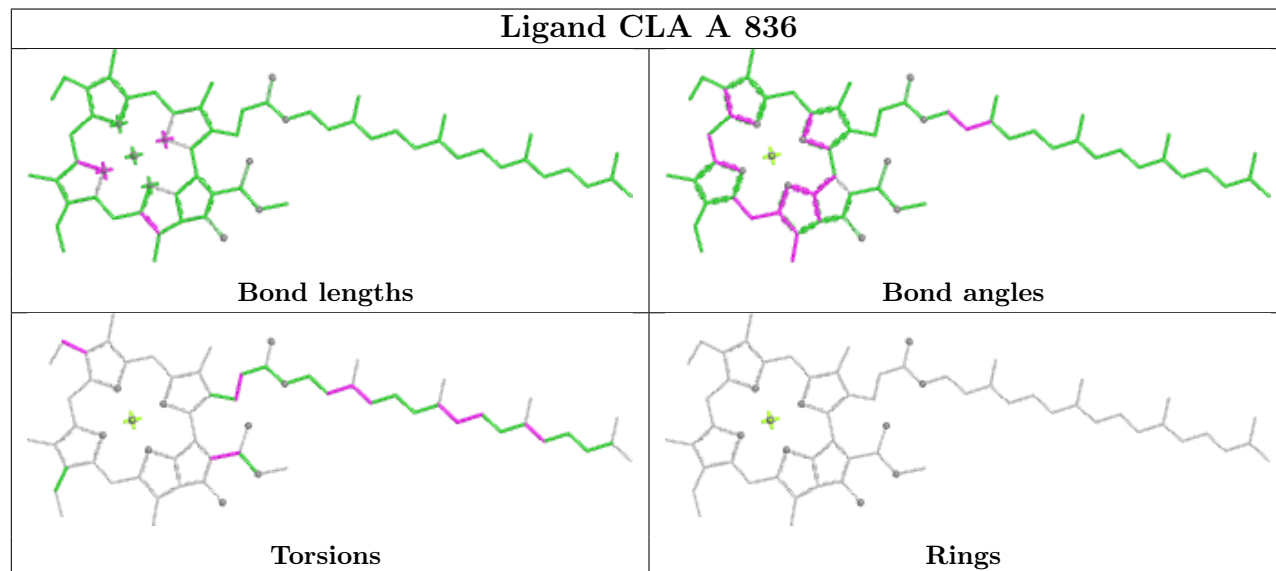


Torsions

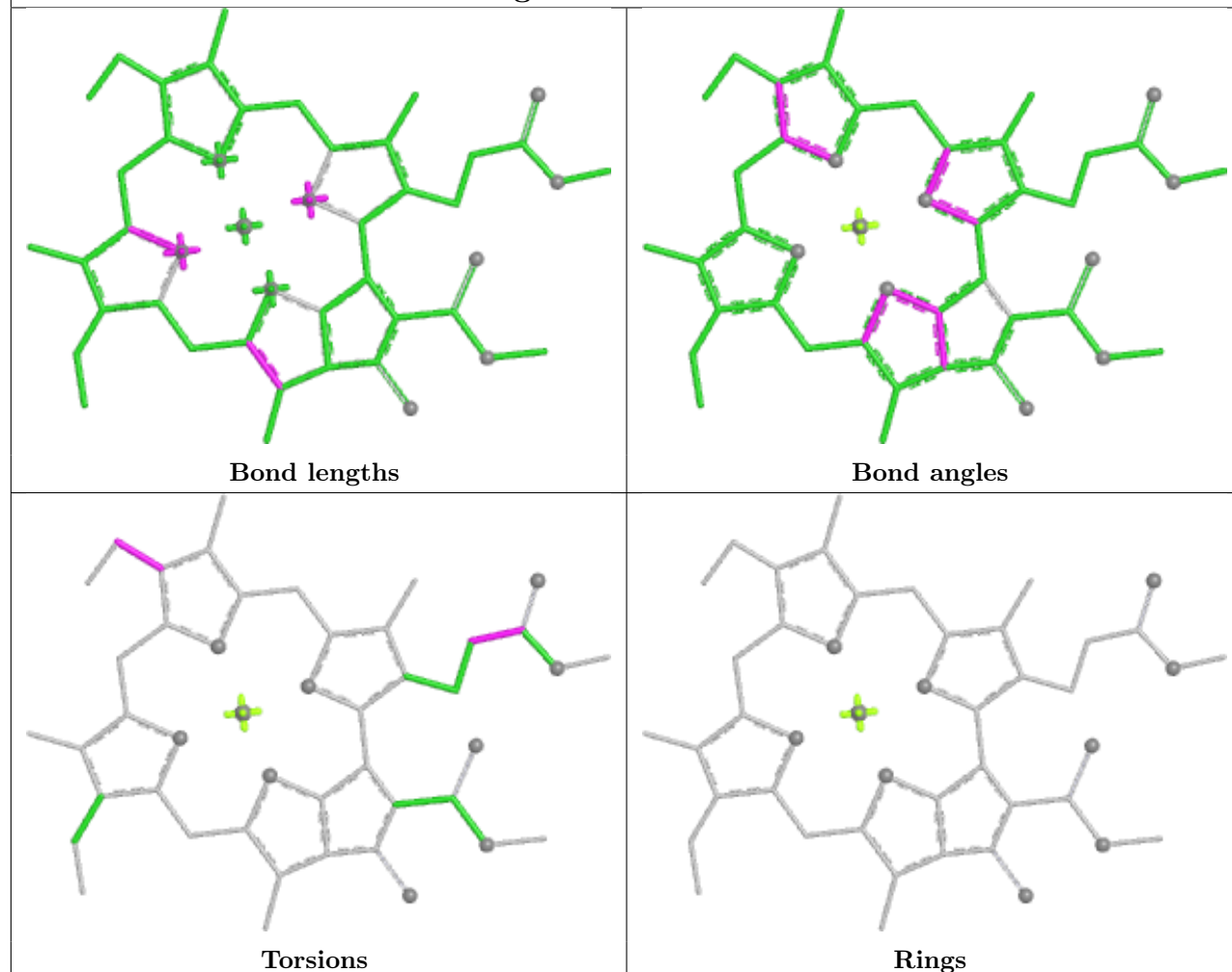


Rings

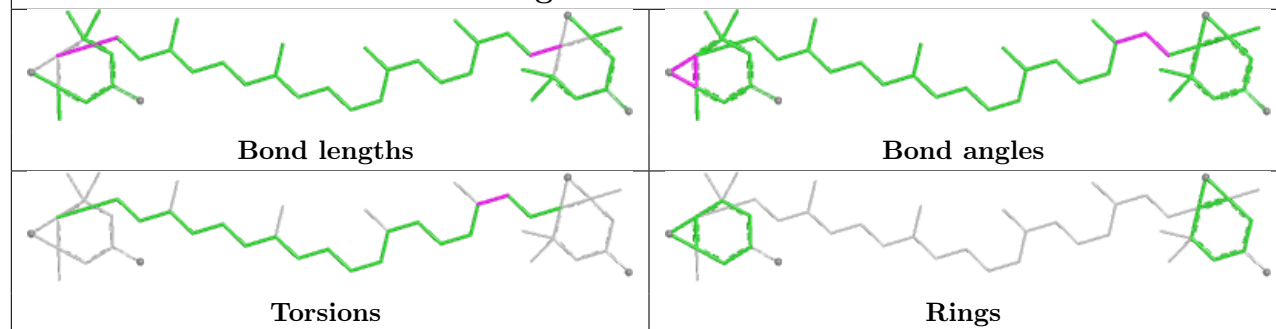


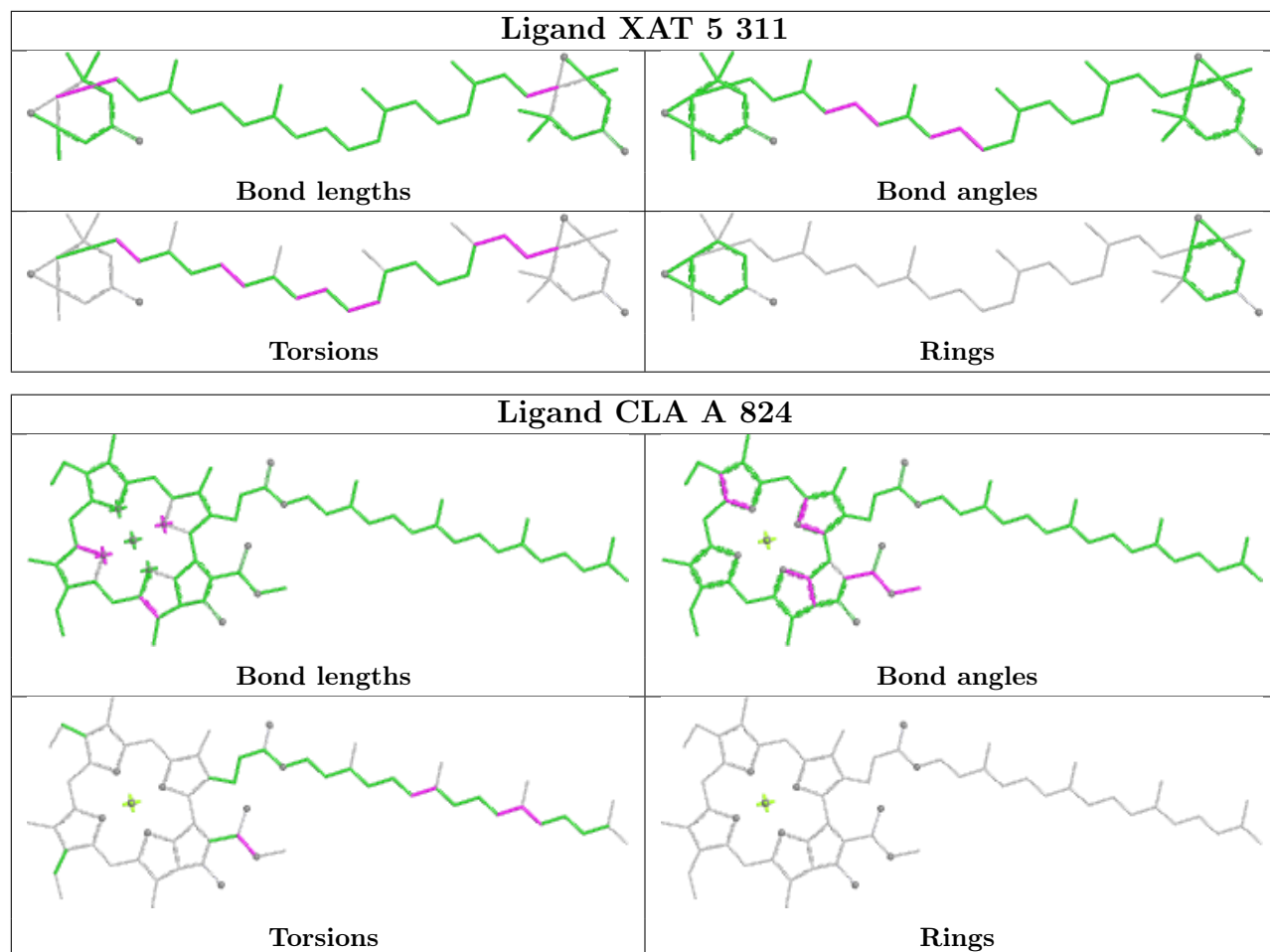
Ligand CLA 8 301**Ligand CLA A 836**

Ligand CLA B 818

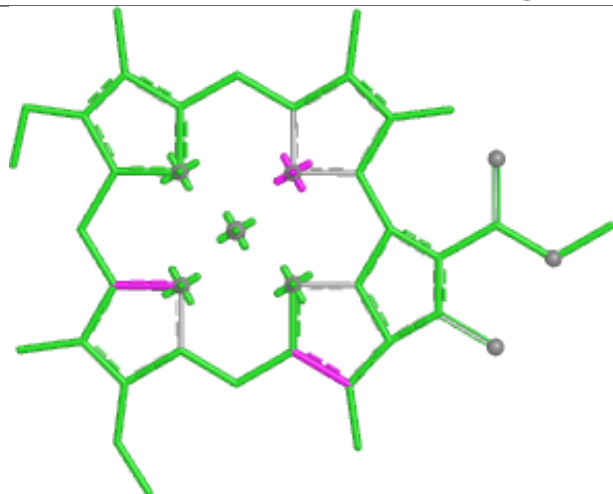


Ligand XAT 8 311

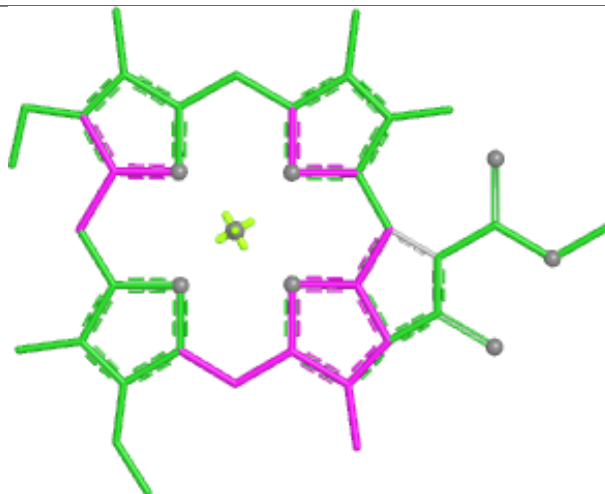




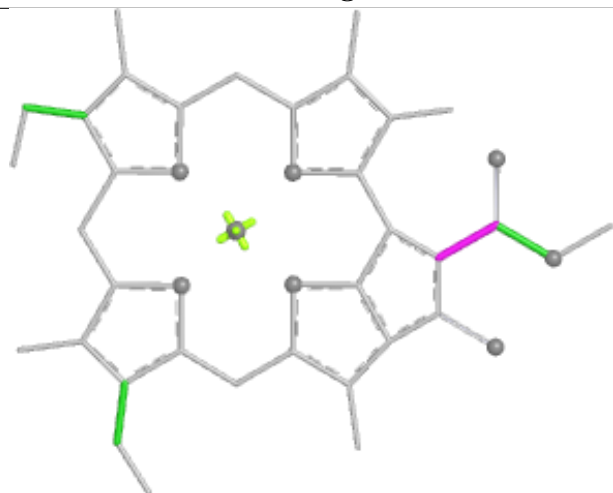
Ligand CLA 5 306



Bond lengths



Bond angles

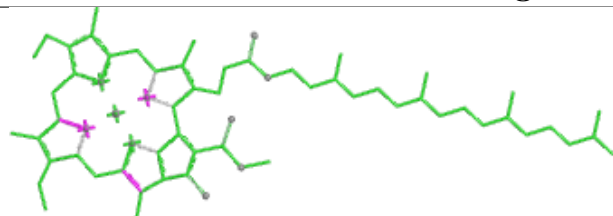


Torsions

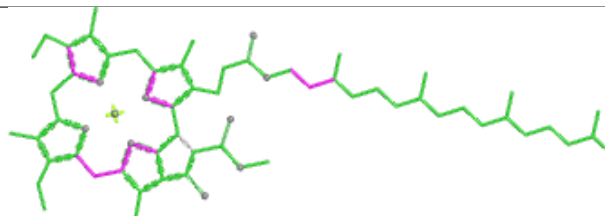


Rings

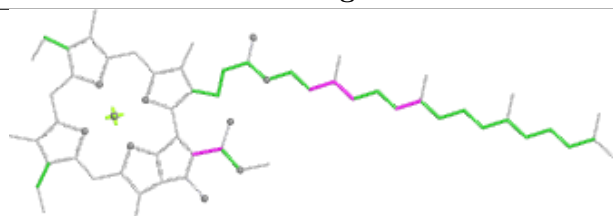
Ligand CLA B 826



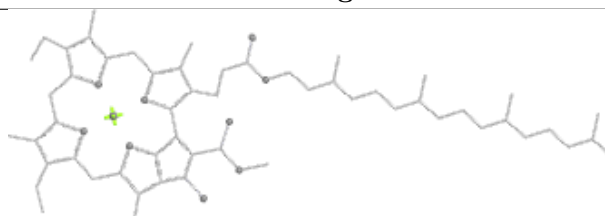
Bond lengths



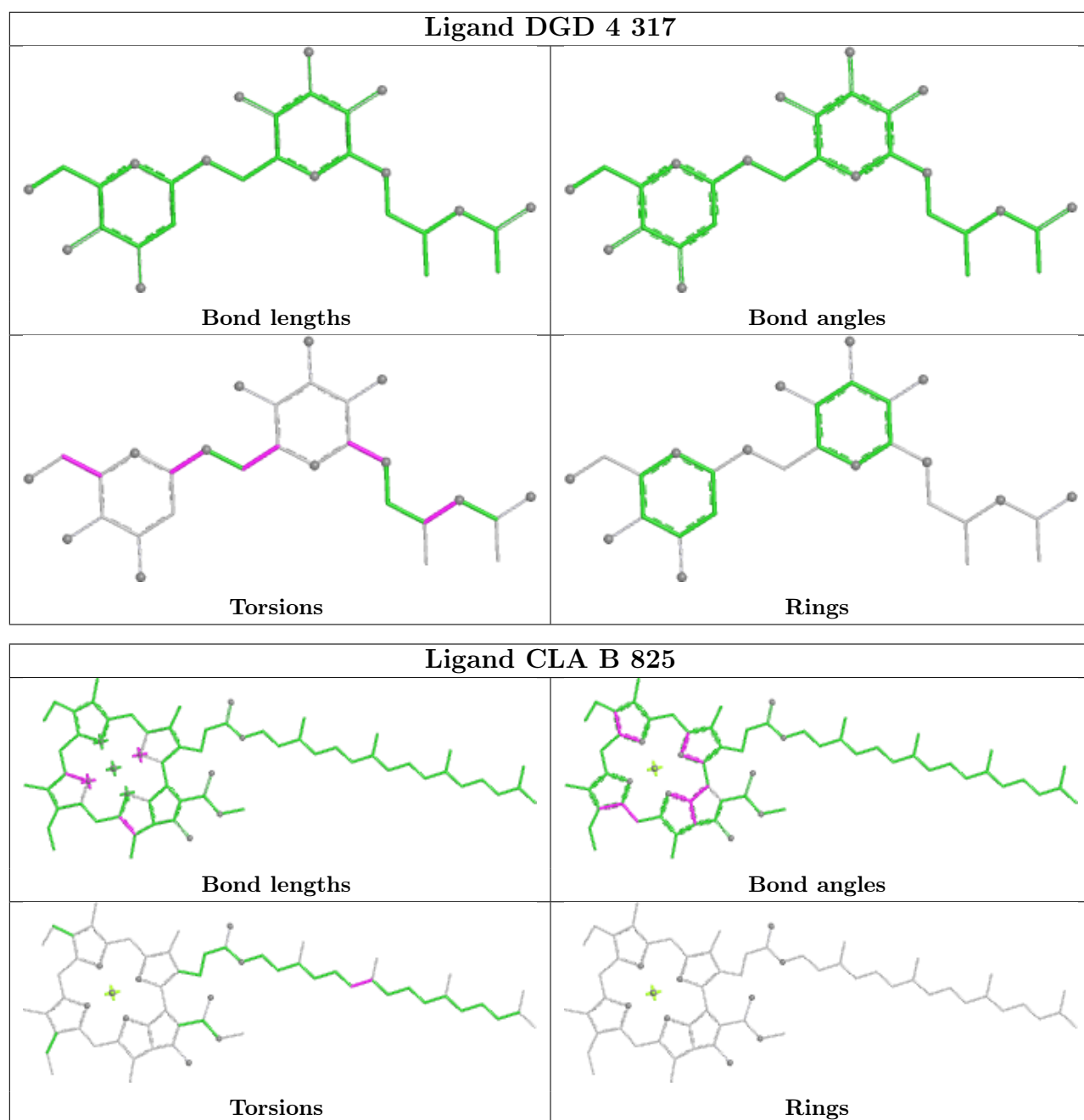
Bond angles

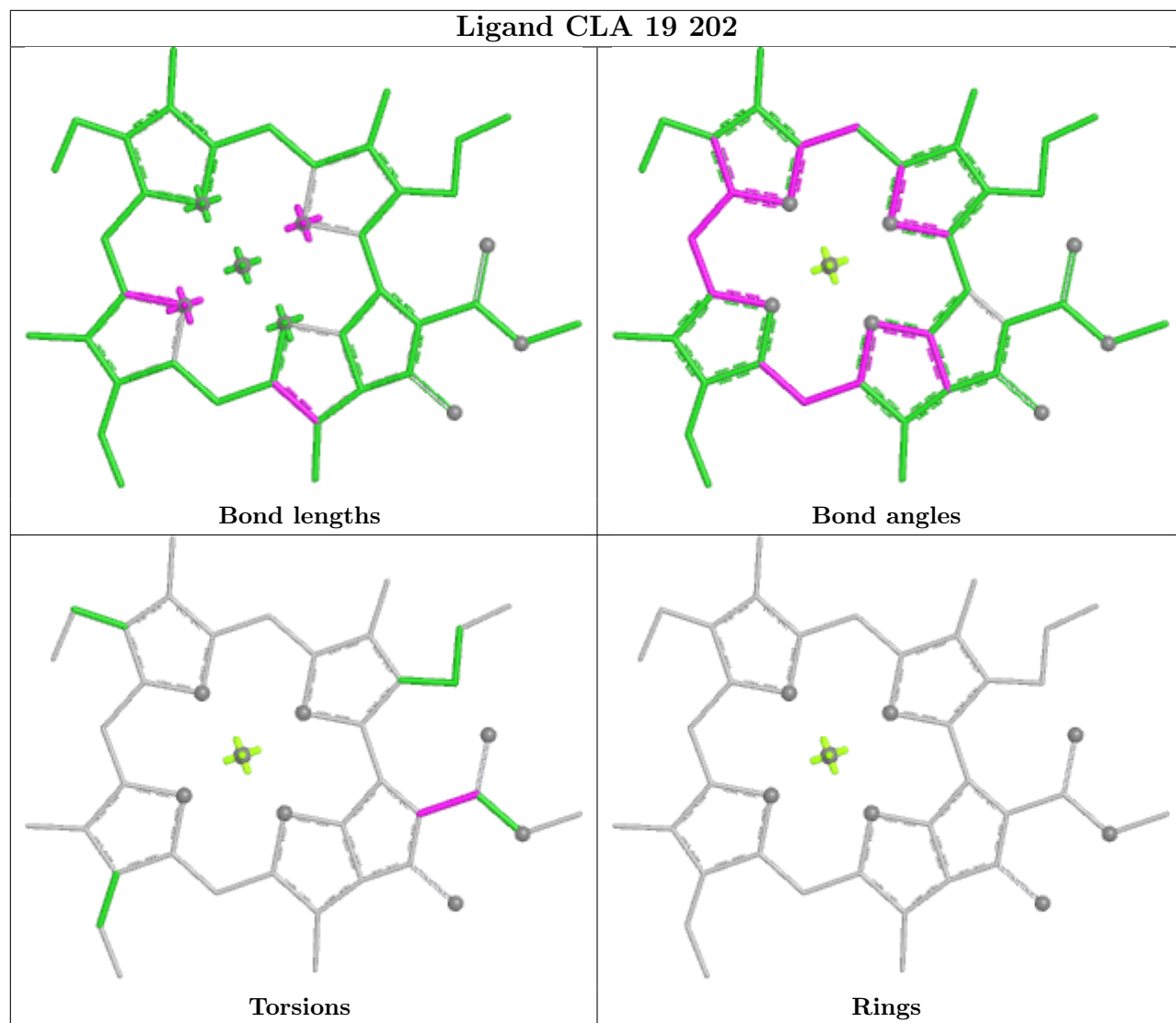


Torsions

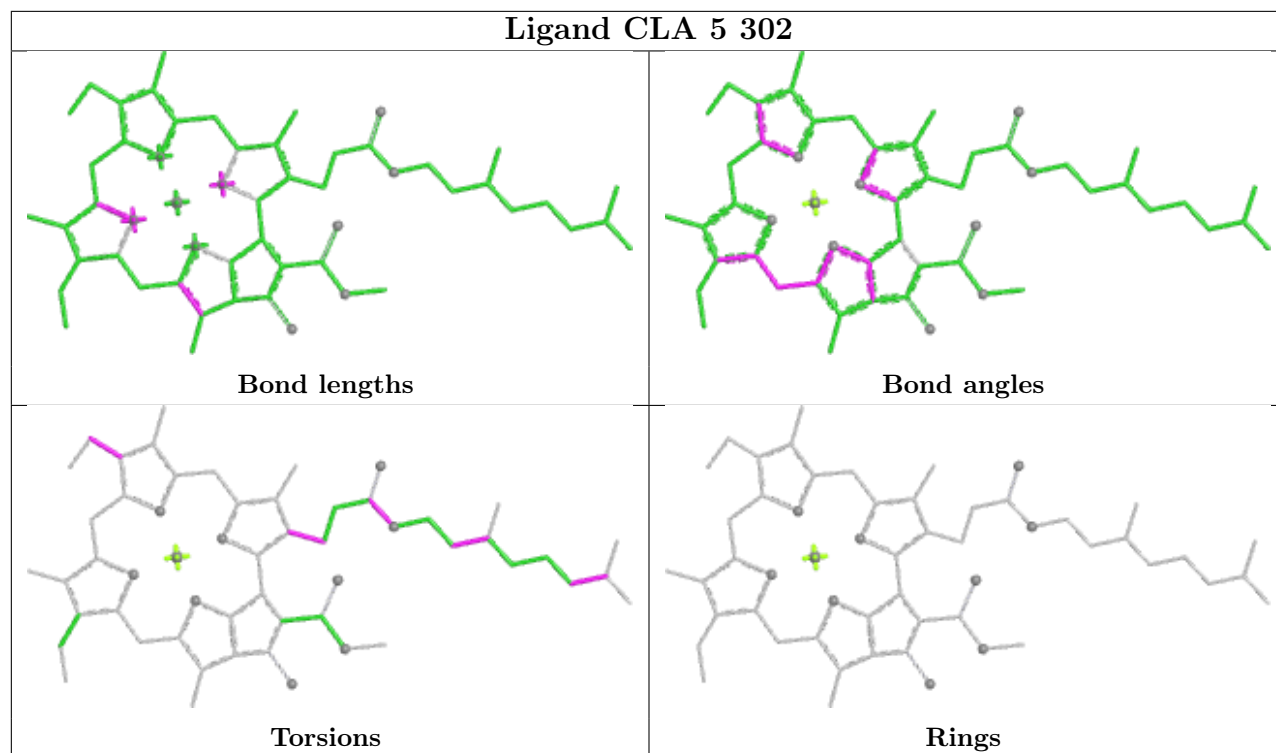


Rings

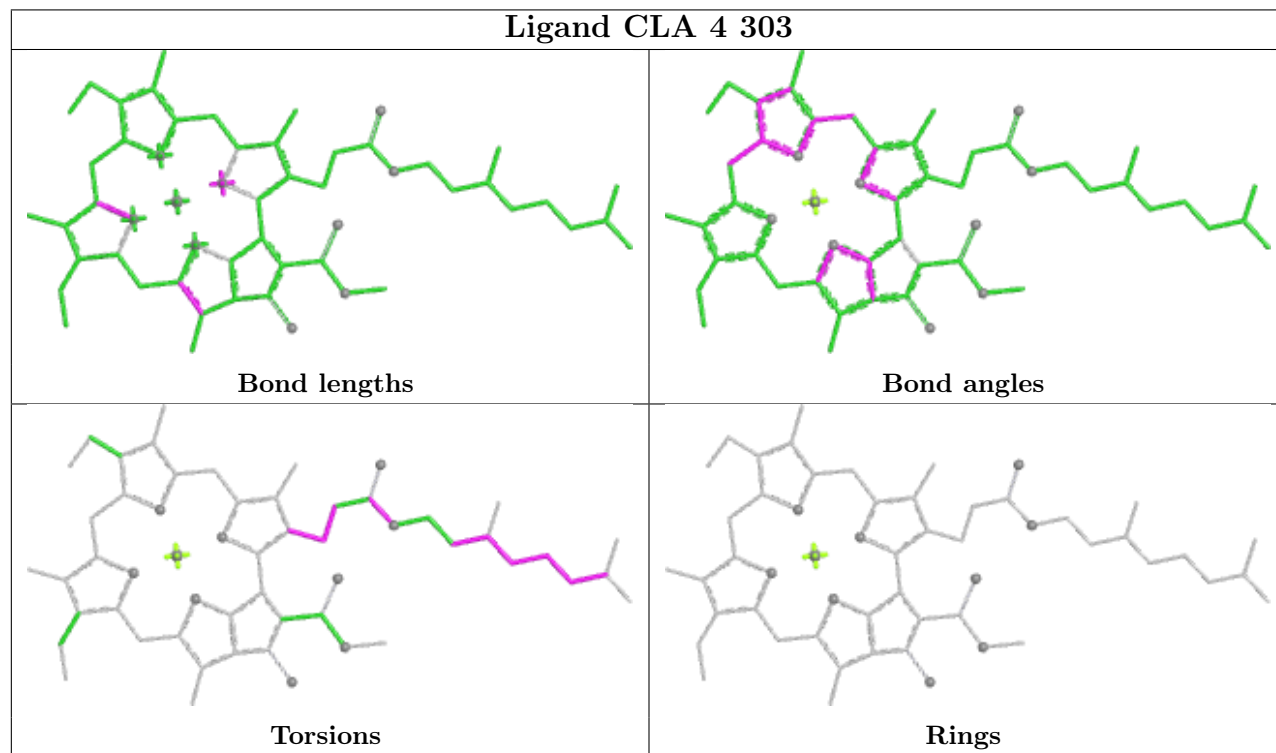


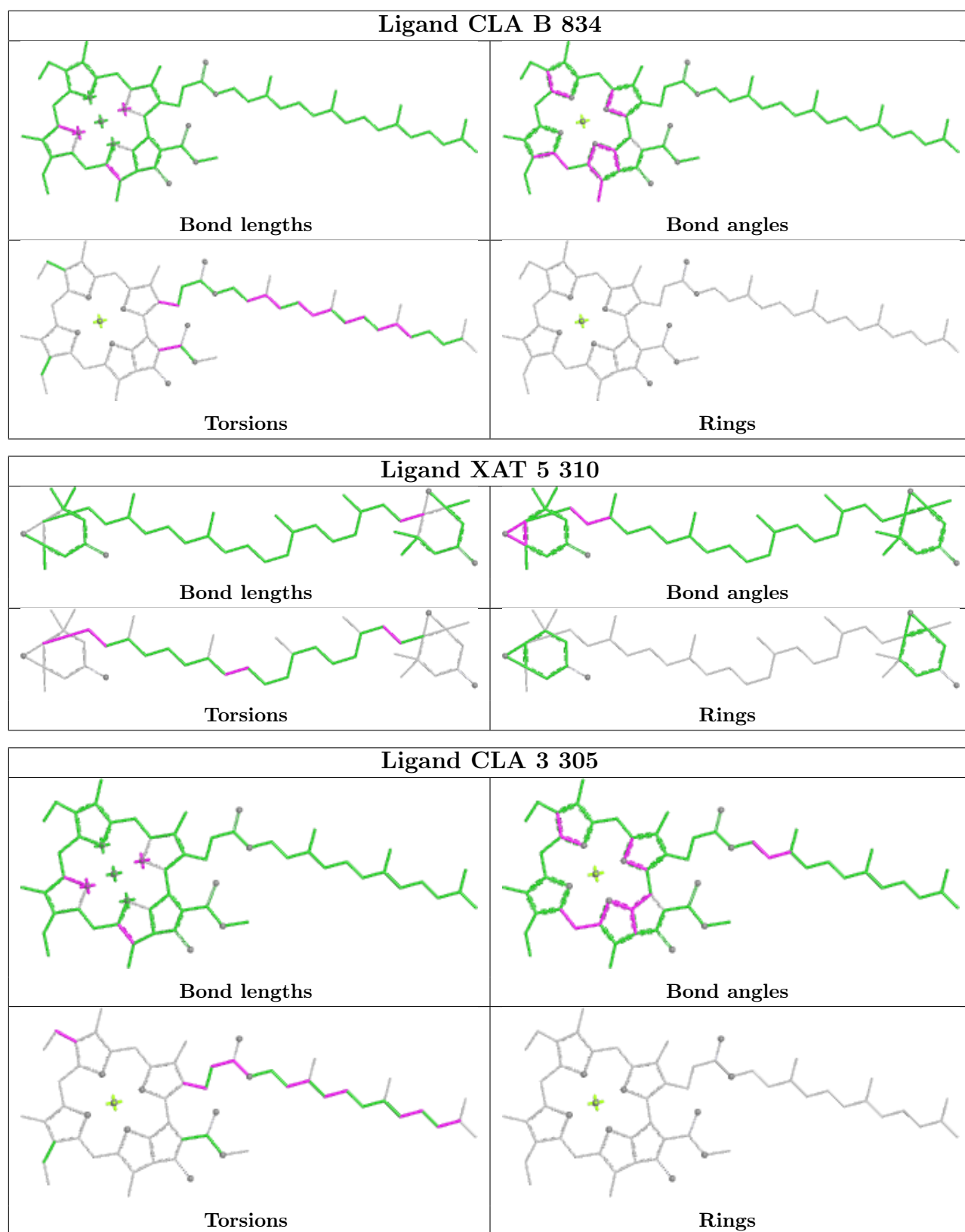


Ligand CLA 5 302

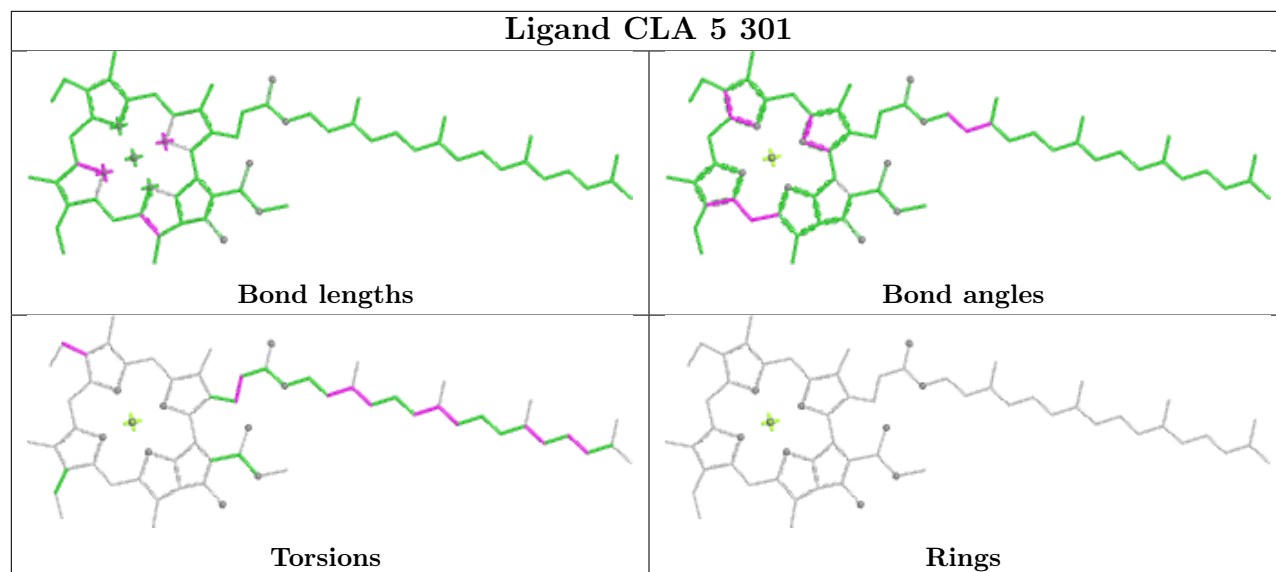


Ligand CLA 4 303

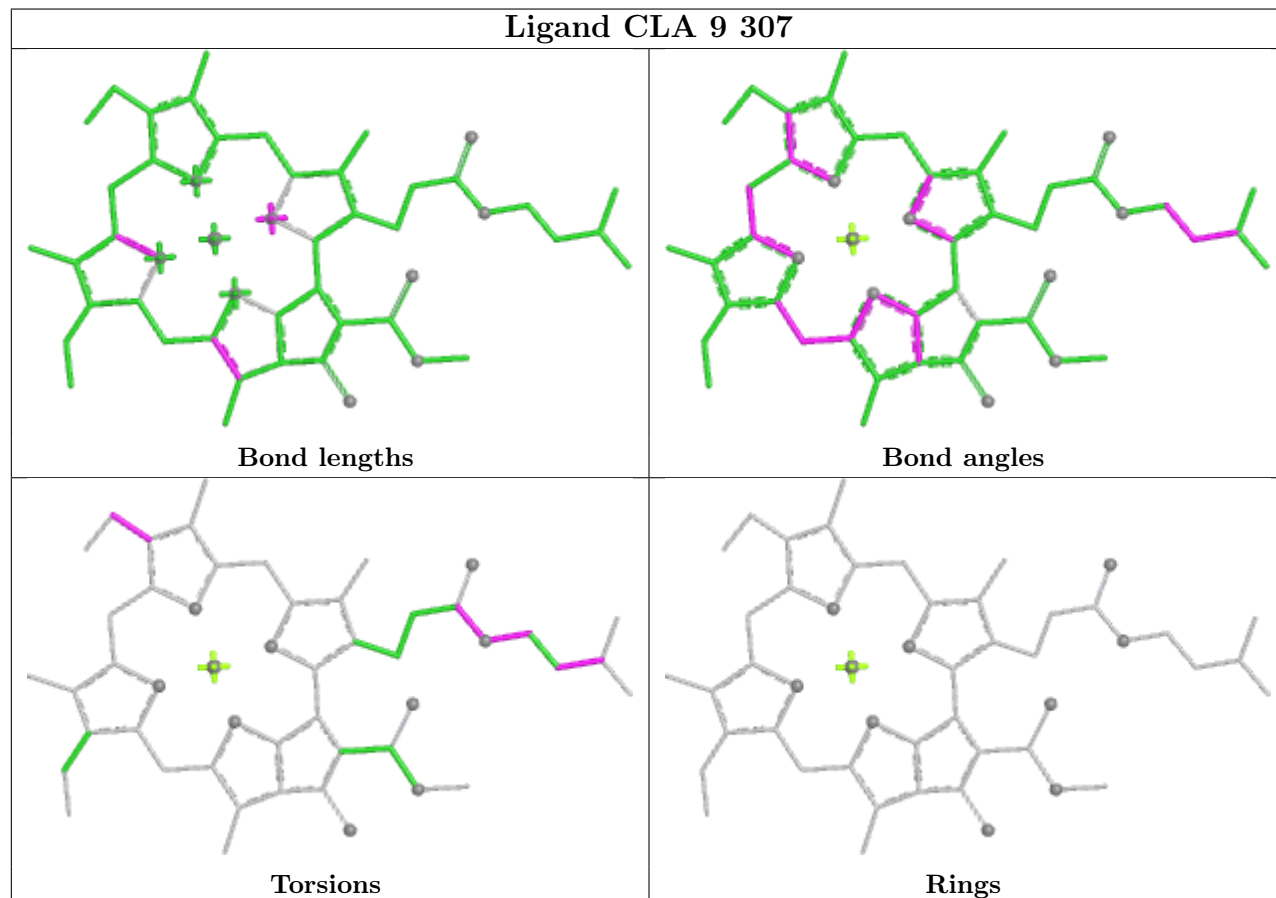


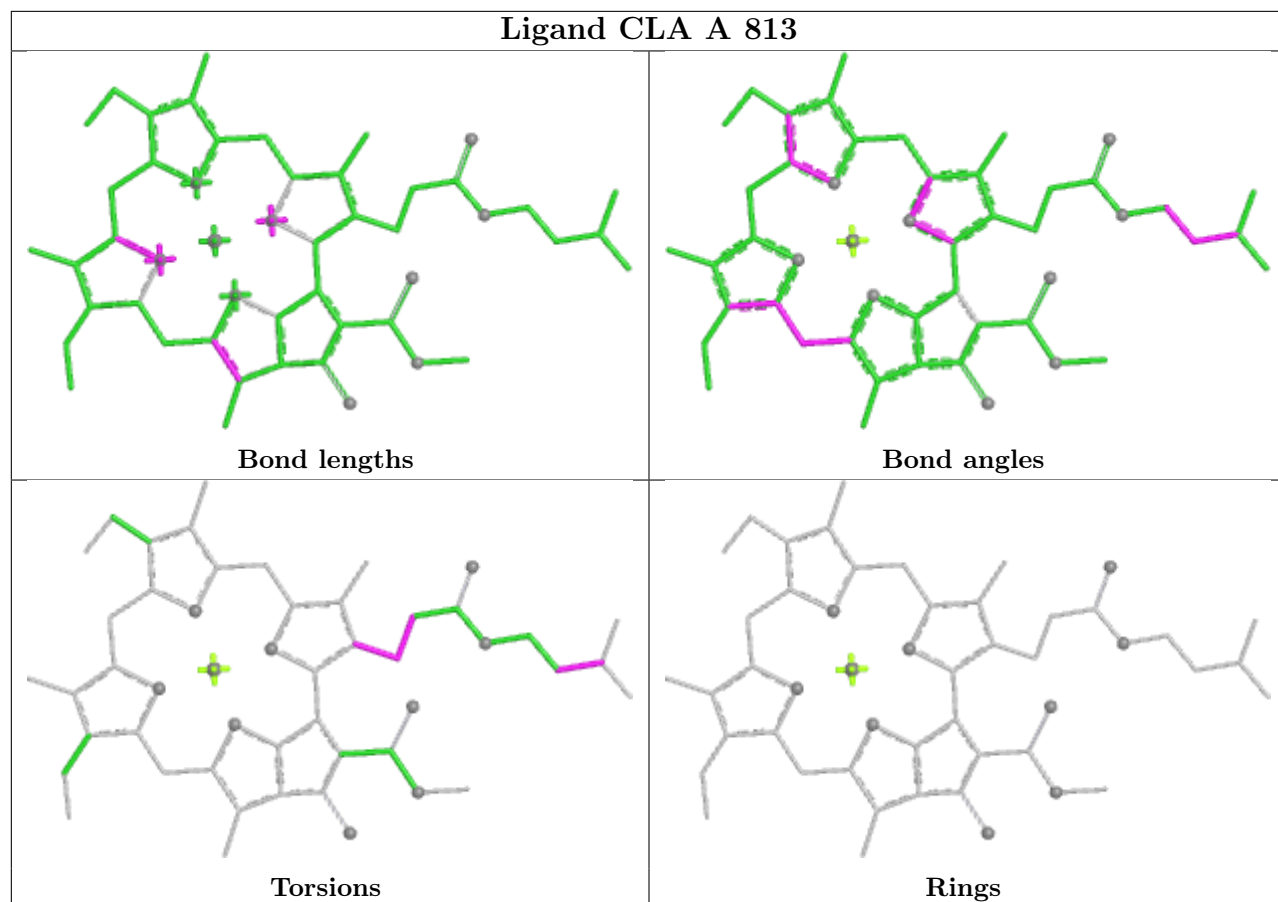


Ligand CLA 5 301

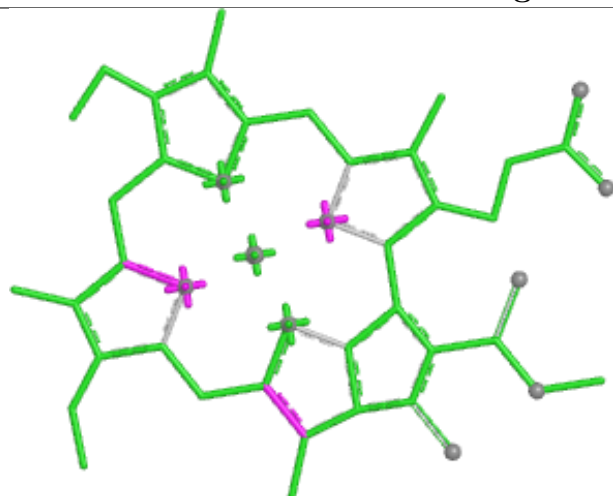


Ligand CLA 9 307

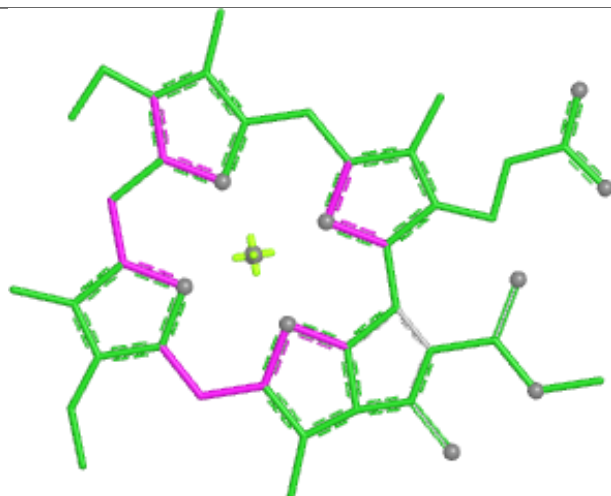




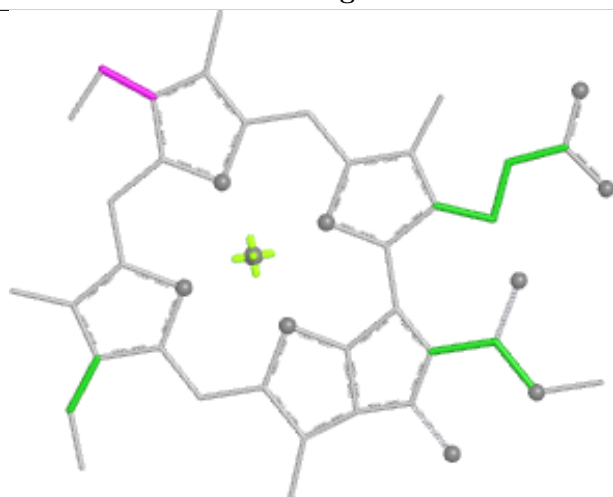
Ligand CLA A 832



Bond lengths



Bond angles

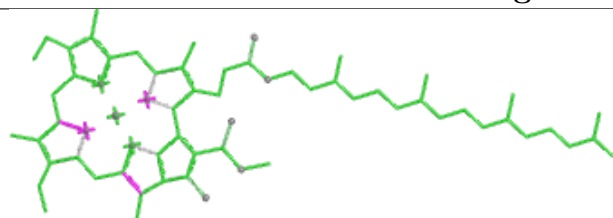


Torsions

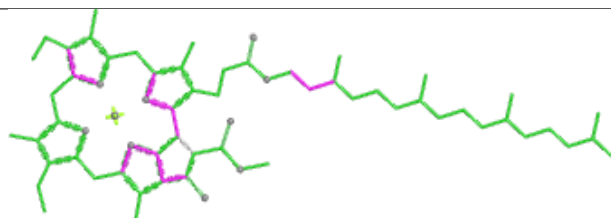


Rings

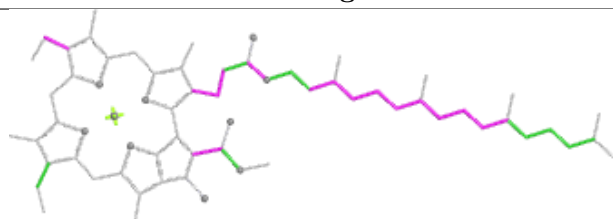
Ligand CLA A 815



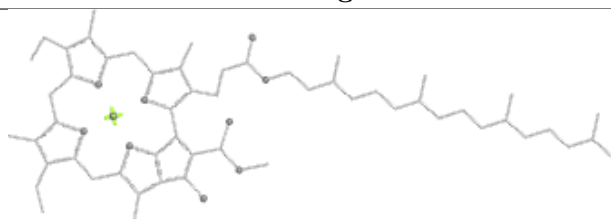
Bond lengths



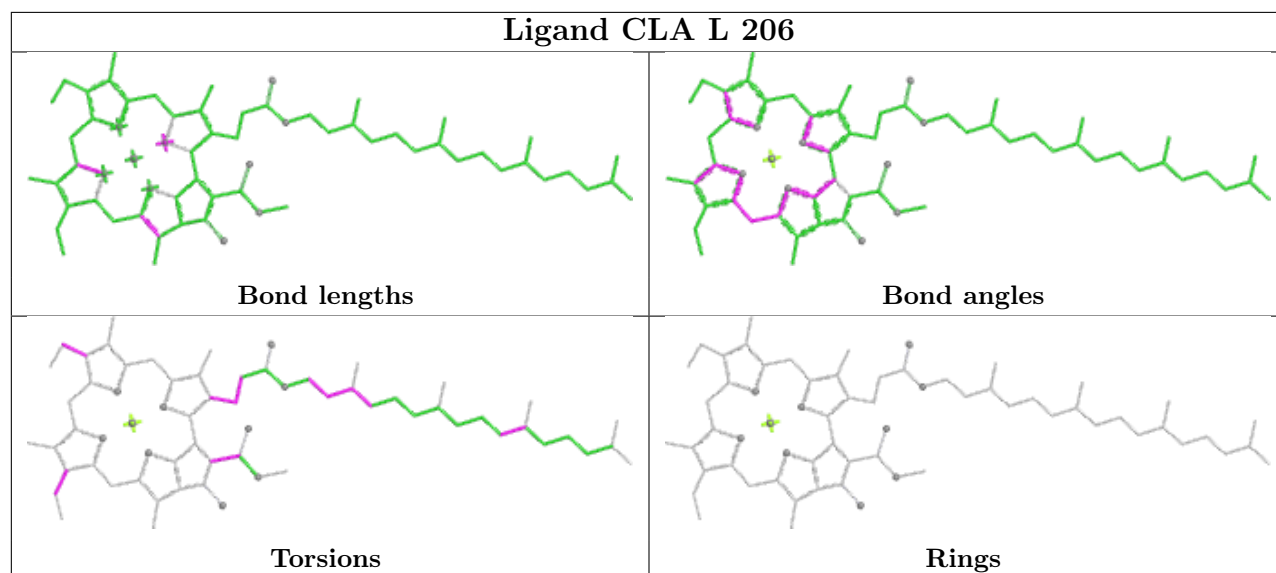
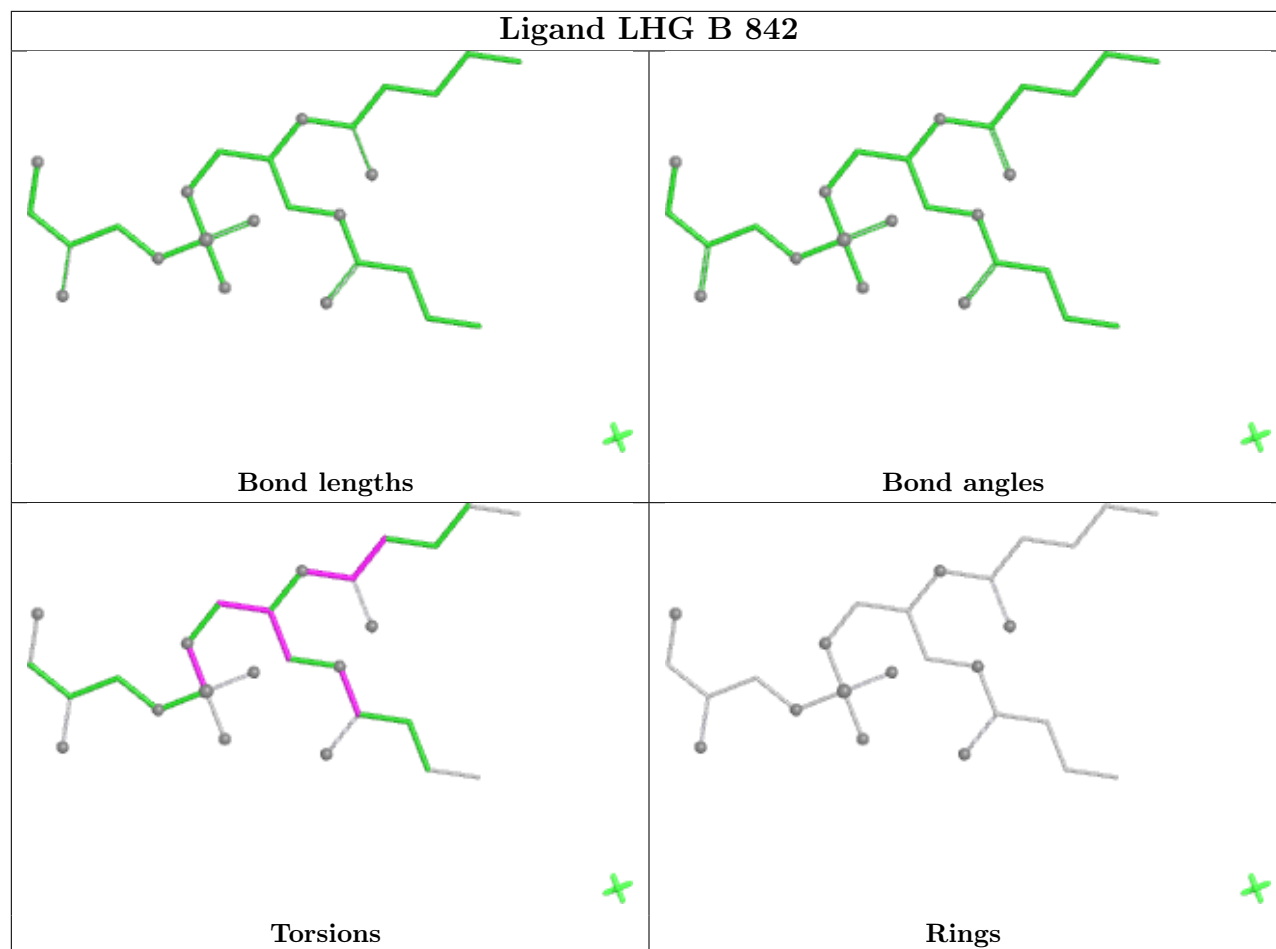
Bond angles

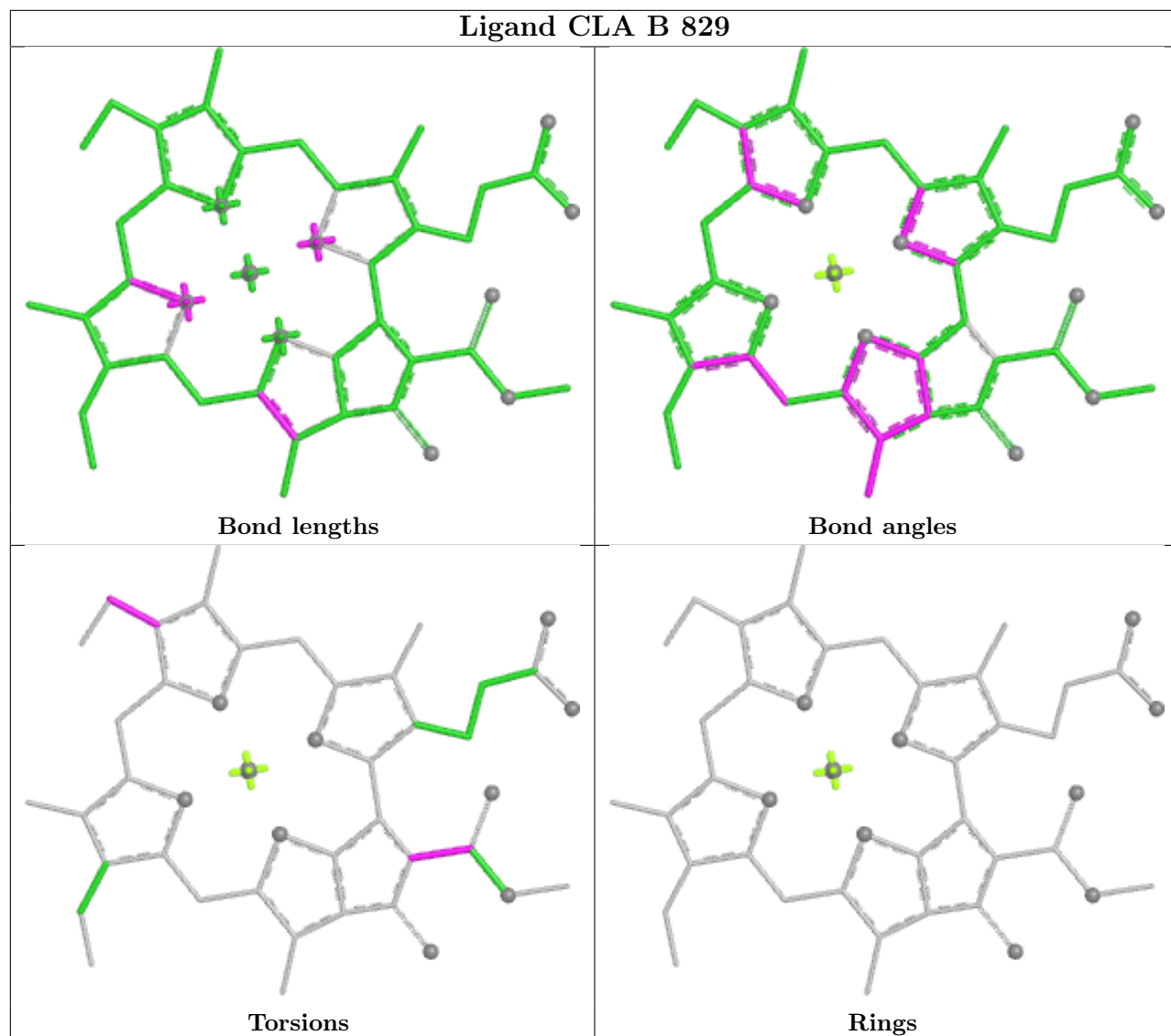


Torsions

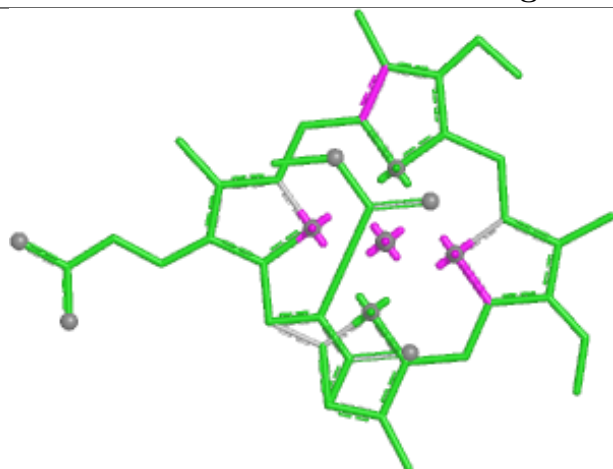


Rings

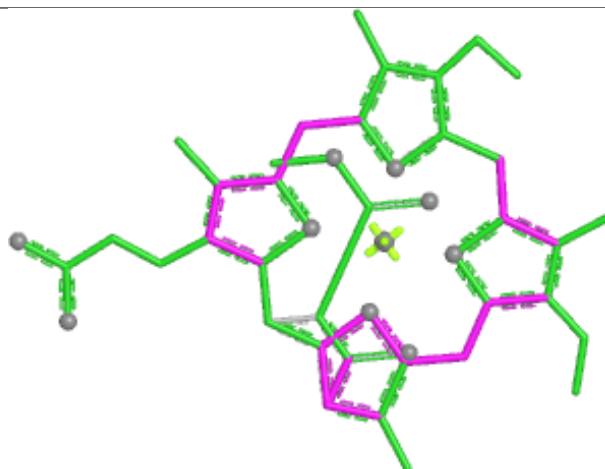




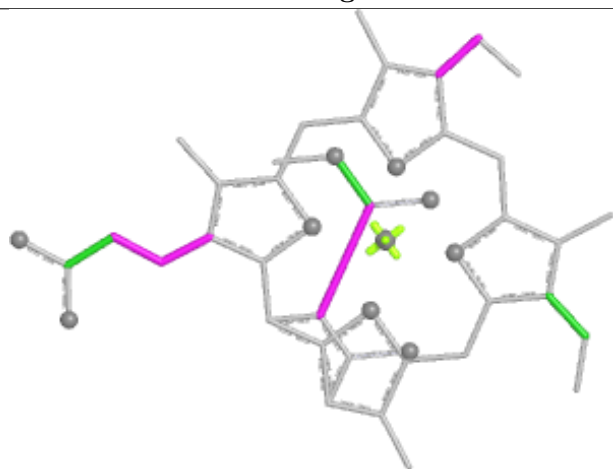
Ligand KC1 1 306



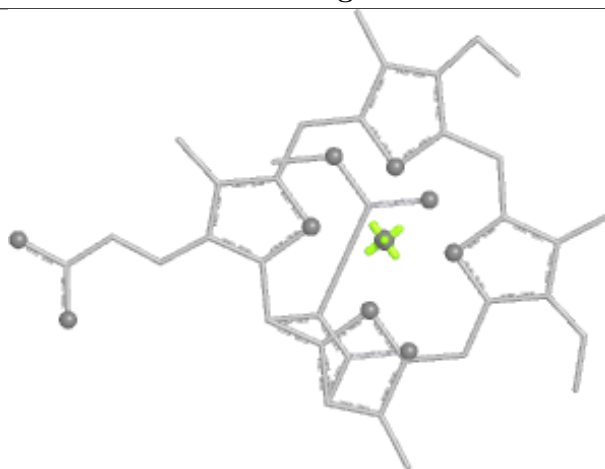
Bond lengths



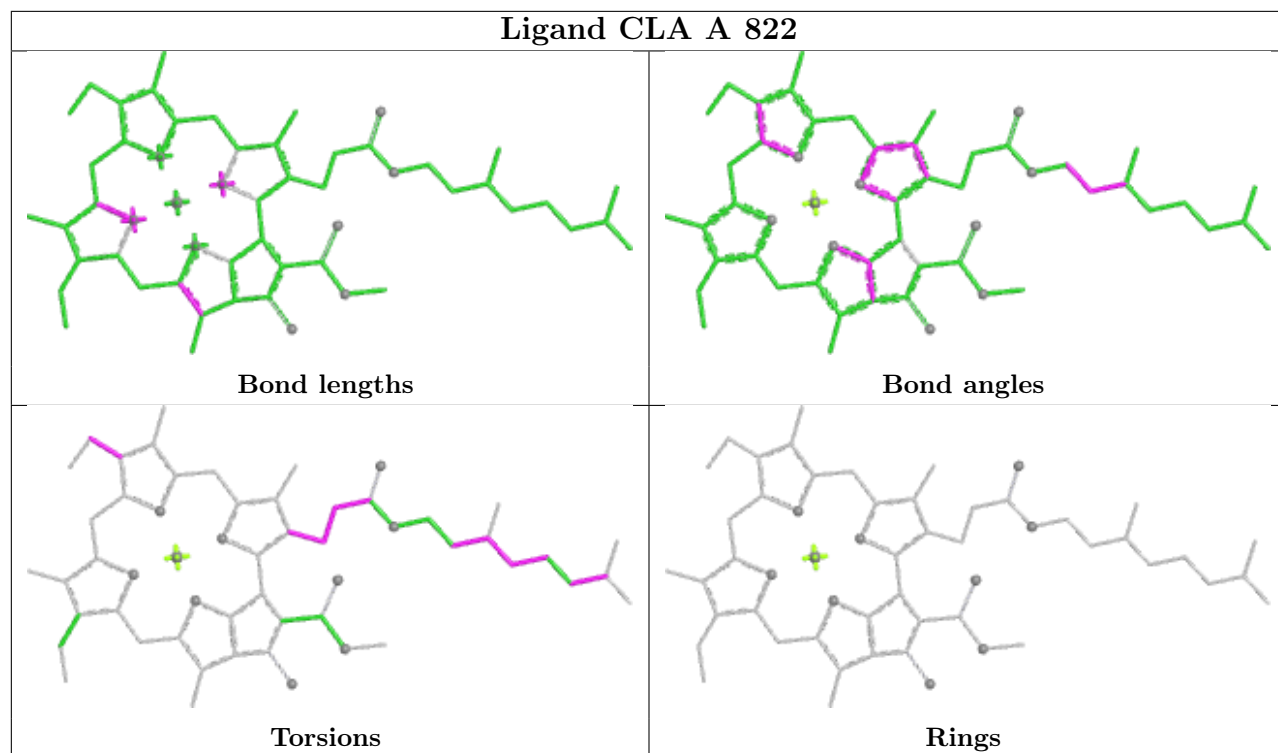
Bond angles

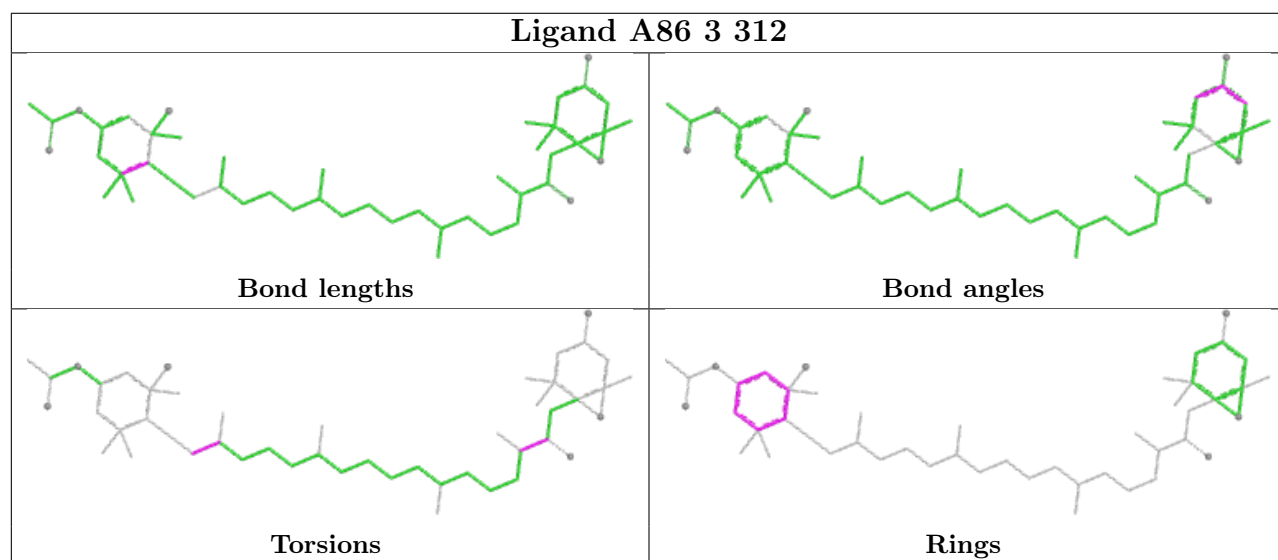
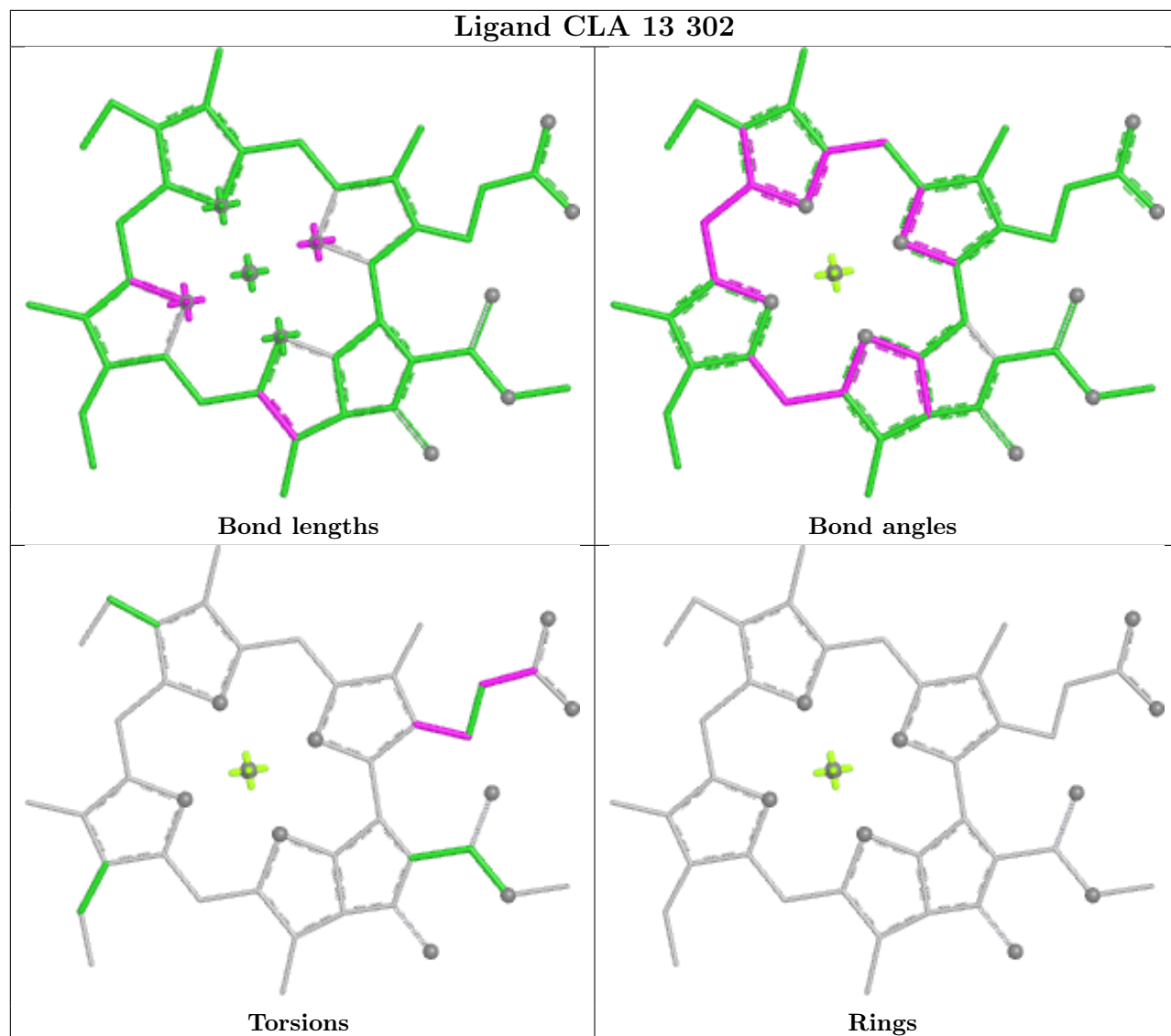


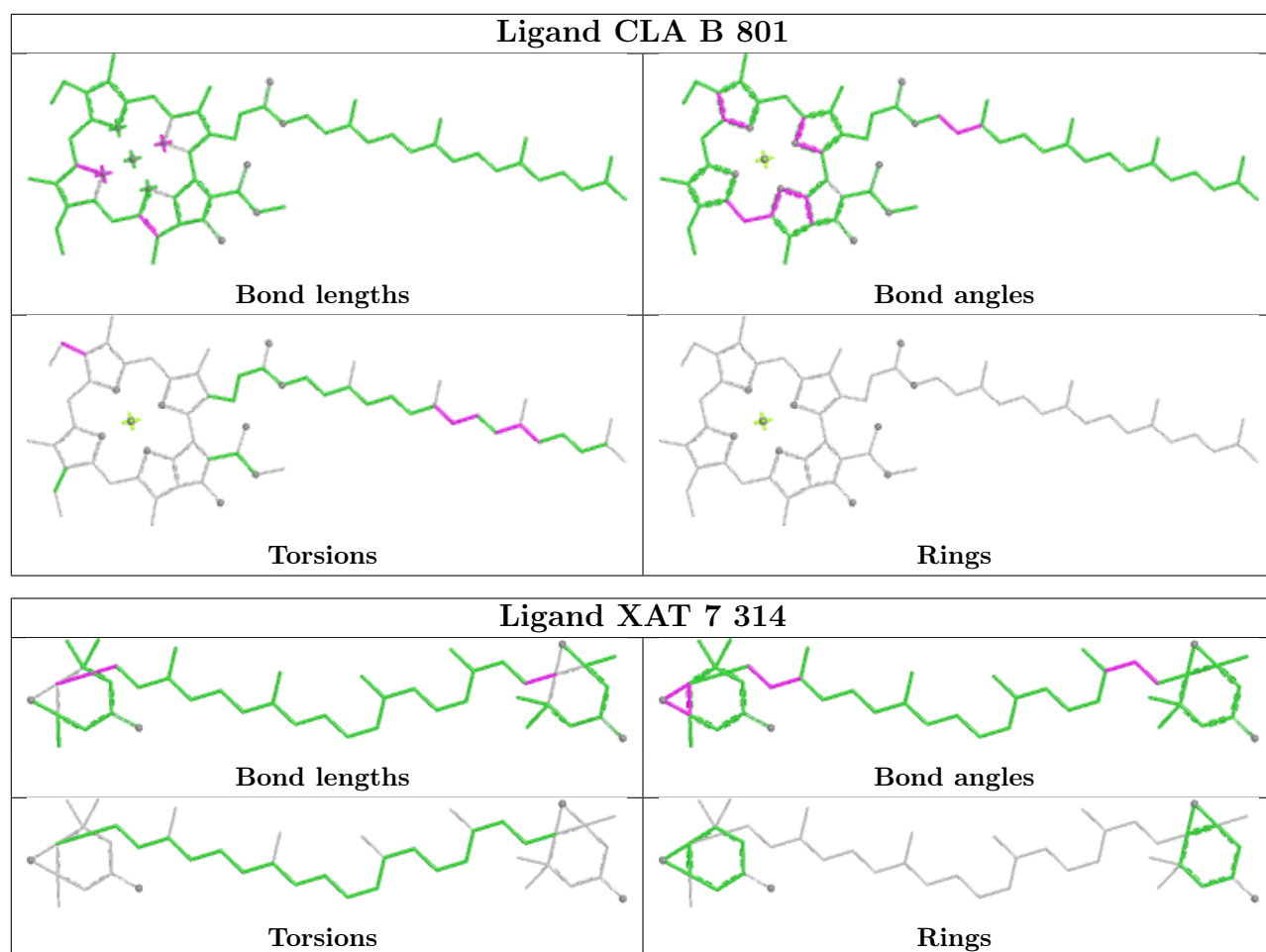
Torsions



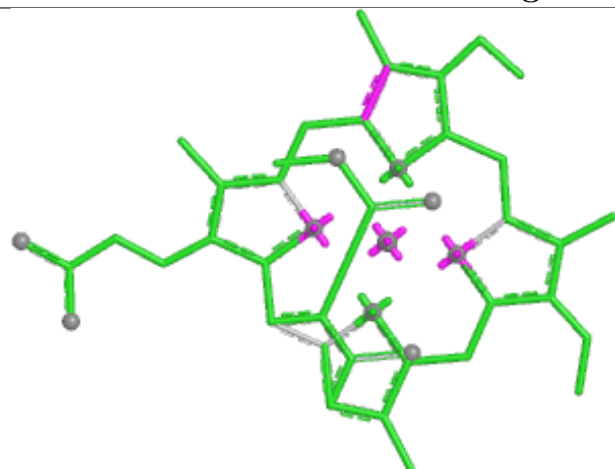
Rings



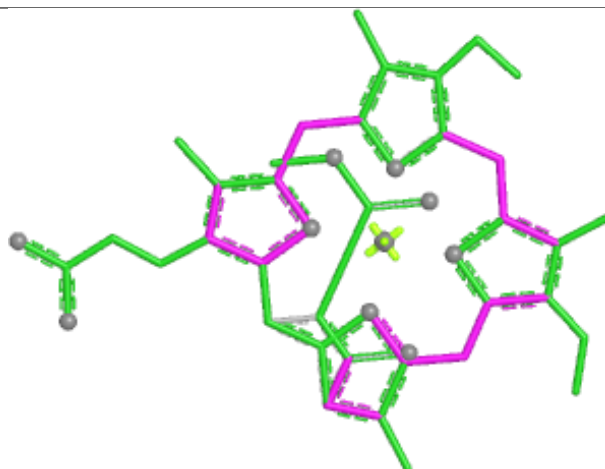




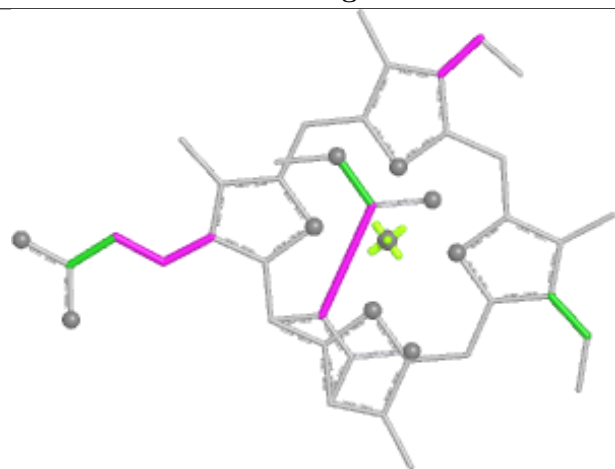
Ligand KC1 5 308



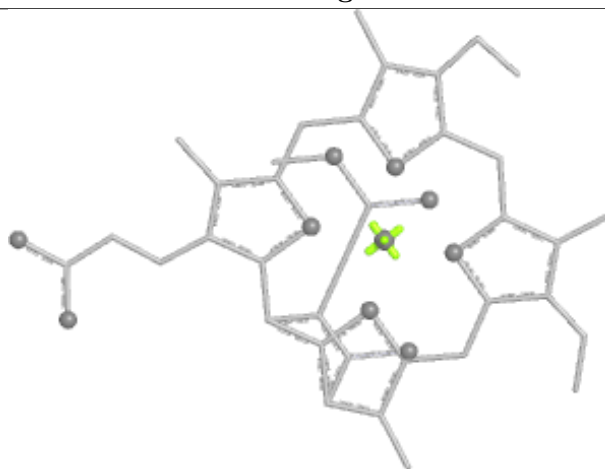
Bond lengths



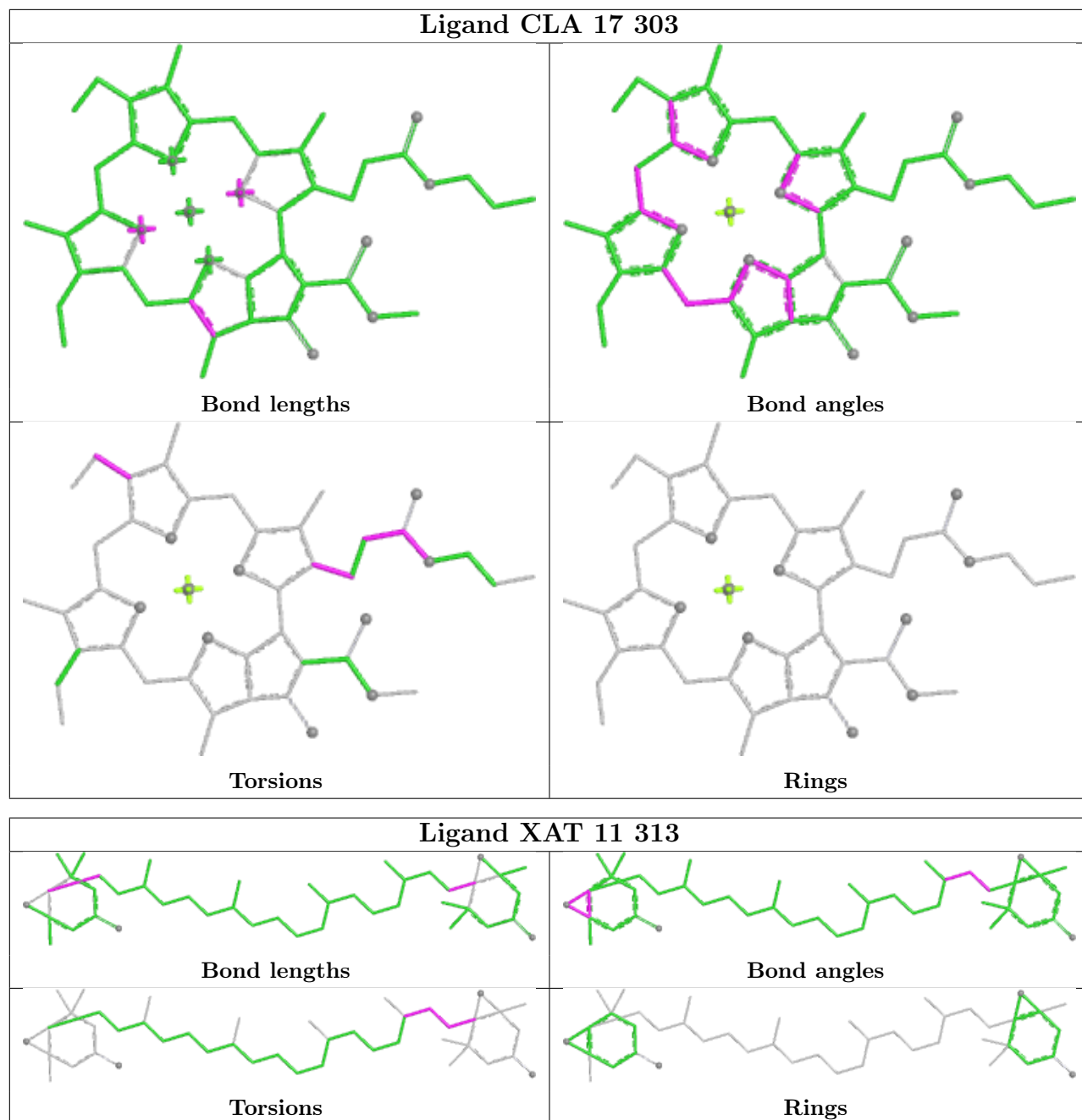
Bond angles

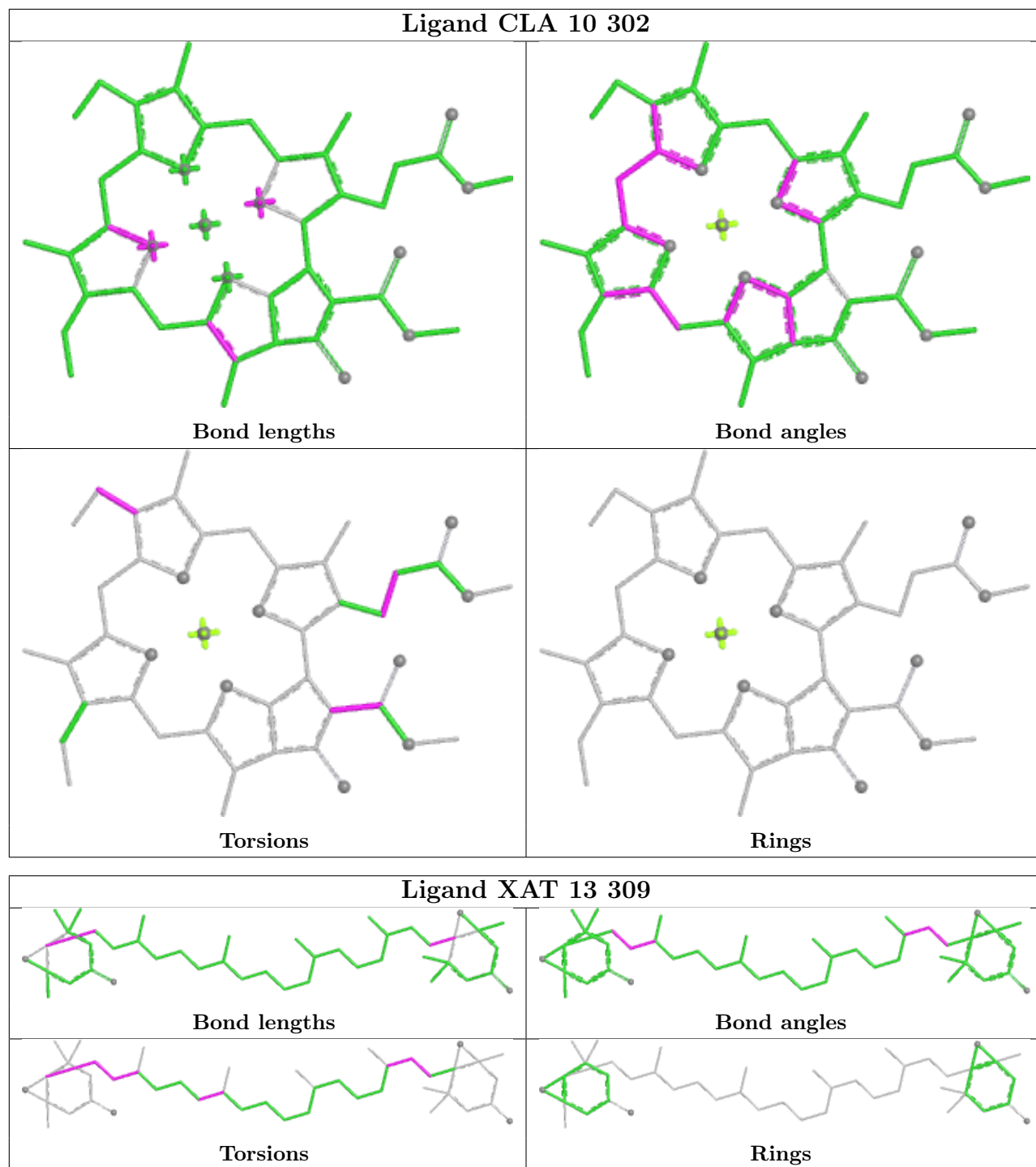


Torsions

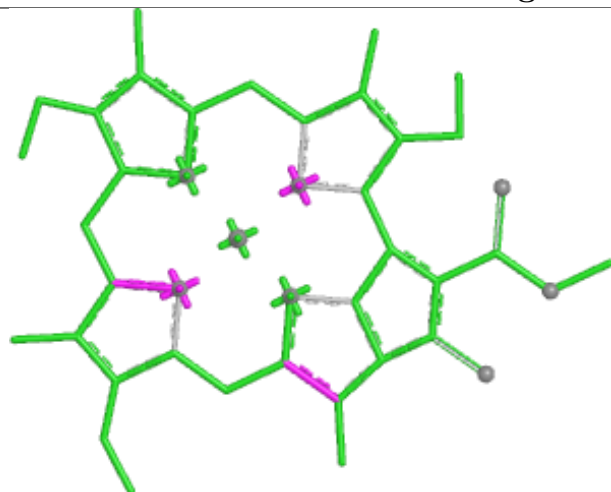


Rings

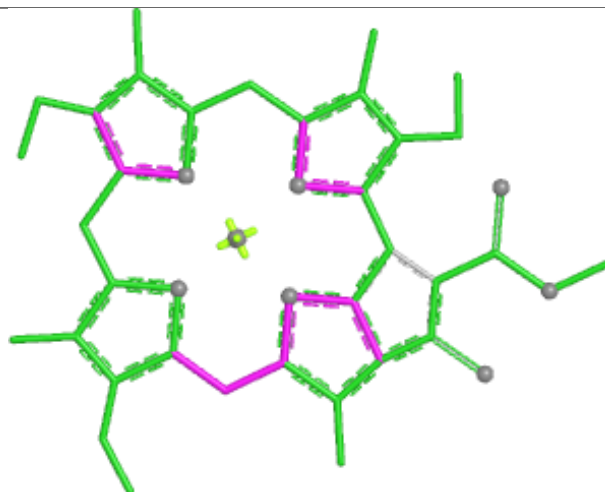




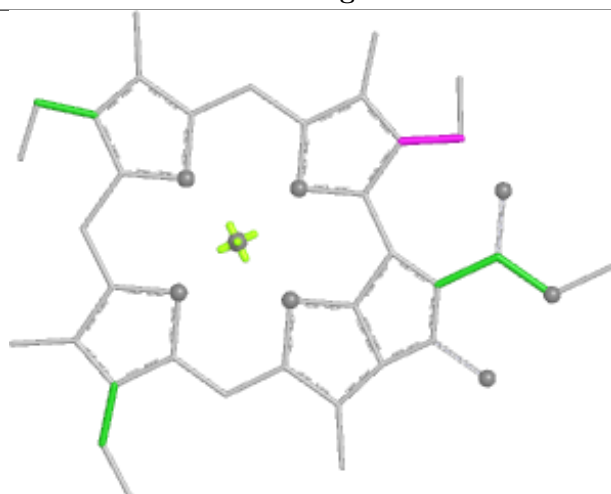
Ligand CLA J 103



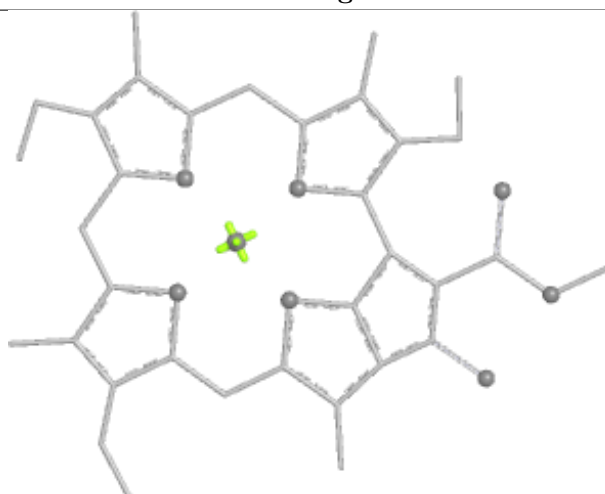
Bond lengths



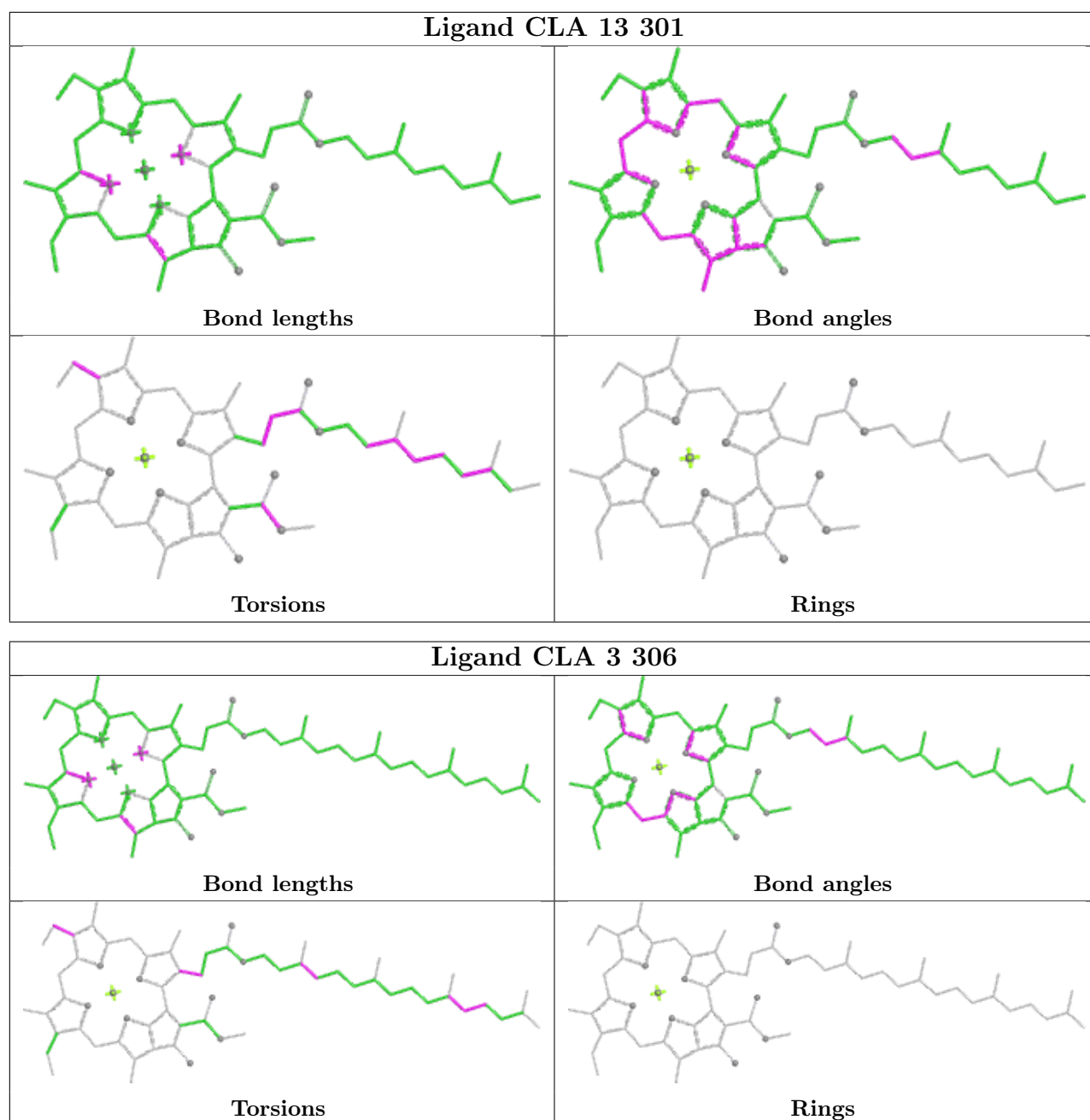
Bond angles

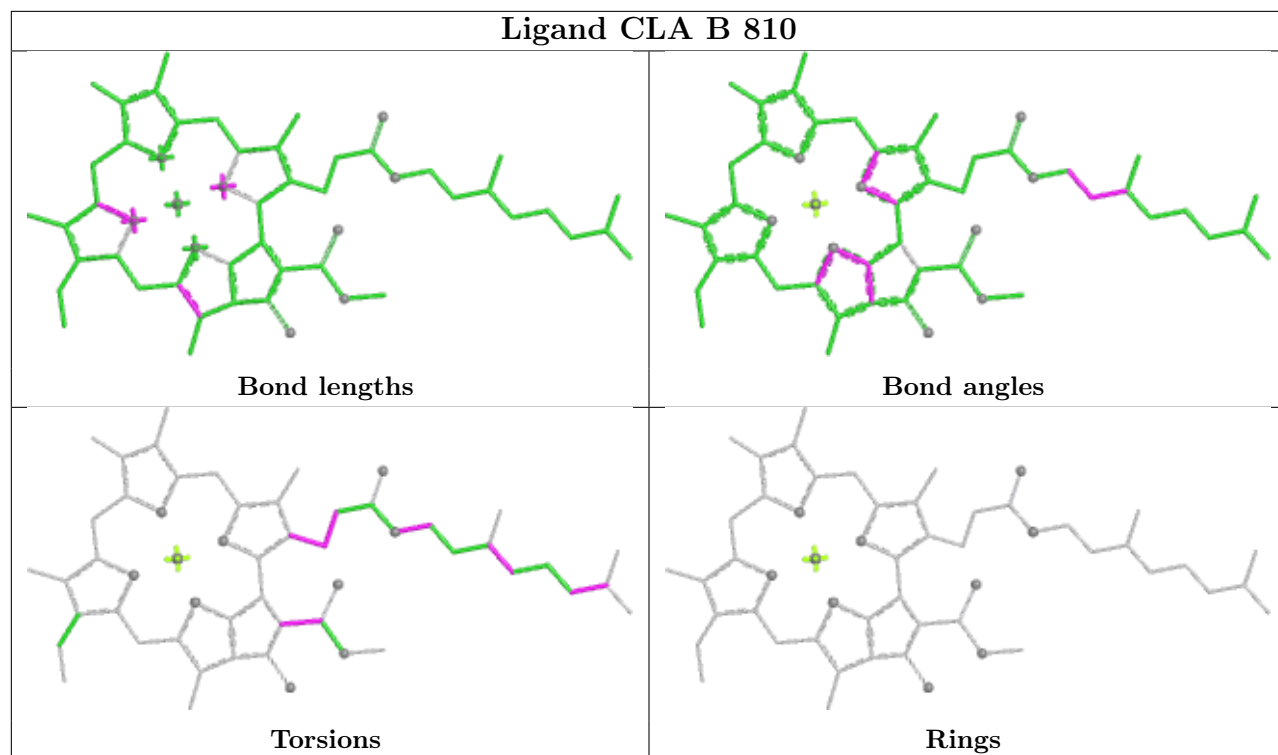


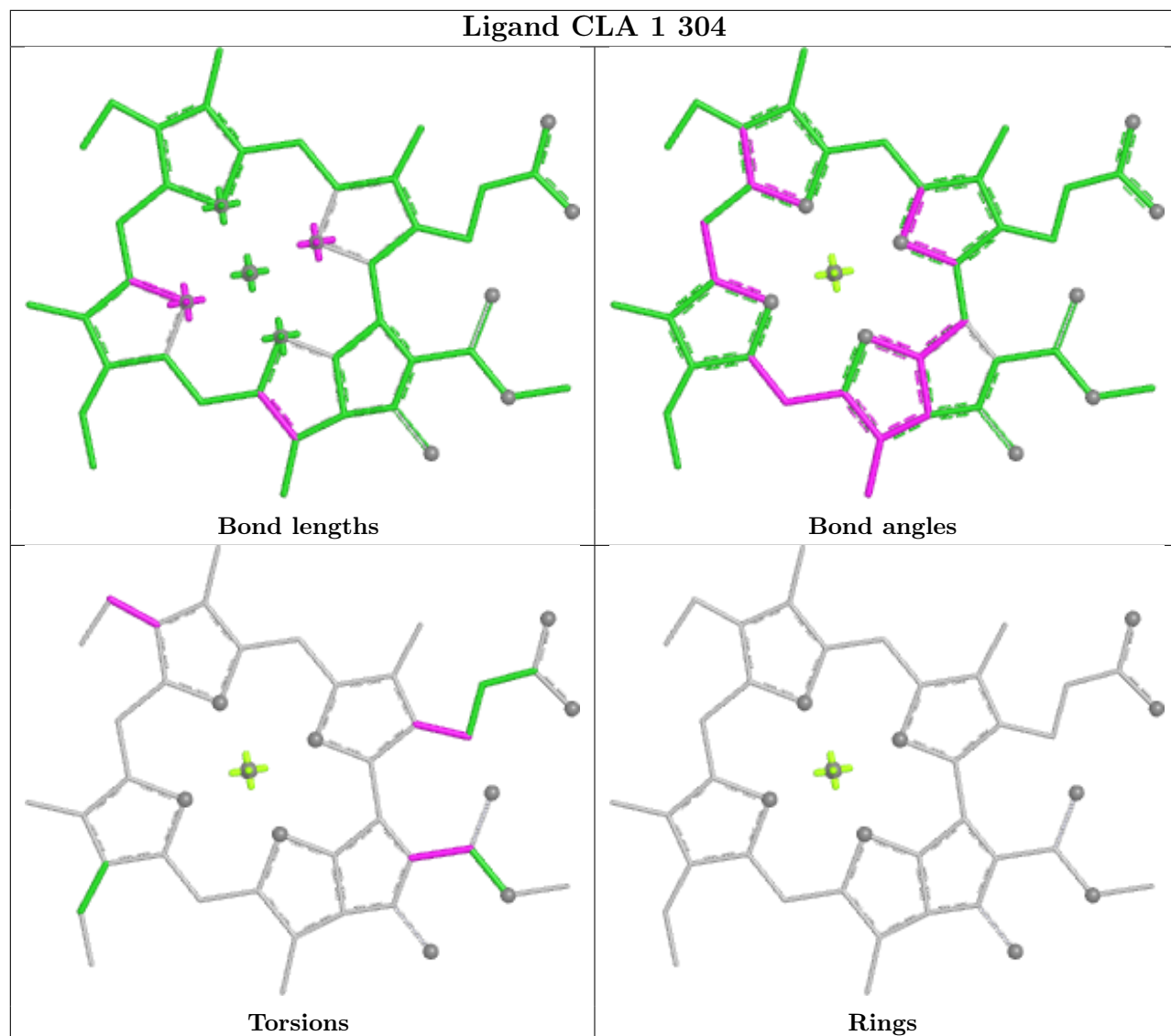
Torsions

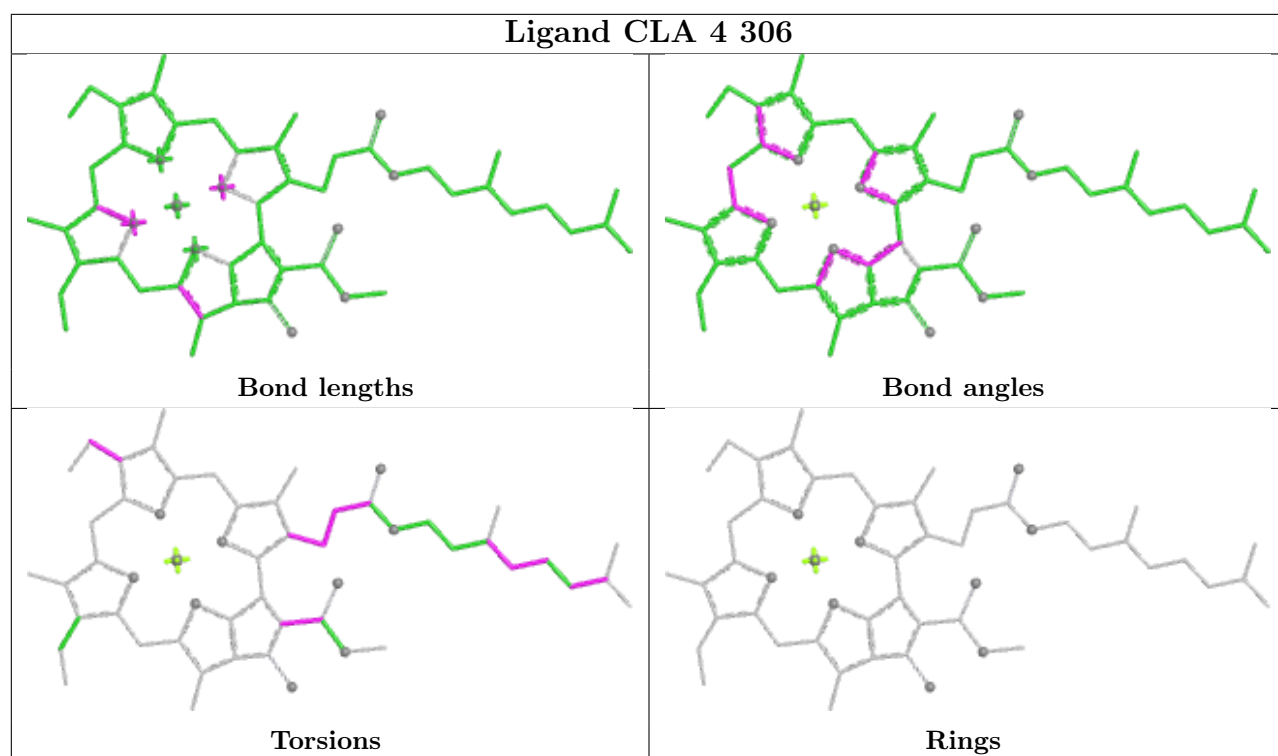


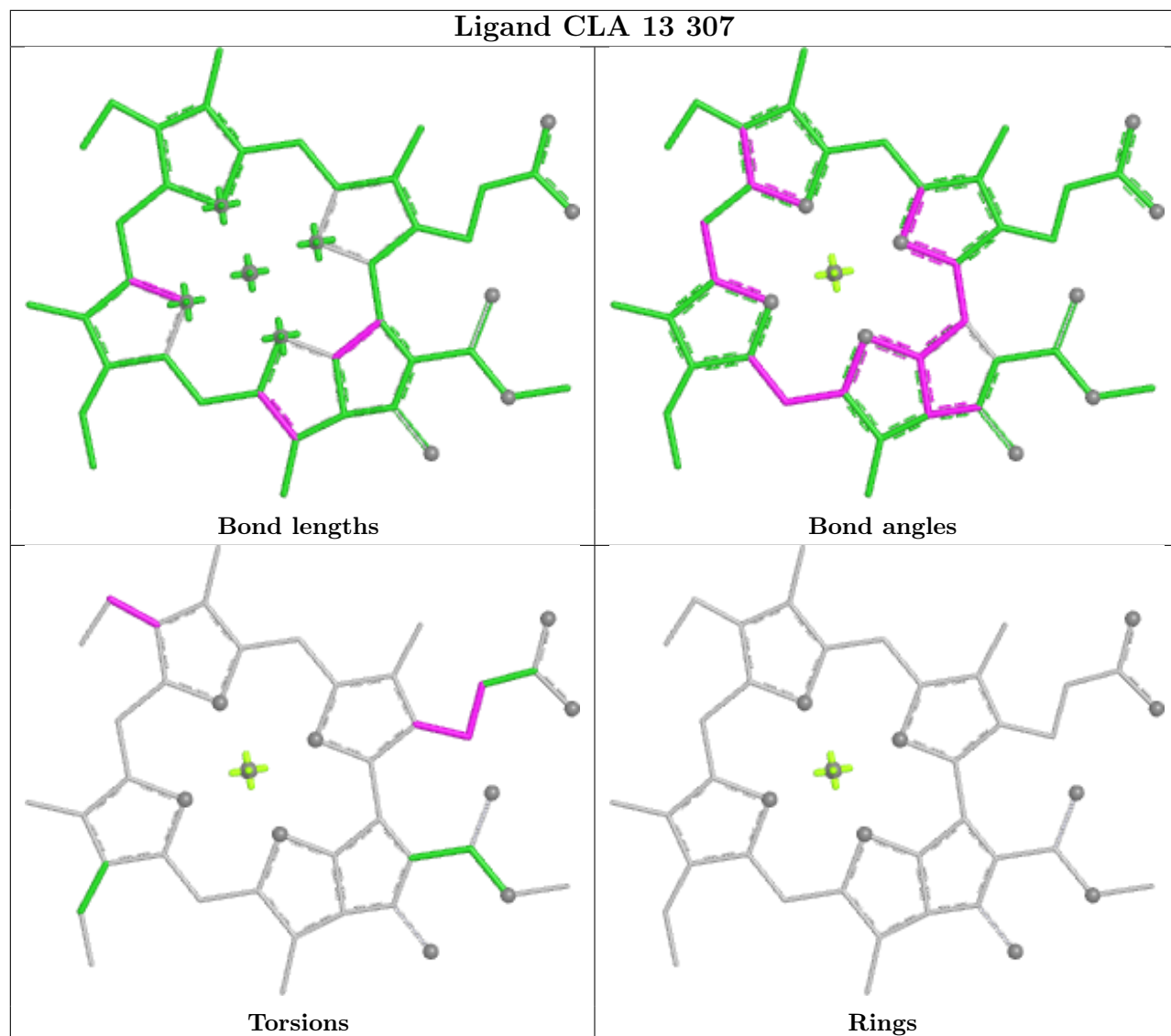
Rings

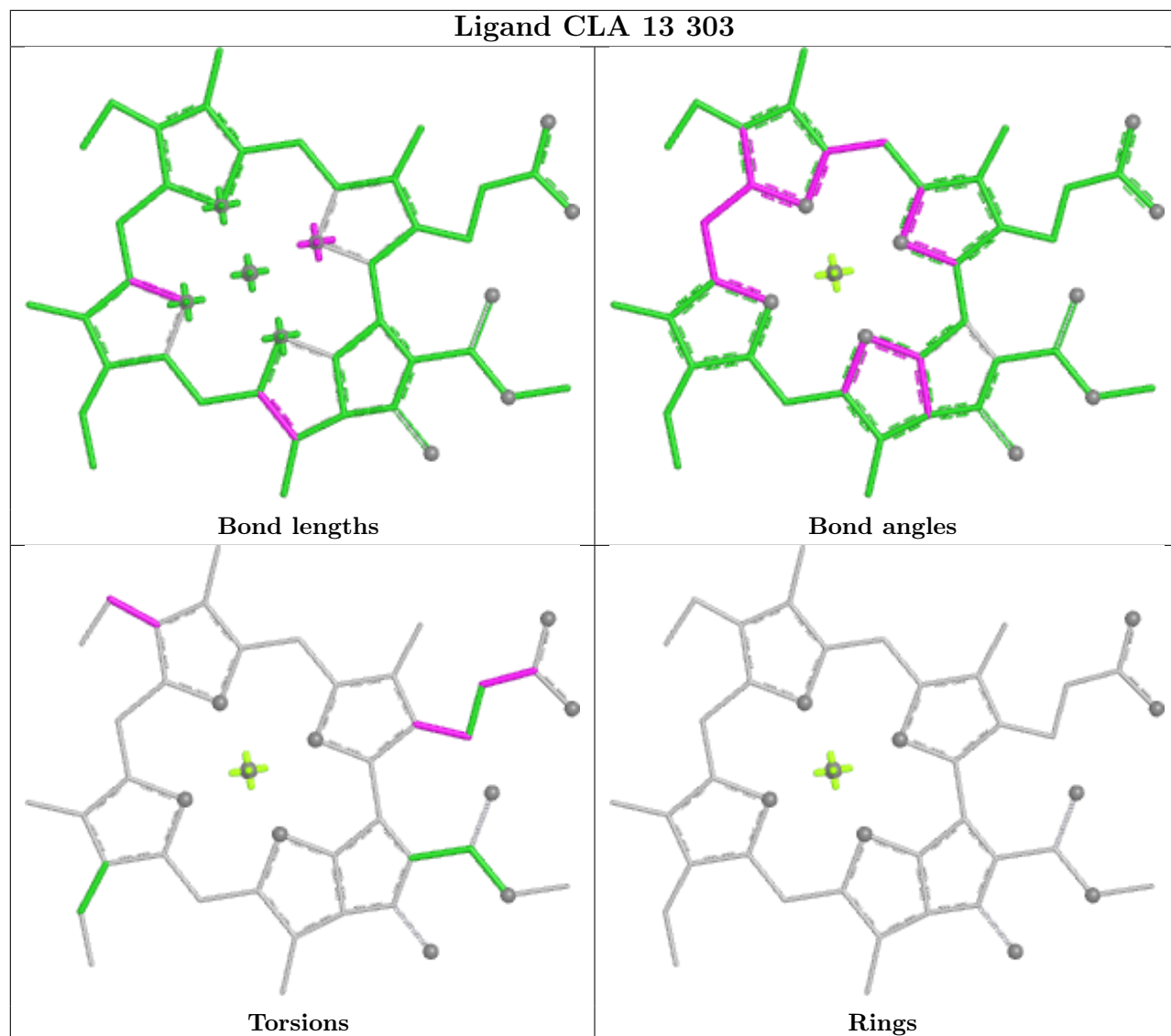




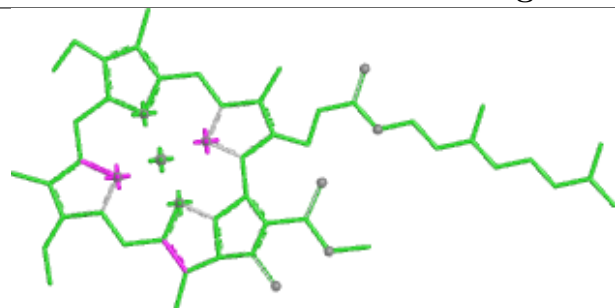




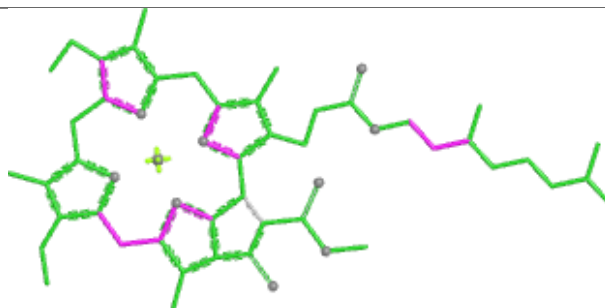




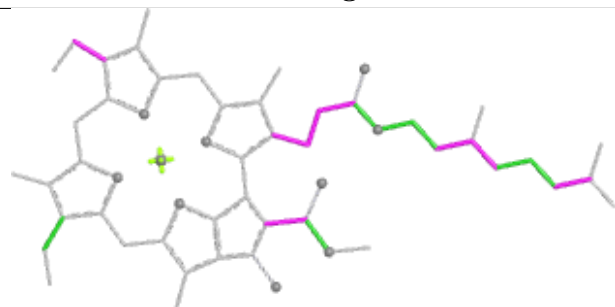
Ligand CLA B 811



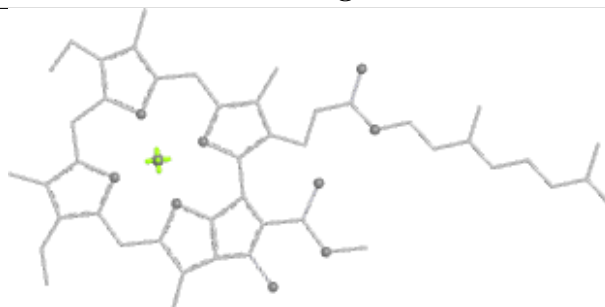
Bond lengths



Bond angles

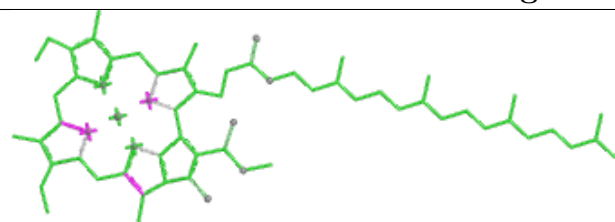


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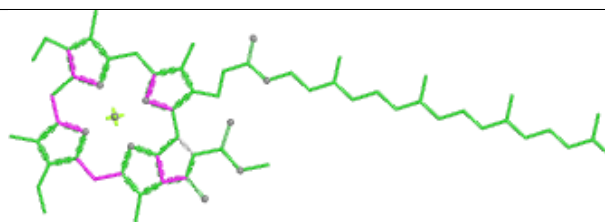


Rings

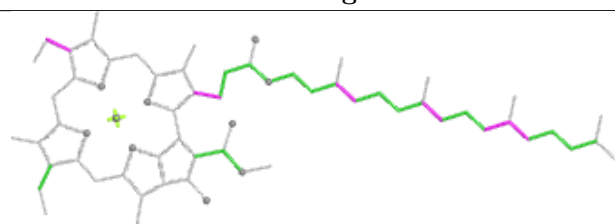
Ligand CLA 5 303



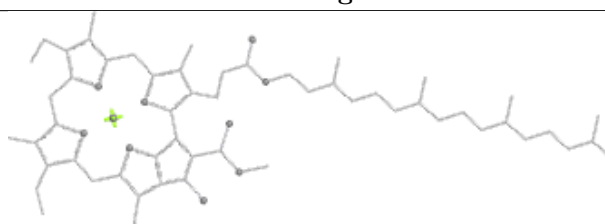
Bond lengths



Bond angles

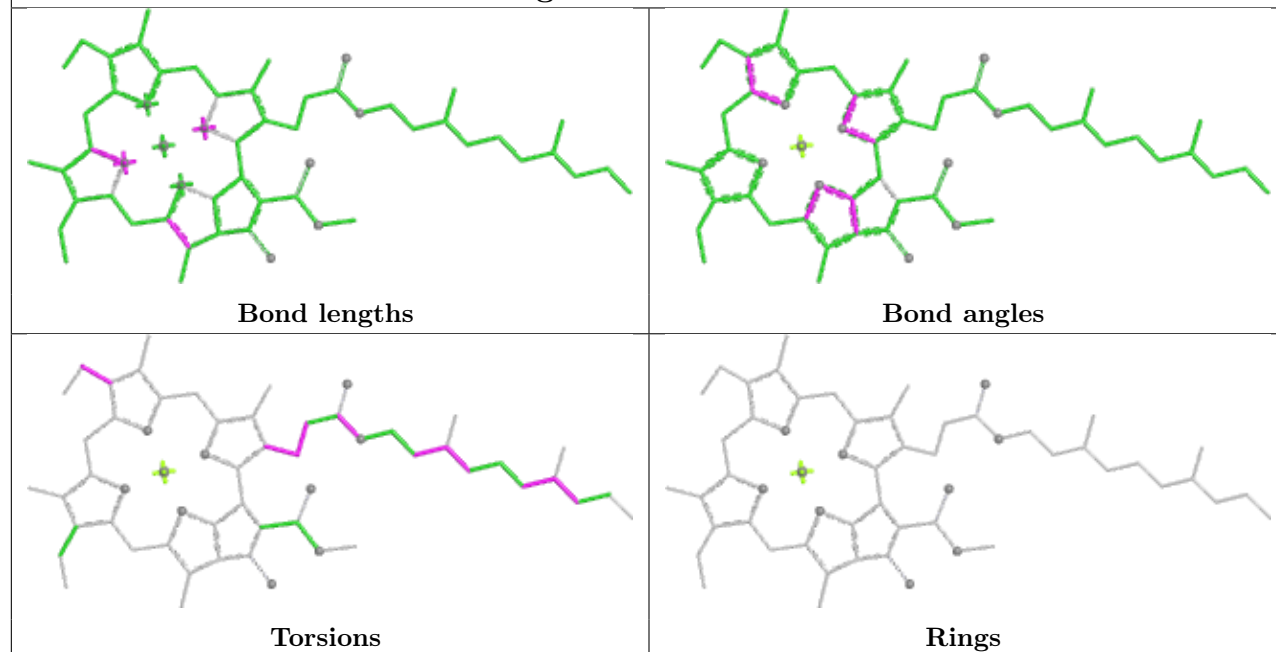


Torsions

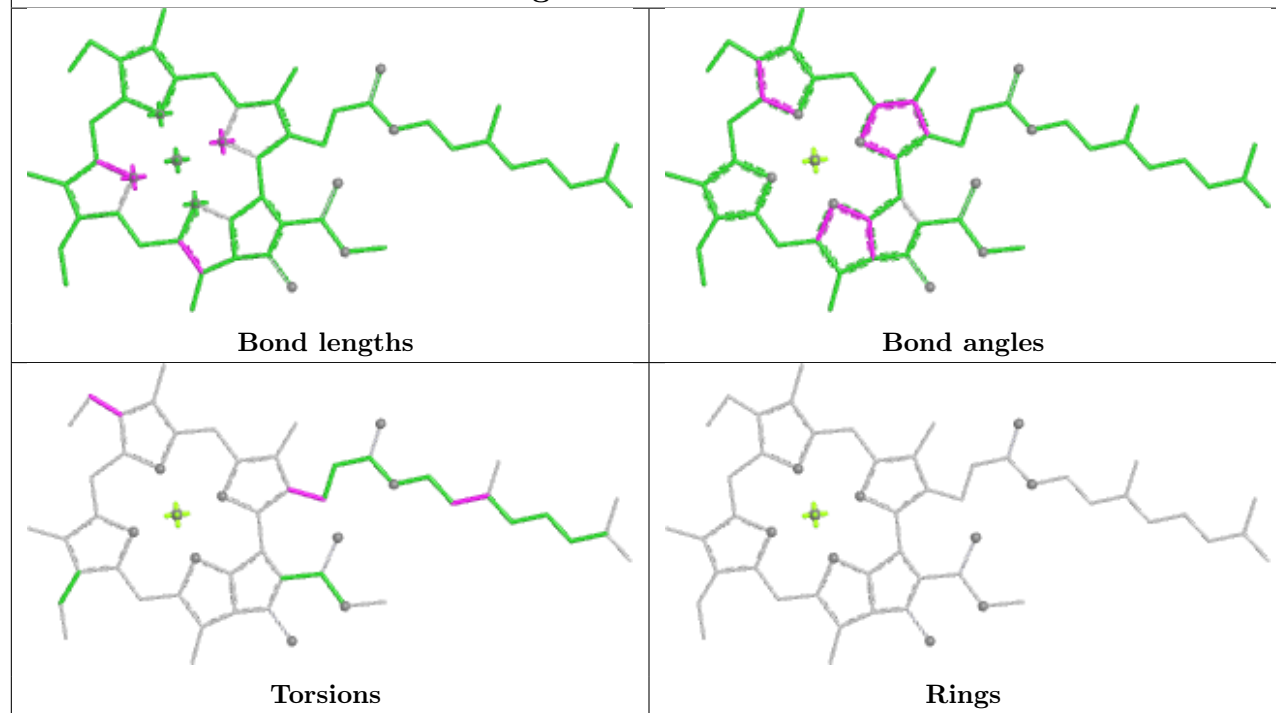


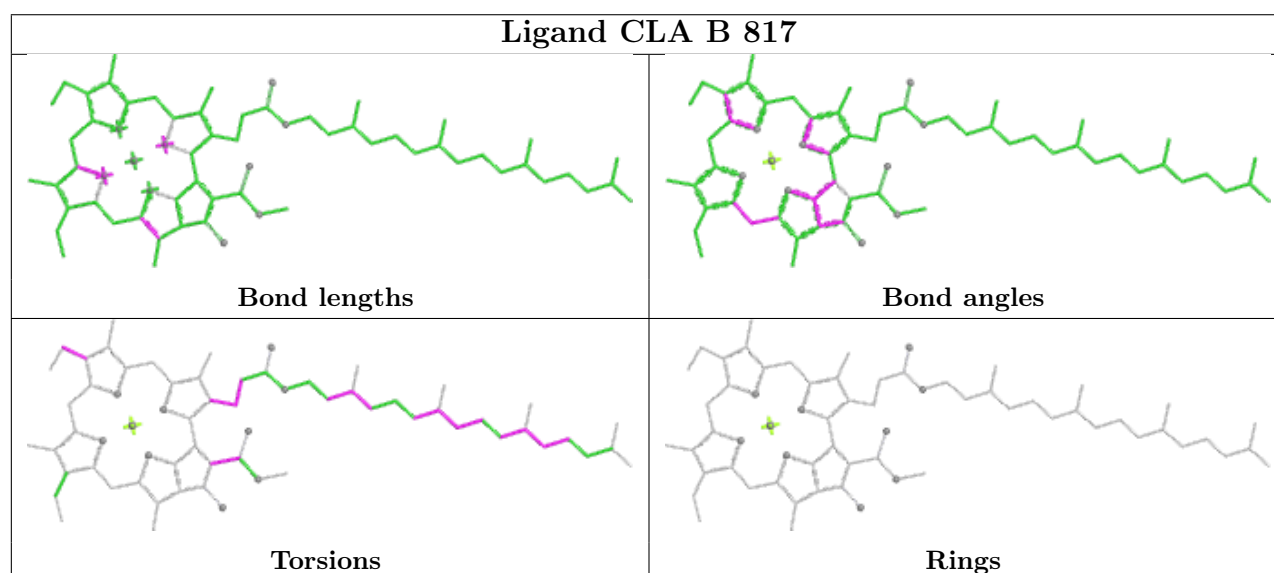
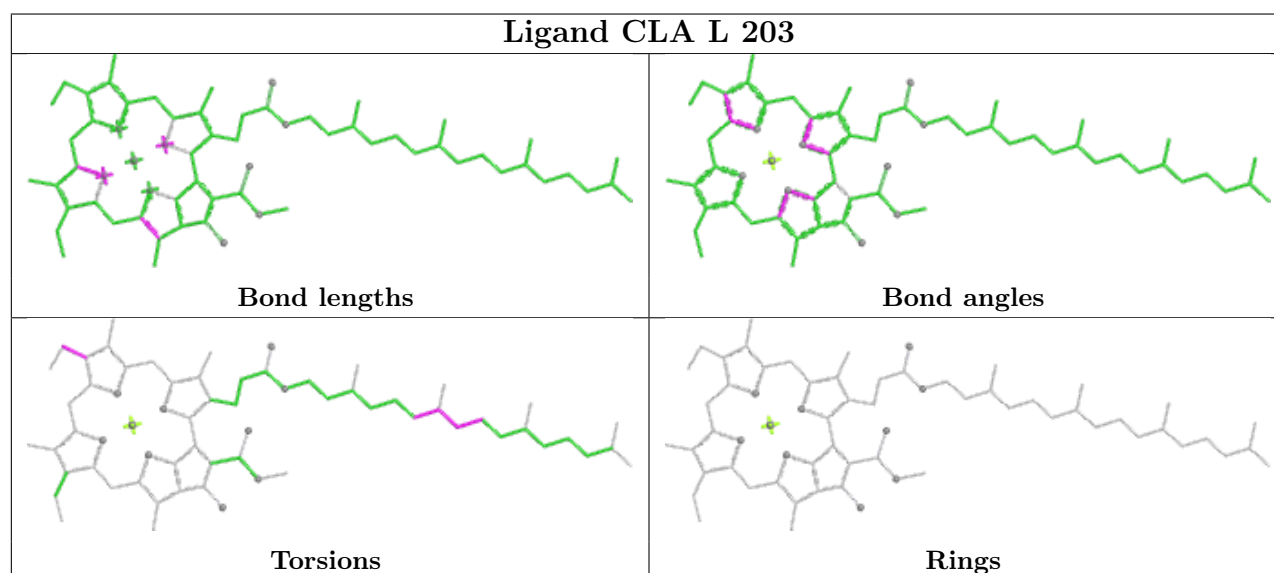
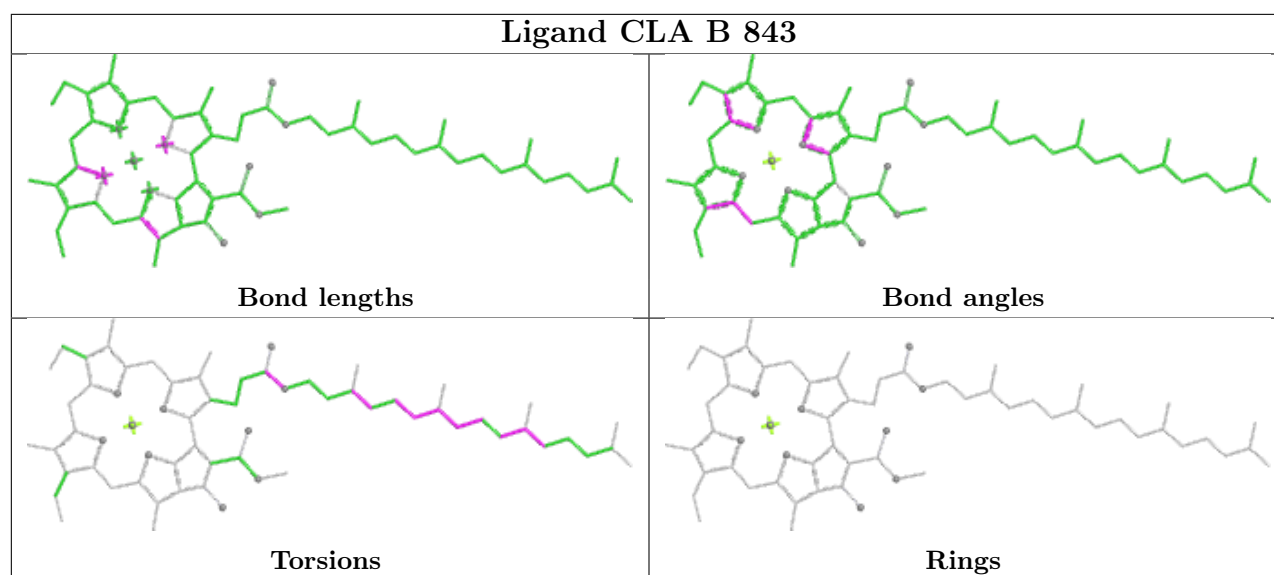
Rings

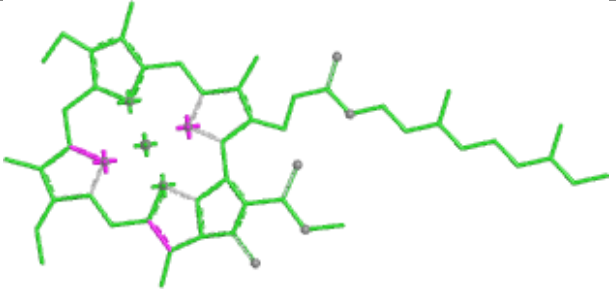
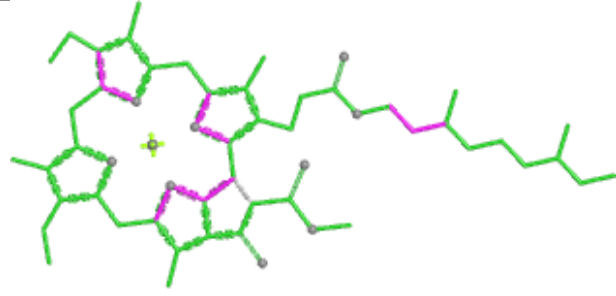
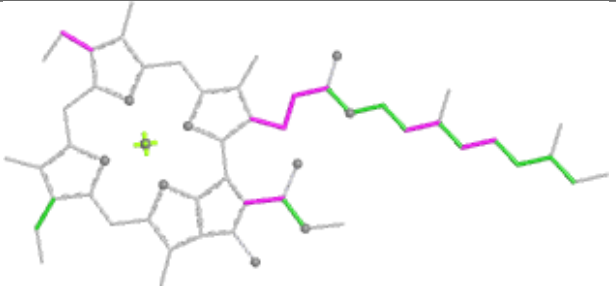
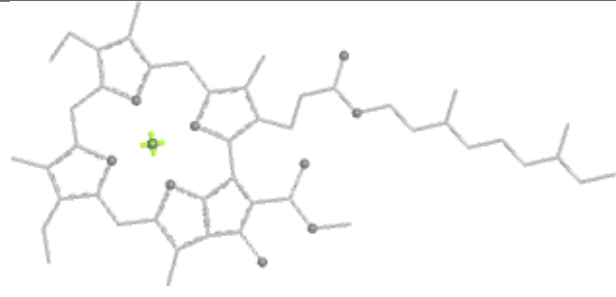
Ligand CLA 8 303

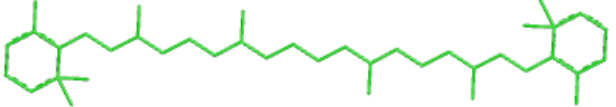
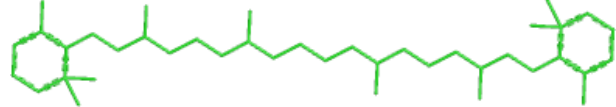

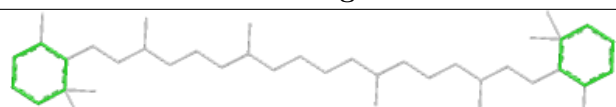


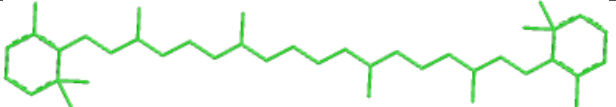
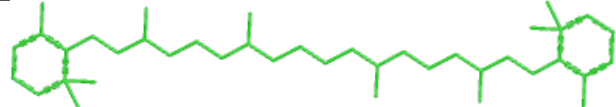
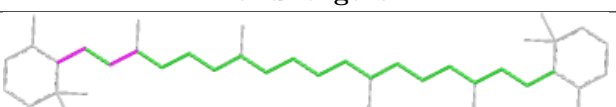
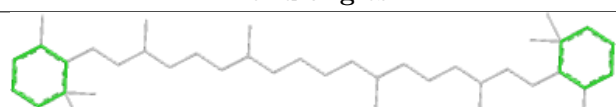
Ligand CLA B 819



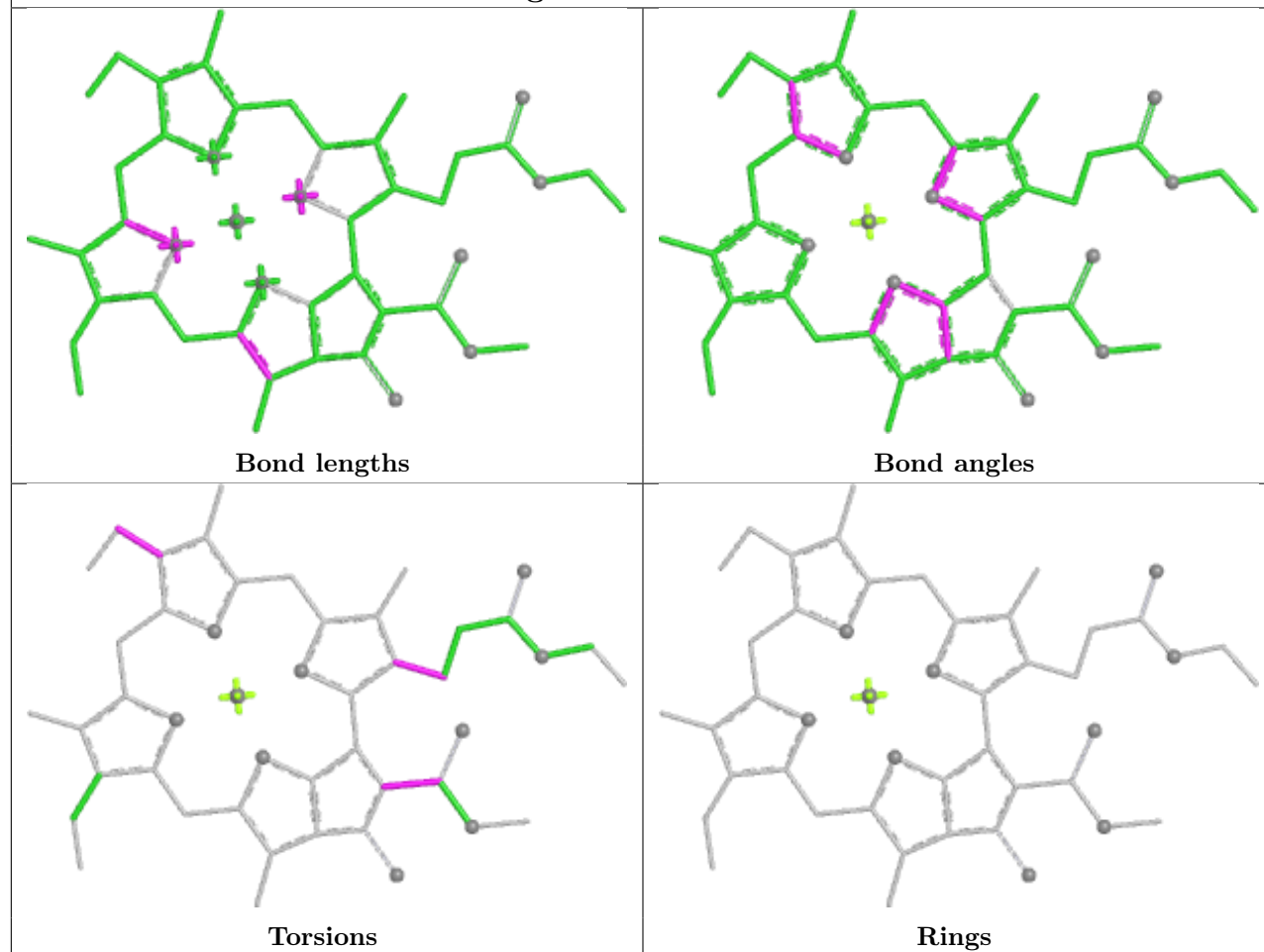


Ligand CLA 10 306	
	
Bond lengths	Bond angles
	
Torsions	Rings

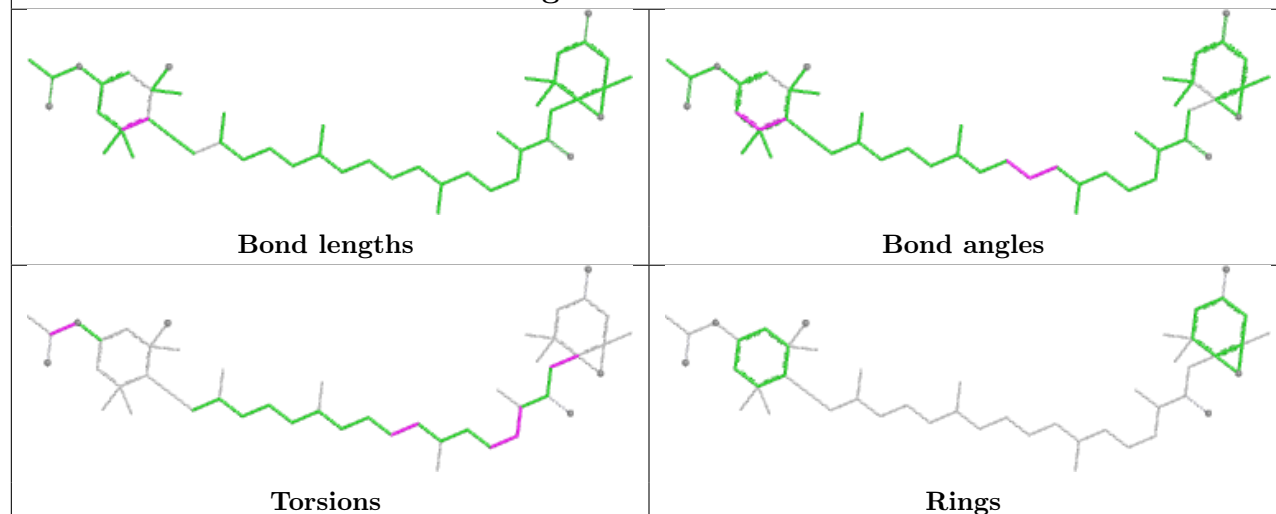
Ligand BCR B 846	
	
Bond lengths	Bond angles
	
Torsions	Rings

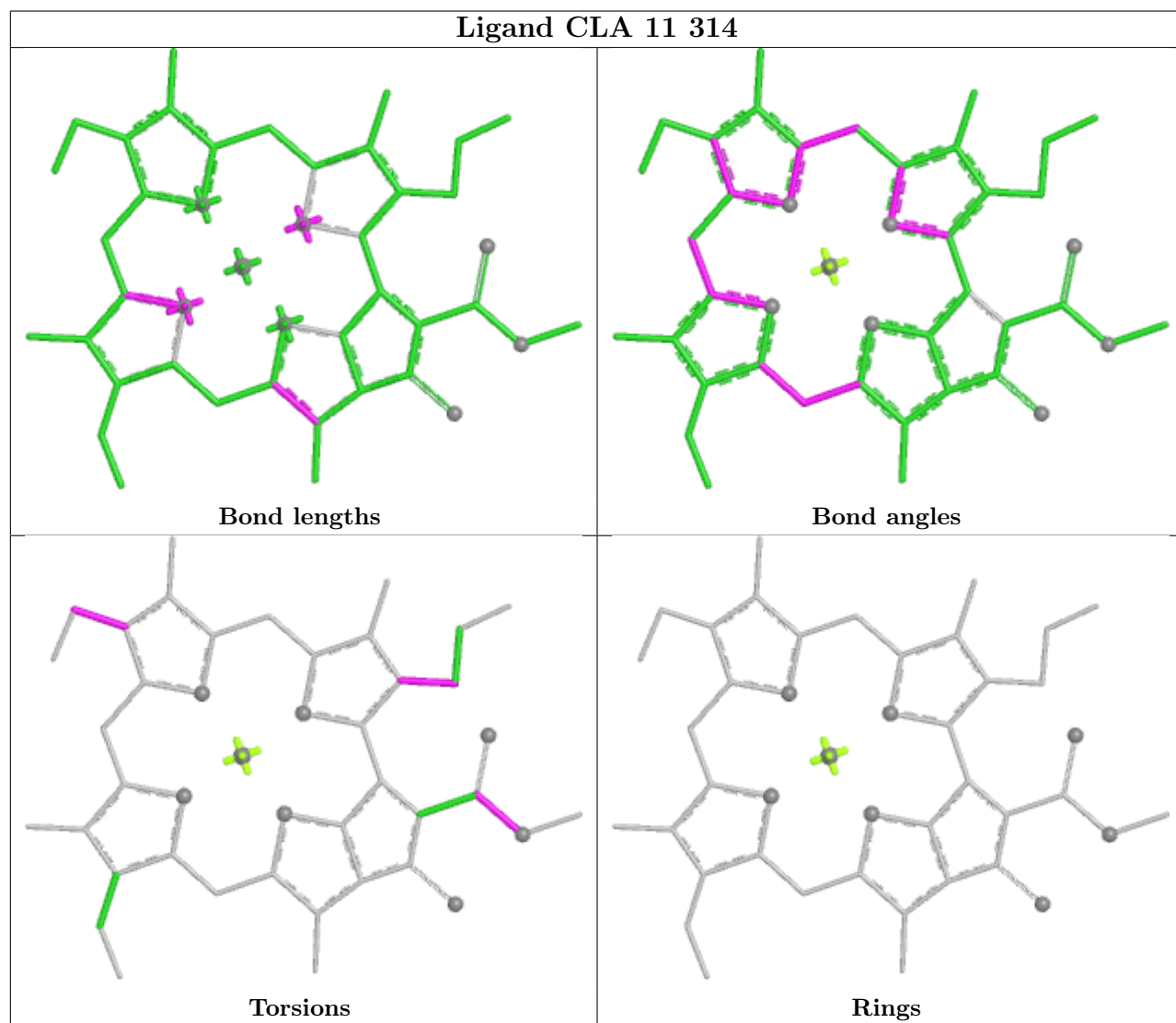
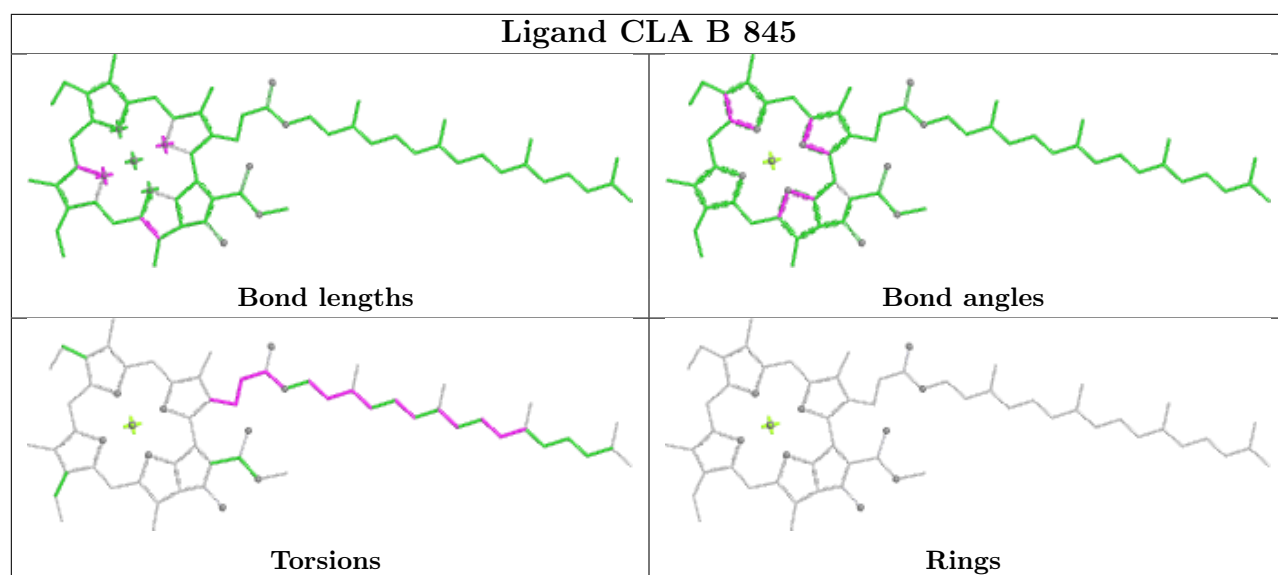
Ligand BCR 1 312	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 846

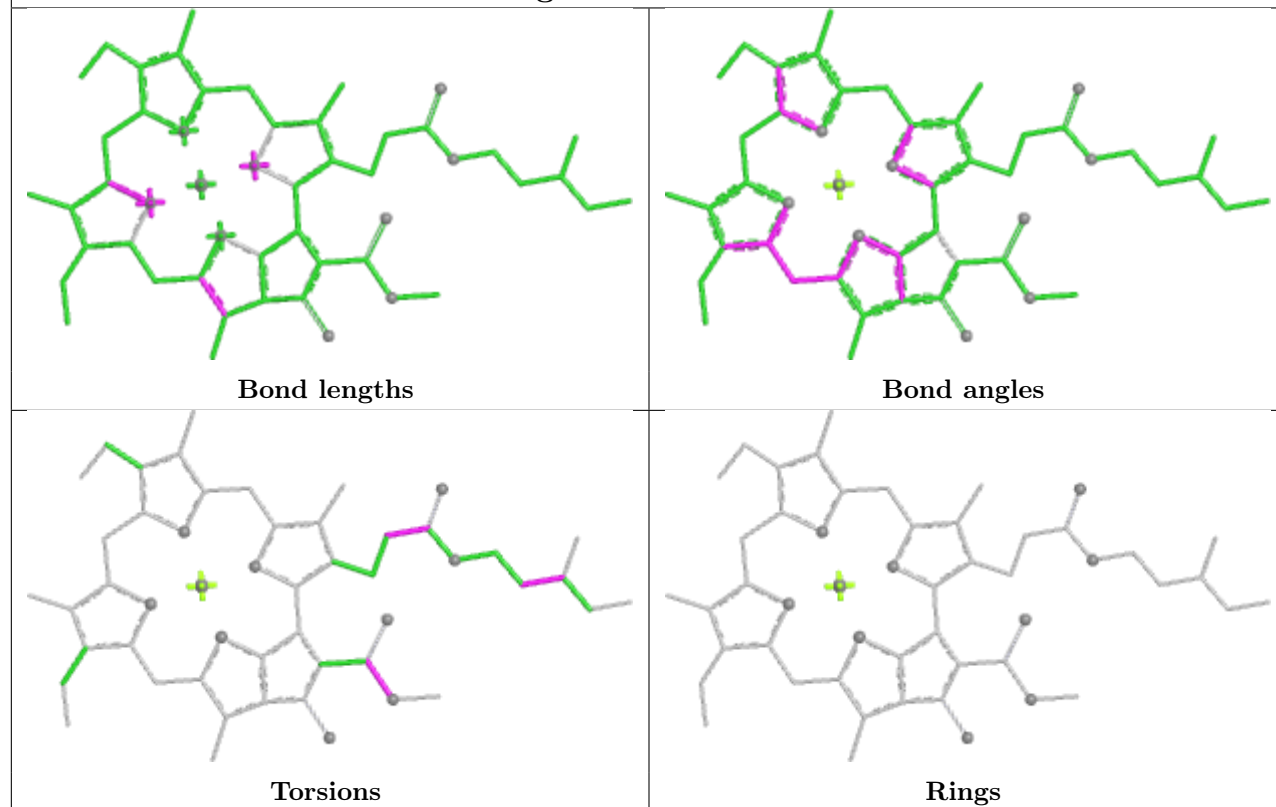


Ligand A86 6 314

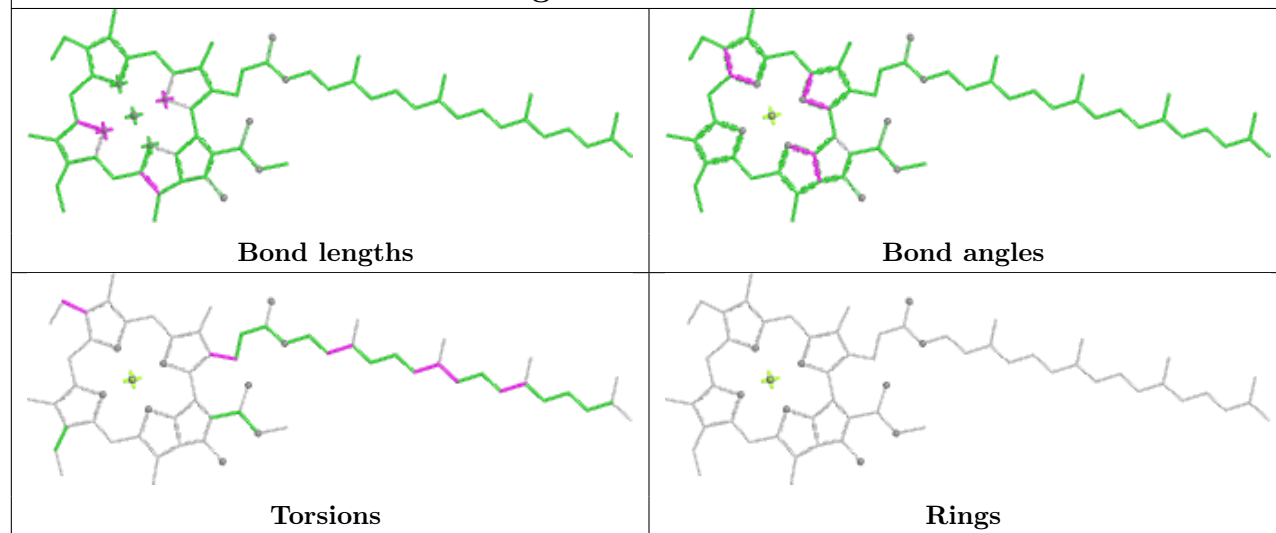




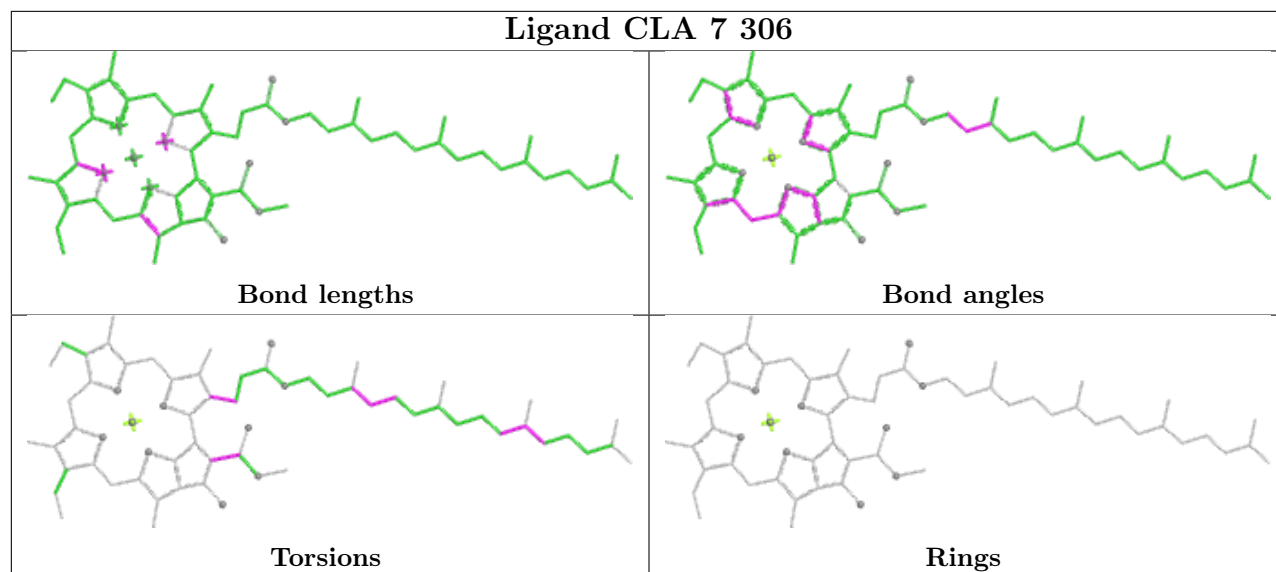
Ligand CLA 4 304



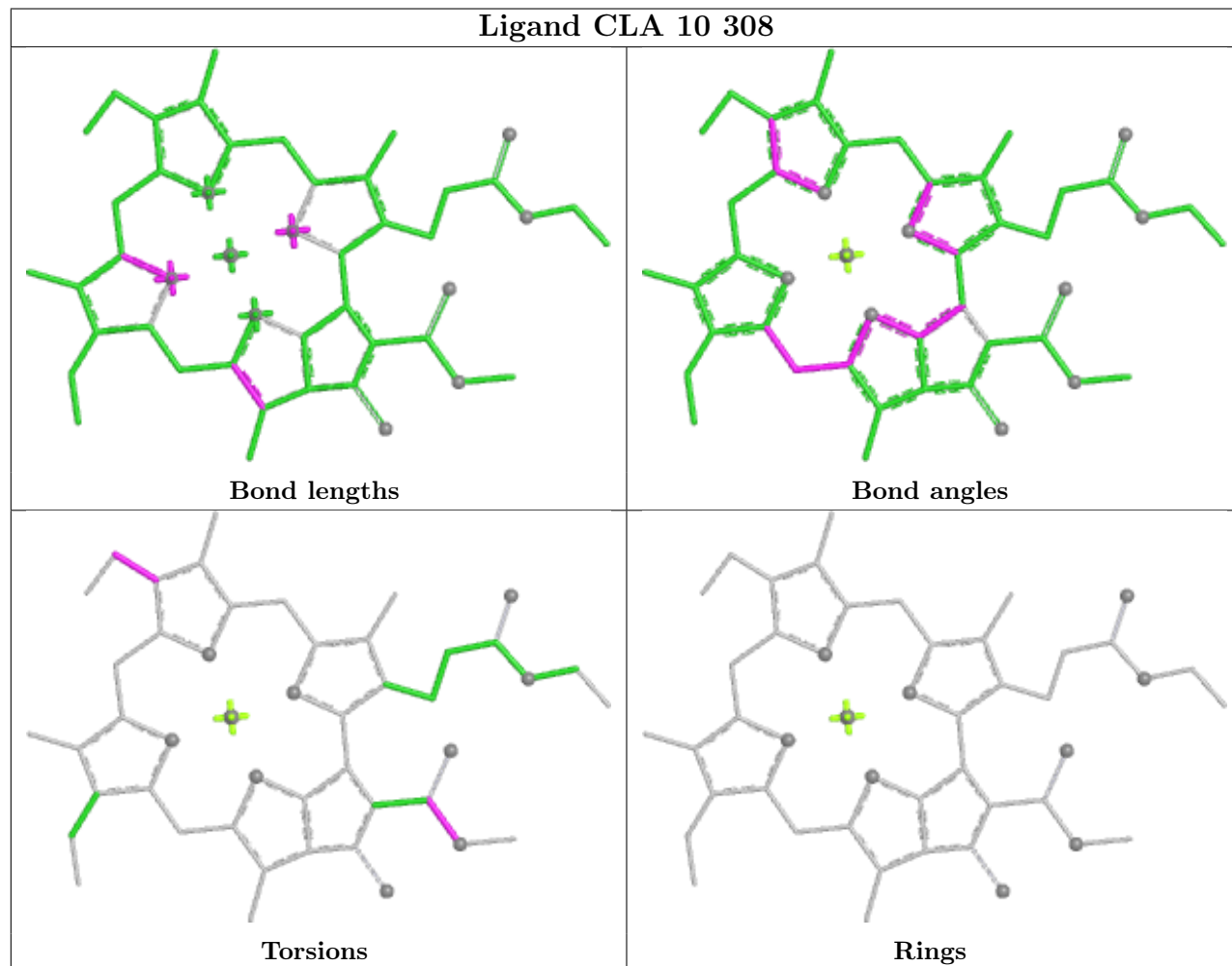
Ligand CLA B 816



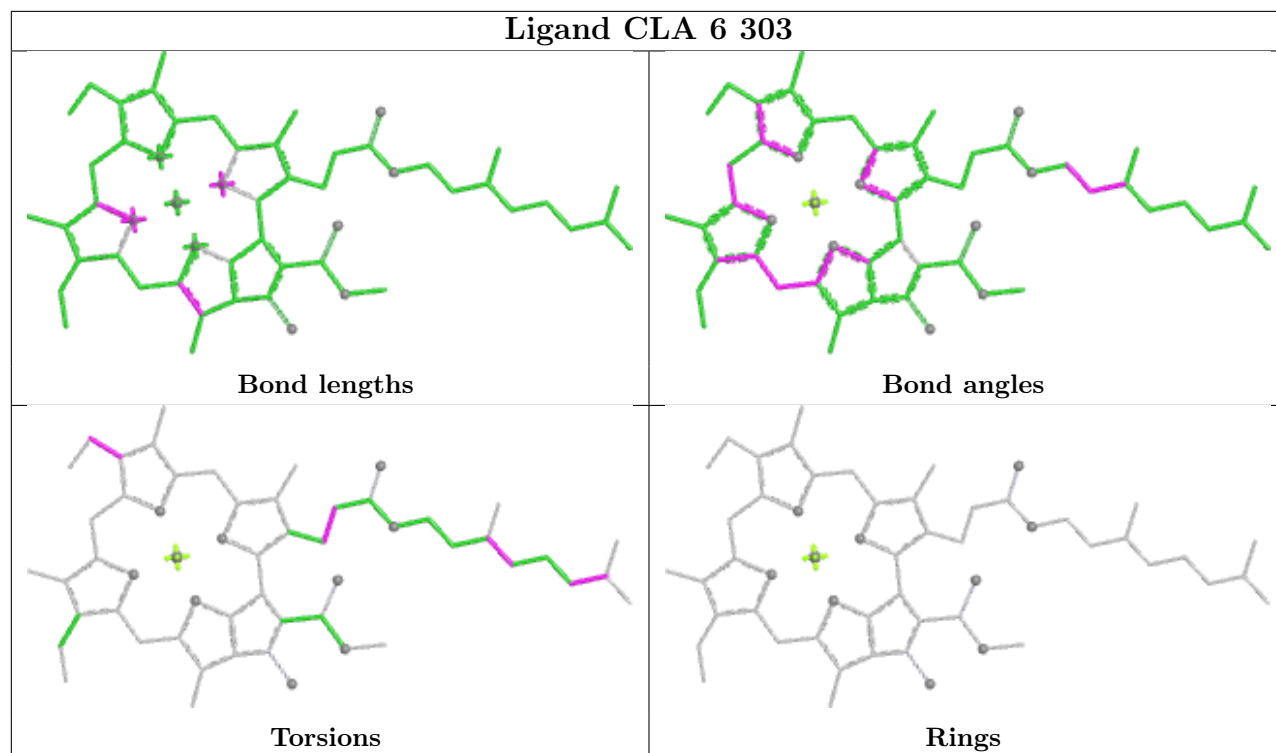
Ligand CLA 7 306



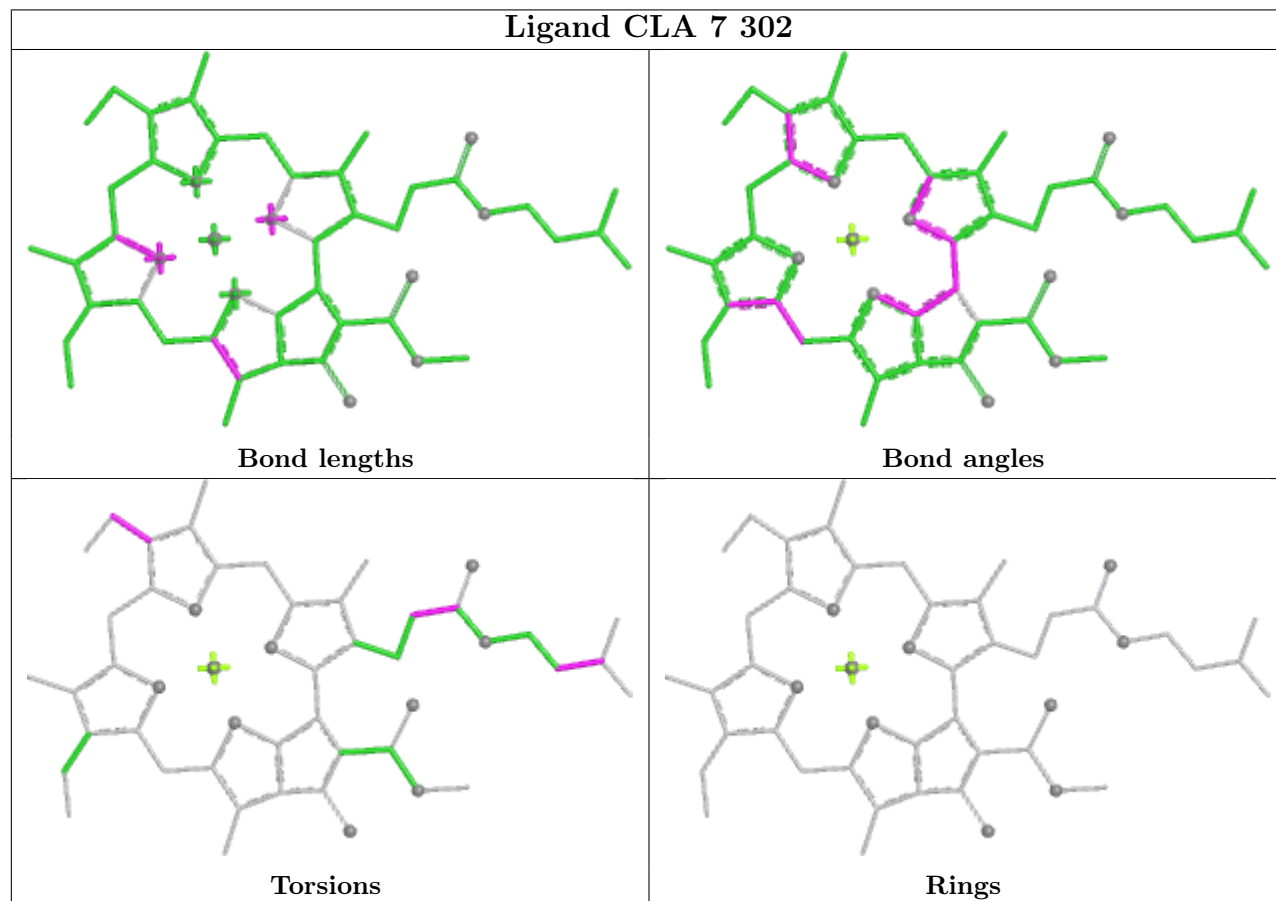
Ligand CLA 10 308

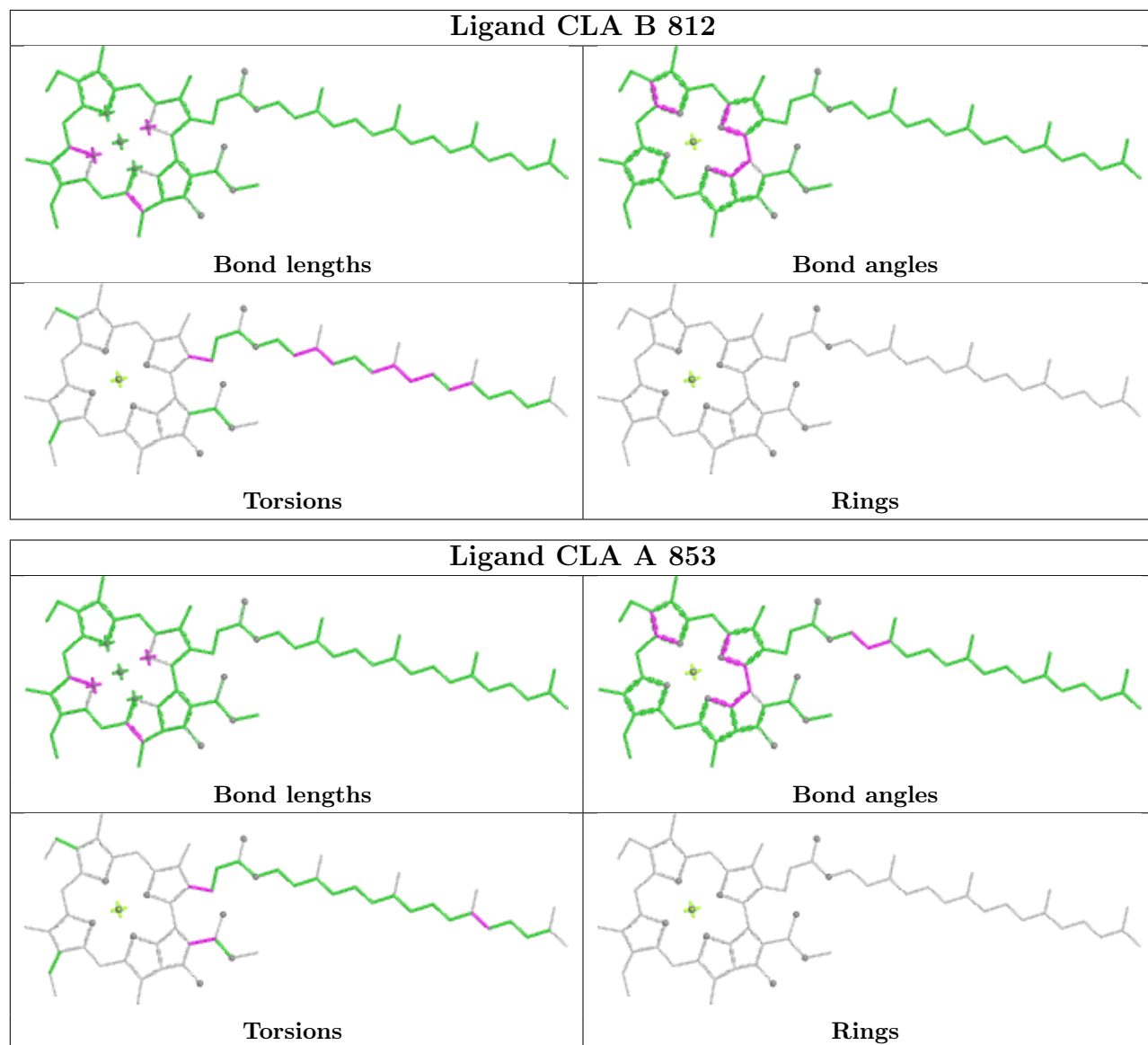


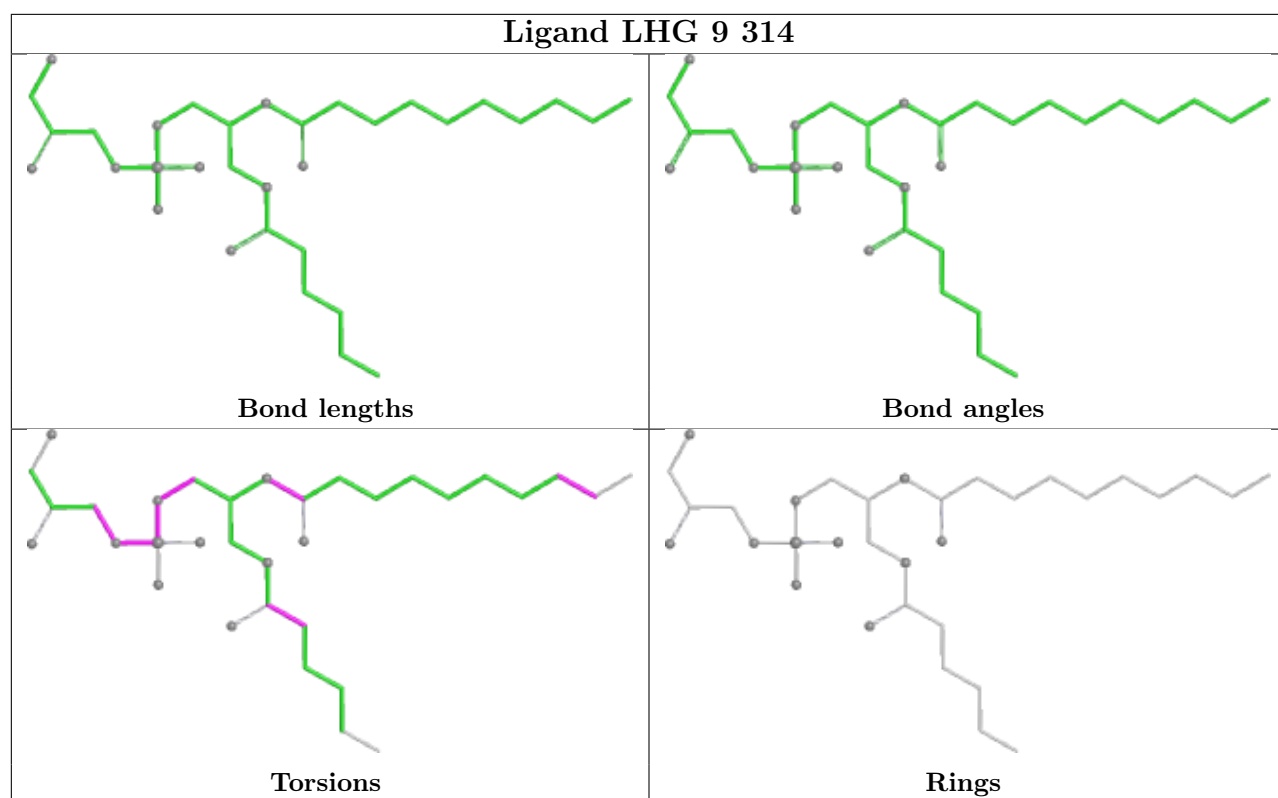
Ligand CLA 6 303



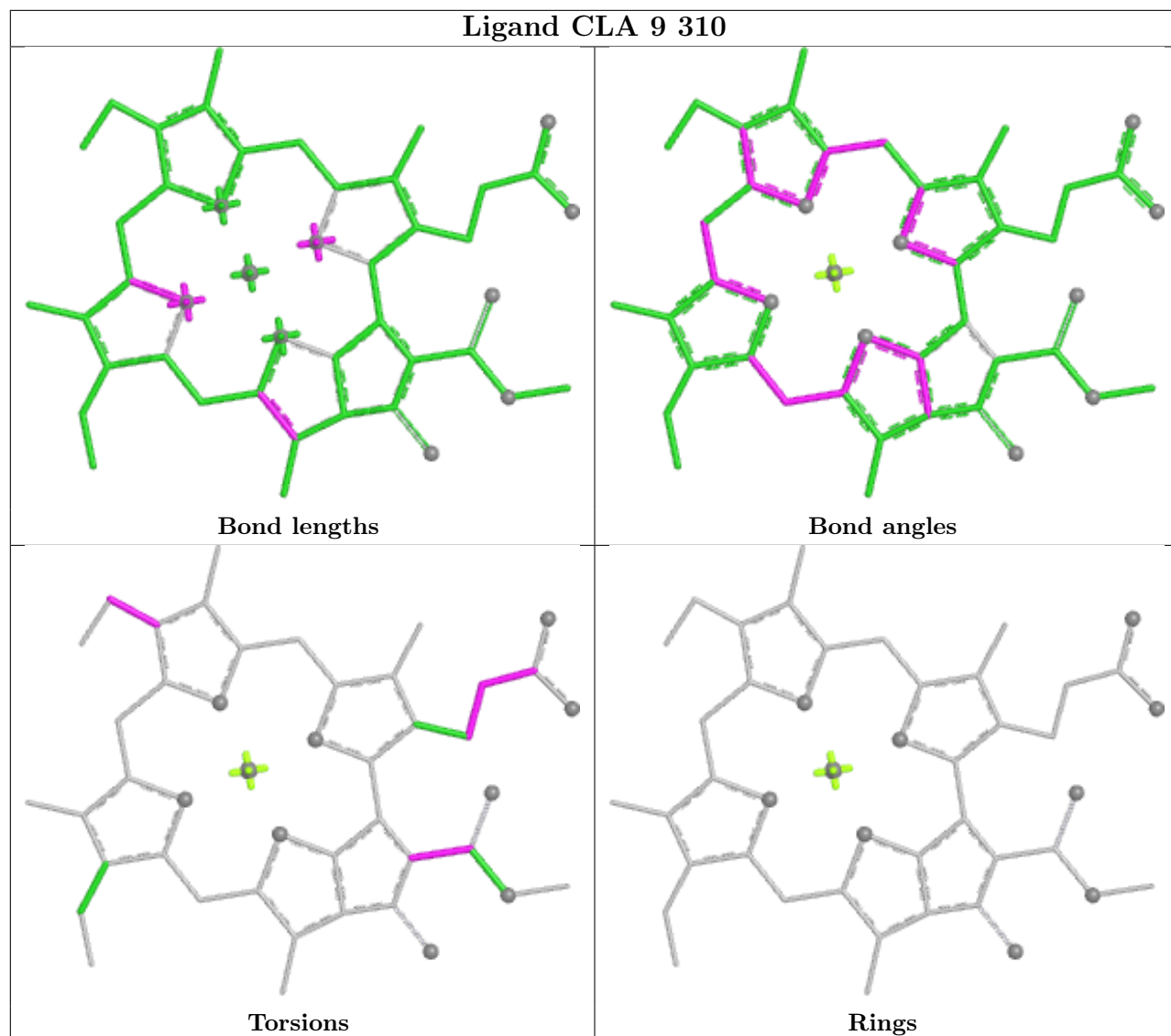
Ligand CLA 7 302



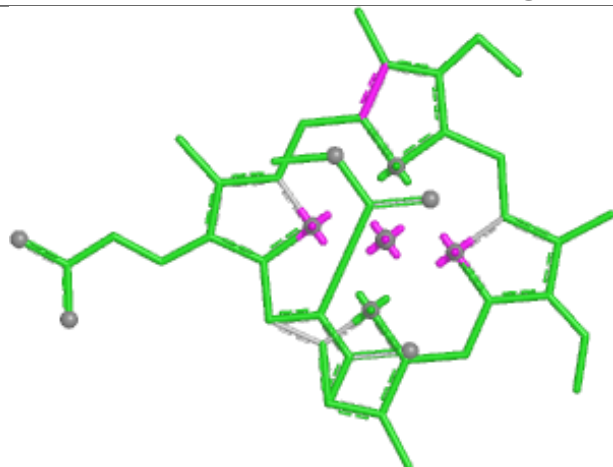




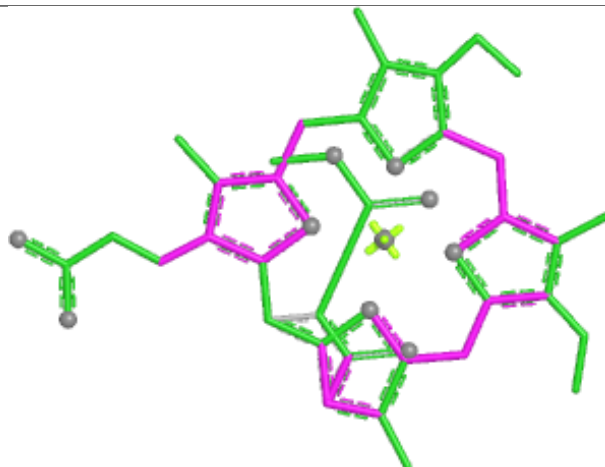
Ligand CLA 9 310



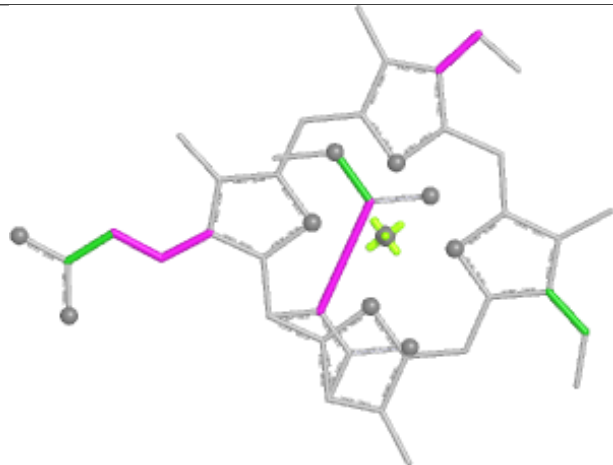
Ligand KC1 9 306



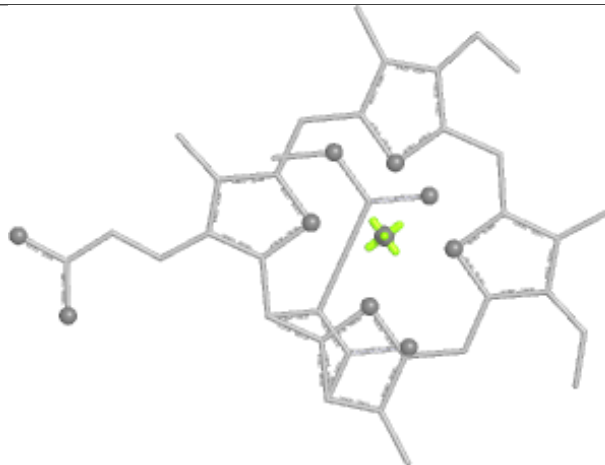
Bond lengths



Bond angles

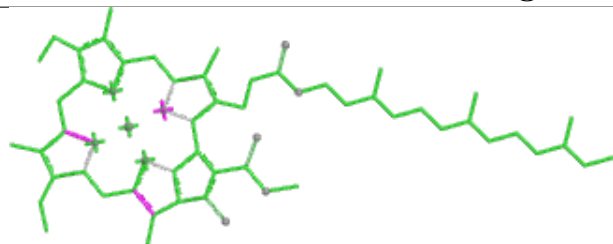


Torsions

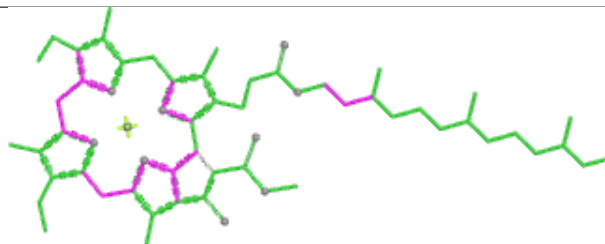


Rings

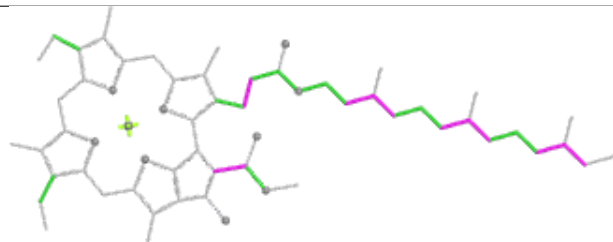
Ligand CLA 4 316



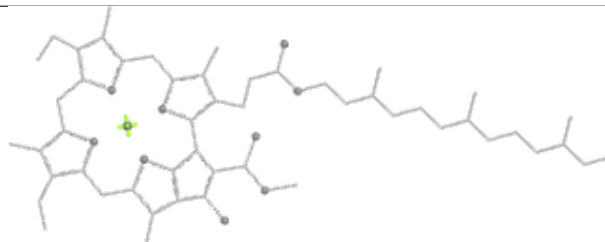
Bond lengths



Bond angles

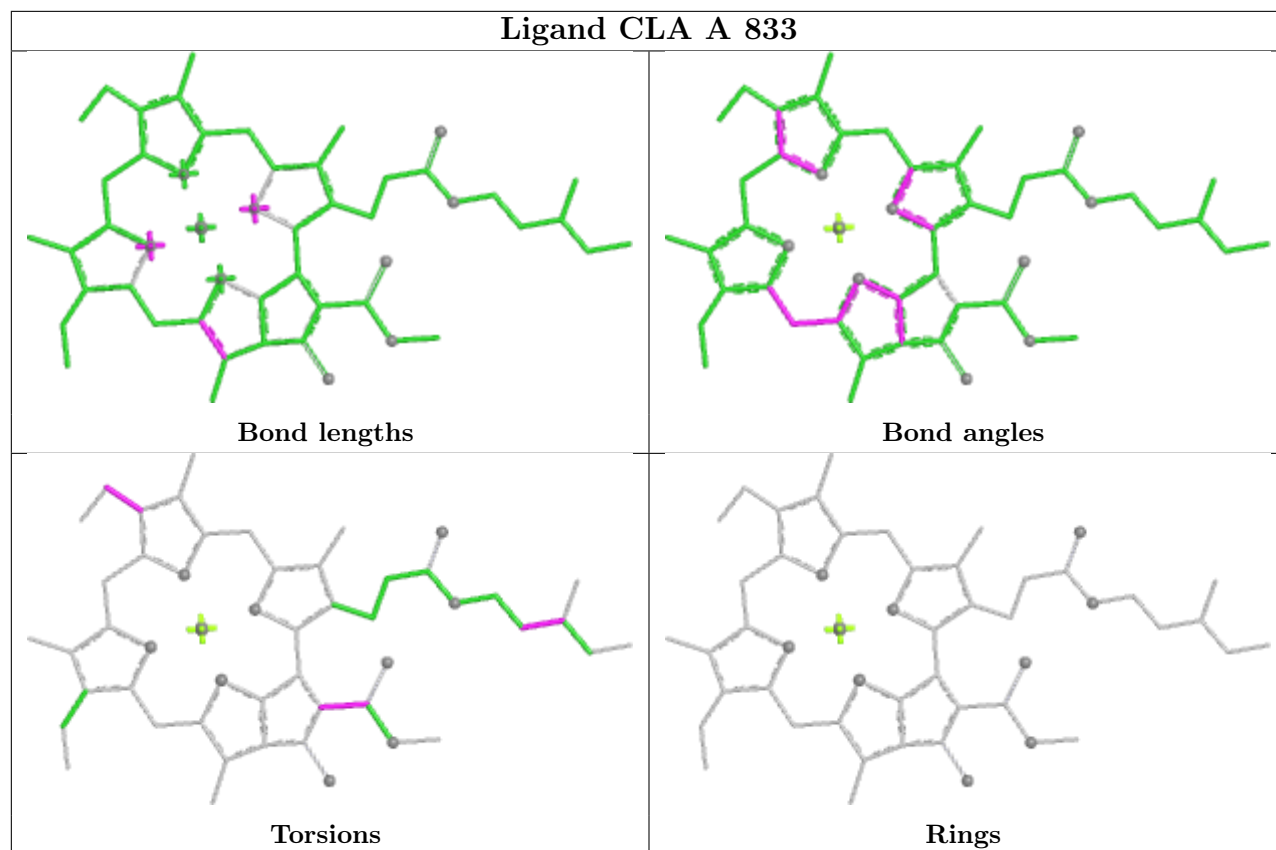


Torsions

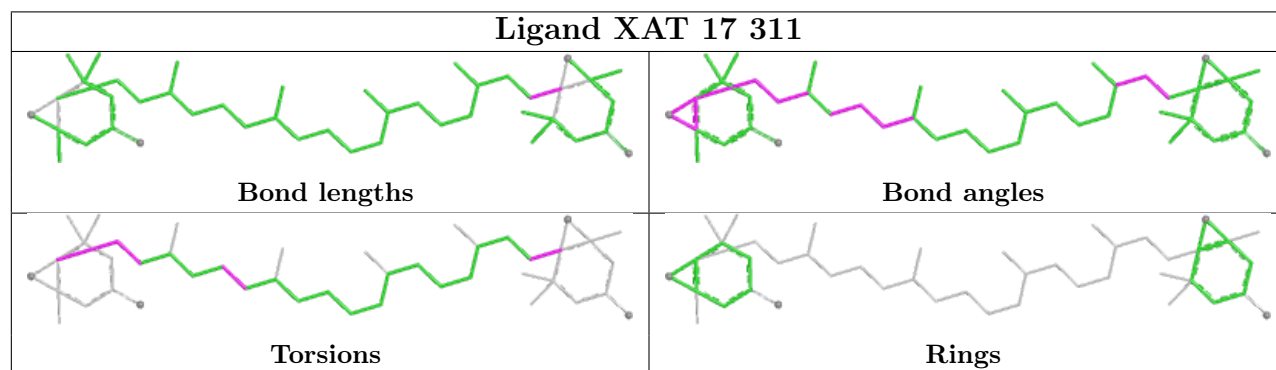


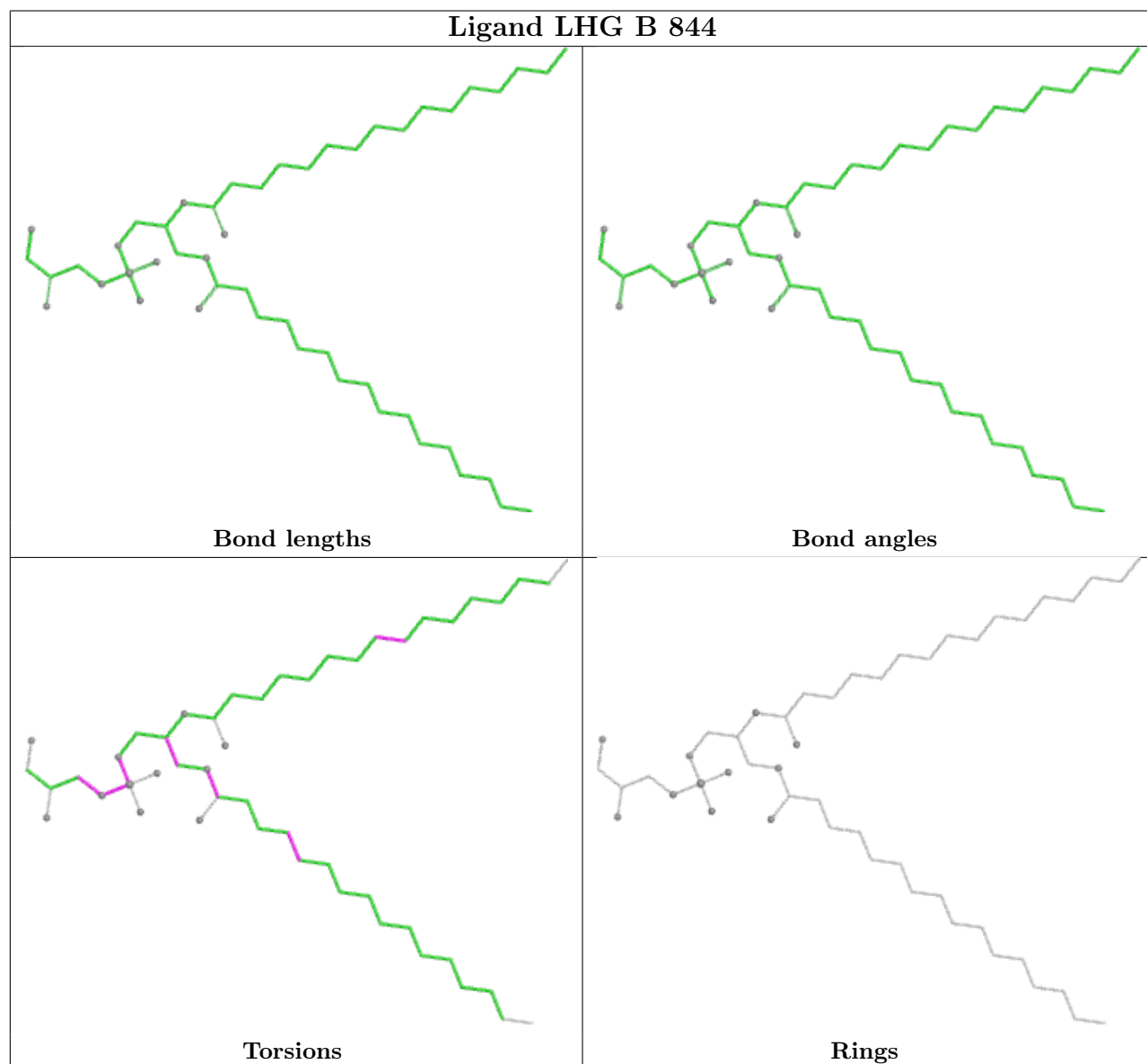
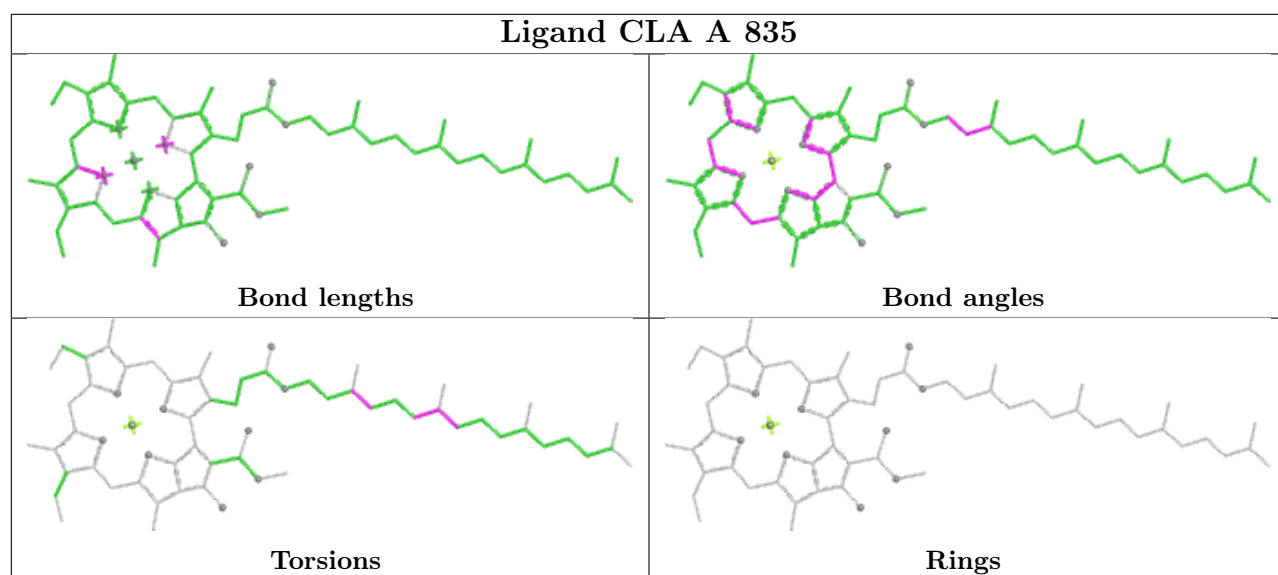
Rings

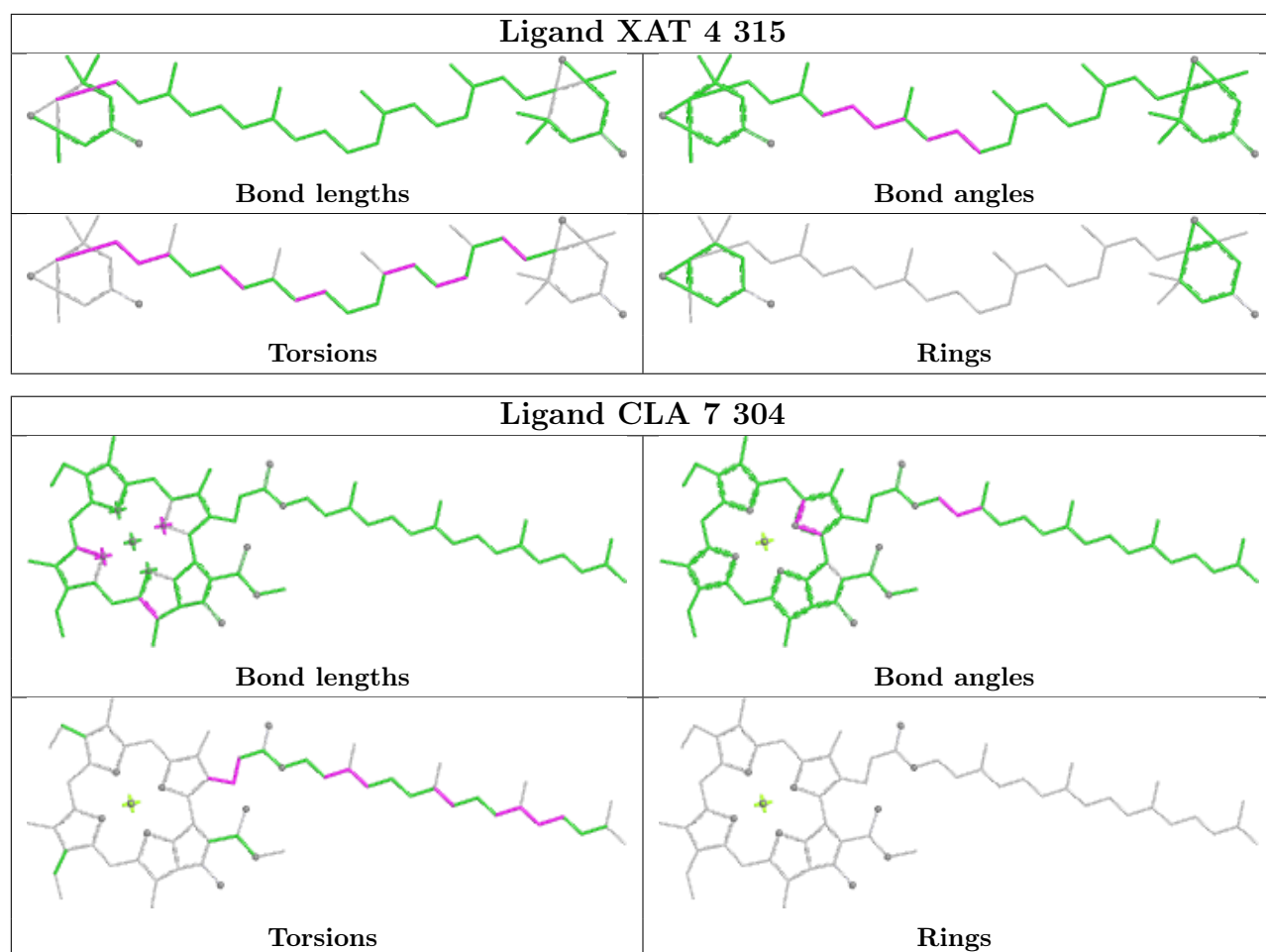
Ligand CLA A 833



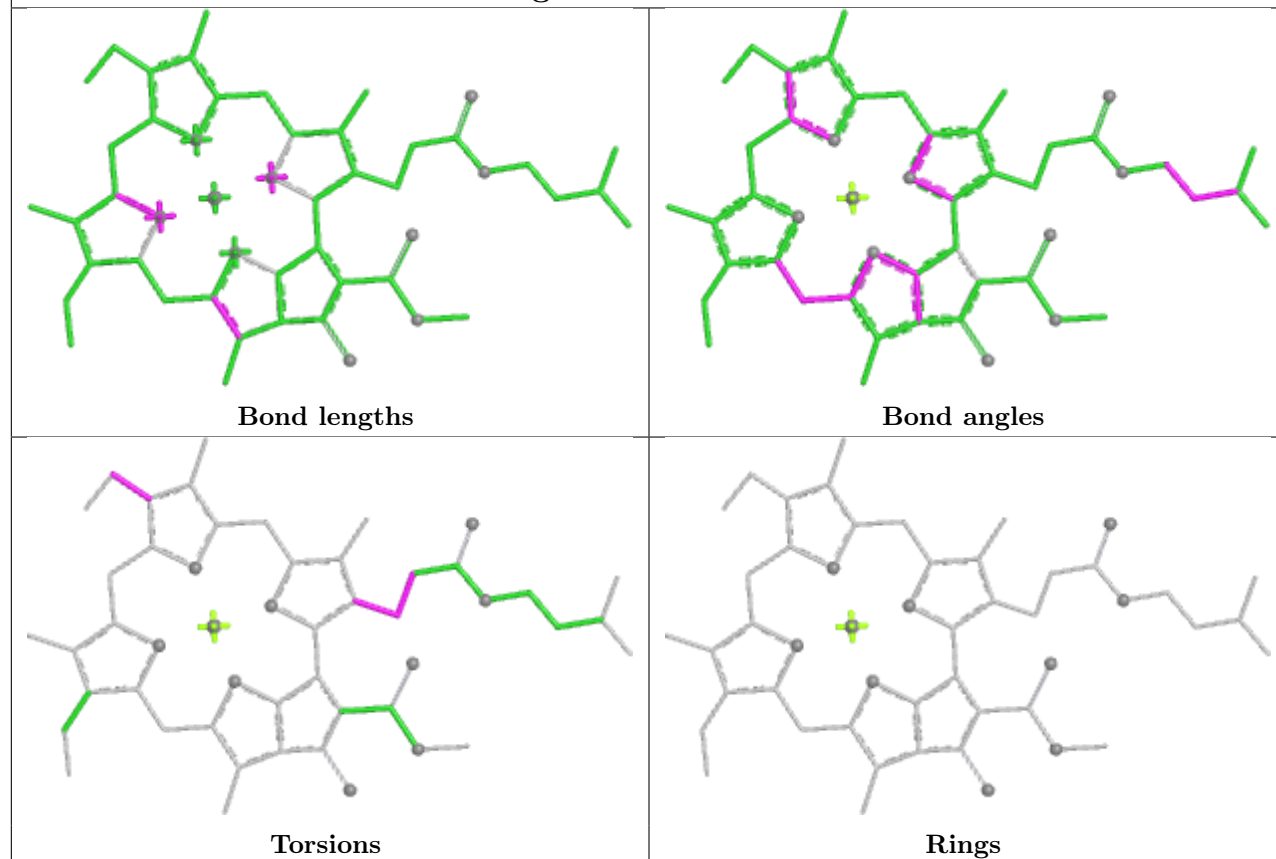
Ligand XAT 17 311



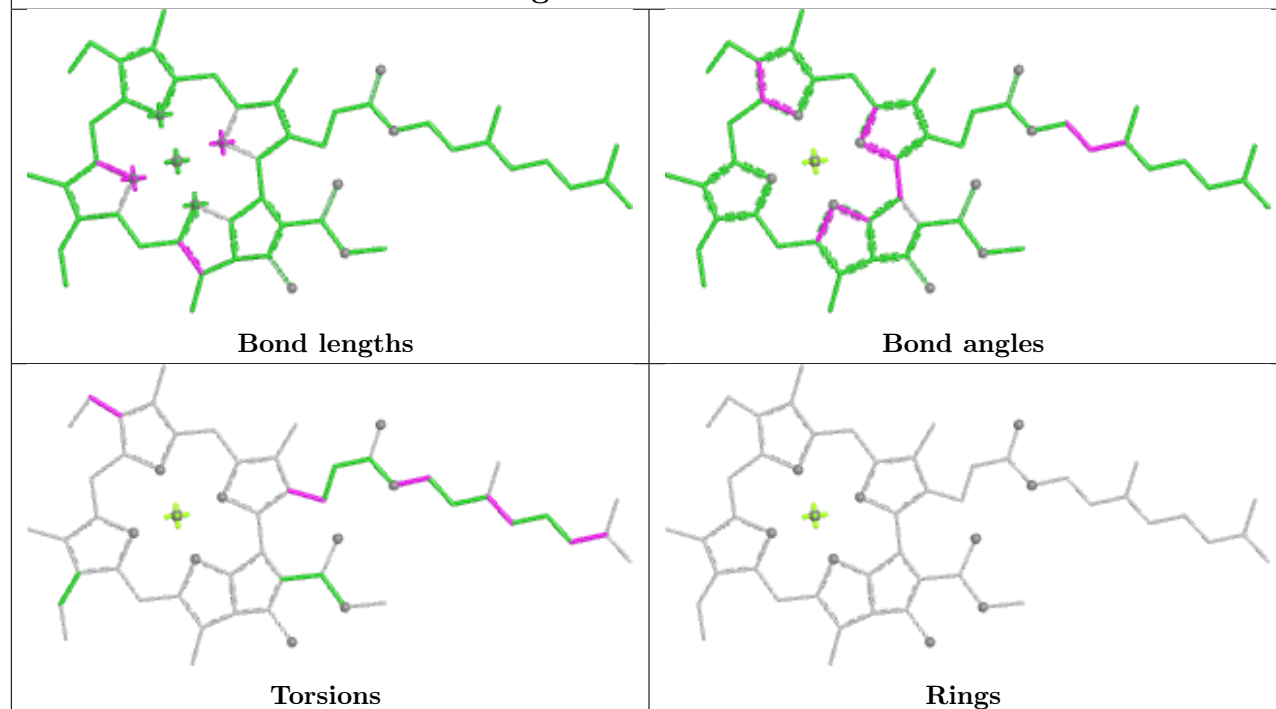


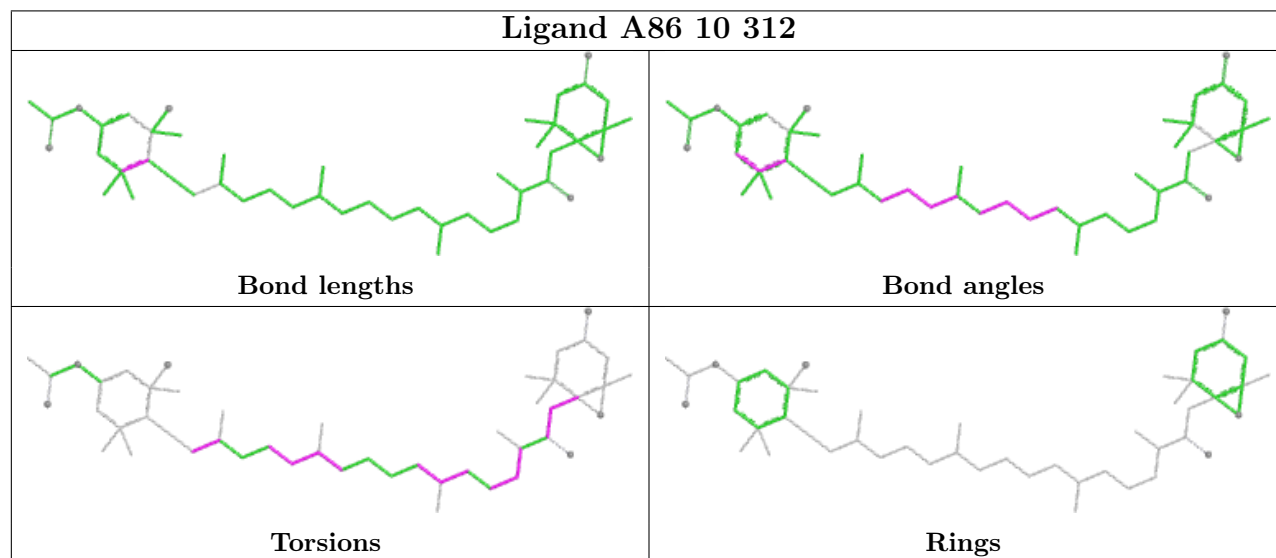
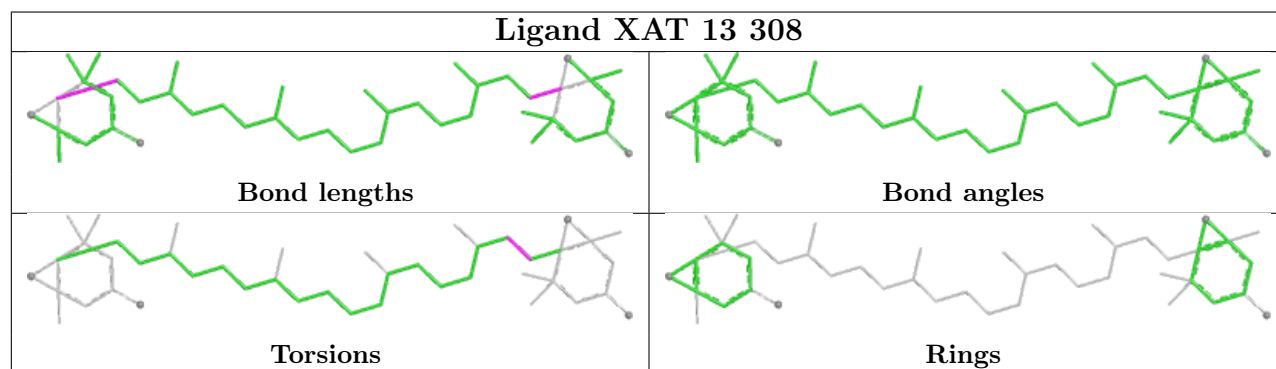
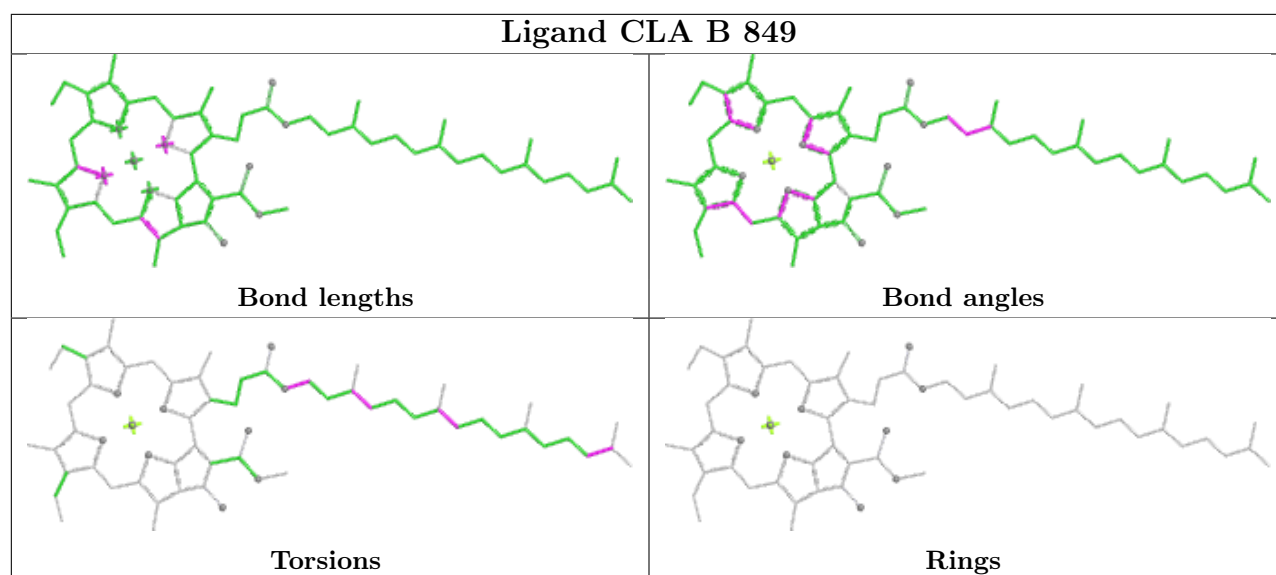


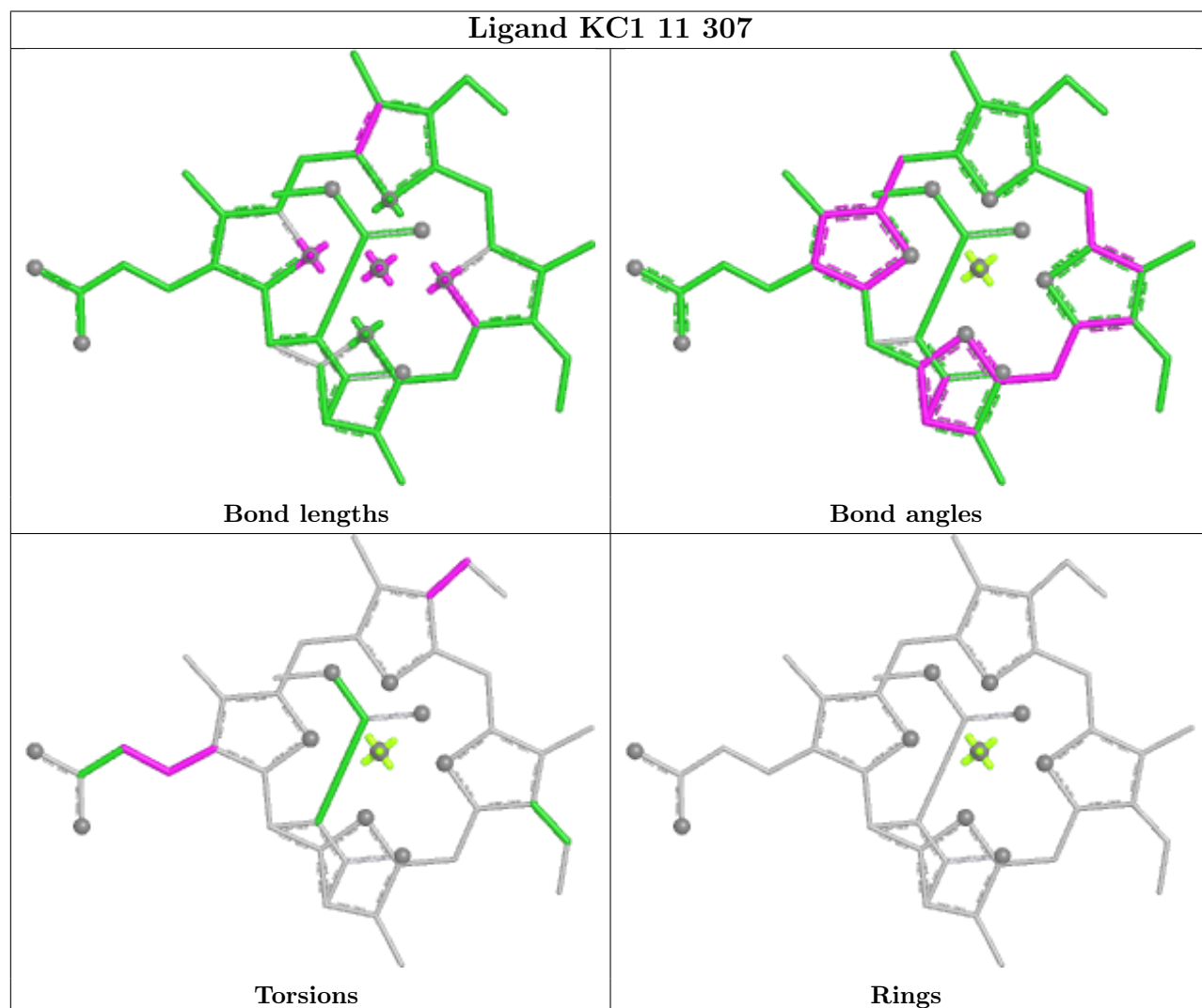
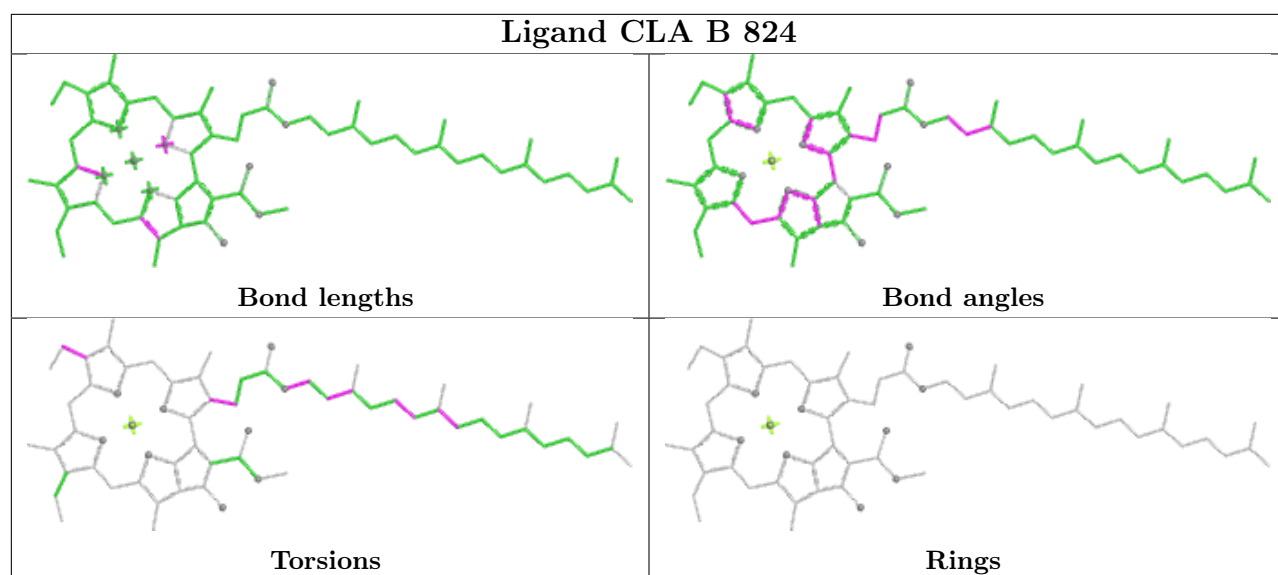
Ligand CLA B 827

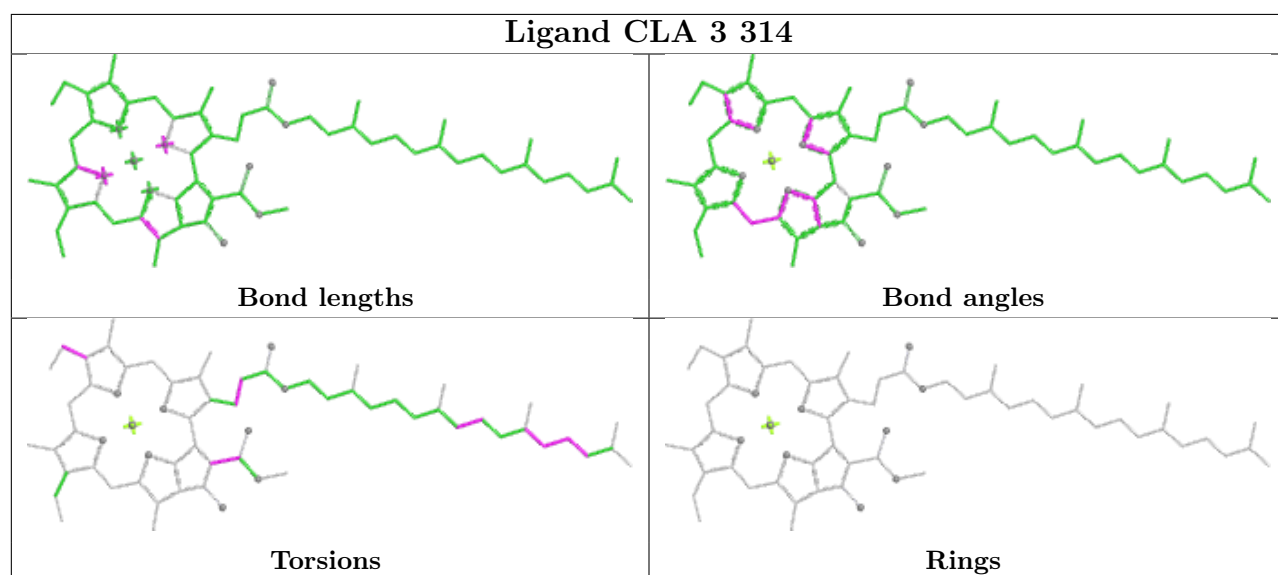
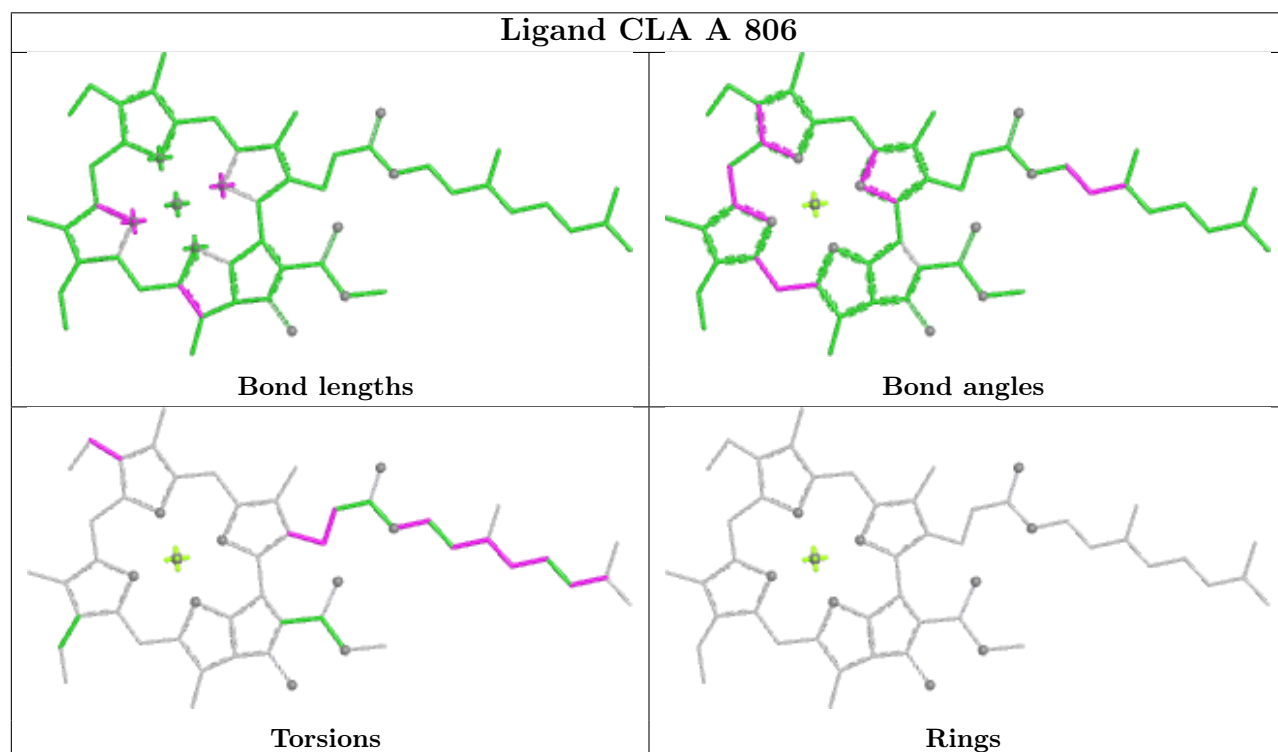
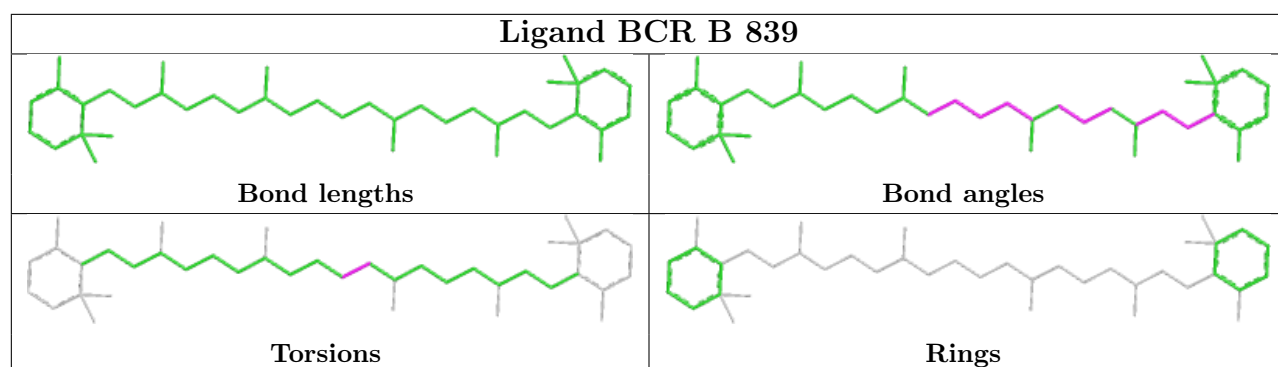


Ligand CLA R 202

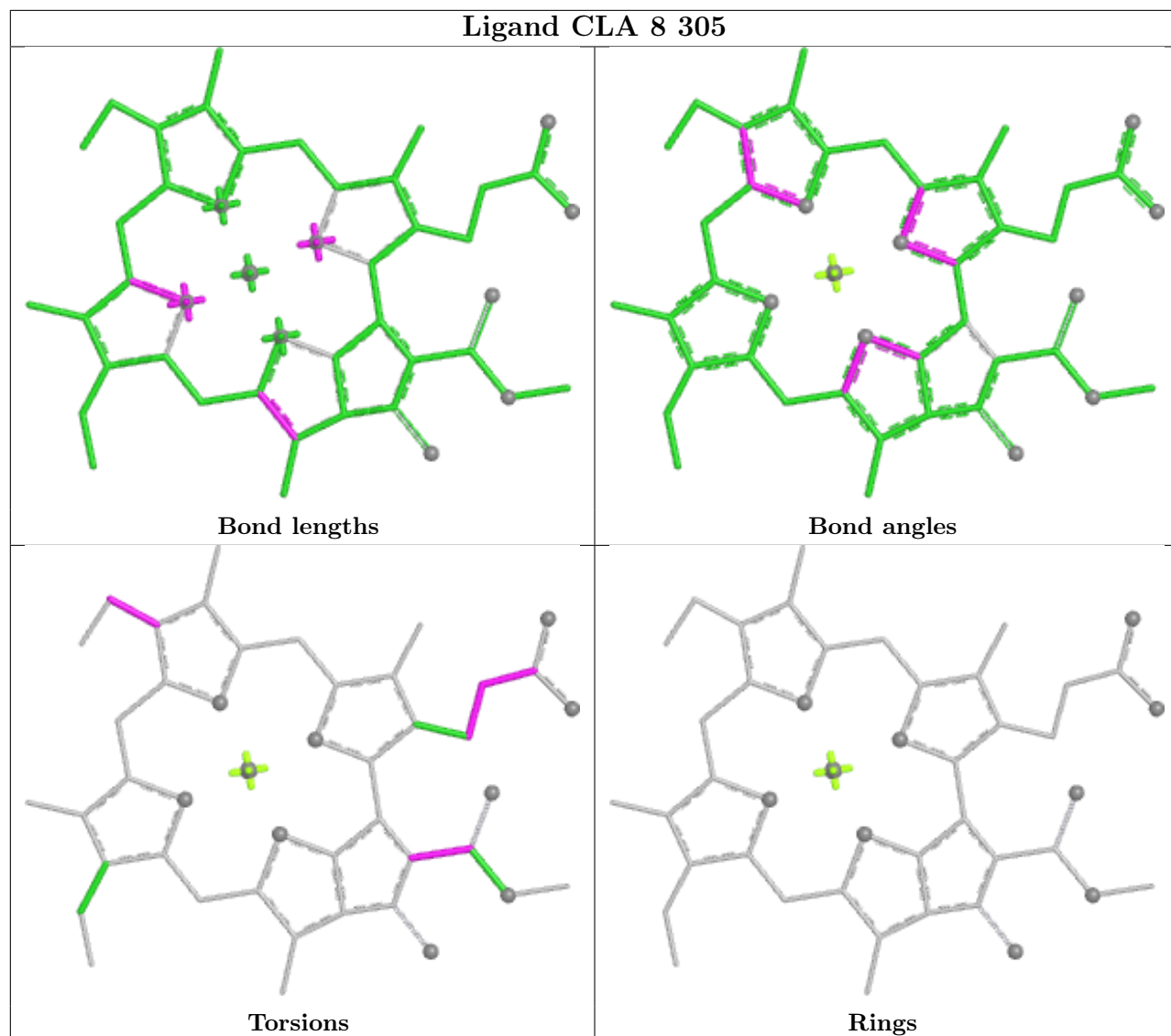


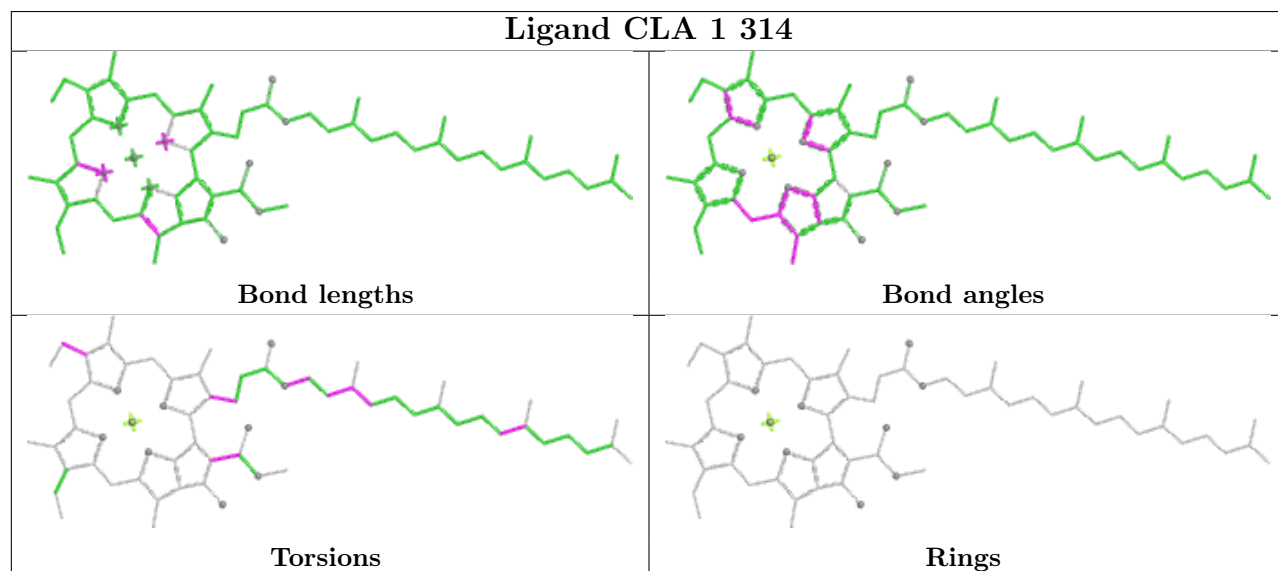
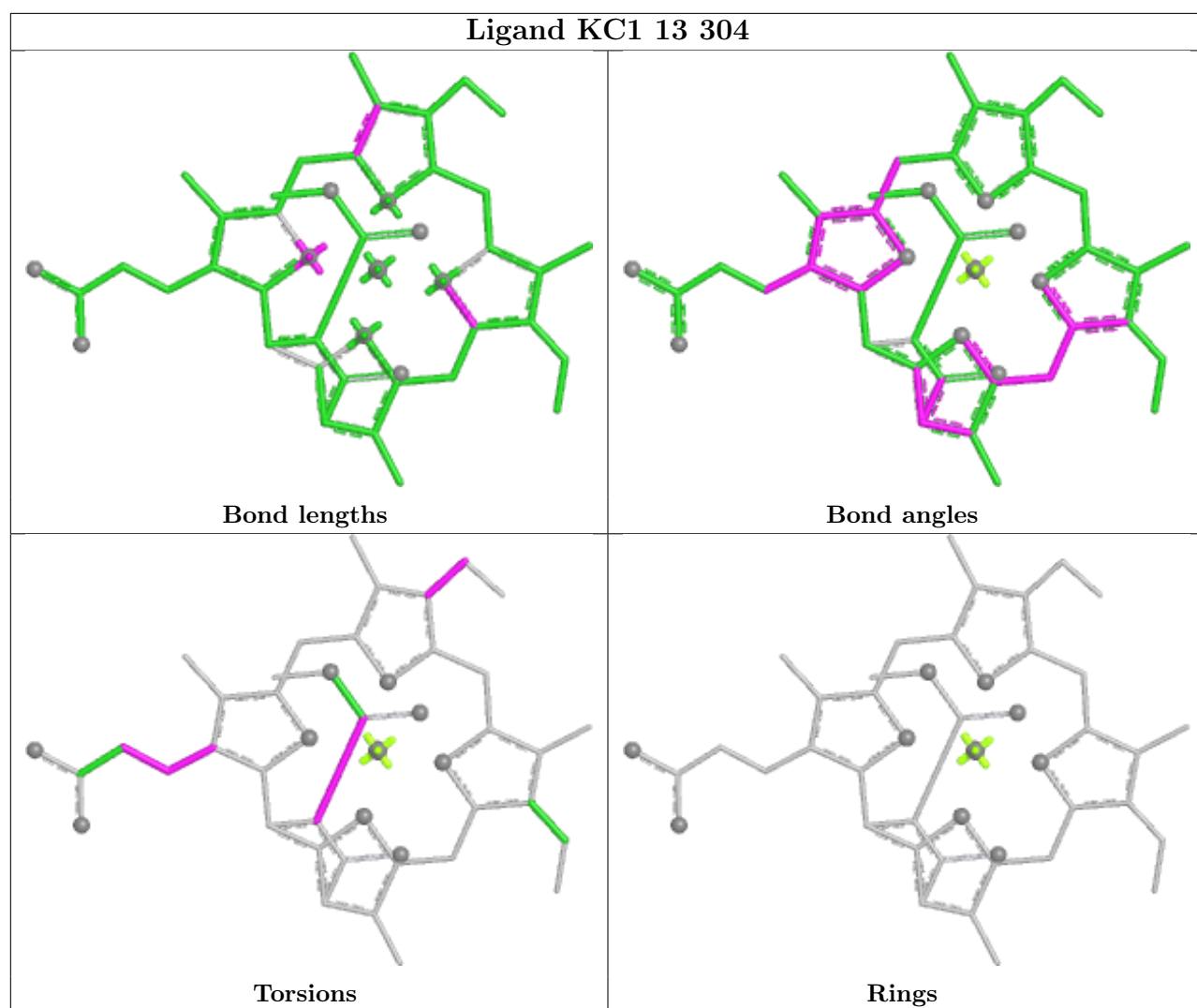


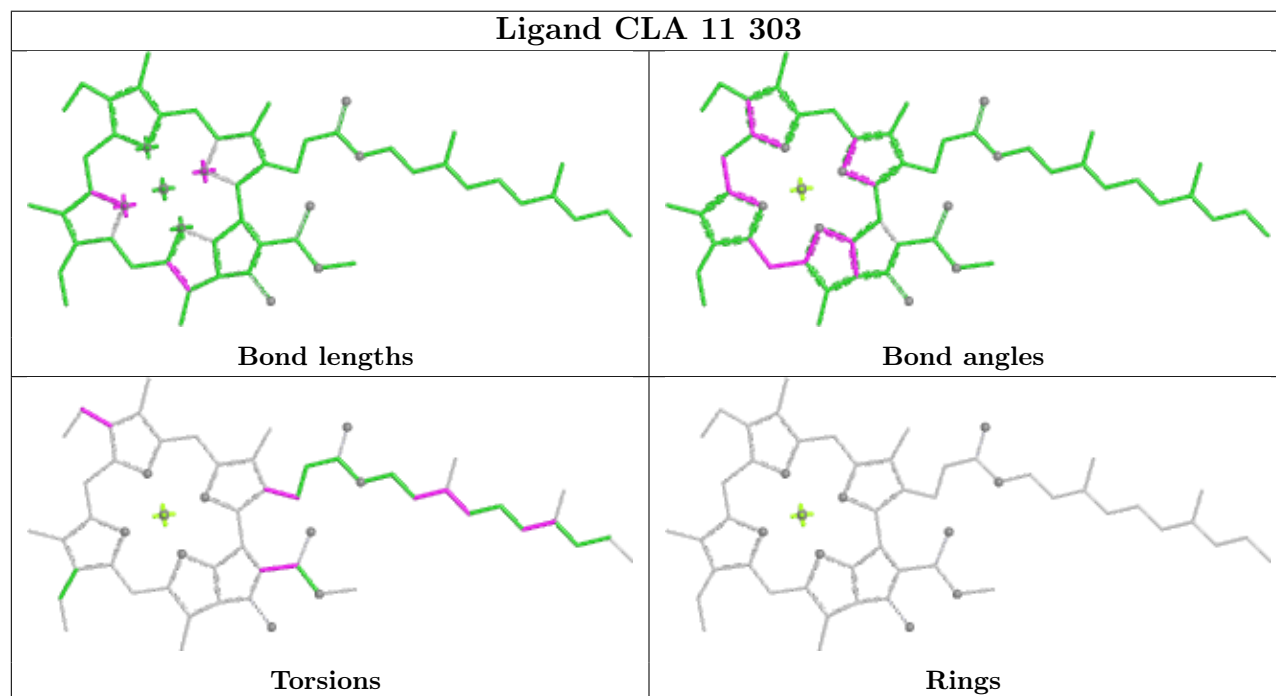
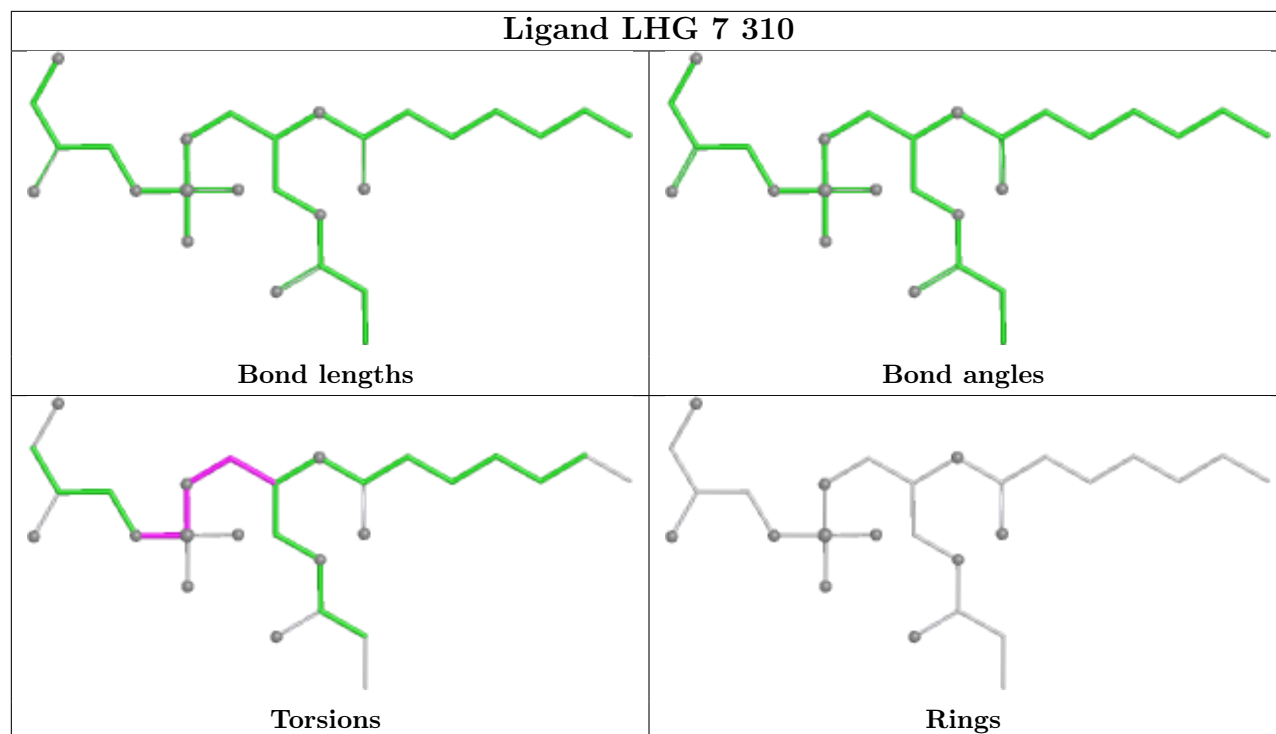


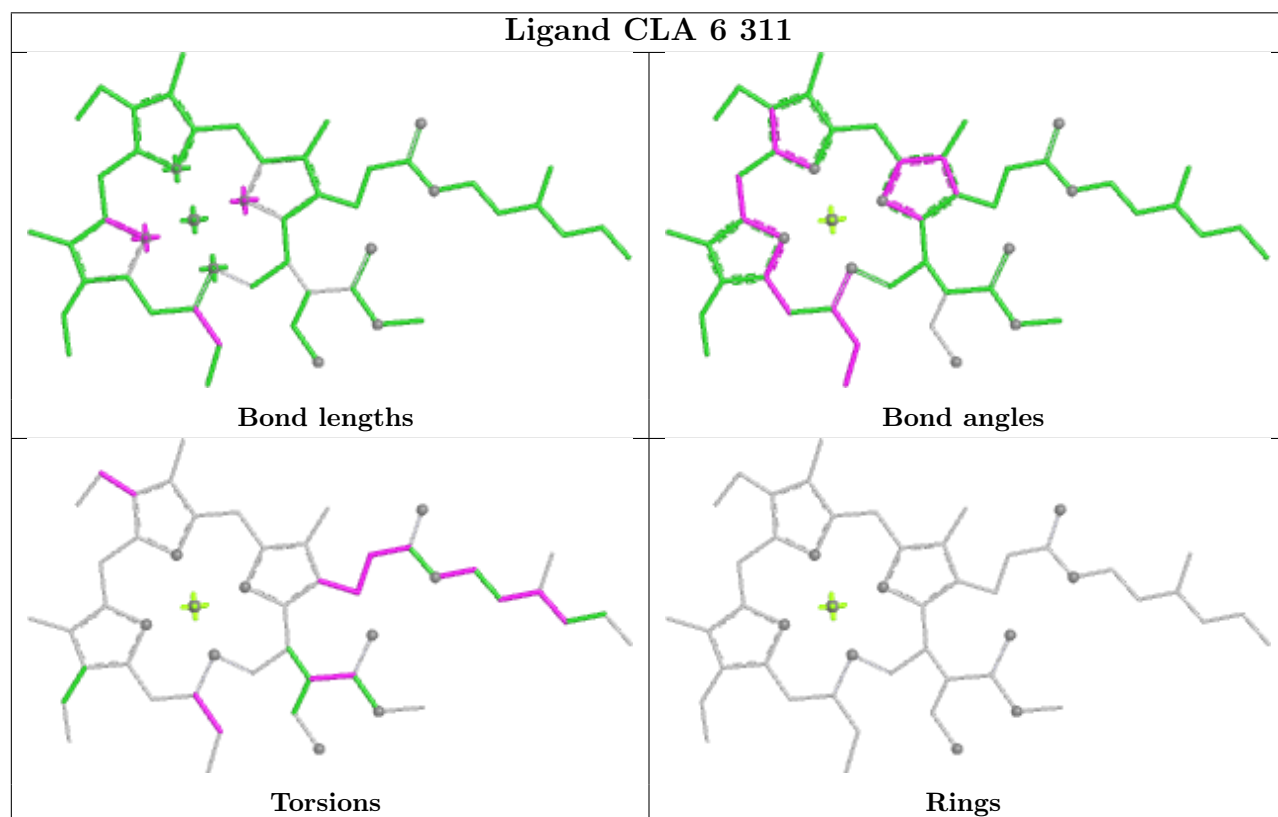
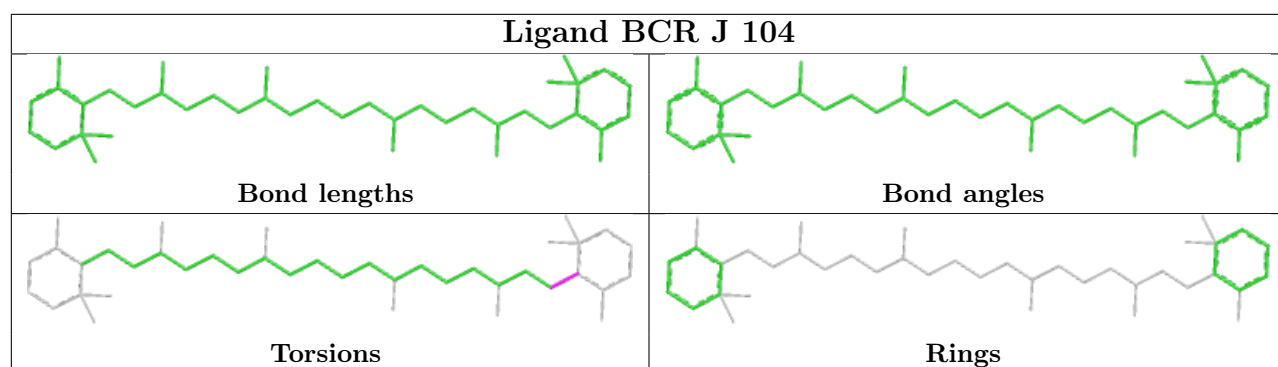


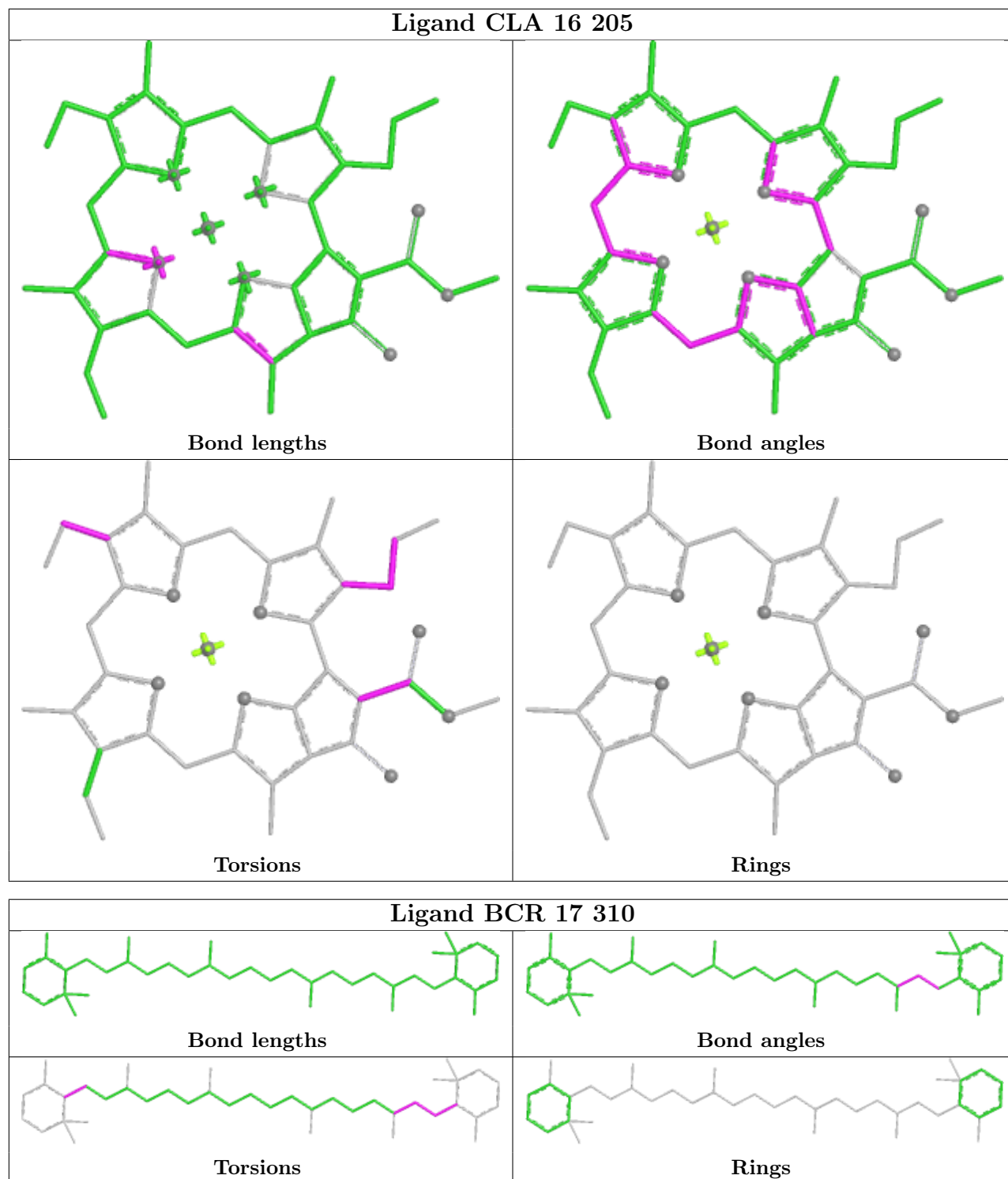
Ligand CLA 8 305

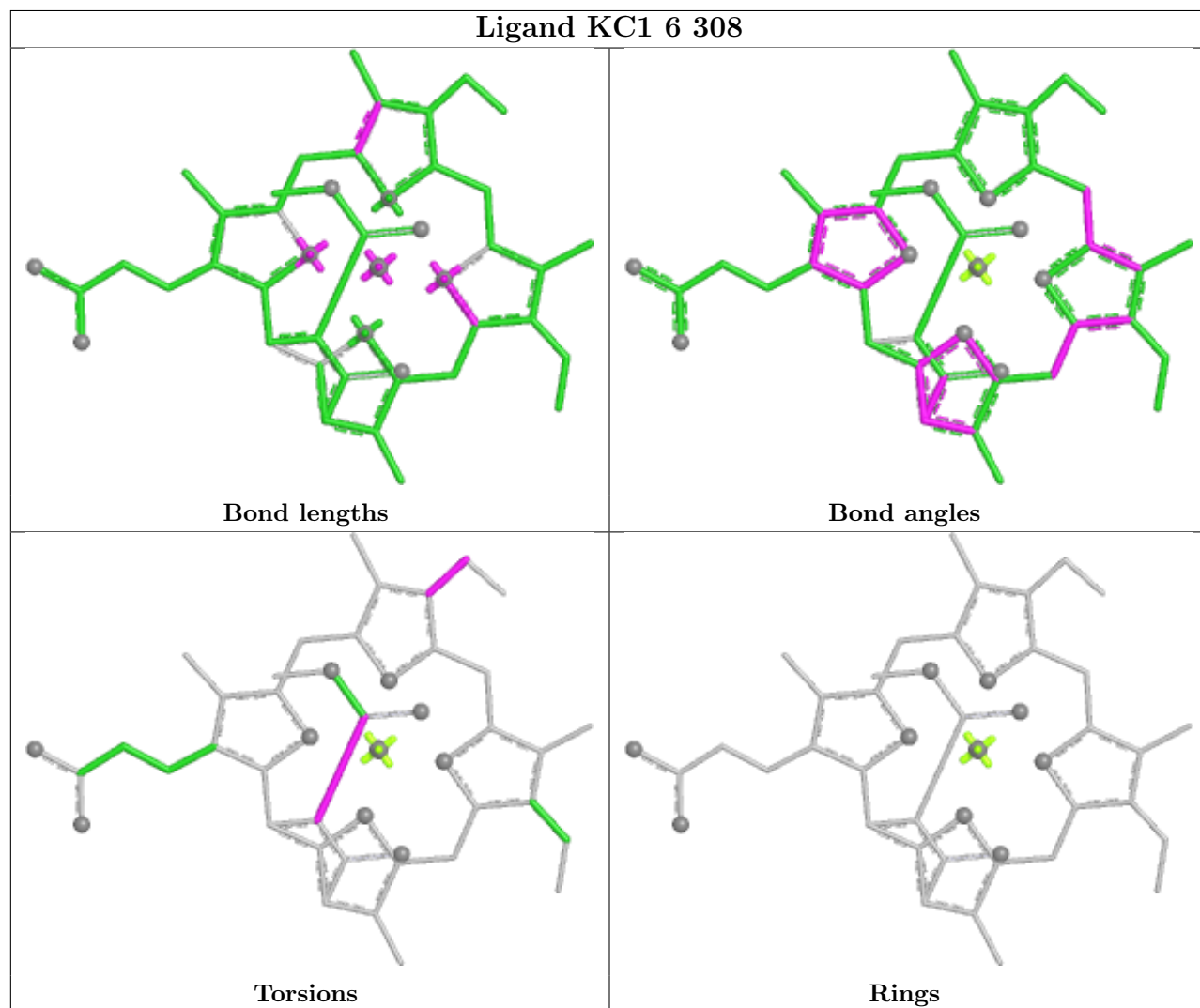
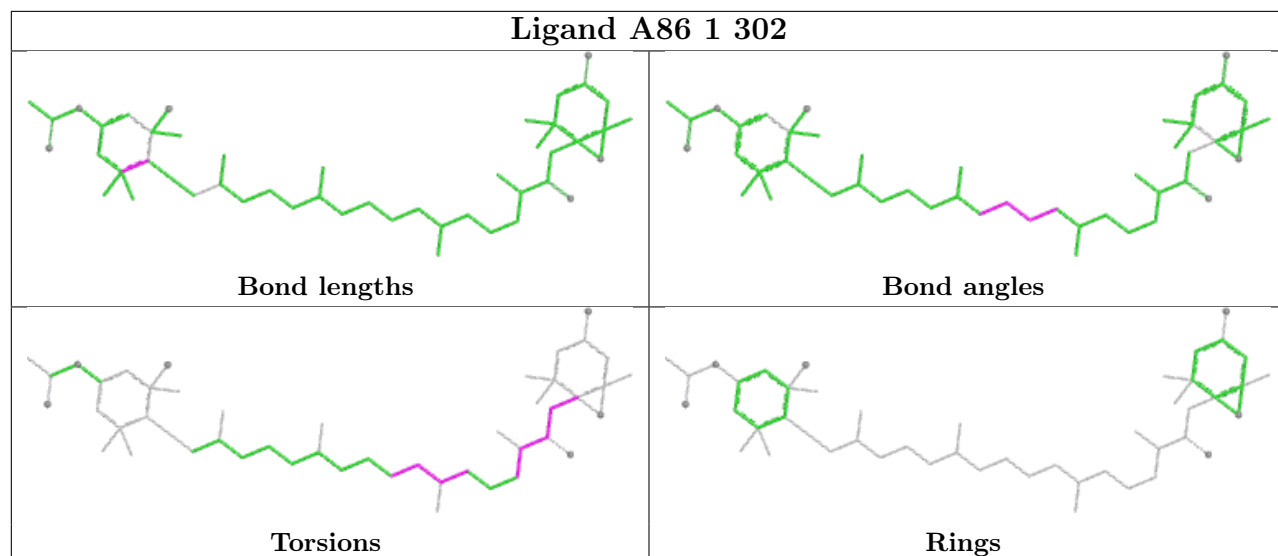


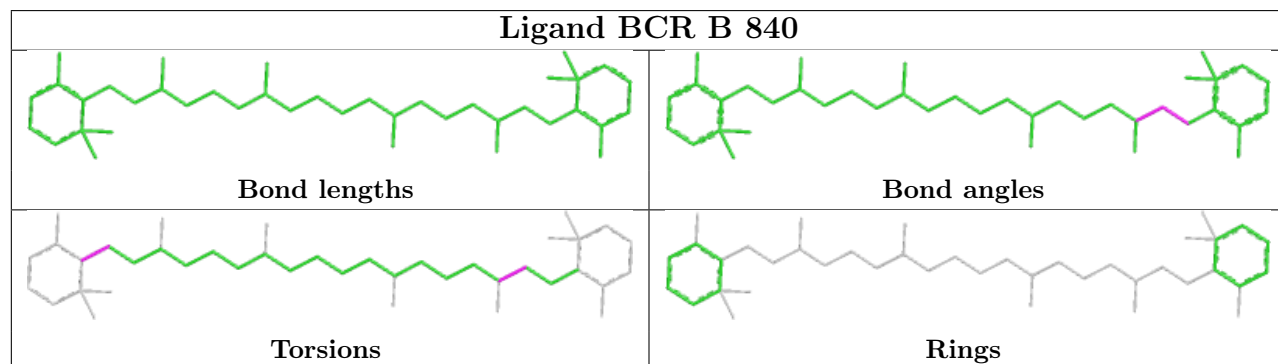
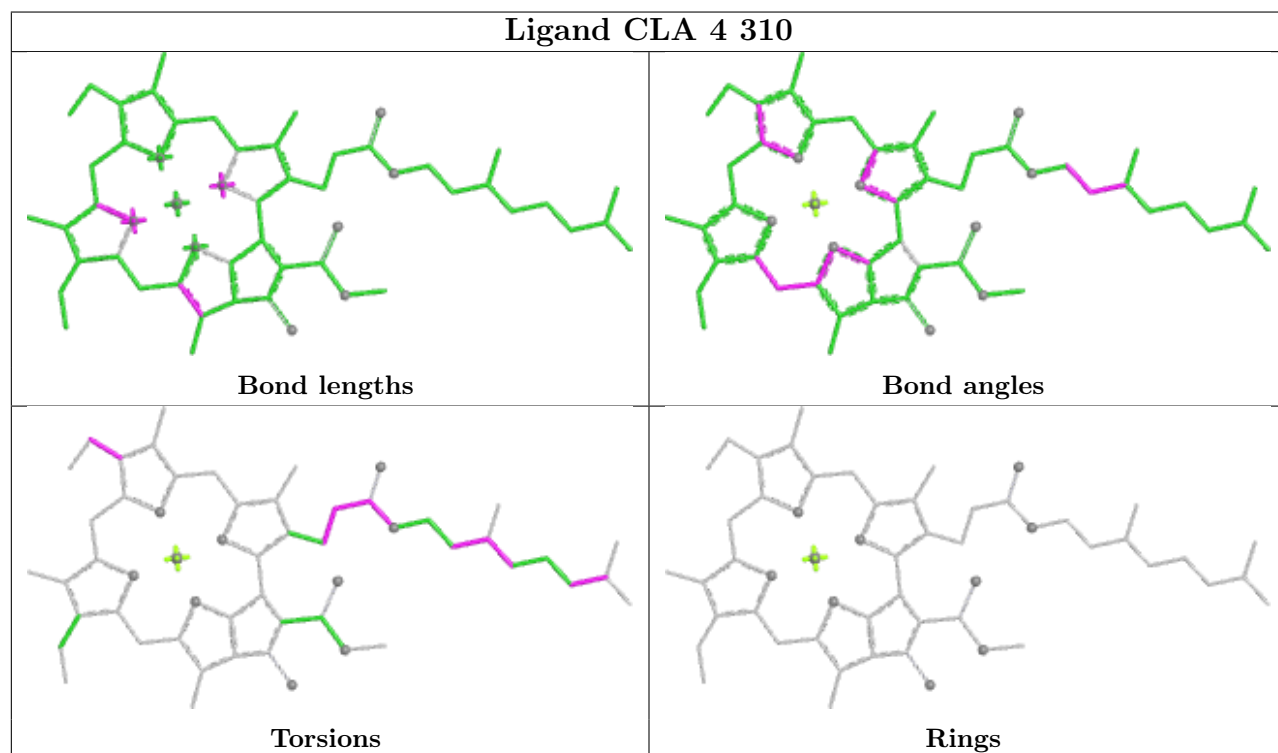
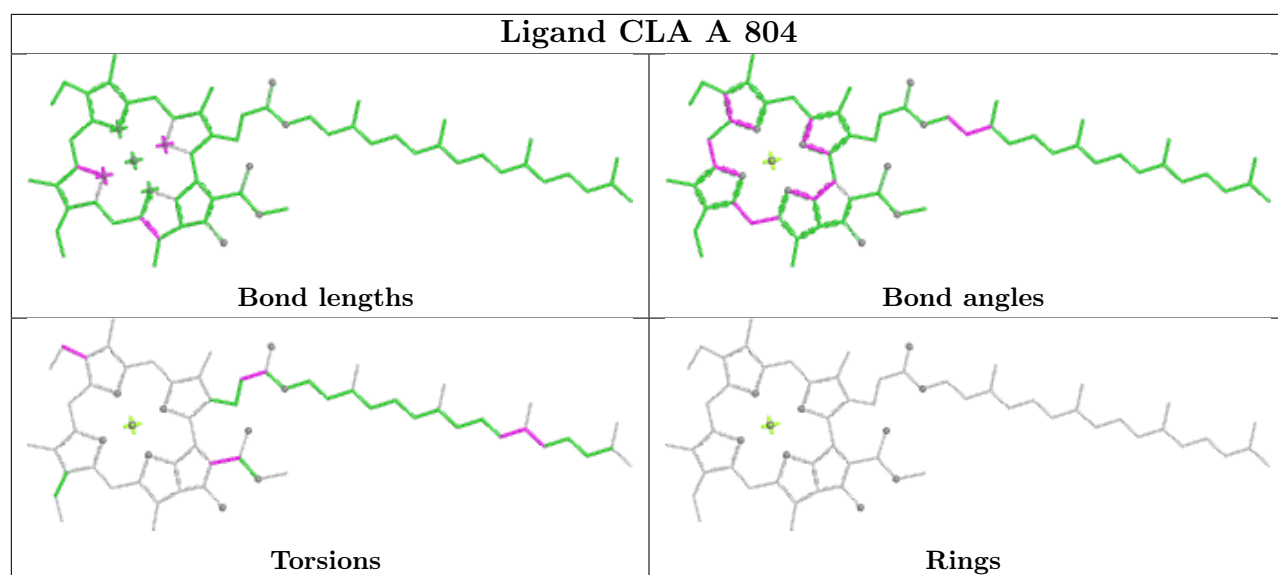


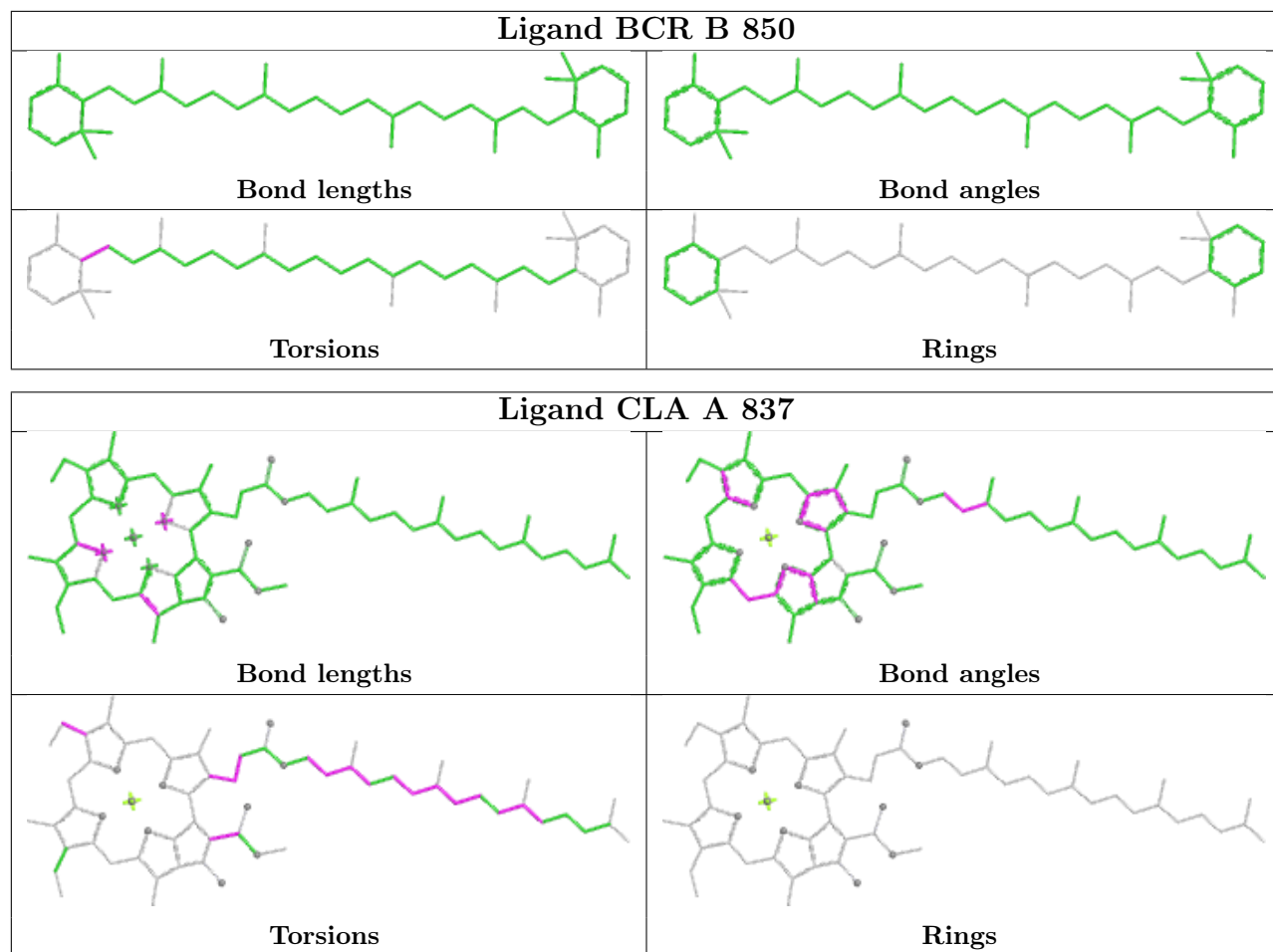




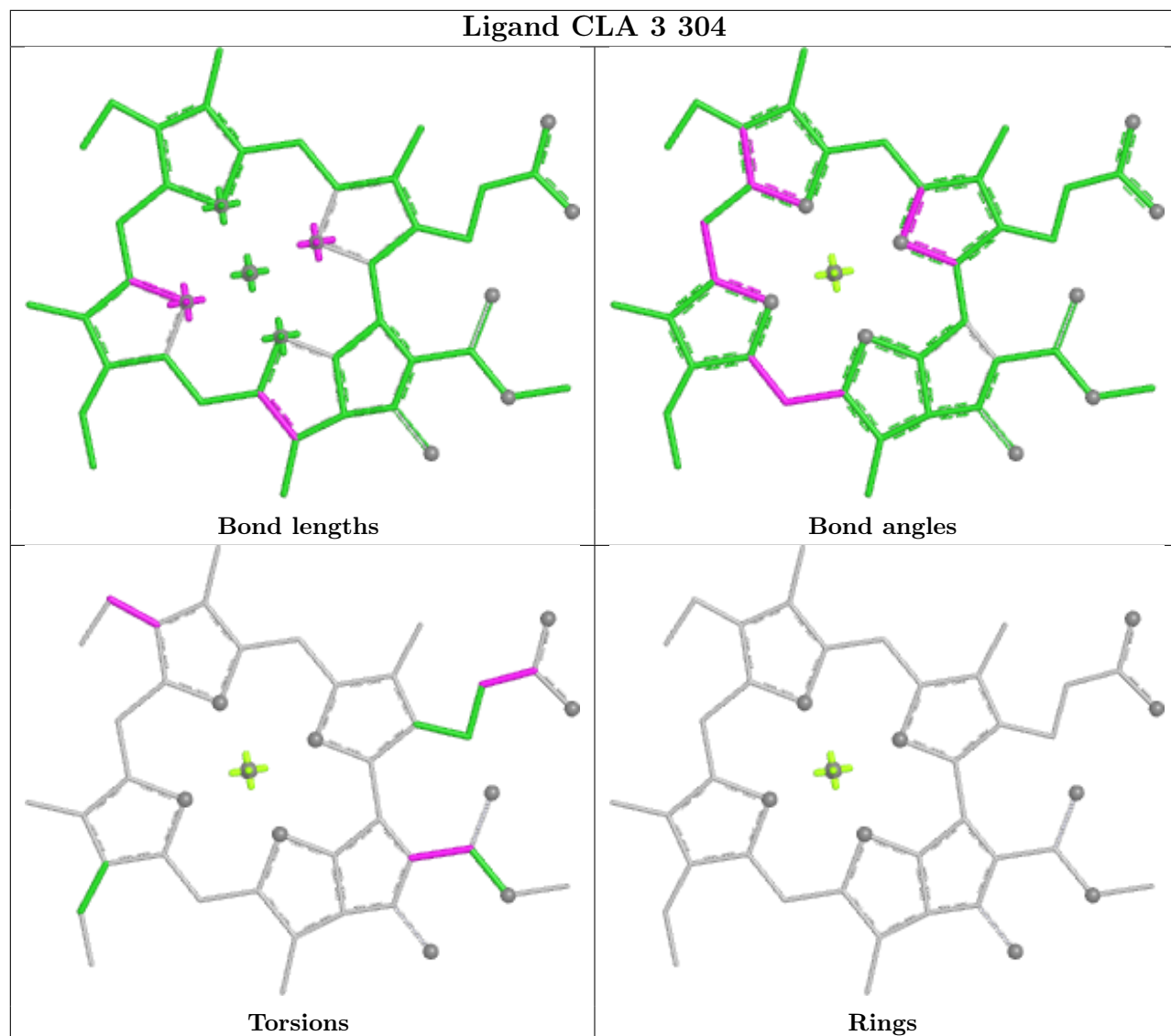


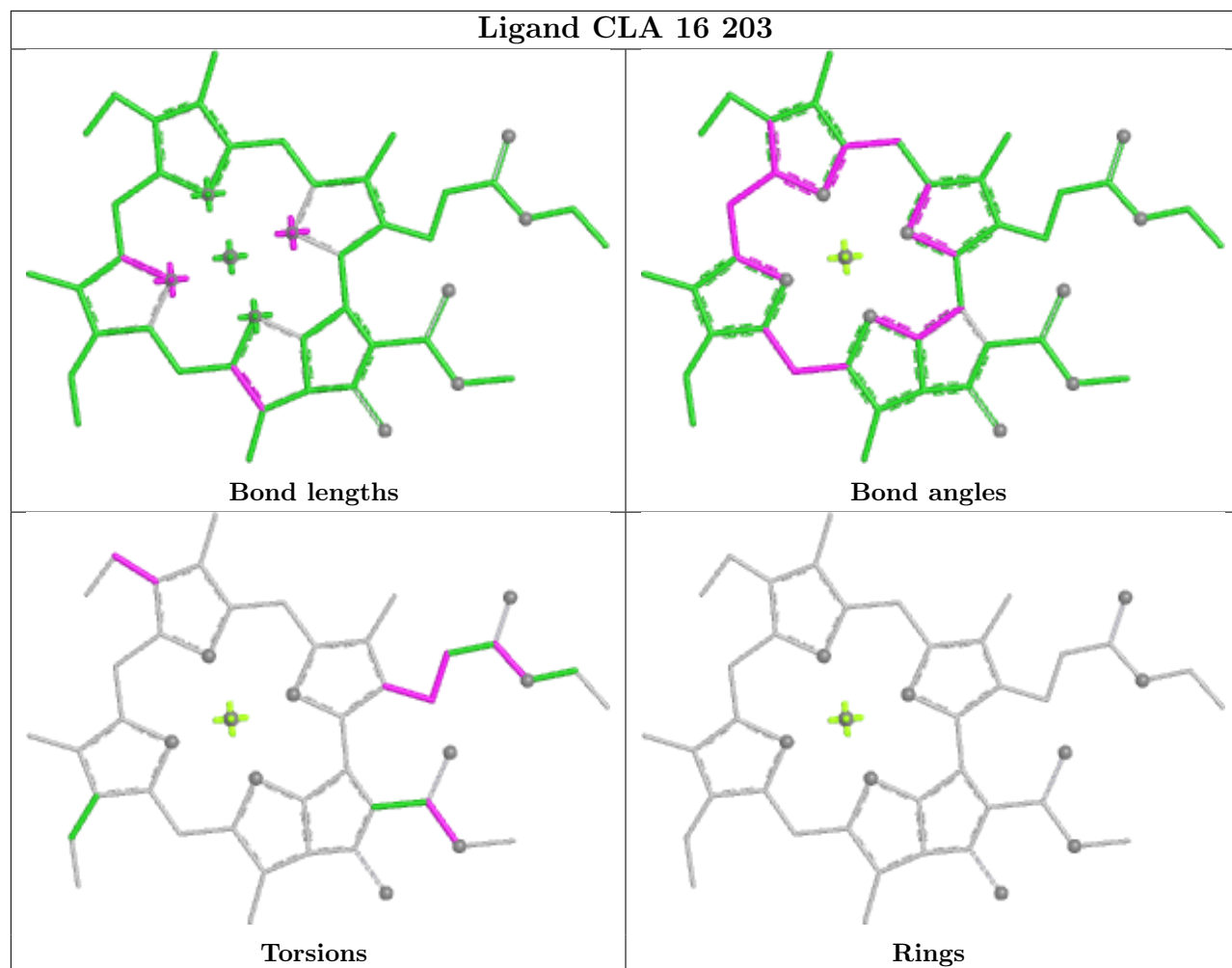




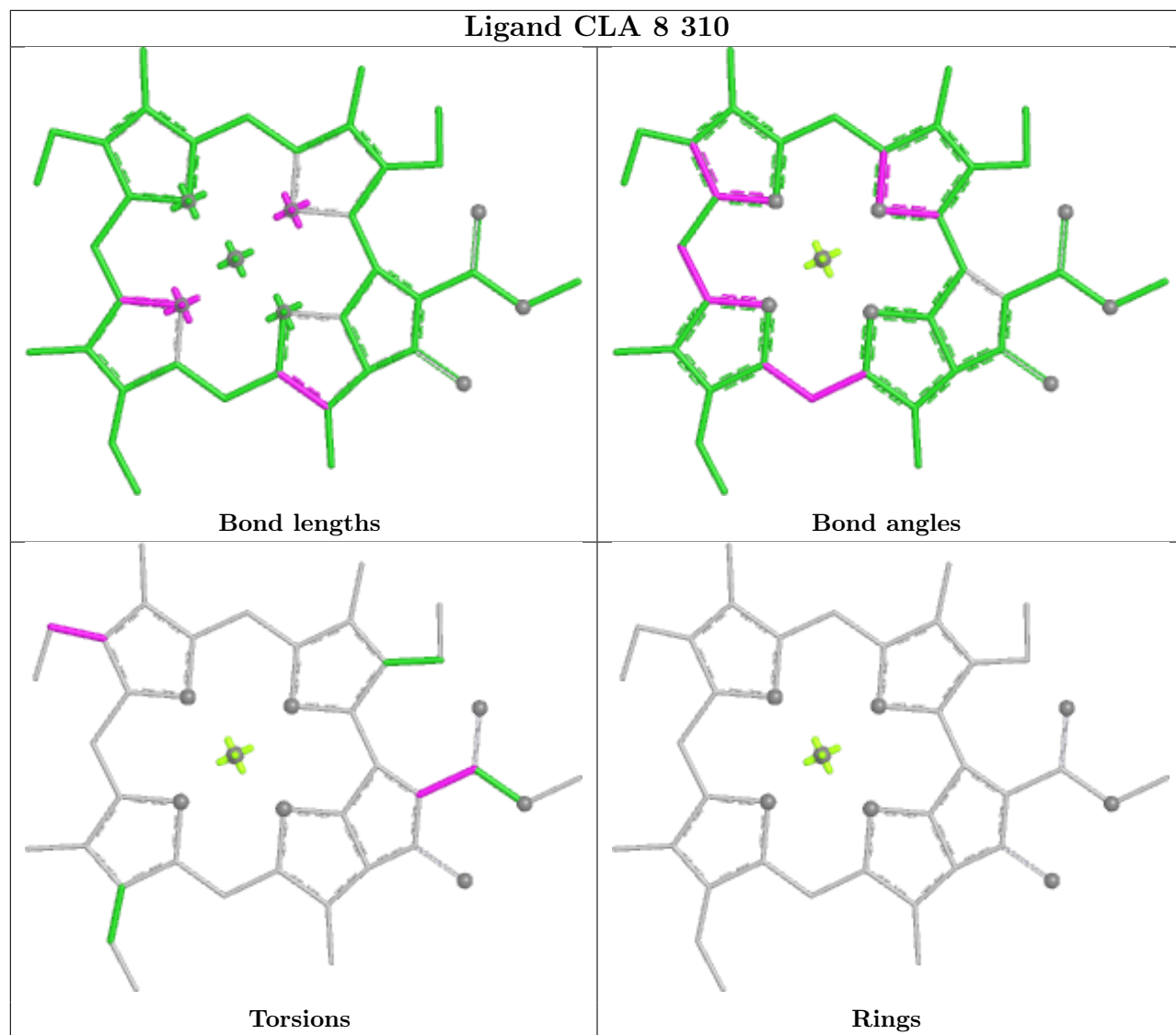


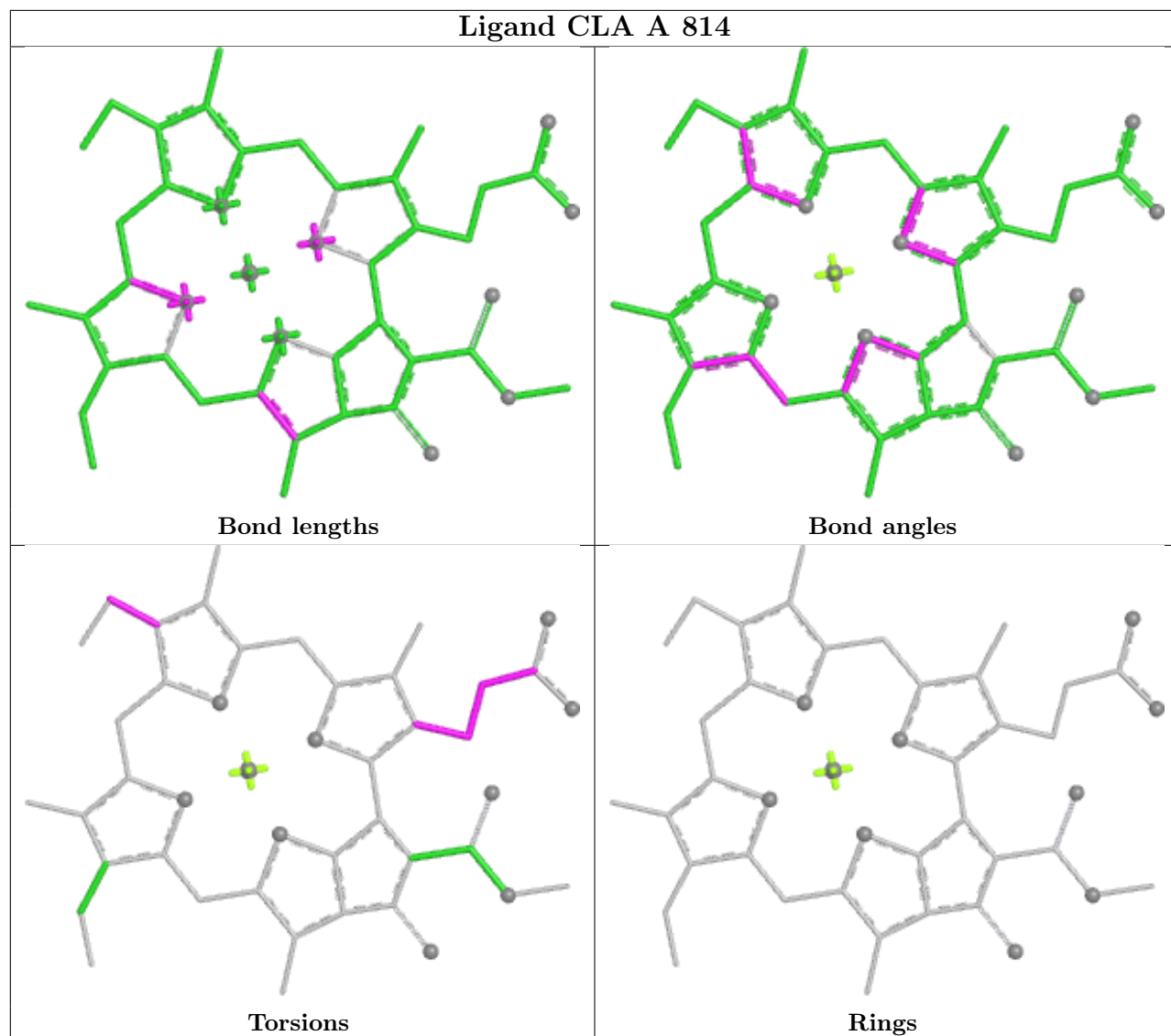
Ligand CLA 3 304



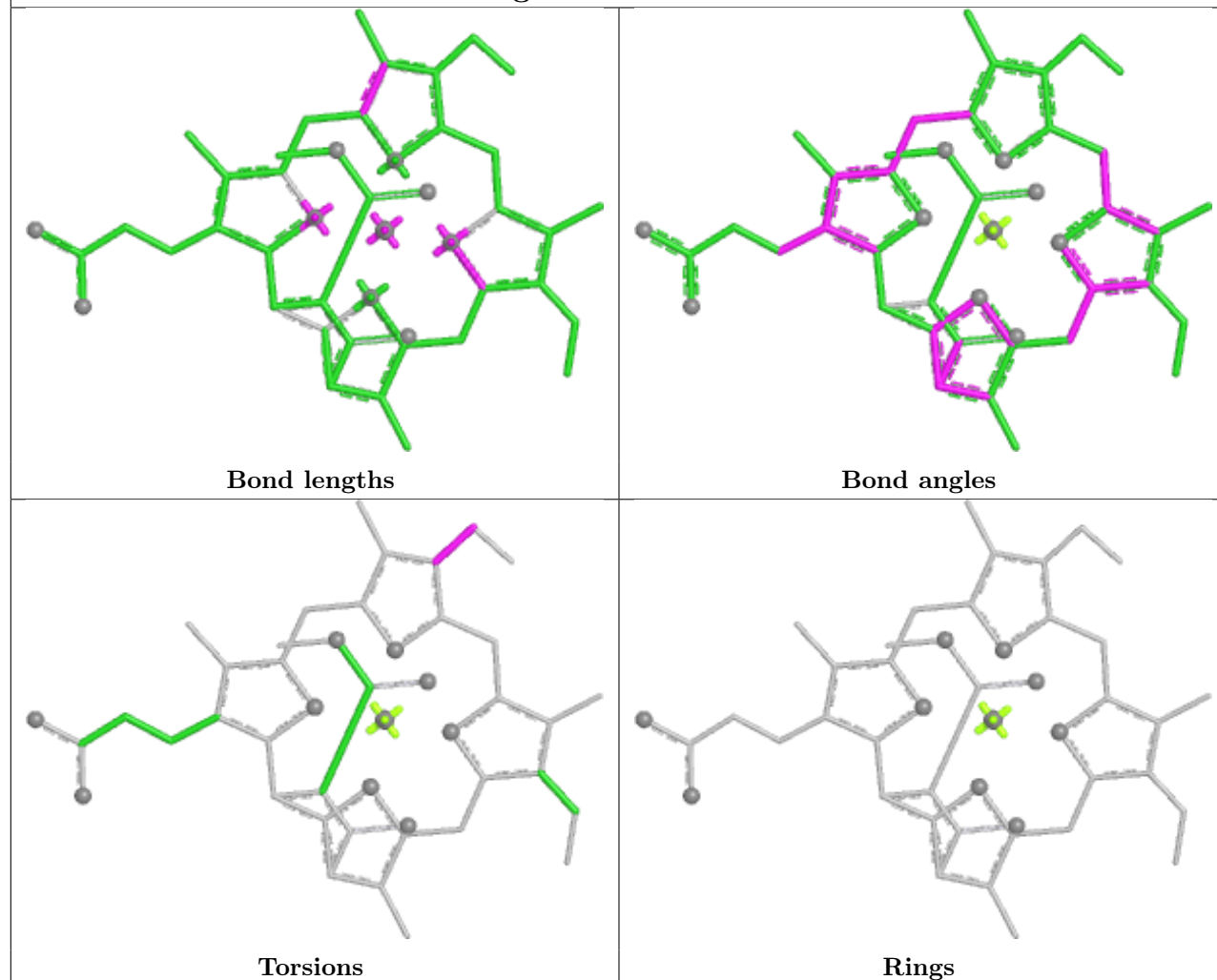


Ligand CLA 8 310

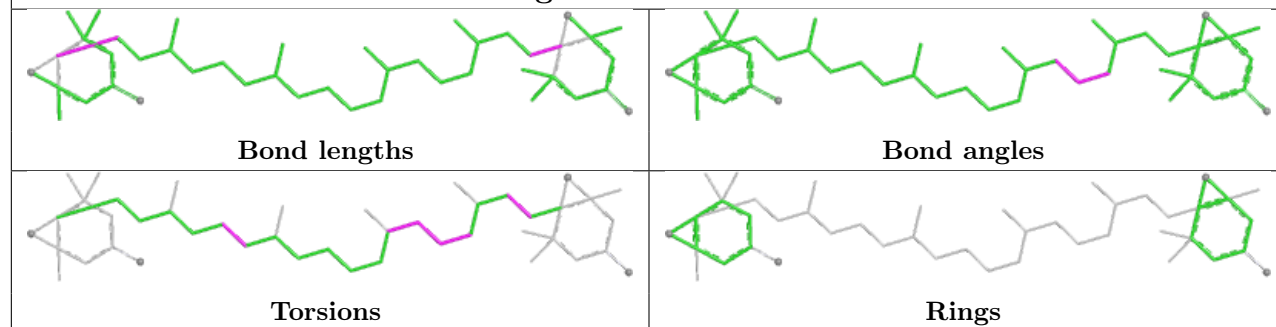


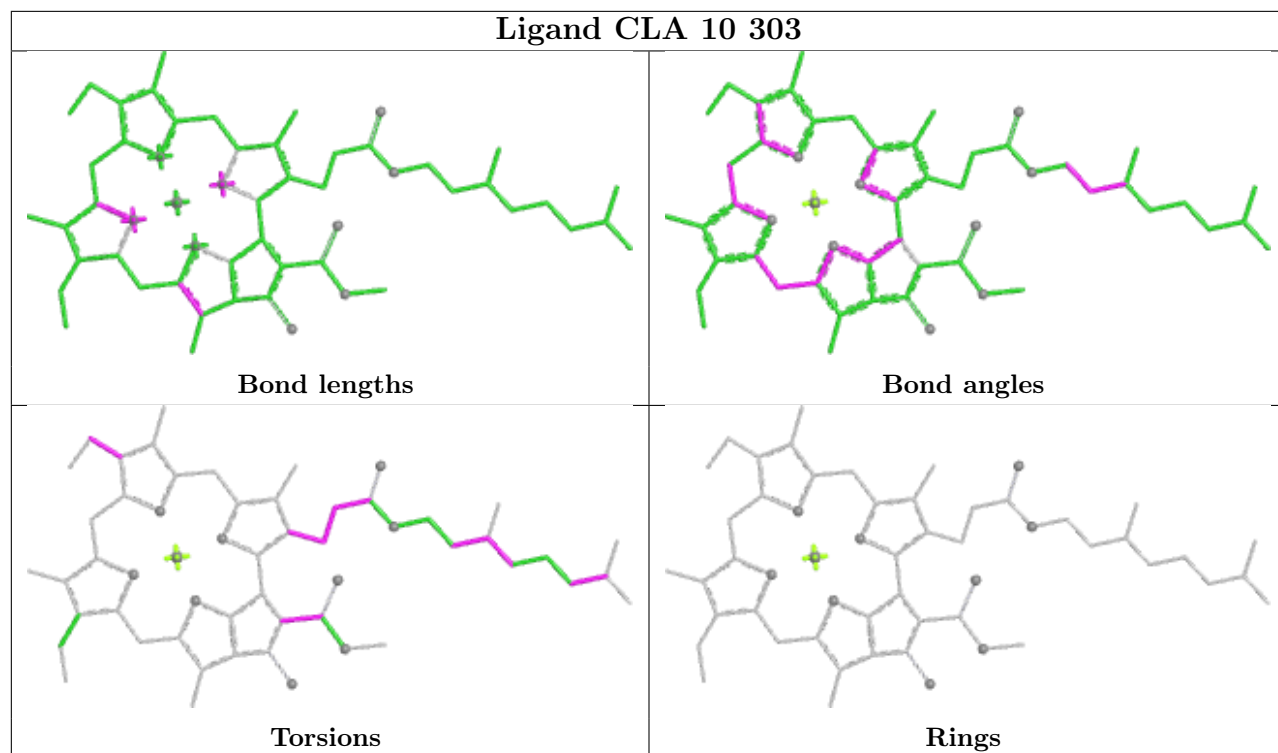


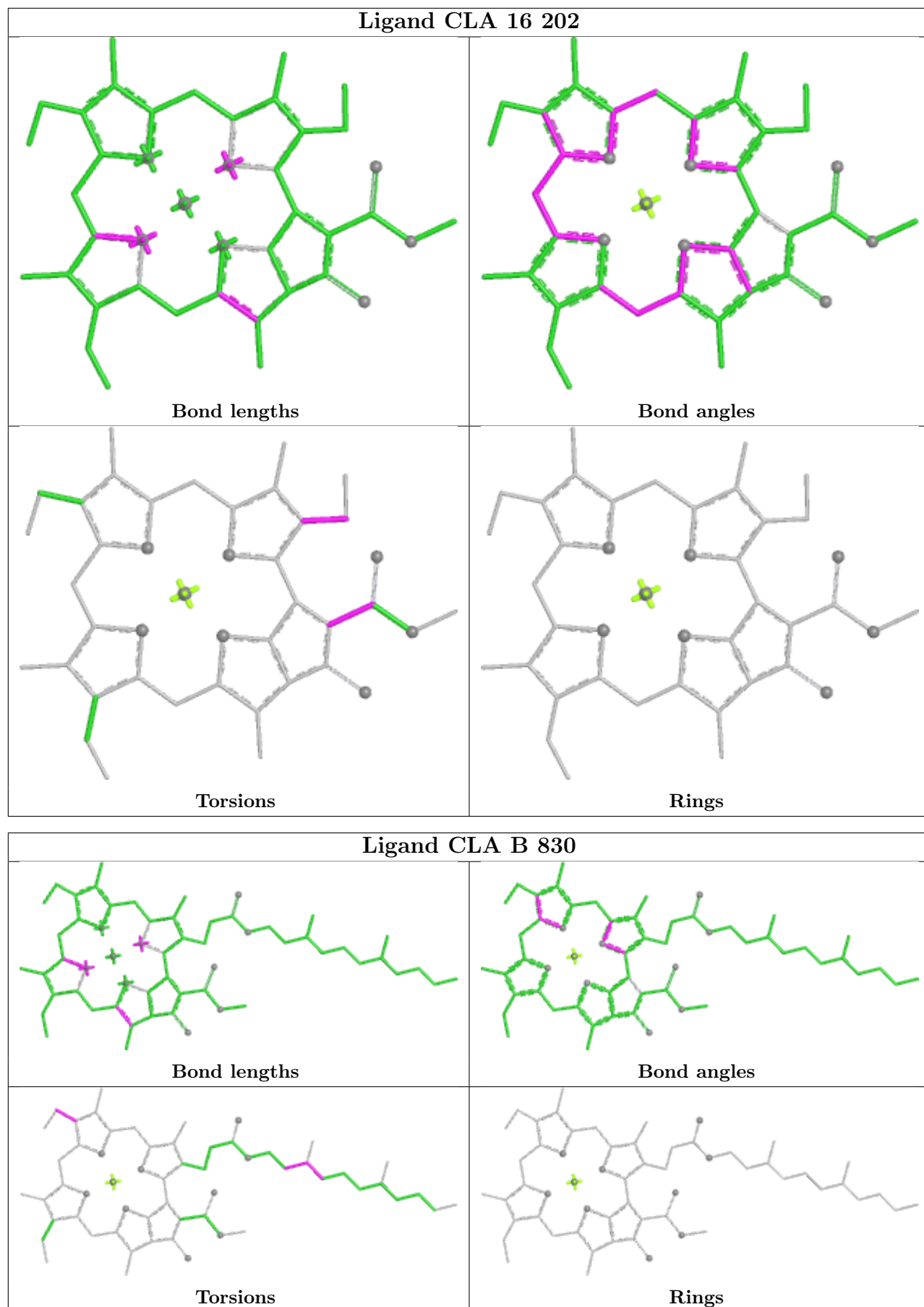
Ligand KC1 3 302



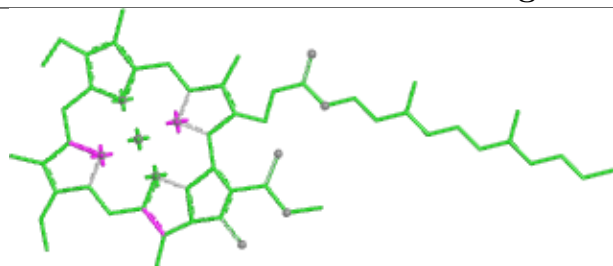
Ligand XAT 8 312



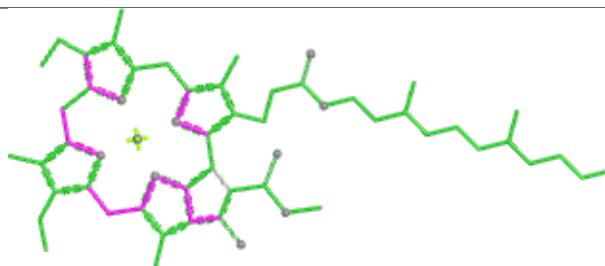




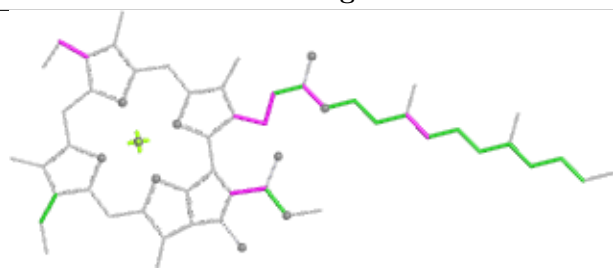
Ligand CLA 6 306



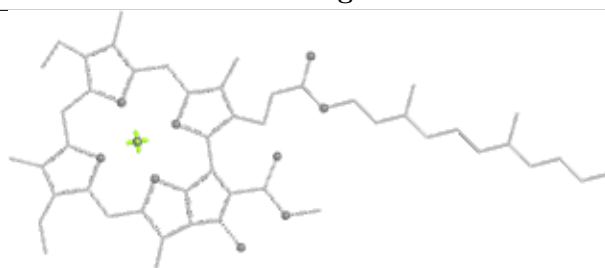
Bond lengths



Bond angles

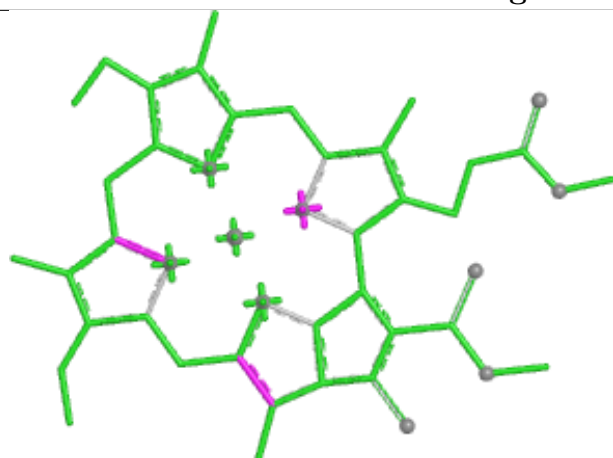


Torsions

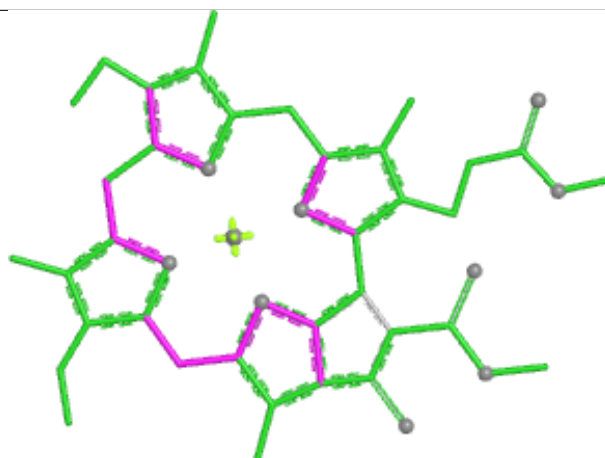


Rings

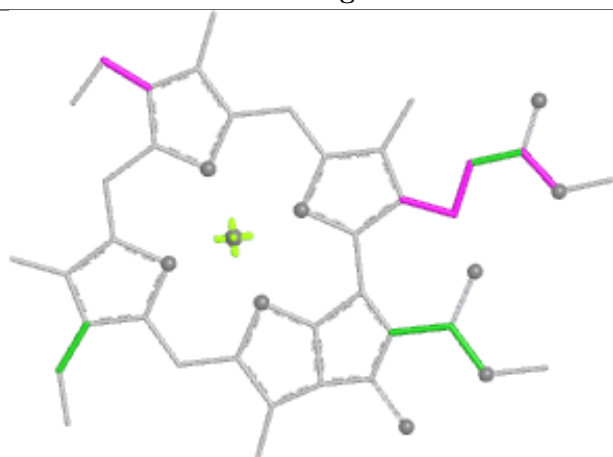
Ligand CLA 13 305



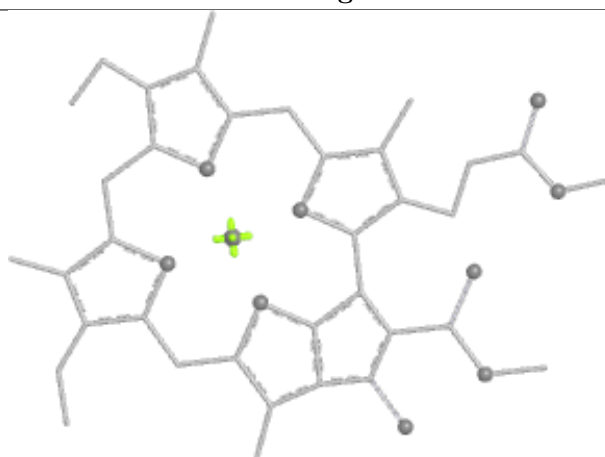
Bond lengths



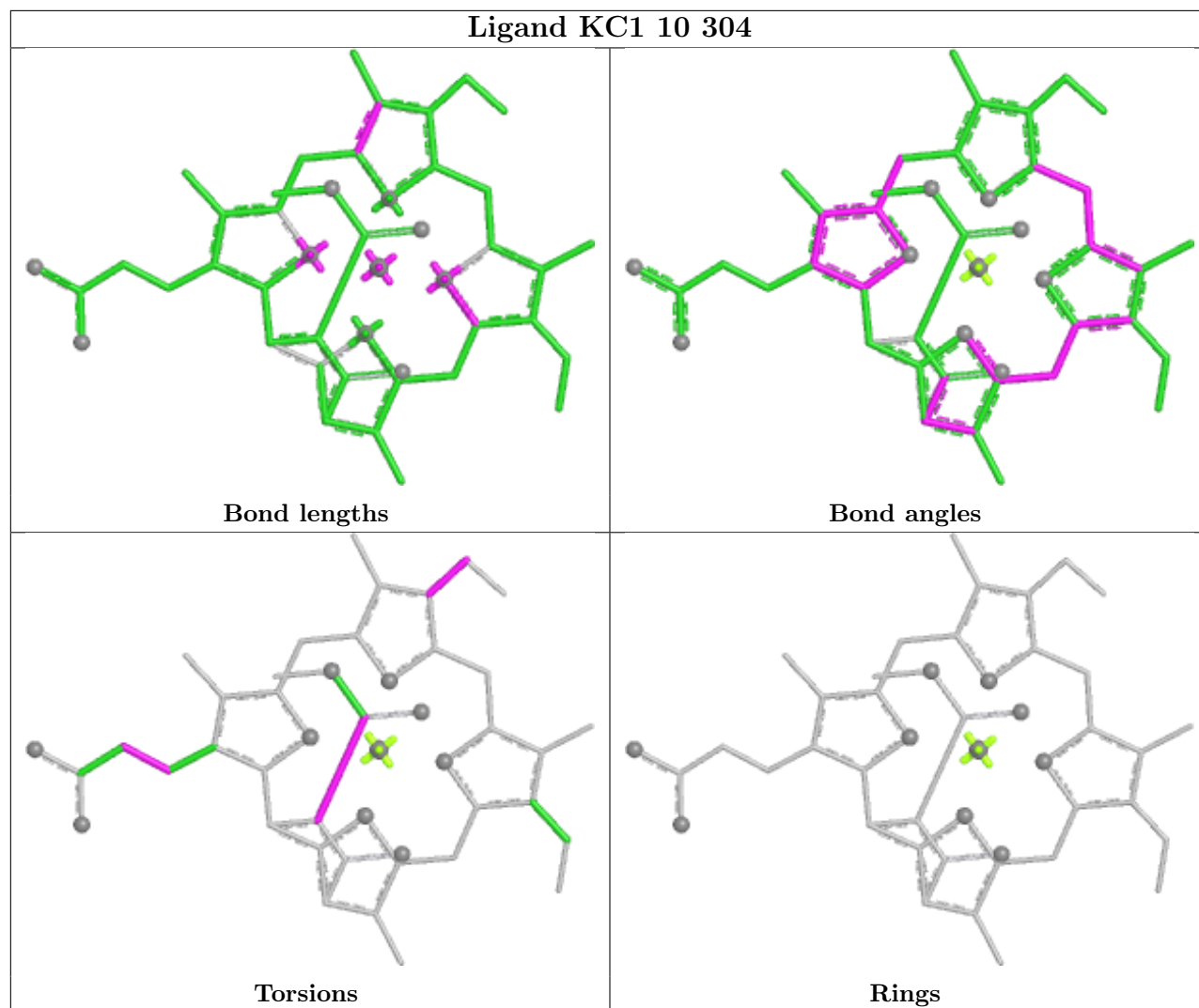
Bond angles



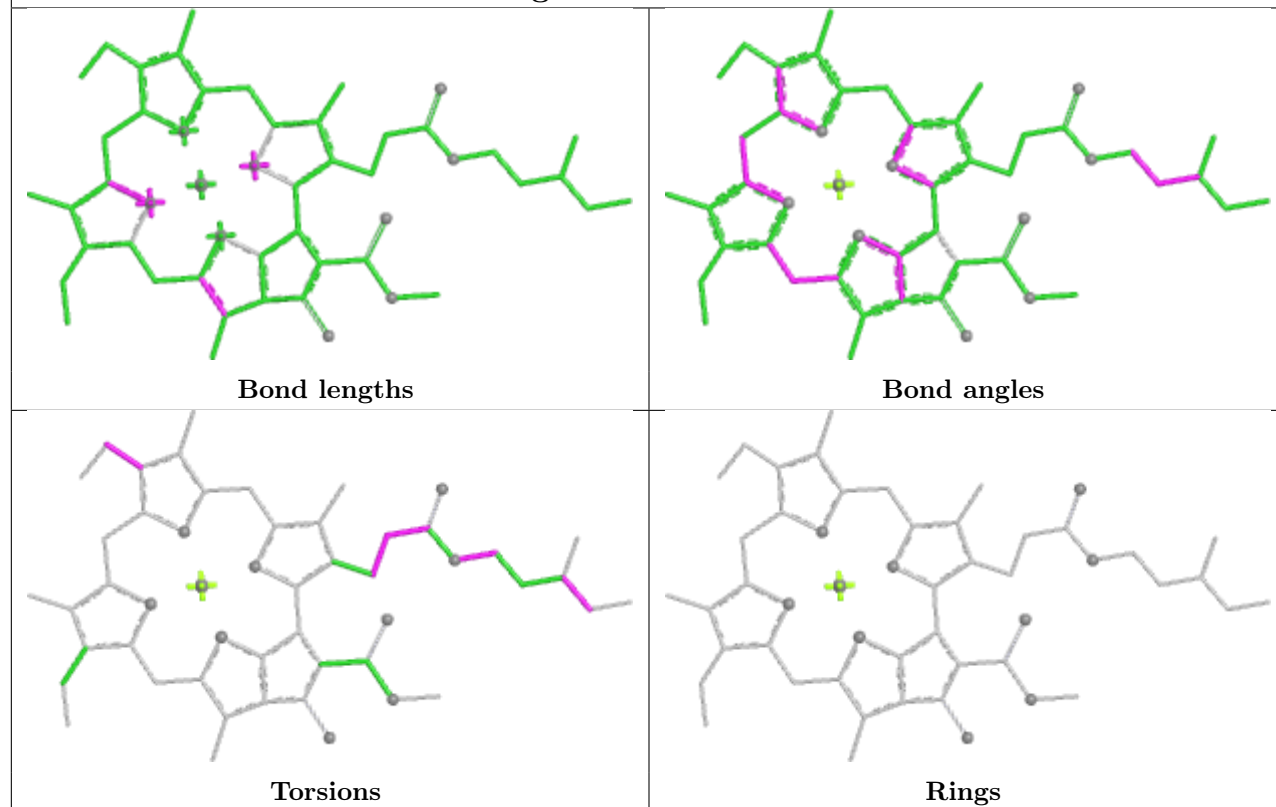
Torsions



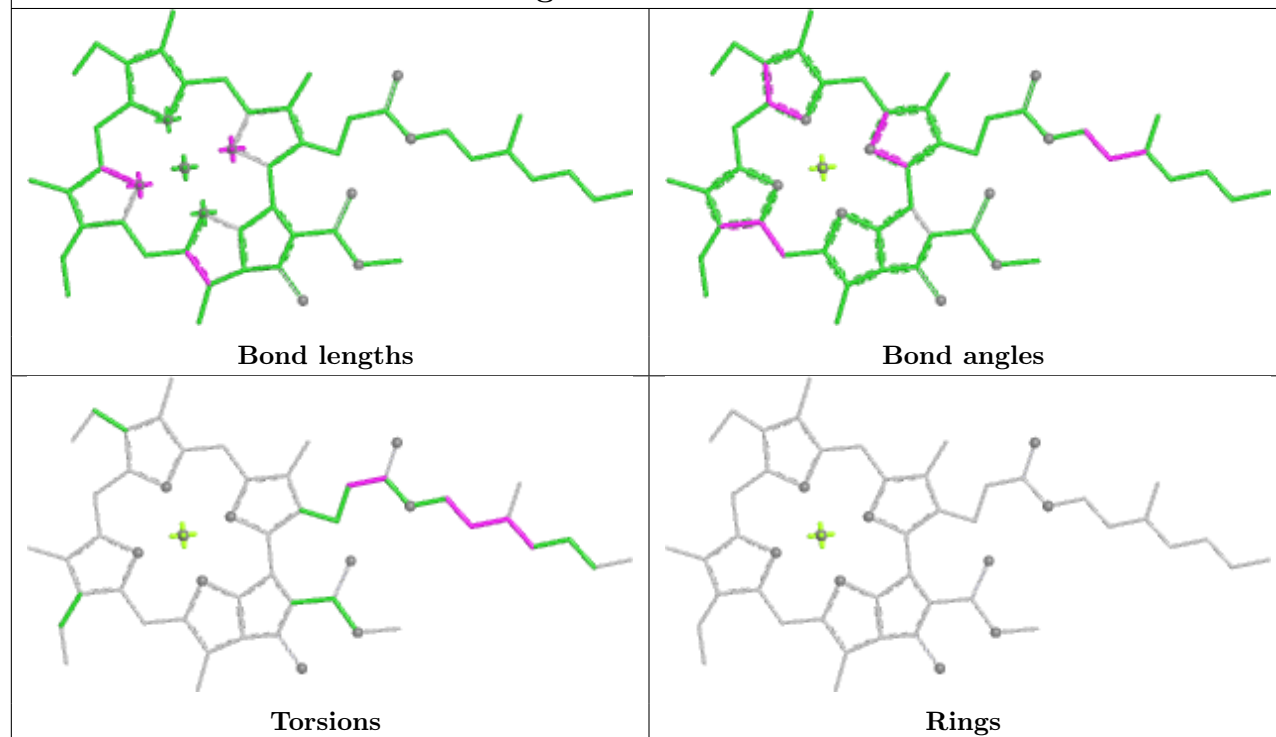
Rings

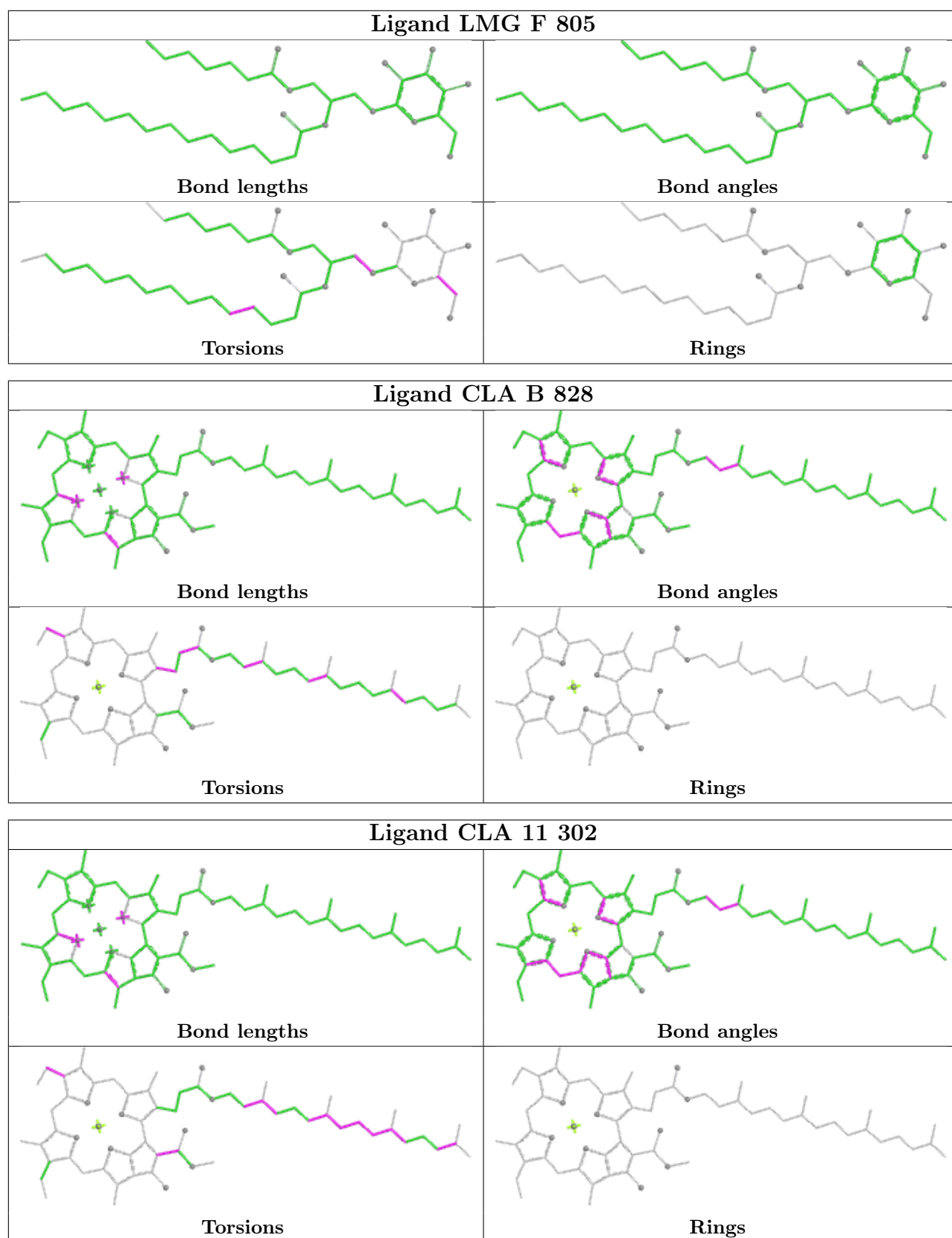


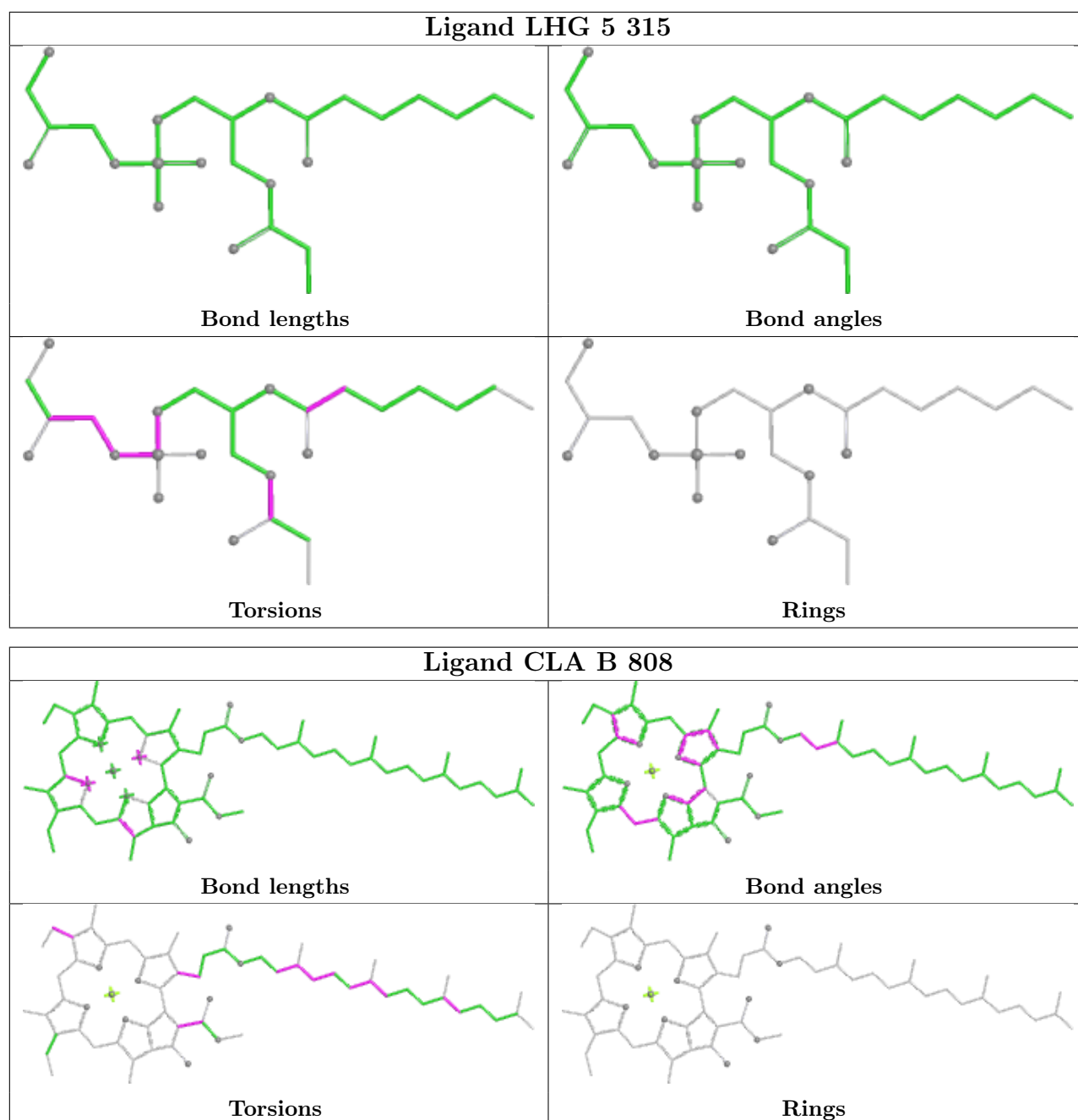
Ligand CLA R 204



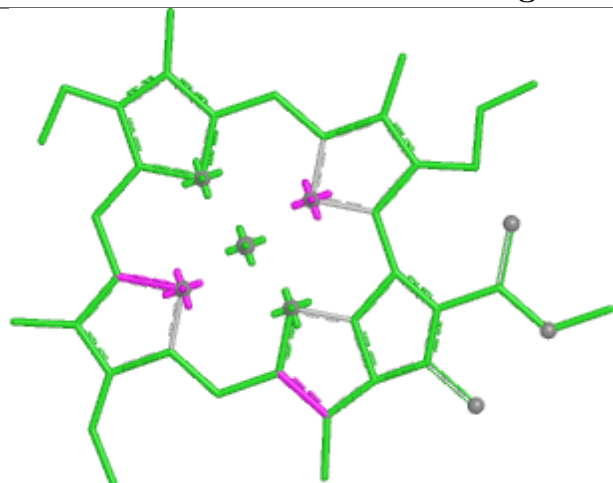
Ligand CLA 6 302



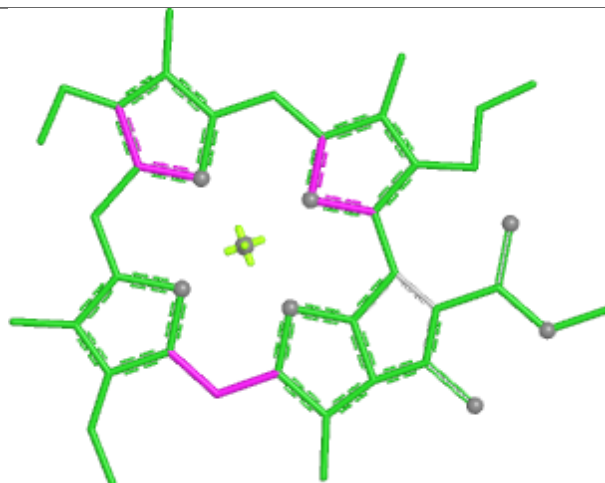




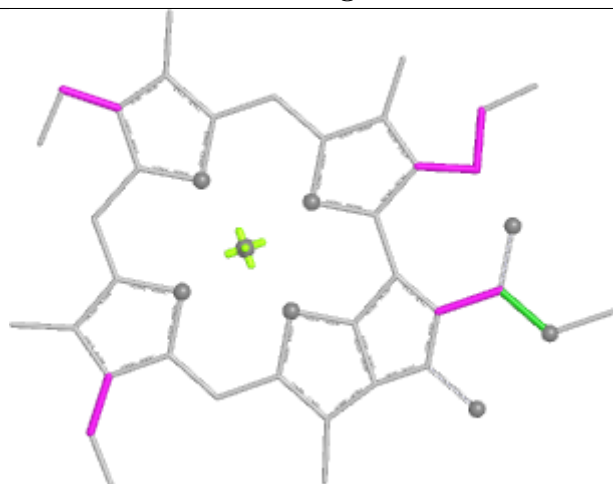
Ligand CLA 7 308



Bond lengths



Bond angles

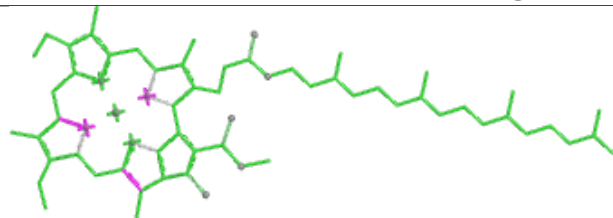


Torsions

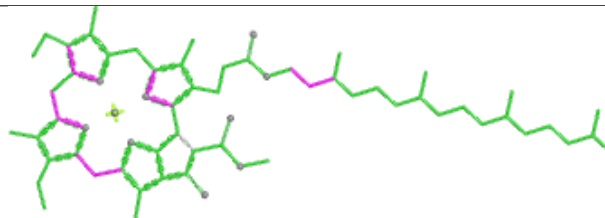


Rings

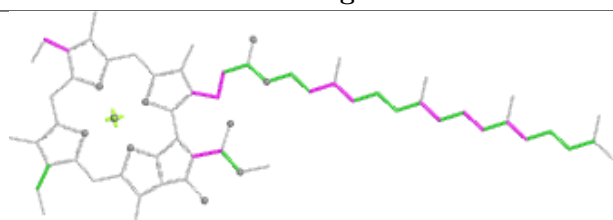
Ligand CLA 11 301



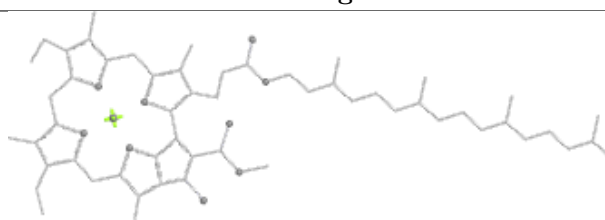
Bond lengths



Bond angles

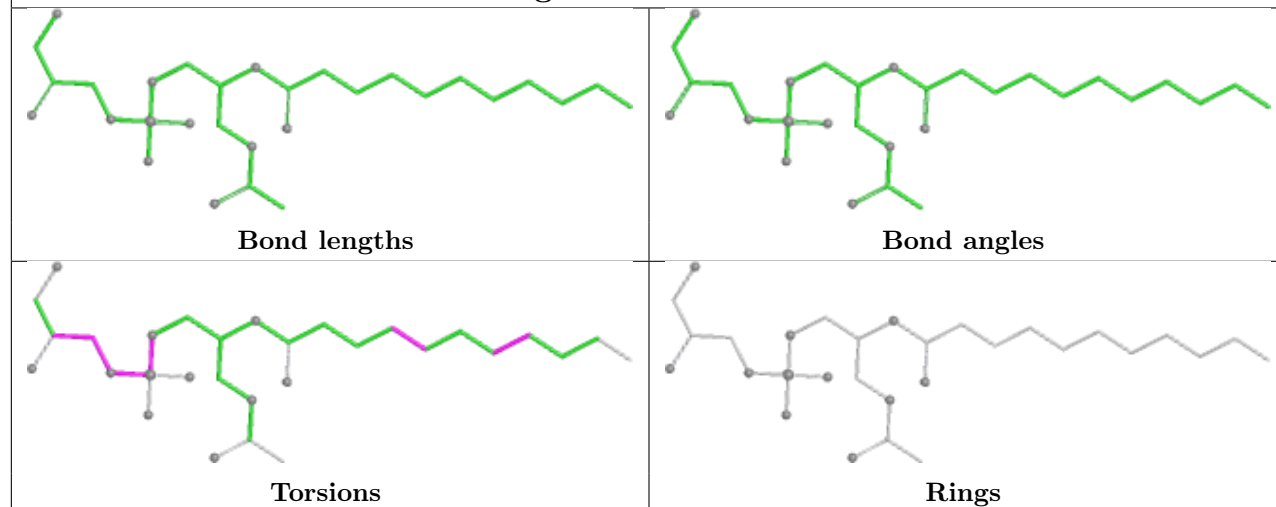


Torsions

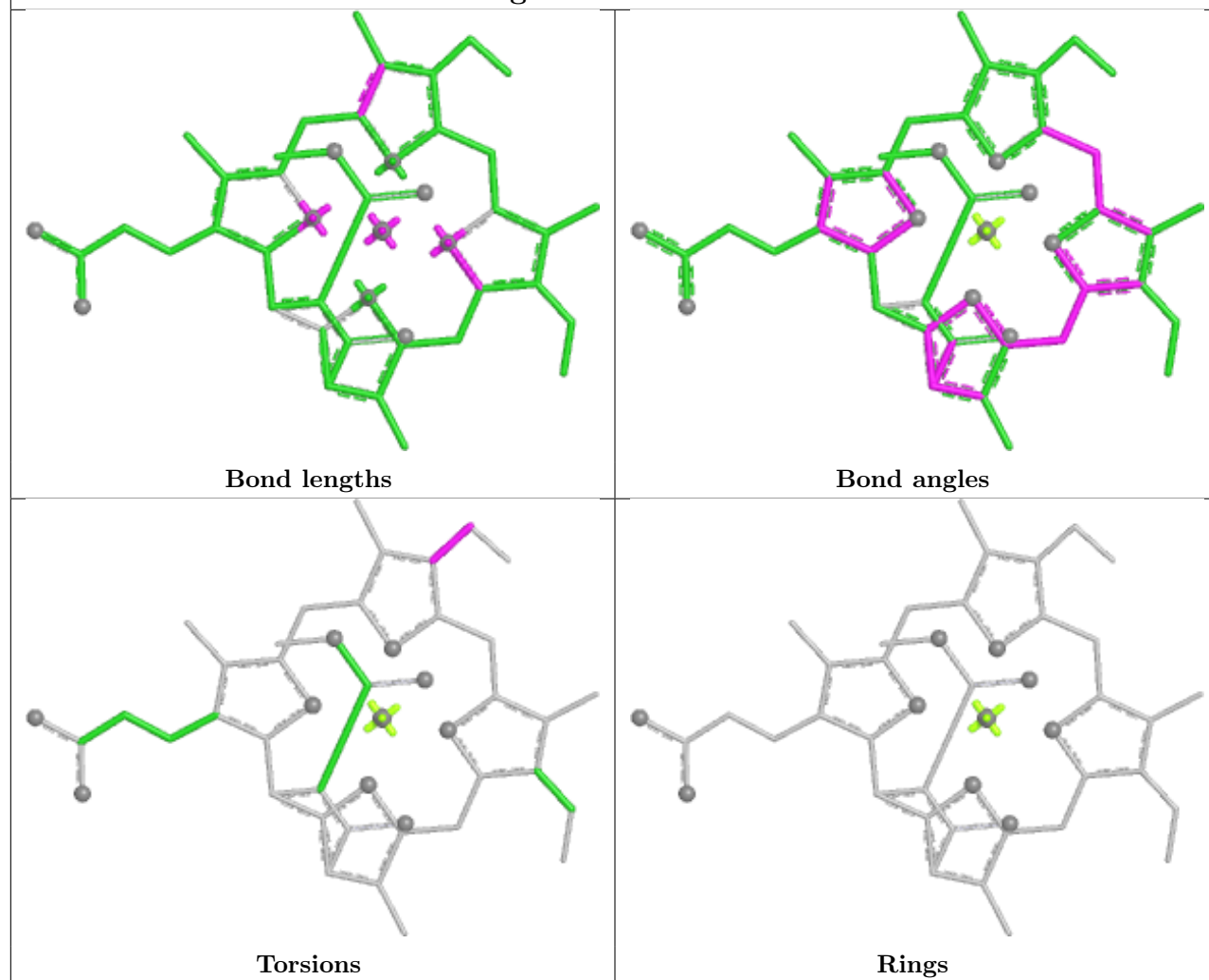


Rings

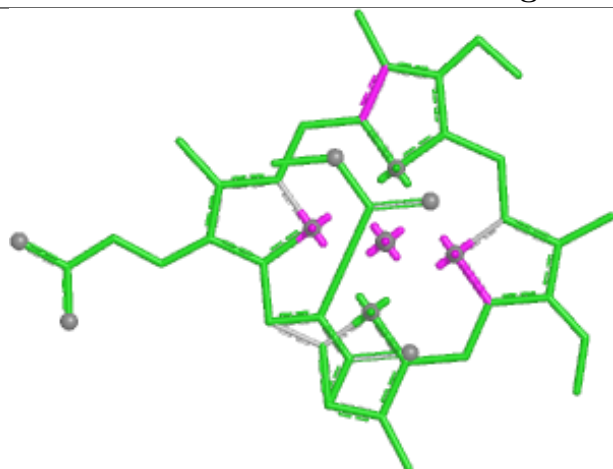
Ligand LHG 9 302



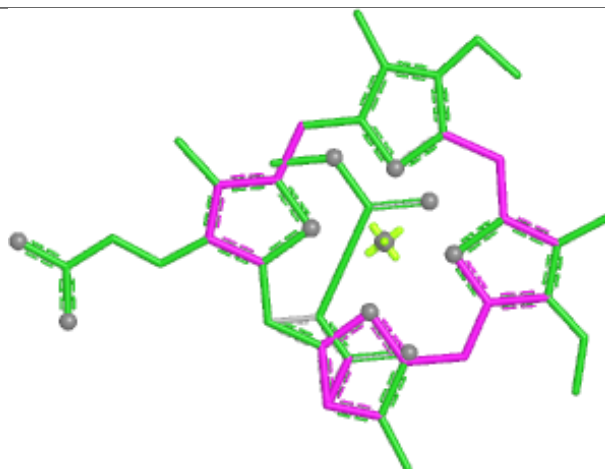
Ligand KC1 a 205



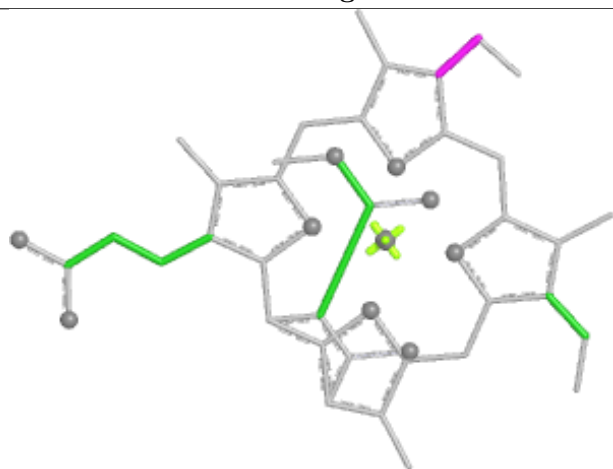
Ligand KC1 8 306



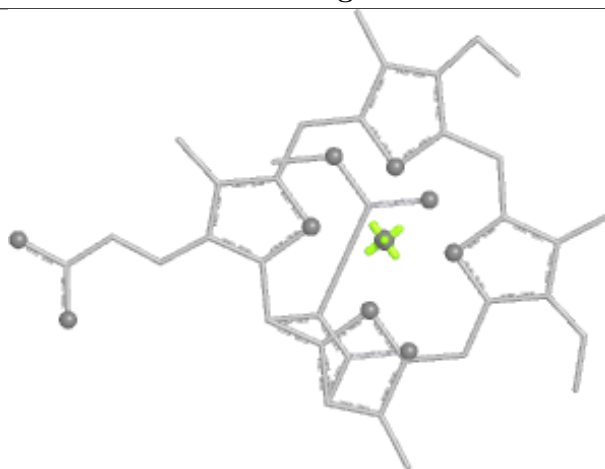
Bond lengths



Bond angles

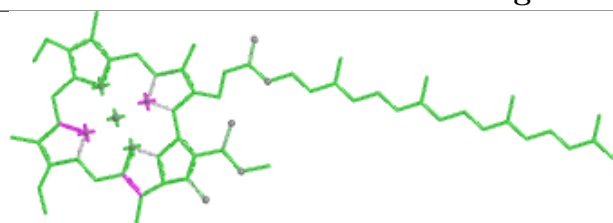


Torsions

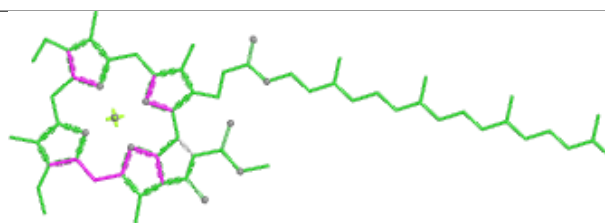


Rings

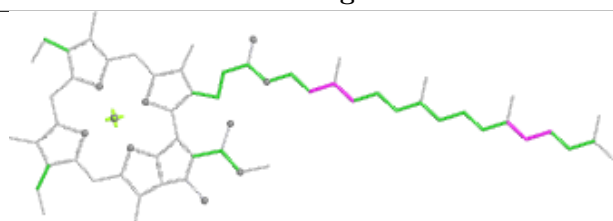
Ligand CLA A 825



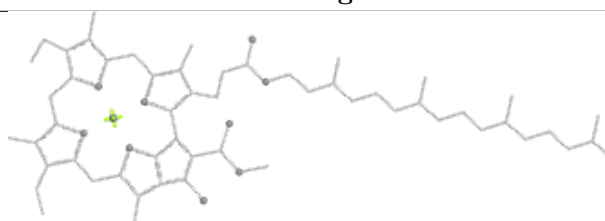
Bond lengths



Bond angles

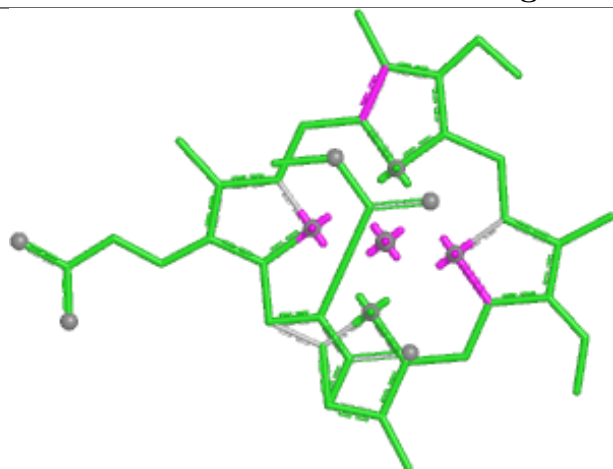


Torsions

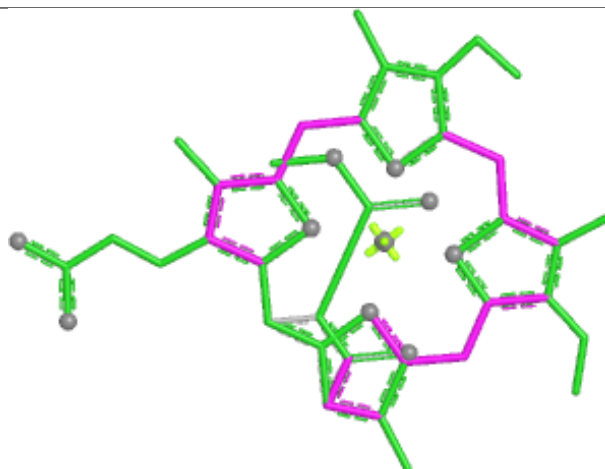


Rings

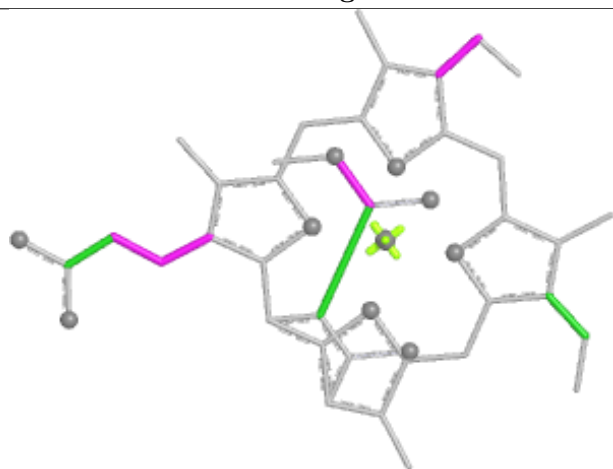
Ligand KC1 6 309



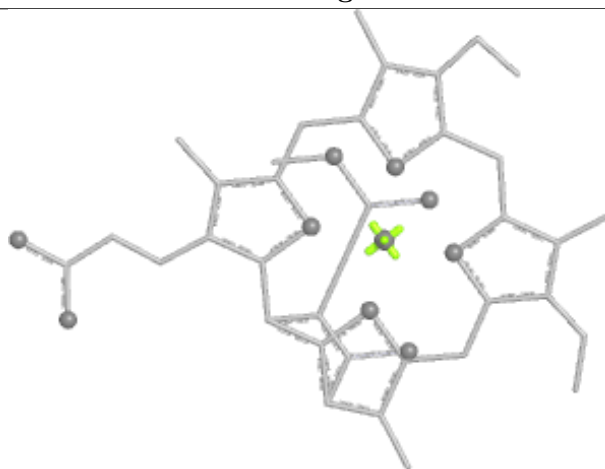
Bond lengths



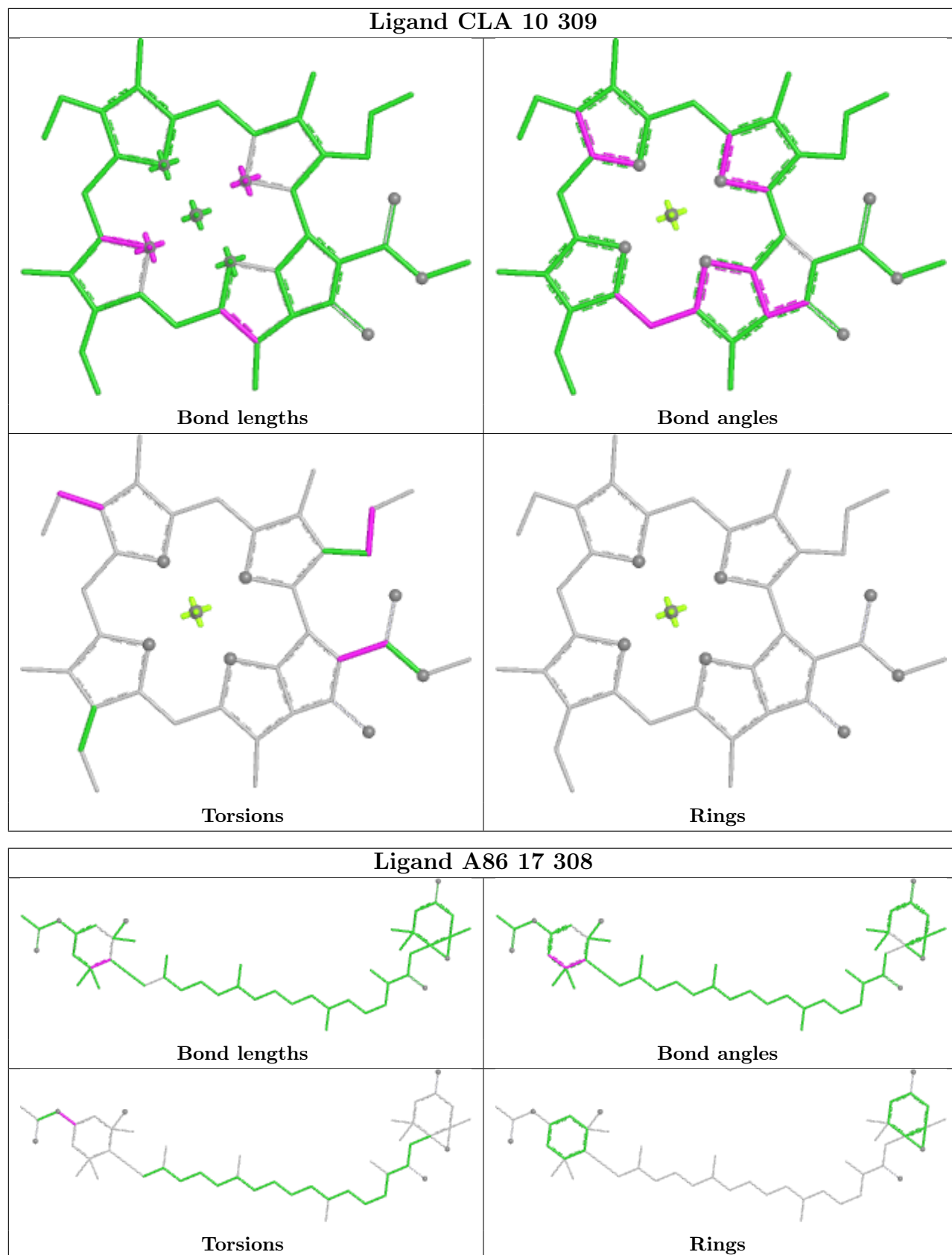
Bond angles



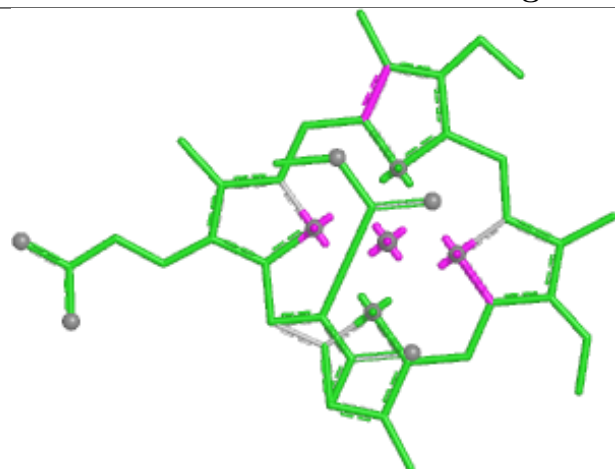
Torsions



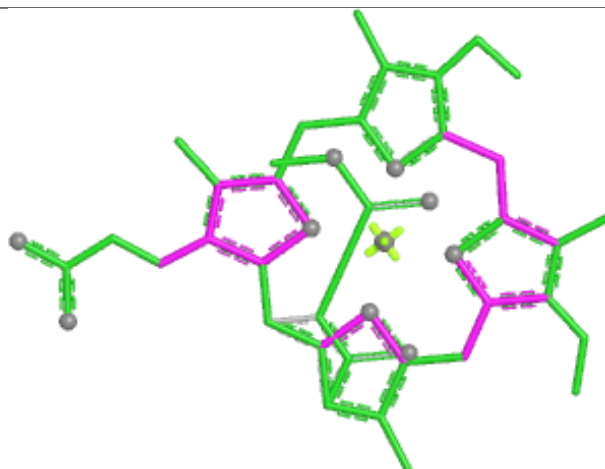
Rings



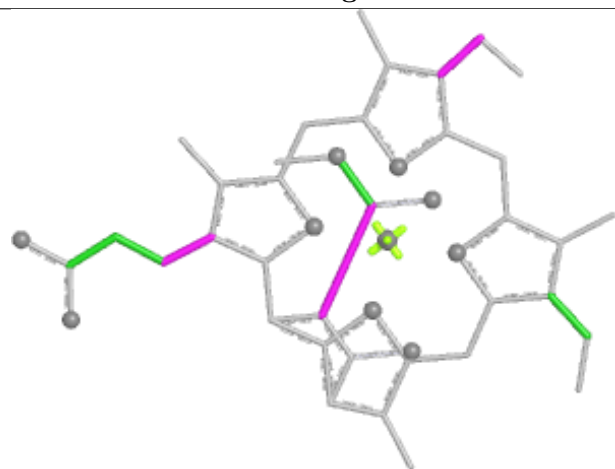
Ligand KC1 4 308



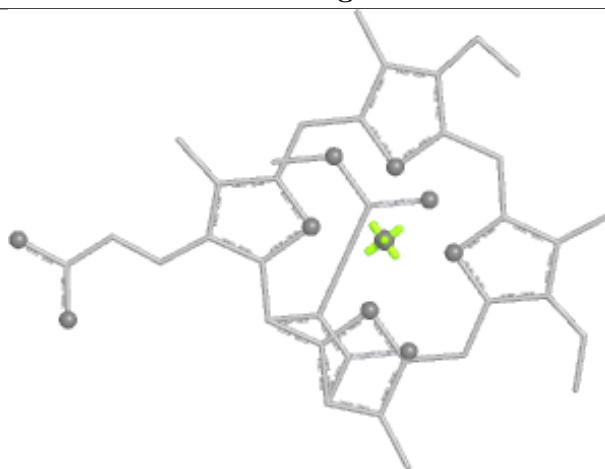
Bond lengths



Bond angles

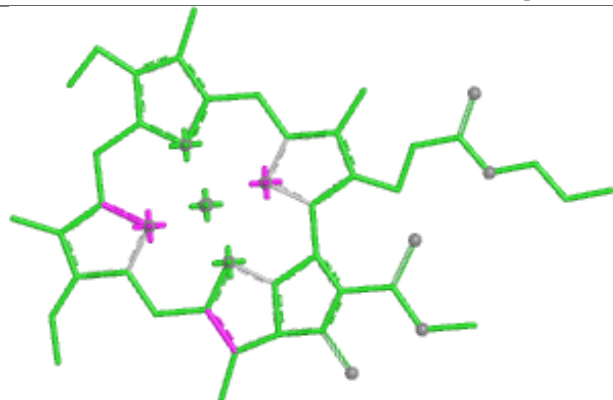


Torsions

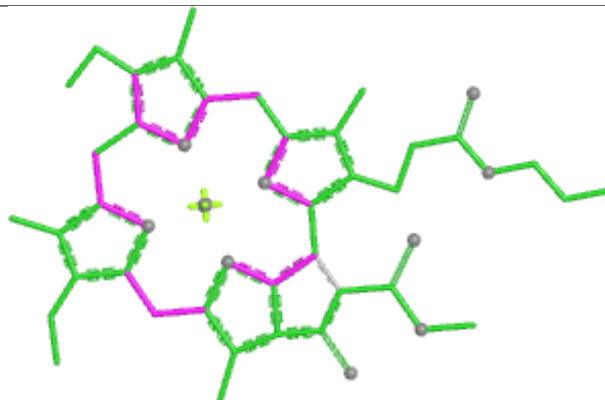


Rings

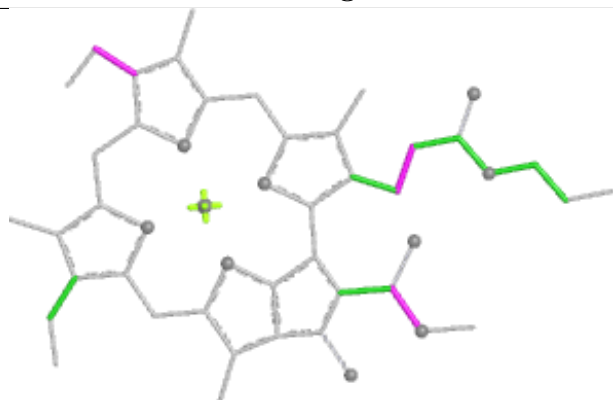
Ligand CLA 1 308



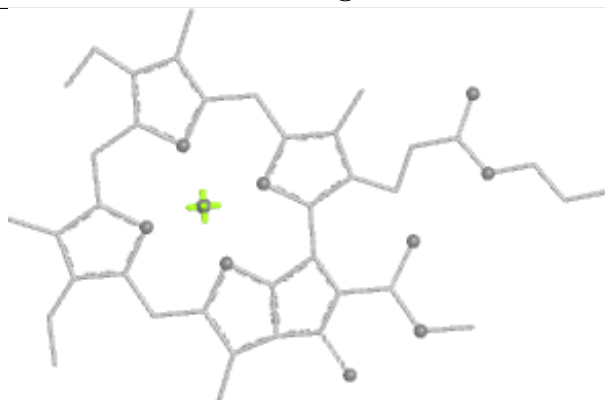
Bond lengths



Bond angles

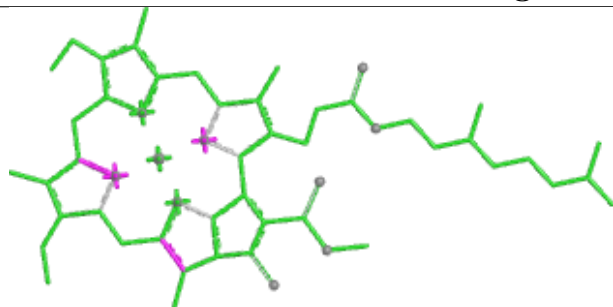


Torsions

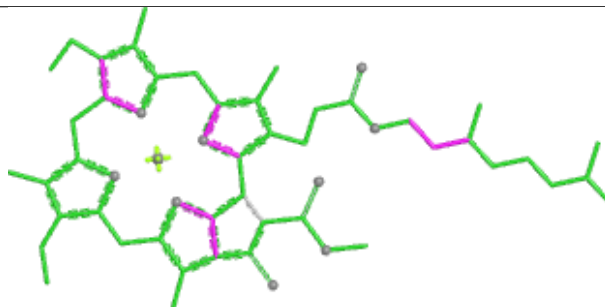


Rings

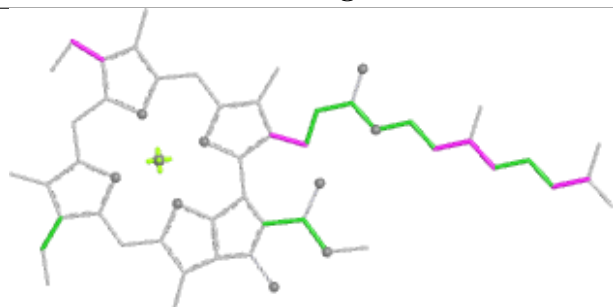
Ligand CLA A 834



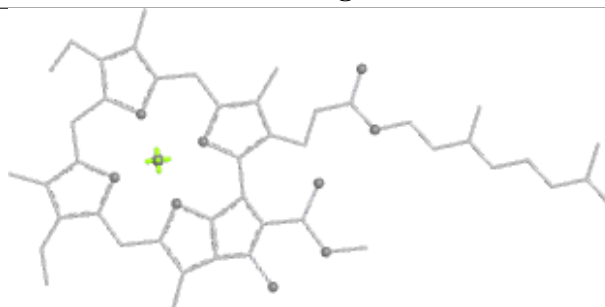
Bond lengths



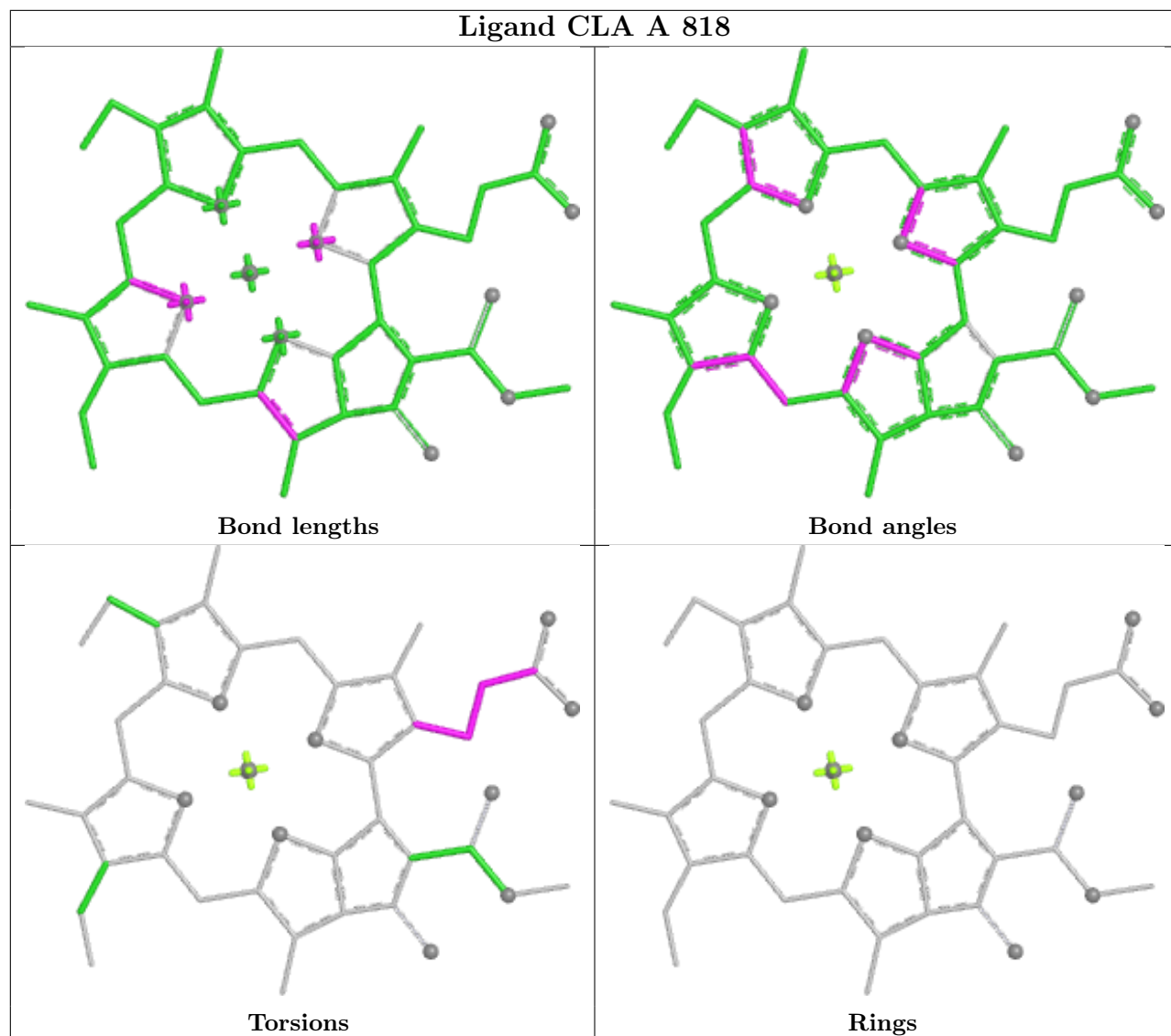
Bond angles



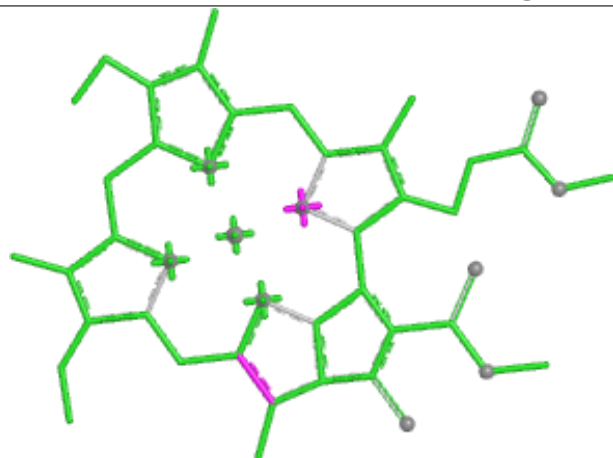
Torsions



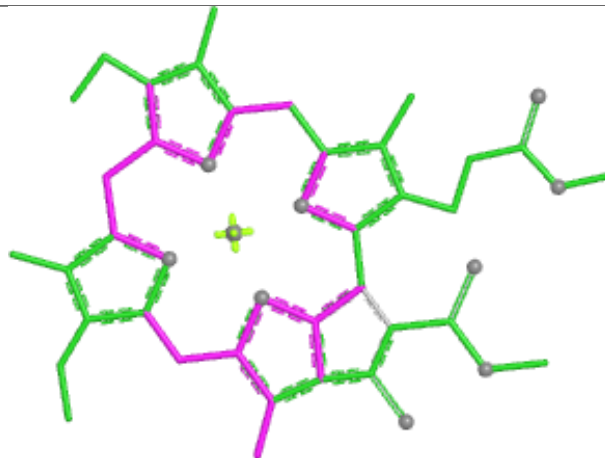
Rings



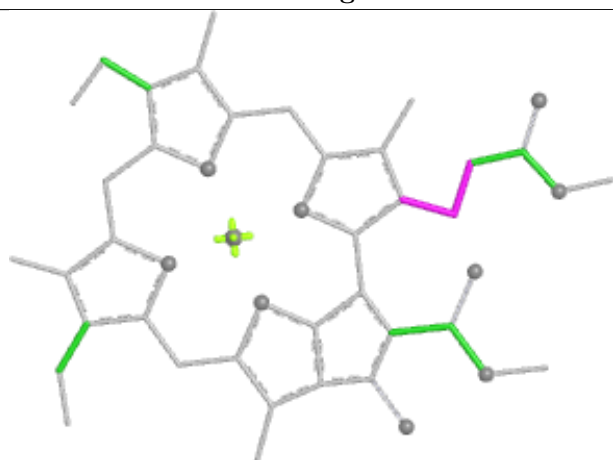
Ligand CLA 9 308



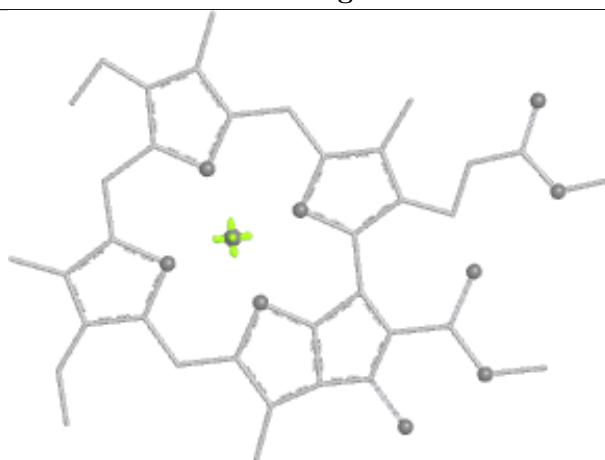
Bond lengths



Bond angles

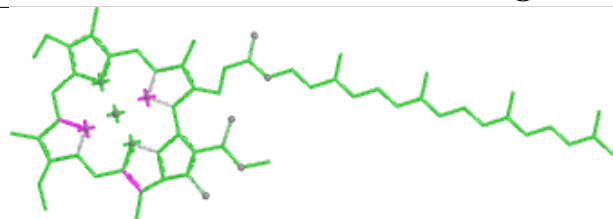


Torsions

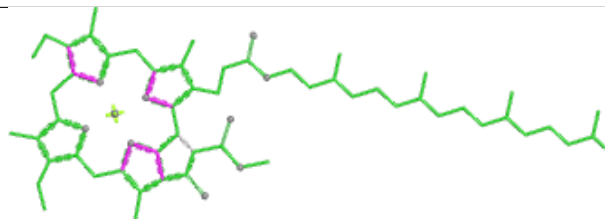


Rings

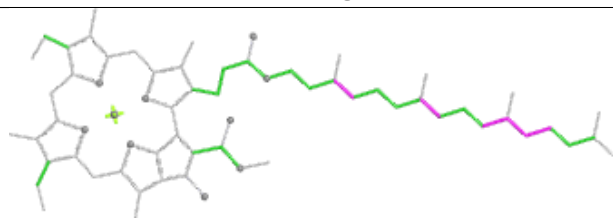
Ligand CLA B 835



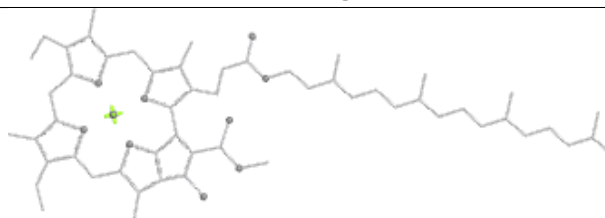
Bond lengths



Bond angles

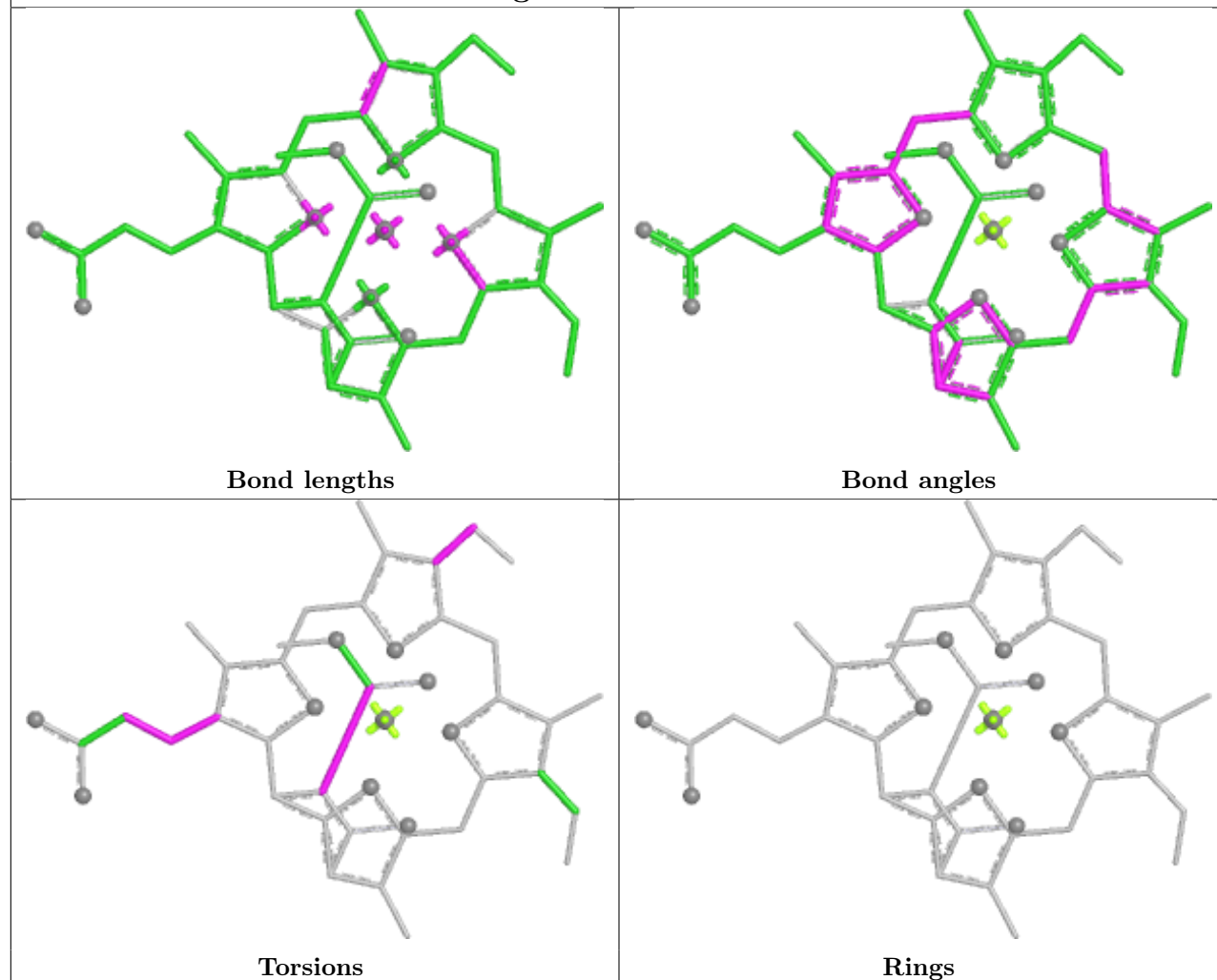


Torsions

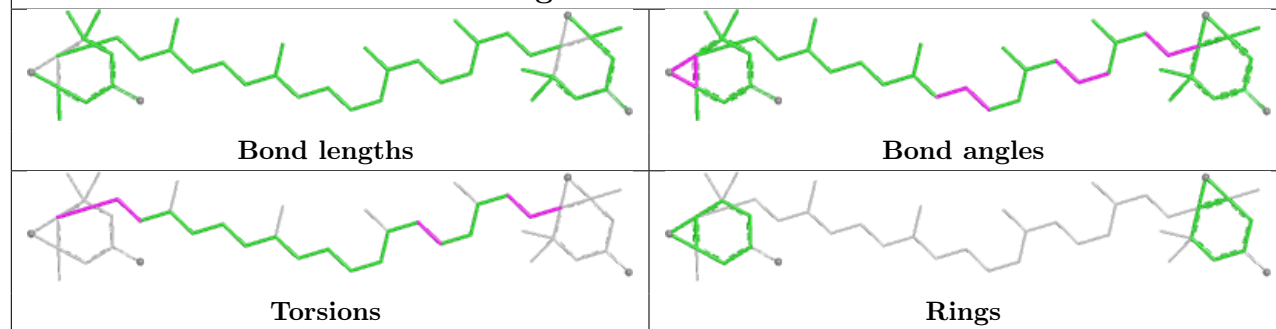


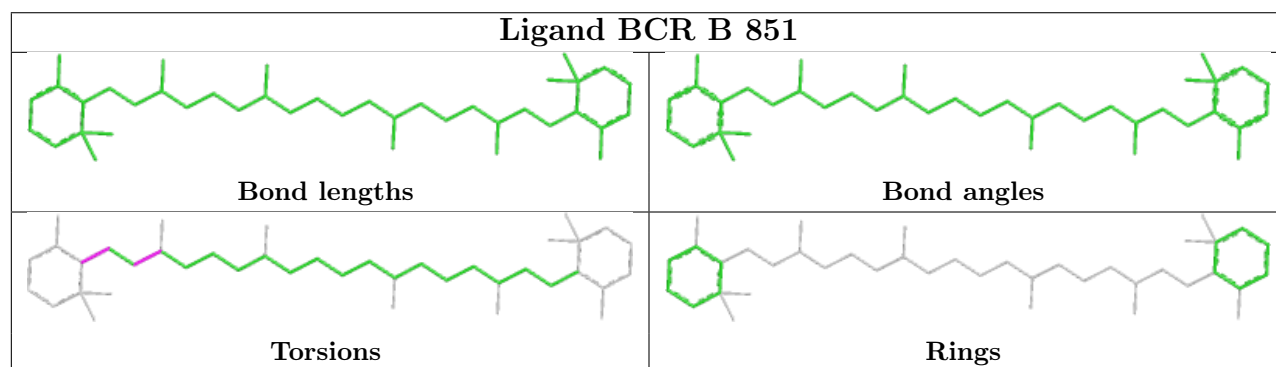
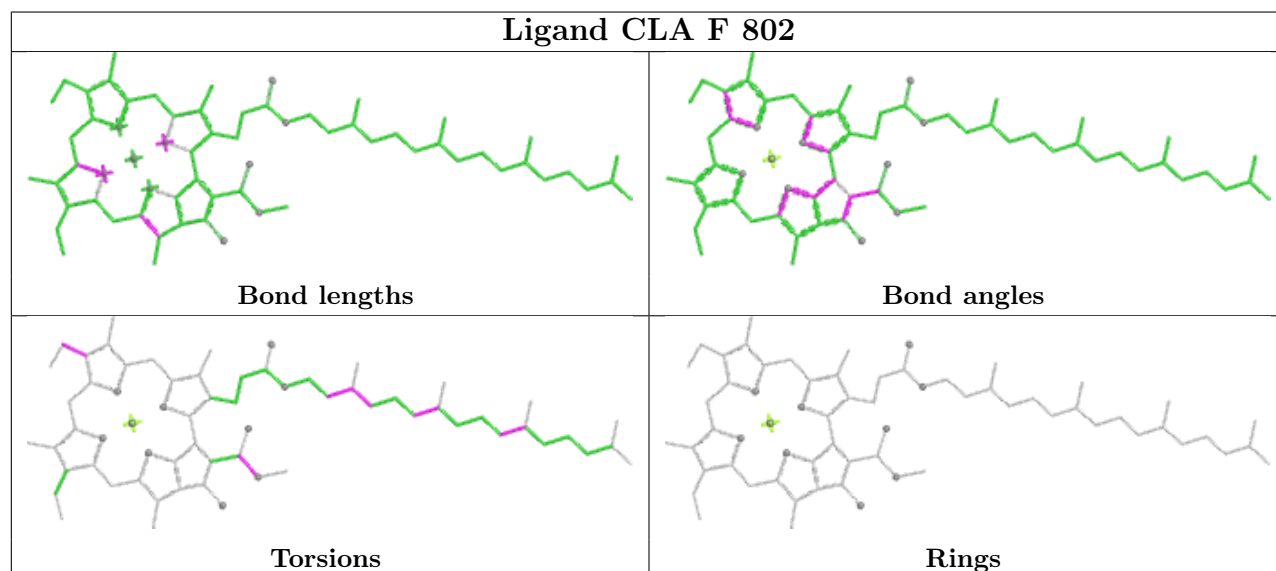
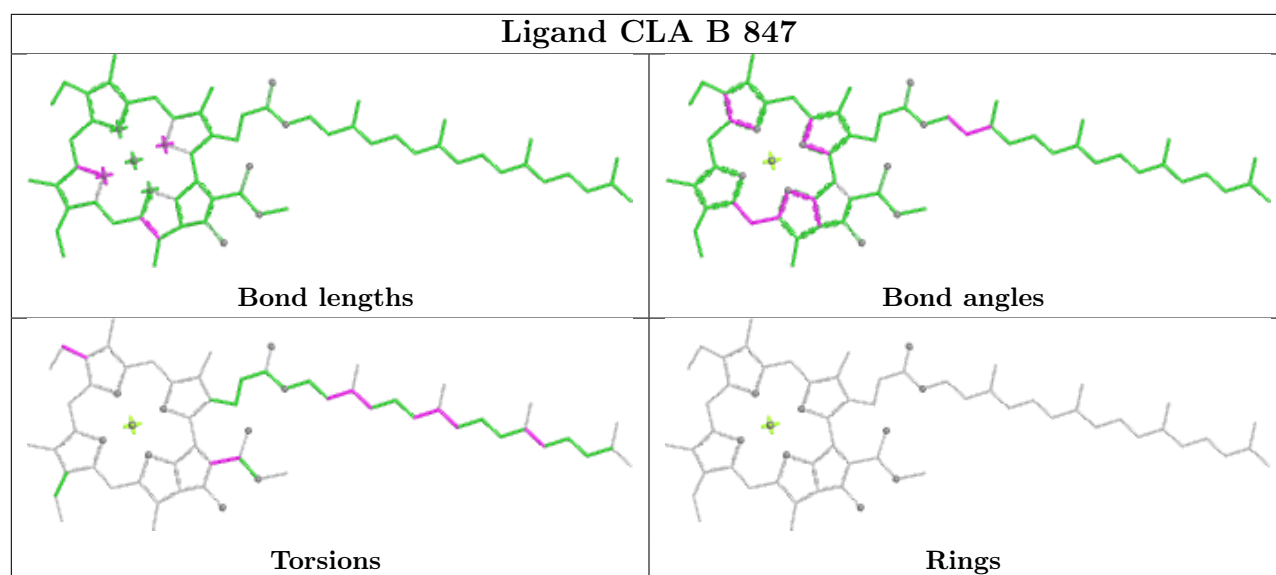
Rings

Ligand KC1 6 310

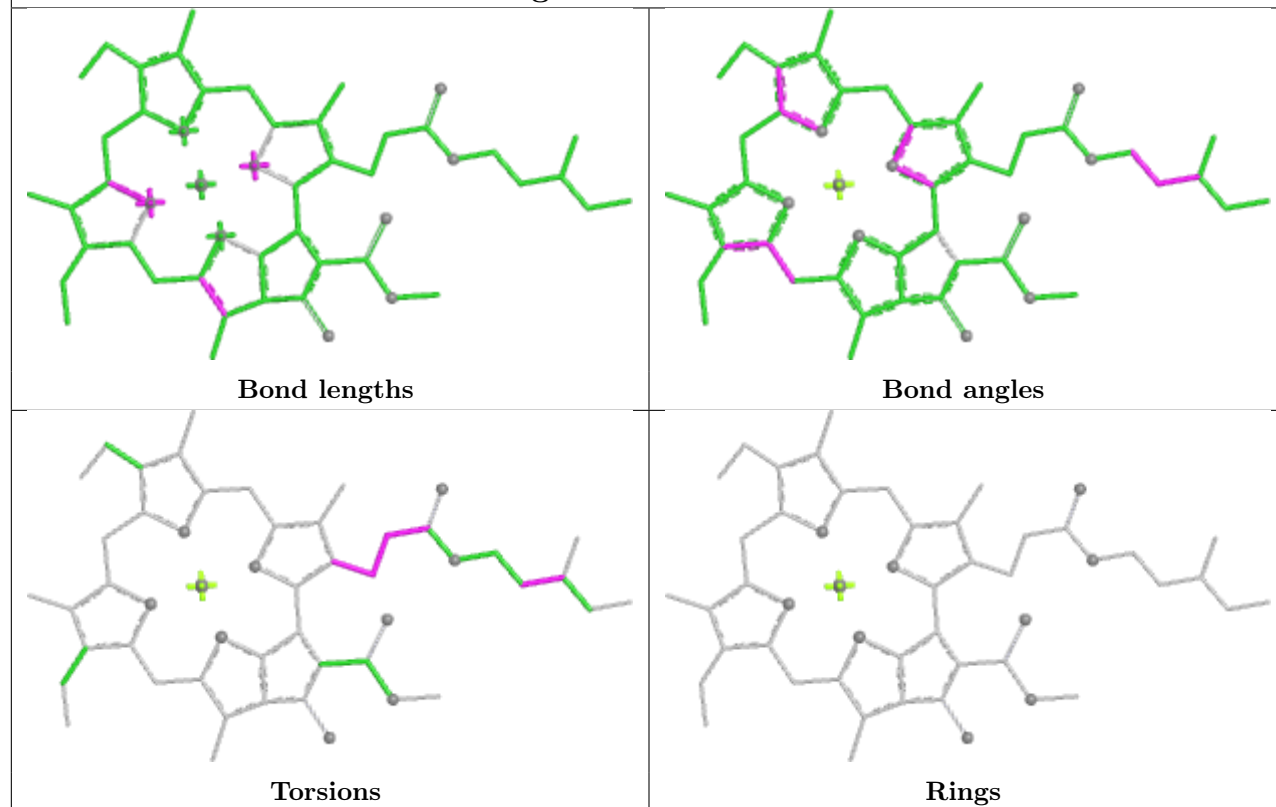


Ligand XAT 4 318

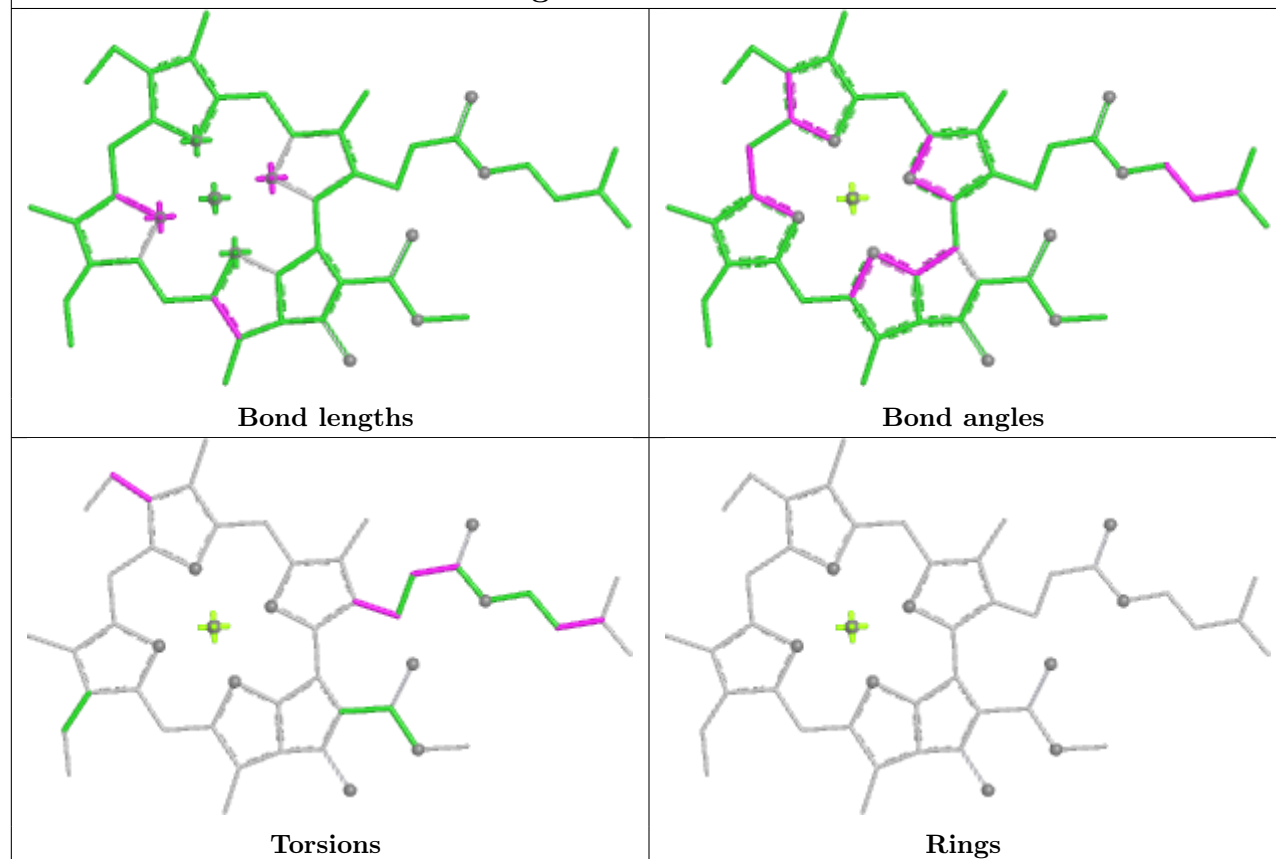


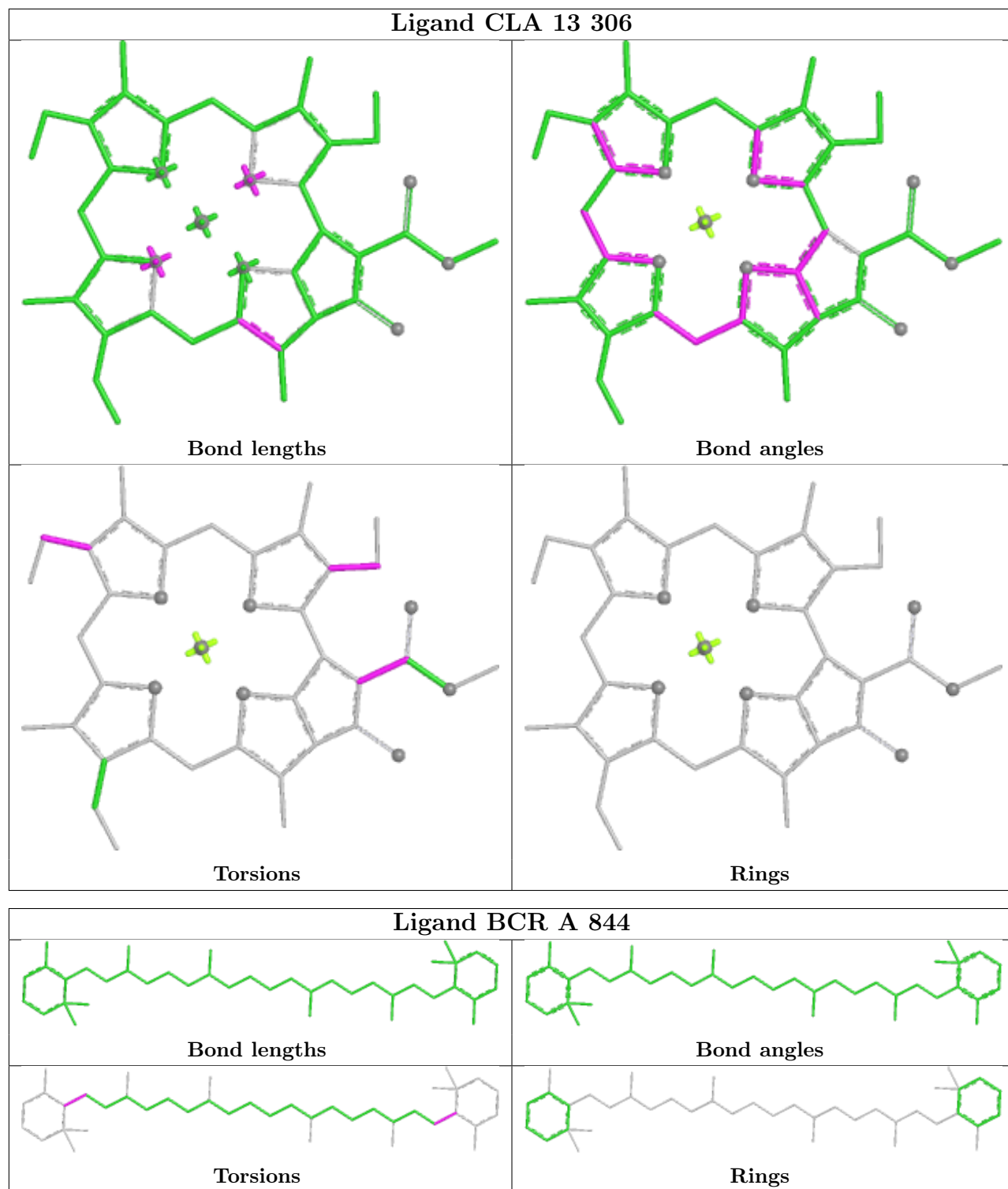


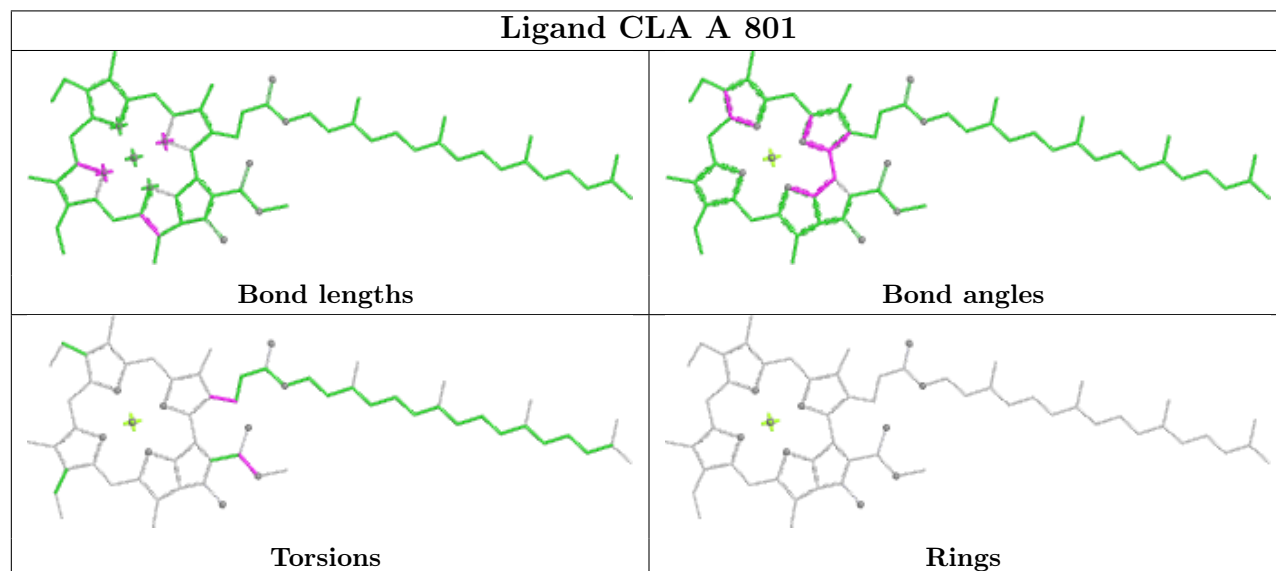
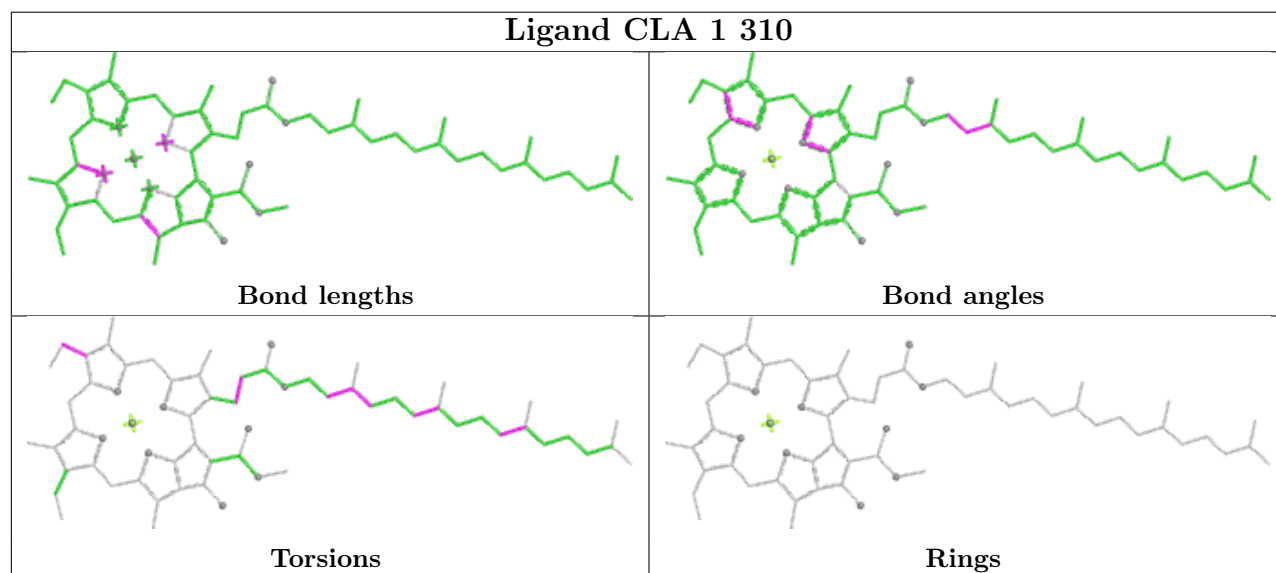
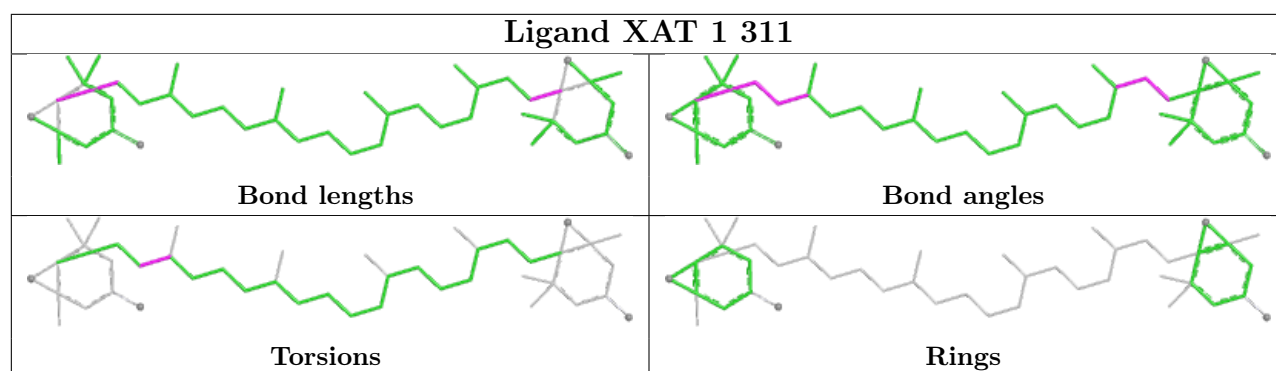
Ligand CLA A 821

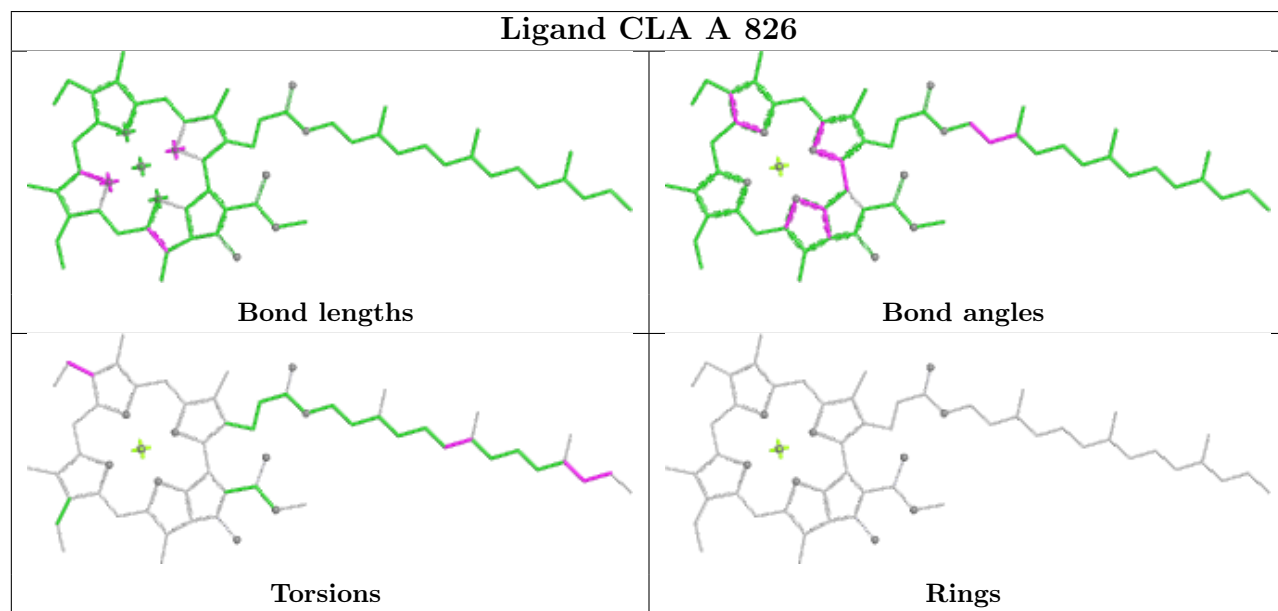
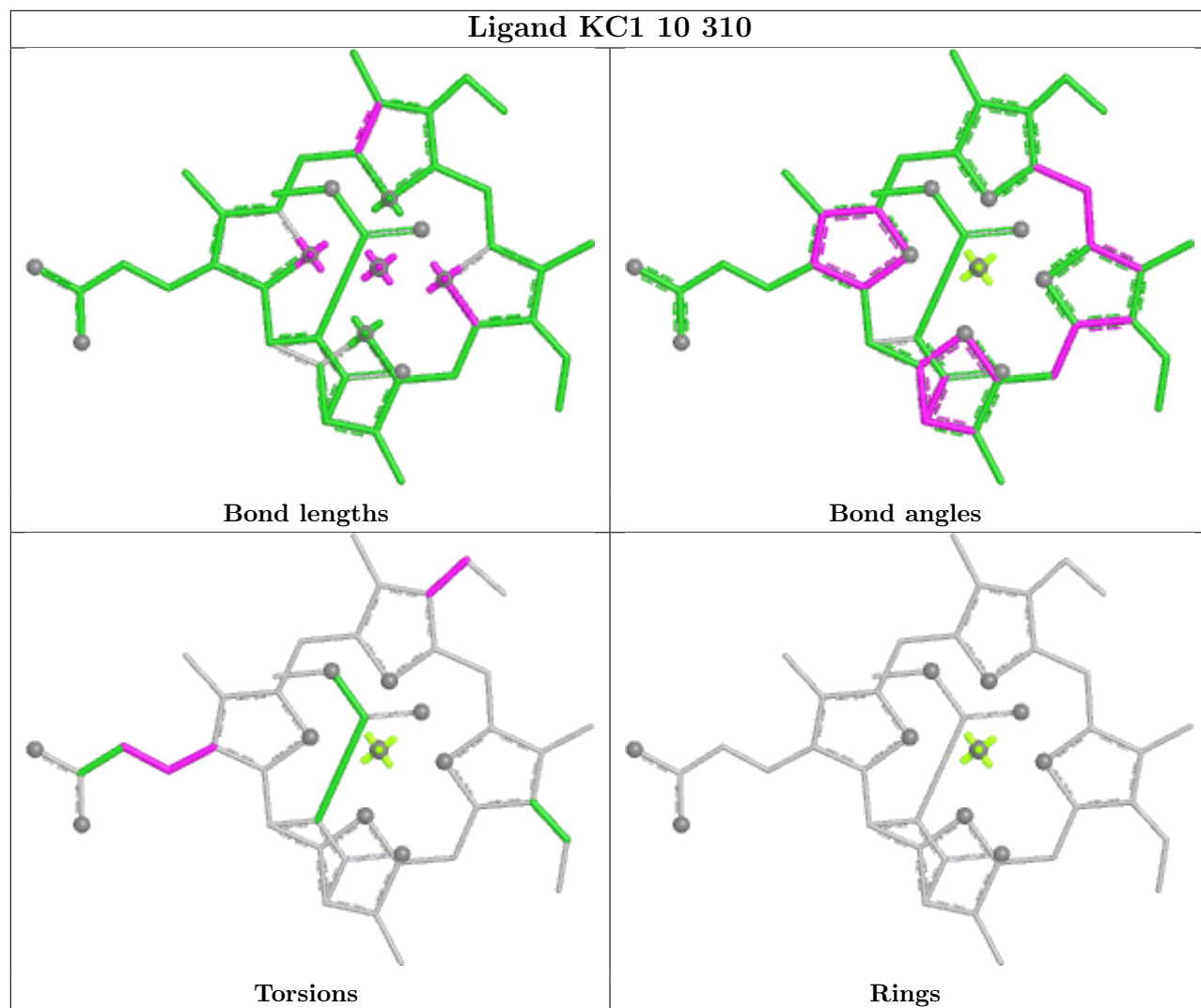


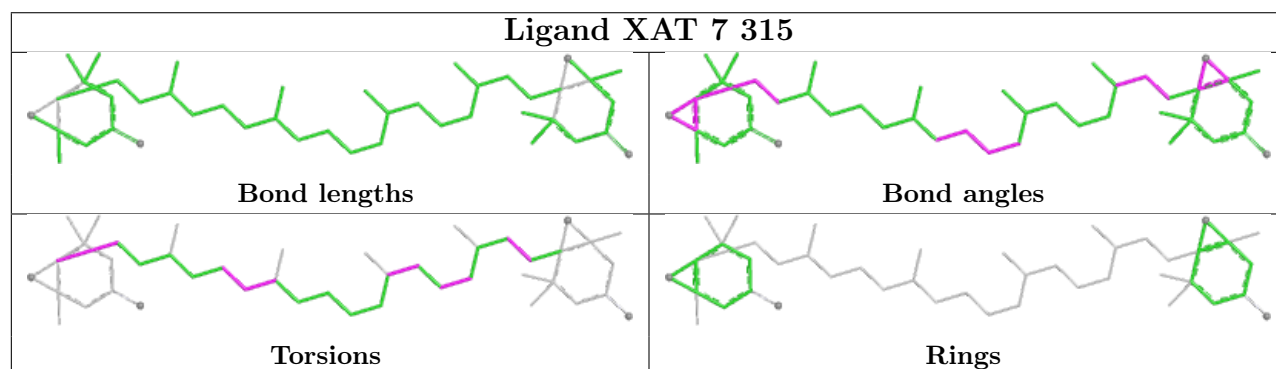
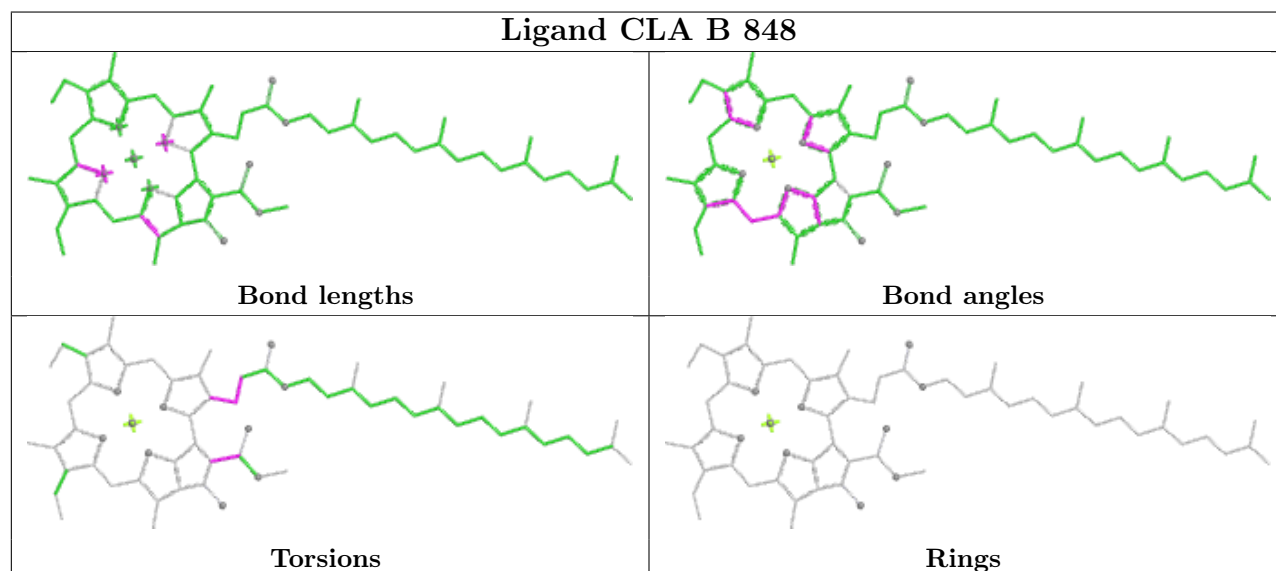
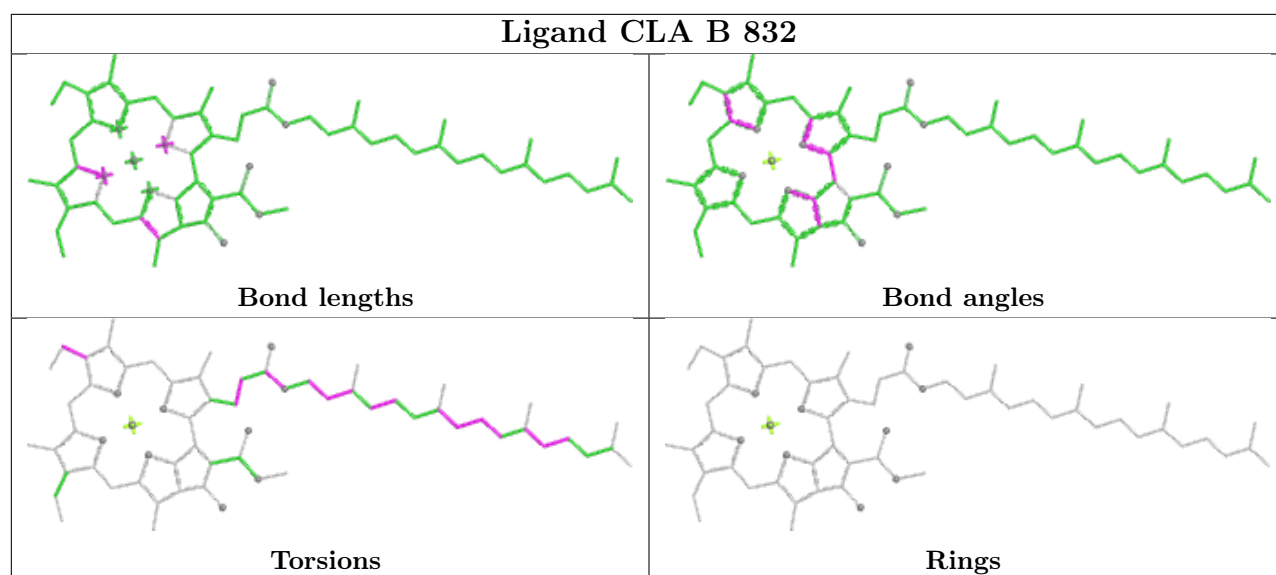
Ligand CLA A 829



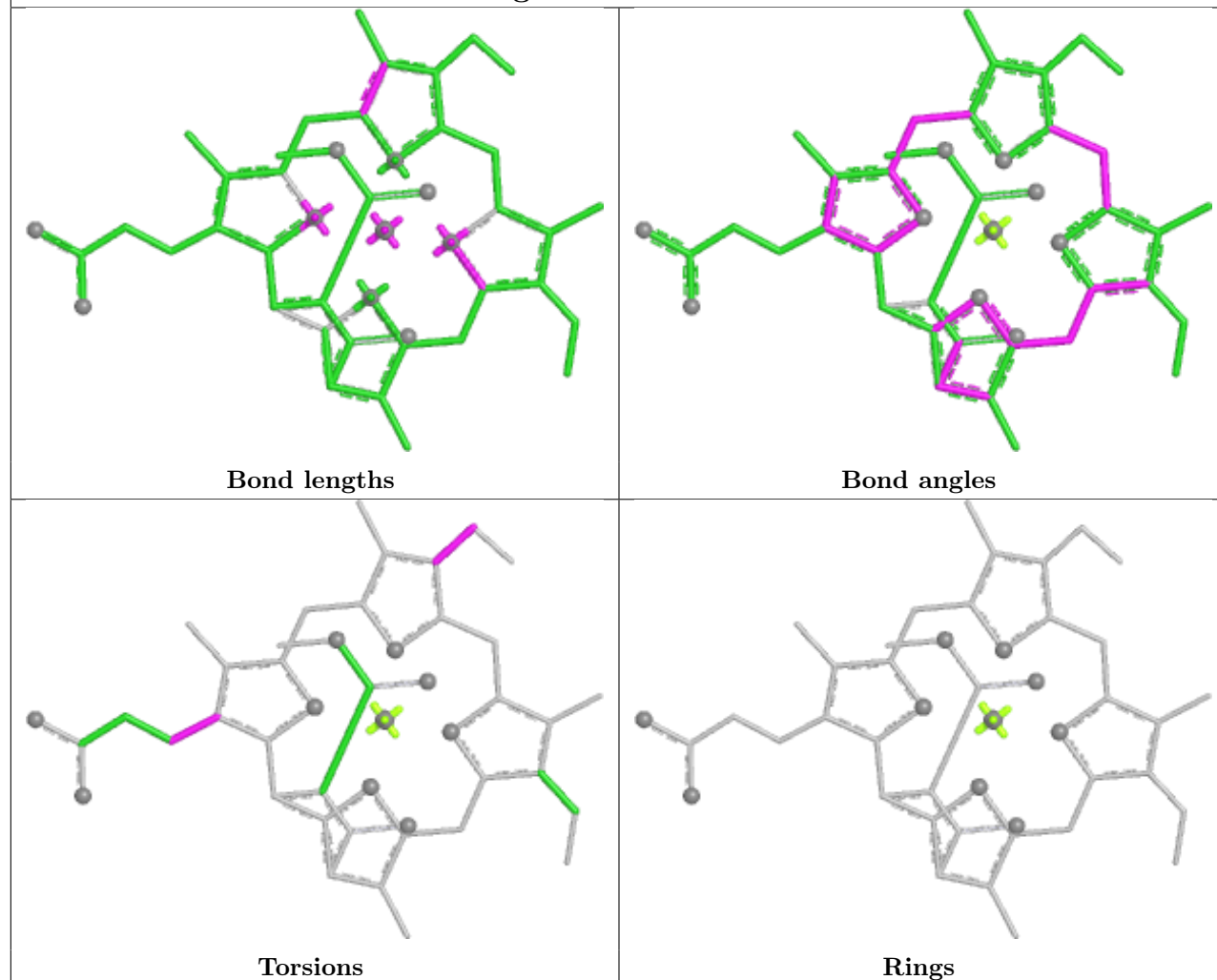




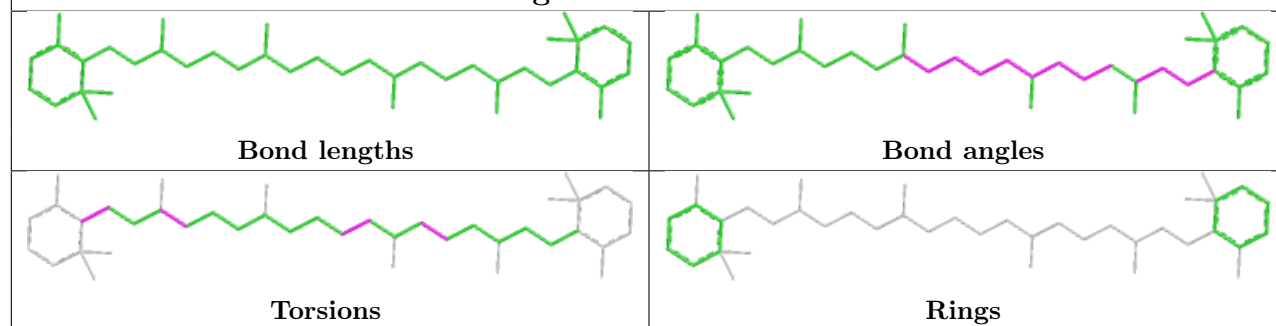




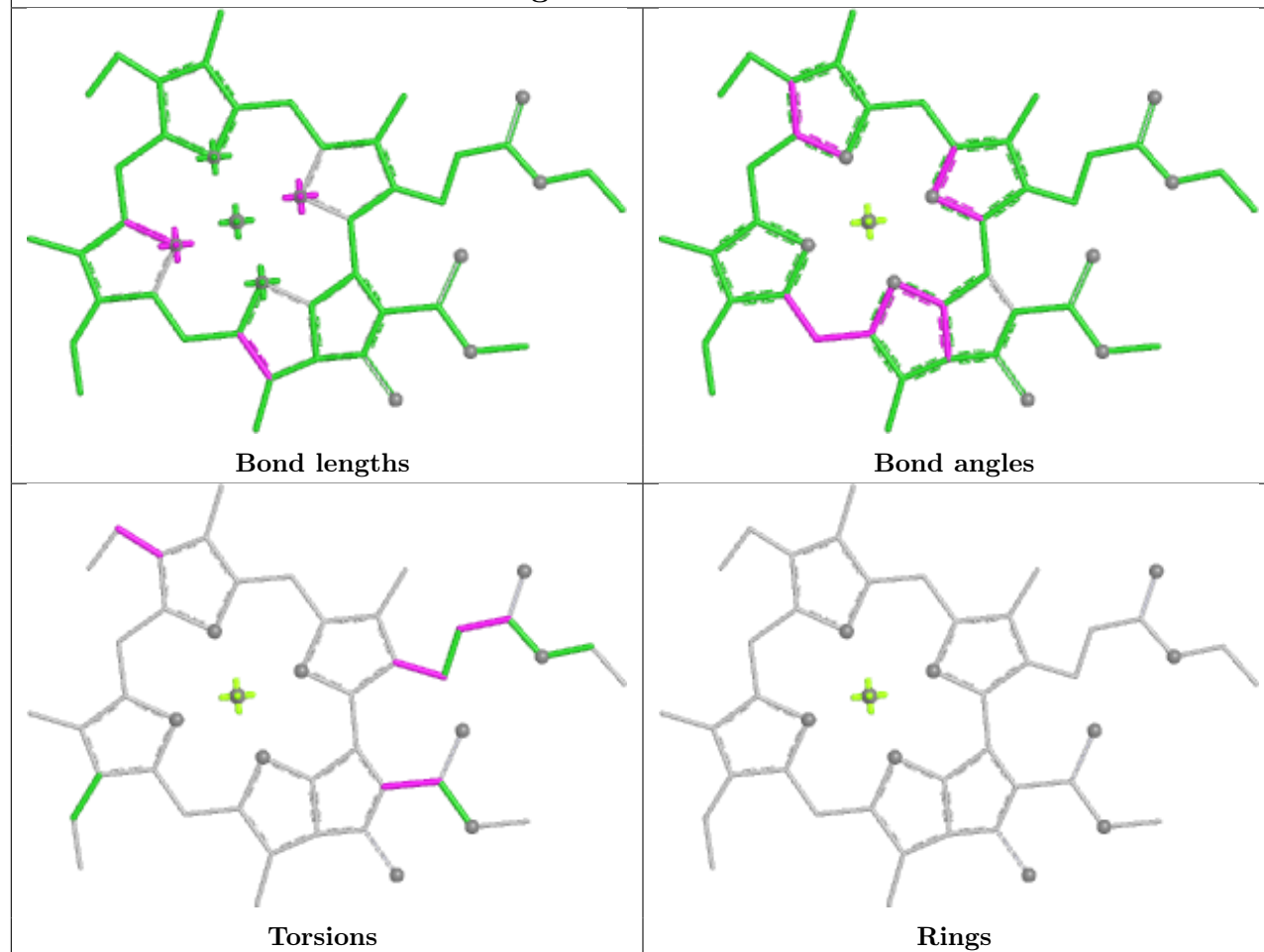
Ligand KC1 9 309



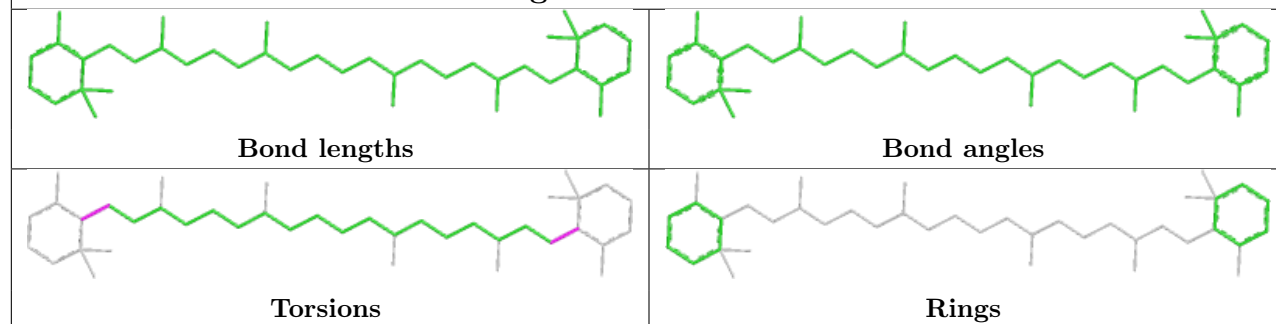
Ligand BCR L 202

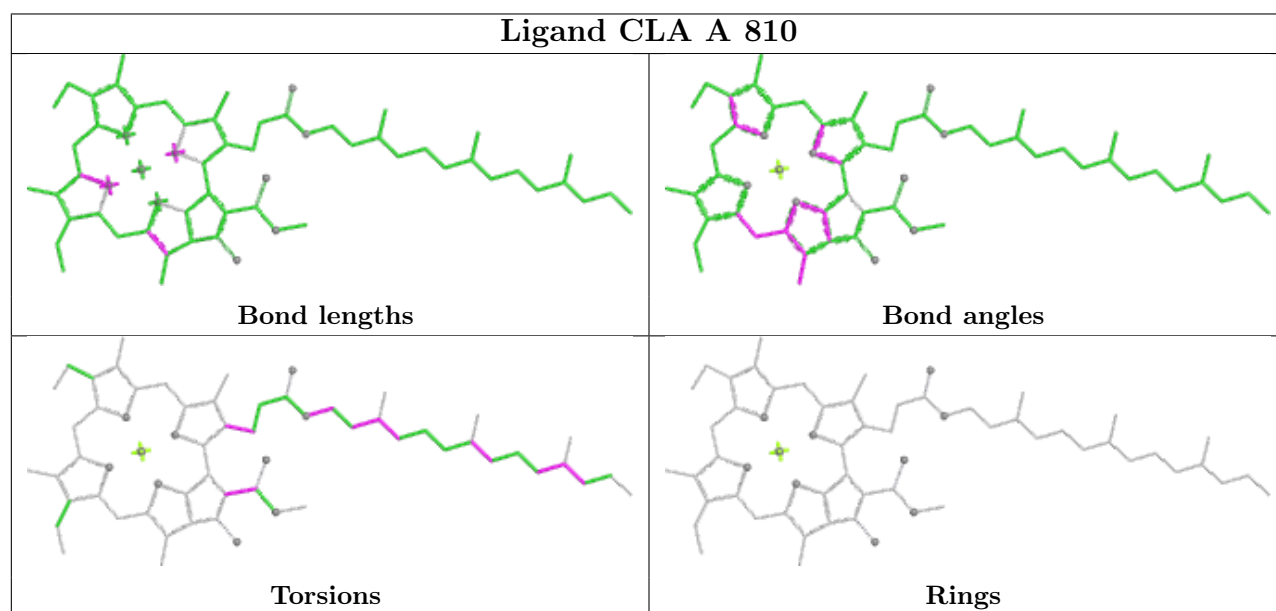
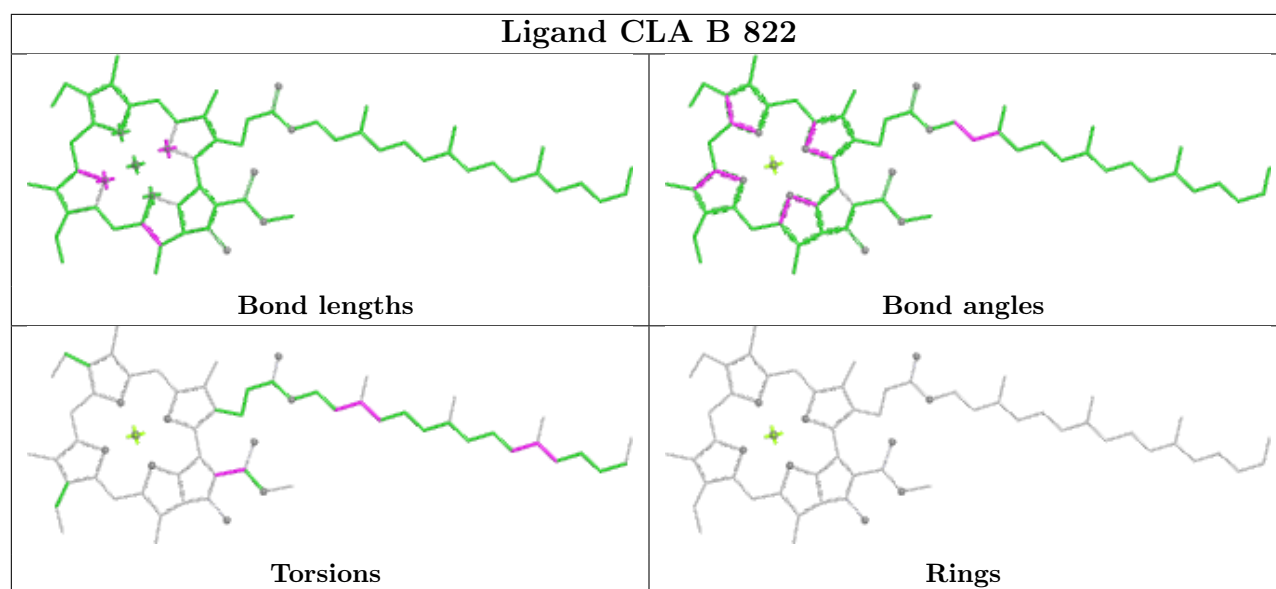


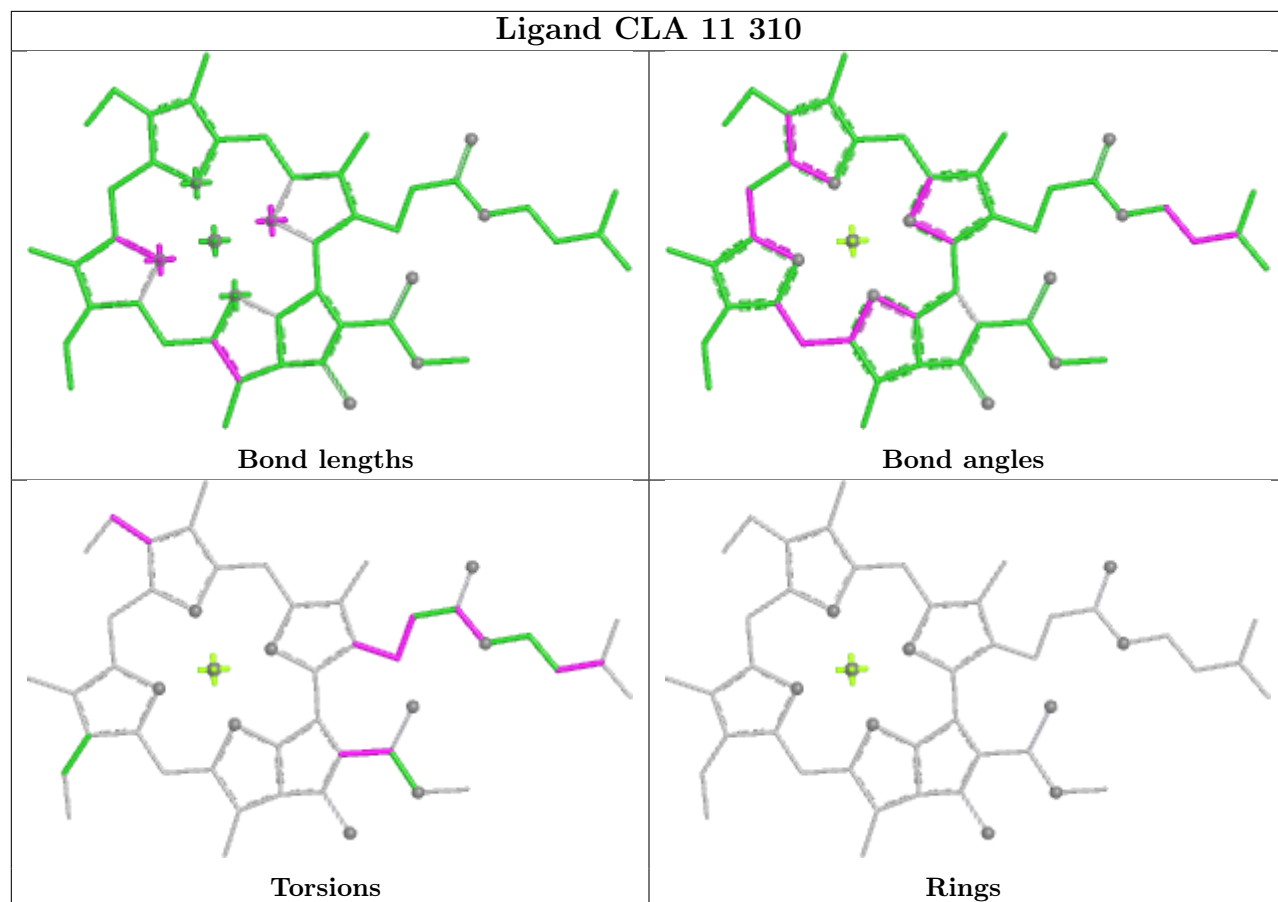
Ligand CLA 5 304

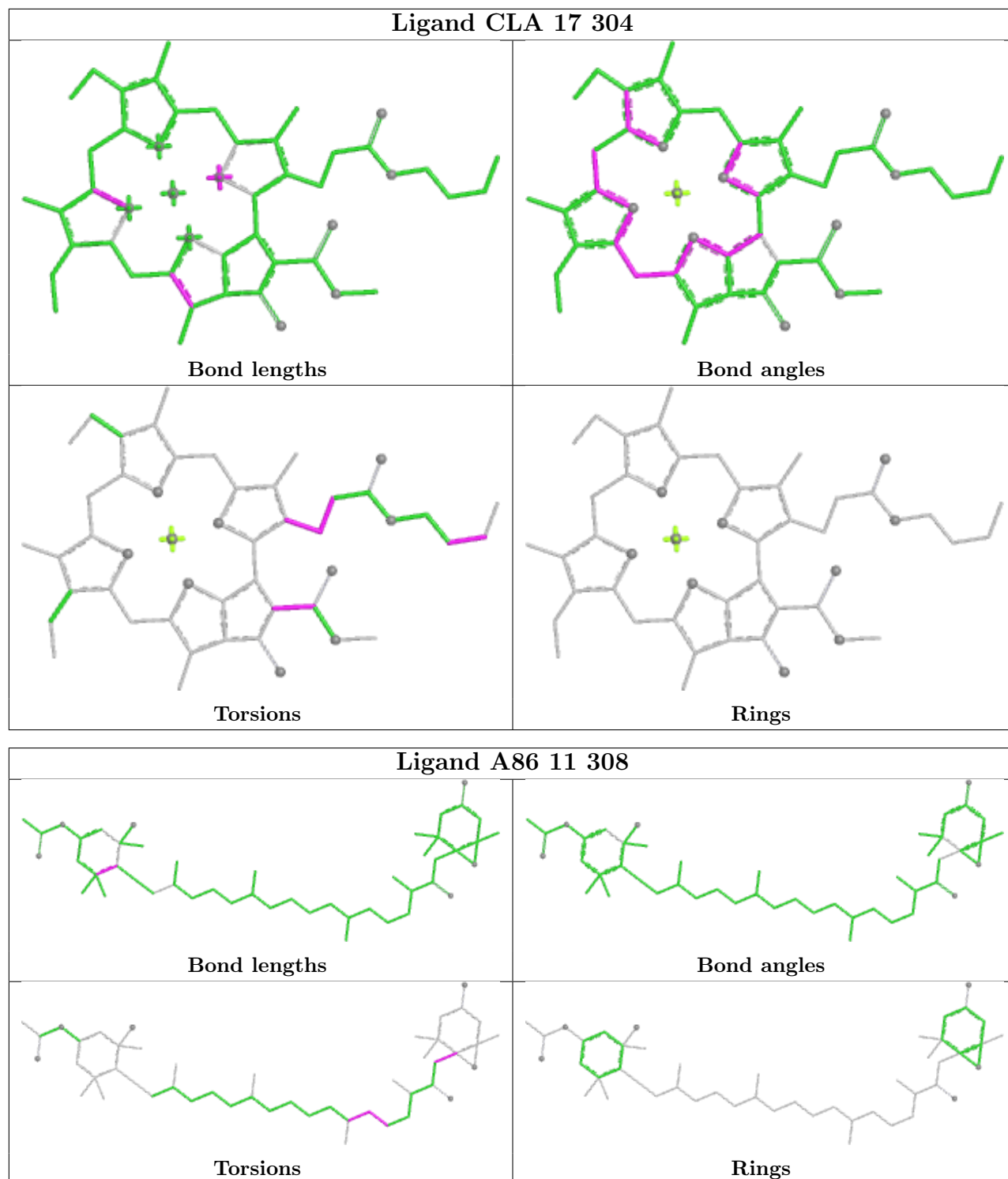


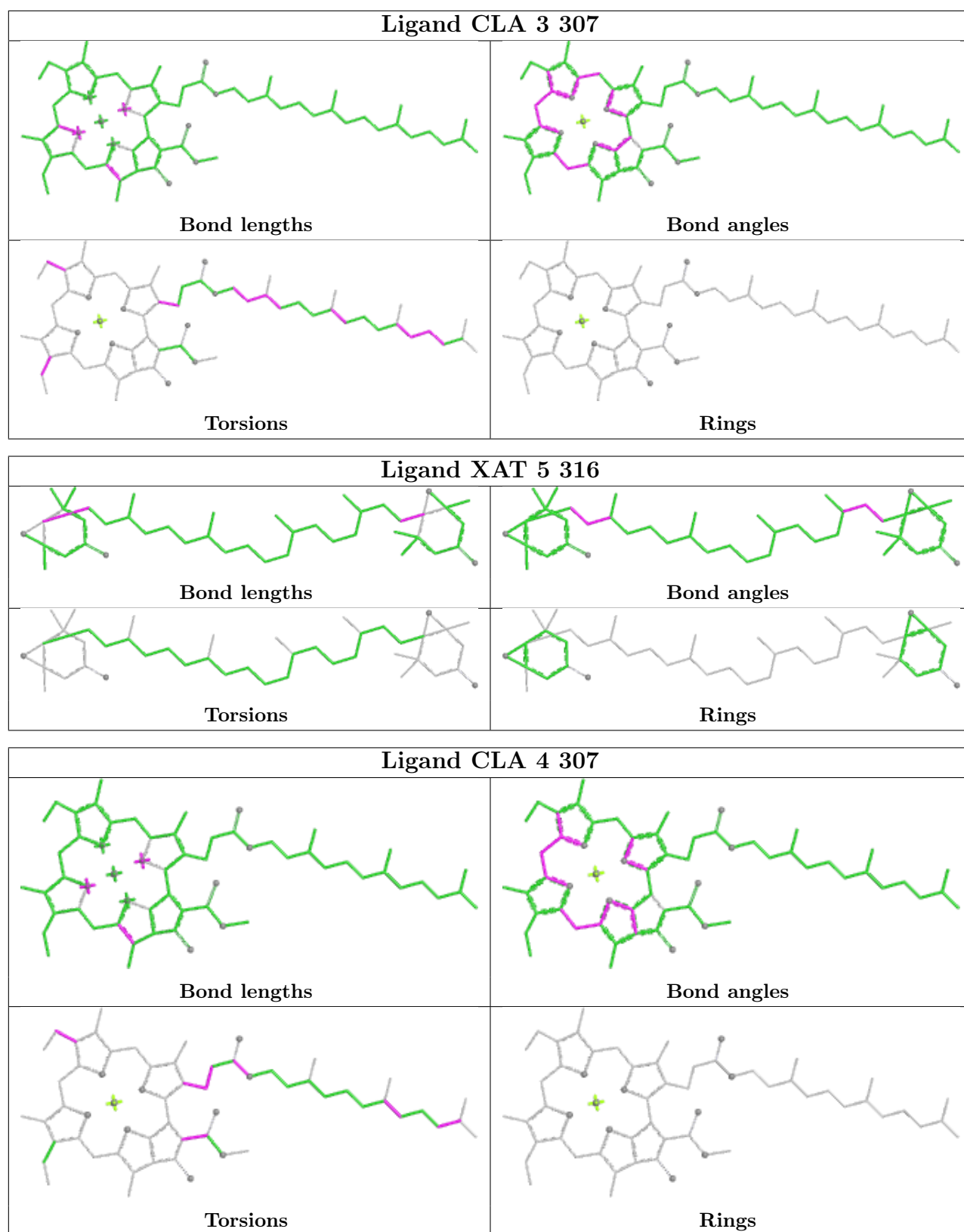
Ligand BCR A 841

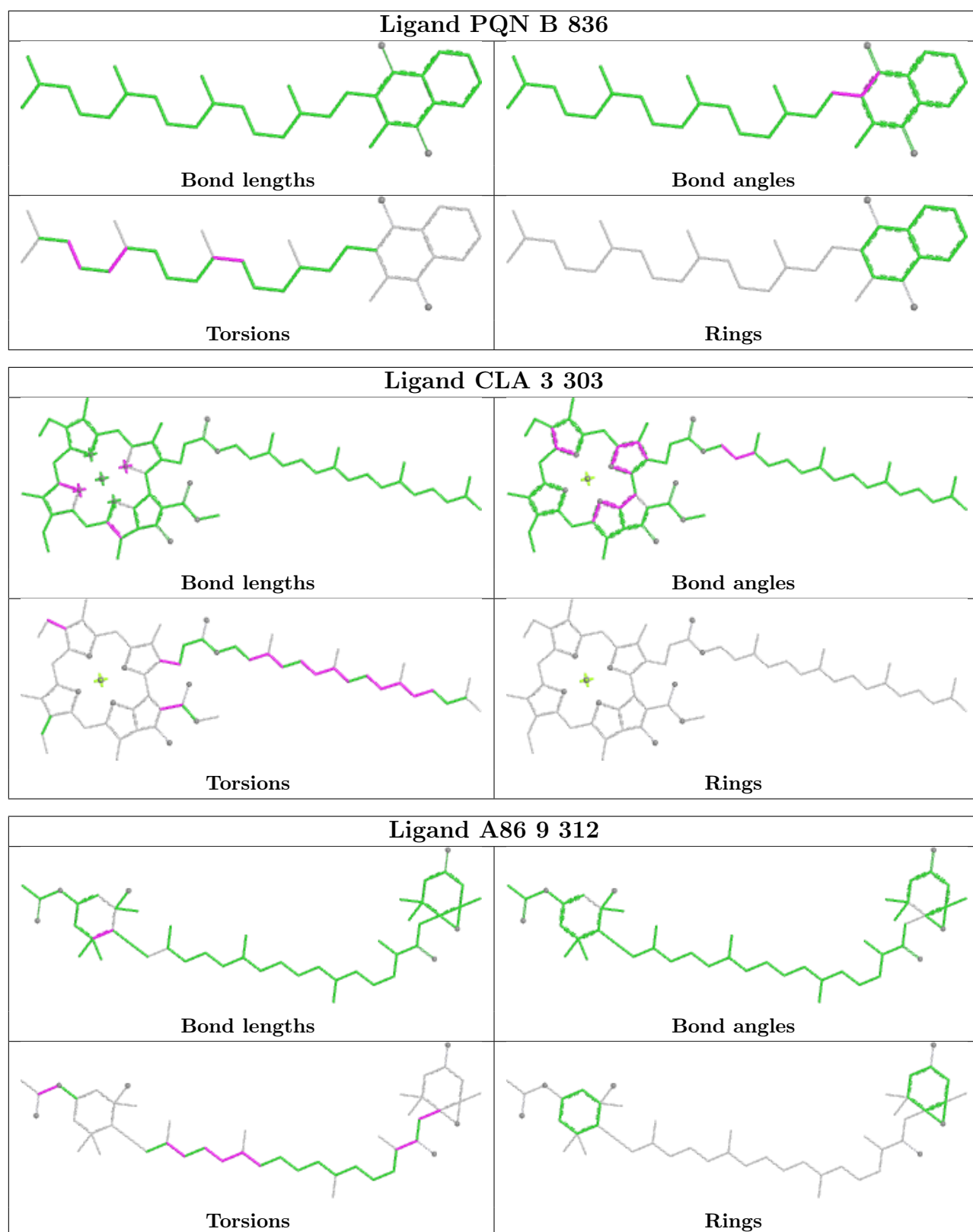


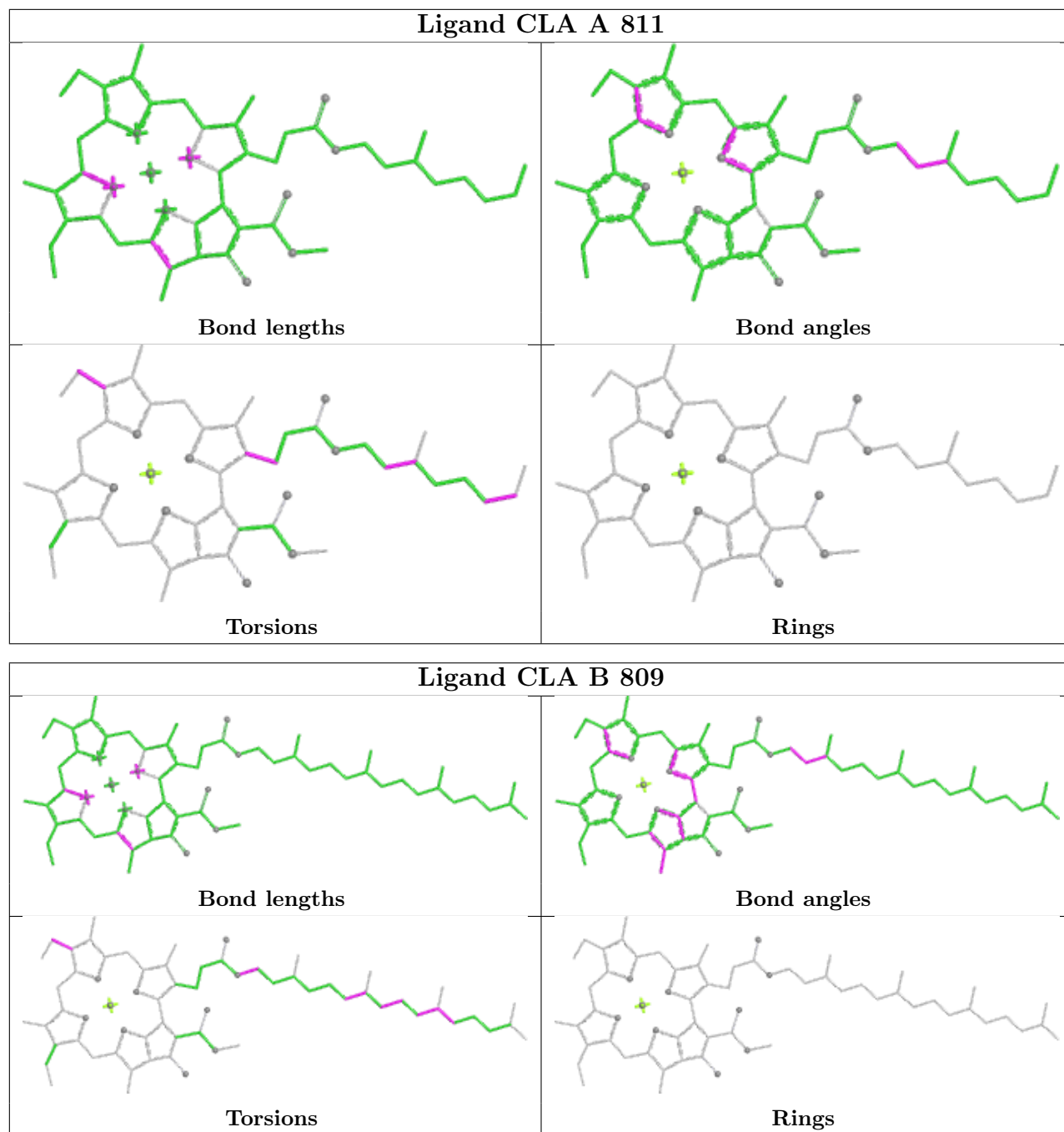




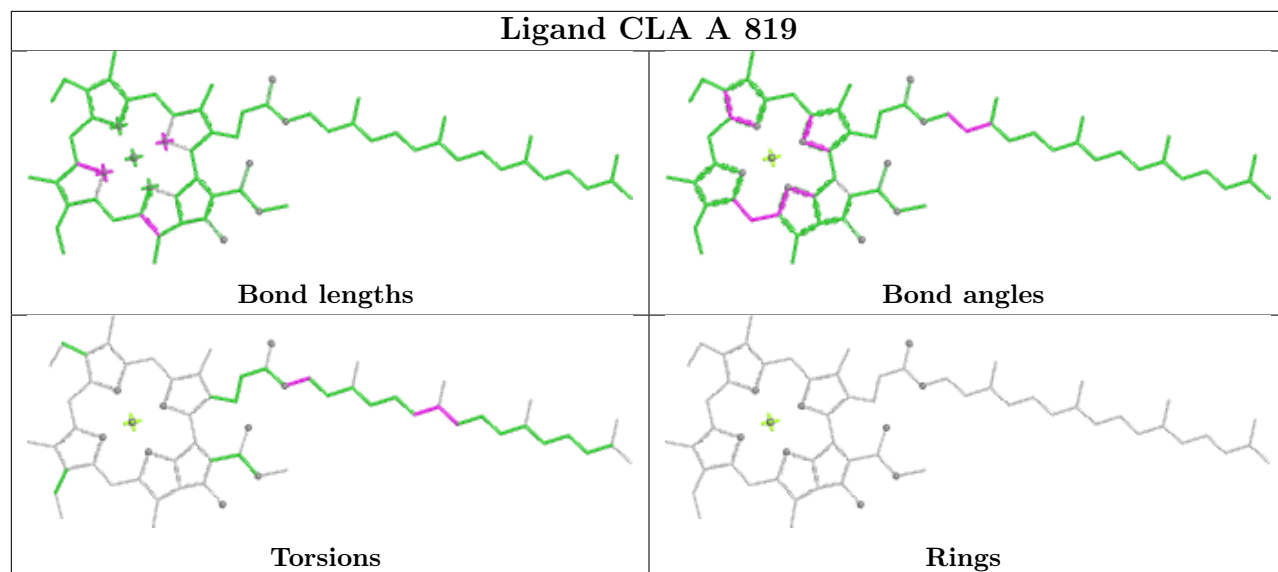




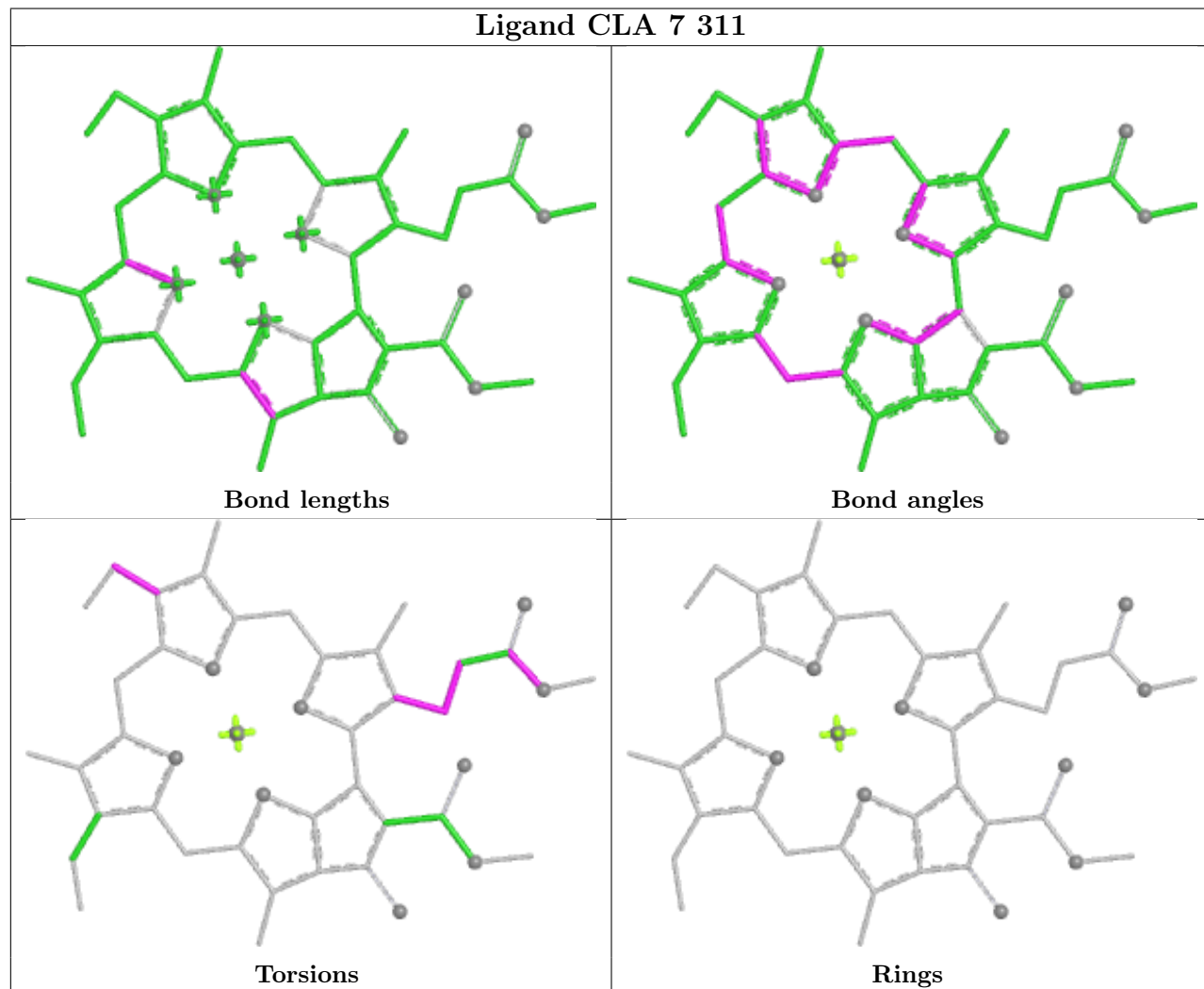


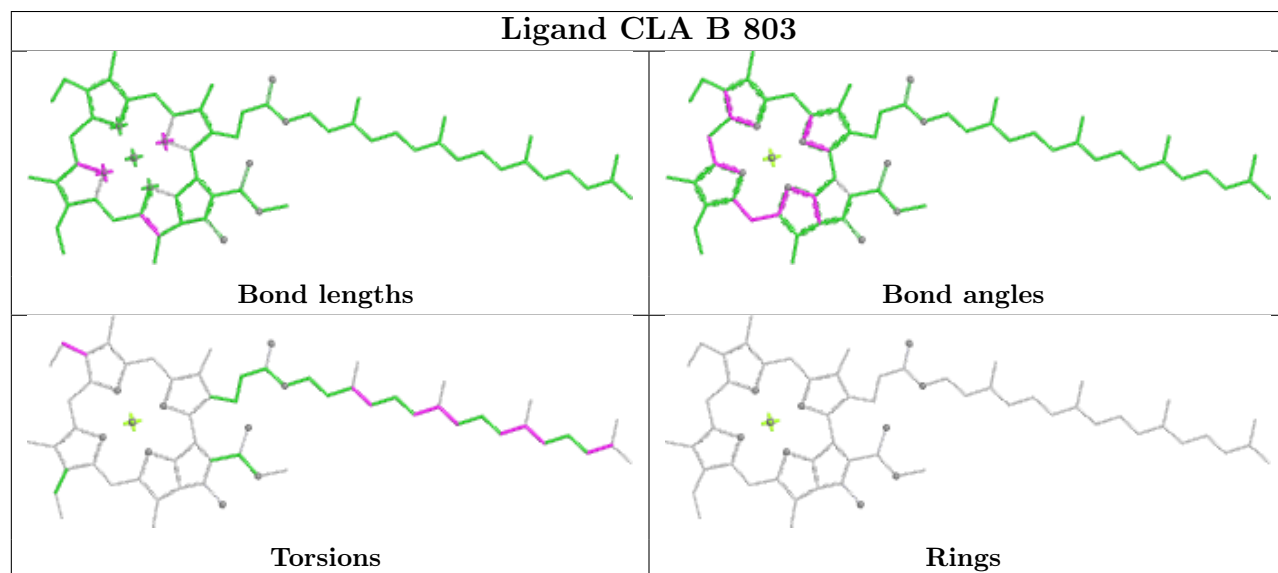
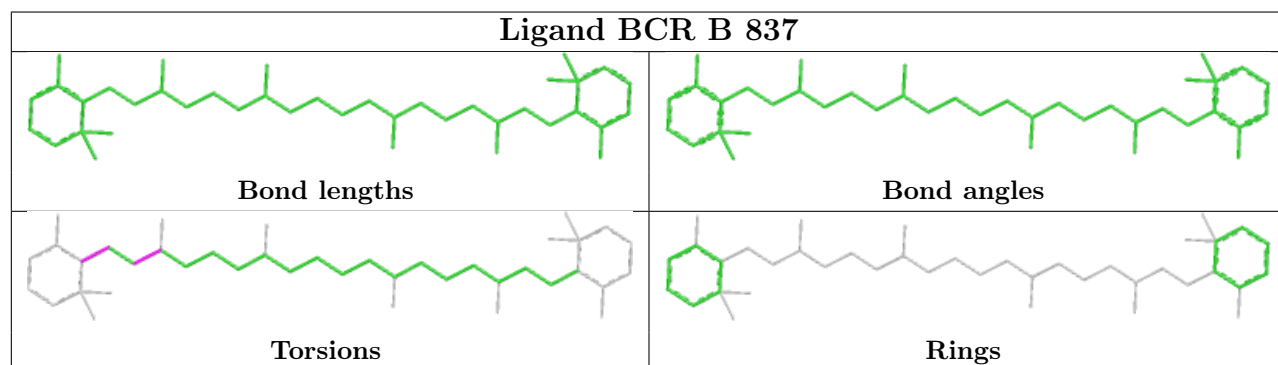
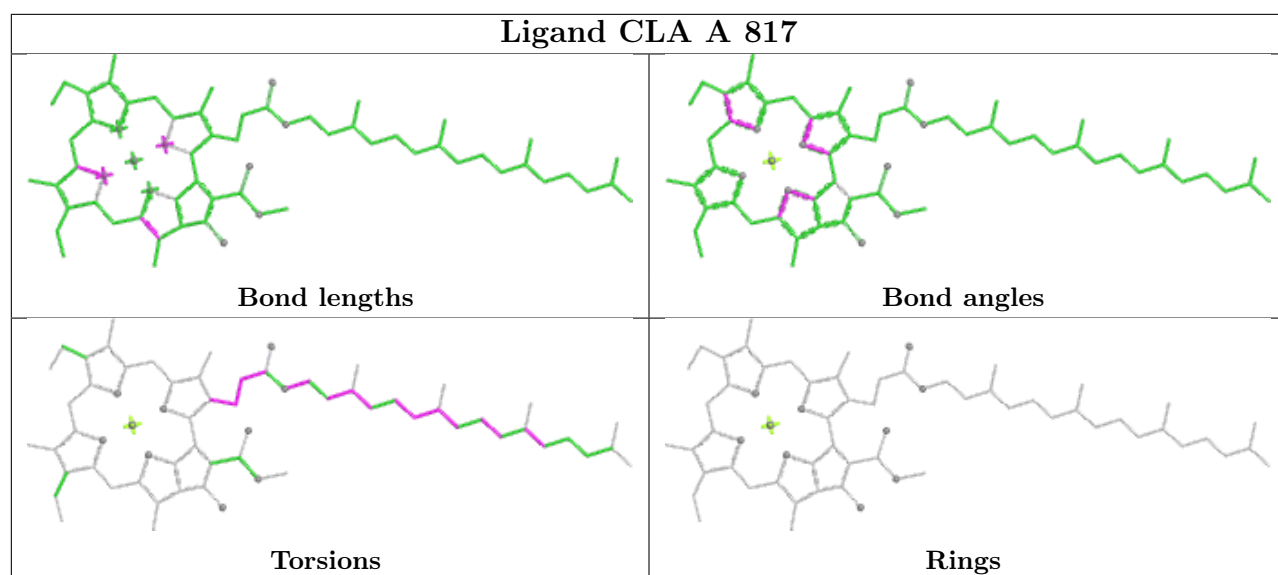


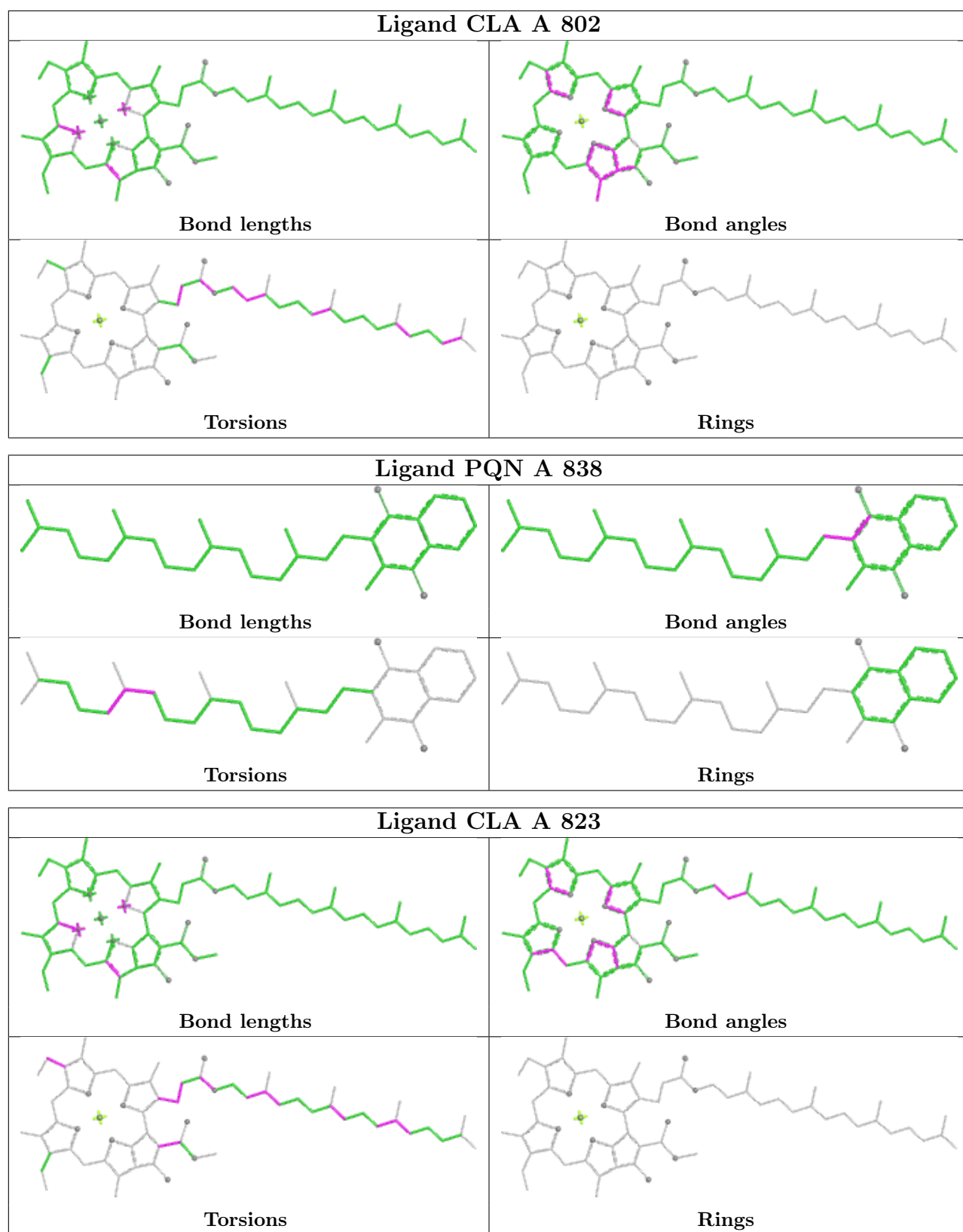
Ligand CLA A 819



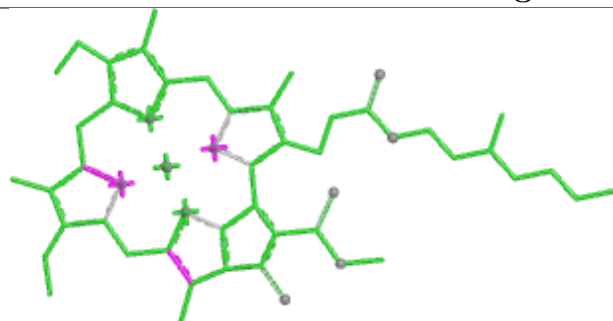
Ligand CLA 7 311



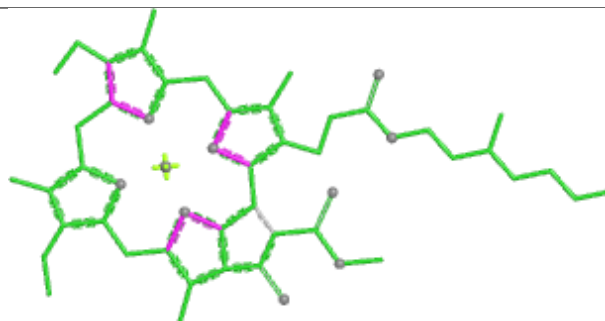




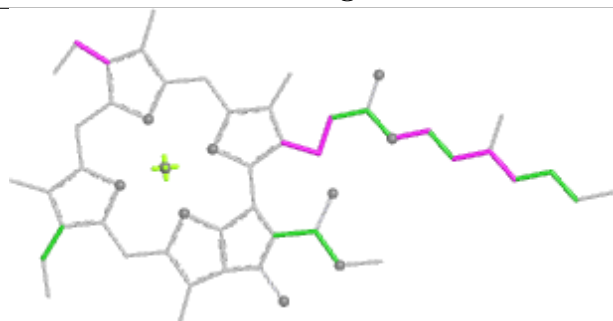
Ligand CLA B 820



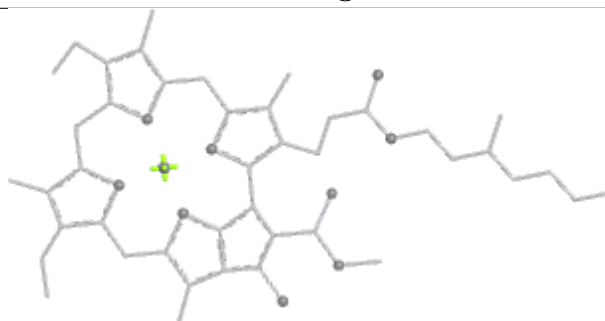
Bond lengths



Bond angles

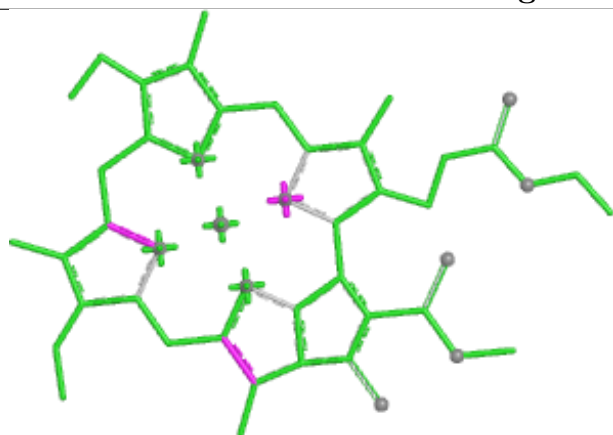


Torsions

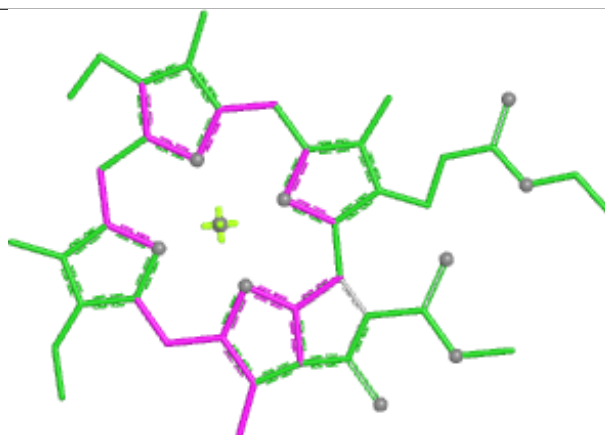


Rings

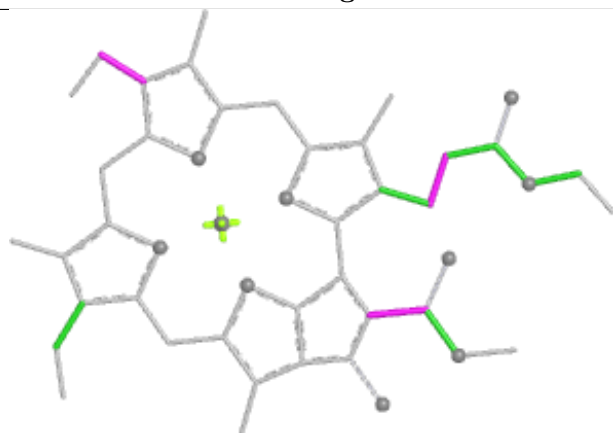
Ligand CLA 9 303



Bond lengths



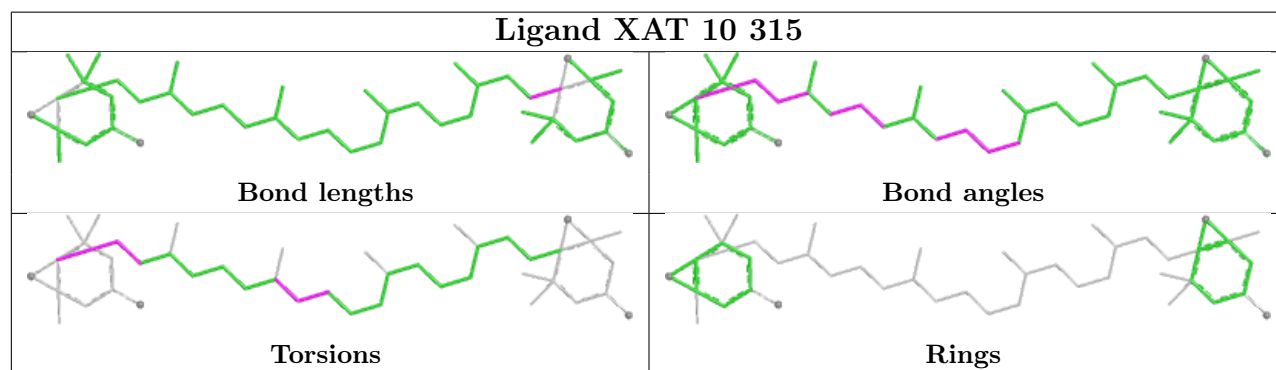
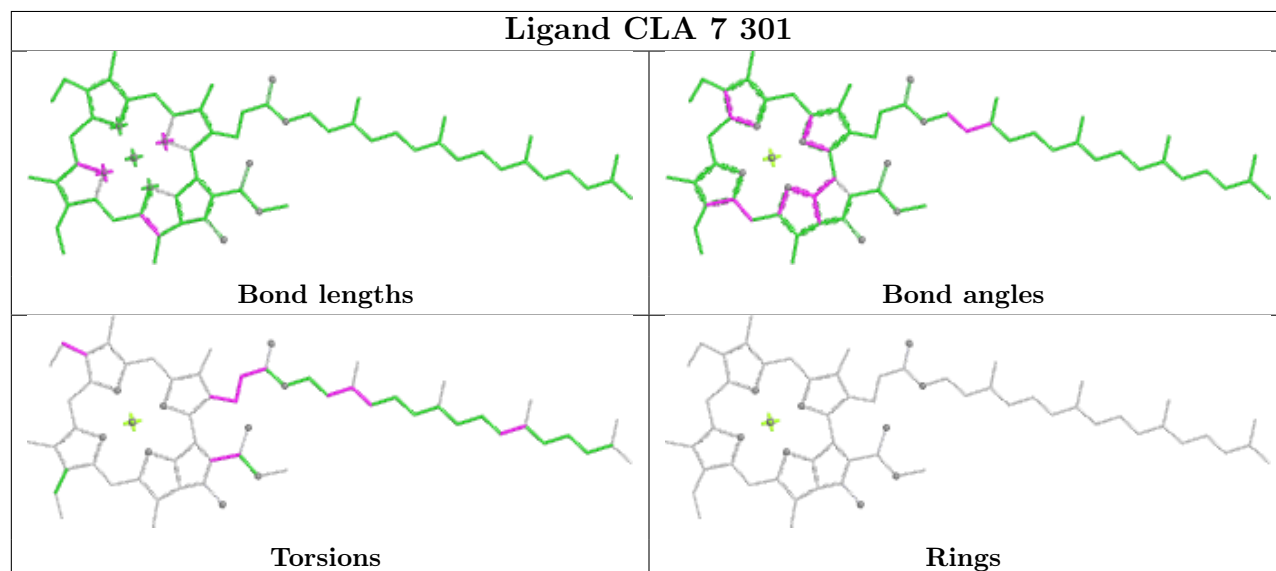
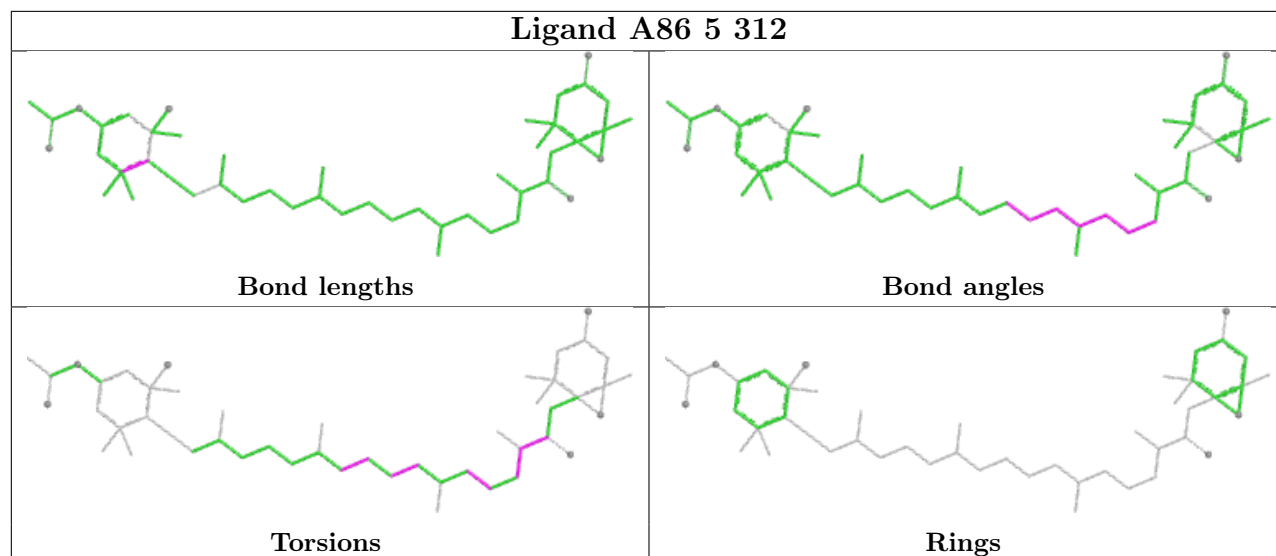
Bond angles

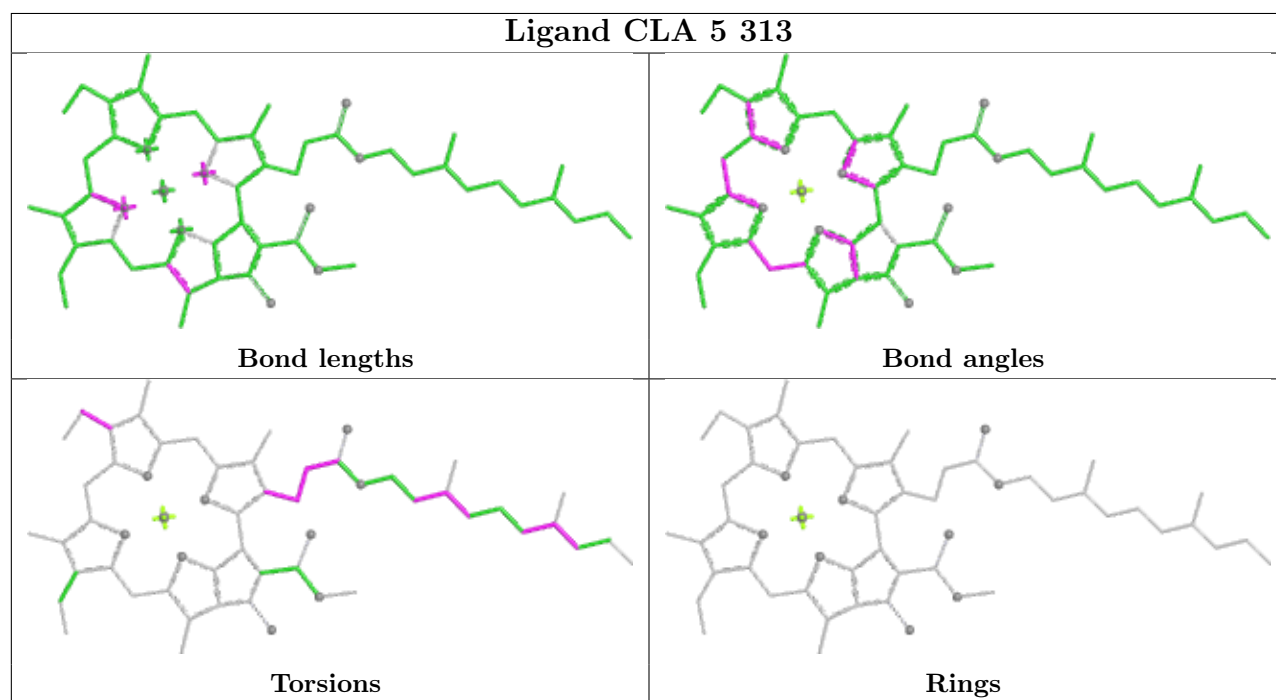
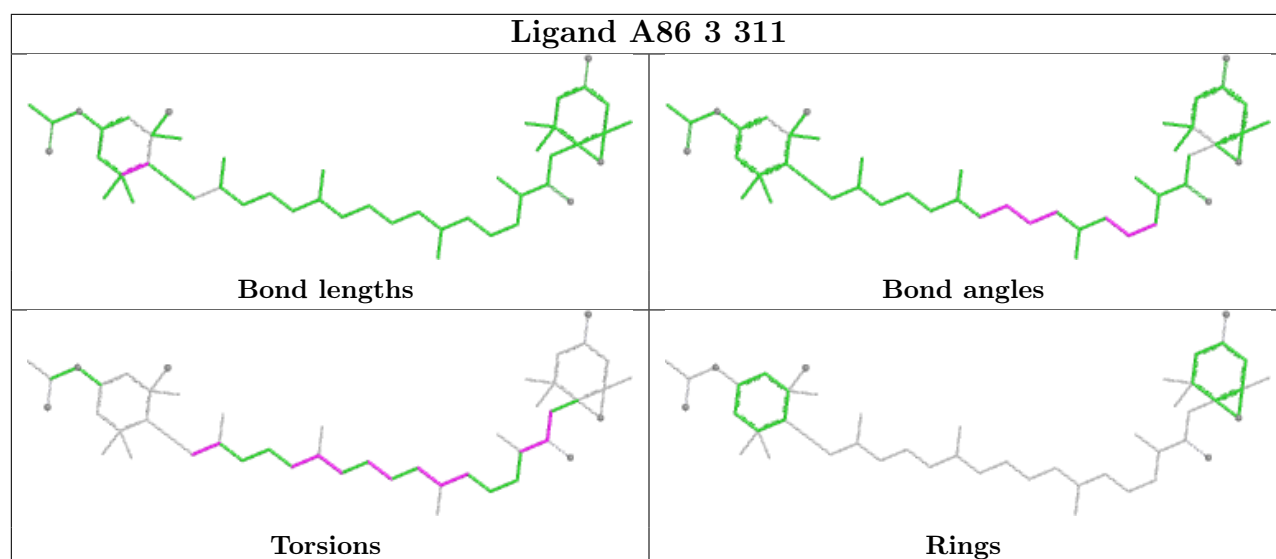


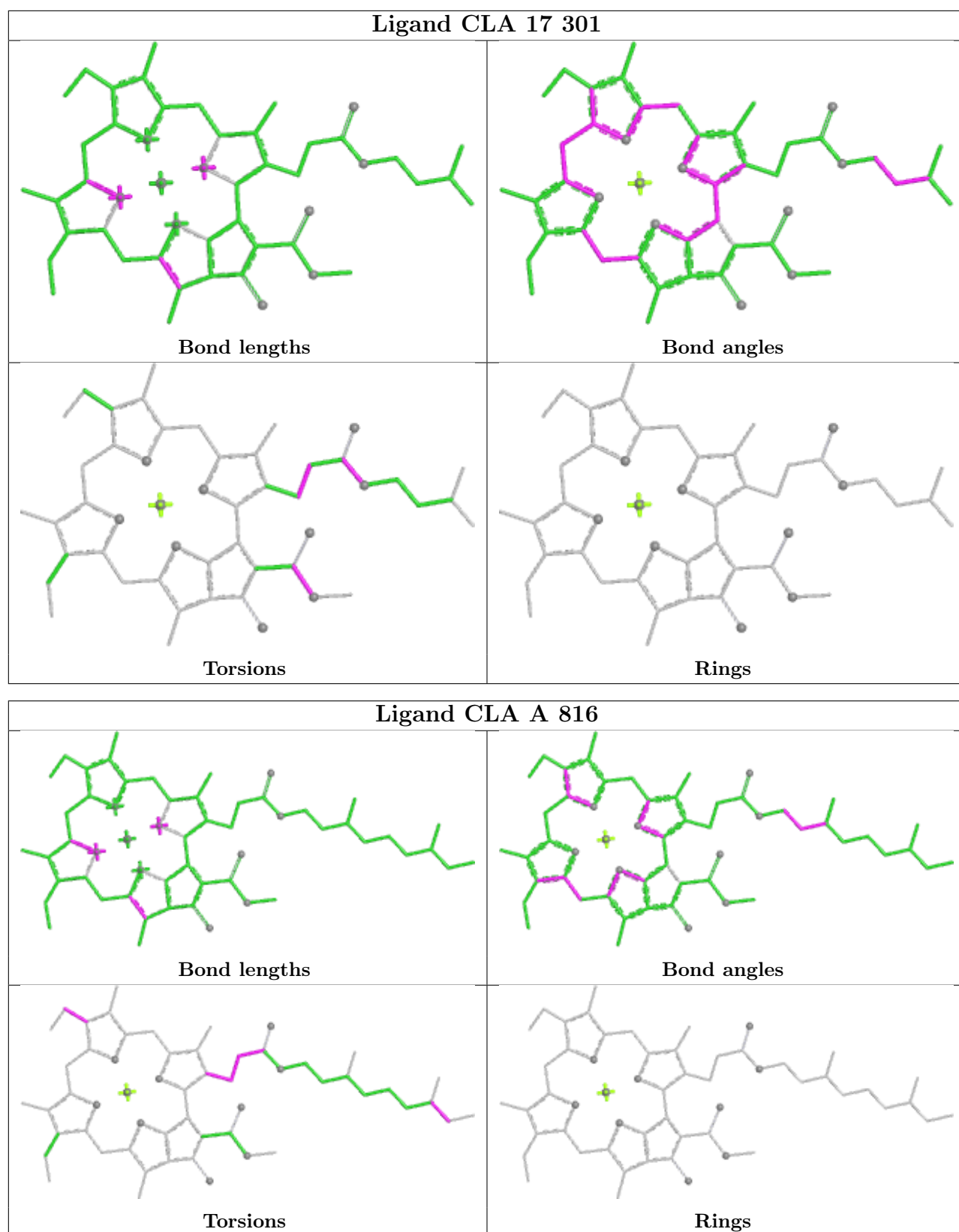
Torsions



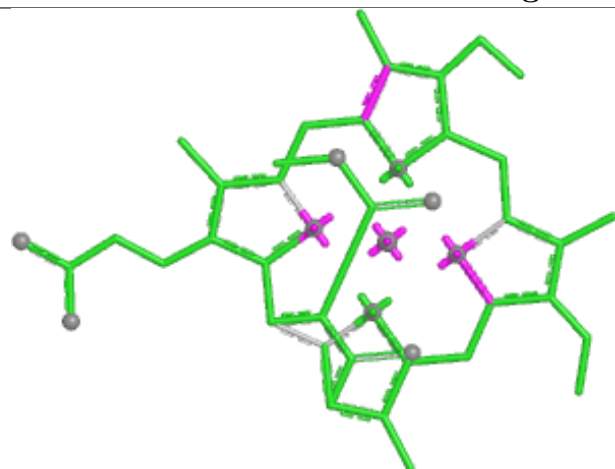
Rings



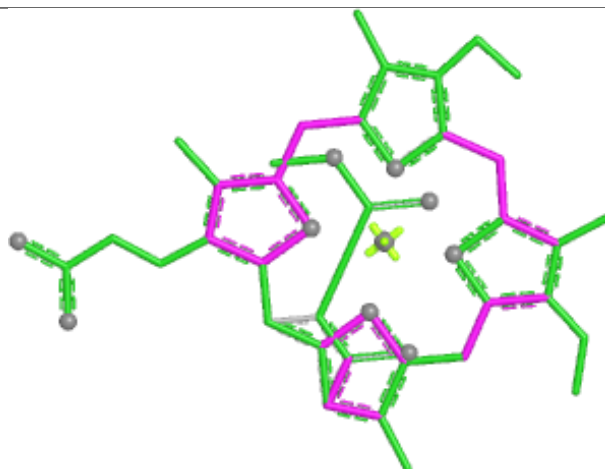




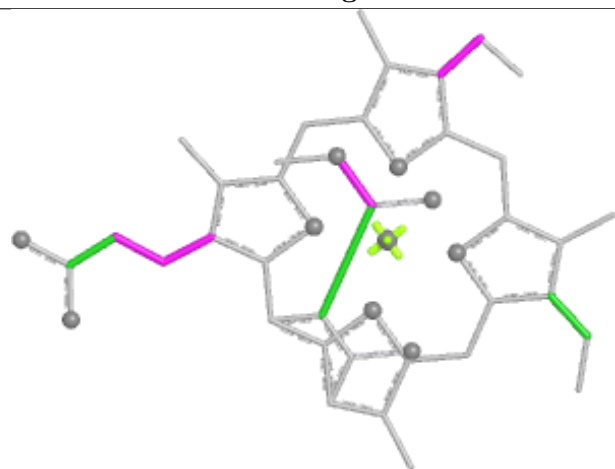
Ligand KC1 4 309



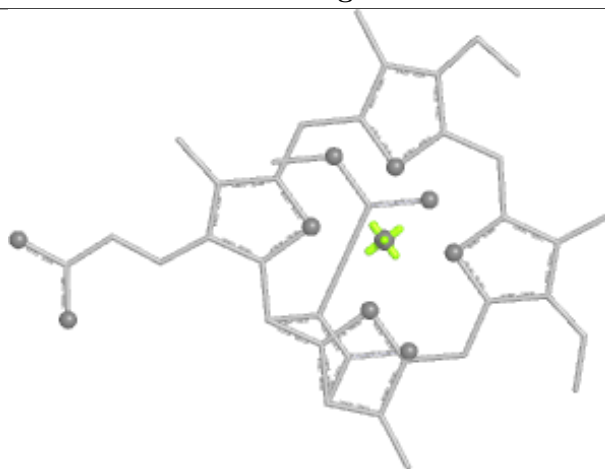
Bond lengths



Bond angles

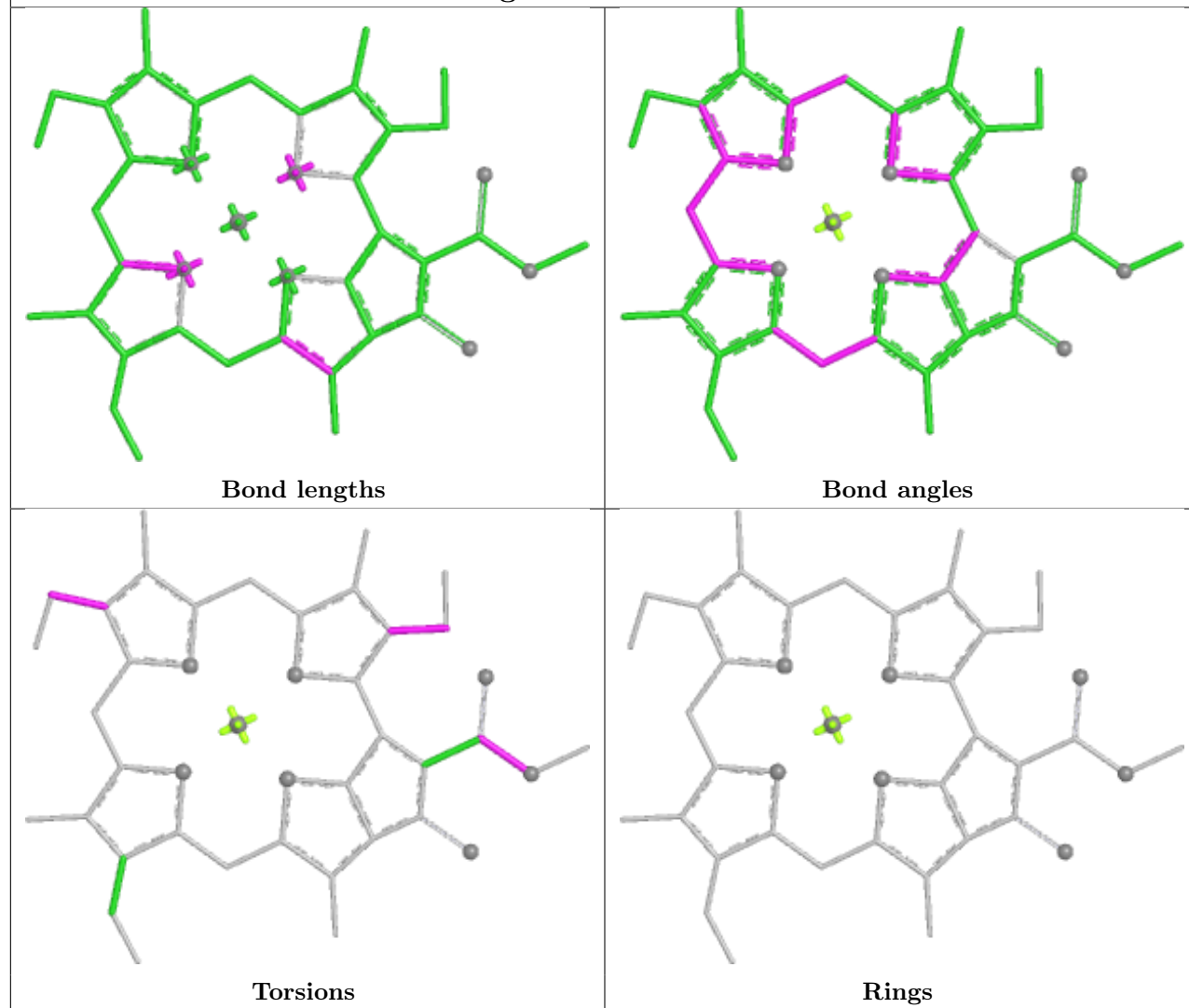


Torsions

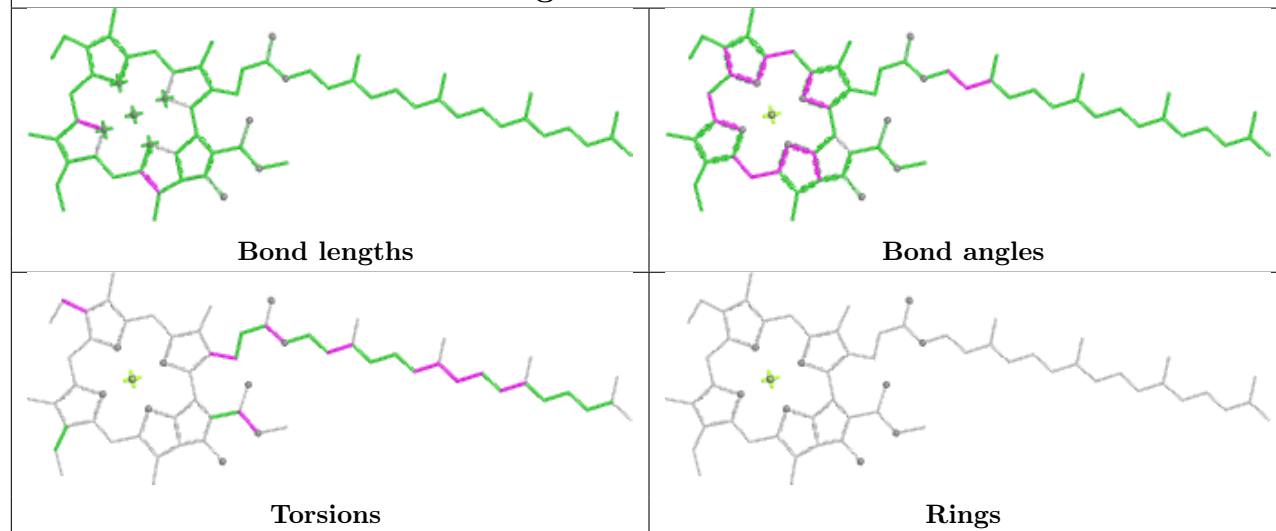


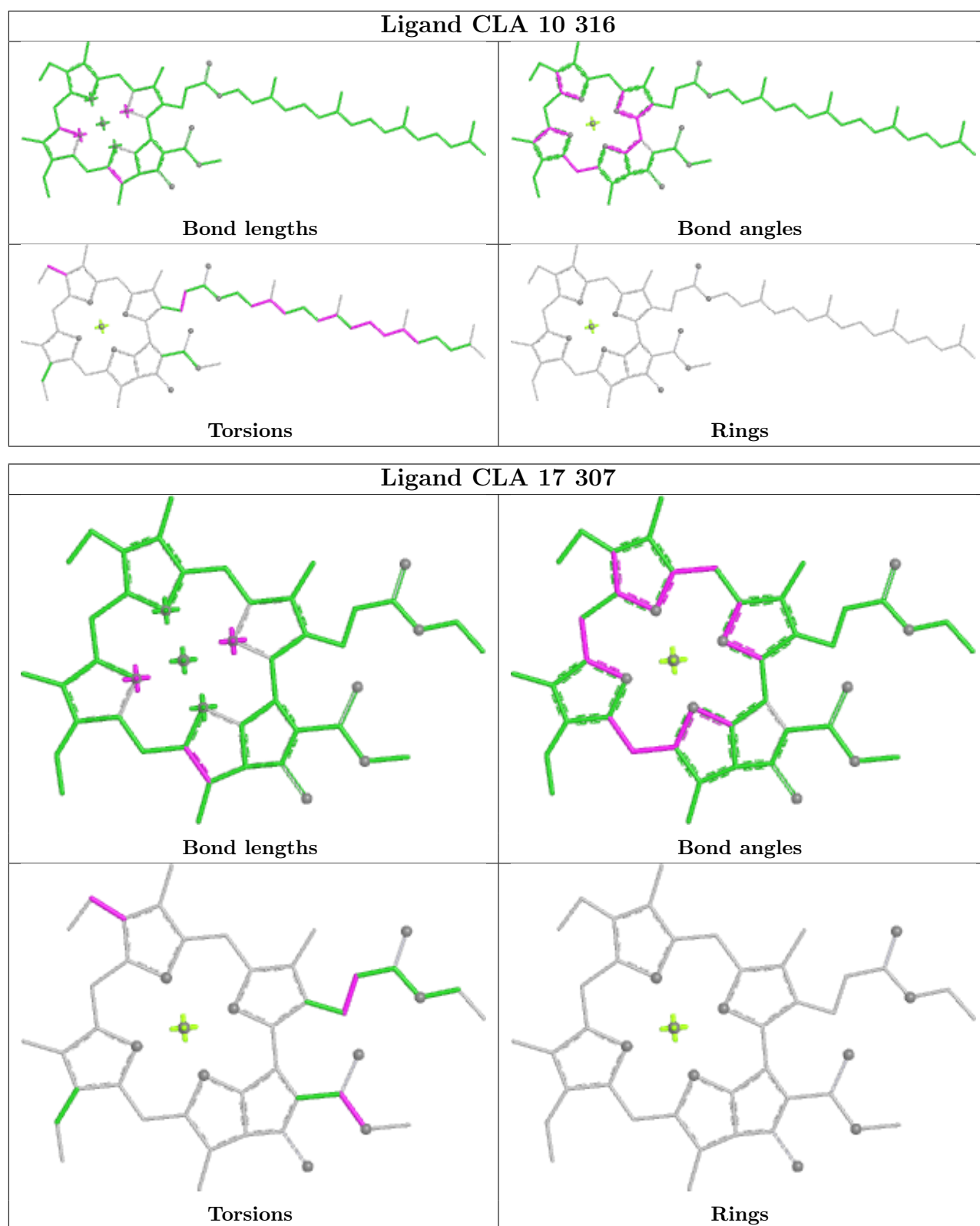
Rings

Ligand CLA a 202



Ligand CLA 1 303





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
24	2	2
20	15	1
23	19	1
27	a	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	2	49:UNK	C	70:UNK	N	27.51
1	2	85:UNK	C	111:UNK	N	21.06
1	15	55:UNK	C	61:UNK	N	20.22
1	19	57:UNK	C	71:UNK	N	7.85
1	a	99:UNK	C	102:UNK	N	5.58

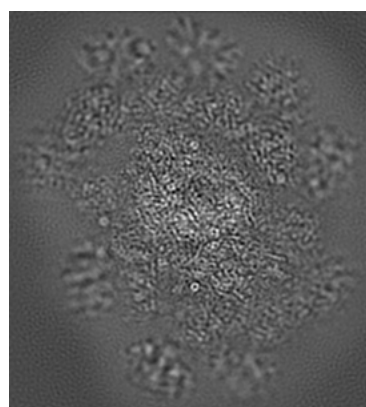
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-72770. These allow visual inspection of the internal detail of the map and identification of artifacts.

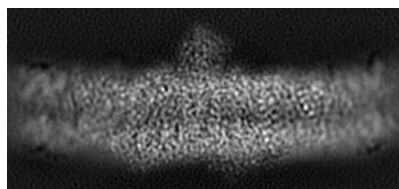
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

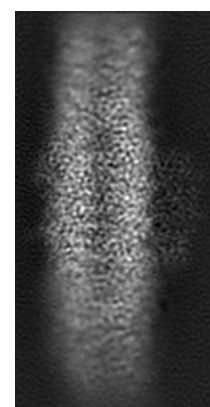
6.1.1 Primary map



X



Y

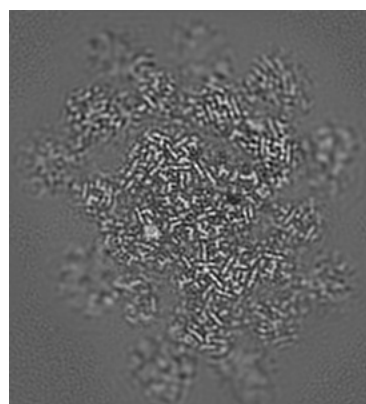


Z

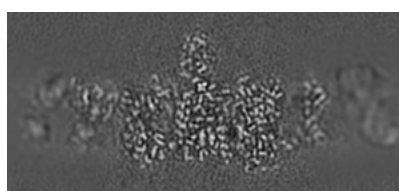
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

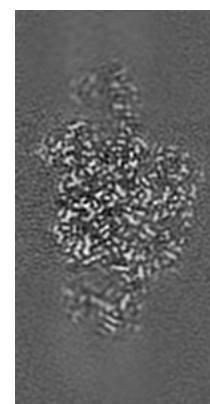
6.2.1 Primary map



X Index: 49



Y Index: 96

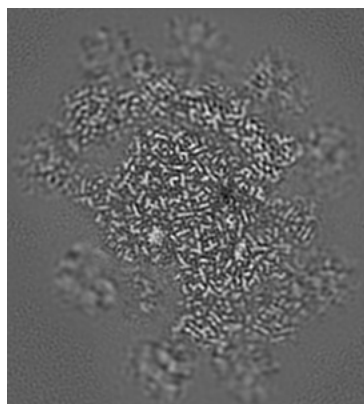


Z Index: 107

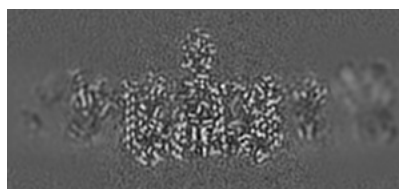
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

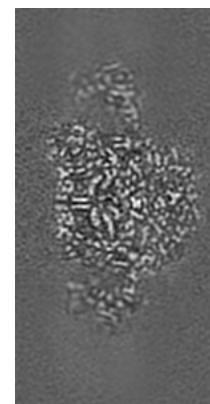
6.3.1 Primary map



X Index: 52



Y Index: 99

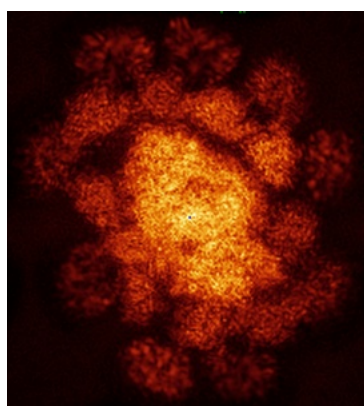


Z Index: 104

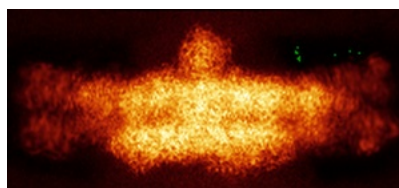
The images above show the largest variance slices of the map in three orthogonal directions.

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

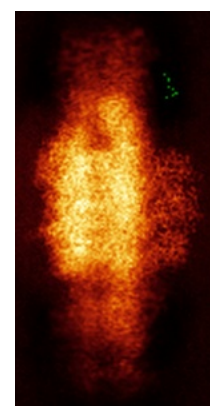
6.4.1 Primary map



X



Y

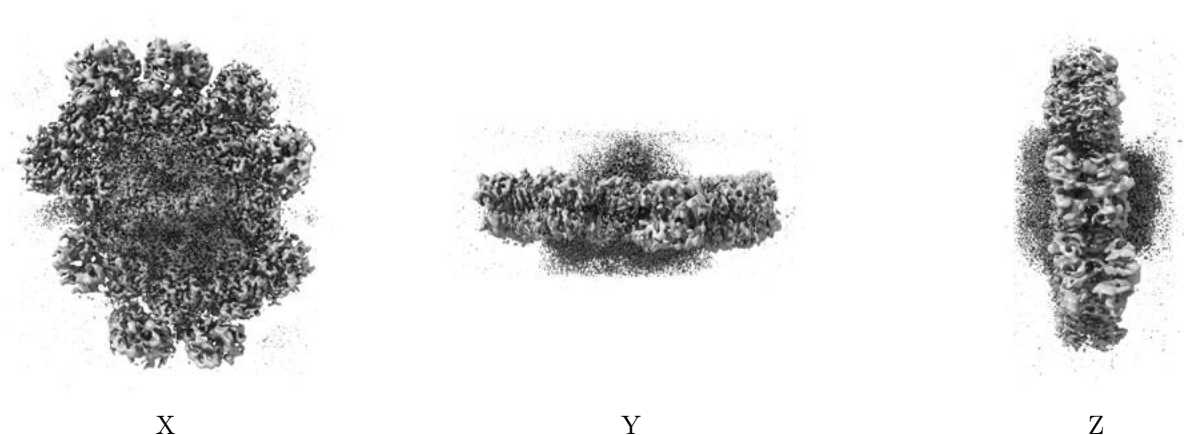


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.45. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

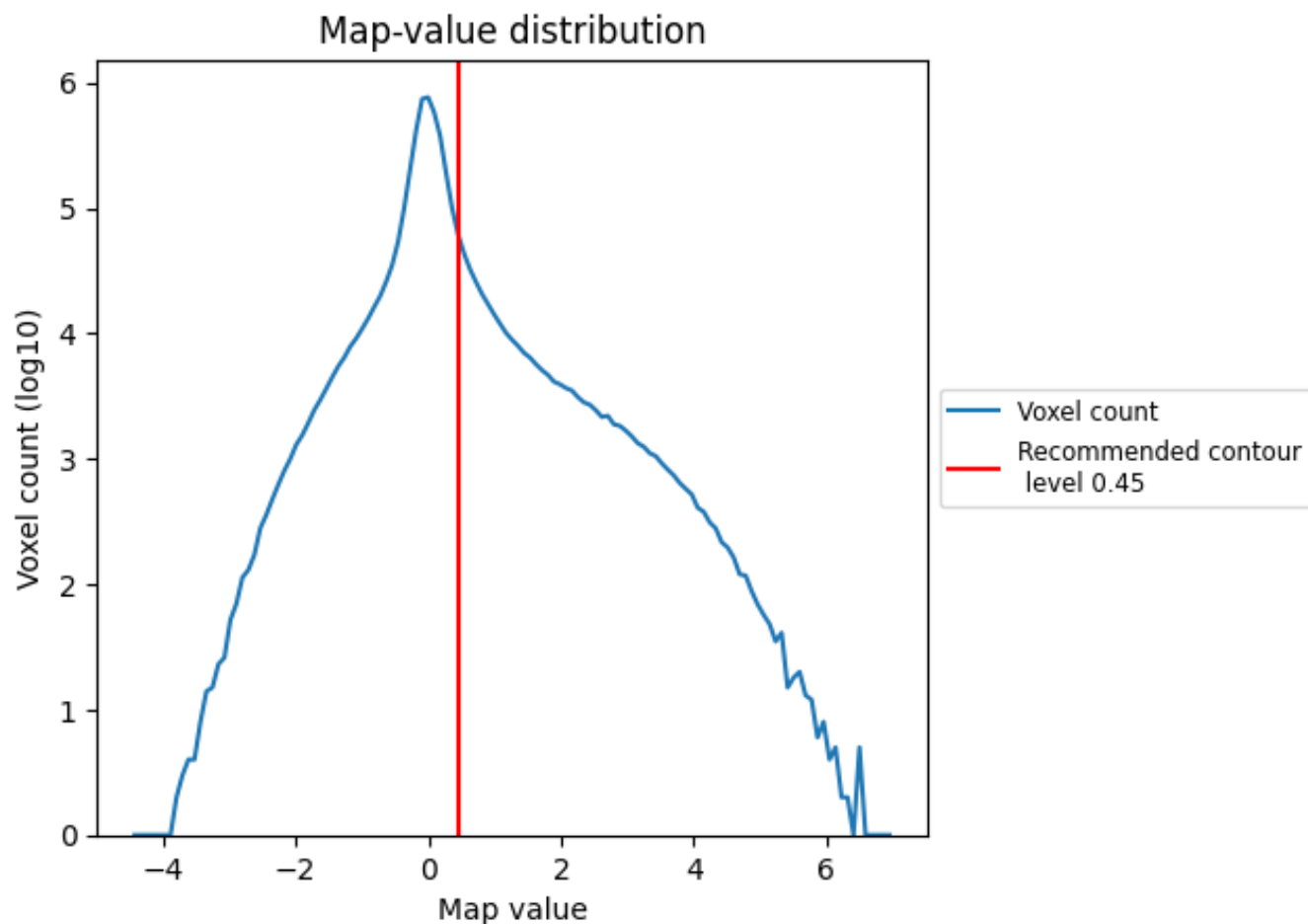
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

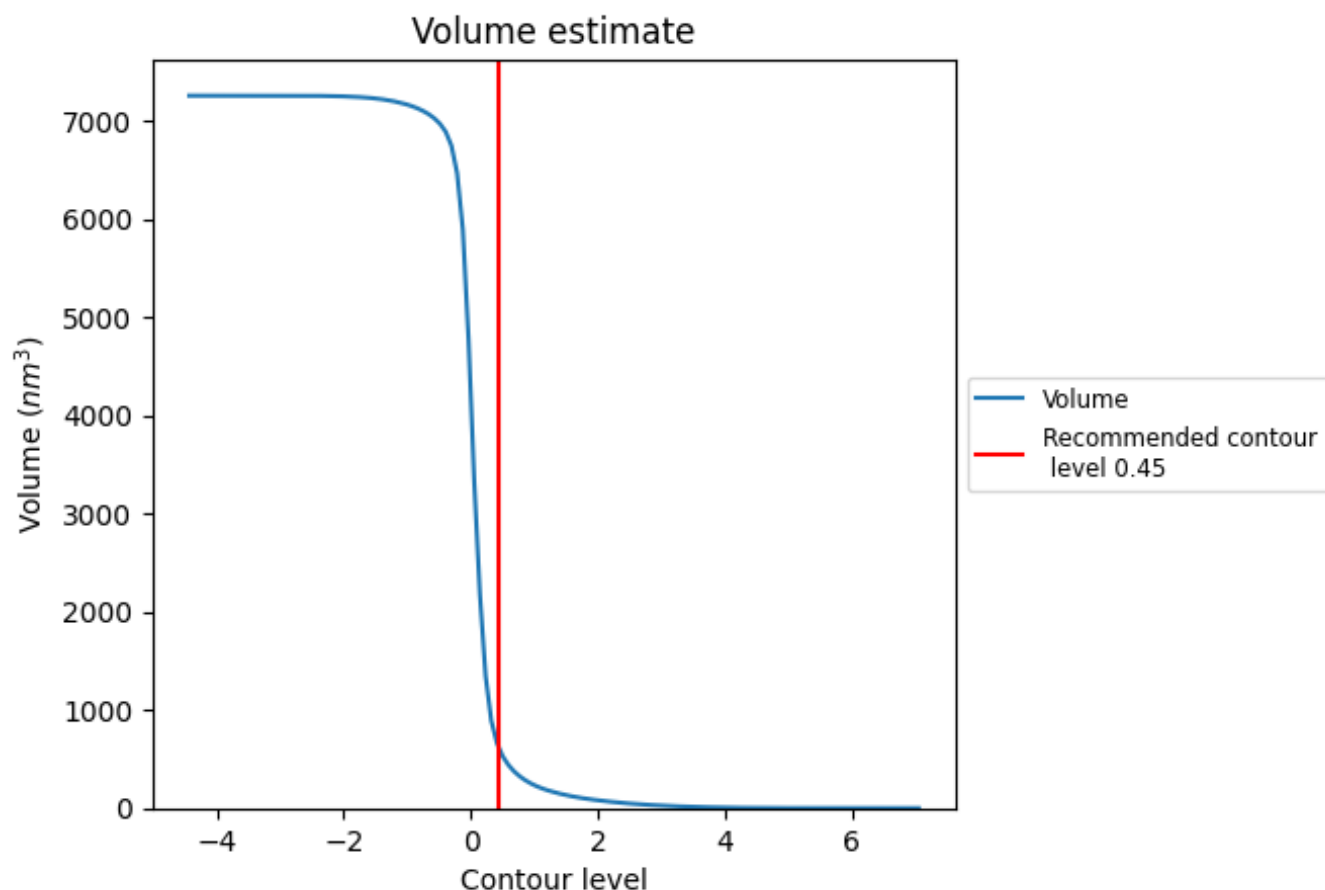
This section contains the results of statistical analysis of the map.

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 604 nm³; this corresponds to an approximate mass of 546 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](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

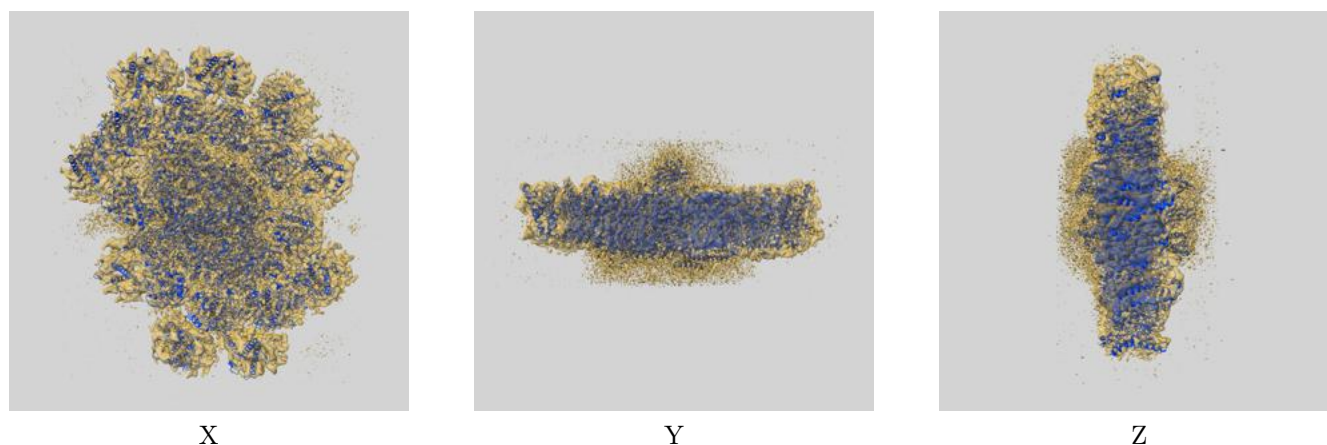
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

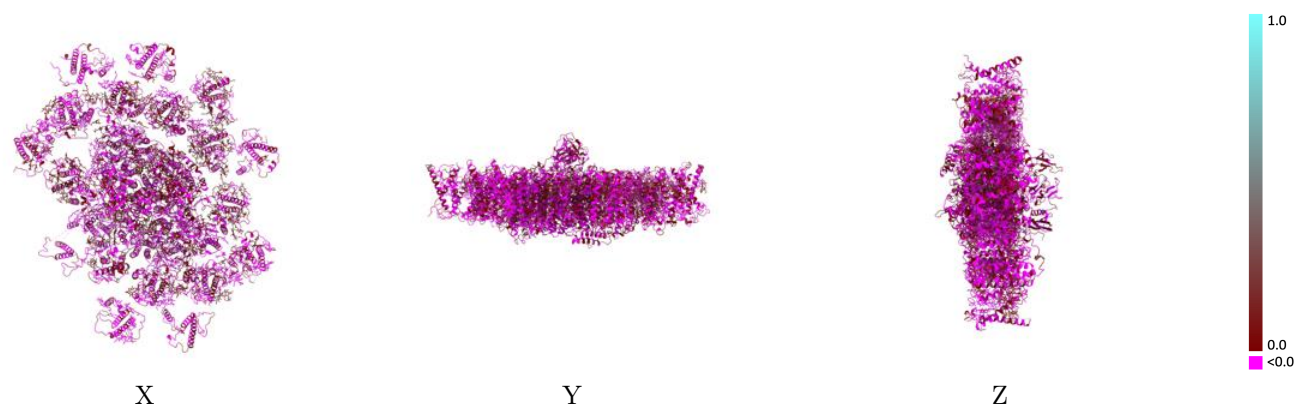
This section contains information regarding the fit between EMDB map EMD-72770 and PDB model 9YGV. Per-residue inclusion information can be found in section [3](#) on page [29](#).

9.1 Map-model overlay [i](#)



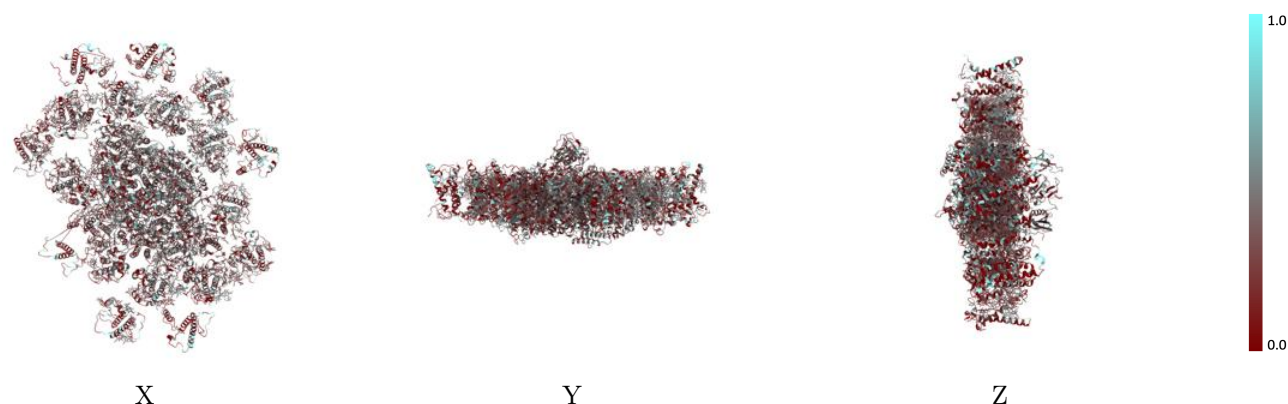
The images above show the 3D surface view of the map at the recommended contour level 0.45 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



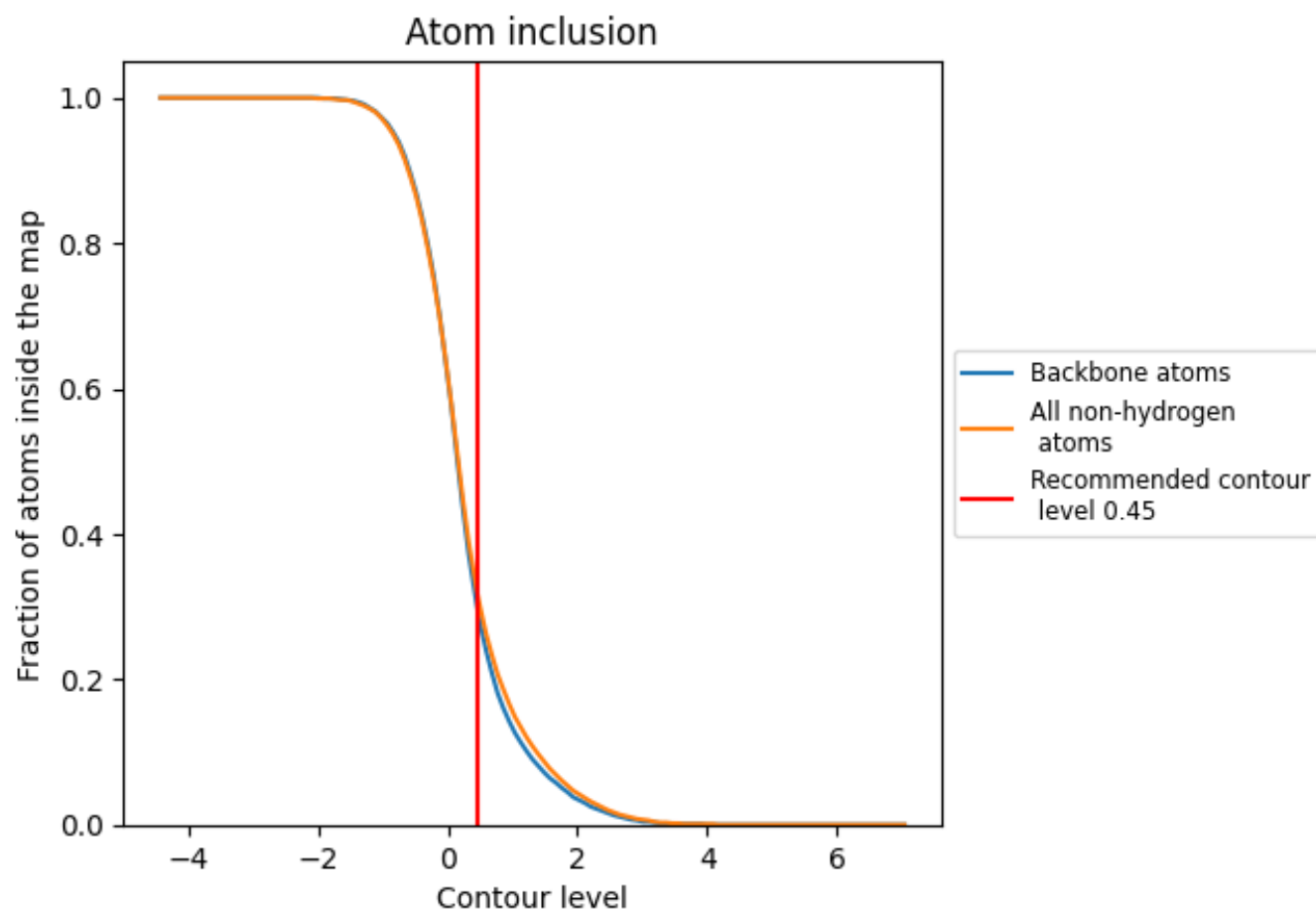
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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 (0.45).





























































9.4 Atom inclusion [i](#)



At the recommended contour level, 30% of all backbone atoms, 32% 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 (0.45) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.3210	 -0.0080
1	 0.2830	 -0.0090
10	 0.3030	 0.0020
11	 0.3100	 -0.0050
13	 0.2660	 -0.0010
15	 0.2510	 -0.0300
16	 0.2700	 -0.0600
17	 0.3330	 0.0360
19	 0.3170	 -0.0250
2	 0.3190	 -0.0170
3	 0.2980	 0.0110
4	 0.3030	 -0.0250
5	 0.3330	 0.0140
6	 0.3680	 0.0300
7	 0.3600	 0.0230
8	 0.3110	 0.0270
9	 0.2830	 -0.0220
A	 0.3430	 -0.0160
B	 0.3490	 -0.0100
C	 0.3280	 -0.0490
D	 0.2890	 -0.0160
E	 0.3890	 0.0370
F	 0.3510	 -0.0030
I	 0.2560	 -0.0410
J	 0.3040	 -0.0400
L	 0.2840	 -0.0320
M	 0.2450	 -0.0070
R	 0.2790	 -0.0530
a	 0.2950	 -0.0730
b	 0.2420	 -0.0390

