



wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 07:53 AM UTC

PDB ID : 8ASL / pdb_00008asl
EMDB ID : EMD-15618
Title : RCII/PSI complex, class 2
Authors : Zhao, Z.; Vercellino, I.; Knoppova, J.; Sobotka, R.; Murray, J.W.; Nixon, P.J.;
Sazanov, L.A.; Komenda, J.
Deposited on : 2022-08-19
Resolution : 3.15 Å (reported)
Based on initial models : 2XBG, 6WJ6, 5OY0

This is a wwPDB EM Validation Summary 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

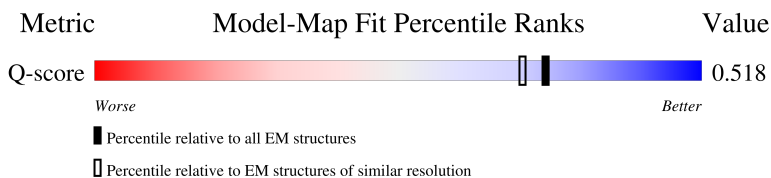
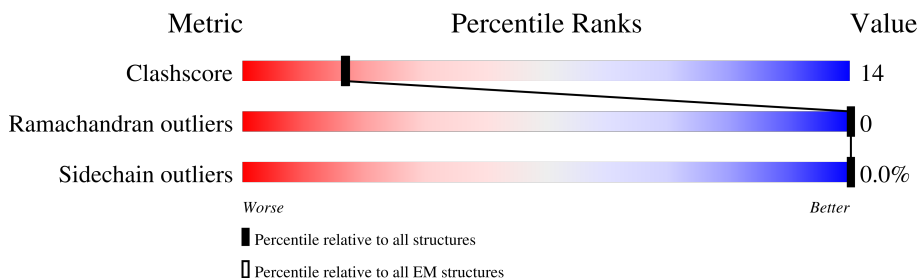
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.15 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.



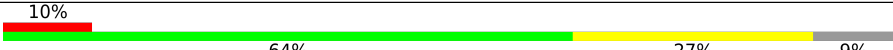
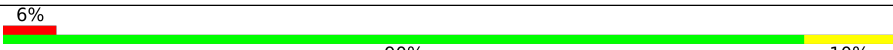
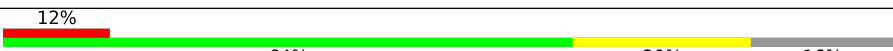
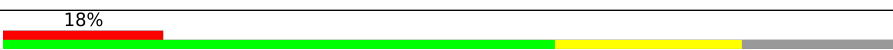
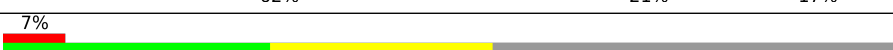
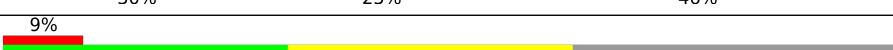
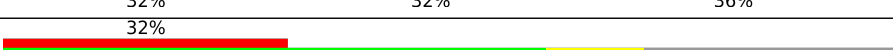
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14486 (2.65 - 3.65)

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

Mol	Chain	Length	Quality of chain
1	a	751	 73% 26% .
2	b	731	 79% 21%
3	c	81	 68% 31% .
4	d	141	 78% 21% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	e	74	
6	f	165	
7	i	40	
8	j	40	
9	k	86	
10	l	157	
11	m	31	
12	A	344	
13	D	336	
14	E	81	
15	F	44	
16	I	38	
17	S	342	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	CL0	a	801	X	-	-	-
19	CLA	A	402	X	-	-	-
19	CLA	A	403	X	-	-	-
19	CLA	A	405	X	-	-	-
19	CLA	D	401	X	-	-	-
19	CLA	D	403	X	-	-	-
19	CLA	D	404	X	-	-	-
19	CLA	a	802	X	-	-	-
19	CLA	a	803	X	-	-	-
19	CLA	a	804	X	-	-	-
19	CLA	a	805	X	-	-	-
19	CLA	a	806	X	-	-	-
19	CLA	a	807	X	-	-	-
19	CLA	a	808	X	-	-	-
19	CLA	a	809	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	a	810	X	-	-	-
19	CLA	a	811	X	-	-	-
19	CLA	a	812	X	-	-	-
19	CLA	a	813	X	-	-	-
19	CLA	a	815	X	-	-	-
19	CLA	a	816	X	-	-	-
19	CLA	a	817	X	-	-	-
19	CLA	a	818	X	-	-	-
19	CLA	a	819	X	-	-	-
19	CLA	a	820	X	-	-	-
19	CLA	a	821	X	-	-	-
19	CLA	a	822	X	-	-	-
19	CLA	a	823	X	-	-	-
19	CLA	a	824	X	-	-	-
19	CLA	a	825	X	-	-	-
19	CLA	a	826	X	-	-	-
19	CLA	a	827	X	-	-	-
19	CLA	a	828	X	-	-	-
19	CLA	a	829	X	-	-	-
19	CLA	a	830	X	-	-	-
19	CLA	a	831	X	-	-	-
19	CLA	a	832	X	-	-	-
19	CLA	a	833	X	-	-	-
19	CLA	a	834	X	-	-	-
19	CLA	a	835	X	-	-	-
19	CLA	a	836	X	-	-	-
19	CLA	a	837	X	-	-	-
19	CLA	a	839	X	-	-	-
19	CLA	a	840	X	-	-	-
19	CLA	a	841	X	-	-	-
19	CLA	a	842	X	-	-	-
19	CLA	a	843	X	-	-	-
19	CLA	a	855	X	-	-	-
19	CLA	a	856	X	-	-	-
19	CLA	a	858	X	-	-	-
19	CLA	b	3002	X	-	-	-
19	CLA	b	3003	X	-	-	-
19	CLA	b	3004	X	-	-	-
19	CLA	b	3005	X	-	-	-
19	CLA	b	3006	X	-	-	-
19	CLA	b	3007	X	-	-	-
19	CLA	b	3008	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	b	3009	X	-	-	-
19	CLA	b	3010	X	-	-	-
19	CLA	b	3011	X	-	-	-
19	CLA	b	3012	X	-	-	-
19	CLA	b	3013	X	-	-	-
19	CLA	b	3014	X	-	-	-
19	CLA	b	3015	X	-	-	-
19	CLA	b	3016	X	-	-	-
19	CLA	b	3017	X	-	-	-
19	CLA	b	3018	X	-	-	-
19	CLA	b	3019	X	-	-	-
19	CLA	b	3020	X	-	-	-
19	CLA	b	3021	X	-	-	-
19	CLA	b	3022	X	-	-	-
19	CLA	b	3023	X	-	-	-
19	CLA	b	3024	X	-	-	-
19	CLA	b	3025	X	-	-	-
19	CLA	b	3026	X	-	-	-
19	CLA	b	3027	X	-	-	-
19	CLA	b	3028	X	-	-	-
19	CLA	b	3029	X	-	-	-
19	CLA	b	3030	X	-	-	-
19	CLA	b	3031	X	-	-	-
19	CLA	b	3032	X	-	-	-
19	CLA	b	3033	X	-	-	-
19	CLA	b	3034	X	-	-	-
19	CLA	b	3035	X	-	-	-
19	CLA	b	3036	X	-	-	-
19	CLA	b	3037	X	-	-	-
19	CLA	b	3038	X	-	-	-
19	CLA	b	3039	X	-	-	-
19	CLA	b	3040	X	-	-	-
19	CLA	b	3041	X	-	-	-
19	CLA	f	201	X	-	-	-
19	CLA	f	203	X	-	-	-
19	CLA	f	204	X	-	-	-
19	CLA	j	102	X	-	-	-
19	CLA	j	103	X	-	-	-
19	CLA	k	4002	X	-	-	-
19	CLA	k	4003	X	-	-	-
19	CLA	l	1501	X	-	-	-
19	CLA	l	1502	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	1	1503	X	-	-	-

2 Entry composition

There are 32 unique types of molecules in this entry. The entry contains 32739 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 Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	a	741	Total	C	N	O	S	0	0
			5795	3797	984	987	27		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	b	729	Total	C	N	O	S	0	0
			5770	3798	967	990	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	c	80	Total	C	N	O	S	0	0
			600	369	103	117	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	d	139	Total	C	N	O	S	0	0
			1087	688	188	208	3		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
5	e	69	Total	C	N	O	0	0
			538	337	95	106		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	f	142	Total	C	N	O	S	0	0
			1108	715	184	204	5		

- Molecule 7 is a protein called Photosystem I reaction center subunit VIII.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	i	40	Total	C	N	O	S	0	0
			311	209	44	55	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	j	40	Total	C	N	O	S	0	0
			319	215	47	54	3		

- Molecule 9 is a protein called Photosystem I reaction center subunit PsaK 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	k	75	Total	C	N	O	S	0	0
			524	343	87	90	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	l	143	Total	C	N	O	S	0	0
			1069	697	173	197	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	m	31	Total	C	N	O	S	0	0
			238	159	36	42	1		

- Molecule 12 is a protein called Photosystem II protein D1 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	A	289	Total	C	N	O	S	0	0
			2248	1478	366	389	15		

- Molecule 13 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	D	278	Total	C	N	O	S	0	0
			2188	1465	351	360	12		

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-5	MET	-	initiating methionine	UNP P09192
D	-4	HIS	-	expression tag	UNP P09192
D	-3	HIS	-	expression tag	UNP P09192
D	-2	HIS	-	expression tag	UNP P09192
D	-1	HIS	-	expression tag	UNP P09192
D	0	HIS	-	expression tag	UNP P09192
D	1	HIS	-	expression tag	UNP P09192

- Molecule 14 is a protein called Cytochrome b559 subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	E	44	Total	C	N	O	S	0	0
			360	245	54	60	1		

- Molecule 15 is a protein called Cytochrome b559 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	F	28	Total	C	N	O	S	0	0
			222	149	39	33	1		

- Molecule 16 is a protein called Photosystem II reaction center protein I.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	I	27	Total	C	N	O		0	0
			211	149	28	34			

- Molecule 17 is a protein called Photosystem II assembly lipoprotein Ycf48.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	S	303	Total	C	N	O	S	0	0
			2328	1481	393	451	3		

- Molecule 18 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					AltCon
18	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 19 is CHLOROPHYLL A (CCD ID: CLA) (formula: $\text{C}_{55}\text{H}_{72}\text{MgN}_4\text{O}_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltCon
19	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	a	1	Total 65	C 55	Mg 1	N 4	O 5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
19	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	a	1	Total 51	C 41	Mg 1	N 4	O 5	0
19	a	1	Total 50	C 40	Mg 1	N 4	O 5	0
19	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
19	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	a	1	Total 46	C 36	Mg 1	N 4	O 5	0
19	a	1	Total 46	C 36	Mg 1	N 4	O 5	0
19	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	a	1	Total 65	C 55	Mg 1	N 4	O 5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
19	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
19	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	a	1	Total 56	C 46	Mg 1	N 4	O 5	0
19	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
19	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	a	1	Total 51	C 41	Mg 1	N 4	O 5	0
19	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	a	1	Total 56	C 46	Mg 1	N 4	O 5	0
19	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	a	1	Total 65	C 55	Mg 1	N 4	O 5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
19	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	b	1	Total 56	C 46	Mg 1	N 4	O 5	0
19	b	1	Total 56	C 46	Mg 1	N 4	O 5	0
19	b	1	Total 50	C 40	Mg 1	N 4	O 5	0
19	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	b	1	Total 55	C 45	Mg 1	N 4	O 5	0
19	b	1	Total 56	C 46	Mg 1	N 4	O 5	0
19	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	b	1	Total 60	C 50	Mg 1	N 4	O 5	0
19	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	b	1	Total 60	C 50	Mg 1	N 4	O 5	0

Continued on next page...

Continued from previous page...

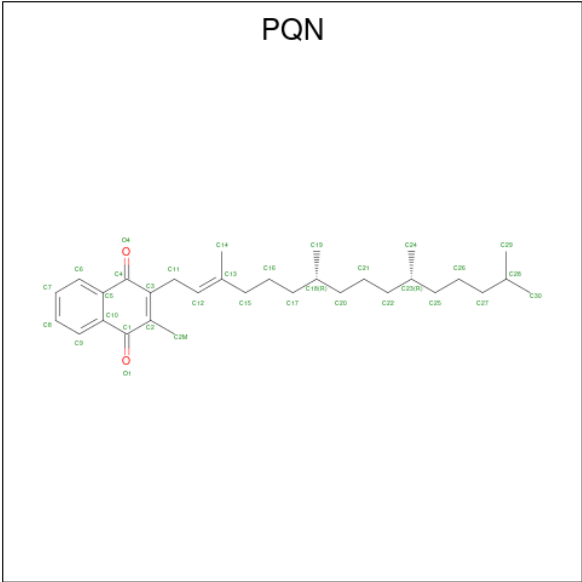
Mol	Chain	Residues	Atoms					AltConf
19	b	1	Total 46	C 36	Mg 1	N 4	O 5	0
19	b	1	Total 57	C 47	Mg 1	N 4	O 5	0
19	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	b	1	Total 55	C 45	Mg 1	N 4	O 5	0
19	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	b	1	Total 51	C 41	Mg 1	N 4	O 5	0
19	b	1	Total 50	C 40	Mg 1	N 4	O 5	0
19	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	b	1	Total 50	C 40	Mg 1	N 4	O 5	0
19	b	1	Total 52	C 42	Mg 1	N 4	O 5	0
19	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	b	1	Total 50	C 40	Mg 1	N 4	O 5	0
19	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	b	1	Total 46	C 36	Mg 1	N 4	O 5	0
19	f	1	Total 65	C 55	Mg 1	N 4	O 5	0

Continued on next page...

Continued from previous page...

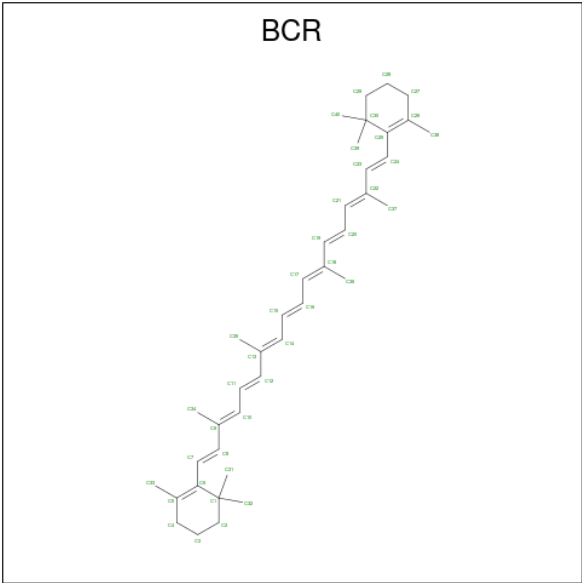
Mol	Chain	Residues	Atoms					AltConf
19	f	1	Total 50	C 40	Mg 1	N 4	O 5	0
19	f	1	Total 50	C 40	Mg 1	N 4	O 5	0
19	j	1	Total 55	C 45	Mg 1	N 4	O 5	0
19	j	1	Total 46	C 36	Mg 1	N 4	O 5	0
19	k	1	Total 46	C 36	Mg 1	N 4	O 5	0
19	k	1	Total 45	C 35	Mg 1	N 4	O 5	0
19	l	1	Total 50	C 40	Mg 1	N 4	O 5	0
19	l	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	l	1	Total 52	C 42	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 46	C 36	Mg 1	N 4	O 5	0
19	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
19	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	D	1	Total 55	C 45	Mg 1	N 4	O 5	0
19	D	1	Total 46	C 36	Mg 1	N 4	O 5	0

- Molecule 20 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



Mol	Chain	Residues	Atoms			AltConf
20	a	1	Total	C	O	0
			33	31	2	
20	b	1	Total	C	O	0
			33	31	2	

- Molecule 21 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



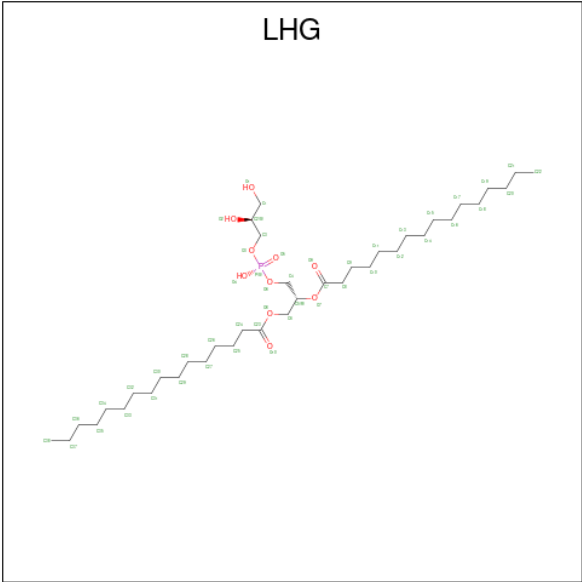
Mol	Chain	Residues	Atoms		AltConf
21	a	1	Total	C	0
			40	40	
21	a	1	Total	C	0
			40	40	

Continued on next page...

Continued from previous page...

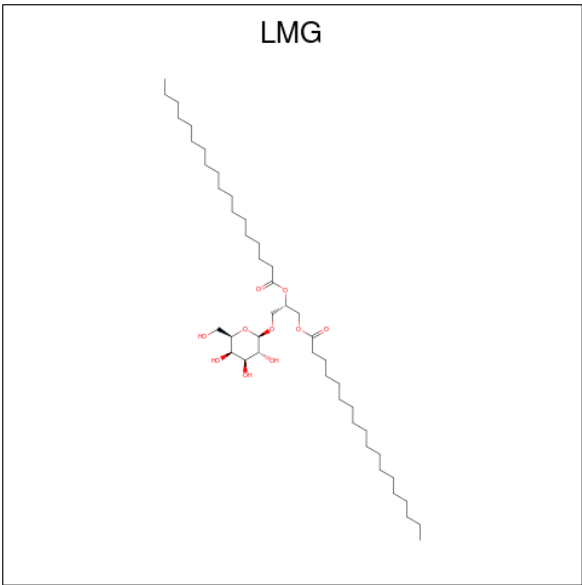
Mol	Chain	Residues	Atoms	AltConf
21	a	1	Total C 40 40	0
21	a	1	Total C 40 40	0
21	a	1	Total C 25 25	0
21	b	1	Total C 40 40	0
21	b	1	Total C 40 40	0
21	b	1	Total C 40 40	0
21	b	1	Total C 40 40	0
21	b	1	Total C 40 40	0
21	b	1	Total C 40 40	0
21	f	1	Total C 40 40	0
21	i	1	Total C 40 40	0
21	j	1	Total C 40 40	0
21	j	1	Total C 40 40	0
21	k	1	Total C 40 40	0
21	k	1	Total C 40 40	0
21	l	1	Total C 40 40	0
21	A	1	Total C 40 40	0

- Molecule 22 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



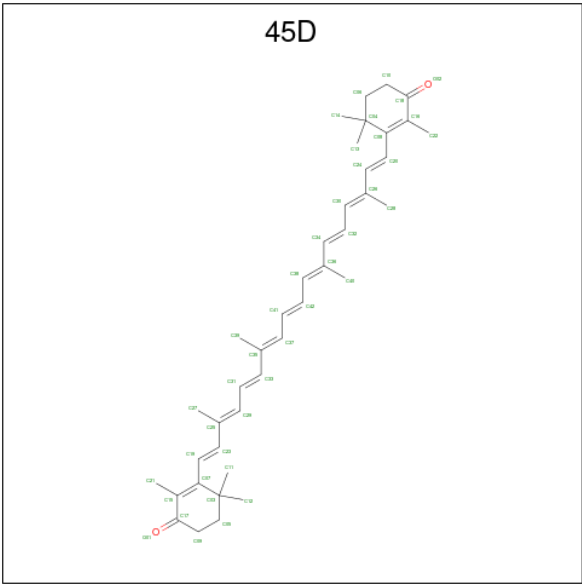
Mol	Chain	Residues	Atoms				AltConf
22	a	1	Total	C	O	P	0
			49	38	10	1	
22	a	1	Total	C	O	P	0
			49	38	10	1	
22	a	1	Total	C	O	P	0
			49	38	10	1	
22	b	1	Total	C	O	P	0
			38	27	10	1	
22	f	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 23 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀).



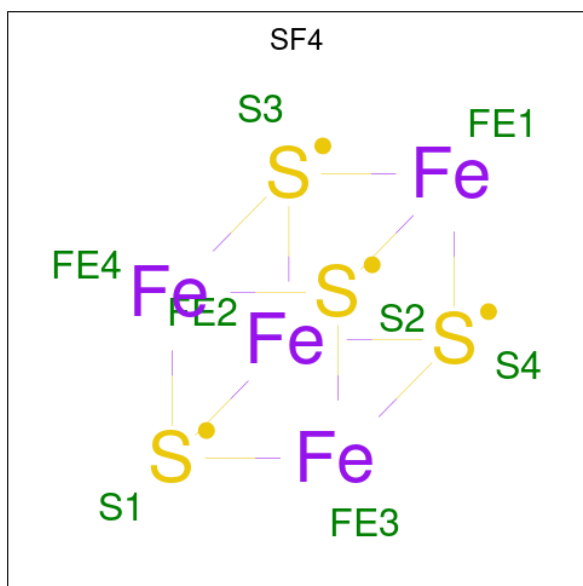
Mol	Chain	Residues	Atoms			AltConf
23	a	1	Total	C	O	0
			50	40	10	
23	a	1	Total	C	O	0
			40	30	10	
23	b	1	Total	C	O	0
			55	45	10	
23	b	1	Total	C	O	0
			55	45	10	

- Molecule 24 is beta,beta-carotene-4,4'-dione (CCD ID: 45D) (formula: C₄₀H₅₂O₂).



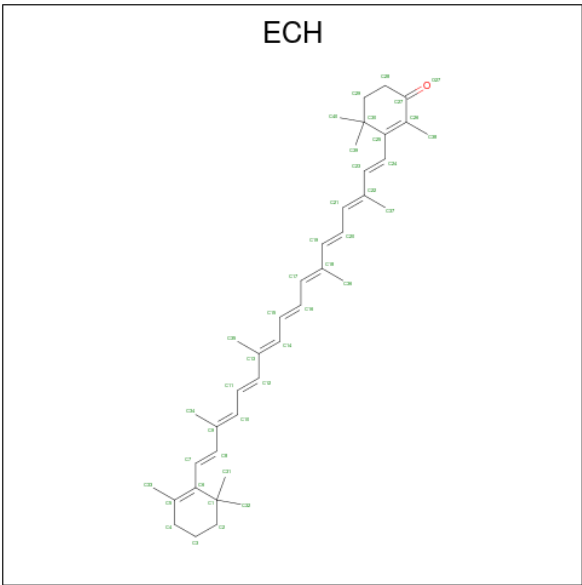
Mol	Chain	Residues	Atoms			AltConf
24	a	1	Total	C	O	0
			42	40	2	

- Molecule 25 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



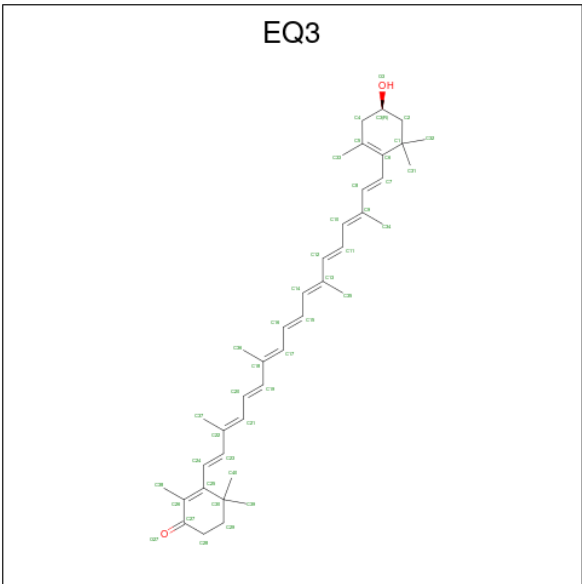
Mol	Chain	Residues	Atoms			AltConf
25	b	1	Total	Fe	S	0
			8	4	4	
25	c	1	Total	Fe	S	0
			8	4	4	
25	c	1	Total	Fe	S	0
			8	4	4	

- Molecule 26 is beta,beta-caroten-4-one (CCD ID: ECH) (formula: $\text{C}_{40}\text{H}_{54}\text{O}$).



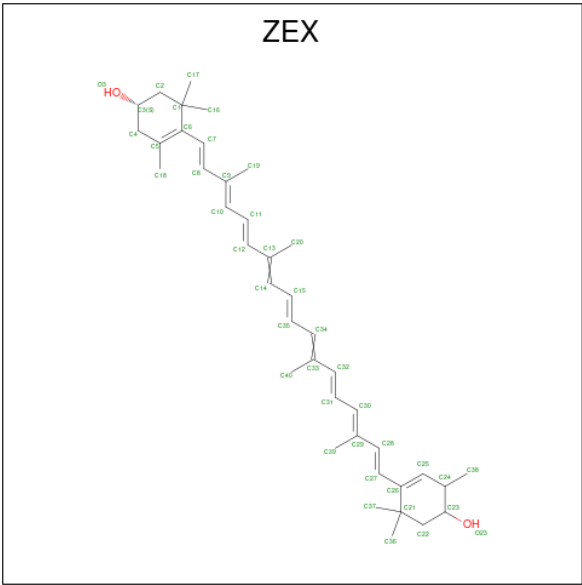
Mol	Chain	Residues	Atoms			AltConf
26	b	1	Total	C	O	0
			41	40	1	
26	m	1	Total	C	O	0
			41	40	1	

- Molecule 27 is (3'R)-3'-hydroxy-beta,beta-caroten-4-one (CCD ID: EQ3) (formula: C₄₀H₅₄O₂).



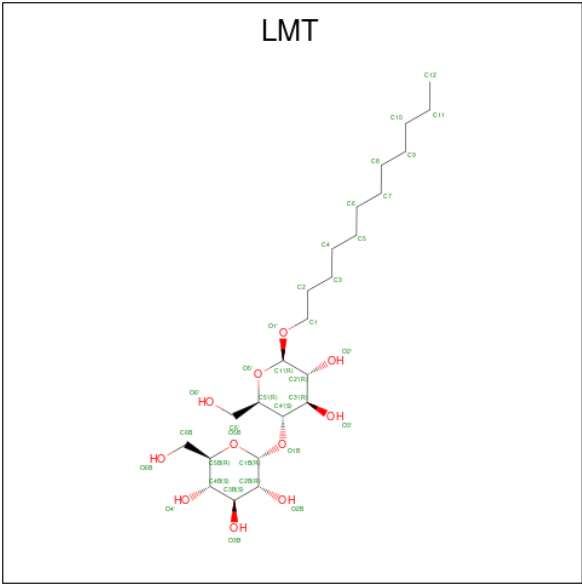
Mol	Chain	Residues	Atoms			AltConf
27	b	1	Total	C	O	0
			42	40	2	

- Molecule 28 is (1R,2S)-4-{(1E,3E,5E,7E,9E,11E,13E,15E,17E)-18-[(4S)-4-hydroxy-2,6,6-trimethylcyclohex-1-en-1-yl]-3,7,12,16-tetramethyloctadeca-1,3,5,7,9,11,13,15,17-nonaen-1-yl}-2,5,5-trimethylcyclohex-3-en-1-ol (CCD ID: ZEX) (formula: C₄₀H₅₆O₂).



Mol	Chain	Residues	Atoms			AltConf
28	b	1	Total	C	O	0
			42	40	2	
28	f	1	Total	C	O	0
			42	40	2	

- Molecule 29 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).

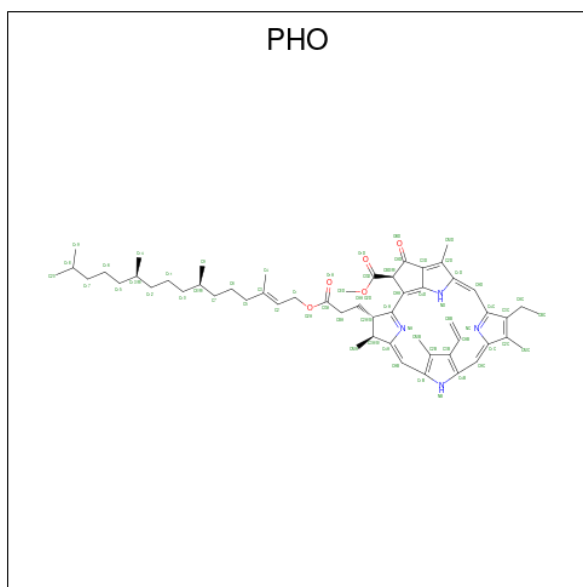


Mol	Chain	Residues	Atoms			AltConf
29	f	1	Total	C	O	0
			35	24	11	

- Molecule 30 is FE (II) ION (CCD ID: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms			AltConf
30	A	1	Total	Fe		0
			1	1		

- Molecule 31 is PHEOPHYTIN A (CCD ID: PHO) (formula: C₅₅H₇₄N₄O₅).



Mol	Chain	Residues	Atoms				AltConf
31	A	1	Total	C	N	O	0
			64	55	4	5	
31	D	1	Total	C	N	O	0
			64	55	4	5	

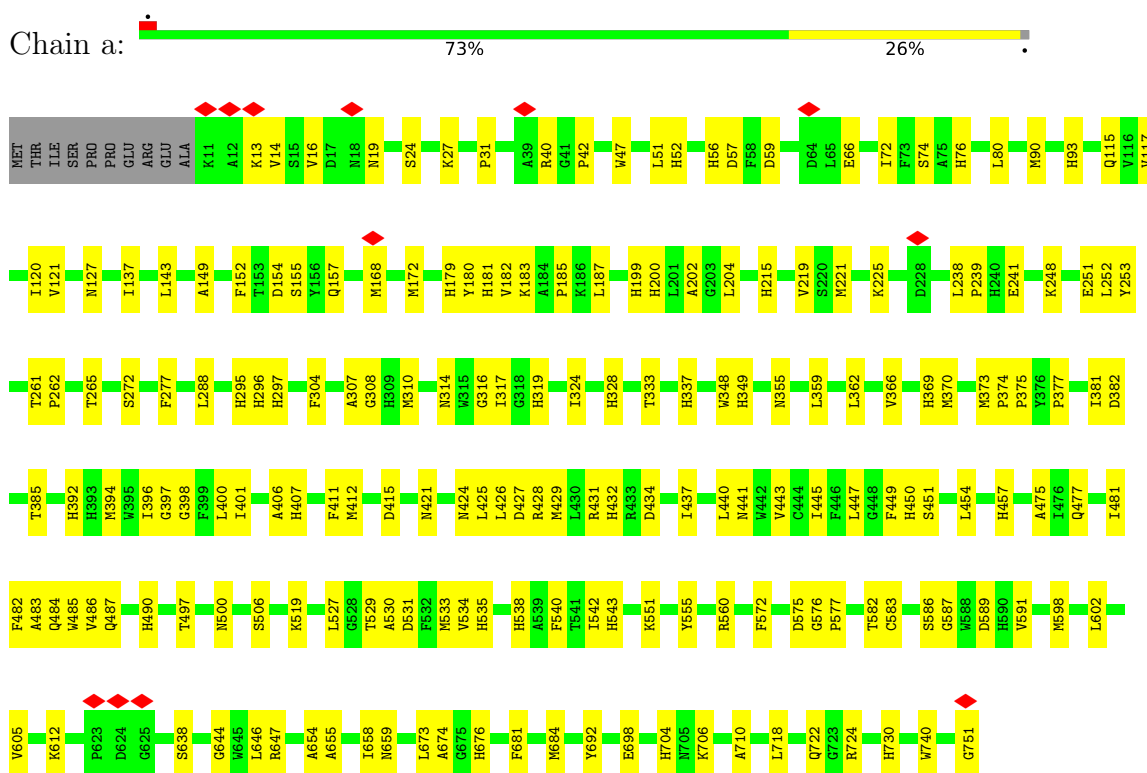
- Molecule 32 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: C₃₄H₃₂FeN₄O₄).



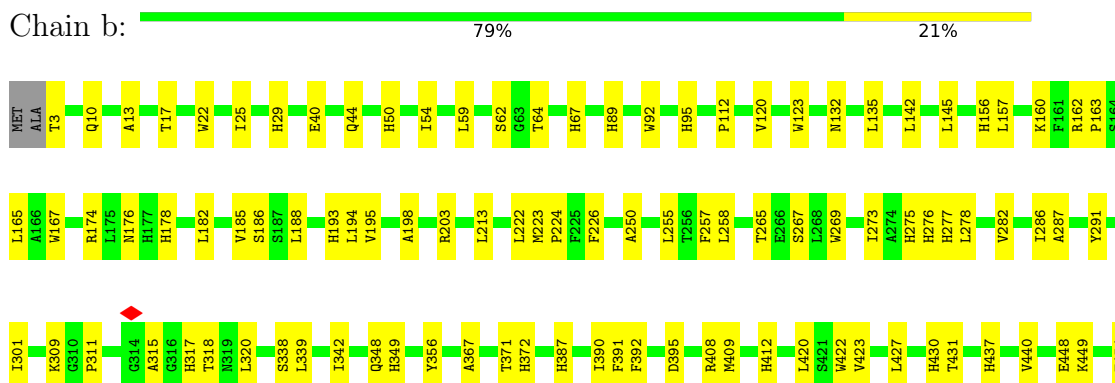
3 Residue-property plots

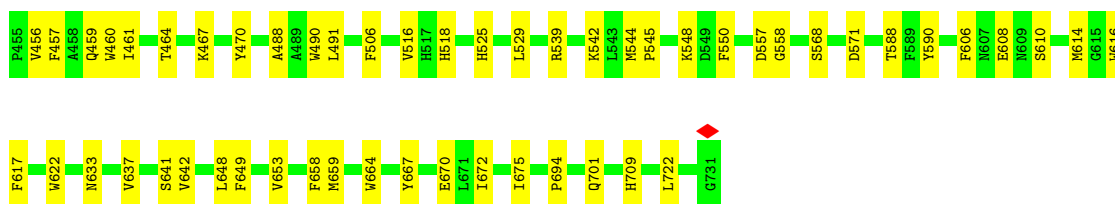
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

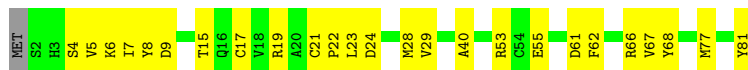


- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

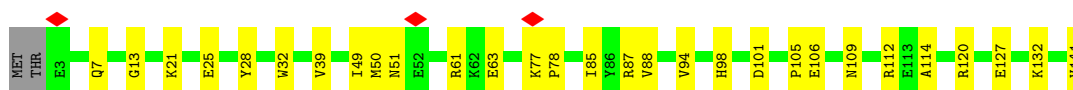
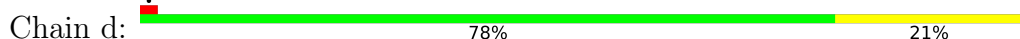




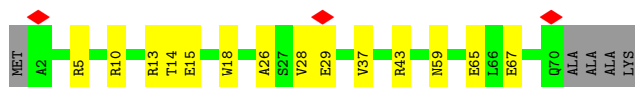
• Molecule 3: Photosystem I iron-sulfur center



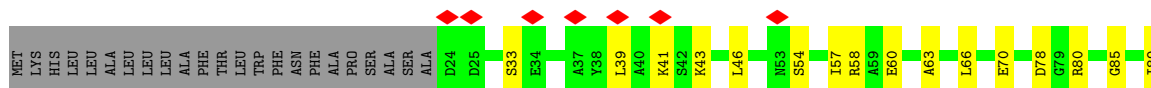
• Molecule 4: Photosystem I reaction center subunit II



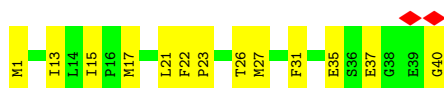
• Molecule 5: Photosystem I reaction center subunit IV



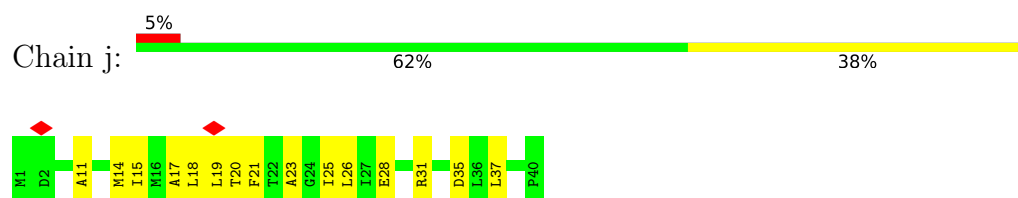
• Molecule 6: Photosystem I reaction center subunit III



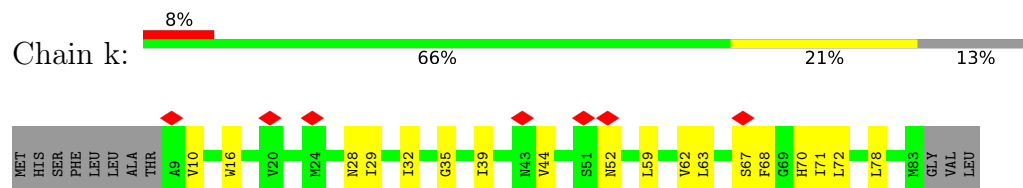
• Molecule 7: Photosystem I reaction center subunit VIII



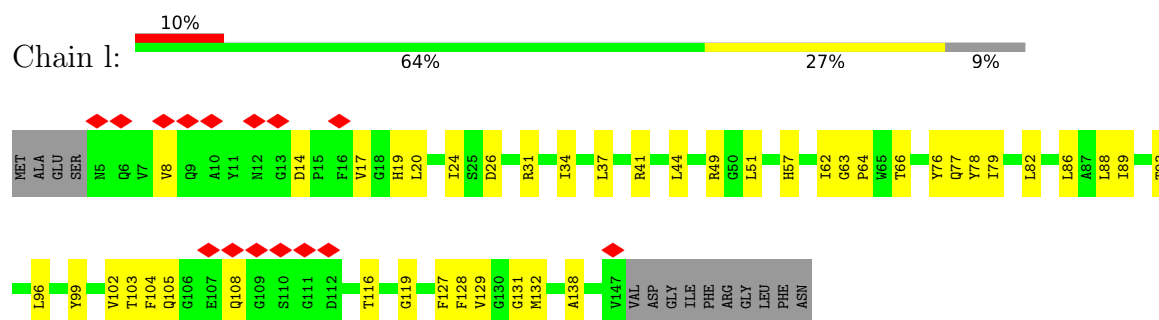
• Molecule 8: Photosystem I reaction center subunit IX



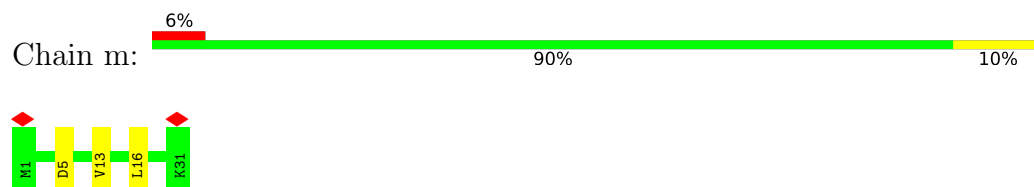
- Molecule 9: Photosystem I reaction center subunit PsaK 1



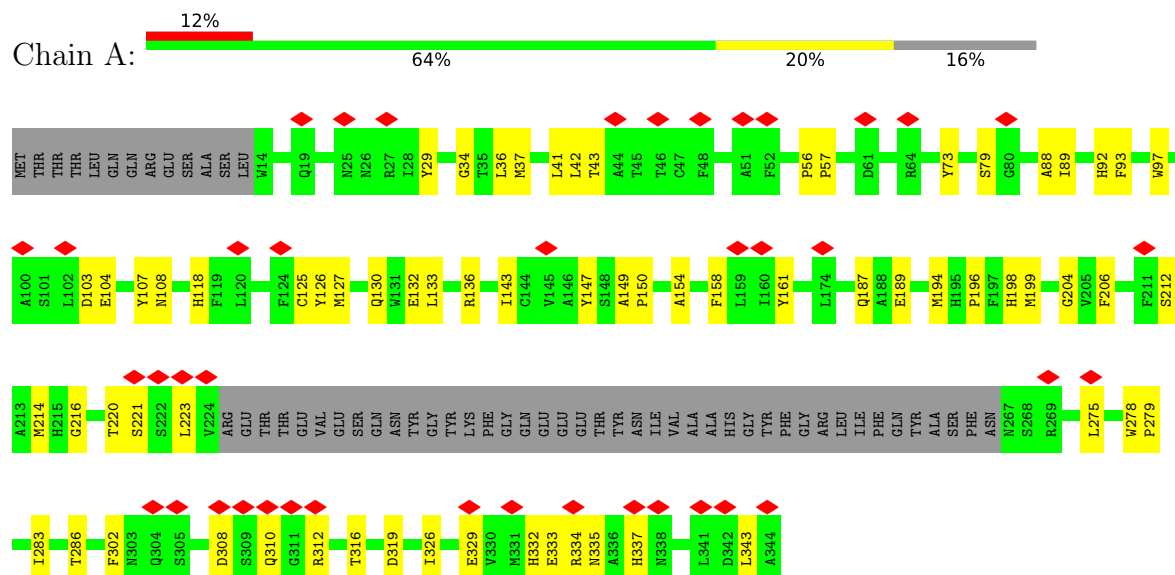
- Molecule 10: Photosystem I reaction center subunit XI

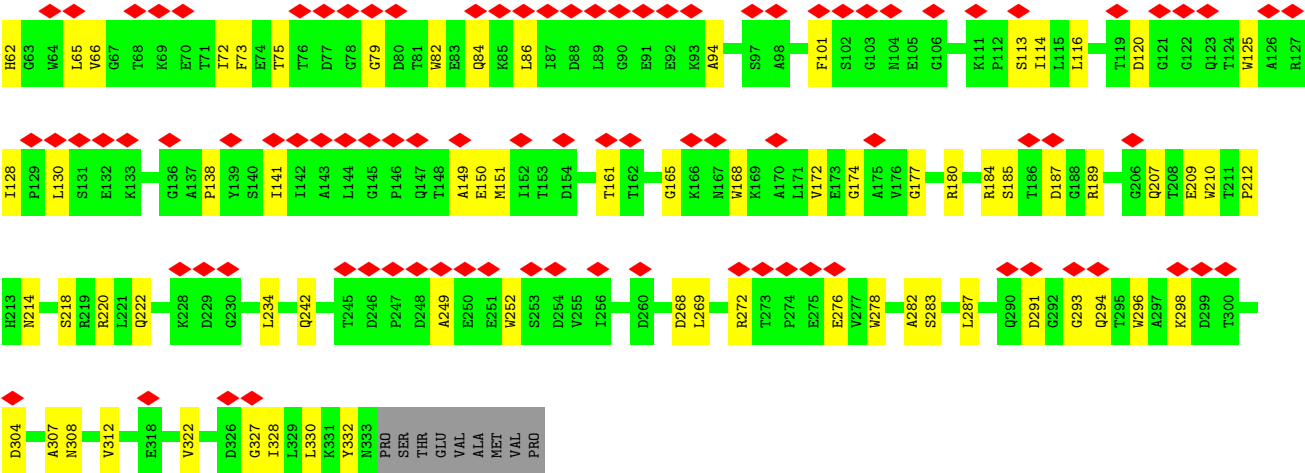


- Molecule 11: Photosystem I reaction center subunit XII



- Molecule 12: Photosystem II protein D1 2





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	178513	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	90.9	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	120000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.510	Depositor
Minimum map value	-0.112	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.0801	Depositor
Map size (Å)	488.0, 488.0, 488.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.22, 1.22, 1.22	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FE2, BCR, 45D, ZEX, PHO, LHG, HEM, CL0, LMG, SF4, LMT, CLA, EQ3, ECH, PQN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	a	0.19	0/5993	0.28	0/8169
2	b	0.18	0/5981	0.29	0/8178
3	c	0.18	0/610	0.36	0/826
4	d	0.15	0/1111	0.29	0/1497
5	e	0.15	0/547	0.33	0/741
6	f	0.14	0/1138	0.28	0/1546
7	i	0.16	0/322	0.36	0/438
8	j	0.14	0/328	0.29	0/443
9	k	0.13	0/535	0.27	0/726
10	l	0.15	0/1097	0.29	0/1493
11	m	0.15	0/241	0.21	0/326
12	A	0.13	0/2322	0.29	0/3169
13	D	0.12	0/2266	0.26	0/3086
14	E	0.14	0/374	0.32	0/513
15	F	0.19	0/228	0.46	0/309
16	I	0.12	0/216	0.29	0/293
17	S	0.11	0/2390	0.27	0/3258
All	All	0.16	0/25699	0.29	0/35011

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	a	5795	0	5653	182	0
2	b	5770	0	5547	143	0
3	c	600	0	581	21	0
4	d	1087	0	1082	22	0
5	e	538	0	514	9	0
6	f	1108	0	1100	31	0
7	i	311	0	304	12	0
8	j	319	0	328	13	0
9	k	524	0	547	17	0
10	l	1069	0	1044	34	0
11	m	238	0	260	2	0
12	A	2248	0	2170	52	0
13	D	2188	0	2129	57	0
14	E	360	0	352	15	0
15	F	222	0	230	10	0
16	I	211	0	227	4	0
17	S	2328	0	2227	54	0
18	a	65	0	72	4	0
19	A	161	0	144	10	0
19	D	166	0	154	14	0
19	a	2811	0	2986	226	0
19	b	2410	0	2456	160	0
19	f	165	0	150	7	0
19	j	101	0	82	6	0
19	k	91	0	66	4	0
19	l	167	0	154	6	0
20	a	33	0	46	1	0
20	b	33	0	46	1	0
21	A	40	0	56	2	0
21	a	185	0	257	19	0
21	b	200	0	280	21	0
21	f	40	0	56	5	0
21	i	40	0	56	2	0
21	j	80	0	112	10	0
21	k	80	0	112	6	0
21	l	40	0	56	4	0
22	a	147	0	222	11	0
22	b	38	0	49	2	0
22	f	49	0	74	6	0
23	a	90	0	123	5	0
23	b	110	0	172	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	a	42	0	52	5	0
25	b	8	0	0	0	0
25	c	16	0	0	2	0
26	b	41	0	54	5	0
26	m	41	0	54	4	0
27	b	42	0	0	0	0
28	b	42	0	56	3	0
28	f	42	0	56	0	0
29	f	35	0	45	4	0
30	A	1	0	0	0	0
31	A	64	0	74	5	0
31	D	64	0	74	5	0
32	F	43	0	30	4	0
All	All	32739	0	32771	910	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 14.

The worst 5 of 910 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)
1:a:392:HIS:HE1	19:a:829:CLA:ND	1.66	0.93
19:b:3020:CLA:HBB1	21:b:3043:BCR:H14C	1.56	0.88
2:b:156:HIS:HE1	19:b:3011:CLA:NC	1.72	0.86
13:D:186:GLN:HB2	19:D:403:CLA:HBC1	1.60	0.83
2:b:275:HIS:HE1	19:b:3016:CLA:ND	1.81	0.79

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	a	739/751 (98%)	711 (96%)	28 (4%)	0	100	100
2	b	727/731 (100%)	707 (97%)	20 (3%)	0	100	100
3	c	78/81 (96%)	73 (94%)	5 (6%)	0	100	100
4	d	137/141 (97%)	128 (93%)	9 (7%)	0	100	100
5	e	67/74 (90%)	64 (96%)	3 (4%)	0	100	100
6	f	140/165 (85%)	135 (96%)	5 (4%)	0	100	100
7	i	38/40 (95%)	38 (100%)	0	0	100	100
8	j	38/40 (95%)	38 (100%)	0	0	100	100
9	k	73/86 (85%)	72 (99%)	1 (1%)	0	100	100
10	l	141/157 (90%)	137 (97%)	4 (3%)	0	100	100
11	m	29/31 (94%)	29 (100%)	0	0	100	100
12	A	285/344 (83%)	273 (96%)	12 (4%)	0	100	100
13	D	274/336 (82%)	268 (98%)	6 (2%)	0	100	100
14	E	42/81 (52%)	42 (100%)	0	0	100	100
15	F	26/44 (59%)	24 (92%)	2 (8%)	0	100	100
16	I	25/38 (66%)	24 (96%)	1 (4%)	0	100	100
17	S	301/342 (88%)	295 (98%)	6 (2%)	0	100	100
All	All	3160/3482 (91%)	3058 (97%)	102 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	a	593/603 (98%)	593 (100%)	0	100	100
2	b	582/583 (100%)	582 (100%)	0	100	100
3	c	68/69 (99%)	68 (100%)	0	100	100
4	d	114/116 (98%)	114 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	e	57/60 (95%)	57 (100%)	0	100	100
6	f	119/137 (87%)	119 (100%)	0	100	100
7	i	32/32 (100%)	32 (100%)	0	100	100
8	j	35/35 (100%)	35 (100%)	0	100	100
9	k	53/62 (86%)	53 (100%)	0	100	100
10	l	107/118 (91%)	106 (99%)	1 (1%)	70	77
11	m	25/25 (100%)	25 (100%)	0	100	100
12	A	235/283 (83%)	235 (100%)	0	100	100
13	D	220/271 (81%)	220 (100%)	0	100	100
14	E	38/73 (52%)	38 (100%)	0	100	100
15	F	22/37 (60%)	22 (100%)	0	100	100
16	I	24/34 (71%)	24 (100%)	0	100	100
17	S	239/279 (86%)	239 (100%)	0	100	100
All	All	2563/2817 (91%)	2562 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	l	19	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
3	c	16	GLN
12	A	337	HIS
4	d	38	GLN
17	S	167	ASN
12	A	165	GLN

5.3.3 RNA ⓘ

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](#)

Of 145 ligands modelled in this entry, 1 is monoatomic - leaving 144 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
21	BCR	a	849	-	25,25,41	1.21	1 (4%)	33,33,56	1.34	5 (15%)
19	CLA	a	855	-	69,73,73	1.15	9 (13%)	82,113,113	1.21	6 (7%)
19	CLA	a	802	-	69,73,73	1.15	9 (13%)	82,113,113	1.28	7 (8%)
19	CLA	a	811	-	54,58,73	1.29	8 (14%)	64,95,113	1.48	6 (9%)
19	CLA	b	3004	-	69,73,73	1.16	9 (13%)	82,113,113	1.29	6 (7%)
19	CLA	b	3018	-	69,73,73	1.15	9 (13%)	82,113,113	1.27	7 (8%)
19	CLA	b	3019	-	64,68,73	1.19	8 (12%)	76,107,113	1.29	6 (7%)
19	CLA	a	818	-	69,73,73	1.13	8 (11%)	82,113,113	1.33	6 (7%)
21	BCR	l	1504	-	41,41,41	1.16	2 (4%)	56,56,56	1.29	9 (16%)
19	CLA	b	3014	-	69,73,73	1.15	8 (11%)	82,113,113	1.32	7 (8%)
19	CLA	b	3037	-	69,73,73	1.14	9 (13%)	82,113,113	1.28	6 (7%)
19	CLA	a	816	-	50,54,73	1.34	9 (18%)	59,90,113	1.42	4 (6%)
19	CLA	a	858	-	69,73,73	1.17	9 (13%)	82,113,113	1.25	5 (6%)
22	LHG	a	854	-	48,48,48	0.62	1 (2%)	51,54,54	1.27	6 (11%)
19	CLA	b	3012	-	54,58,73	1.29	9 (16%)	64,95,113	1.36	6 (9%)
19	CLA	a	827	-	69,73,73	1.16	9 (13%)	82,113,113	1.27	5 (6%)
19	CLA	b	3036	-	56,60,73	1.28	9 (16%)	65,97,113	1.38	8 (12%)
19	CLA	a	813	-	64,68,73	1.21	8 (12%)	76,107,113	1.27	4 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	LMG	b	3049	-	55,55,55	0.69	1 (1%)	63,63,63	1.40	8 (12%)
19	CLA	b	3003	-	69,73,73	1.15	9 (13%)	82,113,113	1.31	8 (9%)
19	CLA	f	201	-	69,73,73	1.16	8 (11%)	82,113,113	1.27	5 (6%)
19	CLA	b	3029	-	69,73,73	1.16	9 (13%)	82,113,113	1.36	7 (8%)
19	CLA	a	856	-	69,73,73	1.16	9 (13%)	82,113,113	1.26	4 (4%)
19	CLA	b	3011	-	60,64,73	1.23	9 (15%)	71,102,113	1.36	5 (7%)
25	SF4	c	101	3	0,12,12	-	-	-	-	-
19	CLA	a	804	-	69,73,73	1.15	9 (13%)	82,113,113	1.29	7 (8%)
19	CLA	a	815	-	69,73,73	1.16	9 (13%)	82,113,113	1.29	6 (7%)
19	CLA	a	838	-	55,59,73	1.29	8 (14%)	64,96,113	1.43	9 (14%)
19	CLA	k	4002	-	50,54,73	1.36	9 (18%)	59,90,113	1.39	4 (6%)
21	BCR	b	3048	-	41,41,41	1.14	2 (4%)	56,56,56	1.19	6 (10%)
19	CLA	b	3016	-	60,64,73	1.23	9 (15%)	71,102,113	1.32	5 (7%)
19	CLA	b	3008	-	69,73,73	1.14	9 (13%)	82,113,113	1.29	7 (8%)
21	BCR	a	848	-	41,41,41	1.23	3 (7%)	56,56,56	1.29	7 (12%)
19	CLA	a	840	-	69,73,73	1.16	8 (11%)	82,113,113	1.30	5 (6%)
19	CLA	a	806	-	69,73,73	1.14	9 (13%)	82,113,113	1.36	6 (7%)
19	CLA	a	829	-	69,73,73	1.15	9 (13%)	82,113,113	1.31	7 (8%)
19	CLA	a	834	-	69,73,73	1.15	8 (11%)	82,113,113	1.31	8 (9%)
18	CL0	a	801	-	58,73,73	2.19	12 (20%)	60,113,113	1.65	14 (23%)
19	CLA	b	3013	-	69,73,73	1.15	9 (13%)	82,113,113	1.36	7 (8%)
19	CLA	b	3006	-	69,73,73	1.15	8 (11%)	82,113,113	1.29	6 (7%)
32	HEM	F	101	15,14	50,50,50	1.38	8 (16%)	67,82,82	1.06	1 (1%)
19	CLA	a	842	-	69,73,73	1.16	9 (13%)	82,113,113	1.31	5 (6%)
19	CLA	a	833	-	64,68,73	1.20	9 (14%)	76,107,113	1.30	5 (6%)
19	CLA	b	3031	-	54,58,73	1.29	9 (16%)	64,95,113	1.36	7 (10%)
21	BCR	A	406	-	41,41,41	1.18	2 (4%)	56,56,56	1.24	7 (12%)
21	BCR	j	101	-	41,41,41	1.17	2 (4%)	56,56,56	1.28	7 (12%)
23	LMG	b	3051	-	55,55,55	0.76	1 (1%)	63,63,63	1.34	8 (12%)
19	CLA	b	3023	-	61,65,73	1.23	9 (14%)	72,103,113	1.31	6 (8%)
19	CLA	a	823	-	69,73,73	1.15	9 (13%)	82,113,113	1.27	6 (7%)
19	CLA	a	809	1	69,73,73	1.14	9 (13%)	82,113,113	1.30	6 (7%)
25	SF4	c	102	3	0,12,12	-	-	-	-	-
19	CLA	b	3041	22	50,54,73	1.33	8 (16%)	59,90,113	1.38	6 (10%)
19	CLA	b	3030	-	55,59,73	1.30	9 (16%)	64,96,113	1.36	5 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	BCR	a	846	-	41,41,41	1.19	3 (7%)	56,56,56	1.23	6 (10%)
19	CLA	a	808	-	69,73,73	1.15	9 (13%)	82,113,113	1.30	8 (9%)
19	CLA	a	822	-	69,73,73	1.16	9 (13%)	82,113,113	1.28	6 (7%)
19	CLA	b	3007	-	69,73,73	1.14	8 (11%)	82,113,113	1.26	6 (7%)
19	CLA	b	3021	-	64,68,73	1.20	8 (12%)	76,107,113	1.30	8 (10%)
19	CLA	l	1503	-	56,60,73	1.28	8 (14%)	65,97,113	1.40	5 (7%)
21	BCR	b	3047	-	41,41,41	1.22	3 (7%)	56,56,56	1.20	7 (12%)
19	CLA	b	3039	-	69,73,73	1.15	9 (13%)	82,113,113	1.30	6 (7%)
31	PHO	D	402	-	58,69,69	2.18	11 (18%)	55,99,99	1.53	8 (14%)
19	CLA	b	3038	-	54,58,73	1.30	8 (14%)	64,95,113	1.35	6 (9%)
19	CLA	a	805	-	69,73,73	1.16	9 (13%)	82,113,113	1.26	6 (7%)
19	CLA	j	102	8	59,63,73	1.26	8 (13%)	70,101,113	1.35	6 (8%)
19	CLA	D	404	-	50,54,73	1.35	8 (16%)	59,90,113	1.43	4 (6%)
19	CLA	b	3024	-	69,73,73	1.15	9 (13%)	82,113,113	1.29	7 (8%)
19	CLA	a	830	-	69,73,73	1.15	9 (13%)	82,113,113	1.23	5 (6%)
22	LHG	b	3050	19	37,37,48	0.71	1 (2%)	40,43,54	1.25	4 (10%)
27	EQ3	b	3052	-	43,43,43	1.40	6 (13%)	55,60,60	1.51	14 (25%)
31	PHO	A	404	-	58,69,69	2.13	10 (17%)	55,99,99	1.40	6 (10%)
20	PQN	a	844	-	34,34,34	0.37	0	43,45,45	0.59	1 (2%)
19	CLA	l	1502	-	69,73,73	1.14	9 (13%)	82,113,113	1.31	6 (7%)
22	LHG	a	850	-	48,48,48	0.64	1 (2%)	51,54,54	1.29	6 (11%)
21	BCR	k	4001	-	41,41,41	1.20	2 (4%)	56,56,56	1.30	6 (10%)
19	CLA	a	817	-	50,54,73	1.34	9 (18%)	59,90,113	1.43	4 (6%)
19	CLA	b	3017	-	69,73,73	1.16	8 (11%)	82,113,113	1.31	6 (7%)
19	CLA	a	810	1	55,59,73	1.29	8 (14%)	64,96,113	1.44	6 (9%)
19	CLA	b	3009	2	69,73,73	1.17	9 (13%)	82,113,113	1.28	6 (7%)
23	LMG	a	853	-	40,40,55	0.81	0	48,48,63	1.33	5 (10%)
19	CLA	D	401	-	69,73,73	1.16	8 (11%)	82,113,113	1.26	4 (4%)
19	CLA	a	807	-	69,73,73	1.15	9 (13%)	82,113,113	1.29	6 (7%)
19	CLA	k	4003	9	49,53,73	1.38	8 (16%)	58,89,113	1.40	5 (8%)
24	45D	a	857	-	43,43,43	1.43	9 (20%)	54,60,60	1.54	10 (18%)
21	BCR	i	101	-	41,41,41	1.20	2 (4%)	56,56,56	1.22	5 (8%)
21	BCR	k	4004	-	41,41,41	1.16	2 (4%)	56,56,56	1.27	7 (12%)
26	ECH	b	3045	-	42,42,42	1.41	8 (19%)	55,58,58	2.22	16 (29%)
21	BCR	b	3044	-	41,41,41	1.17	3 (7%)	56,56,56	1.22	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	a	831	-	69,73,73	1.14	8 (11%)	82,113,113	1.38	8 (9%)
28	ZEX	f	205	-	43,43,43	1.34	8 (18%)	51,60,60	1.40	9 (17%)
29	LMT	f	207	-	36,36,36	1.16	6 (16%)	47,47,47	1.04	3 (6%)
19	CLA	b	3025	-	59,63,73	1.24	9 (15%)	70,101,113	1.35	6 (8%)
19	CLA	a	826	-	69,73,73	1.16	9 (13%)	82,113,113	1.30	8 (9%)
19	CLA	a	835	-	69,73,73	1.15	9 (13%)	82,113,113	1.34	6 (7%)
19	CLA	a	841	-	69,73,73	1.14	9 (13%)	82,113,113	1.30	5 (6%)
19	CLA	b	3032	-	69,73,73	1.17	9 (13%)	82,113,113	1.24	4 (4%)
19	CLA	a	824	-	69,73,73	1.16	9 (13%)	82,113,113	1.30	4 (4%)
21	BCR	b	3046	-	41,41,41	1.16	2 (4%)	56,56,56	1.27	7 (12%)
19	CLA	b	3015	-	59,63,73	1.26	9 (15%)	70,101,113	1.36	6 (8%)
19	CLA	D	403	-	59,63,73	1.24	8 (13%)	70,101,113	1.35	6 (8%)
22	LHG	a	852	19	48,48,48	0.61	1 (2%)	51,54,54	1.30	6 (11%)
19	CLA	b	3027	-	69,73,73	1.14	9 (13%)	82,113,113	1.27	5 (6%)
19	CLA	b	3033	-	69,73,73	1.16	9 (13%)	82,113,113	1.29	6 (7%)
19	CLA	a	821	-	69,73,73	1.17	9 (13%)	82,113,113	1.27	5 (6%)
19	CLA	a	803	-	69,73,73	1.14	9 (13%)	82,113,113	1.30	5 (6%)
19	CLA	f	204	6	54,58,73	1.32	9 (16%)	64,95,113	1.40	7 (10%)
28	ZEX	b	3053	-	43,43,43	1.35	7 (16%)	51,60,60	1.48	10 (19%)
19	CLA	a	836	-	69,73,73	1.15	9 (13%)	82,113,113	1.29	6 (7%)
22	LHG	f	206	-	48,48,48	0.57	0	51,54,54	1.28	6 (11%)
19	CLA	b	3020	-	69,73,73	1.16	9 (13%)	82,113,113	1.25	5 (6%)
19	CLA	a	839	-	69,73,73	1.15	9 (13%)	82,113,113	1.25	6 (7%)
19	CLA	b	3026	-	69,73,73	1.16	9 (13%)	82,113,113	1.27	6 (7%)
19	CLA	b	3002	-	69,73,73	1.16	9 (13%)	82,113,113	1.22	4 (4%)
19	CLA	a	825	-	64,68,73	1.20	9 (14%)	76,107,113	1.33	5 (6%)
19	CLA	A	405	-	54,58,73	1.31	7 (12%)	64,95,113	1.38	5 (7%)
23	LMG	a	851	-	50,50,55	0.76	1 (2%)	58,58,63	1.34	8 (13%)
19	CLA	b	3028	-	69,73,73	1.15	9 (13%)	82,113,113	1.22	4 (4%)
19	CLA	A	402	-	69,73,73	1.16	9 (13%)	82,113,113	1.27	5 (6%)
25	SF4	b	3001	2,1	0,12,12	-	-	-	-	-
21	BCR	a	847	-	41,41,41	1.20	3 (7%)	56,56,56	1.23	6 (10%)
19	CLA	a	820	-	69,73,73	1.15	9 (13%)	82,113,113	1.26	7 (8%)
19	CLA	b	3034	-	69,73,73	1.15	8 (11%)	82,113,113	1.27	7 (8%)
19	CLA	A	403	-	50,54,73	1.34	9 (18%)	59,90,113	1.43	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	BCR	j	104	-	41,41,41	1.21	3 (7%)	56,56,56	1.24	7 (12%)
19	CLA	a	832	-	60,64,73	1.23	8 (13%)	71,102,113	1.34	4 (5%)
19	CLA	j	103	-	50,54,73	1.36	6 (12%)	59,90,113	1.32	5 (8%)
21	BCR	f	202	-	41,41,41	1.21	3 (7%)	56,56,56	1.20	5 (8%)
19	CLA	b	3022	-	50,54,73	1.34	9 (18%)	59,90,113	1.41	4 (6%)
19	CLA	b	3005	-	69,73,73	1.15	9 (13%)	82,113,113	1.32	7 (8%)
20	PQN	b	3042	-	34,34,34	0.40	0	43,45,45	0.55	1 (2%)
26	ECH	m	101	-	42,42,42	1.47	9 (21%)	55,58,58	1.64	14 (25%)
19	CLA	b	3040	-	69,73,73	1.16	8 (11%)	82,113,113	1.31	5 (6%)
19	CLA	b	3035	-	54,58,73	1.32	8 (14%)	64,95,113	1.42	6 (9%)
19	CLA	a	814	-	69,73,73	1.15	9 (13%)	82,113,113	1.32	8 (9%)
19	CLA	b	3010	-	60,64,73	1.25	9 (15%)	71,102,113	1.31	5 (7%)
21	BCR	b	3043	-	41,41,41	1.25	3 (7%)	56,56,56	1.27	6 (10%)
19	CLA	a	828	-	69,73,73	1.16	9 (13%)	82,113,113	1.30	6 (7%)
19	CLA	f	203	-	54,58,73	1.30	8 (14%)	64,95,113	1.39	7 (10%)
19	CLA	l	1501	-	54,58,73	1.33	7 (12%)	64,95,113	1.42	6 (9%)
19	CLA	a	843	22	60,64,73	1.23	9 (15%)	71,102,113	1.33	7 (9%)
19	CLA	a	837	1	69,73,73	1.16	8 (11%)	82,113,113	1.28	6 (7%)
19	CLA	a	819	-	69,73,73	1.16	9 (13%)	82,113,113	1.25	5 (6%)
19	CLA	a	812	-	69,73,73	1.15	9 (13%)	82,113,113	1.25	7 (8%)
21	BCR	a	845	-	41,41,41	1.21	3 (7%)	56,56,56	1.23	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
21	BCR	a	849	-	-	3/18/35/63	0/1/1/2
19	CLA	a	855	-	1/1/15/20	8/39/115/115	-
19	CLA	a	802	-	1/1/15/20	15/39/115/115	-
19	CLA	a	811	-	1/1/12/20	9/21/97/115	-
19	CLA	b	3004	-	1/1/15/20	14/39/115/115	-
19	CLA	b	3018	-	1/1/15/20	9/39/115/115	-
19	CLA	b	3019	-	1/1/14/20	8/33/109/115	-
19	CLA	a	818	-	1/1/15/20	10/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	BCR	l	1504	-	-	11/29/63/63	0/2/2/2
19	CLA	b	3014	-	1/1/15/20	16/39/115/115	-
19	CLA	b	3037	-	1/1/15/20	13/39/115/115	-
19	CLA	a	816	-	1/1/11/20	7/17/93/115	-
19	CLA	a	858	-	1/1/15/20	13/39/115/115	-
22	LHG	a	854	-	-	24/53/53/53	-
19	CLA	b	3012	-	1/1/12/20	5/21/97/115	-
19	CLA	a	827	-	1/1/15/20	12/39/115/115	-
19	CLA	b	3036	-	1/1/12/20	6/24/100/115	-
19	CLA	a	813	-	1/1/14/20	13/33/109/115	-
23	LMG	b	3049	-	-	27/50/70/70	0/1/1/1
19	CLA	b	3003	-	1/1/15/20	18/39/115/115	-
19	CLA	f	201	-	1/1/15/20	20/39/115/115	-
19	CLA	b	3029	-	1/1/15/20	15/39/115/115	-
19	CLA	a	856	-	1/1/15/20	17/39/115/115	-
19	CLA	b	3011	-	1/1/13/20	10/29/105/115	-
25	SF4	c	101	3	-	-	0/6/5/5
19	CLA	a	804	-	1/1/15/20	7/39/115/115	-
19	CLA	a	815	-	1/1/15/20	10/39/115/115	-
19	CLA	a	838	-	-	4/23/99/115	-
19	CLA	k	4002	-	1/1/11/20	7/17/93/115	-
21	BCR	b	3048	-	-	17/29/63/63	0/2/2/2
19	CLA	b	3016	-	1/1/13/20	8/29/105/115	-
19	CLA	b	3008	-	1/1/15/20	11/39/115/115	-
21	BCR	a	848	-	-	7/29/63/63	0/2/2/2
19	CLA	a	840	-	1/1/15/20	12/39/115/115	-
19	CLA	a	806	-	1/1/15/20	9/39/115/115	-
19	CLA	a	829	-	1/1/15/20	7/39/115/115	-
19	CLA	a	834	-	1/1/15/20	7/39/115/115	-
18	CL0	a	801	-	3/3/20/25	10/37/135/135	-
19	CLA	b	3013	-	1/1/15/20	21/39/115/115	-
19	CLA	b	3006	-	1/1/15/20	11/39/115/115	-
32	HEM	F	101	15,14	-	5/14/54/54	-
19	CLA	a	842	-	1/1/15/20	16/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	a	833	-	1/1/14/20	14/33/109/115	-
19	CLA	b	3031	-	1/1/12/20	5/21/97/115	-
21	BCR	A	406	-	-	8/29/63/63	0/2/2/2
21	BCR	j	101	-	-	6/29/63/63	0/2/2/2
23	LMG	b	3051	-	-	29/50/70/70	0/1/1/1
19	CLA	b	3023	-	1/1/13/20	9/30/106/115	-
19	CLA	a	823	-	1/1/15/20	13/39/115/115	-
19	CLA	a	809	1	1/1/15/20	18/39/115/115	-
25	SF4	c	102	3	-	-	0/6/5/5
19	CLA	b	3041	22	1/1/11/20	9/17/93/115	-
19	CLA	b	3030	-	1/1/12/20	9/23/99/115	-
21	BCR	a	846	-	-	5/29/63/63	0/2/2/2
19	CLA	a	808	-	1/1/15/20	13/39/115/115	-
19	CLA	a	822	-	1/1/15/20	12/39/115/115	-
19	CLA	b	3007	-	1/1/15/20	16/39/115/115	-
19	CLA	b	3021	-	1/1/14/20	9/33/109/115	-
19	CLA	l	1503	-	1/1/12/20	7/24/100/115	-
21	BCR	b	3047	-	-	5/29/63/63	0/2/2/2
19	CLA	b	3039	-	1/1/15/20	16/39/115/115	-
31	PHO	D	402	-	-	9/37/103/103	0/5/6/6
19	CLA	b	3038	-	1/1/12/20	6/21/97/115	-
19	CLA	a	805	-	1/1/15/20	11/39/115/115	-
19	CLA	j	102	8	1/1/13/20	10/27/103/115	-
19	CLA	D	404	-	1/1/11/20	5/17/93/115	-
19	CLA	b	3024	-	1/1/15/20	10/39/115/115	-
19	CLA	a	830	-	1/1/15/20	16/39/115/115	-
22	LHG	b	3050	19	-	19/42/42/53	-
27	EQ3	b	3052	-	-	3/29/68/68	0/2/2/2
31	PHO	A	404	-	-	11/37/103/103	0/5/6/6
20	PQN	a	844	-	-	1/23/43/43	0/2/2/2
19	CLA	l	1502	-	1/1/15/20	11/39/115/115	-
22	LHG	a	850	-	-	27/53/53/53	-
21	BCR	k	4001	-	-	8/29/63/63	0/2/2/2
19	CLA	a	817	-	1/1/11/20	7/17/93/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	b	3017	-	1/1/15/20	12/39/115/115	-
19	CLA	a	810	1	1/1/12/20	3/23/99/115	-
19	CLA	b	3009	2	1/1/15/20	14/39/115/115	-
23	LMG	a	853	-	-	14/35/55/70	0/1/1/1
19	CLA	D	401	-	1/1/15/20	15/39/115/115	-
19	CLA	a	807	-	1/1/15/20	14/39/115/115	-
19	CLA	k	4003	9	1/1/11/20	6/15/91/115	-
24	45D	a	857	-	-	4/29/69/69	0/2/2/2
21	BCR	i	101	-	-	6/29/63/63	0/2/2/2
21	BCR	k	4004	-	-	5/29/63/63	0/2/2/2
26	ECH	b	3045	-	-	9/29/66/66	0/2/2/2
21	BCR	b	3044	-	-	7/29/63/63	0/2/2/2
19	CLA	a	831	-	1/1/15/20	17/39/115/115	-
28	ZEX	f	205	-	-	6/29/67/67	0/2/2/2
29	LMT	f	207	-	-	15/21/61/61	0/2/2/2
19	CLA	b	3025	-	1/1/13/20	7/27/103/115	-
19	CLA	a	826	-	1/1/15/20	15/39/115/115	-
19	CLA	a	835	-	1/1/15/20	14/39/115/115	-
19	CLA	a	841	-	1/1/15/20	12/39/115/115	-
19	CLA	b	3032	-	1/1/15/20	7/39/115/115	-
19	CLA	a	824	-	1/1/15/20	17/39/115/115	-
21	BCR	b	3046	-	-	4/29/63/63	0/2/2/2
19	CLA	b	3015	-	1/1/13/20	11/27/103/115	-
19	CLA	D	403	-	1/1/13/20	10/27/103/115	-
22	LHG	a	852	19	-	21/53/53/53	-
19	CLA	b	3027	-	1/1/15/20	11/39/115/115	-
19	CLA	b	3033	-	1/1/15/20	18/39/115/115	-
19	CLA	a	821	-	1/1/15/20	20/39/115/115	-
19	CLA	a	803	-	1/1/15/20	9/39/115/115	-
19	CLA	f	204	6	1/1/12/20	7/21/97/115	-
28	ZEX	b	3053	-	-	4/29/67/67	0/2/2/2
19	CLA	a	836	-	1/1/15/20	12/39/115/115	-
22	LHG	f	206	-	-	28/53/53/53	-
19	CLA	b	3020	-	1/1/15/20	17/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	a	839	-	1/1/15/20	12/39/115/115	-
19	CLA	b	3026	-	1/1/15/20	7/39/115/115	-
19	CLA	b	3002	-	1/1/15/20	13/39/115/115	-
19	CLA	a	825	-	1/1/14/20	11/33/109/115	-
19	CLA	A	405	-	1/1/12/20	5/21/97/115	-
23	LMG	a	851	-	-	27/45/65/70	0/1/1/1
19	CLA	b	3028	-	1/1/15/20	11/39/115/115	-
19	CLA	A	402	-	1/1/15/20	16/39/115/115	-
25	SF4	b	3001	2,1	-	-	0/6/5/5
21	BCR	a	847	-	-	4/29/63/63	0/2/2/2
19	CLA	a	820	-	1/1/15/20	15/39/115/115	-
19	CLA	b	3034	-	1/1/15/20	12/39/115/115	-
19	CLA	A	403	-	1/1/11/20	6/17/93/115	-
21	BCR	j	104	-	-	8/29/63/63	0/2/2/2
19	CLA	a	832	-	1/1/13/20	15/29/105/115	-
19	CLA	j	103	-	1/1/11/20	5/17/93/115	-
21	BCR	f	202	-	-	15/29/63/63	0/2/2/2
19	CLA	b	3022	-	1/1/11/20	3/17/93/115	-
19	CLA	b	3005	-	1/1/15/20	16/39/115/115	-
20	PQN	b	3042	-	-	0/23/43/43	0/2/2/2
26	ECH	m	101	-	-	2/29/66/66	0/2/2/2
19	CLA	b	3040	-	1/1/15/20	8/39/115/115	-
19	CLA	b	3035	-	1/1/12/20	9/21/97/115	-
19	CLA	a	814	-	-	15/39/115/115	-
19	CLA	b	3010	-	1/1/13/20	7/29/105/115	-
21	BCR	b	3043	-	-	10/29/63/63	0/2/2/2
19	CLA	a	828	-	1/1/15/20	17/39/115/115	-
19	CLA	f	203	-	1/1/12/20	4/21/97/115	-
19	CLA	l	1501	-	1/1/12/20	8/21/97/115	-
19	CLA	a	843	22	1/1/13/20	7/29/105/115	-
19	CLA	a	837	1	1/1/15/20	9/39/115/115	-
19	CLA	a	819	-	1/1/15/20	22/39/115/115	-
19	CLA	a	812	-	1/1/15/20	13/39/115/115	-
21	BCR	a	845	-	-	9/29/63/63	0/2/2/2

The worst 5 of 1018 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	D	402	PHO	C1B-C2B	9.73	1.50	1.39
31	A	404	PHO	C1B-C2B	9.52	1.50	1.39
18	a	801	CL0	C1B-C2B	8.71	1.49	1.39
31	D	402	PHO	C3B-C4B	8.62	1.50	1.41
31	A	404	PHO	C3B-C4B	8.32	1.49	1.41

The worst 5 of 869 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	b	3045	ECH	C15-C16-C17	8.17	140.25	123.52
19	a	818	CLA	C4A-NA-C1A	7.42	110.07	106.68
19	a	840	CLA	C4A-NA-C1A	7.32	110.02	106.68
19	a	842	CLA	C4A-NA-C1A	7.30	110.01	106.68
19	a	806	CLA	C4A-NA-C1A	7.29	110.00	106.68

5 of 102 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
18	a	801	CL0	NC
18	a	801	CL0	NA
18	a	801	CL0	ND
19	a	802	CLA	ND
19	a	803	CLA	ND

5 of 1561 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	a	802	CLA	CBD-CGD-O2D-CED
19	a	803	CLA	CBA-CGA-O2A-C1
19	a	803	CLA	O1A-CGA-O2A-C1
19	a	805	CLA	C1A-C2A-CAA-CBA
19	a	805	CLA	C3A-C2A-CAA-CBA

There are no ring outliers.

137 monomers are involved in 516 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	a	855	CLA	1	0
19	a	802	CLA	3	0
19	a	811	CLA	4	0
19	b	3004	CLA	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	b	3018	CLA	6	0
19	b	3019	CLA	3	0
19	a	818	CLA	8	0
21	l	1504	BCR	4	0
19	b	3014	CLA	6	0
19	b	3037	CLA	6	0
19	a	858	CLA	3	0
22	a	854	LHG	5	0
19	b	3012	CLA	1	0
19	a	827	CLA	8	0
19	a	813	CLA	4	0
23	b	3049	LMG	5	0
19	b	3003	CLA	14	0
19	f	201	CLA	5	0
19	b	3029	CLA	11	0
19	a	856	CLA	3	0
19	b	3011	CLA	3	0
25	c	101	SF4	1	0
19	a	804	CLA	5	0
19	a	815	CLA	13	0
19	a	838	CLA	7	0
19	k	4002	CLA	3	0
21	b	3048	BCR	6	0
19	b	3016	CLA	4	0
19	b	3008	CLA	8	0
21	a	848	BCR	3	0
19	a	840	CLA	7	0
19	a	806	CLA	10	0
19	a	829	CLA	13	0
19	a	834	CLA	6	0
18	a	801	CL0	4	0
19	b	3013	CLA	4	0
19	b	3006	CLA	1	0
32	F	101	HEM	4	0
19	a	842	CLA	9	0
19	a	833	CLA	4	0
19	b	3031	CLA	1	0
21	A	406	BCR	2	0
21	j	101	BCR	5	0
23	b	3051	LMG	1	0
19	b	3023	CLA	4	0
19	a	823	CLA	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	a	809	CLA	8	0
25	c	102	SF4	1	0
19	b	3041	CLA	1	0
19	b	3030	CLA	7	0
21	a	846	BCR	4	0
19	a	808	CLA	6	0
19	a	822	CLA	9	0
19	b	3007	CLA	4	0
19	b	3021	CLA	1	0
21	b	3047	BCR	4	0
19	b	3039	CLA	1	0
31	D	402	PHO	5	0
19	b	3038	CLA	3	0
19	a	805	CLA	4	0
19	j	102	CLA	2	0
19	D	404	CLA	3	0
19	b	3024	CLA	5	0
19	a	830	CLA	3	0
22	b	3050	LHG	2	0
31	A	404	PHO	5	0
20	a	844	PQN	1	0
19	l	1502	CLA	5	0
22	a	850	LHG	1	0
21	k	4001	BCR	5	0
19	a	817	CLA	2	0
19	b	3017	CLA	12	0
19	a	810	CLA	2	0
19	b	3009	CLA	3	0
23	a	853	LMG	3	0
19	D	401	CLA	4	0
19	a	807	CLA	2	0
19	k	4003	CLA	1	0
24	a	857	45D	5	0
21	i	101	BCR	2	0
21	k	4004	BCR	1	0
26	b	3045	ECH	5	0
21	b	3044	BCR	4	0
19	a	831	CLA	9	0
29	f	207	LMT	4	0
19	b	3025	CLA	5	0
19	a	826	CLA	3	0
19	a	835	CLA	6	0

Continued on next page...

Continued from previous page...

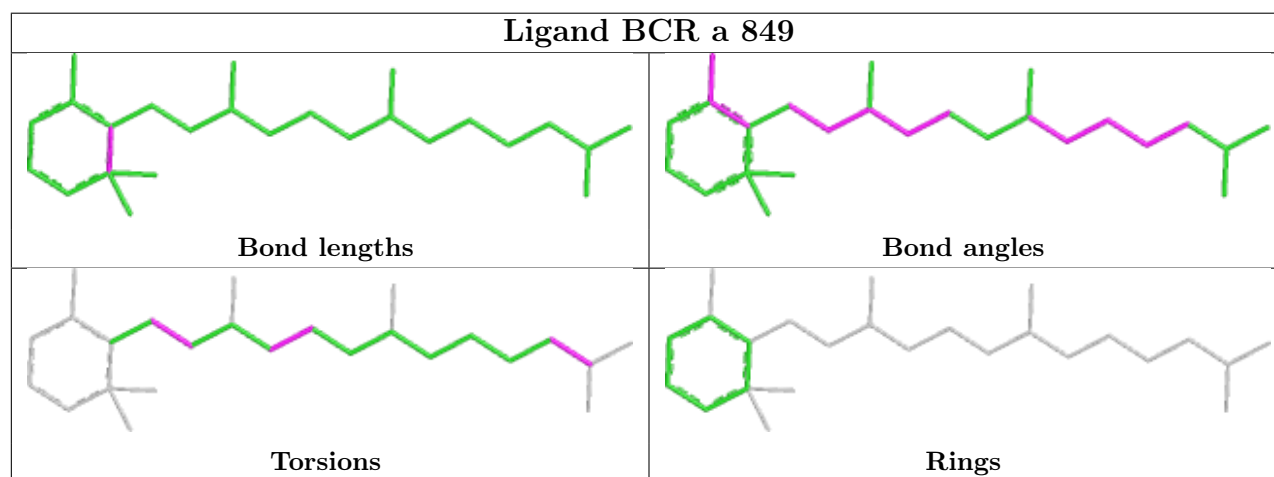
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	a	841	CLA	8	0
19	b	3032	CLA	4	0
19	a	824	CLA	7	0
21	b	3046	BCR	6	0
19	b	3015	CLA	7	0
19	D	403	CLA	7	0
22	a	852	LHG	5	0
19	b	3027	CLA	9	0
19	b	3033	CLA	8	0
19	a	821	CLA	5	0
19	a	803	CLA	5	0
19	f	204	CLA	1	0
28	b	3053	ZEX	3	0
19	a	836	CLA	6	0
22	f	206	LHG	6	0
19	b	3020	CLA	4	0
19	a	839	CLA	2	0
19	b	3026	CLA	7	0
19	b	3002	CLA	1	0
19	a	825	CLA	4	0
19	A	405	CLA	3	0
23	a	851	LMG	2	0
19	b	3028	CLA	3	0
19	A	402	CLA	5	0
21	a	847	BCR	2	0
19	a	820	CLA	2	0
19	b	3034	CLA	4	0
19	A	403	CLA	2	0
21	j	104	BCR	5	0
19	a	832	CLA	6	0
19	j	103	CLA	4	0
21	f	202	BCR	5	0
19	b	3022	CLA	1	0
19	b	3005	CLA	5	0
20	b	3042	PQN	1	0
26	m	101	ECH	4	0
19	b	3040	CLA	5	0
19	b	3035	CLA	2	0
19	a	814	CLA	6	0
19	b	3010	CLA	2	0
21	b	3043	BCR	3	0
19	a	828	CLA	6	0

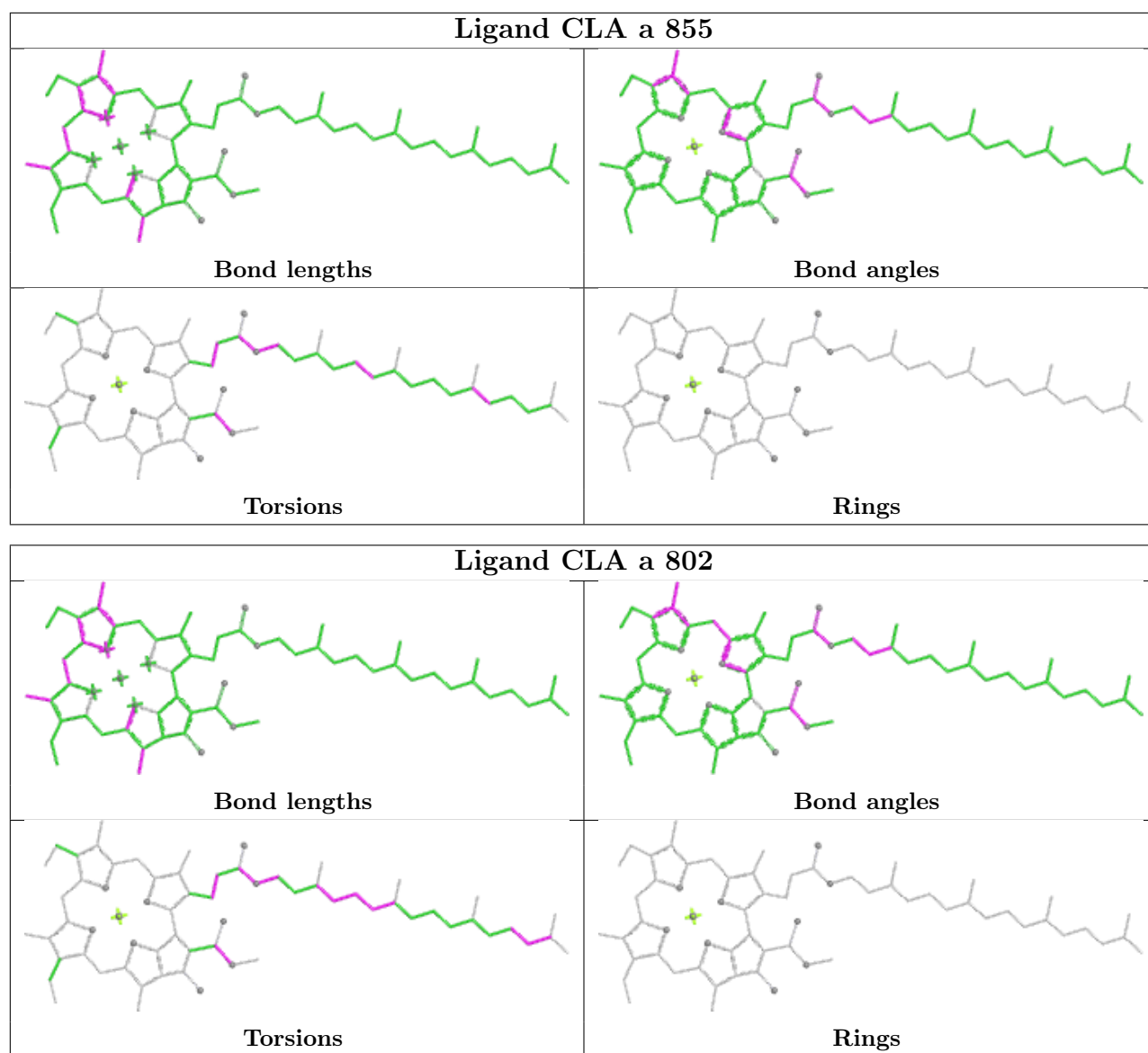
Continued on next page...

Continued from previous page...

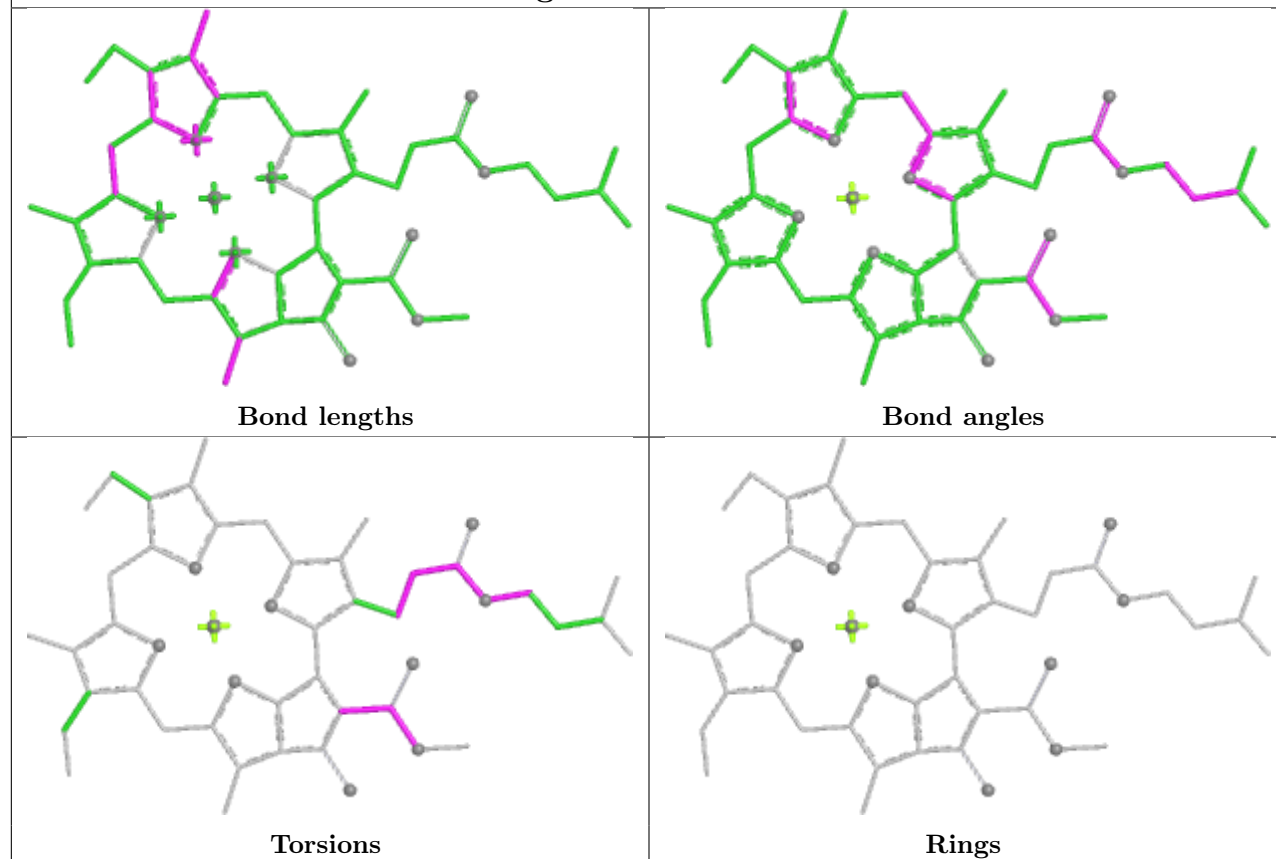
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	f	203	CLA	1	0
19	l	1501	CLA	1	0
19	a	843	CLA	4	0
19	a	837	CLA	7	0
19	a	819	CLA	8	0
19	a	812	CLA	5	0
21	a	845	BCR	10	0

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.

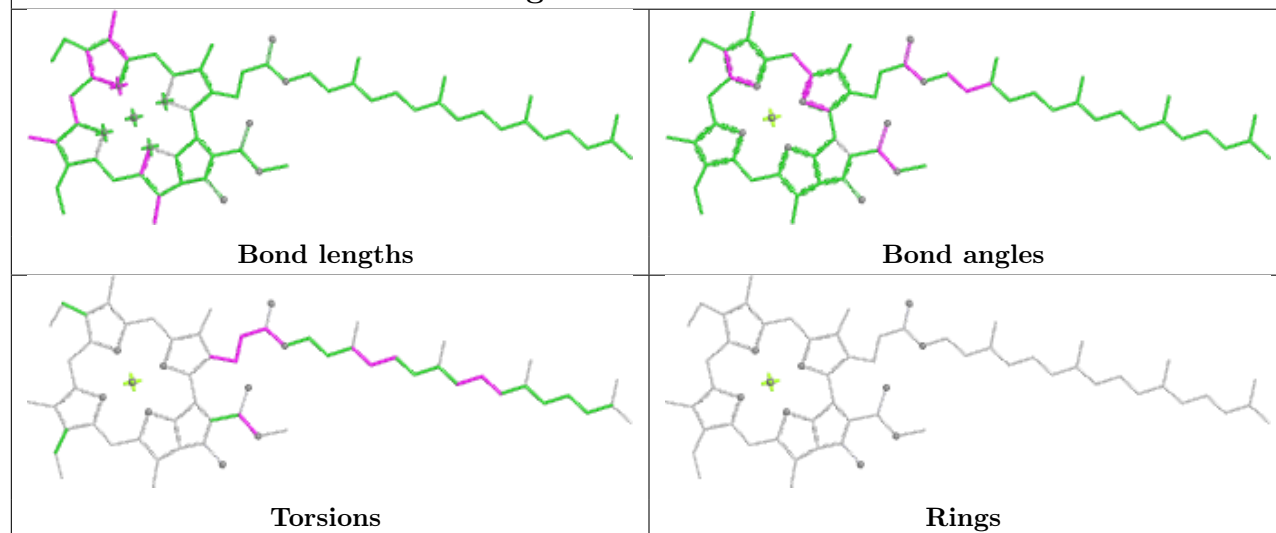


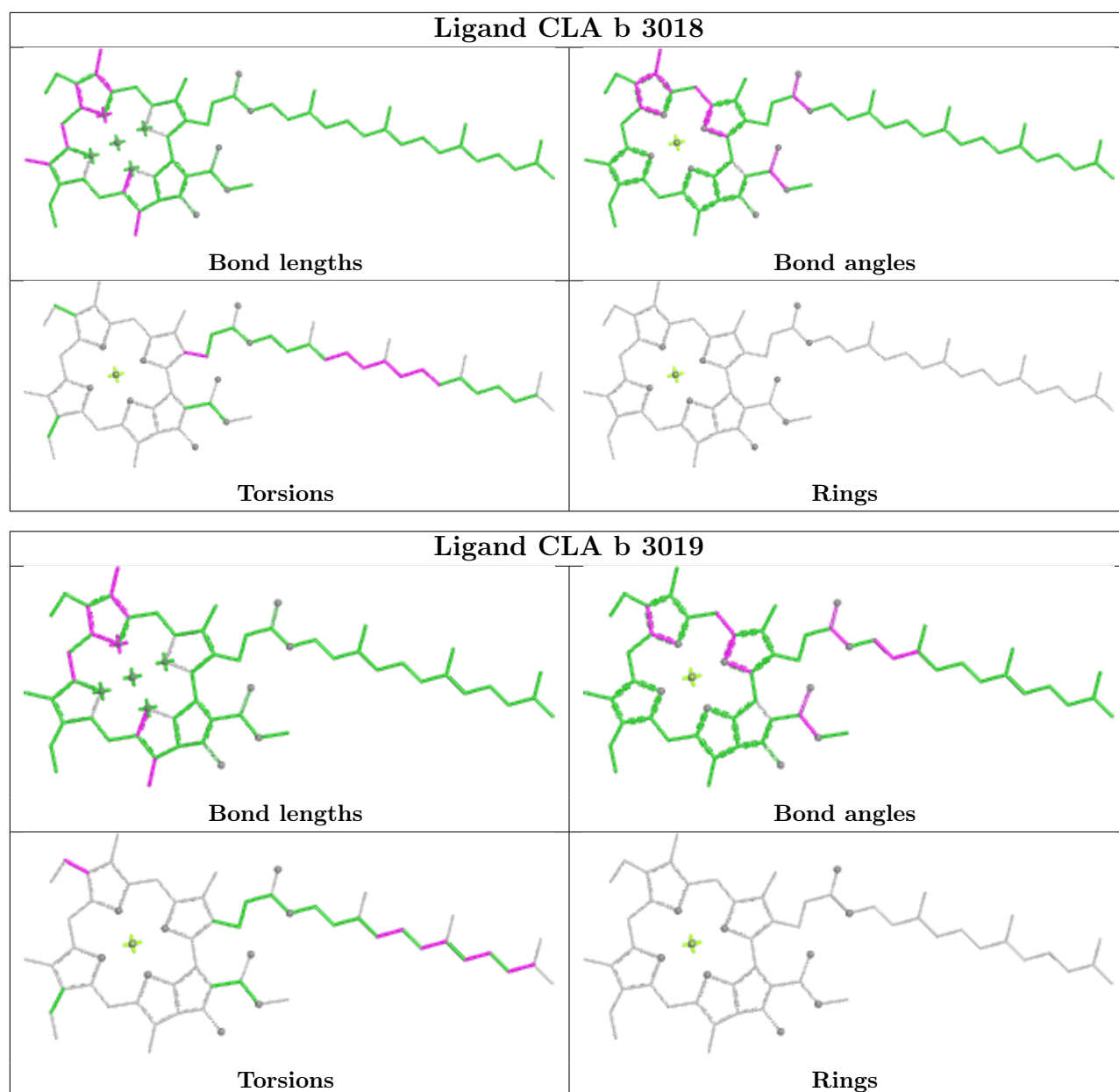


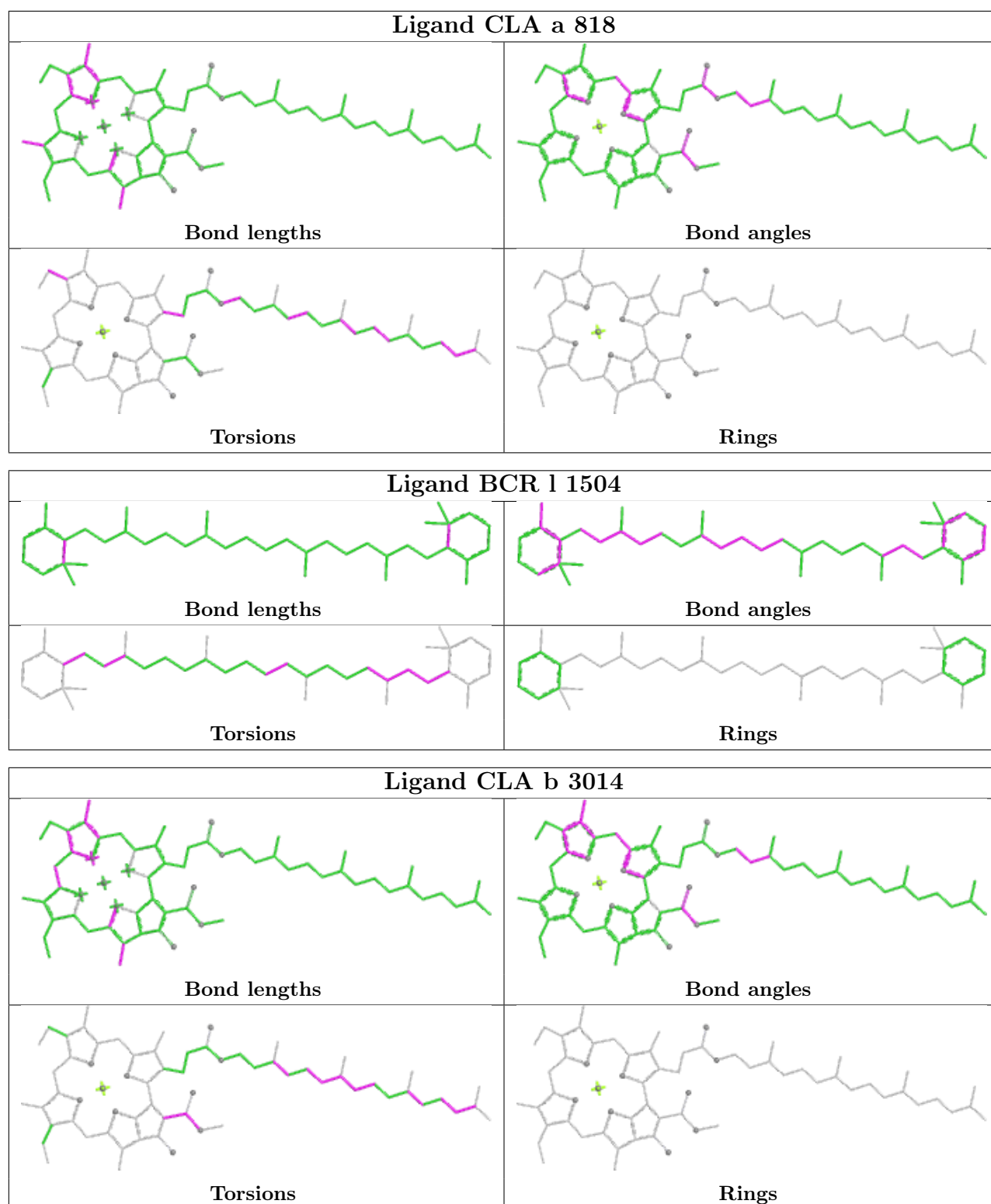
Ligand CLA a 811

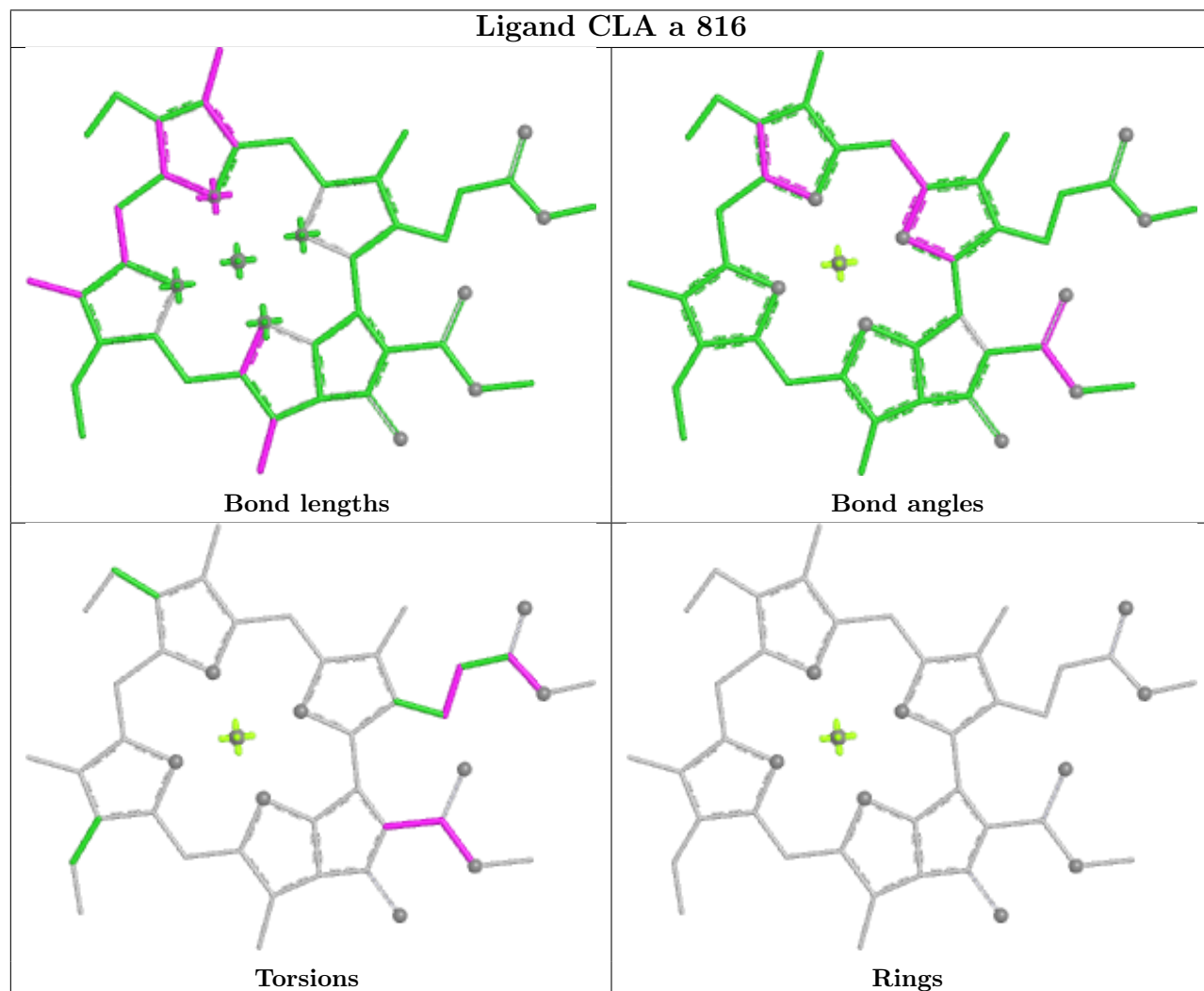
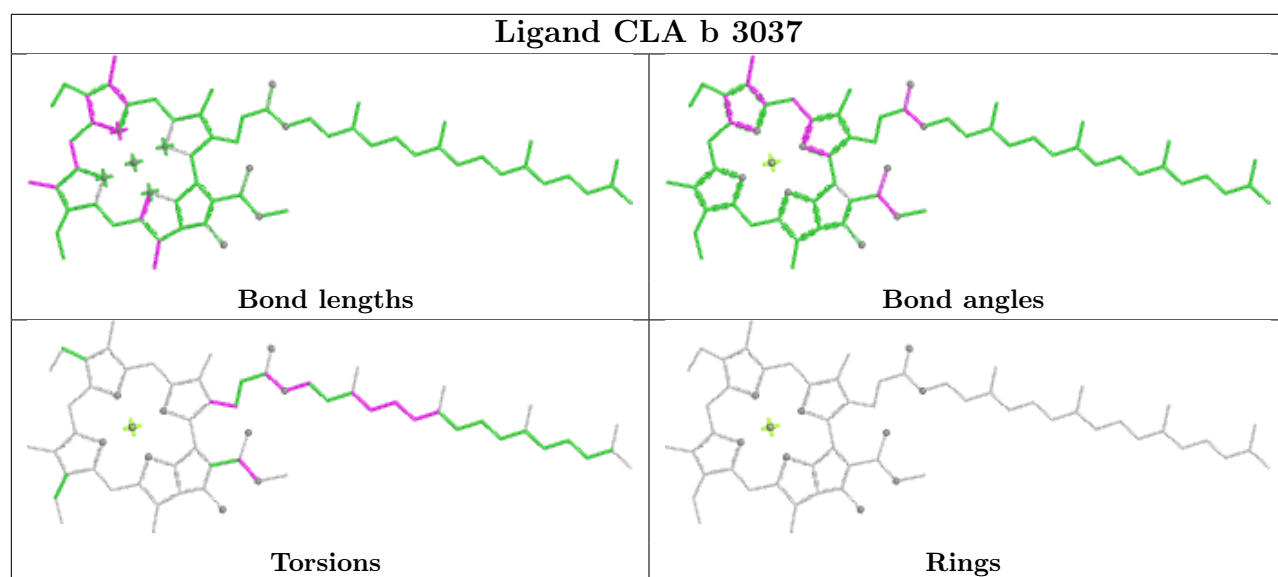


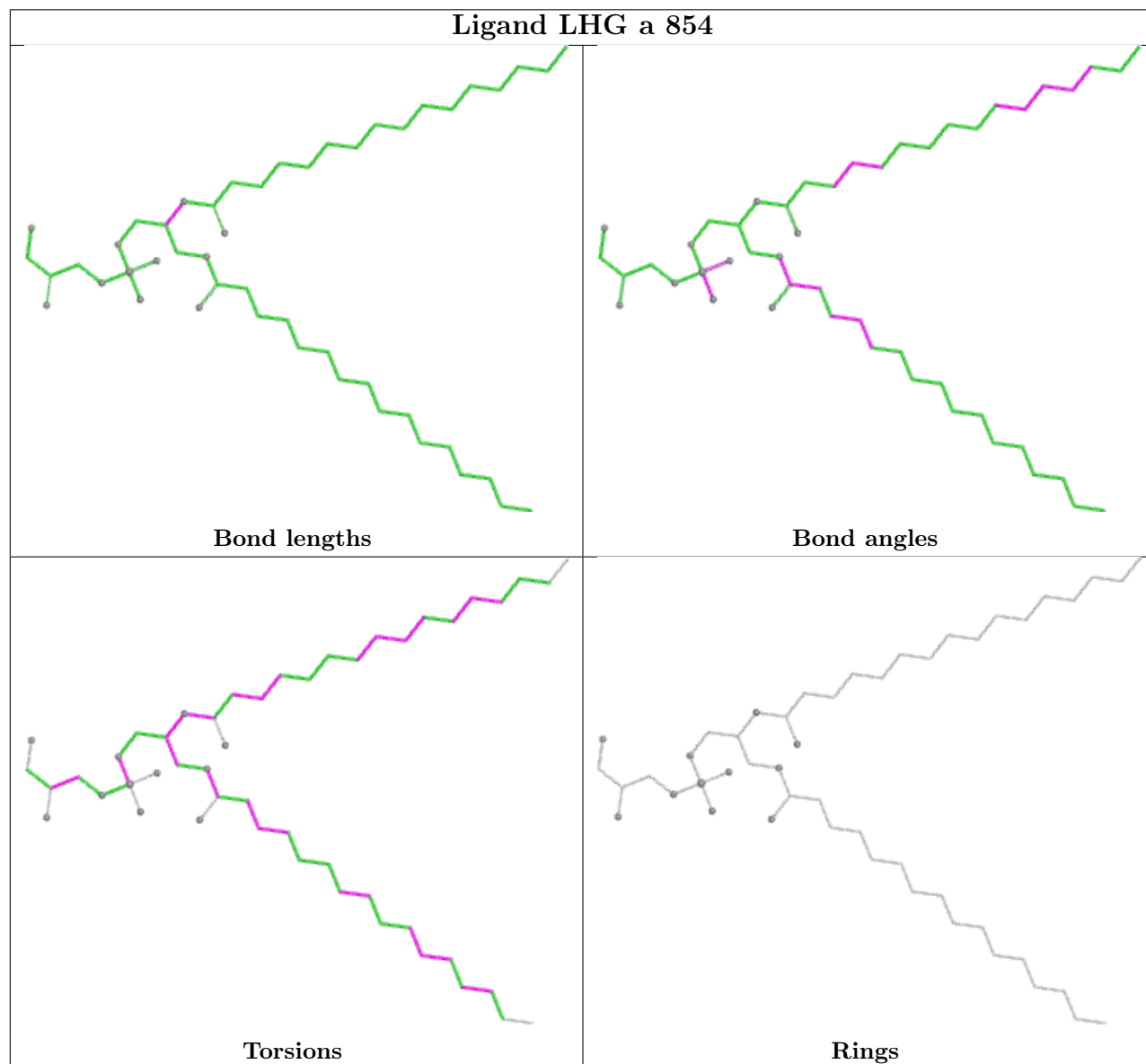
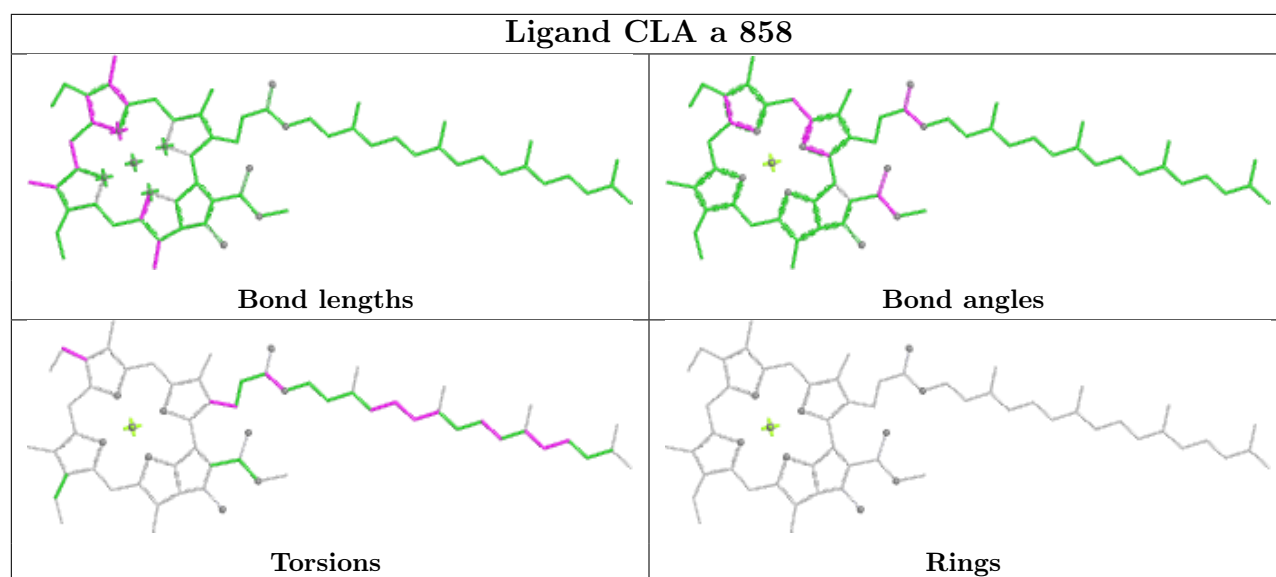
Ligand CLA b 3004

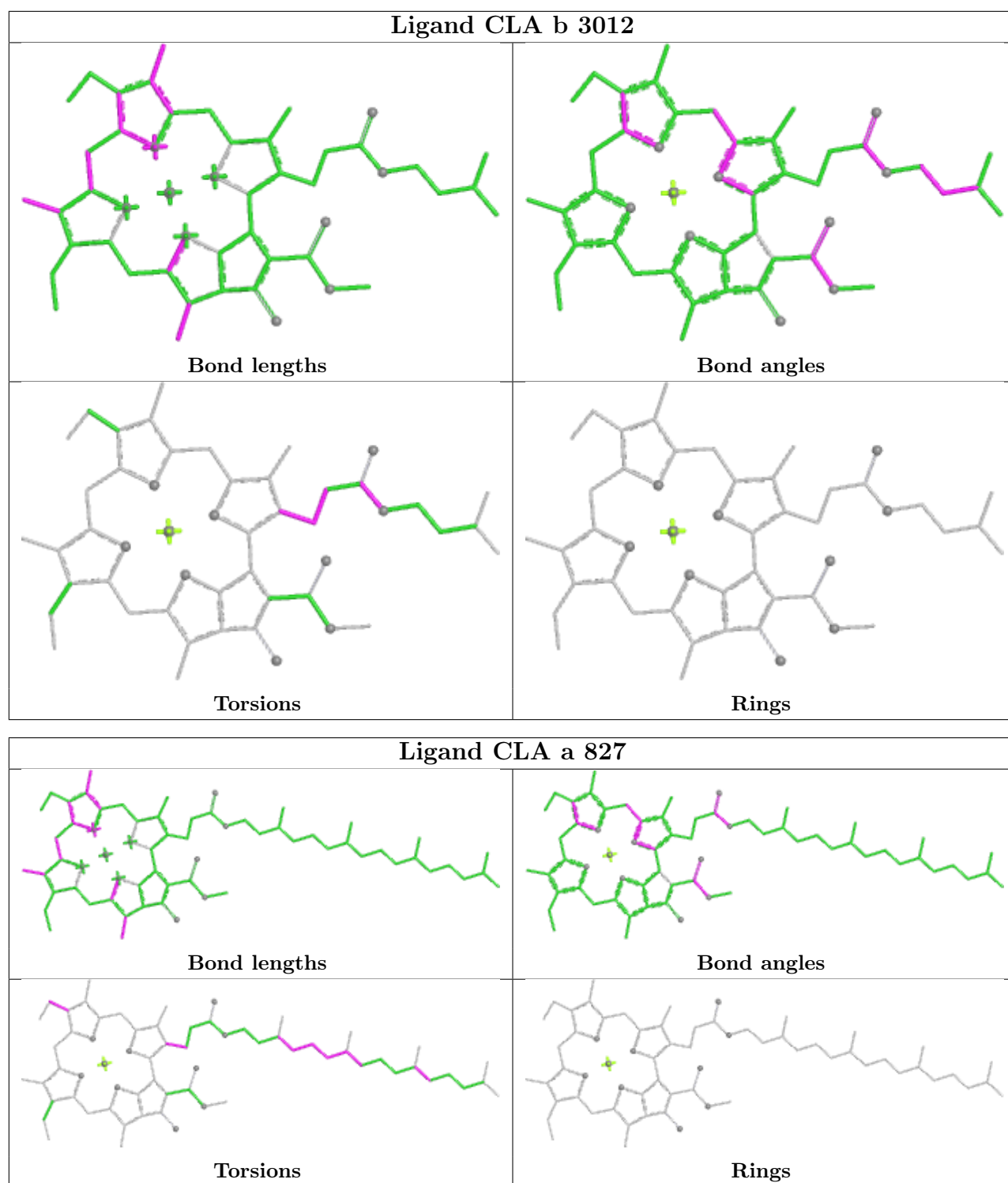


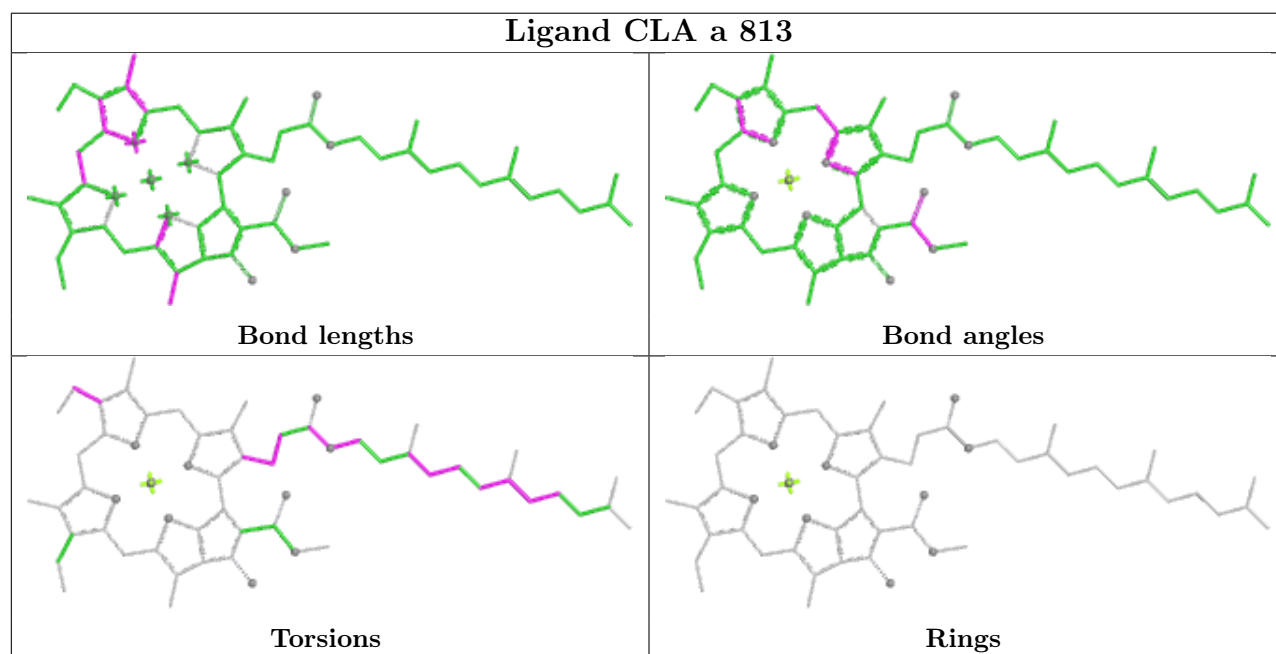
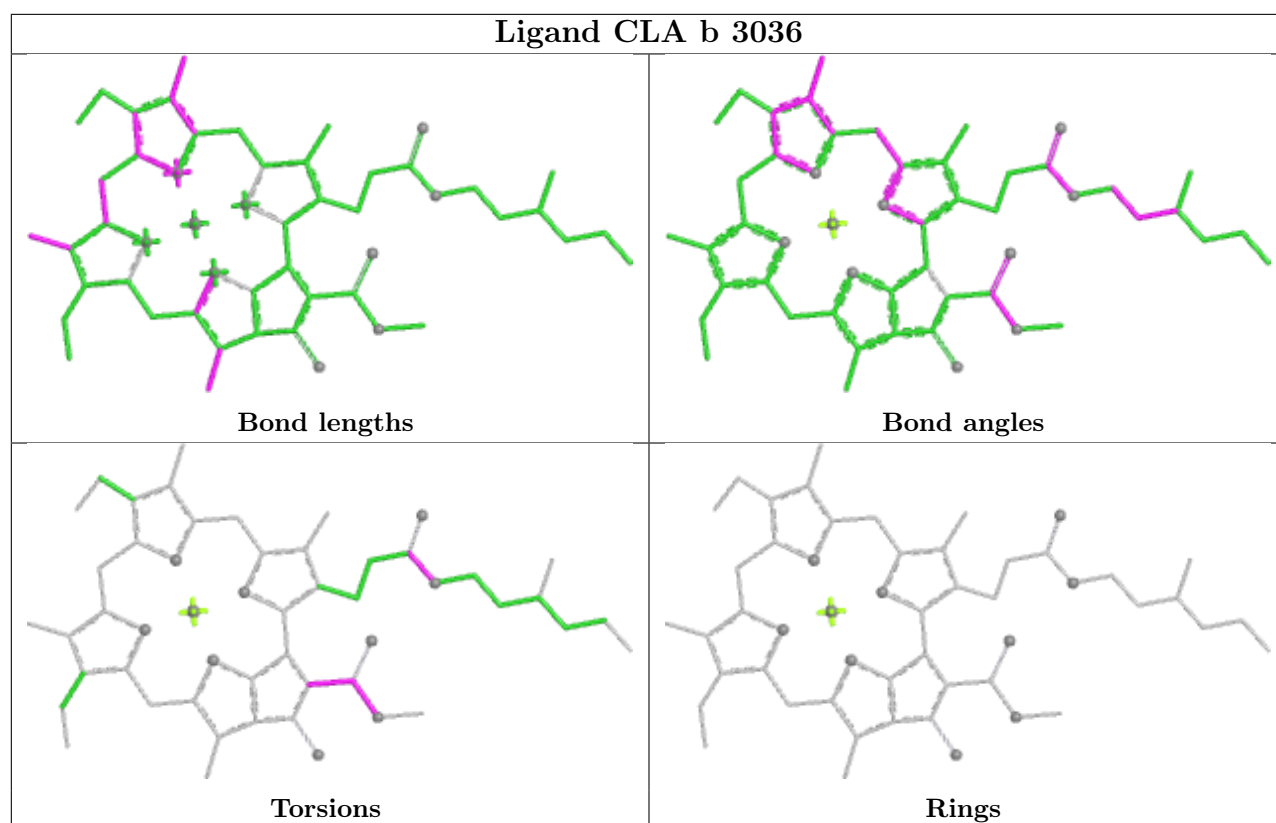


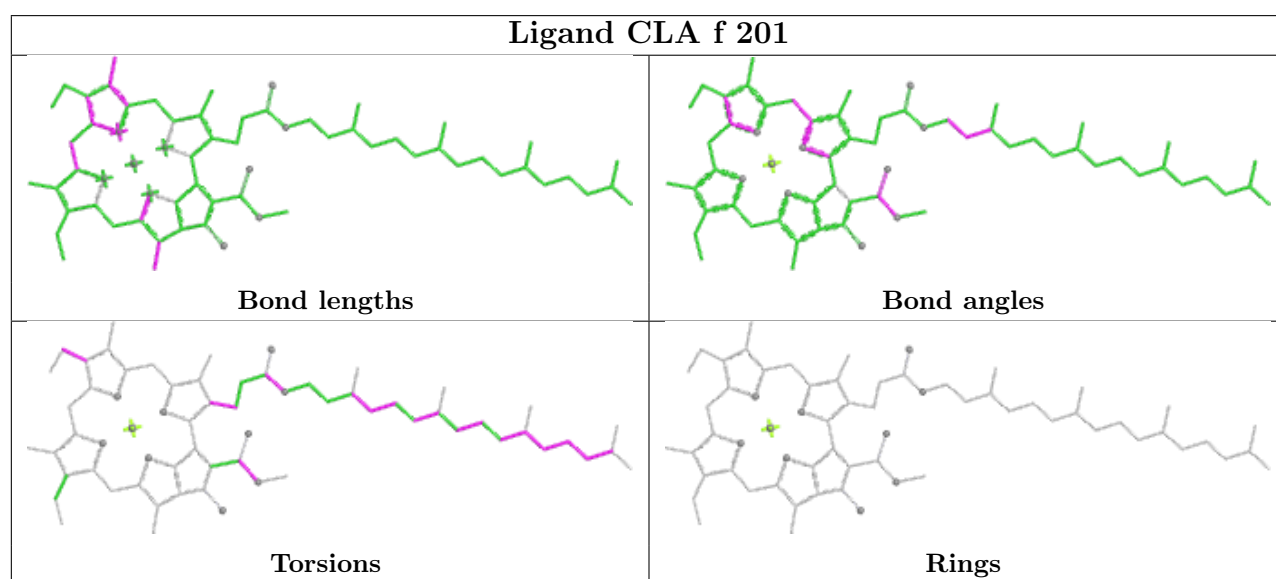
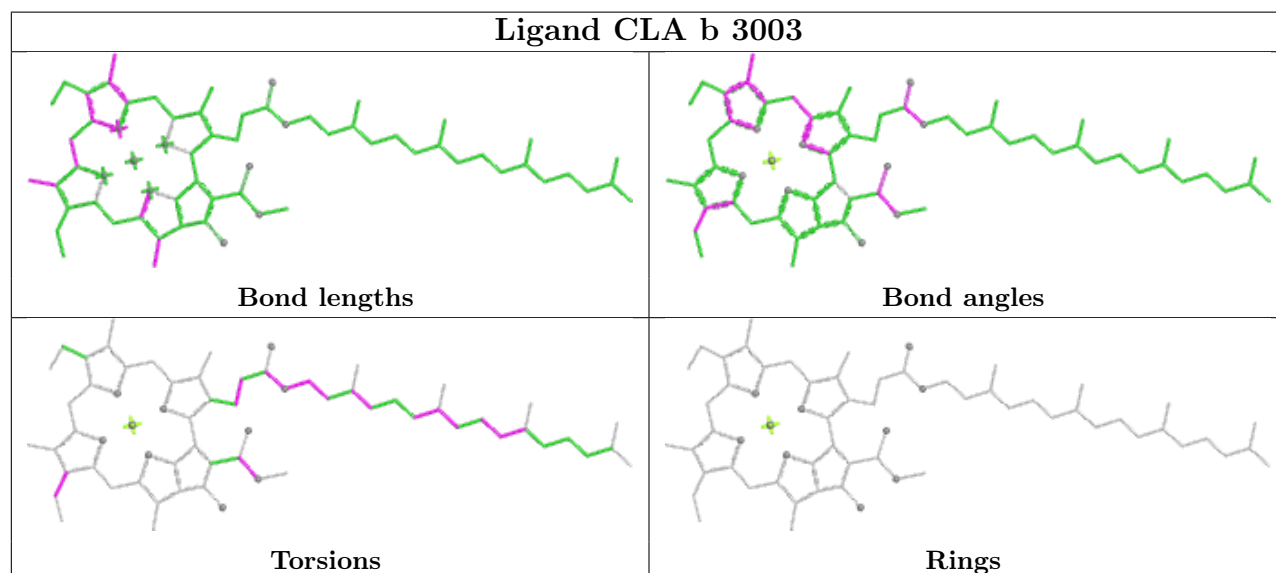
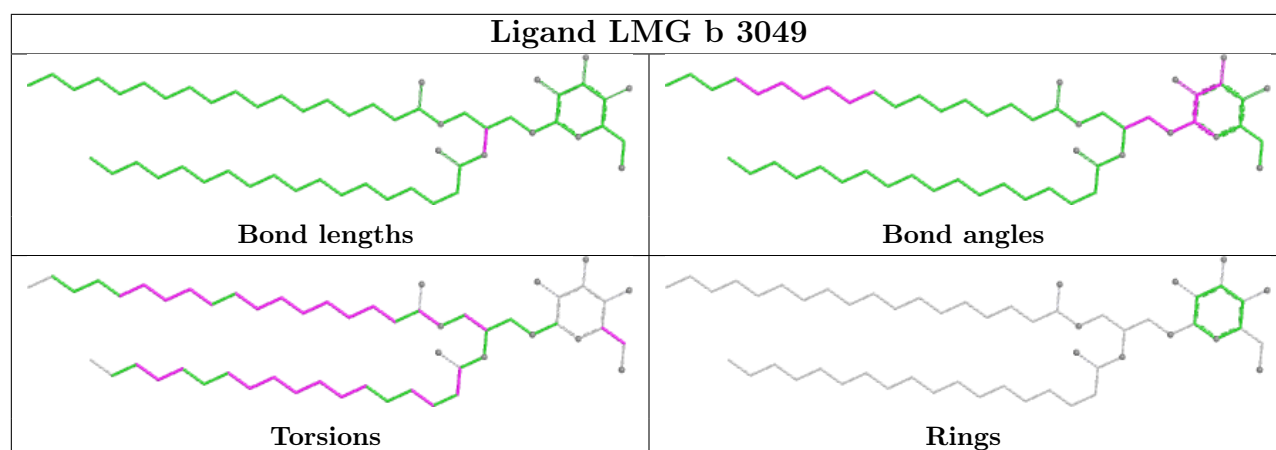


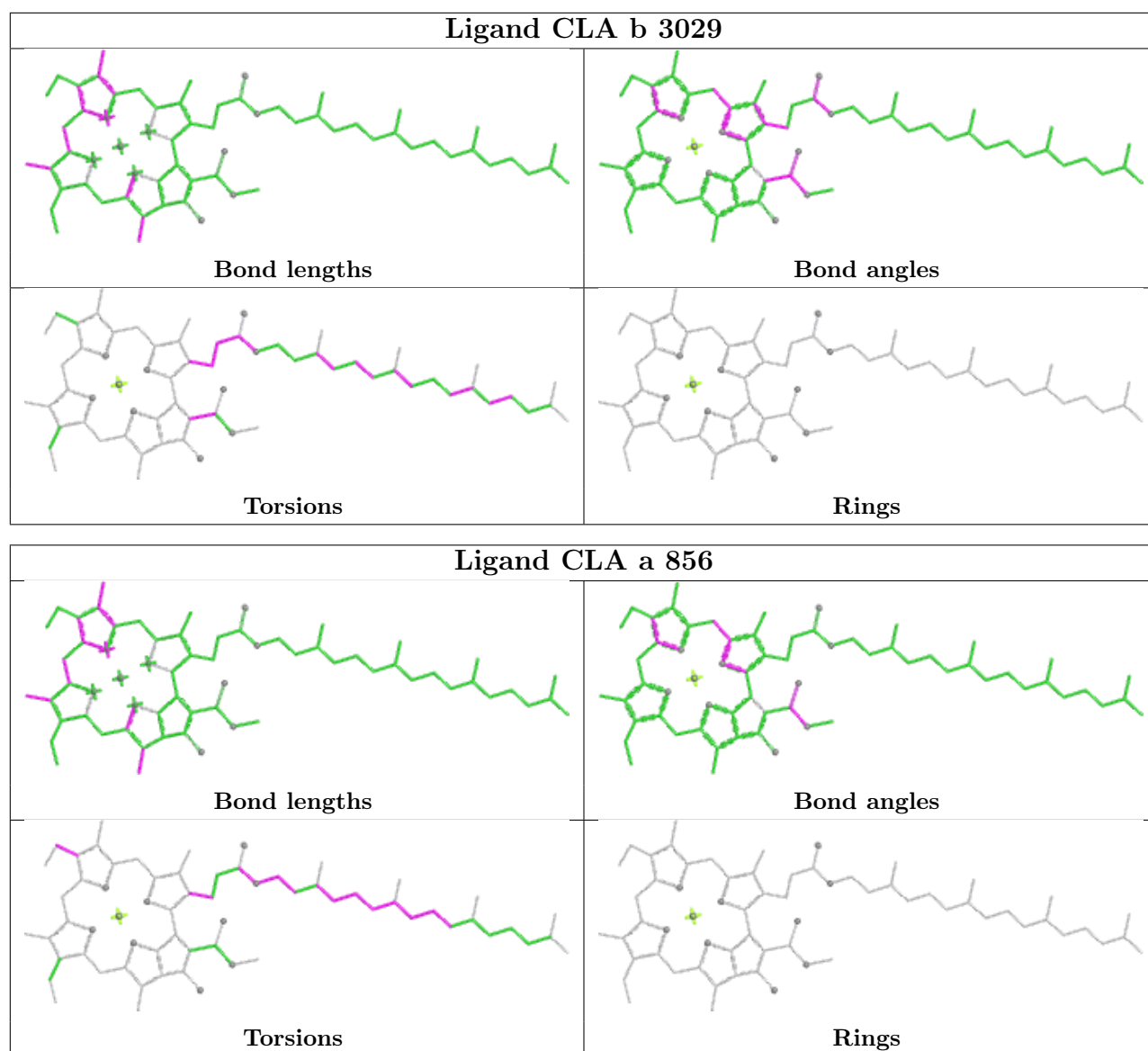


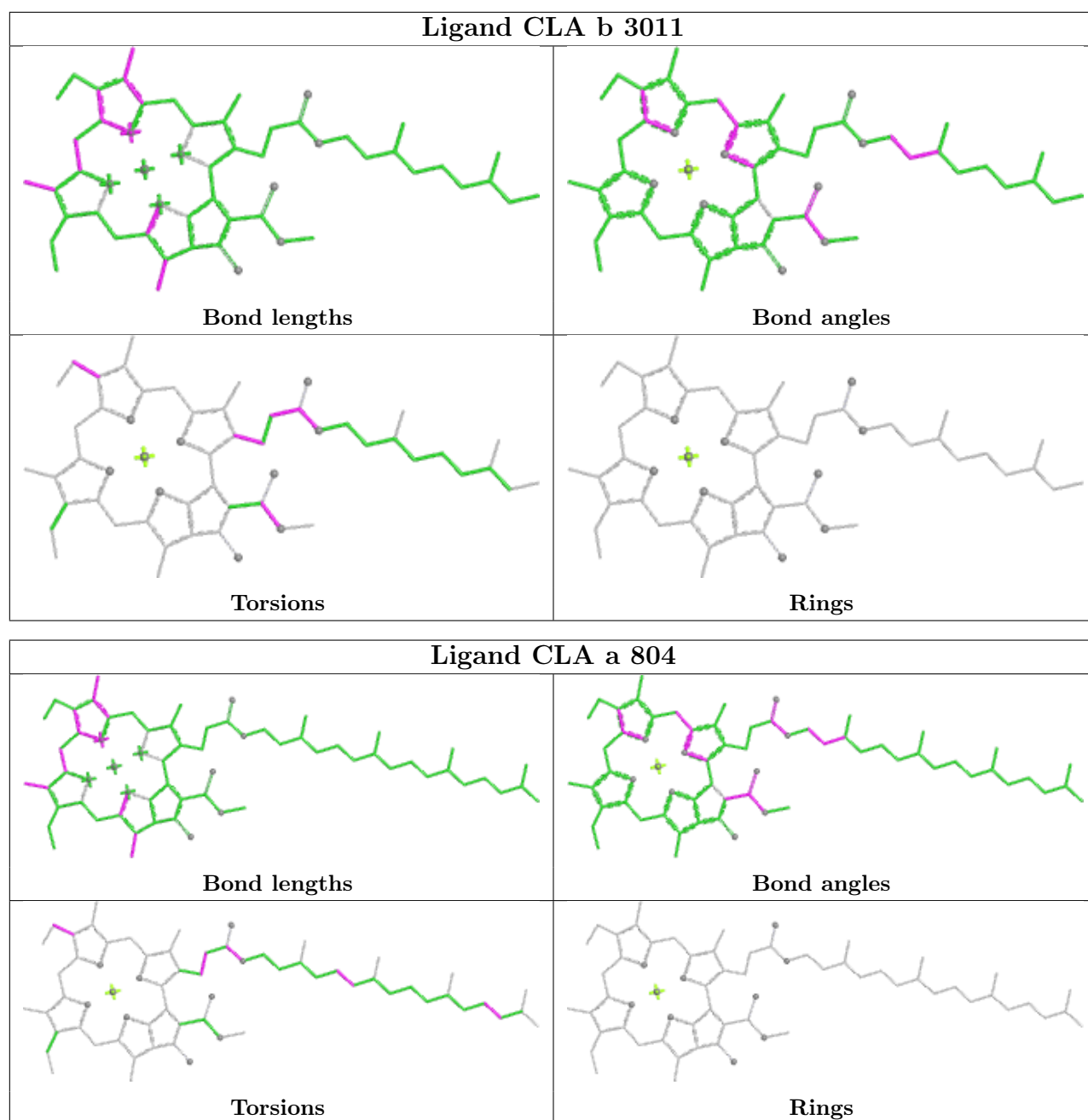


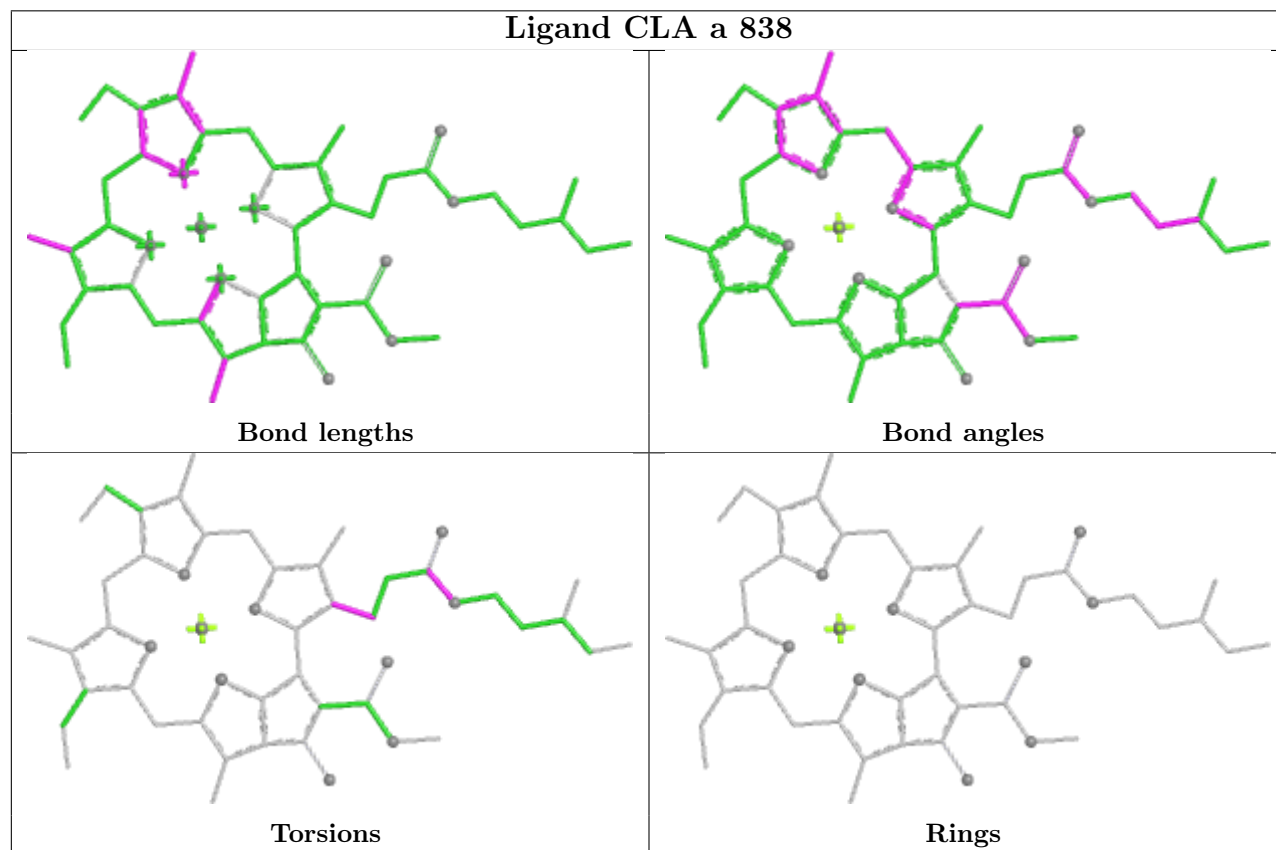
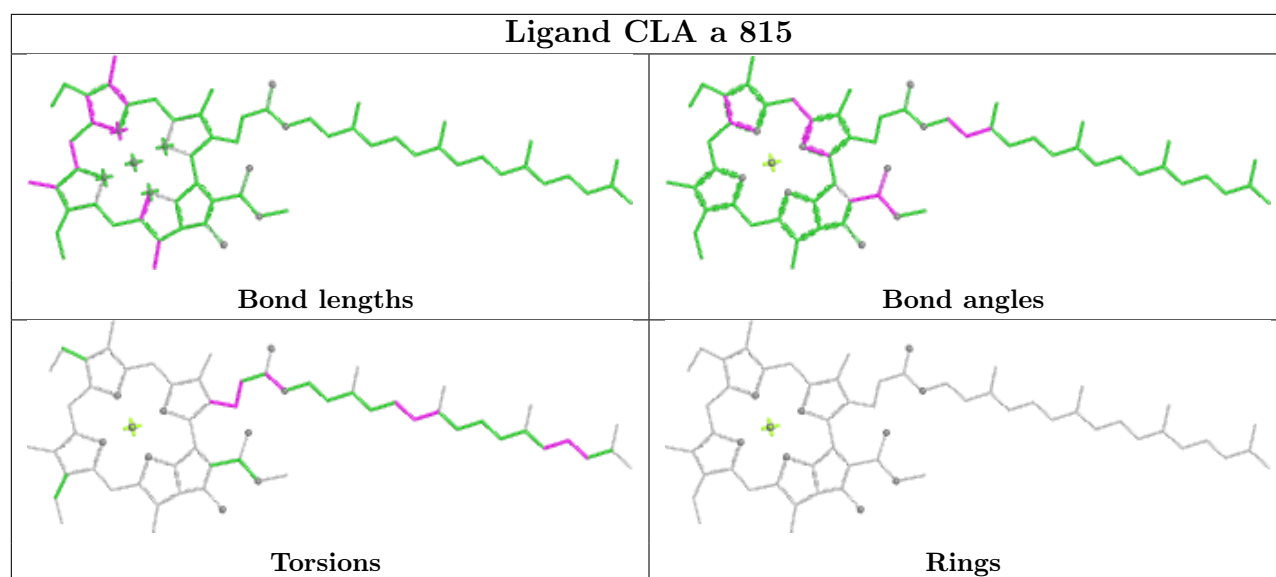


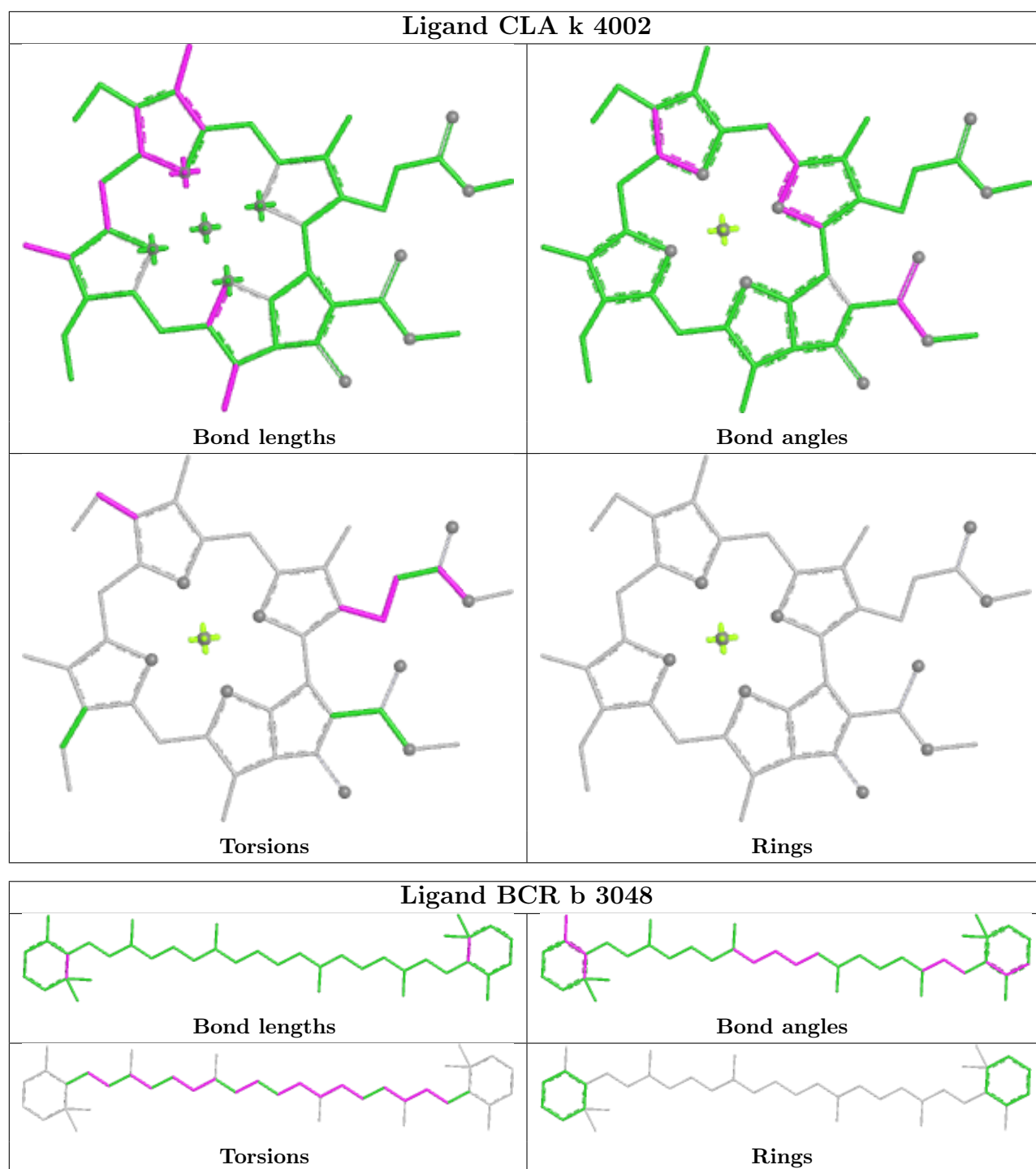


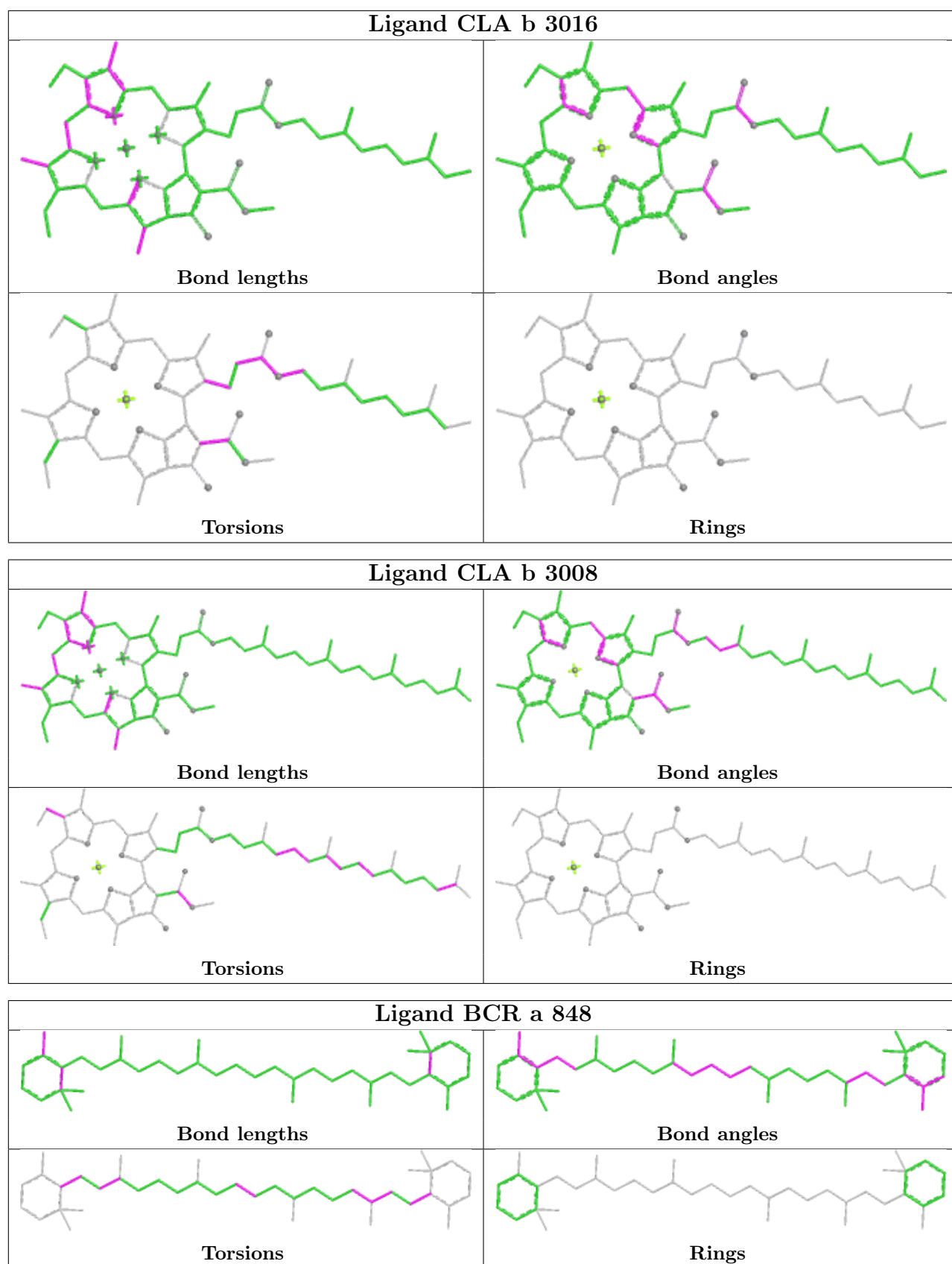


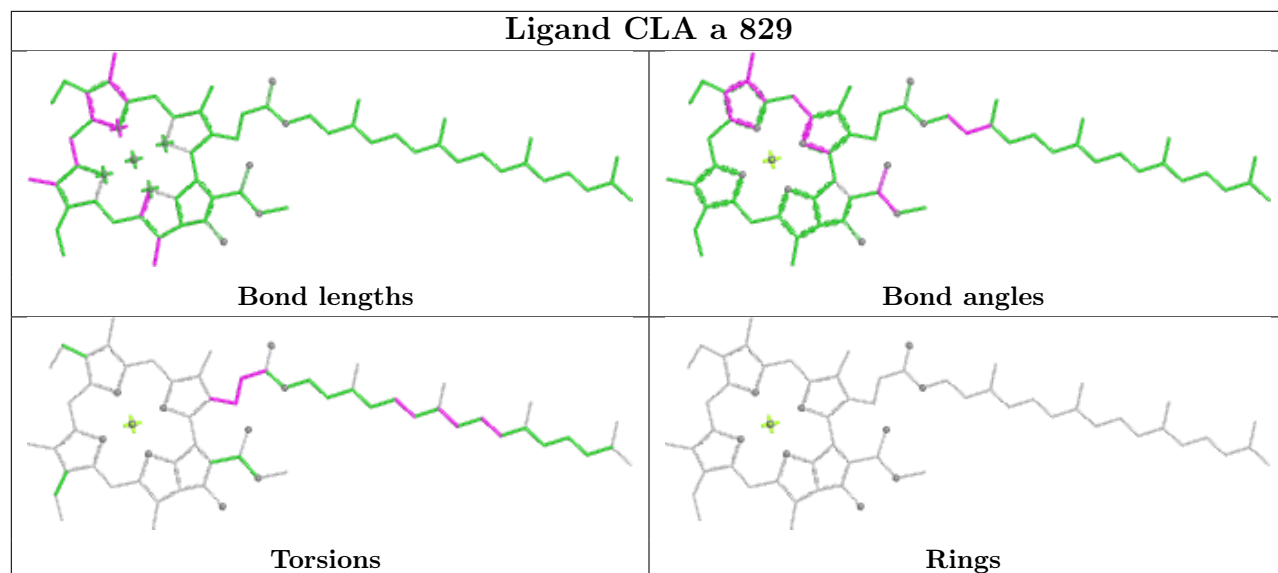
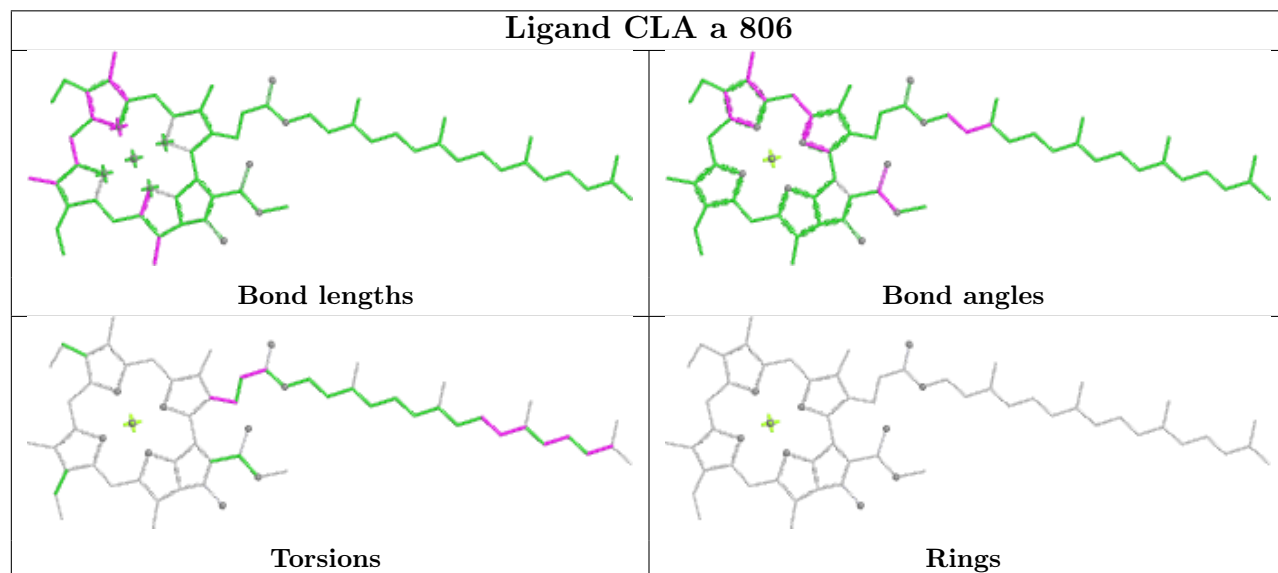
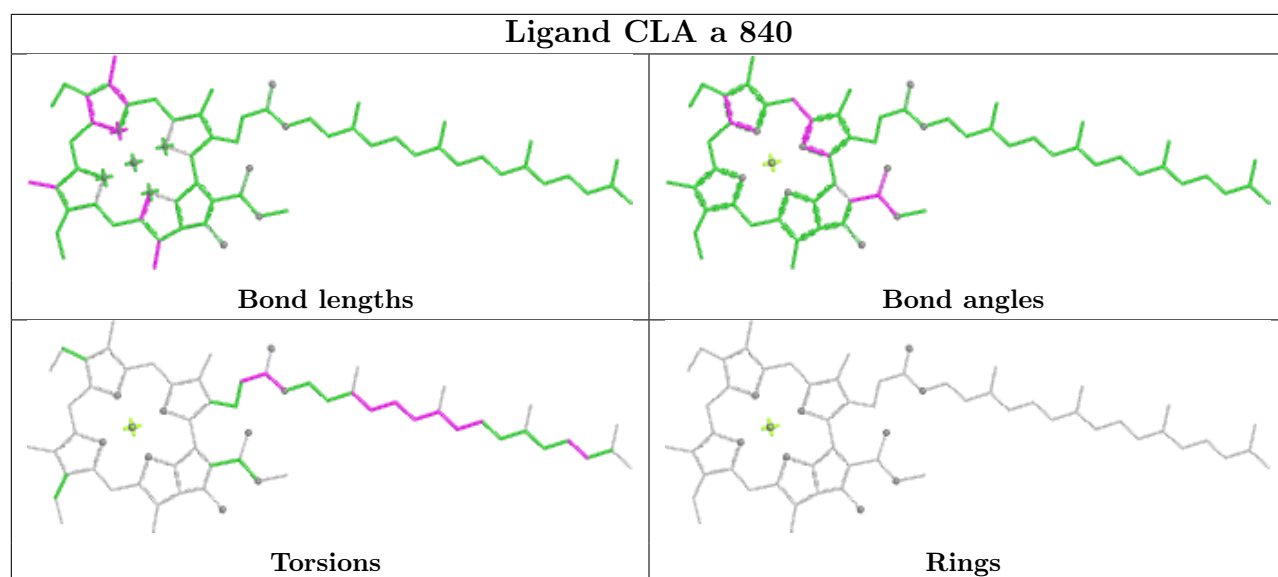


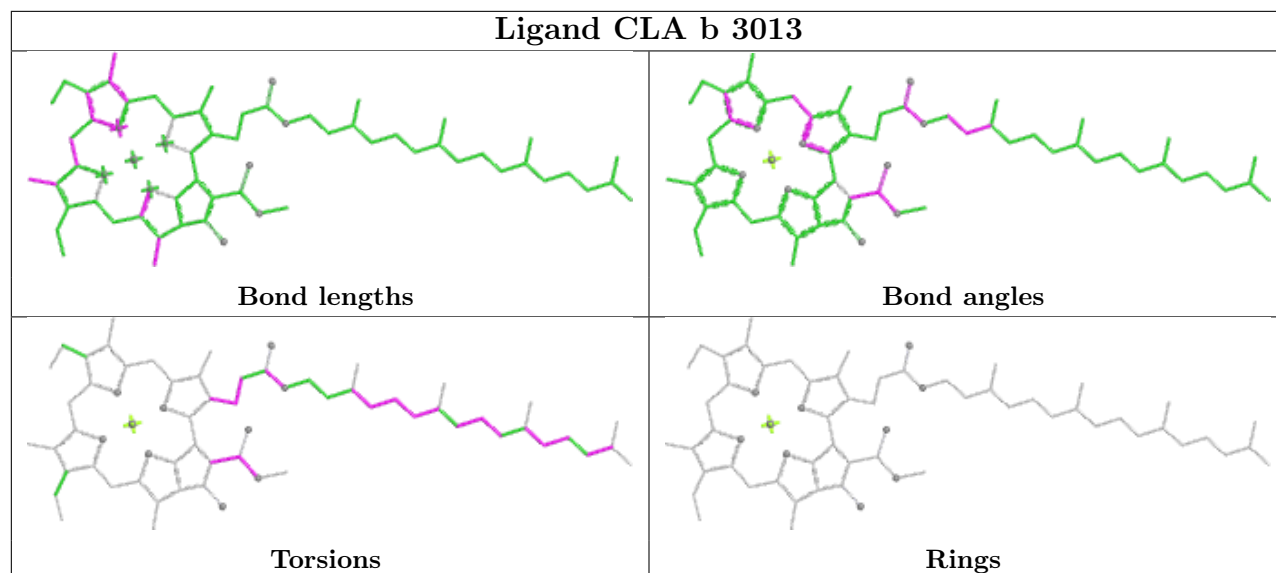
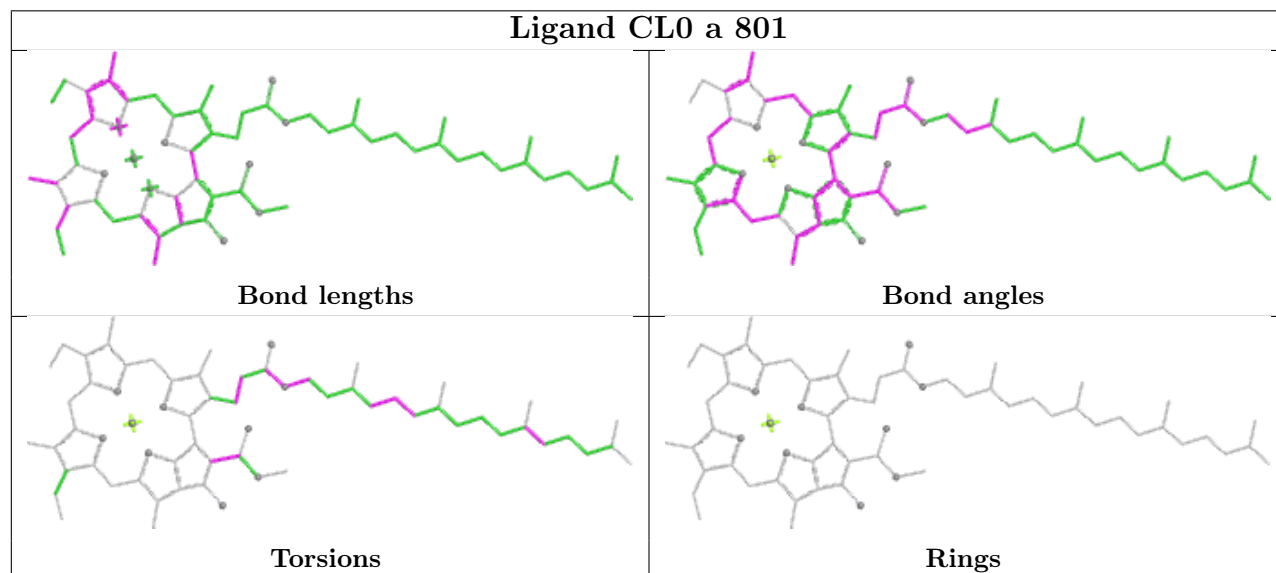
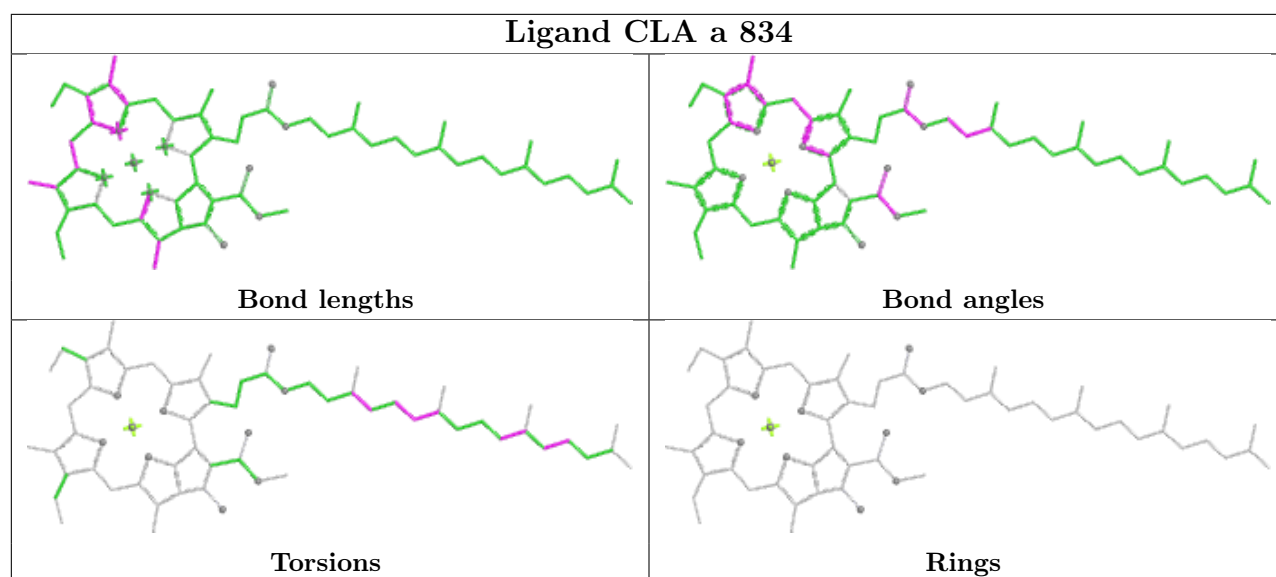


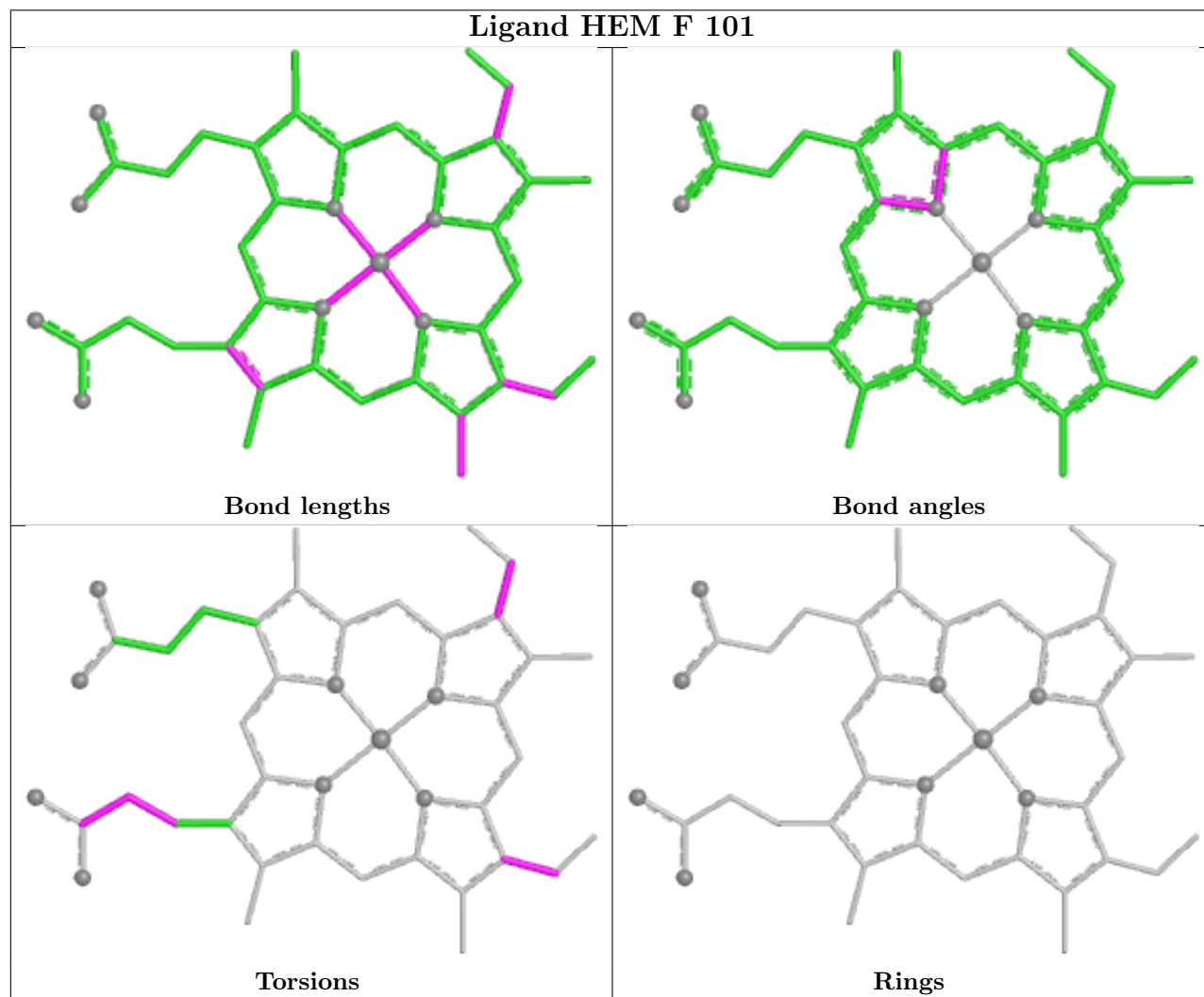
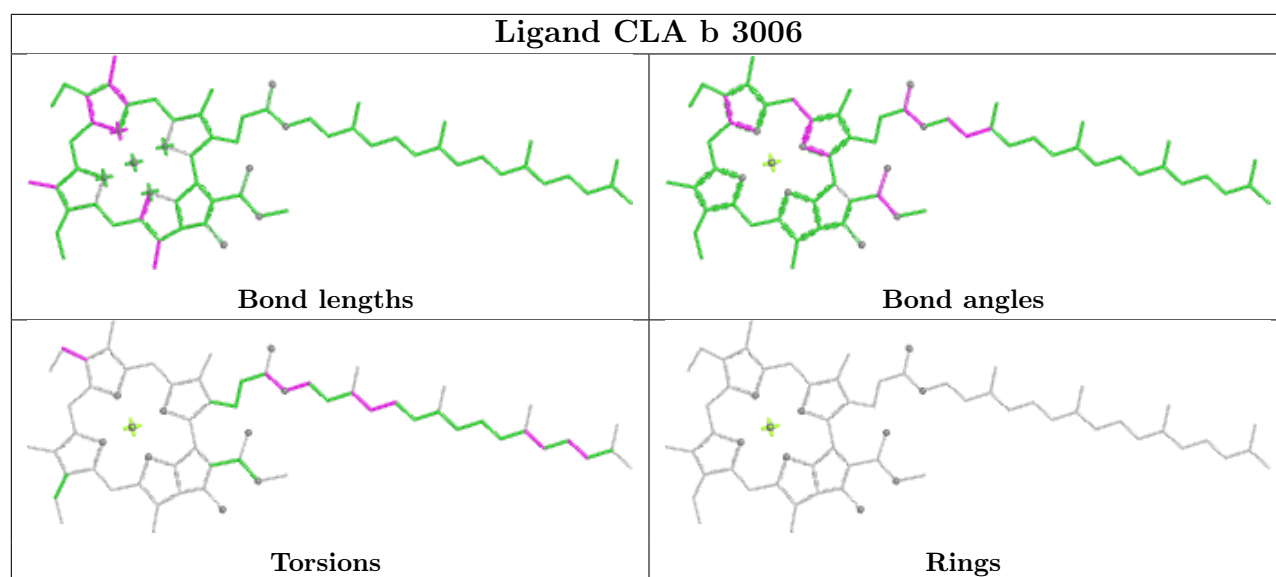


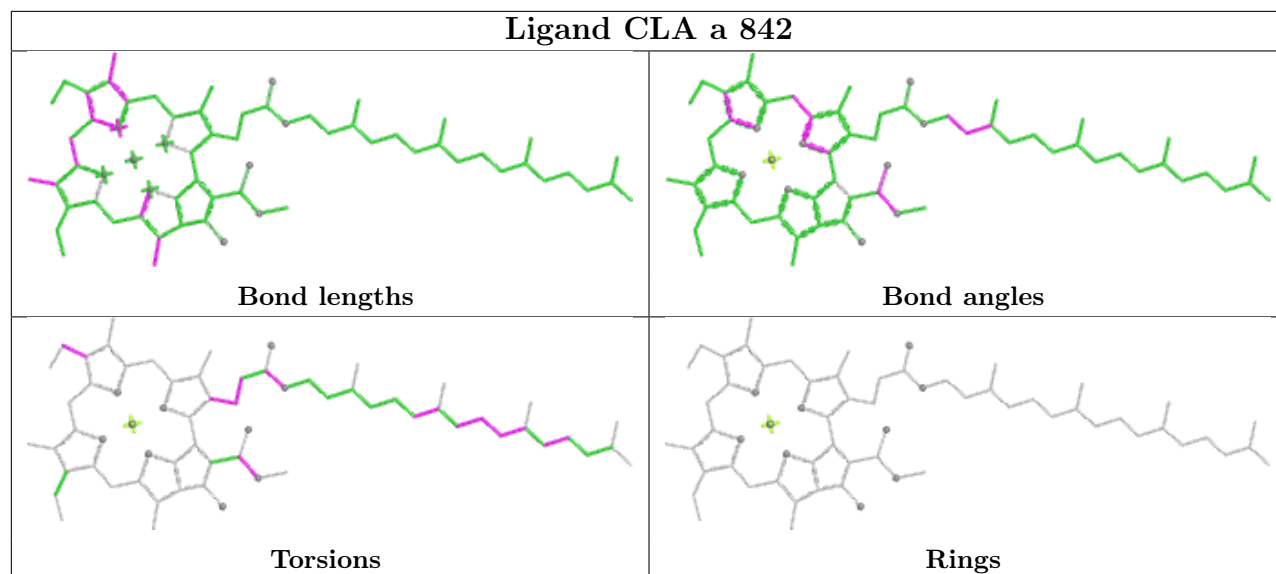
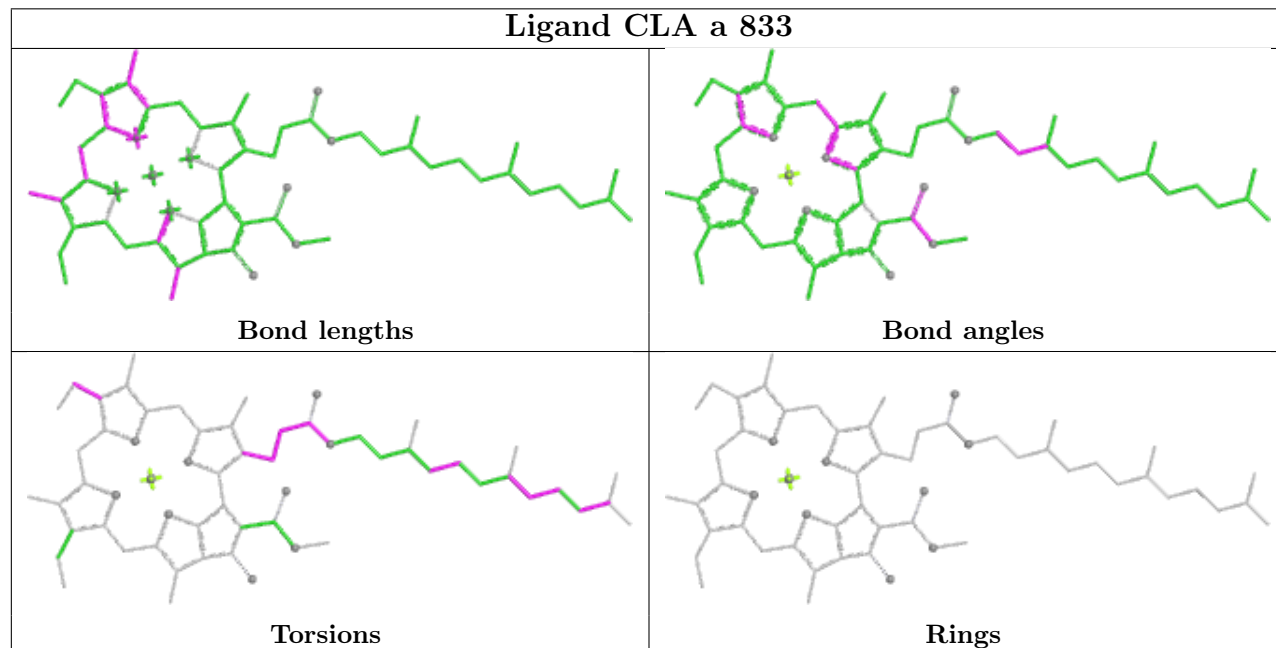


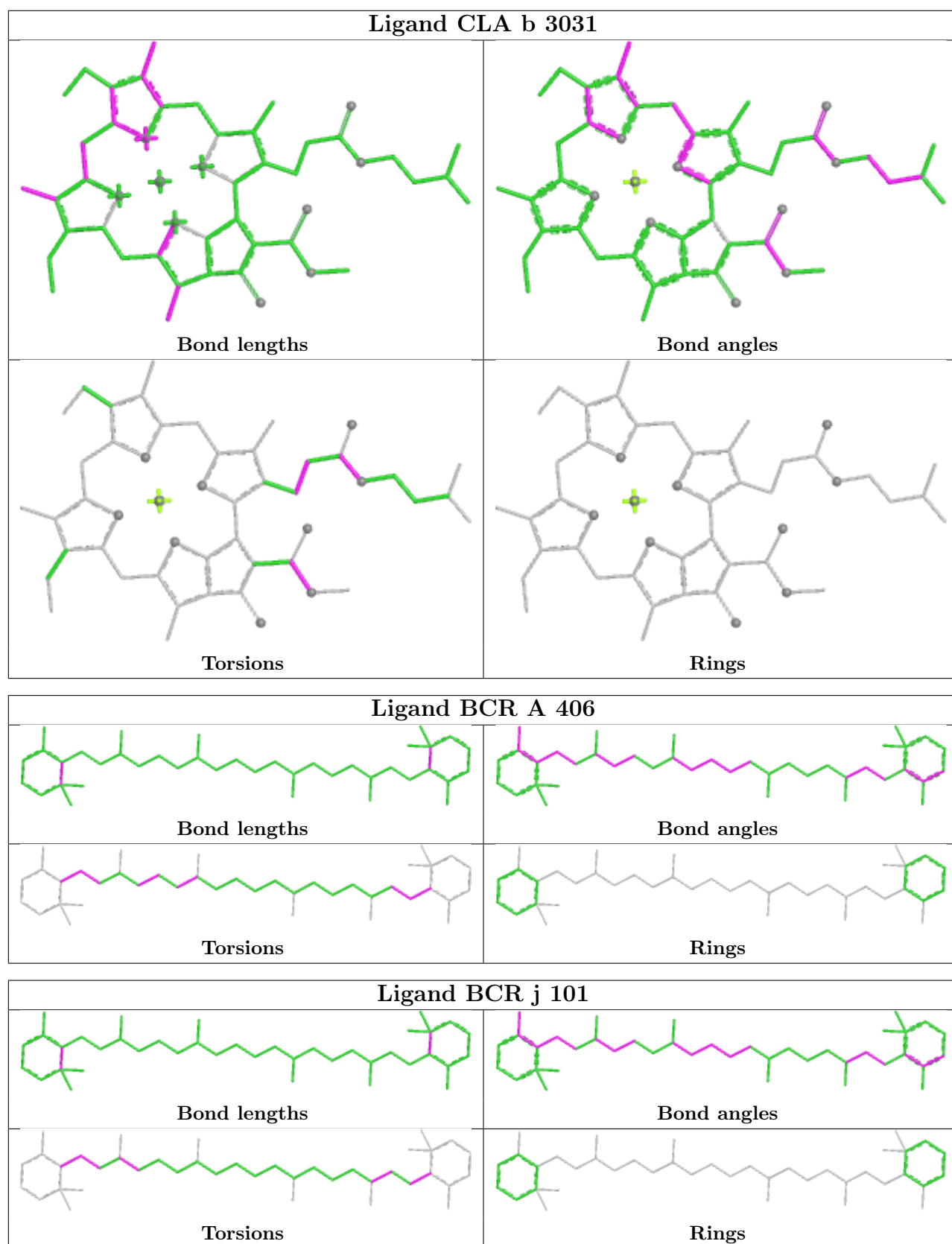


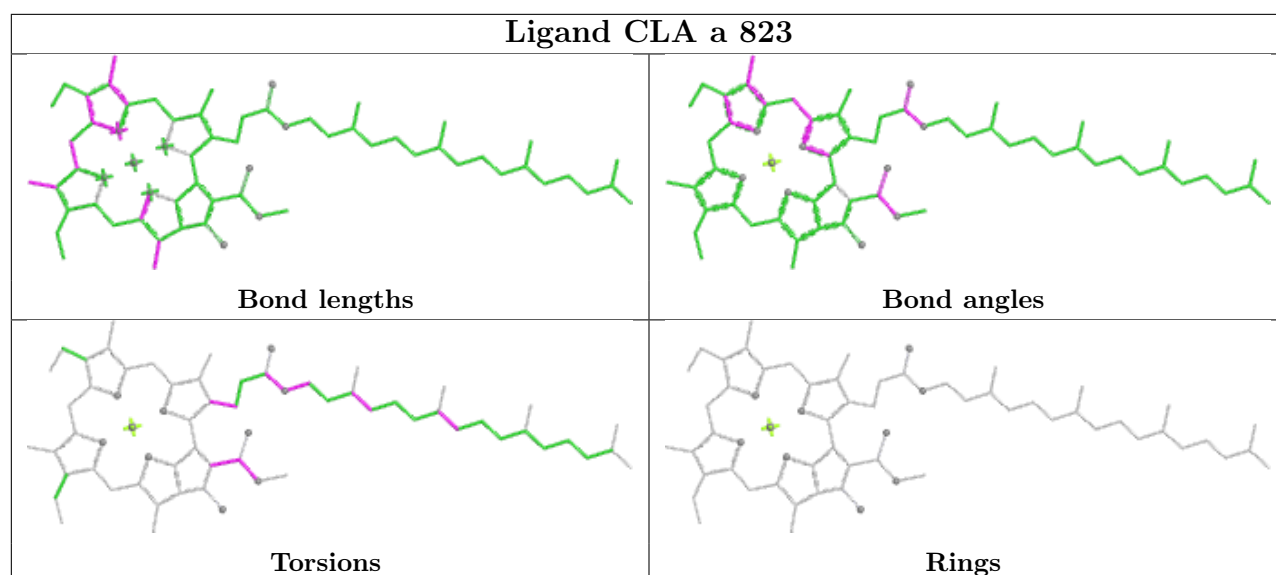
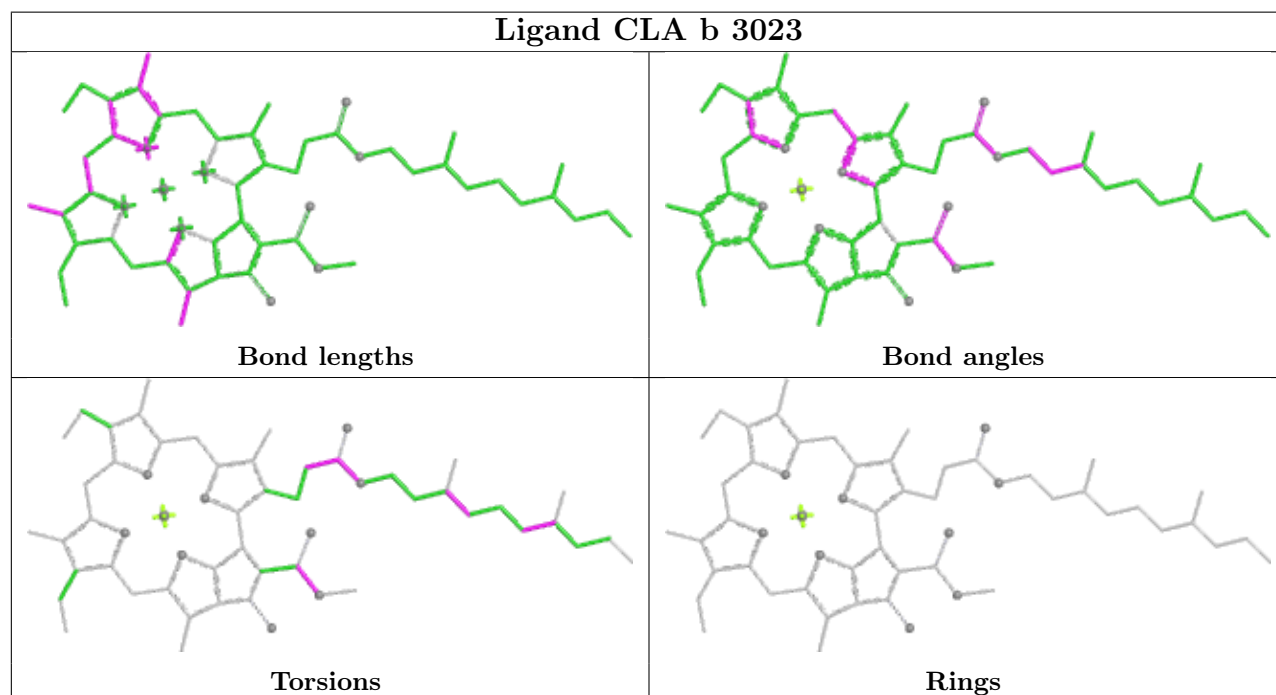
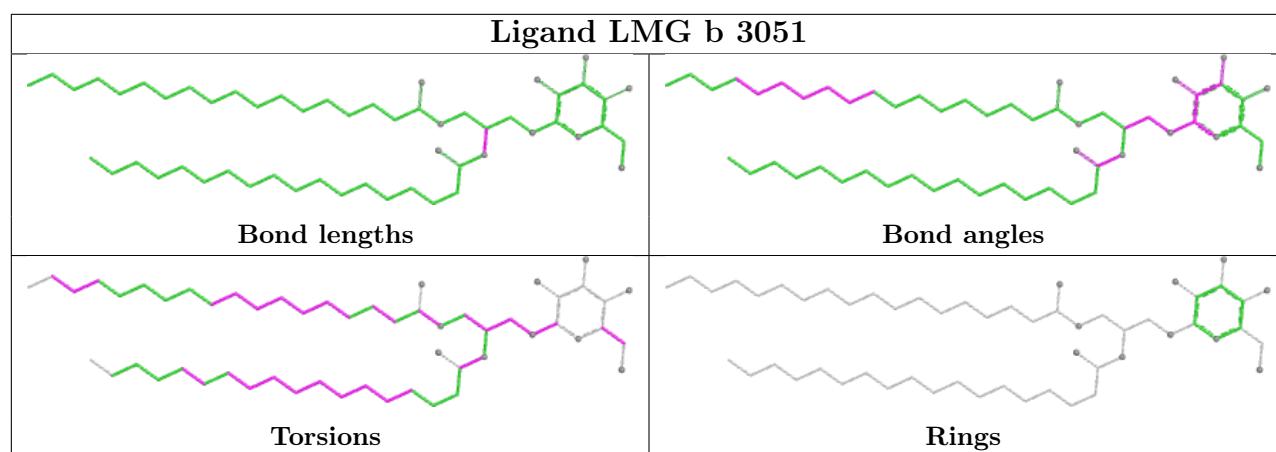




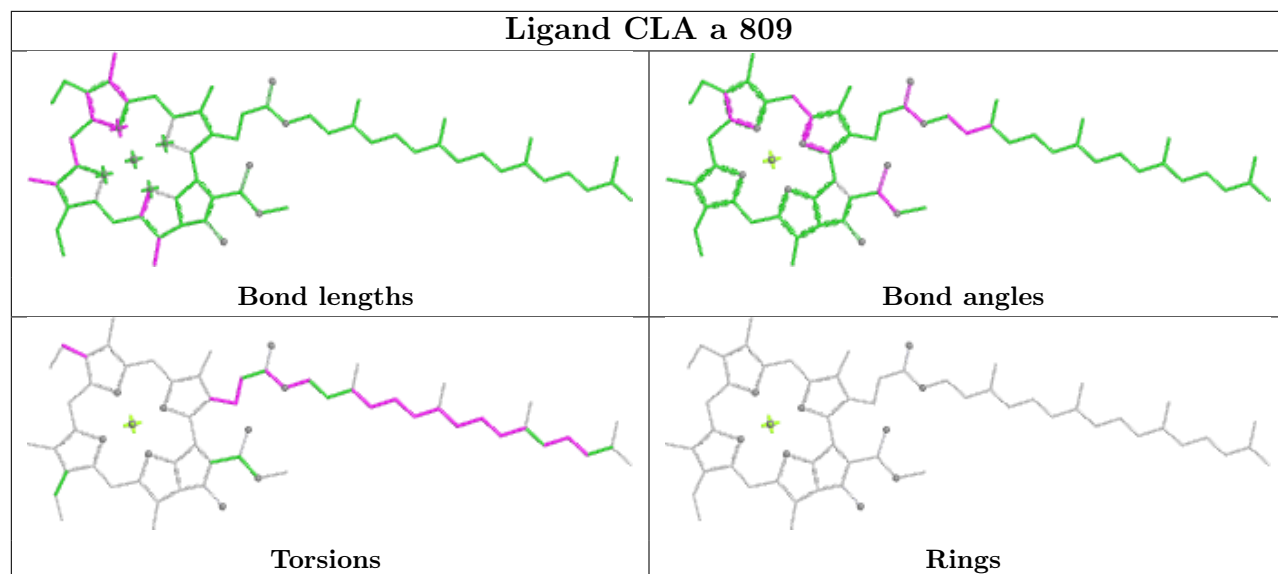


Ligand CLA a 842**Ligand CLA a 833**

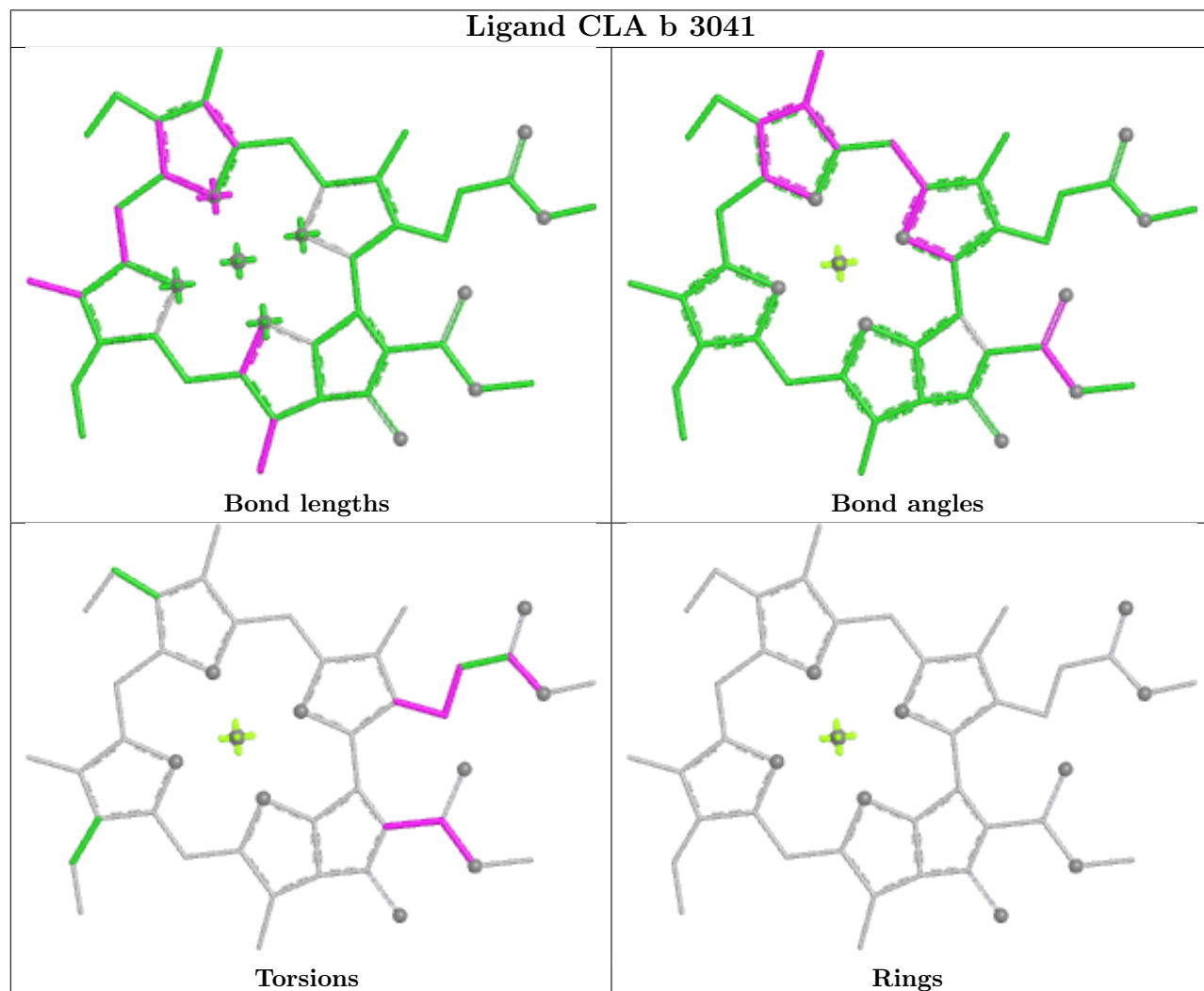


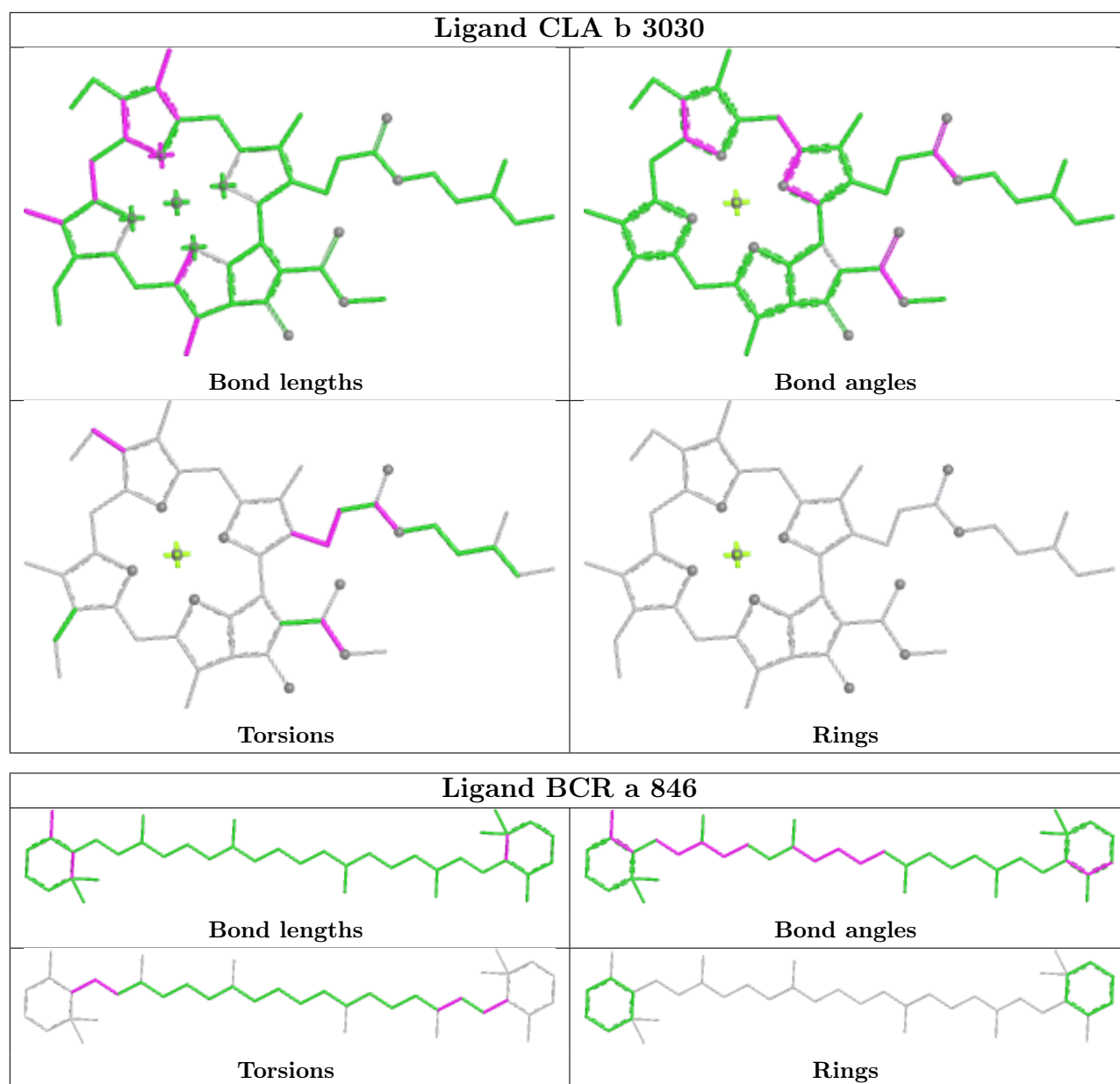


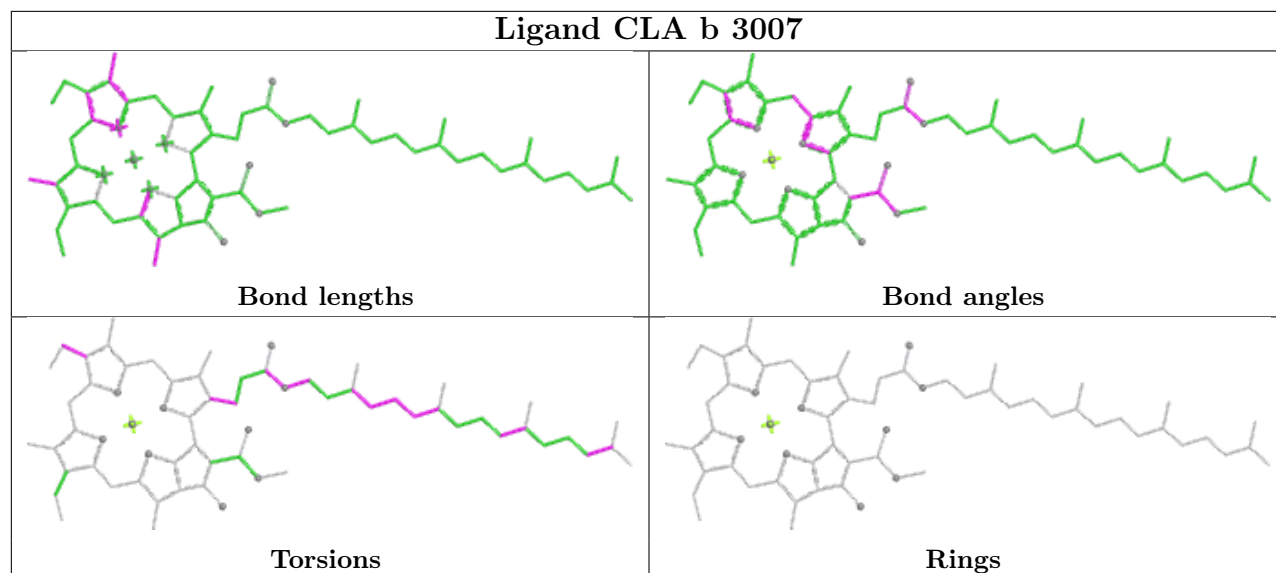
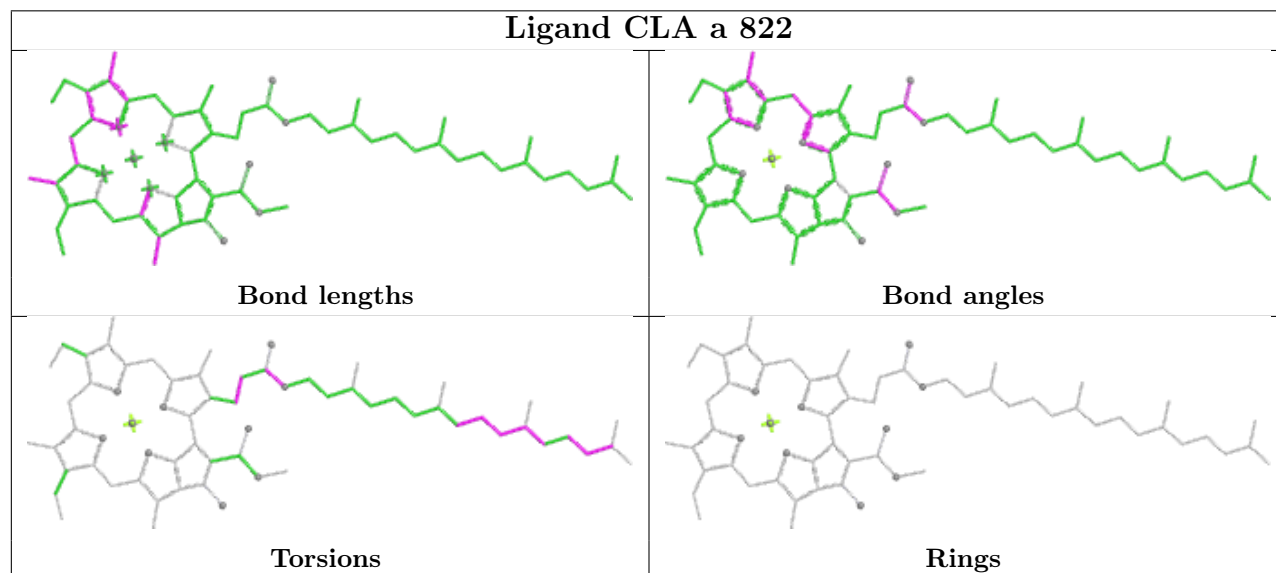
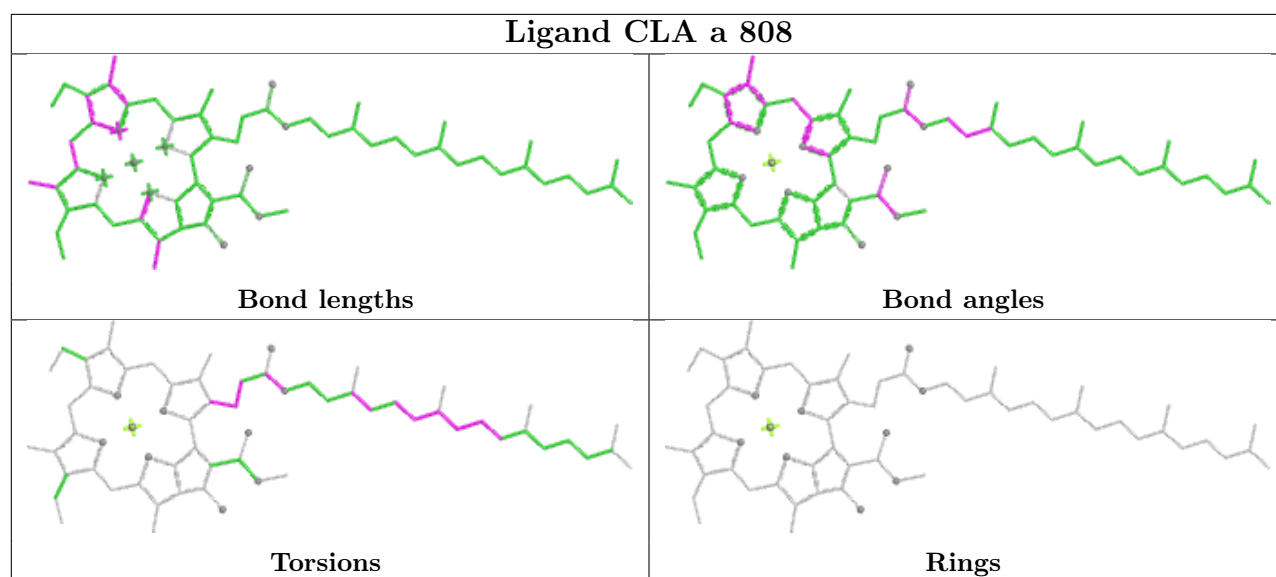
Ligand CLA a 809

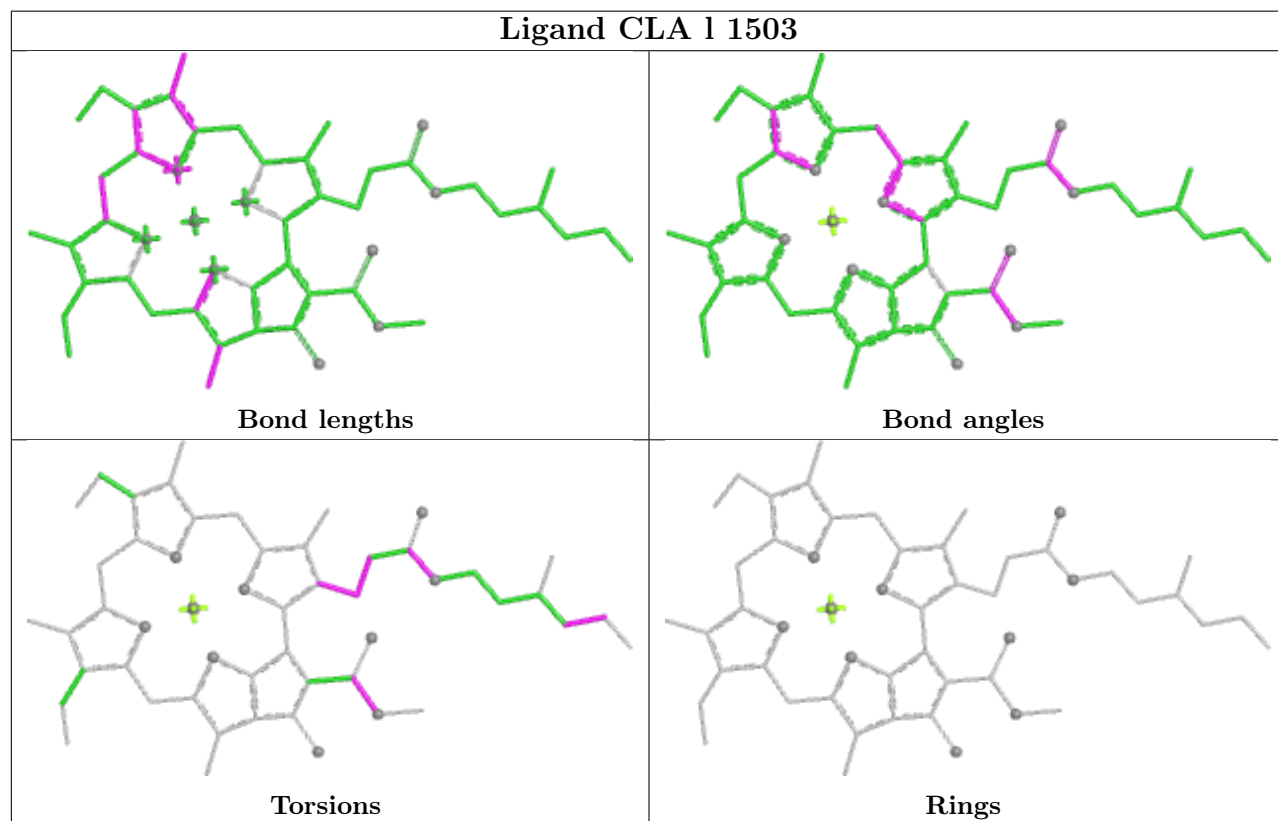
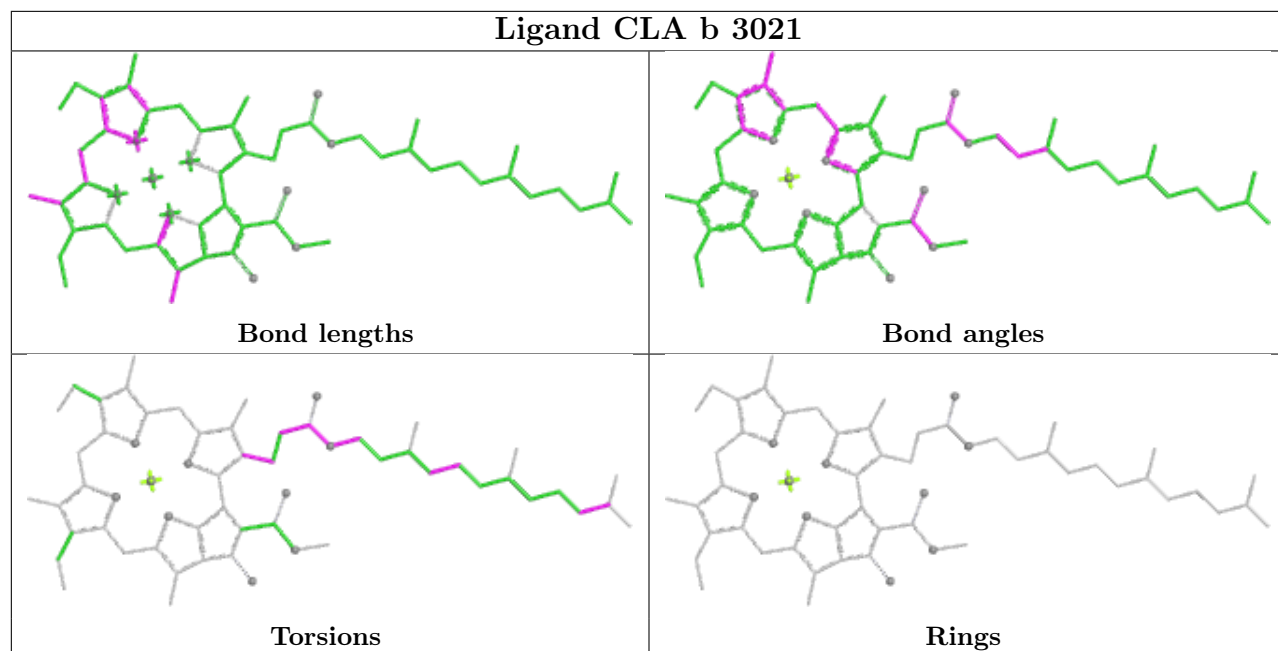


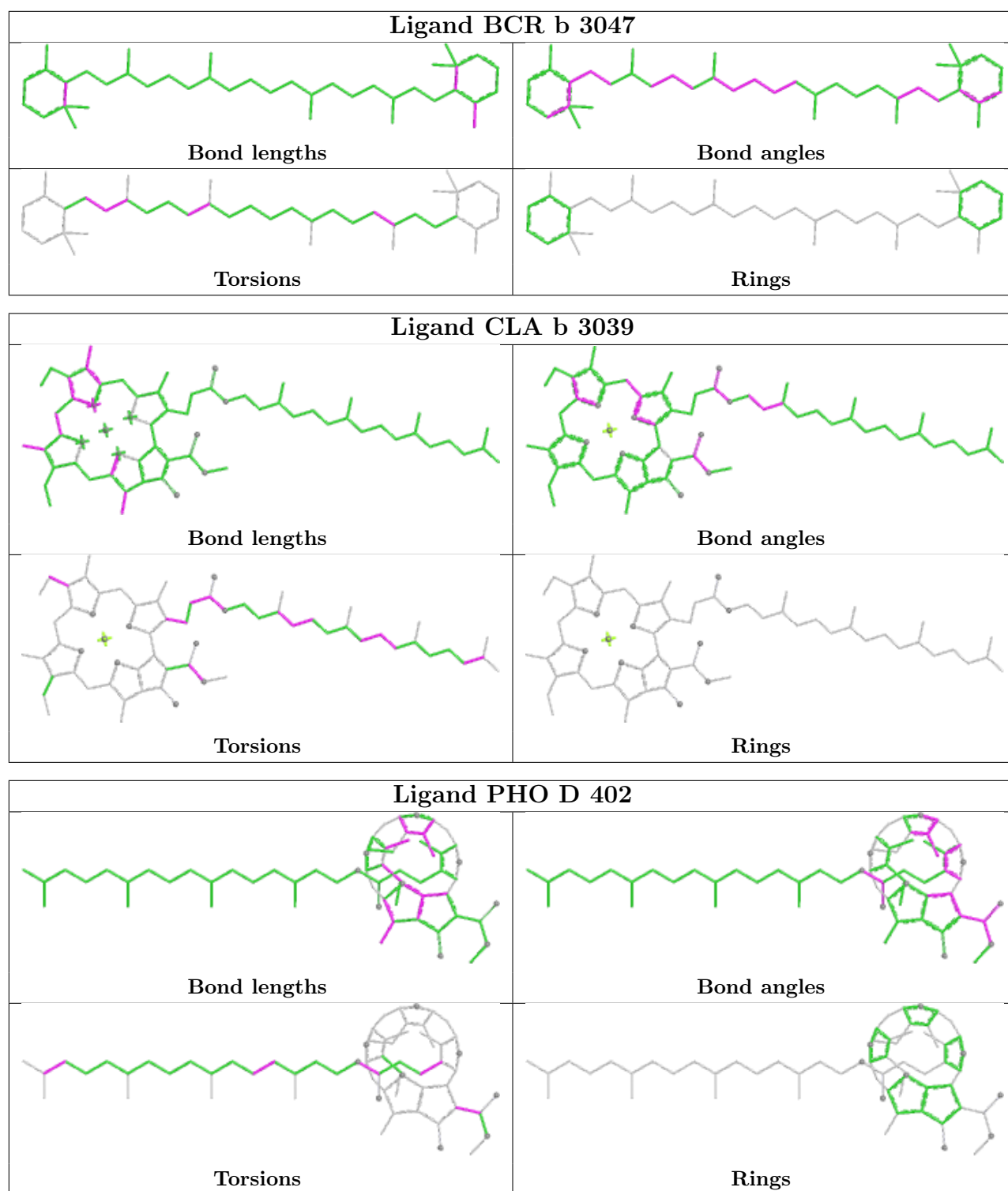
Ligand CLA b 3041



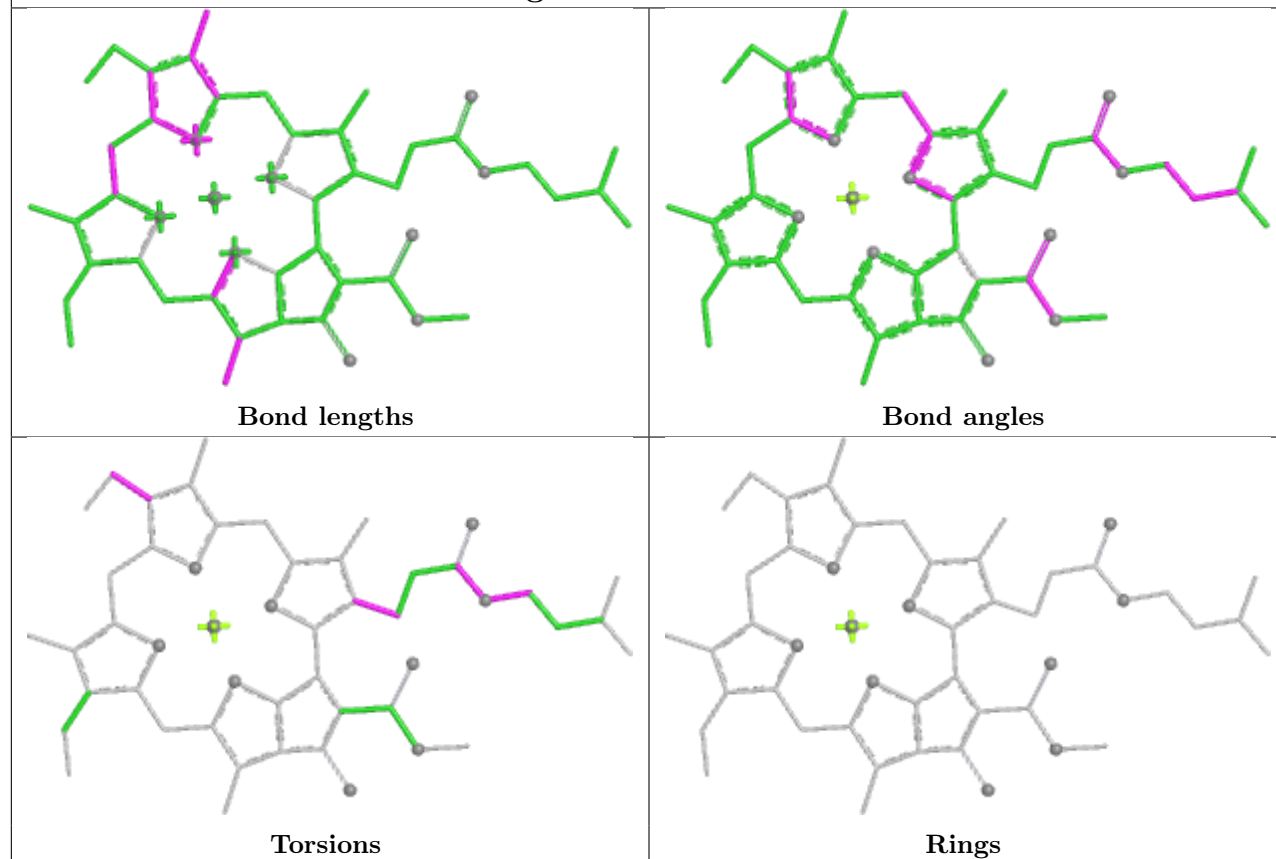




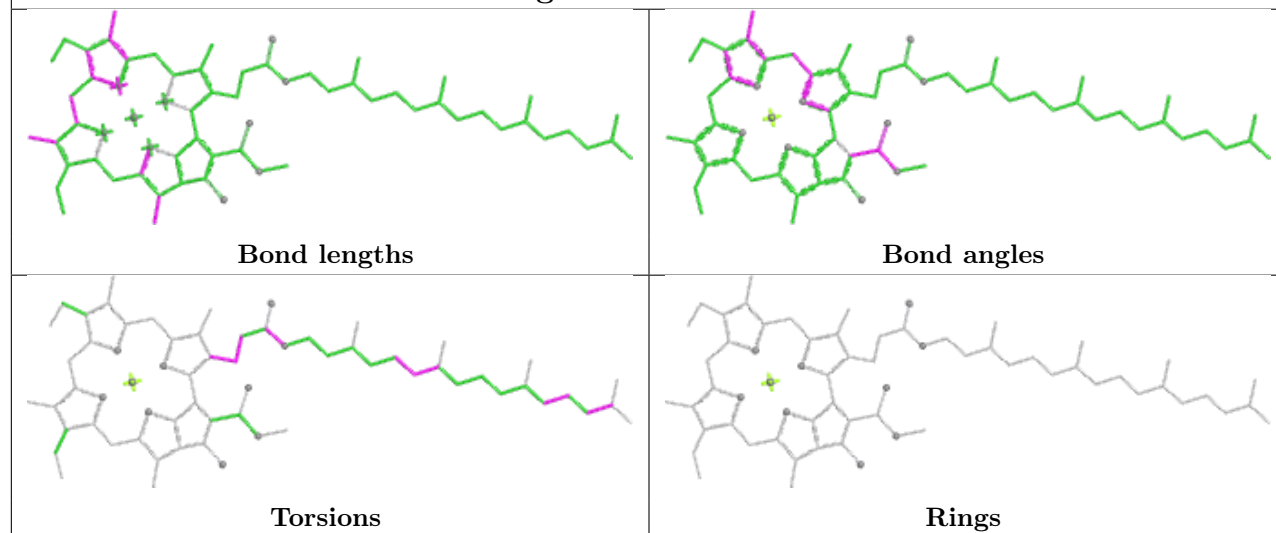


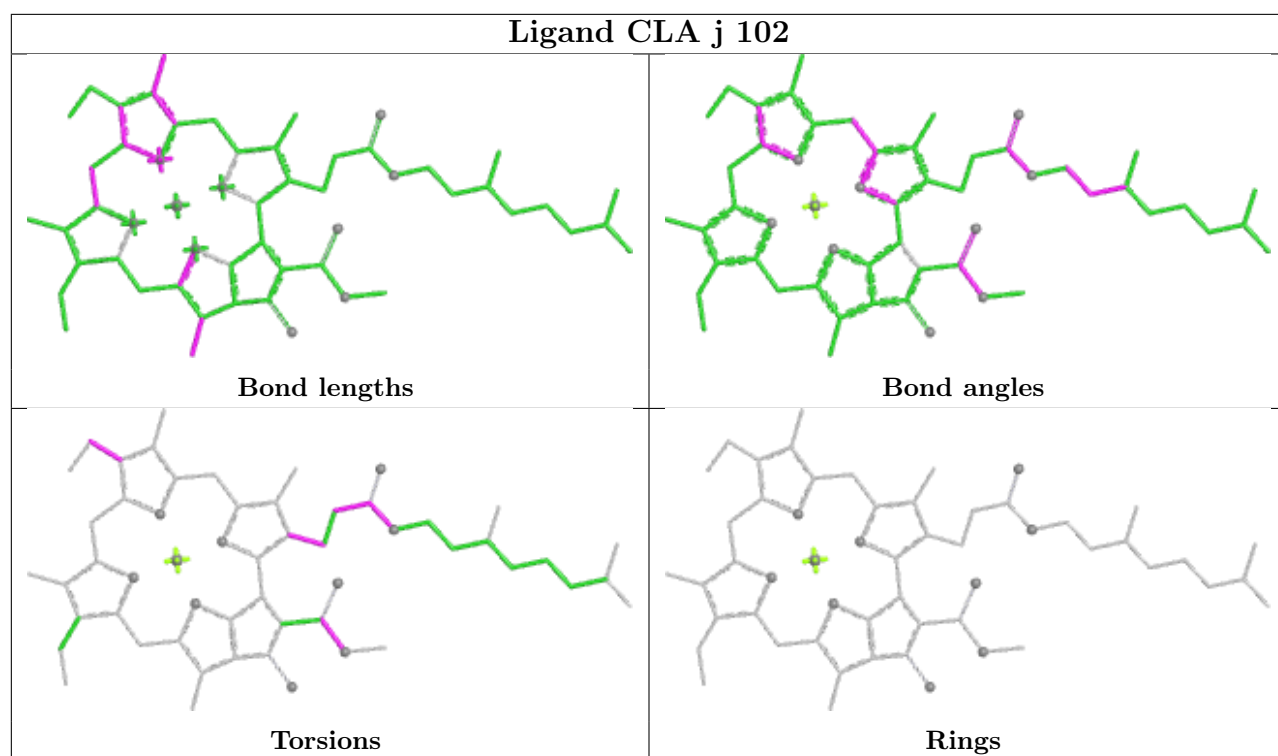


Ligand CLA b 3038

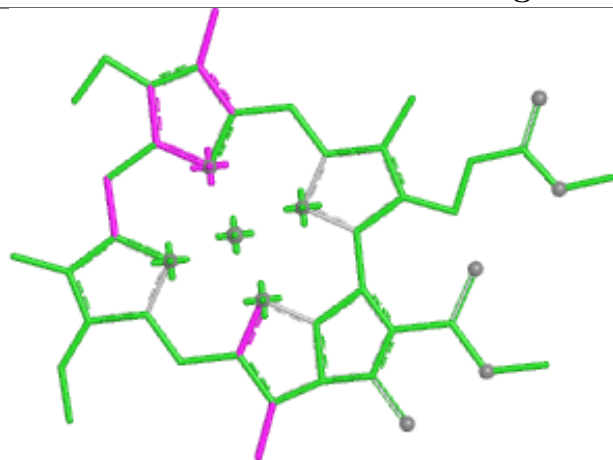


Ligand CLA a 805

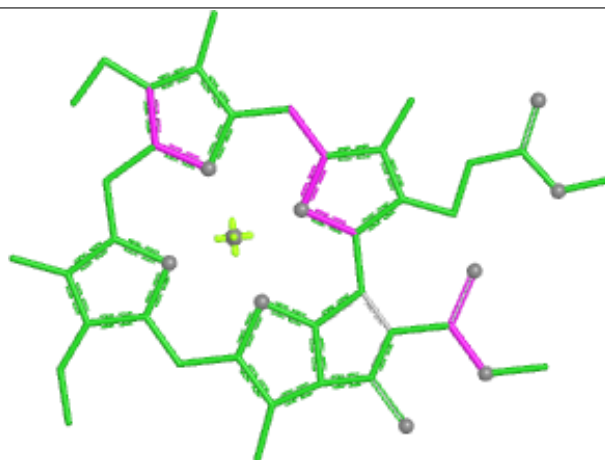




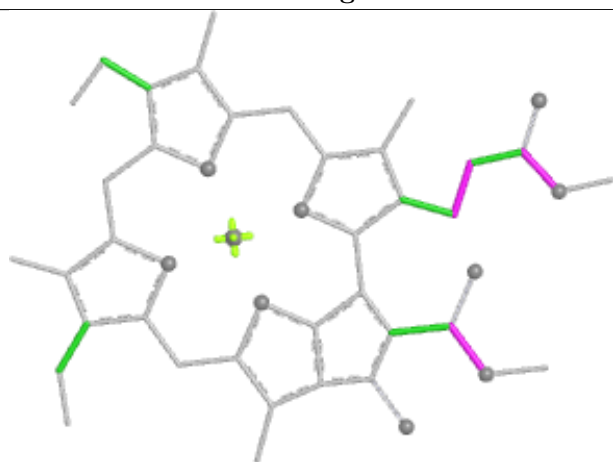
Ligand CLA D 404



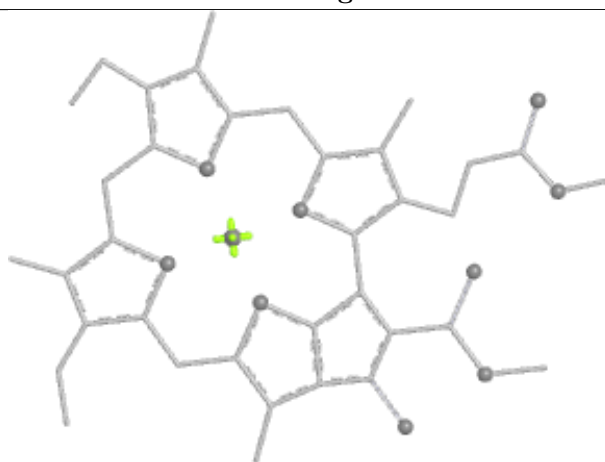
Bond lengths



Bond angles

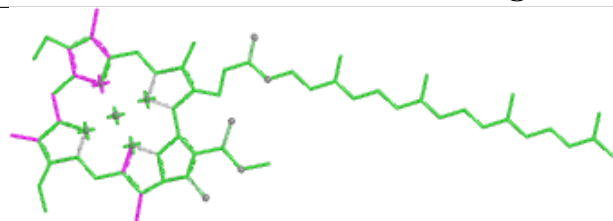


Torsions

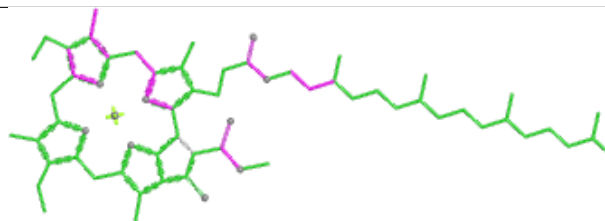


Rings

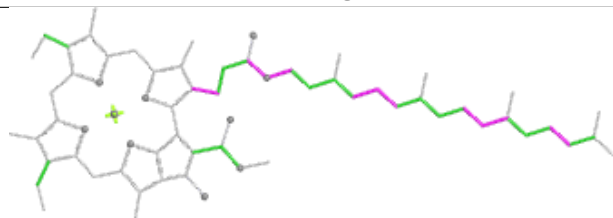
Ligand CLA b 3024



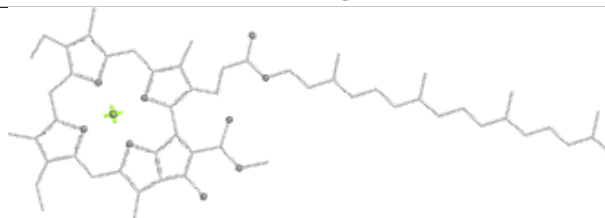
Bond lengths



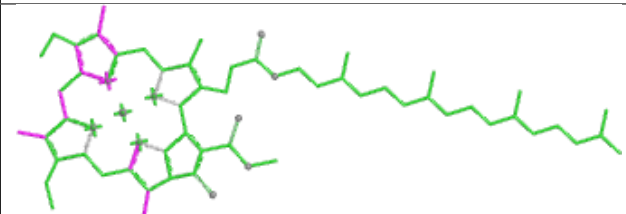
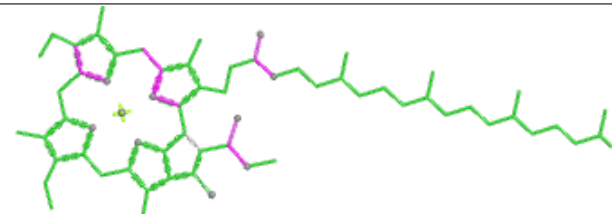
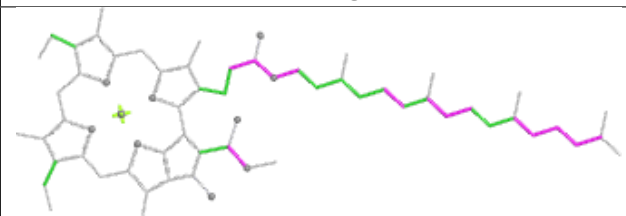
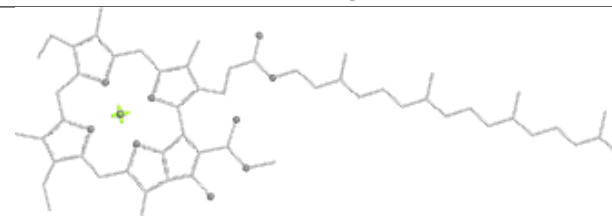
Bond angles

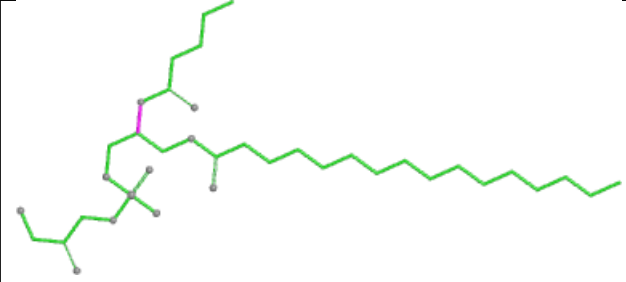
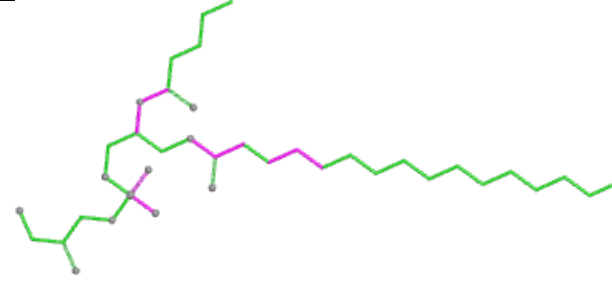
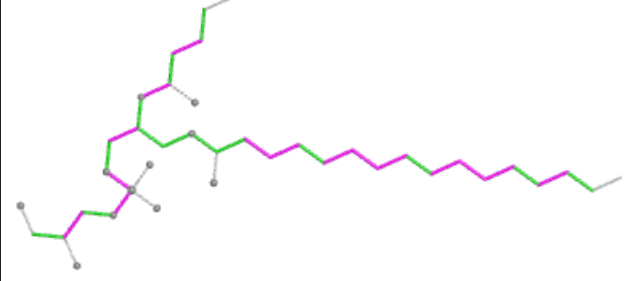
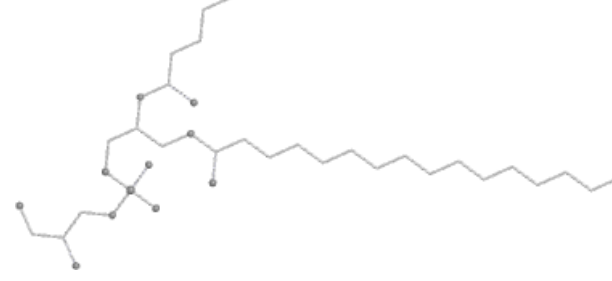


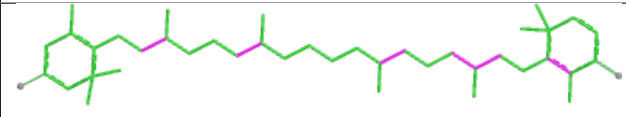
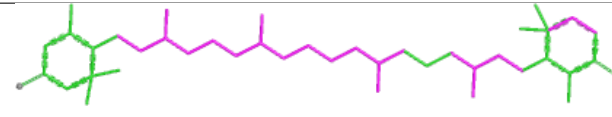
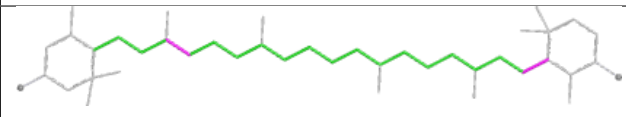
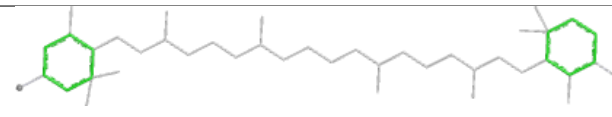
Torsions

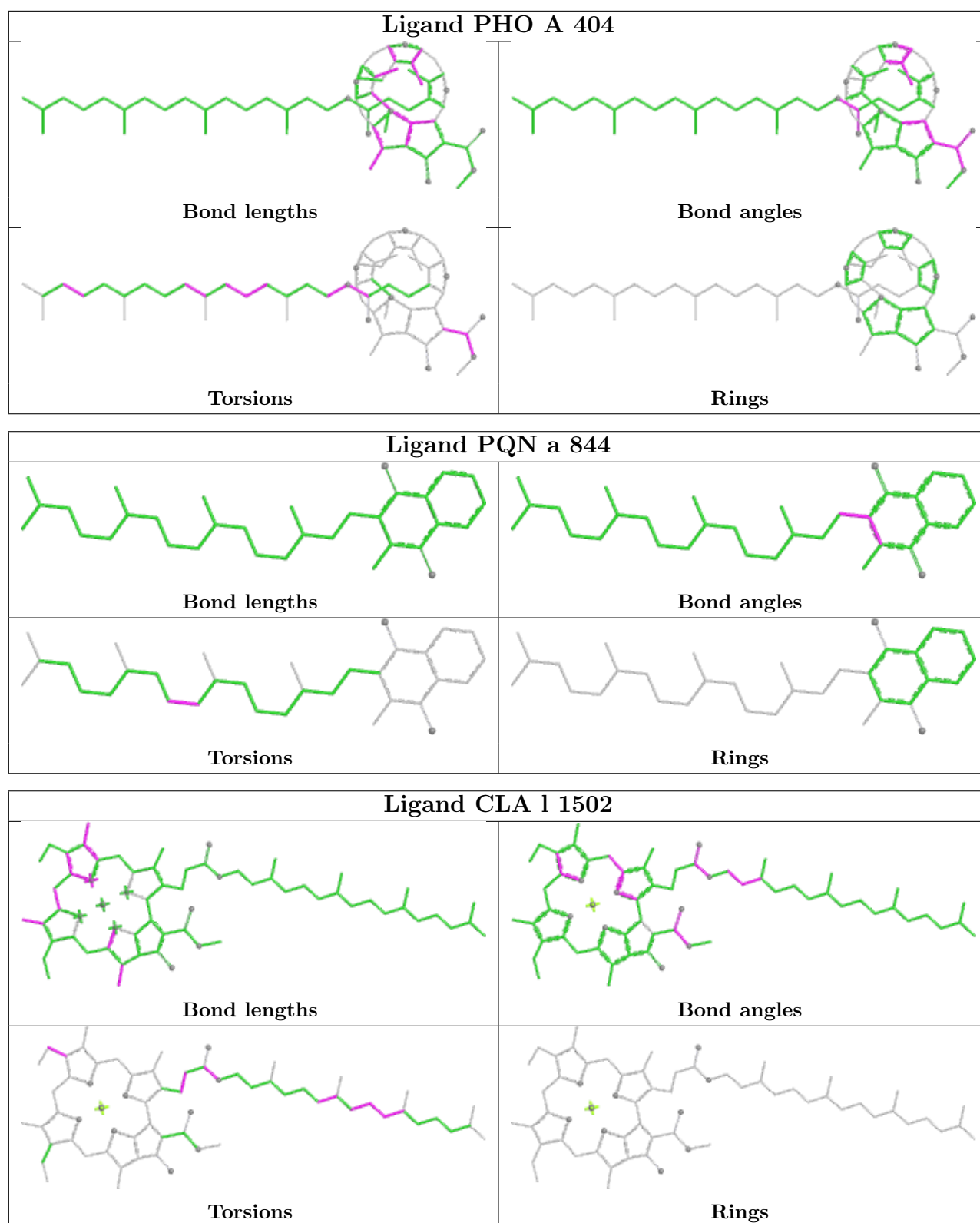


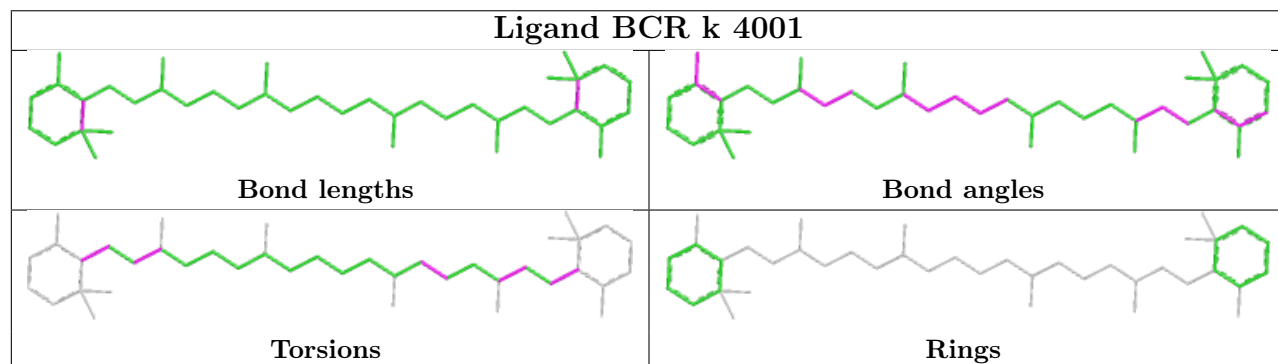
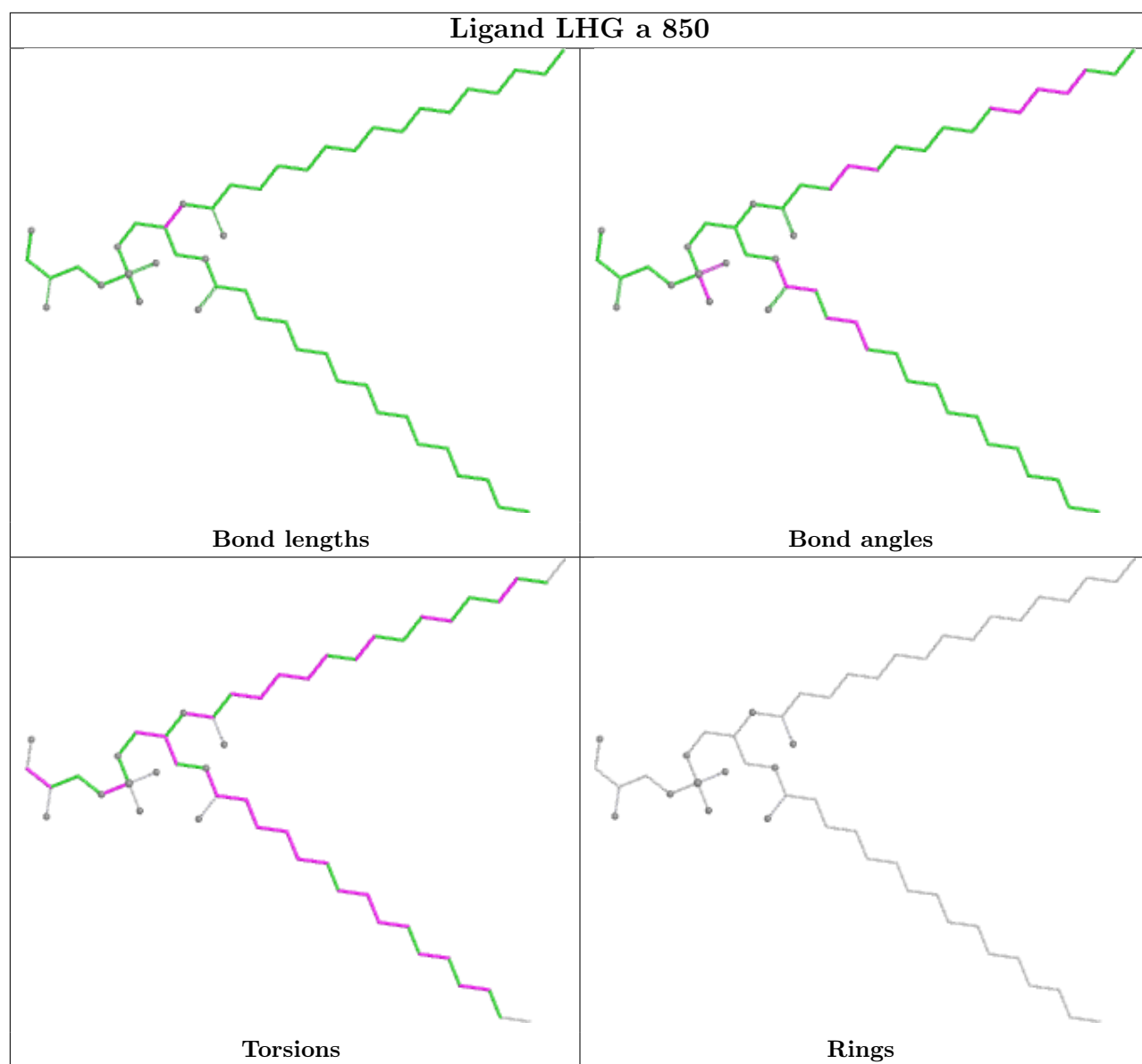
Rings

Ligand CLA a 830	
	
Bond lengths	Bond angles
	
Torsions	Rings

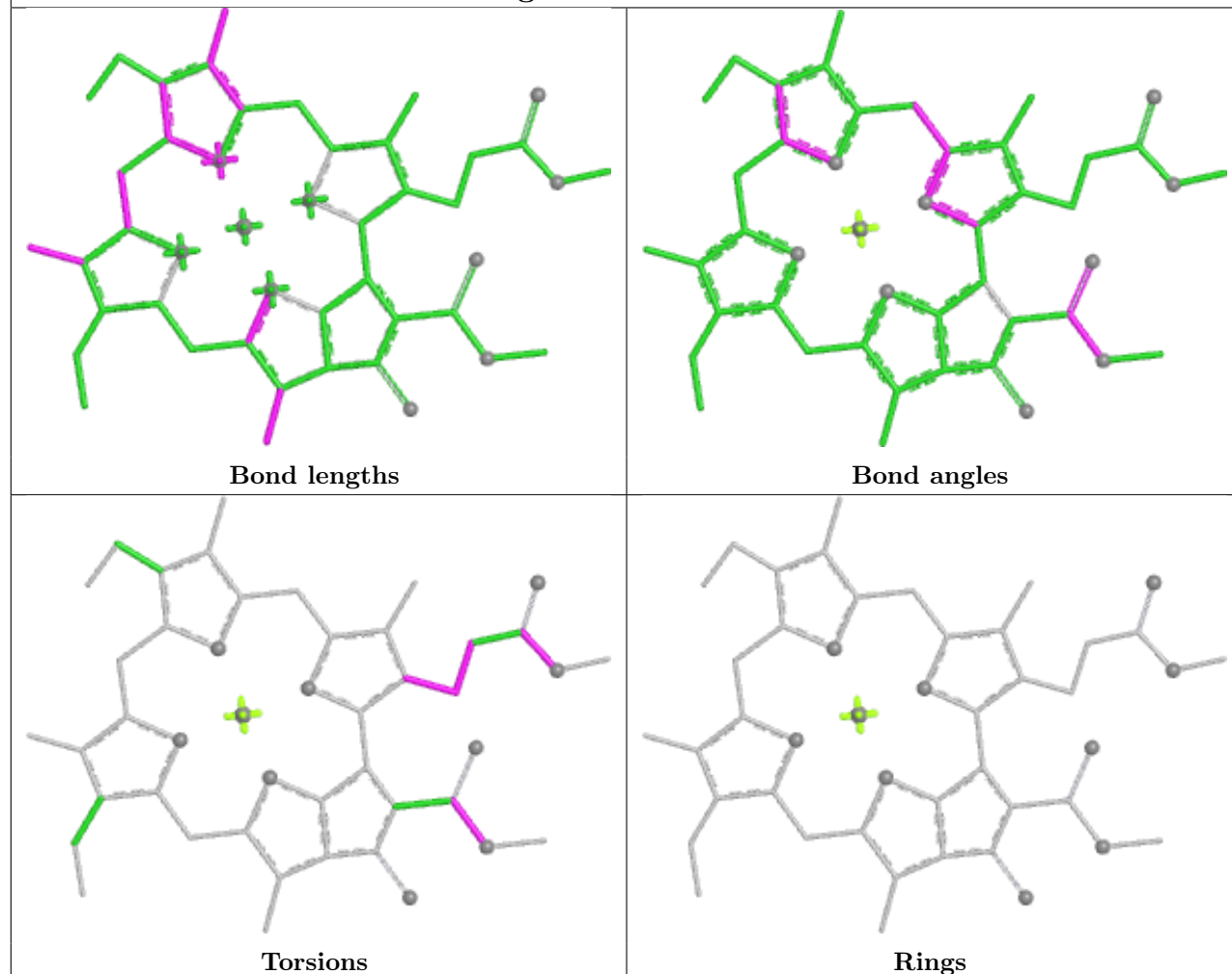
Ligand LHG b 3050	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand EQ3 b 3052	
	
Bond lengths	Bond angles
	
Torsions	Rings

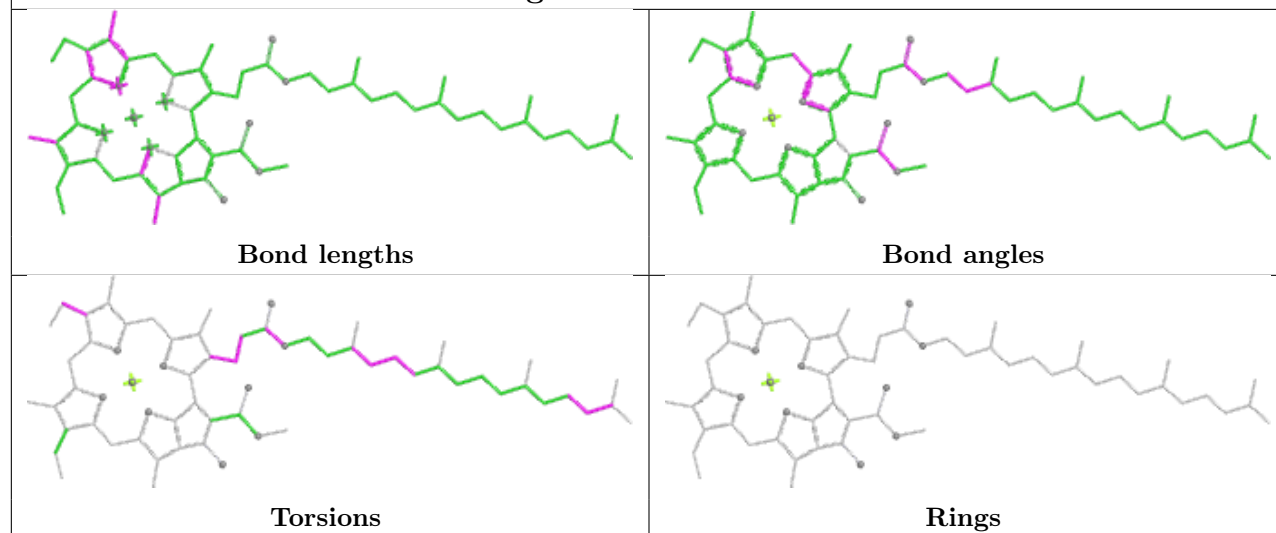




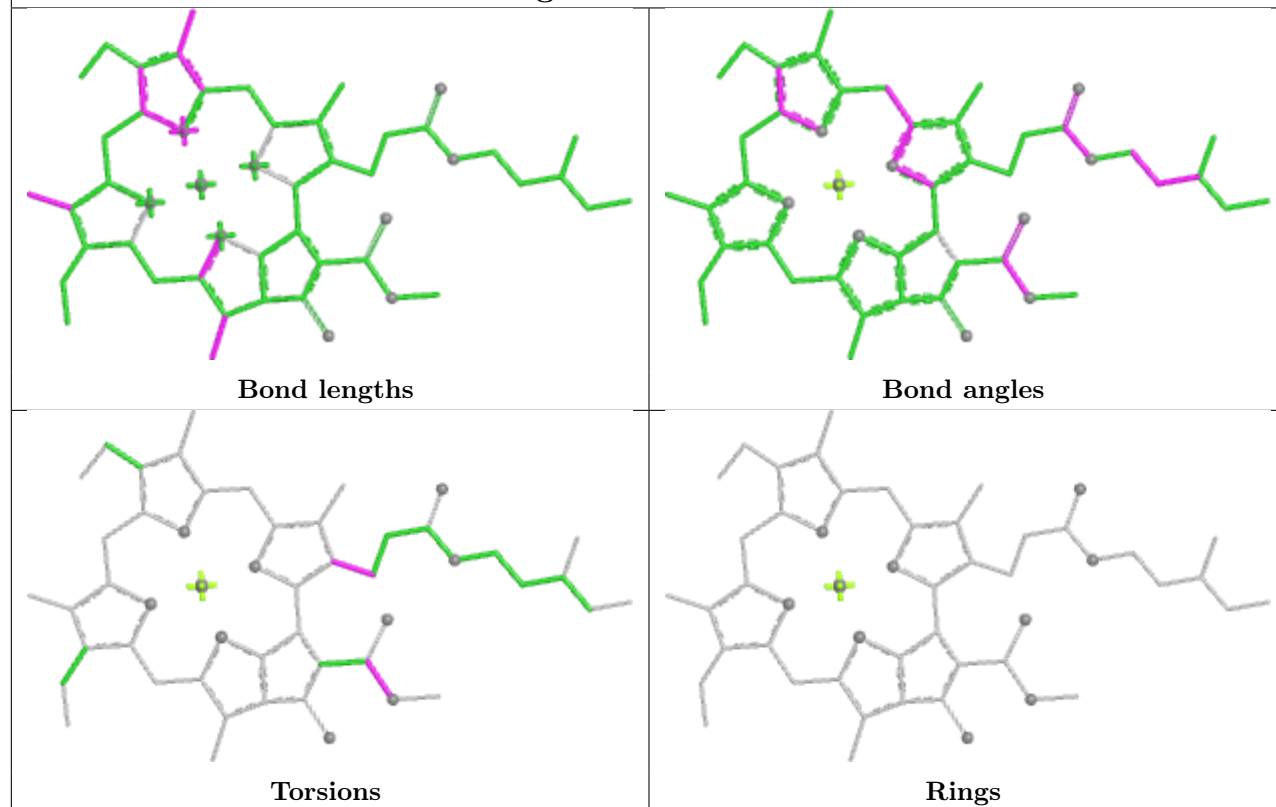
Ligand CLA a 817



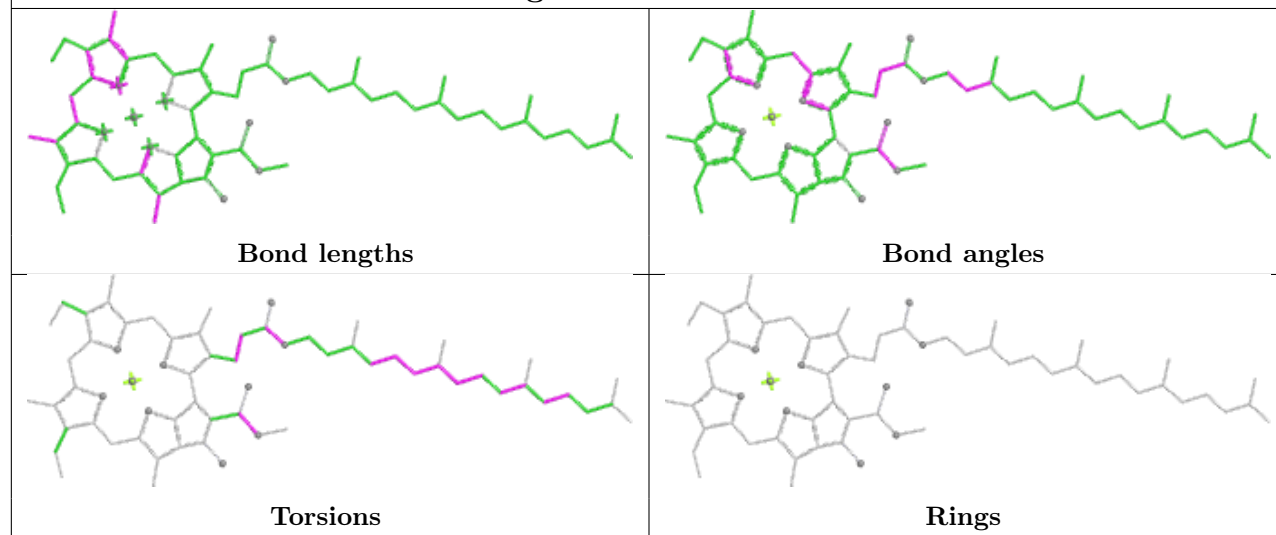
Ligand CLA b 3017

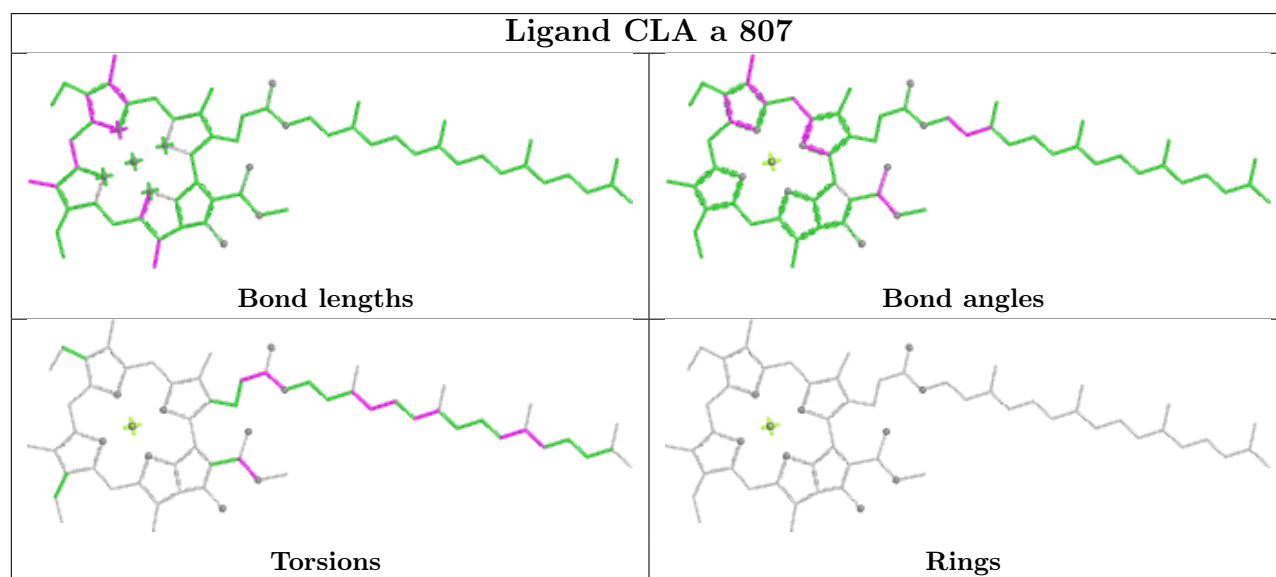
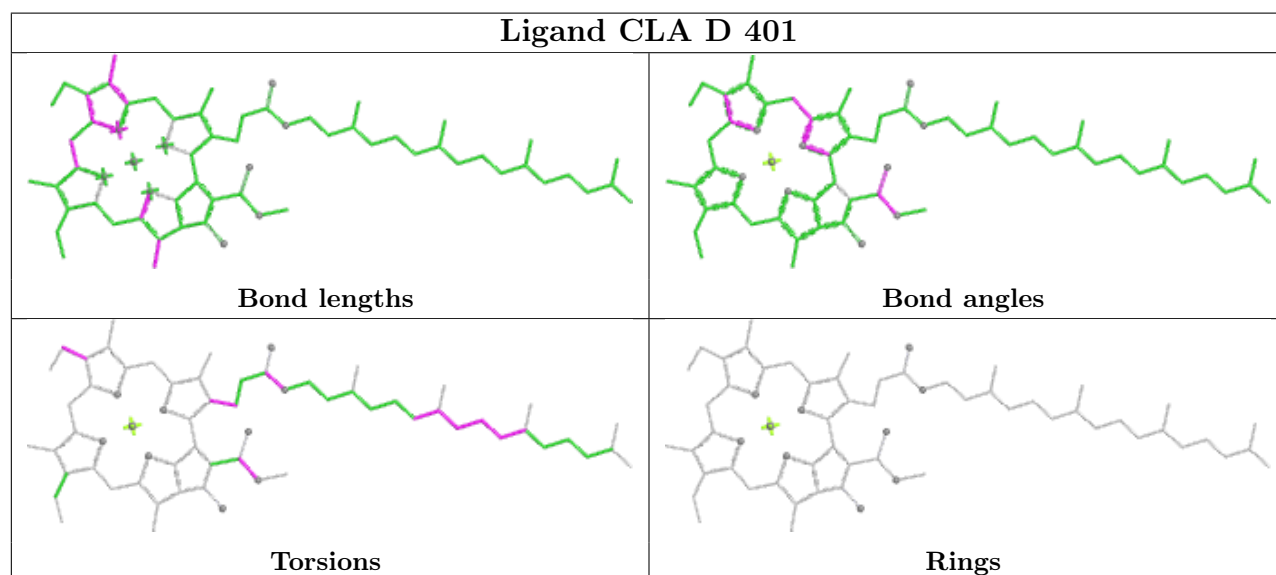
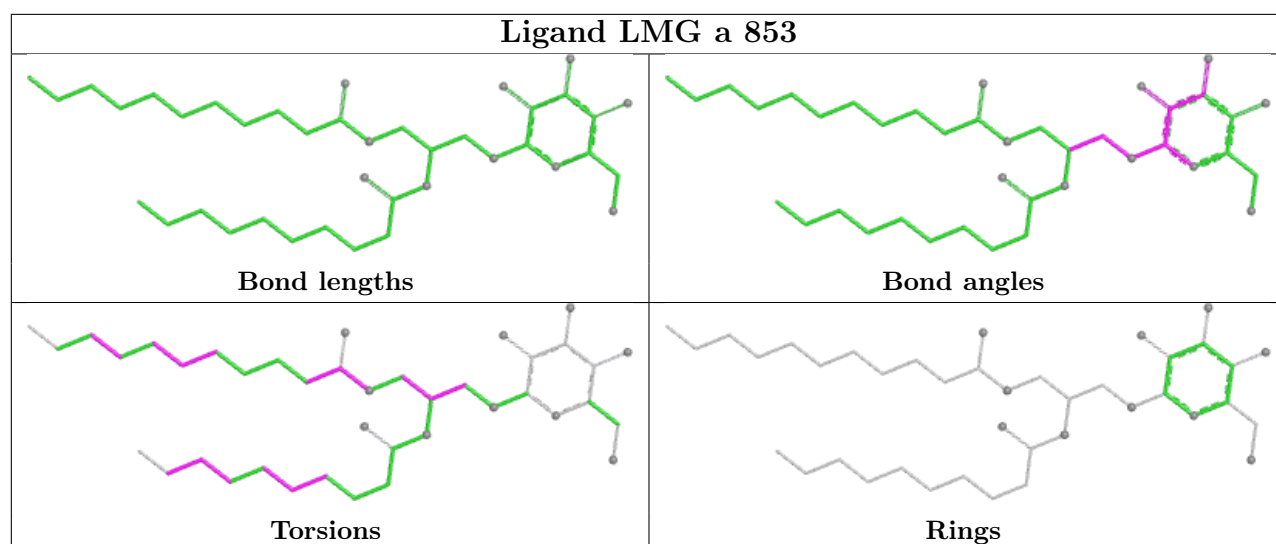


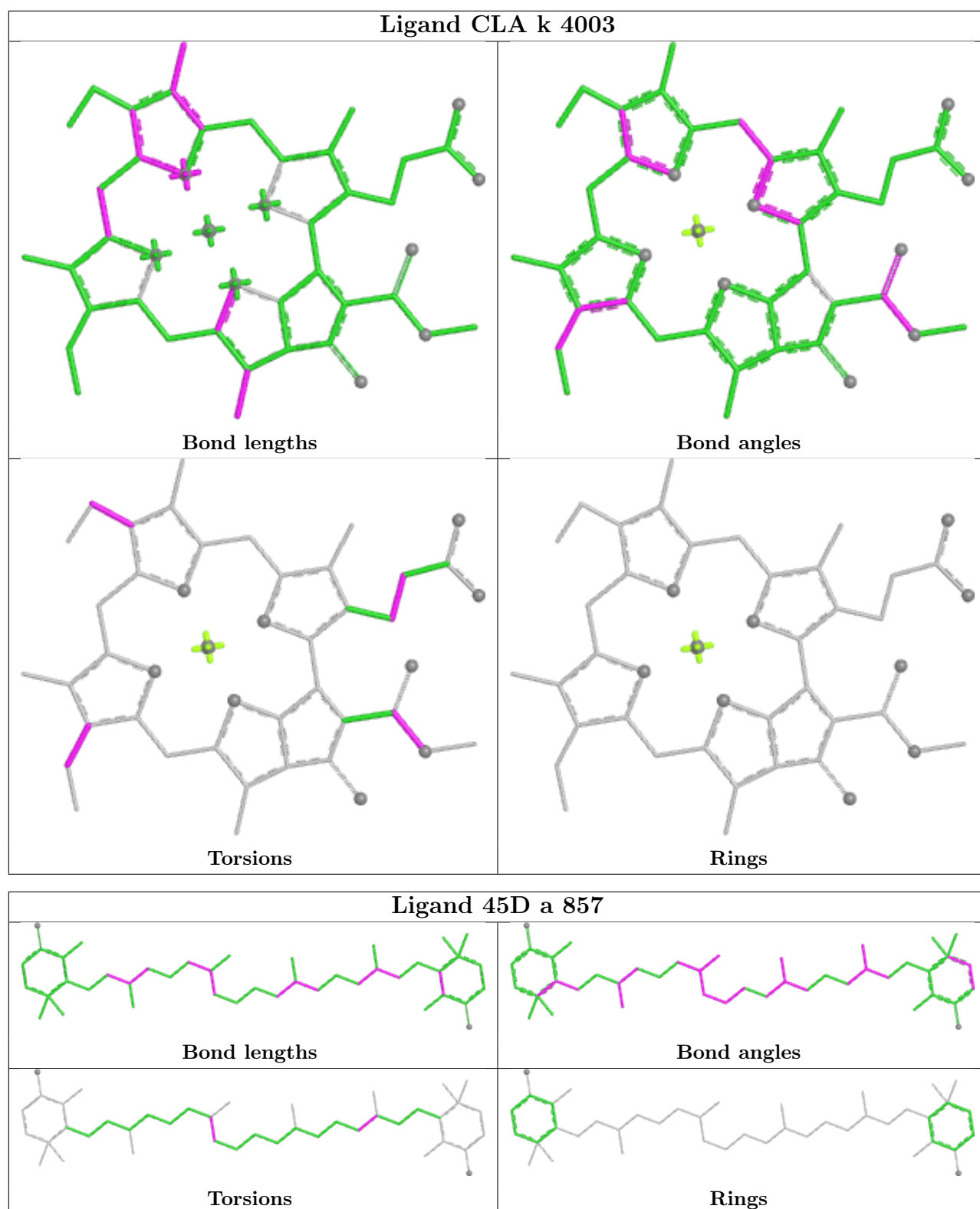
Ligand CLA a 810

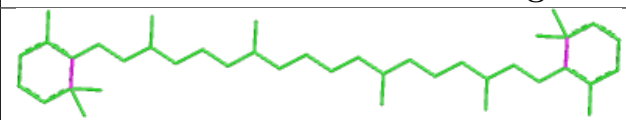
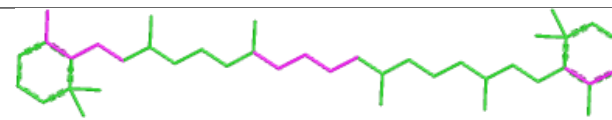
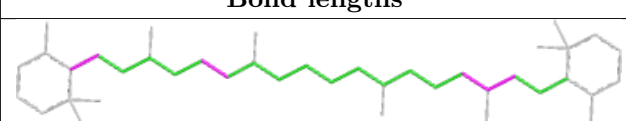
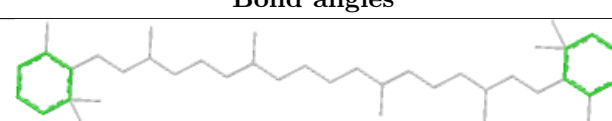


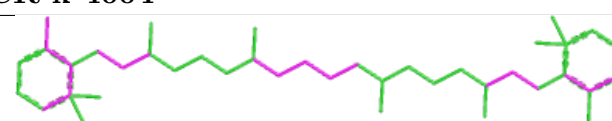
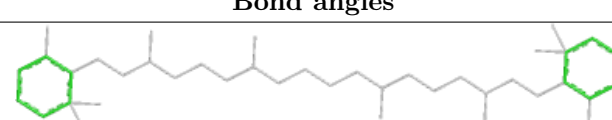
Ligand CLA b 3009

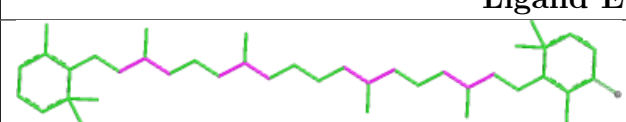
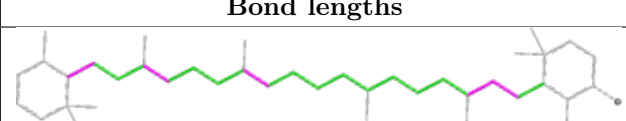
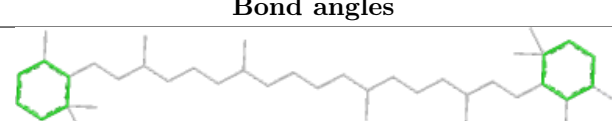


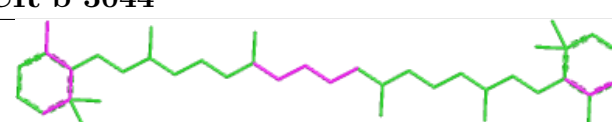
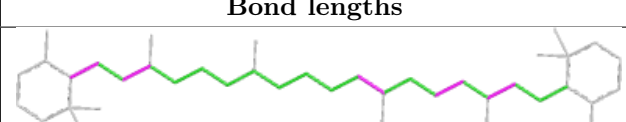
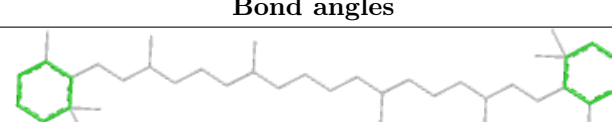


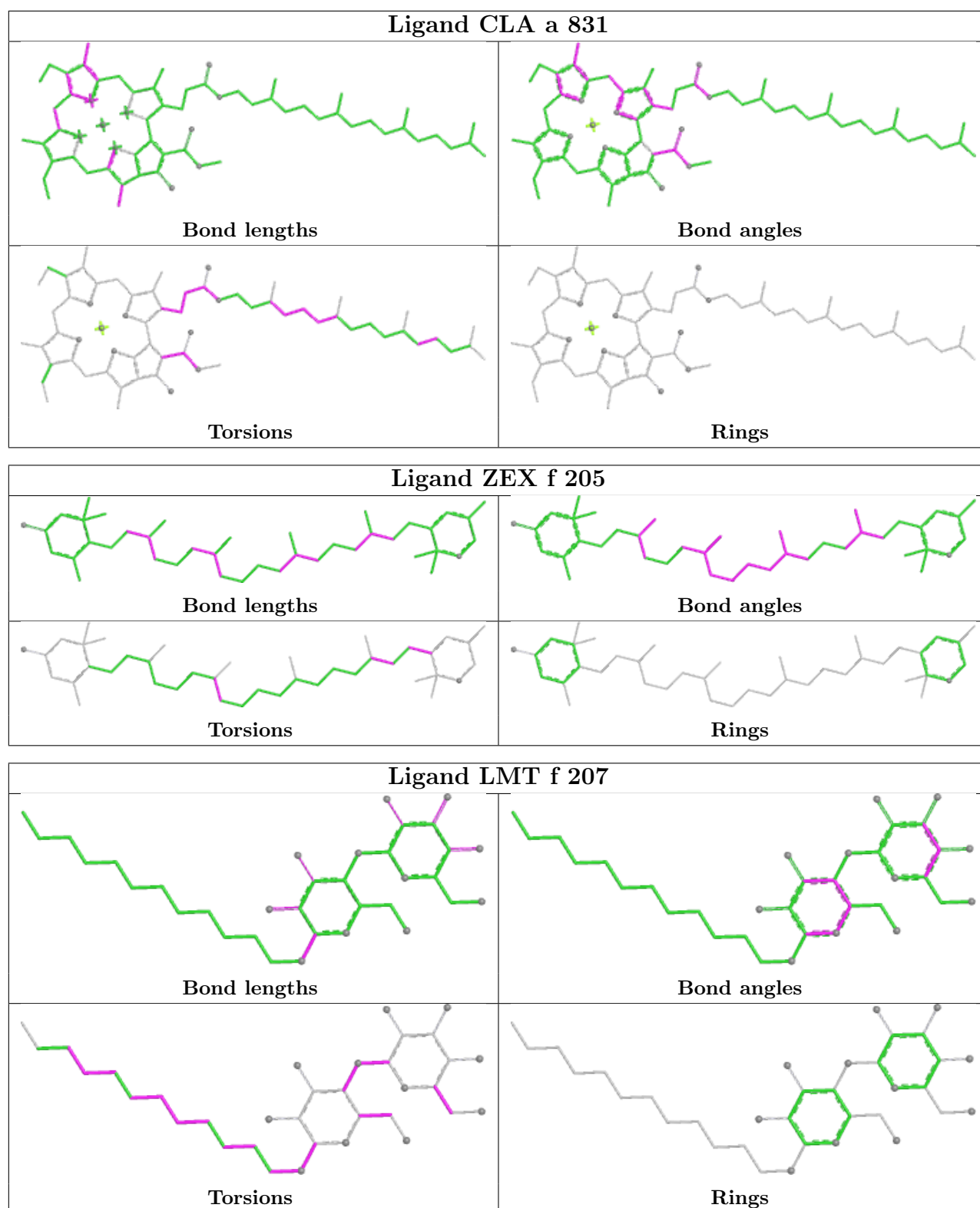


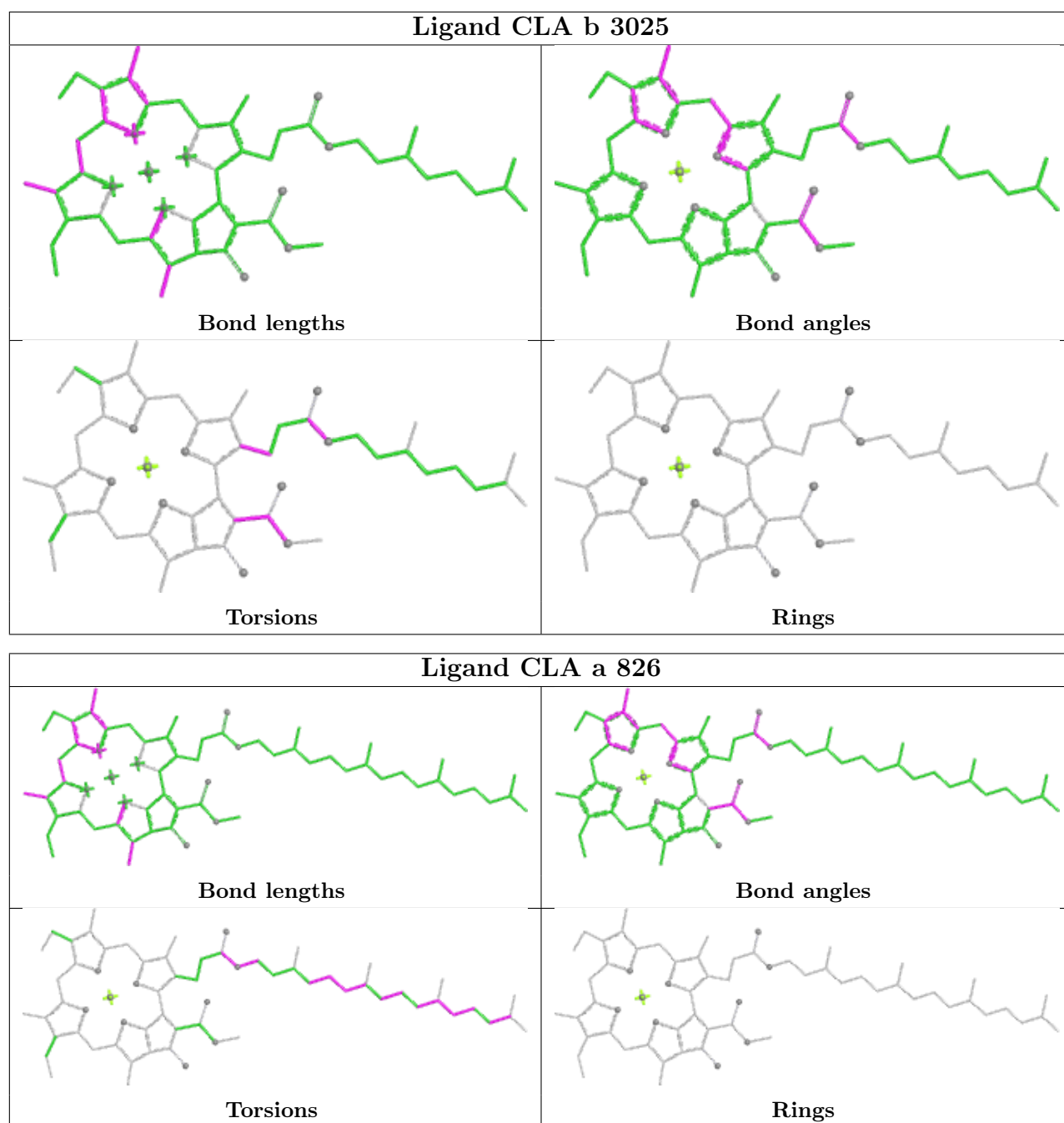
Ligand BCR i 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

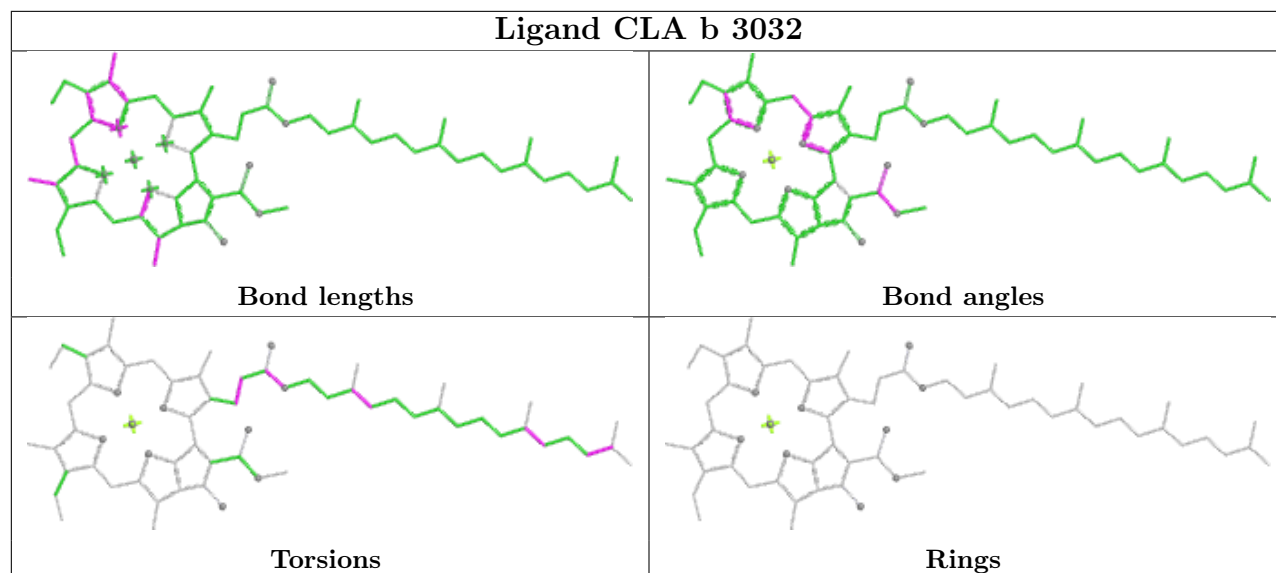
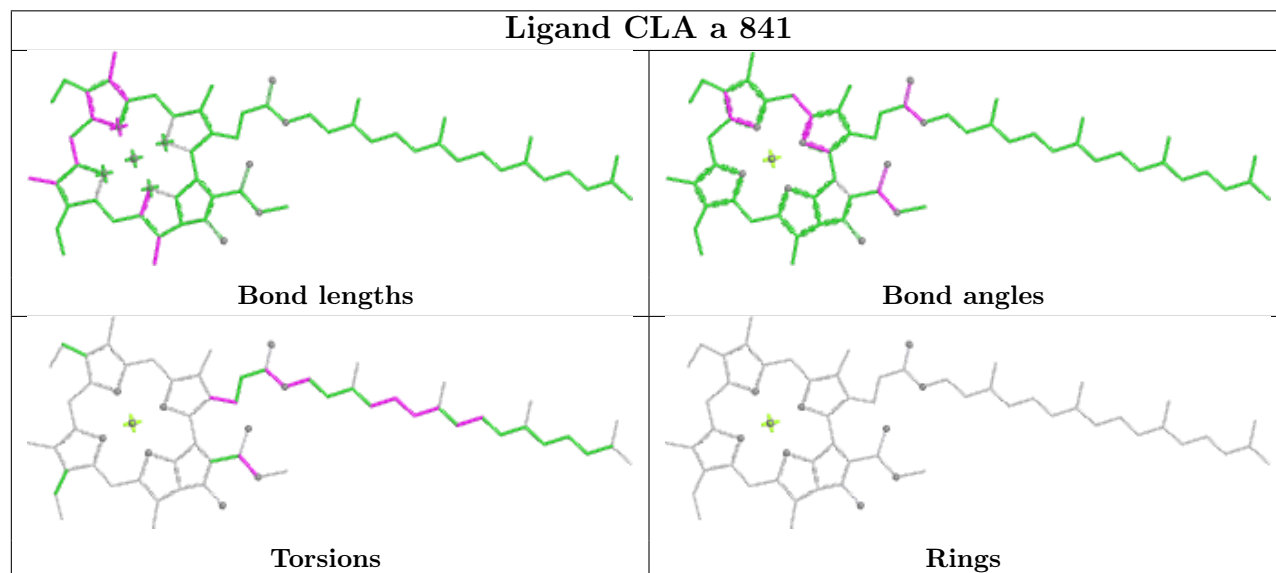
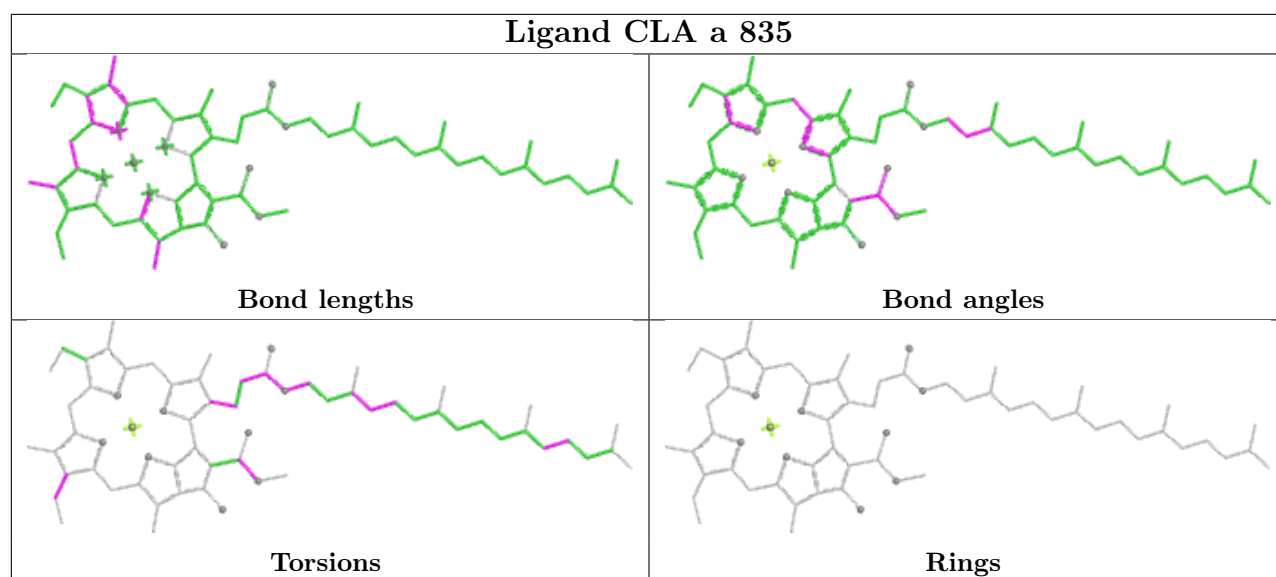
Ligand BCR k 4004	
	
Bond lengths	Bond angles
	
Torsions	Rings

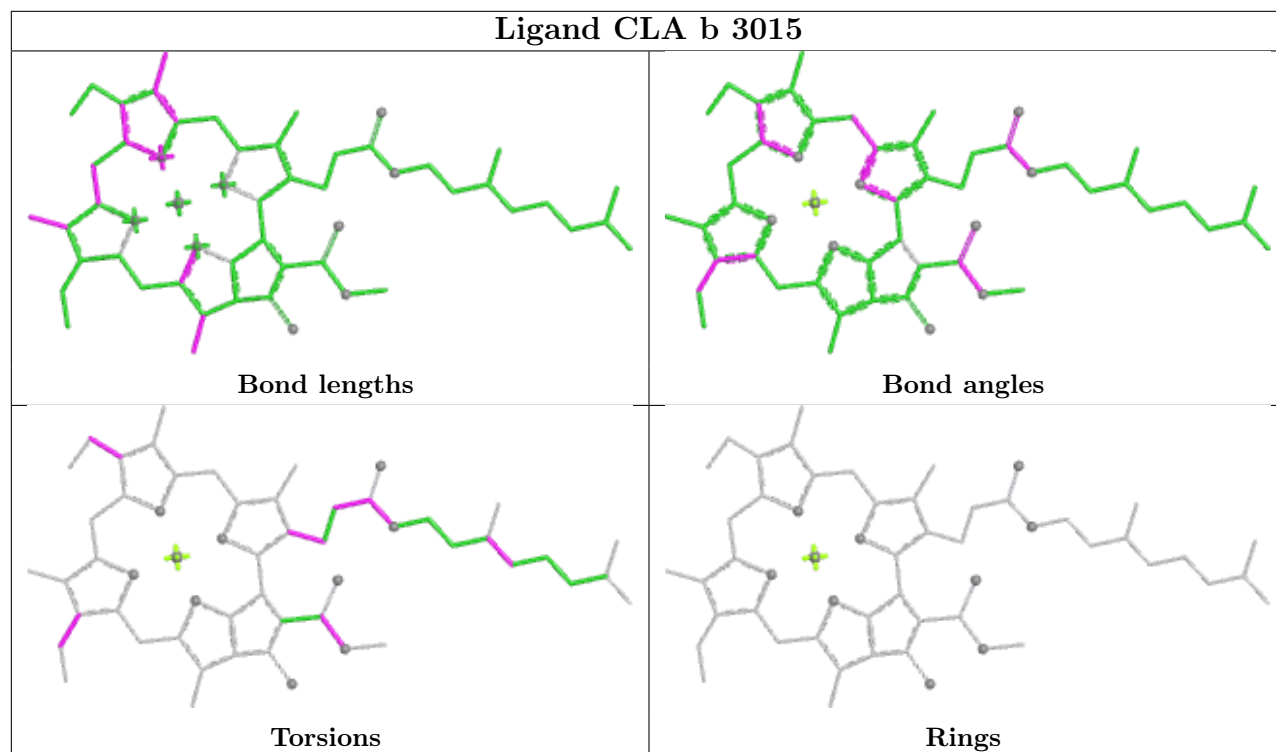
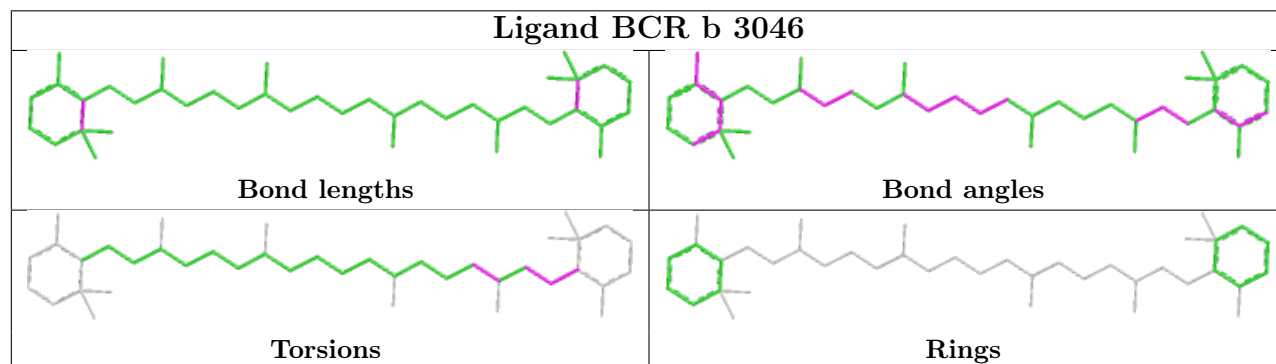
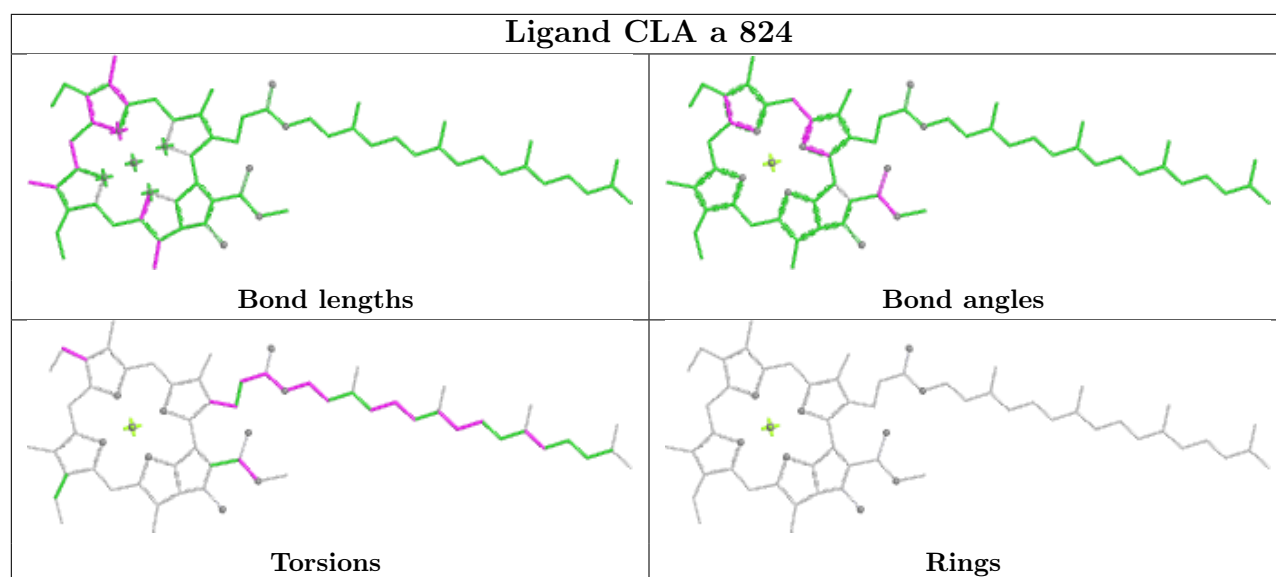
Ligand ECH b 3045	
	
Bond lengths	Bond angles
	
Torsions	Rings

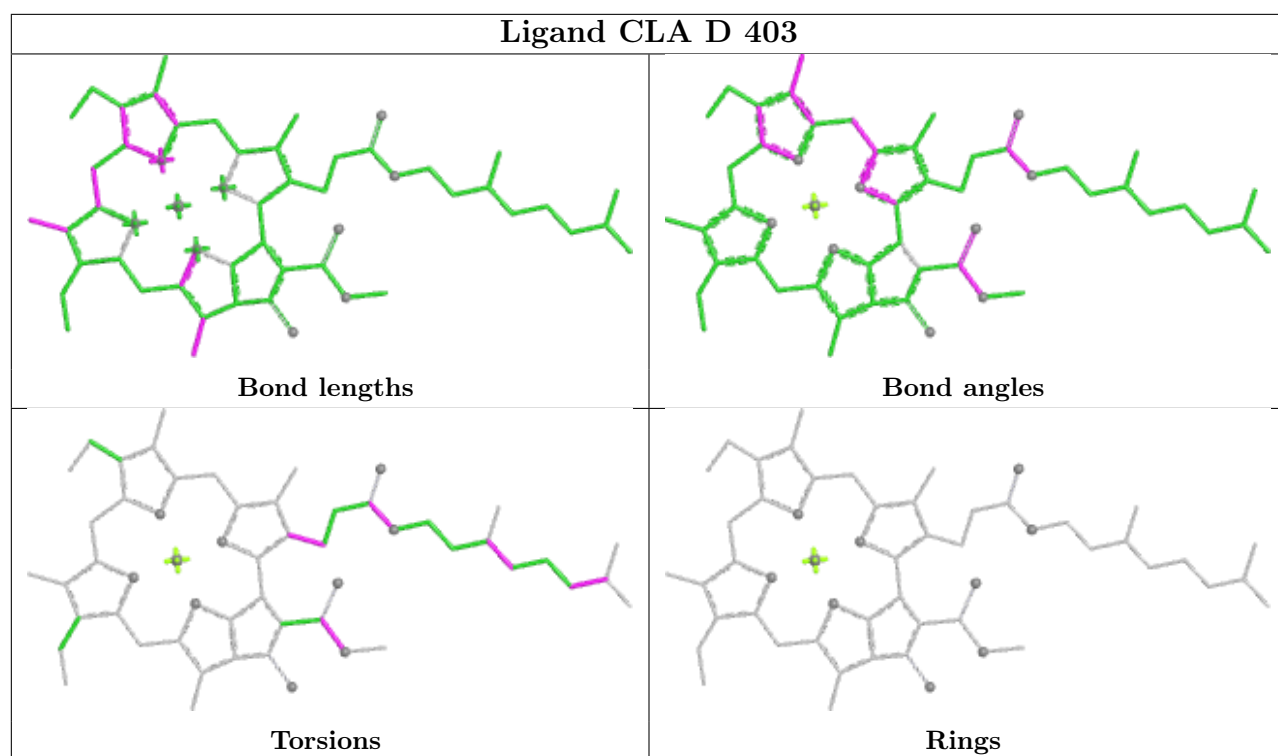
Ligand BCR b 3044	
	
Bond lengths	Bond angles
	
Torsions	Rings

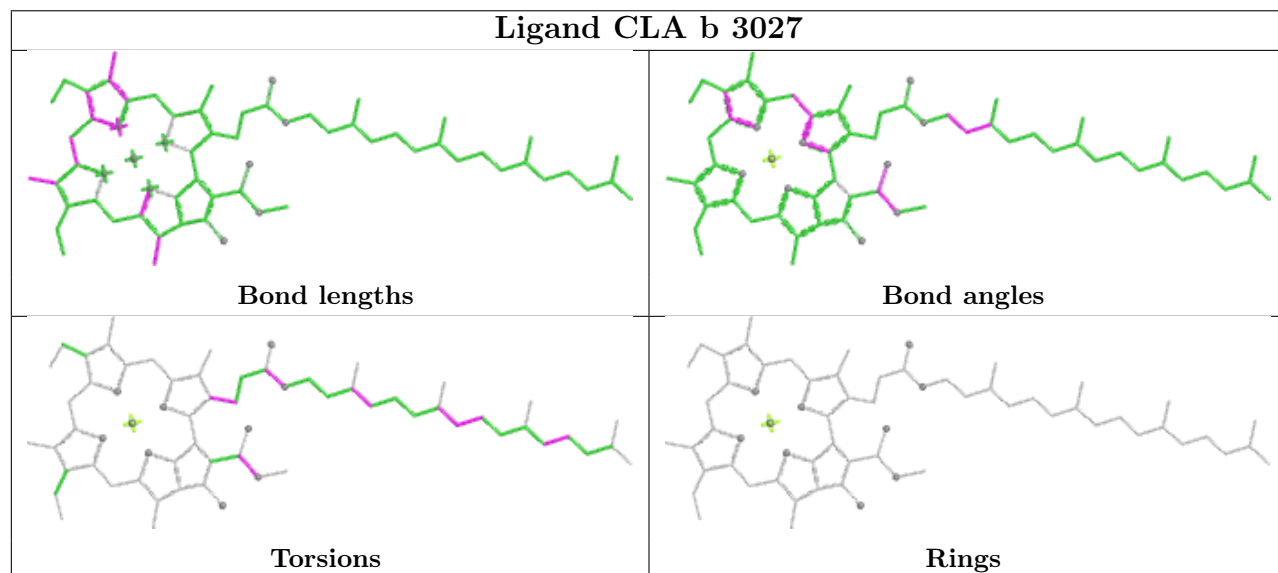
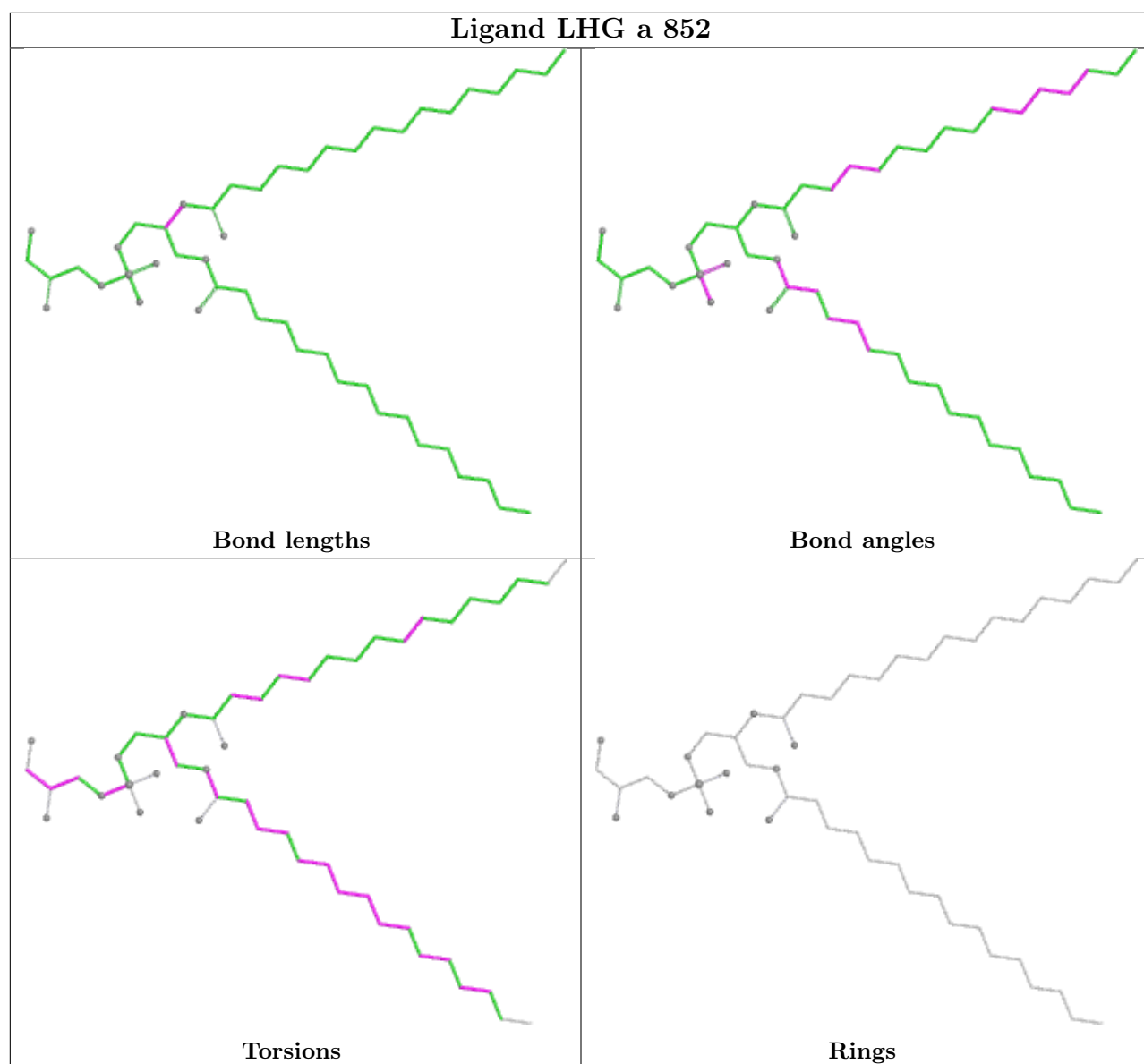


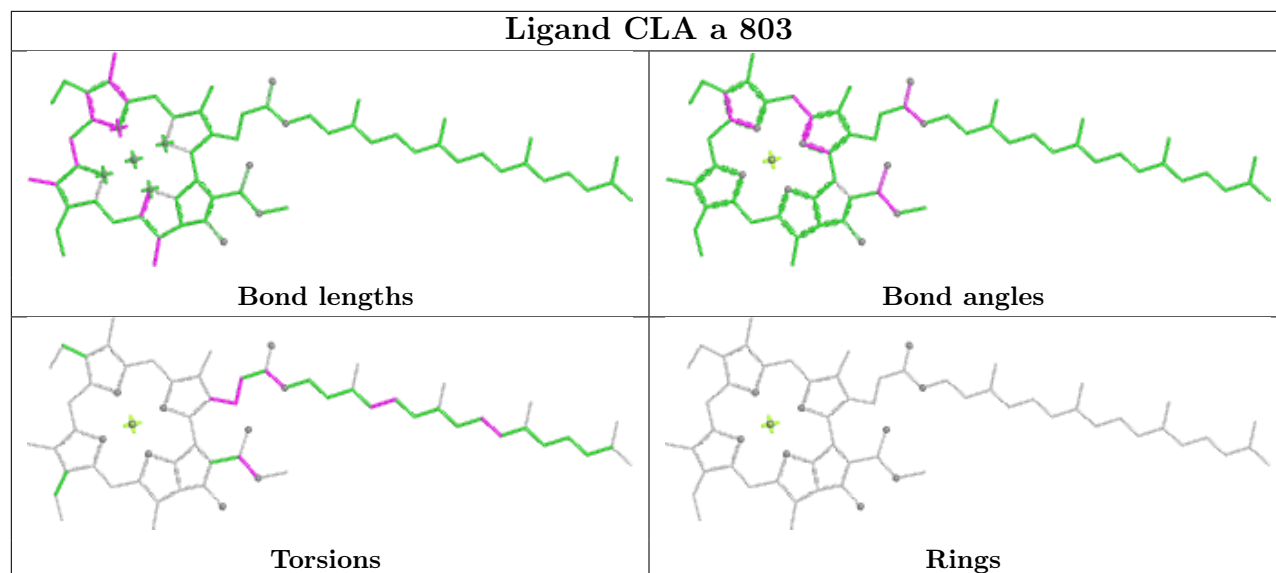
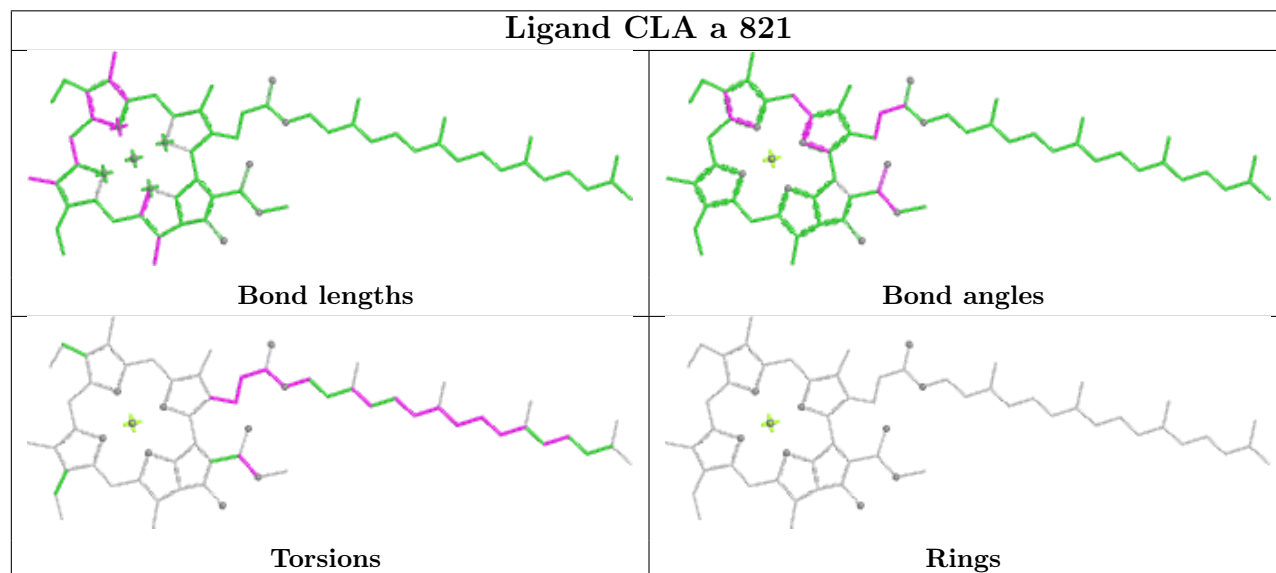
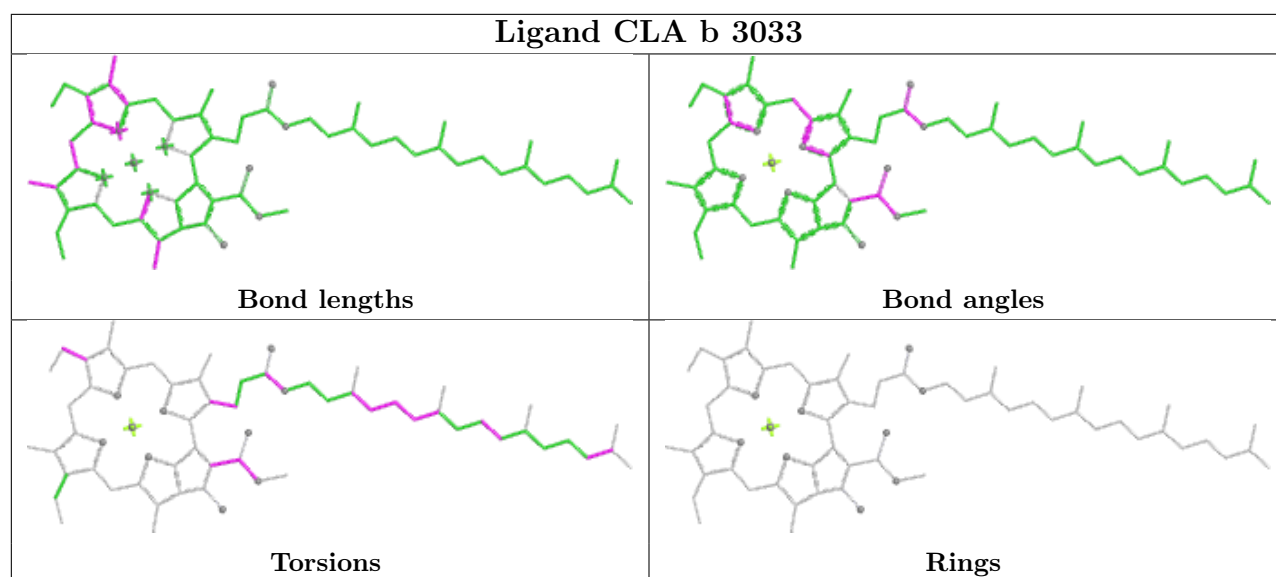


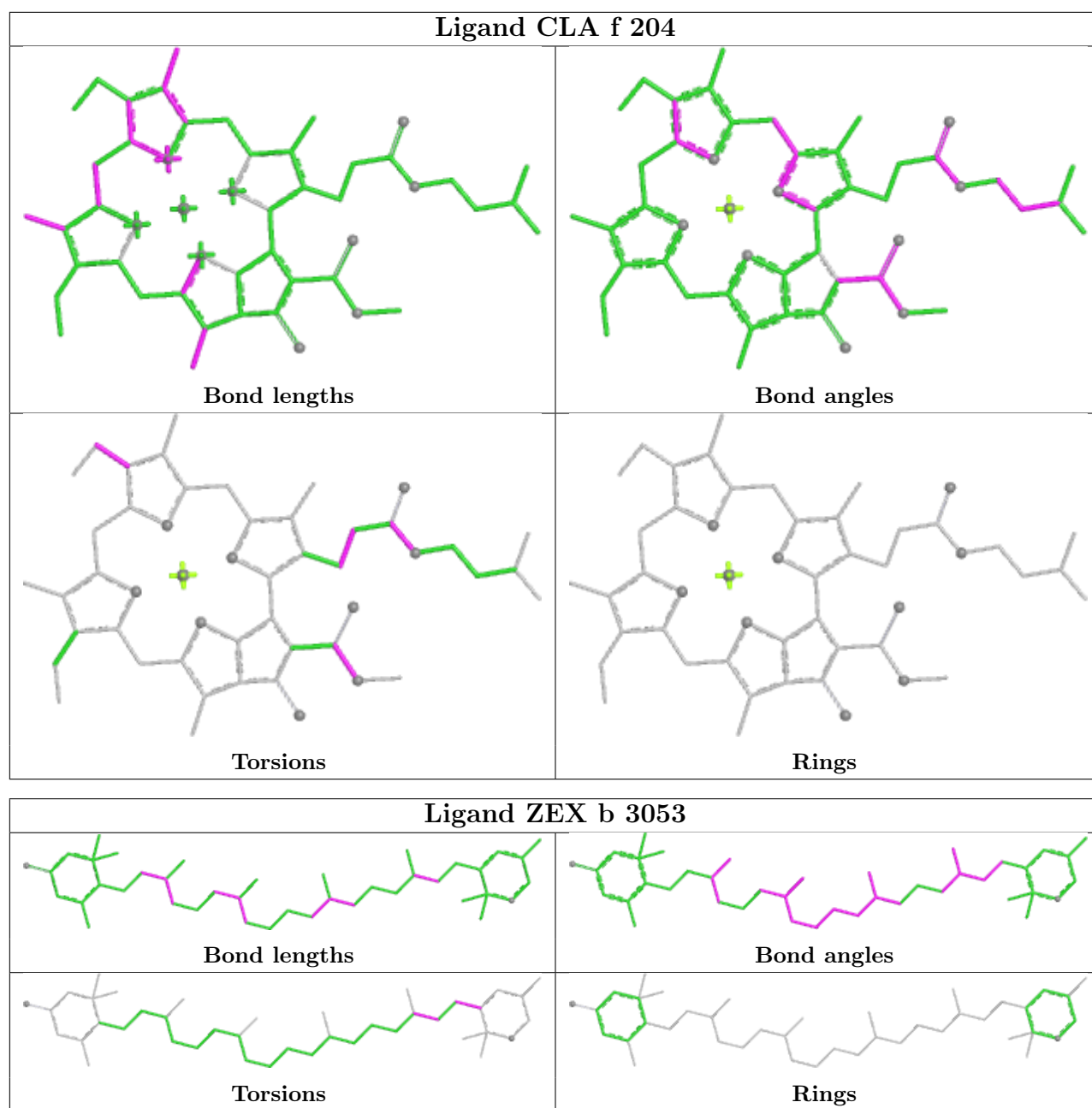


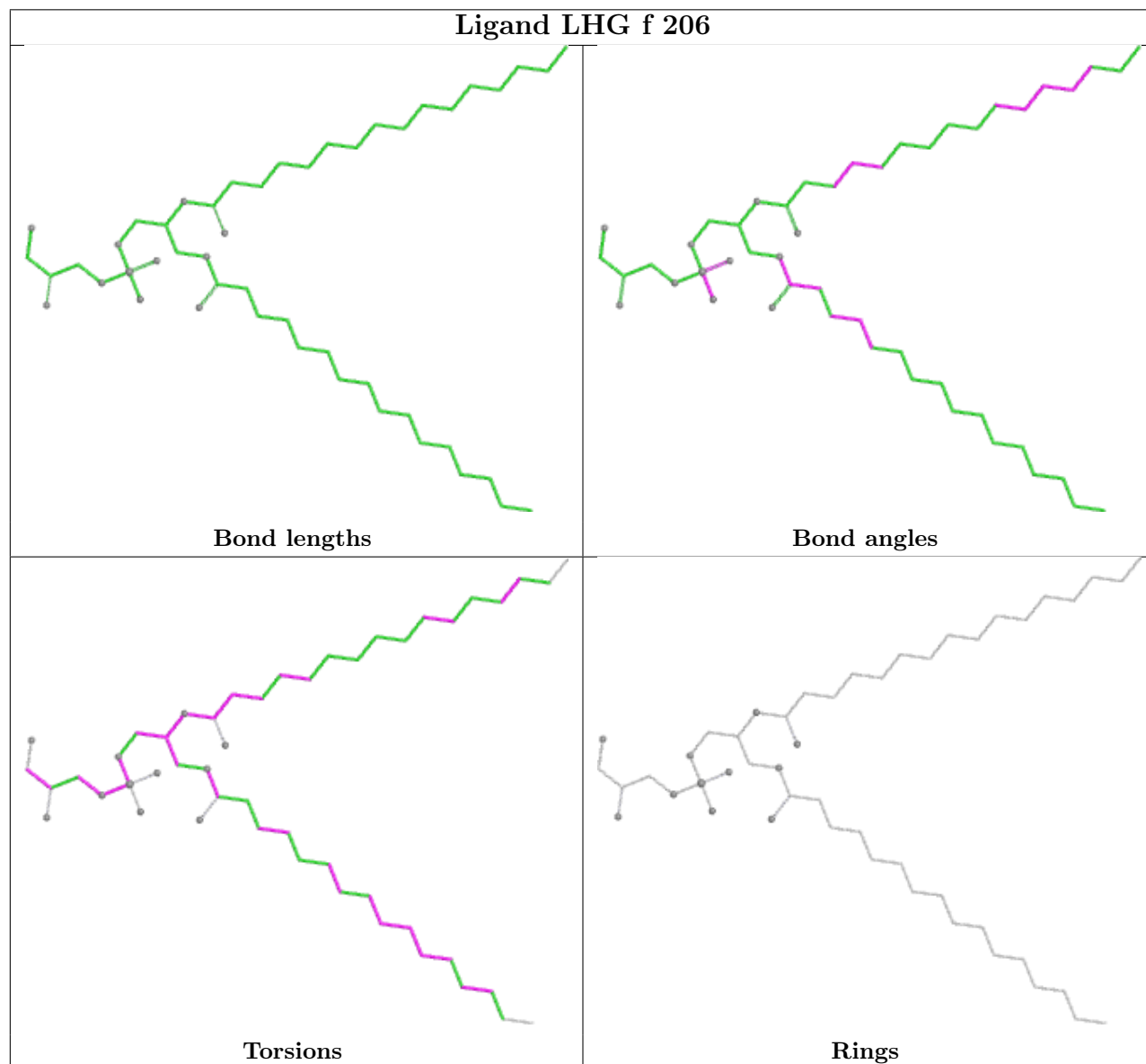
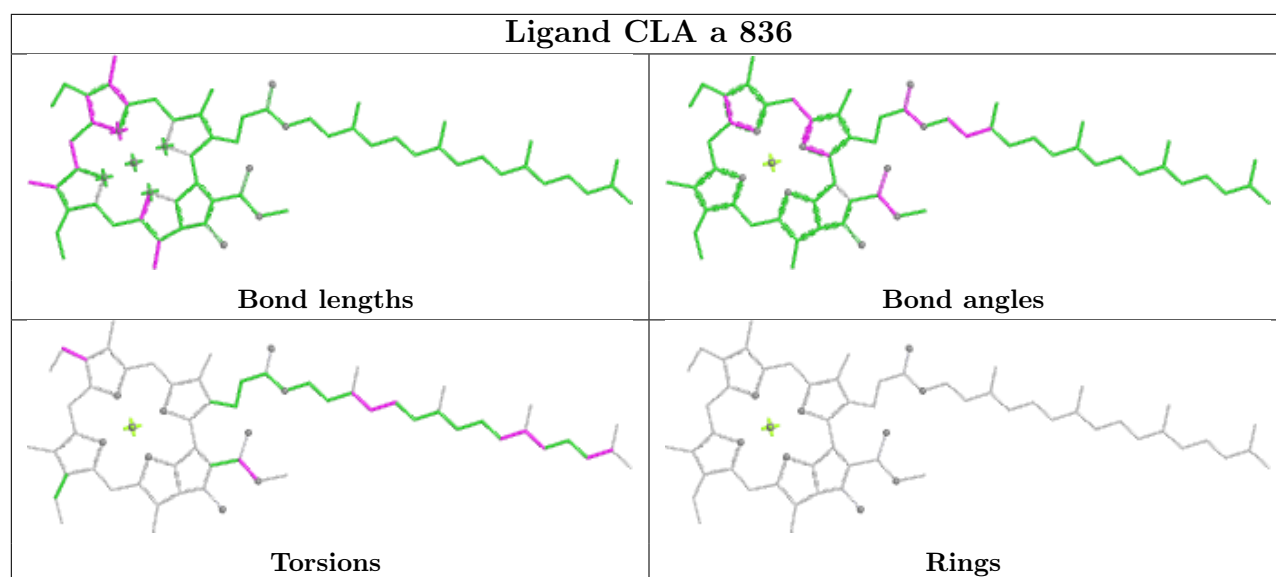


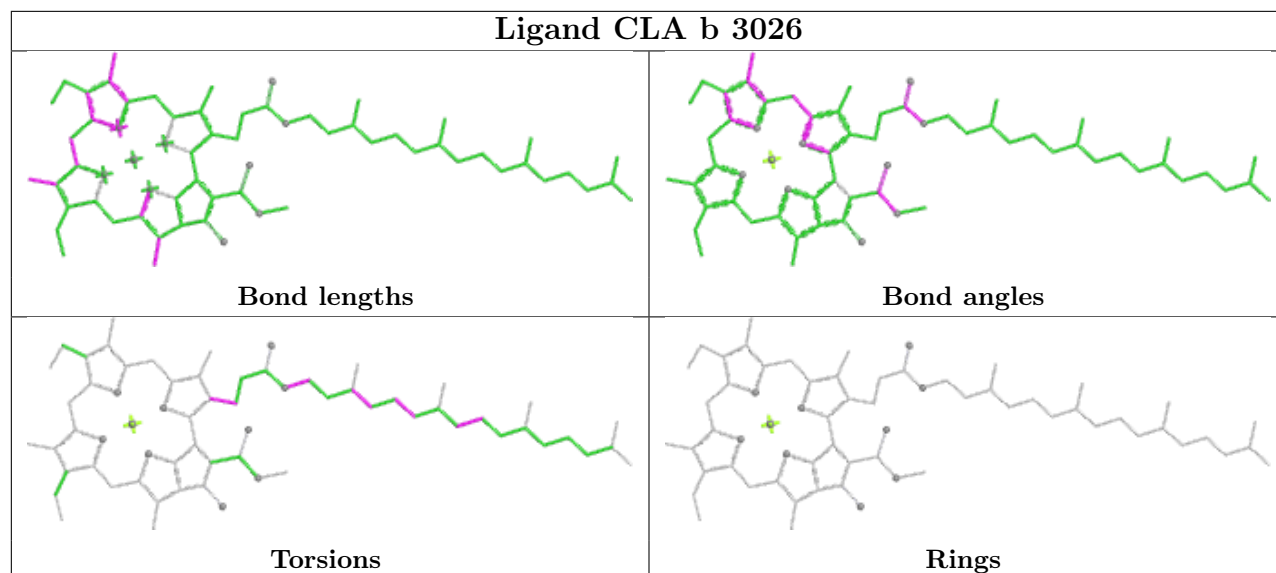
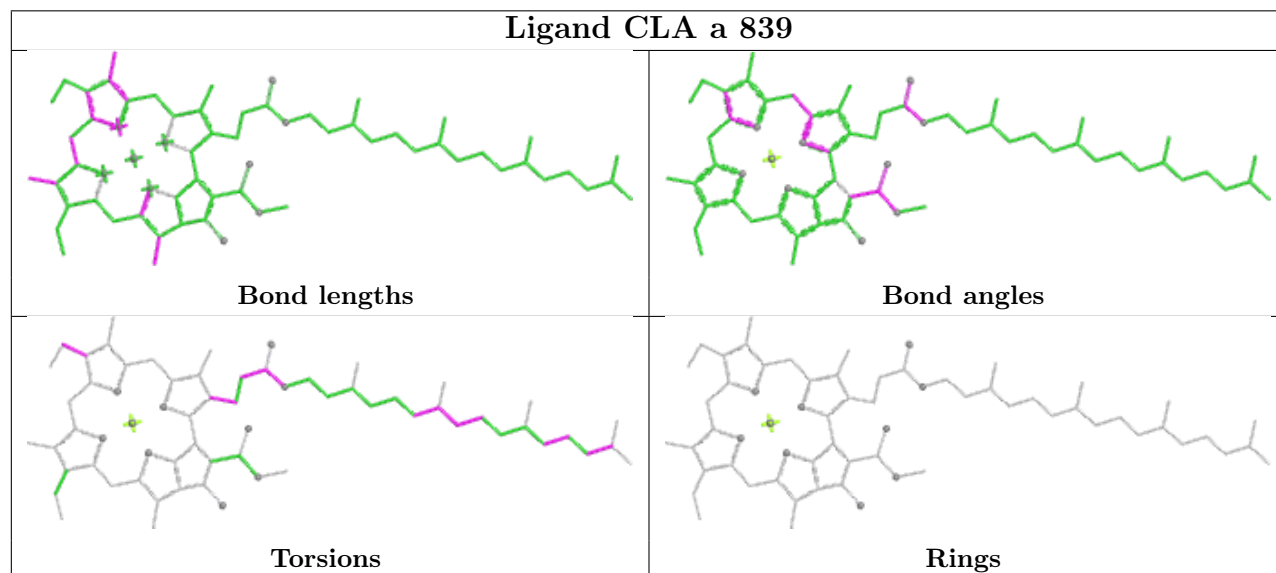
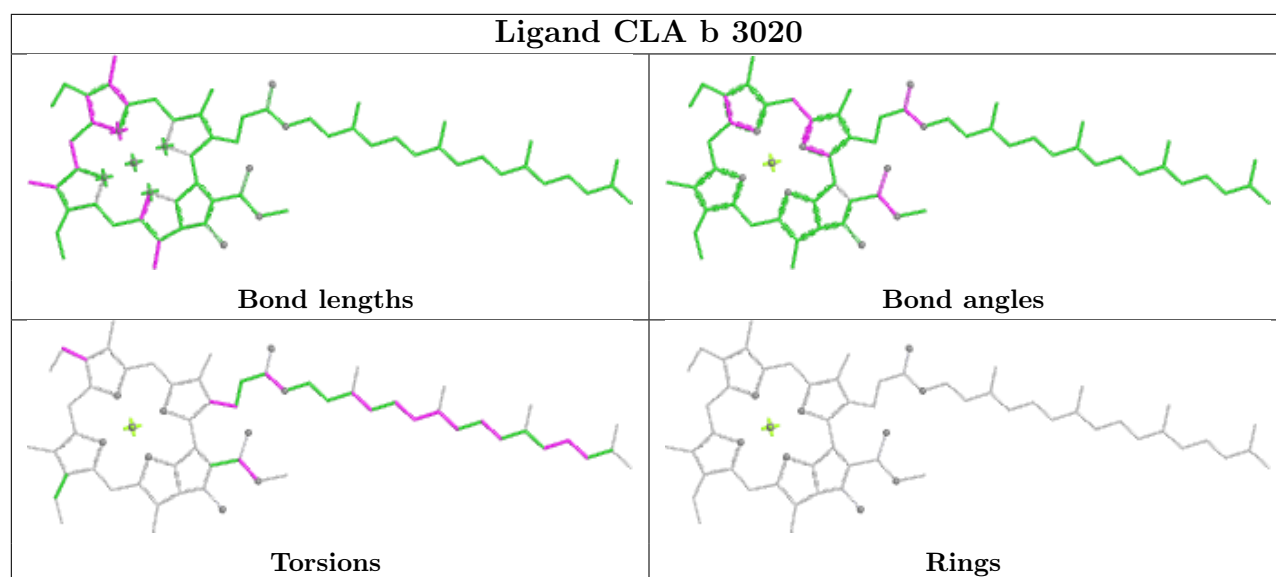


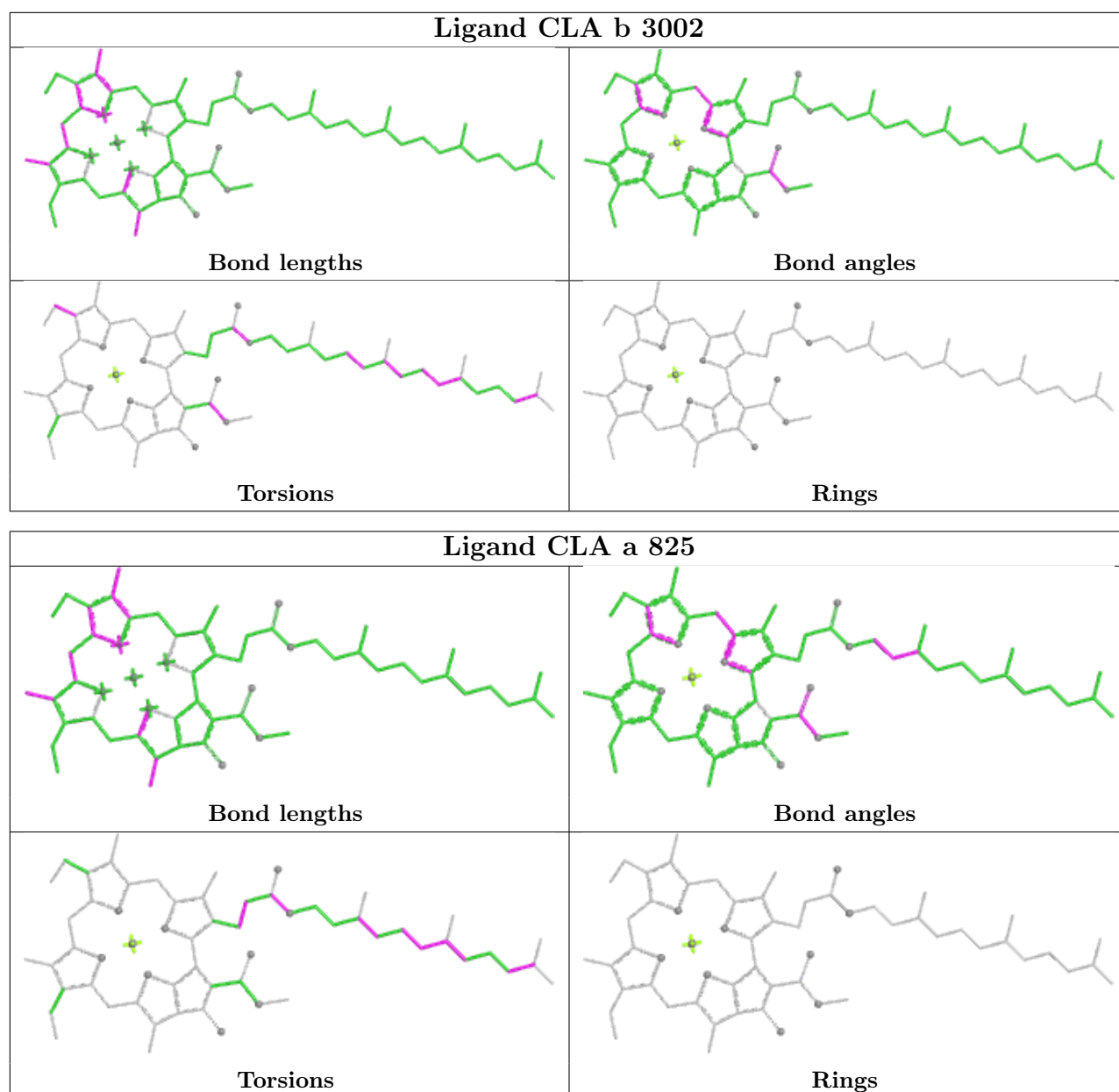




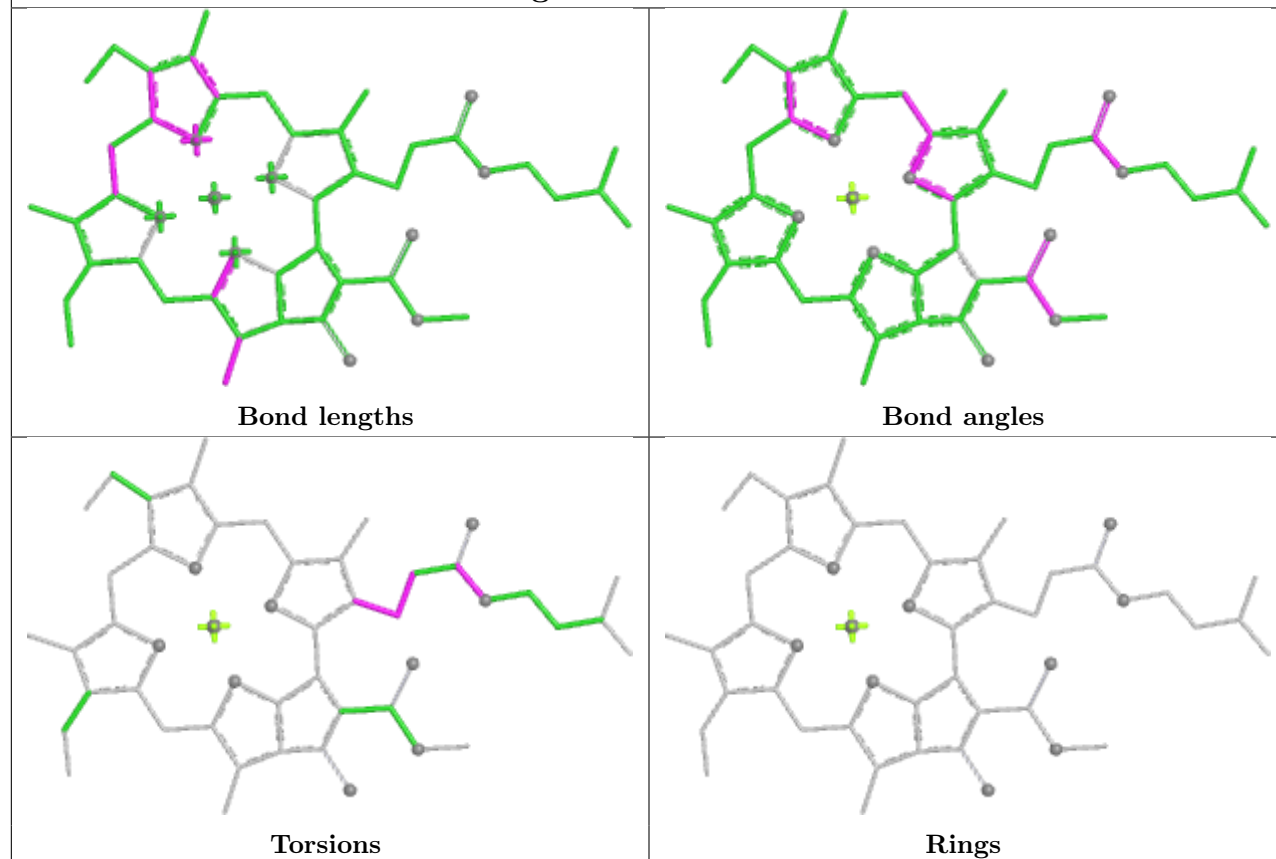




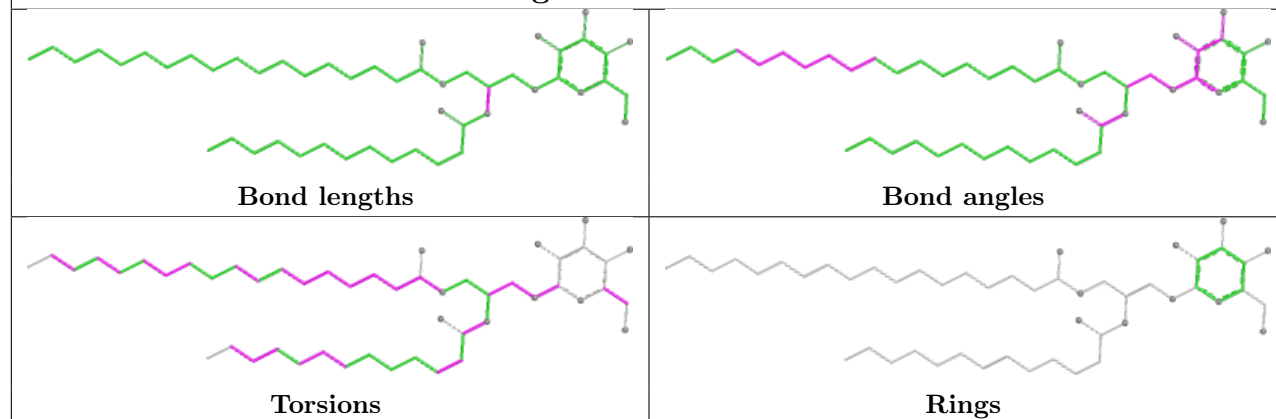


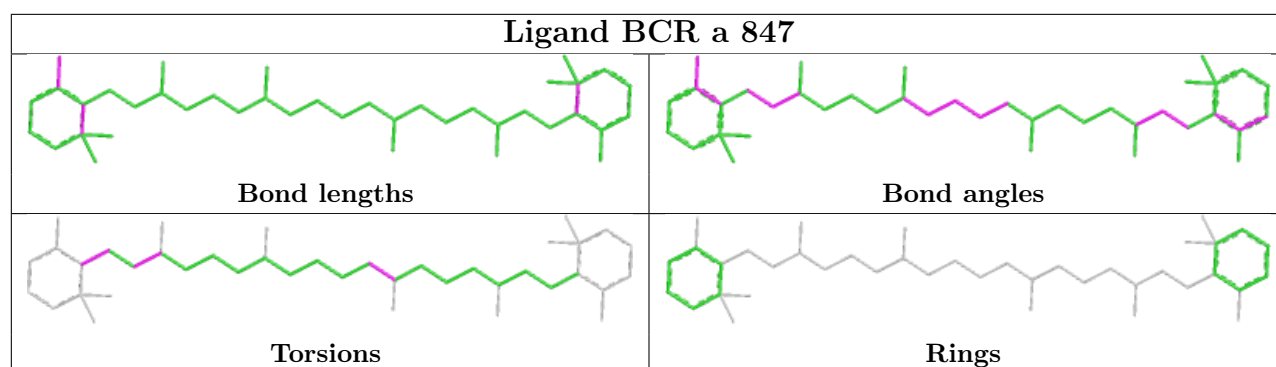
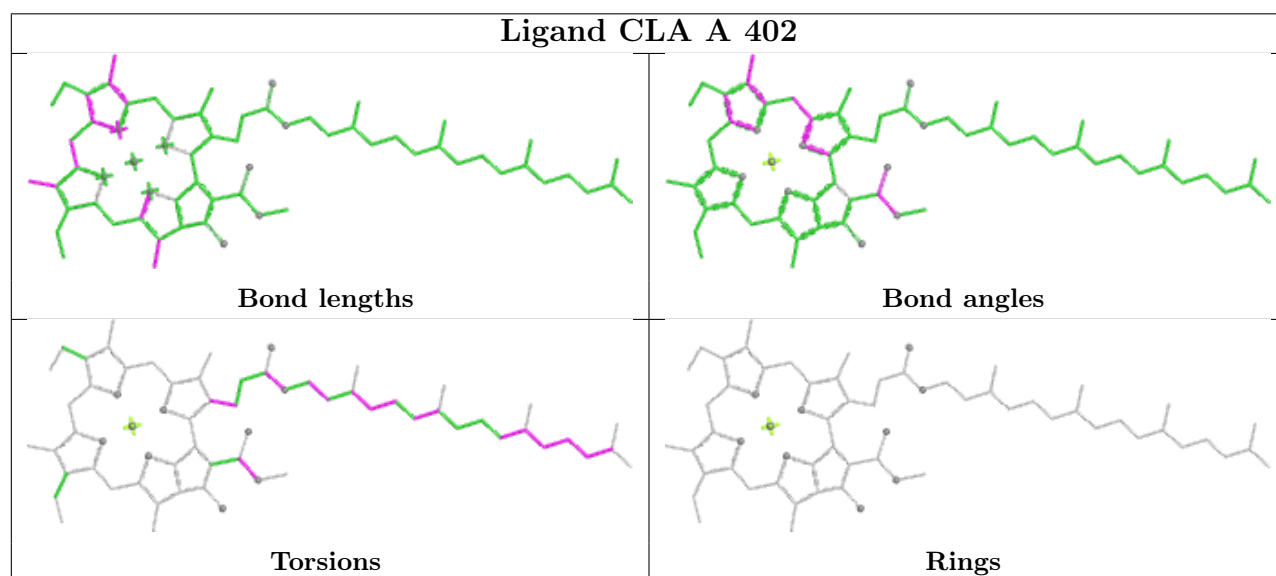
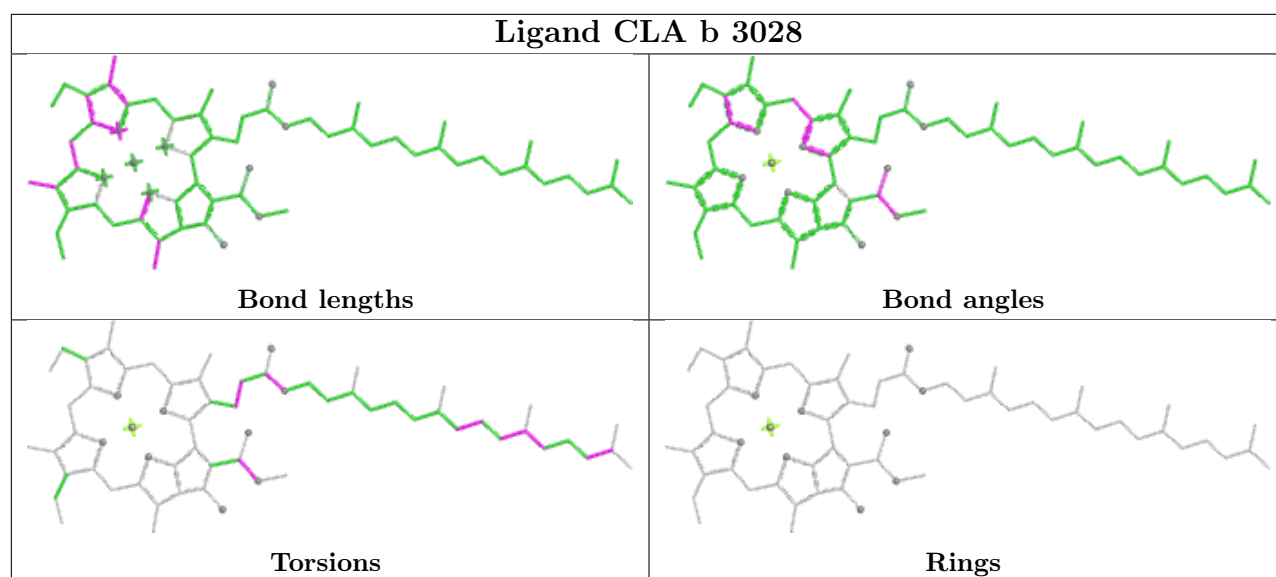


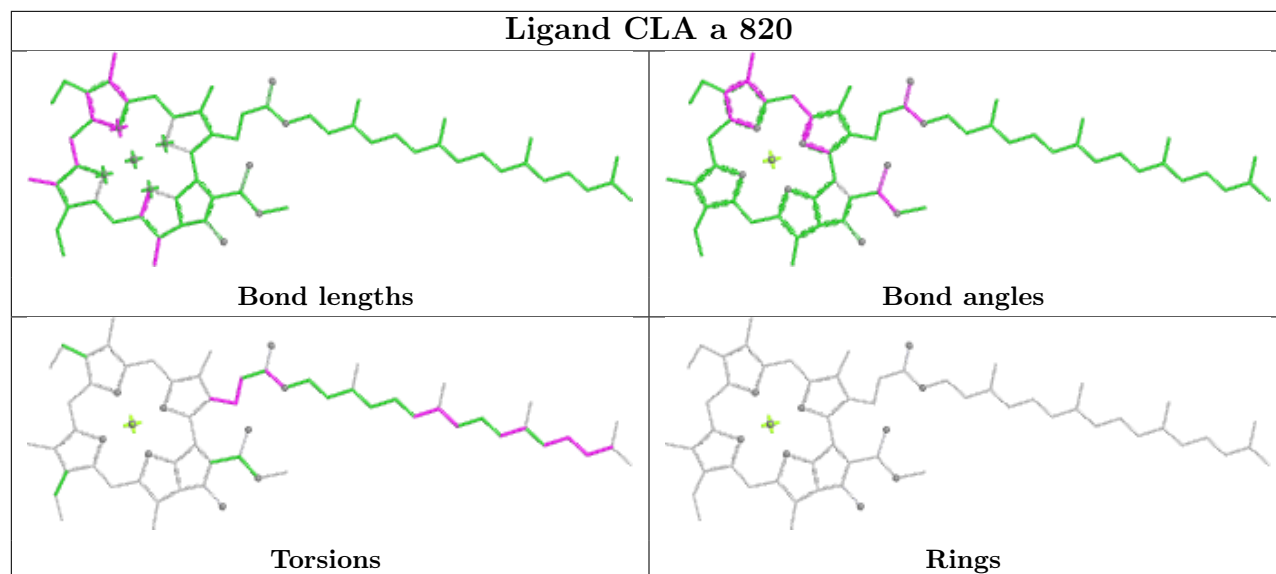
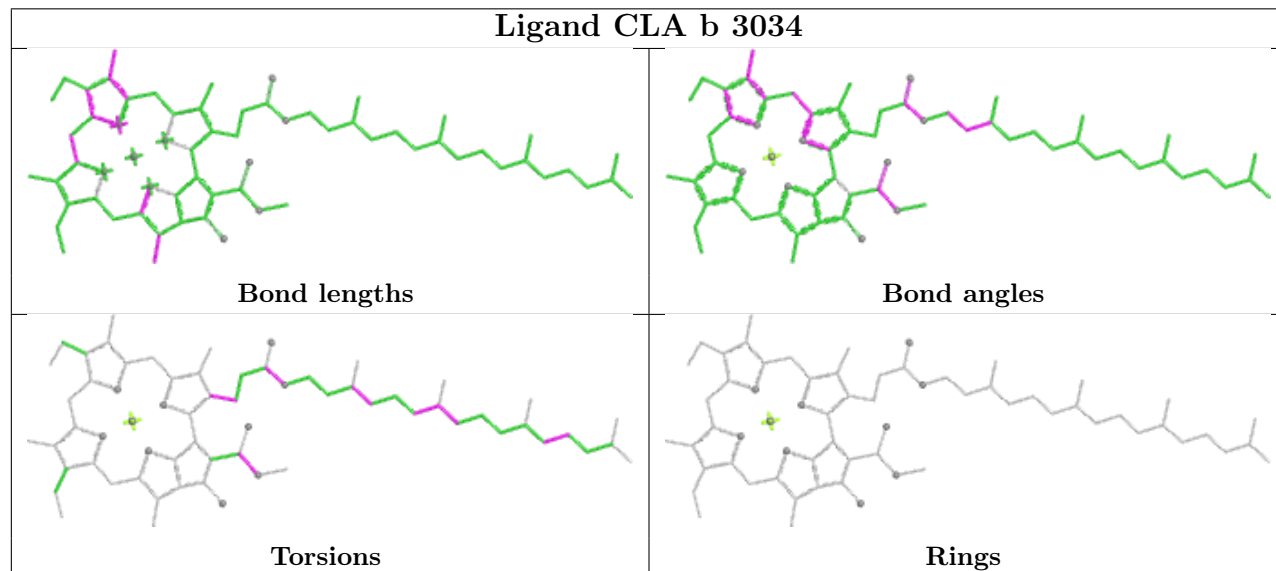
Ligand CLA A 405



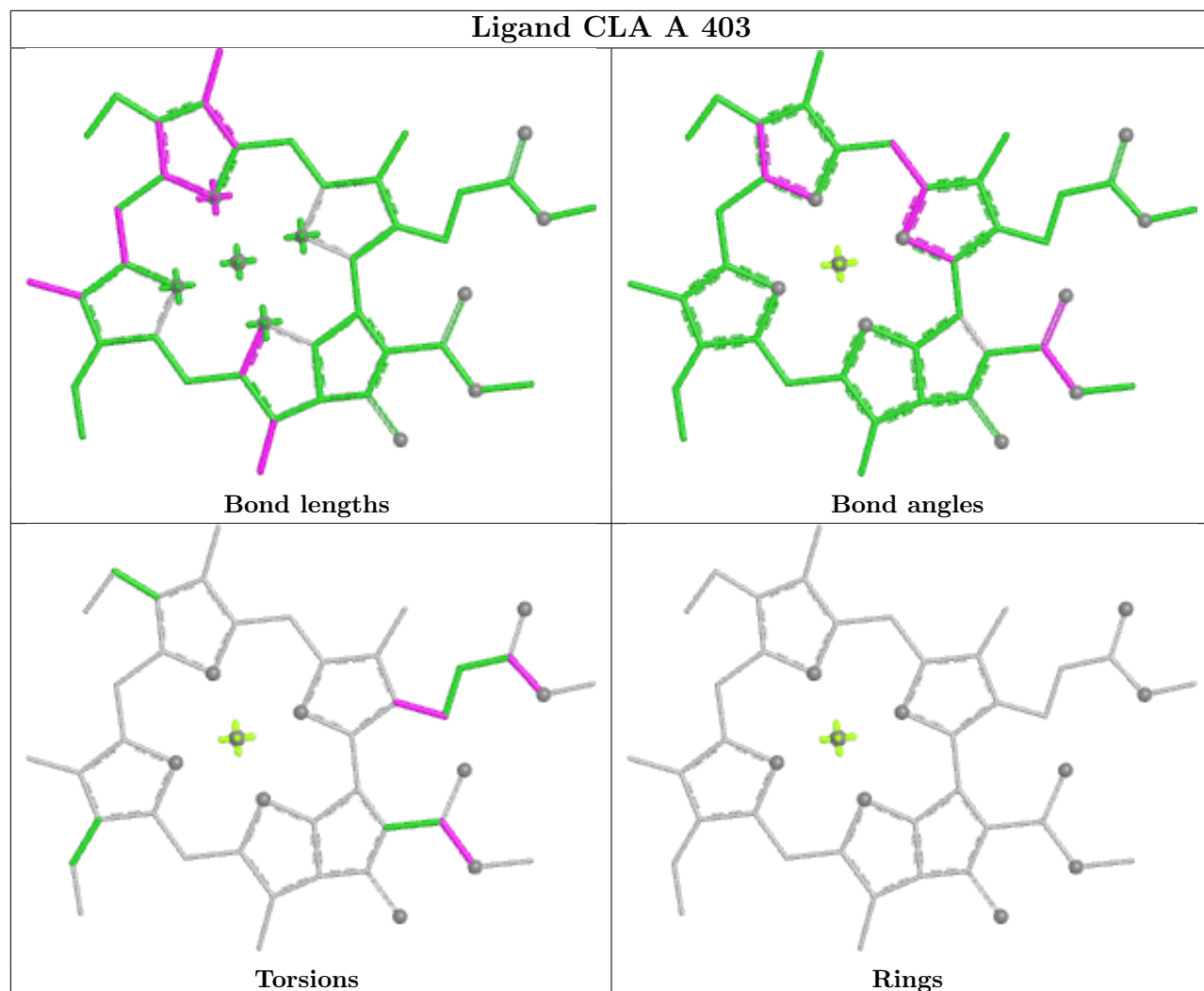
Ligand LMG a 851



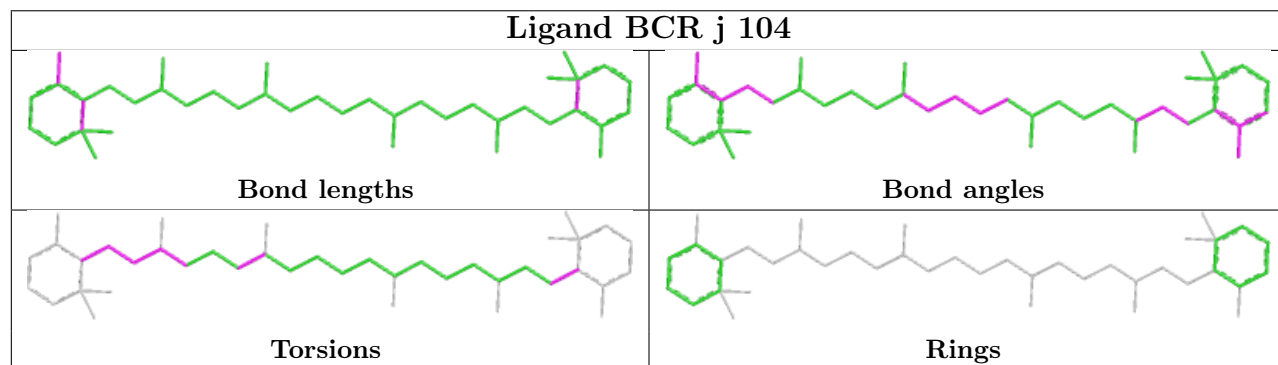


Ligand CLA a 820**Ligand CLA b 3034**

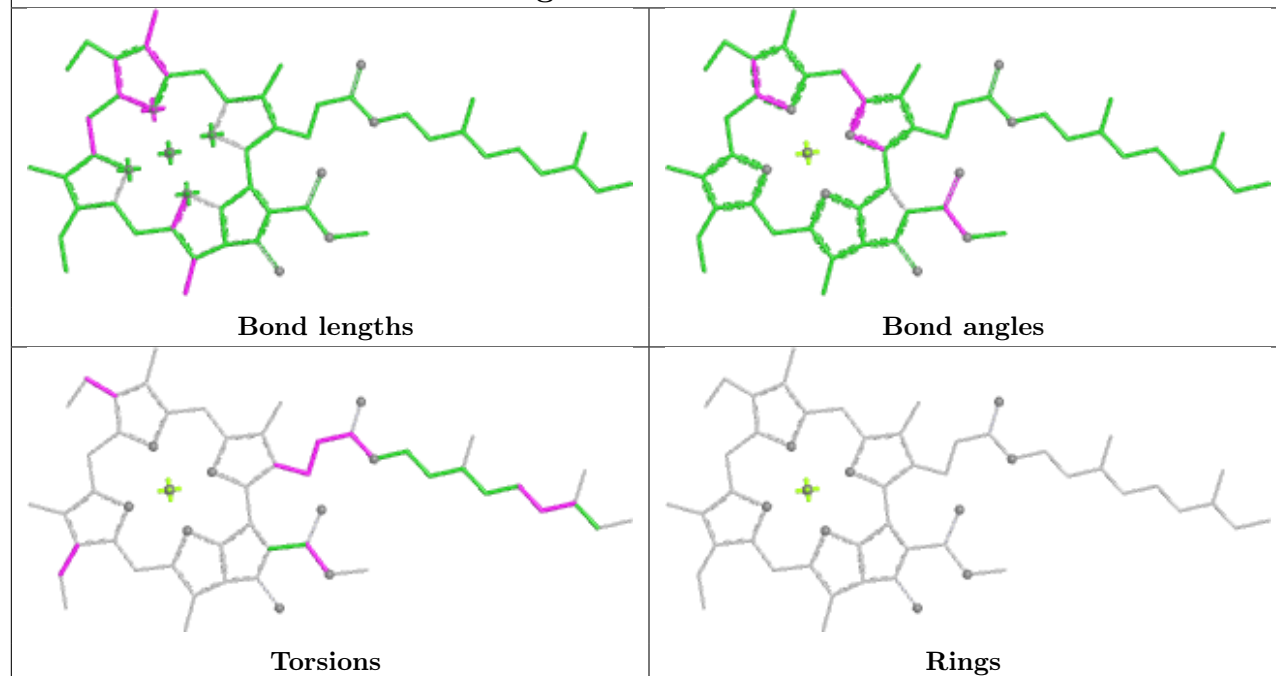
Ligand CLA A 403



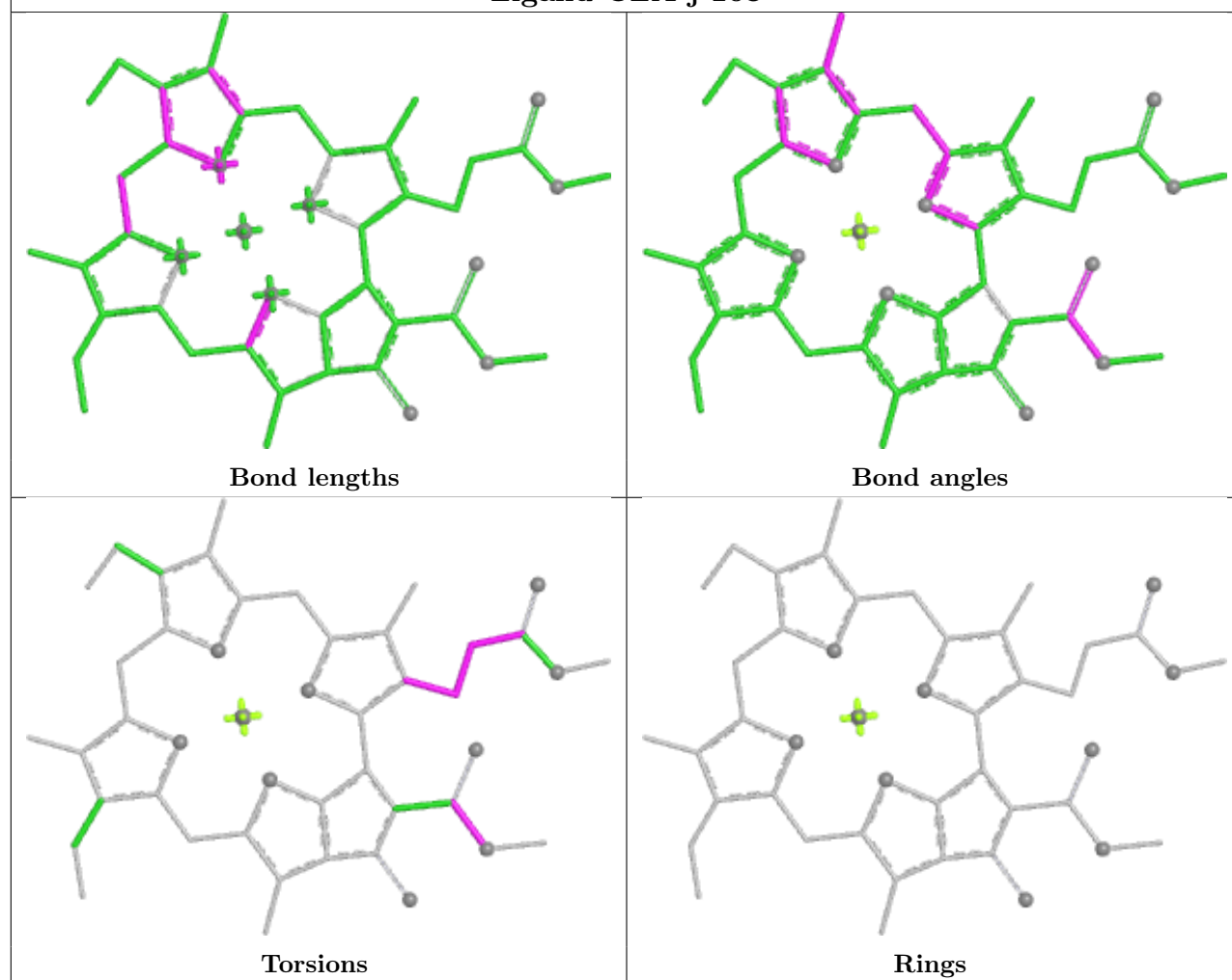
Ligand BCR j 104

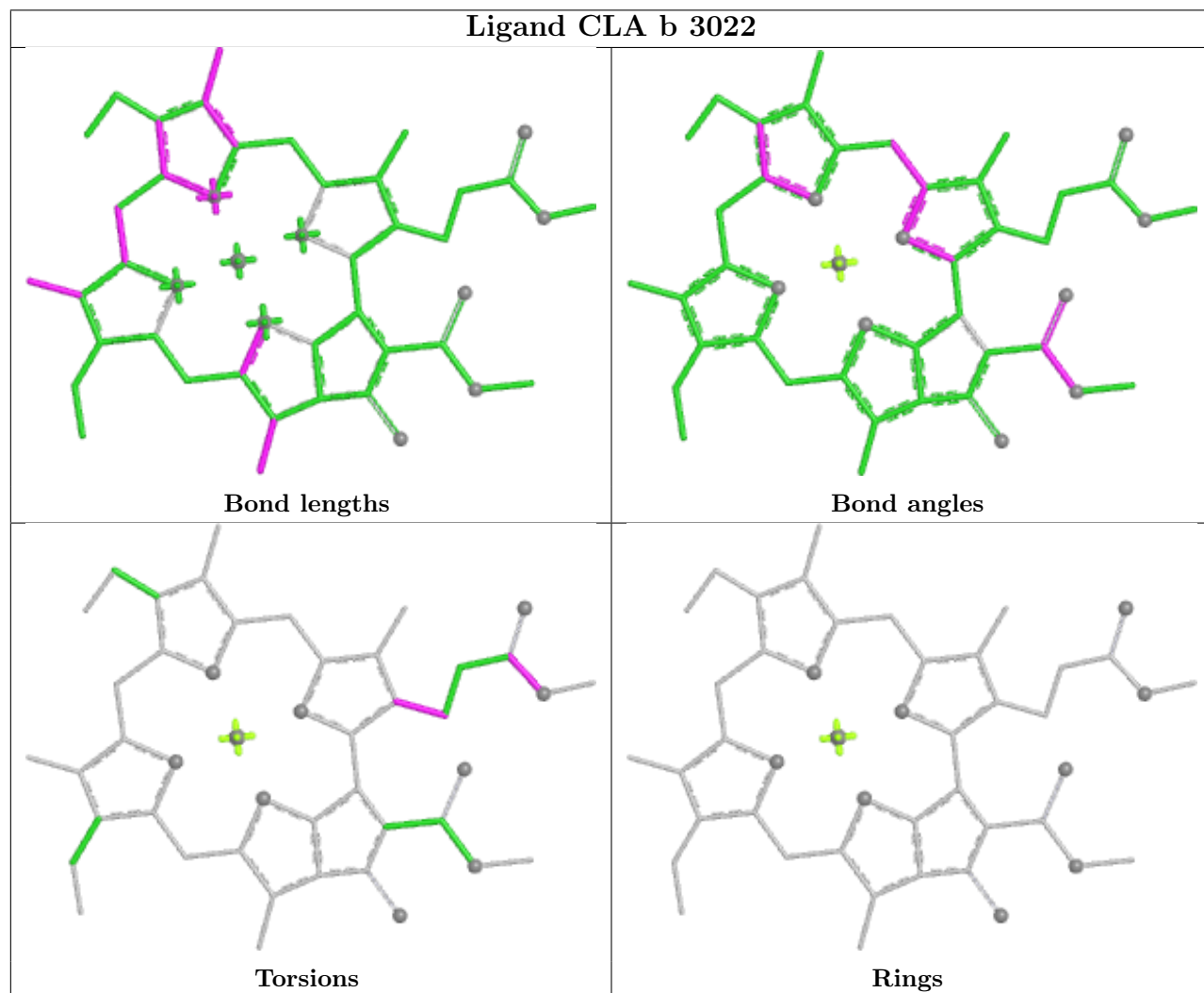
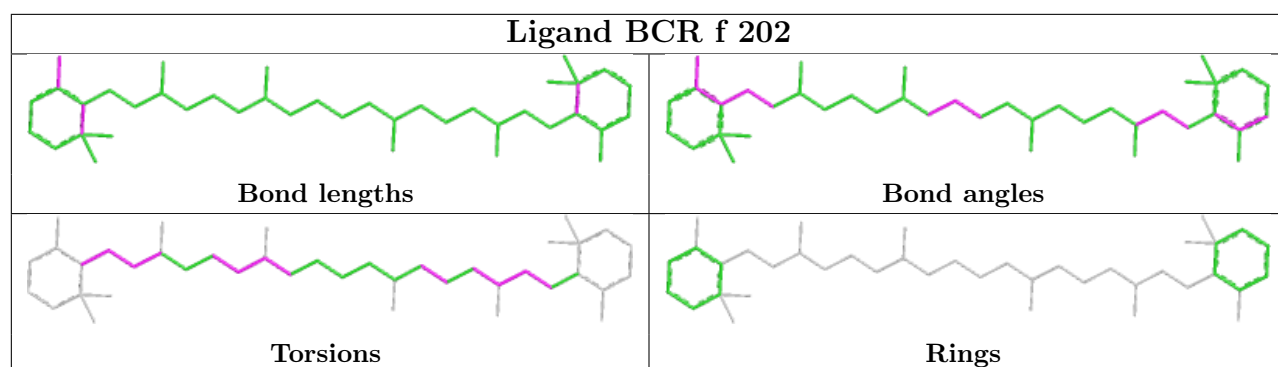


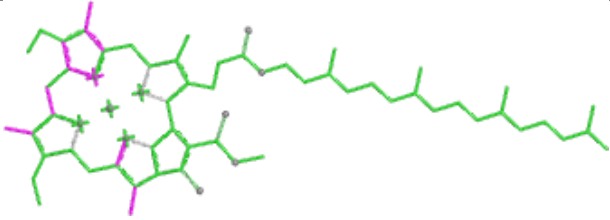
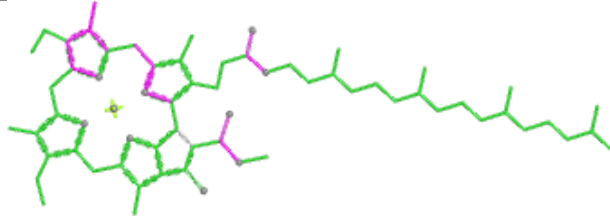
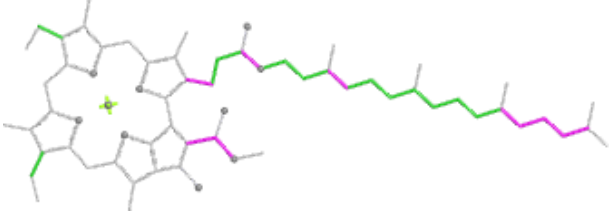
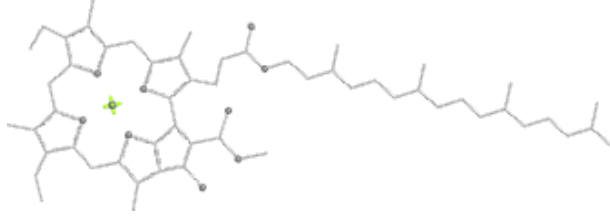
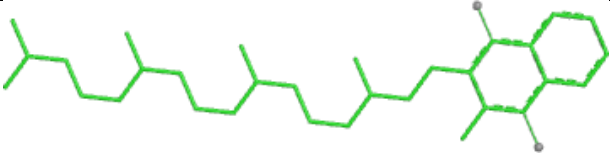
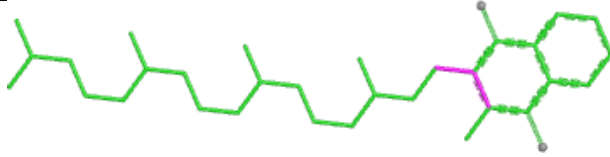
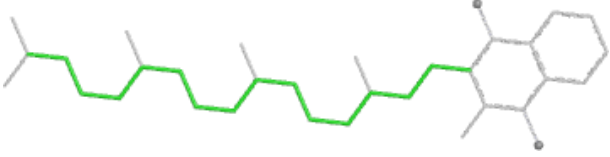
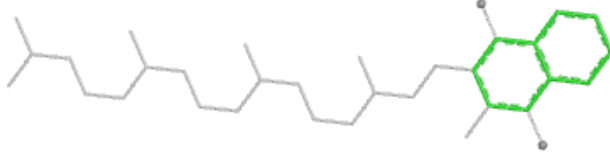
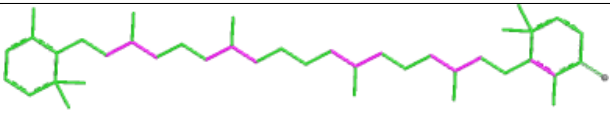
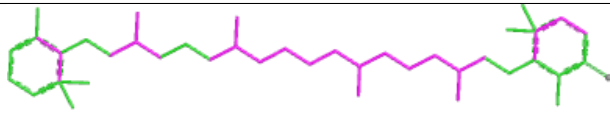
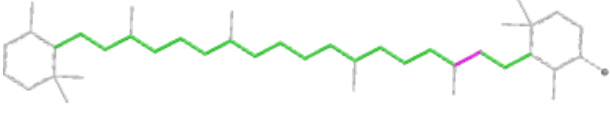
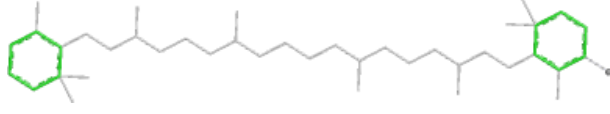
Ligand CLA a 832

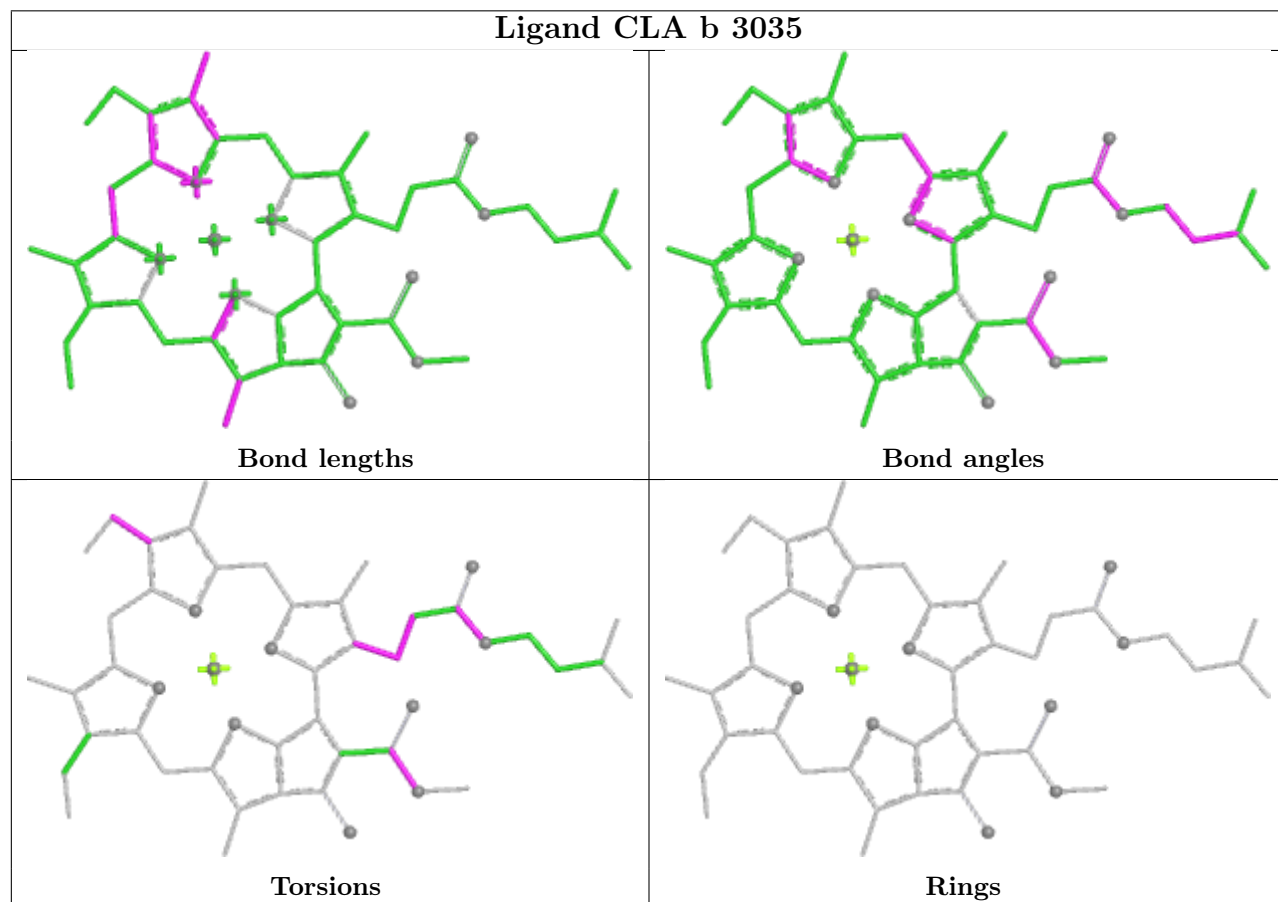
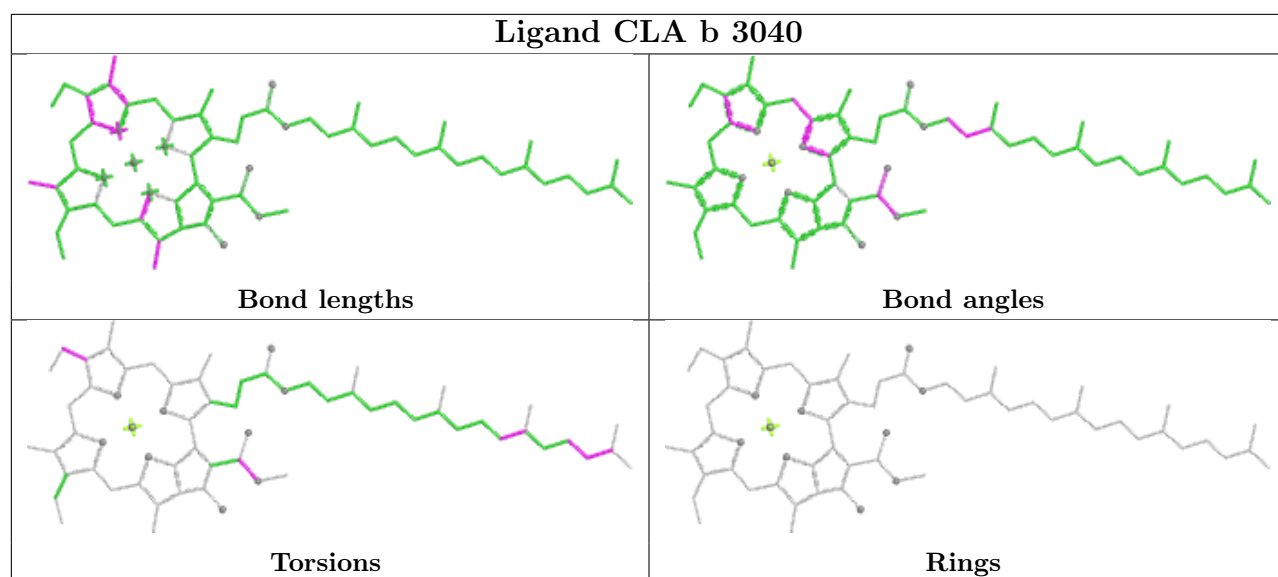


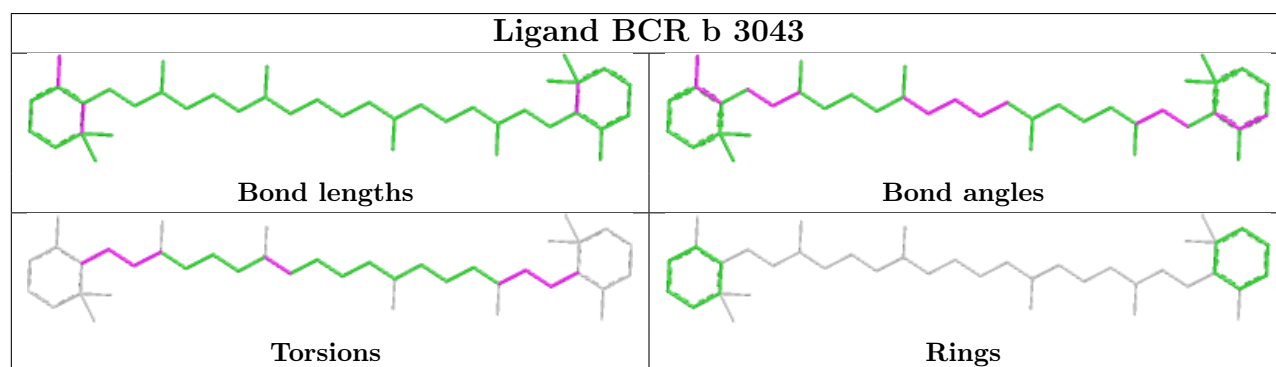
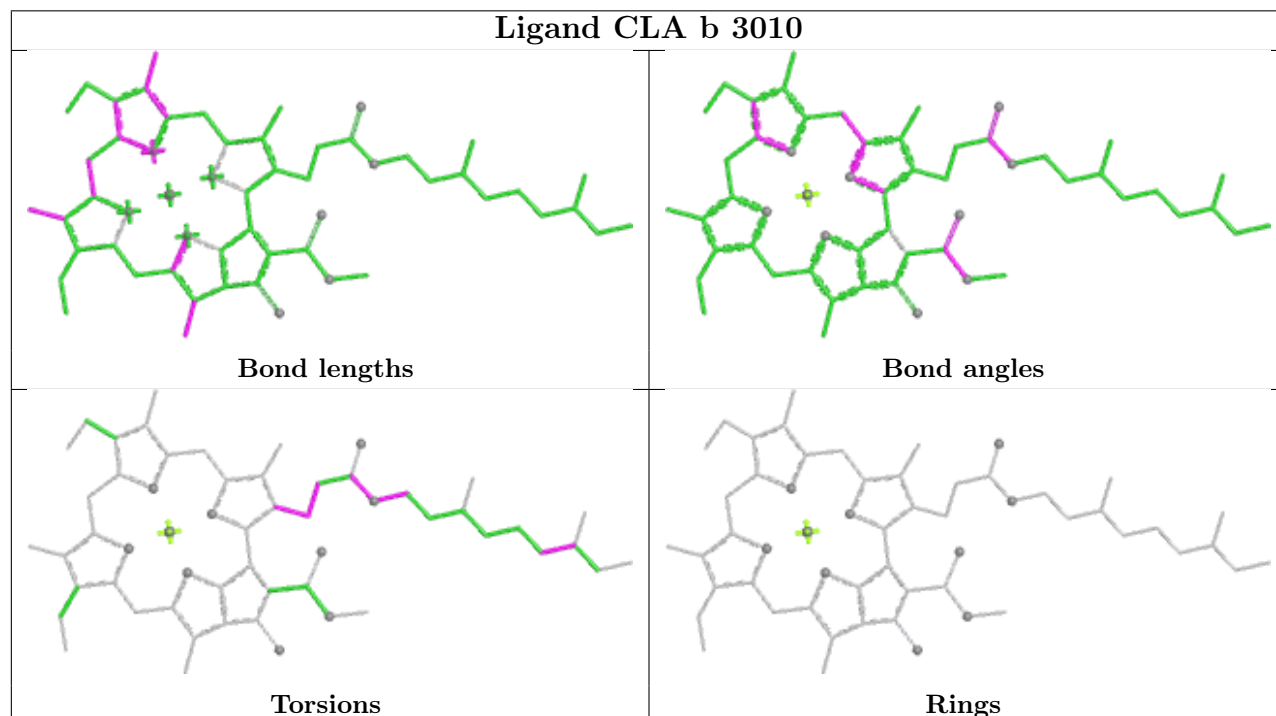
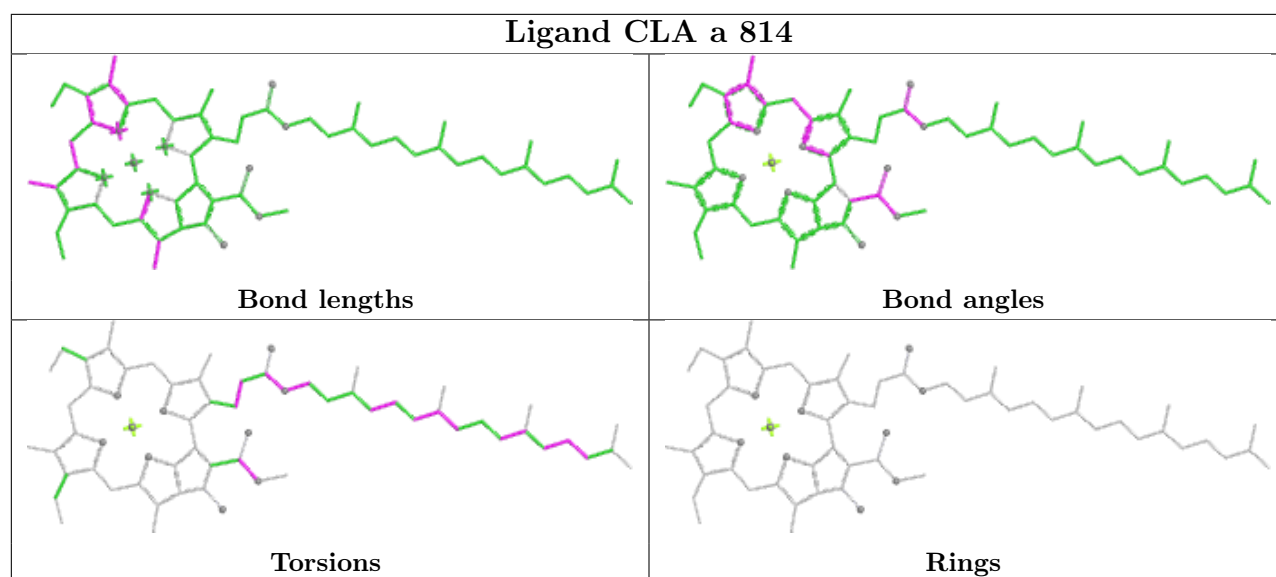
Ligand CLA j 103



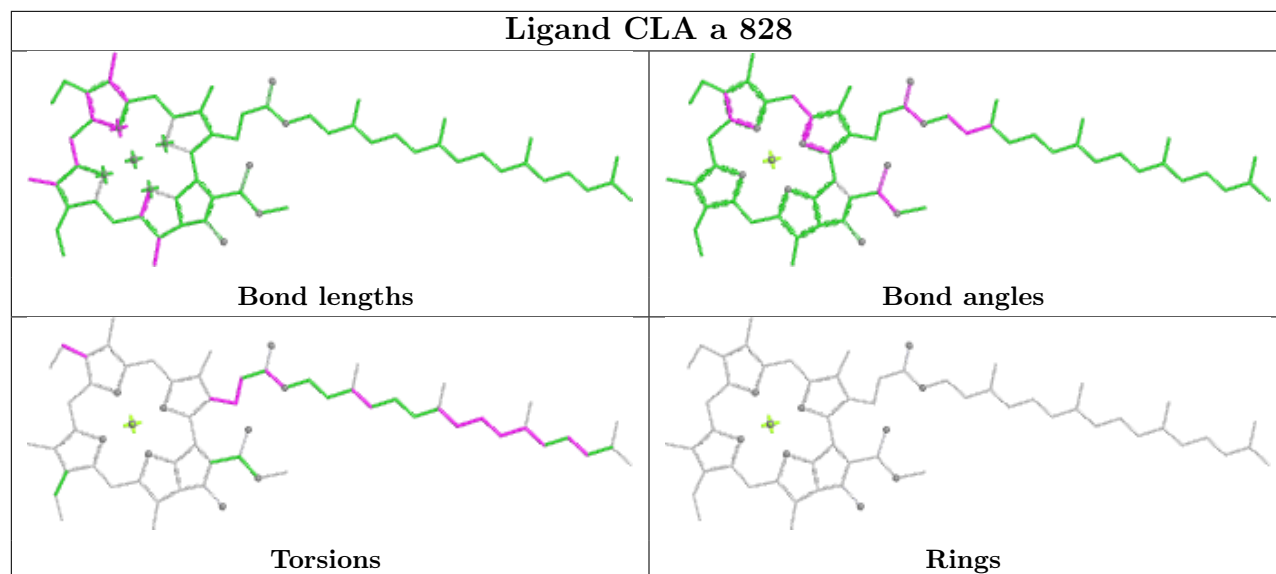


Ligand CLA b 3005	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PQN b 3042	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand ECH m 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

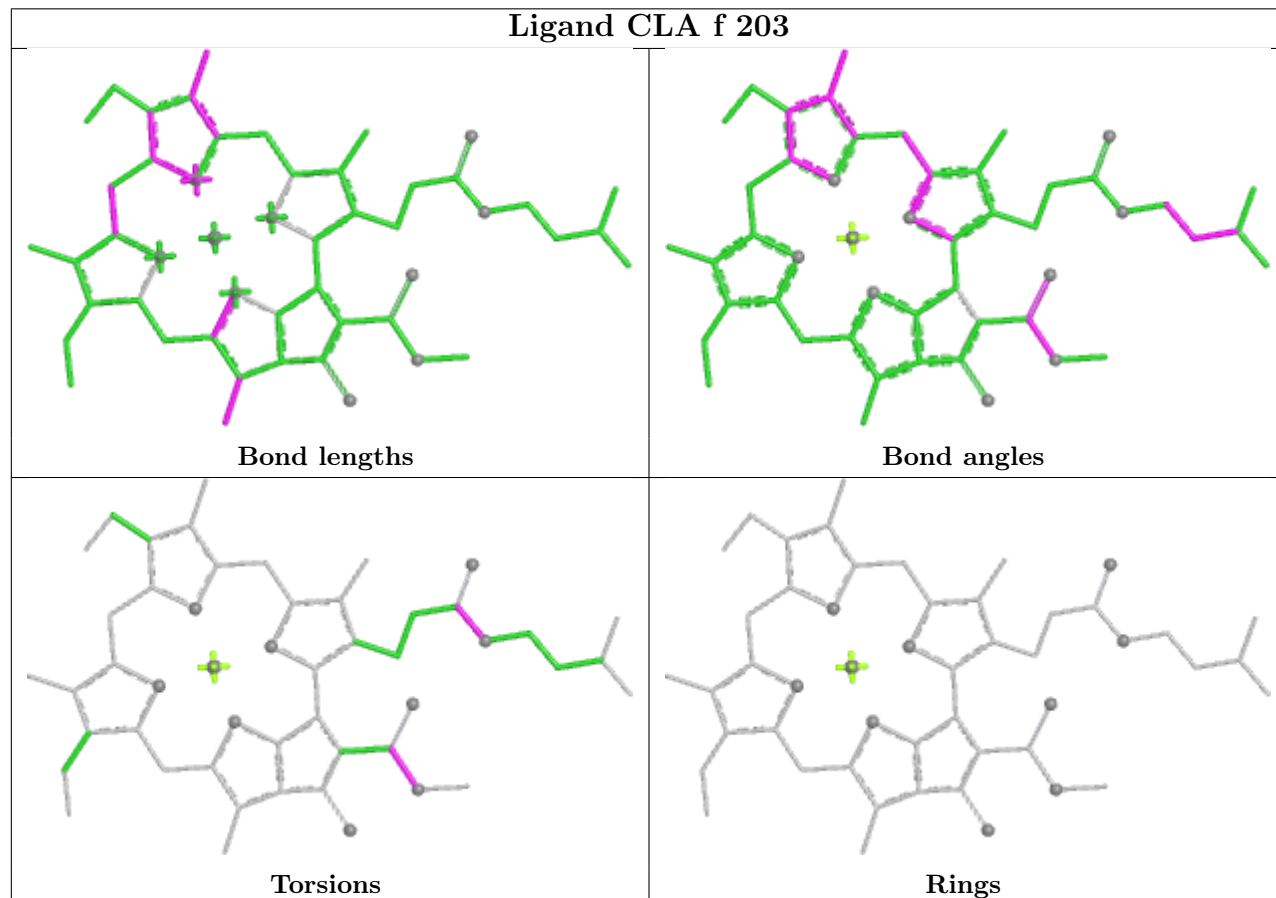




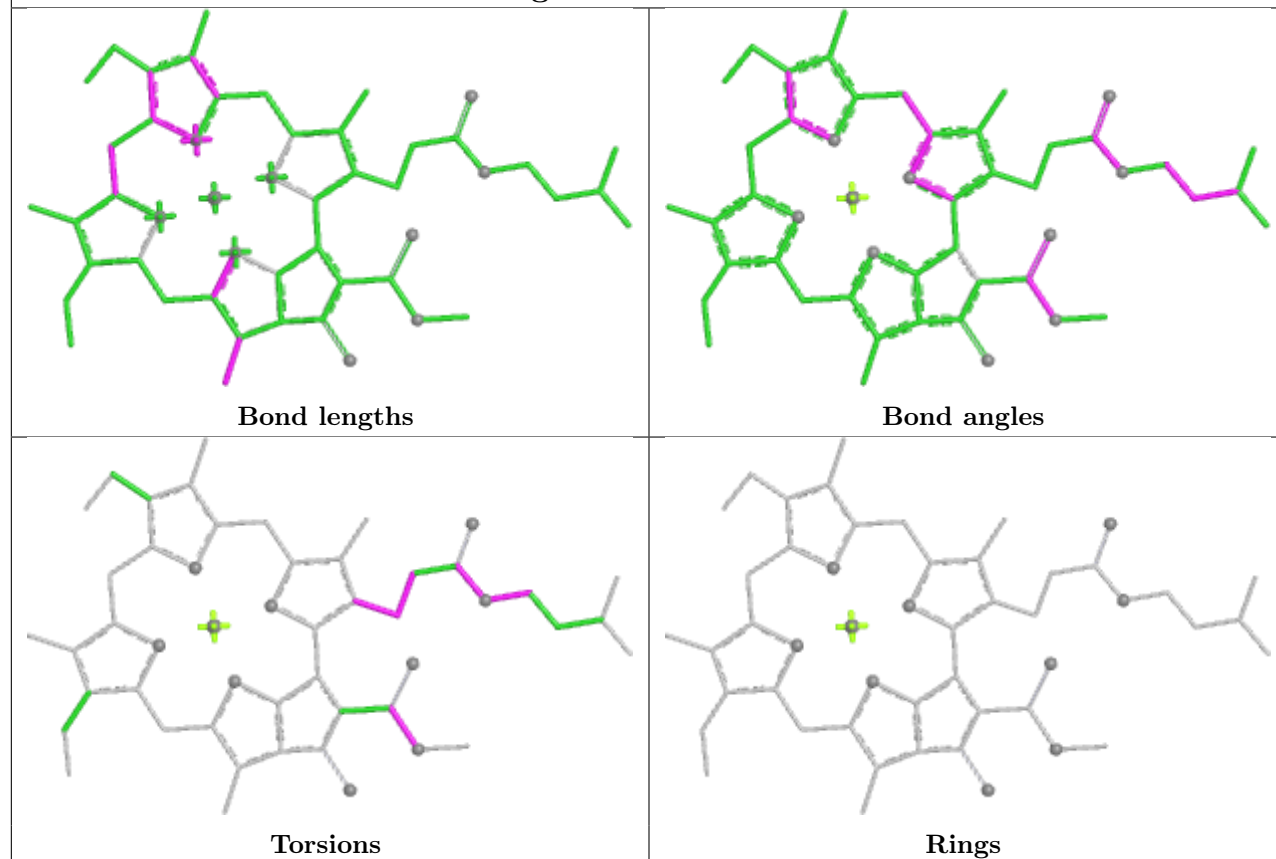
Ligand CLA a 828



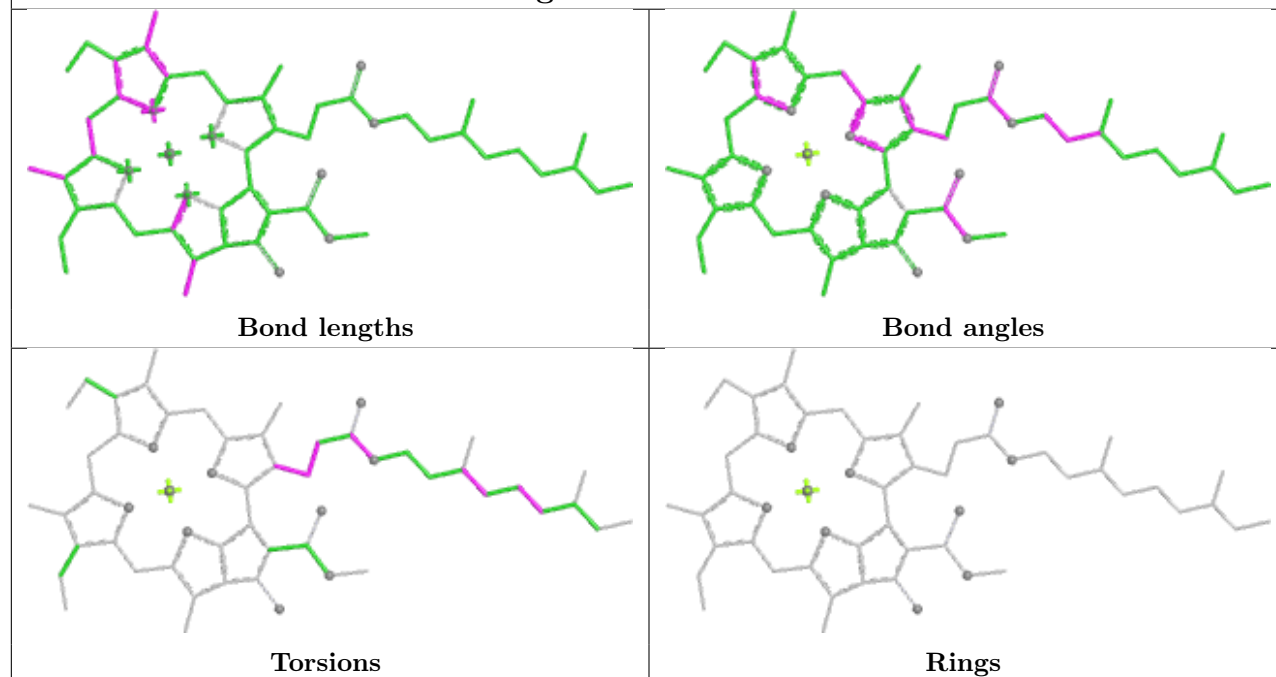
Ligand CLA f 203



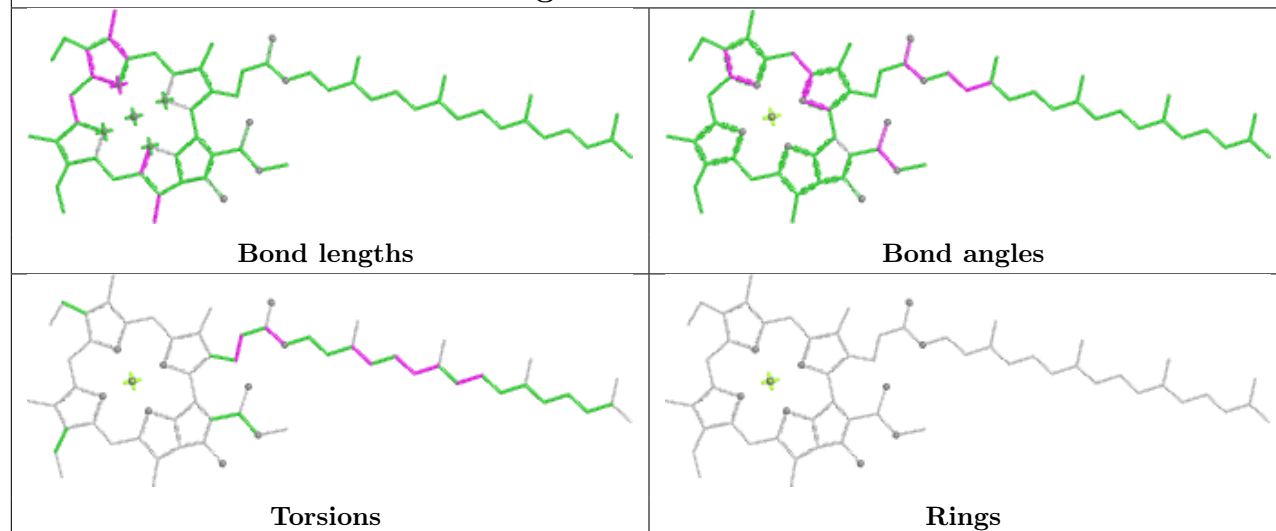
Ligand CLA 1 1501



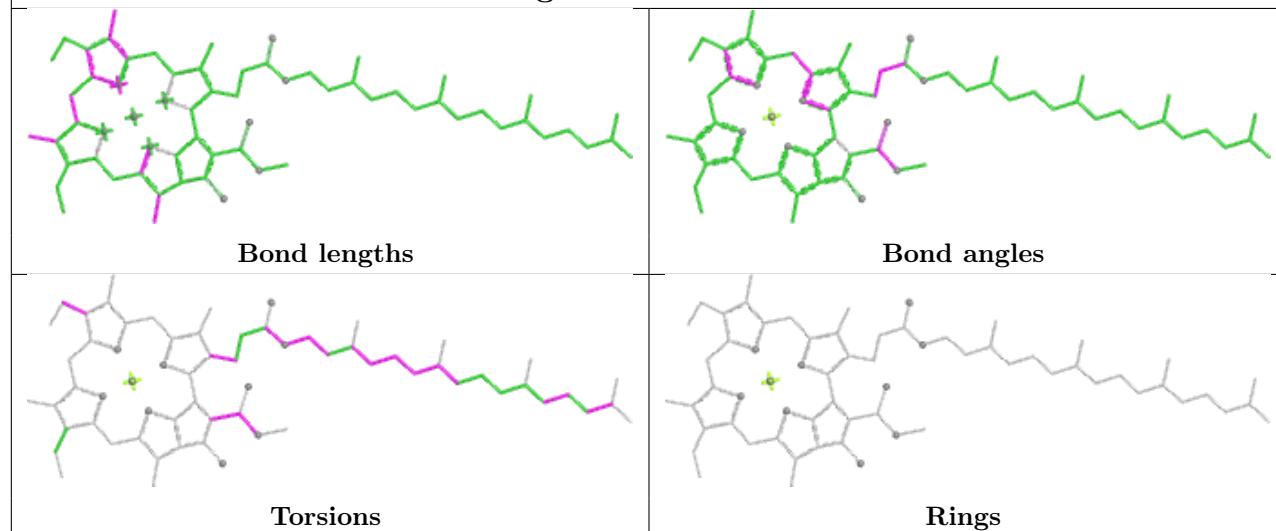
Ligand CLA a 843



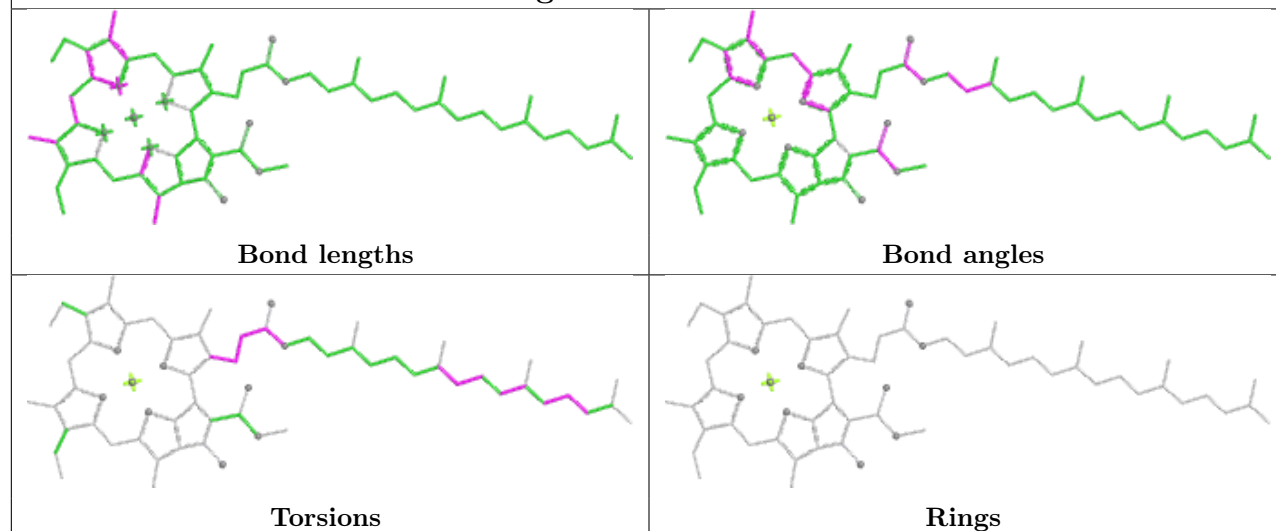
Ligand CLA a 837

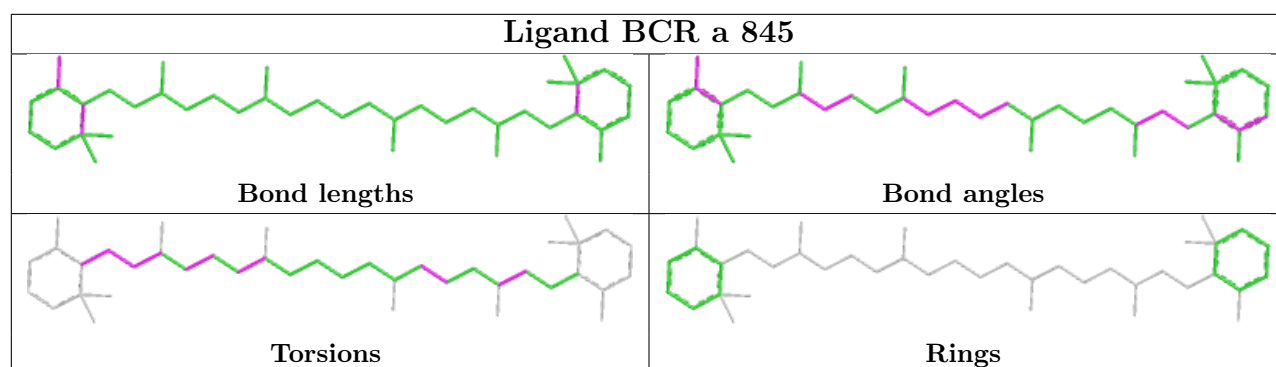


Ligand CLA a 819



Ligand CLA a 812





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

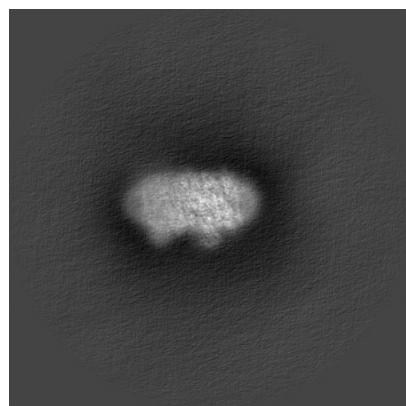
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15618. These allow visual inspection of the internal detail of the map and identification of artifacts.

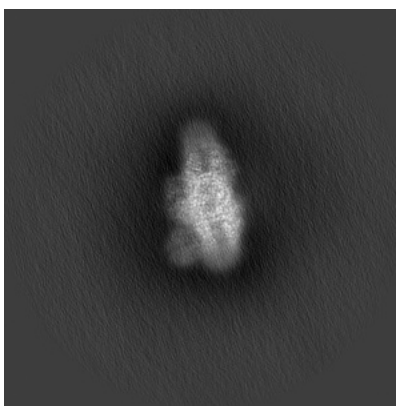
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

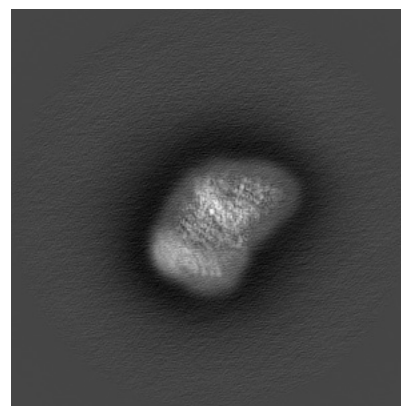
6.1.1 Primary map



X

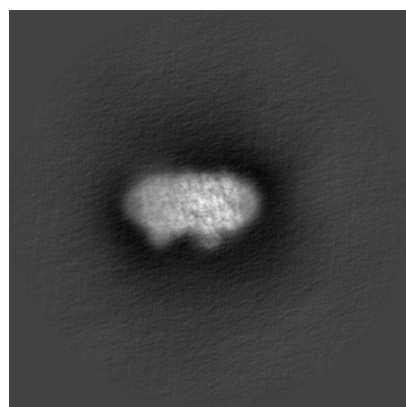


Y

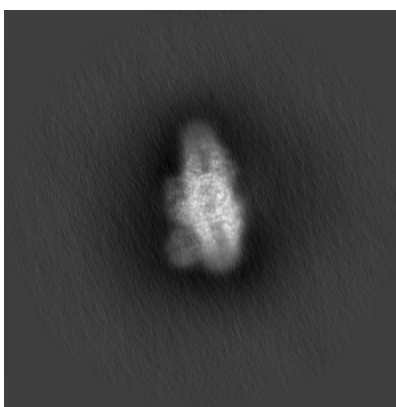


Z

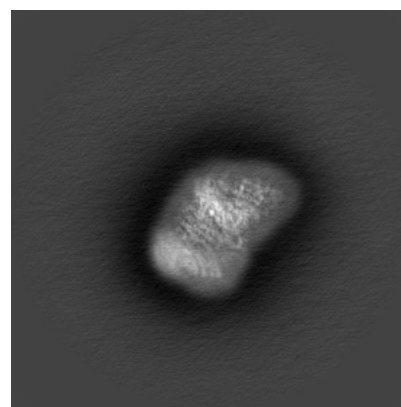
6.1.2 Raw map



X



Y

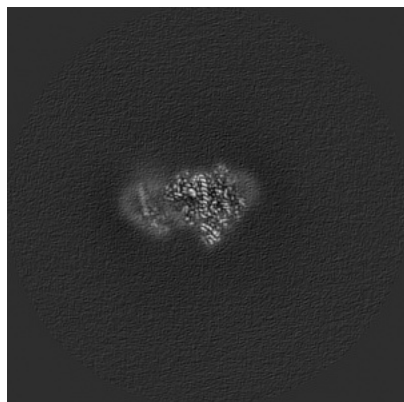


Z

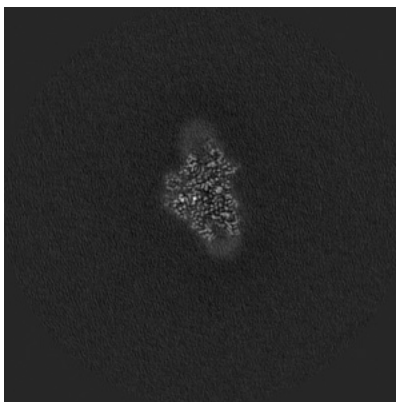
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

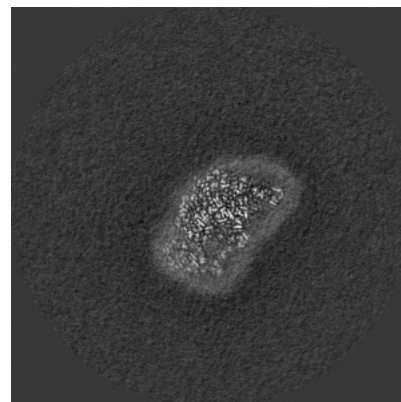
6.2.1 Primary map



X Index: 200

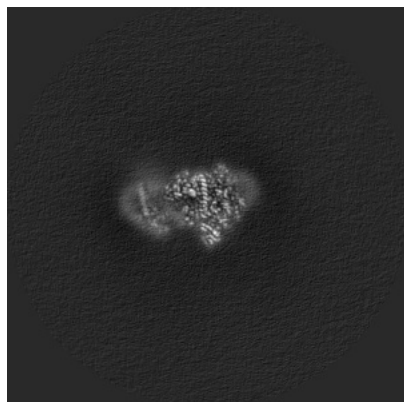


Y Index: 200

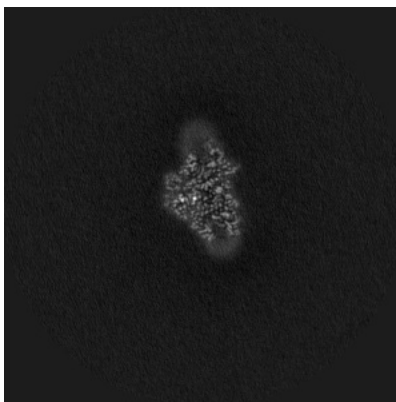


Z Index: 200

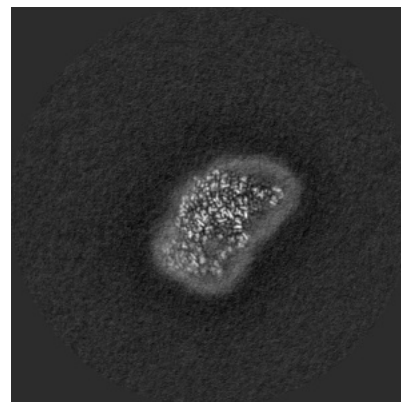
6.2.2 Raw map



X Index: 200



Y Index: 200

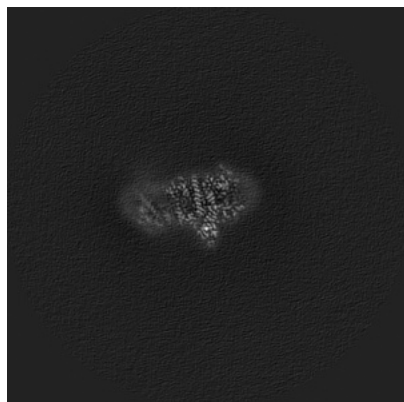


Z Index: 200

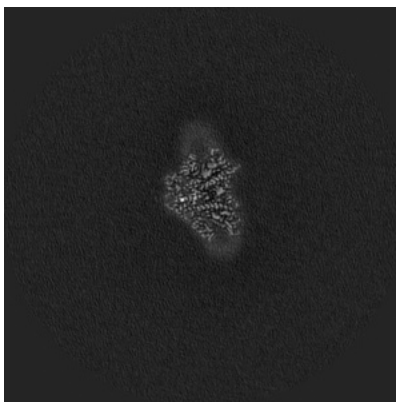
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

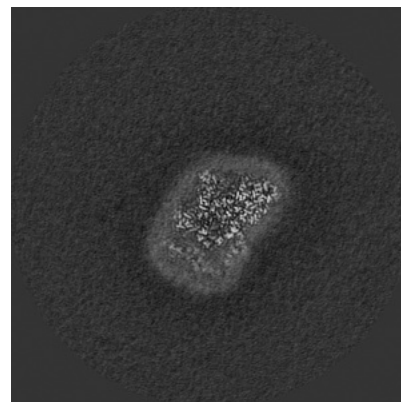
6.3.1 Primary map



X Index: 206

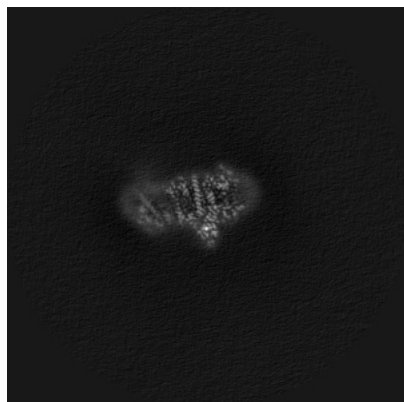


Y Index: 199

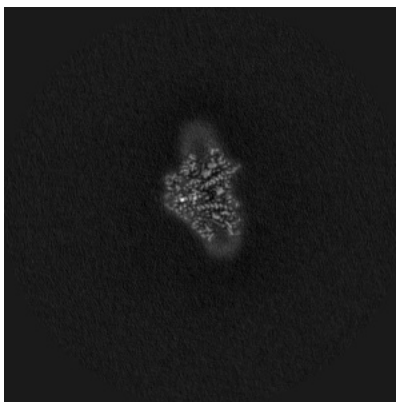


Z Index: 210

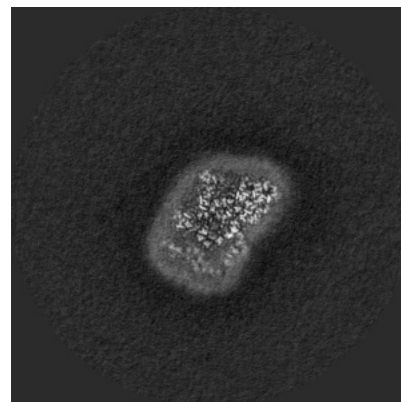
6.3.2 Raw map



X Index: 206



Y Index: 199

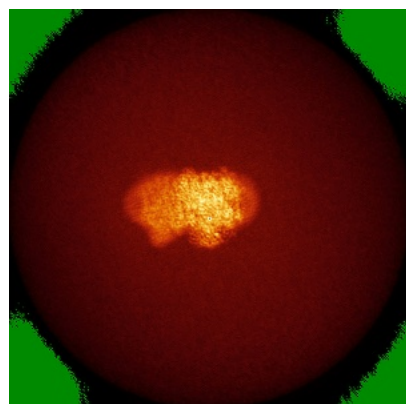


Z Index: 210

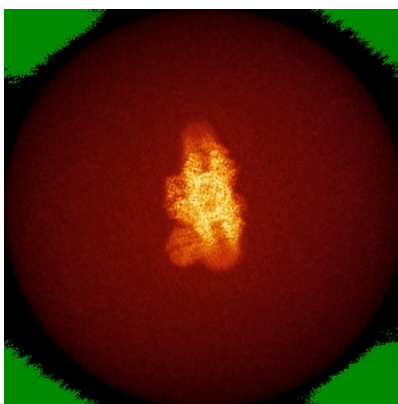
The images above show the largest variance slices of the map in three orthogonal directions.

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

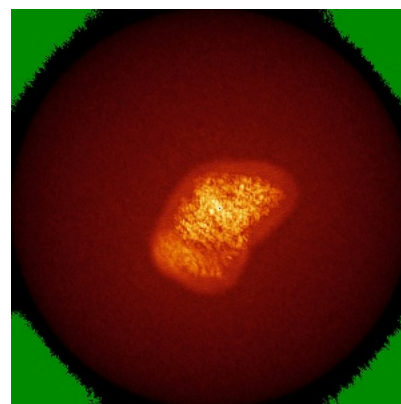
6.4.1 Primary map



X

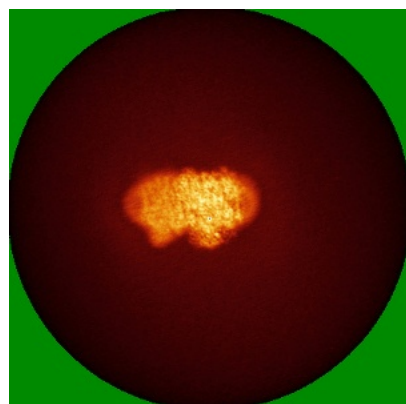


Y

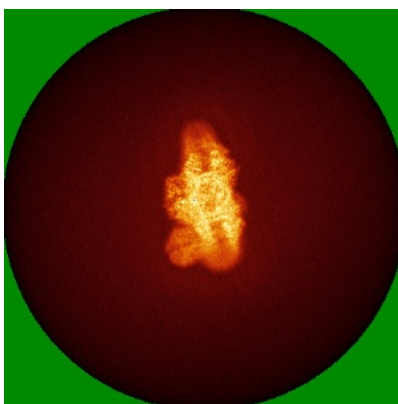


Z

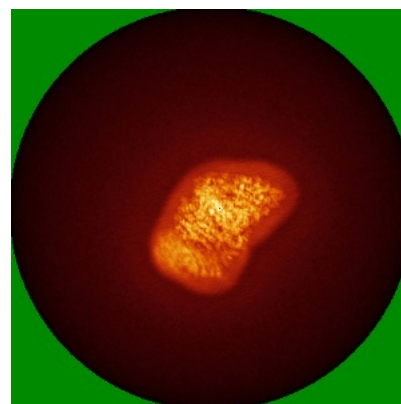
6.4.2 Raw map



X



Y

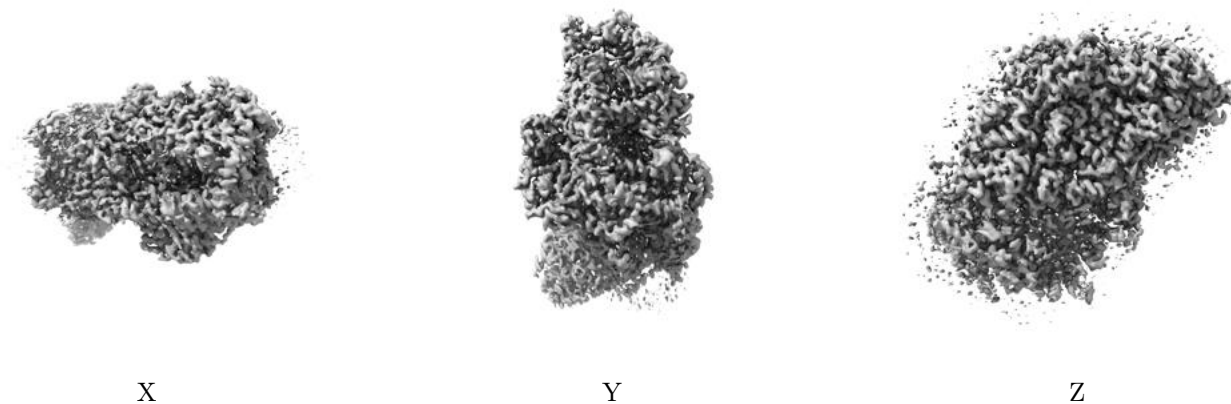


Z

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 0.0801. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

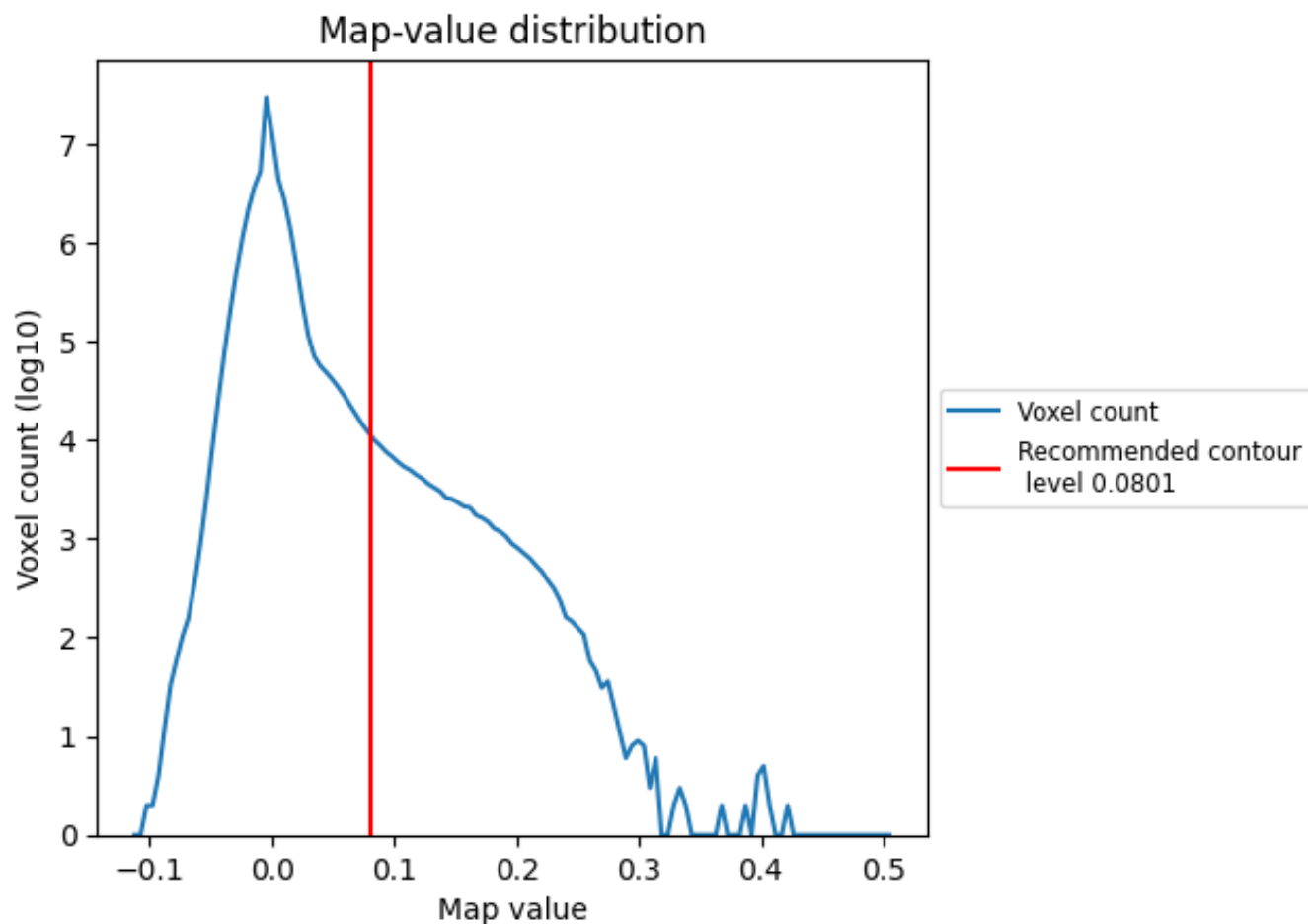
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

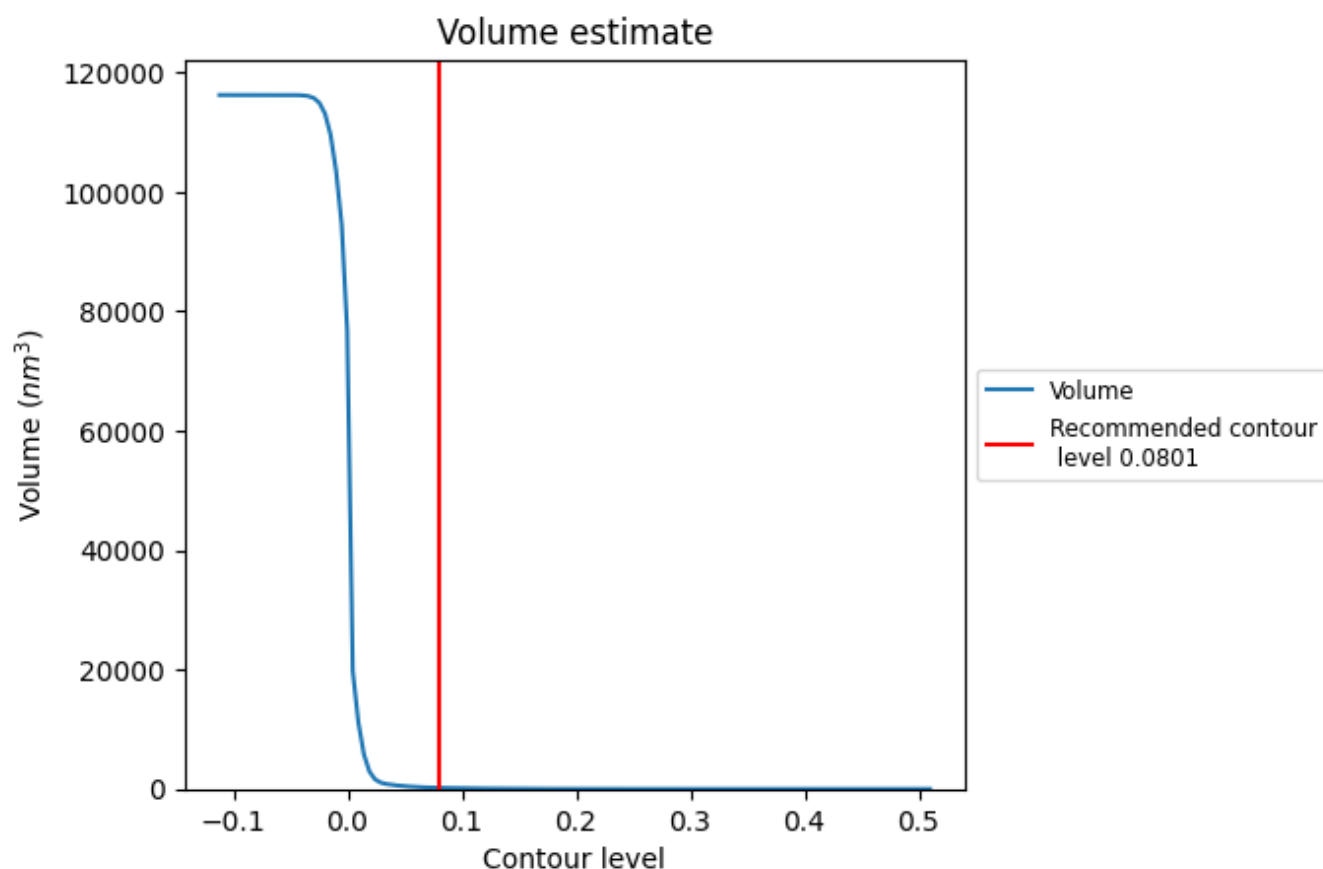
This section contains the results of statistical analysis of the map.

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.

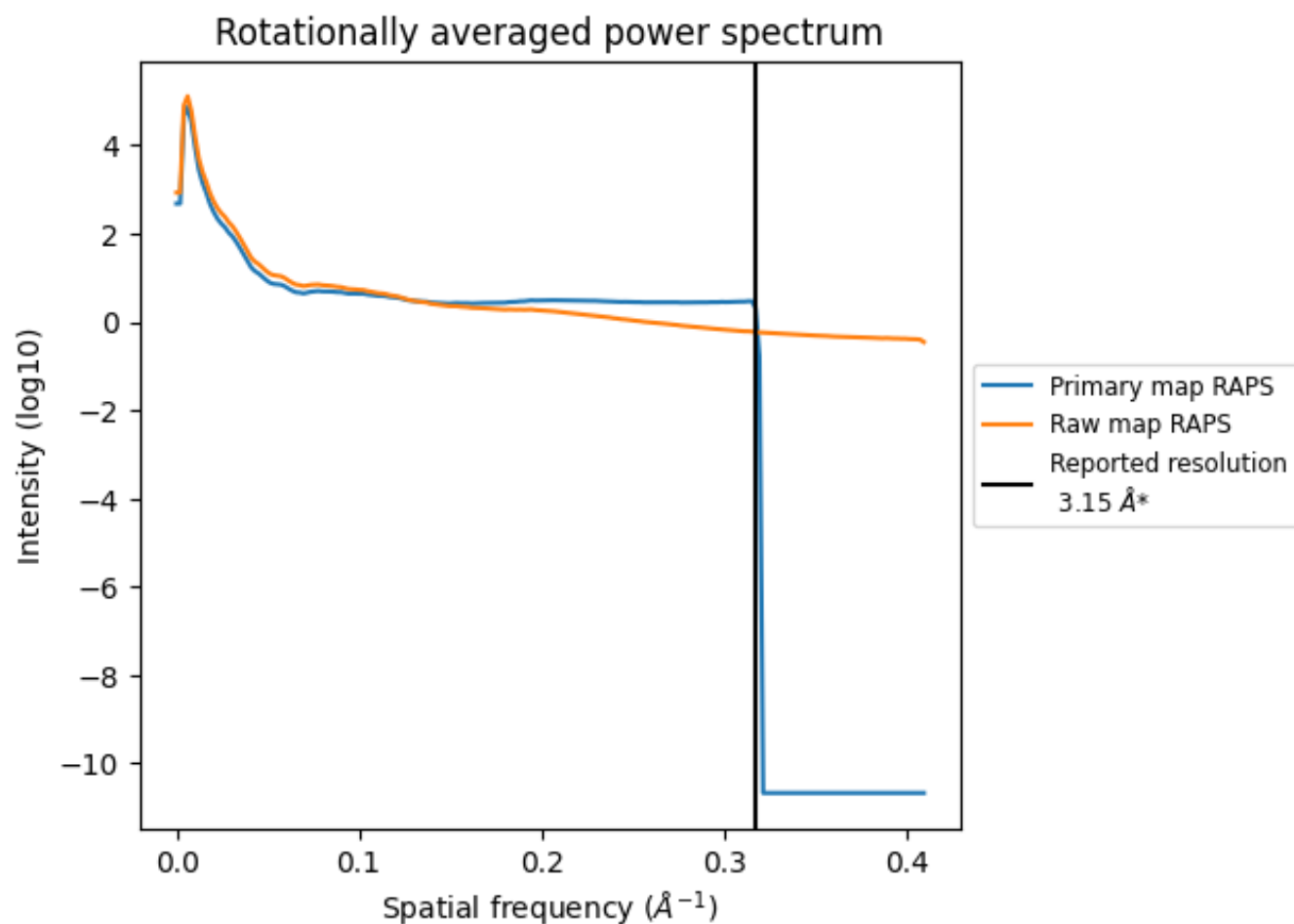
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 187 nm^3 ; this corresponds to an approximate mass of 169 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 ⓘ

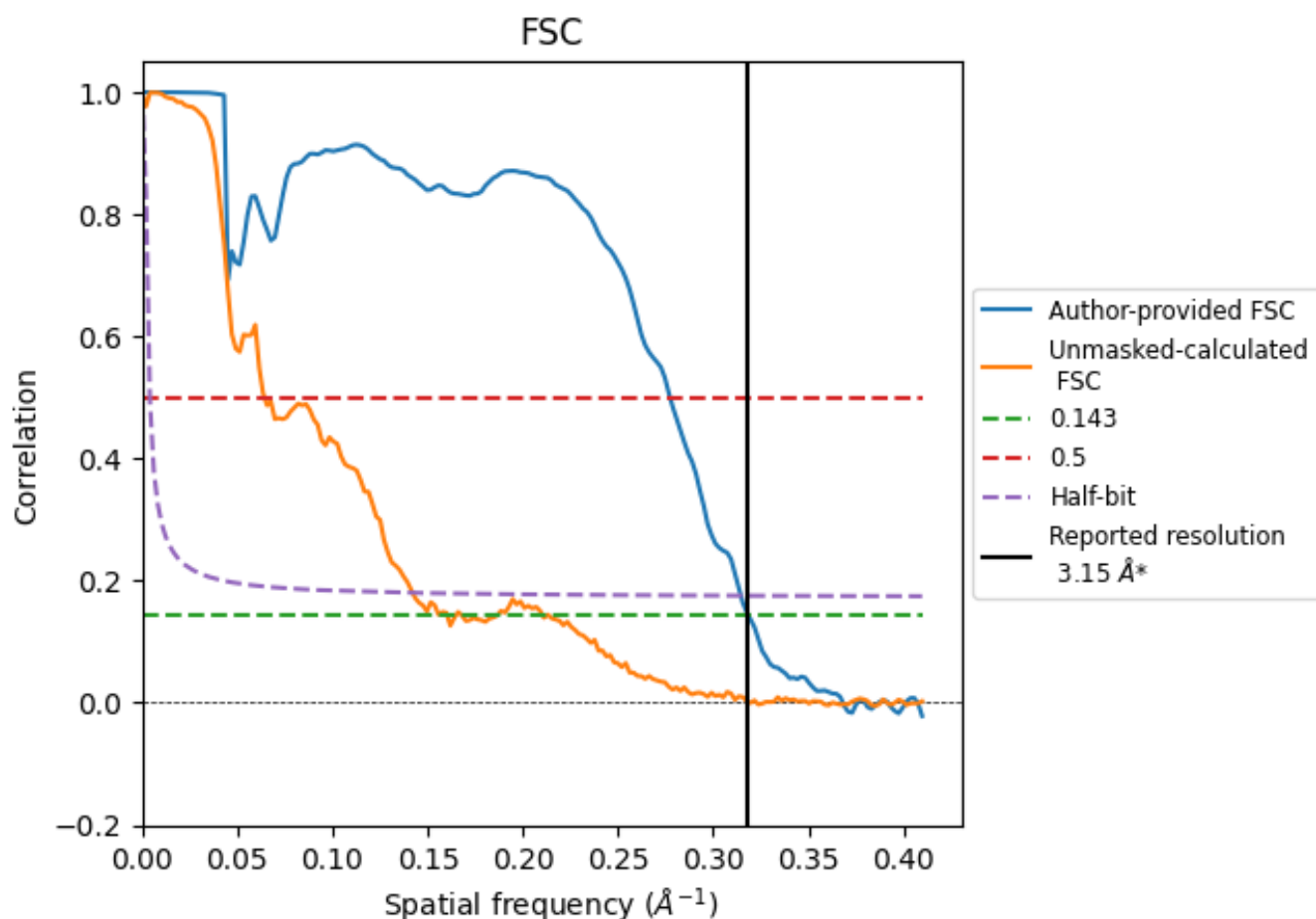


*Reported resolution corresponds to spatial frequency of 0.317 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.317 Å⁻¹

8.2 Resolution estimates [i](#)

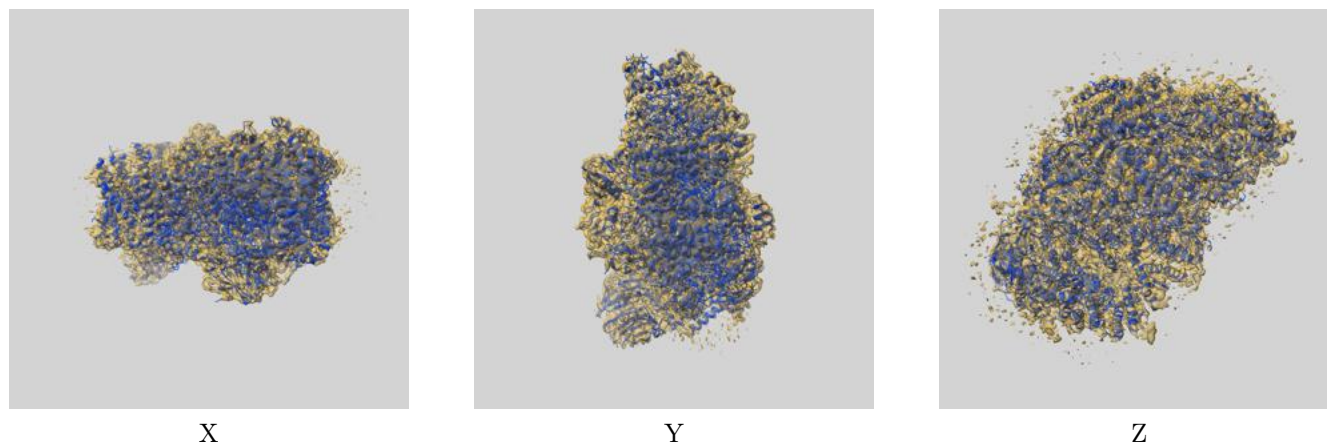
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.15	-	-
Author-provided FSC curve	3.14	3.60	3.18
Unmasked-calculated*	6.24	15.58	7.04

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.24 differs from the reported value 3.15 by more than 10 %

9 Map-model fit [i](#)

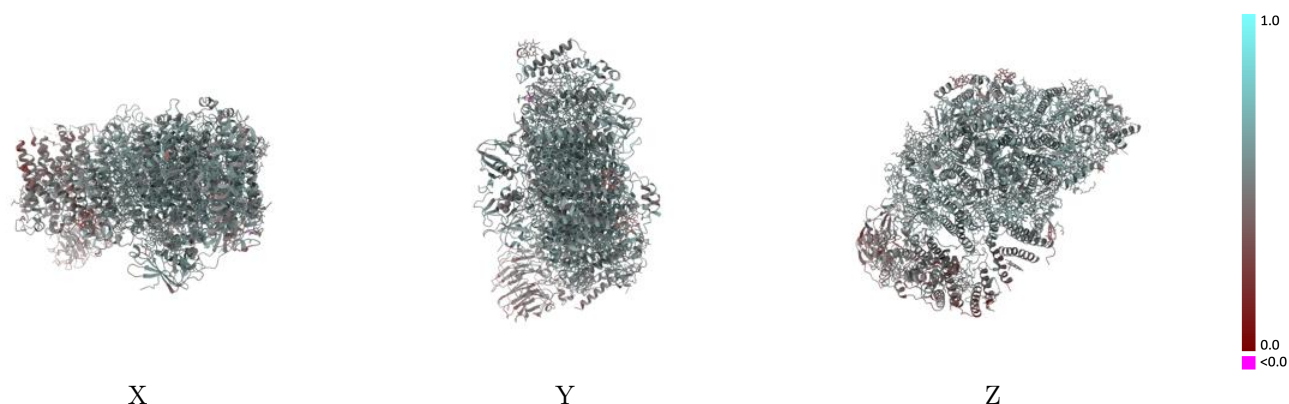
This section contains information regarding the fit between EMDB map EMD-15618 and PDB model 8ASL. Per-residue inclusion information can be found in [section 3](#) on [page 25](#).

9.1 Map-model overlay [i](#)



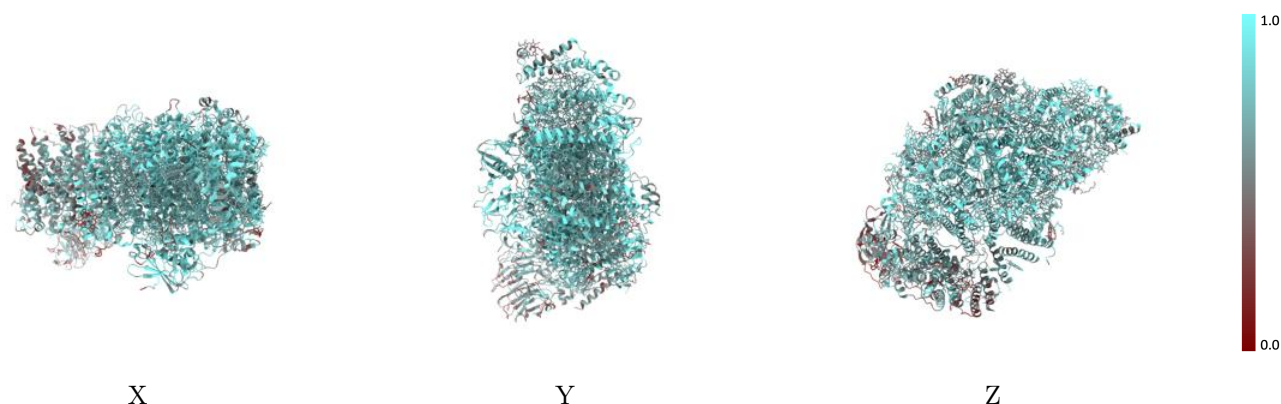
The images above show the 3D surface view of the map at the recommended contour level 0.0801 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



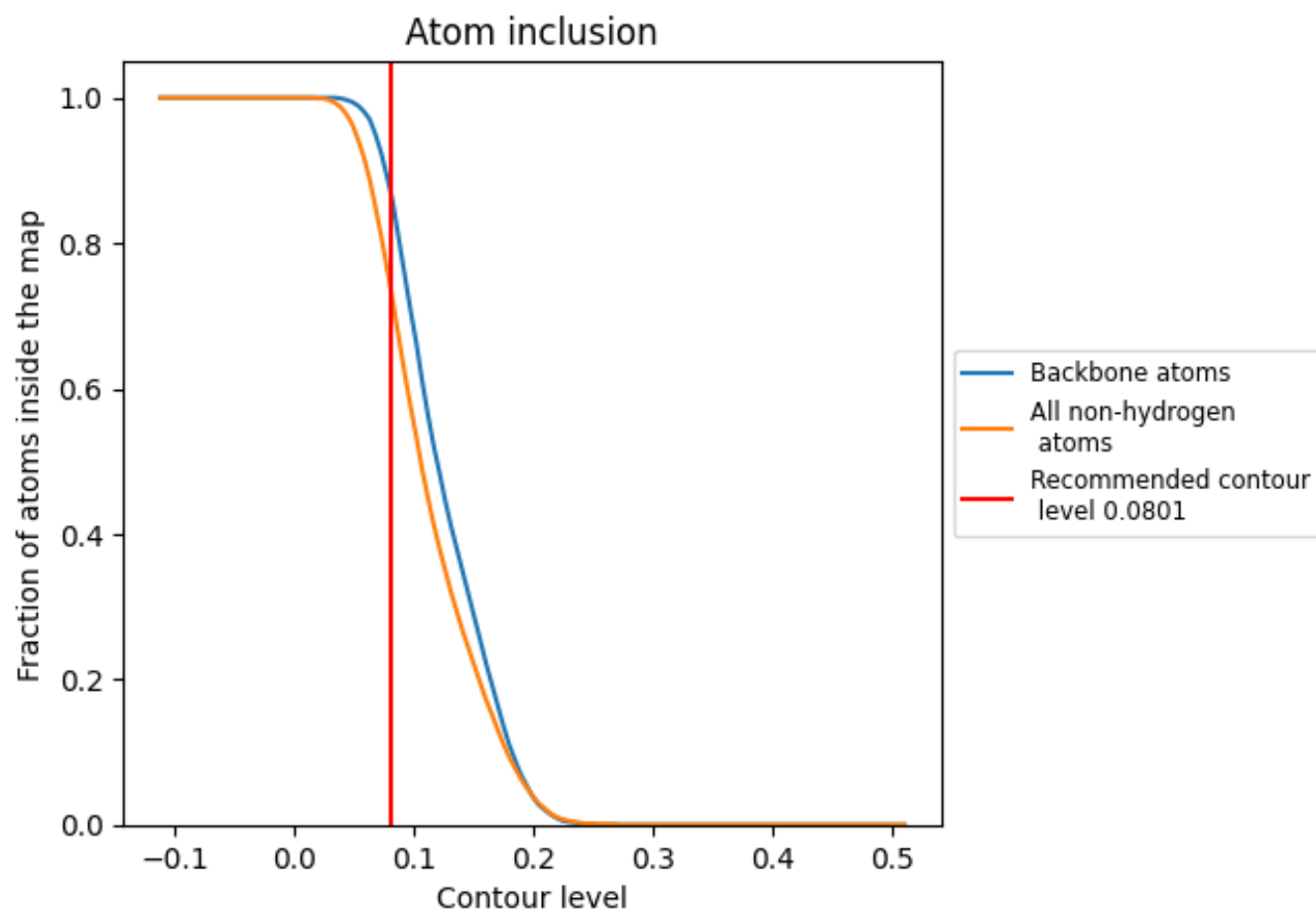
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0801).

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 74% 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 (0.0801) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7400	0.5180
A	0.6210	0.4580
D	0.5850	0.4470
E	0.6500	0.4520
F	0.6210	0.4440
I	0.4290	0.3910
S	0.5100	0.3970
a	0.8130	0.5560
b	0.8260	0.5550
c	0.9200	0.5460
d	0.8060	0.5380
e	0.7670	0.5320
f	0.6810	0.5230
i	0.7550	0.5400
j	0.6140	0.4920
k	0.6310	0.5060
l	0.7110	0.4970
m	0.7360	0.5420

1.0

0.0

<0.0