



wwPDB EM Validation Summary Report ⓘ

Aug 6, 2026 – 03:46 AM JST

PDB ID : 7COY / pdb_00007coy
EMDB ID : EMD-30420
Title : Structure of the far-red light utilizing photosystem I of *Acaryochloris marina*
Authors : Kawakami, K.; Yonekura, K.; Hamaguchi, T.; Kashino, Y.; Shinzawa-Itoh, K.;
Inoue-Kashino, N.; Itoh, S.; Ifuku, K.; Yamashita, E.
Deposited on : 2020-08-05
Resolution : 2.50 Å(reported)

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:

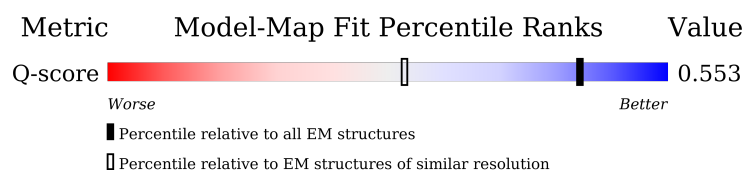
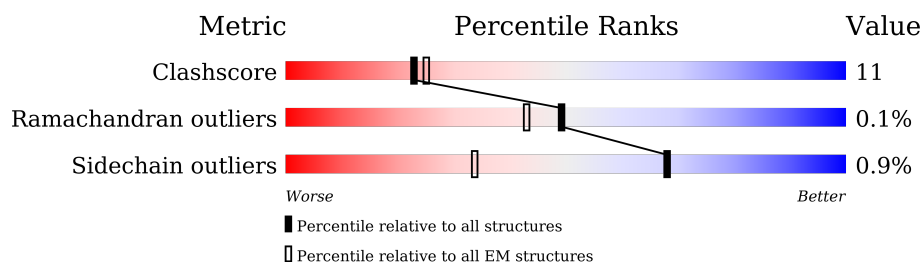
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using 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) : 2.50

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.50 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	7115 (2.00 - 3.00)

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	aA	753	19% 68% 22% 9%
1	bA	753	19% 68% 22% 9%
1	cA	753	19% 68% 22% 9%
2	aB	736	18% 65% 23% 11%

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Mol	Chain	Length	Quality of chain
2	bB	736	
2	cB	736	
3	aC	81	
3	bC	81	
3	cC	81	
4	aD	139	
4	bD	139	
4	cD	139	
5	aE	89	
5	bE	89	
5	cE	89	
6	aF	167	
6	bF	167	
6	cF	167	
7	aI	34	
7	bI	34	
7	cI	34	
8	aJ	51	
8	bJ	51	
8	cJ	51	
9	aK	86	
9	bK	86	
9	cK	86	
10	aL	153	
10	bL	153	

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Mol	Chain	Length	Quality of chain
10	cL	153	
11	aM	31	
11	bM	31	
11	cM	31	

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
12	G9R	aA	3101	X	-	-	-
12	G9R	cA	3101	X	-	-	-
14	CL7	aA	3103	X	-	-	-
14	CL7	aA	3104	X	-	-	-
14	CL7	aA	3105	X	-	-	-
14	CL7	aA	3106	X	-	-	-
14	CL7	aA	3107	X	-	-	-
14	CL7	aA	3108	X	-	-	-
14	CL7	aA	3109	X	-	-	-
14	CL7	aA	3110	X	-	-	-
14	CL7	aA	3111	X	-	-	-
14	CL7	aA	3112	X	-	-	-
14	CL7	aA	3113	X	-	-	-
14	CL7	aA	3114	X	-	-	-
14	CL7	aA	3115	X	-	-	-
14	CL7	aA	3116	X	-	-	-
14	CL7	aA	3117	X	-	-	-
14	CL7	aA	3118	X	-	-	-
14	CL7	aA	3119	X	-	-	-
14	CL7	aA	3120	X	-	-	-
14	CL7	aA	3121	X	-	-	-
14	CL7	aA	3122	X	-	-	-
14	CL7	aA	3123	X	-	-	-
14	CL7	aA	3124	X	-	-	-
14	CL7	aA	3125	X	-	-	-
14	CL7	aA	3126	X	-	-	-
14	CL7	aA	3127	X	-	-	-
14	CL7	aA	3128	X	-	-	-
14	CL7	aA	3129	X	-	-	-
14	CL7	aA	3130	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CL7	aA	3131	X	-	-	-
14	CL7	aA	3132	X	-	-	-
14	CL7	aA	3133	X	-	-	-
14	CL7	aA	3134	X	-	-	-
14	CL7	aA	3140	X	-	-	-
14	CL7	aA	3141	X	-	-	-
14	CL7	aA	3142	X	-	-	-
14	CL7	aA	3143	X	-	-	-
14	CL7	aA	3146	X	-	-	-
14	CL7	aB	3002	X	-	-	-
14	CL7	aB	3003	X	-	-	-
14	CL7	aB	3005	X	-	-	-
14	CL7	aB	3006	X	-	-	-
14	CL7	aB	3007	X	-	-	-
14	CL7	aB	3008	X	-	-	-
14	CL7	aB	3009	X	-	-	-
14	CL7	aB	3010	X	-	-	-
14	CL7	aB	3011	X	-	-	-
14	CL7	aB	3012	X	-	-	-
14	CL7	aB	3013	X	-	-	-
14	CL7	aB	3014	X	-	-	-
14	CL7	aB	3015	X	-	-	-
14	CL7	aB	3016	X	-	-	-
14	CL7	aB	3017	X	-	-	-
14	CL7	aB	3018	X	-	-	-
14	CL7	aB	3019	X	-	-	-
14	CL7	aB	3020	X	-	-	-
14	CL7	aB	3021	X	-	-	-
14	CL7	aB	3022	X	-	-	-
14	CL7	aB	3023	X	-	-	-
14	CL7	aB	3024	X	-	-	-
14	CL7	aB	3025	X	-	-	-
14	CL7	aB	3026	X	-	-	-
14	CL7	aB	3030	X	-	-	-
14	CL7	aB	3031	X	-	-	-
14	CL7	aB	3032	X	-	-	-
14	CL7	aF	201	X	-	-	-
14	CL7	aJ	101	X	-	-	-
14	CL7	aK	101	X	-	-	-
14	CL7	aL	202	X	-	-	-
14	CL7	aL	203	X	-	-	-
14	CL7	aL	204	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CL7	bA	3102	X	-	-	-
14	CL7	bA	3103	X	-	-	-
14	CL7	bA	3104	X	-	-	-
14	CL7	bA	3105	X	-	-	-
14	CL7	bA	3106	X	-	-	-
14	CL7	bA	3107	X	-	-	-
14	CL7	bA	3108	X	-	-	-
14	CL7	bA	3109	X	-	-	-
14	CL7	bA	3110	X	-	-	-
14	CL7	bA	3111	X	-	-	-
14	CL7	bA	3112	X	-	-	-
14	CL7	bA	3113	X	-	-	-
14	CL7	bA	3114	X	-	-	-
14	CL7	bA	3115	X	-	-	-
14	CL7	bA	3116	X	-	-	-
14	CL7	bA	3117	X	-	-	-
14	CL7	bA	3118	X	-	-	-
14	CL7	bA	3119	X	-	-	-
14	CL7	bA	3120	X	-	-	-
14	CL7	bA	3121	X	-	-	-
14	CL7	bA	3122	X	-	-	-
14	CL7	bA	3123	X	-	-	-
14	CL7	bA	3124	X	-	-	-
14	CL7	bA	3125	X	-	-	-
14	CL7	bA	3126	X	-	-	-
14	CL7	bA	3127	X	-	-	-
14	CL7	bA	3128	X	-	-	-
14	CL7	bA	3129	X	-	-	-
14	CL7	bA	3130	X	-	-	-
14	CL7	bA	3131	X	-	-	-
14	CL7	bA	3132	X	-	-	-
14	CL7	bA	3133	X	-	-	-
14	CL7	bA	3139	X	-	-	-
14	CL7	bA	3140	X	-	-	-
14	CL7	bA	3141	X	-	-	-
14	CL7	bA	3142	X	-	-	-
14	CL7	bA	3145	X	-	-	-
14	CL7	bB	803	X	-	-	-
14	CL7	bB	804	X	-	-	-
14	CL7	bB	806	X	-	-	-
14	CL7	bB	807	X	-	-	-
14	CL7	bB	808	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CL7	bB	809	X	-	-	-
14	CL7	bB	810	X	-	-	-
14	CL7	bB	811	X	-	-	-
14	CL7	bB	812	X	-	-	-
14	CL7	bB	813	X	-	-	-
14	CL7	bB	814	X	-	-	-
14	CL7	bB	815	X	-	-	-
14	CL7	bB	816	X	-	-	-
14	CL7	bB	817	X	-	-	-
14	CL7	bB	818	X	-	-	-
14	CL7	bB	819	X	-	-	-
14	CL7	bB	820	X	-	-	-
14	CL7	bB	821	X	-	-	-
14	CL7	bB	822	X	-	-	-
14	CL7	bB	823	X	-	-	-
14	CL7	bB	824	X	-	-	-
14	CL7	bB	825	X	-	-	-
14	CL7	bB	826	X	-	-	-
14	CL7	bB	827	X	-	-	-
14	CL7	bB	831	X	-	-	-
14	CL7	bB	832	X	-	-	-
14	CL7	bB	833	X	-	-	-
14	CL7	bF	201	X	-	-	-
14	CL7	bJ	101	X	-	-	-
14	CL7	bK	101	X	-	-	-
14	CL7	bL	203	X	-	-	-
14	CL7	bL	204	X	-	-	-
14	CL7	bL	205	X	-	-	-
14	CL7	cA	3102	X	-	-	-
14	CL7	cA	3103	X	-	-	-
14	CL7	cA	3104	X	-	-	-
14	CL7	cA	3105	X	-	-	-
14	CL7	cA	3106	X	-	-	-
14	CL7	cA	3107	X	-	-	-
14	CL7	cA	3108	X	-	-	-
14	CL7	cA	3109	X	-	-	-
14	CL7	cA	3110	X	-	-	-
14	CL7	cA	3111	X	-	-	-
14	CL7	cA	3112	X	-	-	-
14	CL7	cA	3113	X	-	-	-
14	CL7	cA	3114	X	-	-	-
14	CL7	cA	3115	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CL7	cA	3116	X	-	-	-
14	CL7	cA	3117	X	-	-	-
14	CL7	cA	3118	X	-	-	-
14	CL7	cA	3119	X	-	-	-
14	CL7	cA	3120	X	-	-	-
14	CL7	cA	3121	X	-	-	-
14	CL7	cA	3122	X	-	-	-
14	CL7	cA	3123	X	-	-	-
14	CL7	cA	3124	X	-	-	-
14	CL7	cA	3125	X	-	-	-
14	CL7	cA	3126	X	-	-	-
14	CL7	cA	3127	X	-	-	-
14	CL7	cA	3128	X	-	-	-
14	CL7	cA	3129	X	-	-	-
14	CL7	cA	3130	X	-	-	-
14	CL7	cA	3131	X	-	-	-
14	CL7	cA	3132	X	-	-	-
14	CL7	cA	3133	X	-	-	-
14	CL7	cA	3139	X	-	-	-
14	CL7	cA	3140	X	-	-	-
14	CL7	cA	3141	X	-	-	-
14	CL7	cA	3142	X	-	-	-
14	CL7	cA	3144	X	-	-	-
14	CL7	cB	803	X	-	-	-
14	CL7	cB	804	X	-	-	-
14	CL7	cB	806	X	-	-	-
14	CL7	cB	807	X	-	-	-
14	CL7	cB	808	X	-	-	-
14	CL7	cB	809	X	-	-	-
14	CL7	cB	810	X	-	-	-
14	CL7	cB	811	X	-	-	-
14	CL7	cB	812	X	-	-	-
14	CL7	cB	813	X	-	-	-
14	CL7	cB	814	X	-	-	-
14	CL7	cB	815	X	-	-	-
14	CL7	cB	816	X	-	-	-
14	CL7	cB	817	X	-	-	-
14	CL7	cB	818	X	-	-	-
14	CL7	cB	819	X	-	-	-
14	CL7	cB	820	X	-	-	-
14	CL7	cB	821	X	-	-	-
14	CL7	cB	822	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CL7	cB	823	X	-	-	-
14	CL7	cB	824	X	-	-	-
14	CL7	cB	825	X	-	-	-
14	CL7	cB	826	X	-	-	-
14	CL7	cB	827	X	-	-	-
14	CL7	cB	831	X	-	-	-
14	CL7	cB	832	X	-	-	-
14	CL7	cB	833	X	-	-	-
14	CL7	cF	201	X	-	-	-
14	CL7	cJ	101	X	-	-	-
14	CL7	cK	101	X	-	-	-
14	CL7	cL	203	X	-	-	-
14	CL7	cL	204	X	-	-	-
14	CL7	cL	205	X	-	-	-

2 Entry composition [i](#)

There are 20 unique types of molecules in this entry. The entry contains 57966 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	aA	685	Total	C	N	O	S	0	0
			5203	3384	909	886	24		
1	bA	685	Total	C	N	O	S	0	0
			5203	3384	909	886	24		
1	cA	685	Total	C	N	O	S	0	0
			5203	3384	909	886	24		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	aB	658	Total	C	N	O	S	0	0
			5007	3292	840	860	15		
2	bB	658	Total	C	N	O	S	0	0
			5007	3292	840	860	15		
2	cB	658	Total	C	N	O	S	0	0
			5007	3292	840	860	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	aC	80	Total	C	N	O	S	0	0
			573	353	102	108	10		
3	bC	80	Total	C	N	O	S	0	0
			573	353	102	108	10		
3	cC	80	Total	C	N	O	S	0	0
			573	353	102	108	10		

- Molecule 4 is a protein called Photosystem I protein PsuD.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	aD	136	Total	C	N	O	S	0	0
			999	631	177	187	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	bD	136	Total	C	N	O	S	0	0
			999	631	177	187	4		
4	cD	136	Total	C	N	O	S	0	0
			999	631	177	187	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	aE	67	Total	C	N	O		0	0
			375	230	70	75			
5	bE	67	Total	C	N	O		0	0
			375	230	70	75			
5	cE	67	Total	C	N	O		0	0
			375	230	70	75			

- Molecule 6 is a protein called Photosystem I protein Psal.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	aF	132	Total	C	N	O	S	0	0
			847	529	157	157	4		
6	bF	132	Total	C	N	O	S	0	0
			847	529	157	157	4		
6	cF	132	Total	C	N	O	S	0	0
			847	529	157	157	4		

- Molecule 7 is a protein called Photosystem I protein Psal27.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	aI	30	Total	C	N	O	S	0	0
			225	151	33	39	2		
7	bI	30	Total	C	N	O	S	0	0
			225	151	33	39	2		
7	cI	30	Total	C	N	O	S	0	0
			225	151	33	39	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	aJ	35	Total	C	N	O		0	0
			264	184	39	41			
8	bJ	35	Total	C	N	O		0	0
			264	184	39	41			

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Mol	Chain	Residues	Atoms				AltConf	Trace
8	cJ	35	Total	C	N	O	0	0
			264	184	39	41		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
9	aK	33	Total	C	N	O	0	0
			161	95	33	33		
9	bK	33	Total	C	N	O	0	0
			161	95	33	33		
9	cK	33	Total	C	N	O	0	0
			161	95	33	33		

- Molecule 10 is a protein called Photosystem I protein PsaL.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	aL	147	Total	C	N	O	S	0	0
			999	638	168	189	4		
10	bL	147	Total	C	N	O	S	0	0
			999	638	168	189	4		
10	cL	147	Total	C	N	O	S	0	0
			999	638	168	189	4		

- Molecule 11 is a protein called Photosystem I protein PsaM.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	aM	29	Total	C	N	O	0	0
			205	136	31	38		
11	bM	29	Total	C	N	O	0	0
			205	136	31	38		
11	cM	29	Total	C	N	O	0	0
			205	136	31	38		

- Molecule 12 is CHLOROPHYLL D ISOMER (CCD ID: G9R) (formula: $C_{54}H_{70}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).

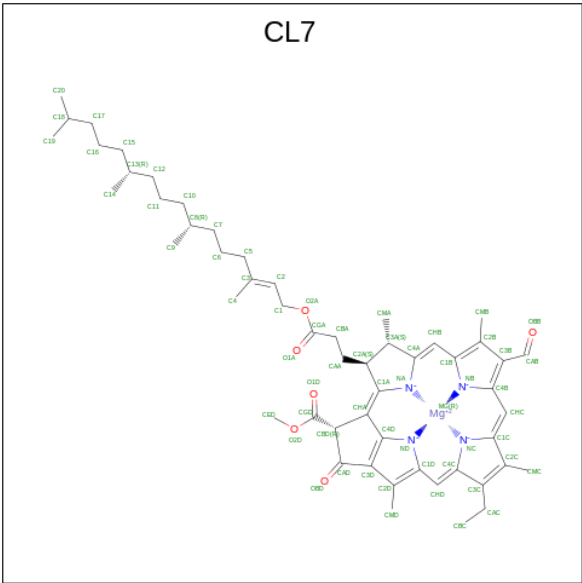


- Molecule 13 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
13	aA	1	Total	C	N	O	0
			64	55	4	5	
13	aB	1	Total	C	N	O	0
			64	55	4	5	
13	bB	1	Total	C	N	O	0
			64	55	4	5	
13	bB	1	Total	C	N	O	0
			64	55	4	5	
13	cB	1	Total	C	N	O	0
			64	55	4	5	
13	cB	1	Total	C	N	O	0
			64	55	4	5	

- Molecule 14 is CHLOROPHYLL D (CCD ID: CL7) (formula: C₅₄H₇₀MgN₄O₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
14	aA	1	Total	C	Mg	N	O
			65	54	1	4	6
14	aA	1	Total	C	Mg	N	O
			41	32	1	4	4
14	aA	1	Total	C	Mg	N	O
			41	32	1	4	4
14	aA	1	Total	C	Mg	N	O
			41	32	1	4	4
14	aA	1	Total	C	Mg	N	O
			65	54	1	4	6

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Mol	Chain	Residues	Atoms					AltConf
14	aA	1	Total 65	C 54	Mg 1	N 4	O 6	0
14	aA	1	Total 42	C 33	Mg 1	N 4	O 4	0
14	aA	1	Total 41	C 32	Mg 1	N 4	O 4	0
14	aA	1	Total 41	C 32	Mg 1	N 4	O 4	0
14	aA	1	Total 38	C 31	Mg 1	N 4	O 2	0
14	aA	1	Total 41	C 32	Mg 1	N 4	O 4	0
14	aA	1	Total 41	C 32	Mg 1	N 4	O 4	0
14	aA	1	Total 65	C 54	Mg 1	N 4	O 6	0
14	aA	1	Total 38	C 31	Mg 1	N 4	O 2	0
14	aA	1	Total 53	C 42	Mg 1	N 4	O 6	0
14	aA	1	Total 38	C 31	Mg 1	N 4	O 2	0
14	aA	1	Total 38	C 31	Mg 1	N 4	O 2	0
14	aA	1	Total 46	C 35	Mg 1	N 4	O 6	0
14	aA	1	Total 51	C 40	Mg 1	N 4	O 6	0
14	aA	1	Total 41	C 32	Mg 1	N 4	O 4	0
14	aA	1	Total 50	C 39	Mg 1	N 4	O 6	0
14	aA	1	Total 51	C 40	Mg 1	N 4	O 6	0
14	aA	1	Total 65	C 54	Mg 1	N 4	O 6	0
14	aA	1	Total 65	C 54	Mg 1	N 4	O 6	0
14	aA	1	Total 53	C 42	Mg 1	N 4	O 6	0
14	aA	1	Total 51	C 40	Mg 1	N 4	O 6	0

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Mol	Chain	Residues	Atoms					AltConf
14	aA	1	Total 65	C 54	Mg 1	N 4	O 6	0
14	aA	1	Total 41	C 32	Mg 1	N 4	O 4	0
14	aA	1	Total 41	C 32	Mg 1	N 4	O 4	0
14	aA	1	Total 41	C 32	Mg 1	N 4	O 4	0
14	aA	1	Total 65	C 54	Mg 1	N 4	O 6	0
14	aA	1	Total 41	C 32	Mg 1	N 4	O 4	0
14	aA	1	Total 65	C 54	Mg 1	N 4	O 6	0
14	aA	1	Total 65	C 54	Mg 1	N 4	O 6	0
14	aA	1	Total 65	C 54	Mg 1	N 4	O 6	0
14	aA	1	Total 65	C 54	Mg 1	N 4	O 6	0
14	aA	1	Total 41	C 32	Mg 1	N 4	O 4	0
14	aB	1	Total 65	C 54	Mg 1	N 4	O 6	0
14	aB	1	Total 65	C 54	Mg 1	N 4	O 6	0
14	aB	1	Total 65	C 54	Mg 1	N 4	O 6	0
14	aB	1	Total 65	C 54	Mg 1	N 4	O 6	0
14	aB	1	Total 65	C 54	Mg 1	N 4	O 6	0
14	aB	1	Total 50	C 39	Mg 1	N 4	O 6	0
14	aB	1	Total 65	C 54	Mg 1	N 4	O 6	0
14	aB	1	Total 41	C 32	Mg 1	N 4	O 4	0
14	aB	1	Total 38	C 31	Mg 1	N 4	O 2	0
14	aB	1	Total 38	C 31	Mg 1	N 4	O 2	0

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Mol	Chain	Residues	Atoms					AltConf
14	aB	1	Total 41	C 32	Mg 1	N 4	O 4	0
14	aB	1	Total 41	C 32	Mg 1	N 4	O 4	0
14	aB	1	Total 50	C 39	Mg 1	N 4	O 6	0
14	aB	1	Total 41	C 32	Mg 1	N 4	O 4	0
14	aB	1	Total 41	C 32	Mg 1	N 4	O 4	0
14	aB	1	Total 56	C 45	Mg 1	N 4	O 6	0
14	aB	1	Total 65	C 54	Mg 1	N 4	O 6	0
14	aB	1	Total 38	C 31	Mg 1	N 4	O 2	0
14	aB	1	Total 41	C 32	Mg 1	N 4	O 4	0
14	aB	1	Total 41	C 32	Mg 1	N 4	O 4	0
14	aB	1	Total 56	C 45	Mg 1	N 4	O 6	0
14	aB	1	Total 38	C 31	Mg 1	N 4	O 2	0
14	aB	1	Total 65	C 54	Mg 1	N 4	O 6	0
14	aB	1	Total 65	C 54	Mg 1	N 4	O 6	0
14	aB	1	Total 54	C 43	Mg 1	N 4	O 6	0
14	aB	1	Total 65	C 54	Mg 1	N 4	O 6	0
14	aB	1	Total 55	C 44	Mg 1	N 4	O 6	0
14	aF	1	Total 38	C 31	Mg 1	N 4	O 2	0
14	aJ	1	Total 42	C 33	Mg 1	N 4	O 4	0
14	aK	1	Total 37	C 30	Mg 1	N 4	O 2	0
14	aL	1	Total 65	C 54	Mg 1	N 4	O 6	0

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Mol	Chain	Residues	Atoms					AltConf
14	aL	1	Total 65	C 54	Mg 1	N 4	O 6	0
14	aL	1	Total 42	C 33	Mg 1	N 4	O 4	0
14	bA	1	Total 65	C 54	Mg 1	N 4	O 6	0
14	bA	1	Total 41	C 32	Mg 1	N 4	O 4	0
14	bA	1	Total 41	C 32	Mg 1	N 4	O 4	0
14	bA	1	Total 41	C 32	Mg 1	N 4	O 4	0
14	bA	1	Total 65	C 54	Mg 1	N 4	O 6	0
14	bA	1	Total 65	C 54	Mg 1	N 4	O 6	0
14	bA	1	Total 42	C 33	Mg 1	N 4	O 4	0
14	bA	1	Total 41	C 32	Mg 1	N 4	O 4	0
14	bA	1	Total 41	C 32	Mg 1	N 4	O 4	0
14	bA	1	Total 38	C 31	Mg 1	N 4	O 2	0
14	bA	1	Total 41	C 32	Mg 1	N 4	O 4	0
14	bA	1	Total 41	C 32	Mg 1	N 4	O 4	0
14	bA	1	Total 65	C 54	Mg 1	N 4	O 6	0
14	bA	1	Total 38	C 31	Mg 1	N 4	O 2	0
14	bA	1	Total 53	C 42	Mg 1	N 4	O 6	0
14	bA	1	Total 38	C 31	Mg 1	N 4	O 2	0
14	bA	1	Total 38	C 31	Mg 1	N 4	O 2	0
14	bA	1	Total 46	C 35	Mg 1	N 4	O 6	0
14	bA	1	Total 51	C 40	Mg 1	N 4	O 6	0

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Mol	Chain	Residues	Atoms					AltConf
14	bA	1	Total 41	C 32	Mg 1	N 4	O 4	0
14	bA	1	Total 50	C 39	Mg 1	N 4	O 6	0
14	bA	1	Total 51	C 40	Mg 1	N 4	O 6	0
14	bA	1	Total 65	C 54	Mg 1	N 4	O 6	0
14	bA	1	Total 65	C 54	Mg 1	N 4	O 6	0
14	bA	1	Total 53	C 42	Mg 1	N 4	O 6	0
14	bA	1	Total 51	C 40	Mg 1	N 4	O 6	0
14	bA	1	Total 65	C 54	Mg 1	N 4	O 6	0
14	bA	1	Total 41	C 32	Mg 1	N 4	O 4	0
14	bA	1	Total 41	C 32	Mg 1	N 4	O 4	0
14	bA	1	Total 41	C 32	Mg 1	N 4	O 4	0
14	bA	1	Total 65	C 54	Mg 1	N 4	O 6	0
14	bA	1	Total 41	C 32	Mg 1	N 4	O 4	0
14	bA	1	Total 65	C 54	Mg 1	N 4	O 6	0
14	bA	1	Total 65	C 54	Mg 1	N 4	O 6	0
14	bA	1	Total 65	C 54	Mg 1	N 4	O 6	0
14	bA	1	Total 41	C 32	Mg 1	N 4	O 4	0
14	bB	1	Total 65	C 54	Mg 1	N 4	O 6	0
14	bB	1	Total 65	C 54	Mg 1	N 4	O 6	0
14	bB	1	Total 65	C 54	Mg 1	N 4	O 6	0

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Mol	Chain	Residues	Atoms					AltConf
14	bB	1	Total 65	C 54	Mg 1	N 4	O 6	0
14	bB	1	Total 65	C 54	Mg 1	N 4	O 6	0
14	bB	1	Total 50	C 39	Mg 1	N 4	O 6	0
14	bB	1	Total 65	C 54	Mg 1	N 4	O 6	0
14	bB	1	Total 41	C 32	Mg 1	N 4	O 4	0
14	bB	1	Total 38	C 31	Mg 1	N 4	O 2	0
14	bB	1	Total 38	C 31	Mg 1	N 4	O 2	0
14	bB	1	Total 41	C 32	Mg 1	N 4	O 4	0
14	bB	1	Total 41	C 32	Mg 1	N 4	O 4	0
14	bB	1	Total 50	C 39	Mg 1	N 4	O 6	0
14	bB	1	Total 41	C 32	Mg 1	N 4	O 4	0
14	bB	1	Total 41	C 32	Mg 1	N 4	O 4	0
14	bB	1	Total 56	C 45	Mg 1	N 4	O 6	0
14	bB	1	Total 65	C 54	Mg 1	N 4	O 6	0
14	bB	1	Total 38	C 31	Mg 1	N 4	O 2	0
14	bB	1	Total 41	C 32	Mg 1	N 4	O 4	0
14	bB	1	Total 41	C 32	Mg 1	N 4	O 4	0
14	bB	1	Total 56	C 45	Mg 1	N 4	O 6	0
14	bB	1	Total 38	C 31	Mg 1	N 4	O 2	0
14	bB	1	Total 65	C 54	Mg 1	N 4	O 6	0
14	bB	1	Total 65	C 54	Mg 1	N 4	O 6	0

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Mol	Chain	Residues	Atoms					AltConf
14	bB	1	Total	C	Mg	N	O	0
			54	43	1	4	6	
14	bB	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
14	bB	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
14	bF	1	Total	C	Mg	N	O	0
			38	31	1	4	2	
14	bJ	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
14	bK	1	Total	C	Mg	N	O	0
			37	30	1	4	2	
14	bL	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
14	bL	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
14	bL	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
14	cA	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
14	cA	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
14	cA	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
14	cA	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
14	cA	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
14	cA	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
14	cA	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
14	cA	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
14	cA	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
14	cA	1	Total	C	Mg	N	O	0
			38	31	1	4	2	
14	cA	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
14	cA	1	Total	C	Mg	N	O	0
			41	32	1	4	4	

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Mol	Chain	Residues	Atoms					AltConf
14	cA	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
14	cA	1	Total	C	Mg	N	O	0
			38	31	1	4	2	
14	cA	1	Total	C	Mg	N	O	0
			53	42	1	4	6	
14	cA	1	Total	C	Mg	N	O	0
			38	31	1	4	2	
14	cA	1	Total	C	Mg	N	O	0
			38	31	1	4	2	
14	cA	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
14	cA	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
14	cA	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
14	cA	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
14	cA	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
14	cA	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
14	cA	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
14	cA	1	Total	C	Mg	N	O	0
			53	42	1	4	6	
14	cA	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
14	cA	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
14	cA	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
14	cA	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
14	cA	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
14	cA	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
14	cA	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
14	cA	1	Total	C	Mg	N	O	0
			65	54	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
14	cA	1	Total 65	C 54	Mg 1	N 4	O 6	0
14	cA	1	Total 65	C 54	Mg 1	N 4	O 6	0
14	cA	1	Total 65	C 54	Mg 1	N 4	O 6	0
14	cA	1	Total 41	C 32	Mg 1	N 4	O 4	0
14	cB	1	Total 65	C 54	Mg 1	N 4	O 6	0
14	cB	1	Total 65	C 54	Mg 1	N 4	O 6	0
14	cB	1	Total 65	C 54	Mg 1	N 4	O 6	0
14	cB	1	Total 65	C 54	Mg 1	N 4	O 6	0
14	cB	1	Total 65	C 54	Mg 1	N 4	O 6	0
14	cB	1	Total 50	C 39	Mg 1	N 4	O 6	0
14	cB	1	Total 65	C 54	Mg 1	N 4	O 6	0
14	cB	1	Total 41	C 32	Mg 1	N 4	O 4	0
14	cB	1	Total 38	C 31	Mg 1	N 4	O 2	0
14	cB	1	Total 38	C 31	Mg 1	N 4	O 2	0
14	cB	1	Total 41	C 32	Mg 1	N 4	O 4	0
14	cB	1	Total 41	C 32	Mg 1	N 4	O 4	0
14	cB	1	Total 50	C 39	Mg 1	N 4	O 6	0
14	cB	1	Total 41	C 32	Mg 1	N 4	O 4	0
14	cB	1	Total 41	C 32	Mg 1	N 4	O 4	0
14	cB	1	Total 56	C 45	Mg 1	N 4	O 6	0
14	cB	1	Total 65	C 54	Mg 1	N 4	O 6	0

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Mol	Chain	Residues	Atoms					AltConf
14	cB	1	Total	C	Mg	N	O	0
			38	31	1	4	2	
14	cB	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
14	cB	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
14	cB	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
14	cB	1	Total	C	Mg	N	O	0
			38	31	1	4	2	
14	cB	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
14	cB	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
14	cB	1	Total	C	Mg	N	O	0
			54	43	1	4	6	
14	cB	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
14	cB	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
14	cF	1	Total	C	Mg	N	O	0
			38	31	1	4	2	
14	cJ	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
14	cK	1	Total	C	Mg	N	O	0
			37	30	1	4	2	
14	cL	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
14	cL	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
14	cL	1	Total	C	Mg	N	O	0
			42	33	1	4	4	

- Molecule 15 is UNKNOWN LIGAND (CCD ID: UNL) (formula:) (labeled as "Ligand of Interest" by depositor).

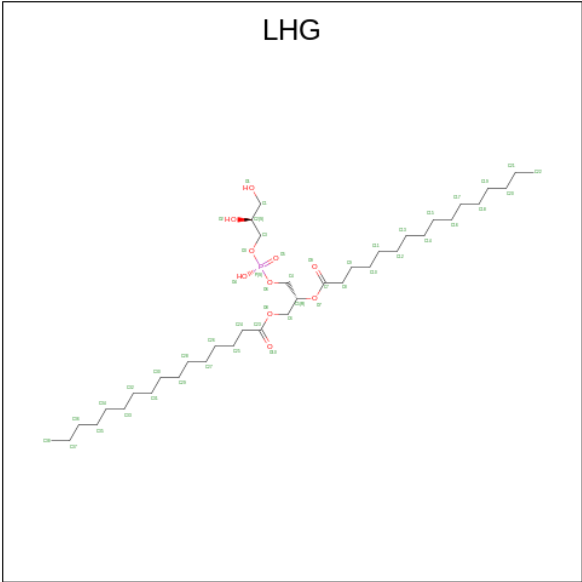
Mol	Chain	Residues	Atoms		AltConf
15	aA	4	Total	C	0
			150	150	
15	aB	3	Total	C	0
			120	120	
15	aI	2	Total	C	0
			80	80	

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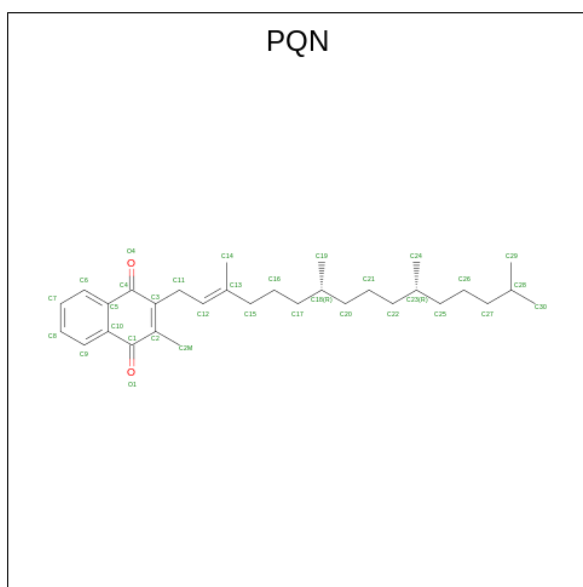
Mol	Chain	Residues	Atoms		AltConf
15	aJ	1	Total 40	C 40	0
15	aL	2	Total 80	C 80	0
15	bA	4	Total 150	C 150	0
15	bB	3	Total 120	C 120	0
15	bI	2	Total 80	C 80	0
15	bJ	1	Total 40	C 40	0
15	bL	2	Total 80	C 80	0
15	cA	3	Total 110	C 110	0
15	cB	3	Total 120	C 120	0
15	cF	1	Total 40	C 40	0
15	cI	2	Total 80	C 80	0
15	cJ	1	Total 40	C 40	0
15	cL	2	Total 80	C 80	0

- Molecule 16 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P) (labeled as "Ligand of Interest" by depositor).



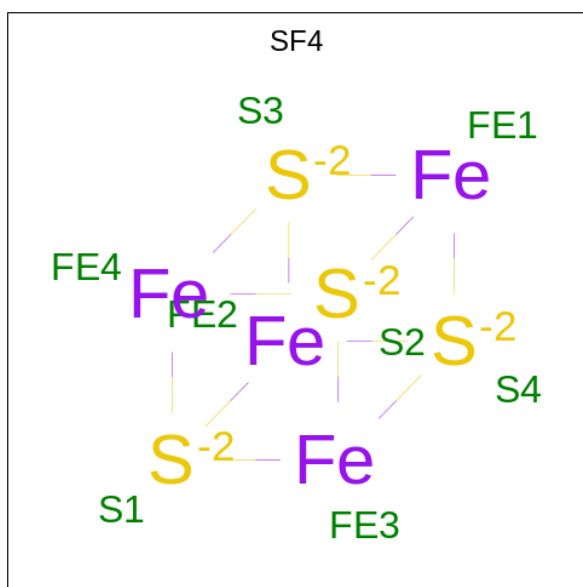
Mol	Chain	Residues	Atoms				AltConf
16	aA	1	Total	C	O	P	0
			49	38	10	1	
16	aA	1	Total	C	O	P	0
			21	12	8	1	
16	bA	1	Total	C	O	P	0
			49	38	10	1	
16	bA	1	Total	C	O	P	0
			21	12	8	1	
16	cA	1	Total	C	O	P	0
			49	38	10	1	
16	cA	1	Total	C	O	P	0
			21	12	8	1	

- Molecule 17 is PHYLLOQUINONE (CCD ID: PQN) (formula: C₃₁H₄₆O₂) (labeled as "Ligand of Interest" by depositor).



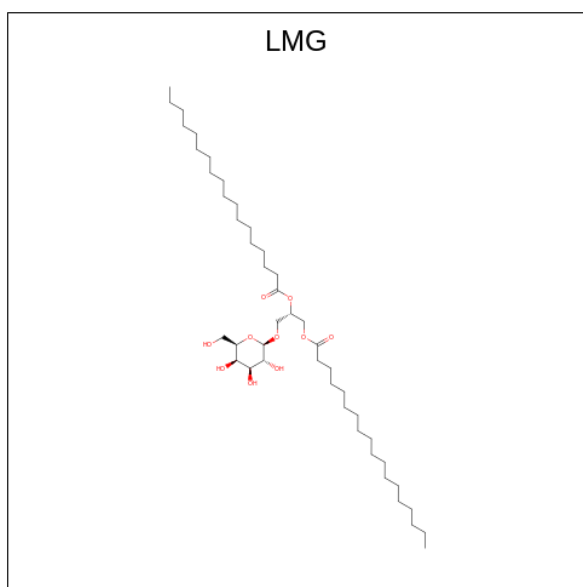
Mol	Chain	Residues	Atoms			AltConf
17	aA	1	Total	C	O	0
			33	31	2	
17	aB	1	Total	C	O	0
			33	31	2	
17	bA	1	Total	C	O	0
			33	31	2	
17	bB	1	Total	C	O	0
			33	31	2	
17	cA	1	Total	C	O	0
			33	31	2	
17	cB	1	Total	C	O	0
			33	31	2	

- Molecule 18 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
18	aB	1	Total	Fe	S	0
			8	4	4	
18	aC	1	Total	Fe	S	0
			8	4	4	
18	aC	1	Total	Fe	S	0
			8	4	4	
18	bB	1	Total	Fe	S	0
			8	4	4	
18	bC	1	Total	Fe	S	0
			8	4	4	
18	bC	1	Total	Fe	S	0
			8	4	4	
18	cB	1	Total	Fe	S	0
			8	4	4	
18	cC	1	Total	Fe	S	0
			8	4	4	
18	cC	1	Total	Fe	S	0
			8	4	4	

- Molecule 19 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
19	aB	1	Total	C	O	0
			52	42	10	
19	bB	1	Total	C	O	0
			52	42	10	
19	cB	1	Total	C	O	0
			52	42	10	

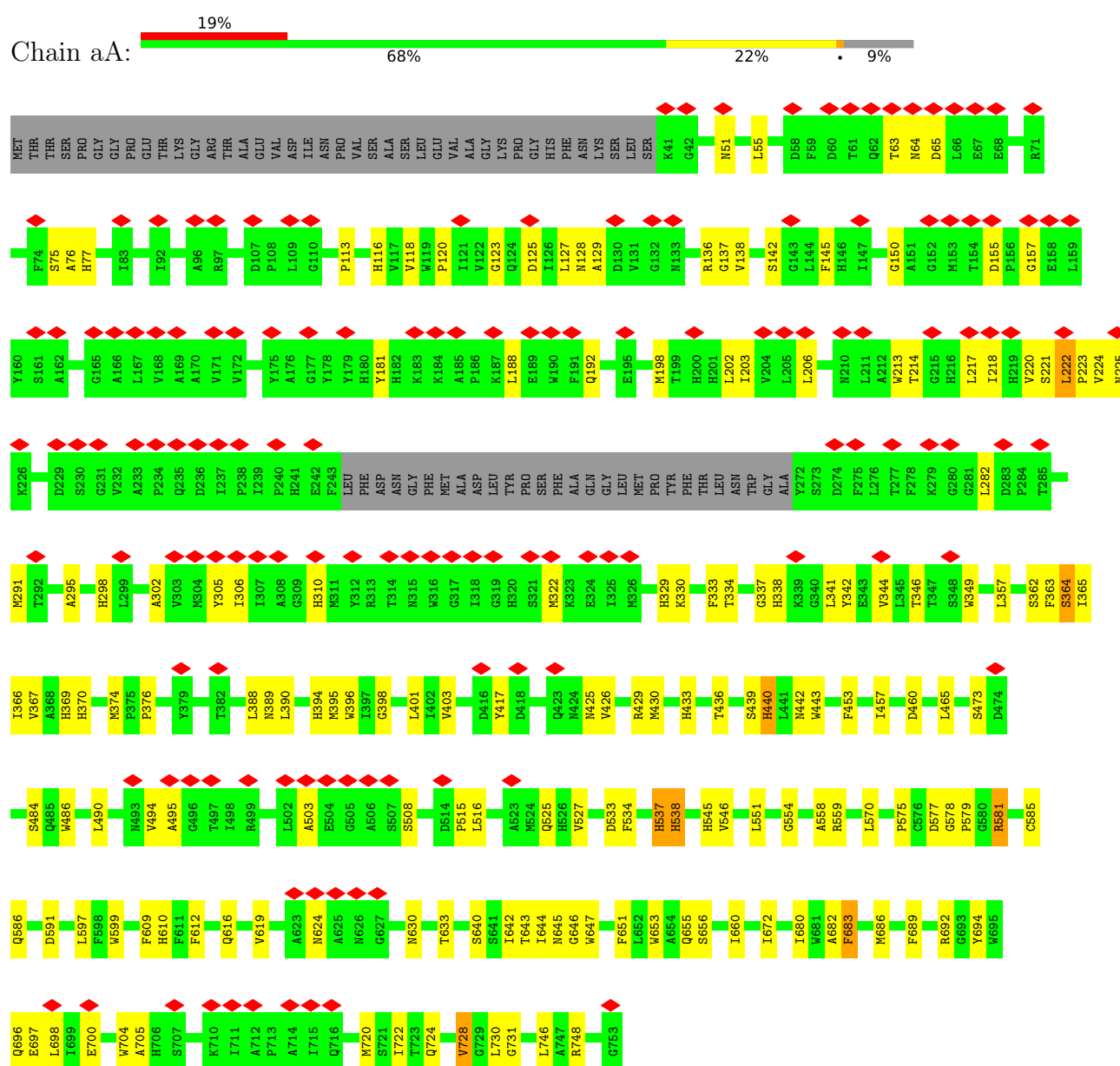
- Molecule 20 is water.

Mol	Chain	Residues	Atoms		AltConf
20	aA	13	Total	O	0
			13	13	
20	aB	12	Total	O	0
			12	12	
20	aL	3	Total	O	0
			3	3	
20	bA	12	Total	O	0
			12	12	
20	bB	13	Total	O	0
			13	13	
20	bL	3	Total	O	0
			3	3	
20	cA	13	Total	O	0
			13	13	
20	cB	12	Total	O	0
			12	12	
20	cL	3	Total	O	0
			3	3	

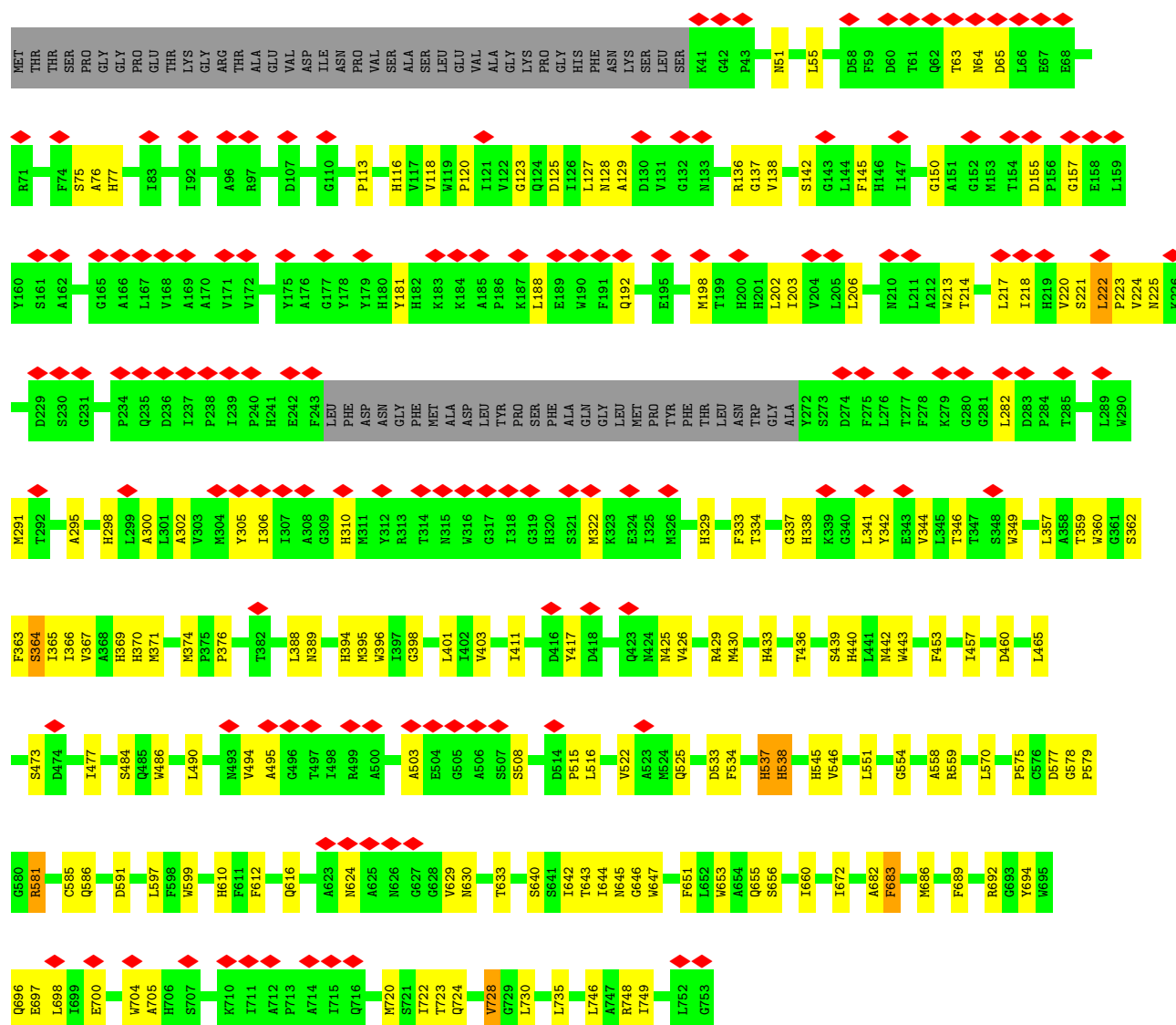
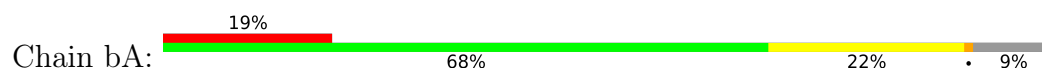
3 Residue-property plots

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.

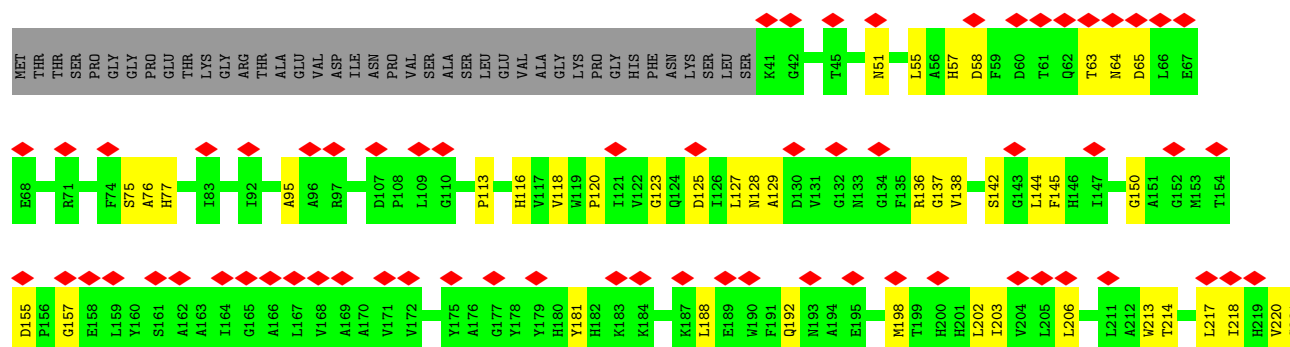
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

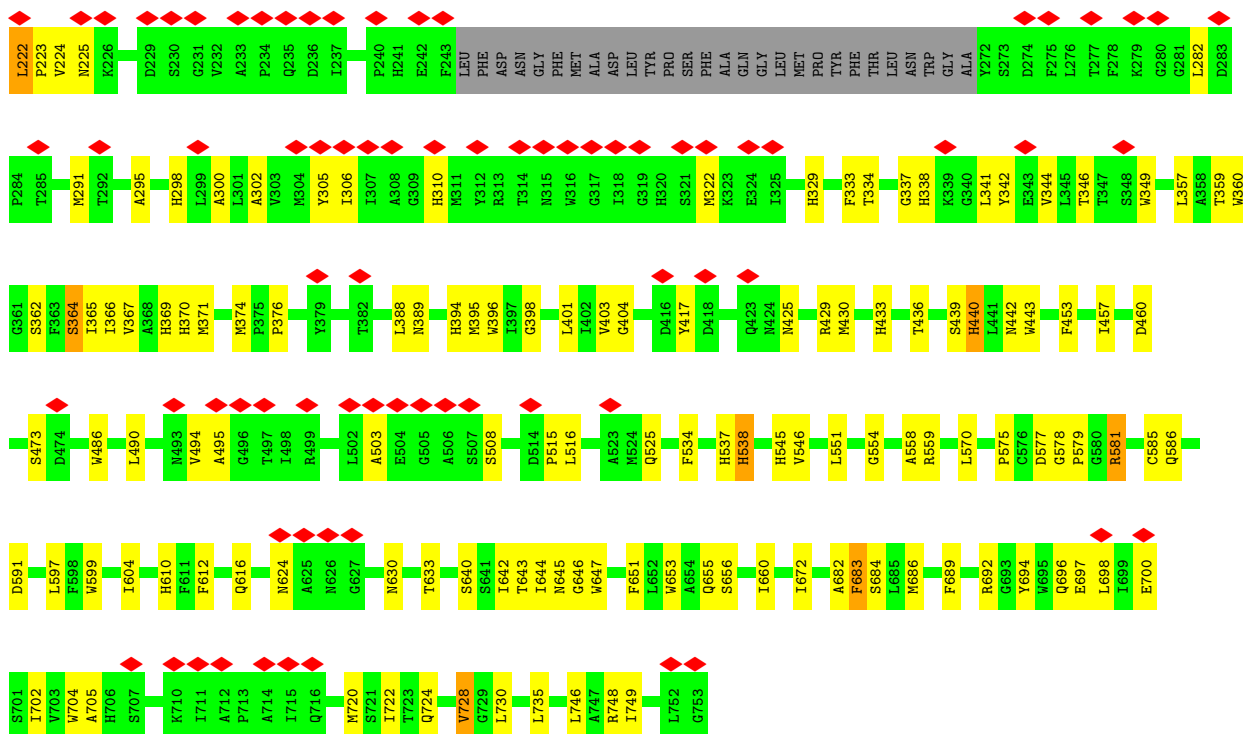


- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

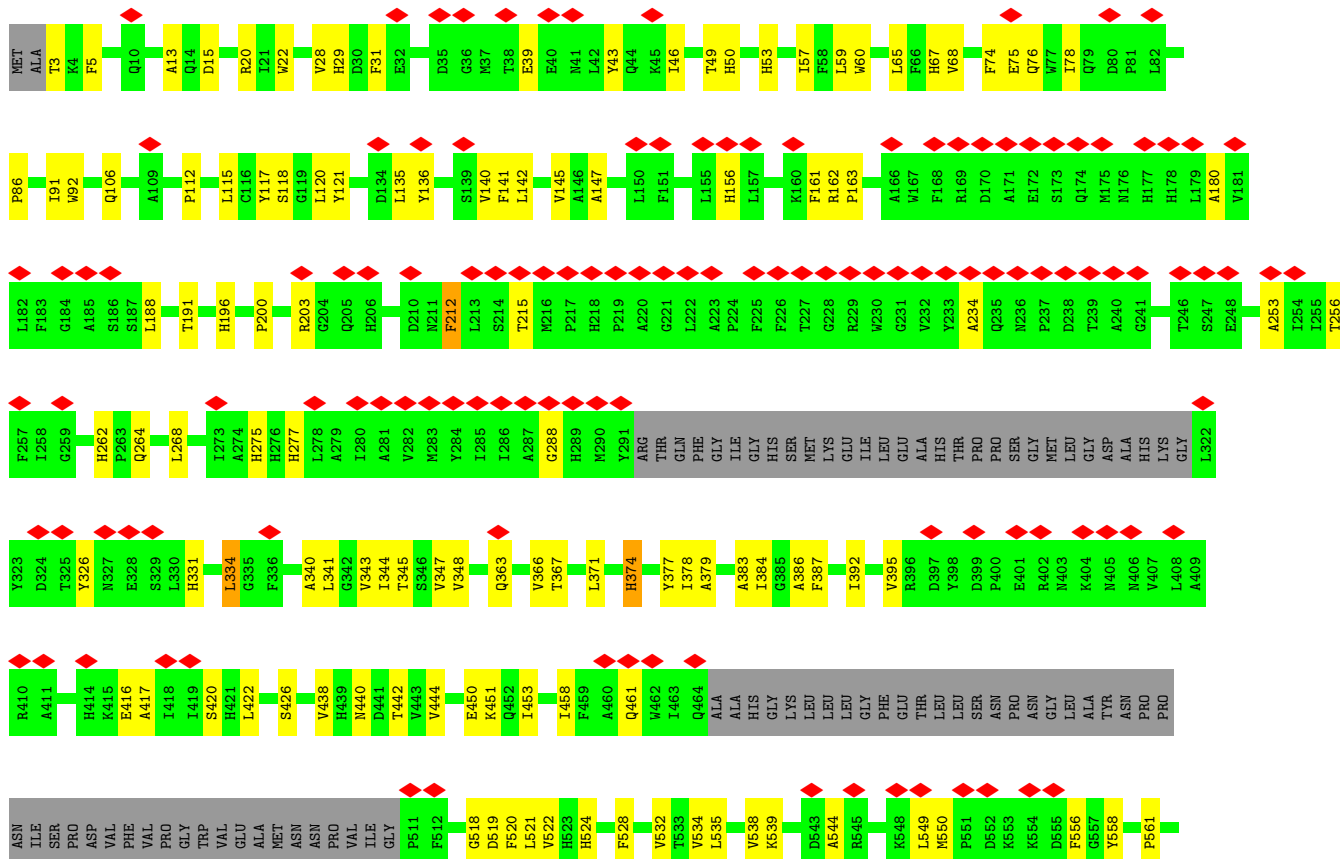


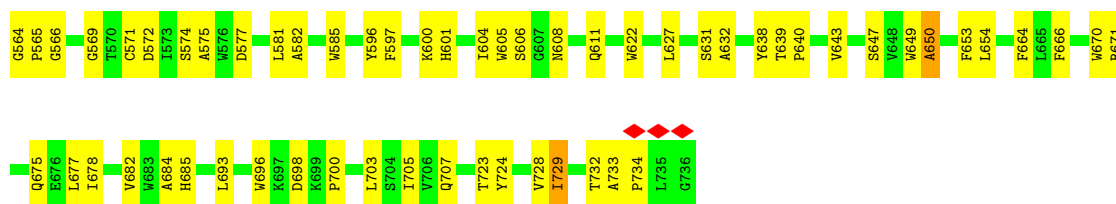
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



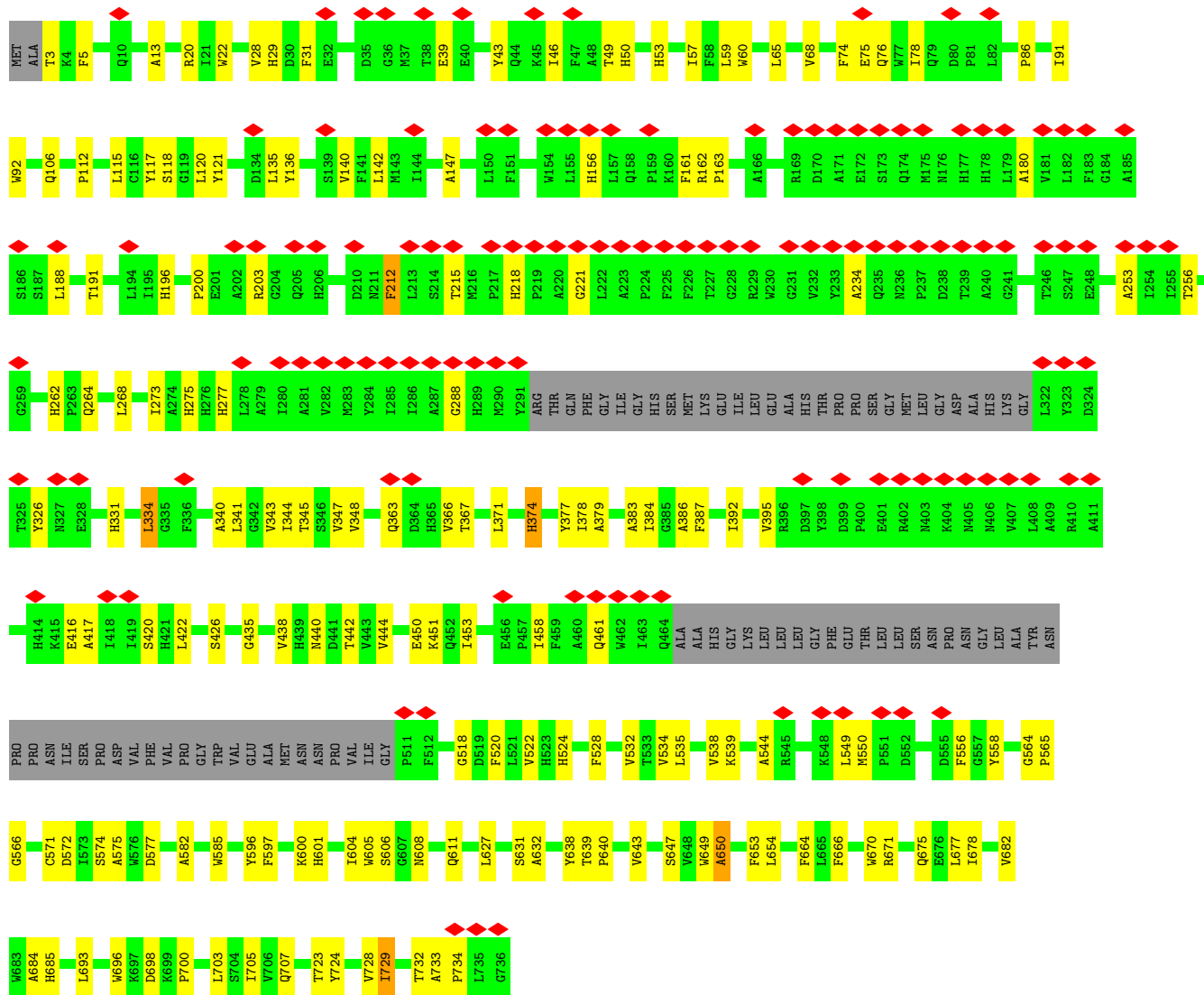


• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

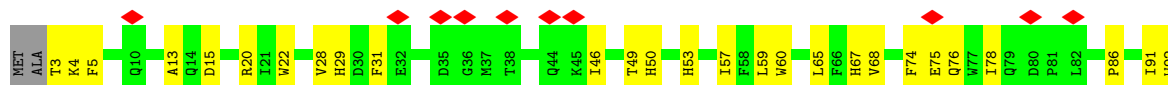


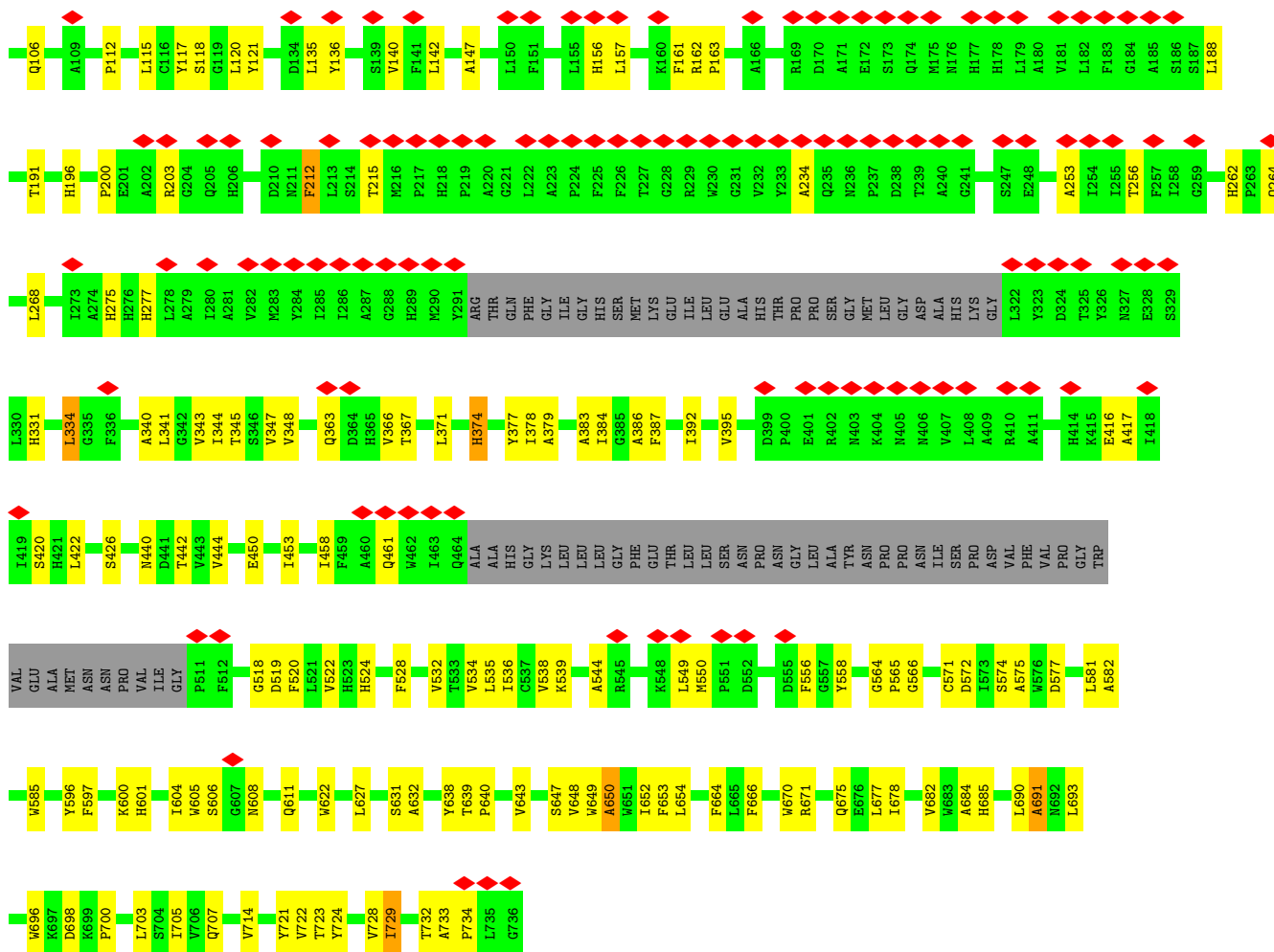


• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

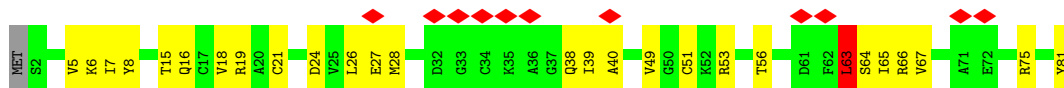


• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

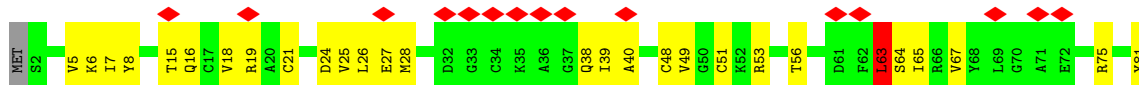




• Molecule 3: Photosystem I iron-sulfur center

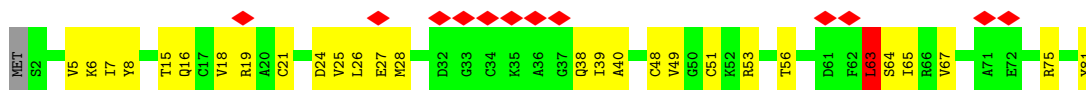


• Molecule 3: Photosystem I iron-sulfur center

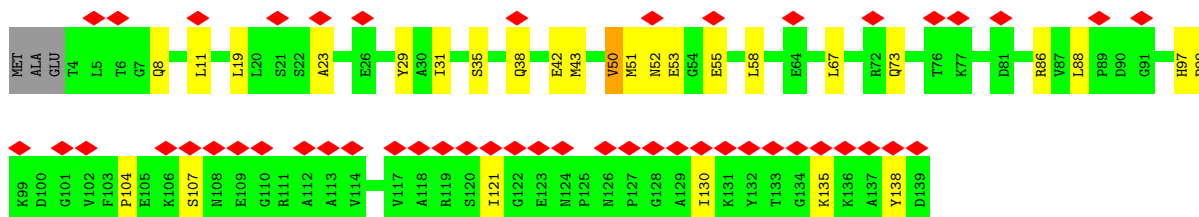
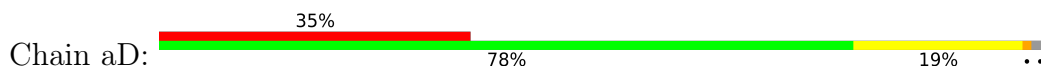


• Molecule 3: Photosystem I iron-sulfur center

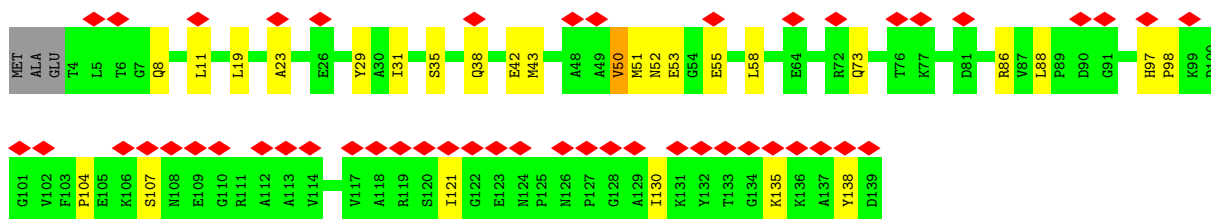
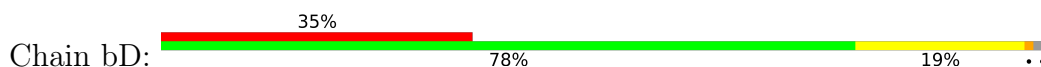




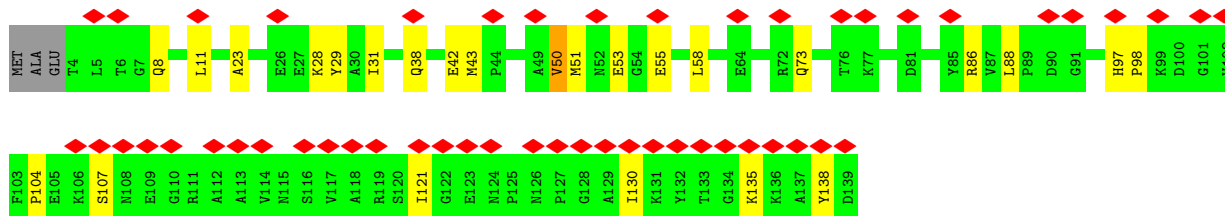
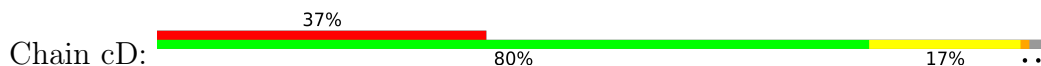
- Molecule 4: Photosystem I protein Psad



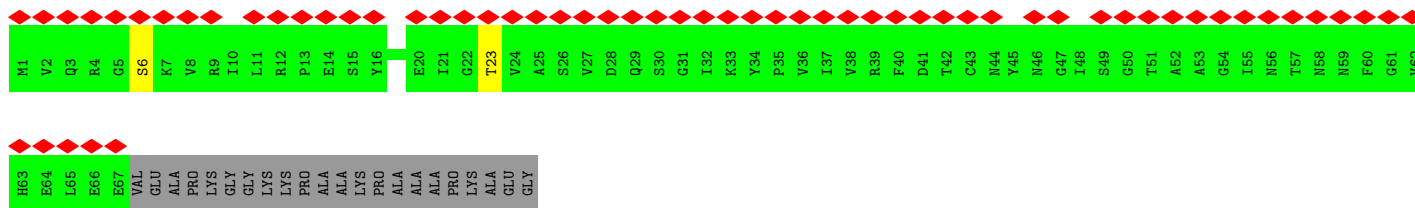
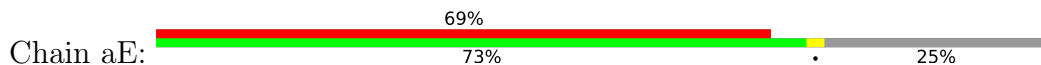
- Molecule 4: Photosystem I protein Psad



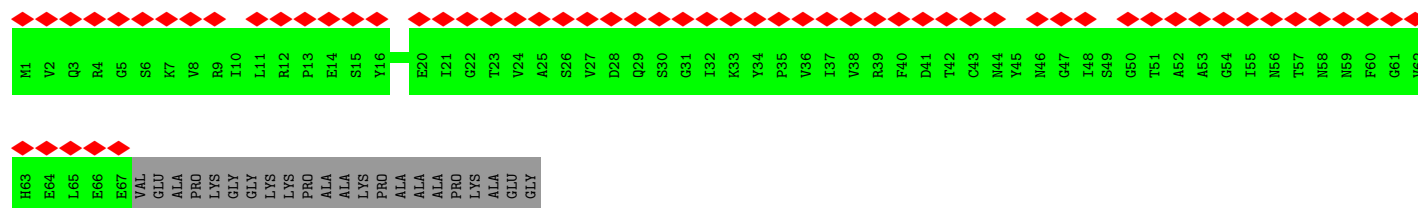
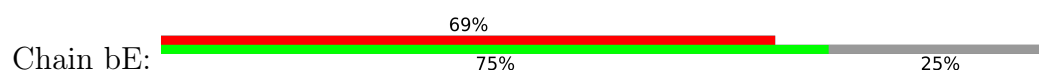
- Molecule 4: Photosystem I protein Psad



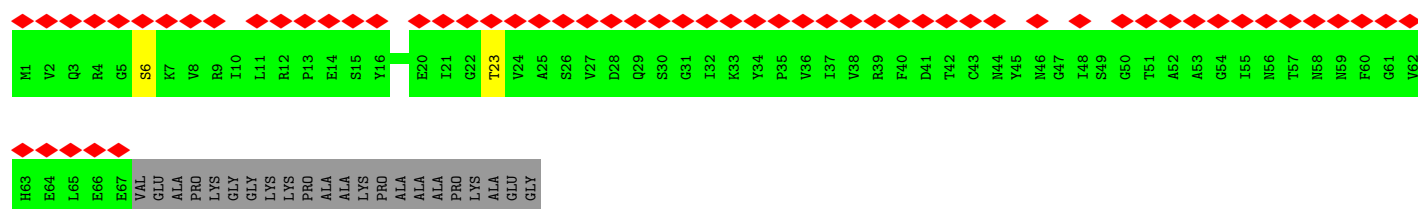
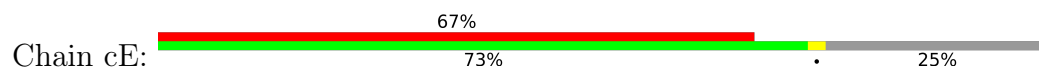
- Molecule 5: Photosystem I reaction center subunit IV



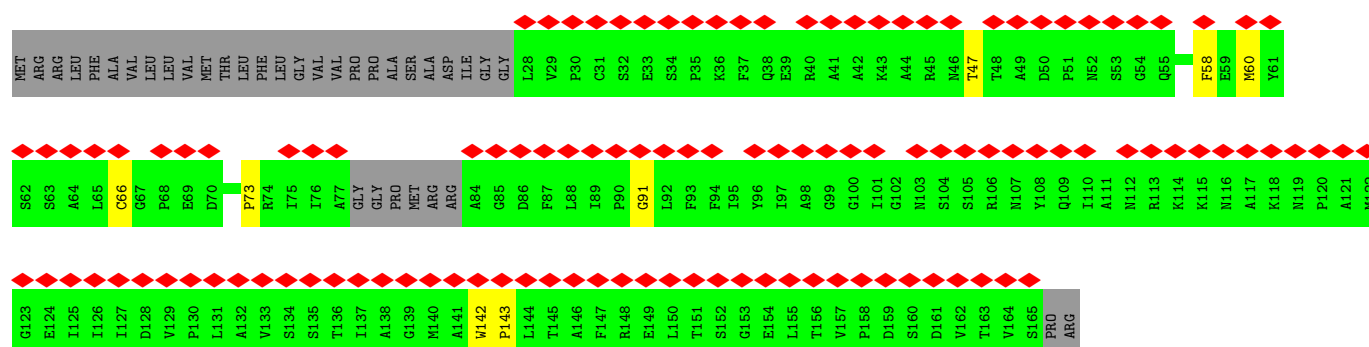
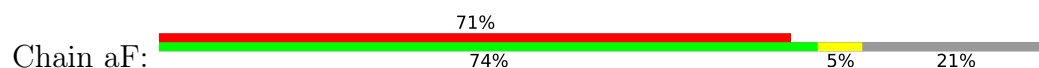
- Molecule 5: Photosystem I reaction center subunit IV



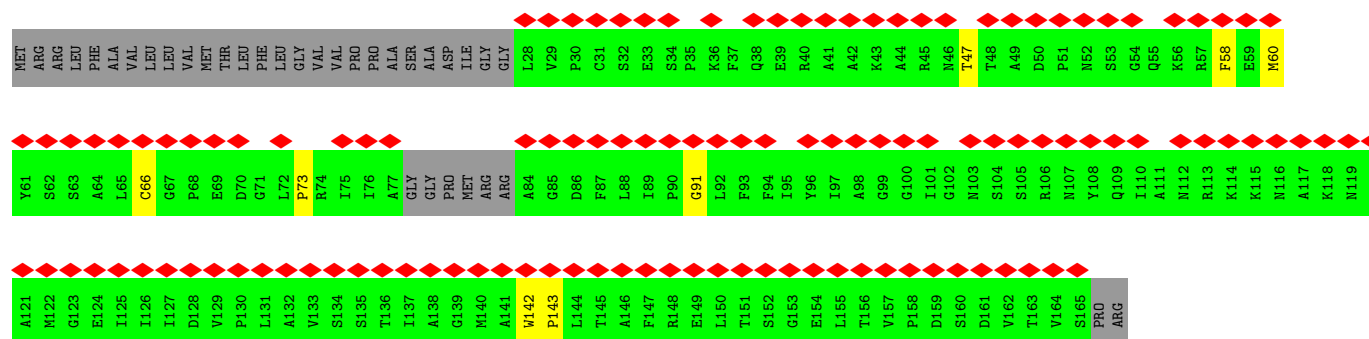
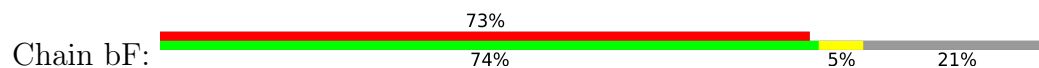
• Molecule 5: Photosystem I reaction center subunit IV



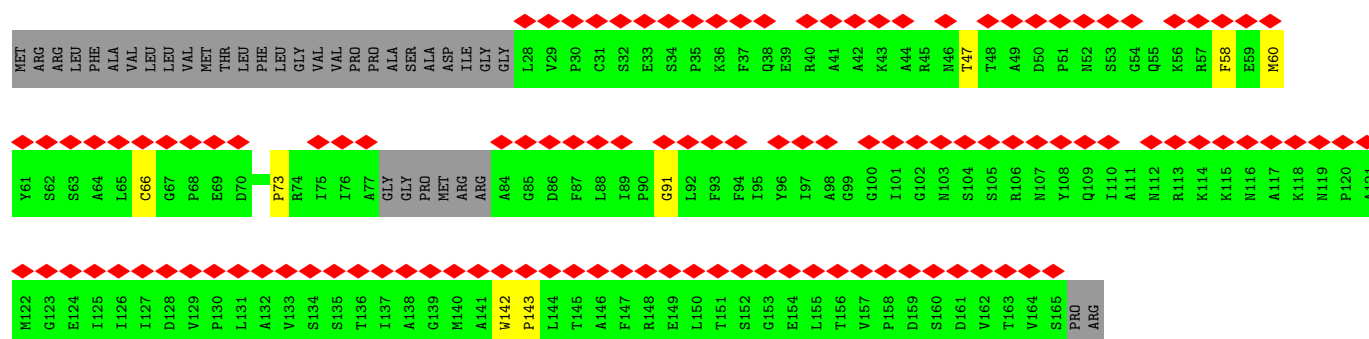
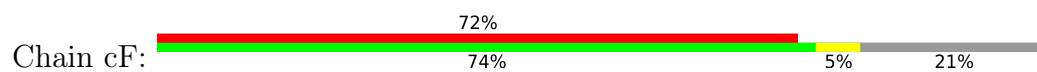
• Molecule 6: Photosystem I protein Psaf



• Molecule 6: Photosystem I protein Psaf



• Molecule 6: Photosystem I protein Psaf



- Molecule 7: Photosystem I protein Psa27



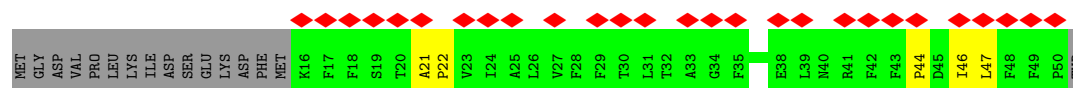
- Molecule 7: Photosystem I protein Psa27



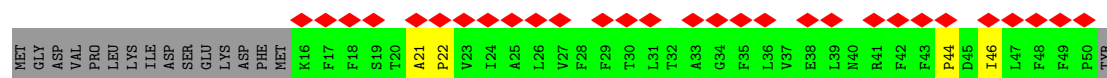
- Molecule 7: Photosystem I protein Psa27



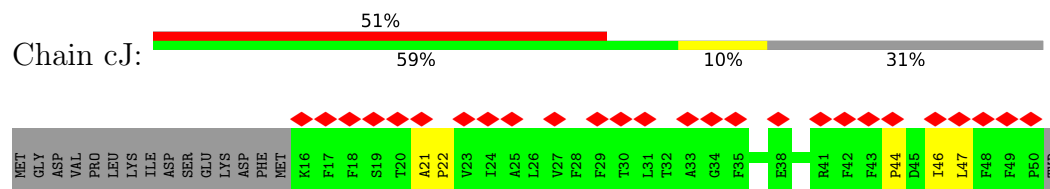
- Molecule 8: Photosystem I reaction center subunit IX



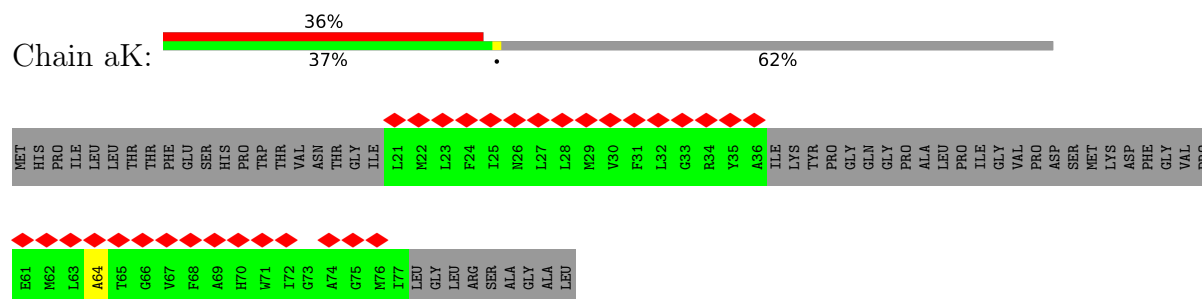
- Molecule 8: Photosystem I reaction center subunit IX



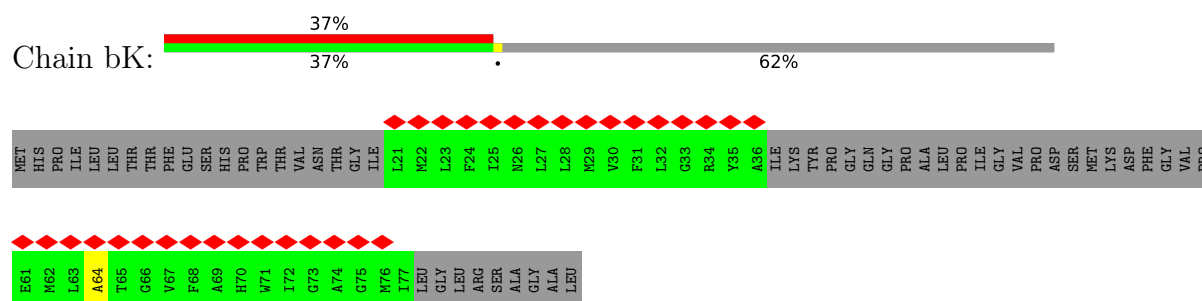
- Molecule 8: Photosystem I reaction center subunit IX



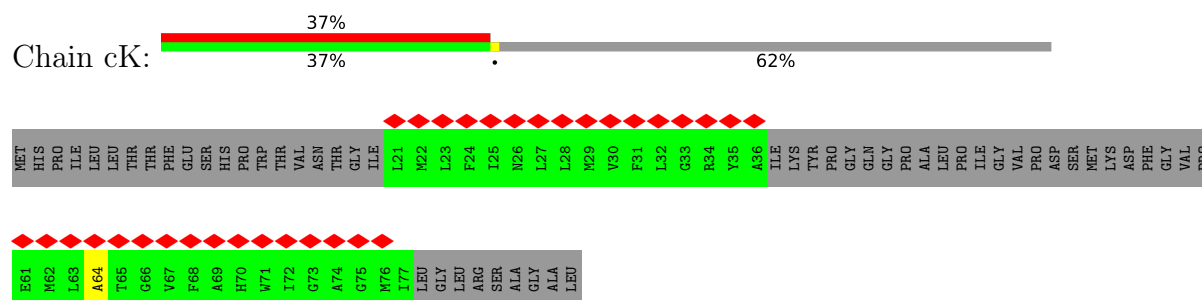
- Molecule 9: Photosystem I reaction center subunit PsaK



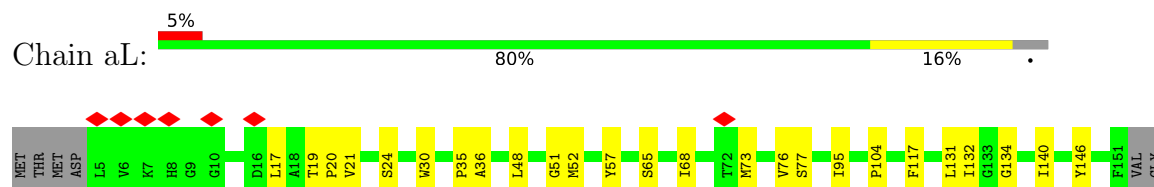
- Molecule 9: Photosystem I reaction center subunit PsaK



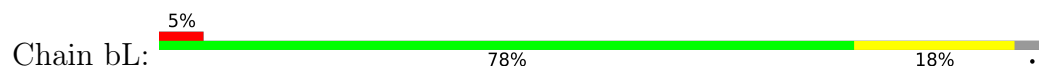
- Molecule 9: Photosystem I reaction center subunit PsaK

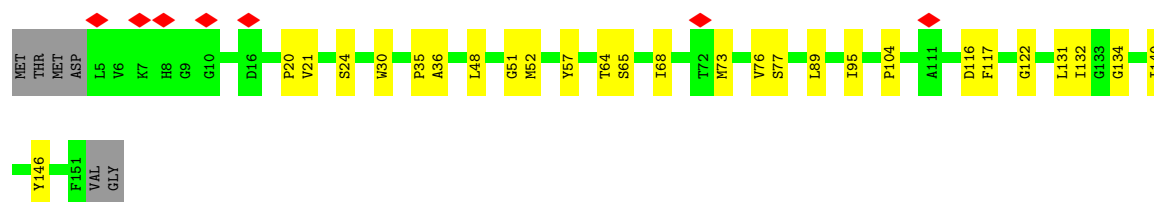


- Molecule 10: Photosystem I protein PsaL

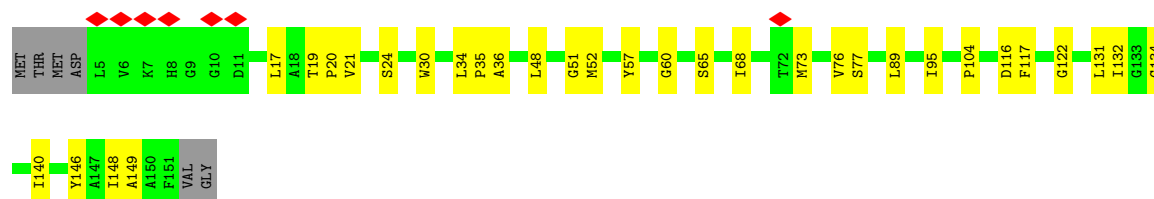
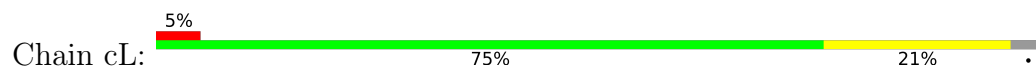


- Molecule 10: Photosystem I protein PsaL





• Molecule 10: Photosystem I protein Psal



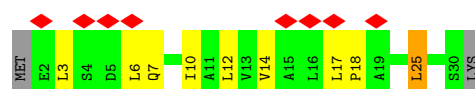
• Molecule 11: Photosystem I protein Psam



• Molecule 11: Photosystem I protein Psam



• Molecule 11: Photosystem I protein Psam



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	86419	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL CRYO ARM 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	85.7	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.075	Depositor
Minimum map value	-0.047	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.00637	Depositor
Map size (Å)	356.40002, 356.40002, 356.40002	wwPDB
Map dimensions	330, 330, 330	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	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: CL7, LHG, LMG, PHO, SF4, G9R, PQN, UNL

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	aA	1.11	6/5369 (0.1%)	1.26	6/7326 (0.1%)
1	bA	1.11	5/5369 (0.1%)	1.26	6/7326 (0.1%)
1	cA	1.11	8/5369 (0.1%)	1.25	4/7326 (0.1%)
2	aB	1.07	3/5185 (0.1%)	1.23	5/7107 (0.1%)
2	bB	1.07	3/5185 (0.1%)	1.23	4/7107 (0.1%)
2	cB	1.07	3/5185 (0.1%)	1.24	6/7107 (0.1%)
3	aC	0.96	0/582	1.18	0/792
3	bC	0.96	0/582	1.18	0/792
3	cC	0.96	0/582	1.18	0/792
4	aD	0.89	0/1018	1.05	0/1379
4	bD	0.90	0/1018	1.05	0/1379
4	cD	0.90	0/1018	1.05	0/1379
5	aE	1.14	0/379	1.24	0/524
5	bE	1.12	0/379	1.25	0/524
5	cE	1.14	0/379	1.24	0/524
6	aF	0.99	0/863	1.30	0/1183
6	bF	0.99	0/863	1.29	0/1183
6	cF	0.98	0/863	1.30	0/1183
7	aI	0.96	0/230	1.31	0/313
7	bI	0.97	0/230	1.31	0/313
7	cI	0.96	0/230	1.32	0/313
8	aJ	0.84	0/273	1.22	0/373
8	bJ	0.84	0/273	1.22	0/373
8	cJ	0.84	0/273	1.22	0/373
9	aK	1.14	0/159	1.71	0/217
9	bK	1.14	0/159	1.71	0/217
9	cK	1.14	0/159	1.71	0/217
10	aL	1.11	0/1020	1.28	1/1394 (0.1%)
10	bL	1.11	0/1020	1.27	1/1394 (0.1%)
10	cL	1.11	0/1020	1.28	1/1394 (0.1%)
11	aM	0.97	0/205	1.37	0/281
11	bM	0.97	0/205	1.38	0/281

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
11	cM	0.97	0/205	1.38	0/281
All	All	1.07	28/45849 (0.1%)	1.24	34/62667 (0.1%)

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	cB	212	PHE	C-N	15.21	1.52	1.33
2	bB	212	PHE	C-N	14.97	1.52	1.33
2	aB	212	PHE	C-N	14.84	1.52	1.33
1	cA	683	PHE	C-N	-9.32	1.21	1.34
1	aA	683	PHE	C-N	-9.00	1.22	1.34

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	aA	538	HIS	CA-CB-CG	-7.26	106.54	113.80
1	cA	538	HIS	CA-CB-CG	-7.21	106.59	113.80
1	bA	538	HIS	CA-CB-CG	-7.17	106.64	113.80
2	cB	723	THR	N-CA-C	-6.06	104.59	111.14
1	bA	581	ARG	N-CA-C	-5.99	105.55	112.86

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	aA	5203	0	4895	131	0
1	bA	5203	0	4895	137	0
1	cA	5203	0	4895	132	0
2	aB	5007	0	4607	151	0
2	bB	5007	0	4607	144	0
2	cB	5007	0	4607	152	0
3	aC	573	0	543	26	0
3	bC	573	0	543	25	0
3	cC	573	0	543	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	aD	999	0	981	23	0
4	bD	999	0	981	20	0
4	cD	999	0	981	19	0
5	aE	375	0	218	1	0
5	bE	375	0	218	0	0
5	cE	375	0	218	1	0
6	aF	847	0	707	7	0
6	bF	847	0	707	7	0
6	cF	847	0	707	7	0
7	aI	225	0	231	11	0
7	bI	225	0	231	12	0
7	cI	225	0	231	13	0
8	aJ	264	0	237	5	0
8	bJ	264	0	237	4	0
8	cJ	264	0	237	5	0
9	aK	161	0	80	1	0
9	bK	161	0	80	1	0
9	cK	161	0	80	1	0
10	aL	999	0	976	20	0
10	bL	999	0	976	23	0
10	cL	999	0	976	28	0
11	aM	205	0	232	11	0
11	bM	205	0	232	10	0
11	cM	205	0	232	10	0
12	aA	65	0	0	0	0
12	bA	65	0	0	0	0
12	cA	65	0	0	0	0
13	aA	64	0	74	7	0
13	aB	64	0	74	9	0
13	bB	128	0	148	17	0
13	cB	128	0	148	19	0
14	aA	1862	0	1586	51	0
14	aB	1410	0	1250	61	0
14	aF	38	0	24	1	0
14	aJ	42	0	28	0	0
14	aK	37	0	23	0	0
14	aL	172	0	169	10	0
14	bA	1862	0	1586	56	0
14	bB	1410	0	1250	59	0
14	bF	38	0	24	1	0
14	bJ	42	0	28	1	0
14	bK	37	0	23	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	bL	172	0	169	12	0
14	cA	1862	0	1586	54	0
14	cB	1410	0	1250	53	0
14	cF	38	0	24	1	0
14	cJ	42	0	28	0	0
14	cK	37	0	23	0	0
14	cL	172	0	169	13	0
15	aA	150	0	0	0	0
15	aB	120	0	0	0	0
15	aI	80	0	0	0	0
15	aJ	40	0	0	0	0
15	aL	80	0	0	1	0
15	bA	150	0	0	0	0
15	bB	120	0	0	0	0
15	bI	80	0	0	1	0
15	bJ	40	0	0	0	0
15	bL	80	0	0	2	0
15	cA	110	0	0	0	0
15	cB	120	0	0	0	0
15	cF	40	0	0	0	0
15	cI	80	0	0	1	0
15	cJ	40	0	0	0	0
15	cL	80	0	0	2	0
16	aA	70	0	91	3	0
16	bA	70	0	90	4	0
16	cA	70	0	90	3	0
17	aA	33	0	46	1	0
17	aB	33	0	46	1	0
17	bA	33	0	46	3	0
17	bB	33	0	46	3	0
17	cA	33	0	46	2	0
17	cB	33	0	46	1	0
18	aB	8	0	0	0	0
18	aC	16	0	0	0	0
18	bB	8	0	0	0	0
18	bC	16	0	0	0	0
18	cB	8	0	0	0	0
18	cC	16	0	0	0	0
19	aB	52	0	77	1	0
19	bB	52	0	77	1	0
19	cB	52	0	77	2	0
20	aA	13	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	aB	12	0	0	0	0
20	aL	3	0	0	0	0
20	bA	12	0	0	1	0
20	bB	13	0	0	0	0
20	bL	3	0	0	0	0
20	cA	13	0	0	1	0
20	cB	12	0	0	0	0
20	cL	3	0	0	0	0
All	All	57966	0	51583	1222	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 11.

The worst 5 of 1222 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)
2:aB:53:HIS:HD1	14:aB:3031:CL7:H3A	1.35	0.91
2:bB:528:PHE:HE1	13:bB:801:PHO:HBA2	1.39	0.88
2:bB:53:HIS:HD1	14:bB:832:CL7:H3A	1.39	0.88
2:cB:528:PHE:HE1	13:cB:801:PHO:HBA2	1.39	0.88
13:aA:3102:PHO:HBA2	2:aB:528:PHE:HE1	1.38	0.87

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	aA	681/753 (90%)	637 (94%)	44 (6%)	0	100	100
1	bA	681/753 (90%)	635 (93%)	46 (7%)	0	100	100
1	cA	681/753 (90%)	637 (94%)	44 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	aB	652/736 (89%)	616 (94%)	36 (6%)	0	100	100
2	bB	652/736 (89%)	616 (94%)	36 (6%)	0	100	100
2	cB	652/736 (89%)	616 (94%)	36 (6%)	0	100	100
3	aC	78/81 (96%)	72 (92%)	5 (6%)	1 (1%)	9	18
3	bC	78/81 (96%)	72 (92%)	5 (6%)	1 (1%)	9	18
3	cC	78/81 (96%)	72 (92%)	5 (6%)	1 (1%)	9	18
4	aD	134/139 (96%)	126 (94%)	8 (6%)	0	100	100
4	bD	134/139 (96%)	126 (94%)	8 (6%)	0	100	100
4	cD	134/139 (96%)	126 (94%)	8 (6%)	0	100	100
5	aE	65/89 (73%)	61 (94%)	4 (6%)	0	100	100
5	bE	65/89 (73%)	61 (94%)	4 (6%)	0	100	100
5	cE	65/89 (73%)	61 (94%)	4 (6%)	0	100	100
6	aF	128/167 (77%)	120 (94%)	8 (6%)	0	100	100
6	bF	128/167 (77%)	120 (94%)	8 (6%)	0	100	100
6	cF	128/167 (77%)	119 (93%)	9 (7%)	0	100	100
7	aI	28/34 (82%)	27 (96%)	1 (4%)	0	100	100
7	bI	28/34 (82%)	27 (96%)	1 (4%)	0	100	100
7	cI	28/34 (82%)	27 (96%)	1 (4%)	0	100	100
8	aJ	33/51 (65%)	31 (94%)	2 (6%)	0	100	100
8	bJ	33/51 (65%)	31 (94%)	2 (6%)	0	100	100
8	cJ	33/51 (65%)	31 (94%)	2 (6%)	0	100	100
9	aK	29/86 (34%)	29 (100%)	0	0	100	100
9	bK	29/86 (34%)	29 (100%)	0	0	100	100
9	cK	29/86 (34%)	29 (100%)	0	0	100	100
10	aL	145/153 (95%)	142 (98%)	3 (2%)	0	100	100
10	bL	145/153 (95%)	142 (98%)	3 (2%)	0	100	100
10	cL	145/153 (95%)	142 (98%)	3 (2%)	0	100	100
11	aM	27/31 (87%)	27 (100%)	0	0	100	100
11	bM	27/31 (87%)	27 (100%)	0	0	100	100
11	cM	27/31 (87%)	27 (100%)	0	0	100	100
All	All	6000/6960 (86%)	5661 (94%)	336 (6%)	3 (0%)	49	68

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	aC	63	LEU
3	cC	63	LEU
3	bC	63	LEU

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	aA	500/606 (82%)	497 (99%)	3 (1%)	78	91
1	bA	500/606 (82%)	497 (99%)	3 (1%)	78	91
1	cA	500/606 (82%)	496 (99%)	4 (1%)	73	88
2	aB	471/594 (79%)	467 (99%)	4 (1%)	73	88
2	bB	471/594 (79%)	467 (99%)	4 (1%)	73	88
2	cB	471/594 (79%)	467 (99%)	4 (1%)	73	88
3	aC	60/69 (87%)	58 (97%)	2 (3%)	33	61
3	bC	60/69 (87%)	58 (97%)	2 (3%)	33	61
3	cC	60/69 (87%)	58 (97%)	2 (3%)	33	61
4	aD	99/112 (88%)	97 (98%)	2 (2%)	48	75
4	bD	99/112 (88%)	97 (98%)	2 (2%)	48	75
4	cD	99/112 (88%)	97 (98%)	2 (2%)	48	75
5	aE	11/69 (16%)	11 (100%)	0	100	100
5	bE	11/69 (16%)	11 (100%)	0	100	100
5	cE	11/69 (16%)	11 (100%)	0	100	100
6	aF	62/133 (47%)	62 (100%)	0	100	100
6	bF	62/133 (47%)	62 (100%)	0	100	100
6	cF	62/133 (47%)	62 (100%)	0	100	100
7	aI	23/26 (88%)	23 (100%)	0	100	100
7	bI	23/26 (88%)	23 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	cI	23/26 (88%)	23 (100%)	0	100	100
8	aJ	23/46 (50%)	23 (100%)	0	100	100
8	bJ	23/46 (50%)	23 (100%)	0	100	100
8	cJ	23/46 (50%)	23 (100%)	0	100	100
10	aL	96/112 (86%)	96 (100%)	0	100	100
10	bL	96/112 (86%)	96 (100%)	0	100	100
10	cL	96/112 (86%)	96 (100%)	0	100	100
11	aM	23/25 (92%)	22 (96%)	1 (4%)	26	51
11	bM	23/25 (92%)	22 (96%)	1 (4%)	26	51
11	cM	23/25 (92%)	22 (96%)	1 (4%)	26	51
All	All	4104/5376 (76%)	4067 (99%)	37 (1%)	68	87

5 of 37 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	cB	57	ILE
4	cD	50	VAL
2	cB	458	ILE
3	cC	39	ILE
1	bA	222	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36 such sidechains are listed below:

Mol	Chain	Res	Type
2	cB	34	HIS
4	cD	52	ASN
2	cB	102	GLN
2	cB	685	HIS
1	bA	80	HIS

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 279 ligands modelled in this entry, 36 are unknown - leaving 243 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$
12	G9R	cA	3101	1	69,73,73	2.21	19 (27%)	83,113,113	3.42	37 (44%)
14	CL7	bA	3126	1	58,61,73	2.36	19 (32%)	66,97,113	1.51	12 (18%)
14	CL7	aA	3142	1	71,73,73	2.21	24 (33%)	80,113,113	1.57	16 (20%)
14	CL7	cA	3113	1	47,49,73	2.59	20 (42%)	51,84,113	1.80	13 (25%)
14	CL7	cL	205	20	48,50,73	2.91	23 (47%)	51,85,113	1.74	12 (23%)
14	CL7	cB	808	2	71,73,73	2.27	25 (35%)	80,113,113	1.97	17 (21%)
14	CL7	cA	3130	1	47,49,73	2.67	20 (42%)	51,84,113	1.65	12 (23%)
14	CL7	bL	203	10	71,73,73	2.33	20 (28%)	80,113,113	1.87	22 (27%)
14	CL7	aA	3120	20	52,54,73	2.65	20 (38%)	57,90,113	2.05	14 (24%)
13	PHO	cB	805	-	58,69,69	3.19	23 (39%)	56,99,99	2.71	17 (30%)
14	CL7	aF	201	2	43,46,73	2.69	20 (46%)	46,80,113	1.74	8 (17%)
14	CL7	cA	3129	1	47,49,73	3.21	24 (51%)	51,84,113	2.43	22 (43%)
14	CL7	bB	827	2	71,73,73	2.50	27 (38%)	80,113,113	1.97	28 (35%)
14	CL7	bA	3103	1	47,49,73	2.60	20 (42%)	51,84,113	1.79	14 (27%)
14	CL7	bA	3129	1	47,49,73	3.23	27 (57%)	51,84,113	2.45	22 (43%)
14	CL7	aK	101	-	45,45,73	2.49	18 (40%)	49,78,113	1.69	12 (24%)
14	CL7	cB	816	2	56,58,73	2.69	22 (39%)	62,95,113	1.98	21 (33%)
14	CL7	aA	3140	-	71,73,73	2.14	17 (23%)	80,113,113	1.53	13 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CL7	aB	3009	2	71,73,73	2.39	27 (38%)	80,113,113	1.82	23 (28%)
14	CL7	bB	825	2	43,46,73	2.77	21 (48%)	46,80,113	1.55	8 (17%)
14	CL7	cA	3139	-	71,73,73	2.20	20 (28%)	80,113,113	1.65	16 (20%)
14	CL7	bA	3118	-	43,46,73	2.65	20 (46%)	46,80,113	1.64	8 (17%)
14	CL7	aA	3122	1	47,49,73	2.67	22 (46%)	51,84,113	1.95	12 (23%)
14	CL7	cB	823	2	47,49,73	2.57	20 (42%)	51,84,113	2.08	18 (35%)
18	SF4	bB	802	2,1	0,12,12	-	-	-		
14	CL7	bB	814	2	47,49,73	2.47	19 (40%)	51,84,113	1.79	14 (27%)
14	CL7	aA	3130	1	47,49,73	3.13	27 (57%)	51,84,113	2.43	20 (39%)
14	CL7	aB	3024	2	43,46,73	2.76	20 (46%)	46,80,113	1.64	11 (23%)
14	CL7	bB	817	-	47,49,73	2.57	21 (44%)	51,84,113	1.92	13 (25%)
14	CL7	aB	3006	2	71,73,73	2.24	25 (35%)	80,113,113	1.81	25 (31%)
14	CL7	bB	832	2	71,73,73	2.32	23 (32%)	80,113,113	1.83	20 (25%)
14	CL7	cA	3124	1	71,73,73	2.46	27 (38%)	80,113,113	2.22	21 (26%)
14	CL7	cA	3106	1	71,73,73	2.43	26 (36%)	80,113,113	1.75	20 (25%)
14	CL7	cB	810	2	71,73,73	2.44	27 (38%)	80,113,113	1.79	23 (28%)
14	CL7	cB	821	2	43,46,73	2.59	20 (46%)	46,80,113	1.58	9 (19%)
14	CL7	aA	3114	1	47,49,73	2.54	20 (42%)	51,84,113	1.72	13 (25%)
14	CL7	aA	3108	1	71,73,73	2.23	20 (28%)	80,113,113	1.63	16 (20%)
14	CL7	cA	3110	1	47,49,73	2.57	21 (44%)	51,84,113	1.80	12 (23%)
14	CL7	bA	3139	-	71,73,73	2.25	18 (25%)	80,113,113	1.62	14 (17%)
14	CL7	cB	833	2	61,63,73	2.57	25 (40%)	68,101,113	1.72	16 (23%)
14	CL7	aA	3110	1	47,49,73	2.52	17 (36%)	51,84,113	1.87	16 (31%)
14	CL7	cA	3122	1	56,58,73	2.51	23 (41%)	62,95,113	2.10	17 (27%)
14	CL7	bA	3105	1	47,49,73	2.87	22 (46%)	51,84,113	2.08	21 (41%)
16	LHG	cA	3137	-	48,48,48	0.97	5 (10%)	51,54,54	1.02	3 (5%)
17	PQN	bB	828	-	34,34,34	2.48	13 (38%)	42,45,45	1.55	6 (14%)
14	CL7	bL	204	10	71,73,73	2.37	21 (29%)	80,113,113	1.99	23 (28%)
14	CL7	cA	3125	1	71,73,73	2.37	24 (33%)	80,113,113	2.00	23 (28%)
14	CL7	aA	3109	1	48,50,73	2.60	18 (37%)	51,85,113	1.87	17 (33%)
18	SF4	bC	102	3	0,12,12	-	-	-		
14	CL7	aA	3117	-	59,61,73	2.31	19 (32%)	65,98,113	1.90	18 (27%)
14	CL7	aB	3021	2	47,49,73	2.67	19 (40%)	51,84,113	2.02	13 (25%)
14	CL7	cB	826	20	71,73,73	2.43	25 (35%)	80,113,113	1.75	22 (27%)
14	CL7	aB	3011	2	43,46,73	2.70	21 (48%)	46,80,113	1.60	10 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	PQN	cB	828	-	34,34,34	2.55	13 (38%)	42,45,45	1.51	6 (14%)
14	CL7	bB	824	2	62,64,73	2.43	20 (32%)	69,102,113	1.72	19 (27%)
14	CL7	cA	3131	-	47,49,73	2.64	19 (40%)	51,84,113	1.82	16 (31%)
14	CL7	aA	3106	1	47,49,73	2.73	21 (44%)	51,84,113	1.96	20 (39%)
14	CL7	cA	3108	1	48,50,73	2.62	20 (41%)	51,85,113	2.04	17 (33%)
13	PHO	aA	3102	-	58,69,69	3.52	18 (31%)	56,99,99	2.32	15 (26%)
14	CL7	cB	815	2	47,49,73	2.63	20 (42%)	51,84,113	1.63	13 (25%)
14	CL7	cB	819	2	62,64,73	2.83	25 (40%)	69,102,113	1.82	15 (21%)
19	LMG	cB	830	-	52,52,55	0.92	3 (5%)	60,60,63	1.35	7 (11%)
14	CL7	cB	820	2	71,73,73	2.41	26 (36%)	80,113,113	1.67	14 (17%)
14	CL7	bA	3123	1	57,59,73	2.60	22 (38%)	63,96,113	2.20	21 (33%)
14	CL7	bA	3116	-	59,61,73	2.38	20 (33%)	65,98,113	1.91	18 (27%)
13	PHO	bB	805	-	58,69,69	3.14	23 (39%)	56,99,99	2.59	16 (28%)
14	CL7	cA	3117	1	43,46,73	2.63	19 (44%)	46,80,113	1.67	12 (26%)
14	CL7	aB	3013	2	47,49,73	2.47	20 (42%)	51,84,113	1.79	14 (27%)
14	CL7	bA	3131	-	47,49,73	2.64	20 (42%)	51,84,113	1.81	15 (29%)
14	CL7	cB	807	2	71,73,73	2.25	24 (33%)	80,113,113	1.77	24 (30%)
16	LHG	bA	3137	-	48,48,48	1.08	5 (10%)	51,54,54	0.97	3 (5%)
14	CL7	aA	3111	1	47,49,73	2.51	20 (42%)	51,84,113	1.79	12 (23%)
14	CL7	cA	3115	1	43,46,73	2.52	17 (39%)	46,80,113	1.65	12 (26%)
14	CL7	aB	3019	2	71,73,73	2.39	26 (36%)	80,113,113	1.77	19 (23%)
14	CL7	aJ	101	8	47,50,73	2.56	18 (38%)	51,85,113	1.52	10 (19%)
17	PQN	aA	3144	-	34,34,34	2.03	11 (32%)	42,45,45	1.34	5 (11%)
14	CL7	bA	3107	1	71,73,73	2.30	21 (29%)	80,113,113	1.67	16 (20%)
13	PHO	bB	801	-	58,69,69	3.59	18 (31%)	56,99,99	2.25	15 (26%)
14	CL7	cA	3114	1	71,73,73	2.20	23 (32%)	80,113,113	1.92	26 (32%)
14	CL7	cF	201	2	43,46,73	2.69	21 (48%)	46,80,113	1.72	7 (15%)
14	CL7	aA	3127	1	58,61,73	2.36	20 (34%)	66,97,113	1.47	12 (18%)
14	CL7	bA	3111	1	43,46,73	2.66	18 (41%)	46,80,113	1.69	9 (19%)
14	CL7	cA	3103	1	47,49,73	2.62	20 (42%)	51,84,113	1.74	16 (31%)
14	CL7	cA	3119	20	52,54,73	2.77	23 (44%)	57,90,113	2.18	15 (26%)
14	CL7	bA	3109	1	47,49,73	2.59	17 (36%)	51,84,113	1.88	17 (33%)
18	SF4	cB	802	2,1	0,12,12	-	-	-	-	-
14	CL7	aB	3022	2	47,49,73	2.56	20 (42%)	51,84,113	2.07	18 (35%)
14	CL7	cB	804	2	71,73,73	2.61	31 (43%)	80,113,113	1.94	20 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CL7	aB	3031	2	71,73,73	2.36	24 (33%)	80,113,113	1.93	20 (25%)
18	SF4	bC	101	3	0,12,12	-	-	-		
14	CL7	bB	808	2	71,73,73	2.30	23 (32%)	80,113,113	1.91	19 (23%)
14	CL7	bJ	101	8	47,50,73	2.56	17 (36%)	51,85,113	1.55	8 (15%)
14	CL7	bK	101	-	45,45,73	2.59	19 (42%)	49,78,113	1.76	12 (24%)
14	CL7	aB	3012	2	43,46,73	2.68	18 (41%)	46,80,113	1.61	11 (23%)
14	CL7	cA	3111	1	43,46,73	2.66	18 (41%)	46,80,113	1.72	10 (21%)
16	LHG	cA	3138	14	20,20,48	1.60	4 (20%)	22,25,54	1.17	2 (9%)
16	LHG	bA	3138	14	20,20,48	1.64	4 (20%)	22,25,54	1.25	2 (9%)
14	CL7	aA	3129	1	71,73,73	2.27	20 (28%)	80,113,113	1.85	24 (30%)
14	CL7	aA	3105	1	47,49,73	2.58	20 (42%)	51,84,113	1.81	12 (23%)
14	CL7	aA	3116	1	43,46,73	2.51	16 (37%)	46,80,113	1.66	12 (26%)
14	CL7	aL	204	20	48,50,73	2.89	23 (47%)	51,85,113	1.70	15 (29%)
14	CL7	cK	101	-	45,45,73	2.55	20 (44%)	49,78,113	1.61	10 (20%)
14	CL7	bB	809	2	56,58,73	2.63	26 (46%)	62,95,113	1.95	19 (30%)
14	CL7	bA	3119	20	52,54,73	2.77	22 (42%)	57,90,113	2.14	16 (28%)
14	CL7	aB	3015	2	56,58,73	2.70	25 (44%)	62,95,113	1.90	13 (20%)
14	CL7	bB	821	2	43,46,73	2.58	19 (44%)	46,80,113	1.55	9 (19%)
12	G9R	aA	3101	1	69,73,73	2.12	21 (30%)	83,113,113	3.44	34 (40%)
14	CL7	cB	831	2	60,62,73	2.31	23 (38%)	66,99,113	1.67	16 (24%)
14	CL7	aB	3020	2	43,46,73	2.59	19 (44%)	46,80,113	1.56	9 (19%)
14	CL7	aL	202	10	71,73,73	2.29	20 (28%)	80,113,113	1.80	19 (23%)
14	CL7	bA	3113	1	47,49,73	2.60	20 (42%)	51,84,113	1.75	13 (25%)
14	CL7	aL	203	10	71,73,73	2.33	24 (33%)	80,113,113	1.92	25 (31%)
14	CL7	cA	3104	1	47,49,73	2.62	20 (42%)	51,84,113	1.83	13 (25%)
14	CL7	bB	826	20	71,73,73	2.41	24 (33%)	80,113,113	1.73	20 (25%)
14	CL7	cB	818	2	47,49,73	2.55	19 (40%)	51,84,113	1.70	14 (27%)
14	CL7	cA	3121	1	47,49,73	2.79	24 (51%)	51,84,113	1.97	14 (27%)
14	CL7	bA	3125	1	71,73,73	2.43	25 (35%)	80,113,113	2.03	18 (22%)
14	CL7	bB	818	2	47,49,73	2.57	20 (42%)	51,84,113	1.82	14 (27%)
14	CL7	cA	3116	-	59,61,73	2.40	20 (33%)	65,98,113	1.99	20 (30%)
14	CL7	cB	822	2	47,49,73	2.66	20 (42%)	51,84,113	2.09	12 (23%)
14	CL7	bB	811	2	47,49,73	2.68	19 (40%)	51,84,113	1.85	14 (27%)
14	CL7	aA	3143	1	71,73,73	2.33	22 (30%)	80,113,113	1.65	16 (20%)
14	CL7	cA	3102	20	71,73,73	2.49	23 (32%)	80,113,113	2.18	28 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CL7	cB	811	2	47,49,73	2.66	17 (36%)	51,84,113	1.76	13 (25%)
14	CL7	bB	815	2	47,49,73	2.63	21 (44%)	51,84,113	1.63	14 (27%)
14	CL7	cA	3142	1	71,73,73	2.39	21 (29%)	80,113,113	1.70	17 (21%)
14	CL7	cA	3105	1	47,49,73	2.88	21 (44%)	51,84,113	2.08	20 (39%)
14	CL7	bB	804	2	71,73,73	2.66	30 (42%)	80,113,113	1.99	23 (28%)
14	CL7	aB	3016	-	47,49,73	2.58	20 (42%)	51,84,113	1.92	13 (25%)
13	PHO	aB	3004	-	58,69,69	3.19	22 (37%)	56,99,99	2.65	17 (30%)
14	CL7	bB	803	20	71,73,73	2.35	26 (36%)	80,113,113	2.02	18 (22%)
14	CL7	cA	3112	1	47,49,73	2.59	20 (42%)	51,84,113	1.78	13 (25%)
14	CL7	bA	3124	1	71,73,73	2.45	28 (39%)	80,113,113	2.19	20 (25%)
14	CL7	bA	3121	1	47,49,73	2.81	25 (53%)	51,84,113	1.98	16 (31%)
14	CL7	cA	3144	-	47,49,73	2.50	19 (40%)	51,84,113	1.77	14 (27%)
14	CL7	bA	3106	1	71,73,73	2.38	25 (35%)	80,113,113	1.76	22 (27%)
14	CL7	cL	204	10	71,73,73	2.43	23 (32%)	80,113,113	1.91	23 (28%)
14	CL7	bB	819	2	62,64,73	2.82	25 (40%)	69,102,113	1.81	17 (24%)
14	CL7	cA	3140	1	71,73,73	2.30	21 (29%)	80,113,113	1.80	21 (26%)
18	SF4	aC	102	3	0,12,12	-	-	-	-	-
14	CL7	bA	3141	1	71,73,73	2.26	25 (35%)	80,113,113	1.59	13 (16%)
14	CL7	bA	3145	-	47,49,73	2.51	19 (40%)	51,84,113	1.79	13 (25%)
14	CL7	cL	203	10	71,73,73	2.30	21 (29%)	80,113,113	1.76	18 (22%)
14	CL7	aB	3030	2	60,62,73	2.34	23 (38%)	66,99,113	1.71	15 (22%)
14	CL7	cB	809	2	56,58,73	2.56	24 (42%)	62,95,113	1.87	15 (24%)
14	CL7	aA	3107	1	71,73,73	2.27	27 (38%)	80,113,113	1.71	20 (25%)
14	CL7	cB	814	2	47,49,73	2.47	19 (40%)	51,84,113	1.77	14 (27%)
14	CL7	bA	3104	1	47,49,73	2.61	20 (42%)	51,84,113	1.80	14 (27%)
18	SF4	aB	3001	2,1	0,12,12	-	-	-	-	-
14	CL7	aA	3103	20	71,73,73	2.40	24 (33%)	80,113,113	1.98	23 (28%)
14	CL7	bL	205	20	48,50,73	2.89	25 (52%)	51,85,113	1.75	14 (27%)
14	CL7	cA	3123	1	57,59,73	2.71	28 (49%)	63,96,113	2.22	18 (28%)
14	CL7	bF	201	2	43,46,73	2.68	21 (48%)	46,80,113	1.69	8 (17%)
17	PQN	bA	3143	-	34,34,34	2.06	12 (35%)	42,45,45	1.67	6 (14%)
14	CL7	aA	3104	1	47,49,73	2.55	20 (42%)	51,84,113	1.73	16 (31%)
14	CL7	aB	3010	2	47,49,73	2.62	18 (38%)	51,84,113	1.84	14 (27%)
14	CL7	cB	827	2	71,73,73	2.51	28 (39%)	80,113,113	1.91	21 (26%)
14	CL7	cB	832	2	71,73,73	2.36	24 (33%)	80,113,113	1.83	20 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	LHG	aA	3138	-	48,48,48	0.97	4 (8%)	51,54,54	0.95	3 (5%)
14	CL7	bA	3132	20	71,73,73	2.62	31 (43%)	80,113,113	1.86	22 (27%)
14	CL7	aB	3005	2	71,73,73	2.52	24 (33%)	80,113,113	1.63	18 (22%)
14	CL7	cB	813	2	43,46,73	2.68	18 (41%)	46,80,113	1.62	9 (19%)
12	G9R	bA	3101	1	69,73,73	2.18	22 (31%)	83,113,113	3.70	38 (45%)
14	CL7	bB	820	2	71,73,73	2.39	28 (39%)	80,113,113	1.74	17 (21%)
14	CL7	aA	3113	1	47,49,73	2.52	20 (42%)	51,84,113	1.77	14 (27%)
14	CL7	bB	810	2	71,73,73	2.41	25 (35%)	80,113,113	1.76	20 (25%)
14	CL7	cA	3107	1	71,73,73	2.28	21 (29%)	80,113,113	1.63	16 (20%)
14	CL7	cA	3118	-	43,46,73	2.60	19 (44%)	46,80,113	1.77	10 (21%)
14	CL7	aA	3128	1	57,59,73	2.60	22 (38%)	63,96,113	1.83	19 (30%)
14	CL7	cA	3109	1	47,49,73	2.58	17 (36%)	51,84,113	1.87	16 (31%)
14	CL7	bA	3108	1	48,50,73	2.72	22 (45%)	51,85,113	1.89	18 (35%)
17	PQN	aB	3027	-	34,34,34	2.53	14 (41%)	42,45,45	1.47	6 (14%)
14	CL7	aA	3125	1	71,73,73	2.33	27 (38%)	80,113,113	2.05	21 (26%)
14	CL7	cA	3127	1	57,59,73	2.67	25 (43%)	63,96,113	1.91	20 (31%)
14	CL7	cB	817	-	47,49,73	2.59	21 (44%)	51,84,113	1.92	14 (27%)
14	CL7	aA	3131	1	47,49,73	2.62	20 (42%)	51,84,113	1.65	12 (23%)
14	CL7	bA	3128	1	71,73,73	2.51	27 (38%)	80,113,113	2.01	28 (35%)
14	CL7	bA	3130	1	47,49,73	2.66	21 (44%)	51,84,113	1.65	12 (23%)
14	CL7	aA	3146	-	47,49,73	2.48	19 (40%)	51,84,113	1.87	14 (27%)
14	CL7	bB	816	2	56,58,73	2.69	23 (41%)	62,95,113	2.06	19 (30%)
19	LMG	aB	3029	-	52,52,55	0.86	1 (1%)	60,60,63	1.22	7 (11%)
19	LMG	bB	830	-	52,52,55	0.97	3 (5%)	60,60,63	1.28	6 (10%)
14	CL7	aB	3018	2	62,64,73	2.82	25 (40%)	69,102,113	1.92	17 (24%)
14	CL7	aB	3017	2	47,49,73	2.56	18 (38%)	51,84,113	1.81	14 (27%)
14	CL7	cA	3126	1	58,61,73	2.36	20 (34%)	66,97,113	1.78	16 (24%)
14	CL7	aA	3123	1	56,58,73	2.44	20 (35%)	62,95,113	2.08	20 (32%)
14	CL7	bA	3115	1	43,46,73	2.53	17 (39%)	46,80,113	1.64	13 (28%)
14	CL7	bB	822	2	47,49,73	2.66	19 (40%)	51,84,113	1.96	10 (19%)
14	CL7	aA	3119	-	43,46,73	2.58	18 (41%)	46,80,113	1.77	10 (21%)
14	CL7	aA	3121	1	57,59,73	2.46	20 (35%)	63,96,113	1.99	16 (25%)
14	CL7	aB	3008	2	56,58,73	2.53	26 (46%)	62,95,113	1.83	19 (30%)
14	CL7	bA	3117	1	43,46,73	2.64	19 (44%)	46,80,113	1.68	12 (26%)
18	SF4	cC	101	3	0,12,12	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CL7	aB	3032	2	61,63,73	2.54	27 (44%)	68,101,113	1.74	17 (25%)
14	CL7	bB	831	2	60,62,73	2.35	23 (38%)	66,99,113	1.68	16 (24%)
14	CL7	aA	3141	1	71,73,73	2.18	21 (29%)	80,113,113	1.63	19 (23%)
14	CL7	bB	823	2	47,49,73	2.56	19 (40%)	51,84,113	2.11	18 (35%)
14	CL7	aA	3134	16	47,49,73	2.52	19 (40%)	51,84,113	1.83	13 (25%)
14	CL7	cB	825	2	43,46,73	2.75	20 (46%)	46,80,113	1.68	11 (23%)
14	CL7	cB	812	2	43,46,73	2.68	21 (48%)	46,80,113	1.63	10 (21%)
14	CL7	cB	824	2	62,64,73	2.42	20 (32%)	69,102,113	1.75	16 (23%)
16	LHG	aA	3139	14	20,20,48	1.51	3 (15%)	22,25,54	1.28	3 (13%)
14	CL7	aB	3002	20	71,73,73	2.33	25 (35%)	80,113,113	1.84	16 (20%)
14	CL7	aB	3014	2	47,49,73	2.56	19 (40%)	51,84,113	1.59	11 (21%)
14	CL7	bA	3140	1	71,73,73	2.31	21 (29%)	80,113,113	1.79	18 (22%)
14	CL7	bB	812	2	43,46,73	2.68	21 (48%)	46,80,113	1.62	10 (21%)
14	CL7	bB	833	2	61,63,73	2.55	25 (40%)	68,101,113	1.69	17 (25%)
14	CL7	cA	3128	1	71,73,73	2.47	25 (35%)	80,113,113	1.91	25 (31%)
14	CL7	bB	807	2	71,73,73	2.24	25 (35%)	80,113,113	1.78	22 (27%)
14	CL7	aA	3124	1	57,59,73	2.60	24 (42%)	63,96,113	2.03	20 (31%)
14	CL7	aA	3132	-	47,49,73	2.58	19 (40%)	51,84,113	1.86	16 (31%)
14	CL7	bA	3122	1	56,58,73	2.51	21 (37%)	62,95,113	2.10	20 (32%)
14	CL7	cA	3133	16	47,49,73	2.57	20 (42%)	51,84,113	1.86	14 (27%)
14	CL7	bA	3102	20	71,73,73	2.52	26 (36%)	80,113,113	2.09	26 (32%)
14	CL7	cB	803	20	71,73,73	2.38	26 (36%)	80,113,113	2.04	22 (27%)
14	CL7	cJ	101	8	47,50,73	2.54	19 (40%)	51,85,113	1.51	8 (15%)
14	CL7	bA	3133	16	47,49,73	2.56	21 (44%)	51,84,113	1.90	13 (25%)
14	CL7	aB	3003	2	71,73,73	2.55	30 (42%)	80,113,113	1.89	20 (25%)
18	SF4	aC	101	3	0,12,12	-	-	-	-	-
14	CL7	aB	3025	20	71,73,73	2.43	24 (33%)	80,113,113	1.85	23 (28%)
14	CL7	cA	3141	1	71,73,73	2.25	22 (30%)	80,113,113	1.66	15 (18%)
14	CL7	aB	3007	2	71,73,73	2.30	27 (38%)	80,113,113	1.94	20 (25%)
14	CL7	bA	3127	1	57,59,73	2.61	23 (40%)	63,96,113	1.92	19 (30%)
14	CL7	bA	3142	1	71,73,73	2.39	21 (29%)	80,113,113	1.70	18 (22%)
14	CL7	bA	3114	1	71,73,73	2.20	23 (32%)	80,113,113	1.93	24 (30%)
14	CL7	cA	3120	1	57,59,73	2.50	23 (40%)	63,96,113	1.83	17 (26%)
14	CL7	aA	3112	1	43,46,73	2.64	17 (39%)	46,80,113	1.64	10 (21%)
14	CL7	aB	3026	2	71,73,73	2.60	28 (39%)	80,113,113	1.91	24 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CL7	bB	806	2	71,73,73	2.53	23 (32%)	80,113,113	1.61	15 (18%)
14	CL7	cB	806	2	71,73,73	2.50	24 (33%)	80,113,113	1.67	17 (21%)
14	CL7	bB	813	2	43,46,73	2.68	18 (41%)	46,80,113	1.62	10 (21%)
17	PQN	cA	3143	-	34,34,34	2.07	10 (29%)	42,45,45	1.62	6 (14%)
14	CL7	aB	3023	2	62,64,73	2.46	21 (33%)	69,102,113	1.70	16 (23%)
14	CL7	aA	3118	1	43,46,73	2.59	19 (44%)	46,80,113	1.63	11 (23%)
14	CL7	bA	3112	1	47,49,73	2.60	21 (44%)	51,84,113	1.78	13 (25%)
14	CL7	bA	3110	1	47,49,73	2.59	20 (42%)	51,84,113	1.78	12 (23%)
13	PHO	cB	801	-	58,69,69	3.57	18 (31%)	56,99,99	2.32	15 (26%)
14	CL7	cA	3132	20	71,73,73	2.58	31 (43%)	80,113,113	1.94	26 (32%)
14	CL7	aA	3126	1	71,73,73	2.32	23 (32%)	80,113,113	1.74	21 (26%)
14	CL7	aA	3115	1	71,73,73	2.11	20 (28%)	80,113,113	1.83	24 (30%)
14	CL7	aA	3133	20	71,73,73	2.54	30 (42%)	80,113,113	1.89	23 (28%)
14	CL7	bA	3120	1	57,59,73	2.48	23 (40%)	63,96,113	1.88	16 (25%)
18	SF4	cC	102	3	0,12,12	-	-	-	-	-

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
12	G9R	cA	3101	1	1/1/15/20	5/39/115/115	-
14	CL7	bA	3126	1	1/1/11/20	12/26/98/115	-
14	CL7	aA	3142	1	2/2/15/20	16/39/115/115	-
14	CL7	cA	3113	1	1/1/10/20	0/10/86/115	-
14	CL7	cL	205	20	2/2/10/20	2/12/88/115	-
14	CL7	cB	808	2	2/2/15/20	16/39/115/115	-
14	CL7	cA	3130	1	2/2/10/20	4/10/86/115	-
14	CL7	bL	203	10	2/2/15/20	23/39/115/115	-
14	CL7	aA	3120	20	2/2/11/20	3/17/93/115	-
14	CL7	aF	201	2	2/2/9/20	0/4/80/115	-
13	PHO	cB	805	-	-	19/37/103/103	0/5/6/6
14	CL7	cA	3129	1	1/1/10/20	2/10/86/115	-
14	CL7	bB	827	2	2/2/15/20	16/39/115/115	-
14	CL7	bA	3103	1	2/2/10/20	4/10/86/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CL7	bA	3129	1	1/1/10/20	2/10/86/115	-
14	CL7	aK	101	-	2/2/8/20	2/4/76/115	-
14	CL7	cB	816	2	2/2/12/20	6/21/97/115	-
14	CL7	aA	3140	-	2/2/15/20	20/39/115/115	-
14	CL7	aB	3009	2	2/2/15/20	19/39/115/115	-
14	CL7	bB	825	2	2/2/9/20	0/4/80/115	-
14	CL7	cA	3139	-	2/2/15/20	18/39/115/115	-
14	CL7	bA	3118	-	2/2/9/20	0/4/80/115	-
14	CL7	aA	3122	1	1/1/10/20	2/10/86/115	-
14	CL7	cB	823	2	2/2/10/20	7/10/86/115	-
18	SF4	bB	802	2,1	-	-	0/6/5/5
14	CL7	bB	814	2	1/1/10/20	3/10/86/115	-
14	CL7	aA	3130	1	1/1/10/20	3/10/86/115	-
14	CL7	aB	3024	2	2/2/9/20	0/4/80/115	-
14	CL7	bB	817	-	2/2/10/20	6/10/86/115	-
14	CL7	aB	3006	2	1/1/15/20	15/39/115/115	-
14	CL7	bB	832	2	2/2/15/20	18/39/115/115	-
14	CL7	cA	3124	1	2/2/15/20	11/39/115/115	-
14	CL7	cA	3106	1	2/2/15/20	18/39/115/115	-
14	CL7	cB	810	2	2/2/15/20	18/39/115/115	-
14	CL7	cB	821	2	1/1/9/20	2/4/80/115	-
14	CL7	aA	3114	1	2/2/10/20	2/10/86/115	-
14	CL7	aA	3108	1	1/1/15/20	16/39/115/115	-
14	CL7	cA	3110	1	1/1/10/20	2/10/86/115	-
14	CL7	bA	3139	-	2/2/15/20	19/39/115/115	-
14	CL7	cB	833	2	2/2/13/20	11/27/103/115	-
14	CL7	aA	3110	1	2/2/10/20	2/10/86/115	-
14	CL7	cA	3122	1	2/2/12/20	10/21/97/115	-
14	CL7	bA	3105	1	2/2/10/20	4/10/86/115	-
16	LHG	cA	3137	-	-	15/53/53/53	-
17	PQN	bB	828	-	-	7/23/43/43	0/2/2/2
14	CL7	bL	204	10	2/2/15/20	12/39/115/115	-
14	CL7	cA	3125	1	2/2/15/20	11/39/115/115	-
14	CL7	aA	3109	1	1/1/10/20	5/12/88/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	SF4	bC	102	3	-	-	0/6/5/5
14	CL7	aA	3117	-	2/2/12/20	10/25/101/115	-
14	CL7	aB	3021	2	1/1/10/20	5/10/86/115	-
14	CL7	cB	826	20	2/2/15/20	18/39/115/115	-
14	CL7	aB	3011	2	2/2/9/20	2/4/80/115	-
17	PQN	cB	828	-	-	8/23/43/43	0/2/2/2
14	CL7	bB	824	2	2/2/13/20	12/29/105/115	-
14	CL7	cA	3131	-	2/2/10/20	7/10/86/115	-
14	CL7	aA	3106	1	2/2/10/20	5/10/86/115	-
14	CL7	cA	3108	1	1/1/10/20	6/12/88/115	-
14	CL7	cB	819	2	2/2/13/20	11/29/105/115	-
14	CL7	cB	815	2	2/2/10/20	1/10/86/115	-
13	PHO	aA	3102	-	-	9/37/103/103	0/5/6/6
19	LMG	cB	830	-	-	18/47/67/70	0/1/1/1
14	CL7	cB	820	2	2/2/15/20	15/39/115/115	-
14	CL7	bA	3123	1	2/2/12/20	6/23/99/115	-
14	CL7	bA	3116	-	2/2/12/20	11/25/101/115	-
13	PHO	bB	805	-	-	19/37/103/103	0/5/6/6
14	CL7	cA	3117	1	2/2/9/20	2/4/80/115	-
14	CL7	aB	3013	2	1/1/10/20	3/10/86/115	-
14	CL7	bA	3131	-	2/2/10/20	6/10/86/115	-
14	CL7	cB	807	2	1/1/15/20	16/39/115/115	-
16	LHG	bA	3137	-	-	17/53/53/53	-
14	CL7	aA	3111	1	1/1/10/20	2/10/86/115	-
14	CL7	cA	3115	1	1/1/9/20	4/4/80/115	-
14	CL7	aB	3019	2	2/2/15/20	18/39/115/115	-
14	CL7	aJ	101	8	1/1/10/20	2/9/85/115	-
17	PQN	aA	3144	-	-	14/23/43/43	0/2/2/2
14	CL7	bA	3107	1	1/1/15/20	14/39/115/115	-
14	CL7	cA	3114	1	1/1/15/20	19/39/115/115	-
14	CL7	cF	201	2	2/2/9/20	0/4/80/115	-
13	PHO	bB	801	-	-	12/37/103/103	0/5/6/6
14	CL7	aA	3127	1	1/1/11/20	13/26/98/115	-
14	CL7	bA	3111	1	2/2/9/20	1/4/80/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CL7	cA	3103	1	2/2/10/20	5/10/86/115	-
14	CL7	cA	3119	20	2/2/11/20	3/17/93/115	-
14	CL7	bA	3109	1	2/2/10/20	4/10/86/115	-
18	SF4	cB	802	2,1	-	-	0/6/5/5
14	CL7	aB	3022	2	2/2/10/20	6/10/86/115	-
14	CL7	cB	804	2	1/1/15/20	6/39/115/115	-
14	CL7	aB	3031	2	2/2/15/20	17/39/115/115	-
18	SF4	bC	101	3	-	-	0/6/5/5
14	CL7	bB	808	2	2/2/15/20	13/39/115/115	-
14	CL7	bJ	101	8	1/1/10/20	6/9/85/115	-
14	CL7	bK	101	-	2/2/8/20	2/4/76/115	-
14	CL7	aB	3012	2	2/2/9/20	0/4/80/115	-
14	CL7	cA	3111	1	2/2/9/20	2/4/80/115	-
16	LHG	cA	3138	14	-	12/23/23/53	-
16	LHG	bA	3138	14	-	11/23/23/53	-
14	CL7	aA	3129	1	2/2/15/20	18/39/115/115	-
14	CL7	aA	3116	1	1/1/9/20	4/4/80/115	-
14	CL7	aA	3105	1	2/2/10/20	5/10/86/115	-
14	CL7	aL	204	20	2/2/10/20	2/12/88/115	-
14	CL7	cK	101	-	2/2/8/20	2/4/76/115	-
14	CL7	bB	809	2	2/2/12/20	7/21/97/115	-
14	CL7	bA	3119	20	2/2/11/20	3/17/93/115	-
14	CL7	aB	3015	2	2/2/12/20	6/21/97/115	-
14	CL7	bB	821	2	1/1/9/20	2/4/80/115	-
12	G9R	aA	3101	1	1/1/15/20	5/39/115/115	-
14	CL7	cB	831	2	2/2/12/20	9/26/102/115	-
14	CL7	aB	3020	2	1/1/9/20	2/4/80/115	-
14	CL7	aL	202	10	2/2/15/20	19/39/115/115	-
14	CL7	bA	3113	1	1/1/10/20	2/10/86/115	-
14	CL7	aL	203	10	2/2/15/20	16/39/115/115	-
14	CL7	cA	3104	1	2/2/10/20	6/10/86/115	-
14	CL7	bB	826	20	2/2/15/20	17/39/115/115	-
14	CL7	cB	818	2	2/2/10/20	5/10/86/115	-
14	CL7	cA	3121	1	2/2/10/20	1/10/86/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CL7	bA	3125	1	2/2/15/20	9/39/115/115	-
14	CL7	bB	818	2	2/2/10/20	8/10/86/115	-
14	CL7	cA	3116	-	2/2/12/20	10/25/101/115	-
14	CL7	cB	822	2	1/1/10/20	5/10/86/115	-
14	CL7	bB	811	2	2/2/10/20	1/10/86/115	-
14	CL7	aA	3143	1	1/1/15/20	20/39/115/115	-
14	CL7	cA	3102	20	1/1/15/20	9/39/115/115	-
14	CL7	cB	811	2	2/2/10/20	4/10/86/115	-
14	CL7	bB	815	2	2/2/10/20	1/10/86/115	-
14	CL7	cA	3142	1	2/2/15/20	17/39/115/115	-
14	CL7	cA	3105	1	2/2/10/20	5/10/86/115	-
14	CL7	bB	804	2	2/2/15/20	7/39/115/115	-
14	CL7	aB	3016	-	2/2/10/20	6/10/86/115	-
13	PHO	aB	3004	-	-	20/37/103/103	0/5/6/6
14	CL7	bB	803	20	2/2/15/20	13/39/115/115	-
14	CL7	cA	3112	1	2/2/10/20	6/10/86/115	-
14	CL7	bA	3124	1	2/2/15/20	11/39/115/115	-
14	CL7	bA	3121	1	2/2/10/20	3/10/86/115	-
14	CL7	cA	3144	-	2/2/10/20	5/10/86/115	-
14	CL7	bA	3106	1	2/2/15/20	22/39/115/115	-
14	CL7	cL	204	10	2/2/15/20	19/39/115/115	-
14	CL7	bB	819	2	2/2/13/20	11/29/105/115	-
14	CL7	cA	3140	1	2/2/15/20	17/39/115/115	-
18	SF4	aC	102	3	-	-	0/6/5/5
14	CL7	bA	3141	1	2/2/15/20	13/39/115/115	-
14	CL7	bA	3145	-	2/2/10/20	5/10/86/115	-
14	CL7	cL	203	10	2/2/15/20	21/39/115/115	-
14	CL7	aB	3030	2	2/2/12/20	9/26/102/115	-
14	CL7	cB	809	2	2/2/12/20	6/21/97/115	-
14	CL7	aA	3107	1	2/2/15/20	21/39/115/115	-
14	CL7	cB	814	2	1/1/10/20	2/10/86/115	-
14	CL7	bA	3104	1	2/2/10/20	6/10/86/115	-
18	SF4	aB	3001	2,1	-	-	0/6/5/5
14	CL7	aA	3103	20	1/1/15/20	10/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CL7	bL	205	20	2/2/10/20	3/12/88/115	-
14	CL7	cA	3123	1	2/2/12/20	5/23/99/115	-
14	CL7	bF	201	2	2/2/9/20	0/4/80/115	-
17	PQN	bA	3143	-	-	15/23/43/43	0/2/2/2
14	CL7	aA	3104	1	2/2/10/20	4/10/86/115	-
14	CL7	aB	3010	2	2/2/10/20	3/10/86/115	-
14	CL7	cB	827	2	1/1/15/20	18/39/115/115	-
14	CL7	cB	832	2	2/2/15/20	20/39/115/115	-
16	LHG	aA	3138	-	-	16/53/53/53	-
14	CL7	bA	3132	20	2/2/15/20	17/39/115/115	-
14	CL7	aB	3005	2	2/2/15/20	8/39/115/115	-
14	CL7	cB	813	2	2/2/9/20	2/4/80/115	-
12	G9R	bA	3101	1	-	9/39/115/115	-
14	CL7	bB	820	2	2/2/15/20	12/39/115/115	-
14	CL7	aA	3113	1	2/2/10/20	5/10/86/115	-
14	CL7	bB	810	2	2/2/15/20	22/39/115/115	-
14	CL7	cA	3107	1	1/1/15/20	15/39/115/115	-
14	CL7	cA	3118	-	1/1/9/20	0/4/80/115	-
14	CL7	aA	3128	1	2/2/12/20	10/23/99/115	-
14	CL7	cA	3109	1	2/2/10/20	3/10/86/115	-
14	CL7	bA	3108	1	1/1/10/20	6/12/88/115	-
17	PQN	aB	3027	-	-	8/23/43/43	0/2/2/2
14	CL7	aA	3125	1	2/2/15/20	9/39/115/115	-
14	CL7	cA	3127	1	2/2/12/20	9/23/99/115	-
14	CL7	cB	817	-	2/2/10/20	6/10/86/115	-
14	CL7	aA	3131	1	1/1/10/20	5/10/86/115	-
14	CL7	bA	3128	1	2/2/15/20	17/39/115/115	-
14	CL7	bA	3130	1	2/2/10/20	6/10/86/115	-
14	CL7	aA	3146	-	2/2/10/20	7/10/86/115	-
14	CL7	bB	816	2	1/1/12/20	3/21/97/115	-
19	LMG	aB	3029	-	-	20/47/67/70	0/1/1/1
19	LMG	bB	830	-	-	18/47/67/70	0/1/1/1
14	CL7	aB	3018	2	2/2/13/20	11/29/105/115	-
14	CL7	aB	3017	2	2/2/10/20	8/10/86/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CL7	cA	3126	1	2/2/11/20	12/26/98/115	-
14	CL7	aA	3123	1	2/2/12/20	9/21/97/115	-
14	CL7	bA	3115	1	1/1/9/20	4/4/80/115	-
14	CL7	bB	822	2	1/1/10/20	4/10/86/115	-
14	CL7	aA	3119	-	1/1/9/20	0/4/80/115	-
14	CL7	aA	3121	1	2/2/12/20	6/23/99/115	-
14	CL7	aB	3008	2	2/2/12/20	6/21/97/115	-
14	CL7	bA	3117	1	2/2/9/20	2/4/80/115	-
18	SF4	cC	101	3	-	-	0/6/5/5
14	CL7	aB	3032	2	2/2/13/20	10/27/103/115	-
14	CL7	bB	831	2	2/2/12/20	8/26/102/115	-
14	CL7	aA	3141	1	2/2/15/20	18/39/115/115	-
14	CL7	bB	823	2	2/2/10/20	7/10/86/115	-
14	CL7	aA	3134	16	2/2/10/20	8/10/86/115	-
14	CL7	cB	825	2	2/2/9/20	0/4/80/115	-
14	CL7	cB	812	2	2/2/9/20	2/4/80/115	-
14	CL7	cB	824	2	2/2/13/20	15/29/105/115	-
16	LHG	aA	3139	14	-	9/23/23/53	-
14	CL7	aB	3002	20	2/2/15/20	21/39/115/115	-
14	CL7	aB	3014	2	1/1/10/20	1/10/86/115	-
14	CL7	bA	3140	1	2/2/15/20	17/39/115/115	-
14	CL7	bB	812	2	2/2/9/20	2/4/80/115	-
14	CL7	bB	833	2	2/2/13/20	11/27/103/115	-
14	CL7	cA	3128	1	2/2/15/20	19/39/115/115	-
14	CL7	bB	807	2	1/1/15/20	15/39/115/115	-
14	CL7	aA	3124	1	2/2/12/20	6/23/99/115	-
14	CL7	aA	3132	-	2/2/10/20	7/10/86/115	-
14	CL7	bA	3122	1	2/2/12/20	9/21/97/115	-
14	CL7	cA	3133	16	2/2/10/20	4/10/86/115	-
14	CL7	bA	3102	20	1/1/15/20	8/39/115/115	-
14	CL7	cB	803	20	2/2/15/20	15/39/115/115	-
14	CL7	cJ	101	8	1/1/10/20	3/9/85/115	-
14	CL7	bA	3133	16	2/2/10/20	5/10/86/115	-
14	CL7	aB	3003	2	2/2/15/20	4/39/115/115	-
18	SF4	aC	101	3	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CL7	aB	3025	20	2/2/15/20	16/39/115/115	-
14	CL7	cA	3141	1	2/2/15/20	16/39/115/115	-
14	CL7	aB	3007	2	2/2/15/20	13/39/115/115	-
14	CL7	bA	3127	1	2/2/12/20	9/23/99/115	-
14	CL7	bA	3142	1	2/2/15/20	16/39/115/115	-
14	CL7	bA	3114	1	2/2/15/20	19/39/115/115	-
14	CL7	cA	3120	1	2/2/12/20	7/23/99/115	-
14	CL7	aA	3112	1	2/2/9/20	2/4/80/115	-
14	CL7	aB	3026	2	2/2/15/20	18/39/115/115	-
14	CL7	bB	806	2	2/2/15/20	15/39/115/115	-
14	CL7	cB	806	2	2/2/15/20	13/39/115/115	-
14	CL7	bB	813	2	2/2/9/20	0/4/80/115	-
17	PQN	cA	3143	-	-	13/23/43/43	0/2/2/2
14	CL7	aB	3023	2	2/2/13/20	16/29/105/115	-
14	CL7	aA	3118	1	2/2/9/20	2/4/80/115	-
14	CL7	bA	3112	1	2/2/10/20	5/10/86/115	-
14	CL7	bA	3110	1	2/2/10/20	3/10/86/115	-
13	PHO	cB	801	-	-	10/37/103/103	0/5/6/6
14	CL7	cA	3132	20	2/2/15/20	19/39/115/115	-
14	CL7	aA	3126	1	2/2/15/20	13/39/115/115	-
14	CL7	aA	3115	1	2/2/15/20	17/39/115/115	-
14	CL7	aA	3133	20	2/2/15/20	17/39/115/115	-
14	CL7	bA	3120	1	2/2/12/20	7/23/99/115	-
18	SF4	cC	102	3	-	-	0/6/5/5

The worst 5 of 4894 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	cB	801	PHO	C3A-C2A	-14.42	1.41	1.54
13	bB	801	PHO	C3A-C2A	-14.37	1.41	1.54
13	aA	3102	PHO	C3A-C2A	-13.81	1.42	1.54
13	aA	3102	PHO	OBD-CAD	11.47	1.38	1.22
13	cB	801	PHO	OBD-CAD	11.30	1.38	1.22

The worst 5 of 3705 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	bA	3101	G9R	C1D-ND-C4D	-14.07	96.34	106.33
12	aA	3101	G9R	C1D-ND-C4D	-12.96	97.13	106.33
12	bA	3101	G9R	C4A-NA-C1A	-12.94	100.89	106.71
12	cA	3101	G9R	C4A-NA-C1A	-11.27	101.64	106.71
13	cB	805	PHO	C4D-CHA-CBD	-11.07	103.51	108.52

5 of 376 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
12	aA	3101	G9R	ND
12	cA	3101	G9R	ND
14	aA	3103	CL7	NC
14	aA	3104	CL7	NA
14	aA	3104	CL7	NC

5 of 2107 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	aA	3102	PHO	CBA-CGA-O2A-C1
13	aA	3102	PHO	O1A-CGA-O2A-C1
13	bB	801	PHO	CBA-CGA-O2A-C1
13	bB	801	PHO	O1A-CGA-O2A-C1
13	bB	805	PHO	CHA-CBD-CGD-O1D

There are no ring outliers.

169 monomers are involved in 415 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	aA	3142	CL7	3	0
14	cA	3113	CL7	1	0
14	cL	205	CL7	1	0
14	cB	808	CL7	5	0
14	bL	203	CL7	5	0
14	aA	3120	CL7	1	0
13	cB	805	PHO	8	0
14	aF	201	CL7	1	0
14	bB	827	CL7	3	0
14	bA	3103	CL7	1	0
14	bA	3129	CL7	1	0
14	cB	816	CL7	1	0
14	aA	3140	CL7	3	0
14	aB	3009	CL7	2	0
14	cA	3139	CL7	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	bA	3118	CL7	1	0
14	aA	3122	CL7	3	0
14	cB	823	CL7	1	0
14	bB	814	CL7	1	0
14	bB	817	CL7	2	0
14	aB	3006	CL7	5	0
14	bB	832	CL7	8	0
14	cA	3124	CL7	2	0
14	cA	3106	CL7	3	0
14	cB	810	CL7	2	0
14	aA	3114	CL7	1	0
14	aA	3108	CL7	2	0
14	bA	3139	CL7	1	0
14	cB	833	CL7	3	0
14	bA	3105	CL7	1	0
16	cA	3137	LHG	2	0
17	bB	828	PQN	3	0
14	bL	204	CL7	7	0
14	cA	3125	CL7	4	0
14	aA	3109	CL7	1	0
14	aA	3117	CL7	2	0
14	aB	3021	CL7	4	0
14	cB	826	CL7	4	0
17	cB	828	PQN	1	0
14	cA	3131	CL7	1	0
14	aA	3106	CL7	1	0
13	aA	3102	PHO	7	0
14	cB	815	CL7	1	0
14	cB	819	CL7	5	0
19	cB	830	LMG	2	0
14	cB	820	CL7	4	0
14	bA	3123	CL7	2	0
14	bA	3116	CL7	2	0
13	bB	805	PHO	9	0
14	aB	3013	CL7	1	0
14	bA	3131	CL7	1	0
14	cB	807	CL7	5	0
16	bA	3137	LHG	3	0
14	aA	3111	CL7	1	0
14	cA	3115	CL7	3	0
14	aB	3019	CL7	9	0
17	aA	3144	PQN	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	bB	801	PHO	8	0
14	cA	3114	CL7	3	0
14	cF	201	CL7	1	0
14	aA	3127	CL7	1	0
14	cA	3103	CL7	1	0
14	cA	3119	CL7	2	0
14	aB	3022	CL7	1	0
14	cB	804	CL7	5	0
14	aB	3031	CL7	6	0
14	bB	808	CL7	4	0
14	bJ	101	CL7	1	0
16	cA	3138	LHG	1	0
16	bA	3138	LHG	1	0
14	aA	3129	CL7	3	0
14	aA	3116	CL7	3	0
14	bB	809	CL7	1	0
14	bA	3119	CL7	2	0
14	cB	831	CL7	1	0
14	aL	202	CL7	4	0
14	bA	3113	CL7	1	0
14	aL	203	CL7	7	0
14	bB	826	CL7	6	0
14	cA	3121	CL7	1	0
14	bA	3125	CL7	4	0
14	cA	3116	CL7	4	0
14	cB	822	CL7	3	0
14	aA	3143	CL7	1	0
14	cA	3102	CL7	2	0
14	bB	815	CL7	1	0
14	cA	3142	CL7	4	0
14	cA	3105	CL7	2	0
14	bB	804	CL7	2	0
14	aB	3016	CL7	2	0
13	aB	3004	PHO	9	0
14	bB	803	CL7	5	0
14	cA	3112	CL7	1	0
14	bA	3124	CL7	3	0
14	bA	3121	CL7	1	0
14	bA	3106	CL7	6	0
14	cL	204	CL7	8	0
14	bB	819	CL7	4	0
14	cA	3140	CL7	5	0

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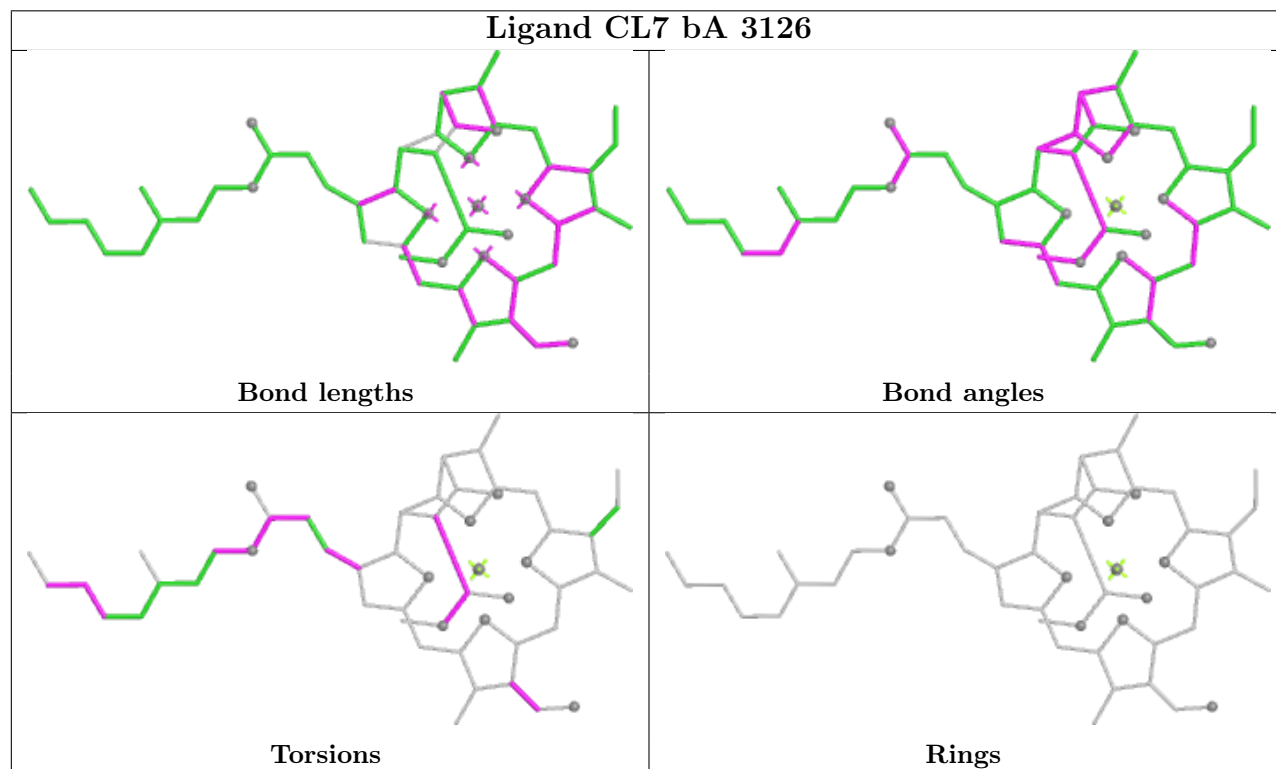
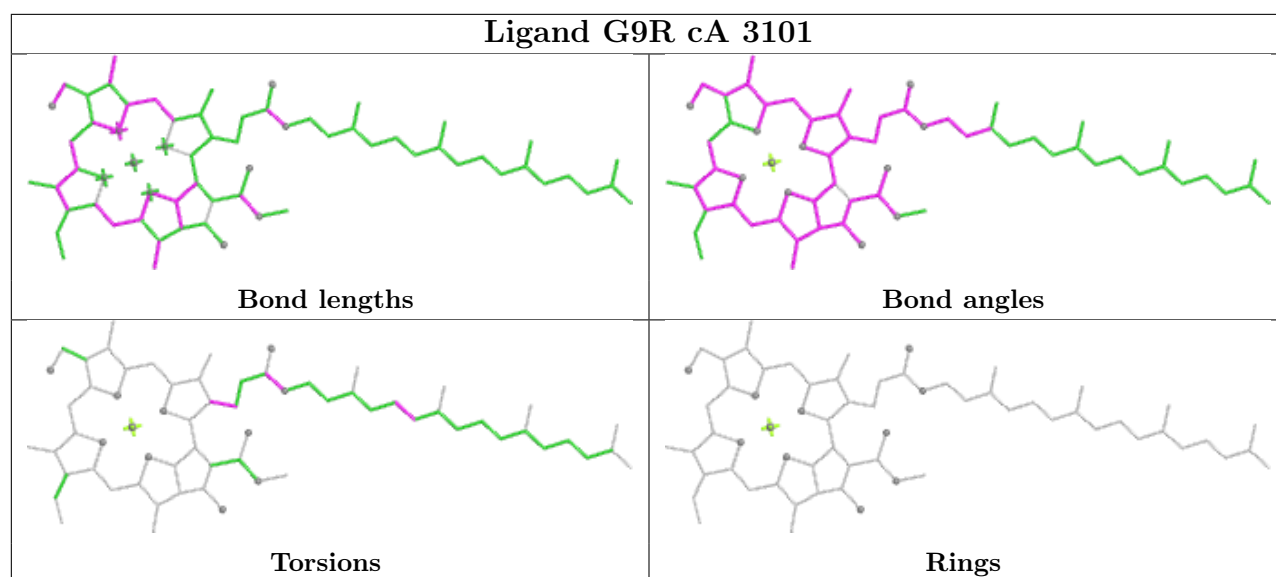
Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	bA	3141	CL7	5	0
14	cL	203	CL7	6	0
14	aB	3030	CL7	2	0
14	cB	809	CL7	1	0
14	aA	3107	CL7	7	0
14	cB	814	CL7	1	0
14	aA	3103	CL7	2	0
14	bL	205	CL7	1	0
14	cA	3123	CL7	4	0
14	bF	201	CL7	1	0
17	bA	3143	PQN	3	0
14	aA	3104	CL7	1	0
14	cB	827	CL7	3	0
14	cB	832	CL7	8	0
16	aA	3138	LHG	2	0
14	bA	3132	CL7	2	0
14	aB	3005	CL7	3	0
14	bB	820	CL7	6	0
14	bB	810	CL7	1	0
14	cA	3107	CL7	1	0
14	cA	3118	CL7	1	0
17	aB	3027	PQN	1	0
14	aA	3125	CL7	2	0
14	cB	817	CL7	2	0
14	bA	3128	CL7	5	0
14	bB	816	CL7	2	0
19	aB	3029	LMG	1	0
19	bB	830	LMG	1	0
14	aB	3018	CL7	6	0
14	cA	3126	CL7	2	0
14	aA	3123	CL7	2	0
14	bA	3115	CL7	3	0
14	bB	822	CL7	4	0
14	aA	3119	CL7	1	0
14	aA	3121	CL7	1	0
14	aB	3008	CL7	2	0
14	aB	3032	CL7	2	0
14	bB	831	CL7	1	0
14	aA	3141	CL7	6	0
14	bB	823	CL7	1	0
14	aA	3134	CL7	1	0
16	aA	3139	LHG	1	0

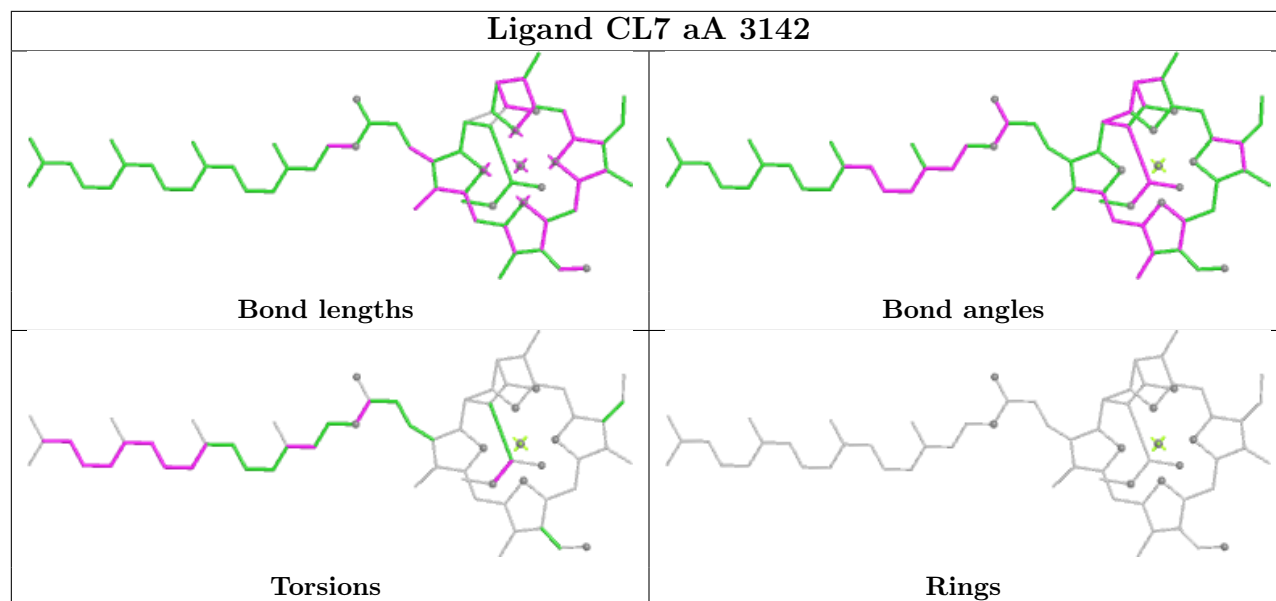
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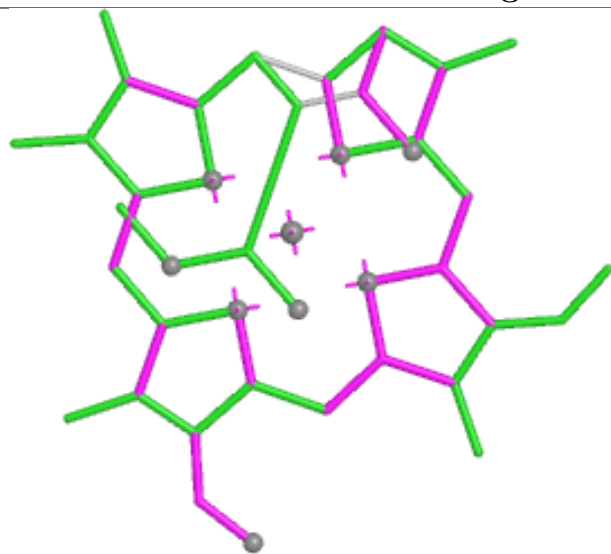
Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	aB	3002	CL7	4	0
14	aB	3014	CL7	1	0
14	bA	3140	CL7	2	0
14	bB	833	CL7	5	0
14	cA	3128	CL7	2	0
14	bB	807	CL7	5	0
14	aA	3124	CL7	2	0
14	bA	3122	CL7	2	0
14	bA	3102	CL7	2	0
14	cB	803	CL7	4	0
14	aB	3003	CL7	3	0
14	aB	3025	CL7	3	0
14	cA	3141	CL7	8	0
14	aB	3007	CL7	7	0
14	bA	3142	CL7	6	0
14	bA	3114	CL7	4	0
14	cA	3120	CL7	2	0
14	aB	3026	CL7	4	0
14	bB	806	CL7	4	0
14	cB	806	CL7	1	0
17	cA	3143	PQN	2	0
14	aB	3023	CL7	1	0
14	bA	3112	CL7	1	0
13	cB	801	PHO	11	0
14	aA	3126	CL7	4	0
14	aA	3115	CL7	2	0
14	aA	3133	CL7	2	0
14	bA	3120	CL7	2	0

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

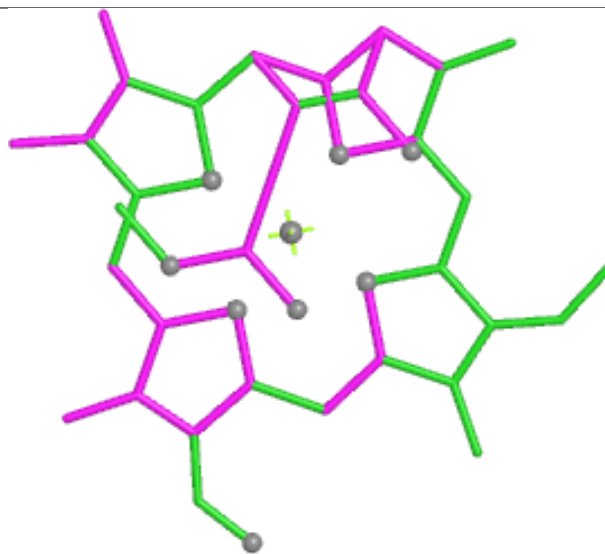




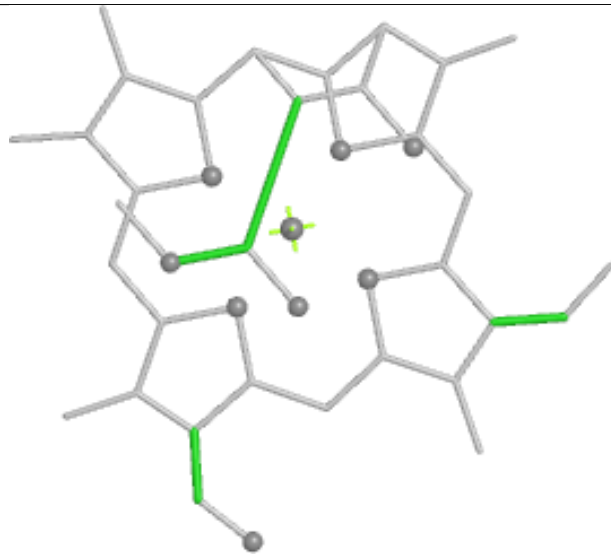
Ligand CL7 cA 3113



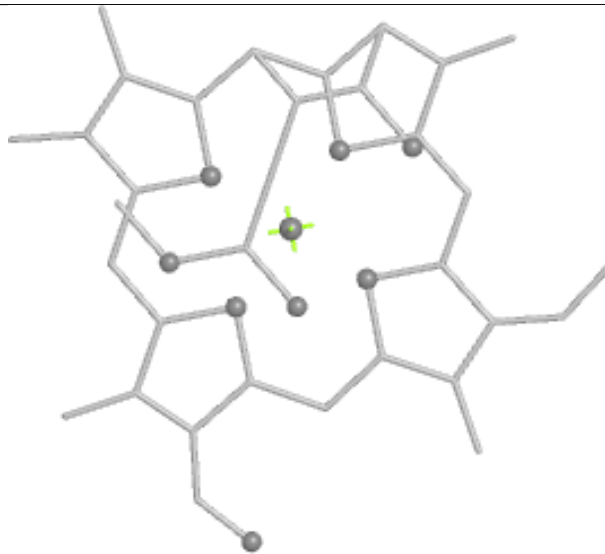
Bond lengths



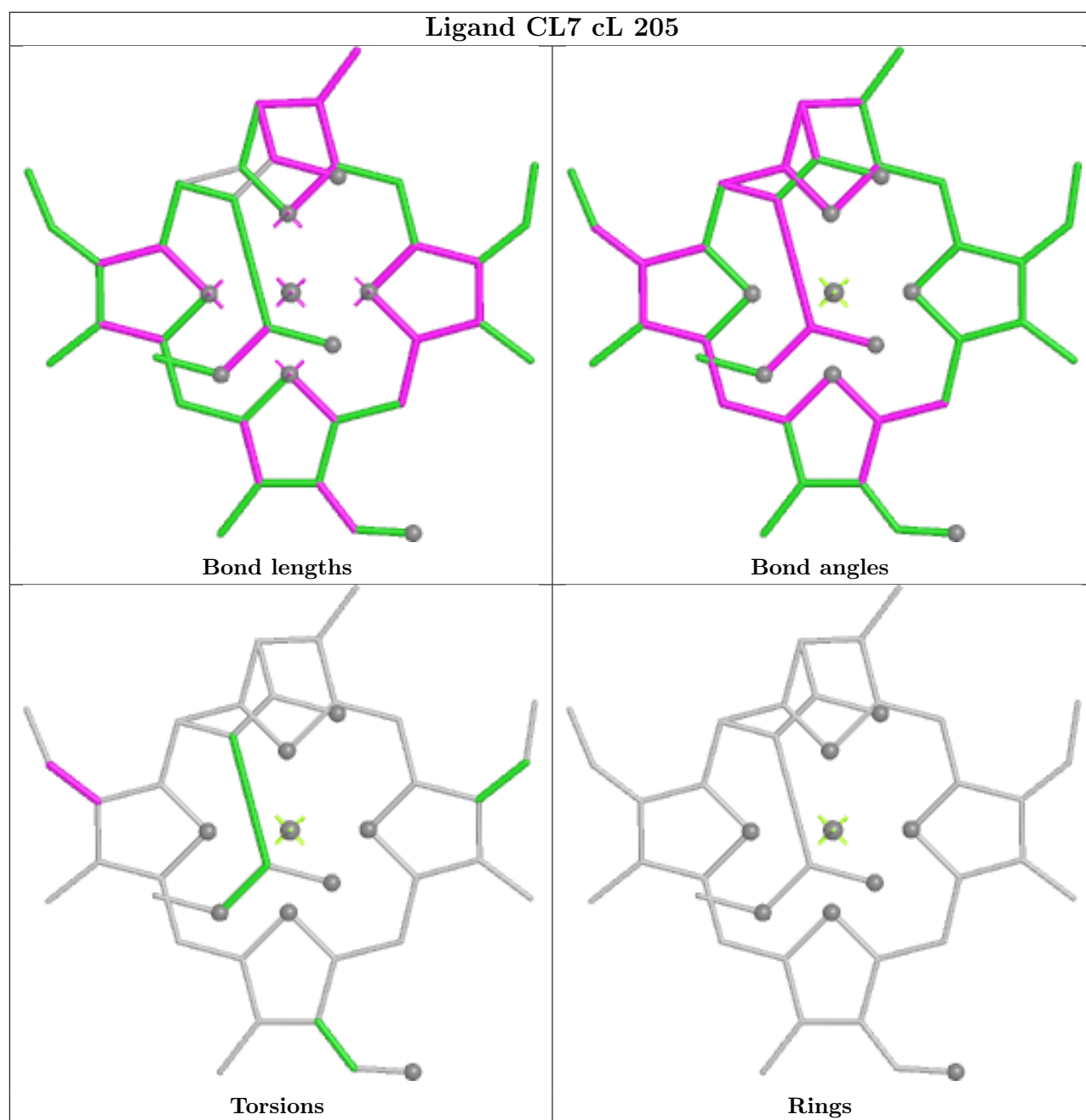
Bond angles

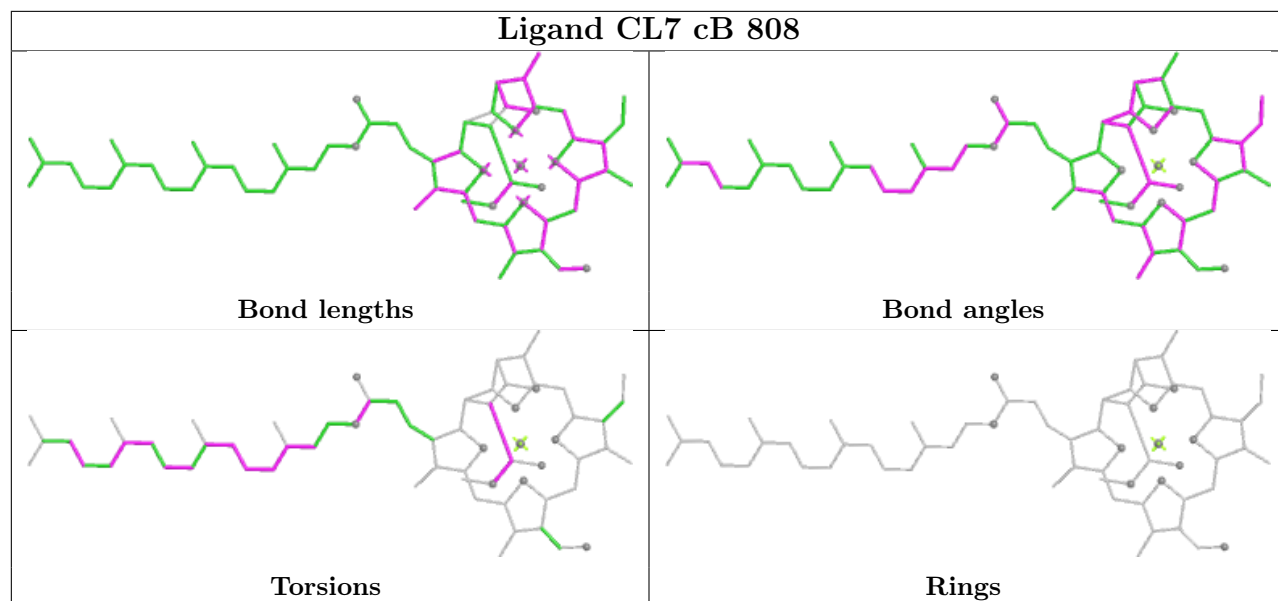


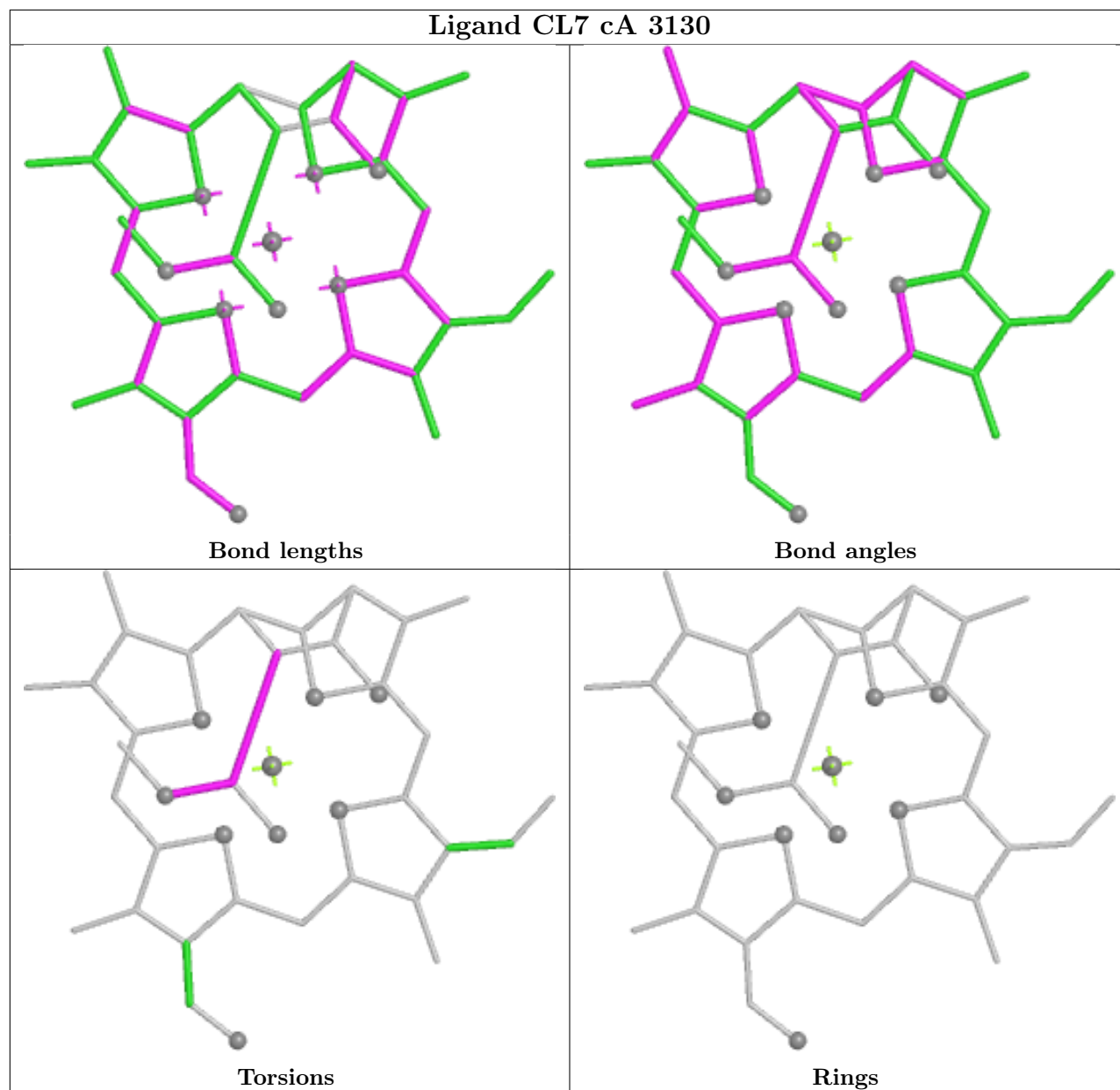
Torsions

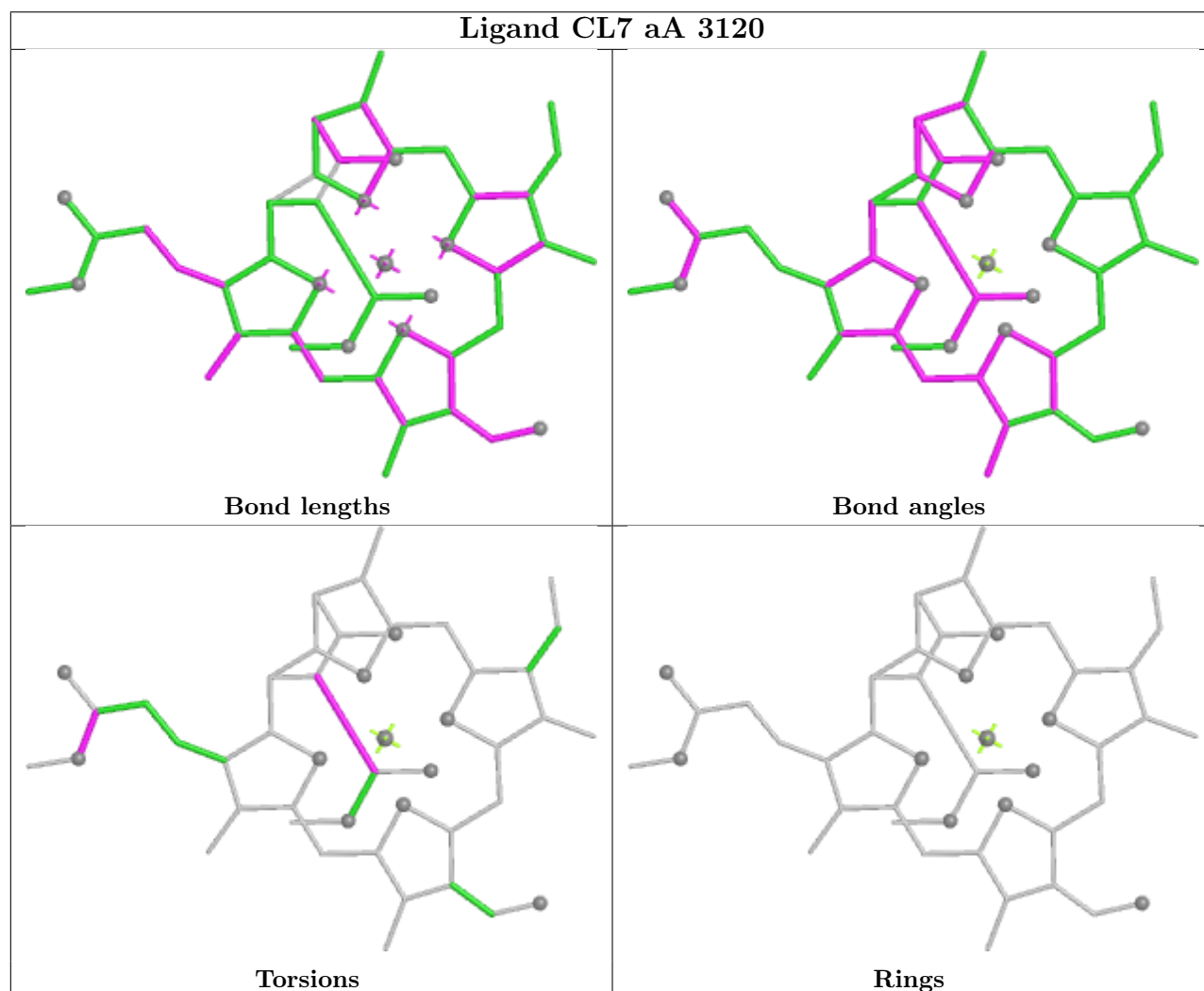
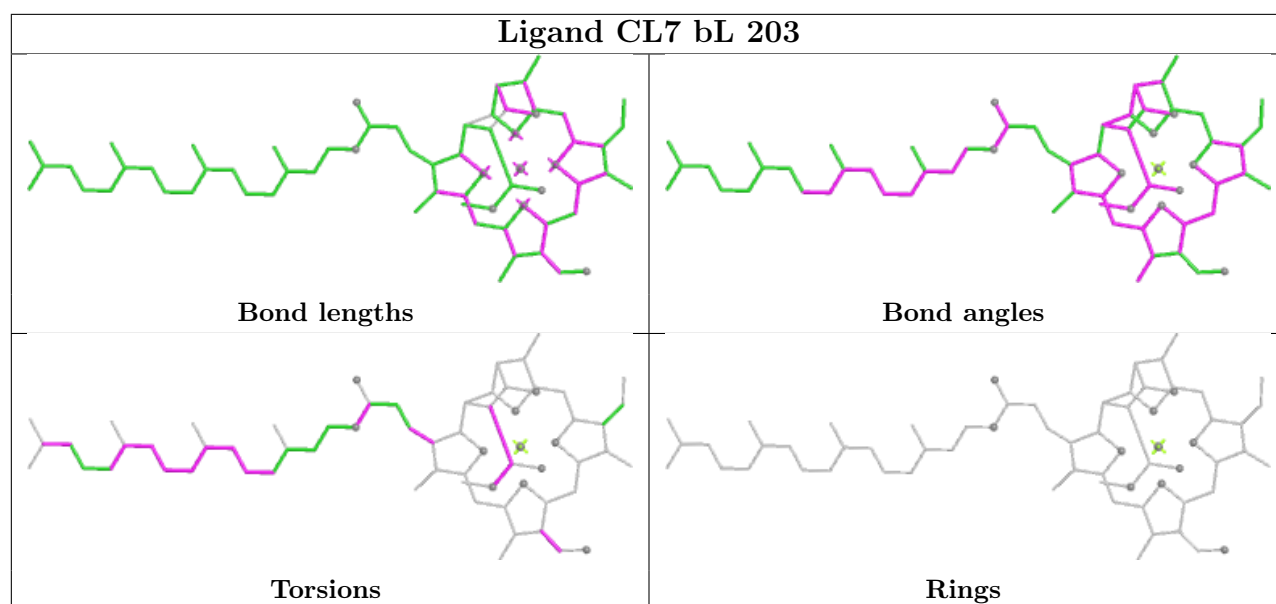


Rings

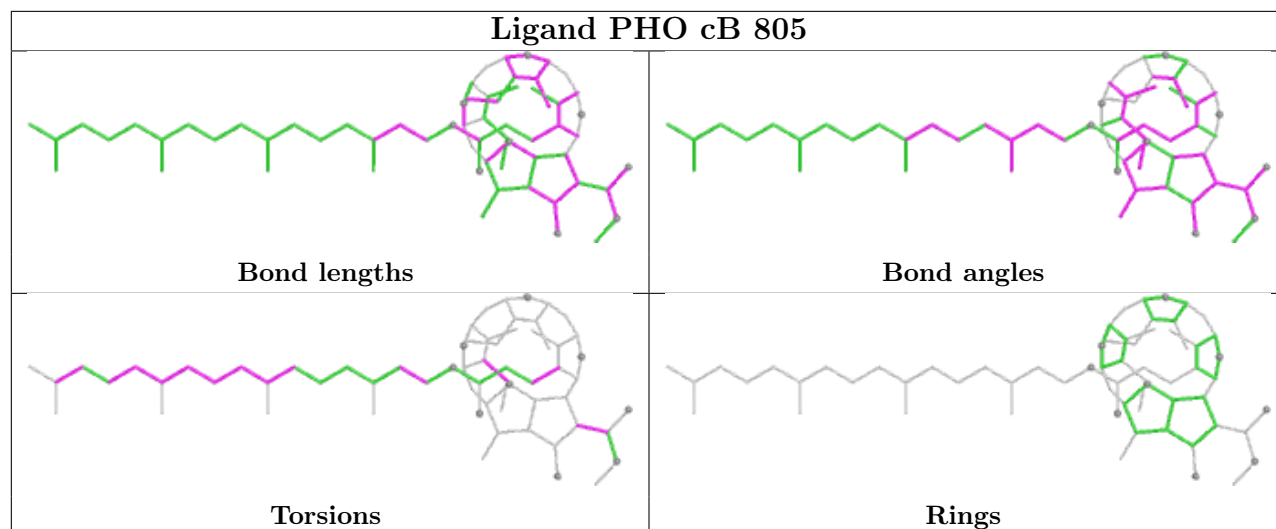




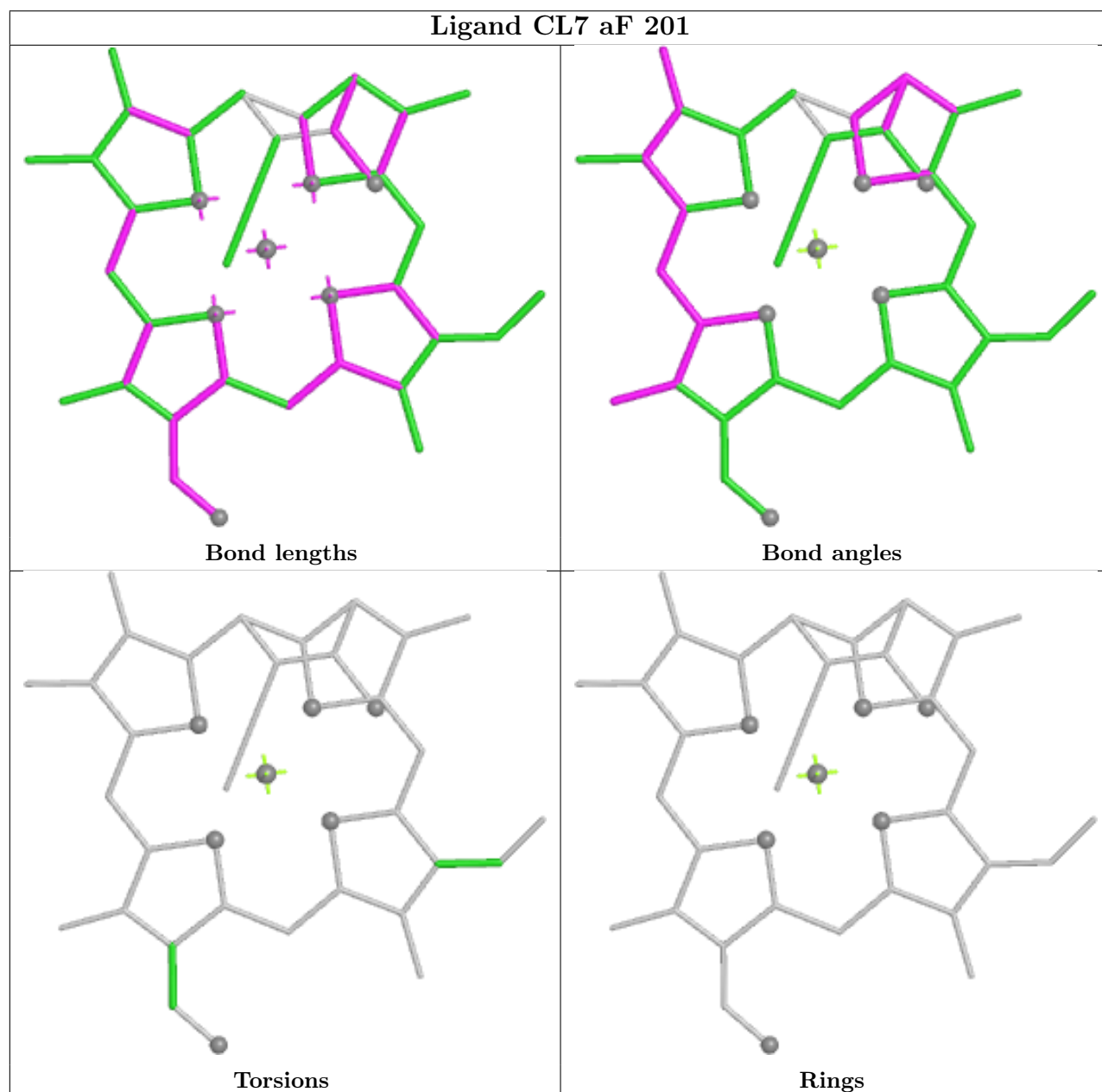




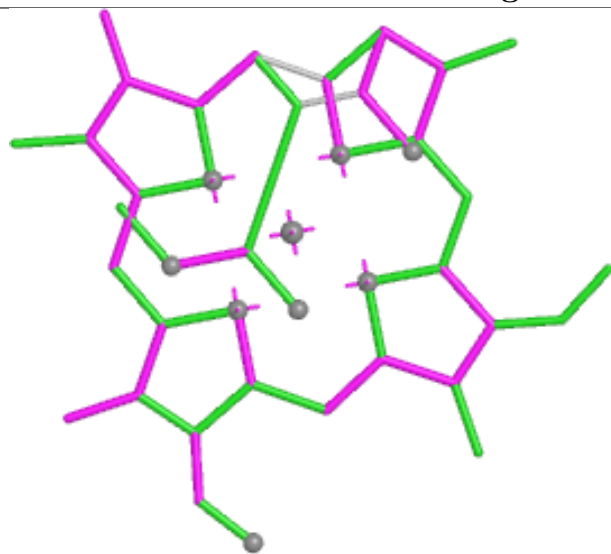
Ligand PHO cB 805



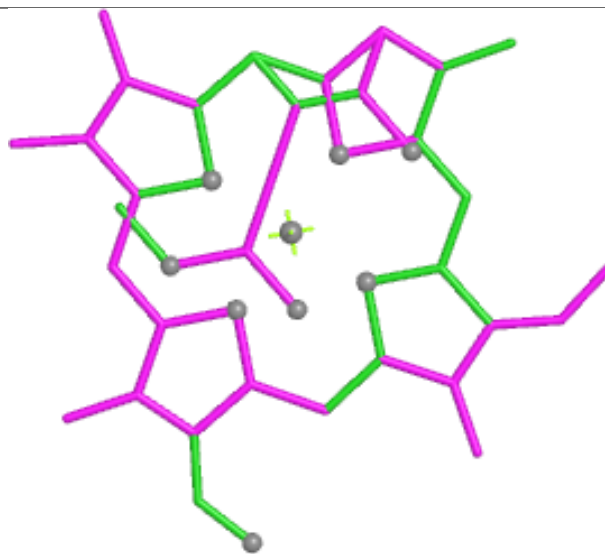
Ligand CL7 aF 201



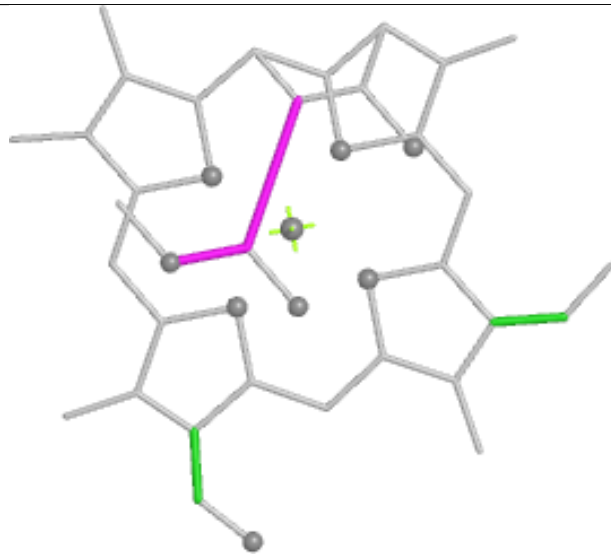
Ligand CL7 cA 3129



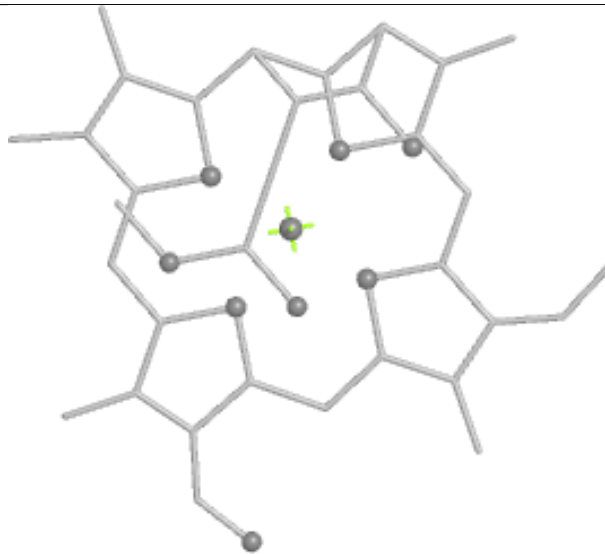
Bond lengths



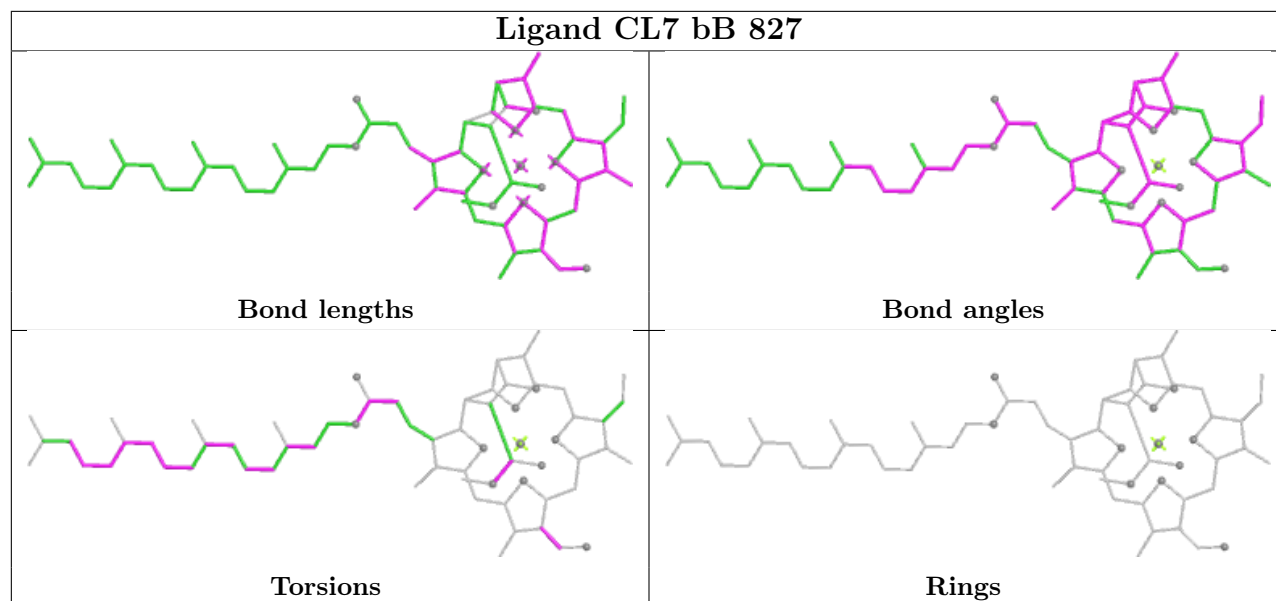
Bond angles



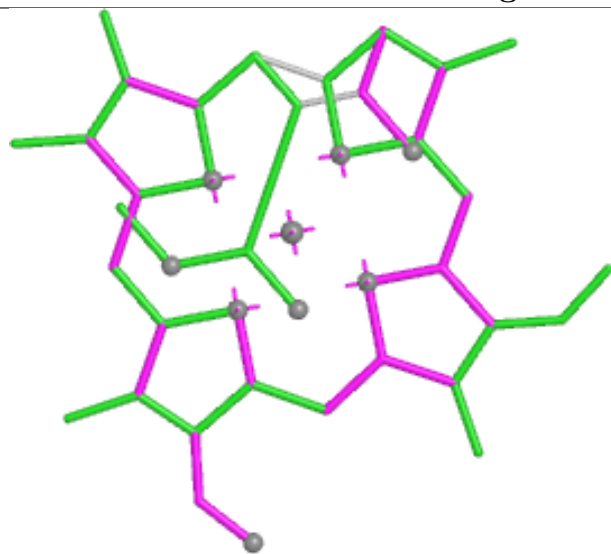
Torsions



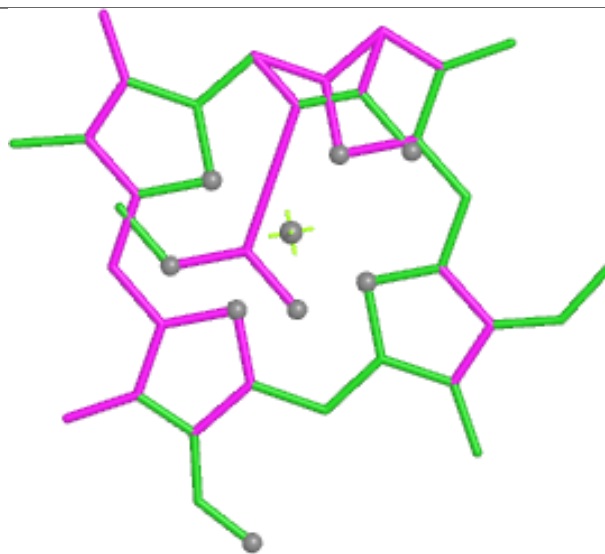
Rings



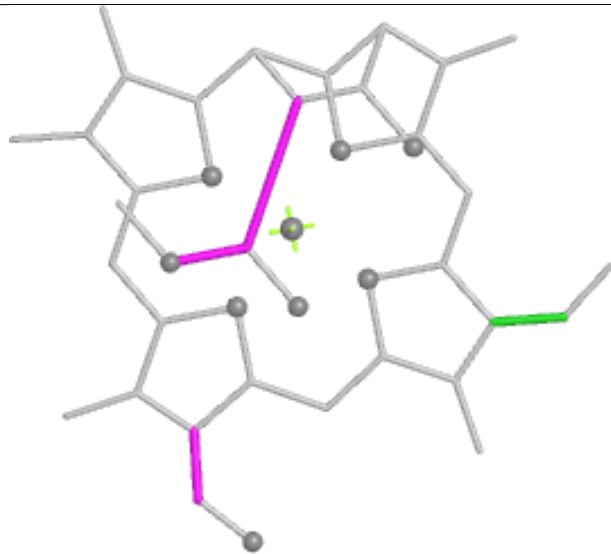
Ligand CL7 bA 3103



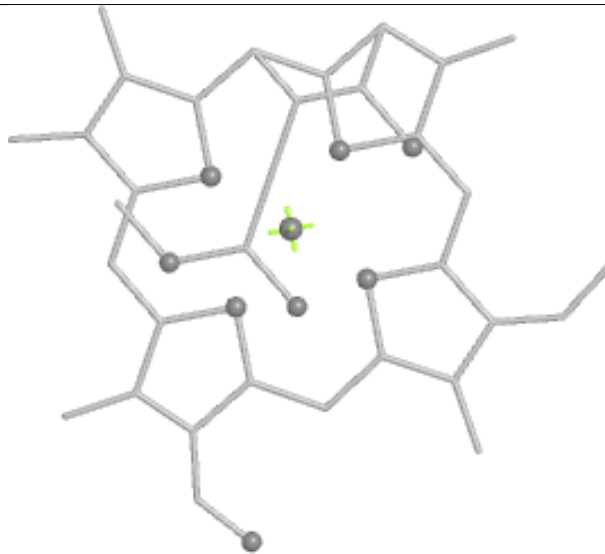
Bond lengths



Bond angles

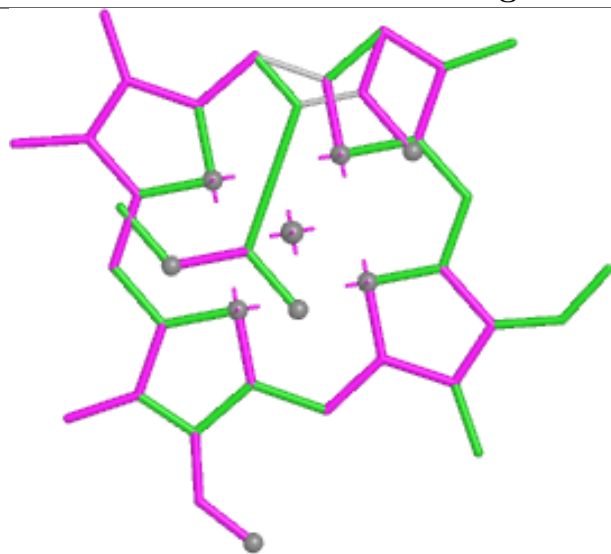


Torsions

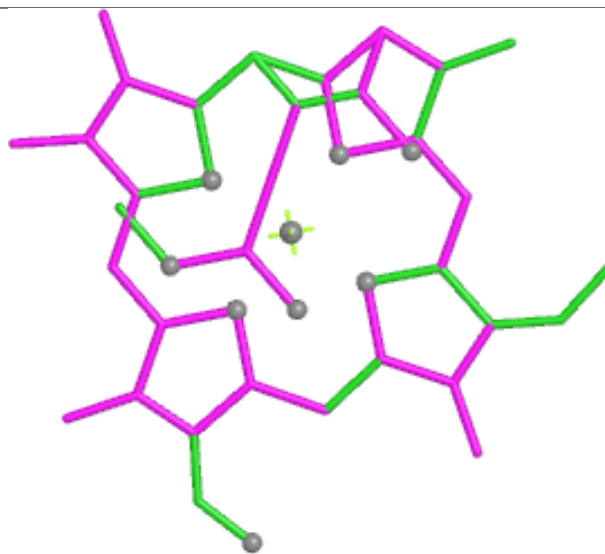


Rings

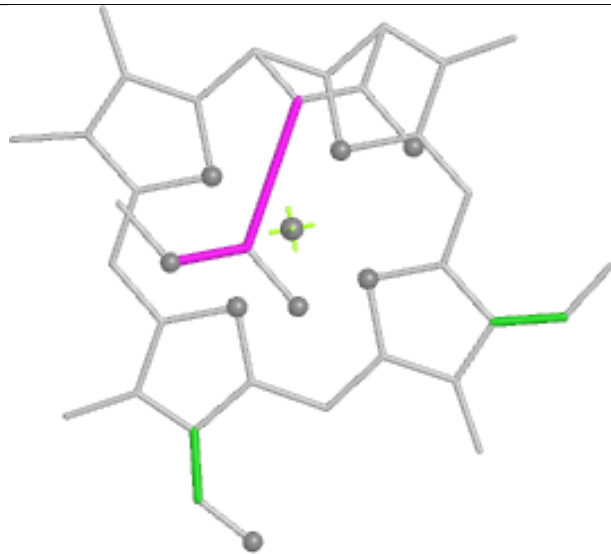
Ligand CL7 bA 3129



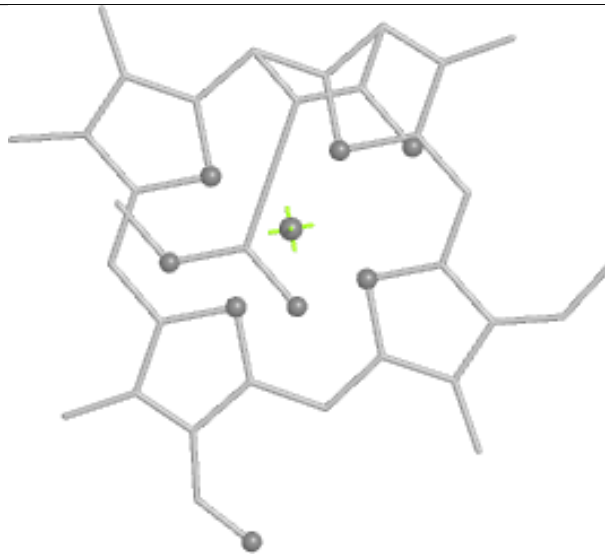
Bond lengths



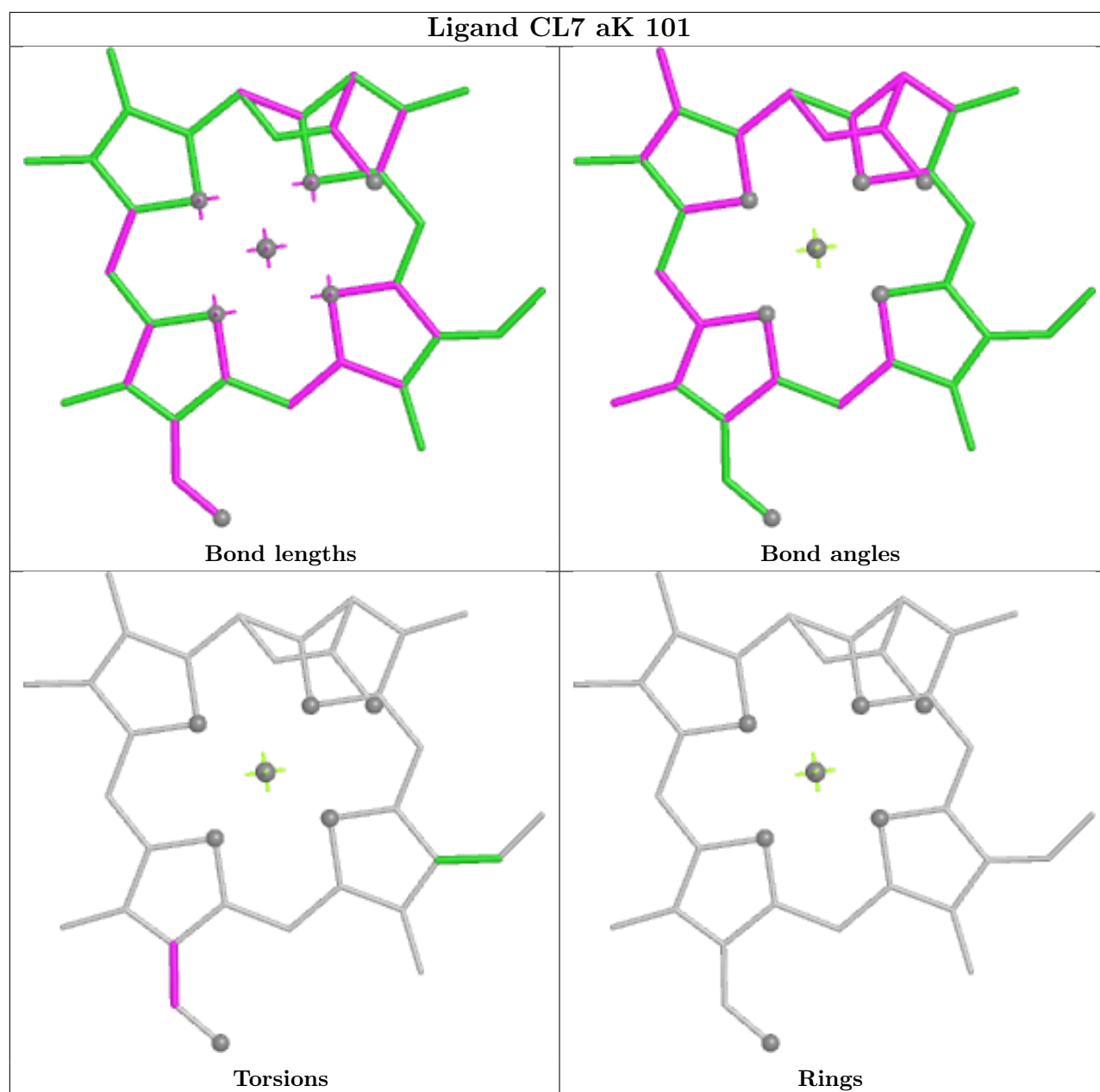
Bond angles

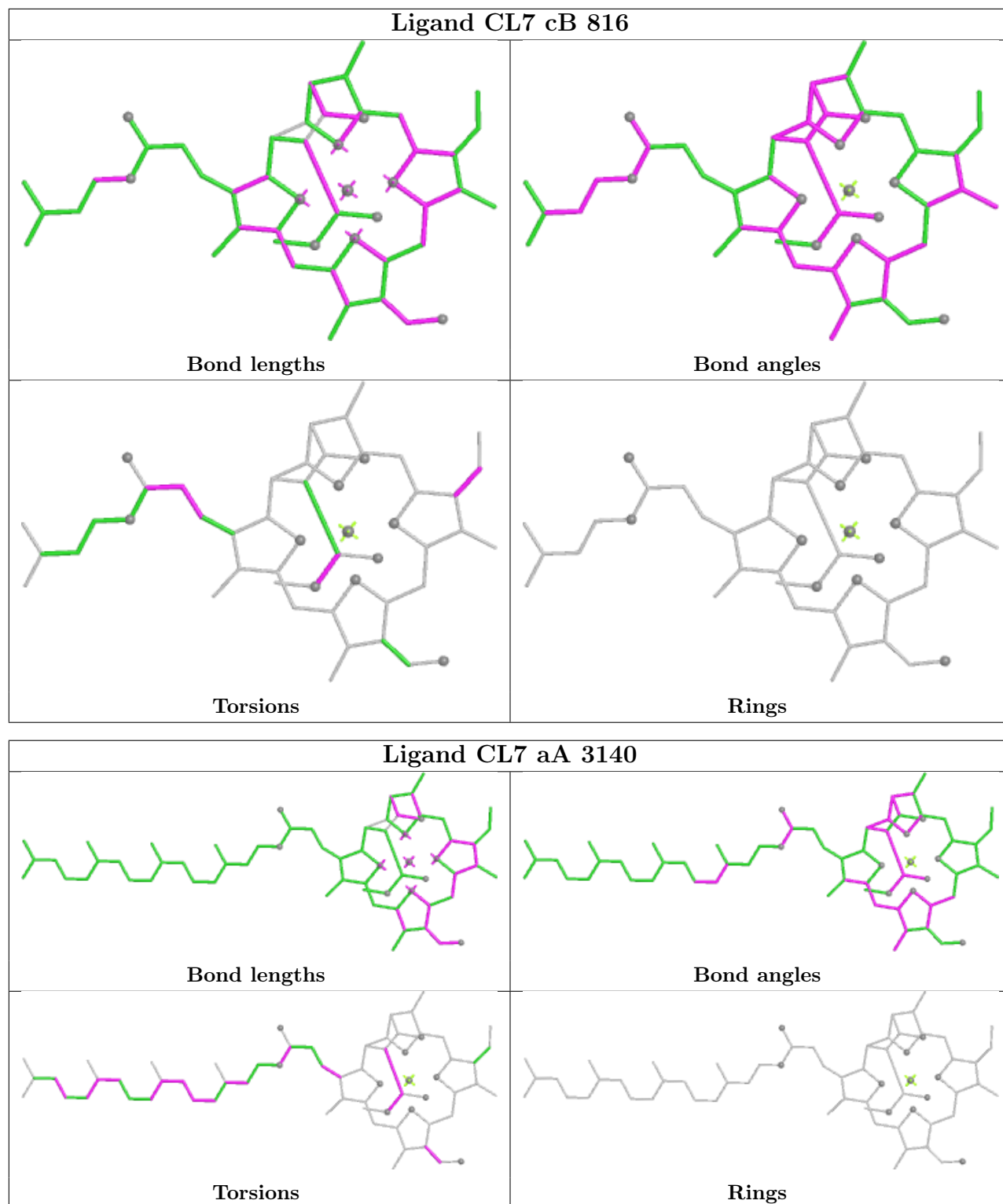


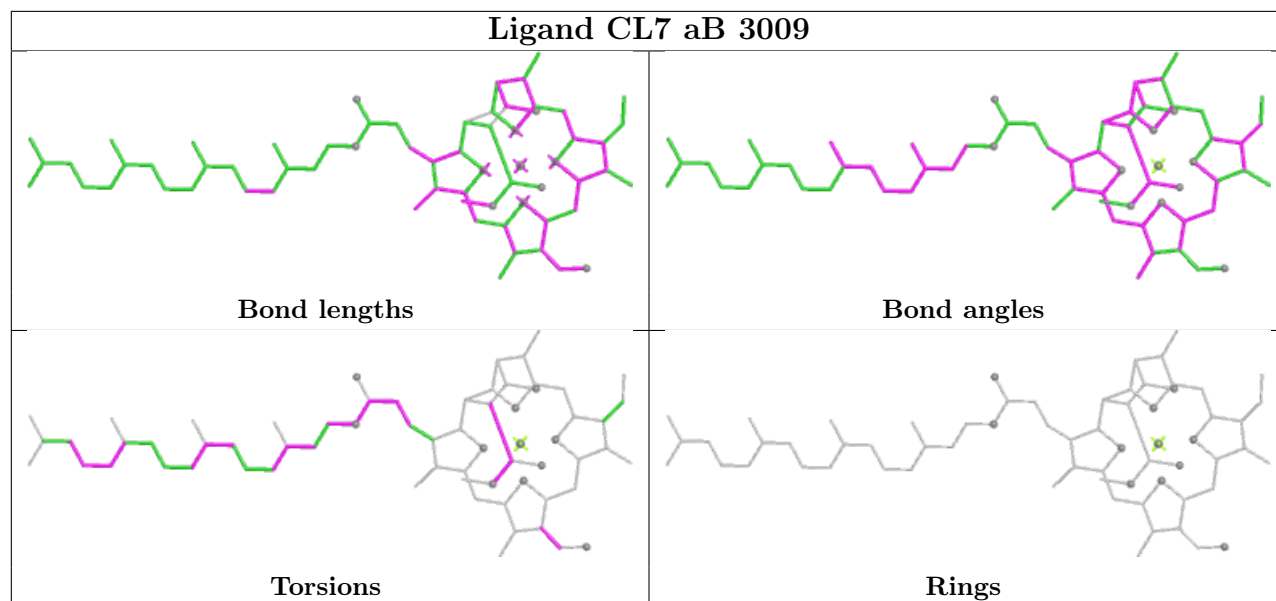
Torsions

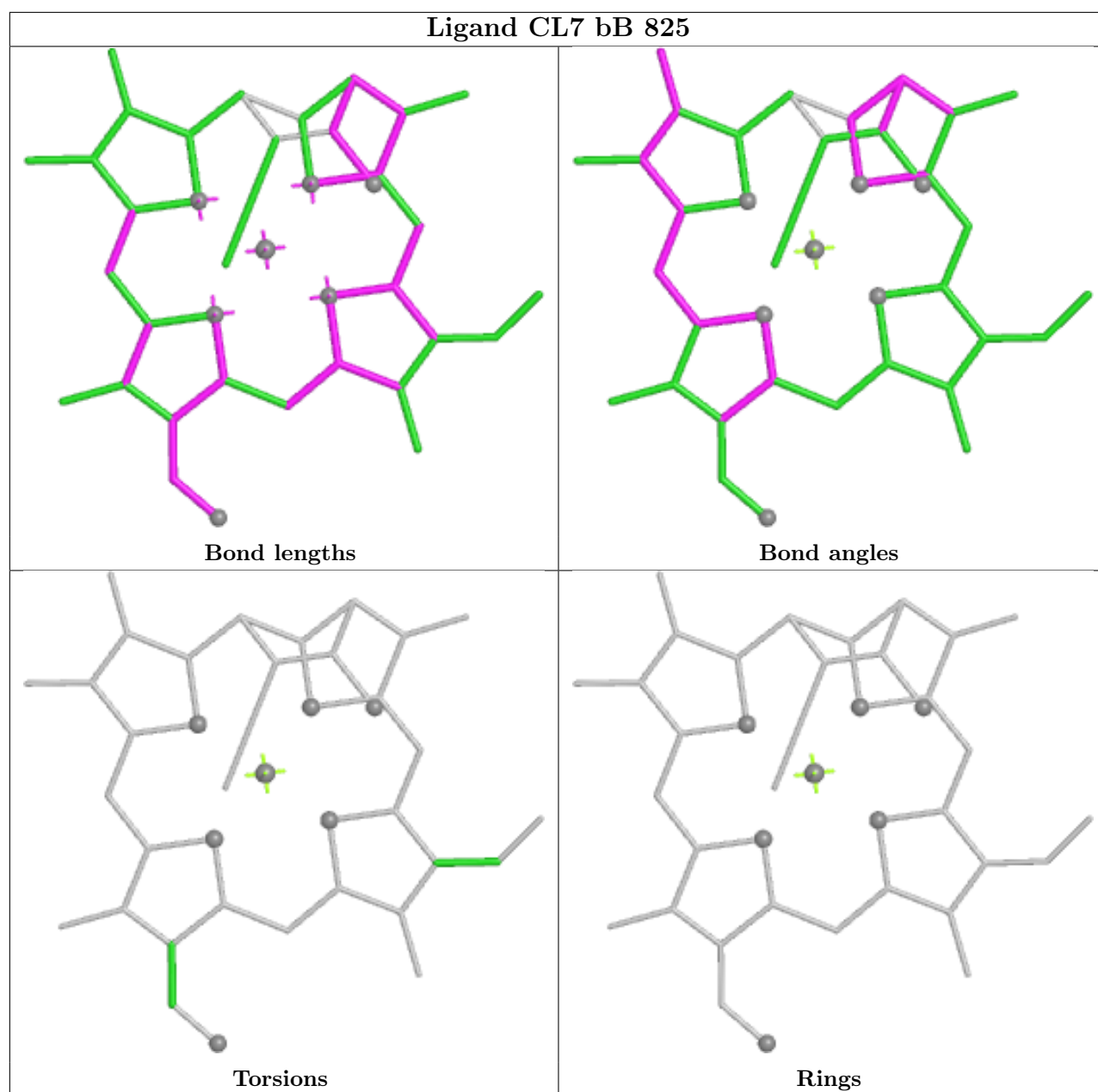


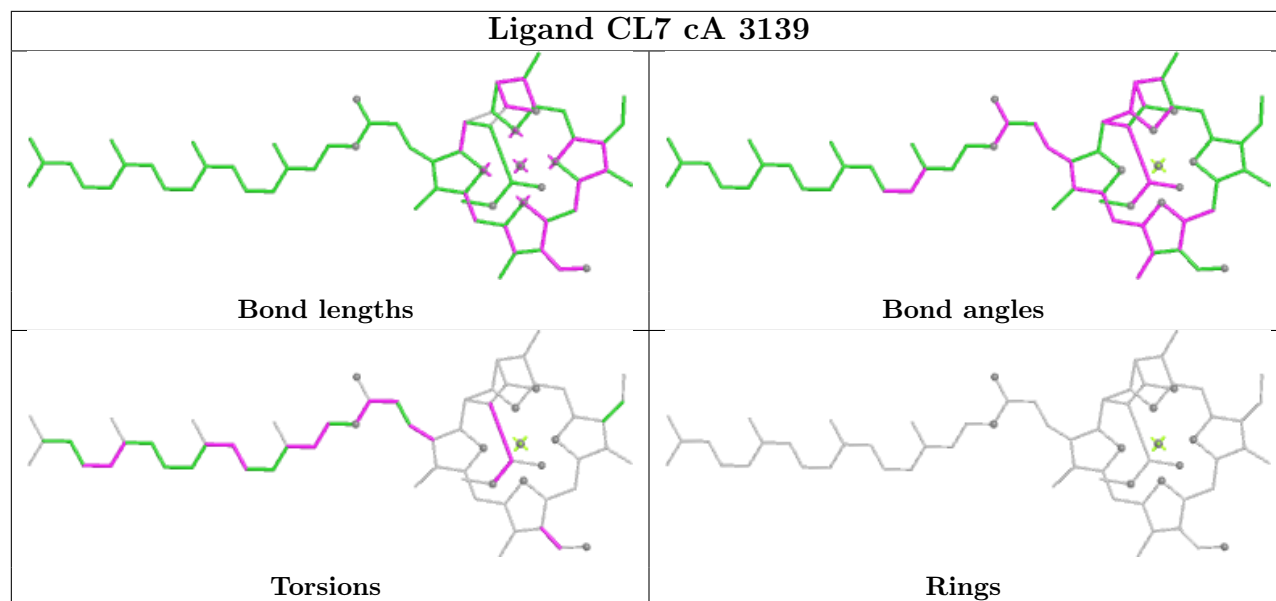
Rings



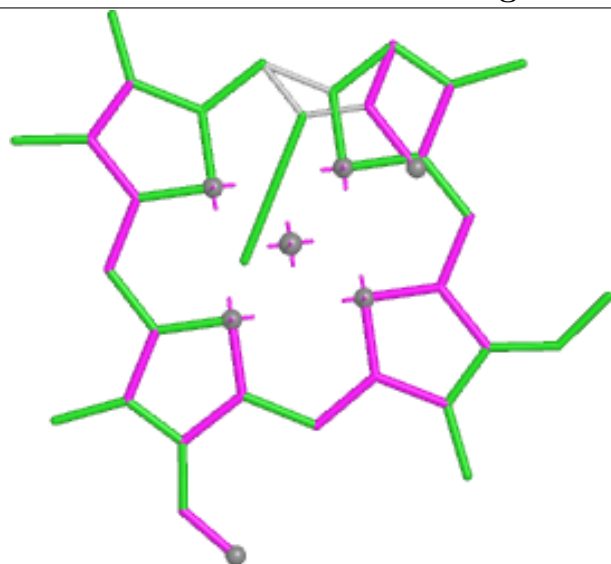




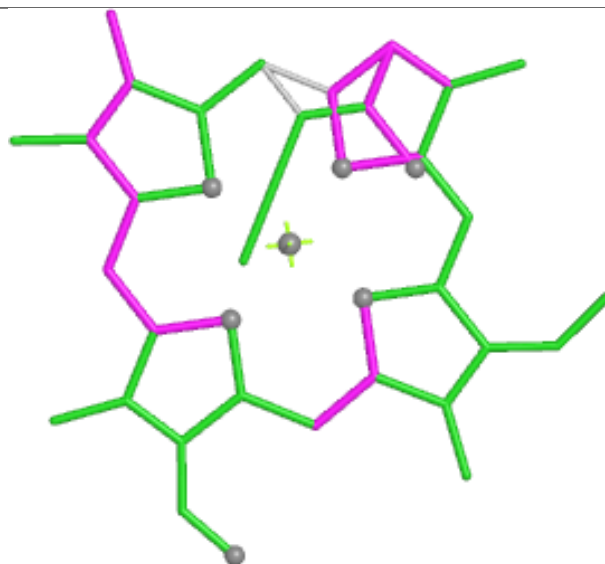




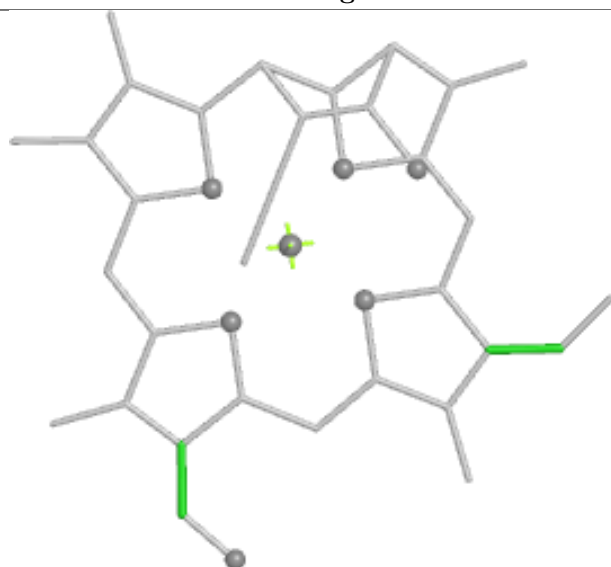
Ligand CL7 bA 3118



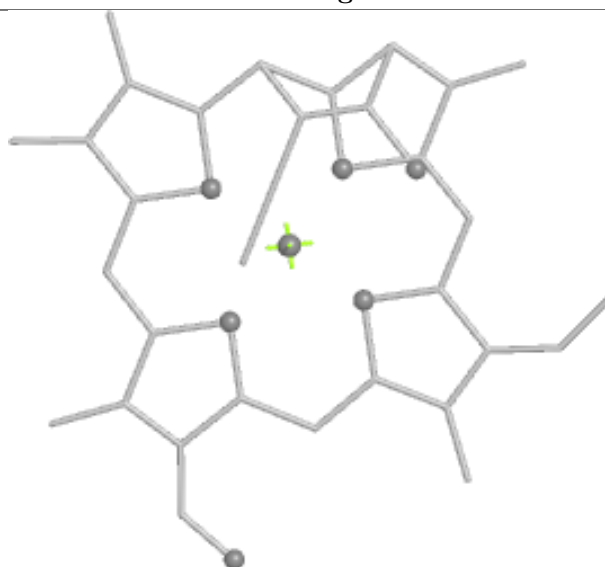
Bond lengths



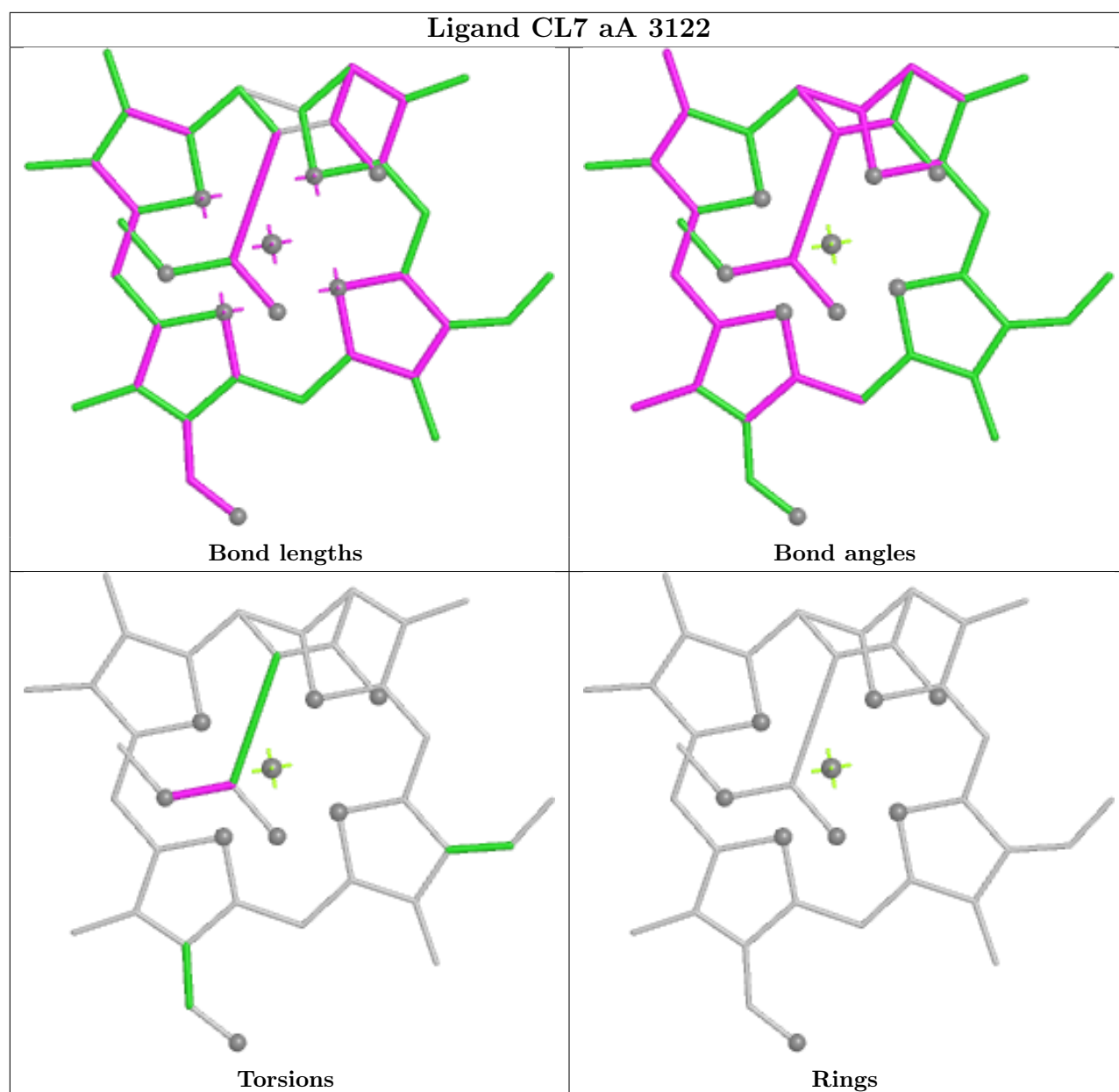
Bond angles

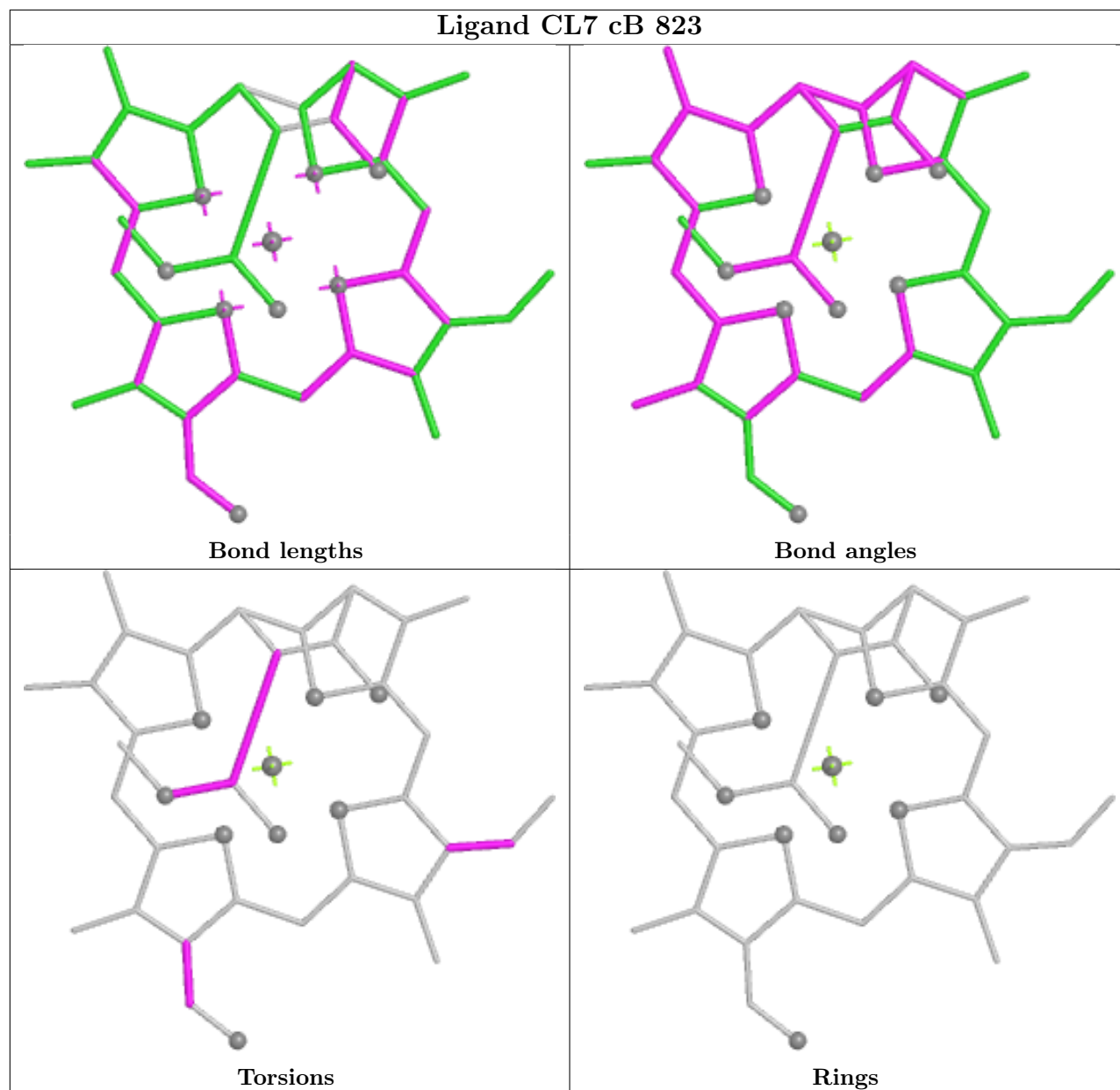


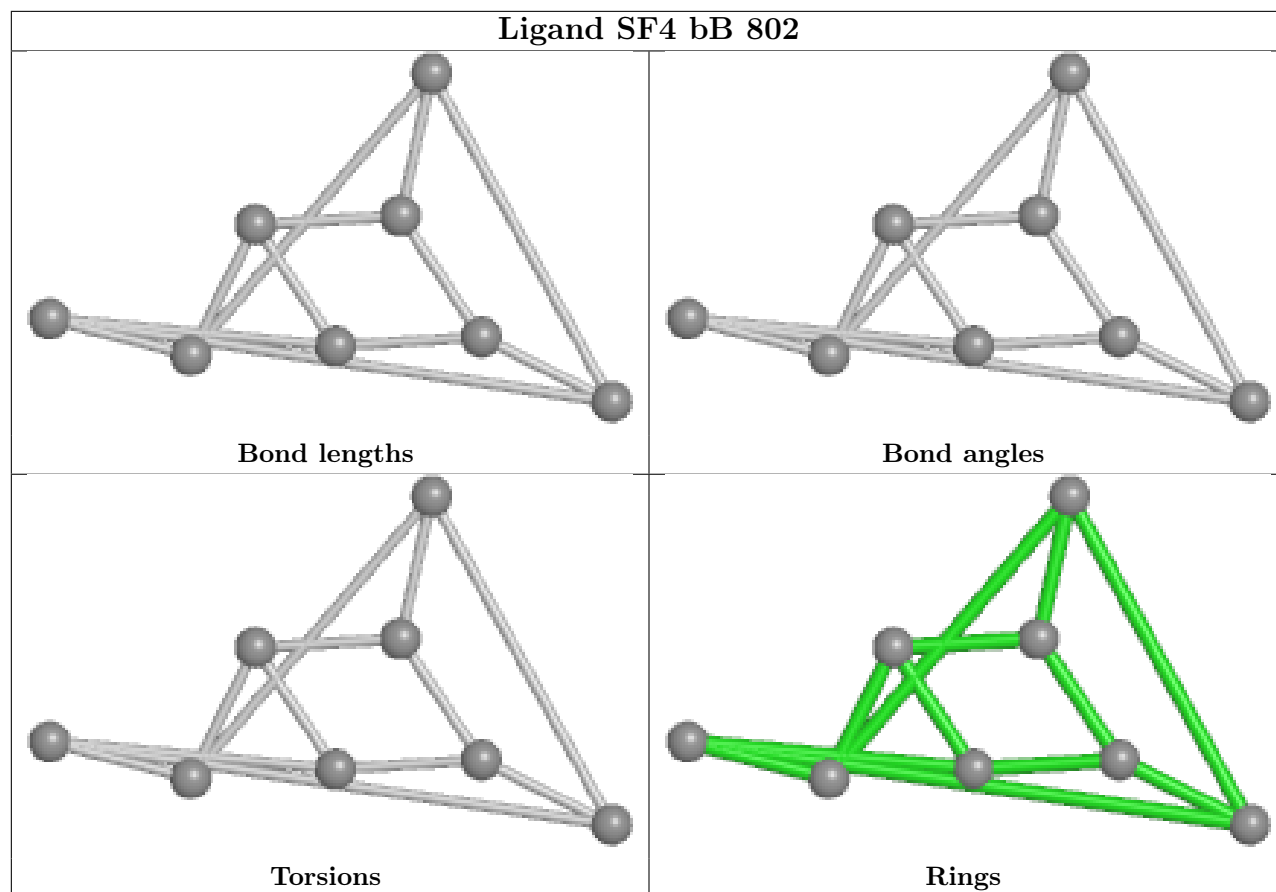
Torsions

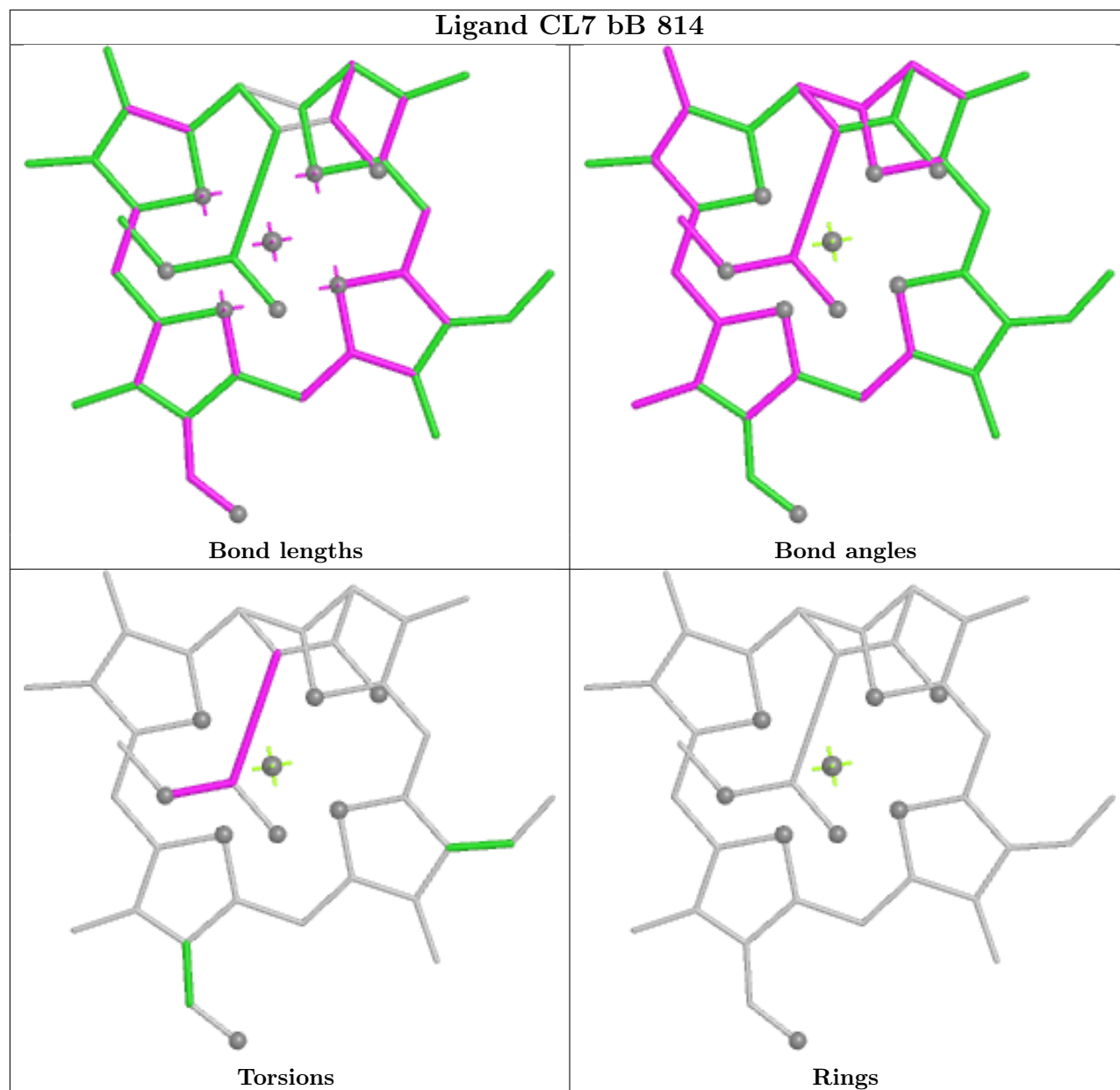


Rings

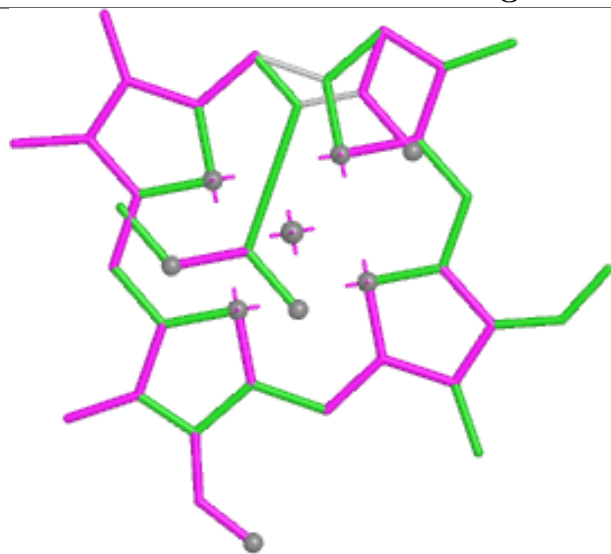




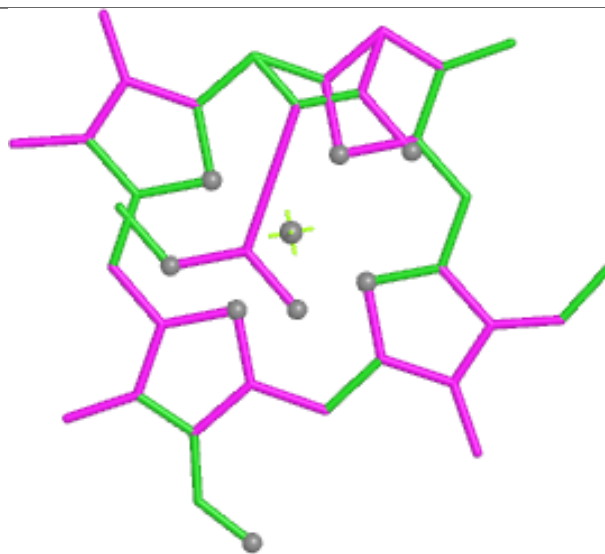




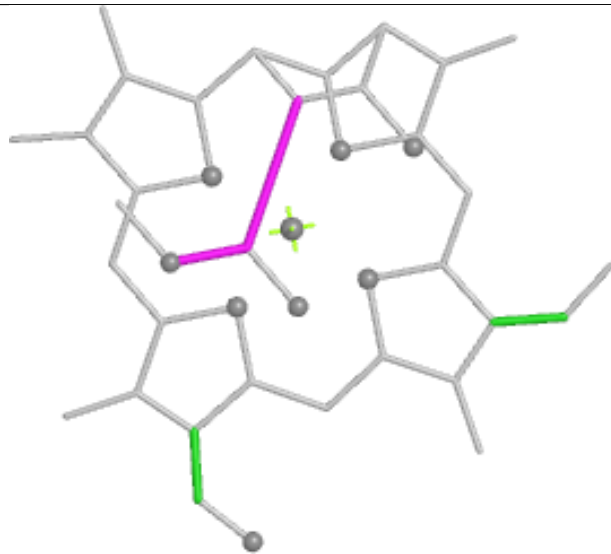
Ligand CL7 aA 3130



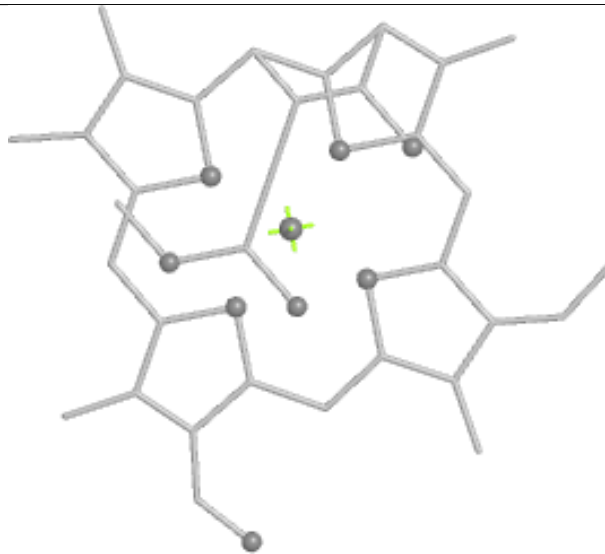
Bond lengths



Bond angles

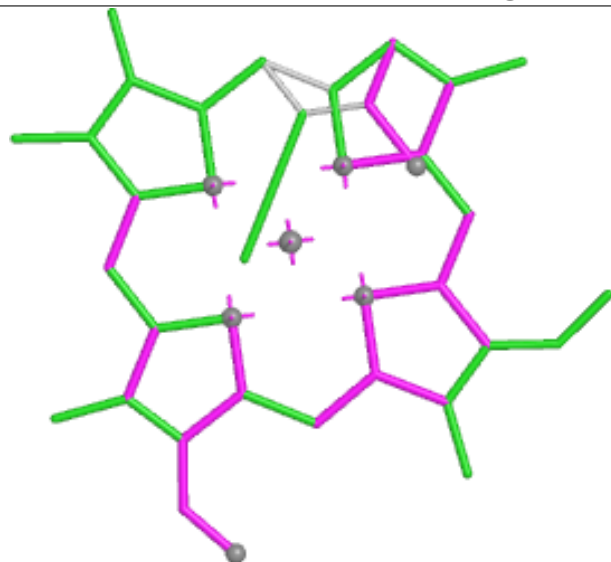


Torsions

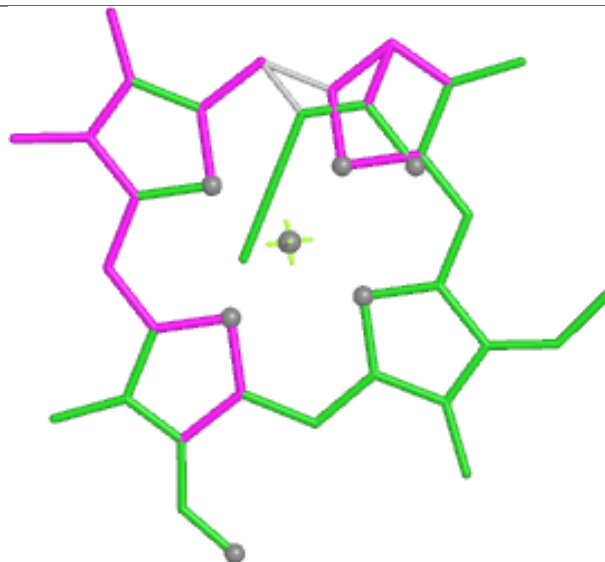


Rings

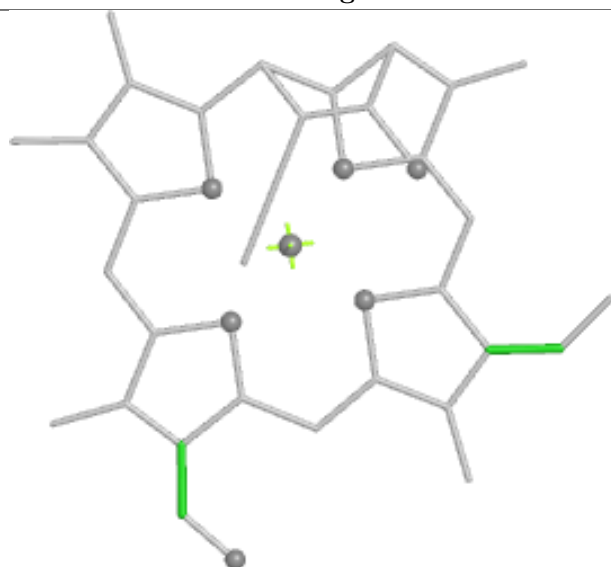
Ligand CL7 aB 3024



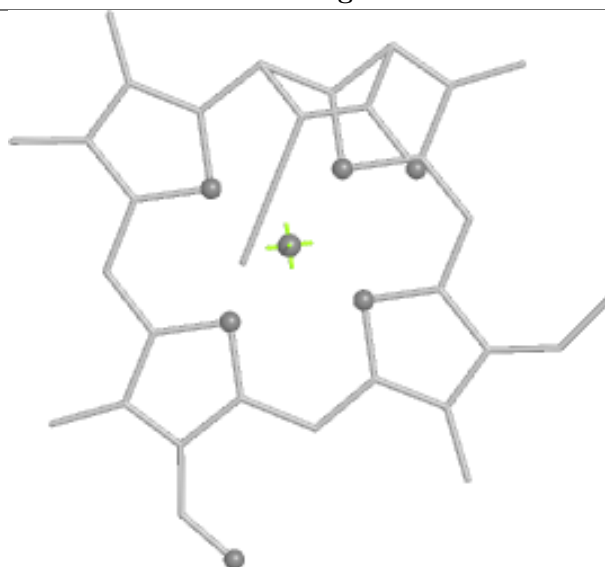
Bond lengths



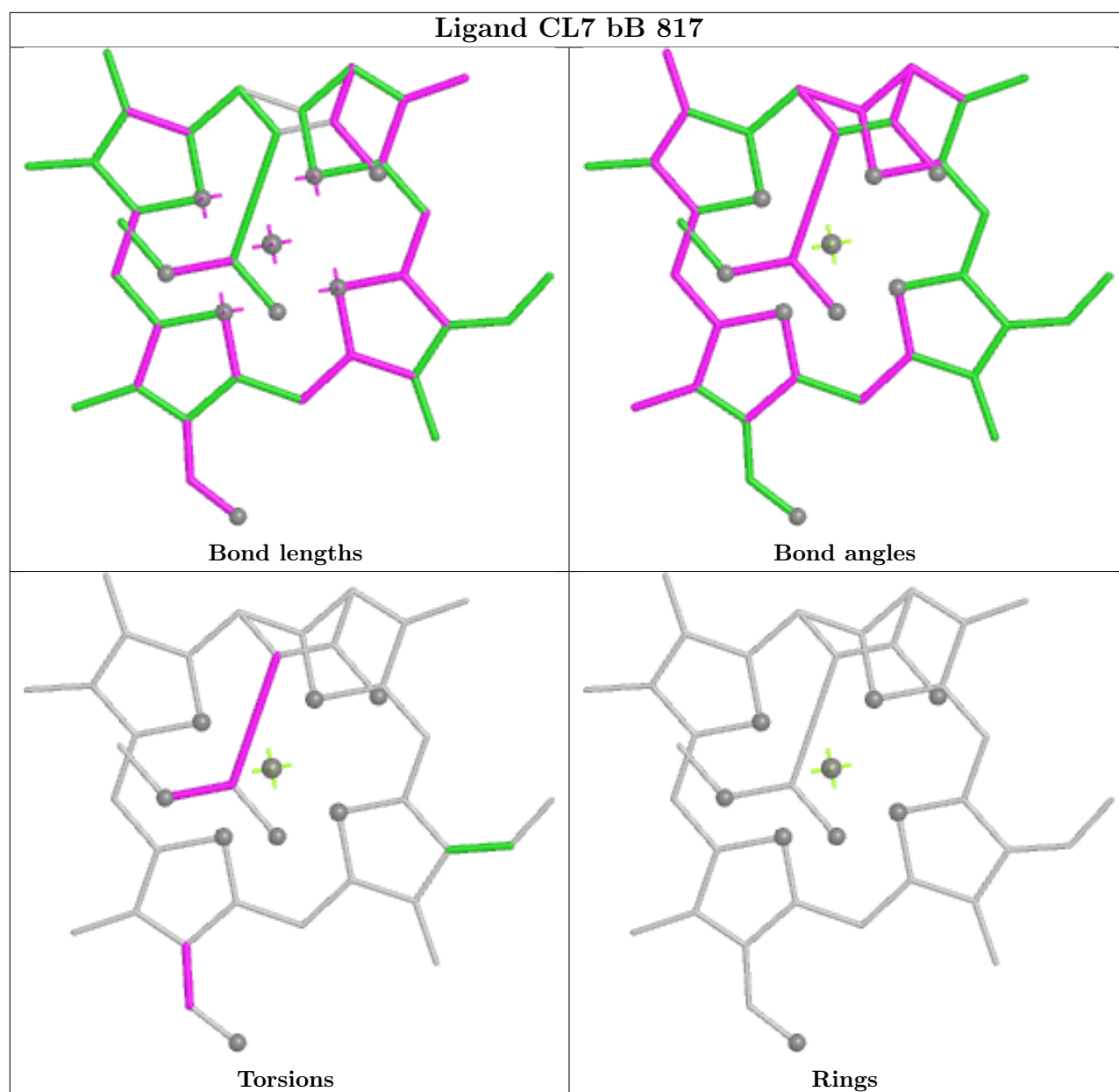
Bond angles

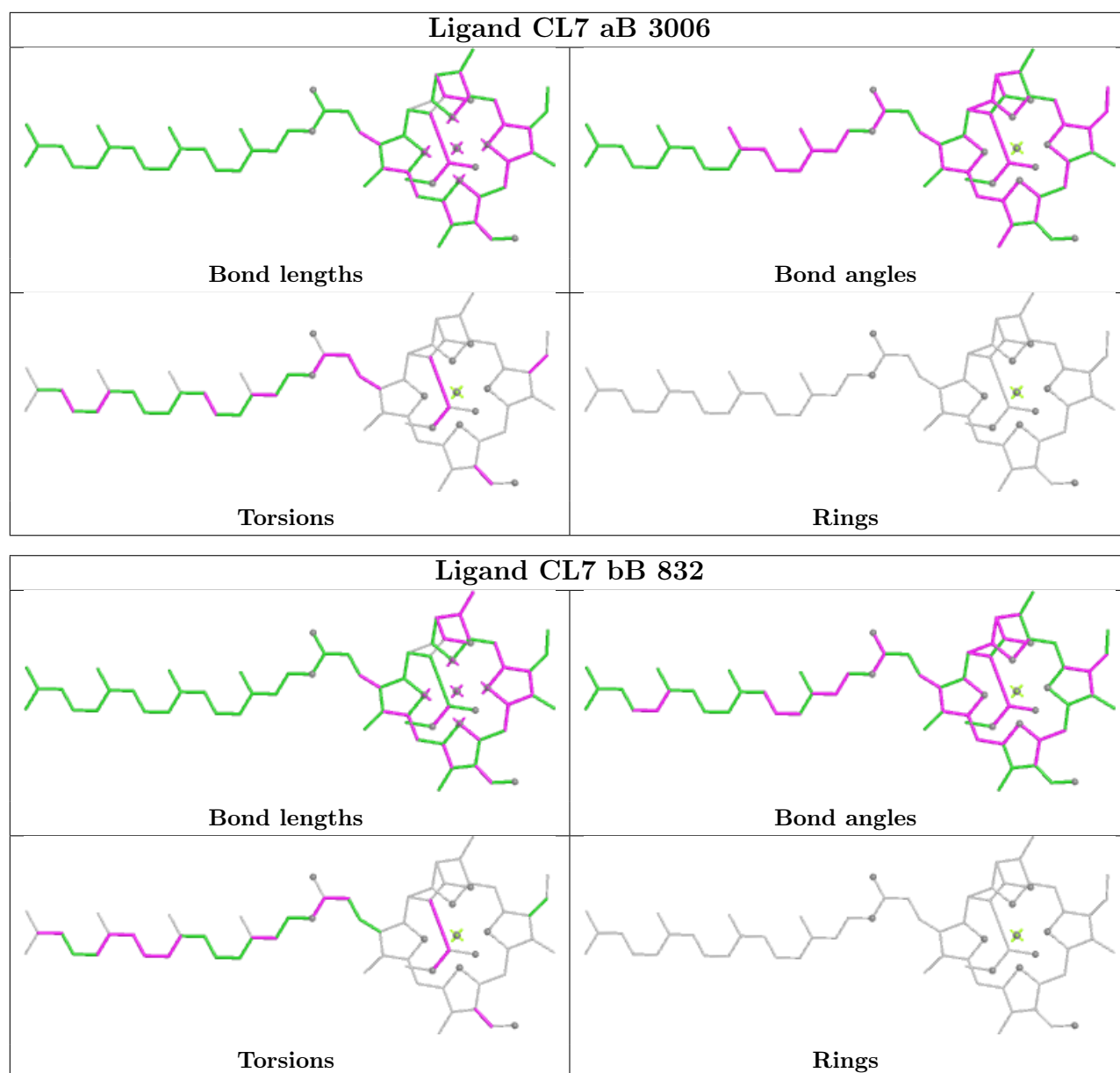


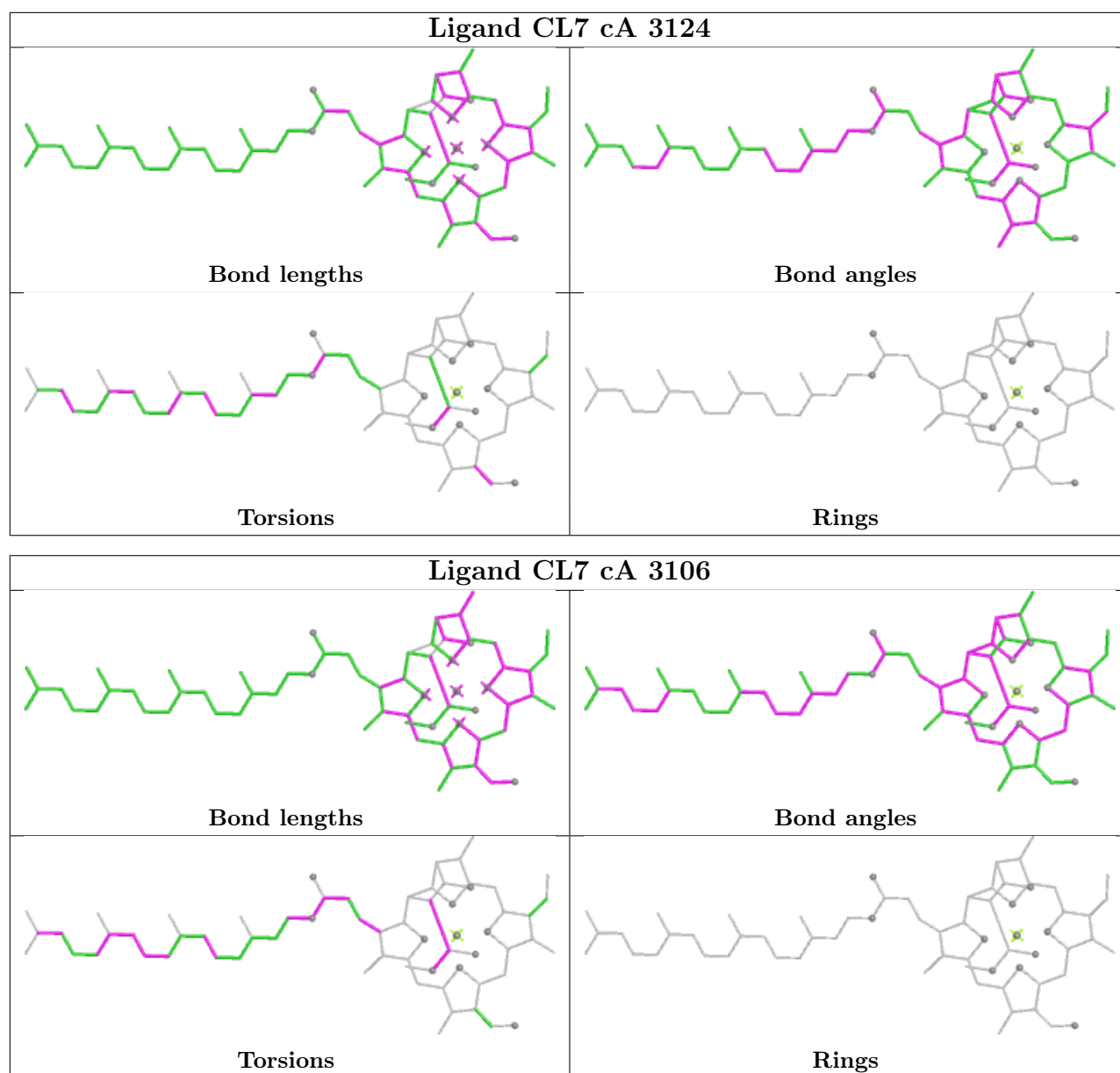
Torsions

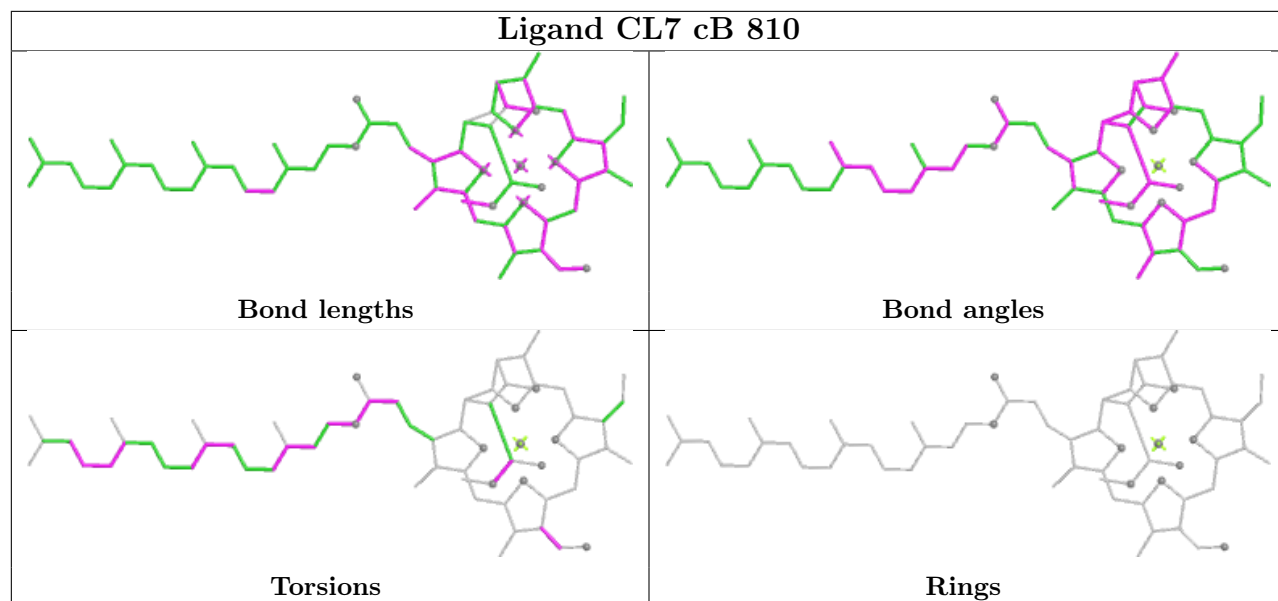


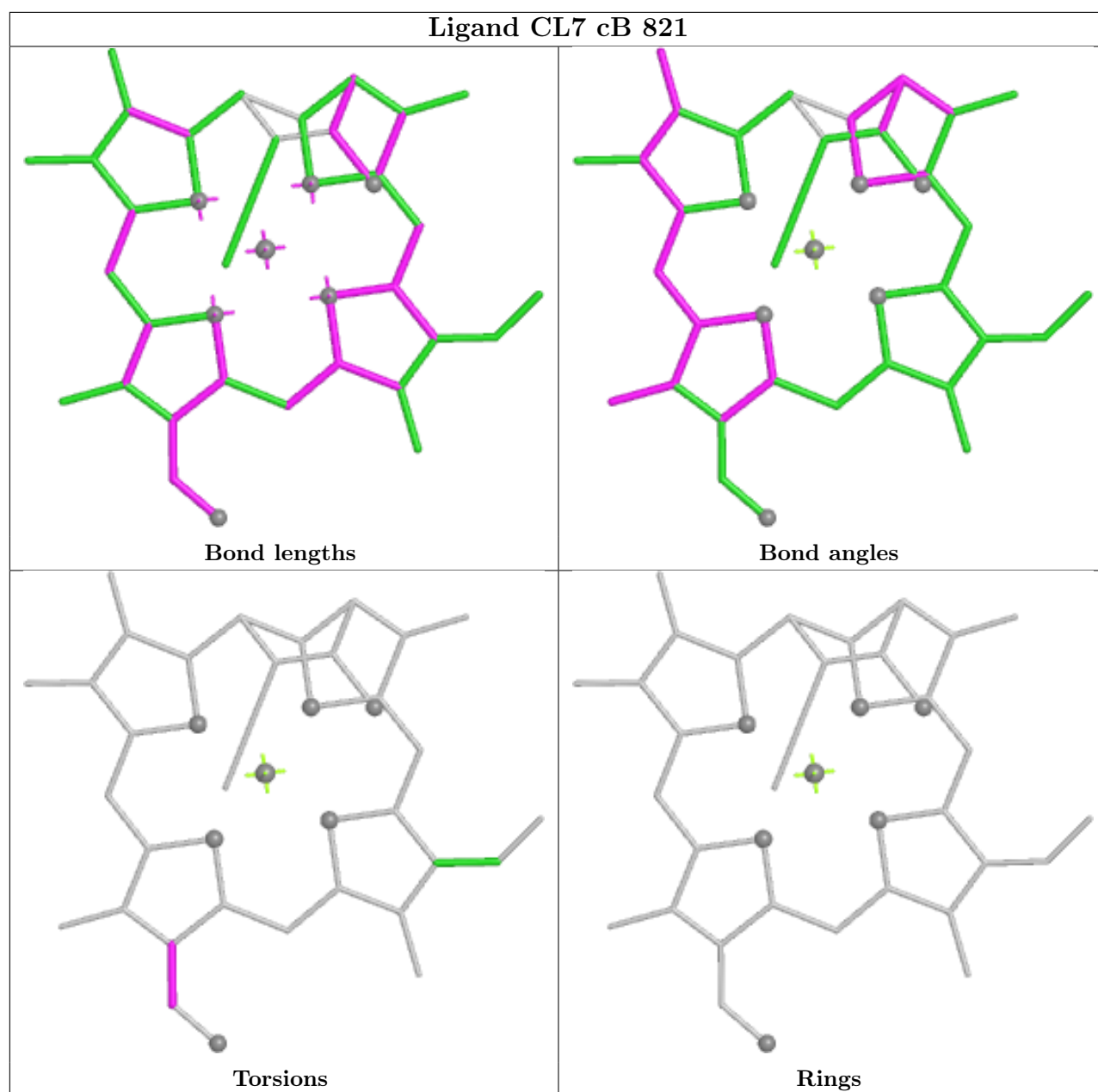
Rings



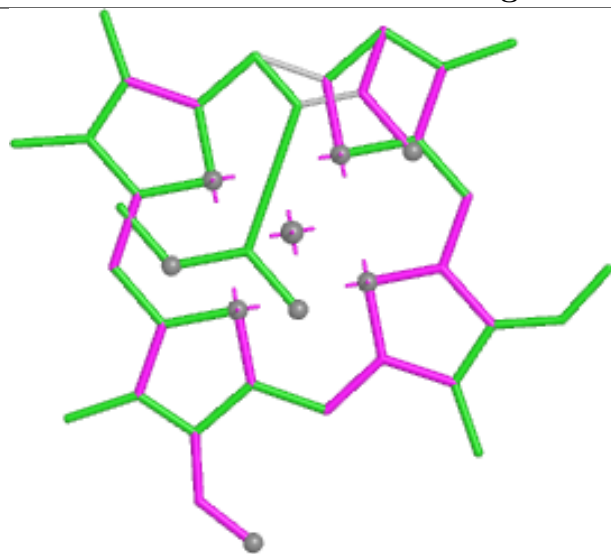




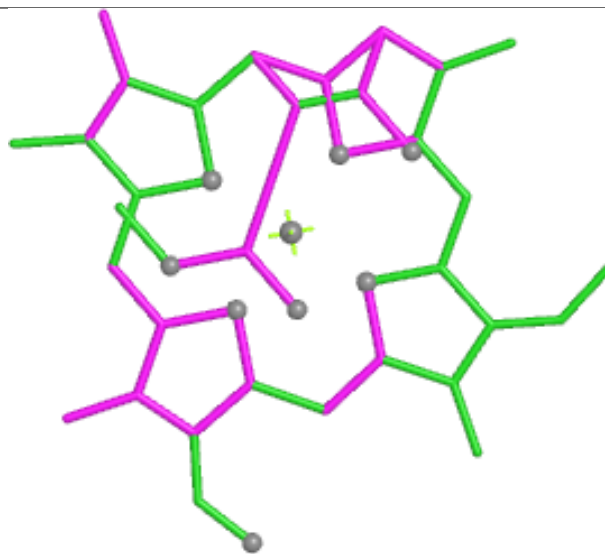




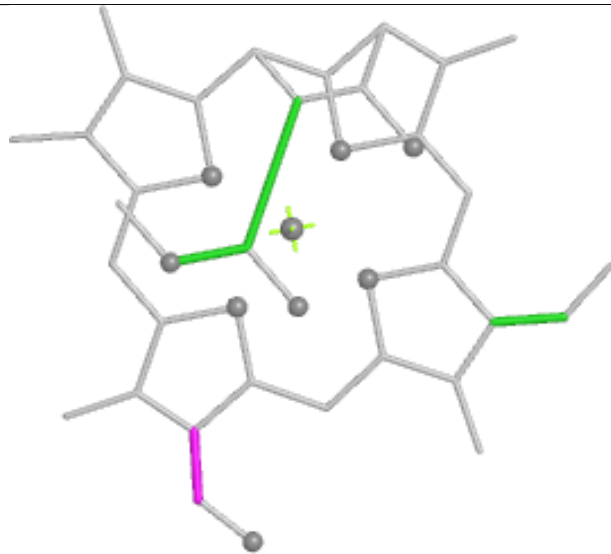
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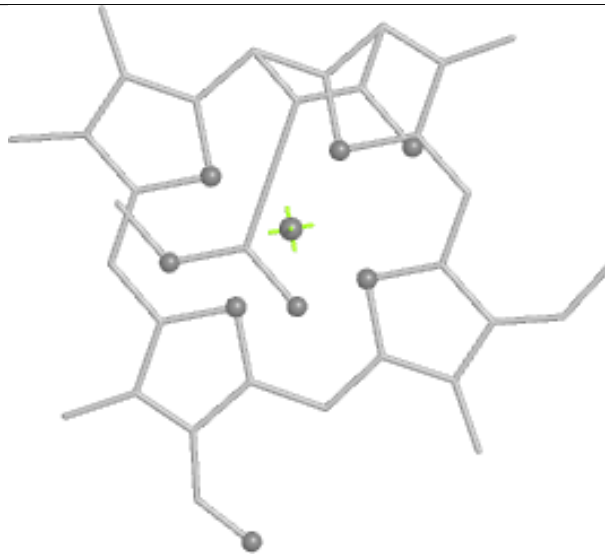
Bond lengths



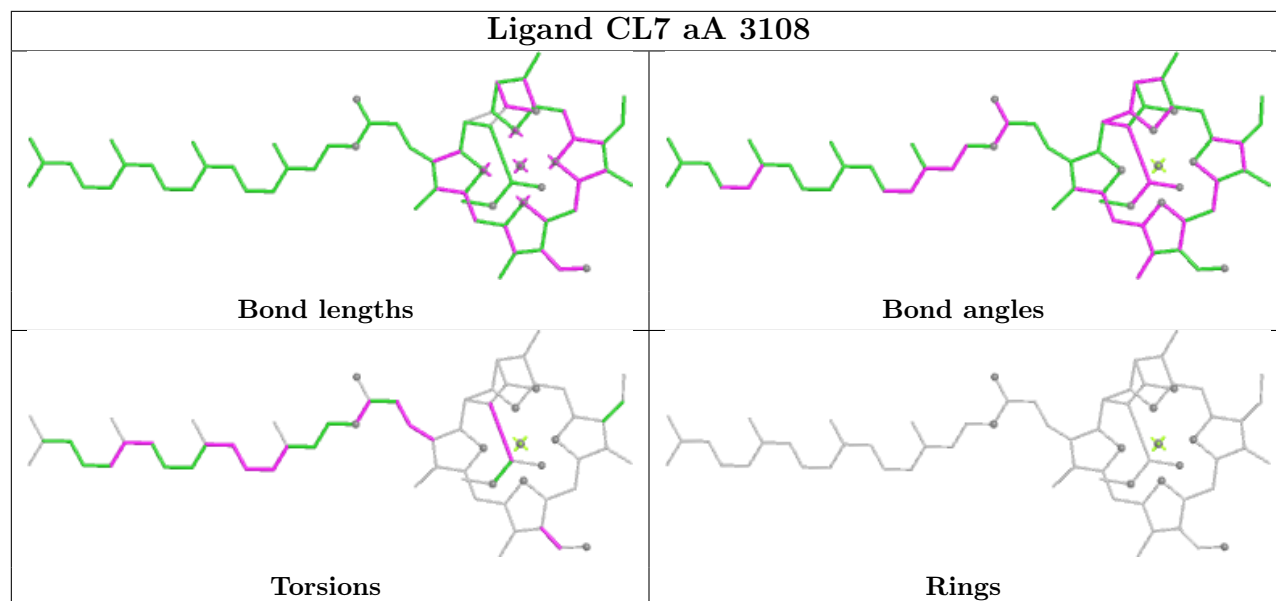
Bond angles

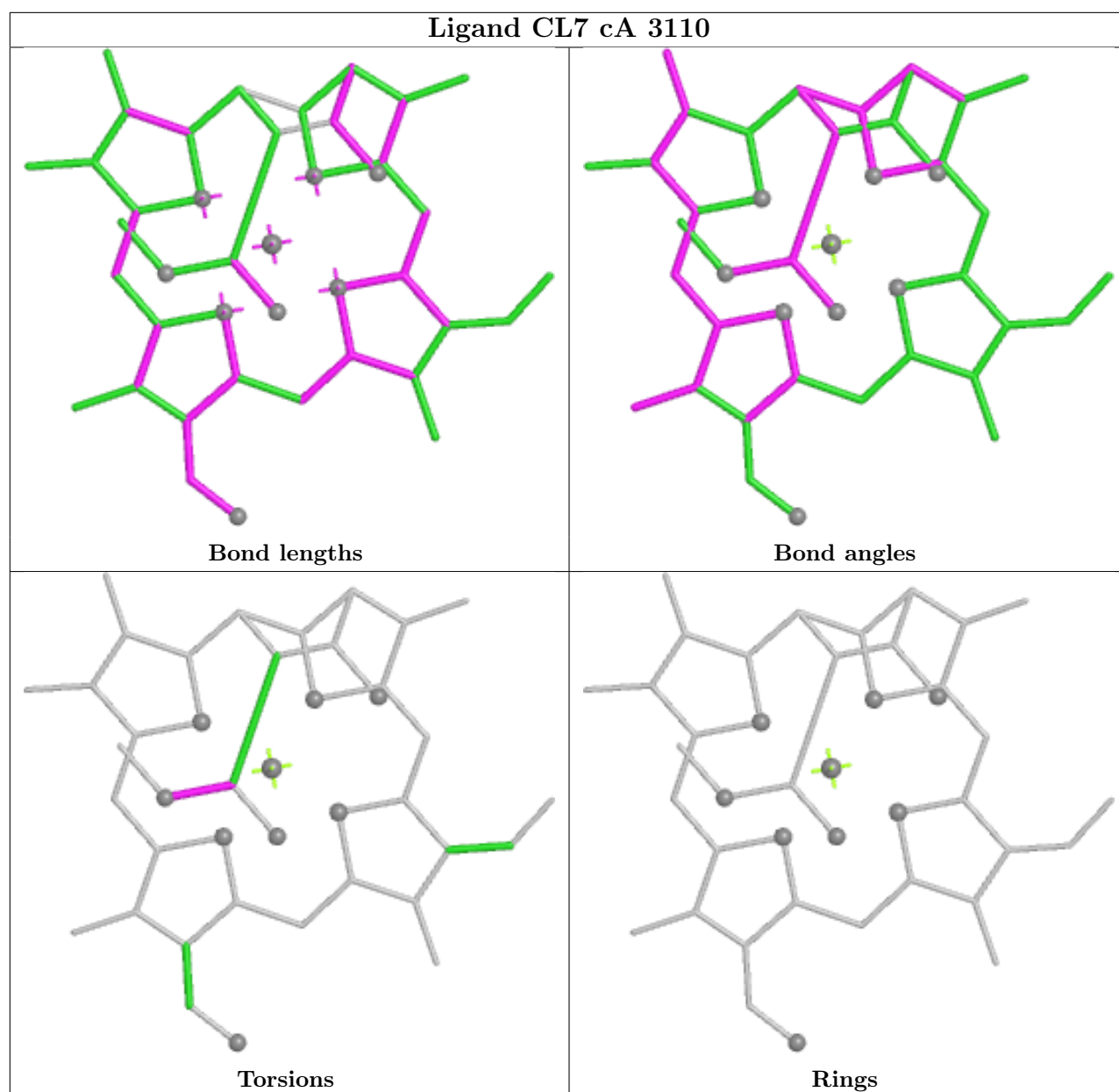


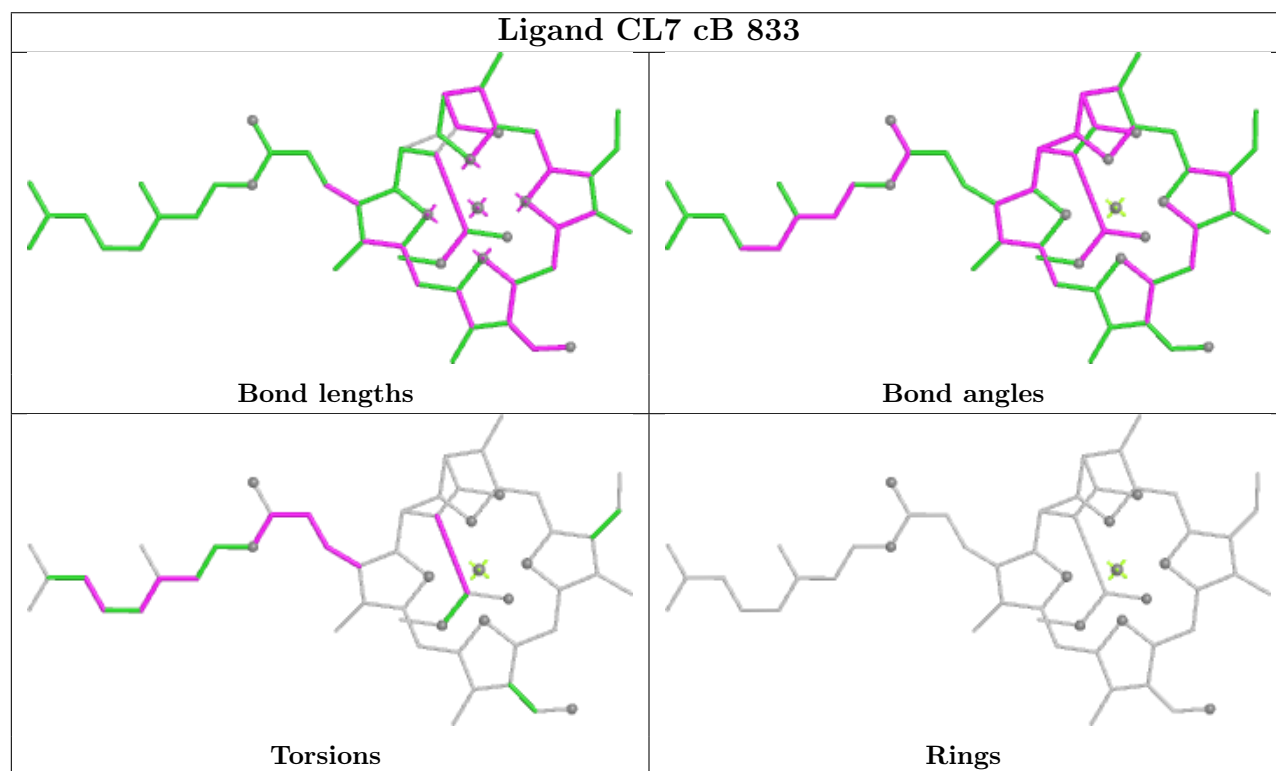
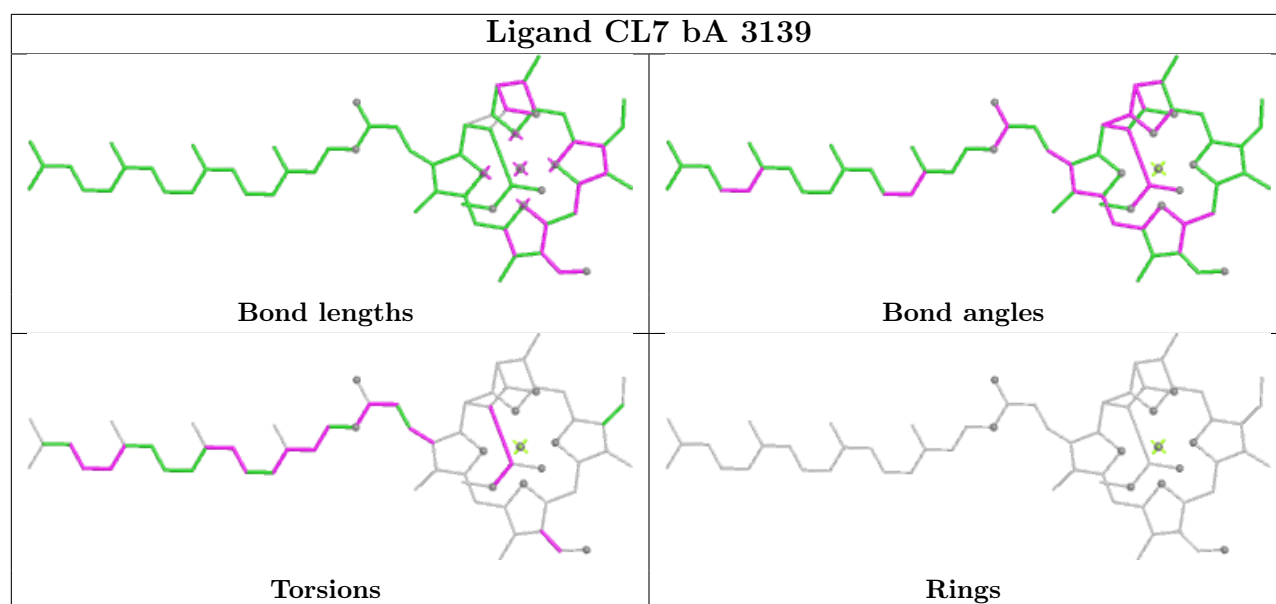
Torsions

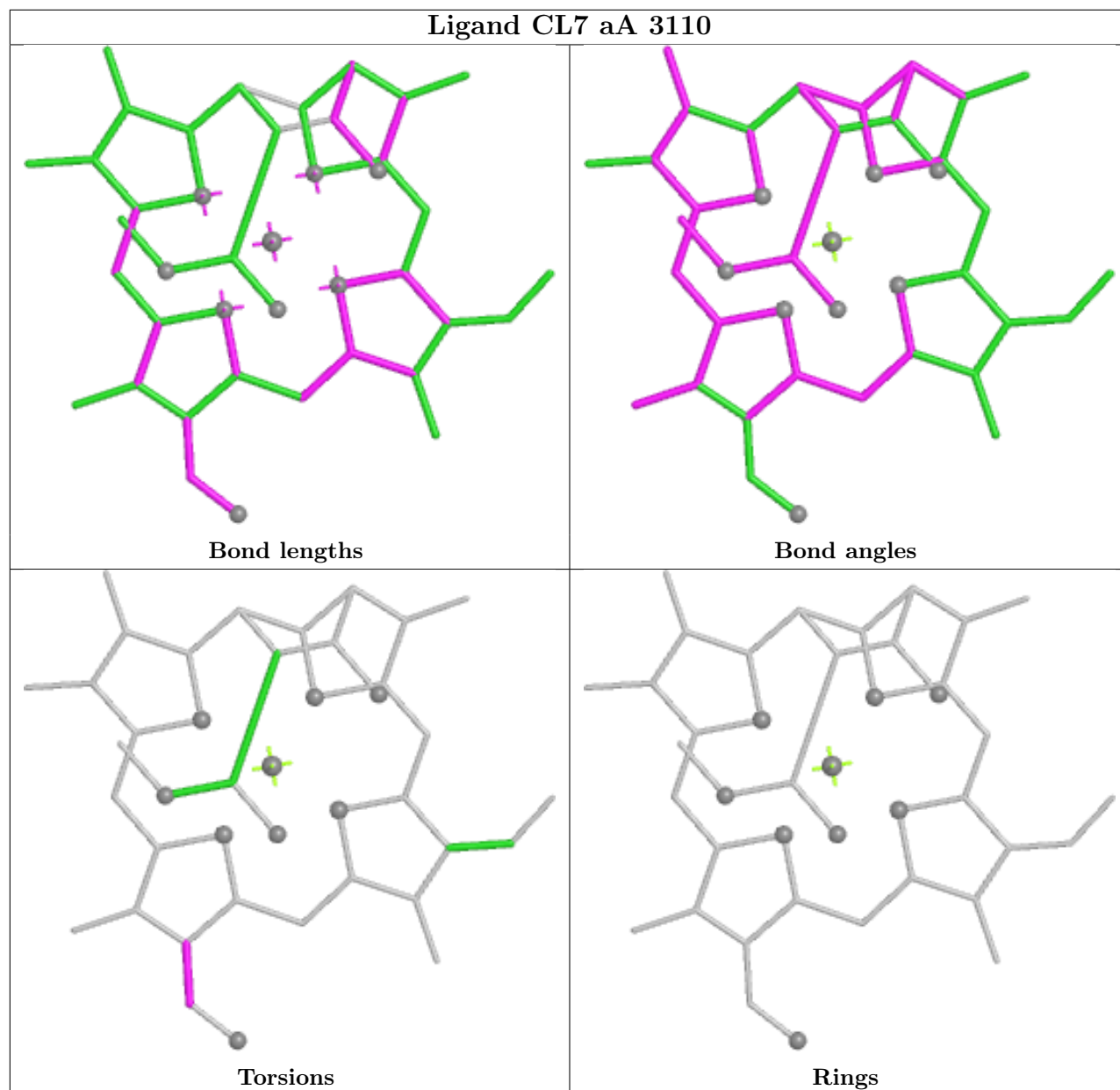


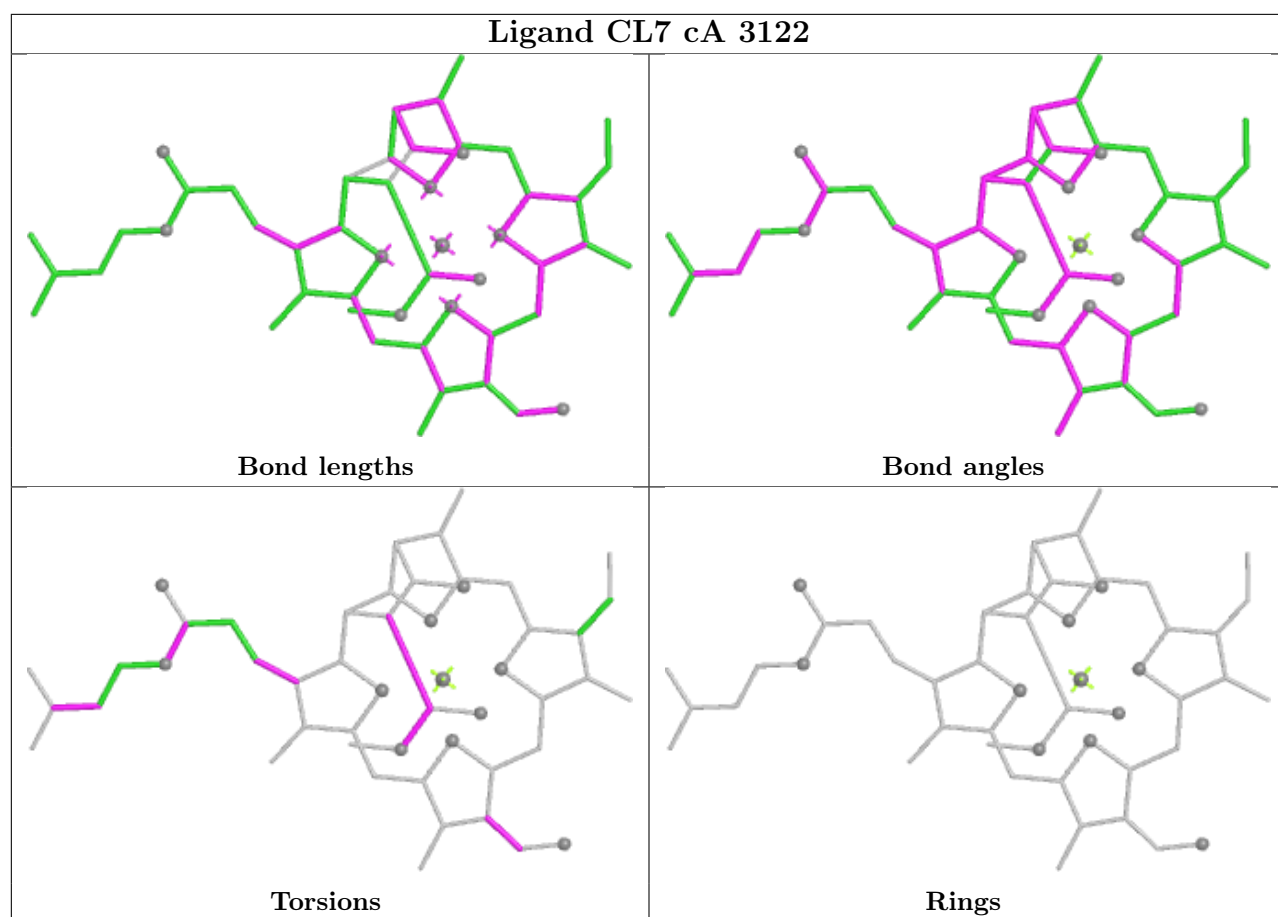
Rings



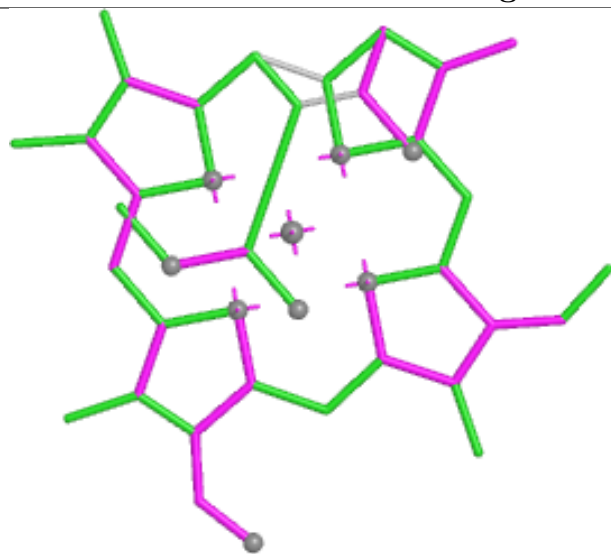




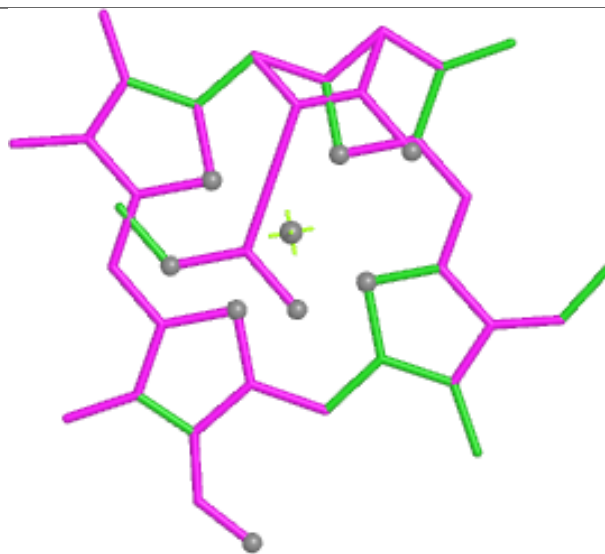




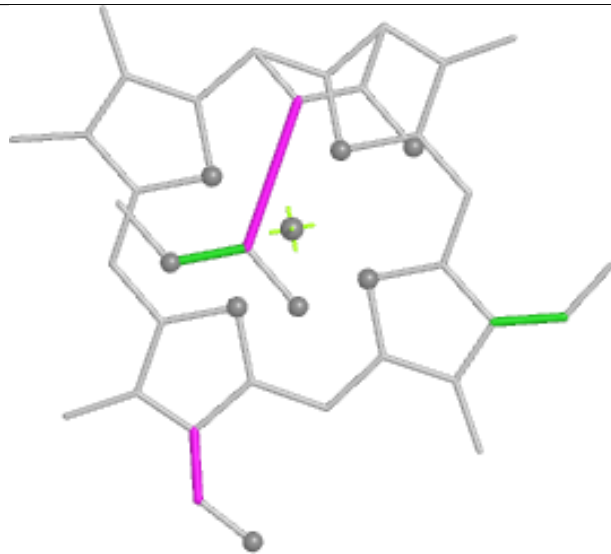
Ligand CL7 bA 3105



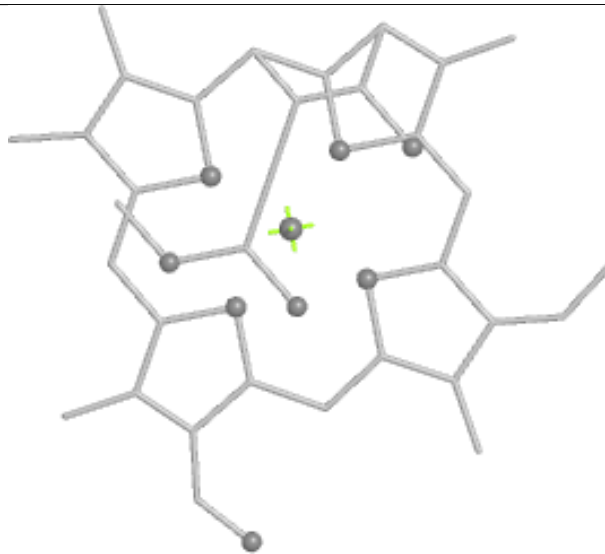
Bond lengths



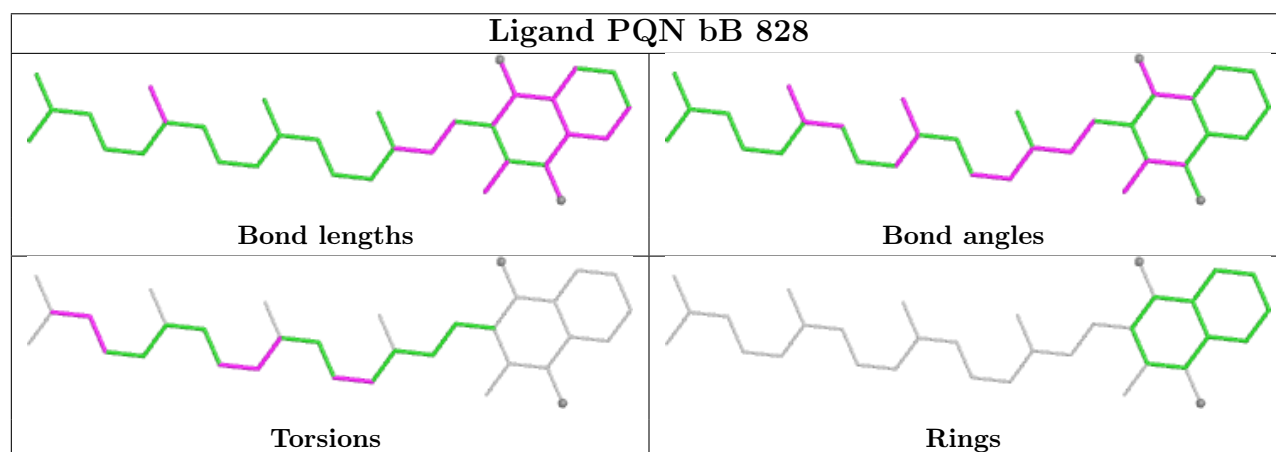
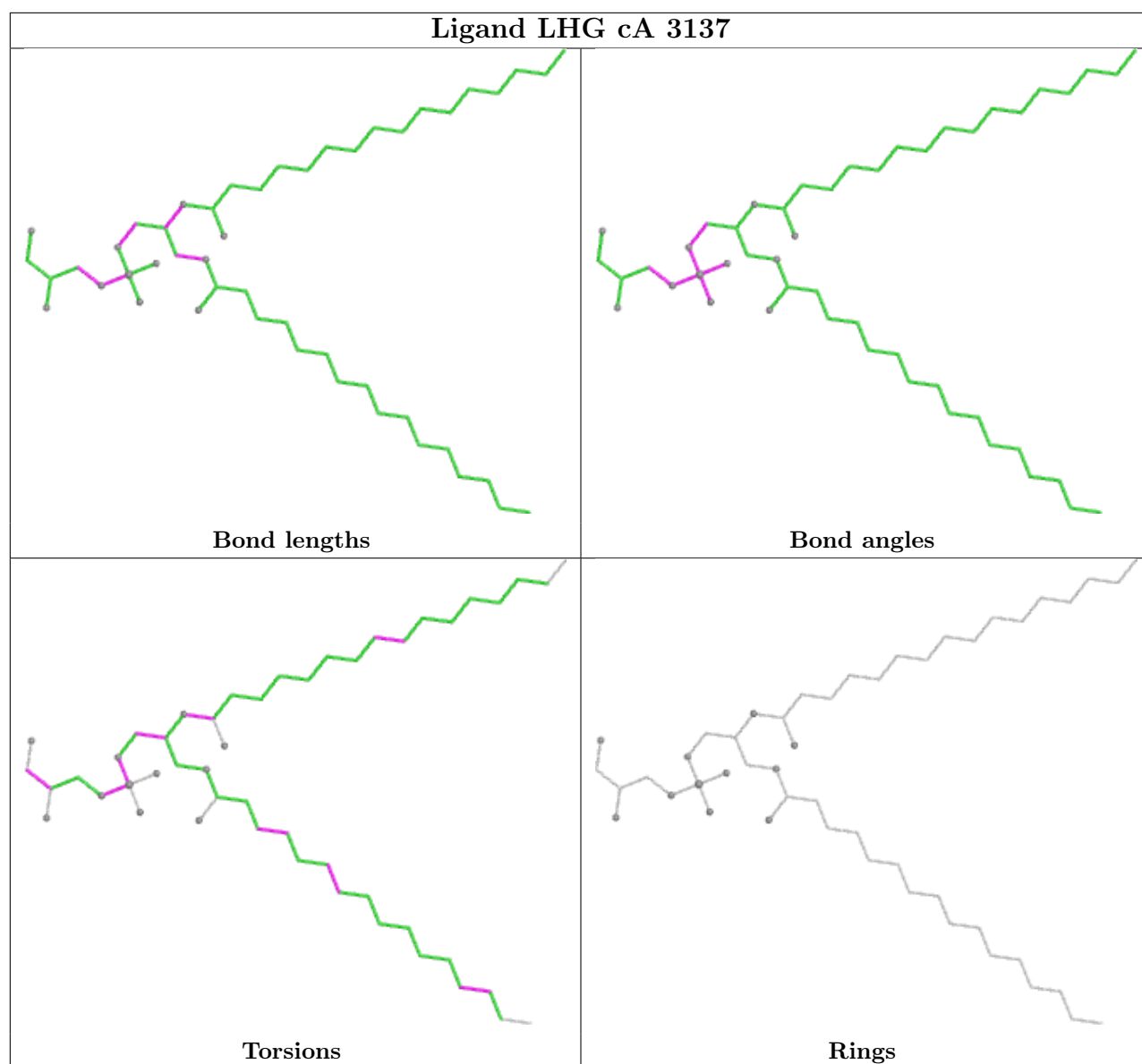
Bond angles

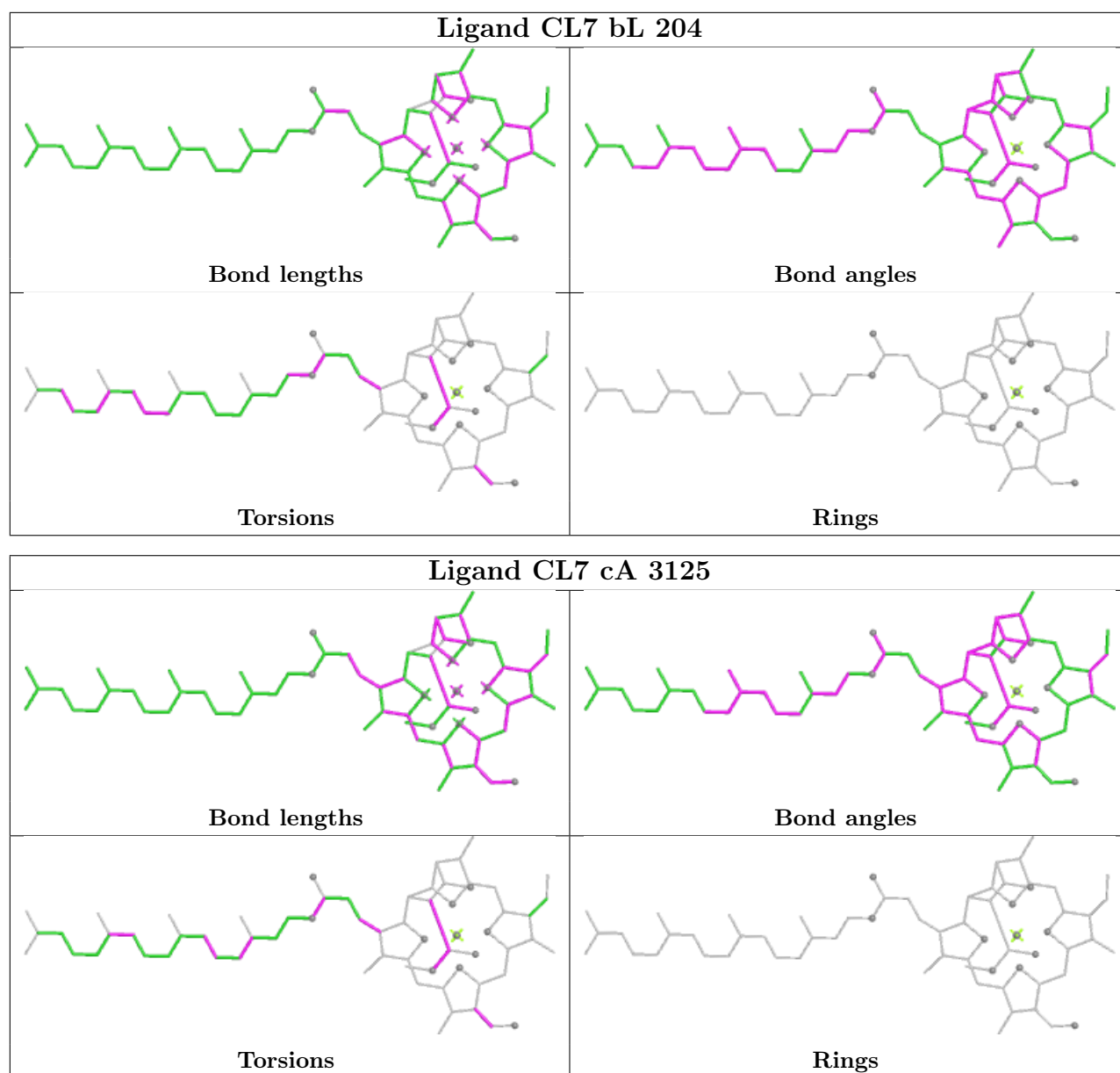


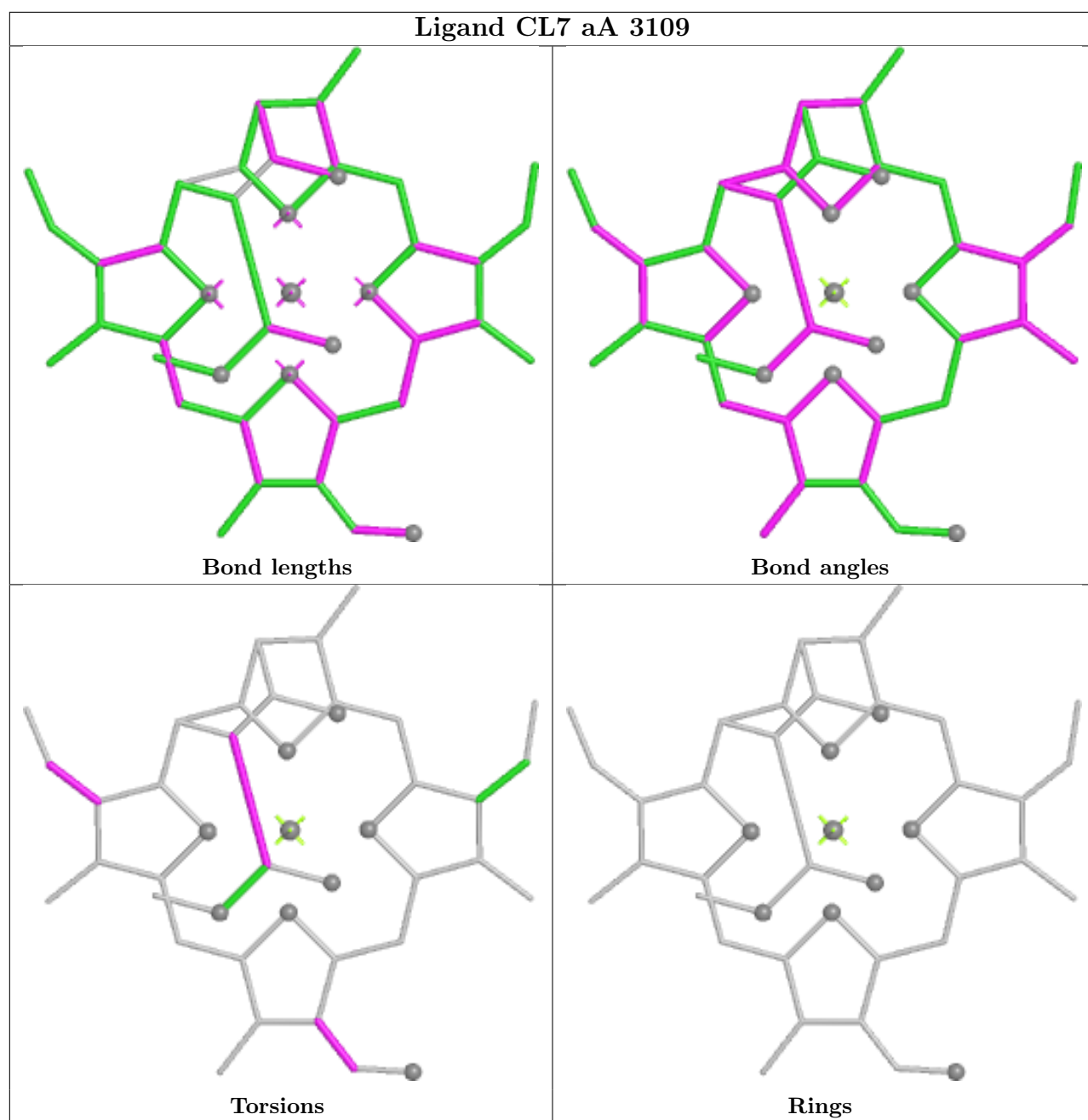
Torsions

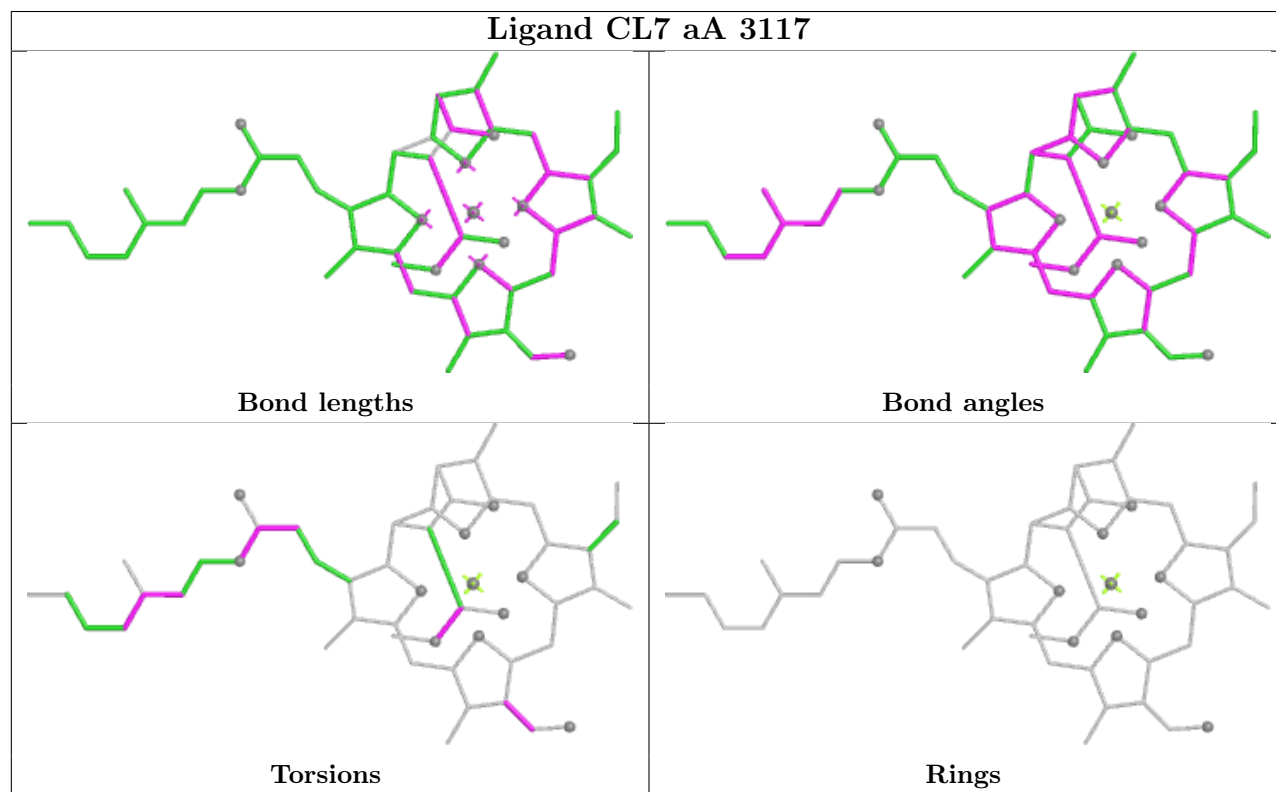
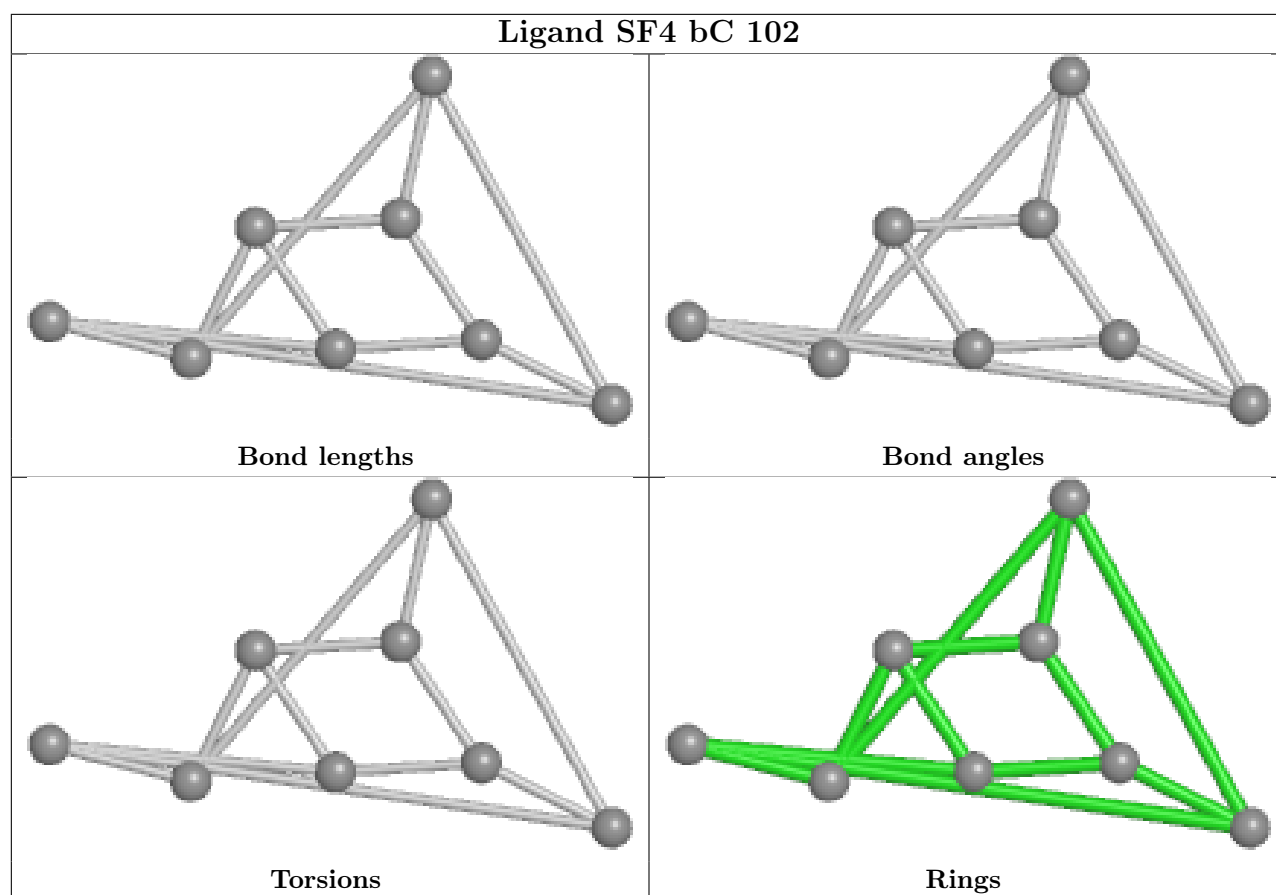


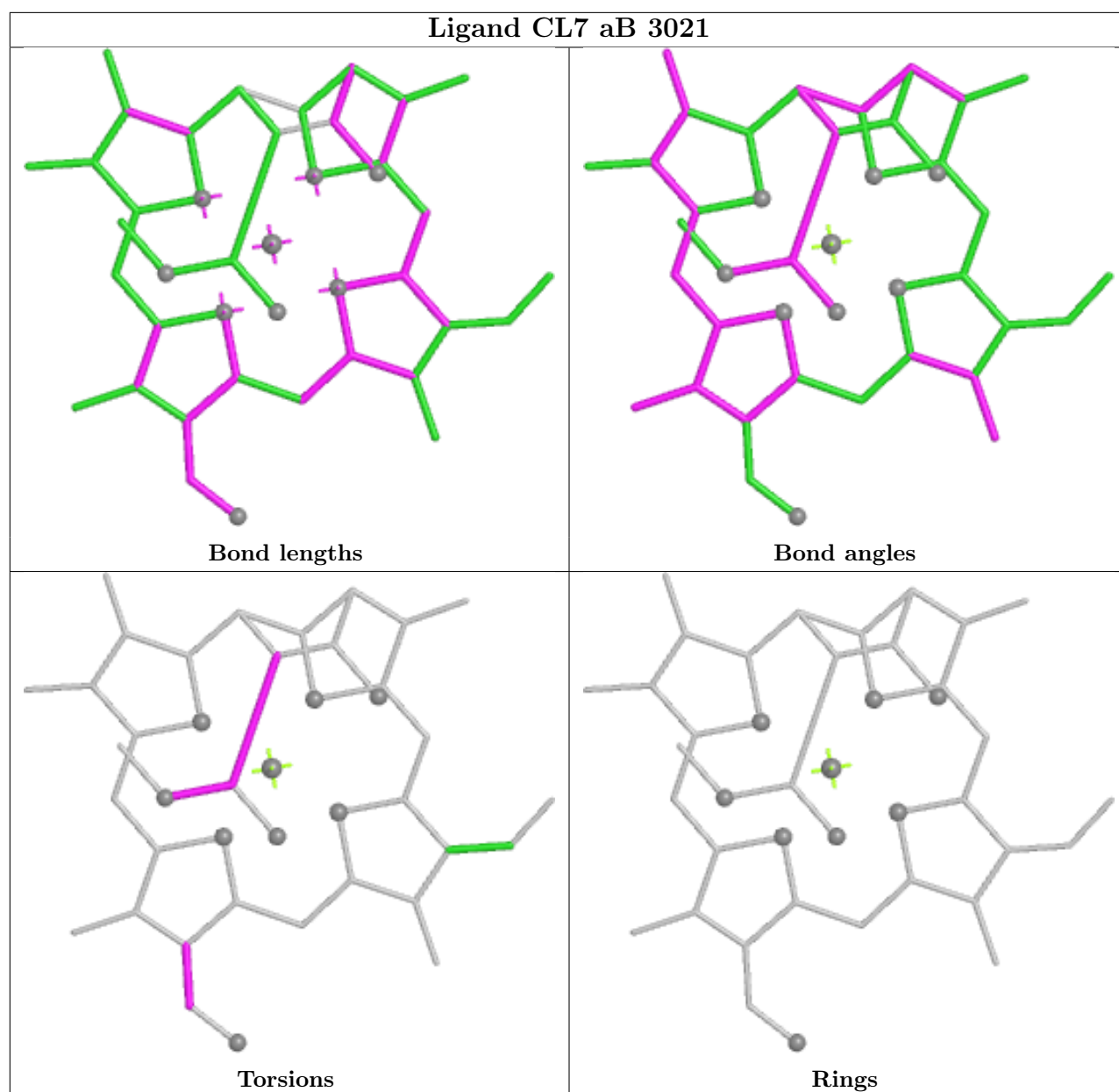
Rings

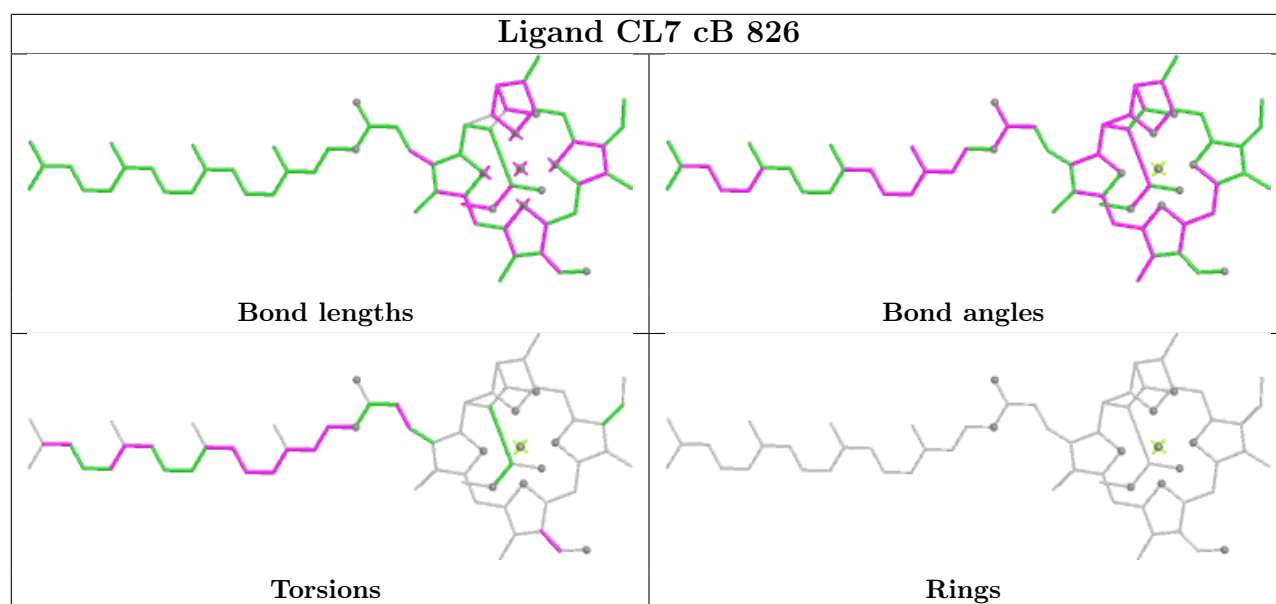


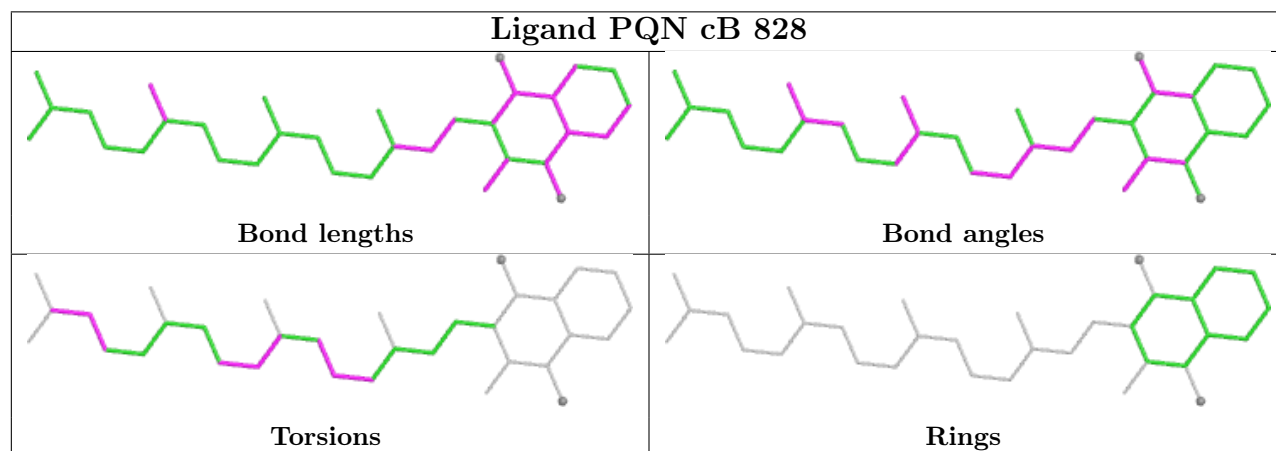
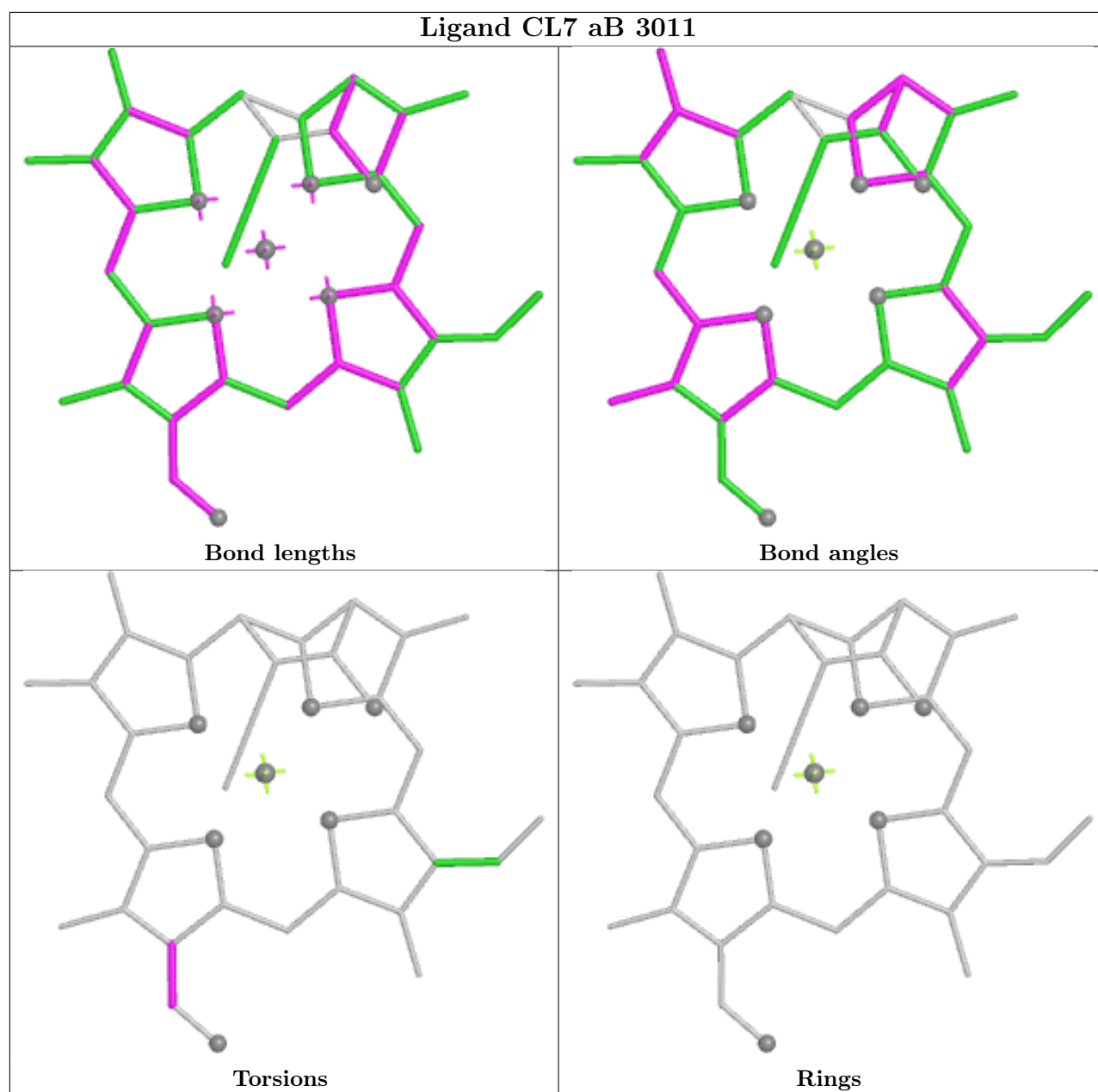


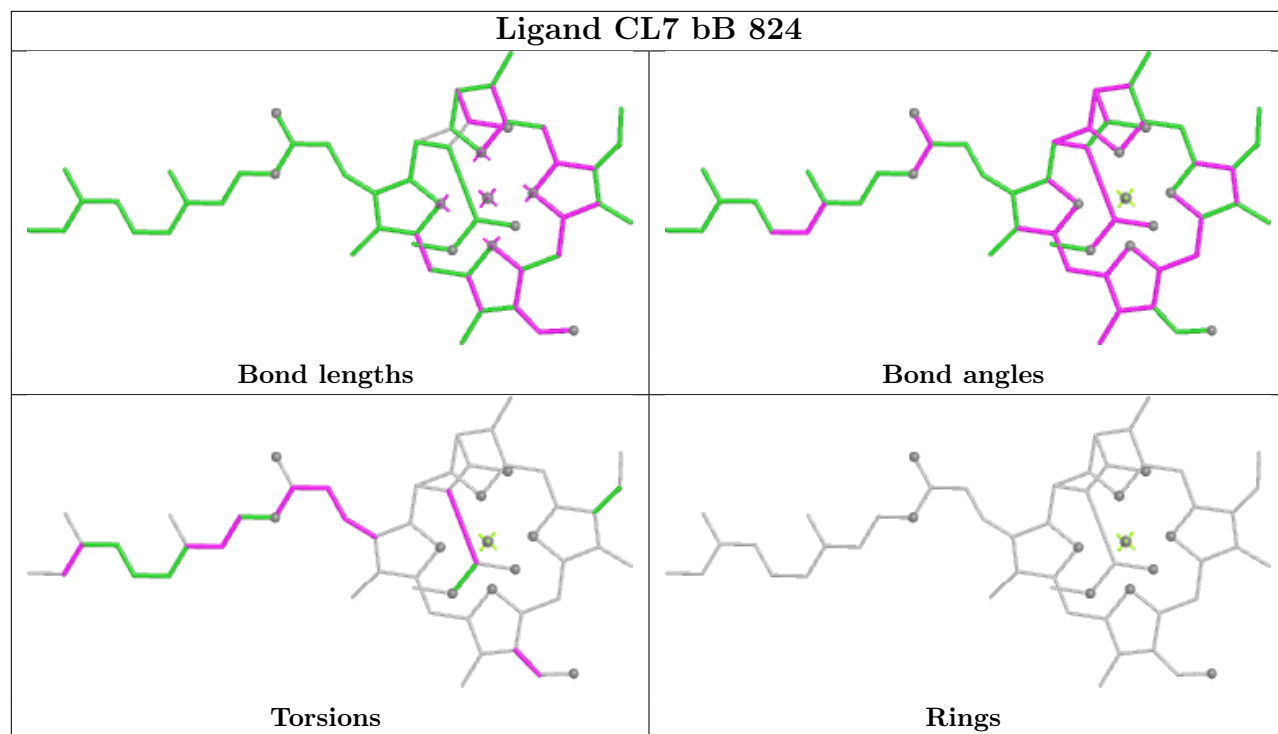




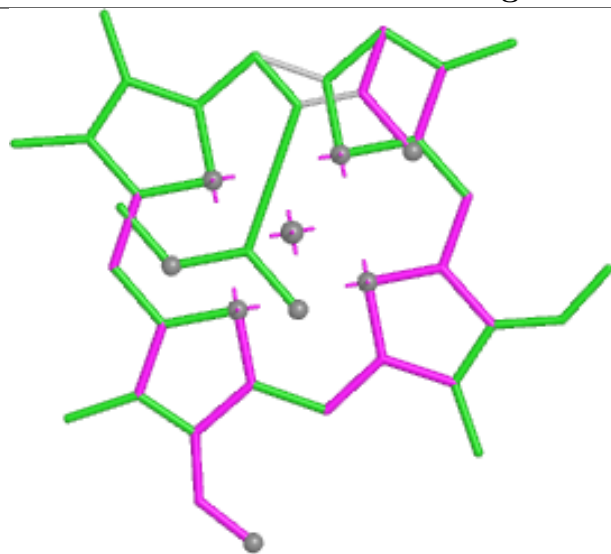




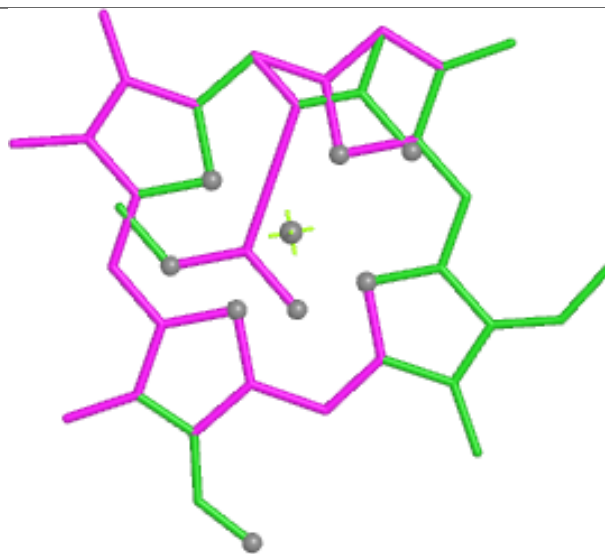




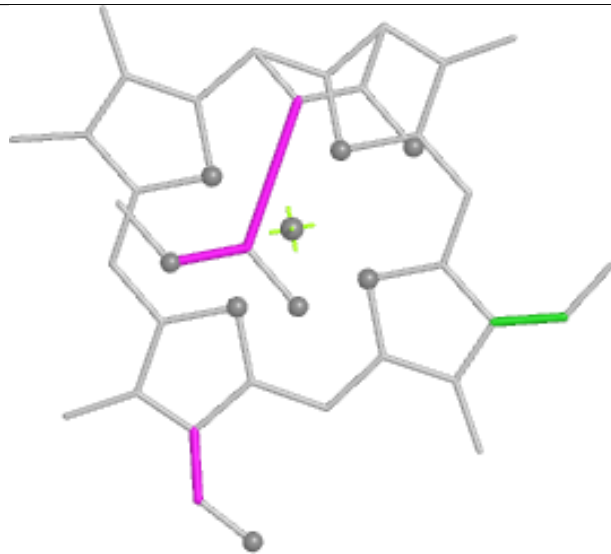
Ligand CL7 cA 3131



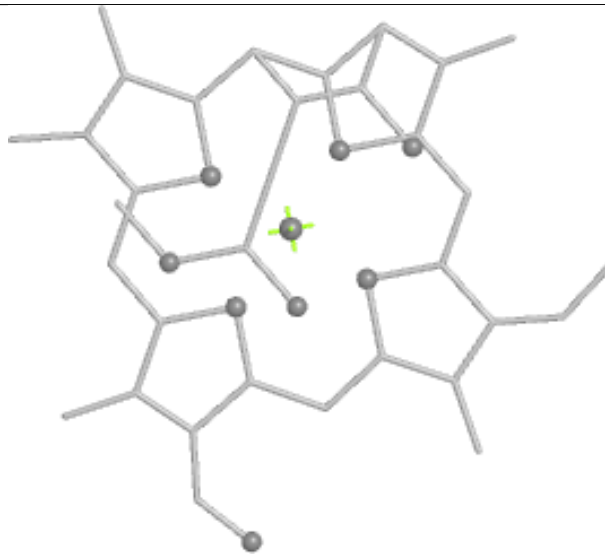
Bond lengths



Bond angles

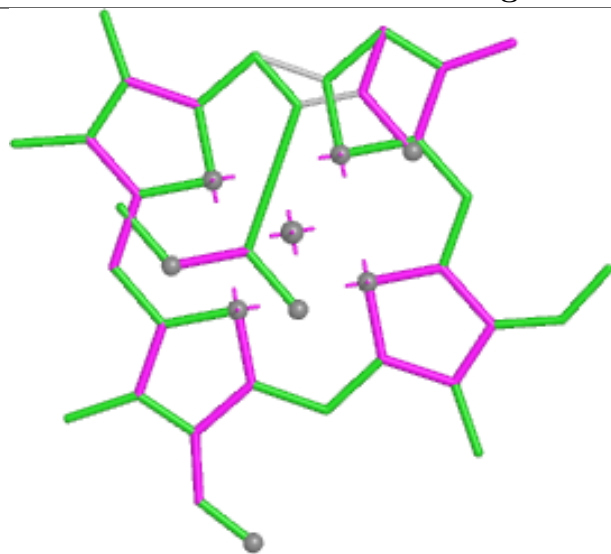


Torsions

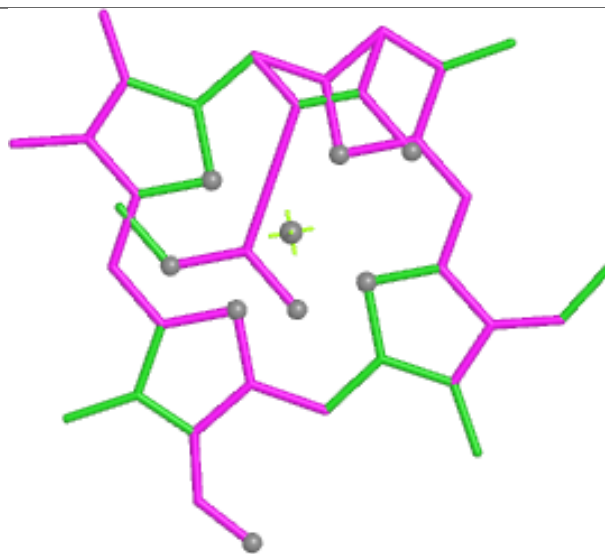


Rings

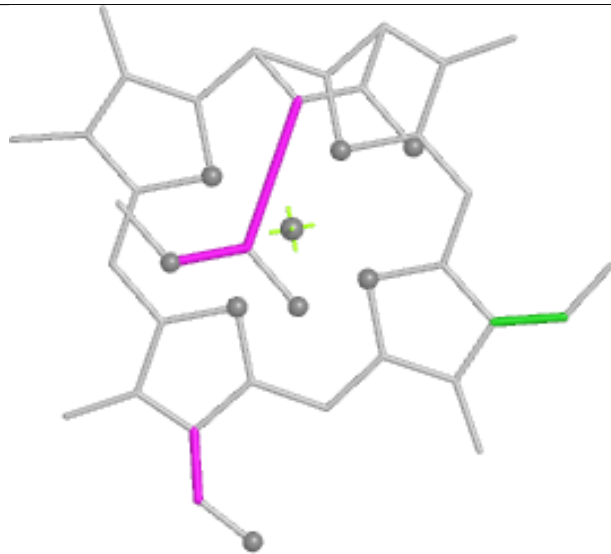
Ligand CL7 aA 3106



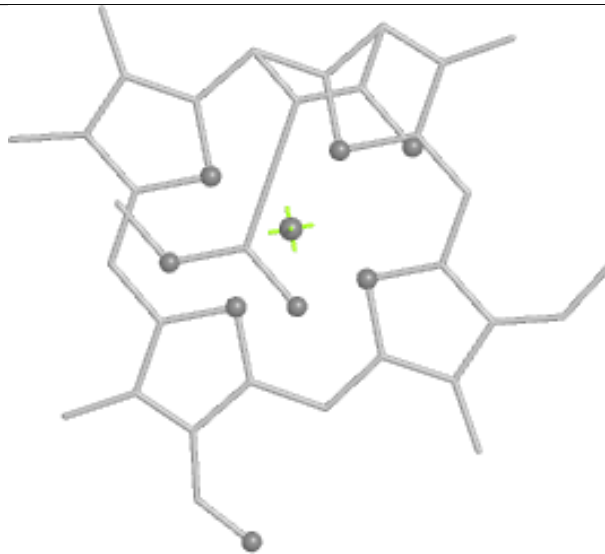
Bond lengths



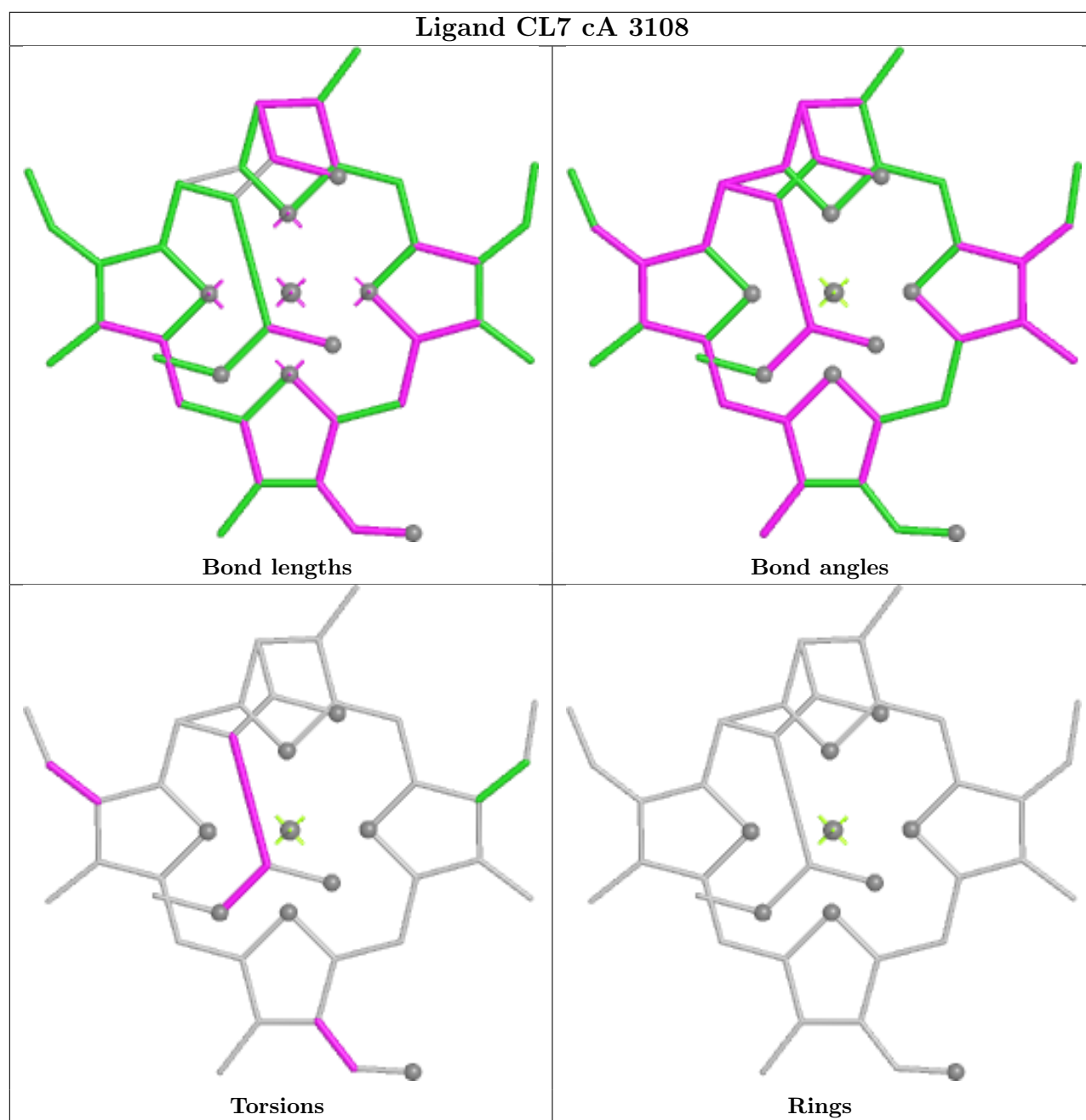
Bond angles



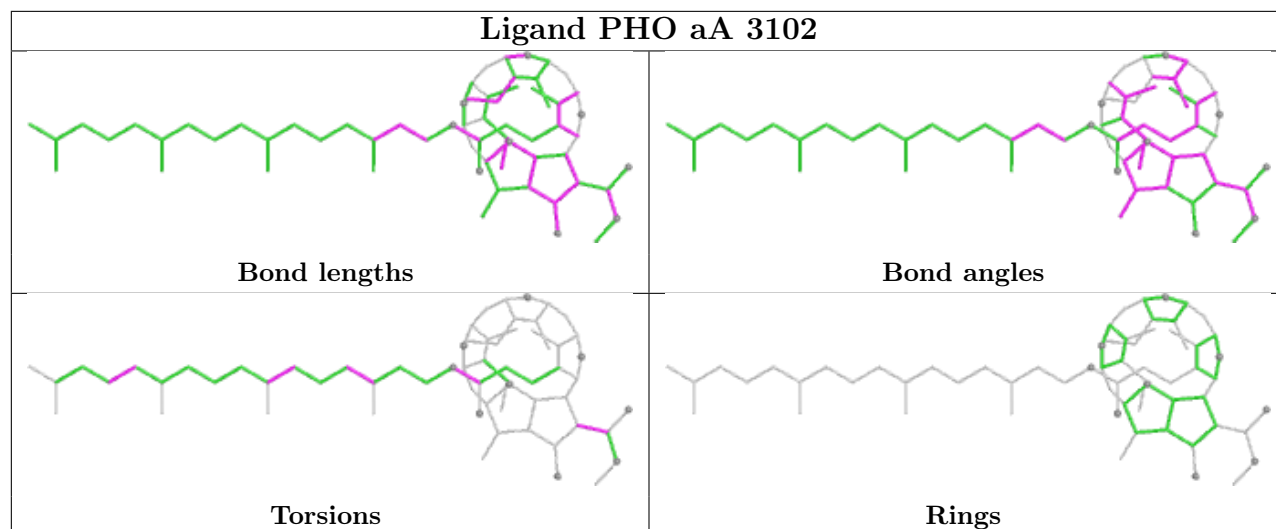
Torsions



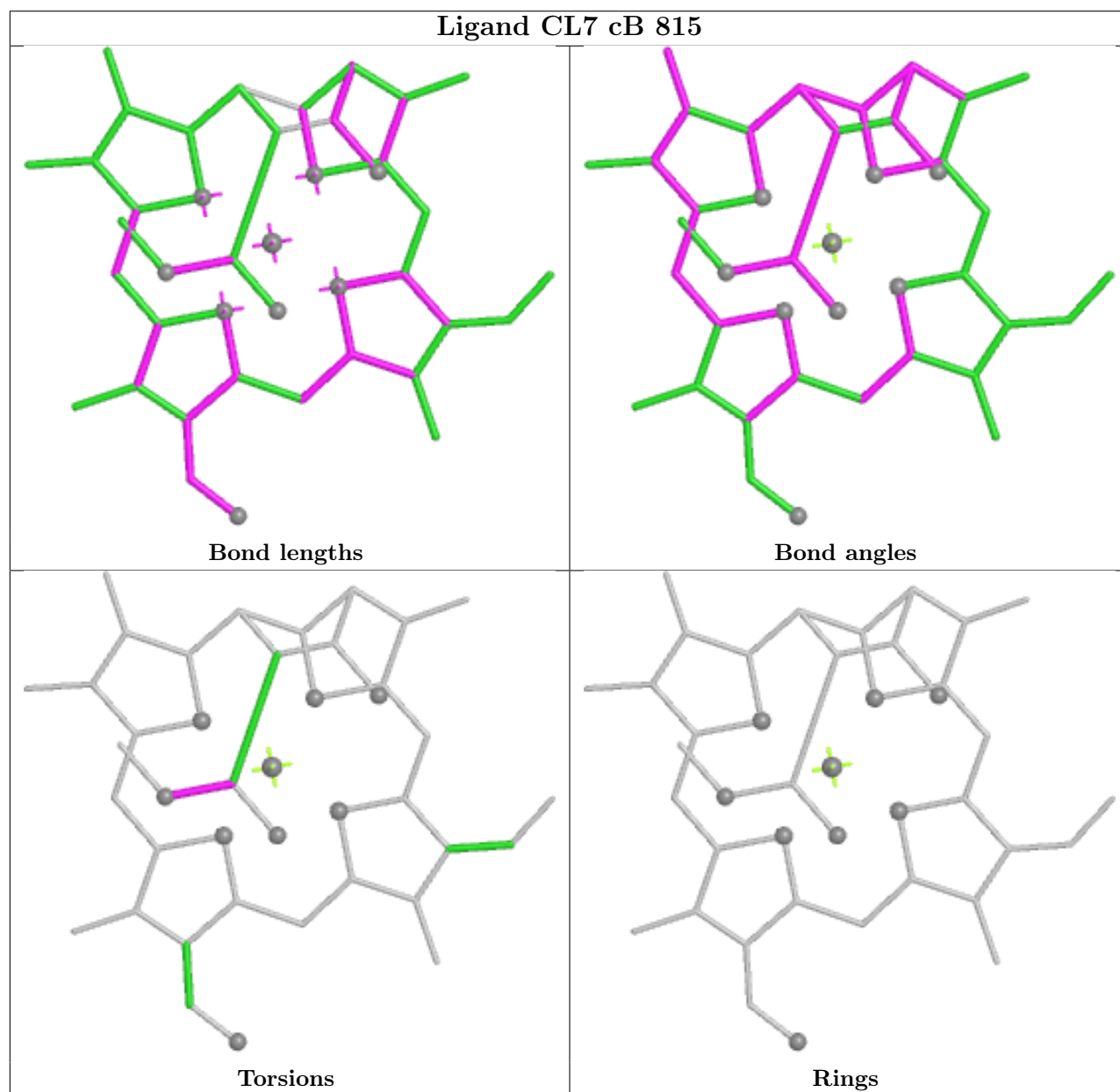
Rings

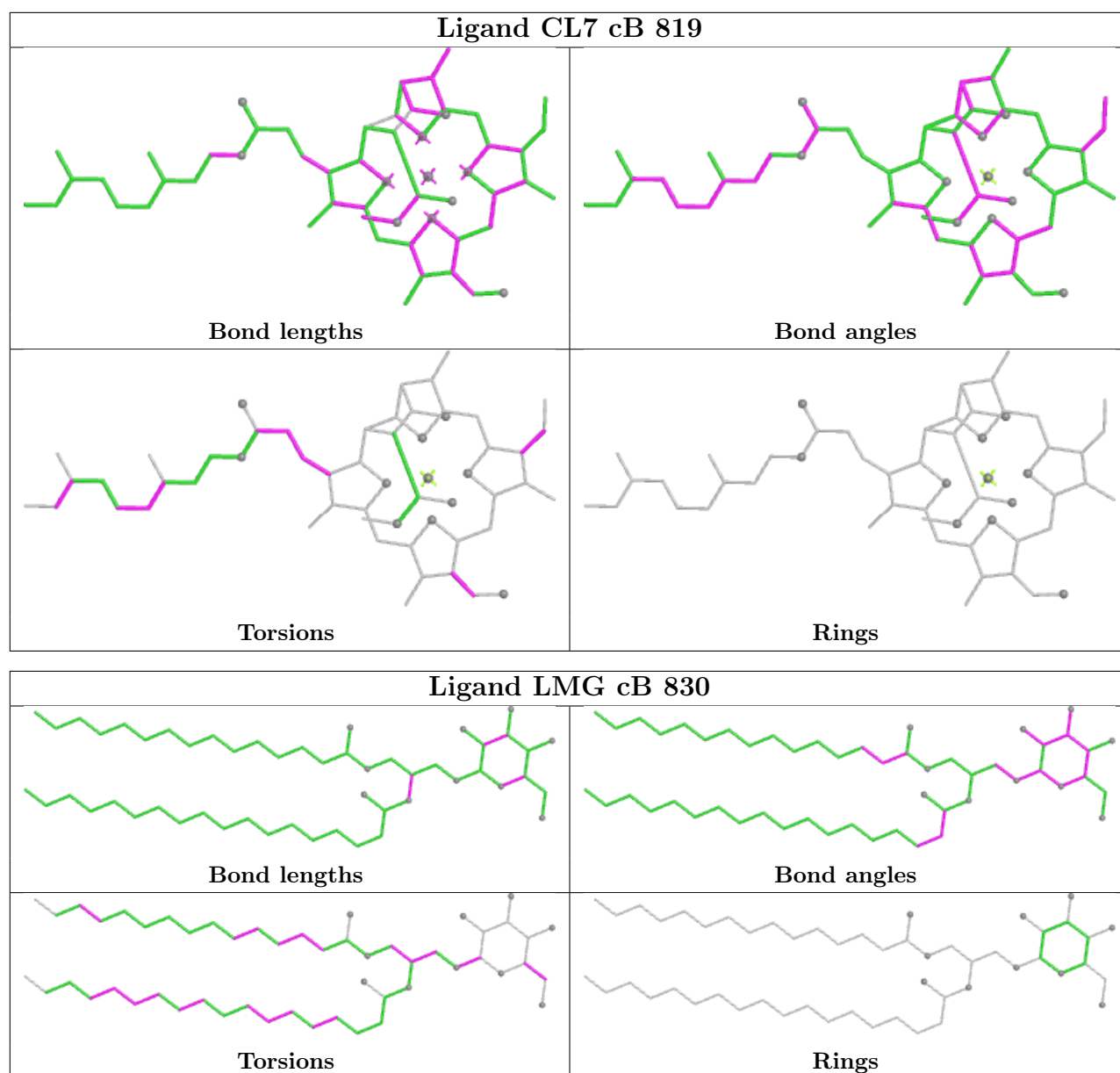


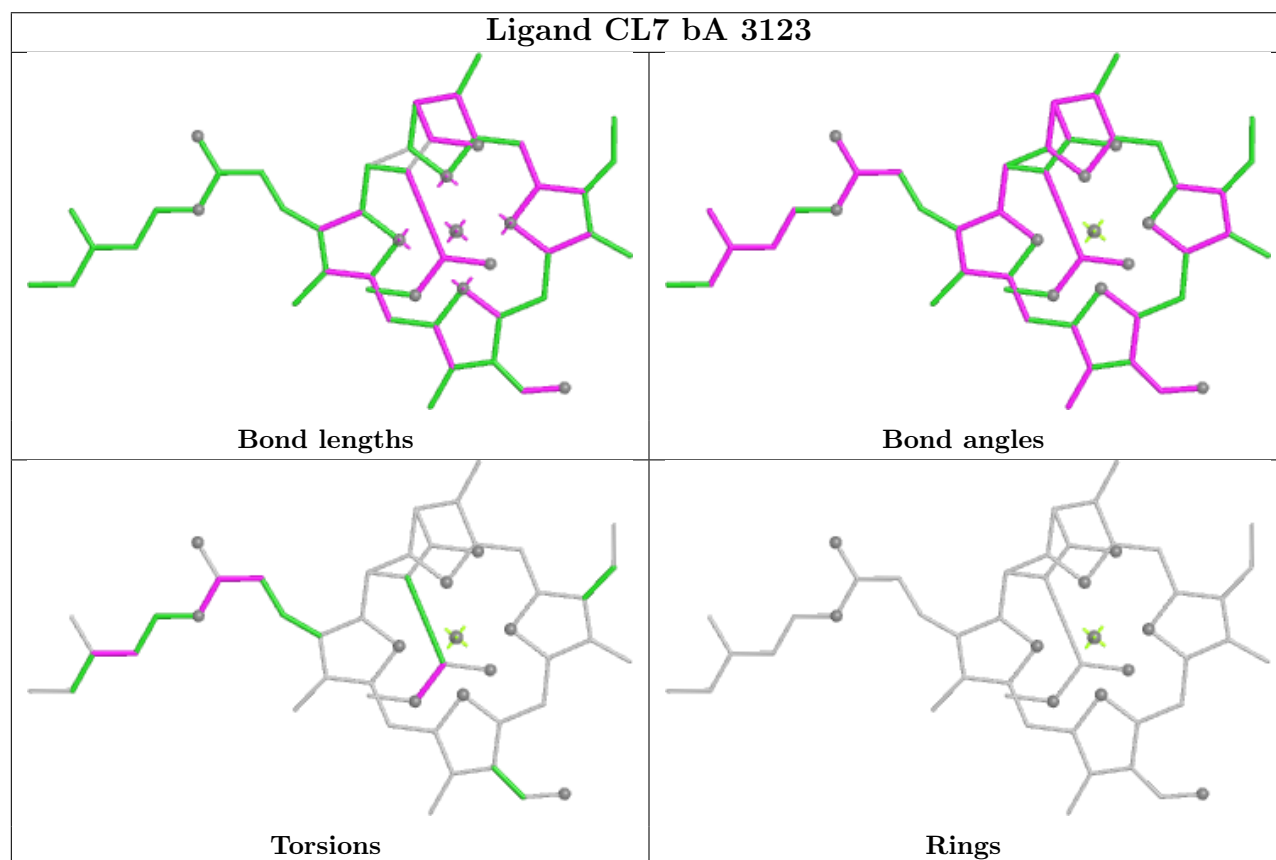
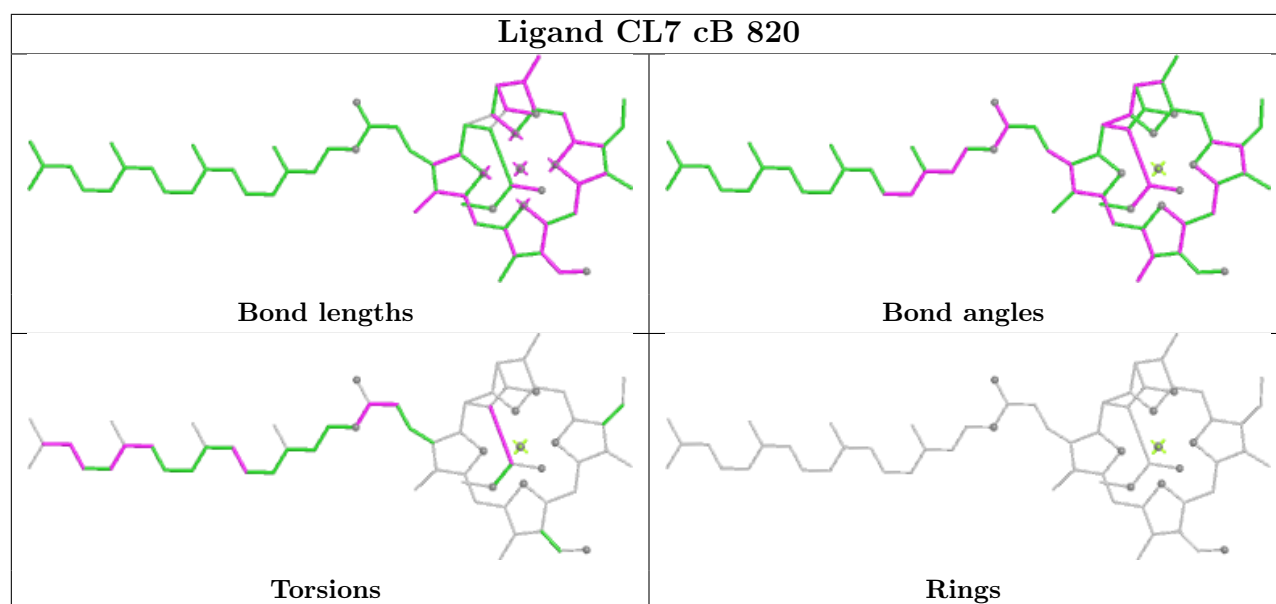
Ligand PHO aA 3102

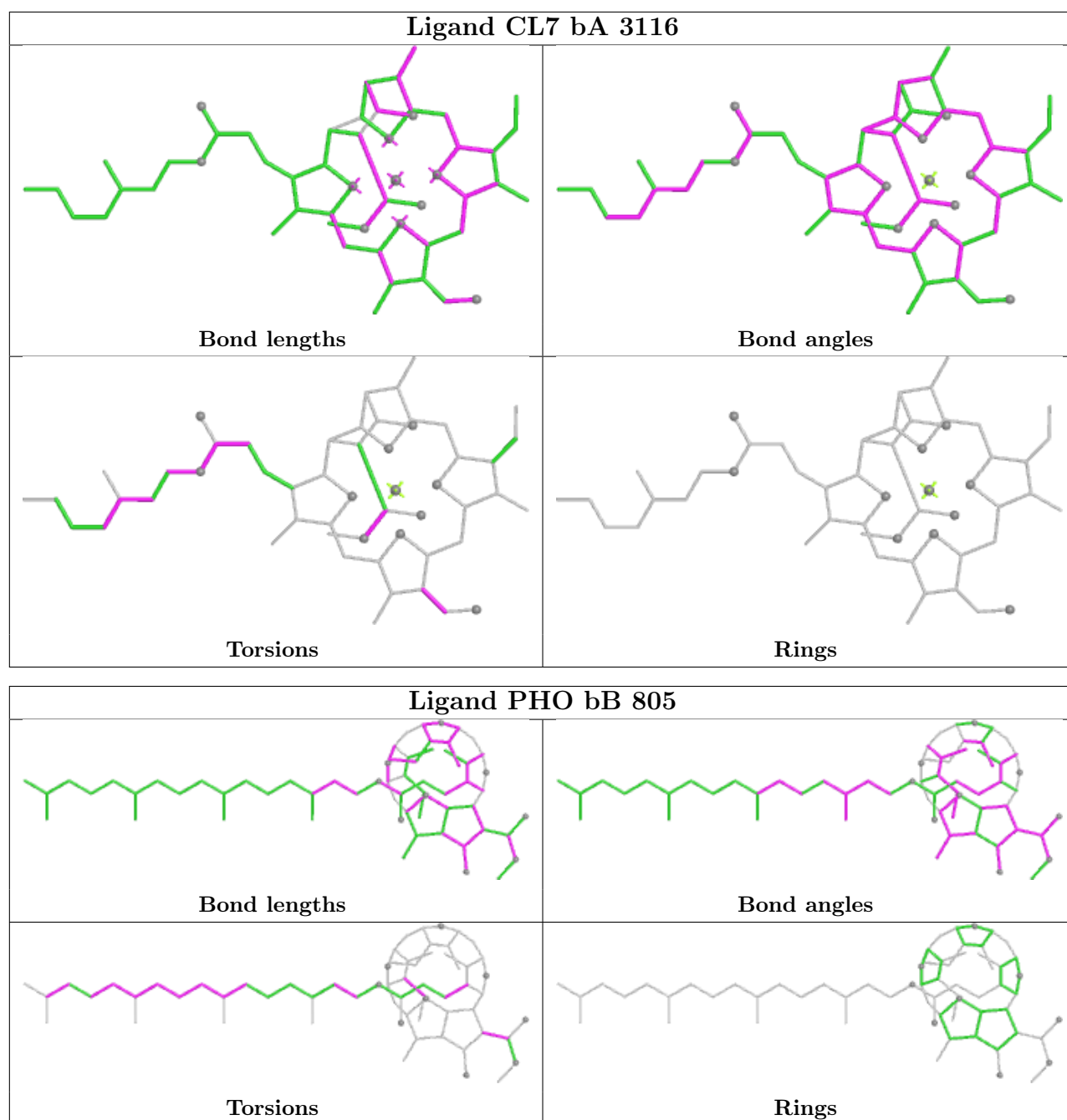


Ligand CL7 cB 815

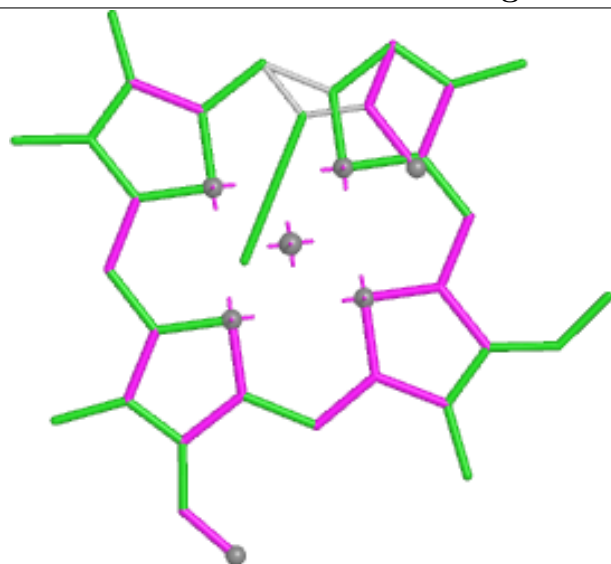




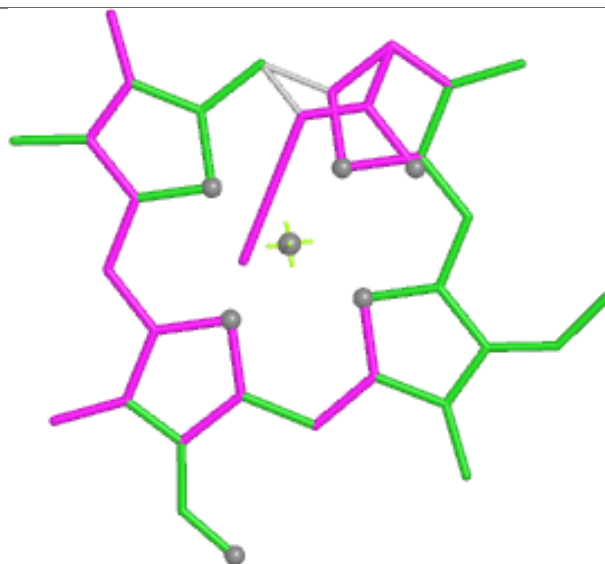




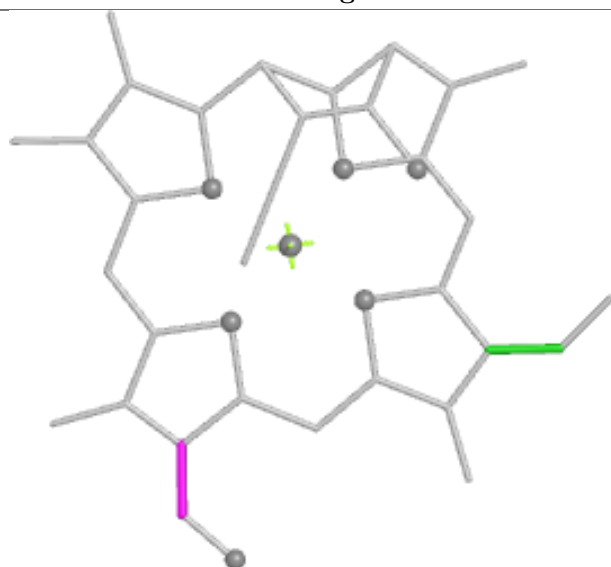
Ligand CL7 cA 3117



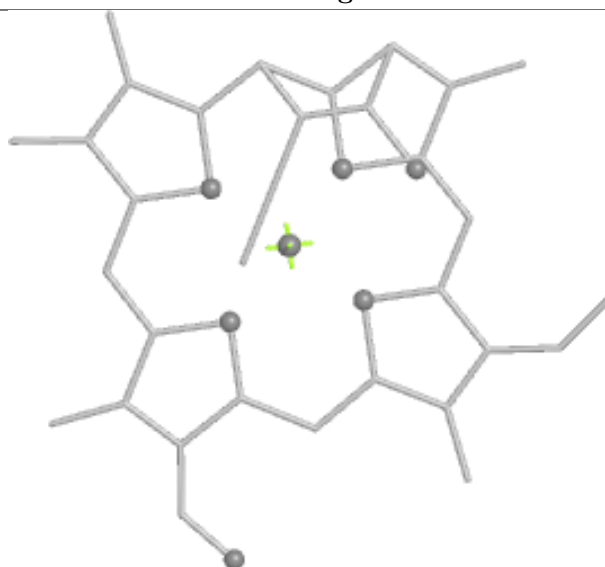
Bond lengths



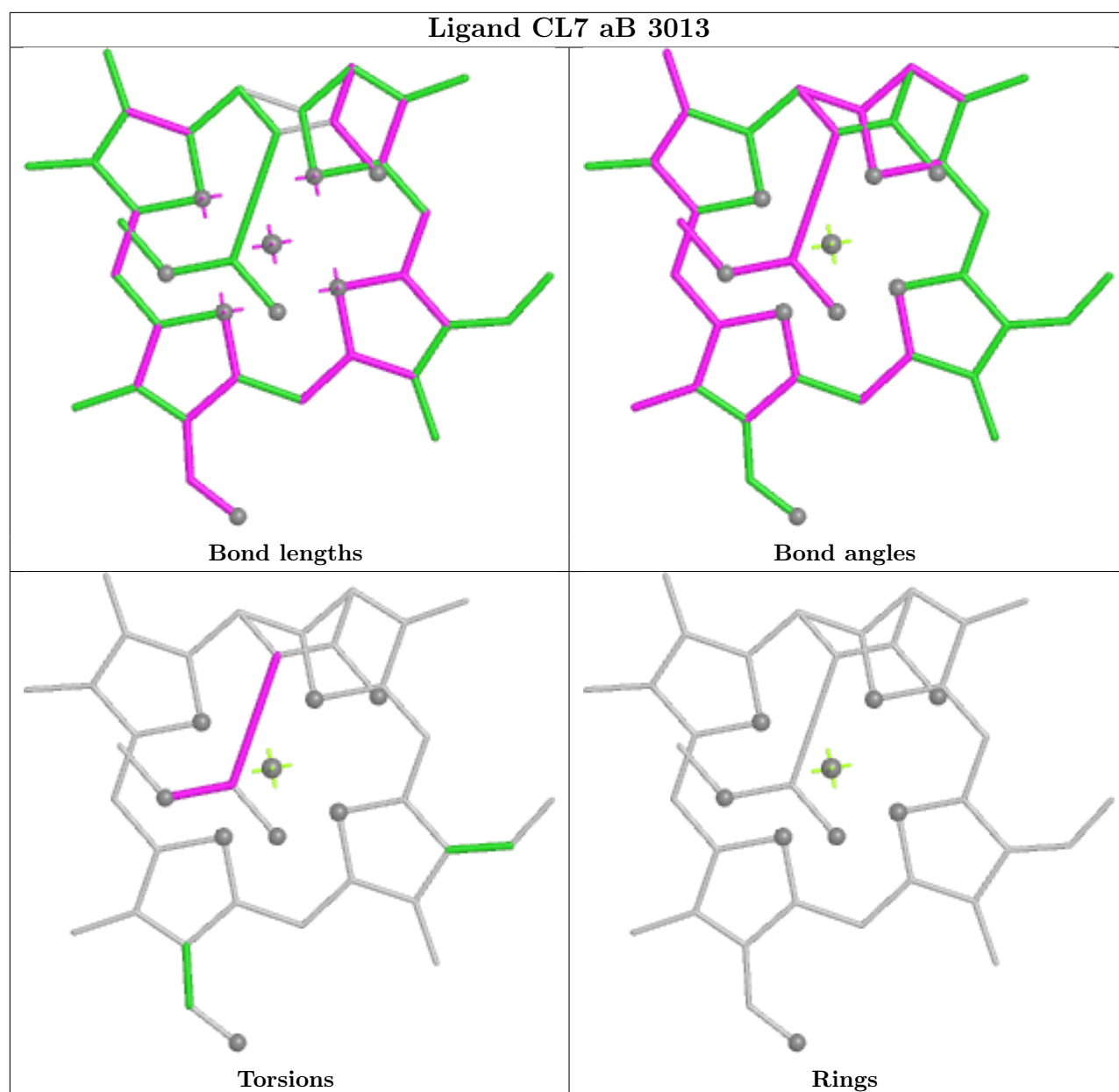
Bond angles



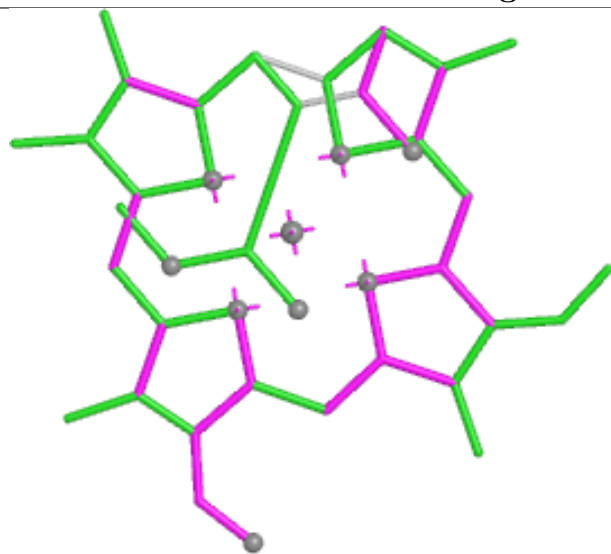
Torsions



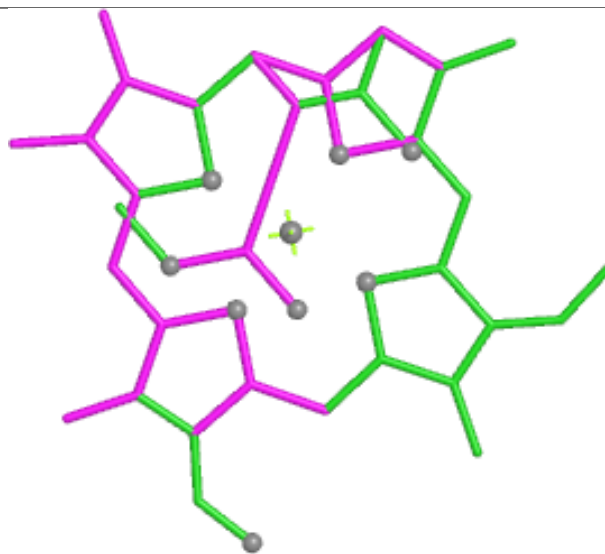
Rings



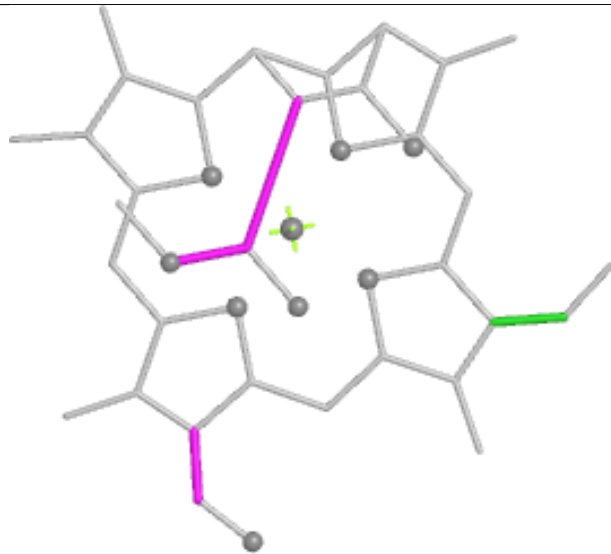
Ligand CL7 bA 3131



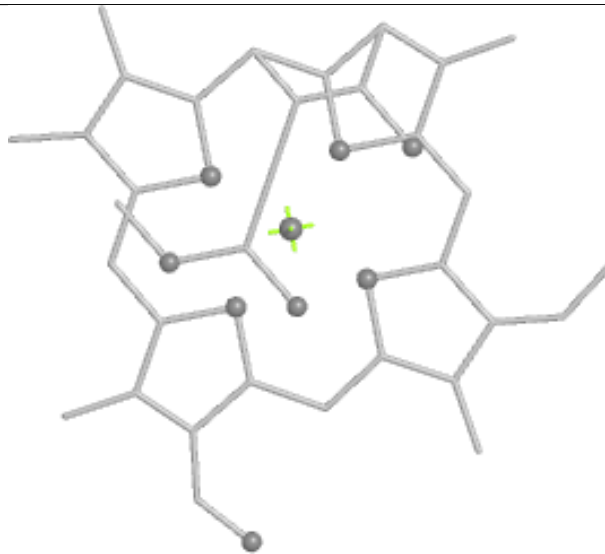
Bond lengths



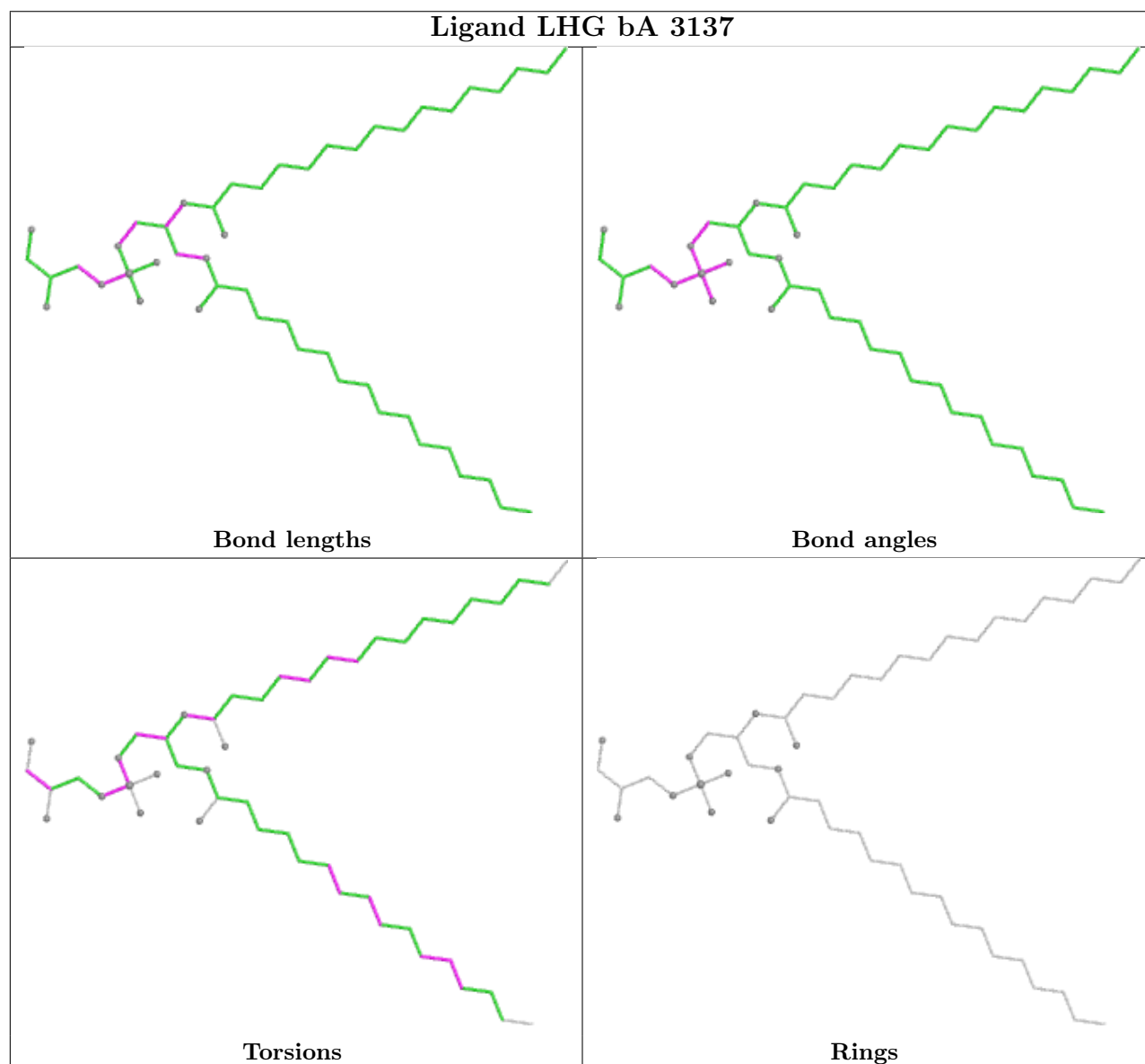
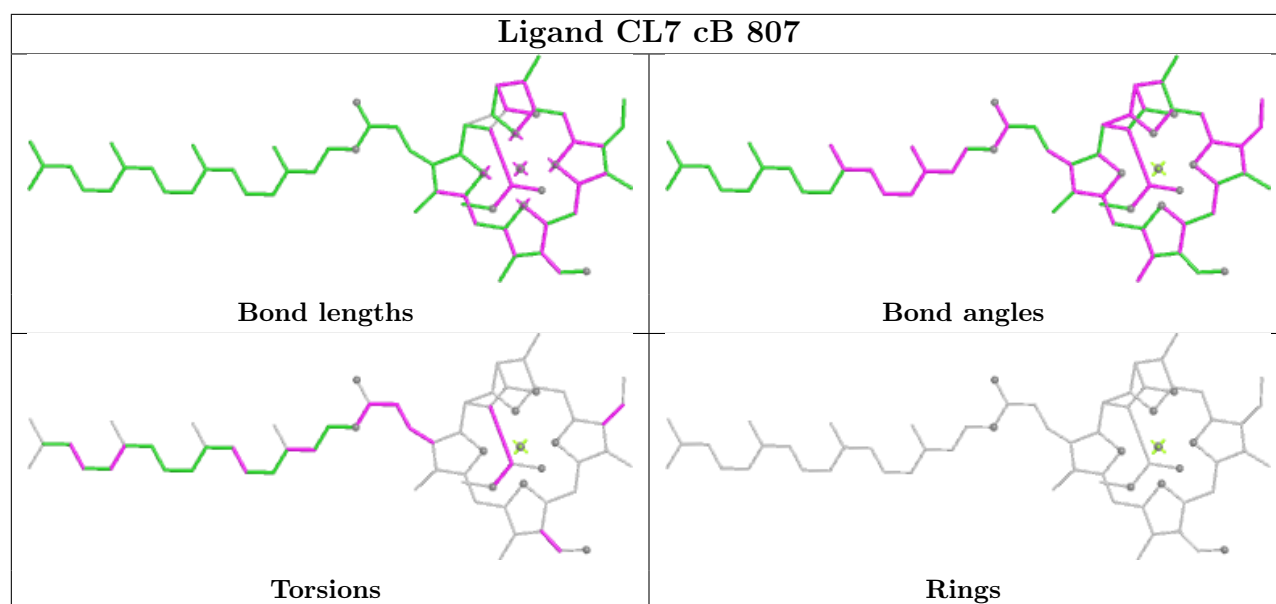
Bond angles



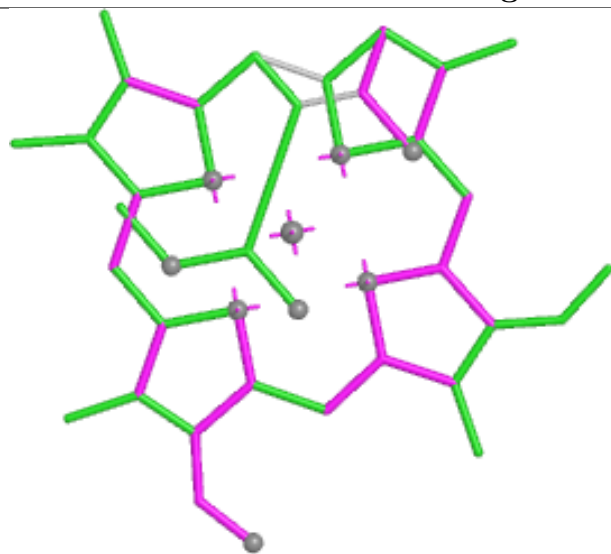
Torsions



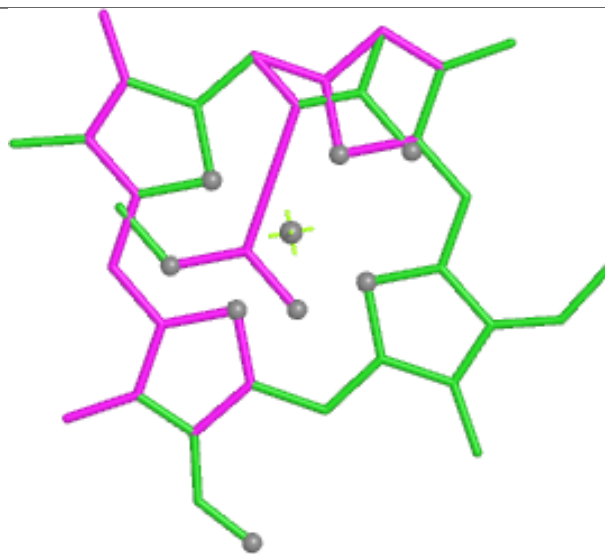
Rings



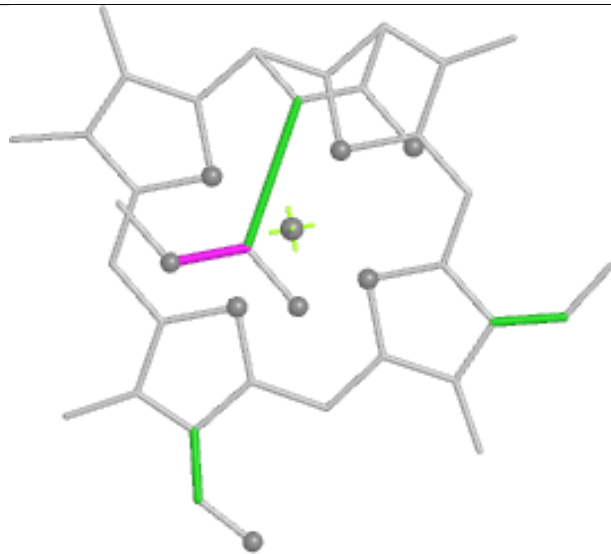
Ligand CL7 aA 3111



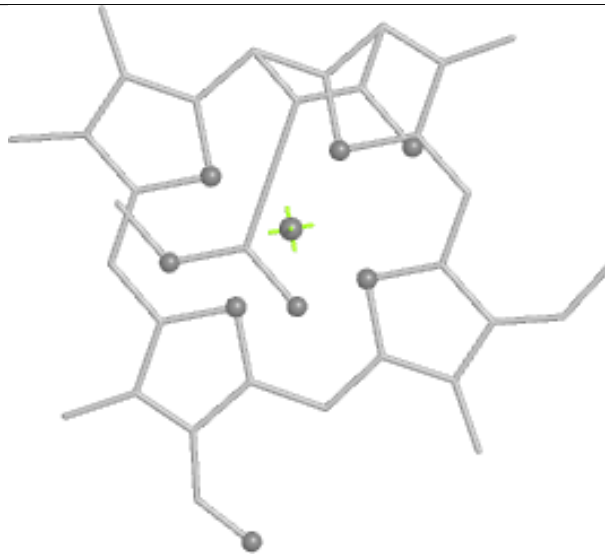
Bond lengths



Bond angles

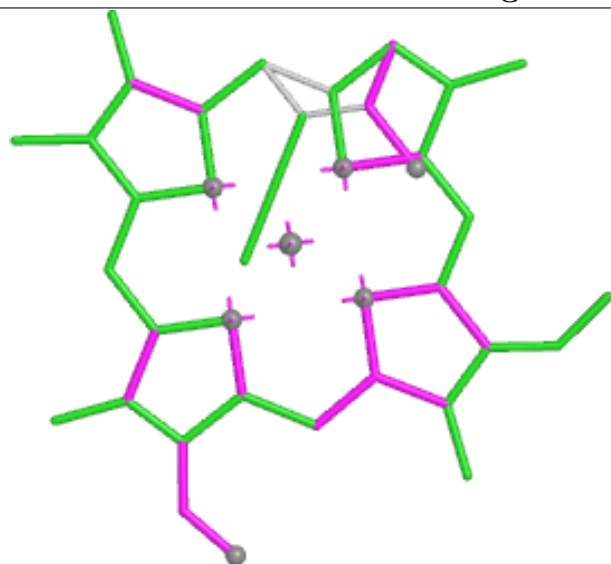


Torsions

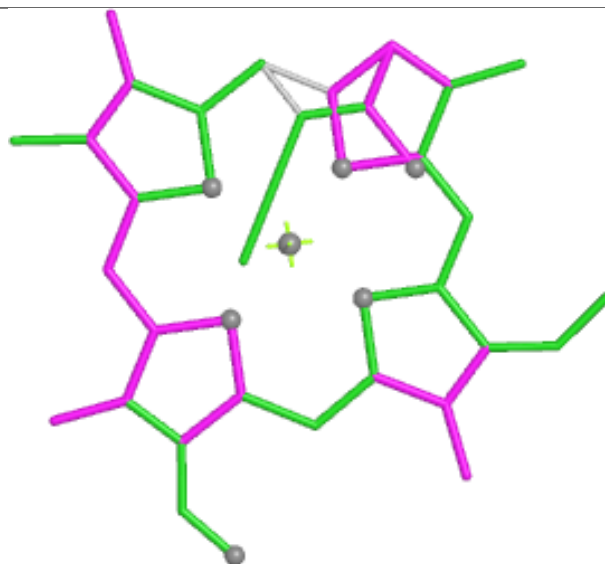


Rings

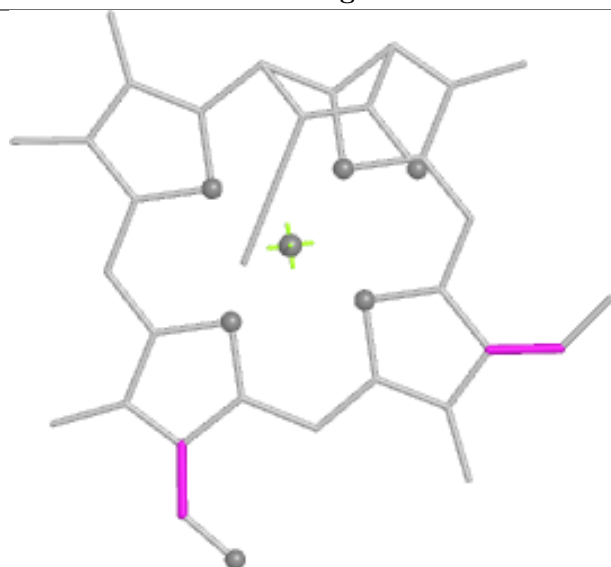
Ligand CL7 cA 3115



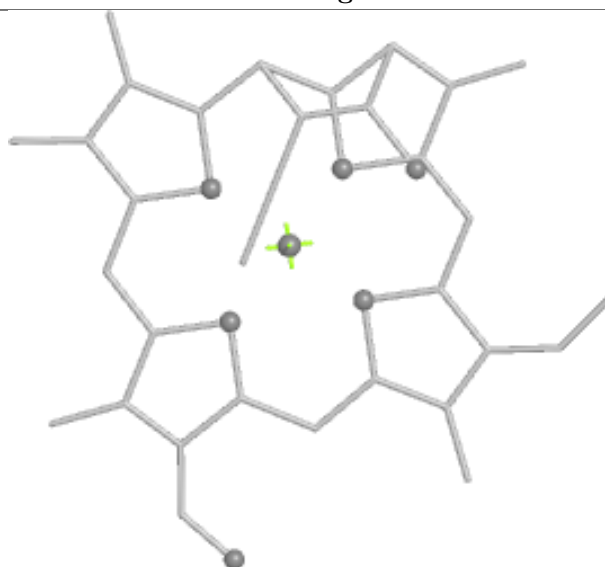
Bond lengths



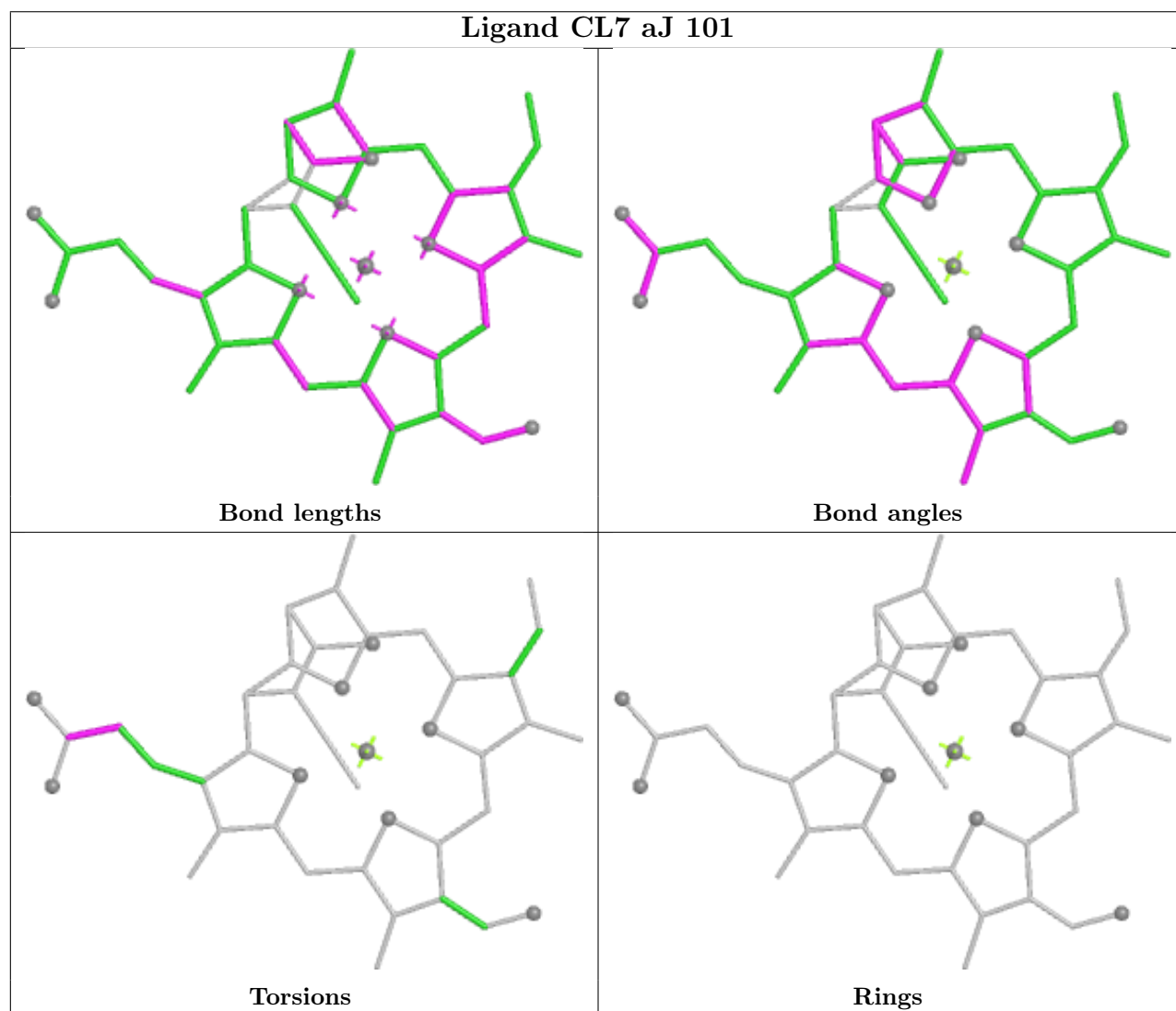
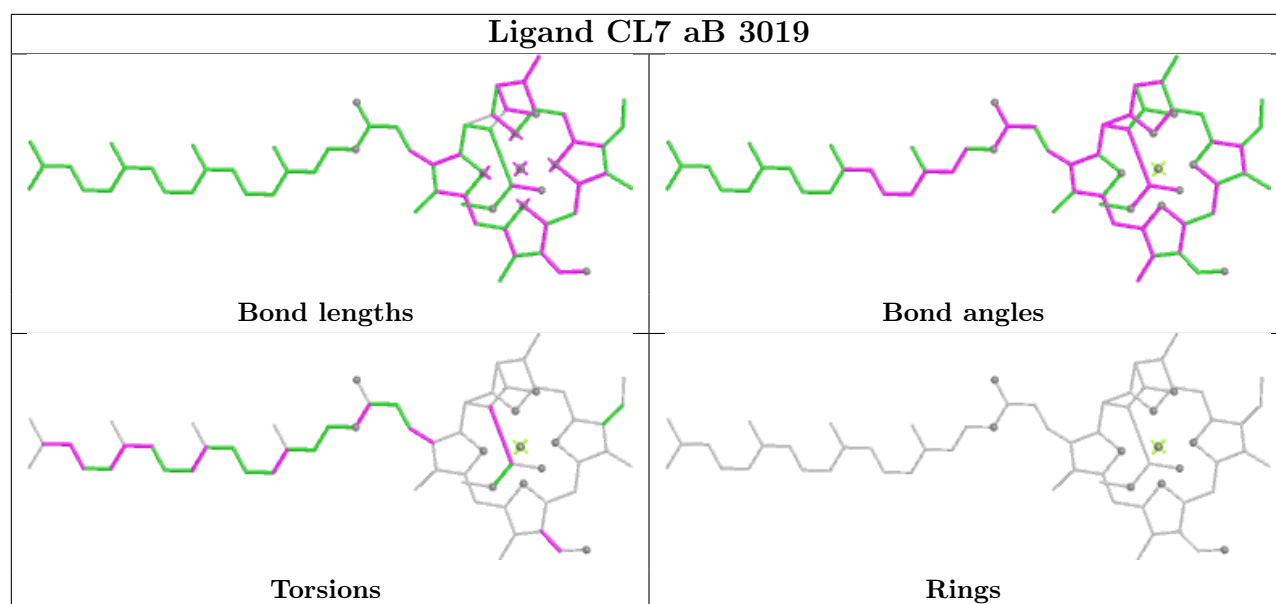
Bond angles

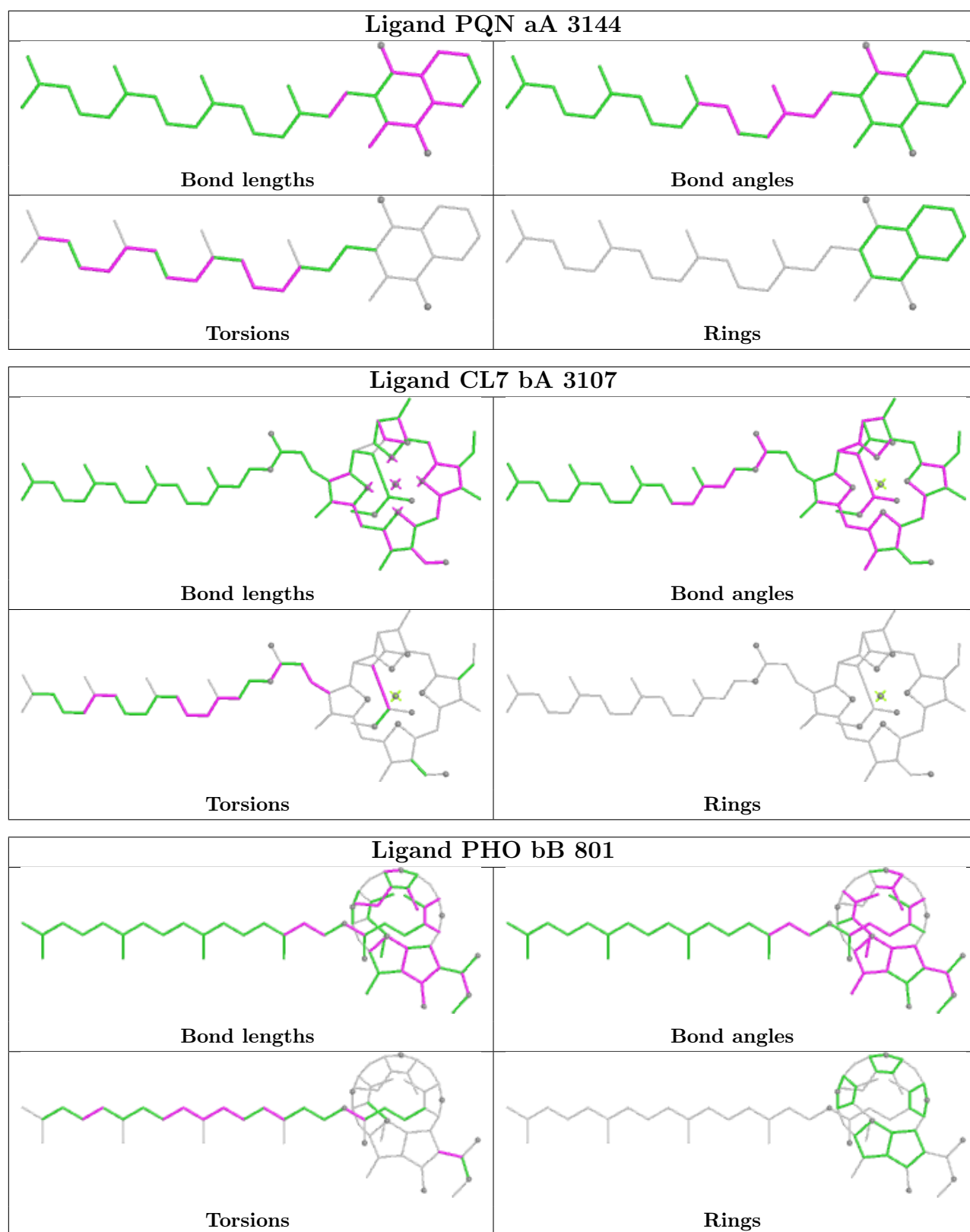


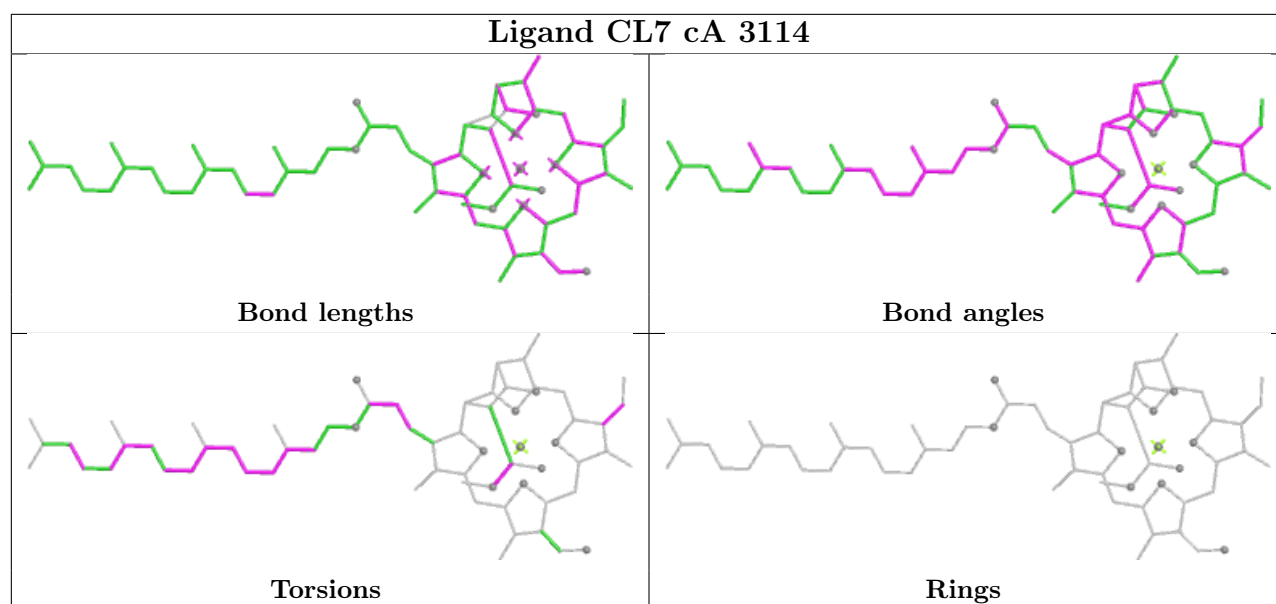
Torsions



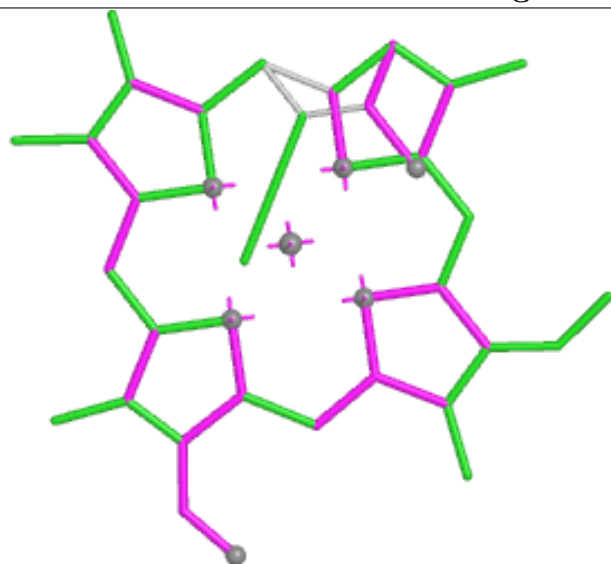
Rings



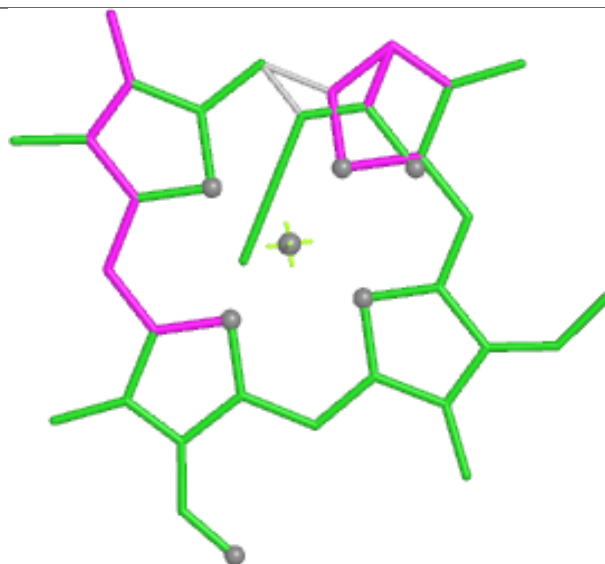




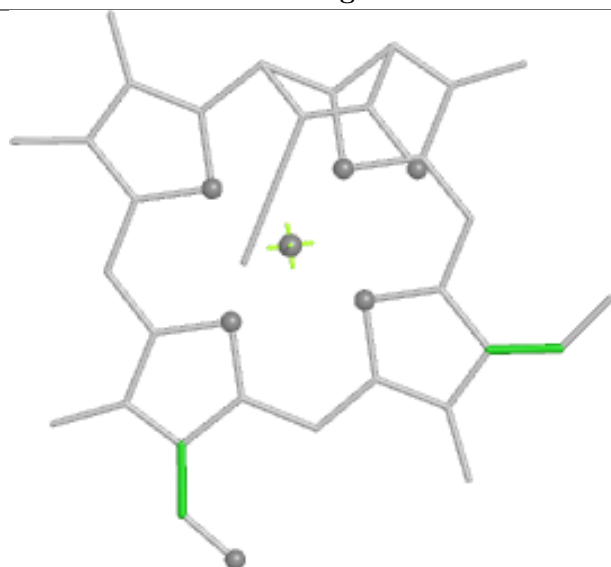
Ligand CL7 cF 201



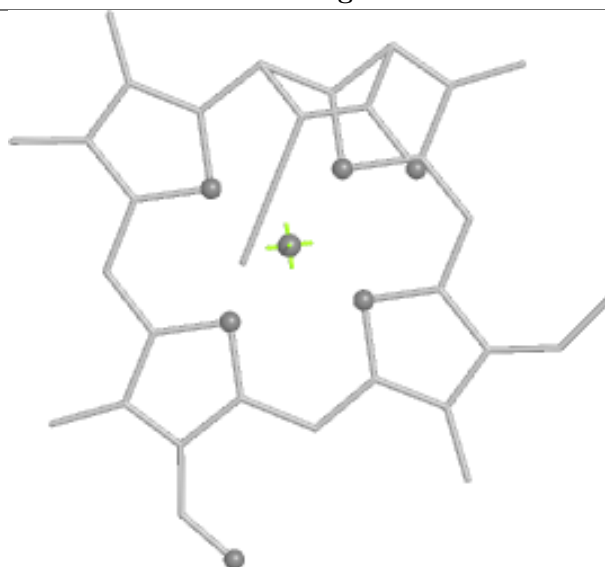
Bond lengths



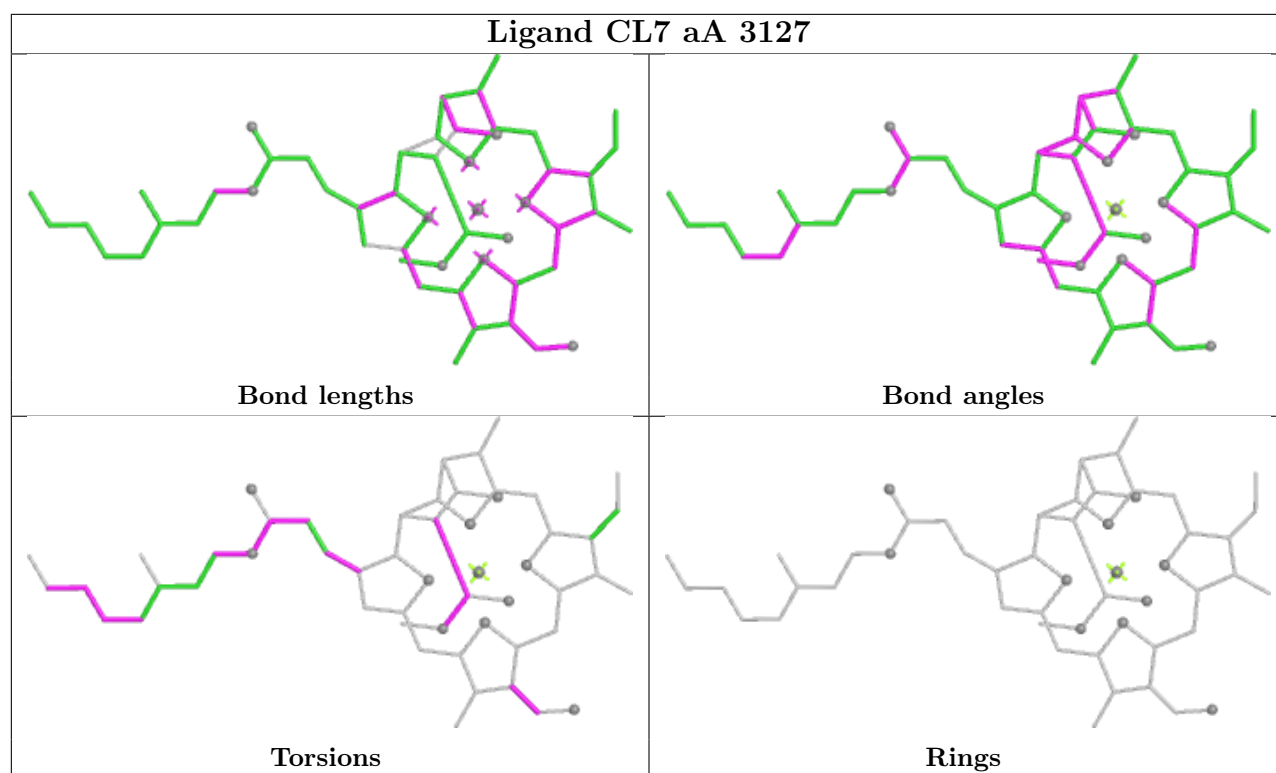
Bond angles



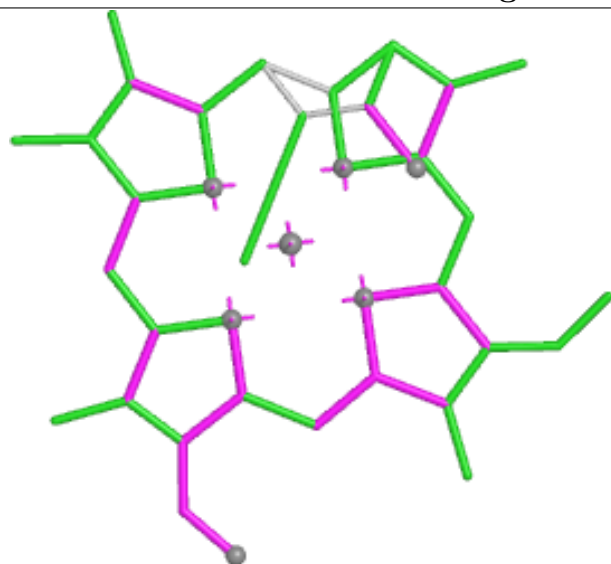
Torsions



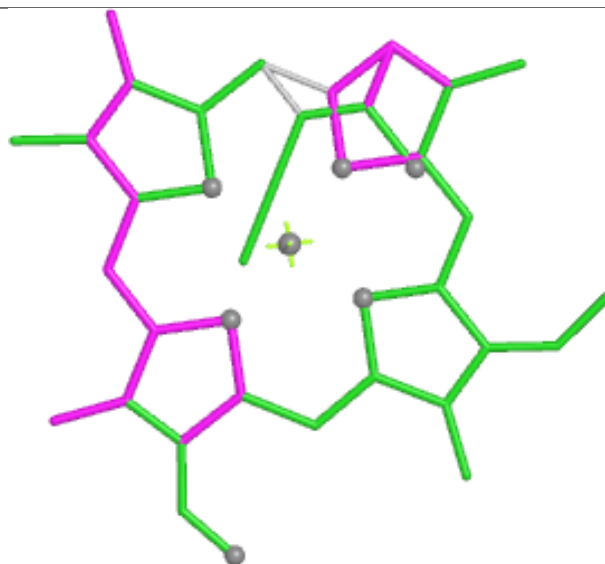
Rings



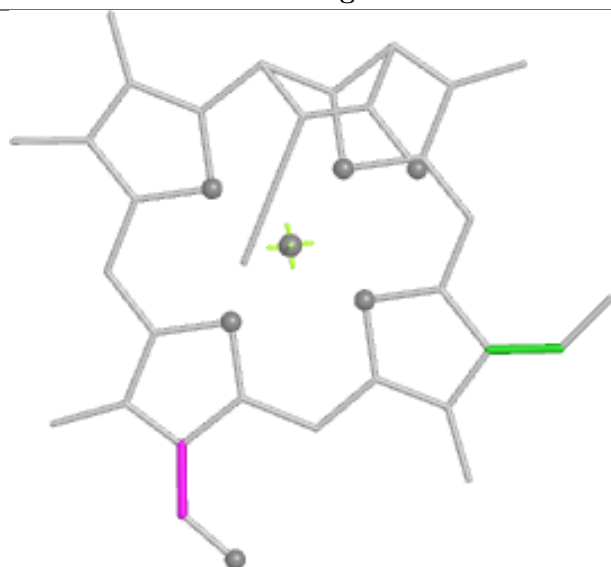
Ligand CL7 bA 3111



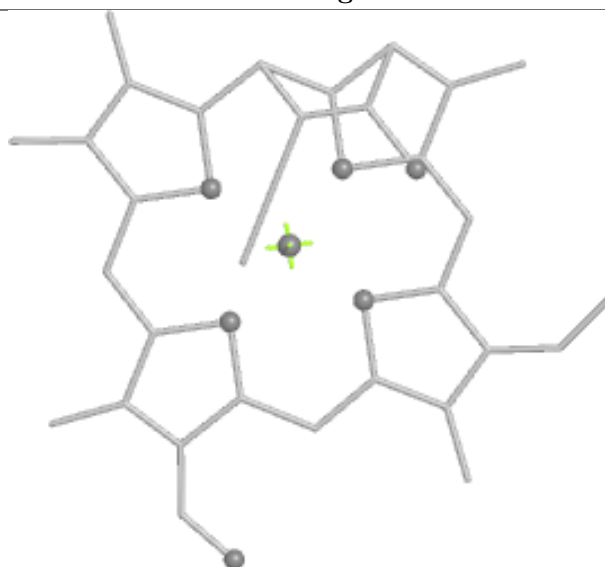
Bond lengths



Bond angles

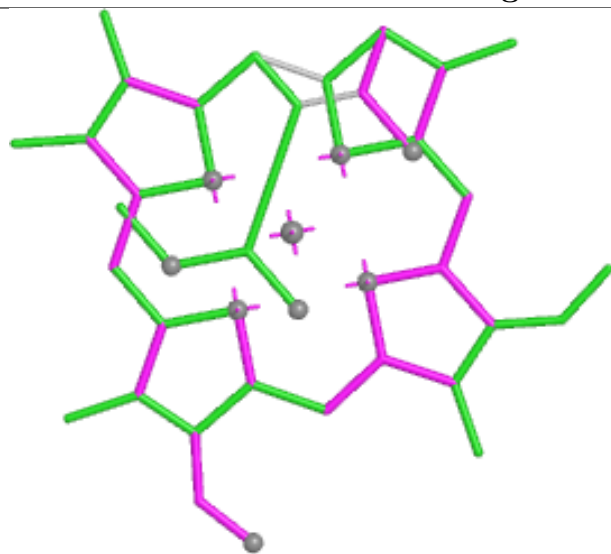


Torsions

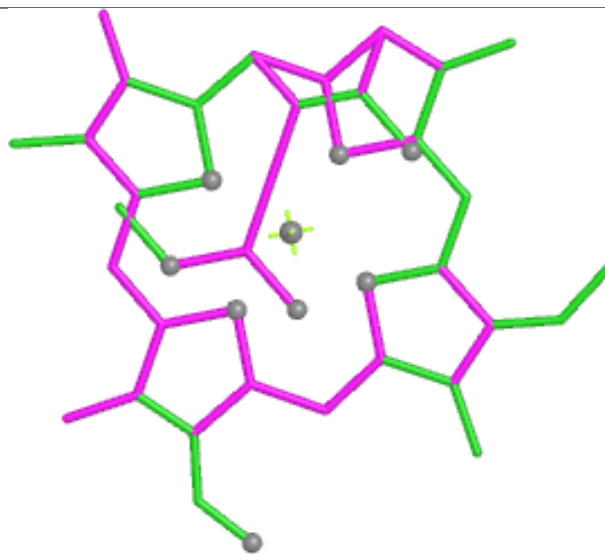


Rings

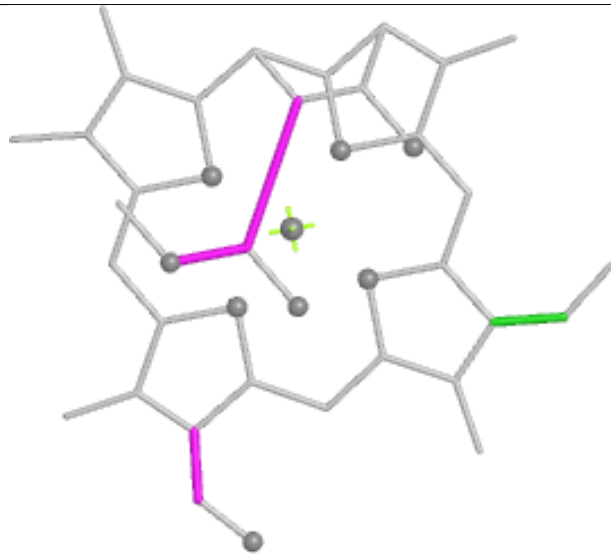
Ligand CL7 cA 3103



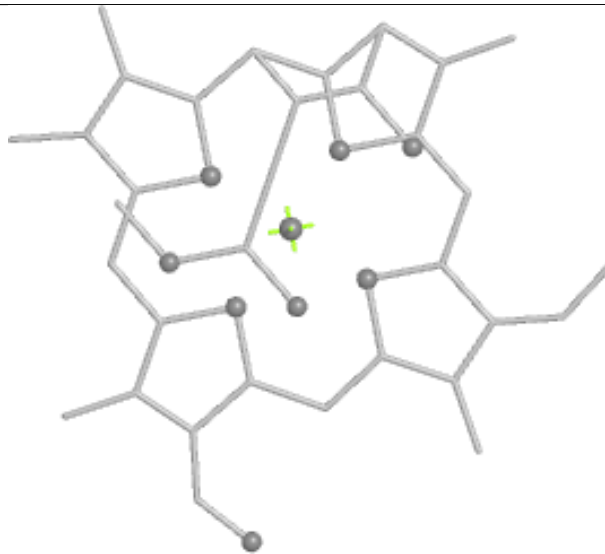
Bond lengths



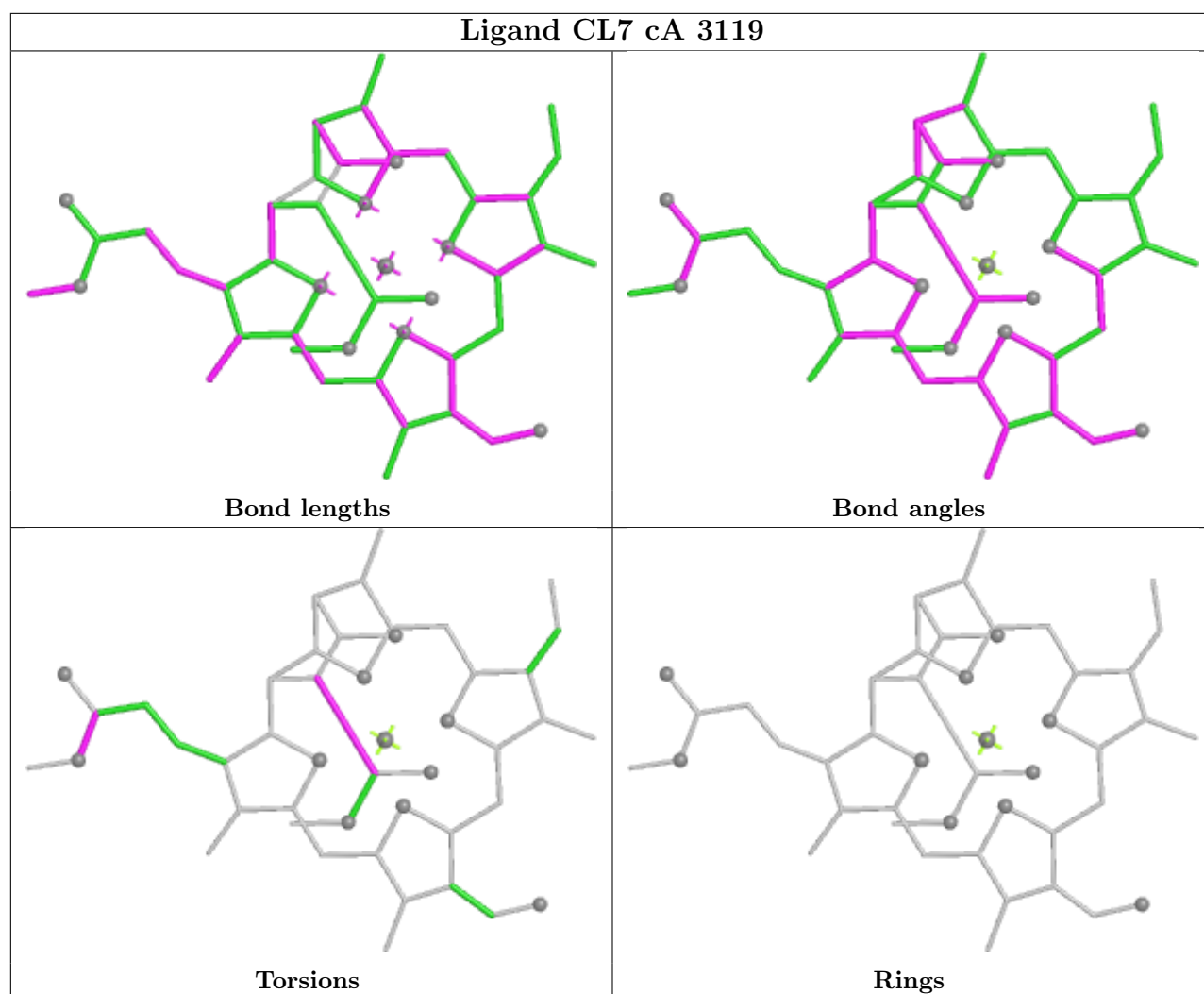
Bond angles



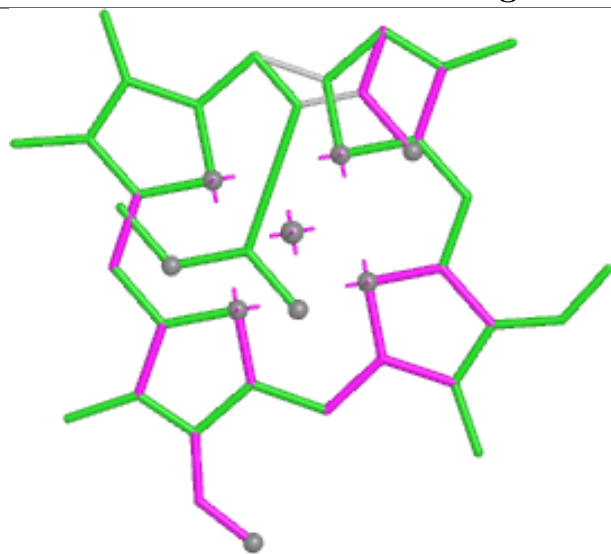
Torsions



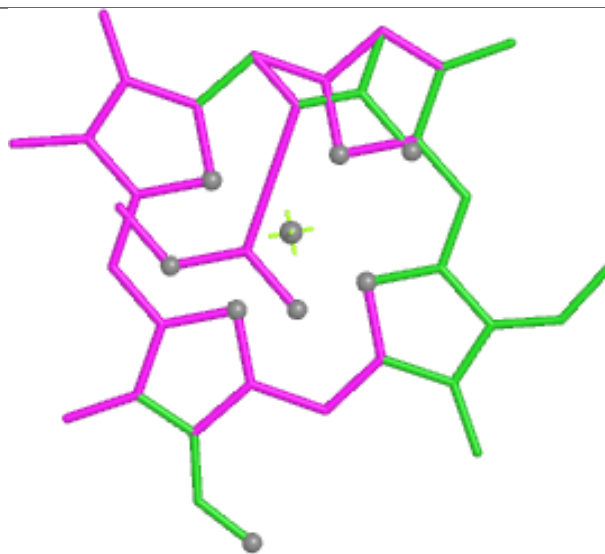
Rings



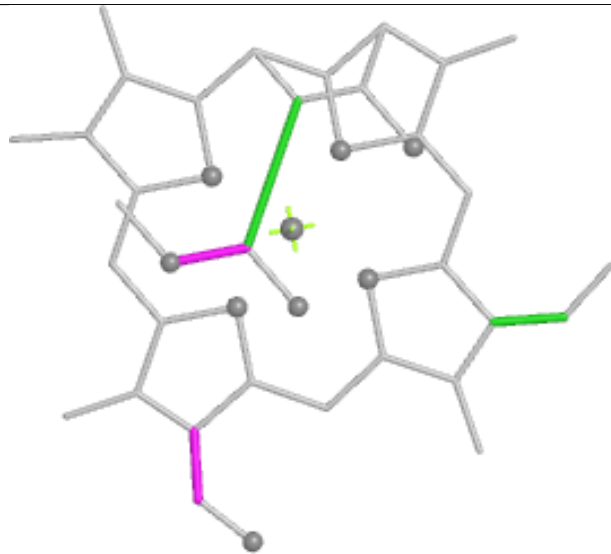
Ligand CL7 bA 3109



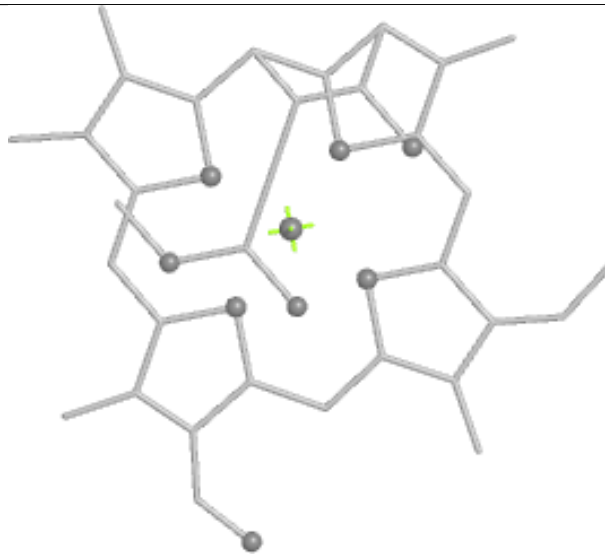
Bond lengths



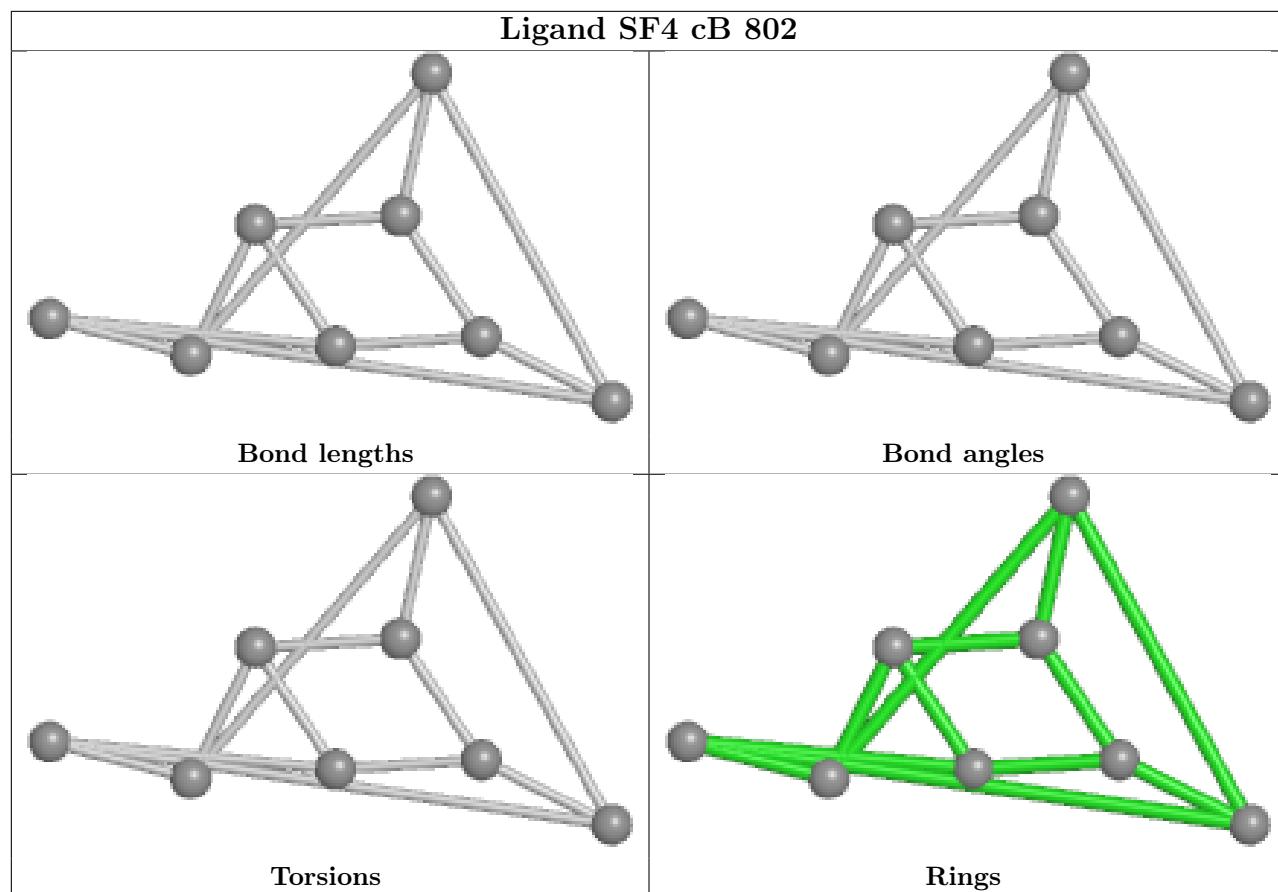
Bond angles

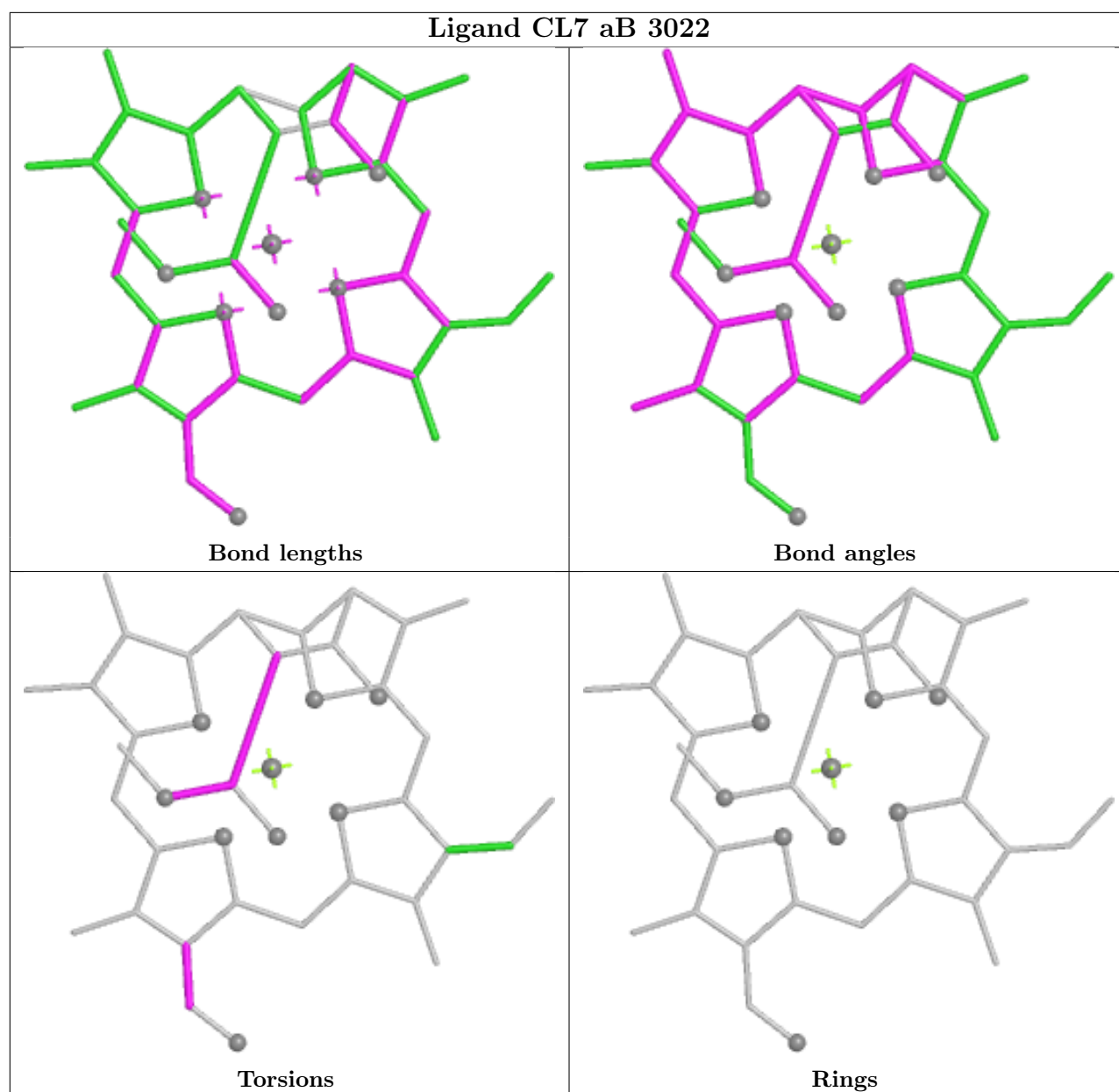


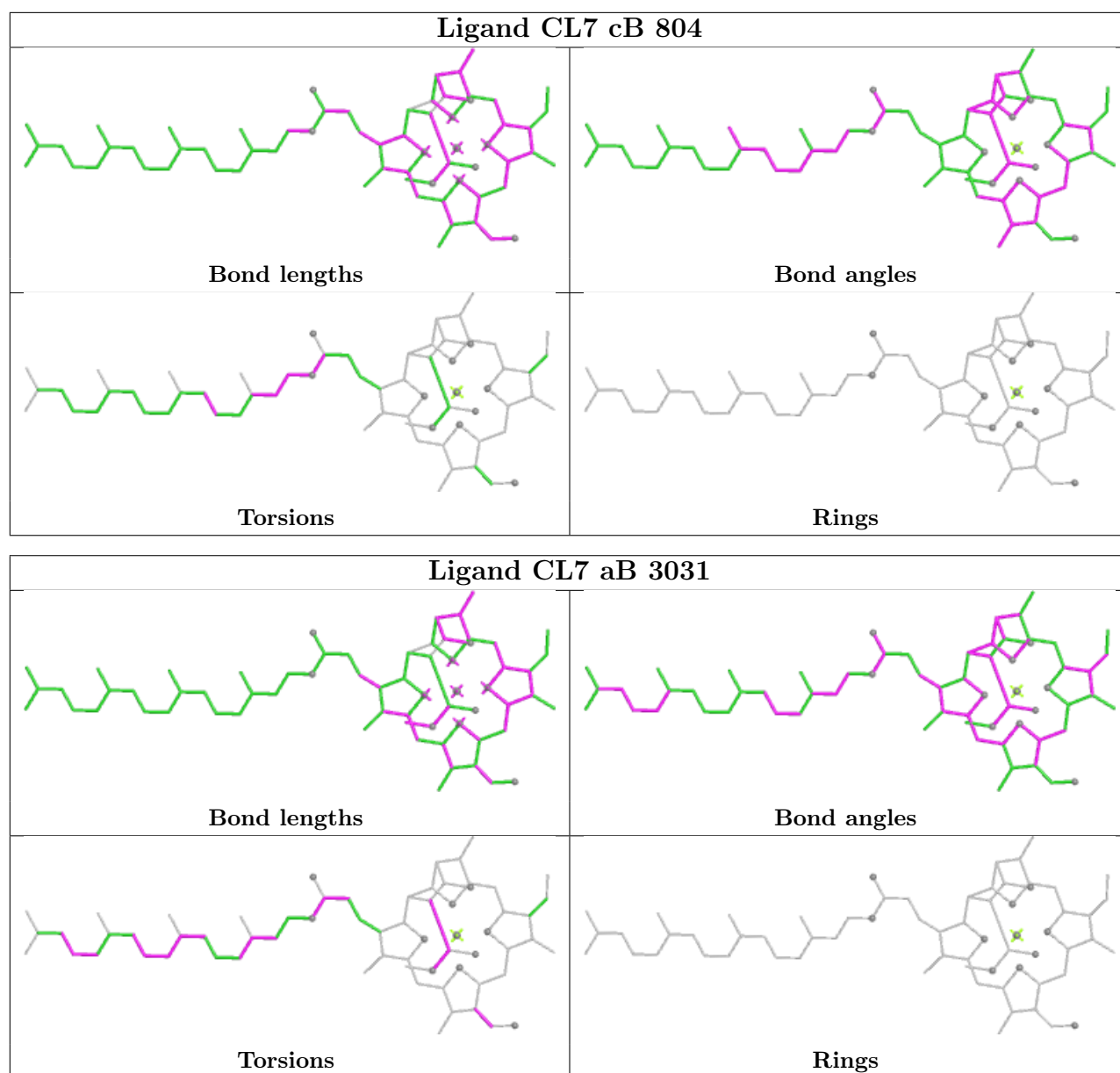
Torsions

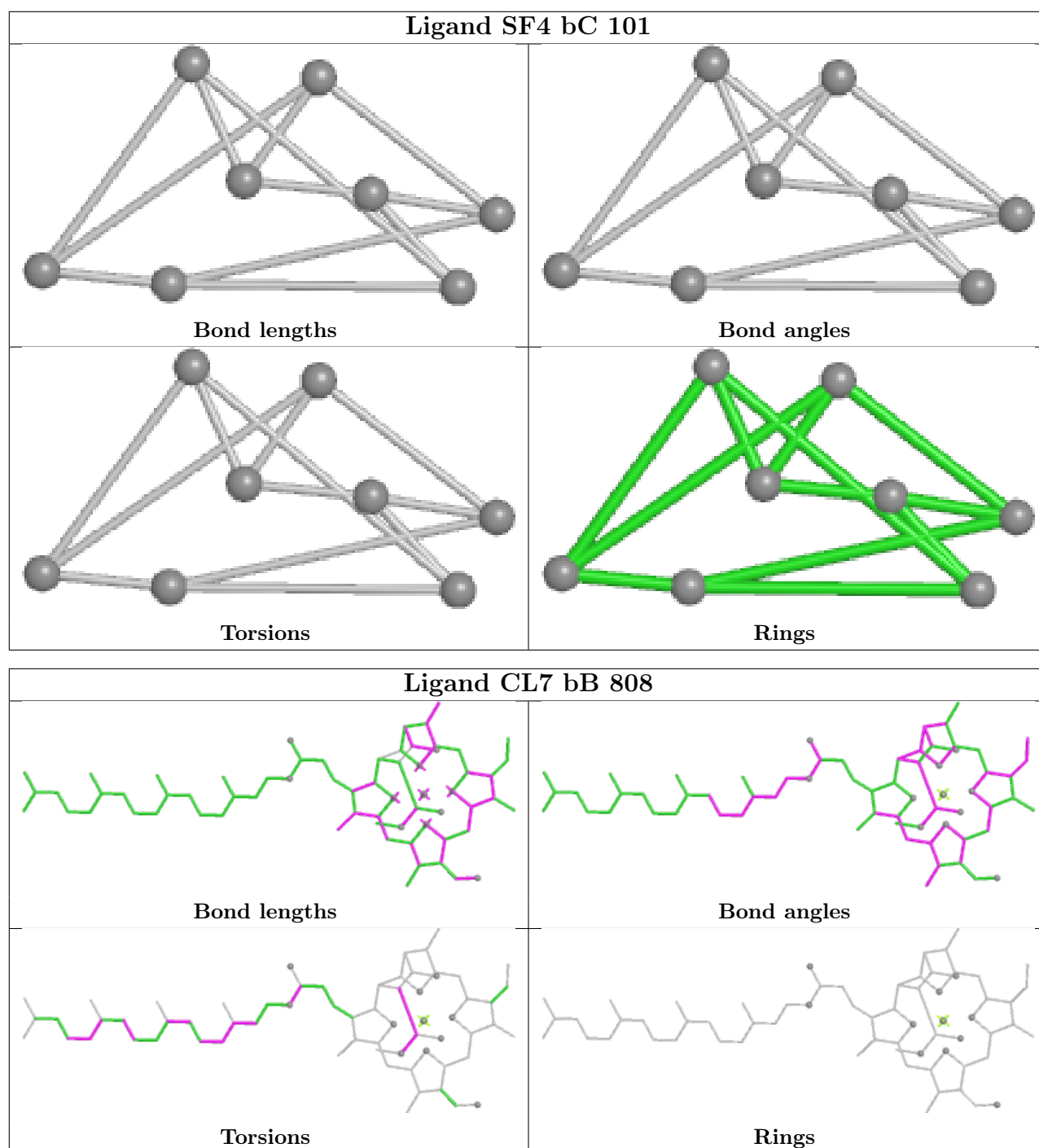


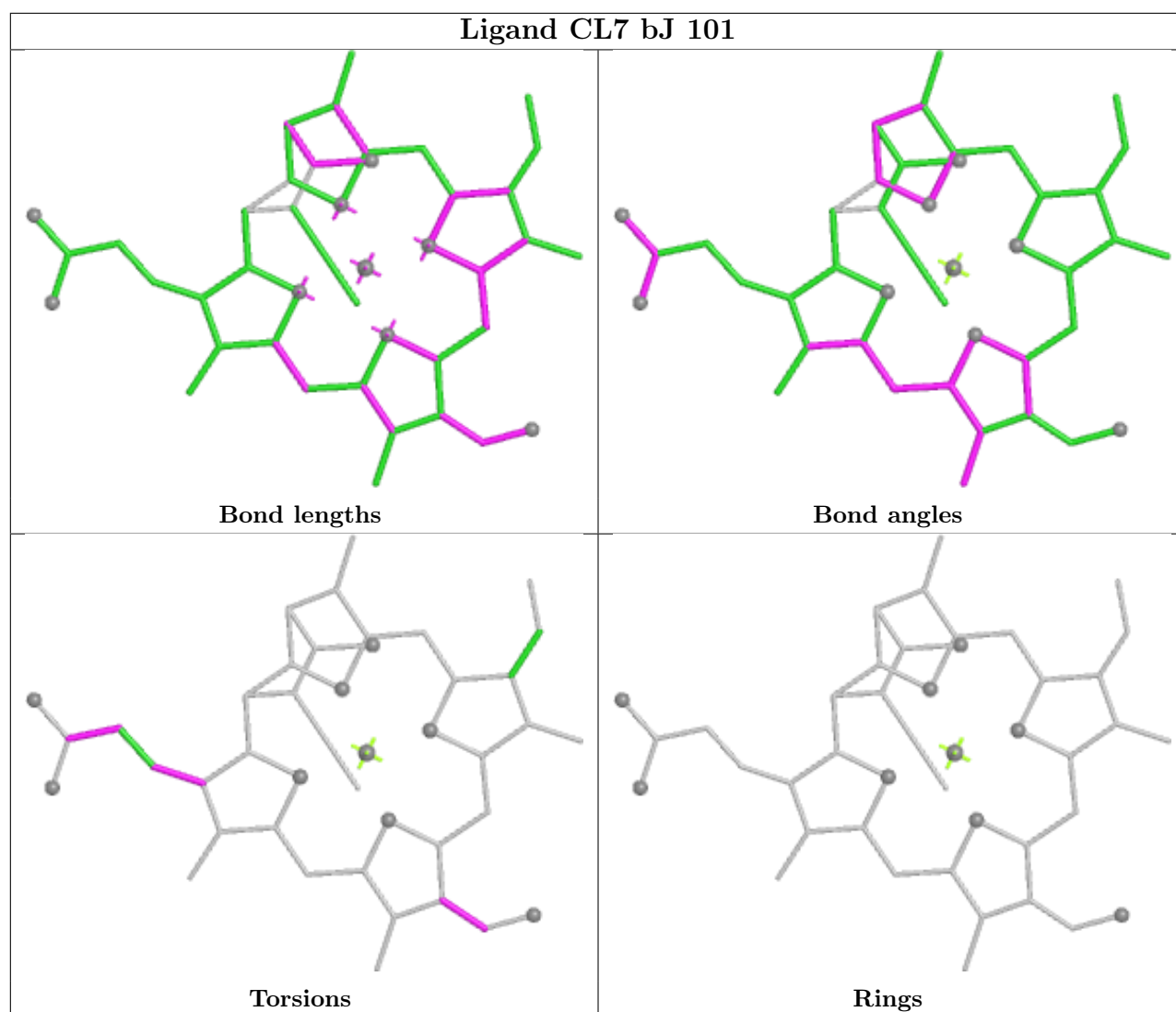
Rings

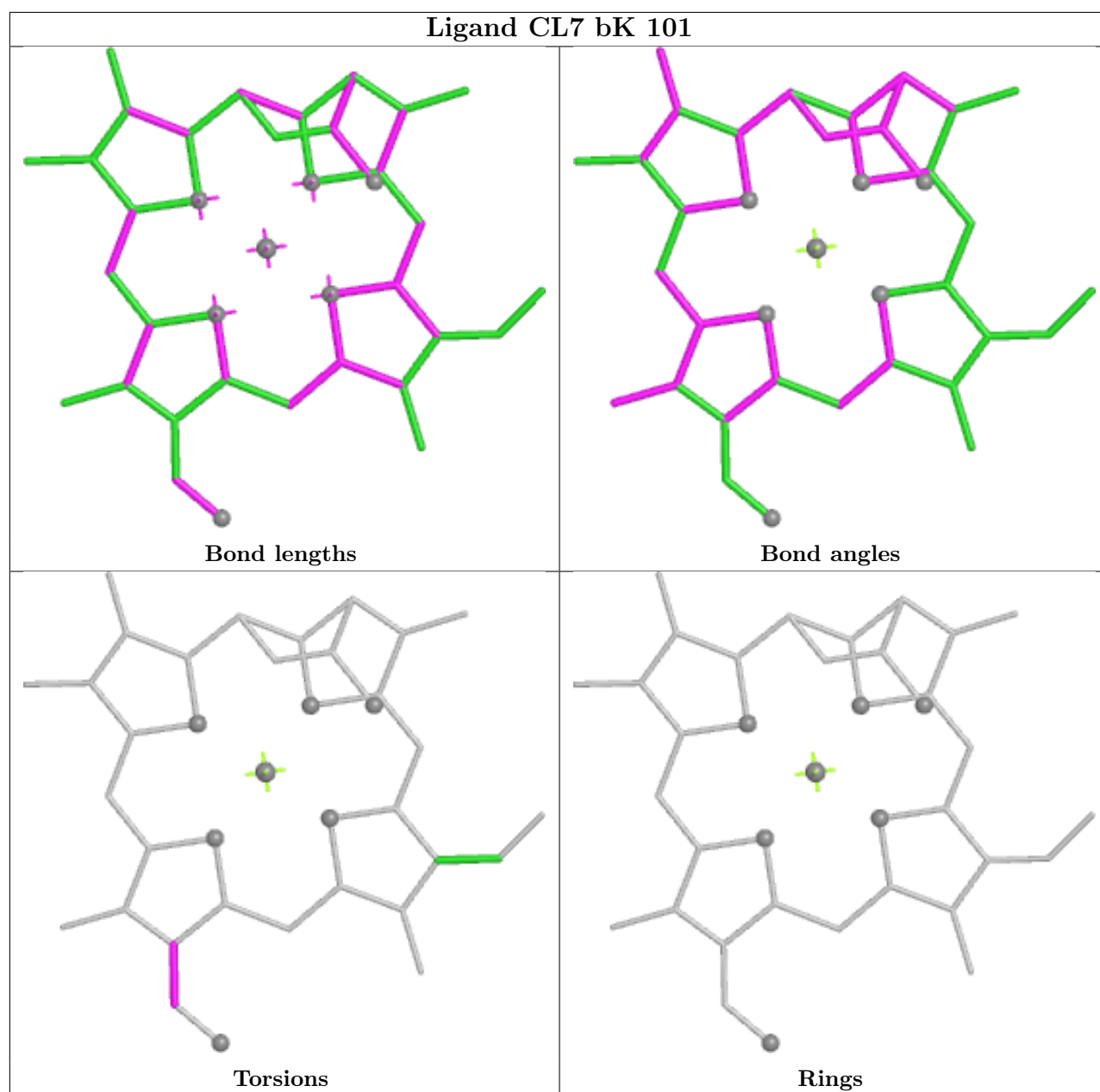




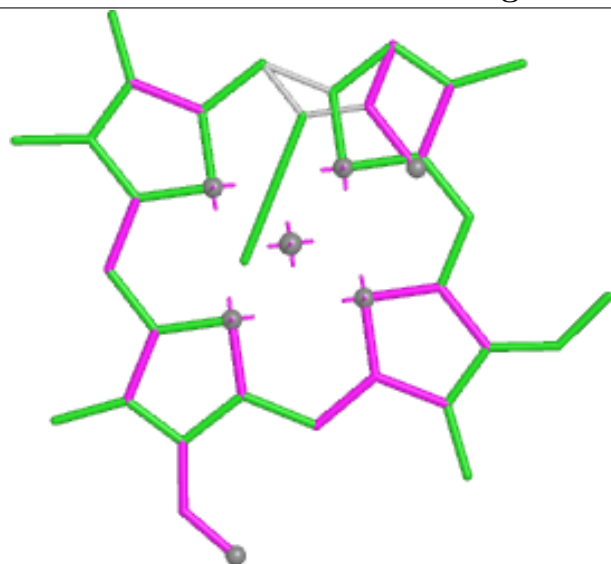




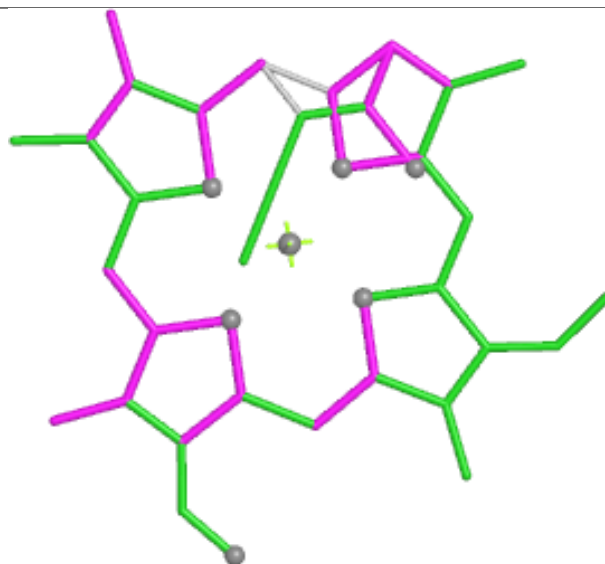




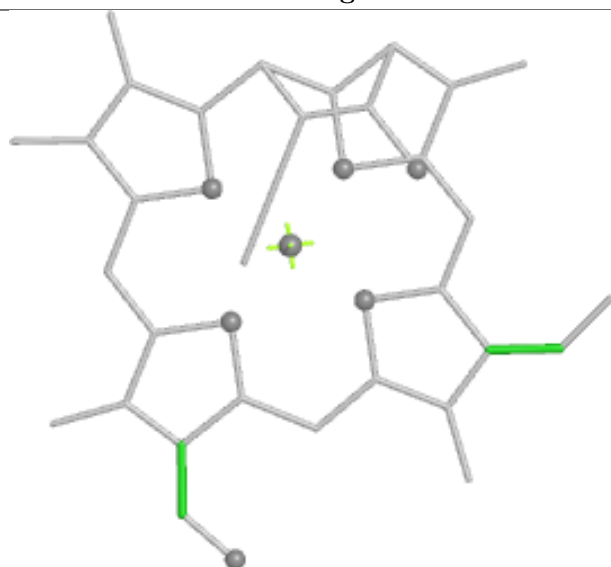
Ligand CL7 aB 3012



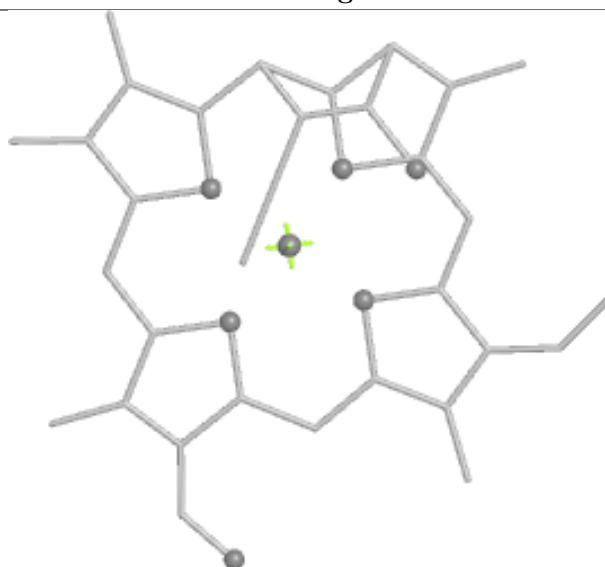
Bond lengths



Bond angles

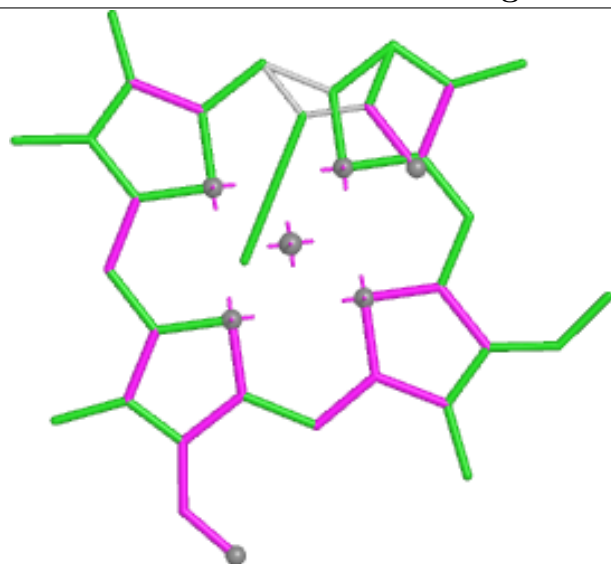


Torsions

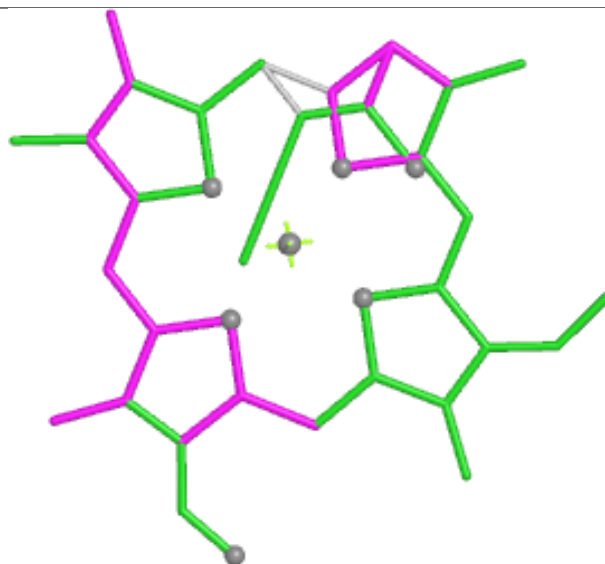


Rings

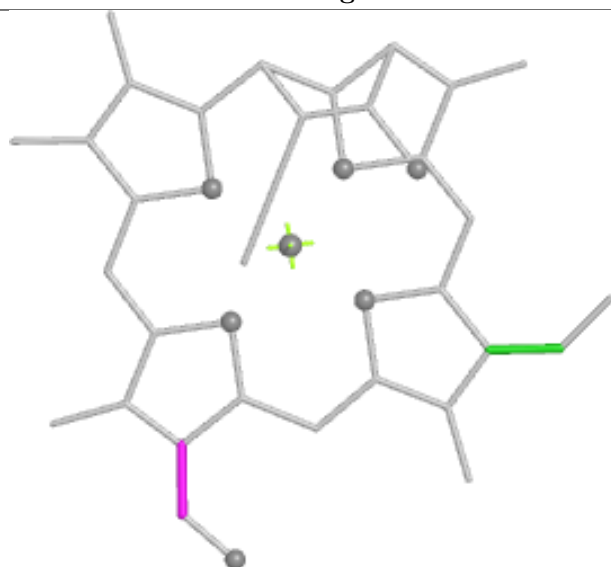
Ligand CL7 cA 3111



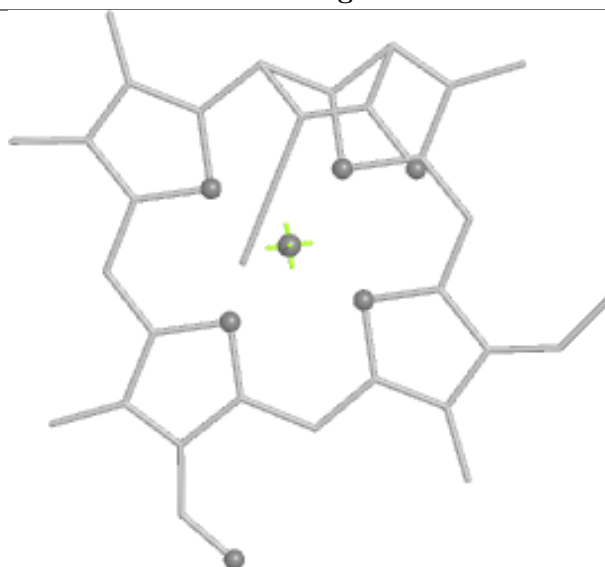
Bond lengths



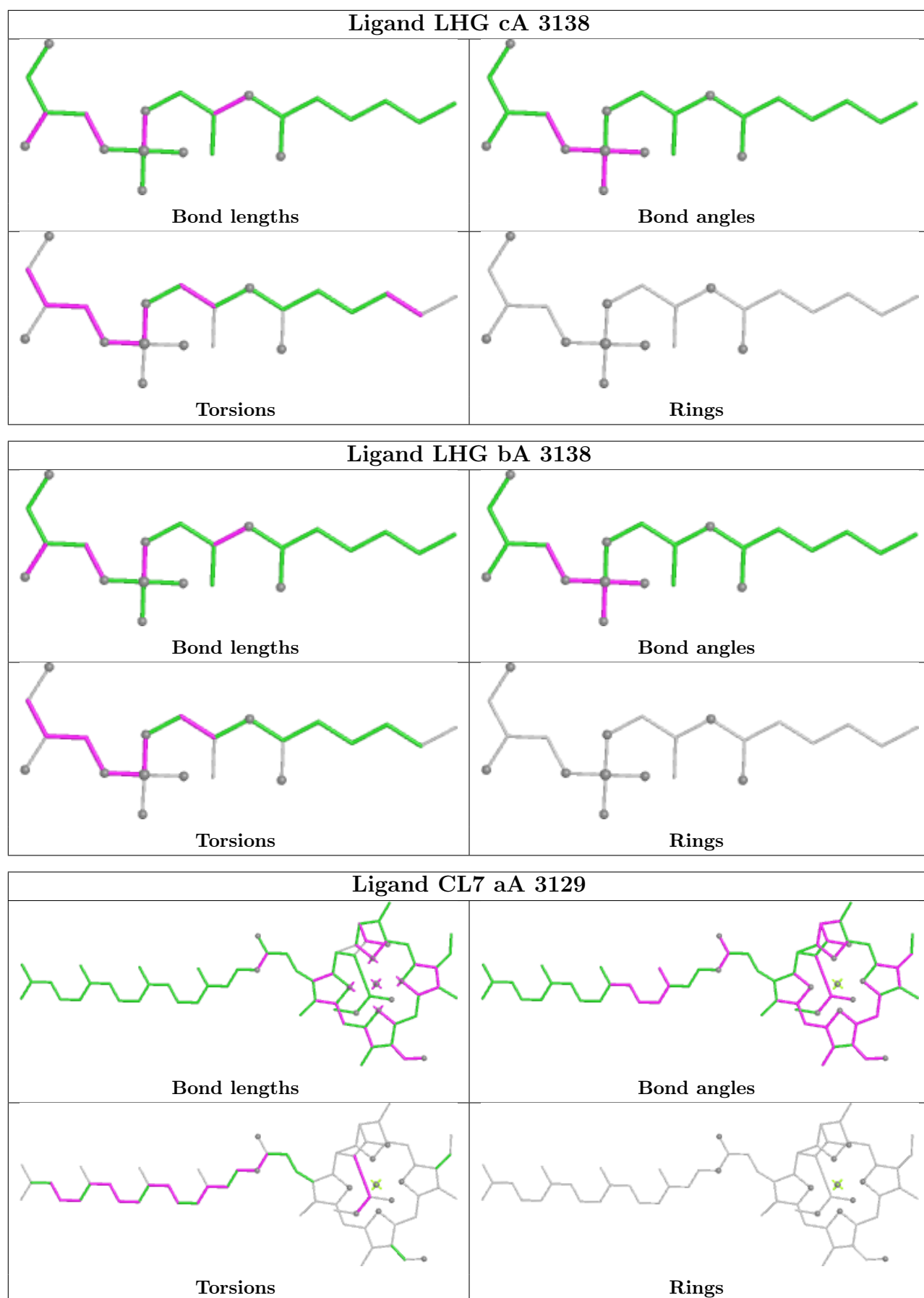
Bond angles

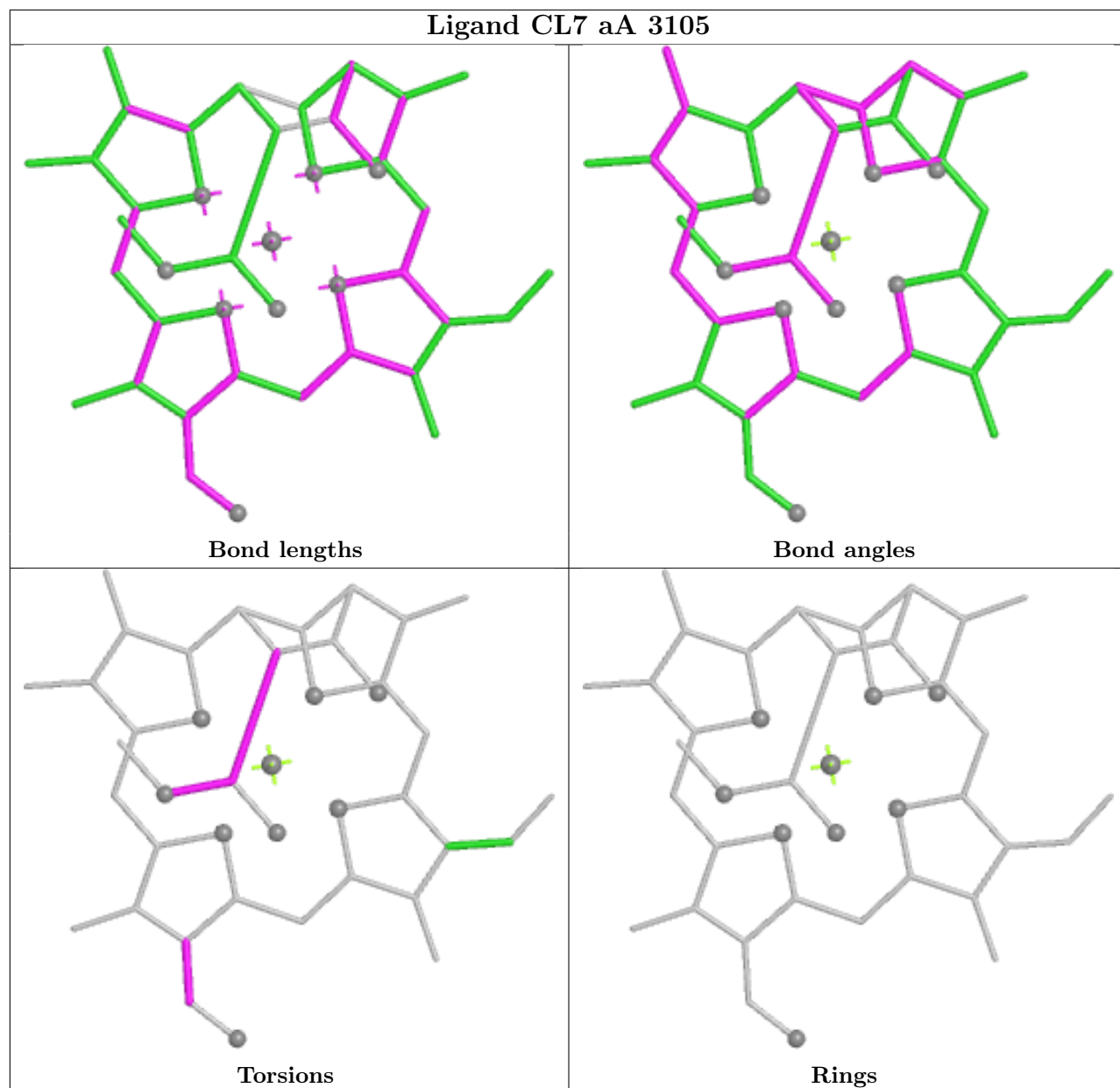


Torsions

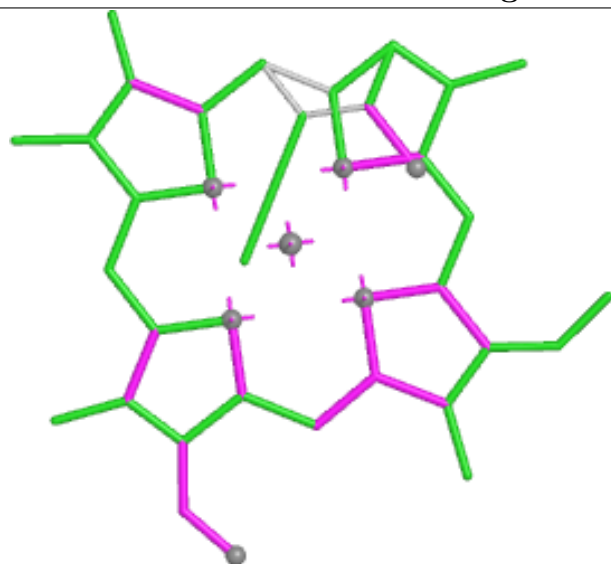


Rings

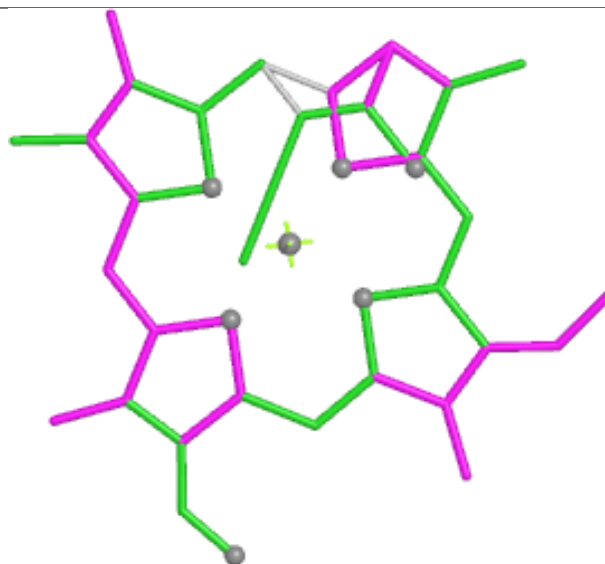




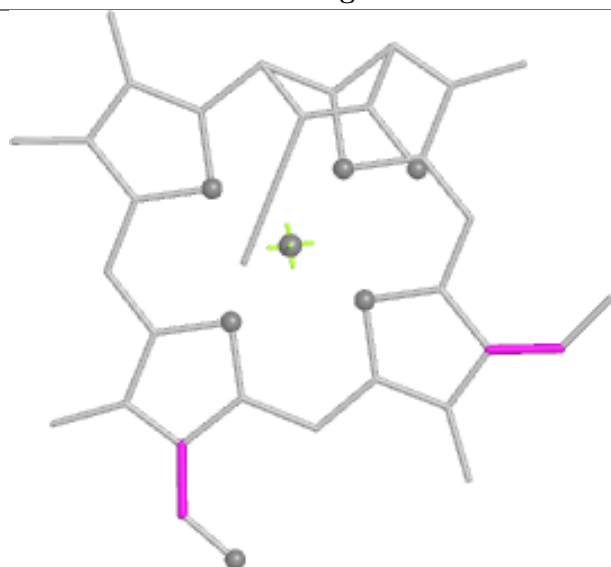
Ligand CL7 aA 3116



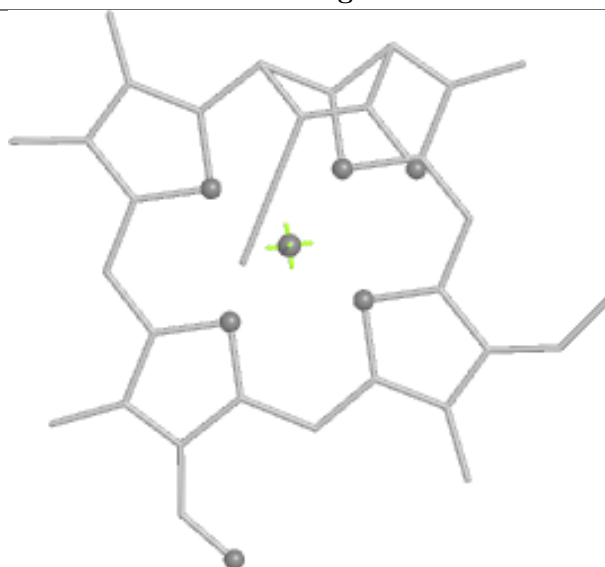
Bond lengths



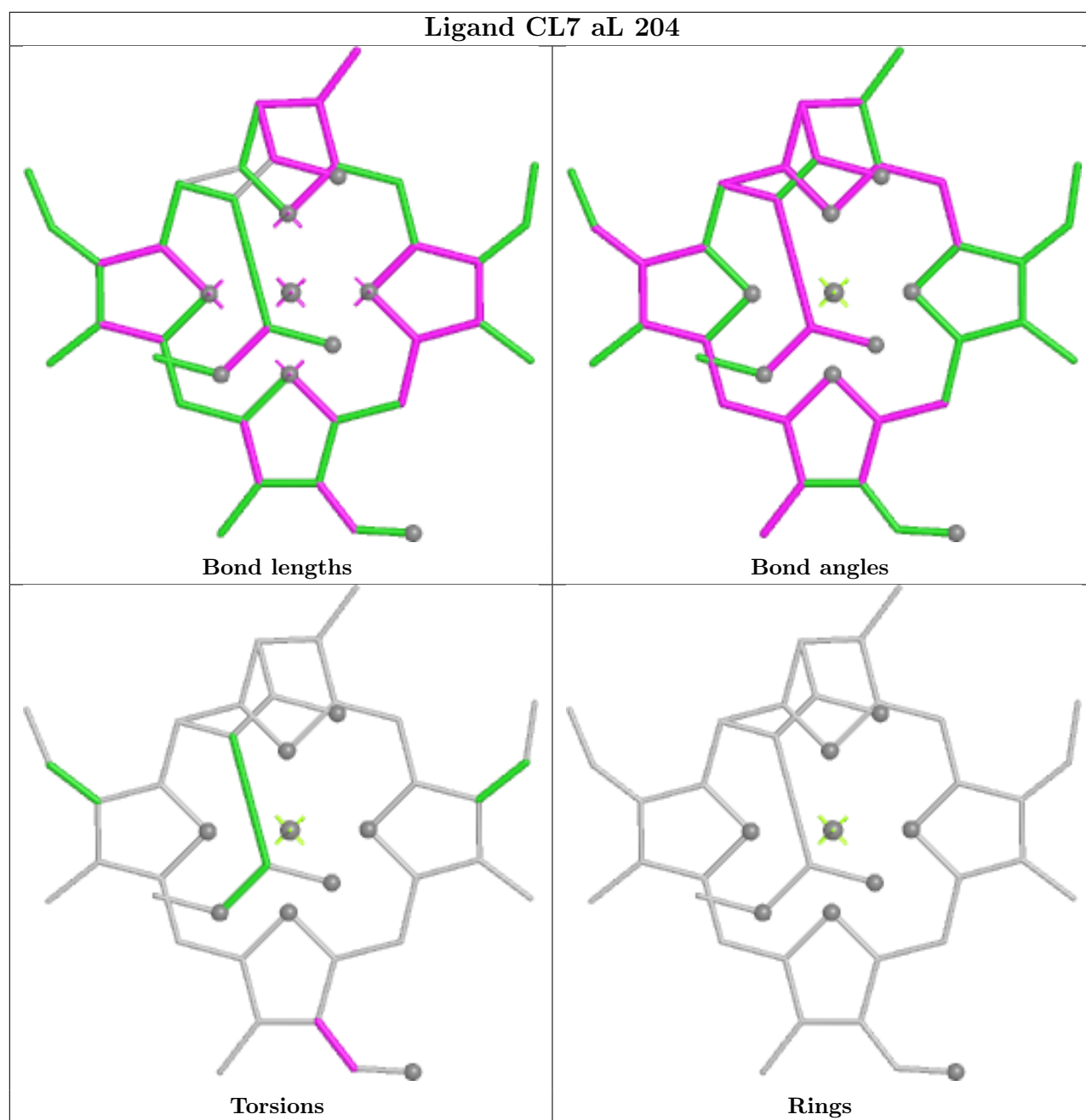
Bond angles

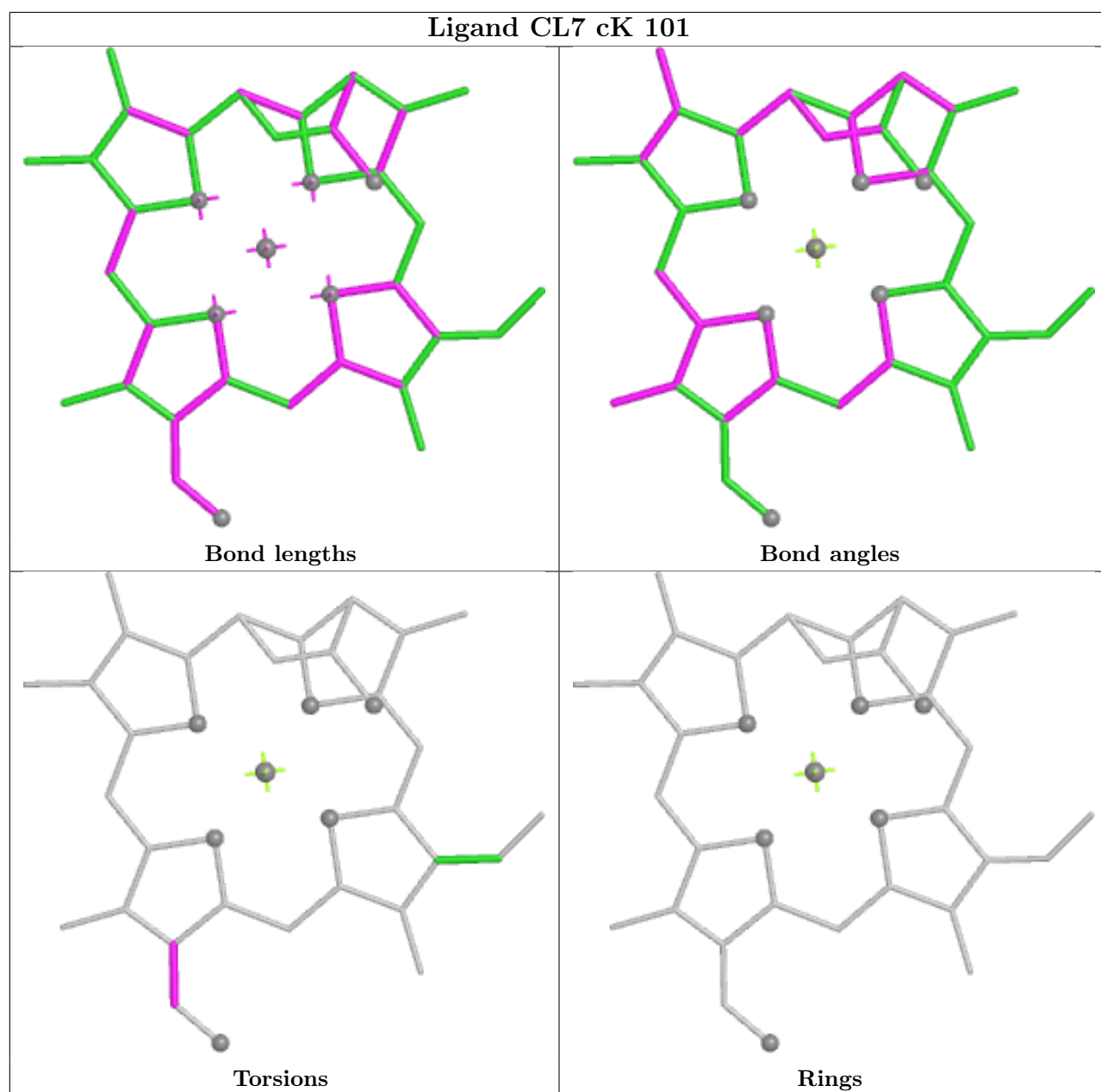


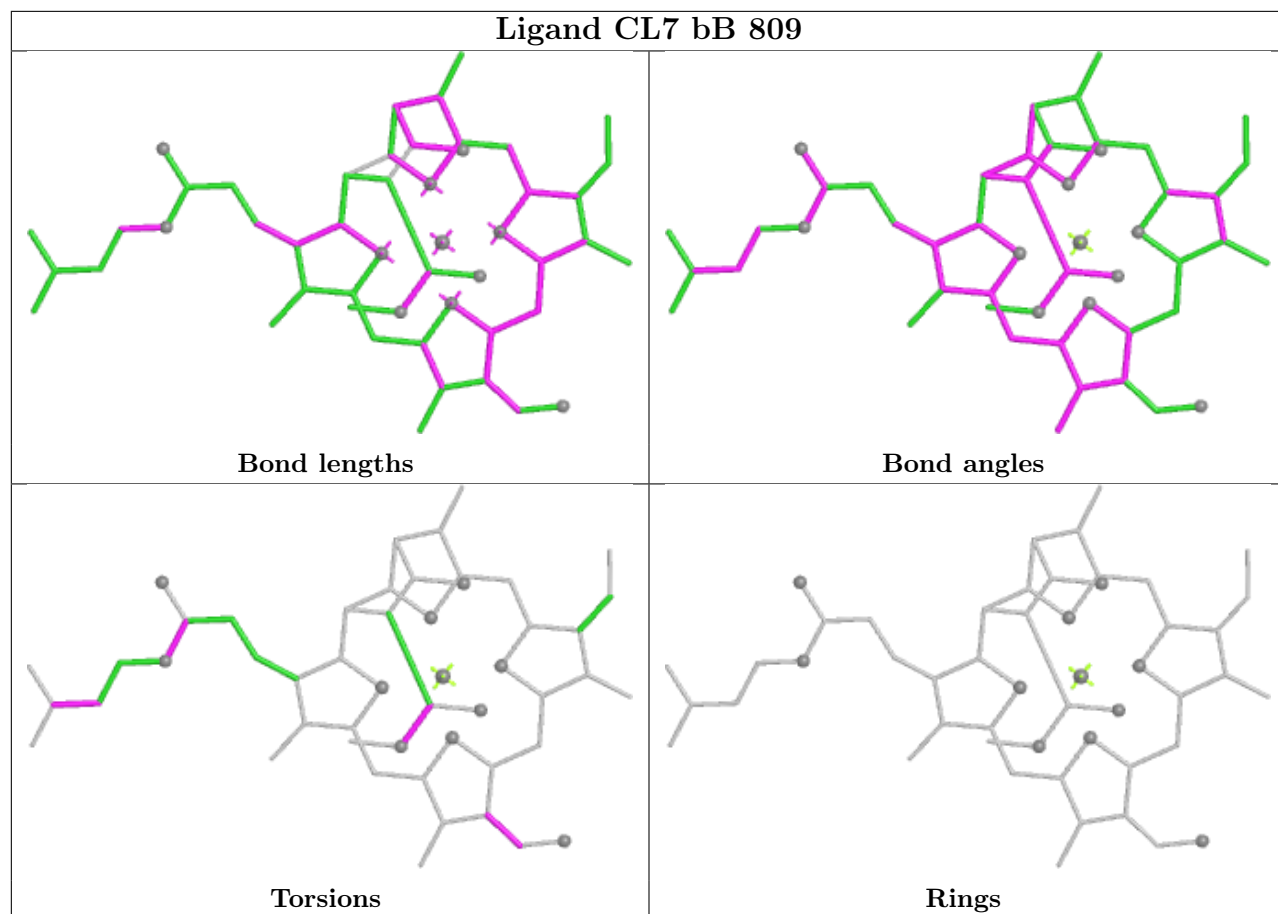
Torsions



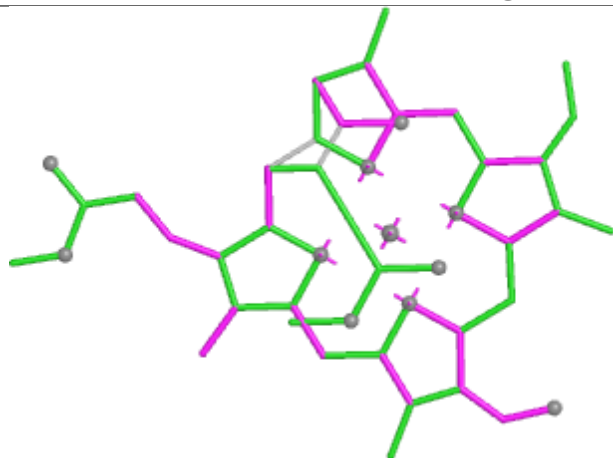
Rings



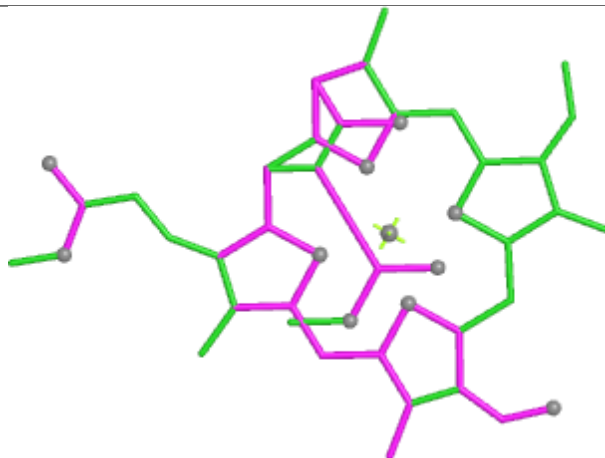




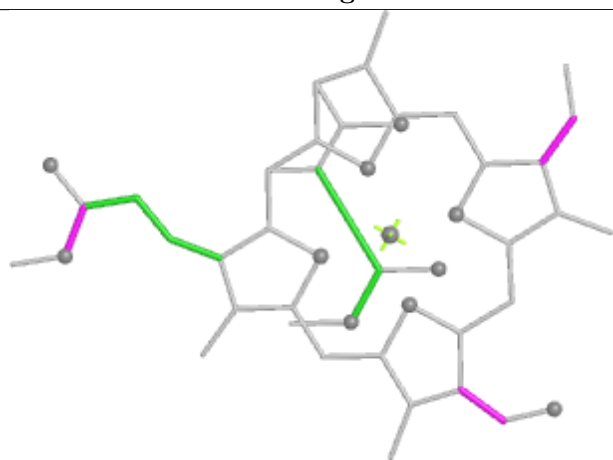
Ligand CL7 bA 3119



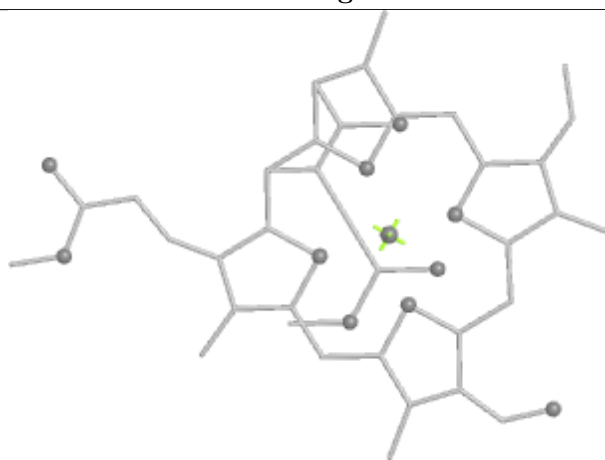
Bond lengths



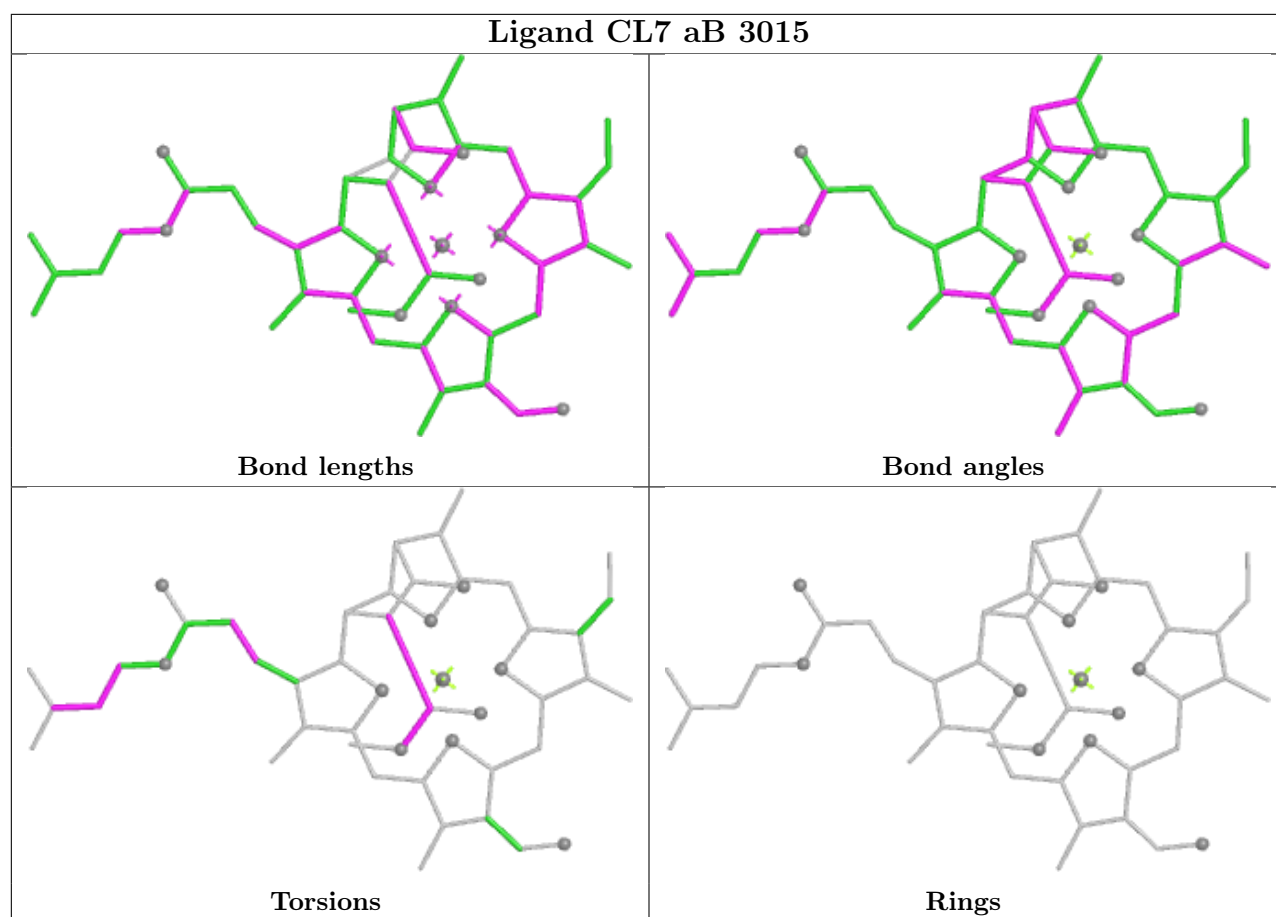
Bond angles

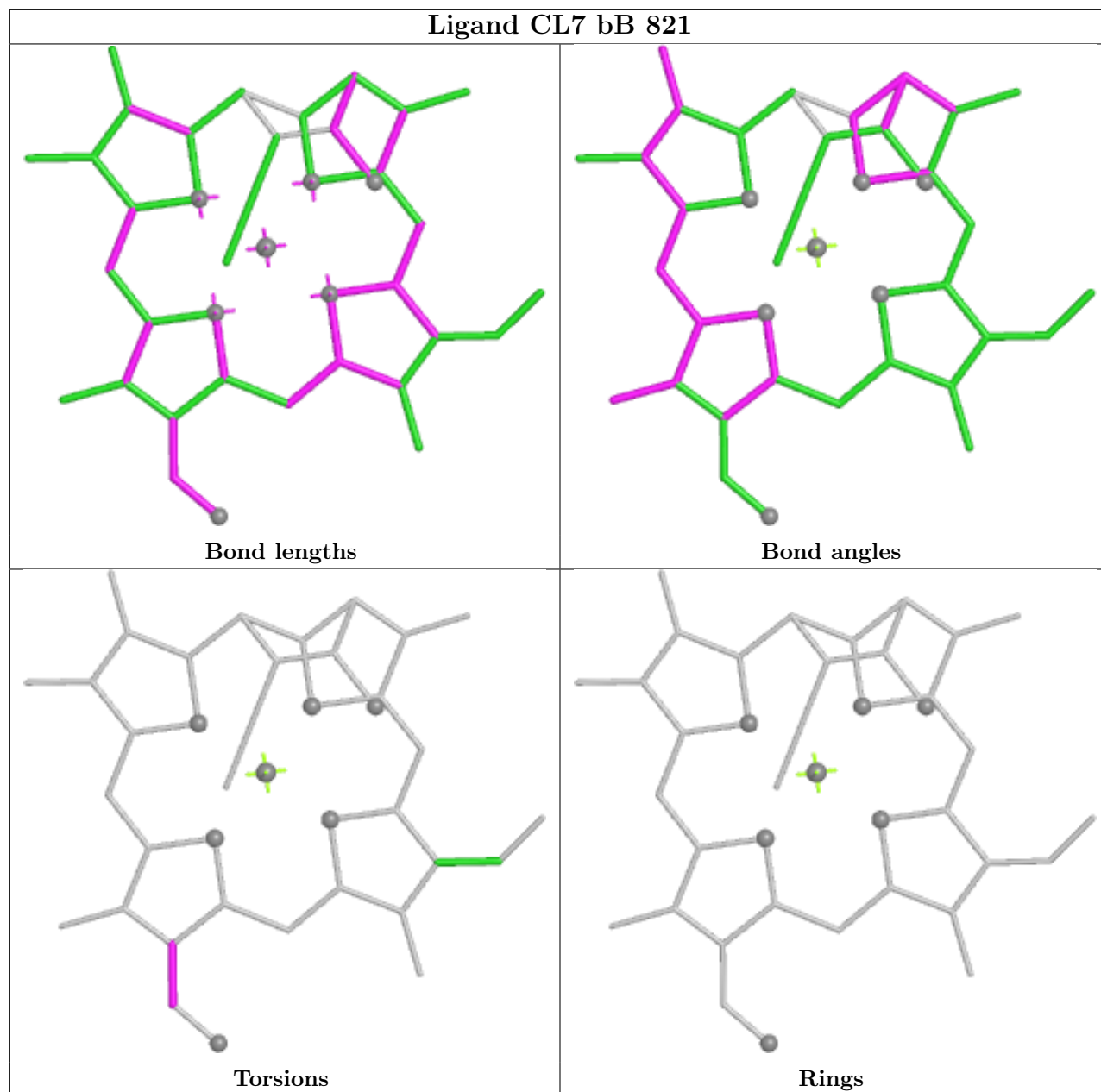


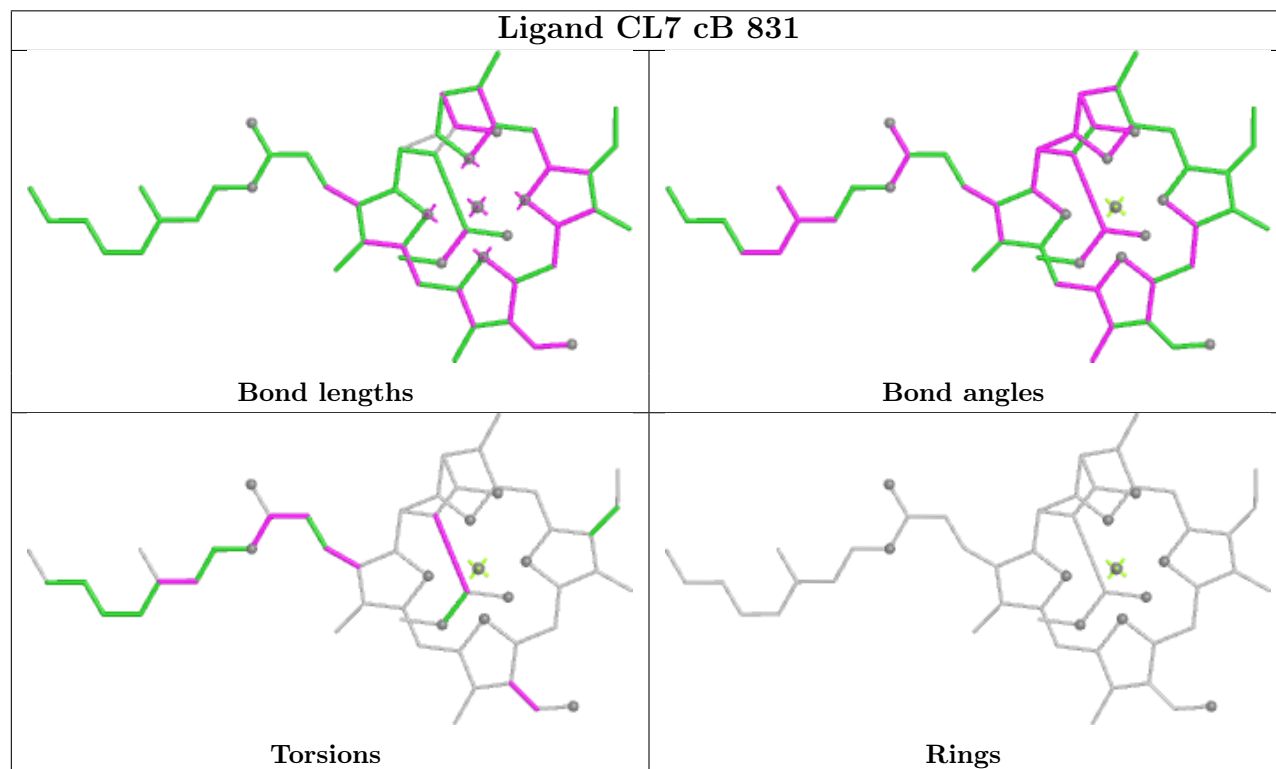
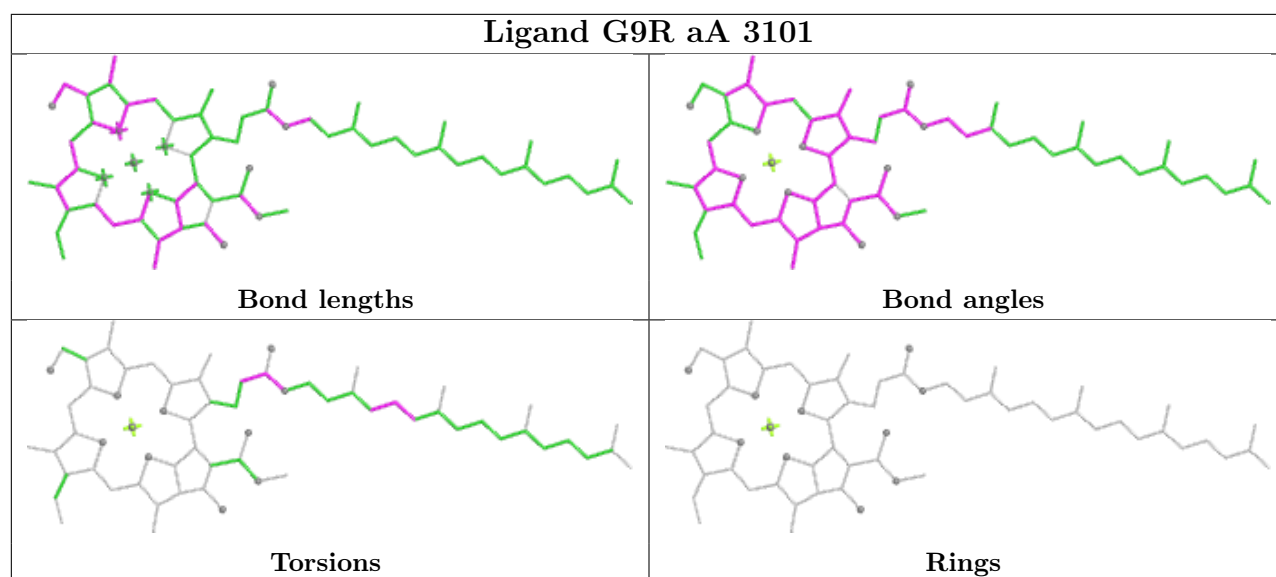
Torsions



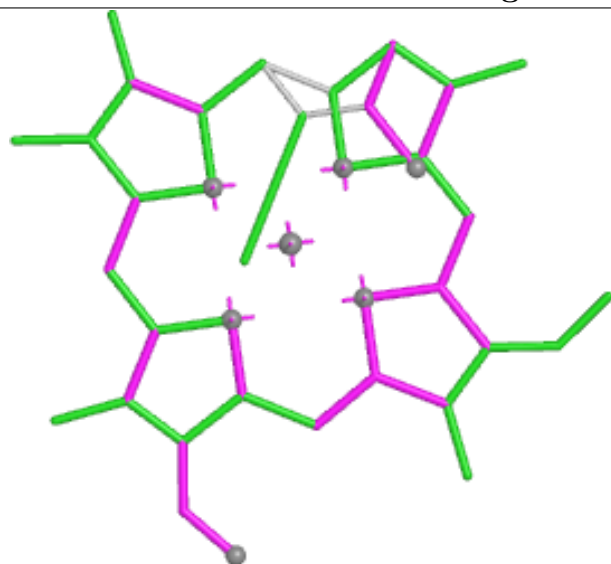
Rings



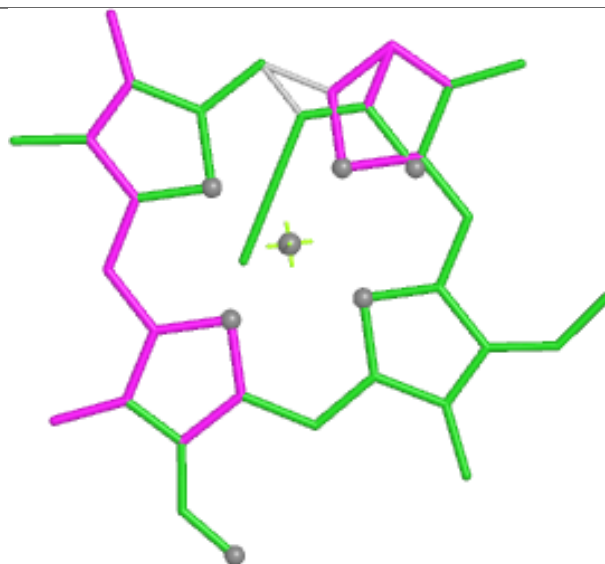




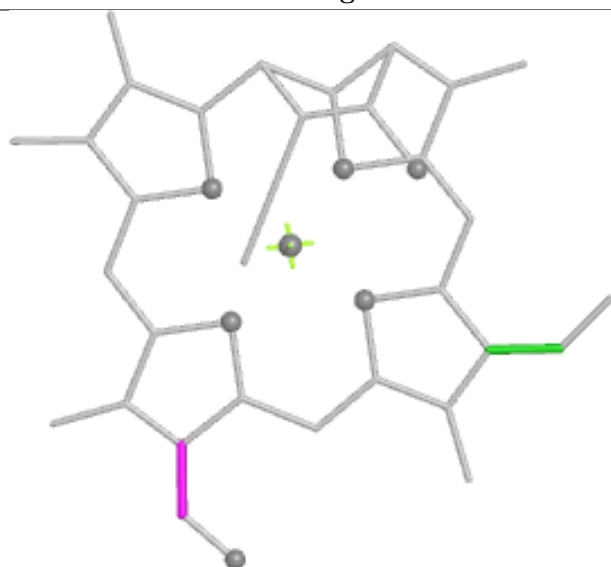
Ligand CL7 aB 3020



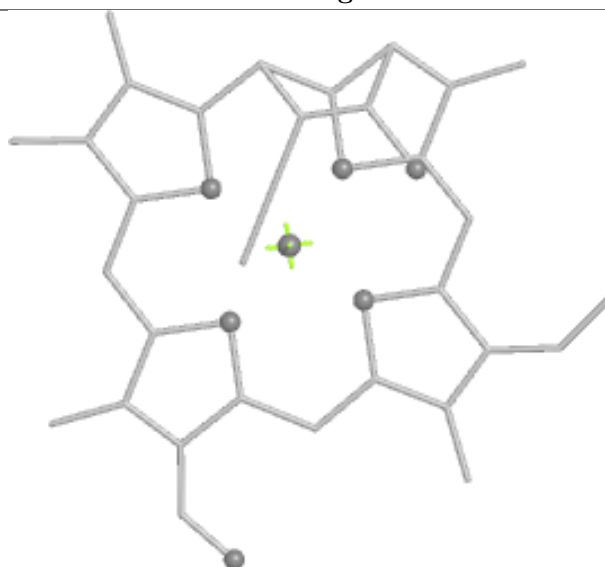
Bond lengths



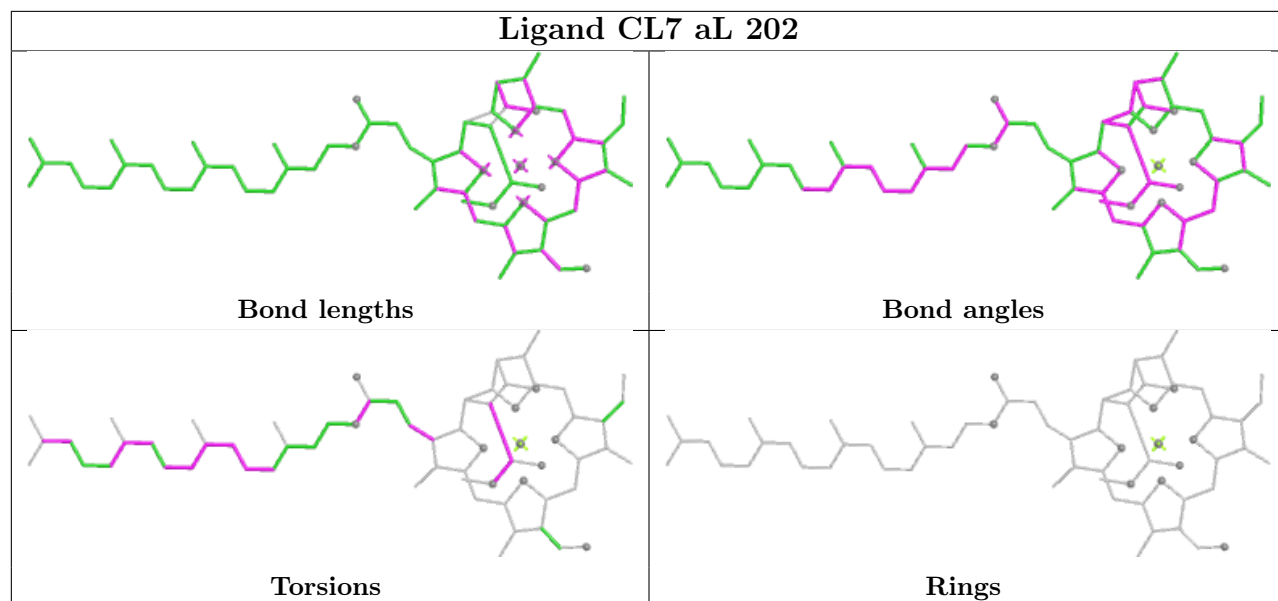
Bond angles



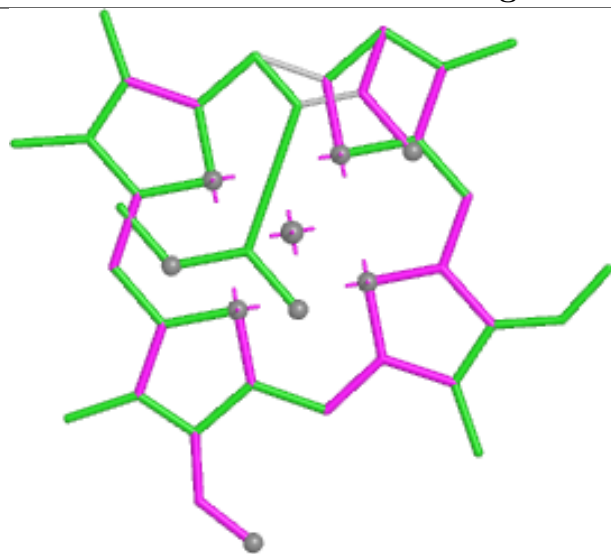
Torsions



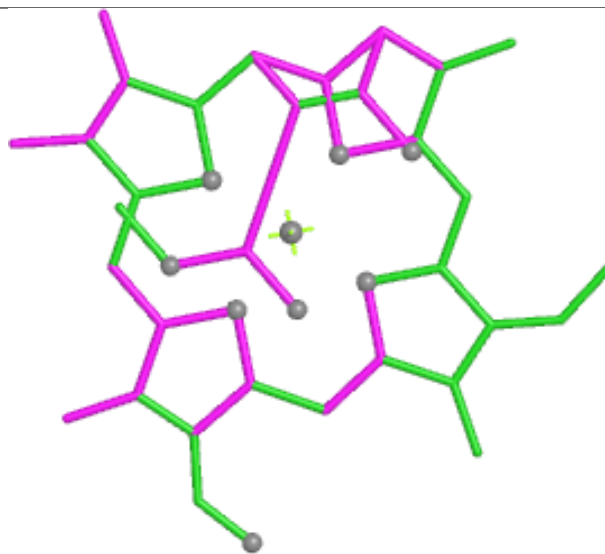
Rings



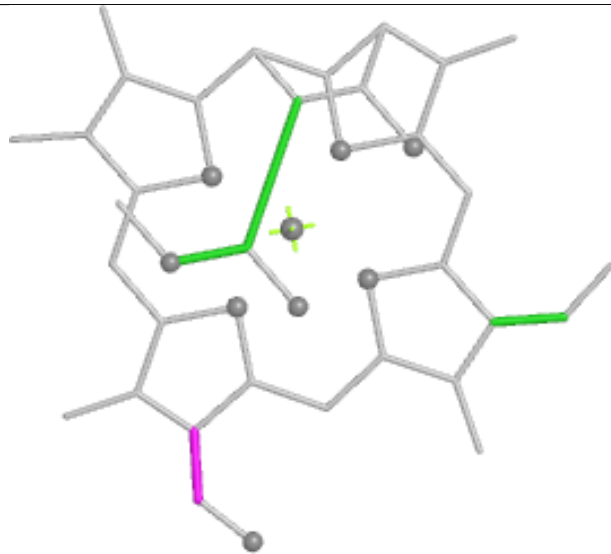
Ligand CL7 bA 3113



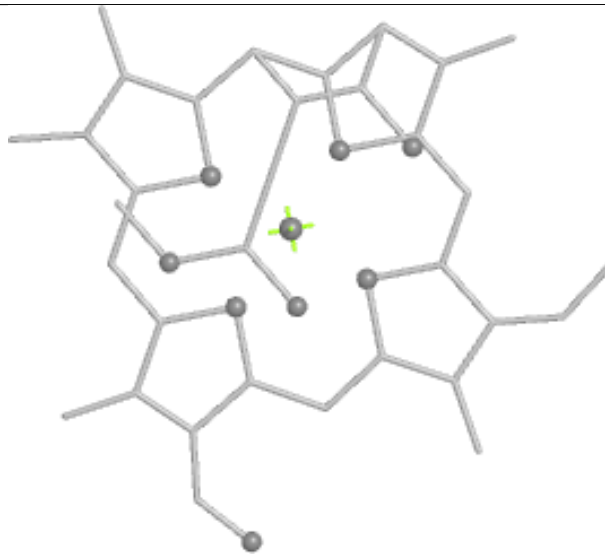
Bond lengths



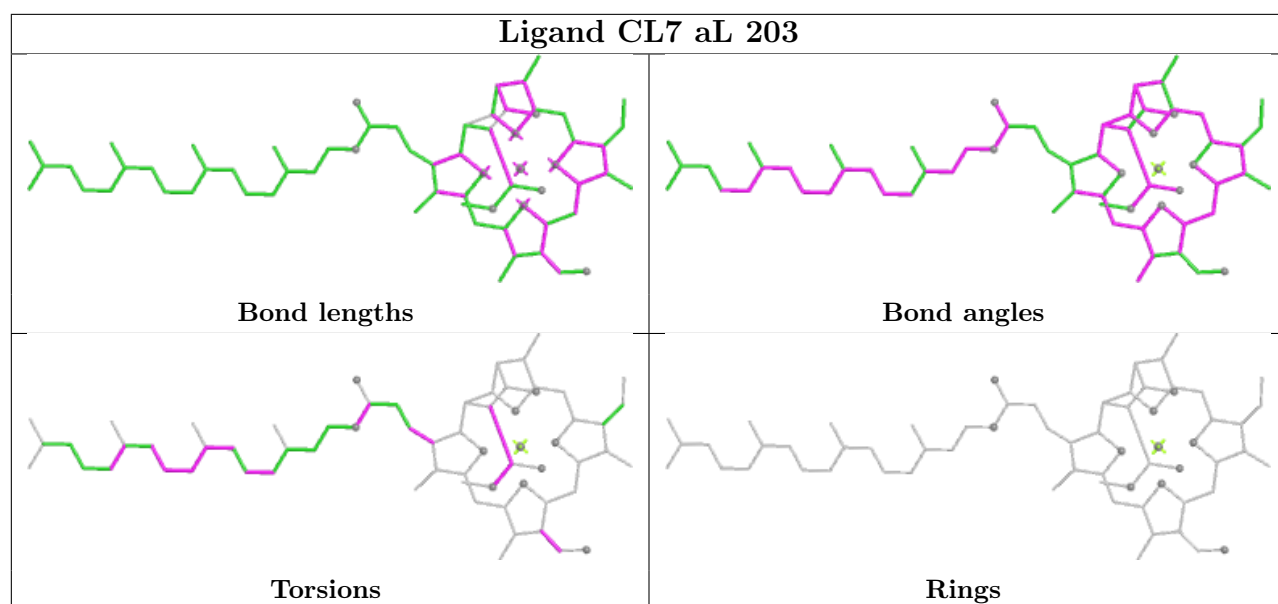
Bond angles



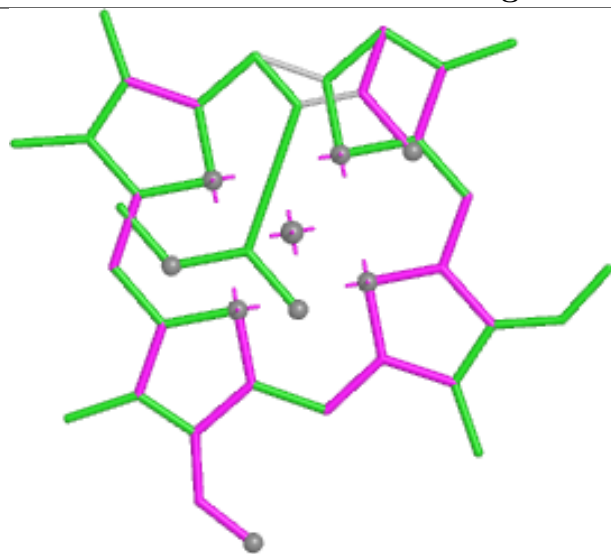
Torsions



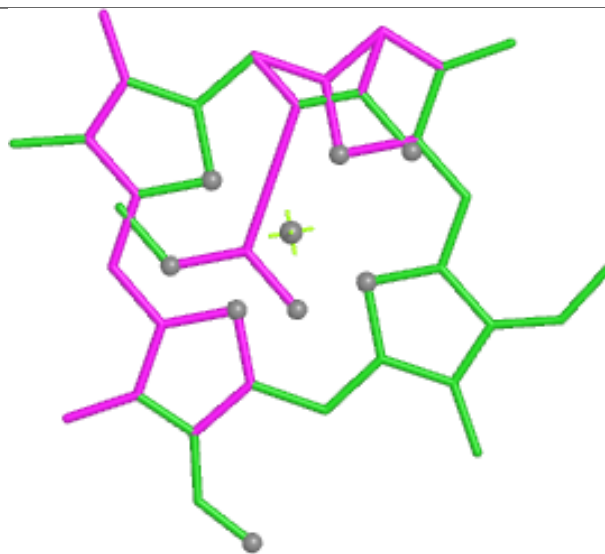
Rings



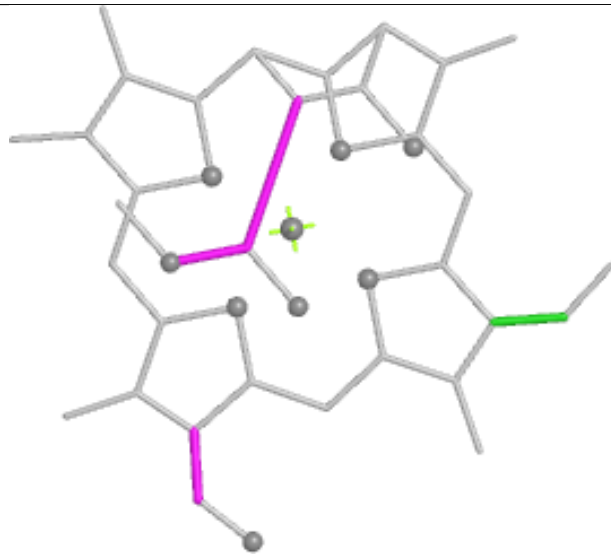
Ligand CL7 cA 3104



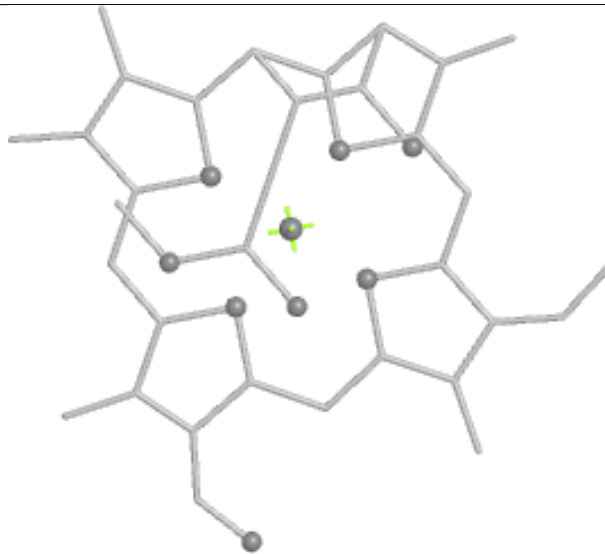
Bond lengths



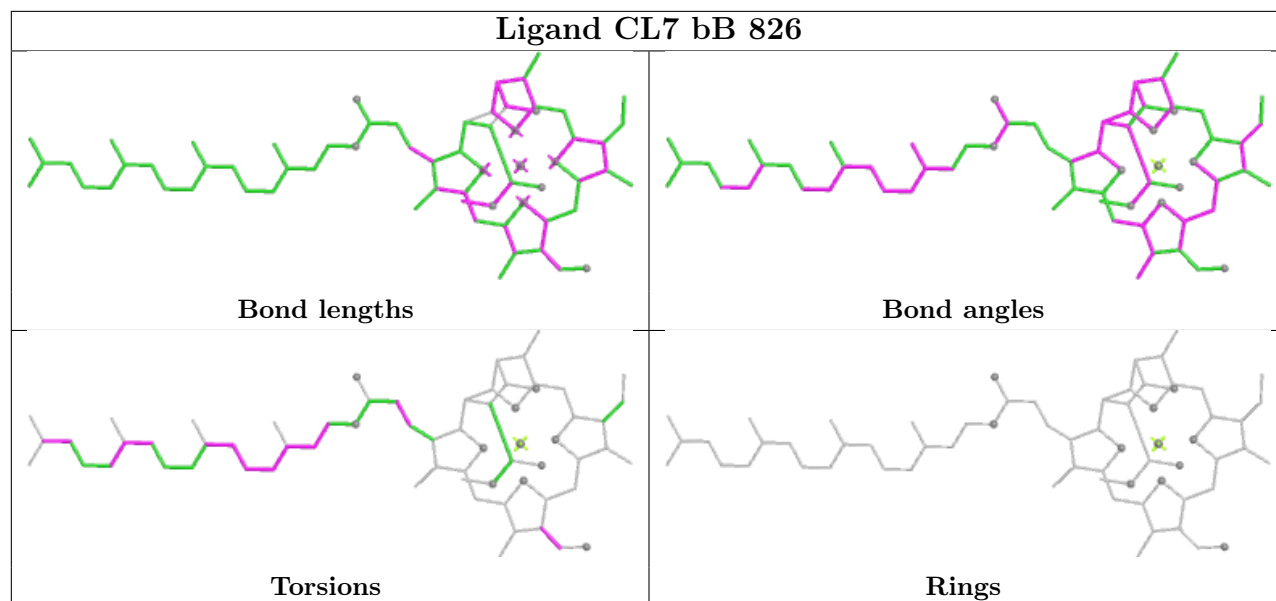
Bond angles

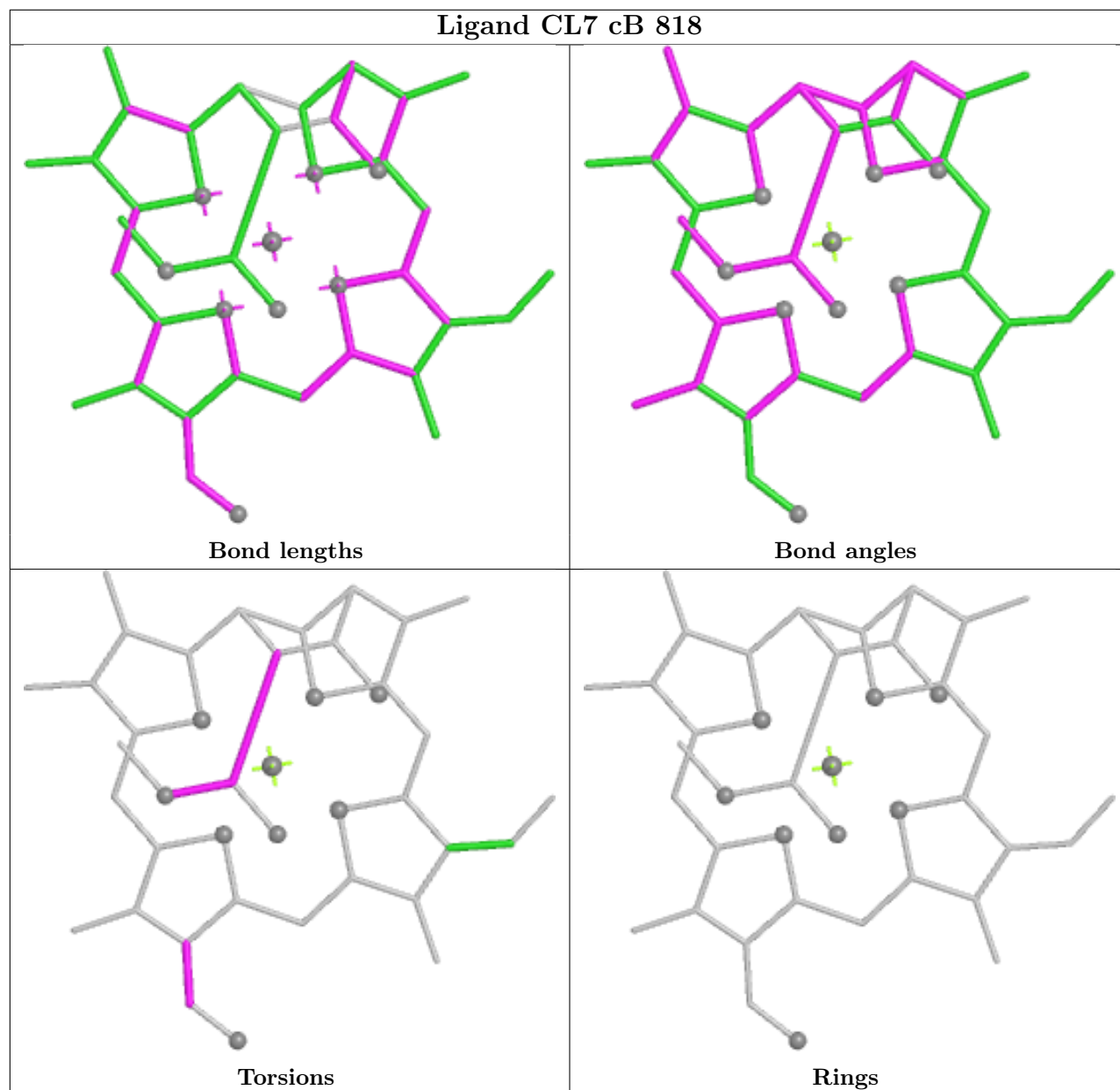


Torsions

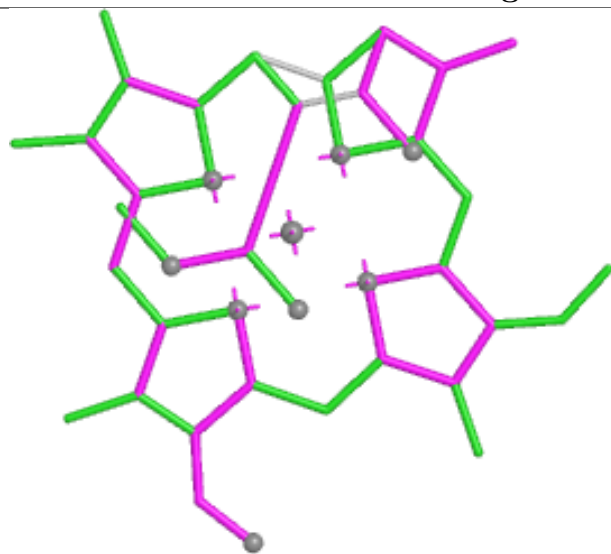


Rings

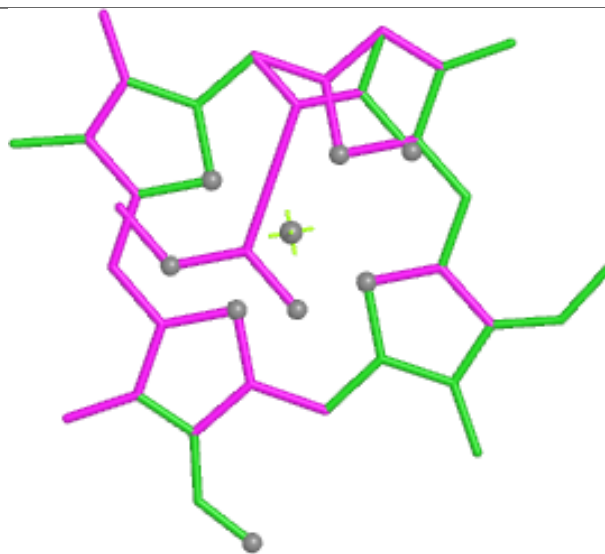




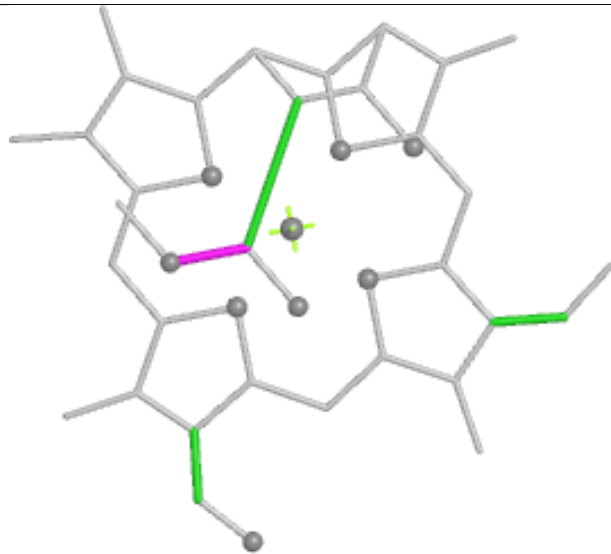
Ligand CL7 cA 3121



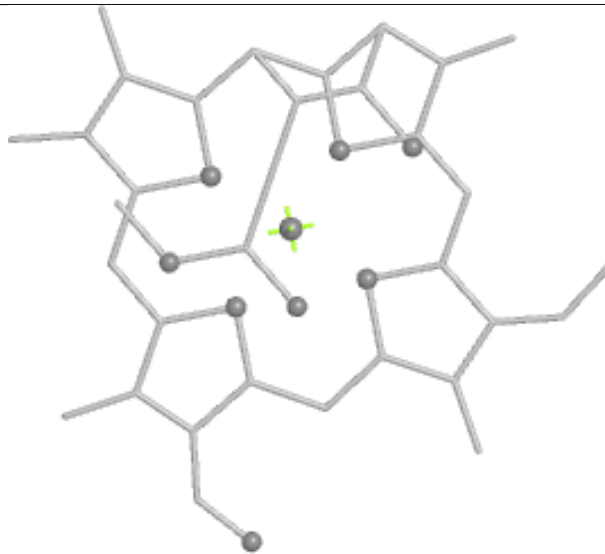
Bond lengths



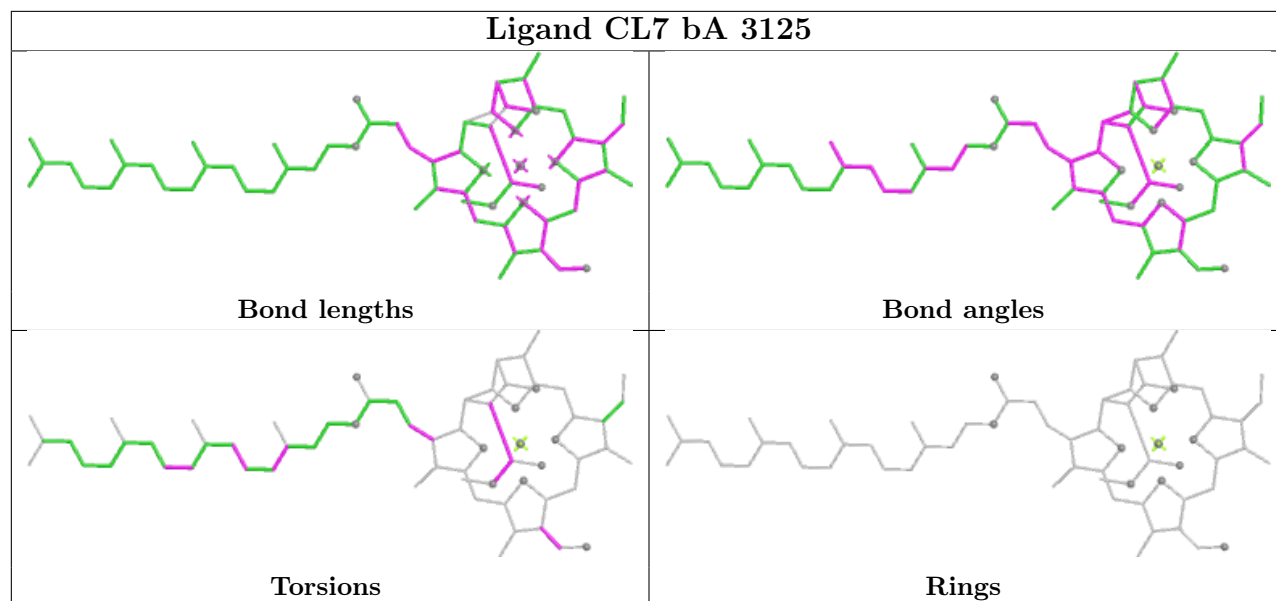
Bond angles

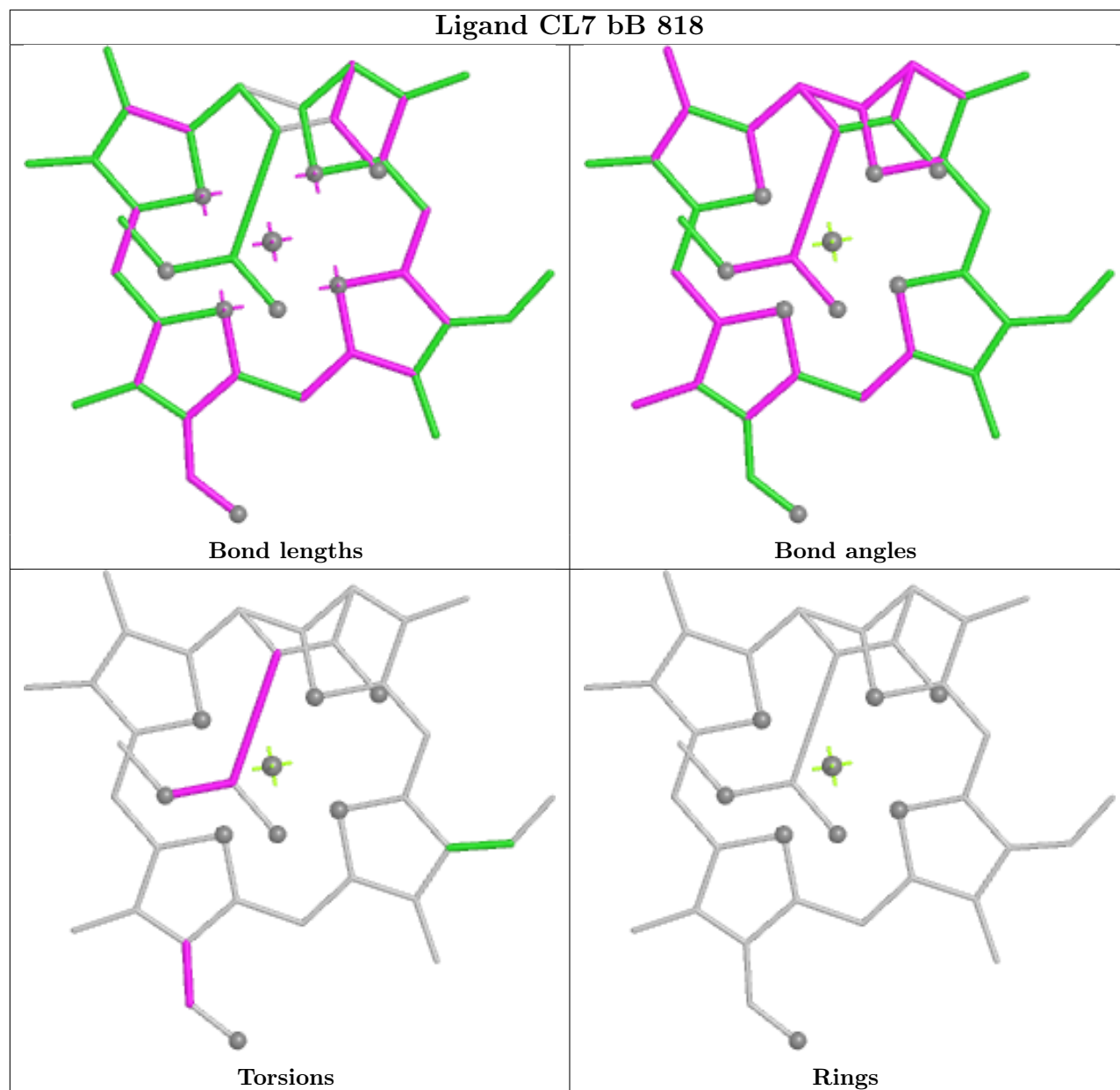


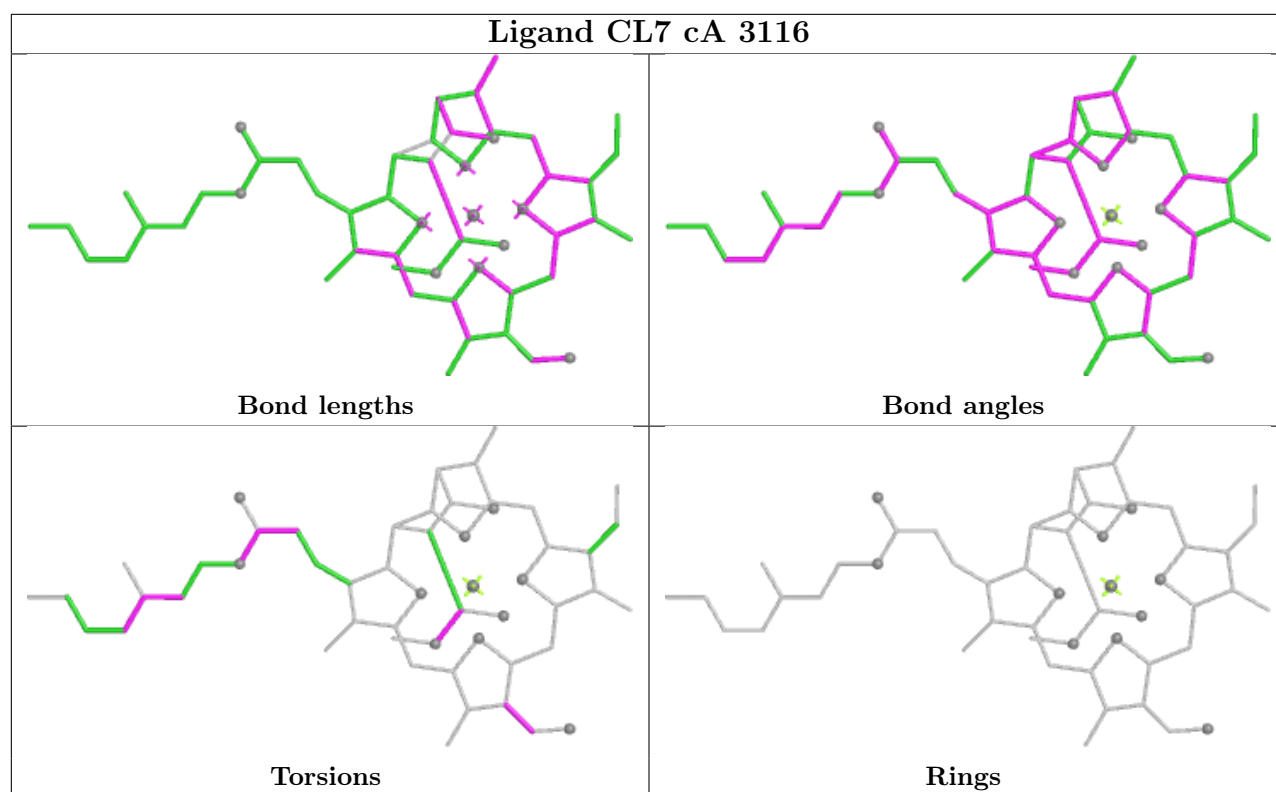
Torsions

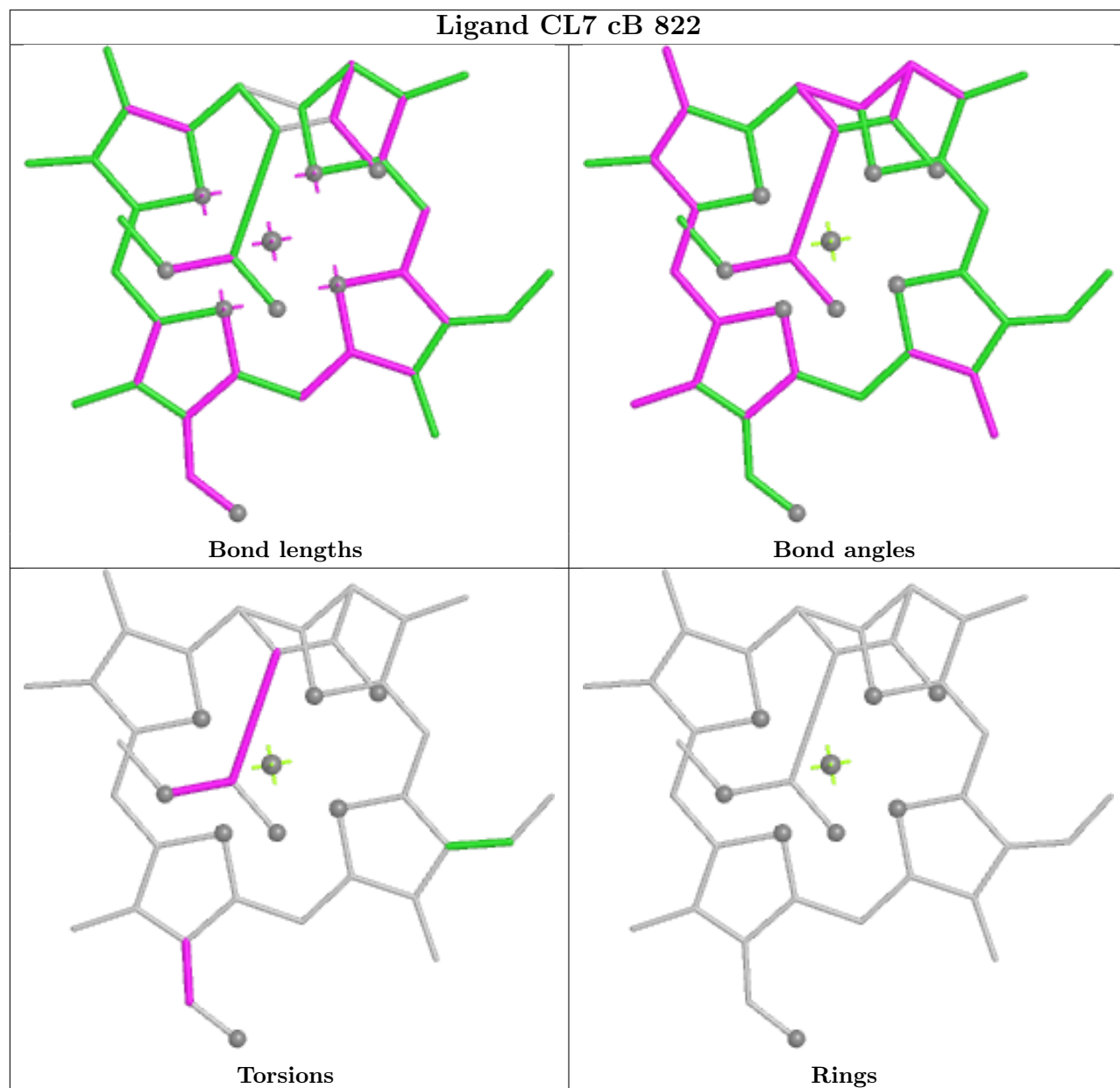


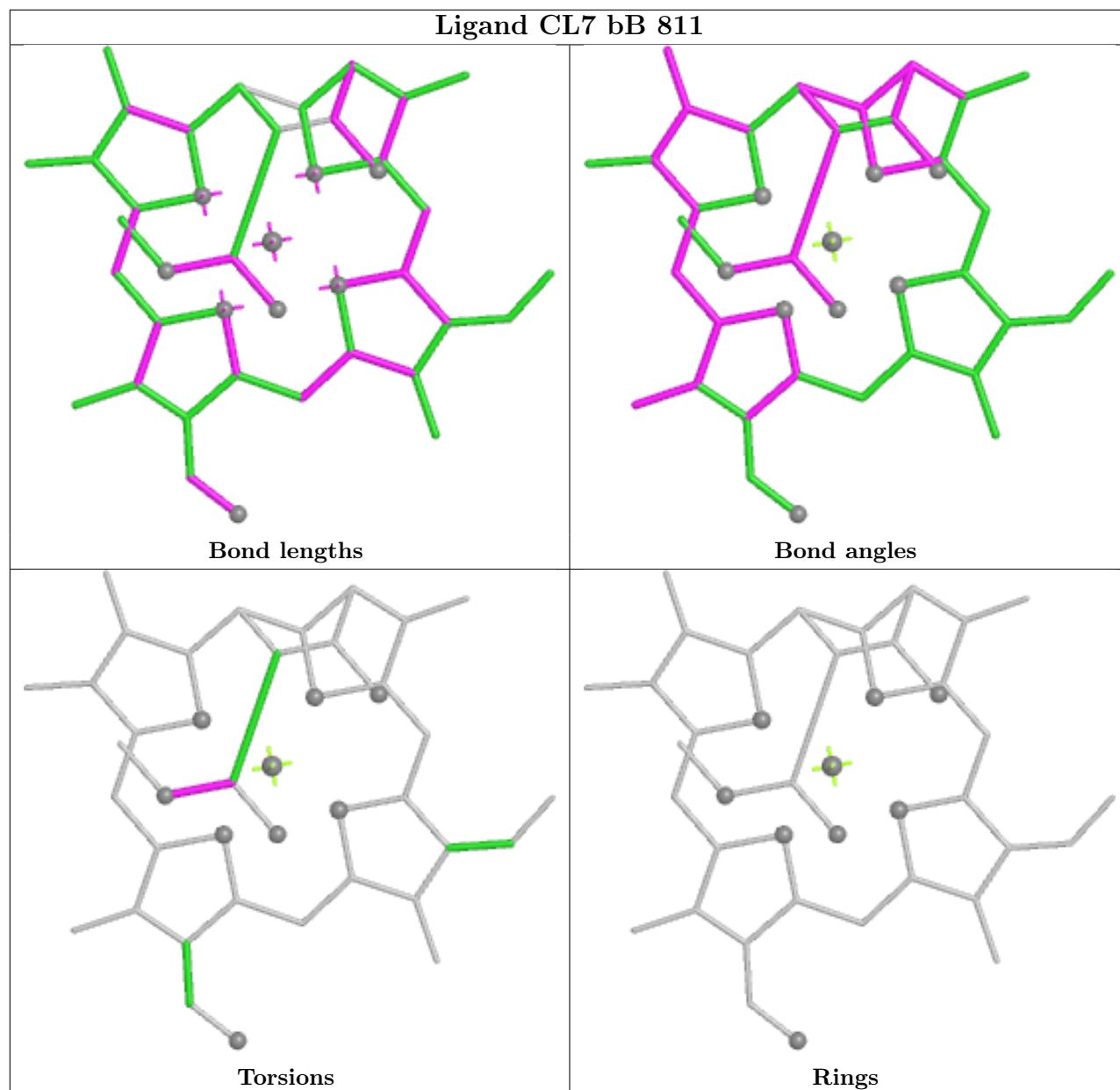
Rings

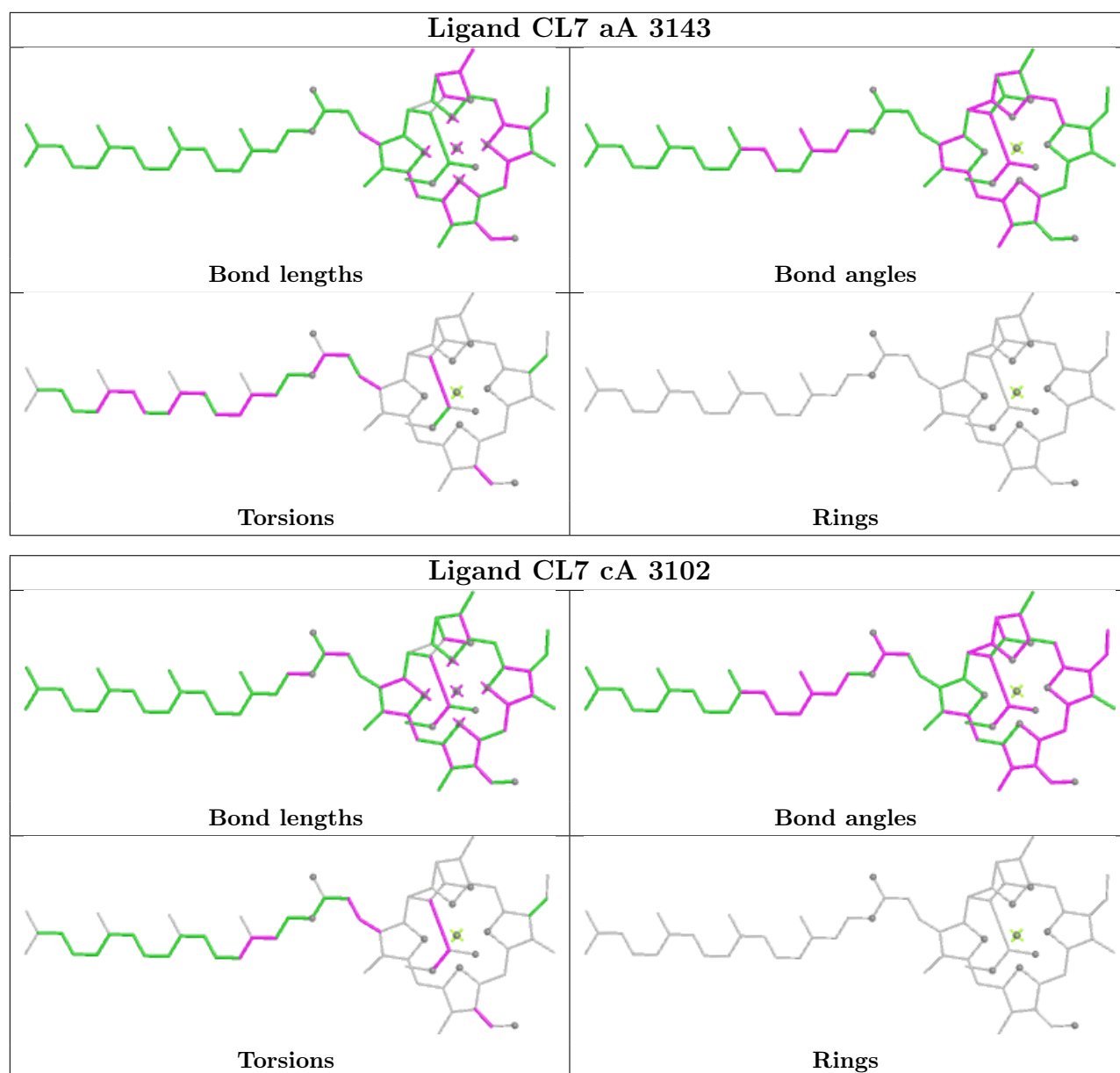


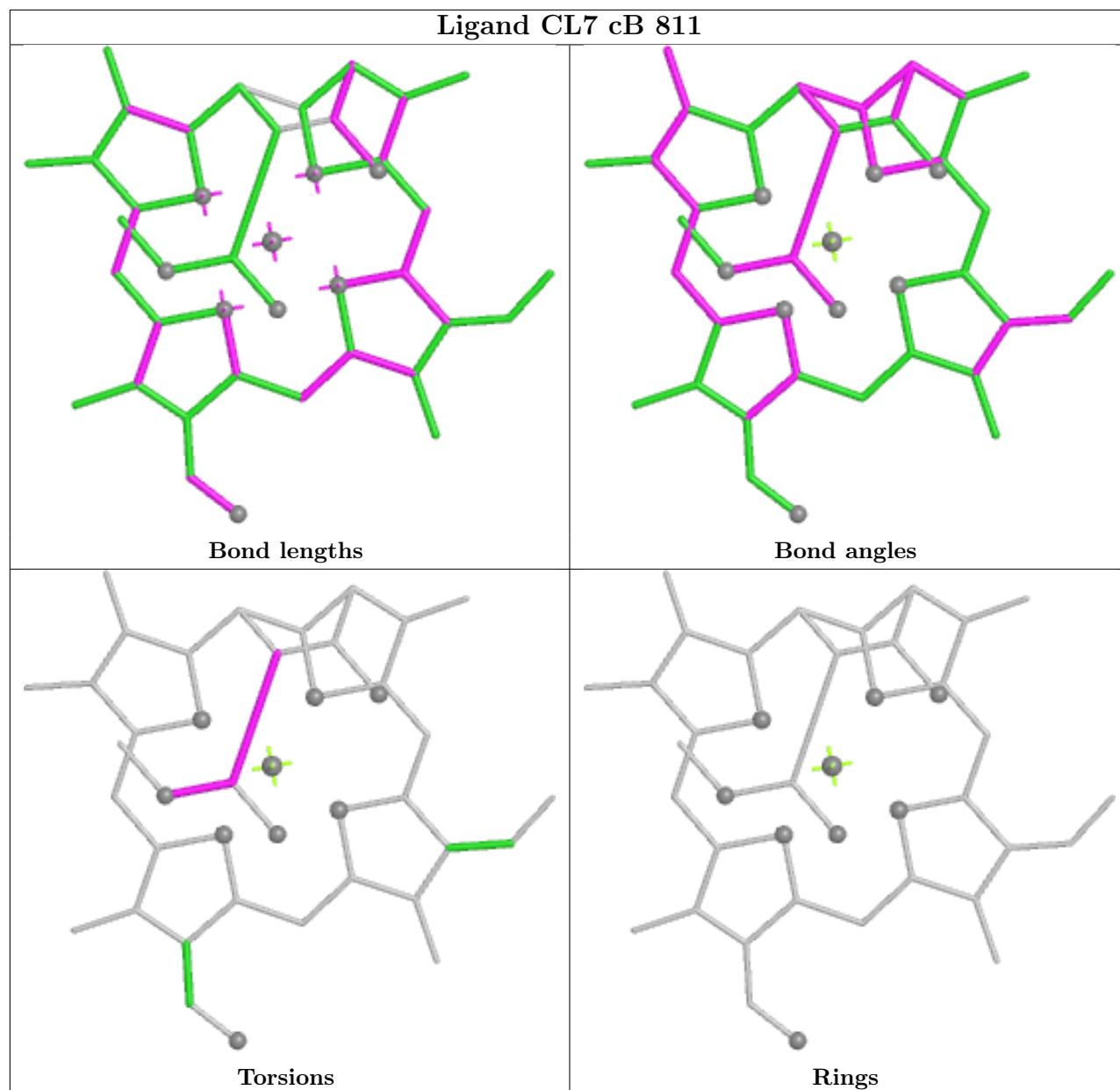


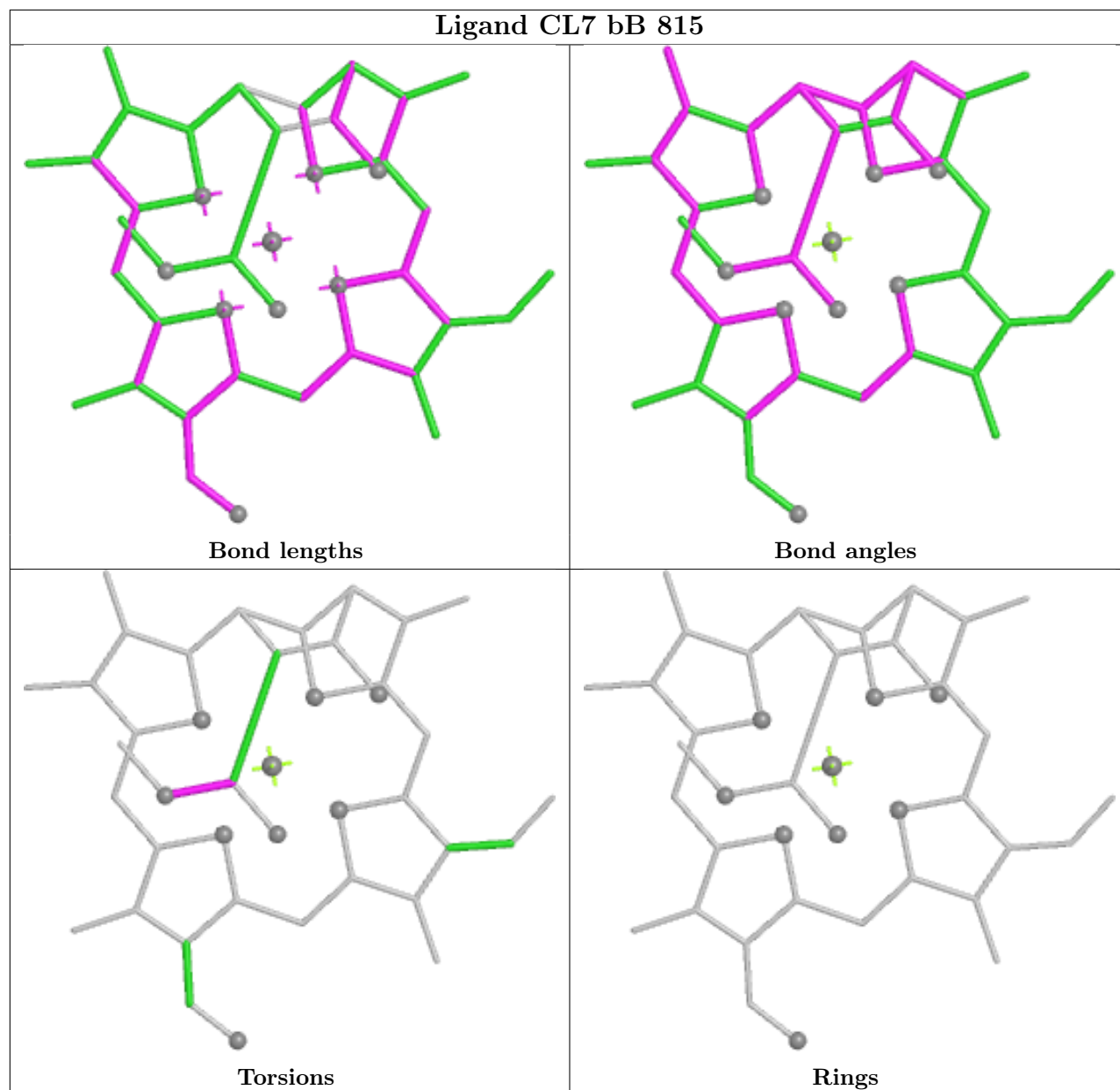


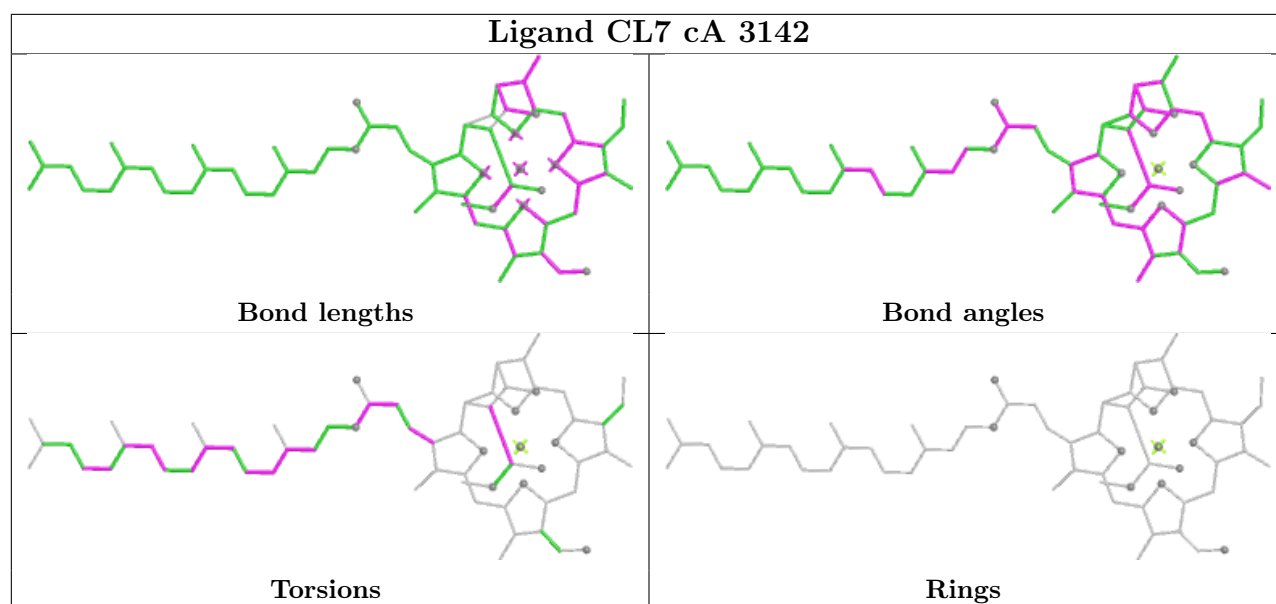




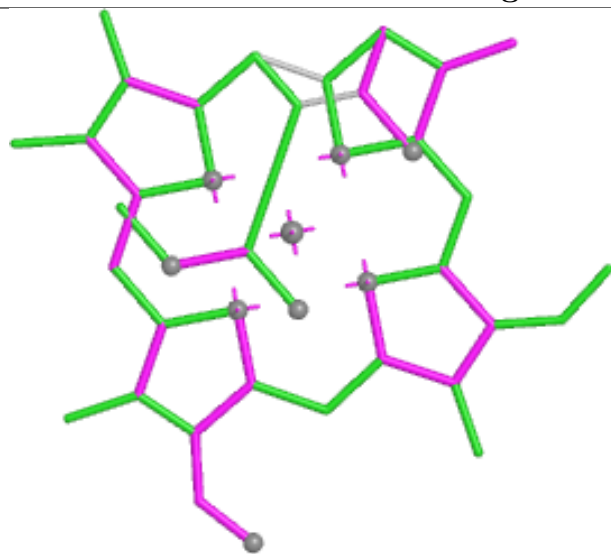




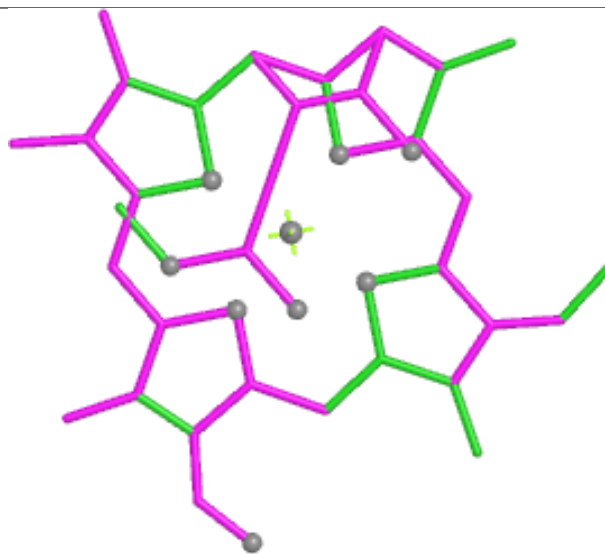




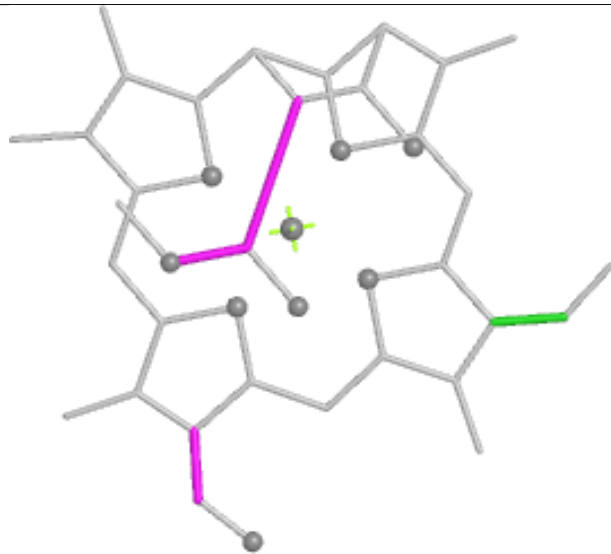
Ligand CL7 cA 3105



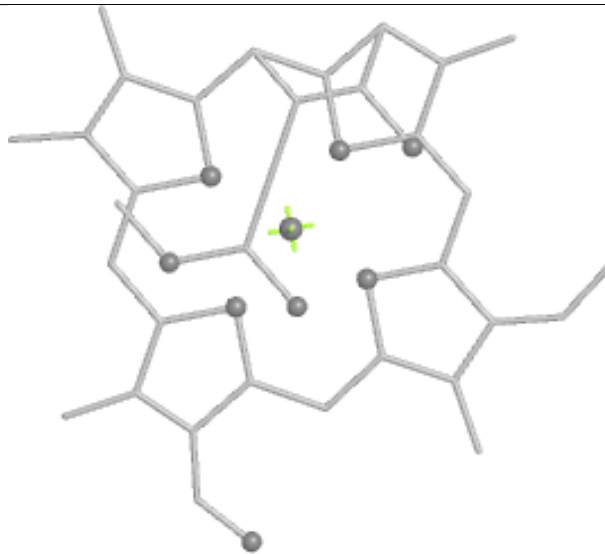
Bond lengths



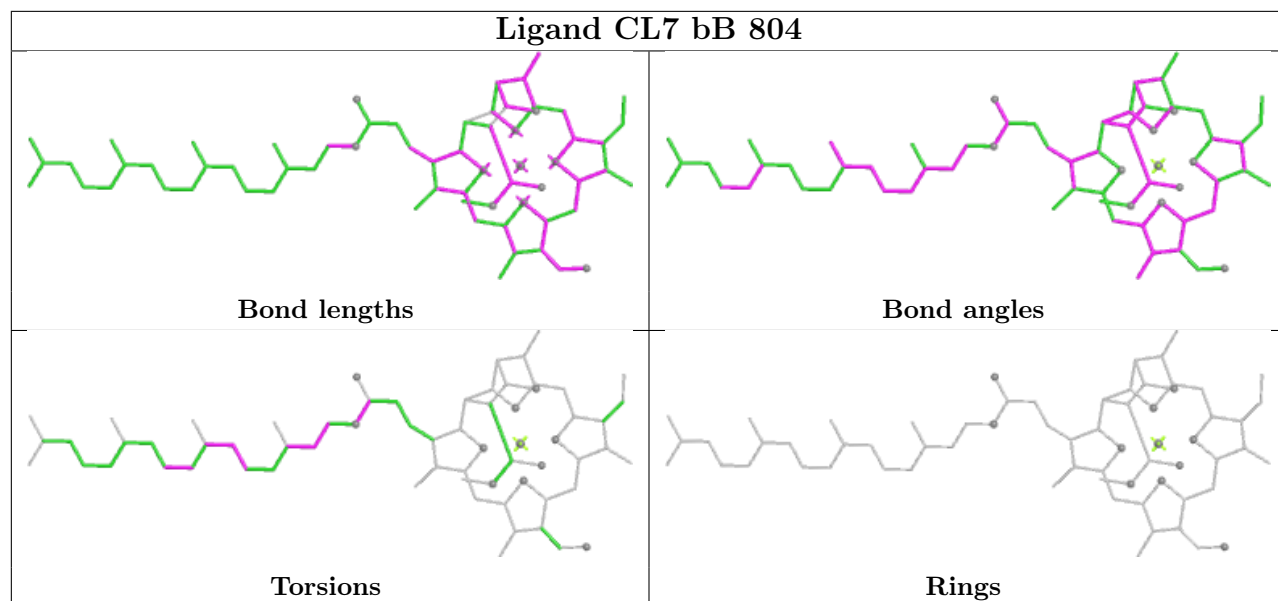
Bond angles



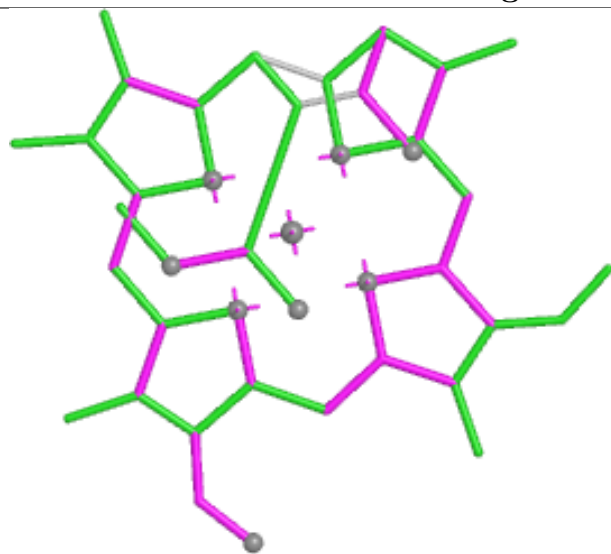
Torsions



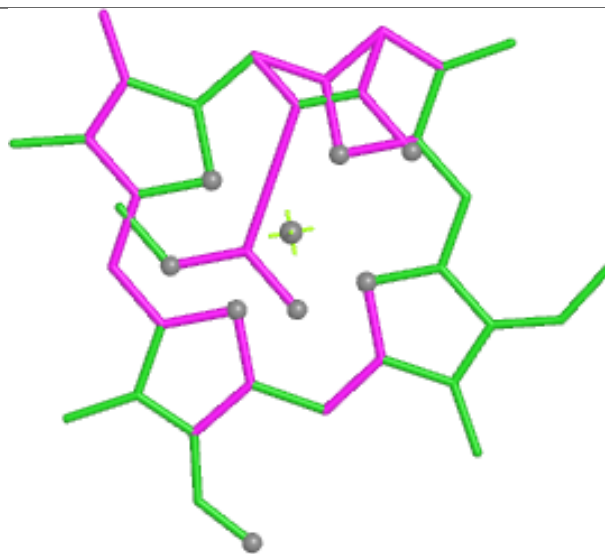
Rings



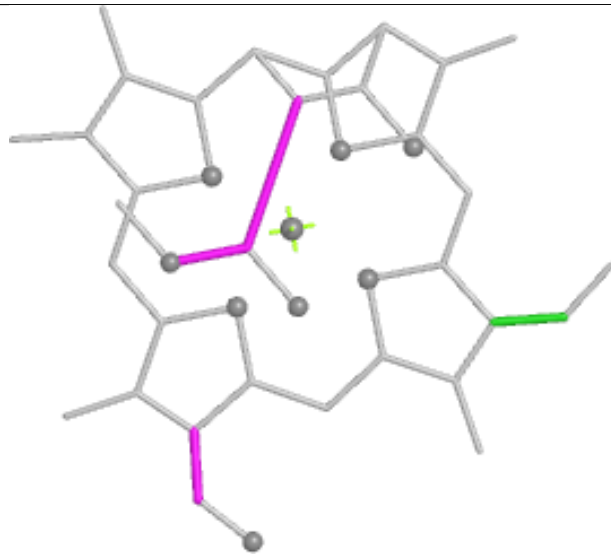
Ligand CL7 aB 3016



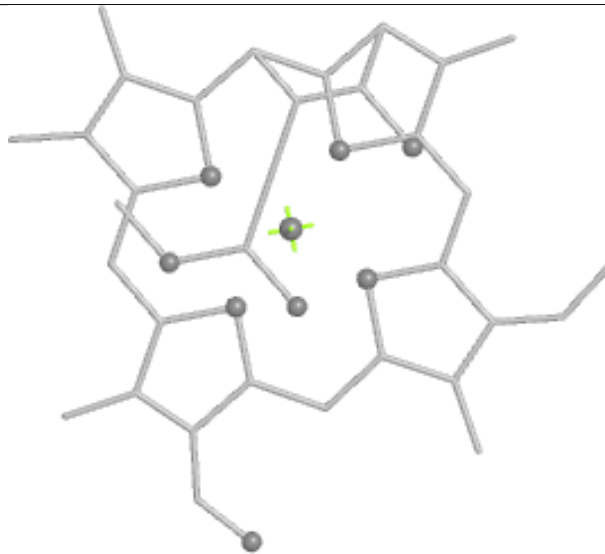
Bond lengths



Bond angles

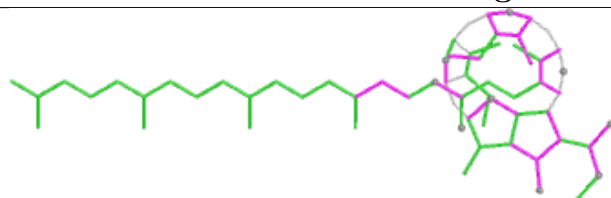


Torsions

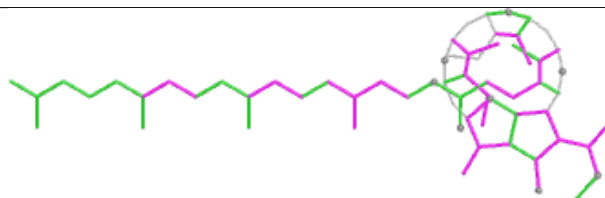


Rings

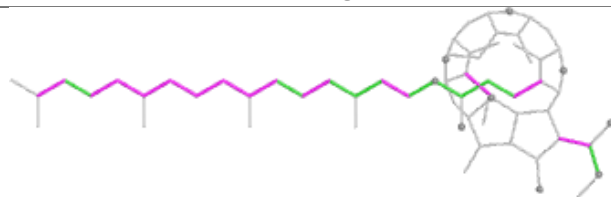
Ligand PHO aB 3004



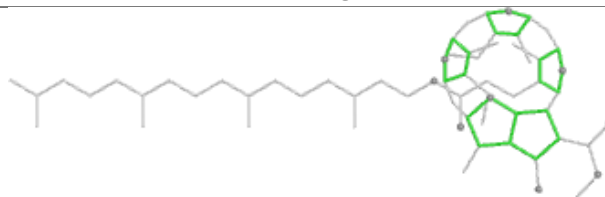
Bond lengths



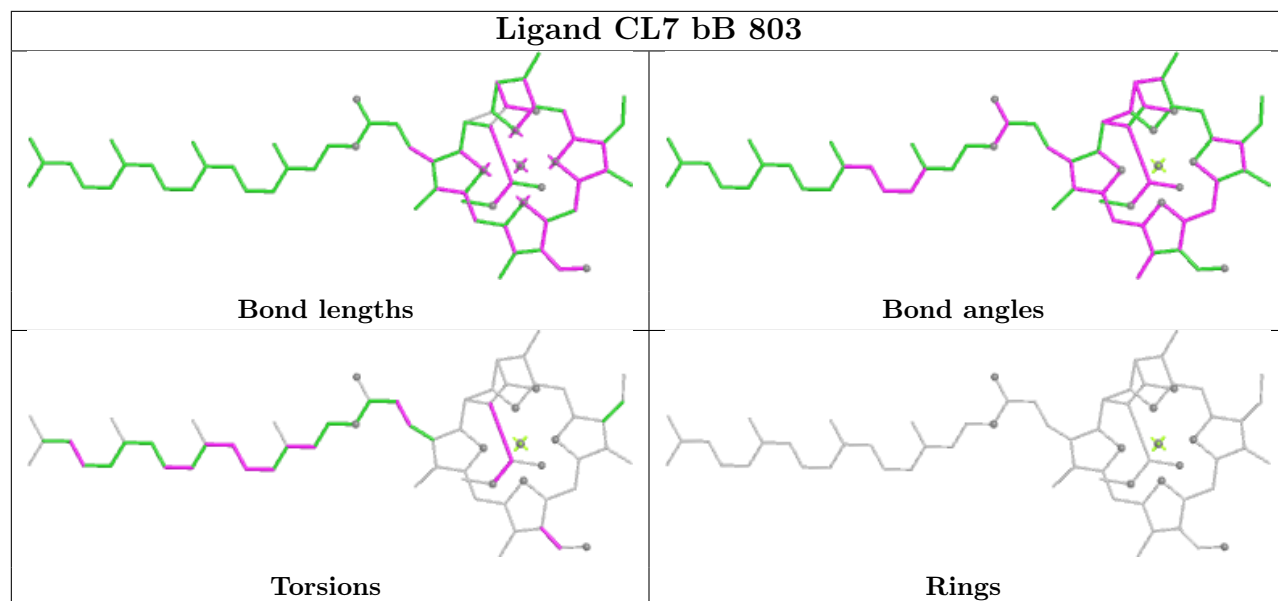
Bond angles



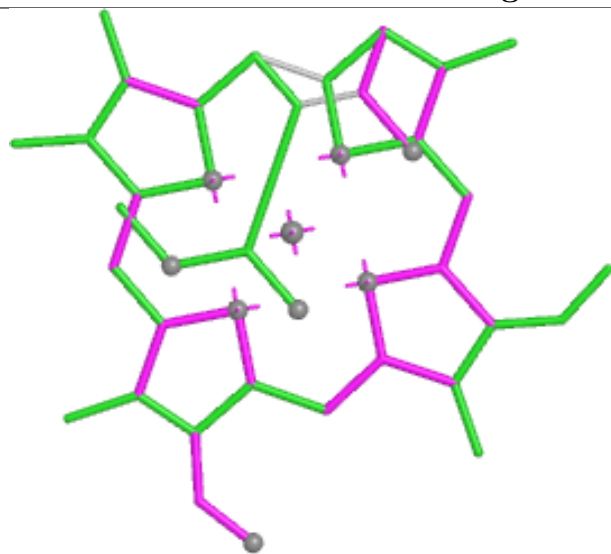
Torsions



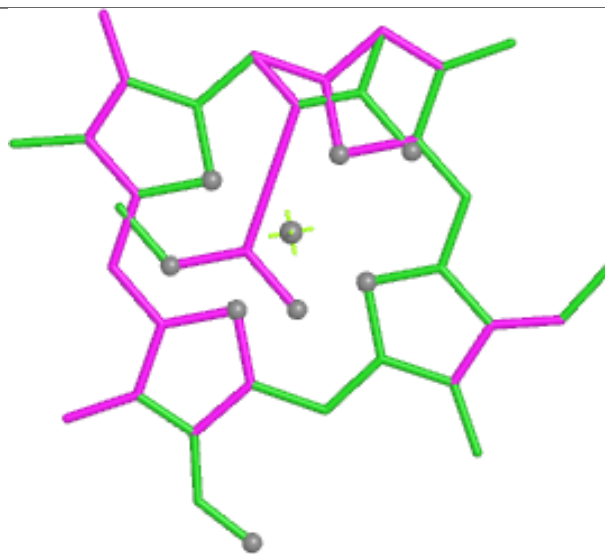
Rings



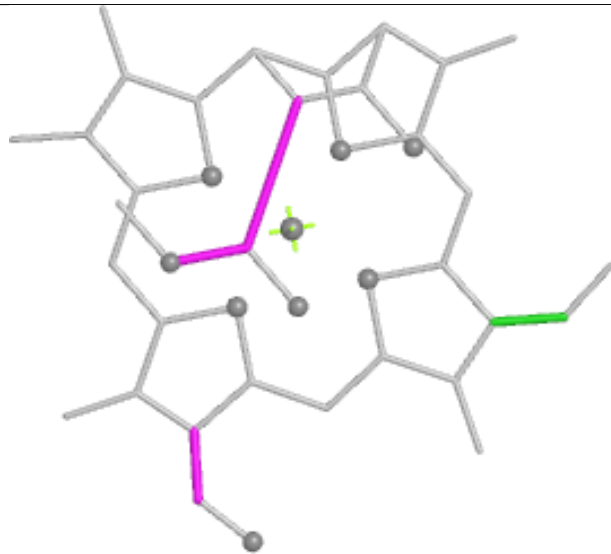
Ligand CL7 cA 3112



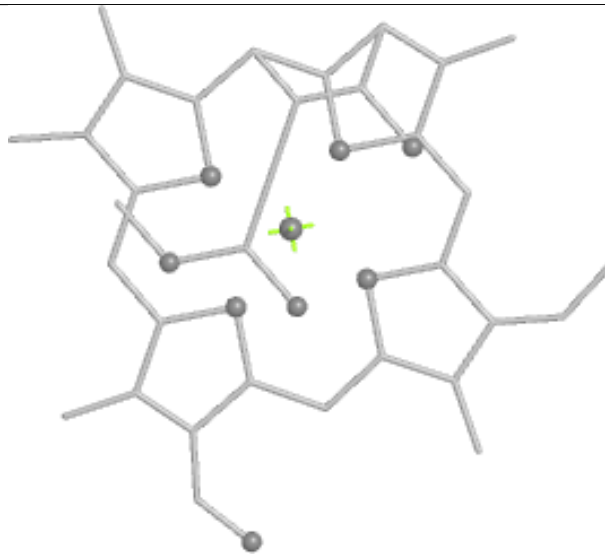
Bond lengths



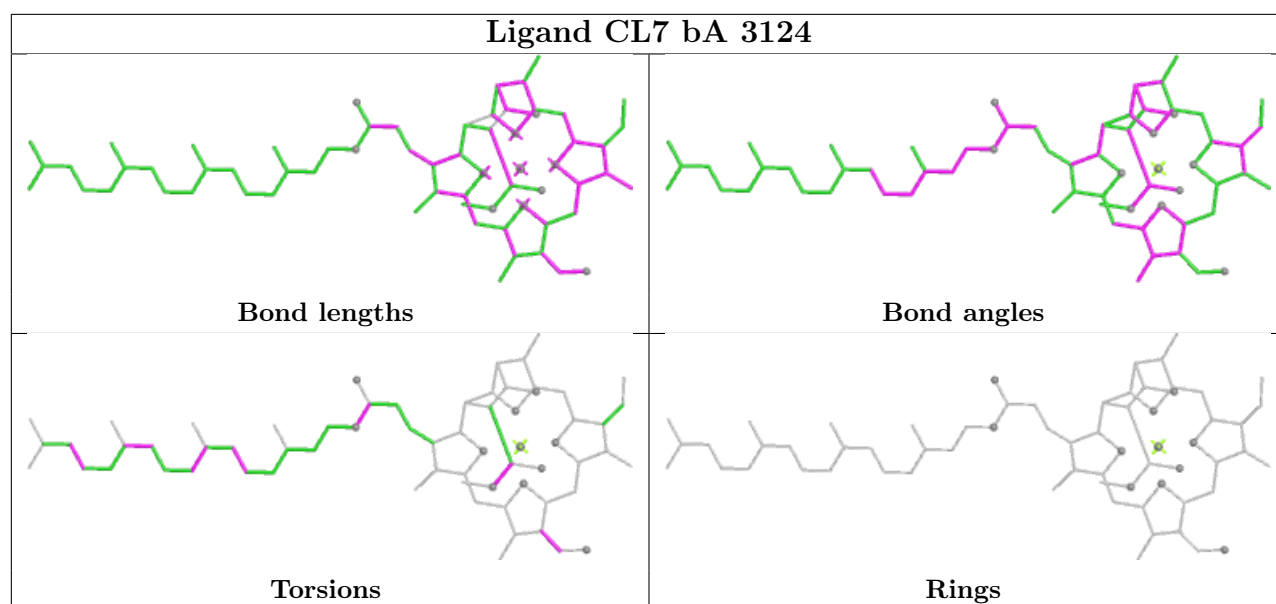
Bond angles



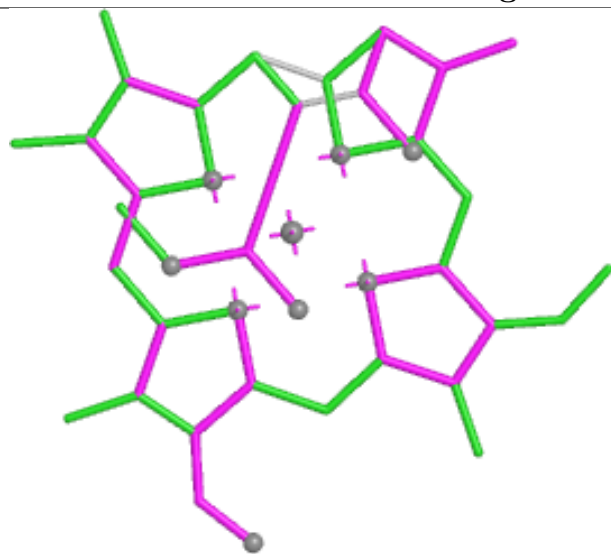
Torsions



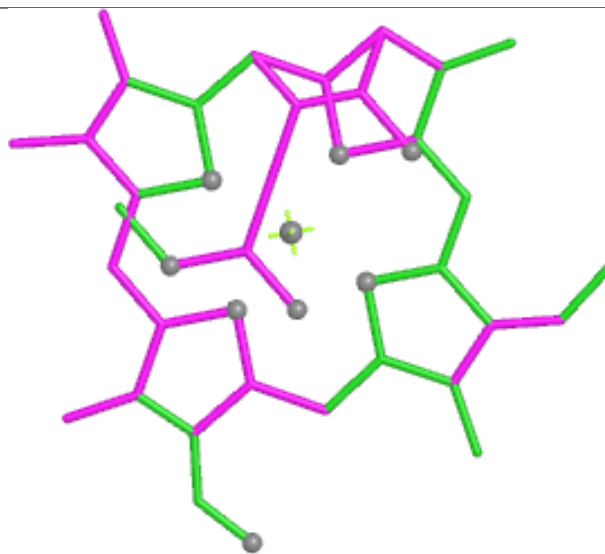
Rings



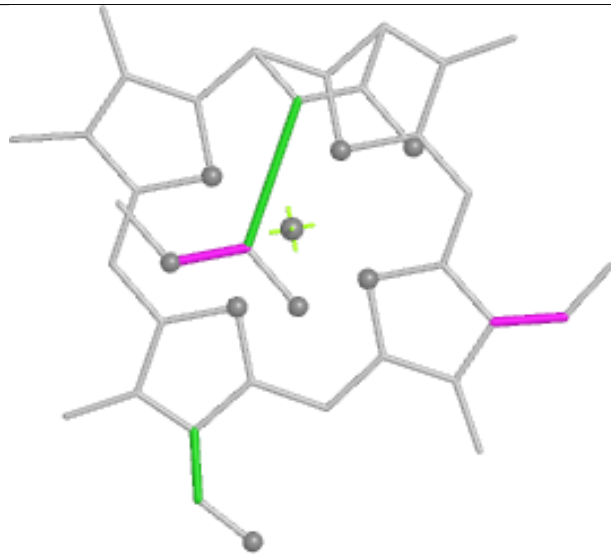
Ligand CL7 bA 3121



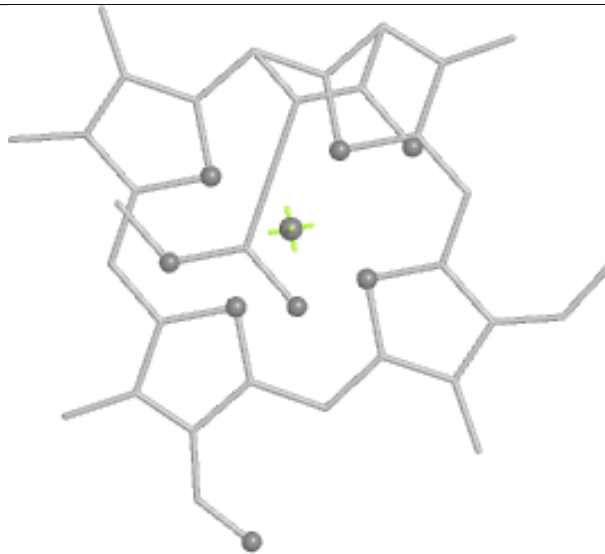
Bond lengths



Bond angles

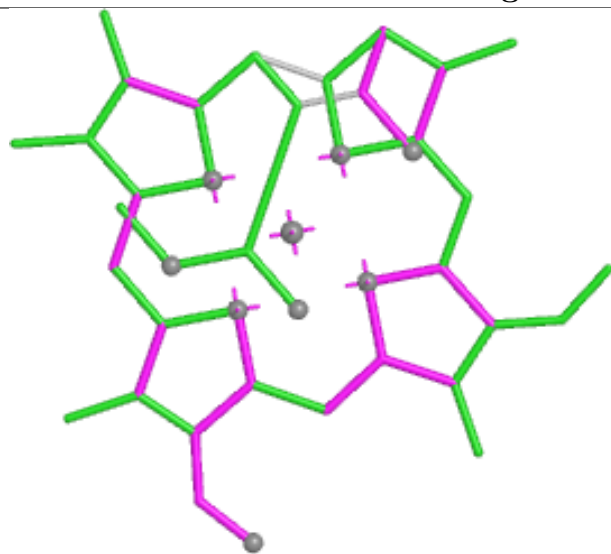


Torsions

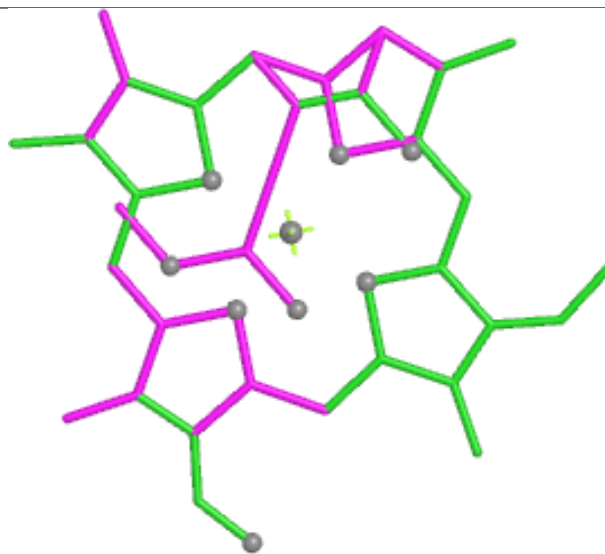


Rings

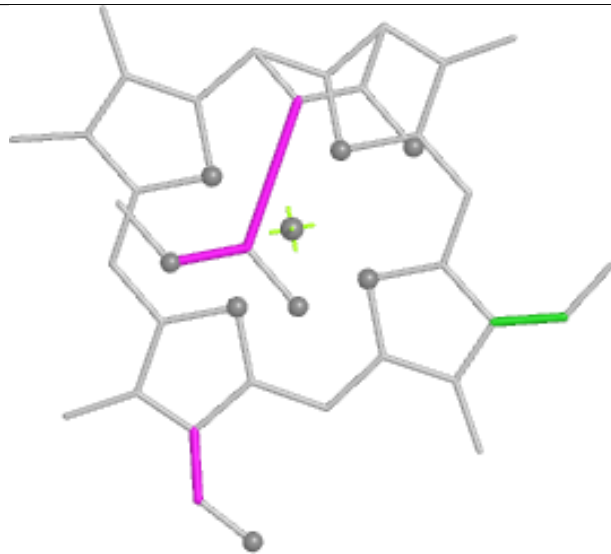
Ligand CL7 cA 3144



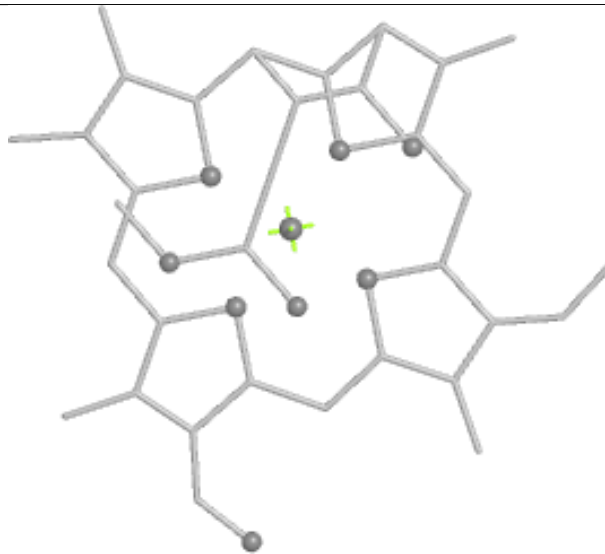
Bond lengths



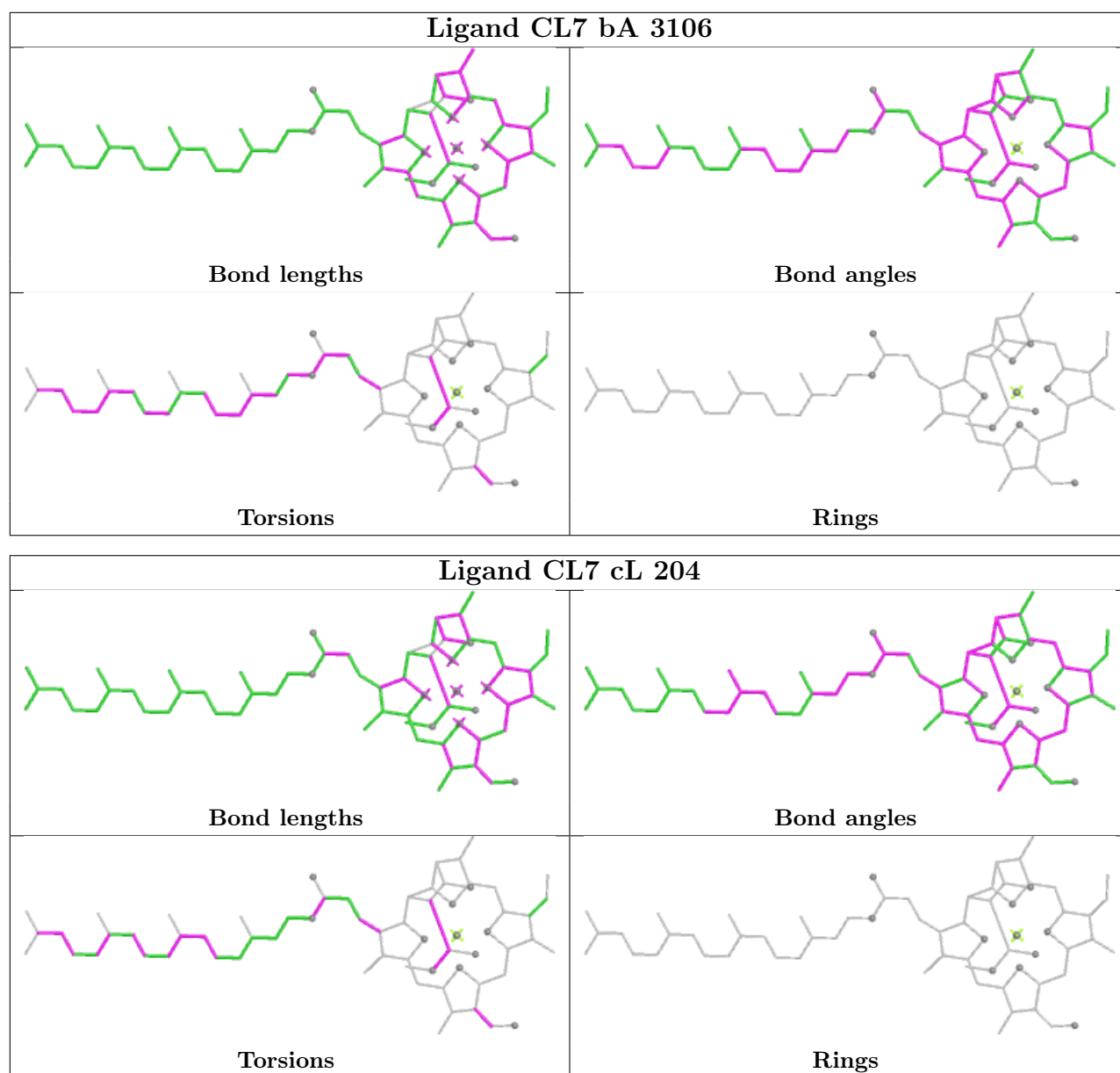
Bond angles

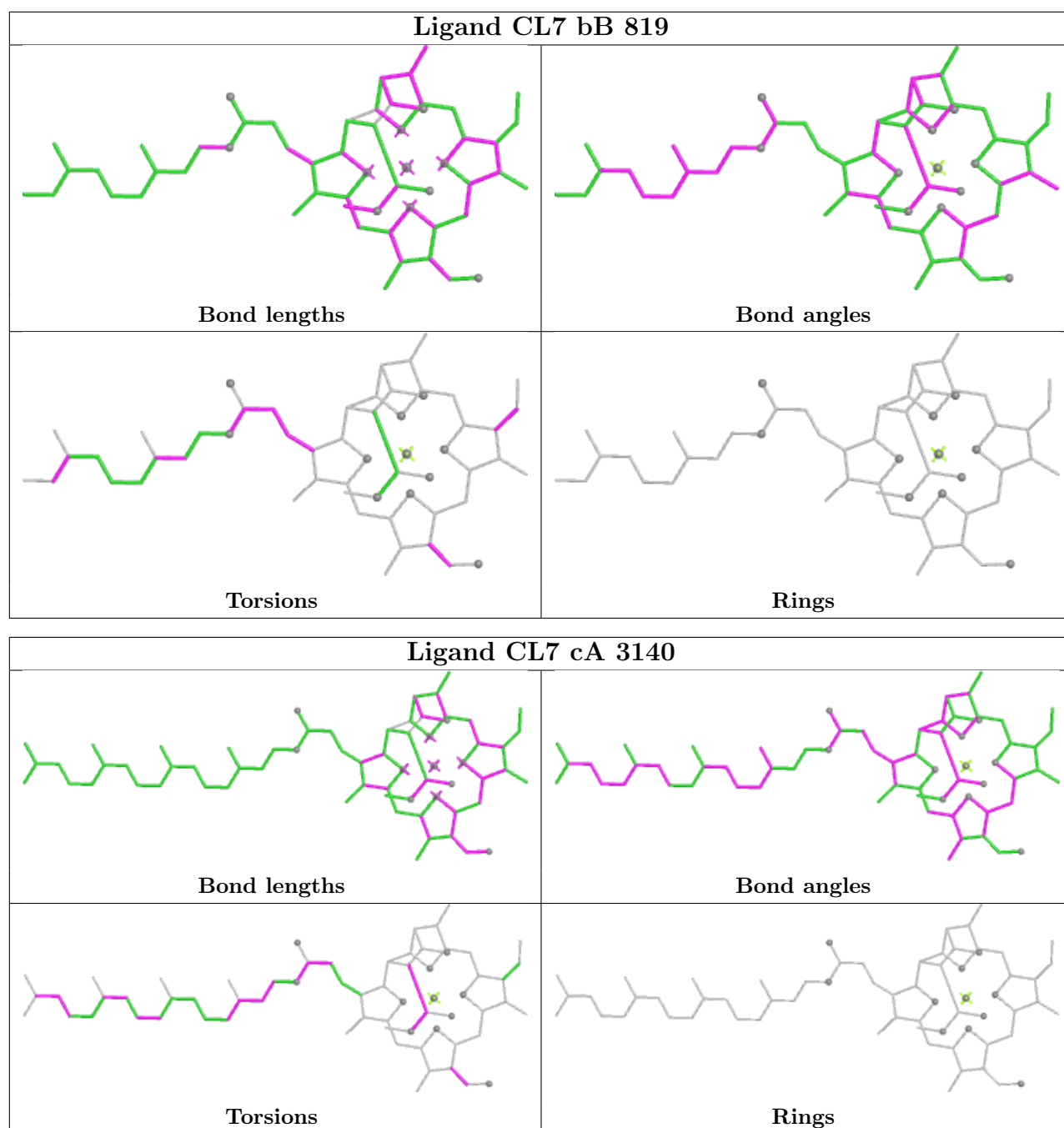


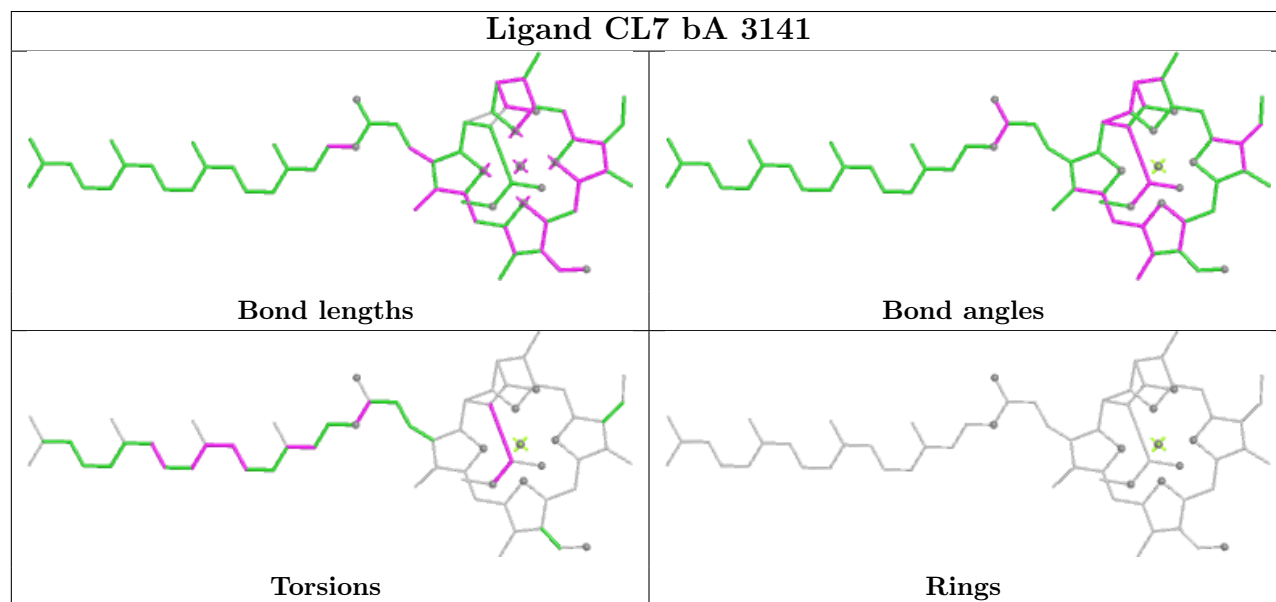
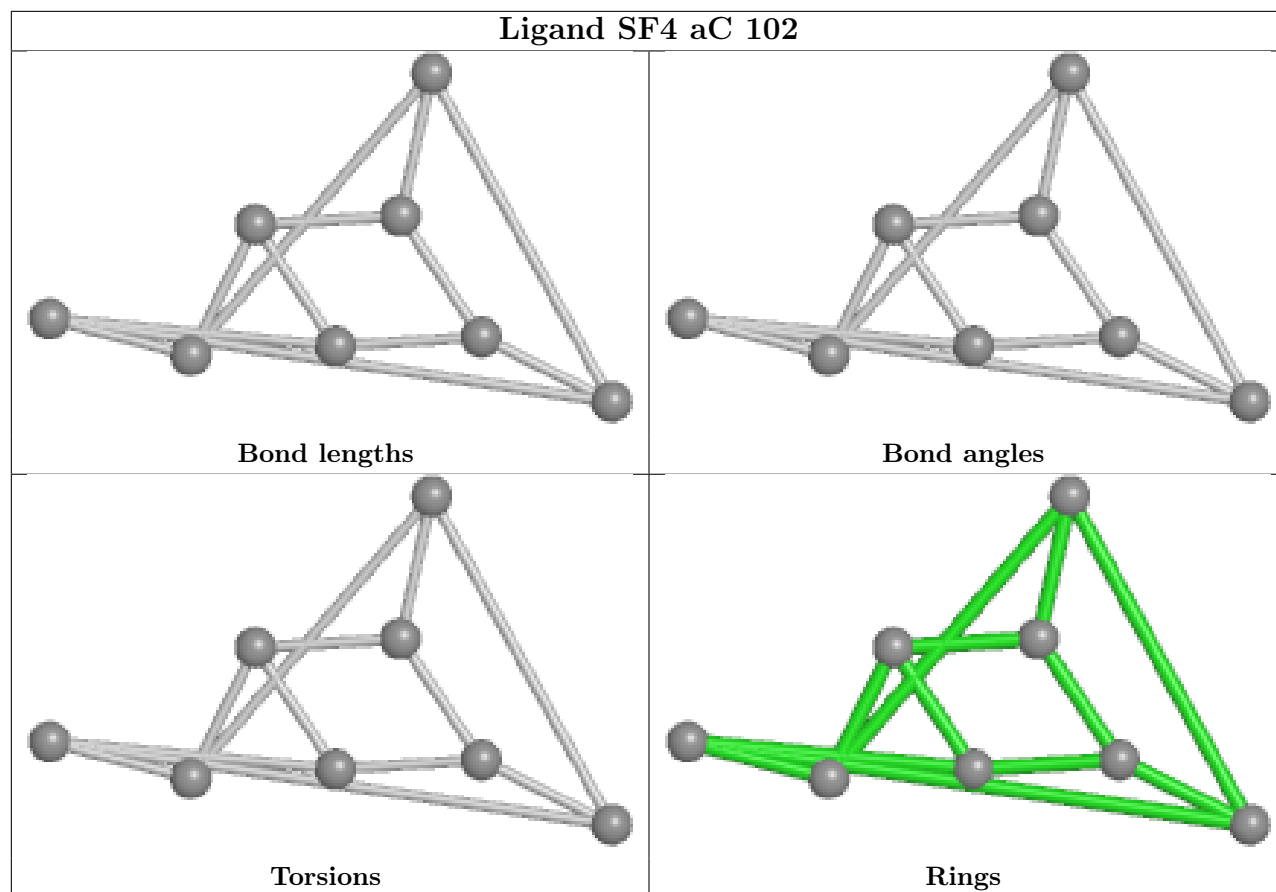
Torsions



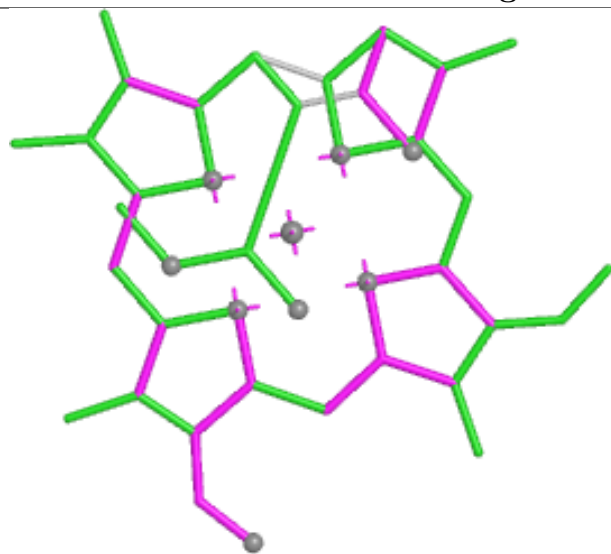
Rings



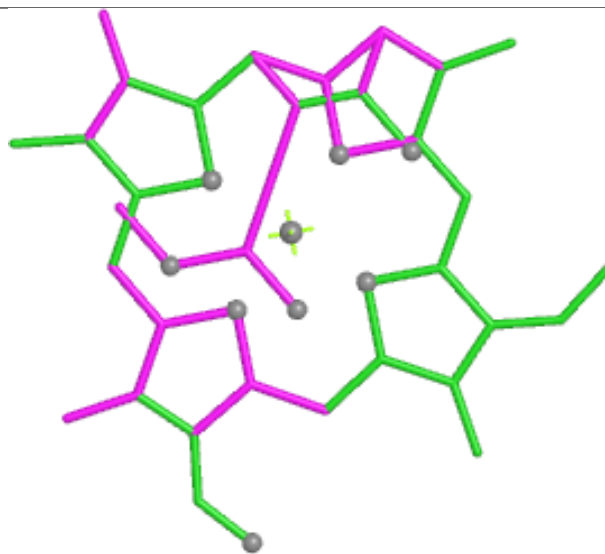




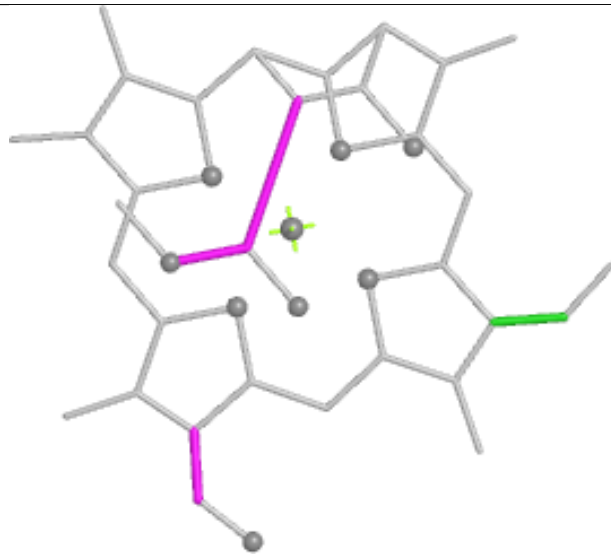
Ligand CL7 bA 3145



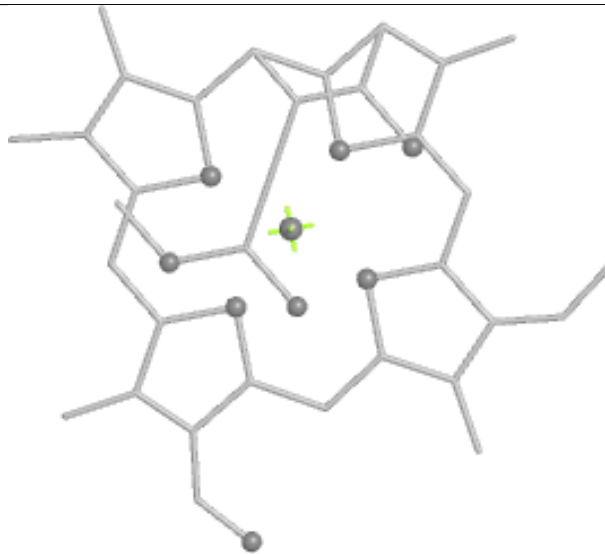
Bond lengths



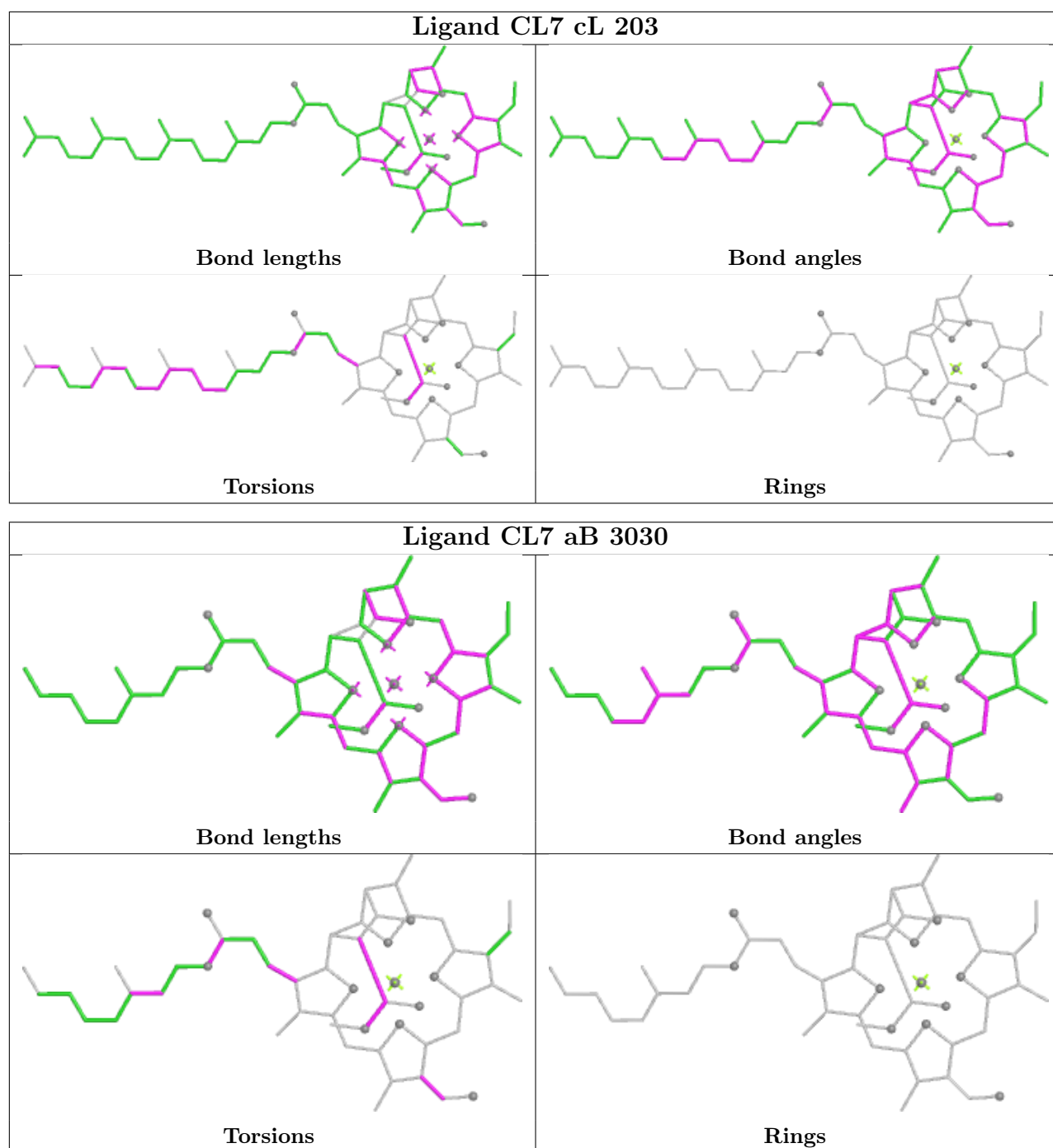
Bond angles

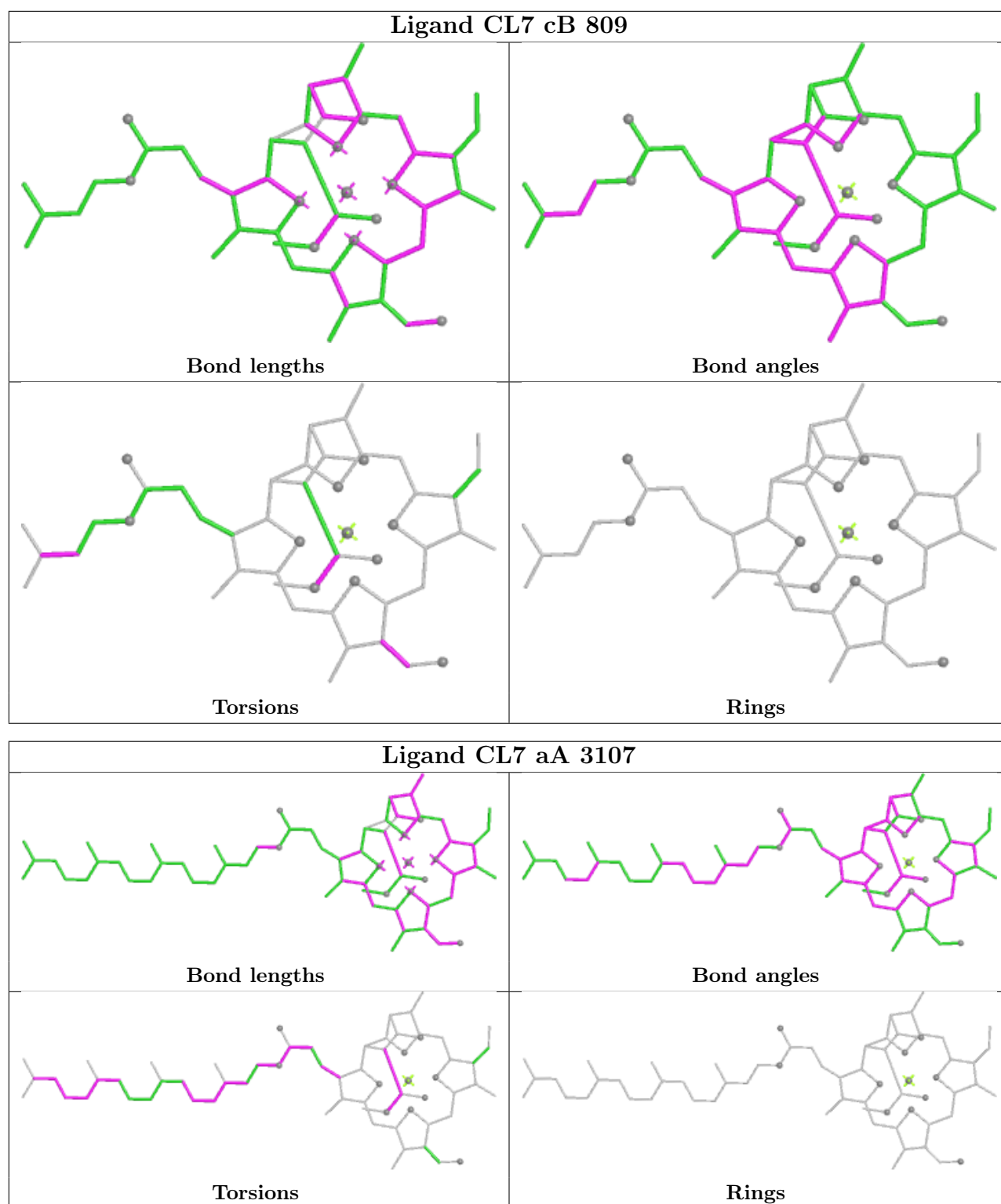


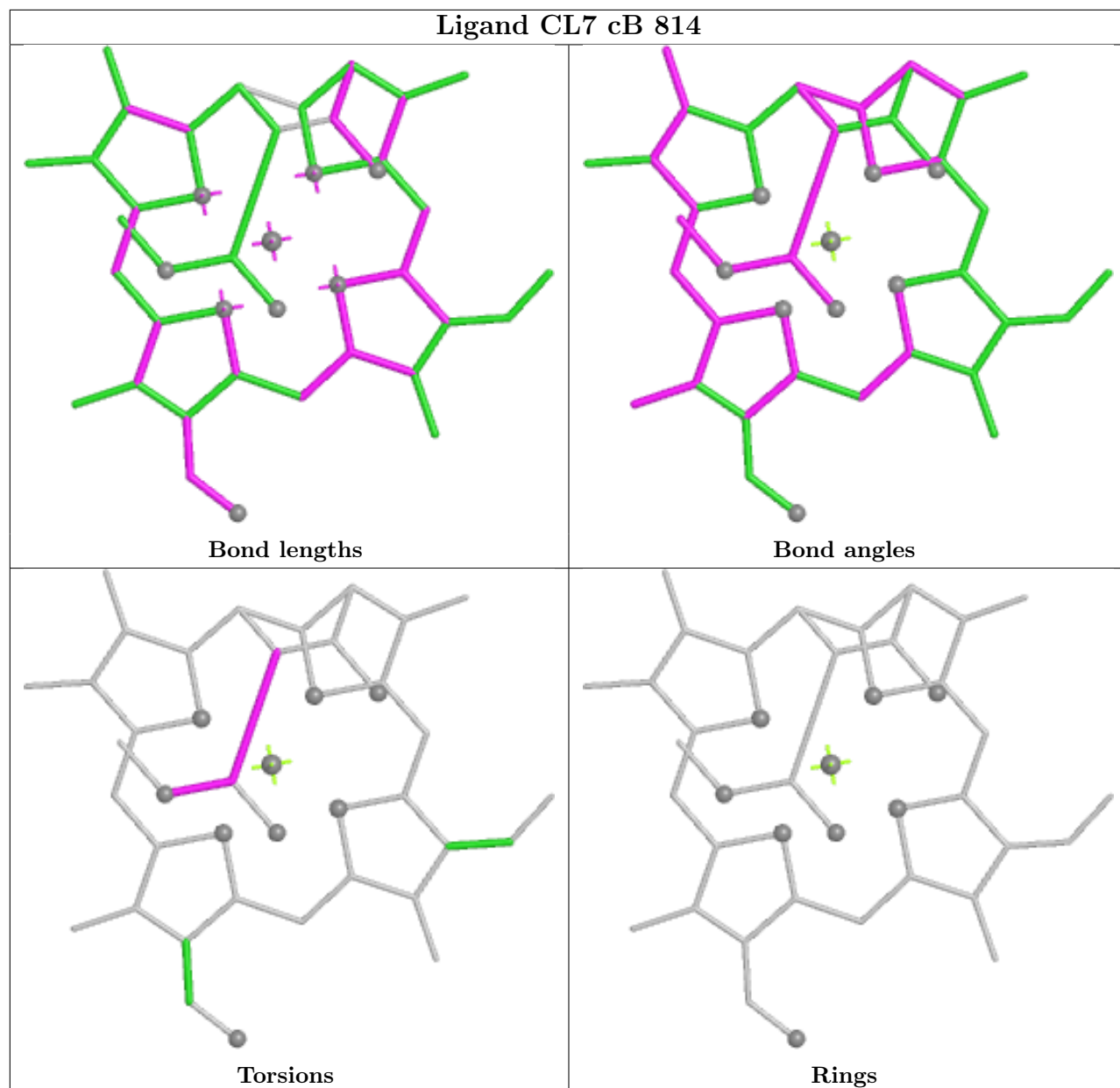
Torsions



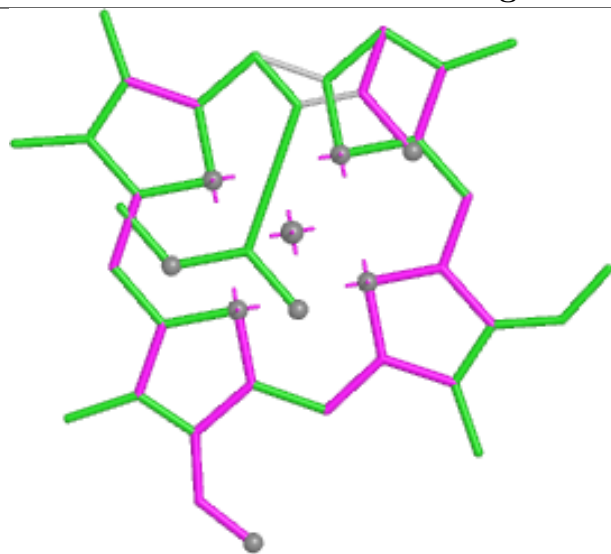
Rings



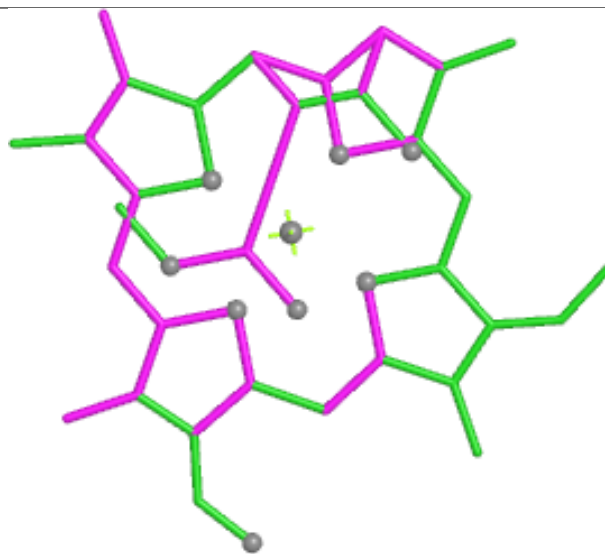




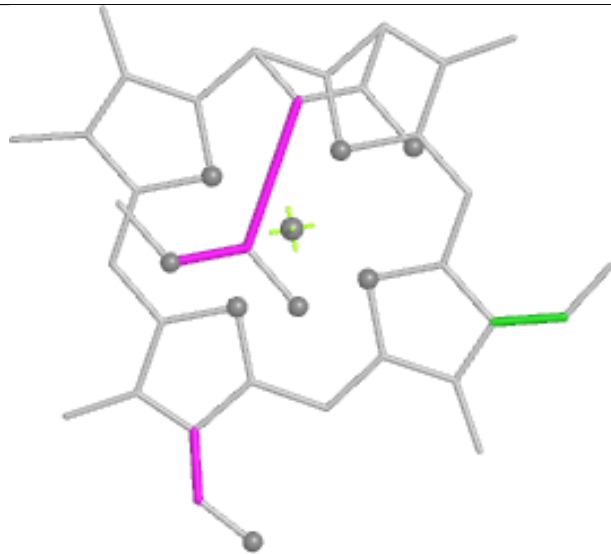
Ligand CL7 bA 3104



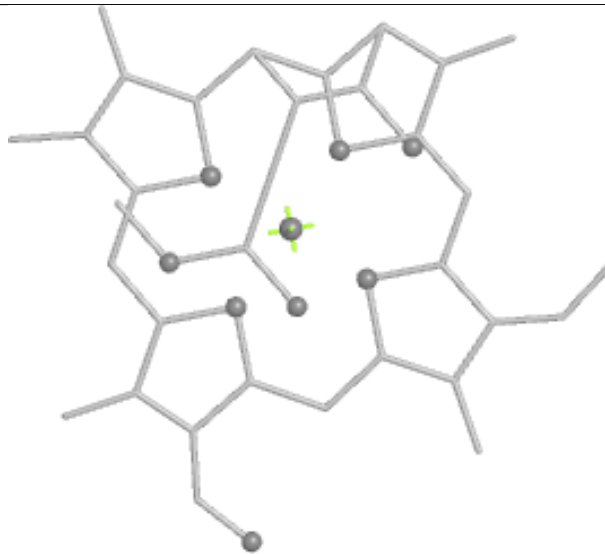
Bond lengths



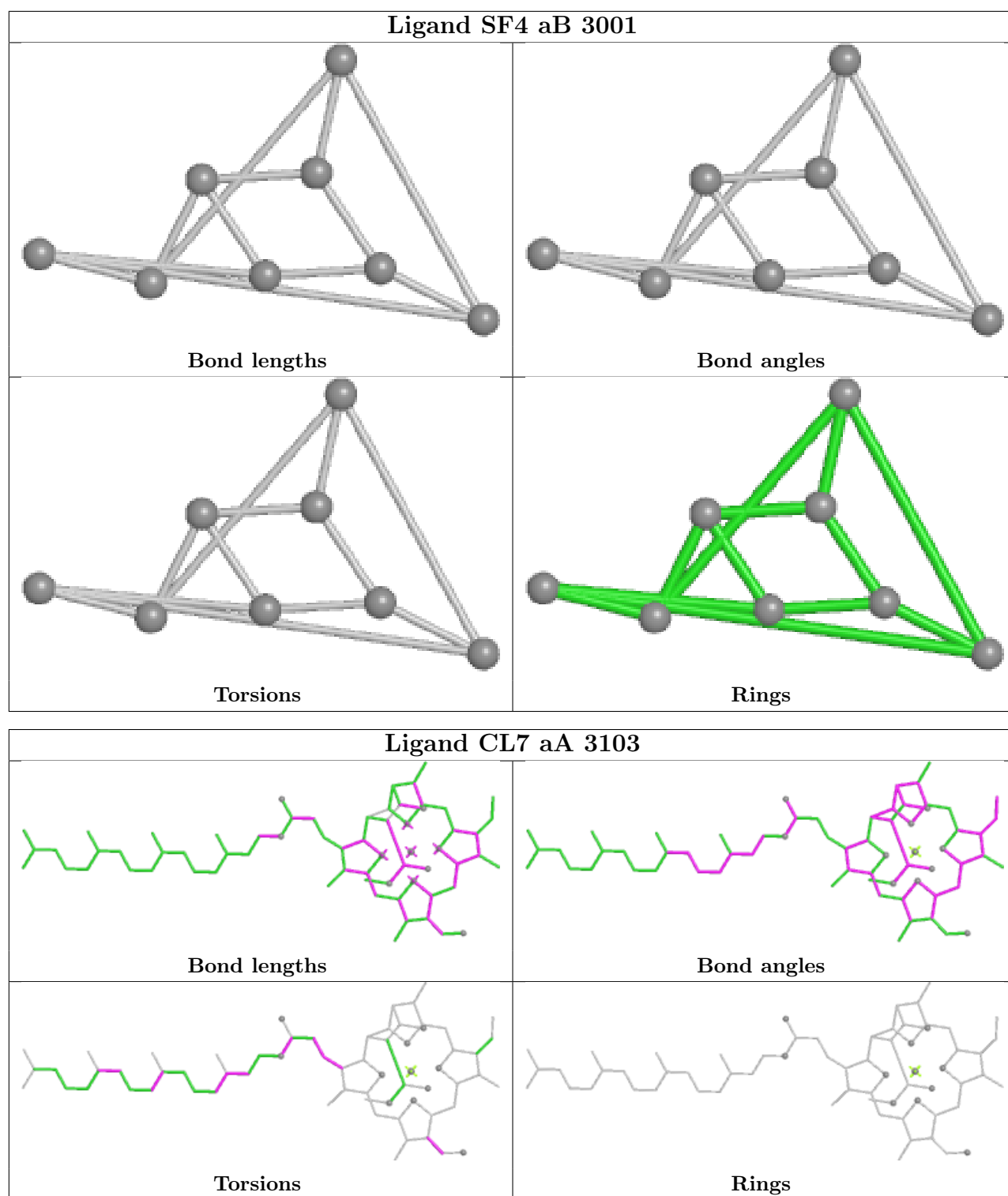
Bond angles

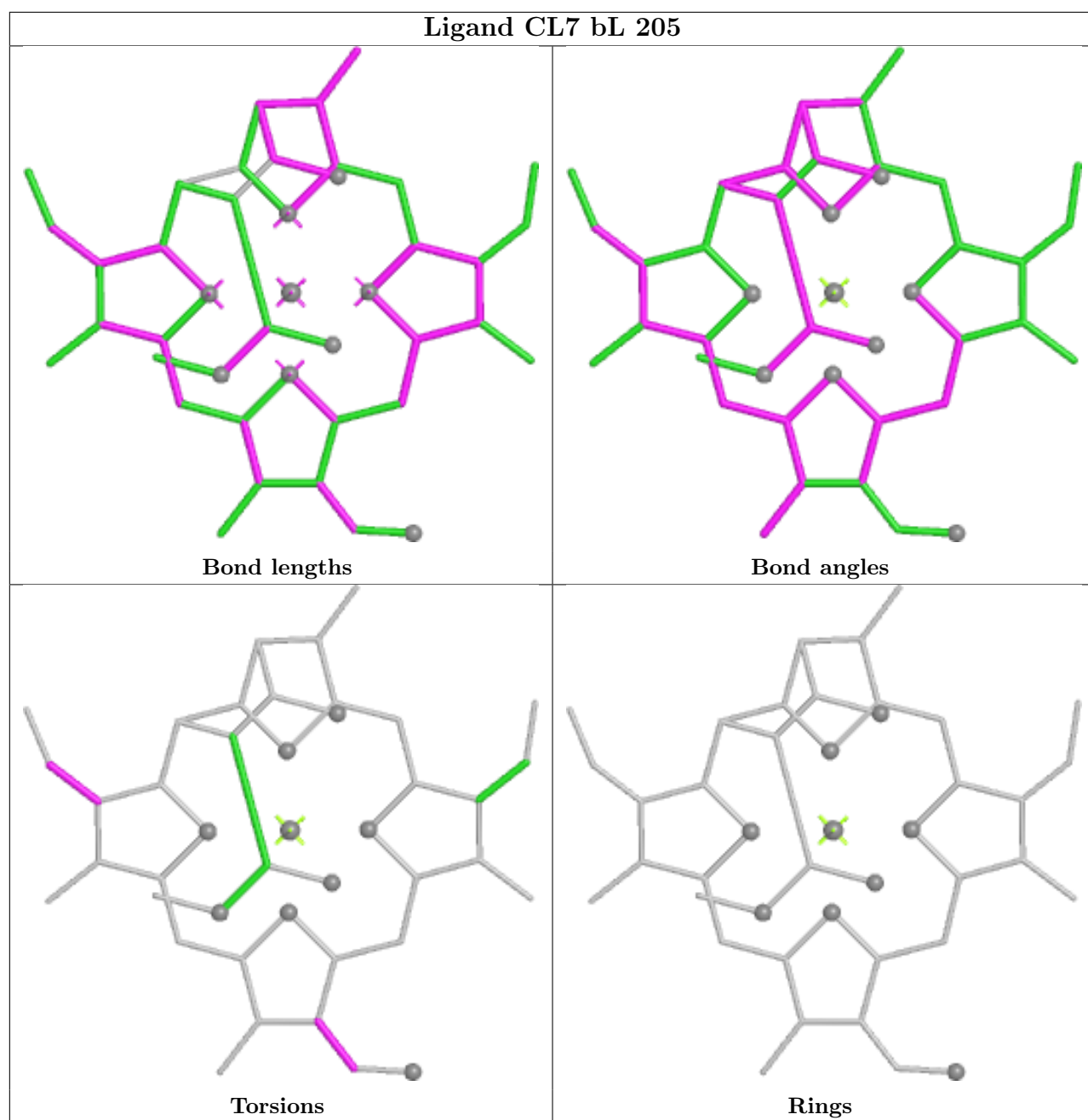


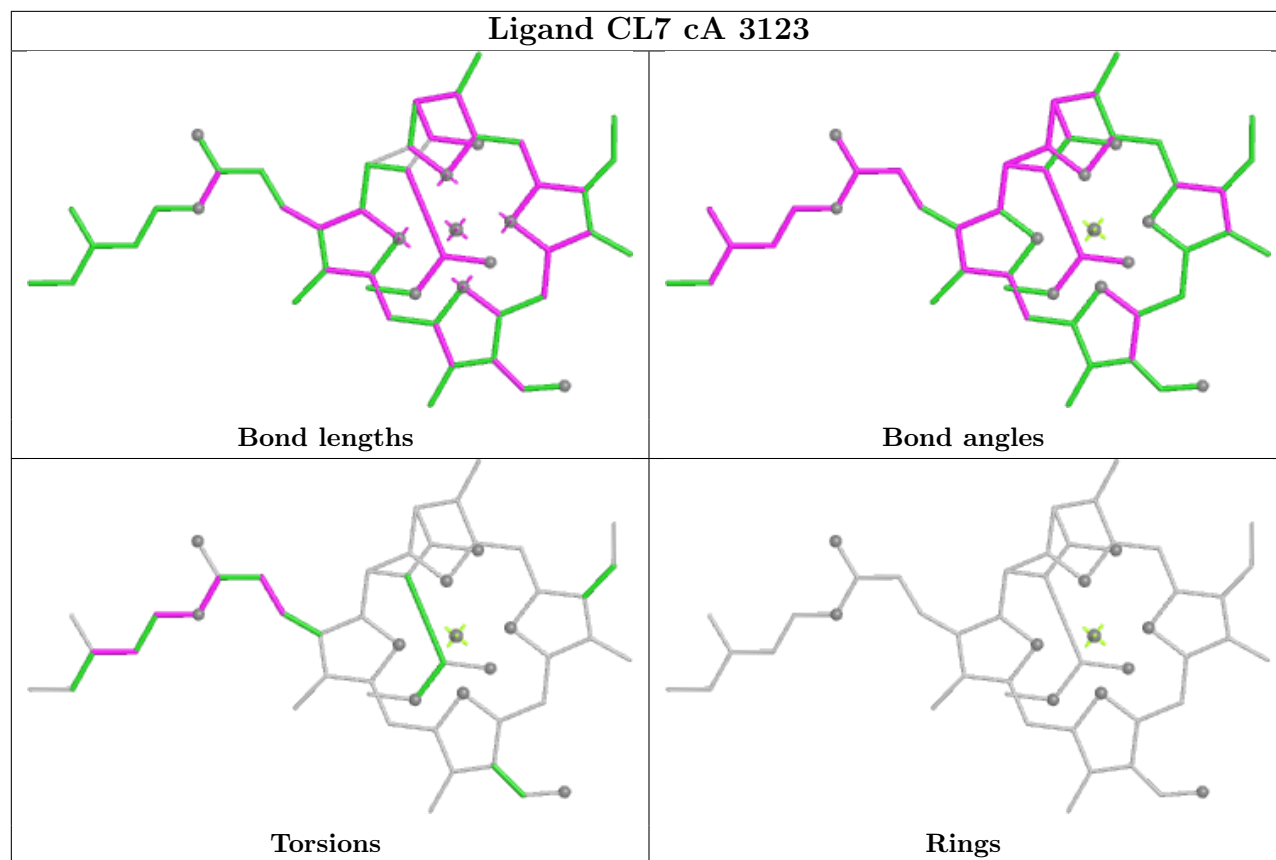
Torsions

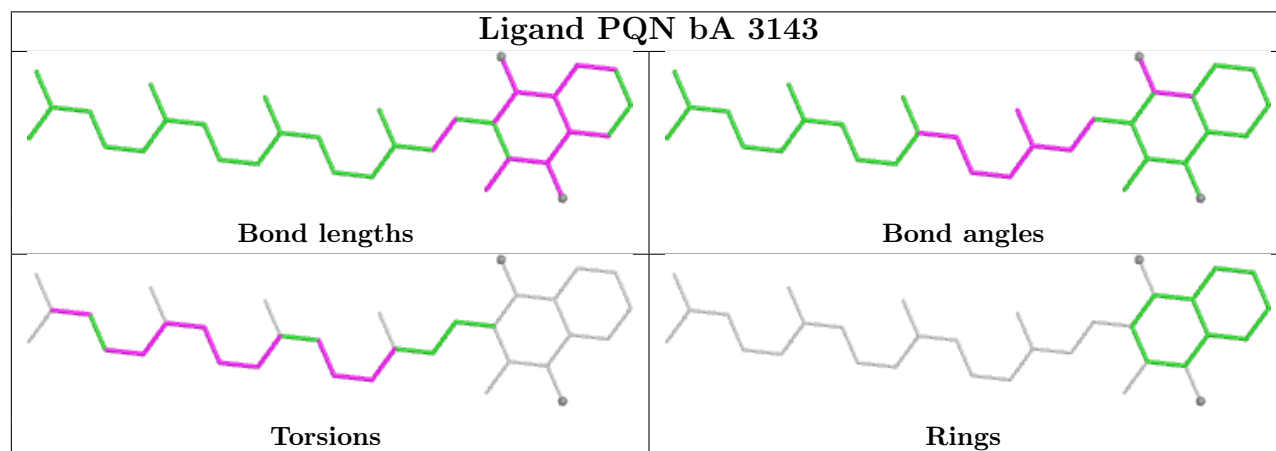
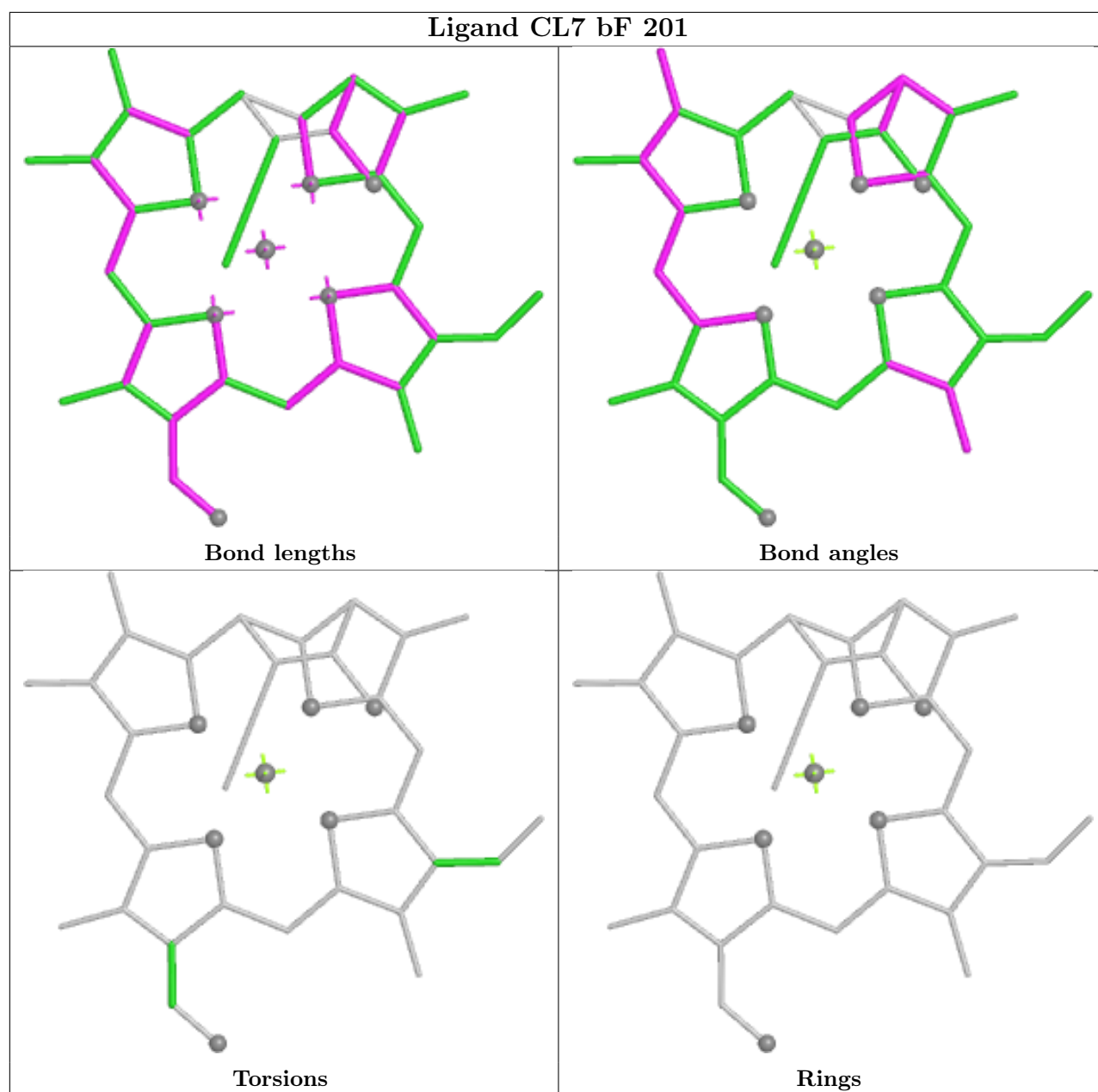


Rings

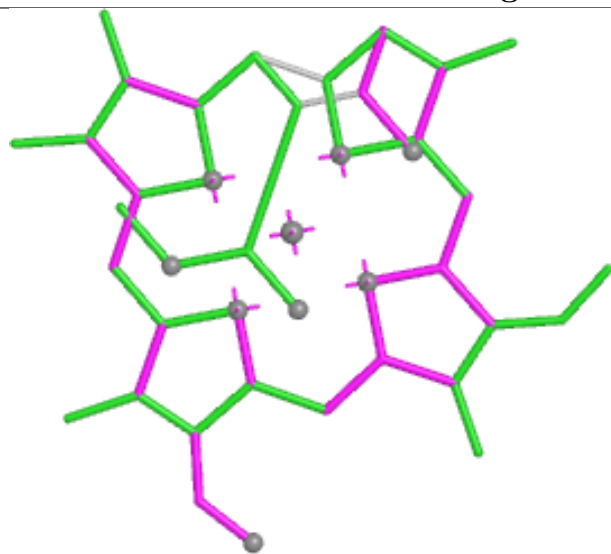




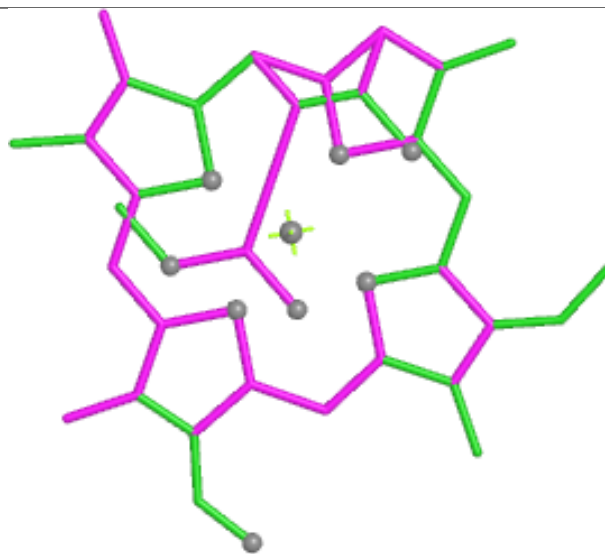




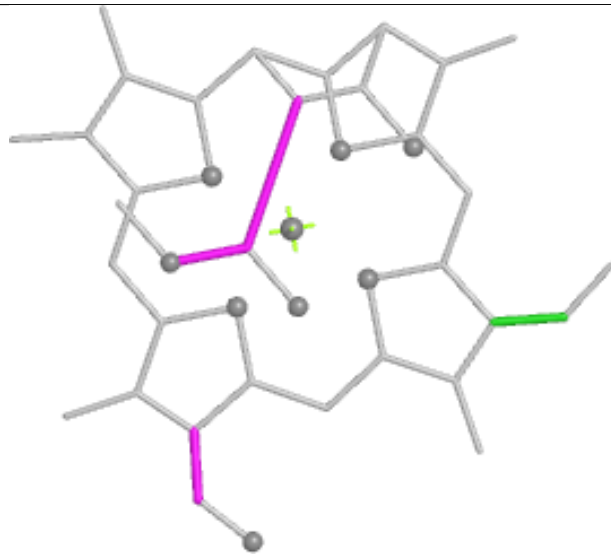
Ligand CL7 aA 3104



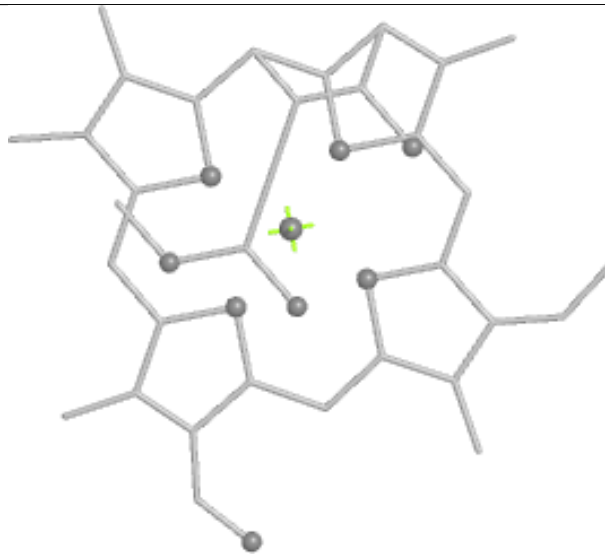
Bond lengths



Bond angles

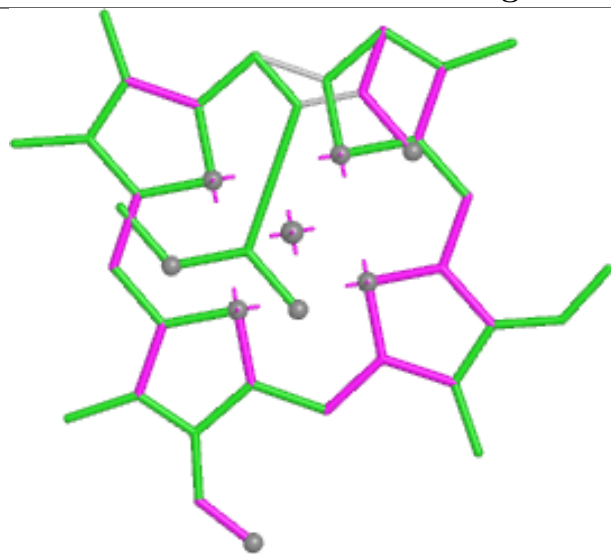


Torsions

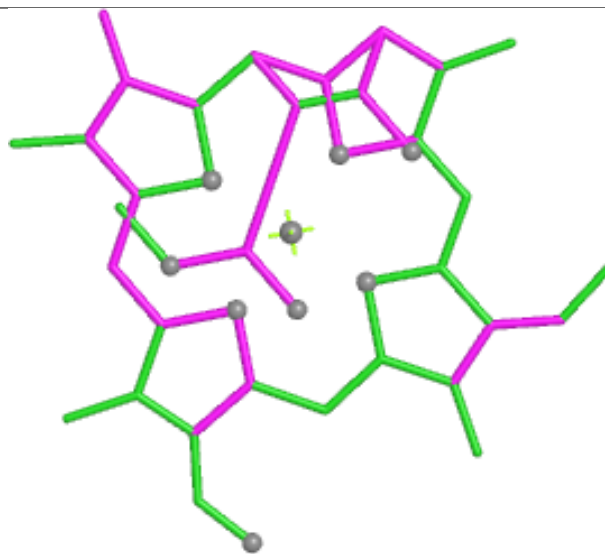


Rings

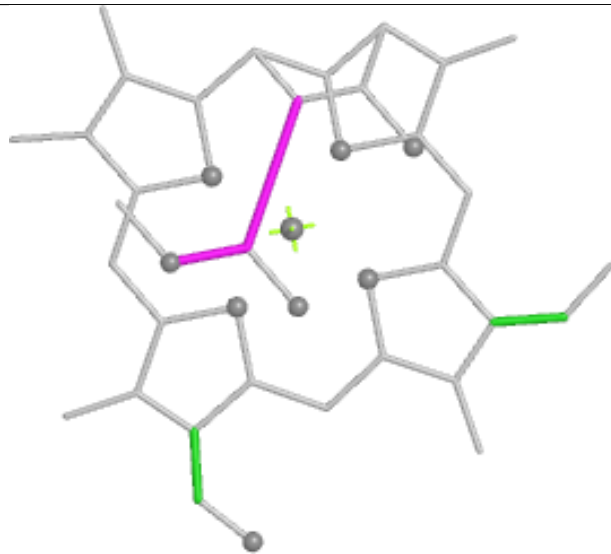
Ligand CL7 aB 3010



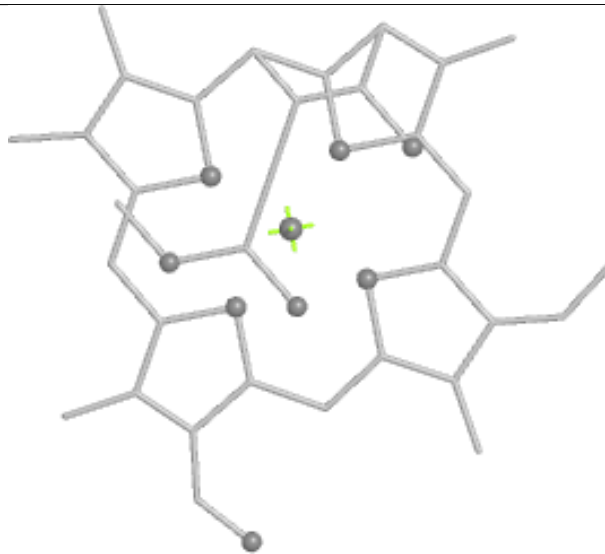
Bond lengths



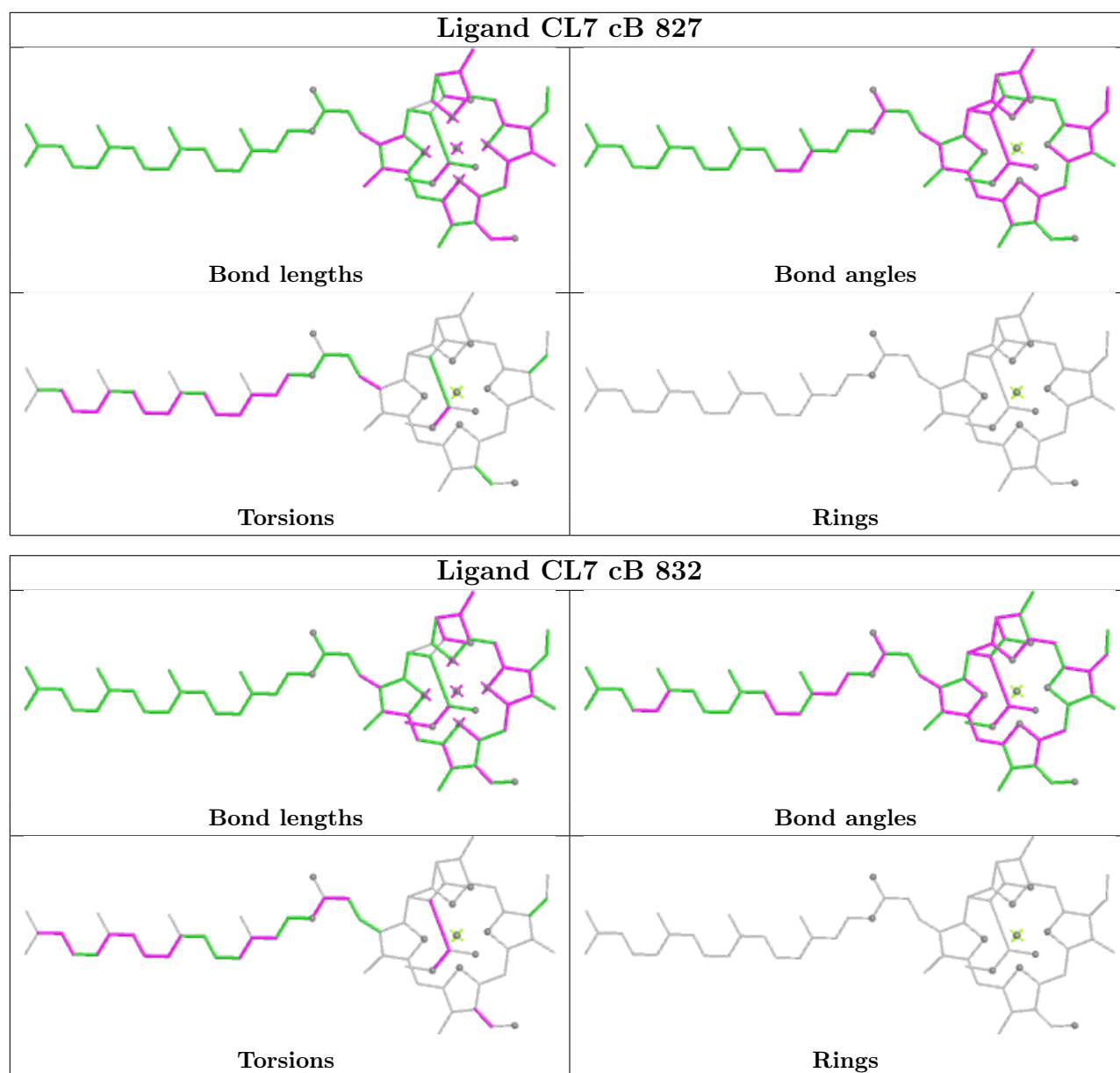
Bond angles

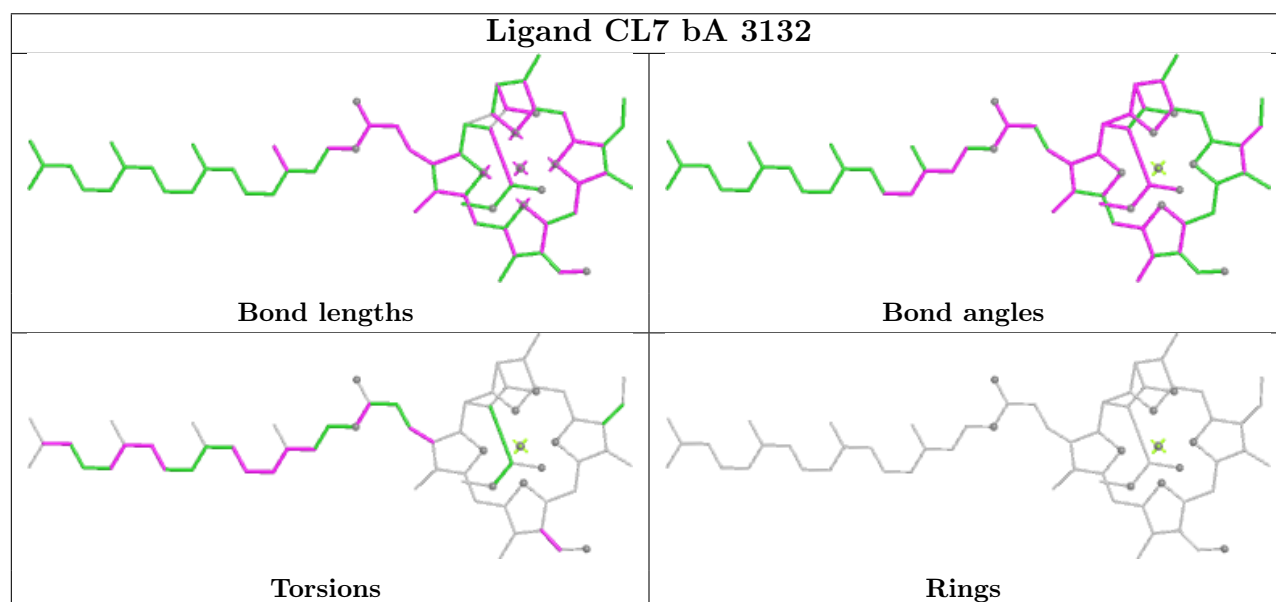
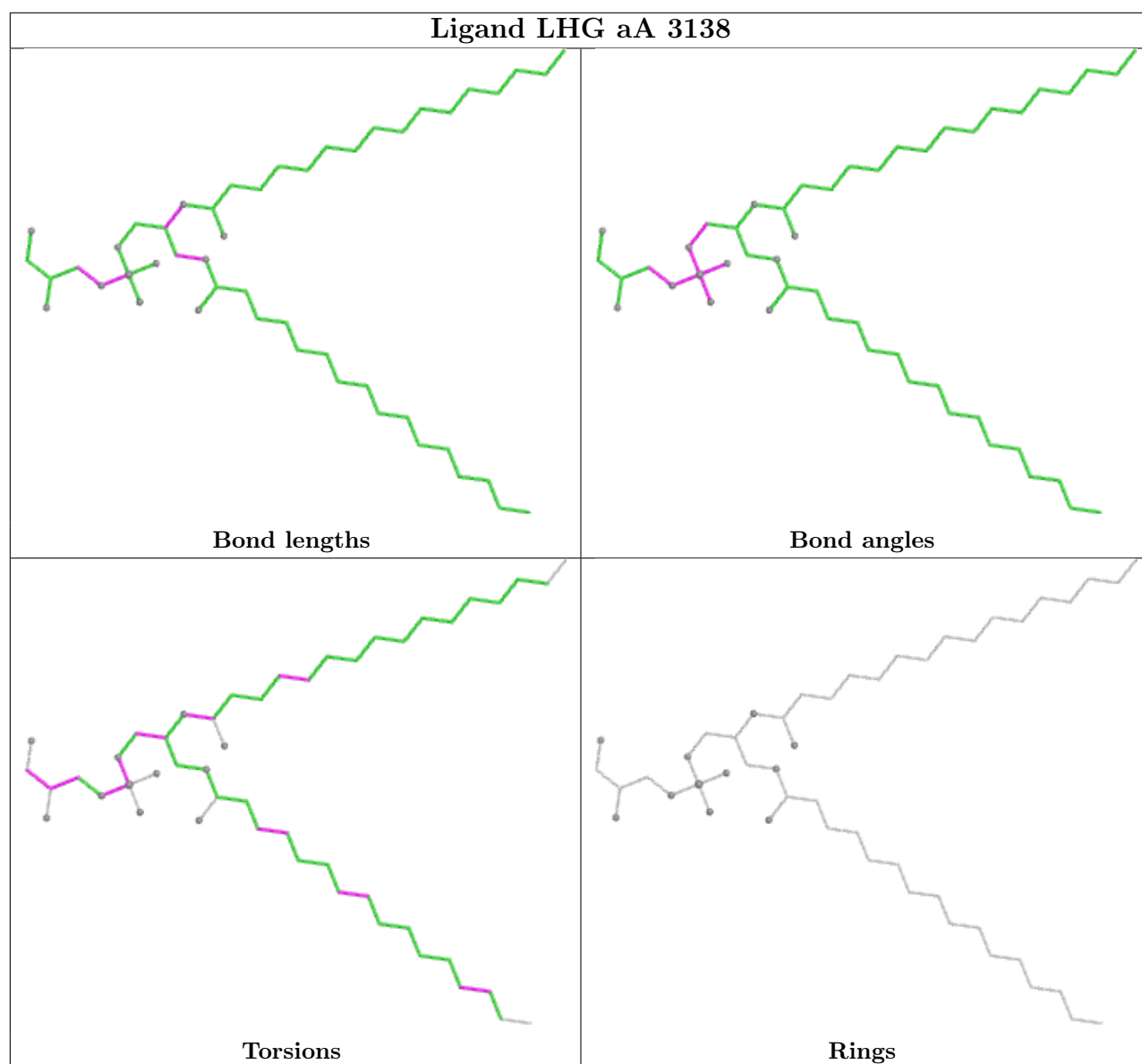


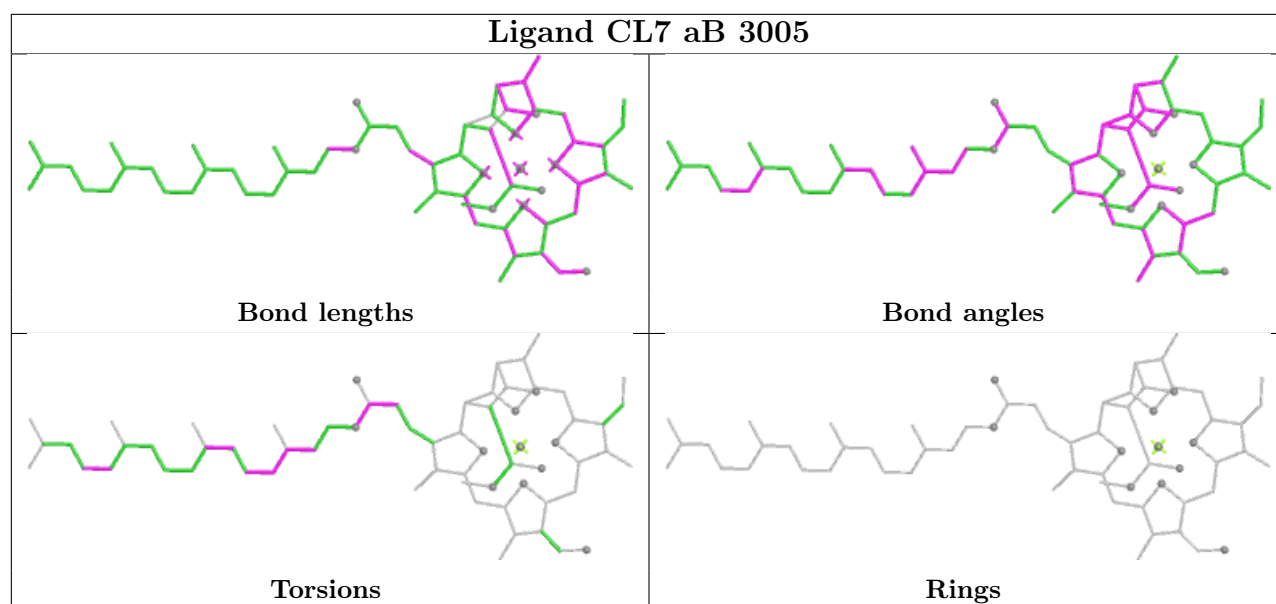
Torsions

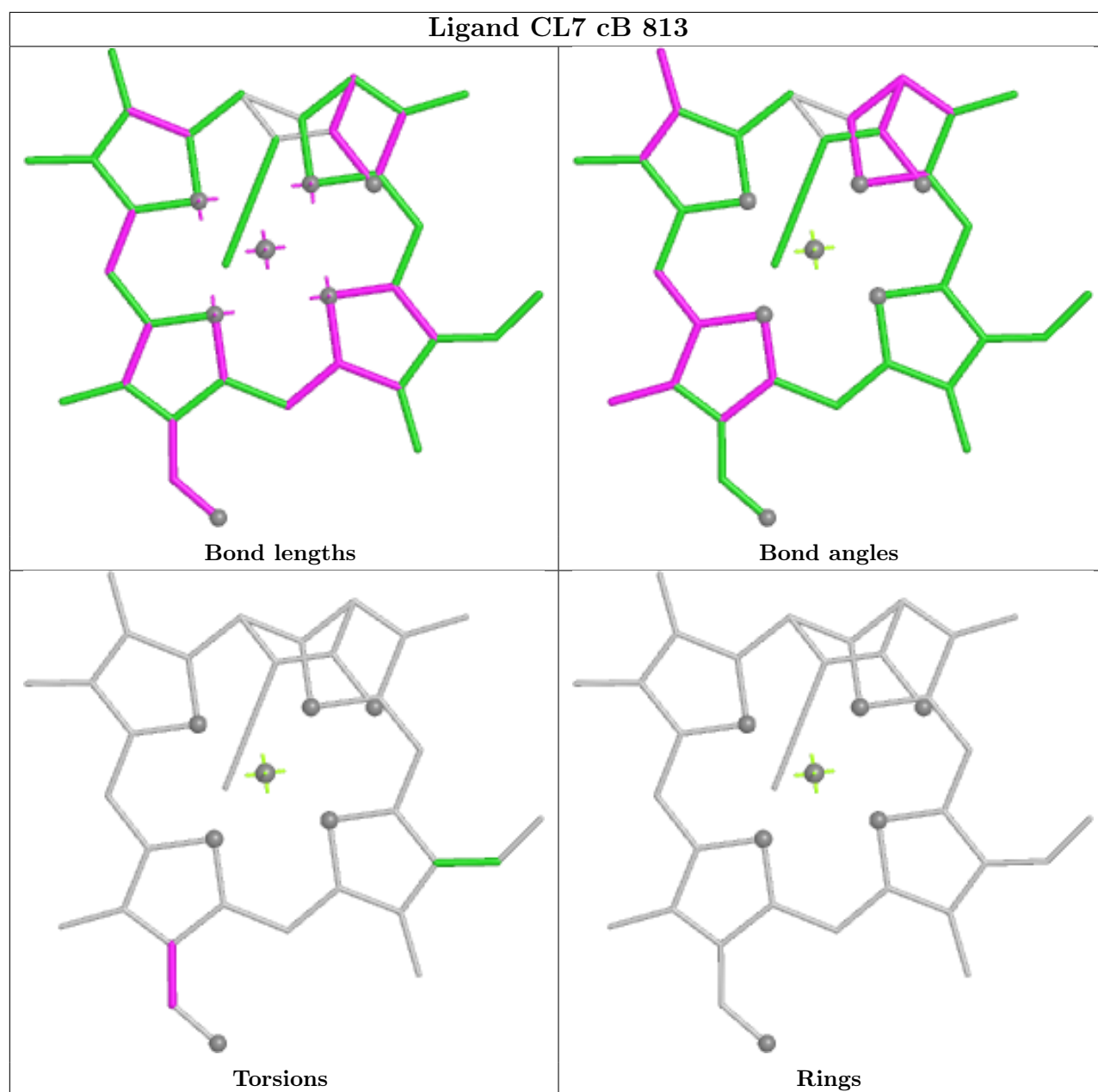


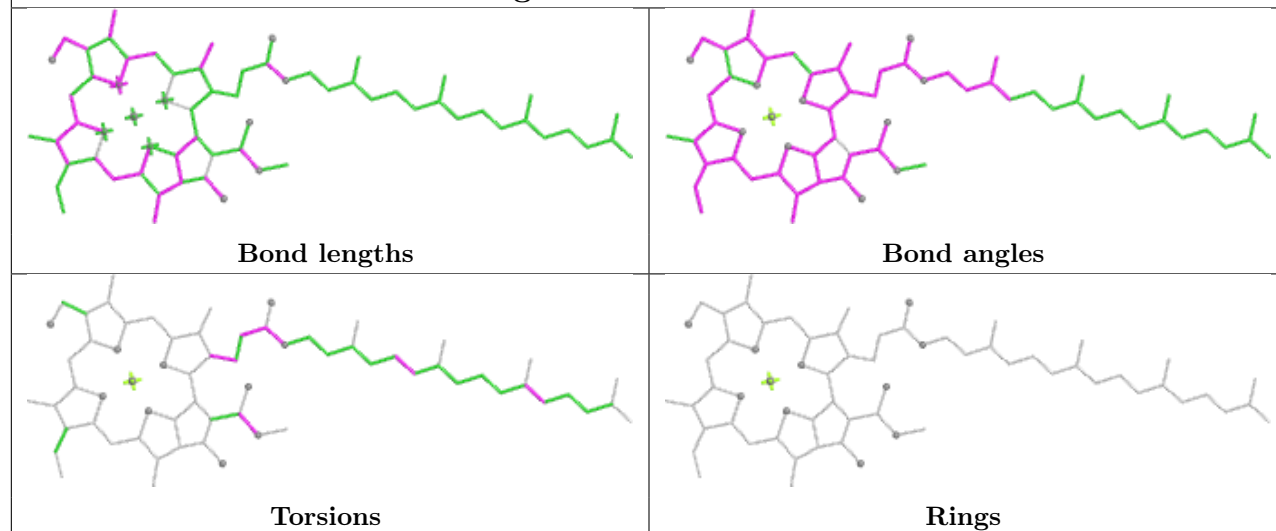
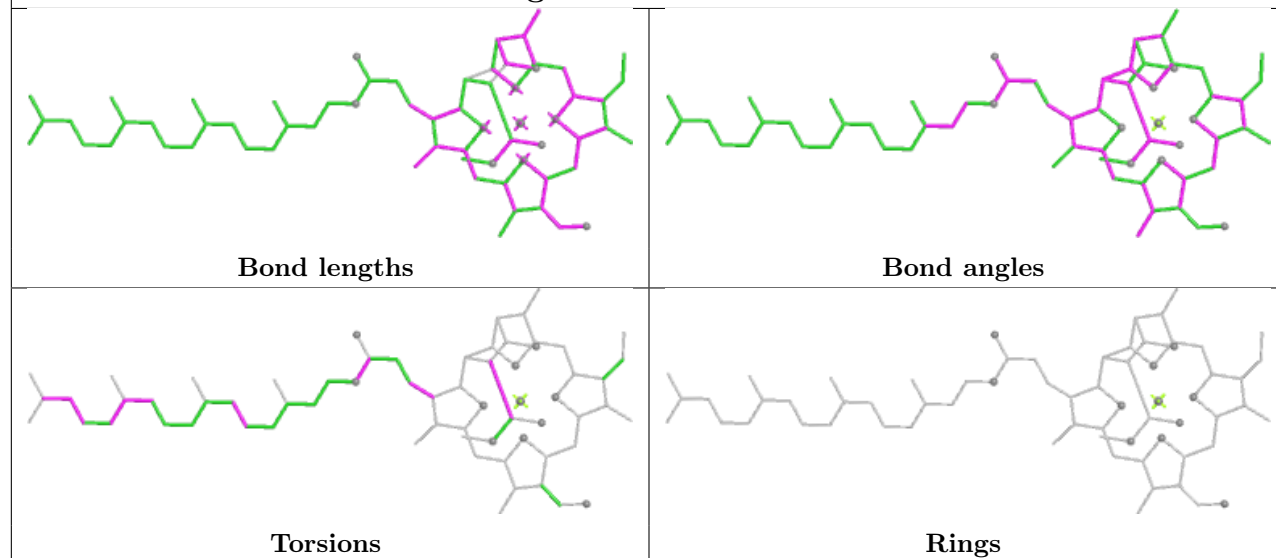
Rings



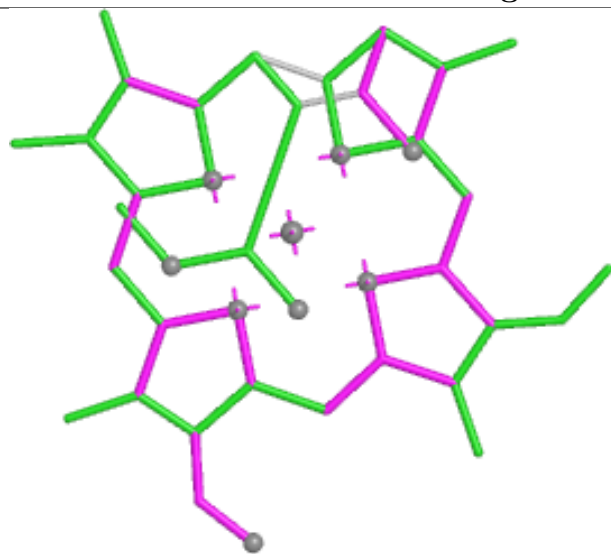




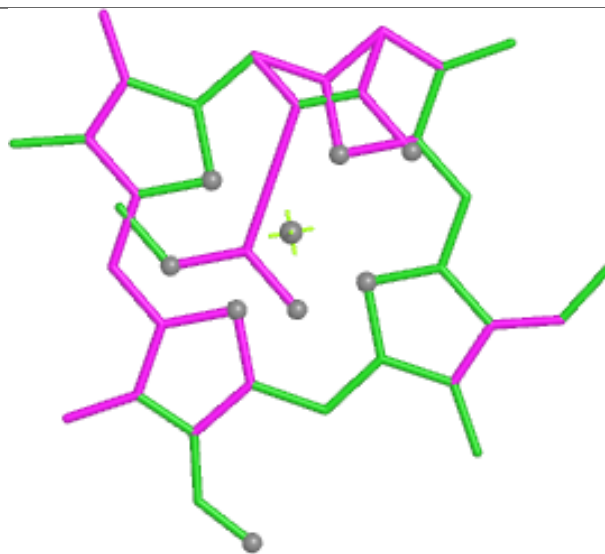


Ligand G9R bA 3101**Ligand CL7 bB 820**

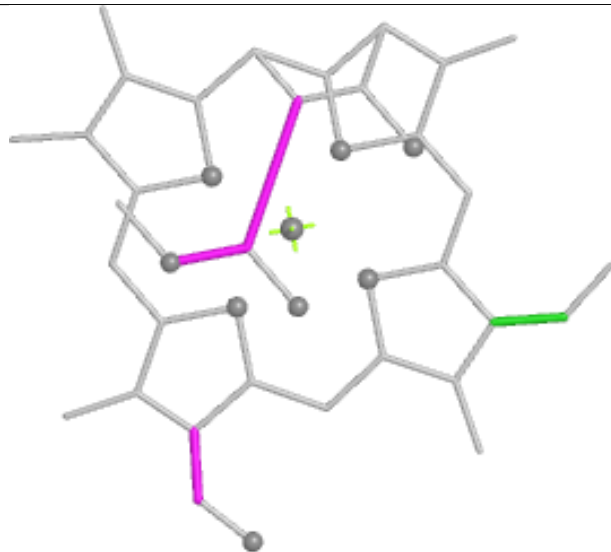
Ligand CL7 aA 3113



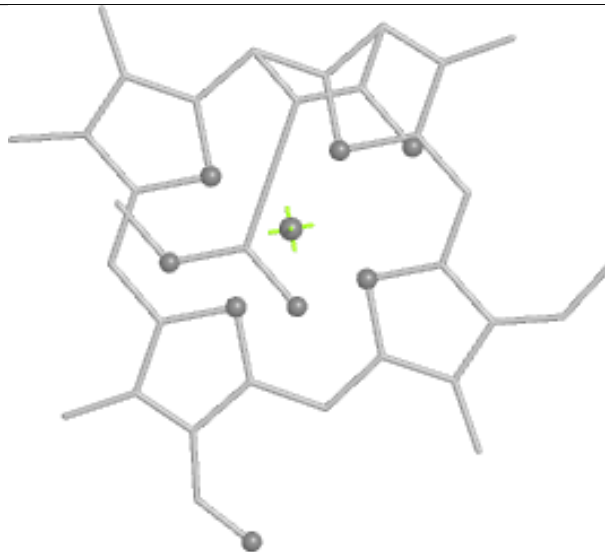
Bond lengths



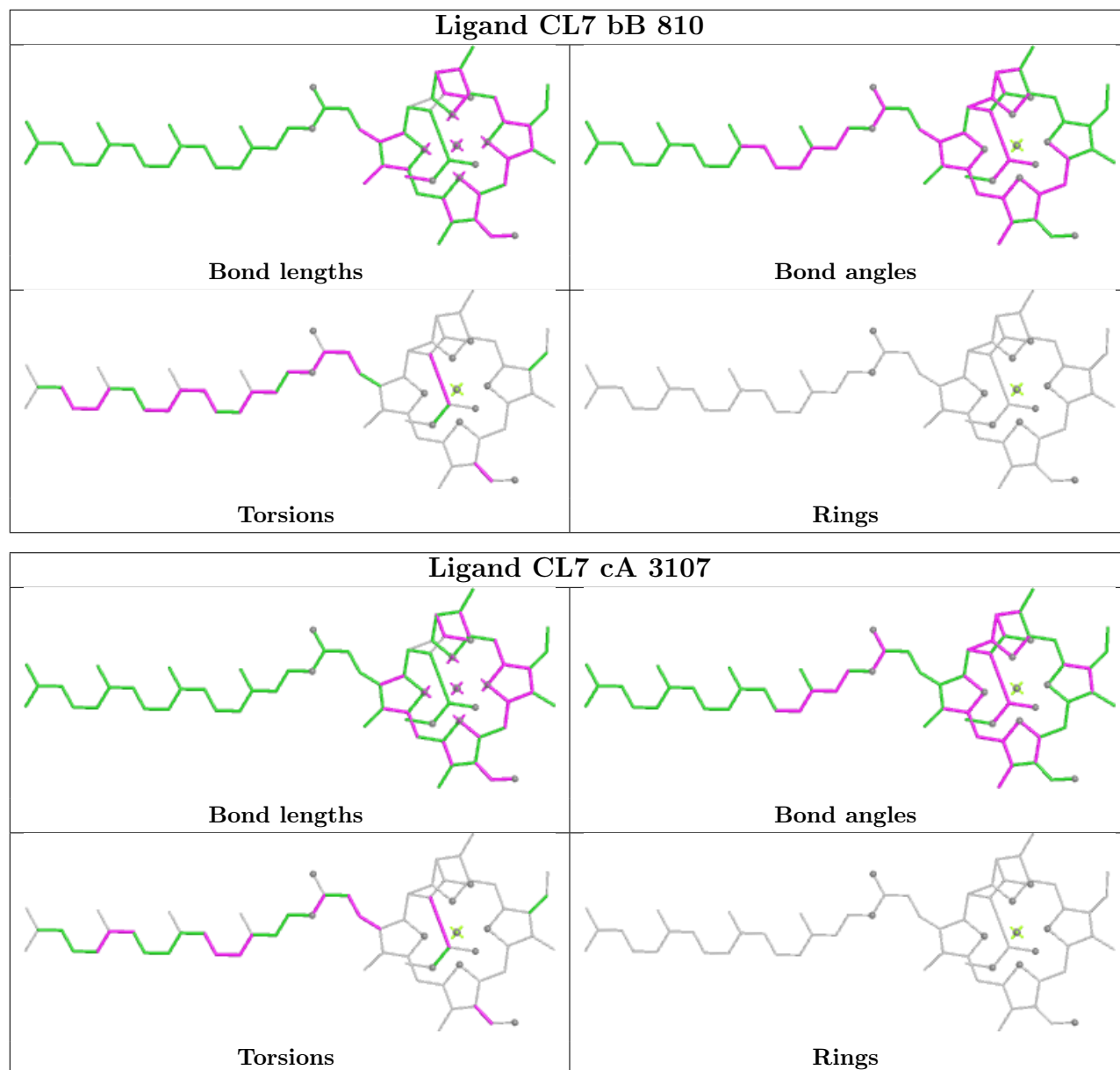
Bond angles



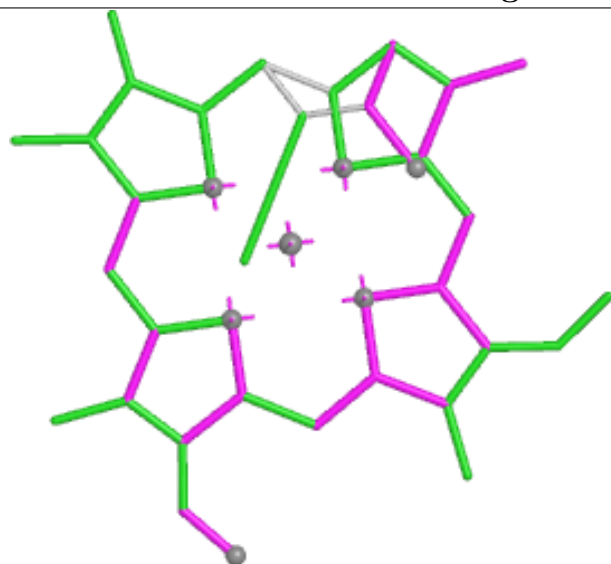
Torsions



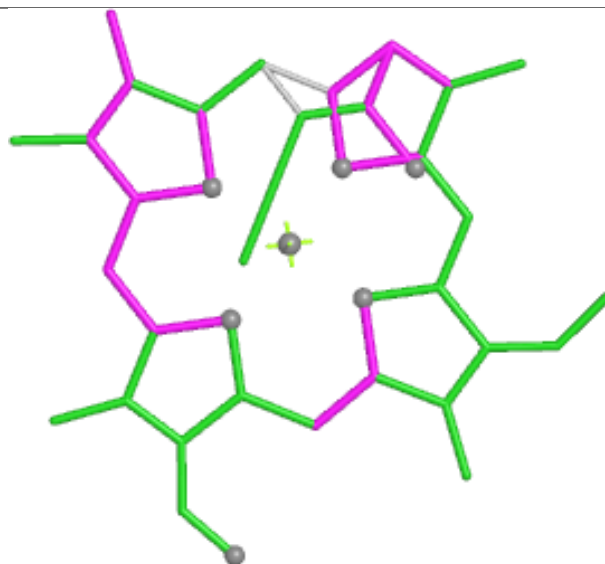
Rings



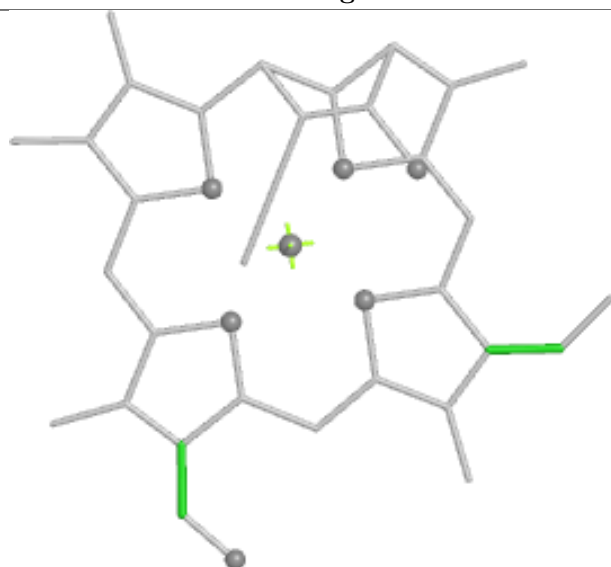
Ligand CL7 cA 3118



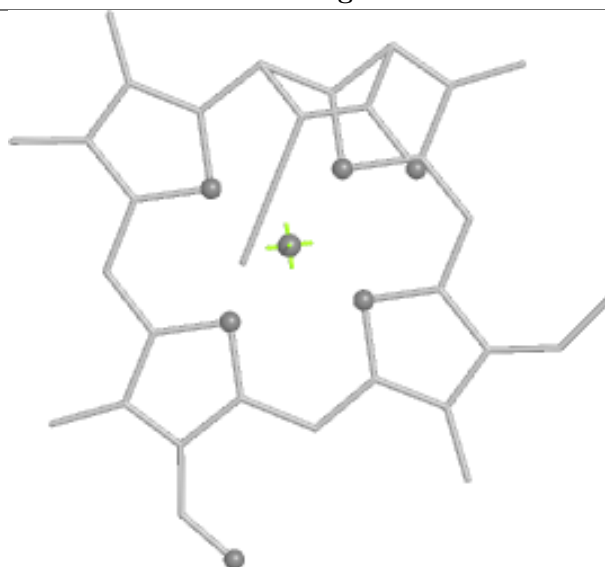
Bond lengths



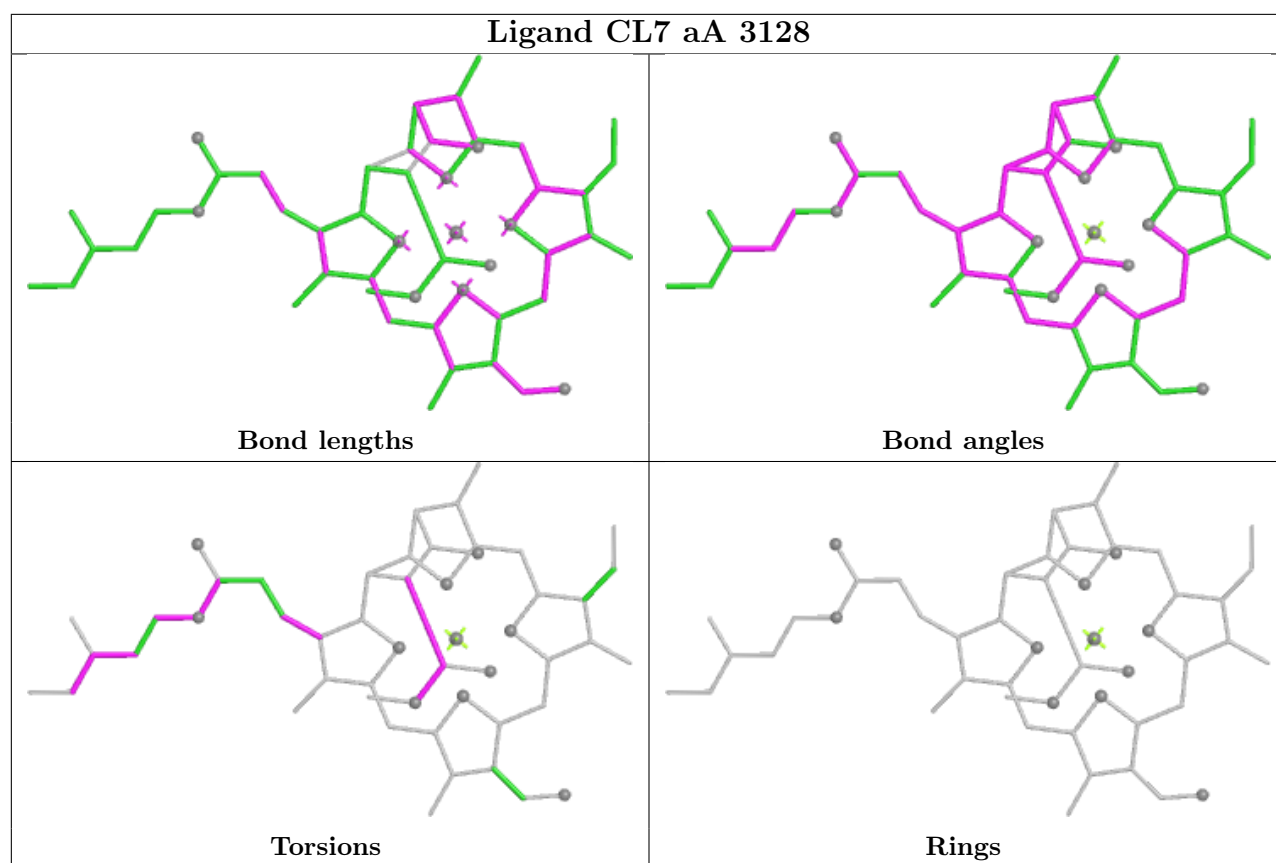
Bond angles



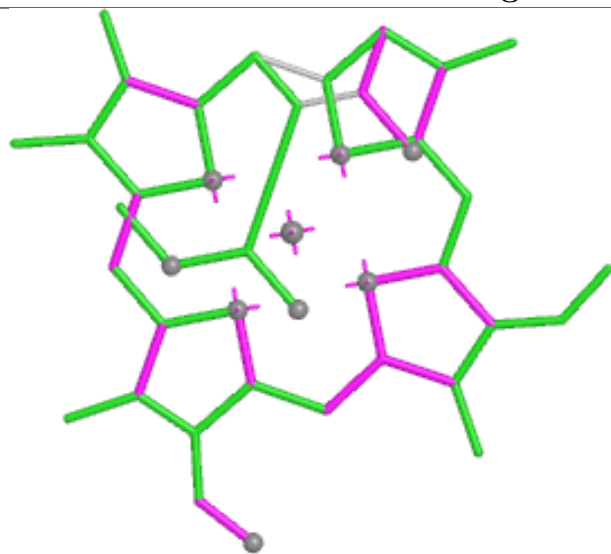
Torsions



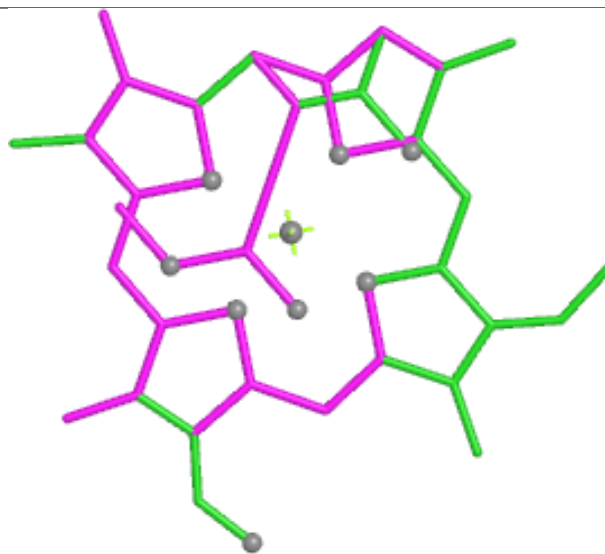
Rings



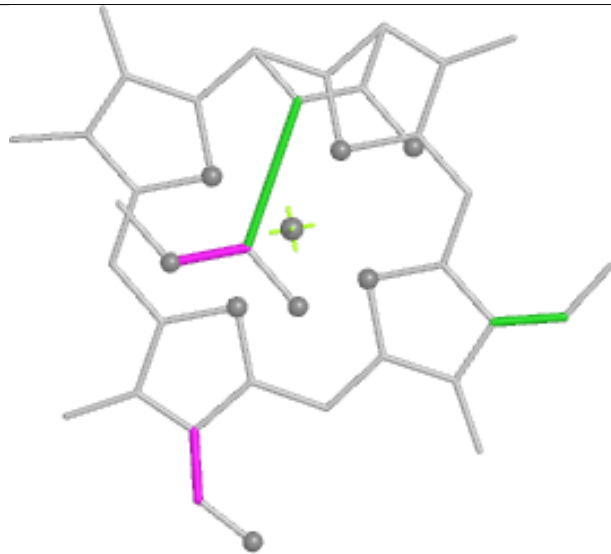
Ligand CL7 cA 3109



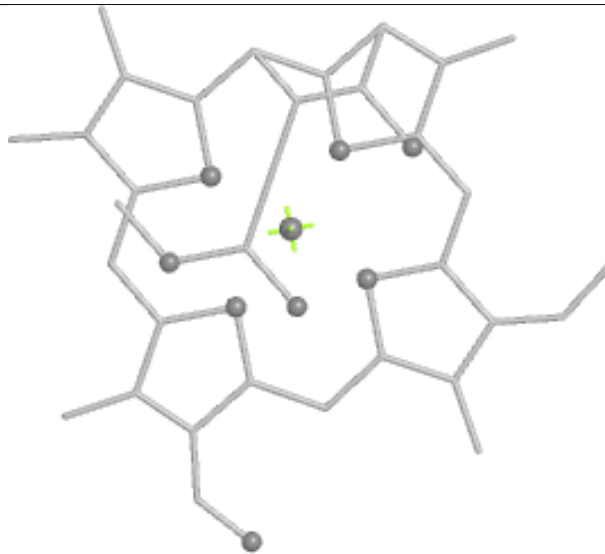
Bond lengths



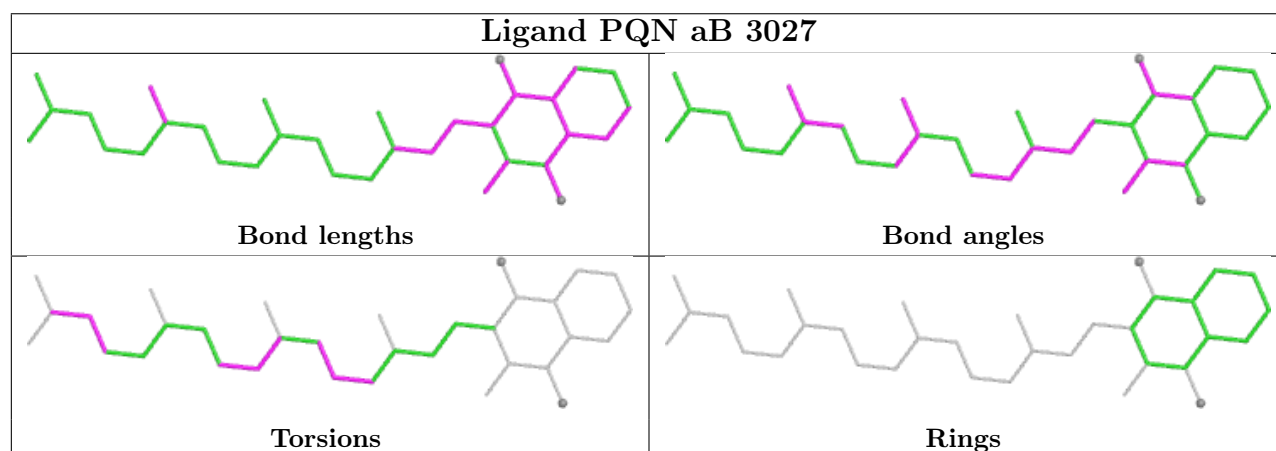
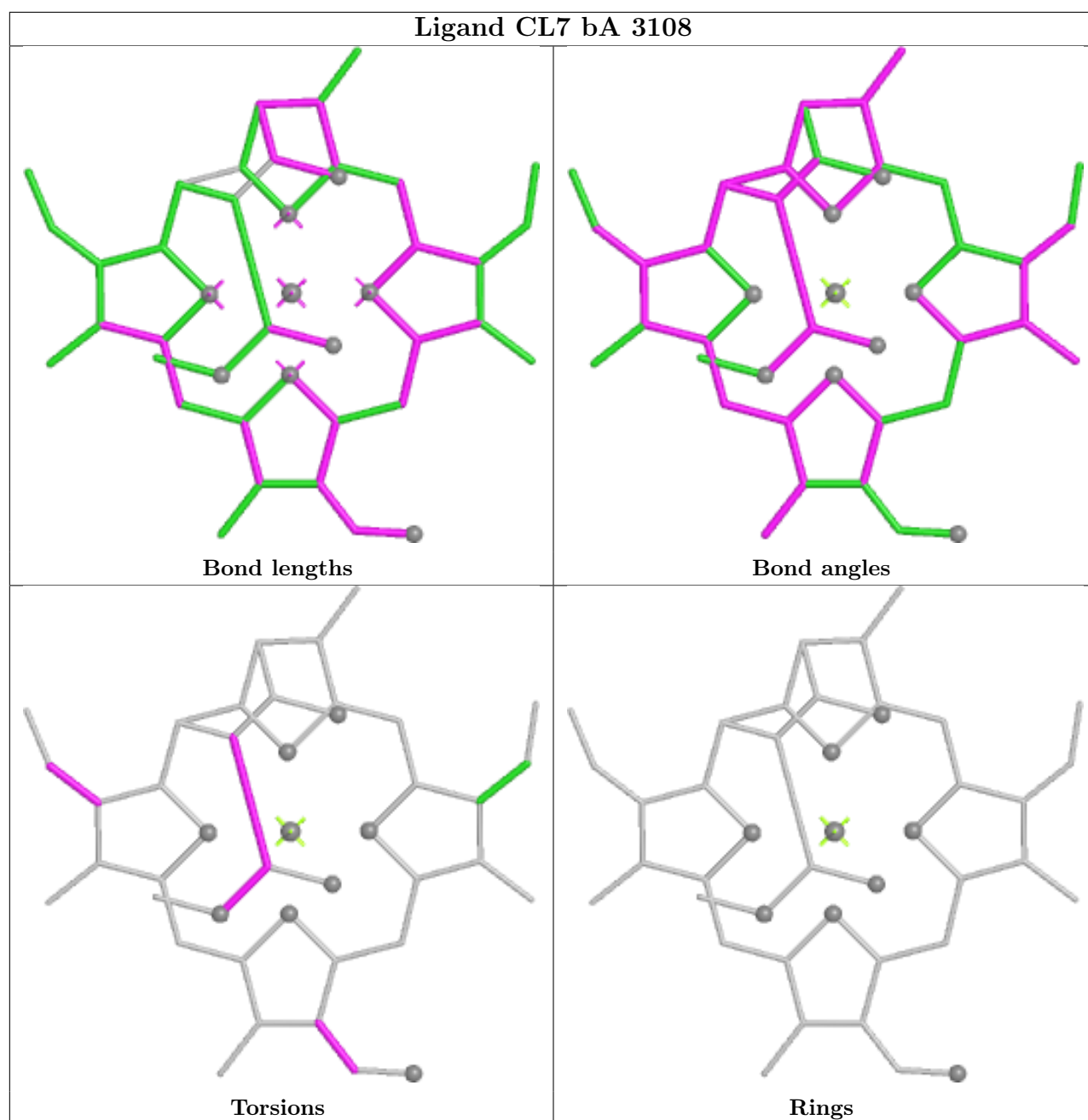
Bond angles

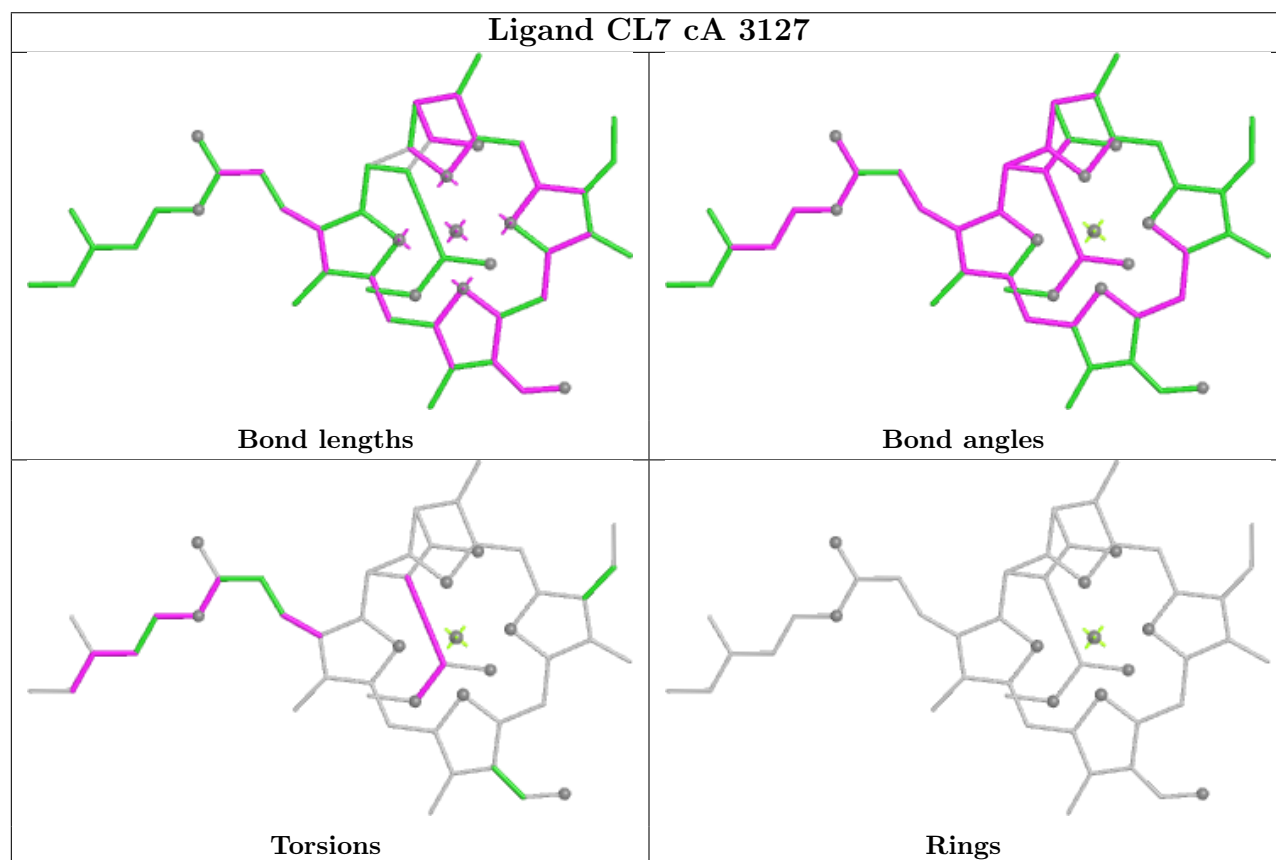
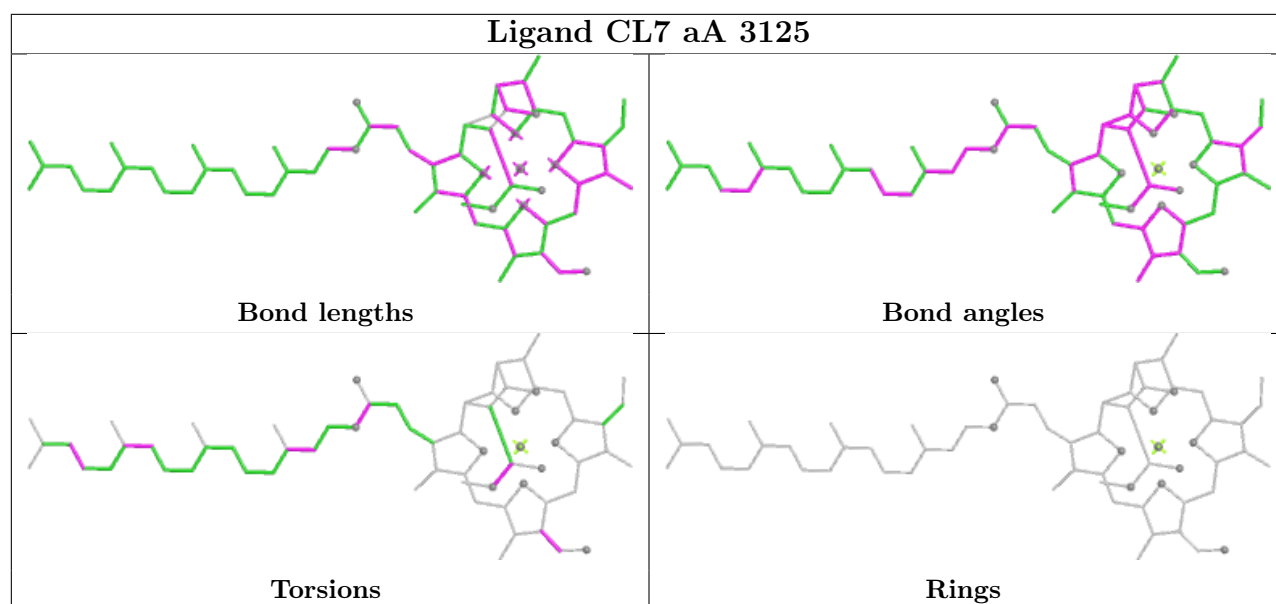


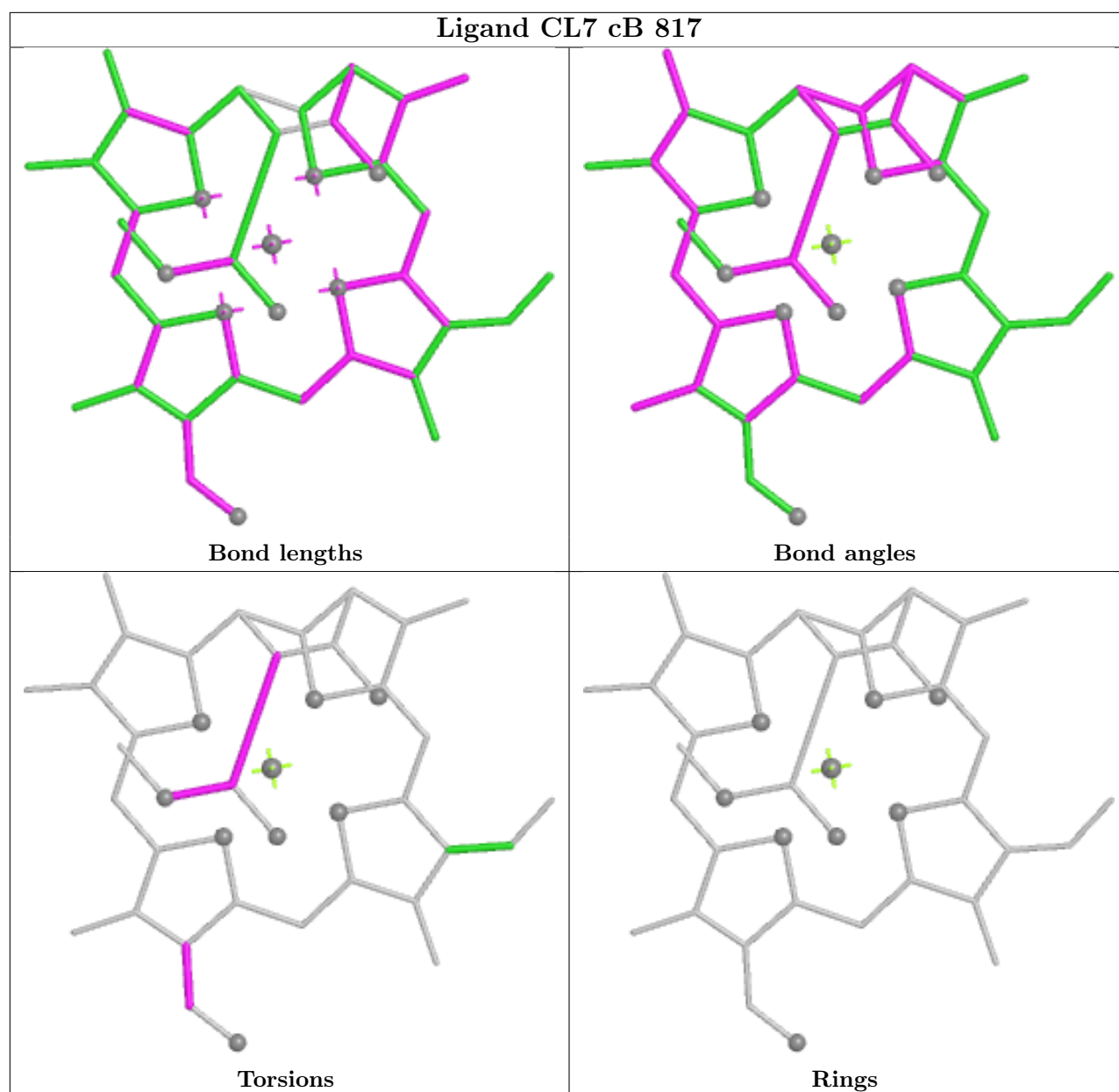
Torsions



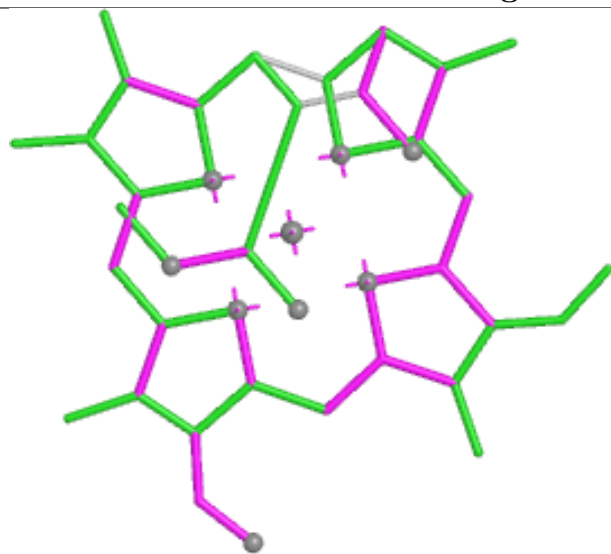
Rings



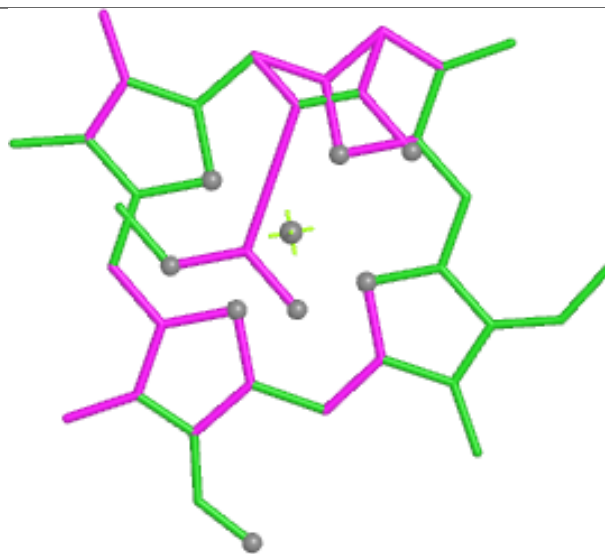




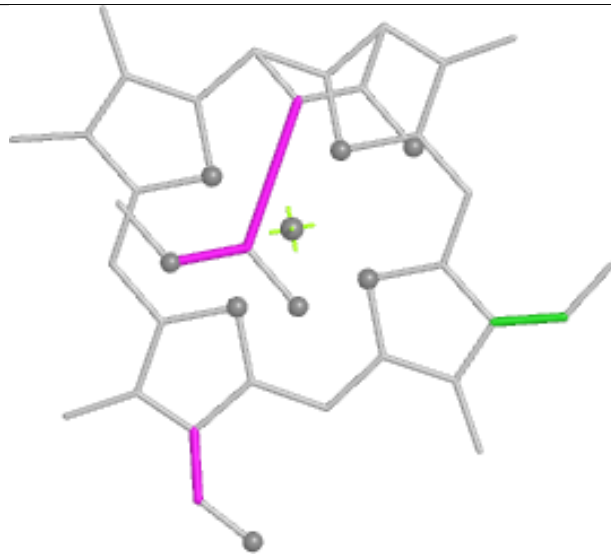
Ligand CL7 aA 3131



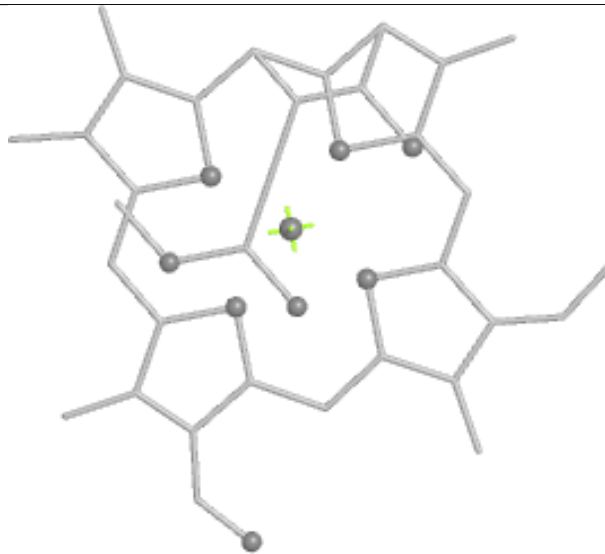
Bond lengths



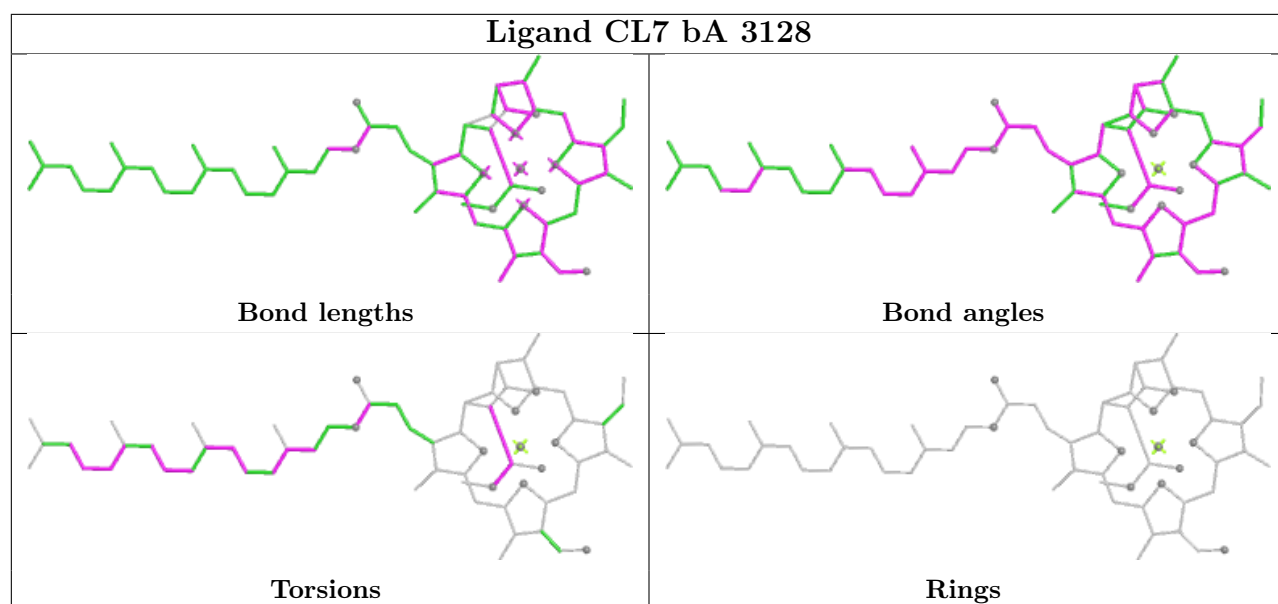
Bond angles



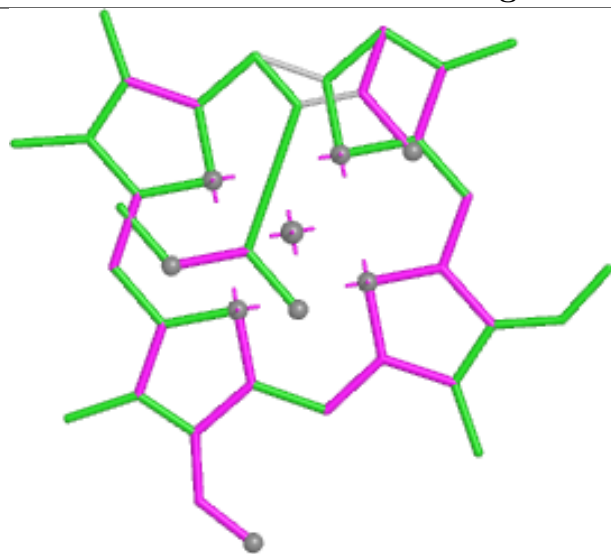
Torsions



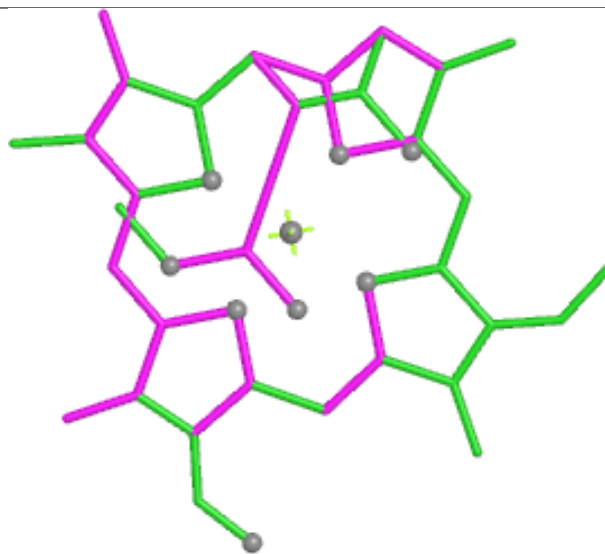
Rings



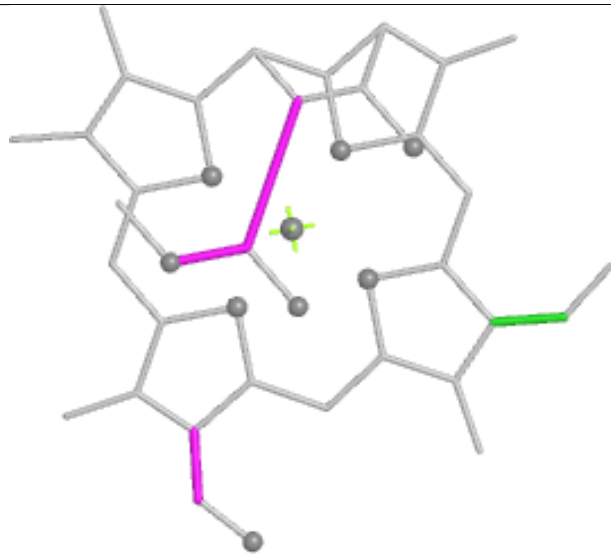
Ligand CL7 bA 3130



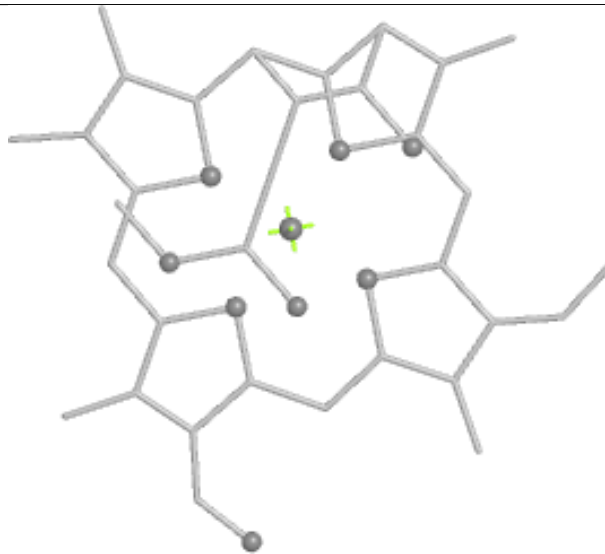
Bond lengths



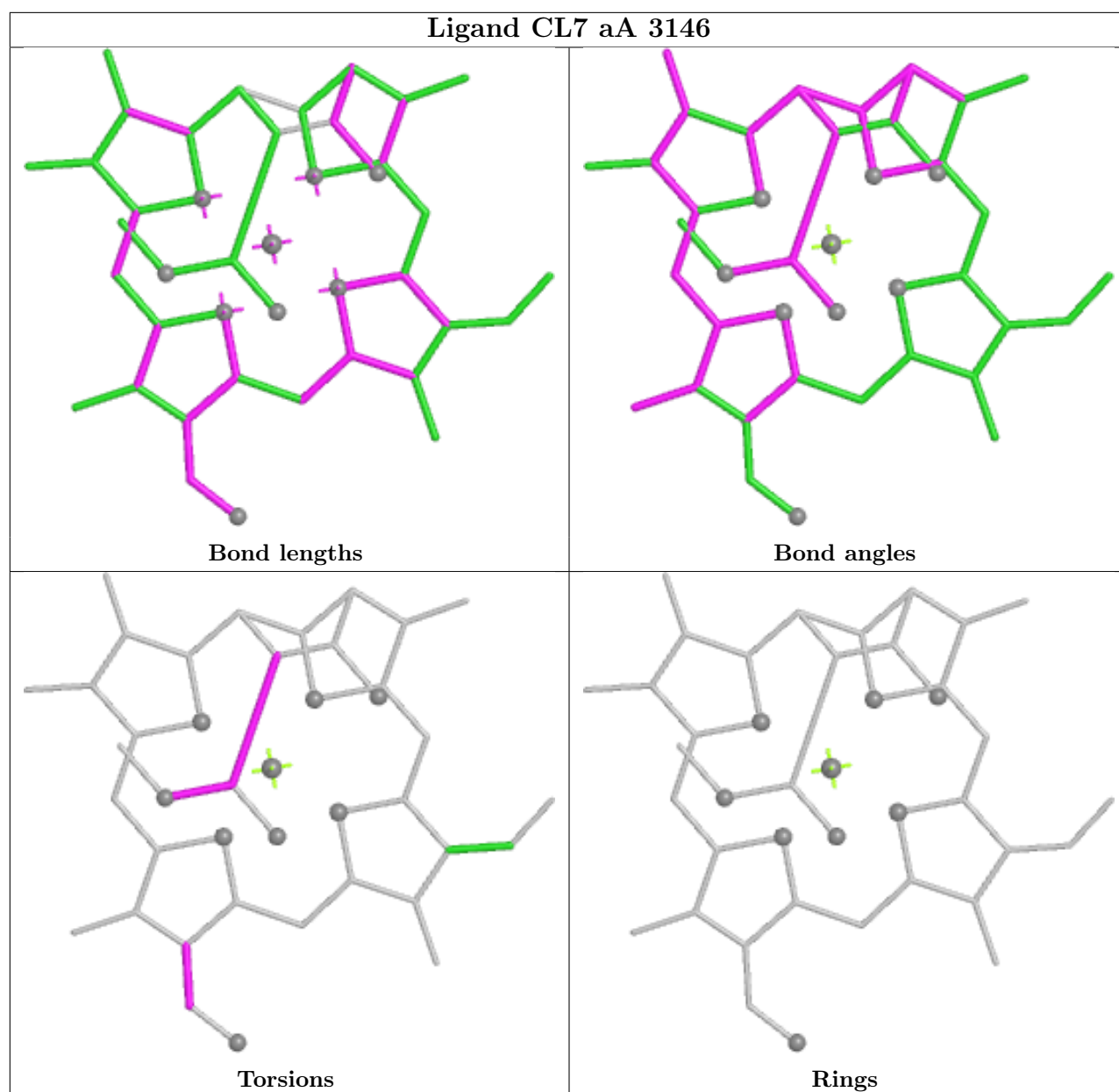
Bond angles

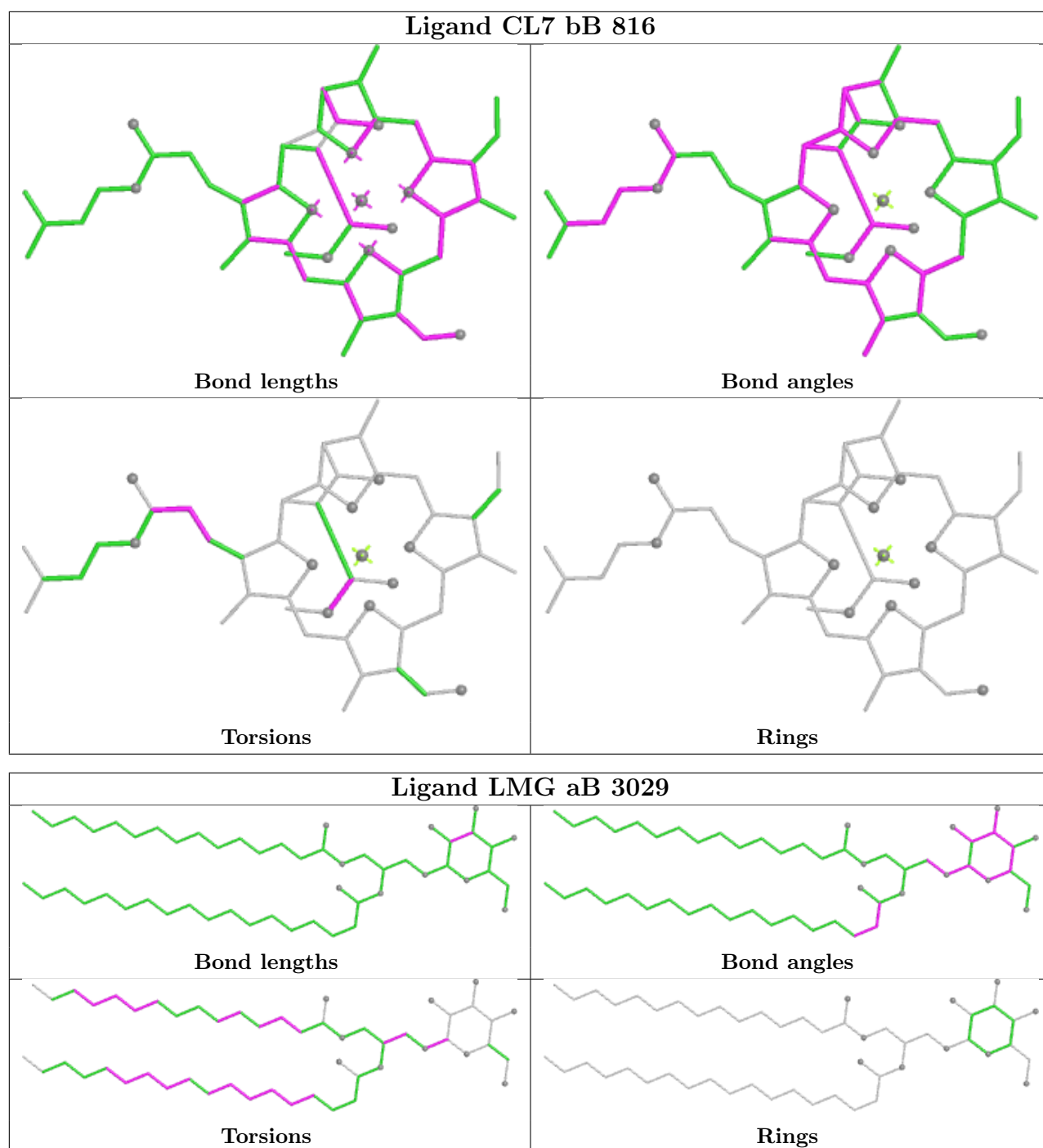


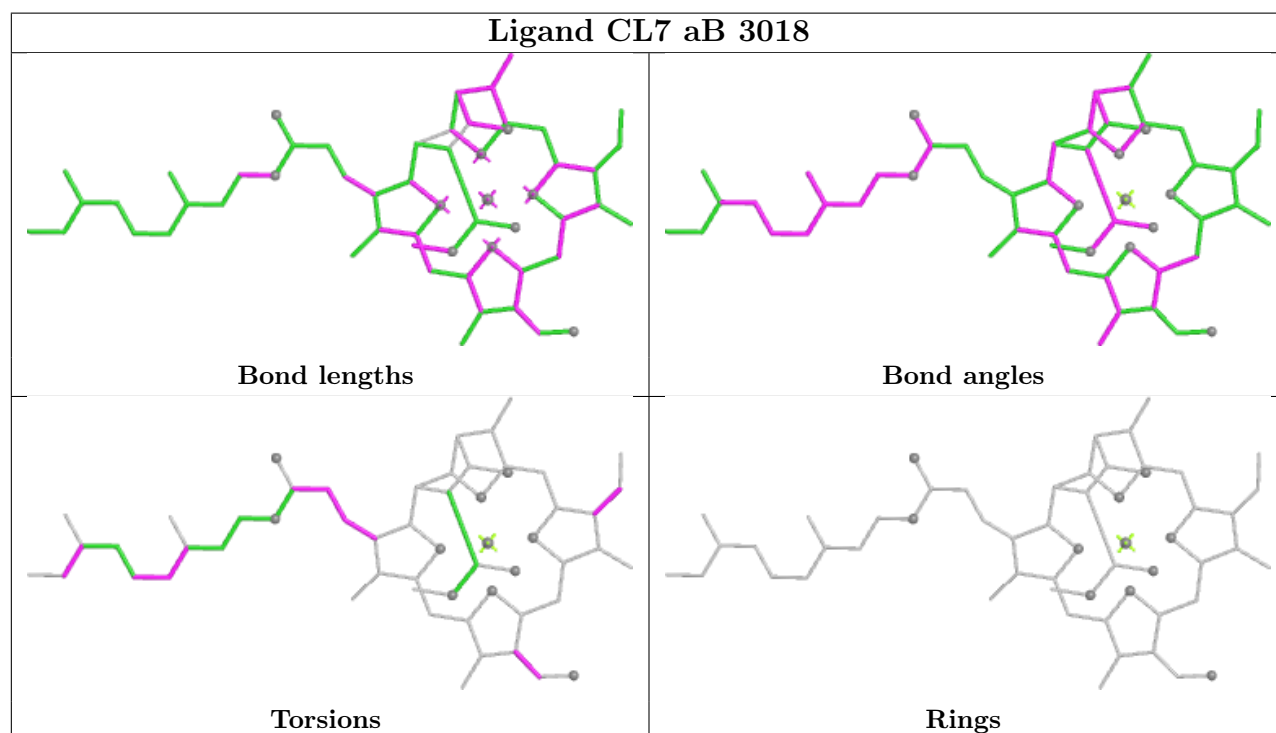
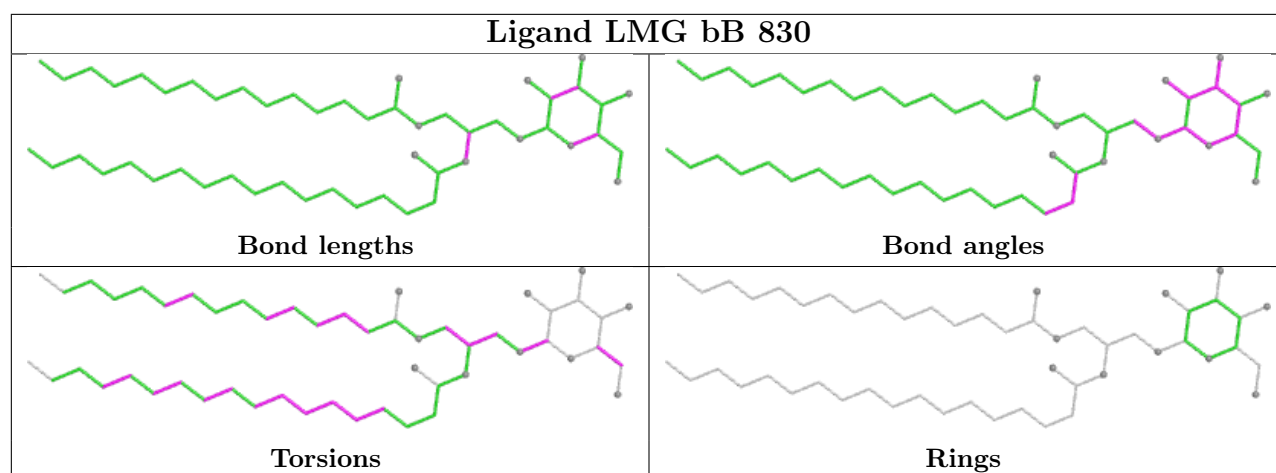
Torsions

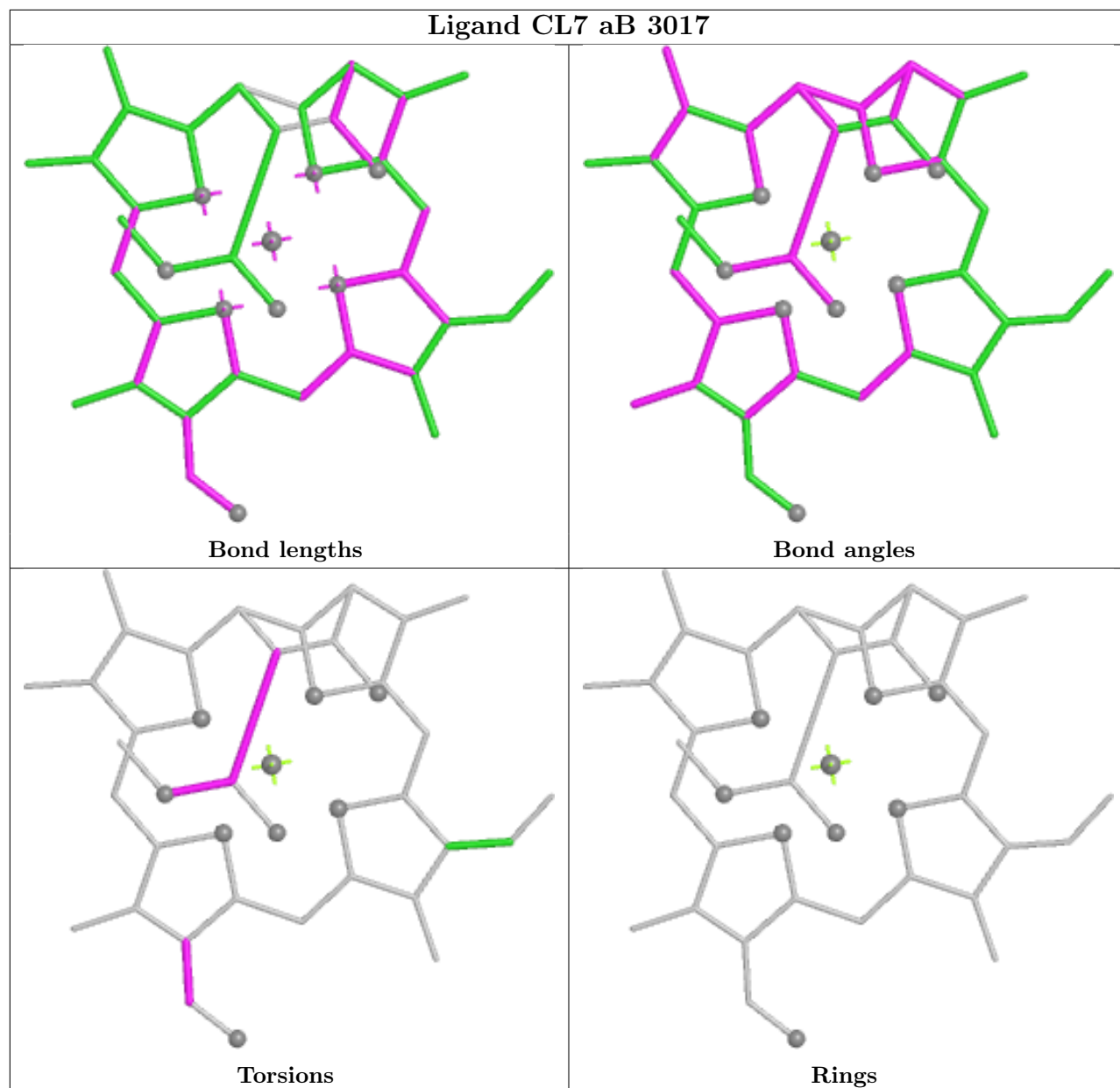


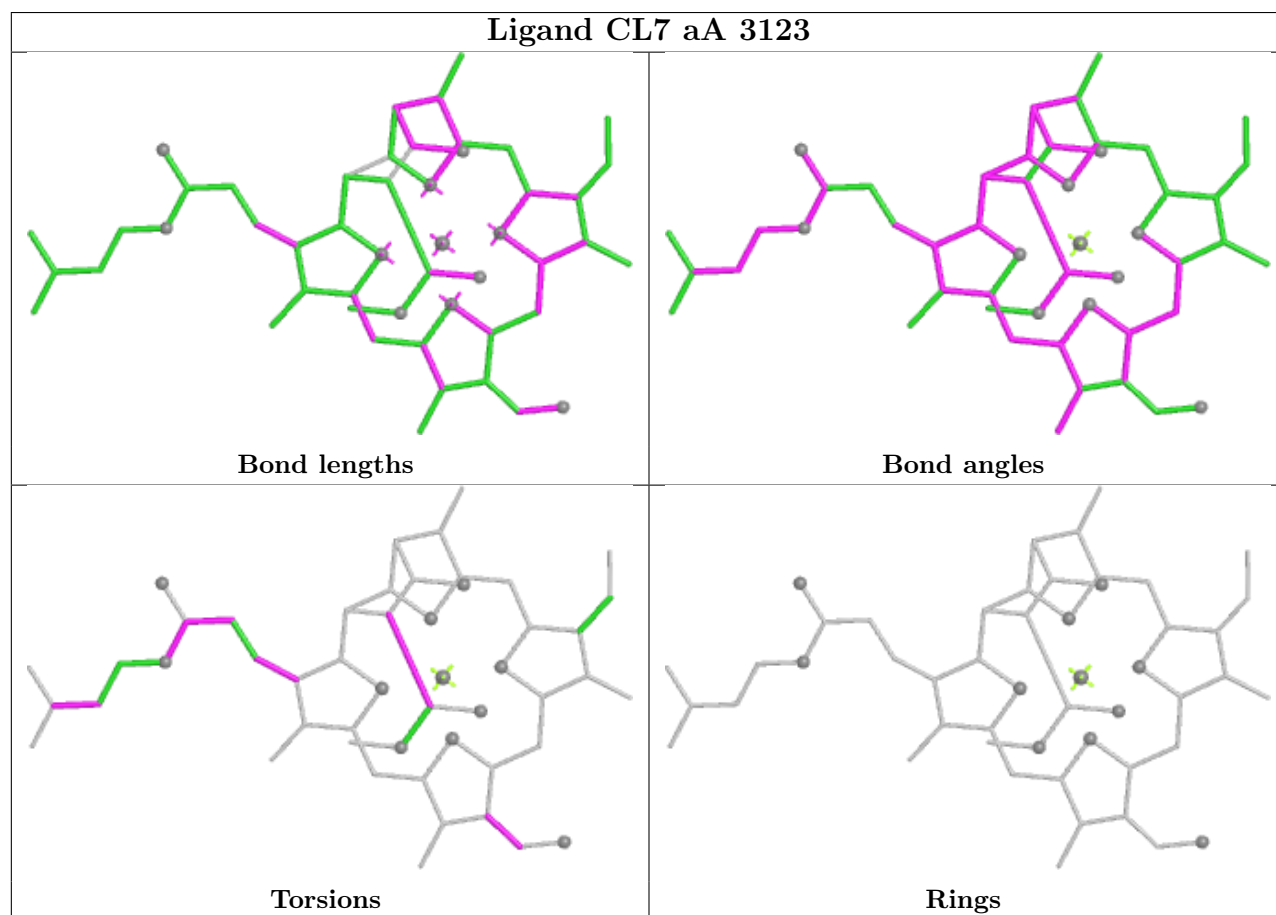
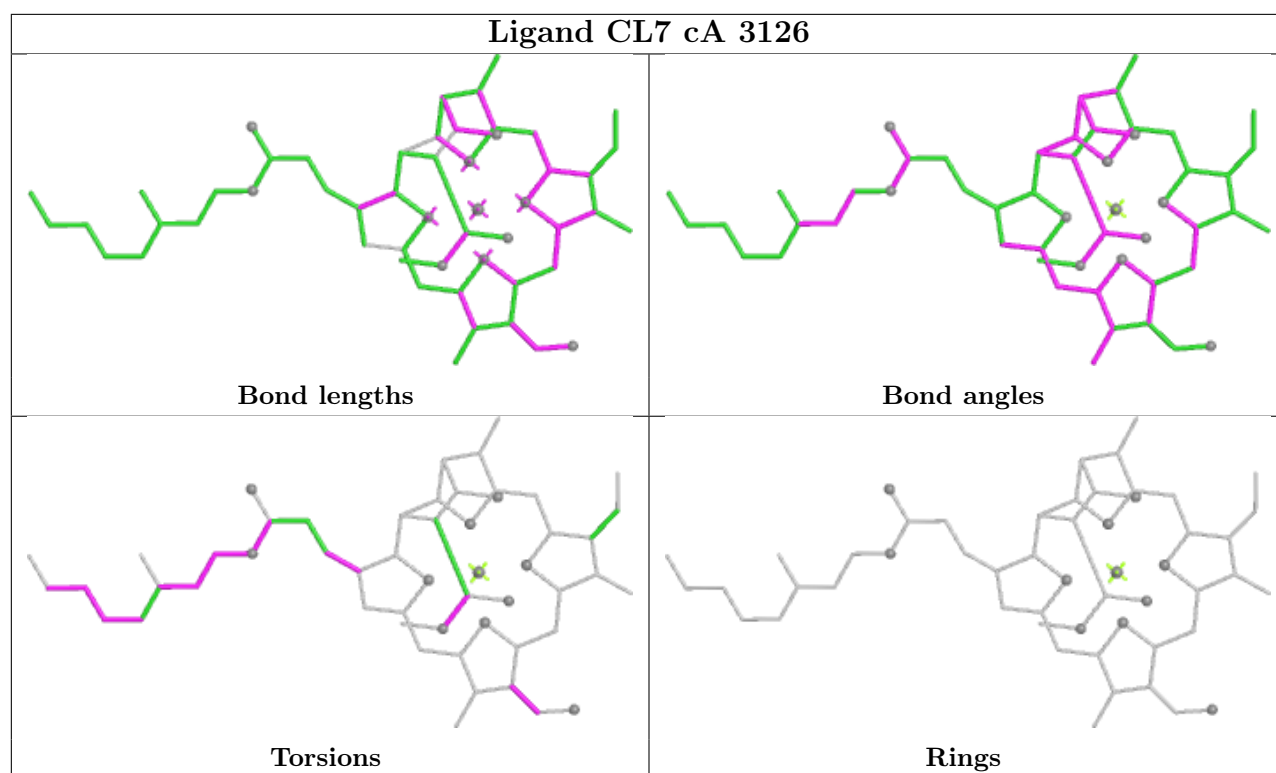
Rings



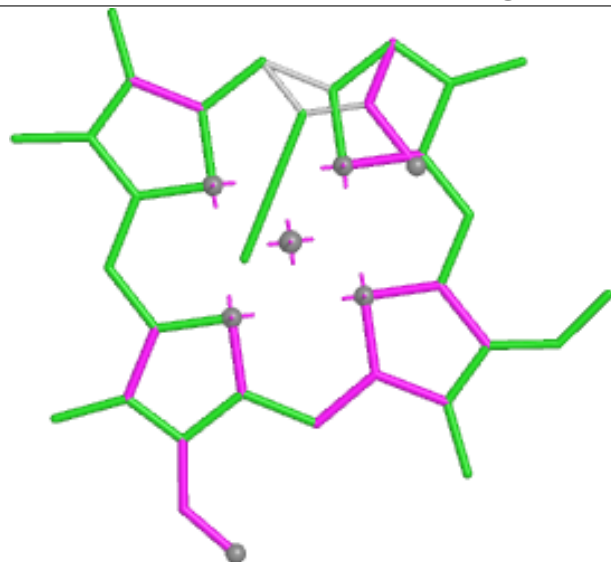




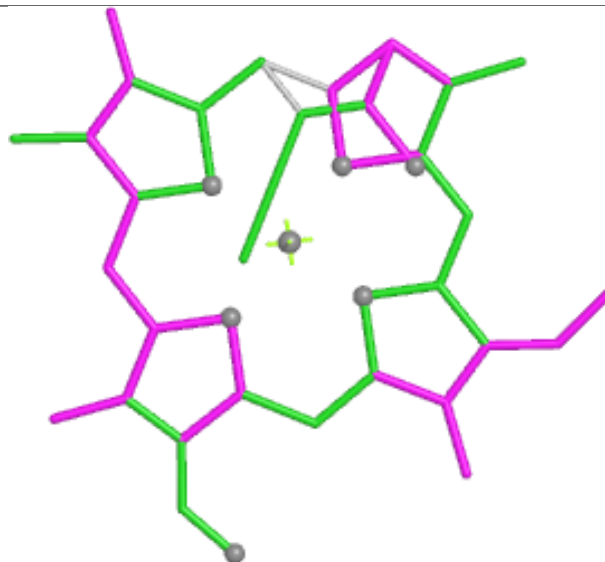




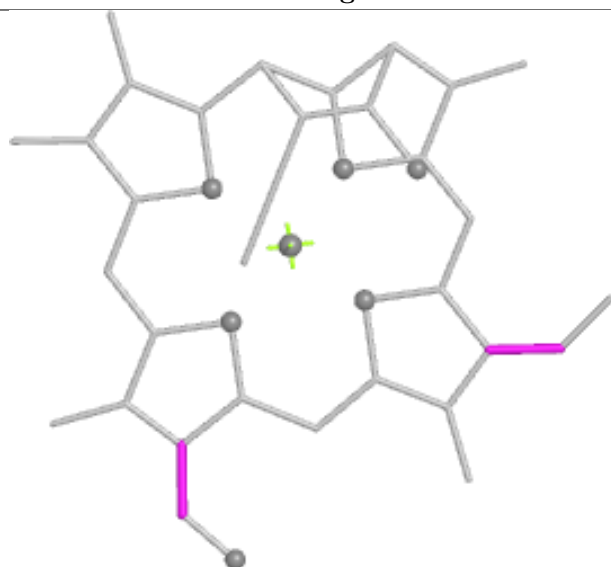
Ligand CL7 bA 3115



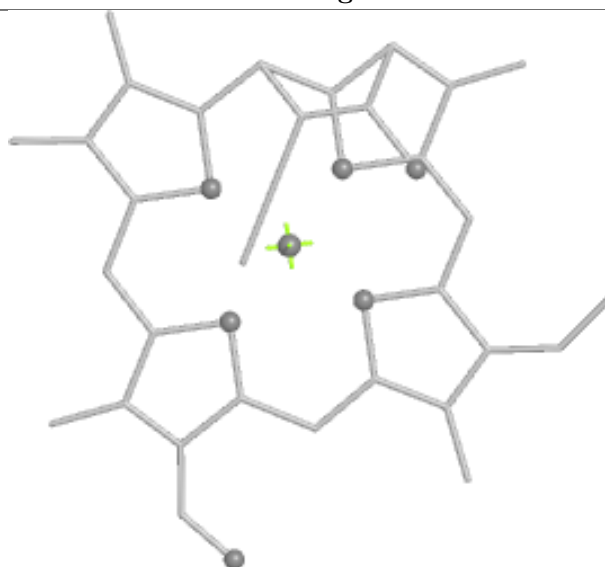
Bond lengths



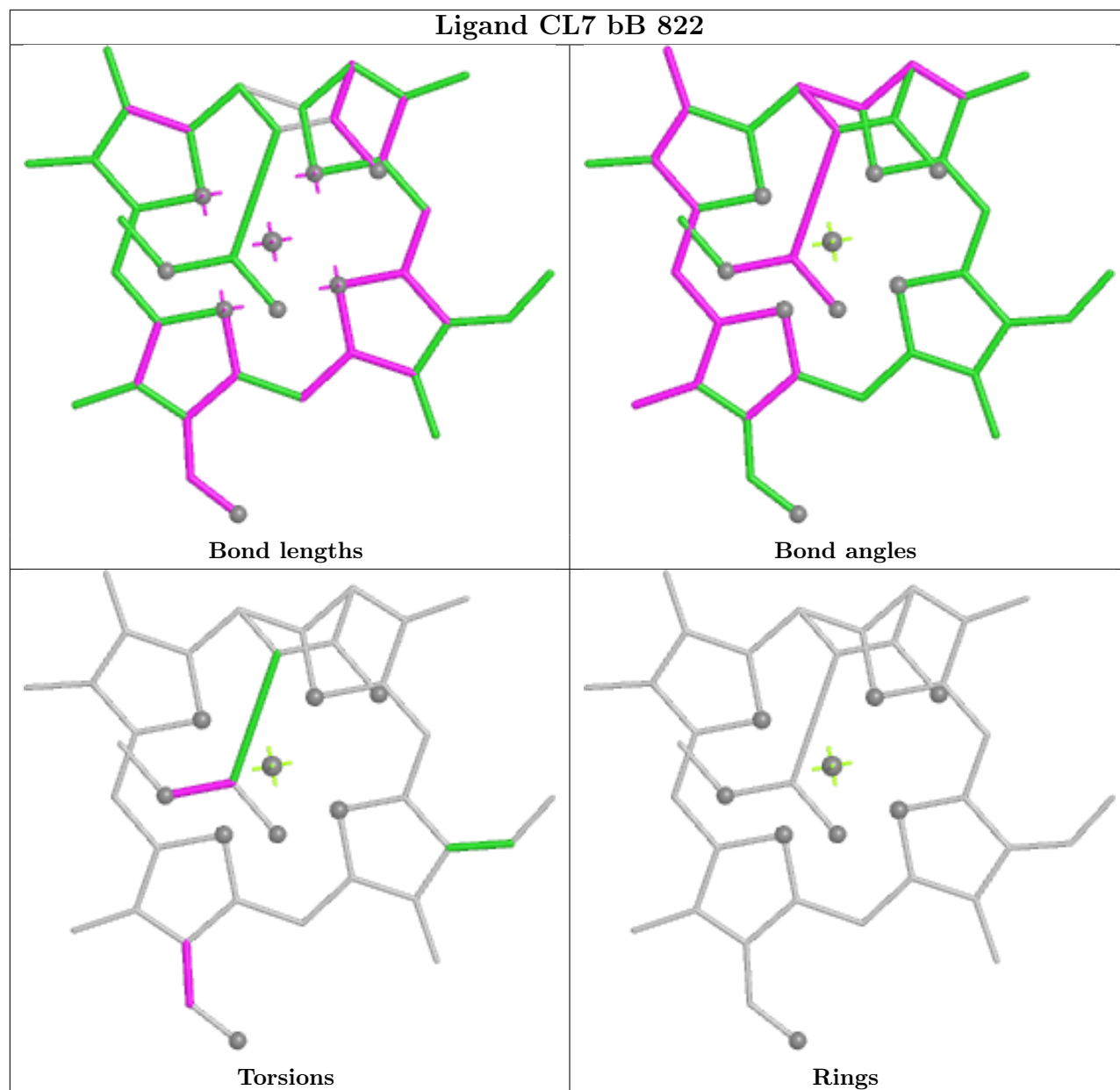
Bond angles



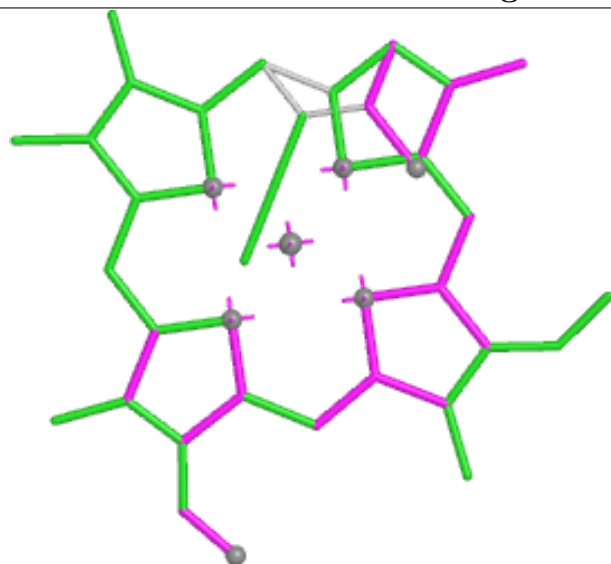
Torsions



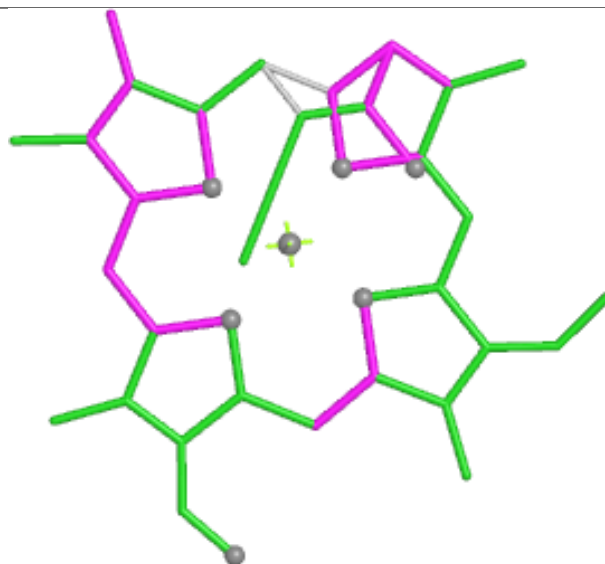
Rings



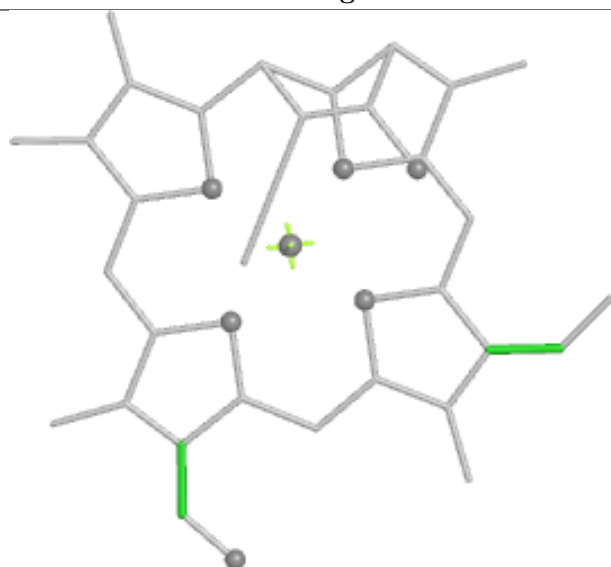
Ligand CL7 aA 3119



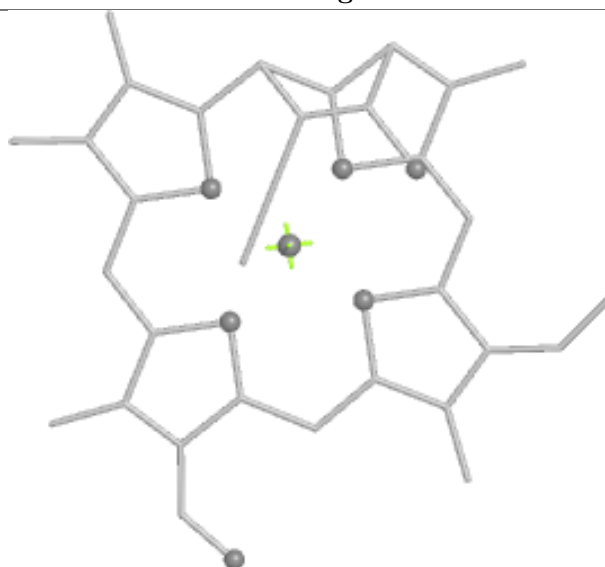
Bond lengths



Bond angles

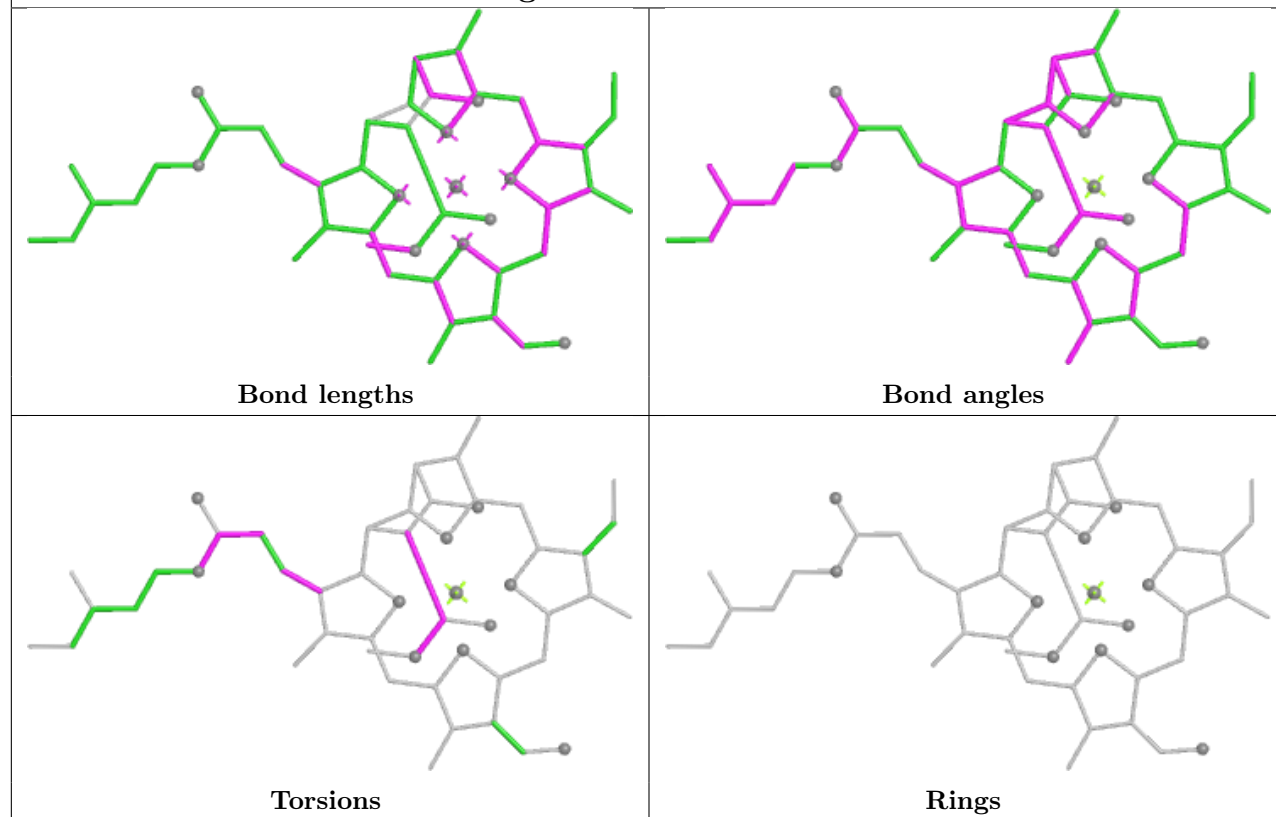


Torsions

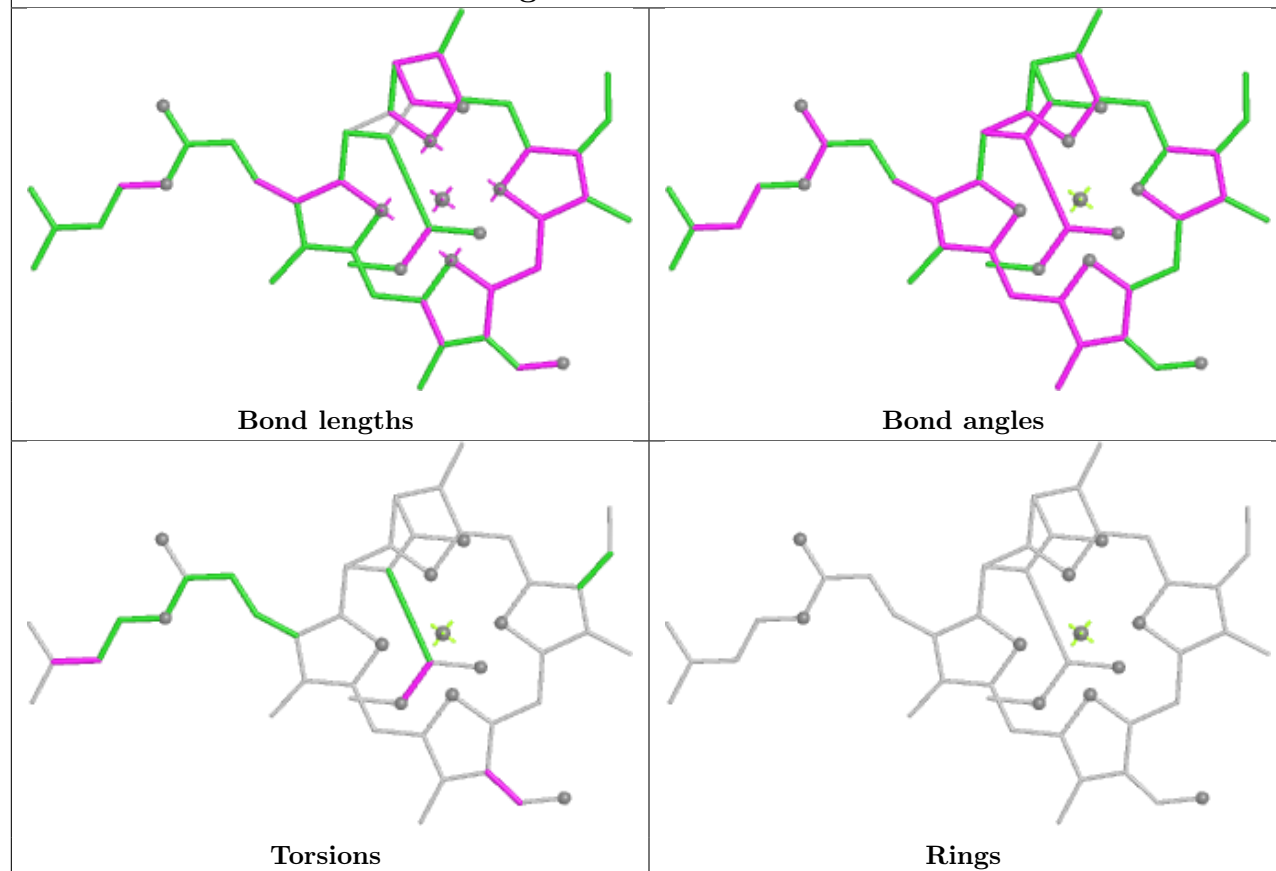


Rings

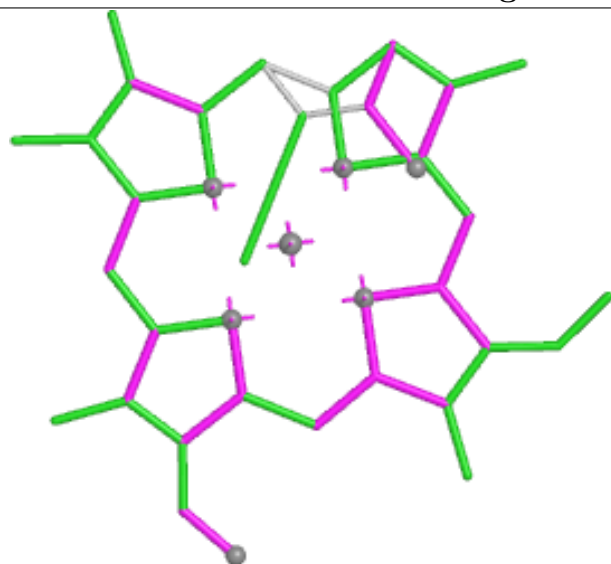
Ligand CL7 aA 3121



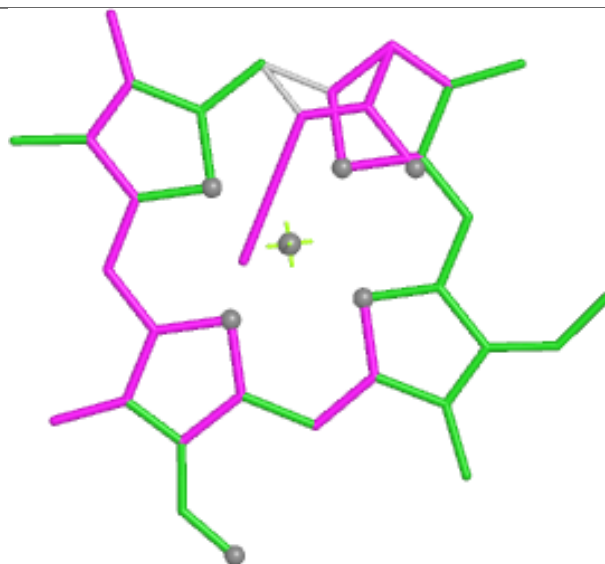
Ligand CL7 aB 3008



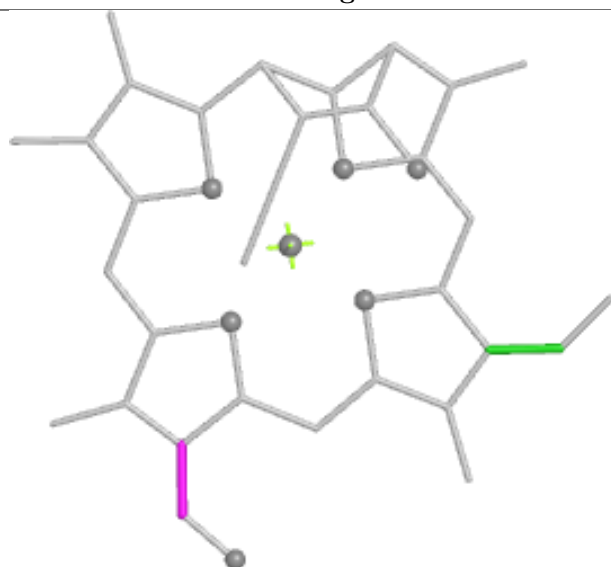
Ligand CL7 bA 3117



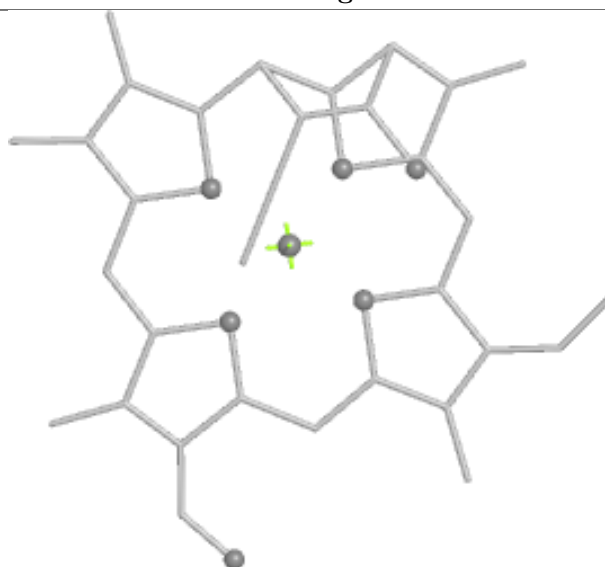
Bond lengths



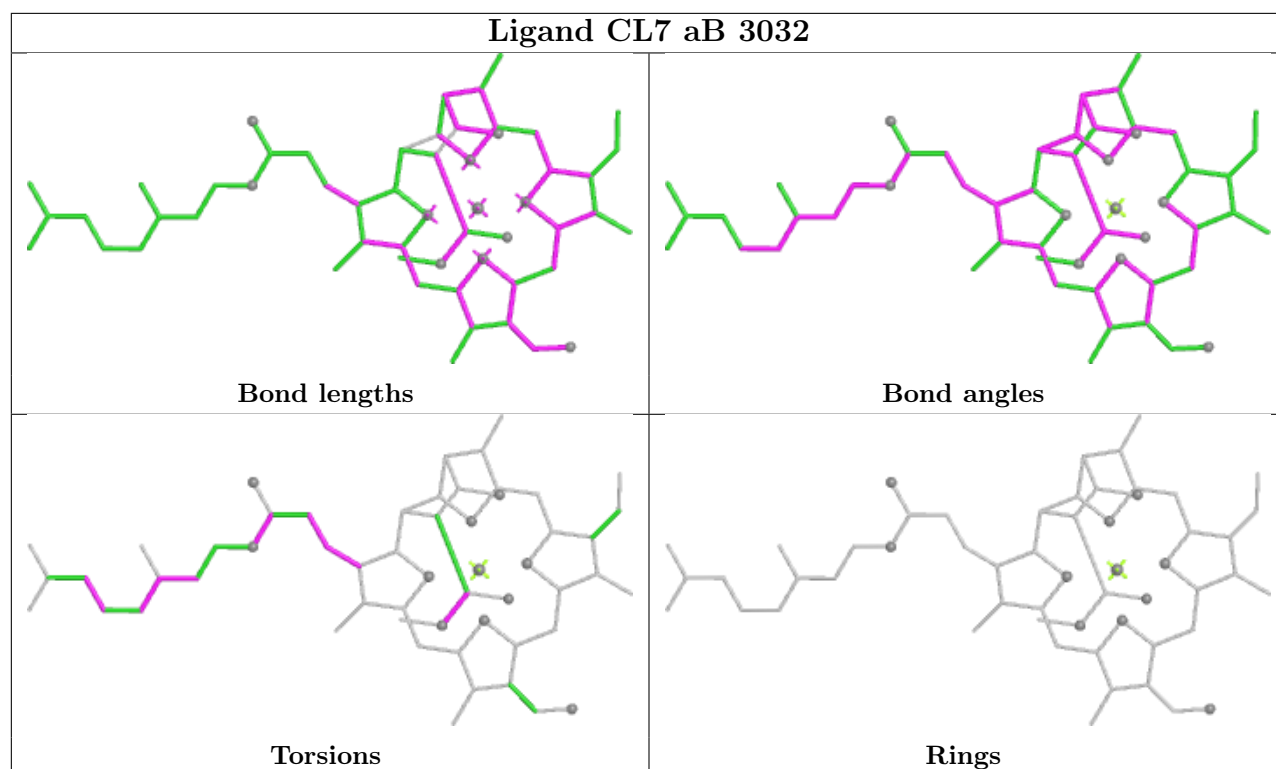
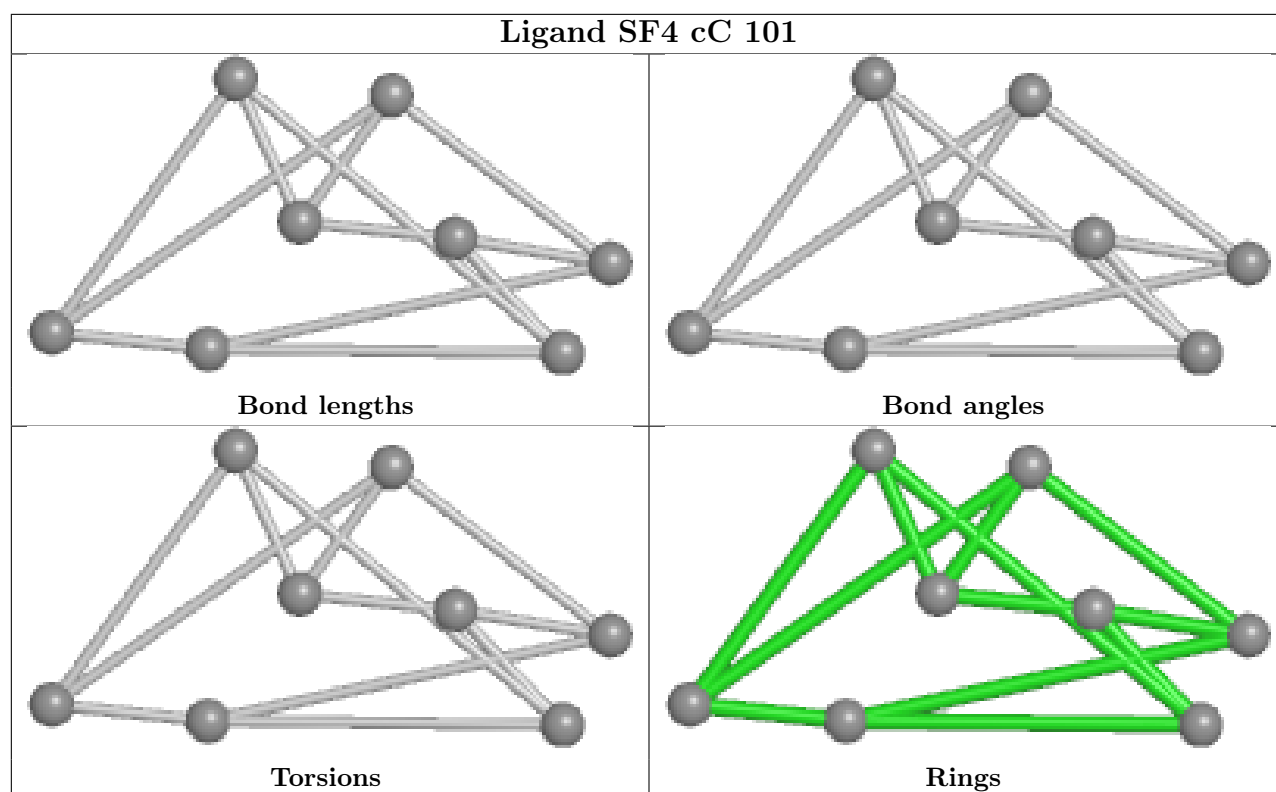
Bond angles

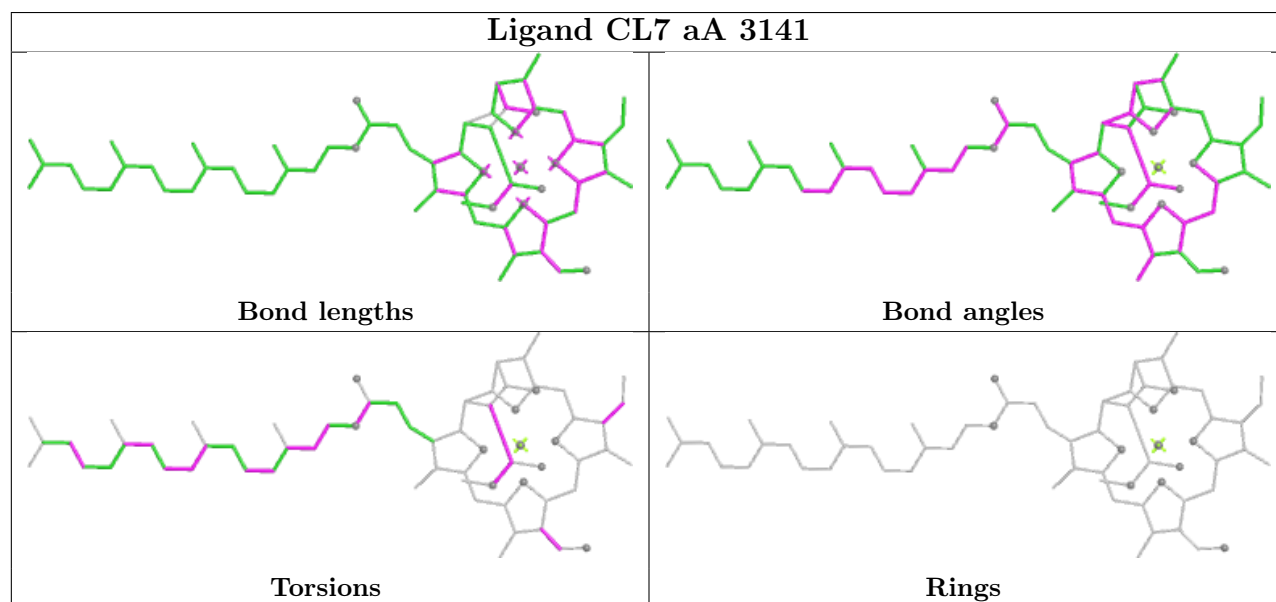
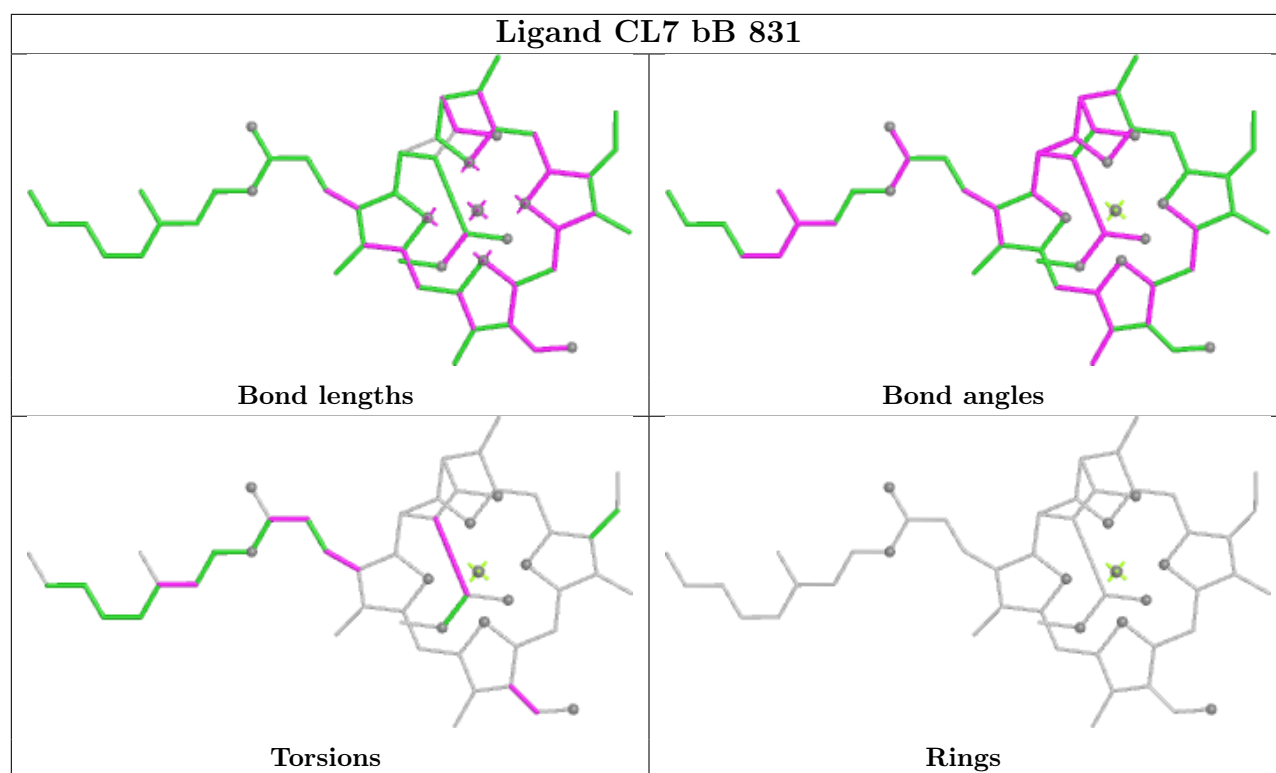


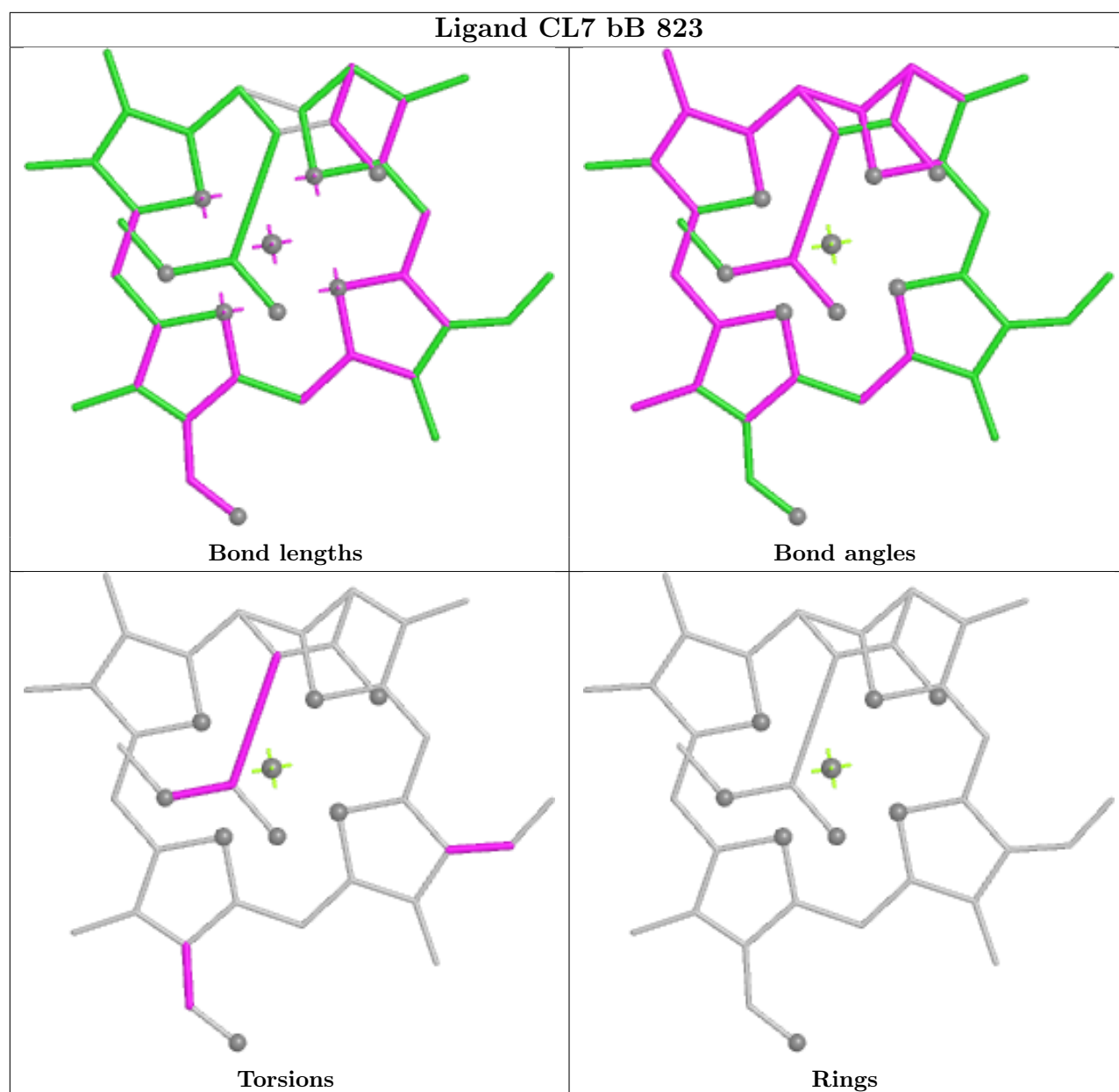
Torsions



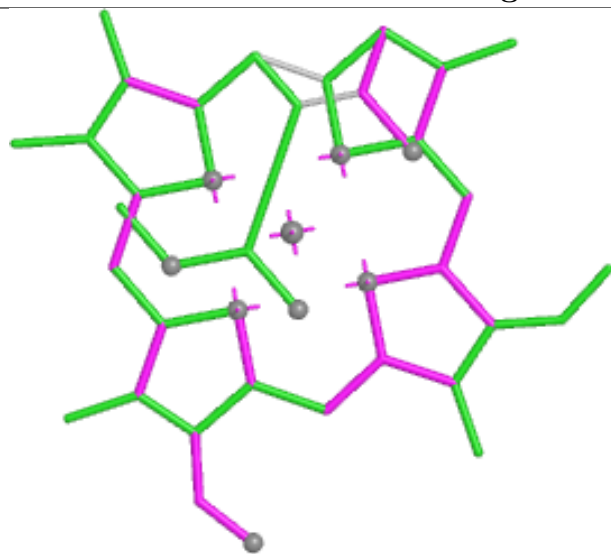
Rings



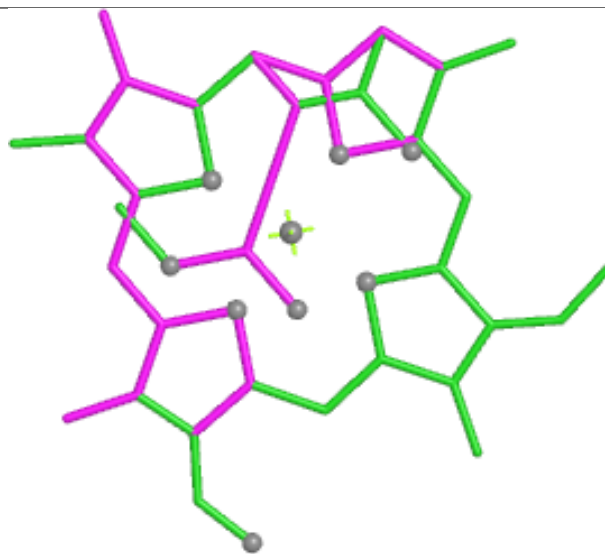




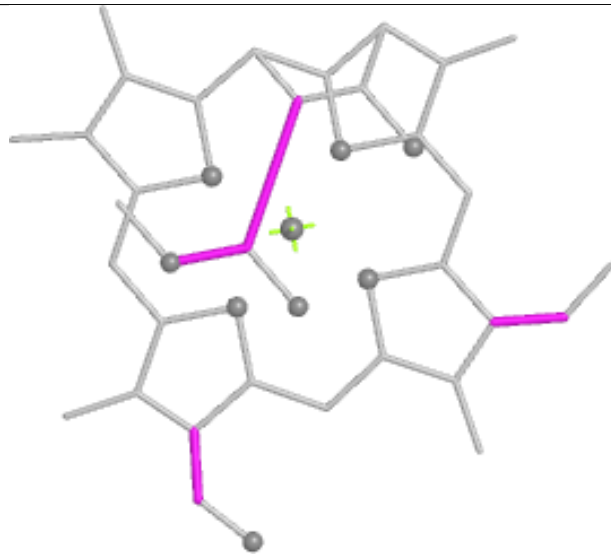
Ligand CL7 aA 3134



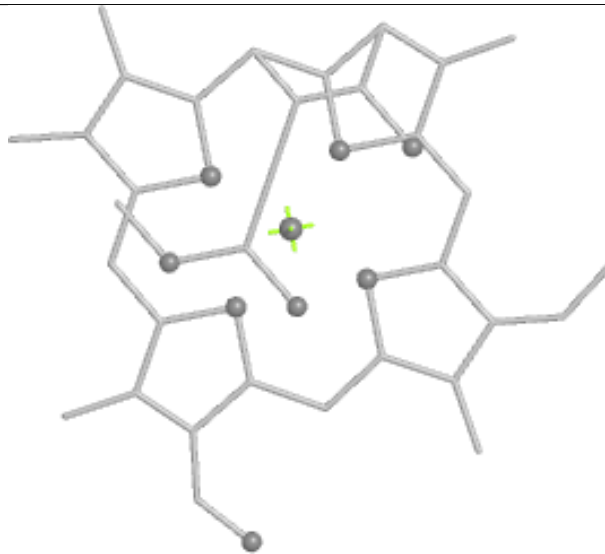
Bond lengths



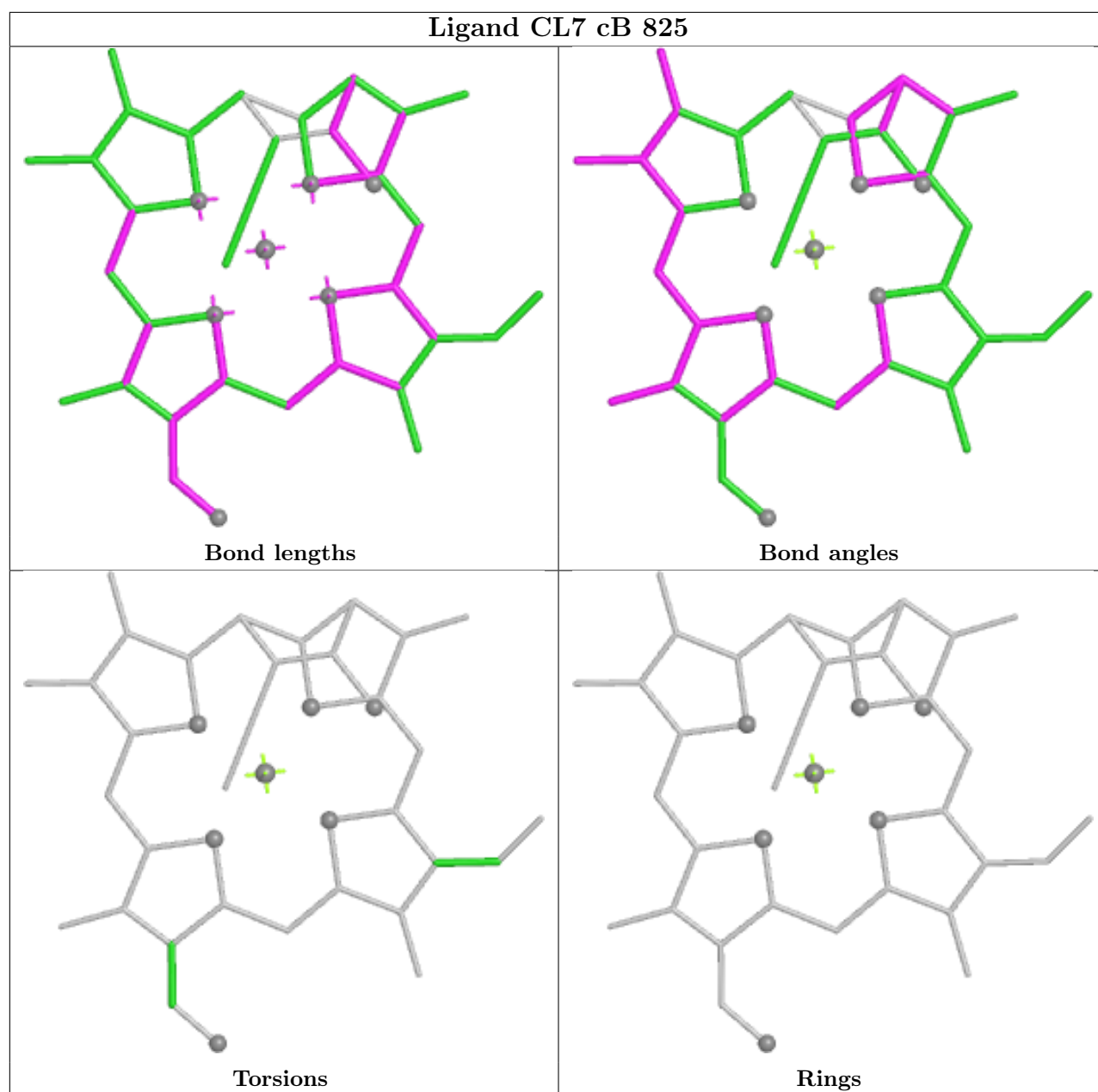
Bond angles

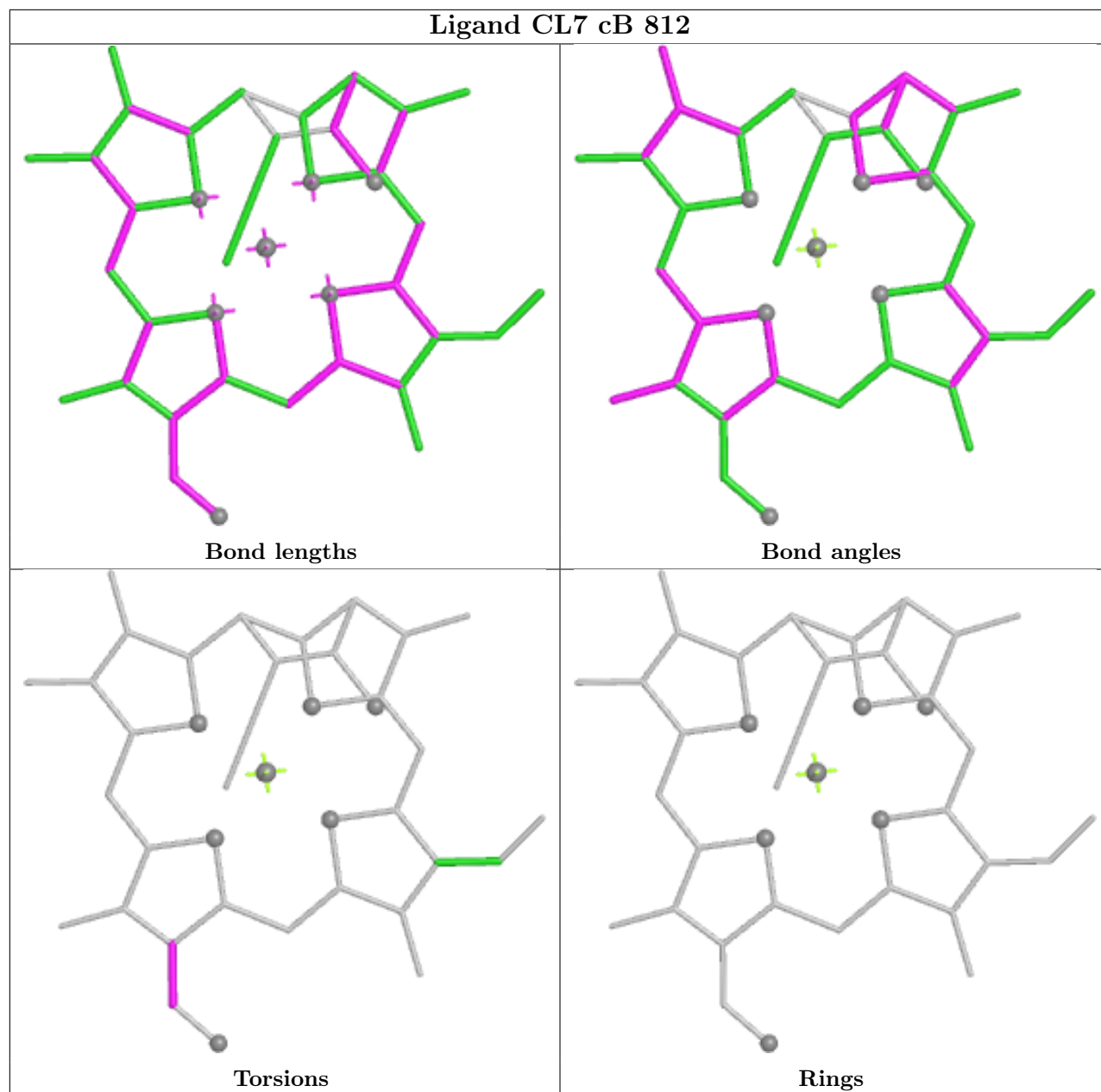


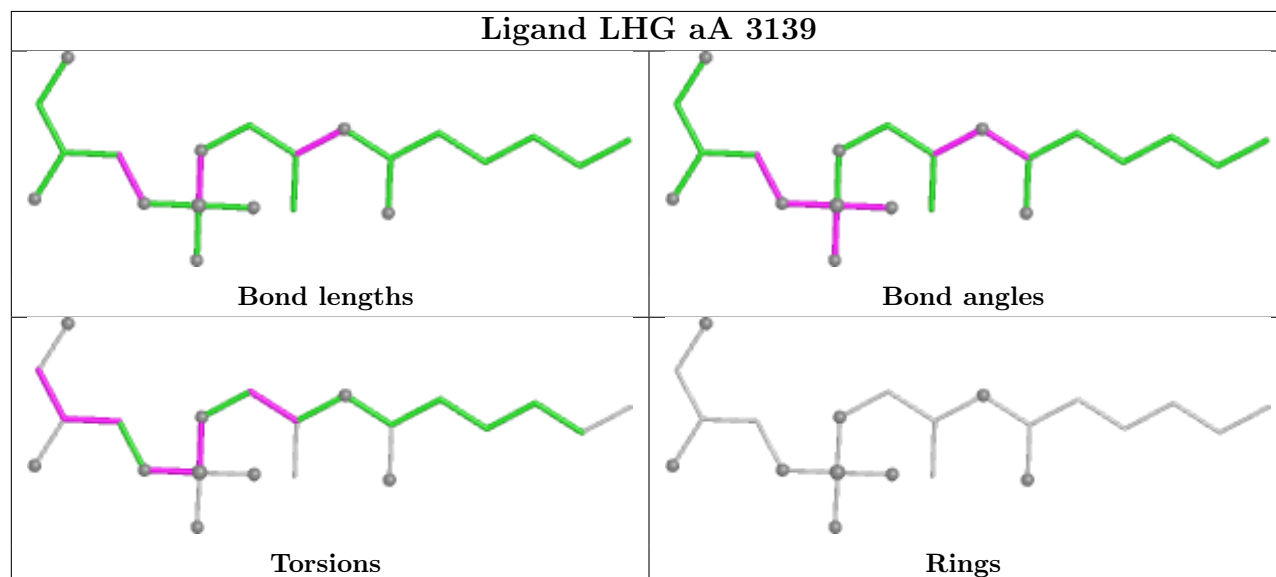
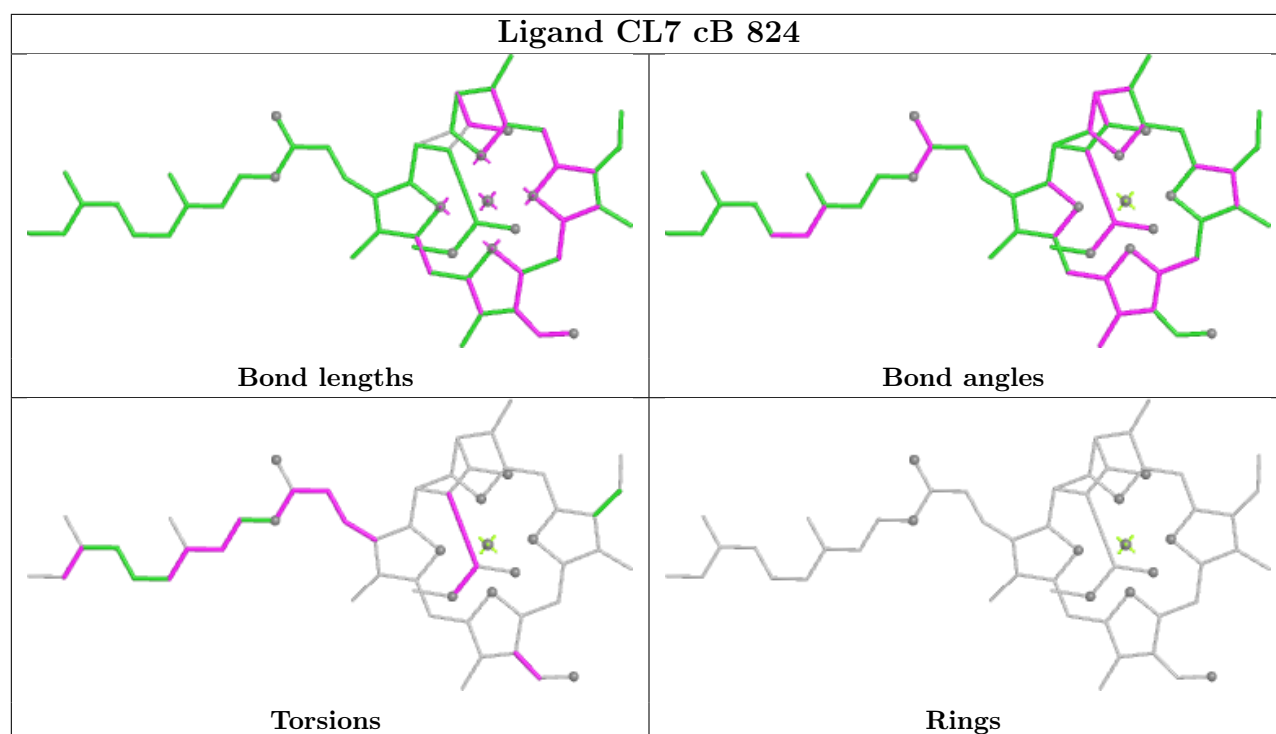
Torsions

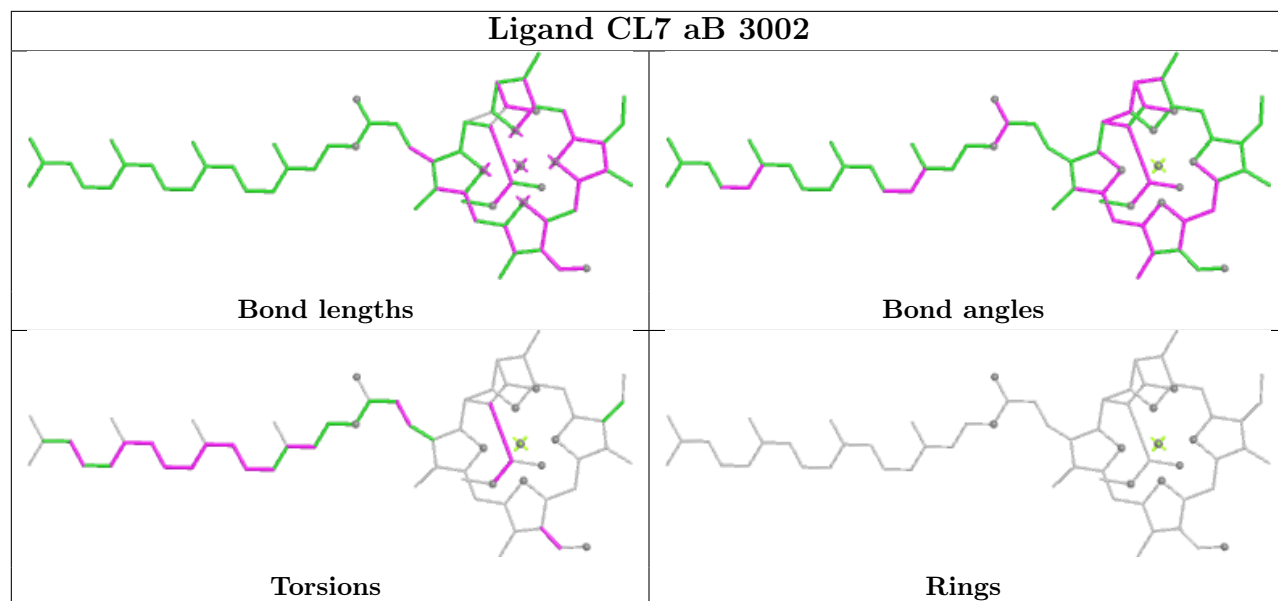


Rings

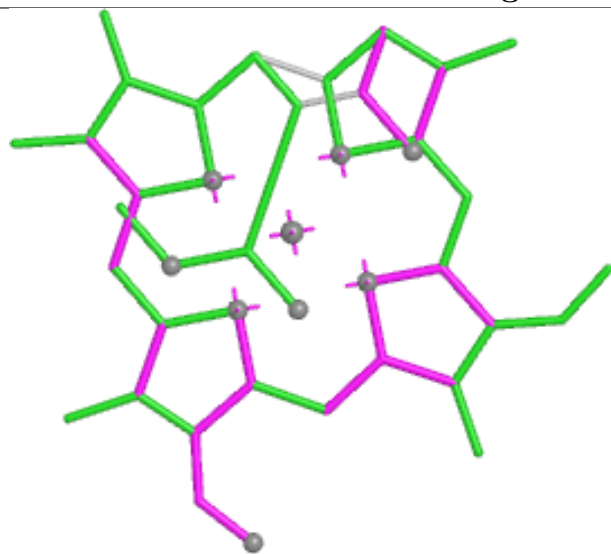




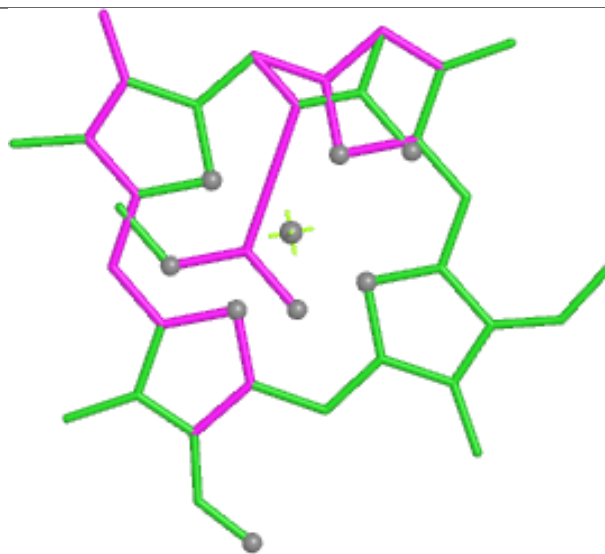




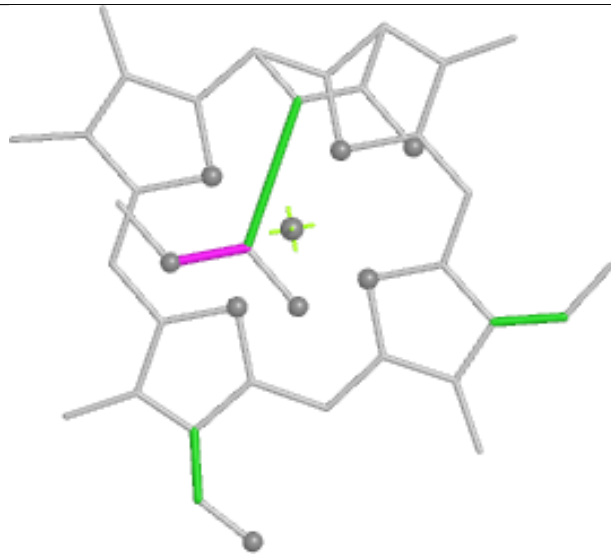
Ligand CL7 aB 3014



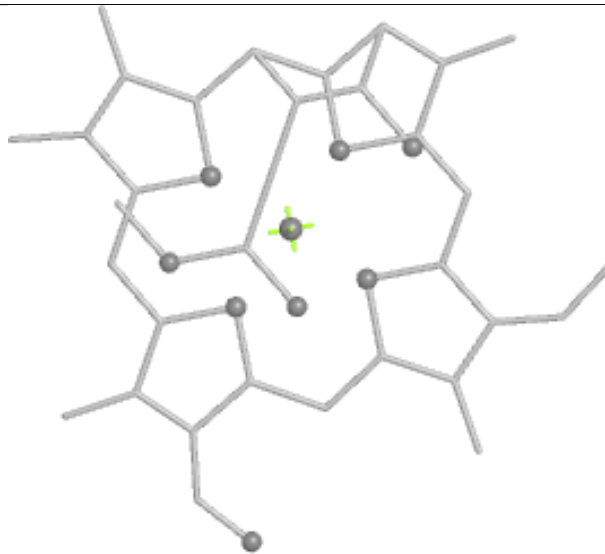
Bond lengths



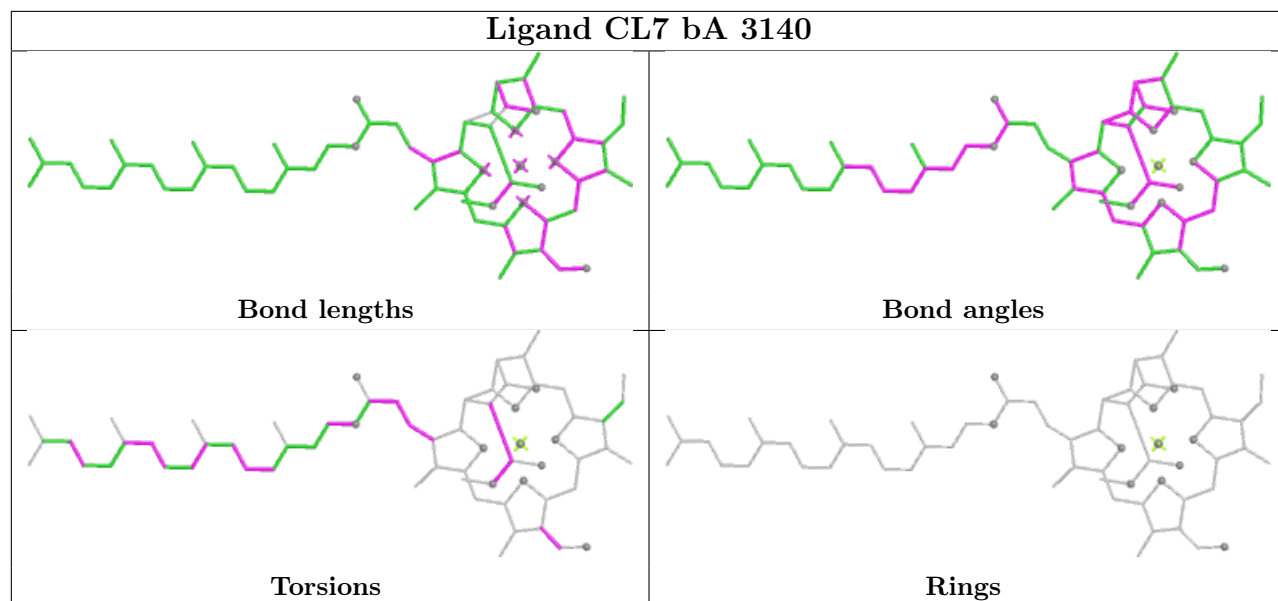
Bond angles

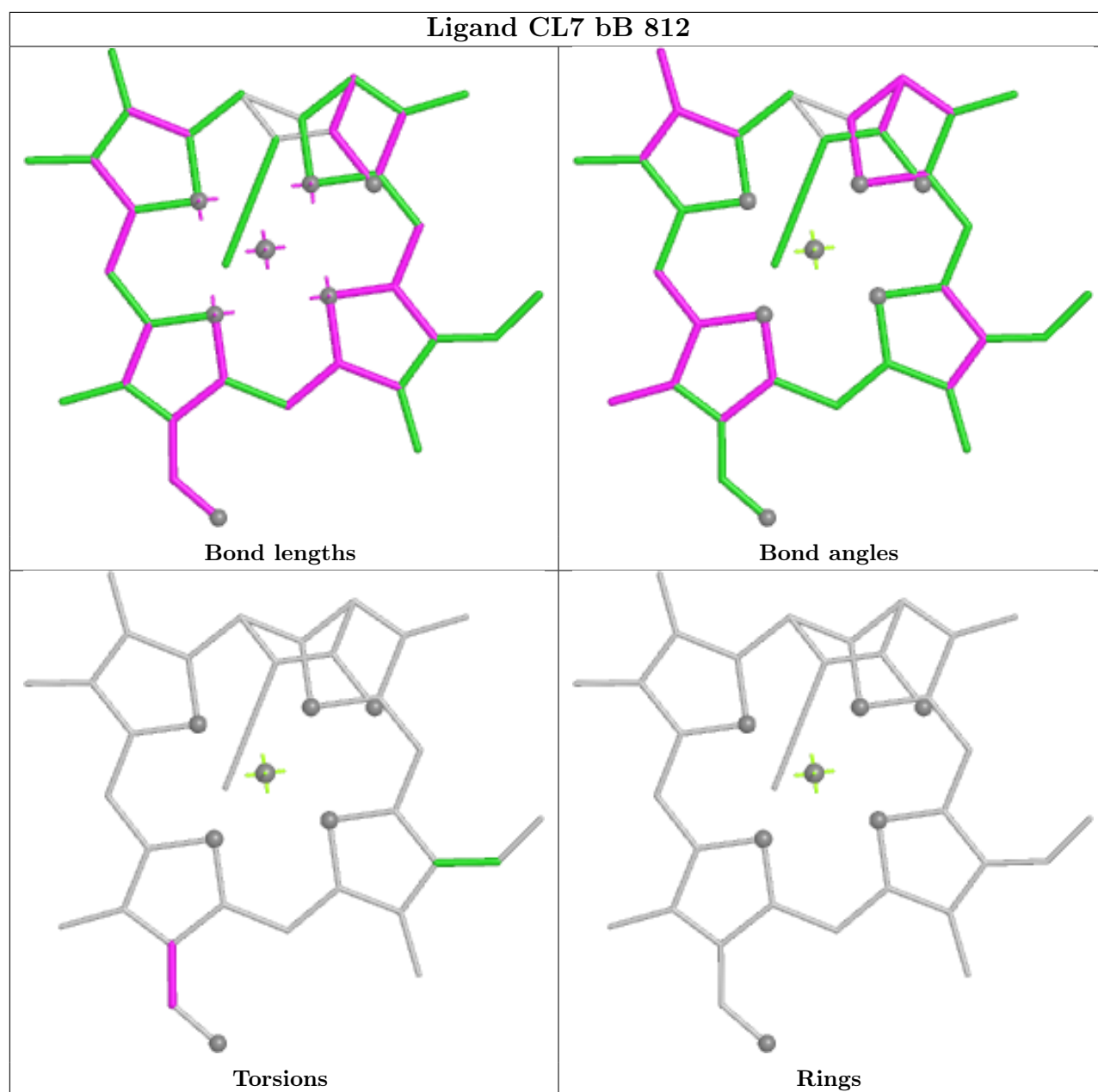


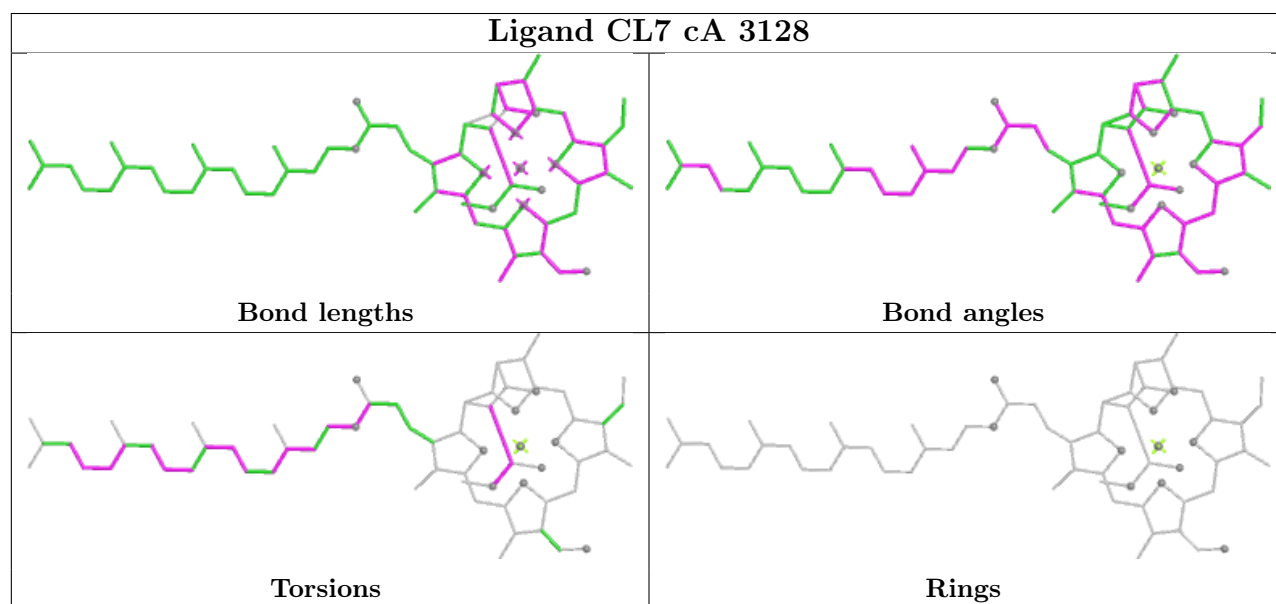
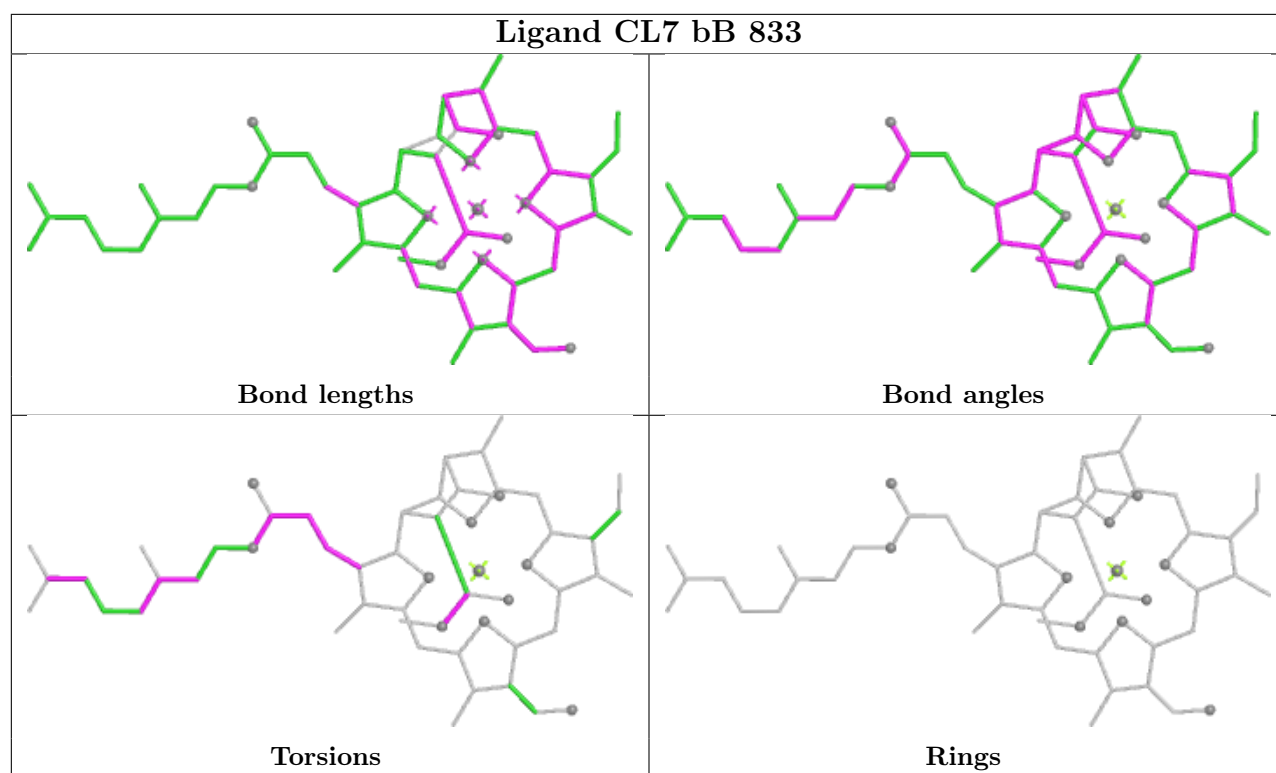
Torsions

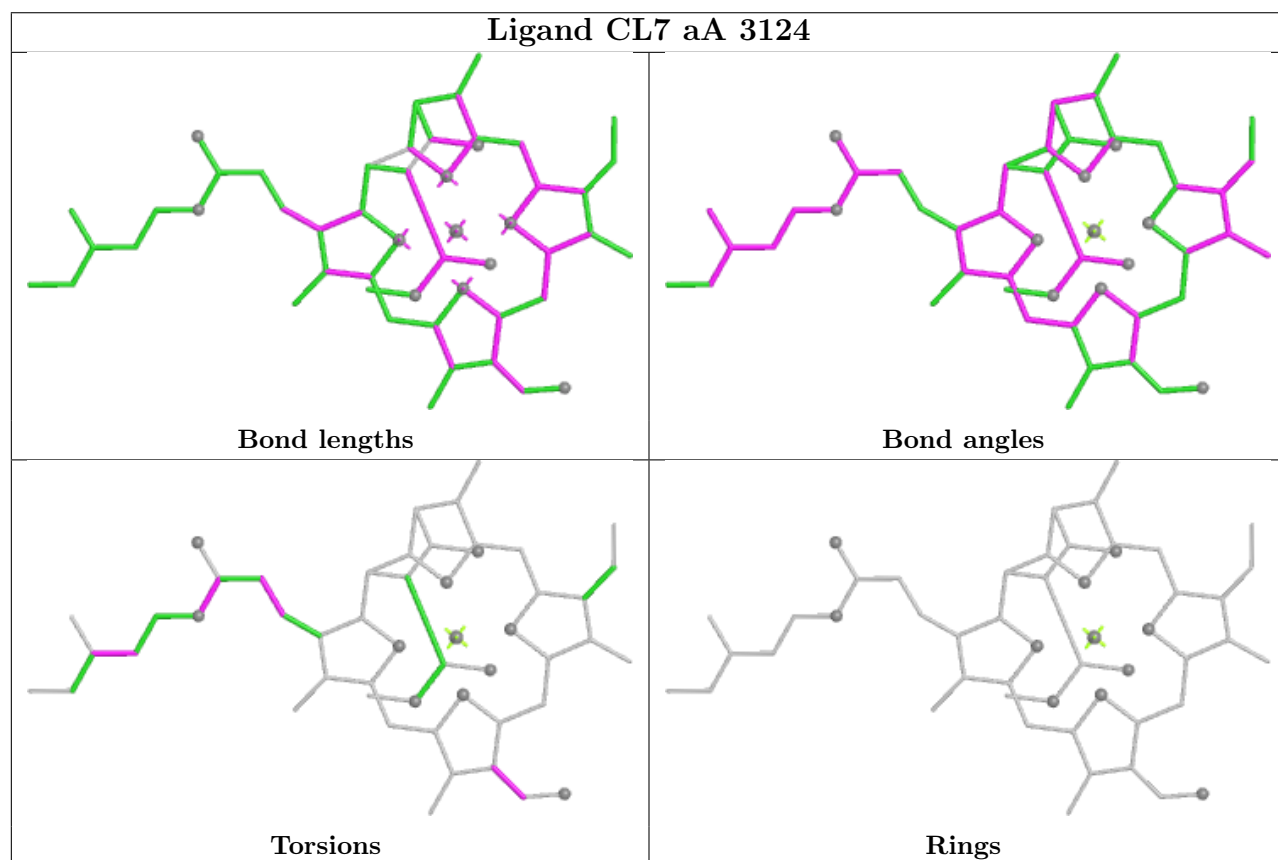
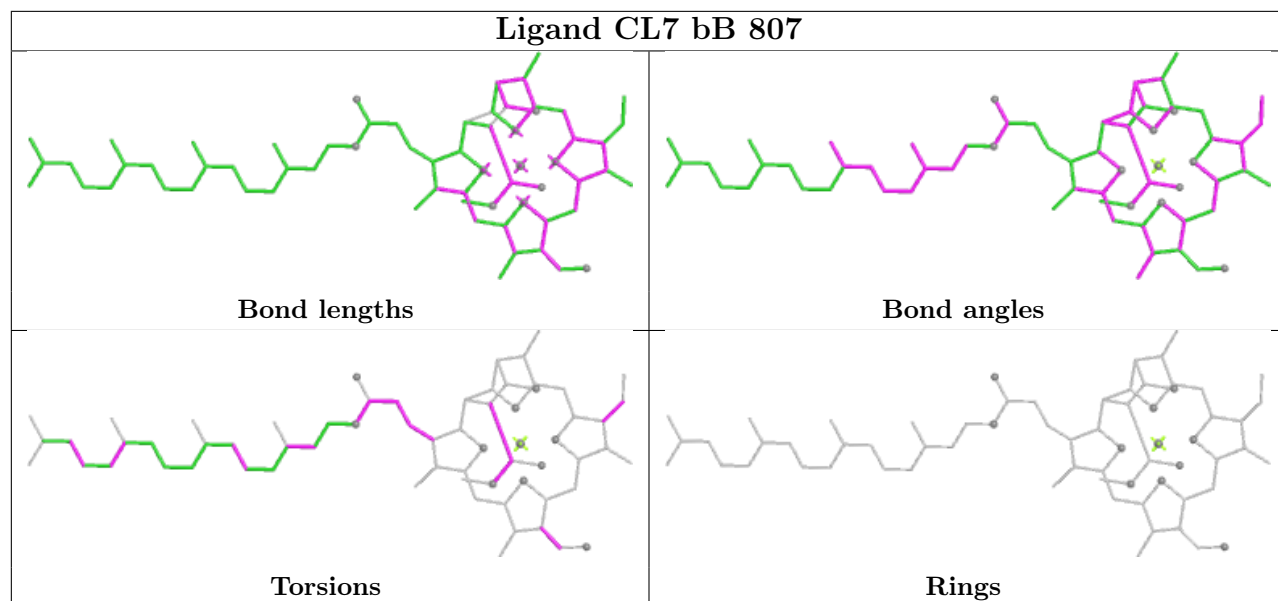


Rings

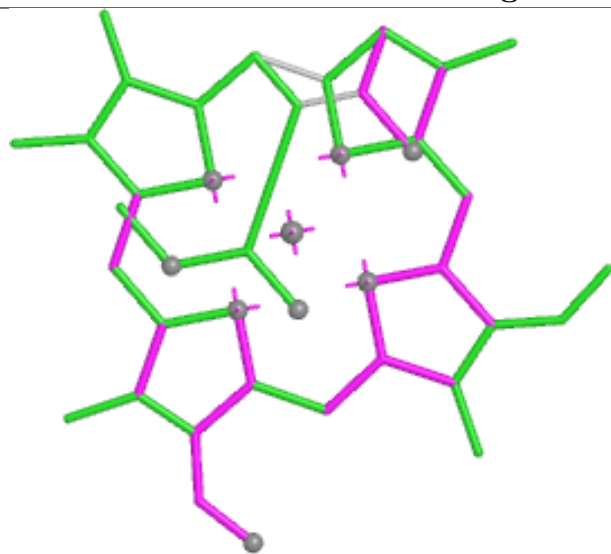




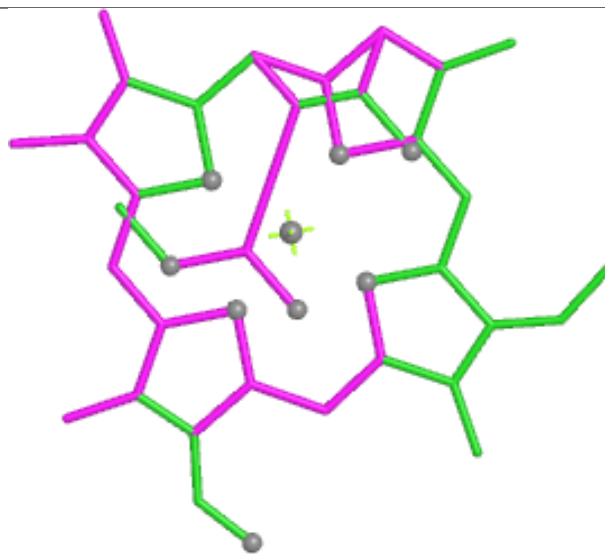




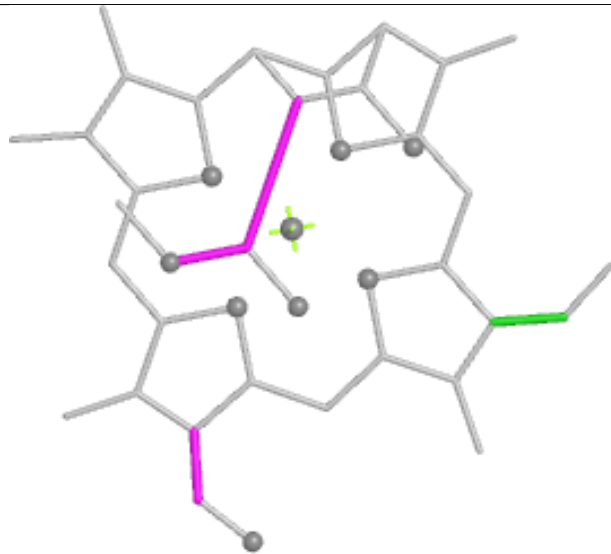
Ligand CL7 aA 3132



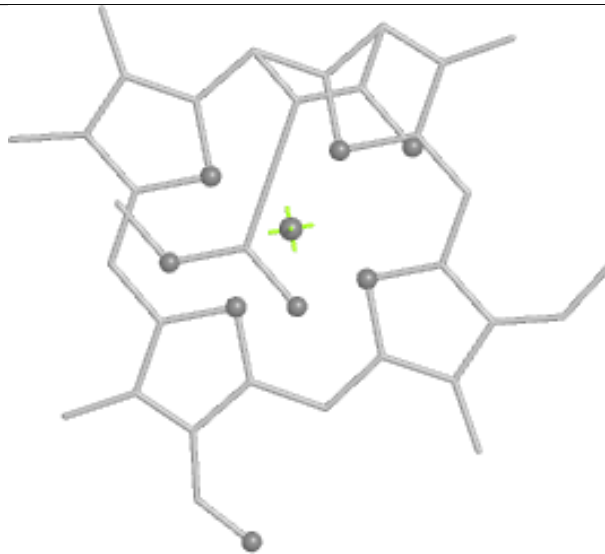
Bond lengths



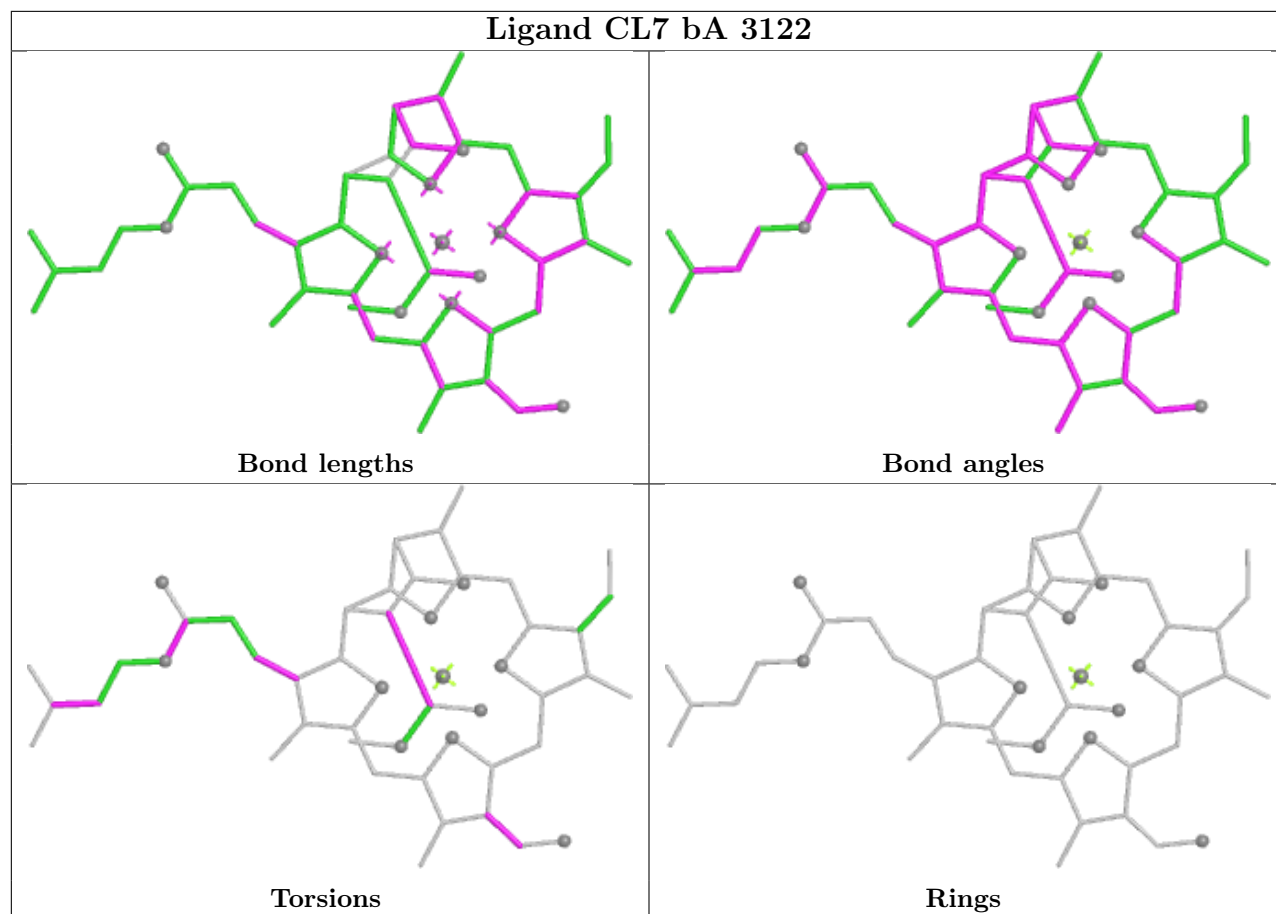
Bond angles

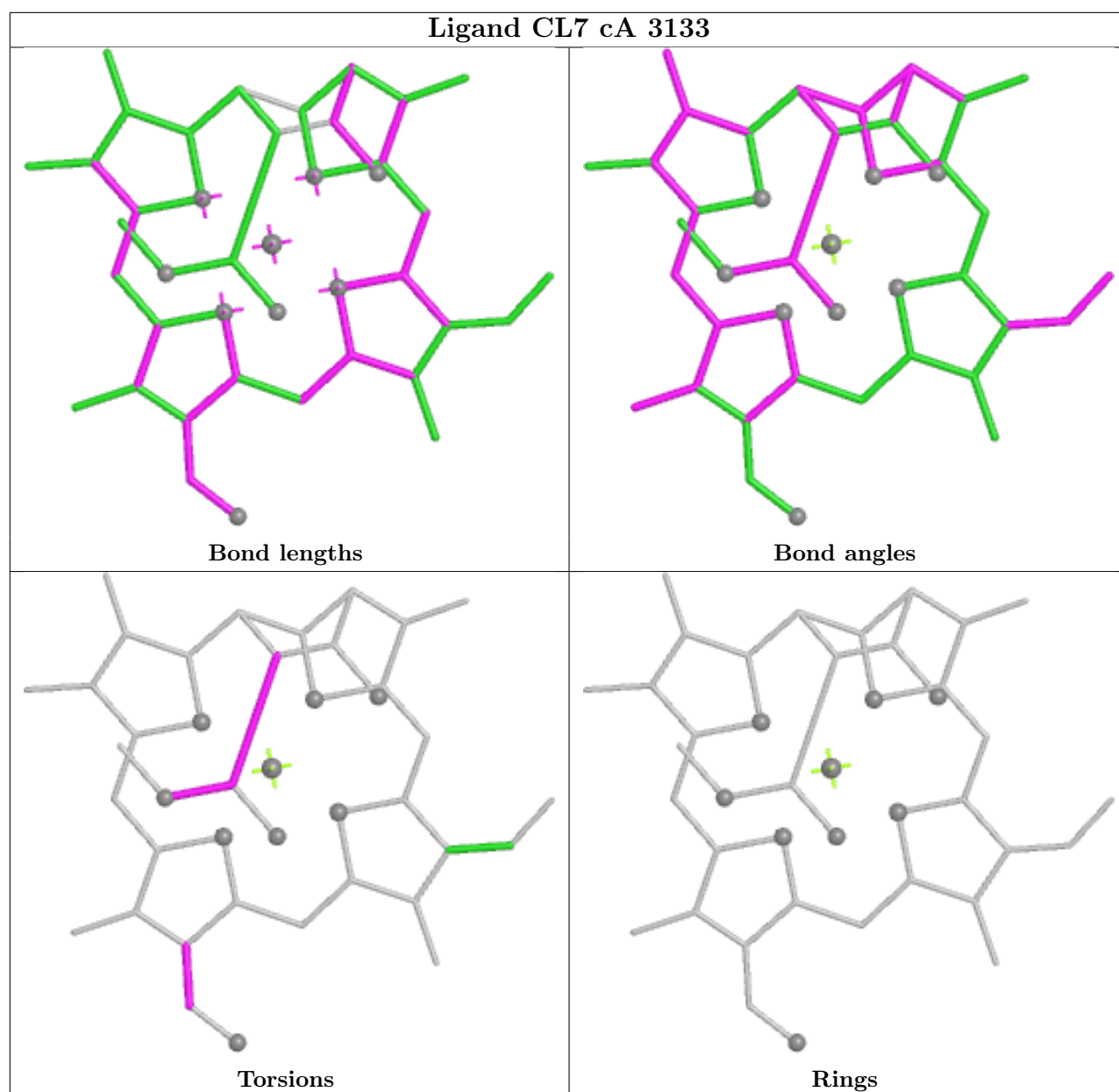


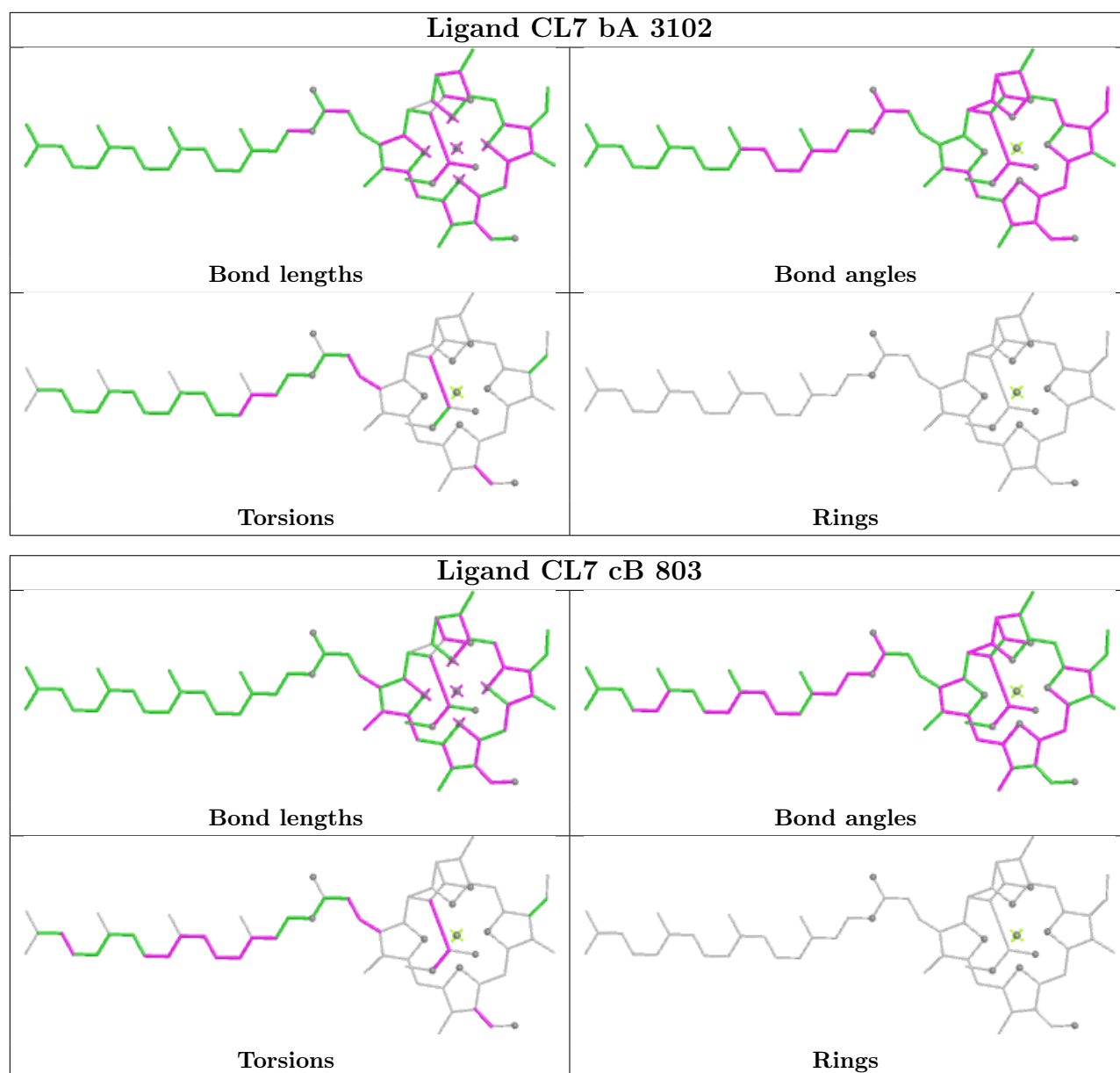
Torsions



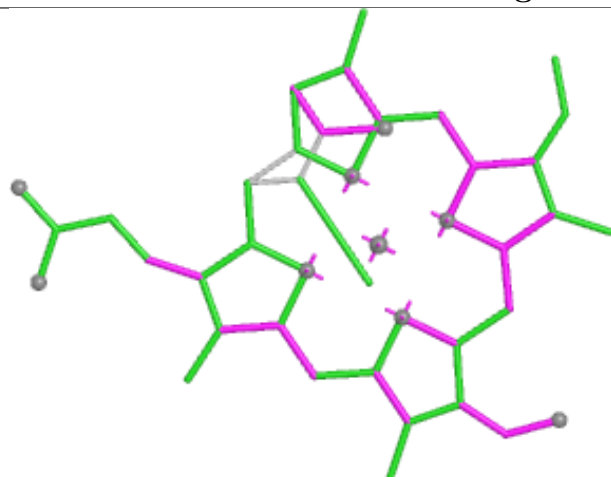
Rings



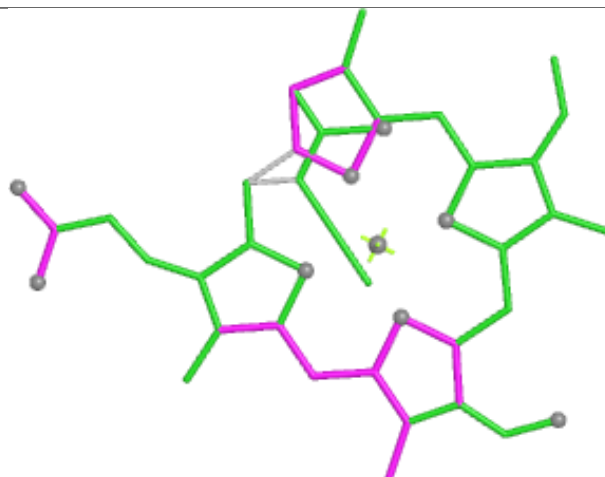




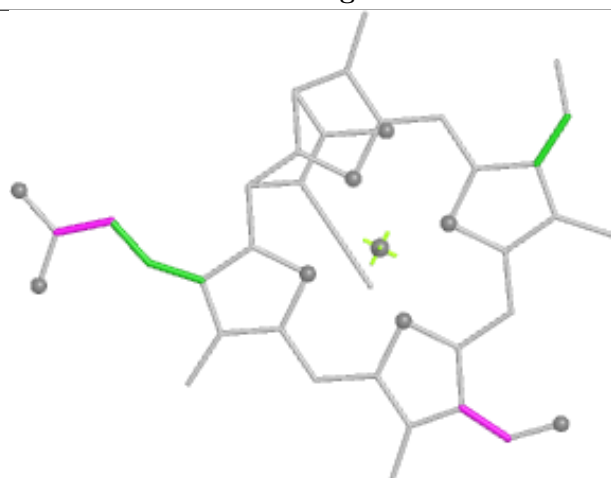
Ligand CL7 cJ 101



Bond lengths



Bond angles

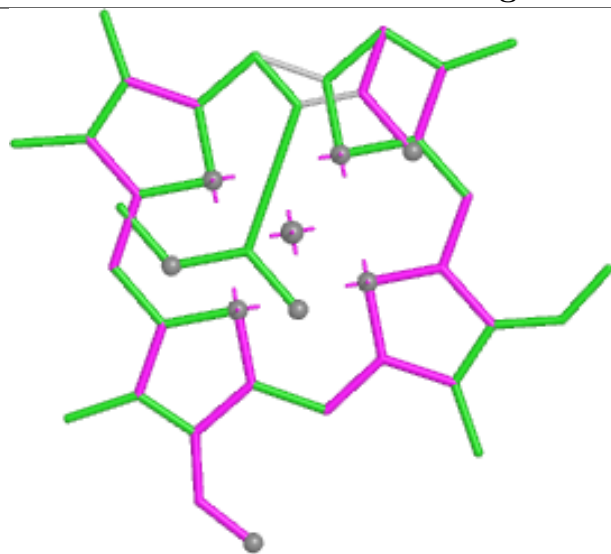


Torsions

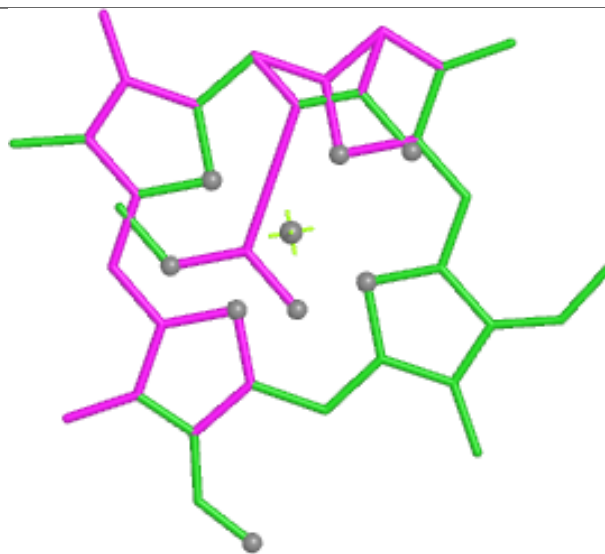


Rings

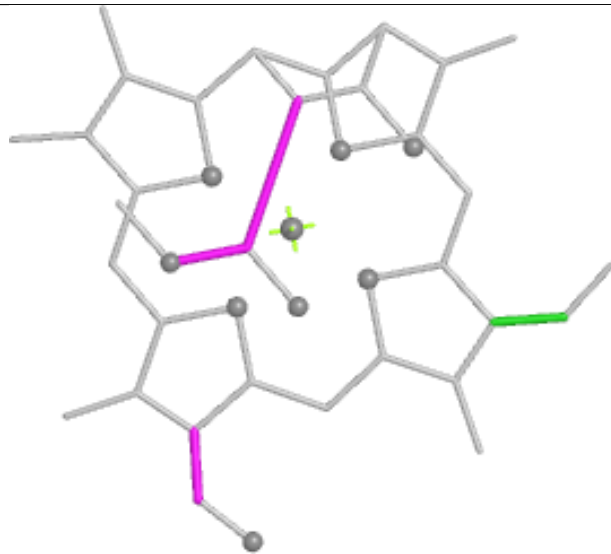
Ligand CL7 bA 3133



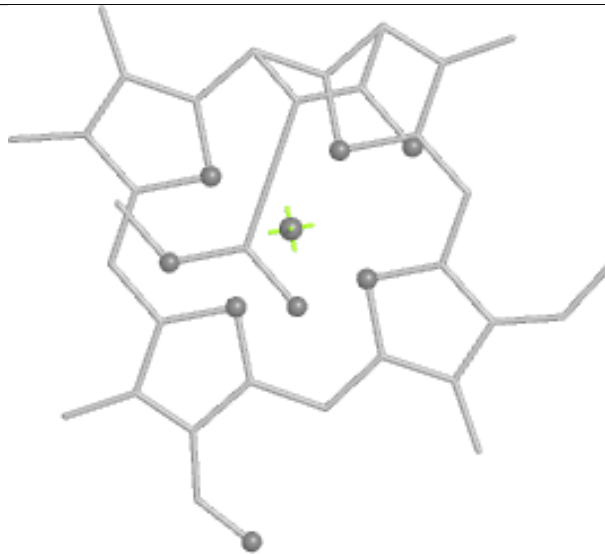
Bond lengths



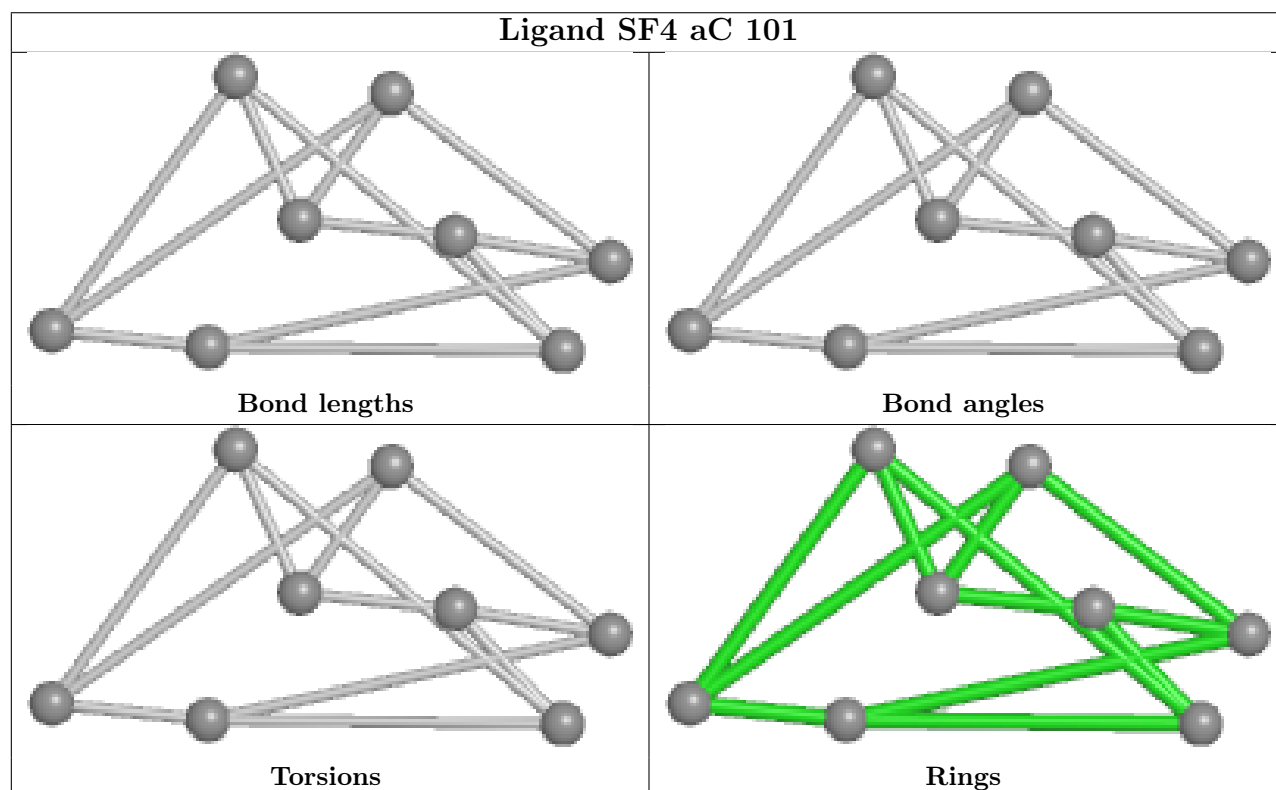
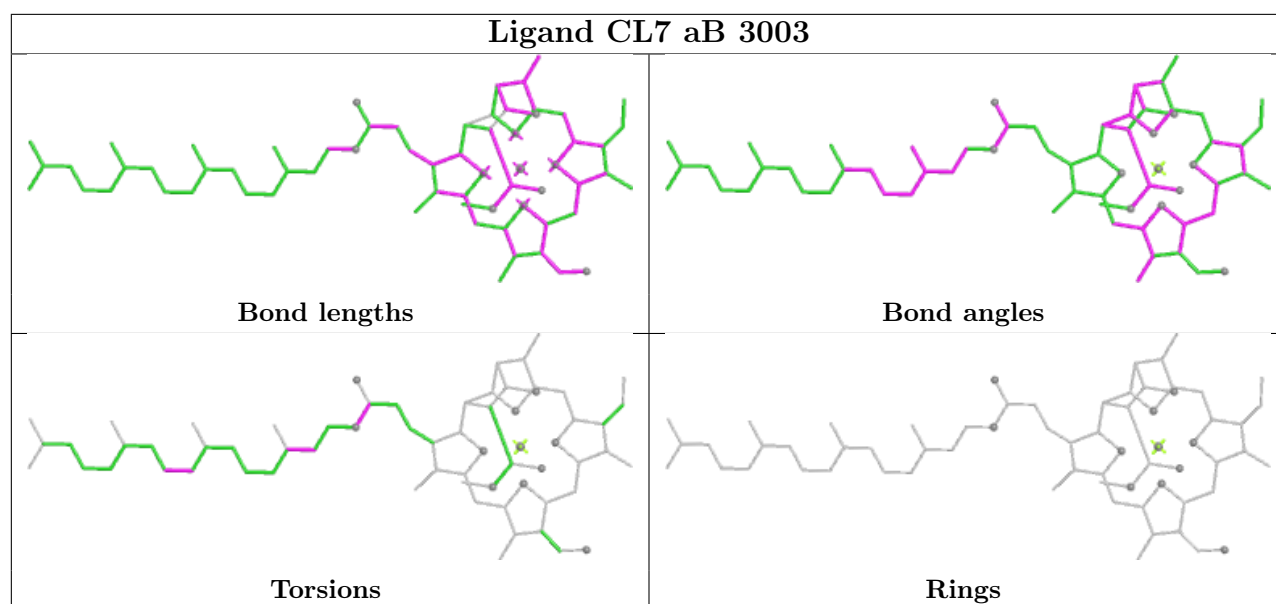
Bond angles

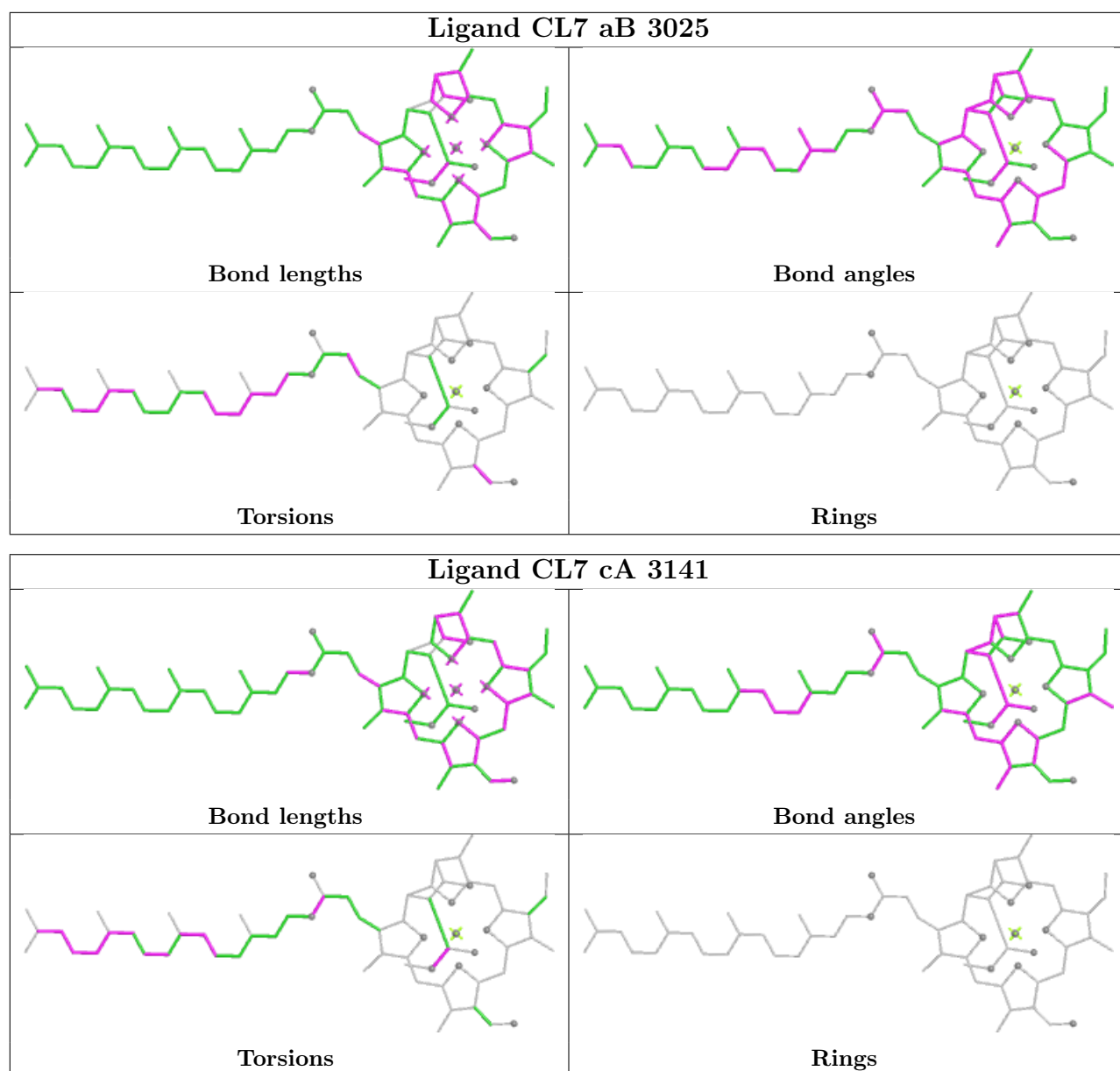


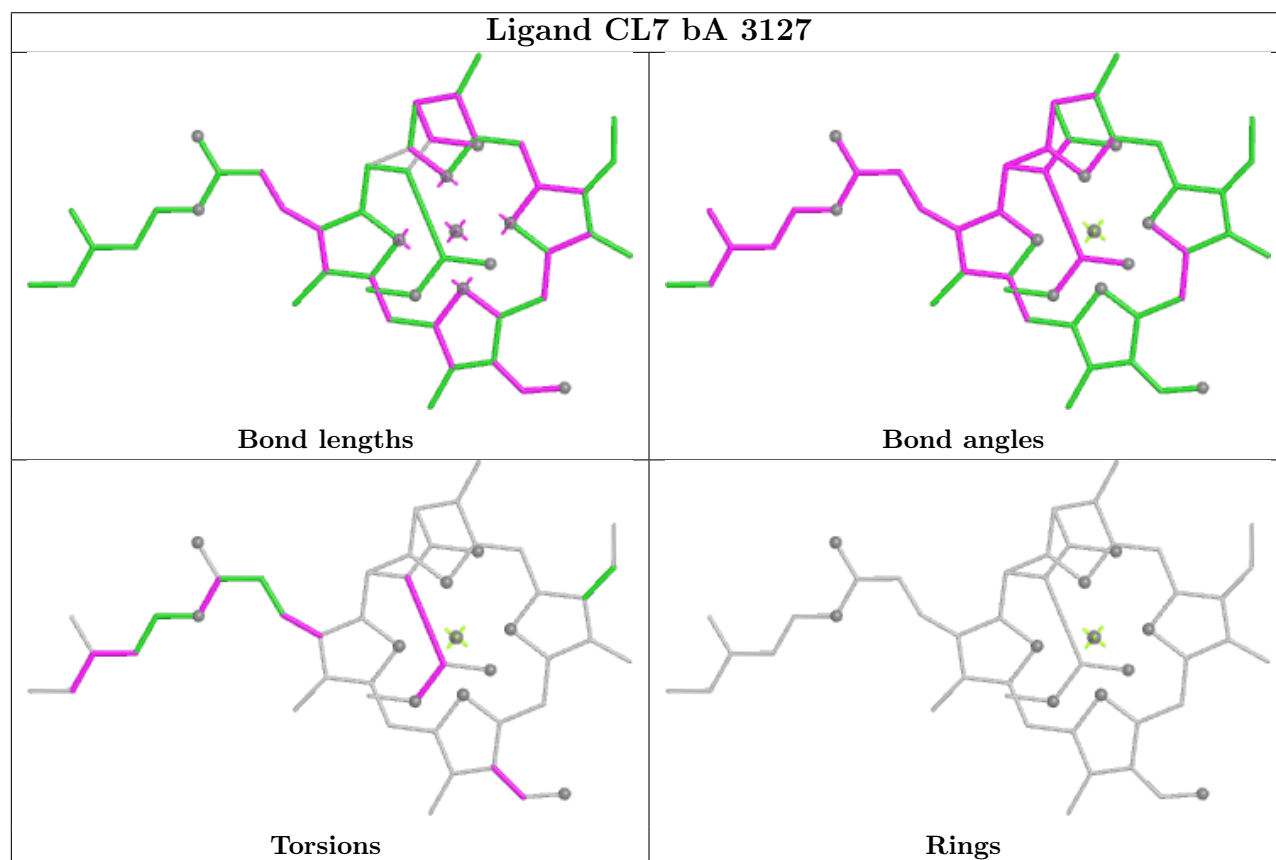
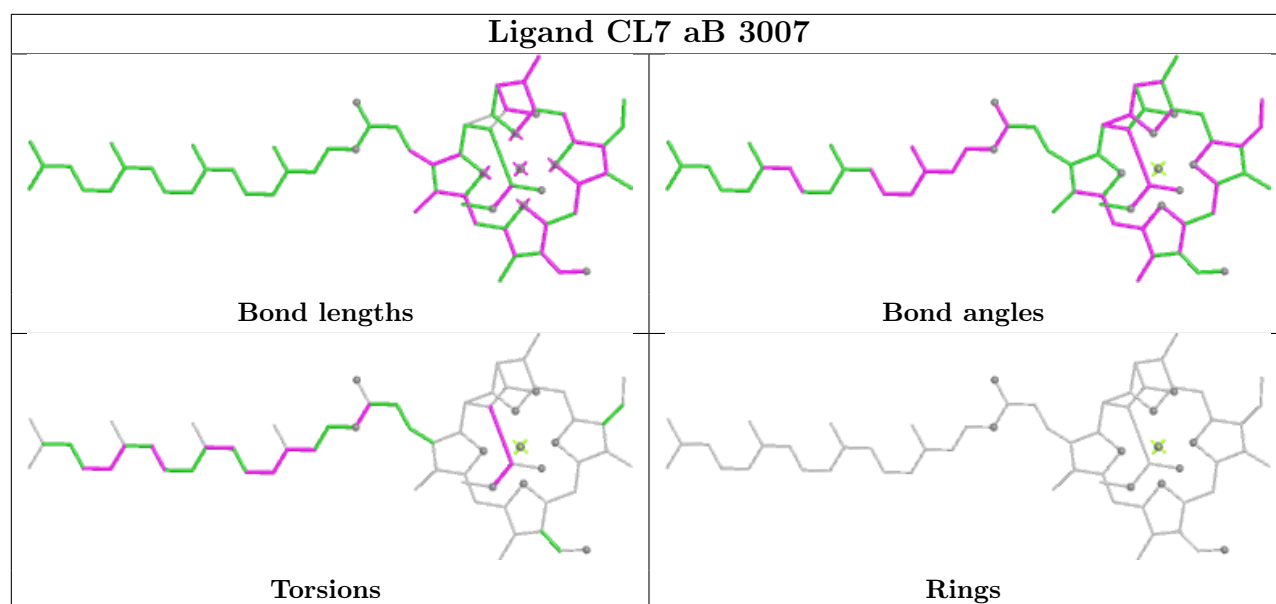
Torsions

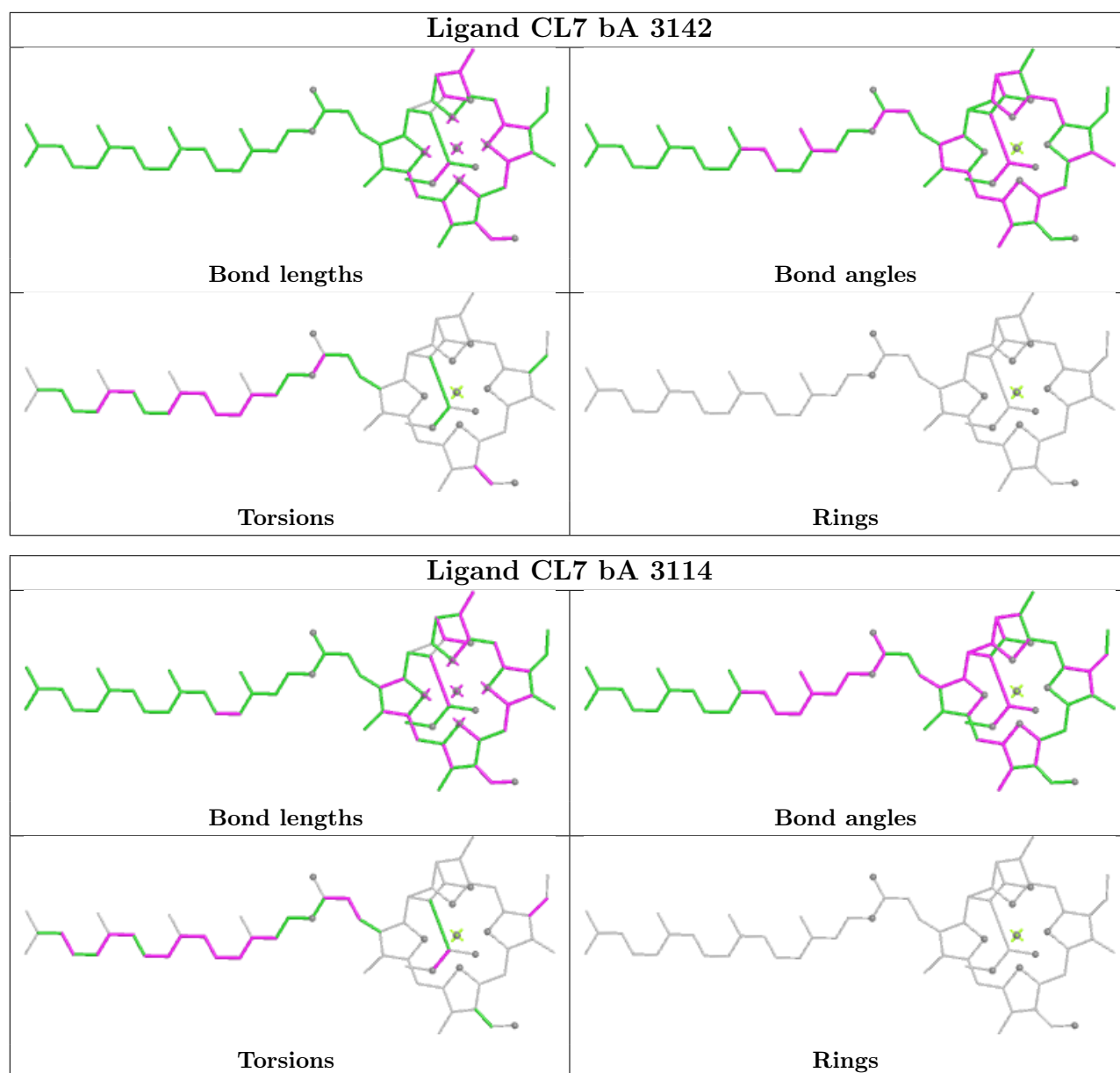


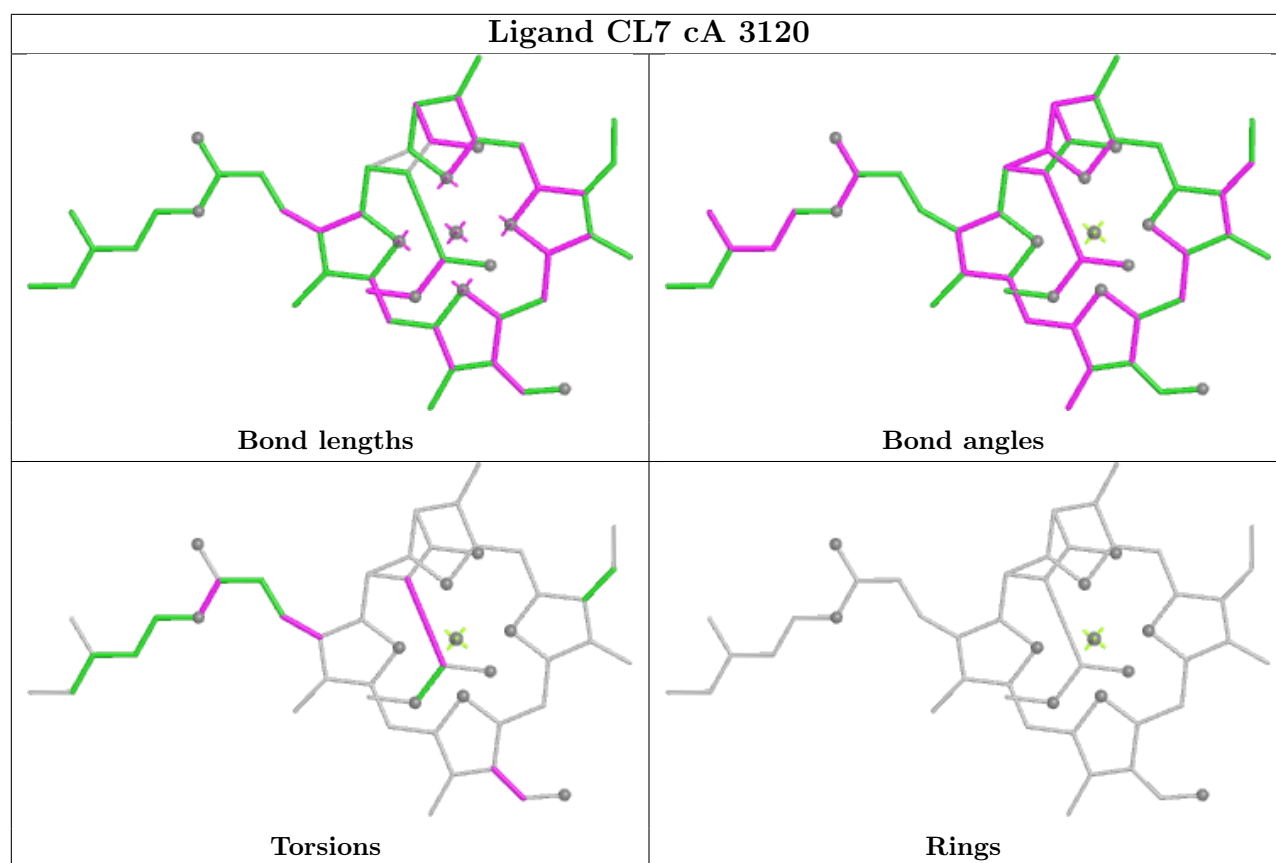
Rings



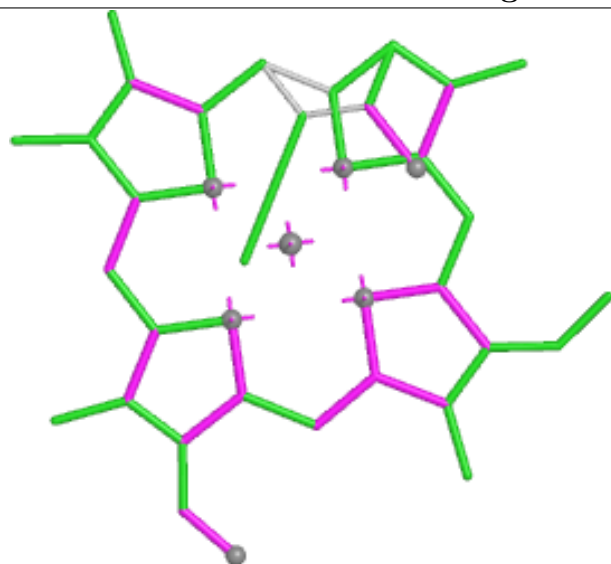




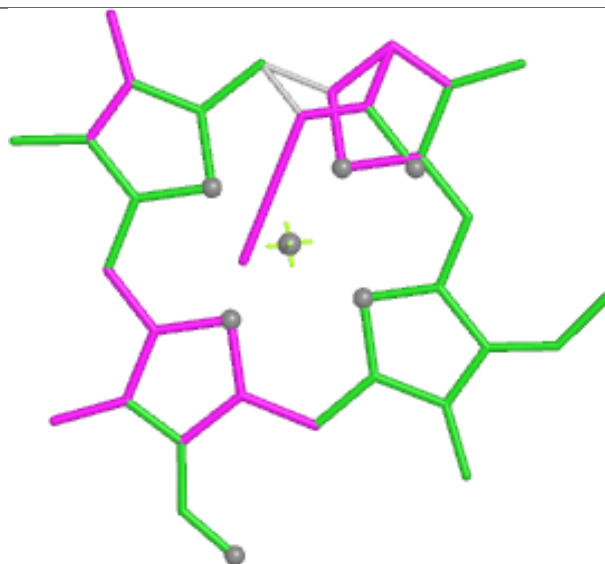




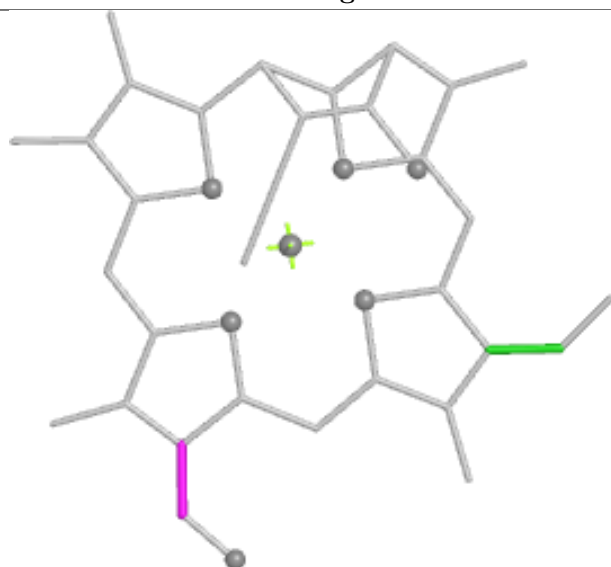
Ligand CL7 aA 3112



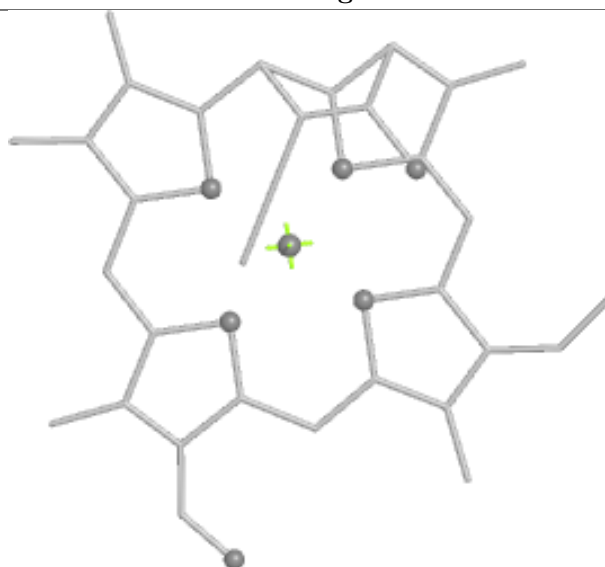
Bond lengths



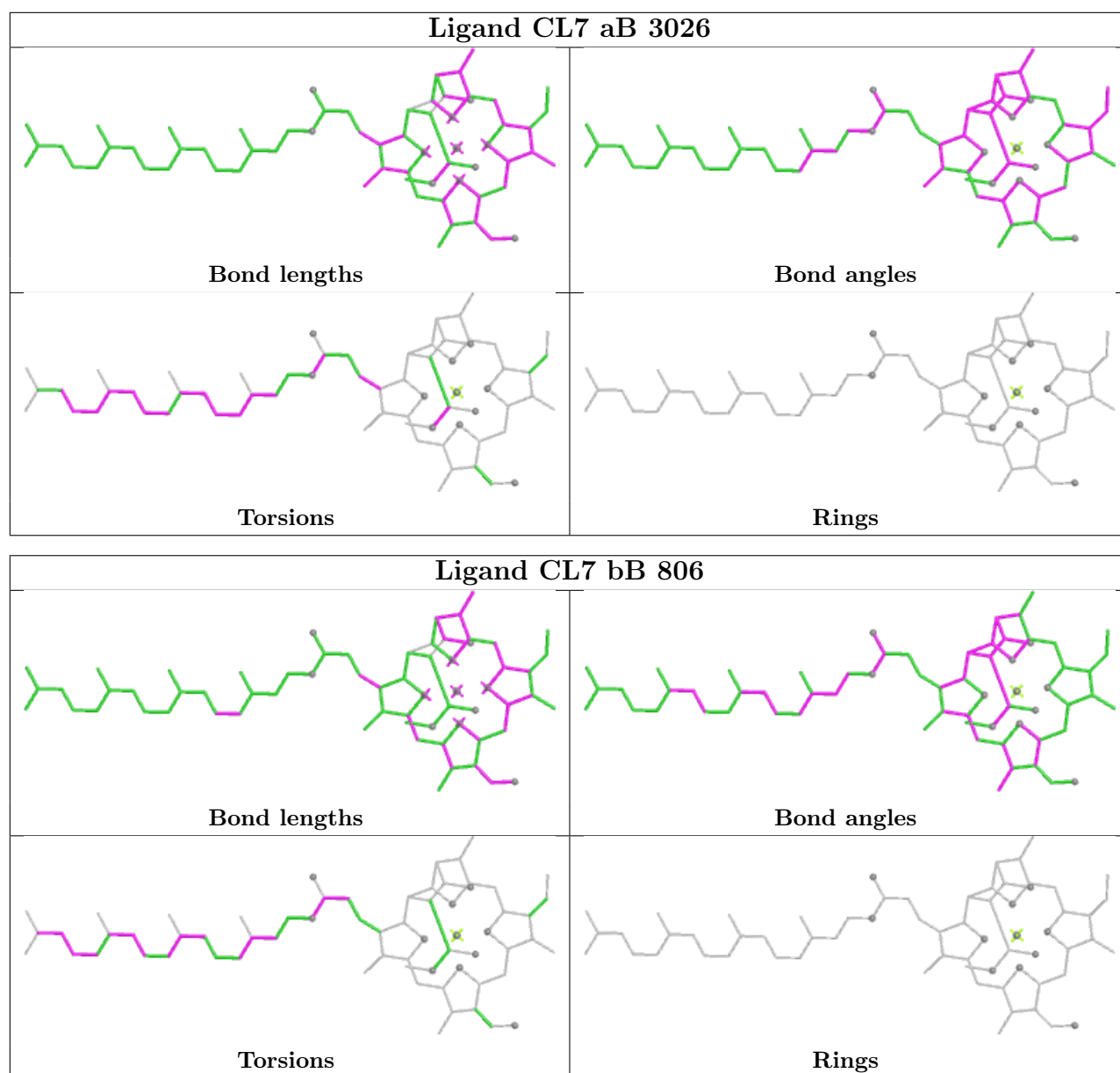
Bond angles

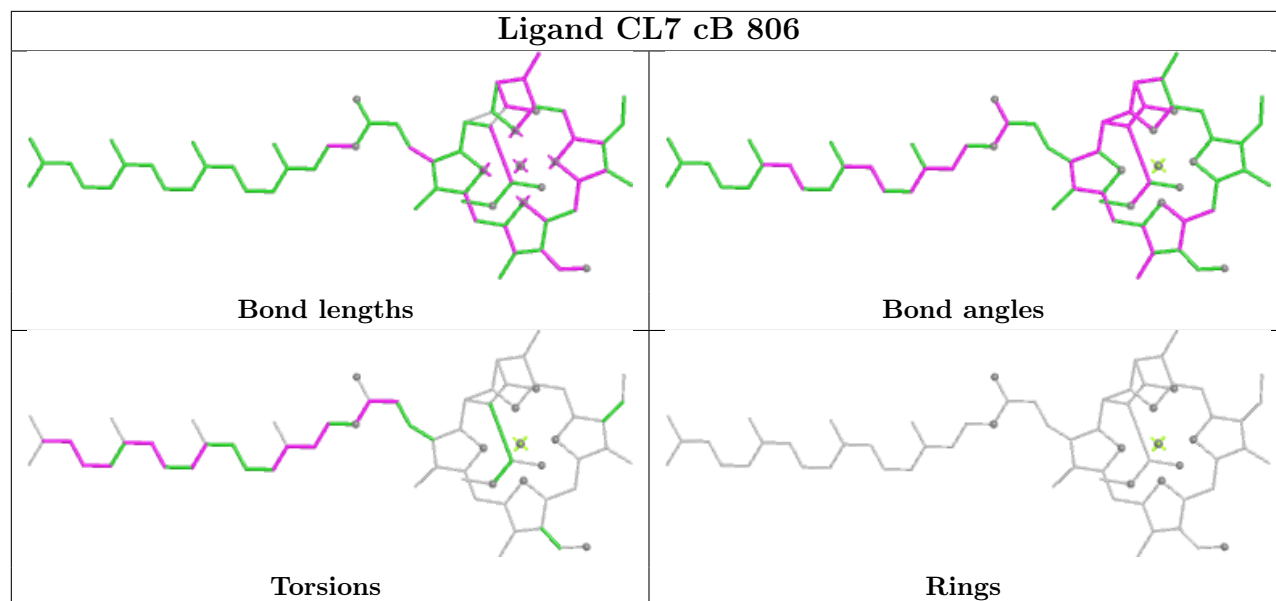


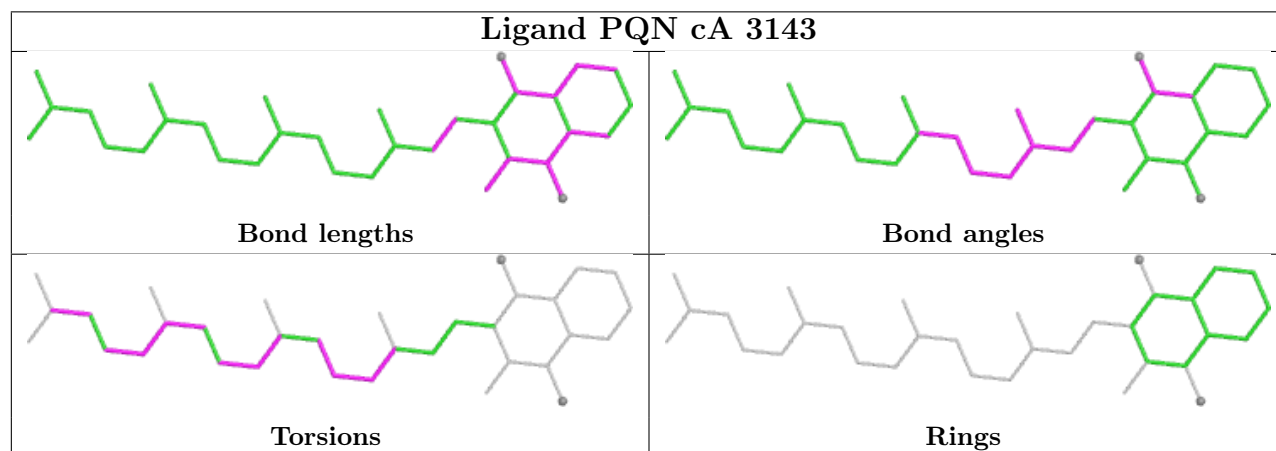
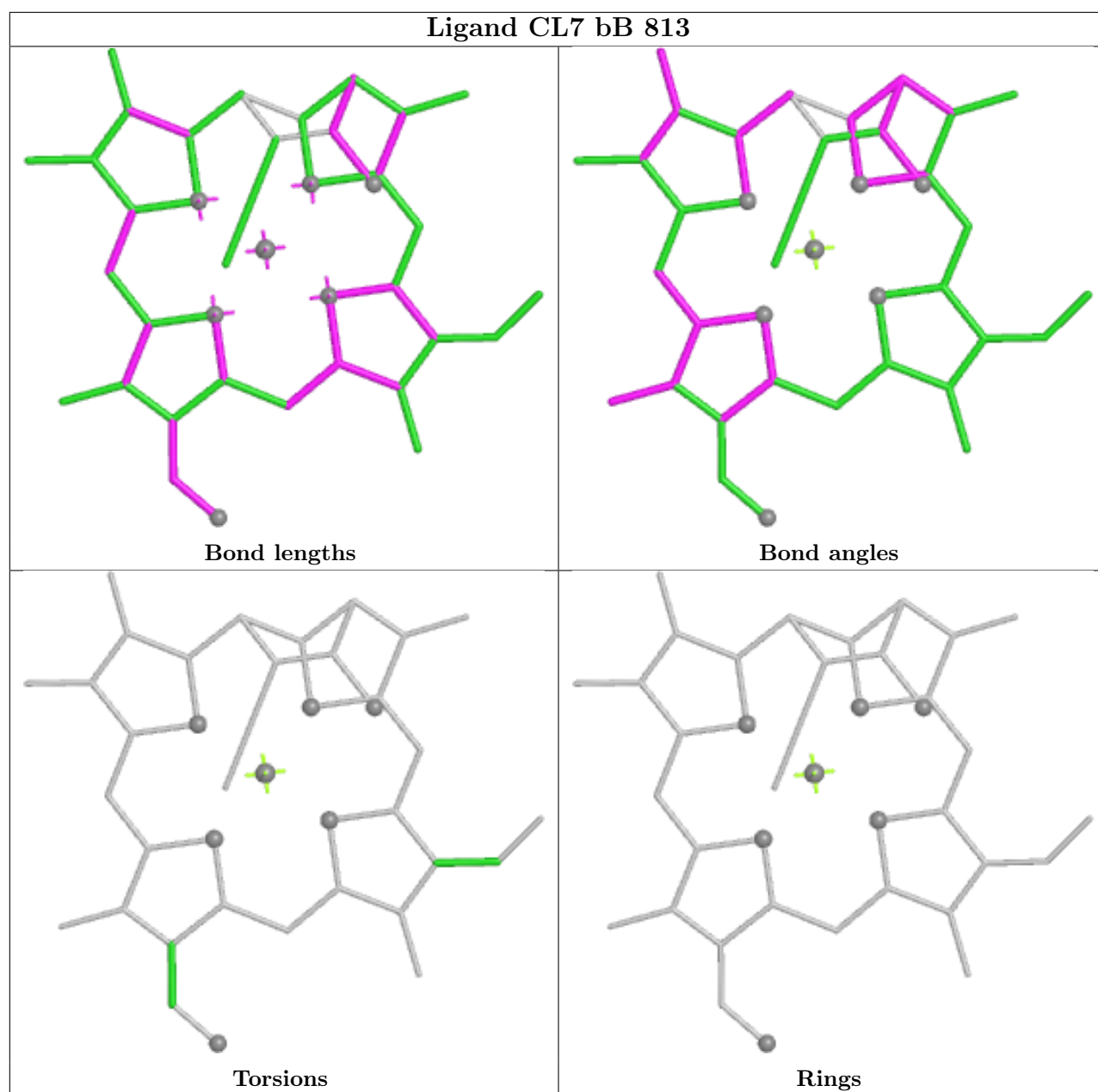
Torsions

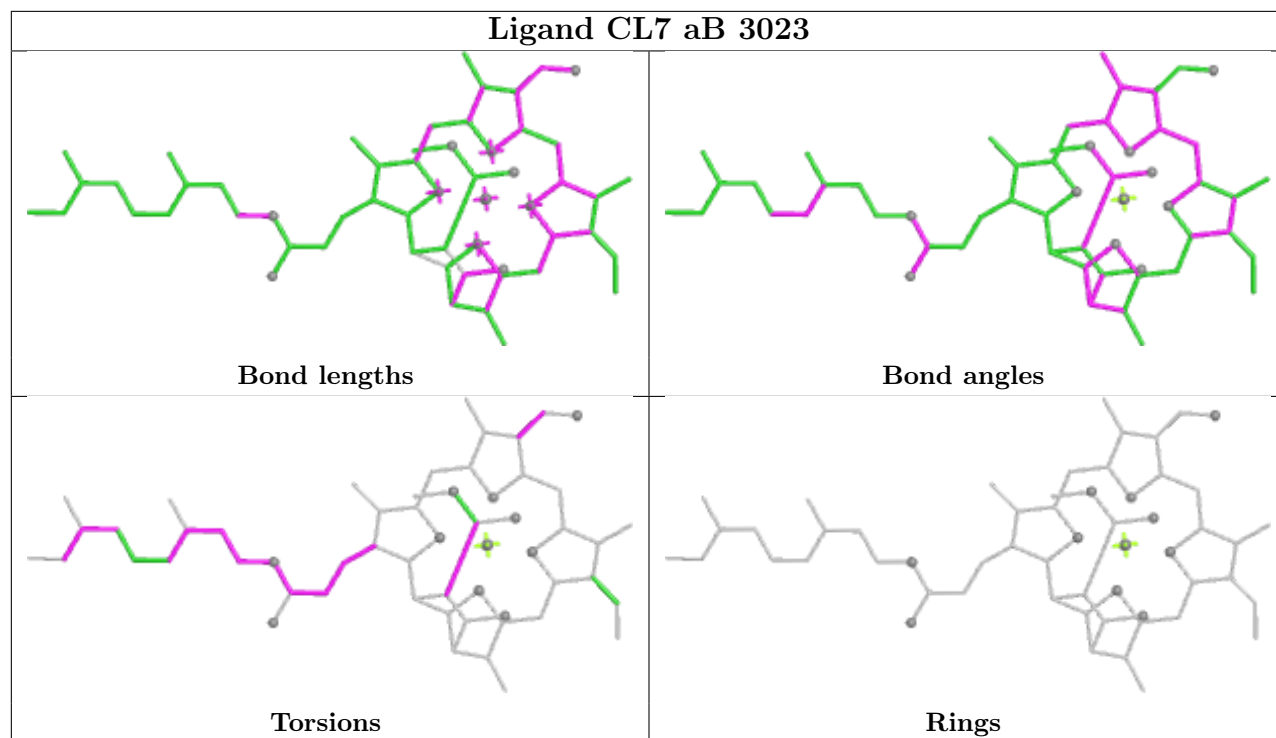


Rings

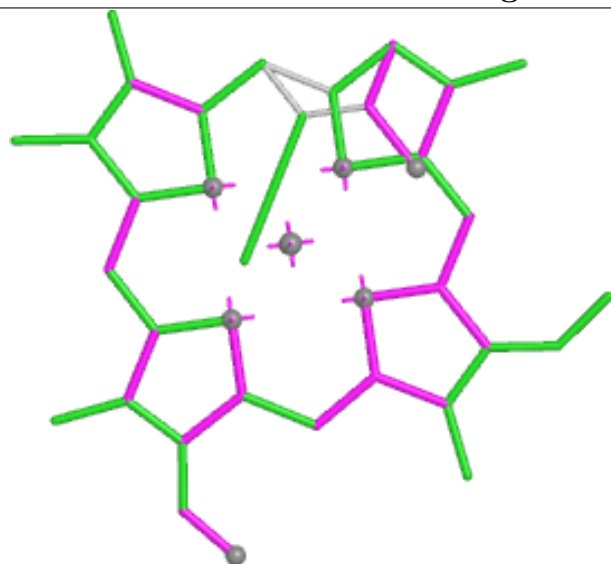




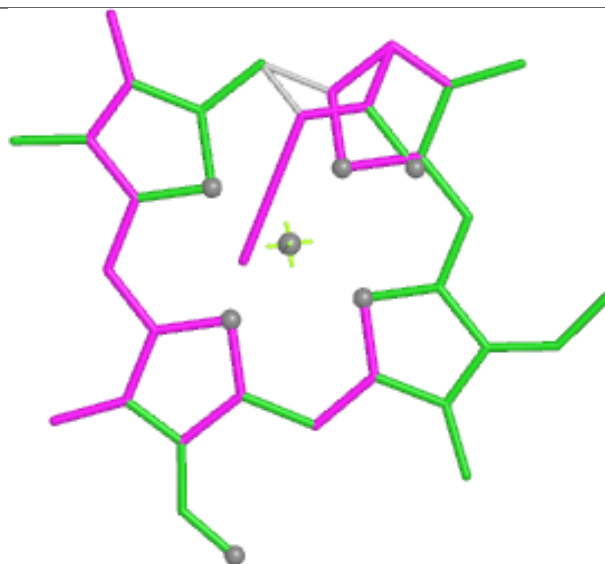




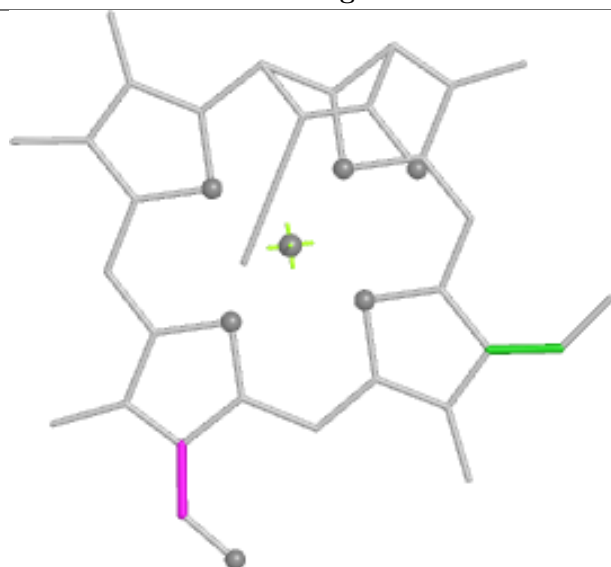
Ligand CL7 aA 3118



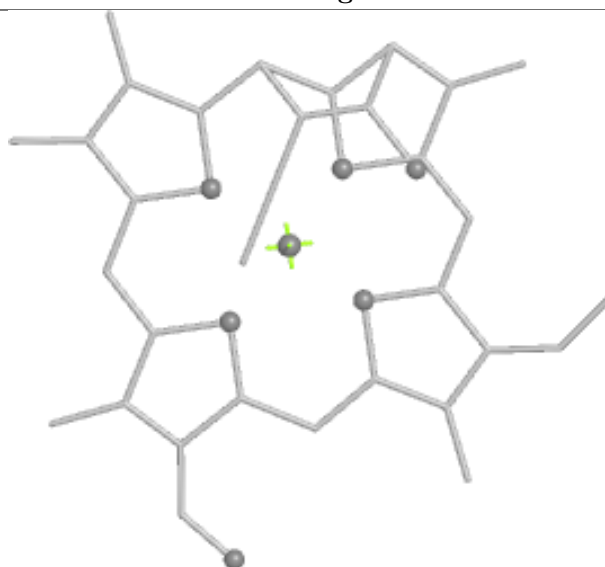
Bond lengths



Bond angles

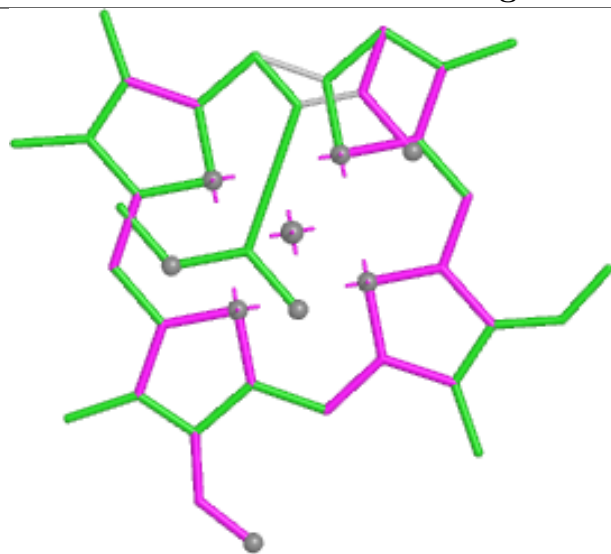


Torsions

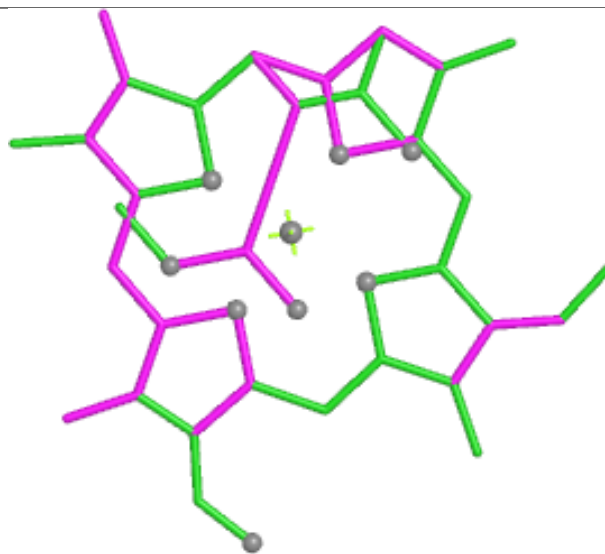


Rings

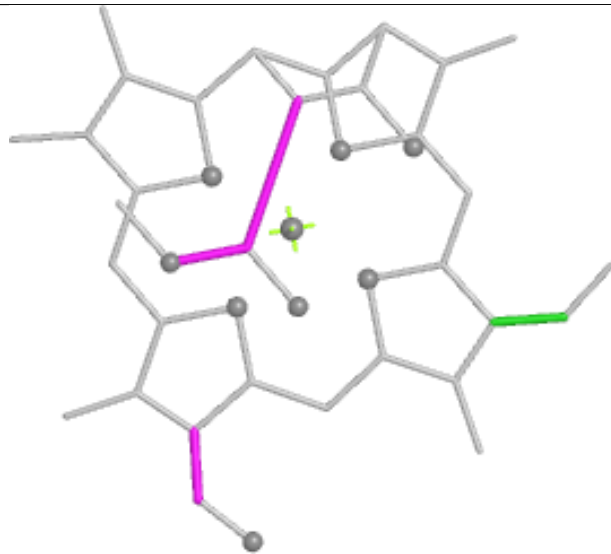
Ligand CL7 bA 3112



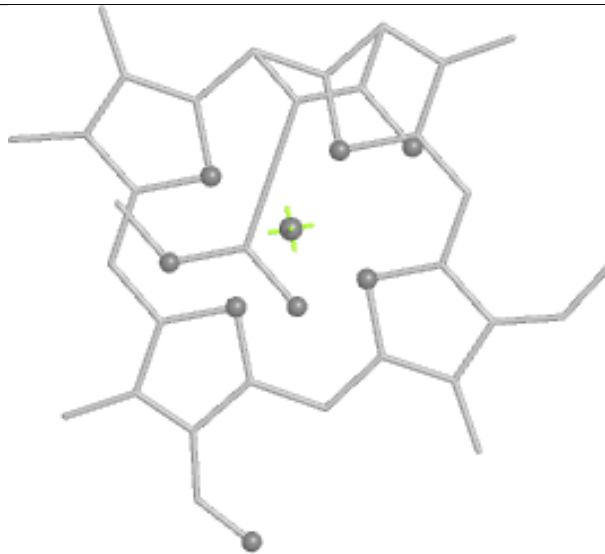
Bond lengths



Bond angles

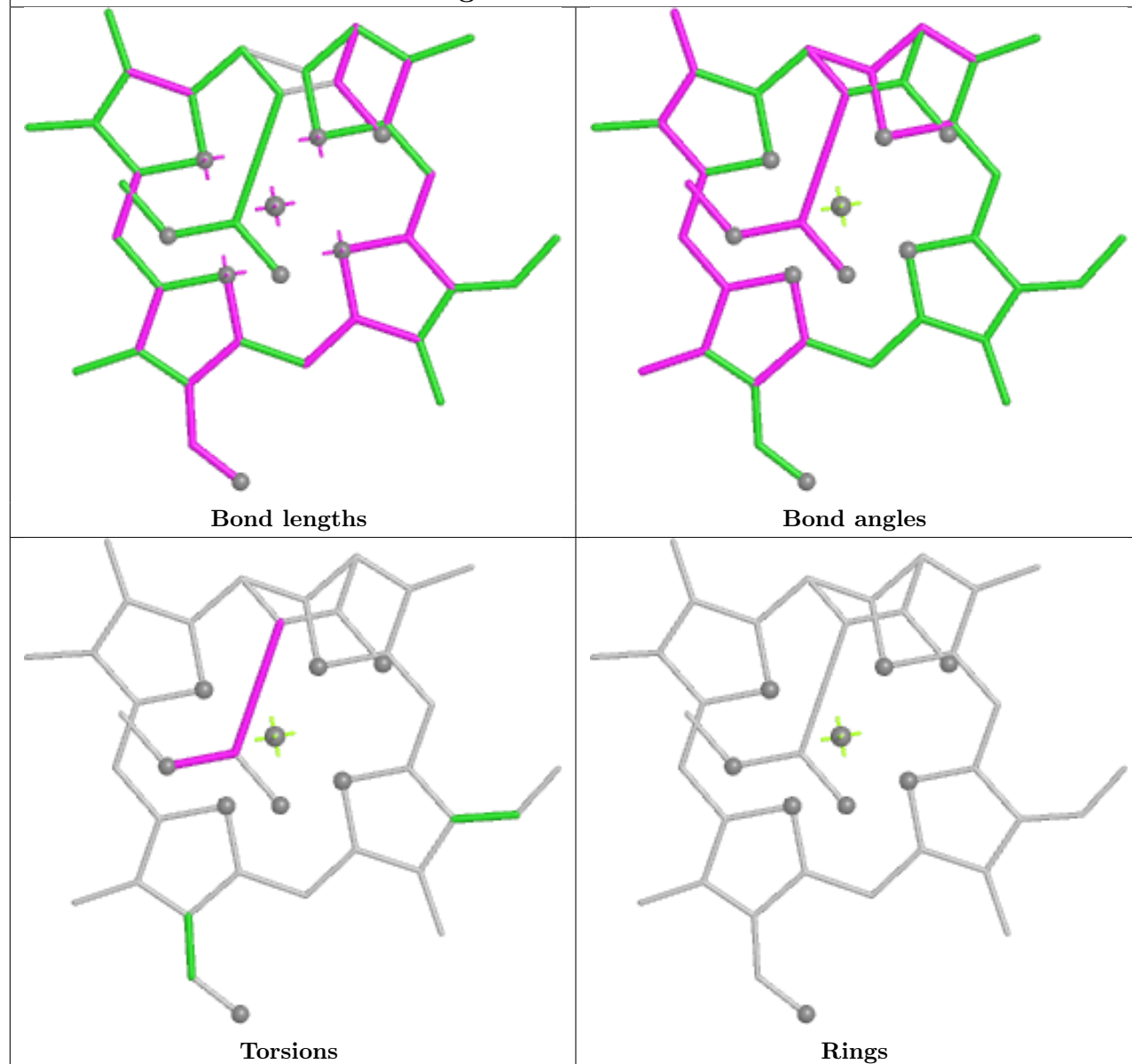


Torsions

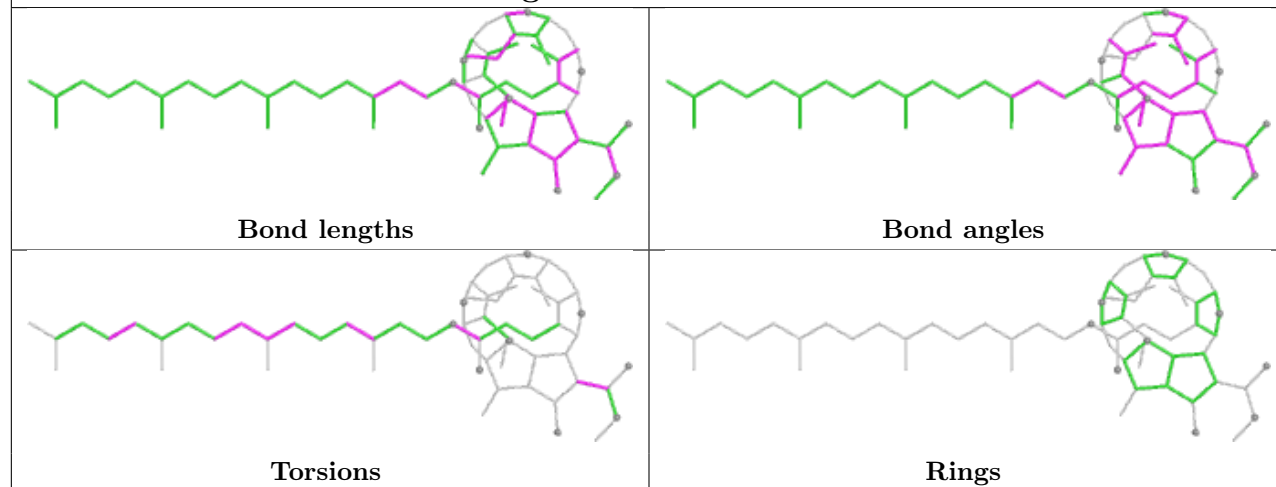


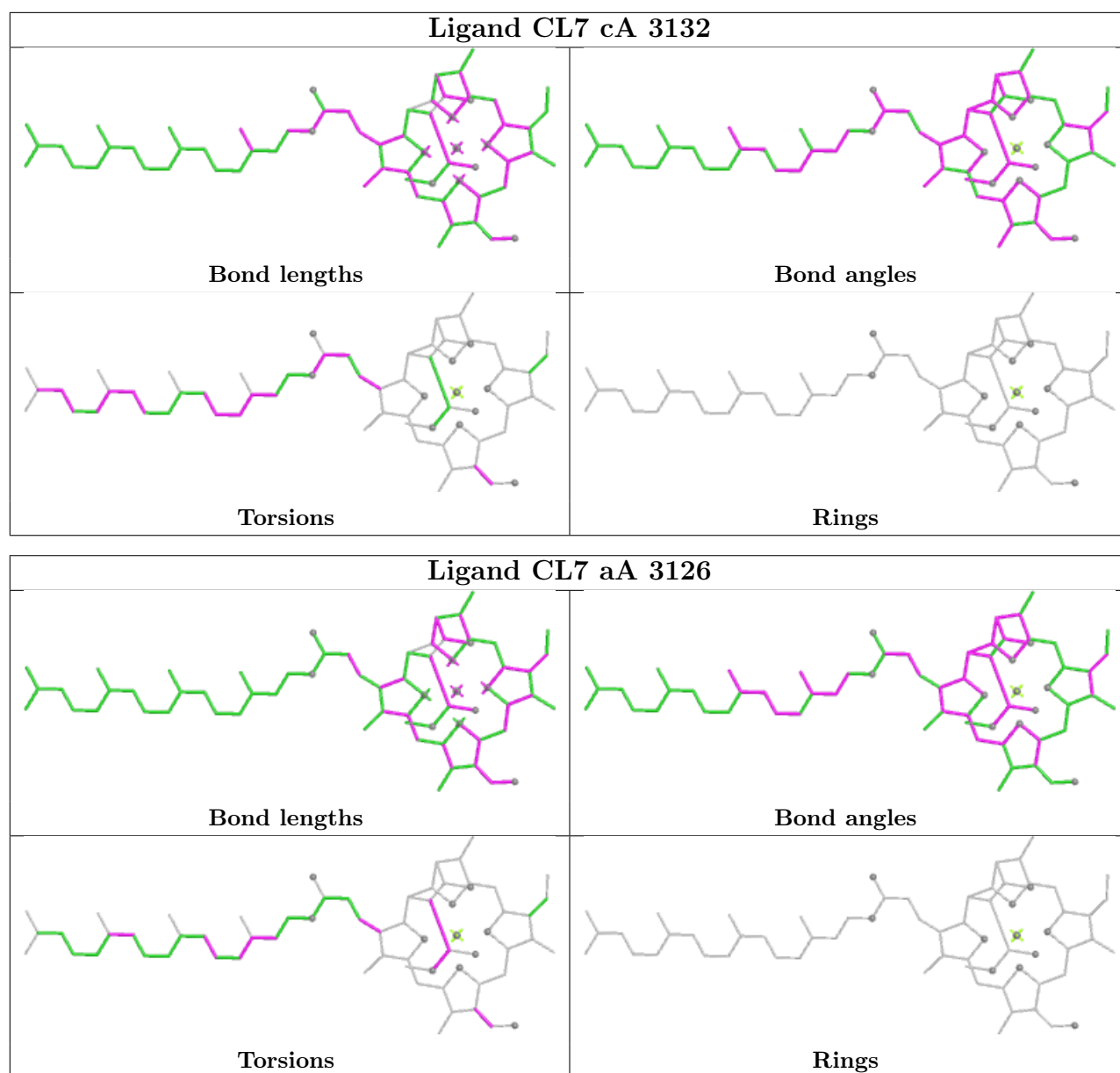
Rings

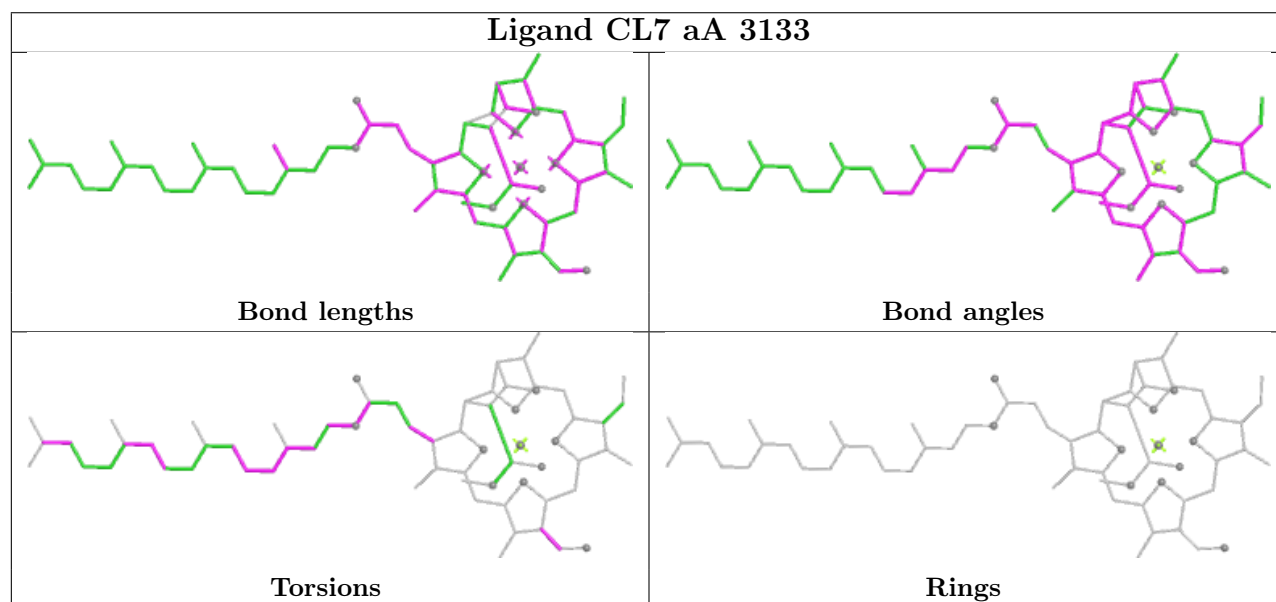
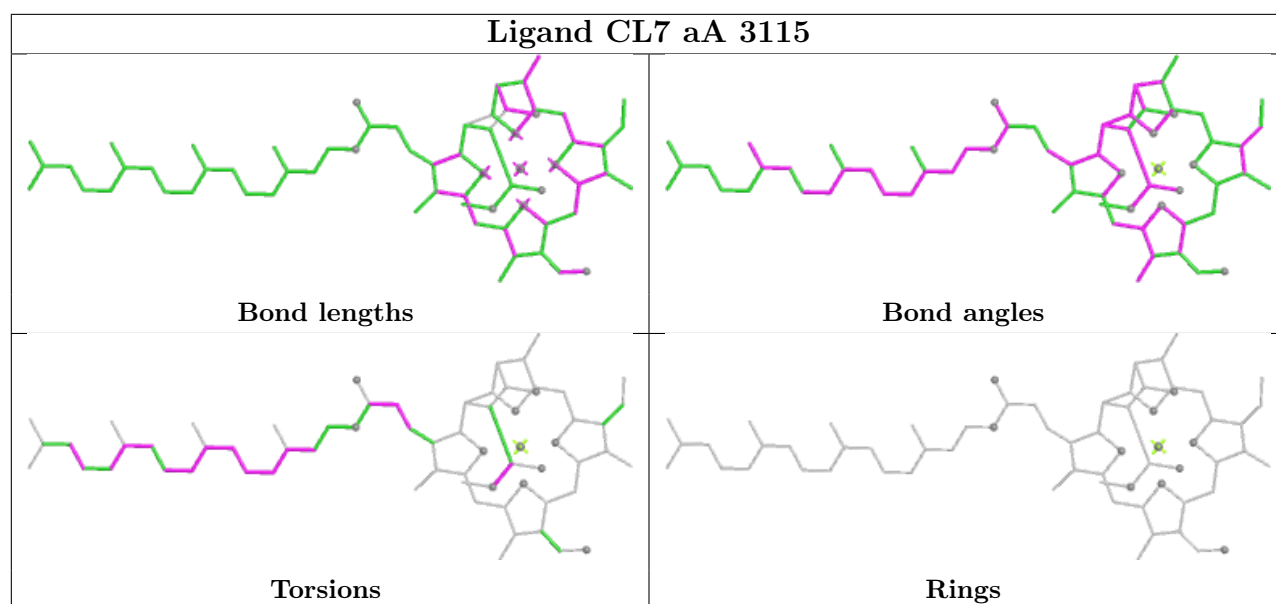
Ligand CL7 bA 3110

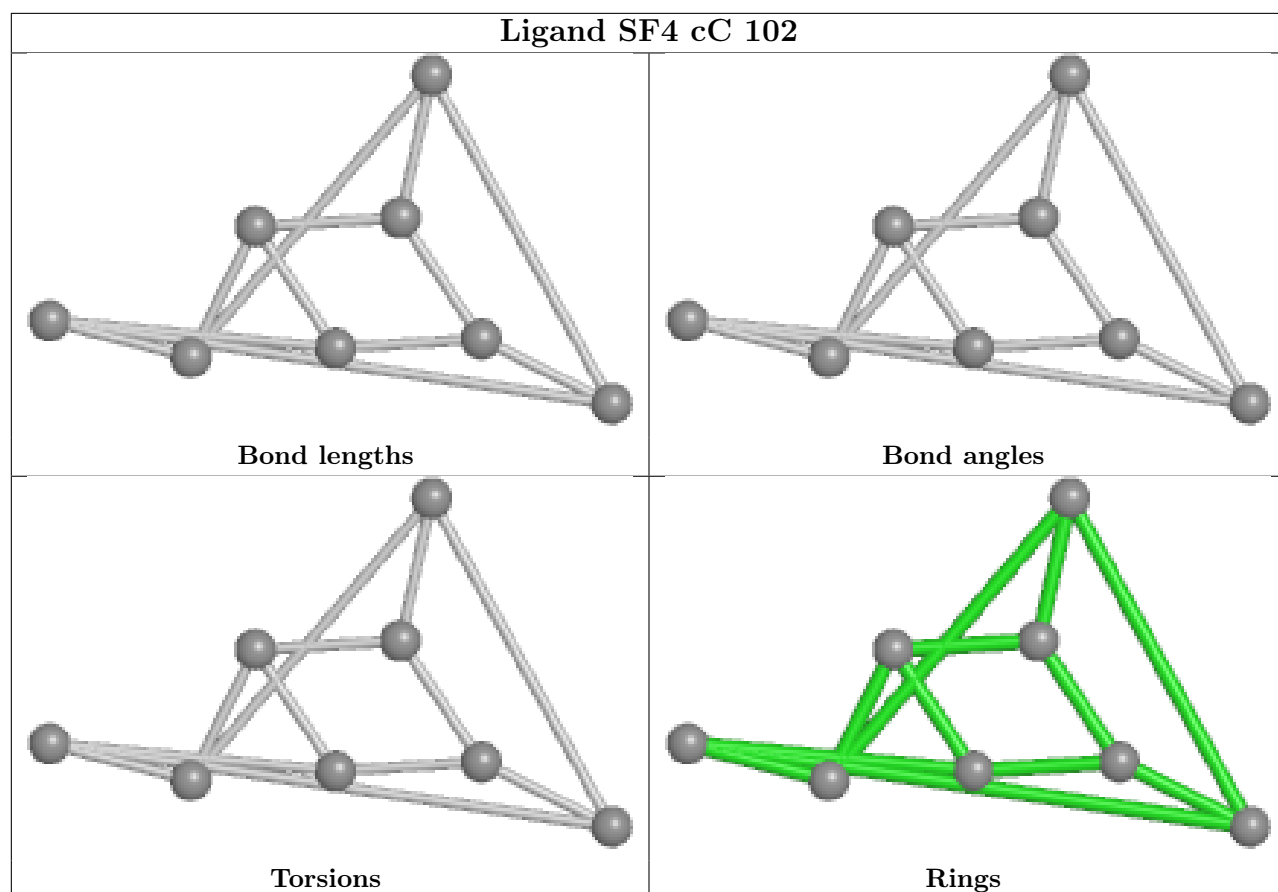
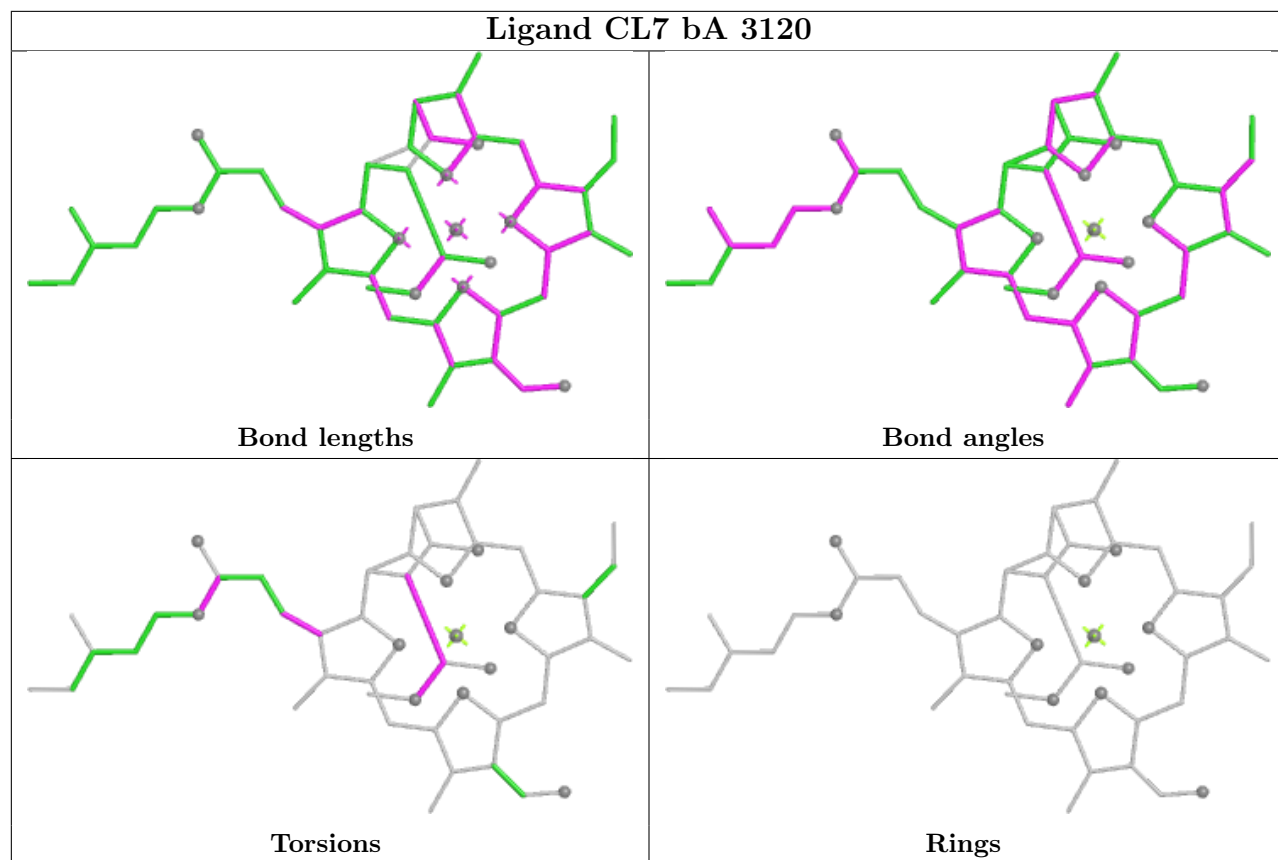


Ligand PHO cB 801









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.

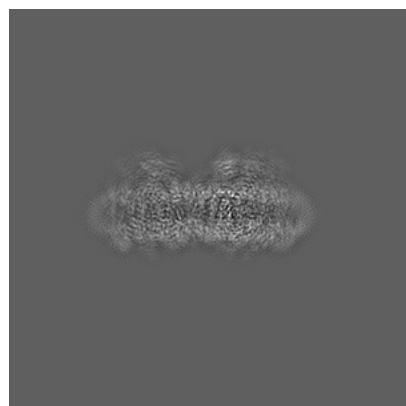
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30420. These allow visual inspection of the internal detail of the map and identification of artifacts.

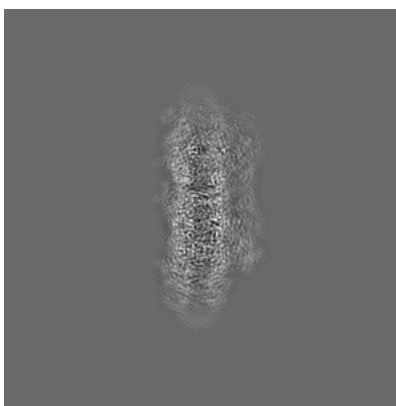
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

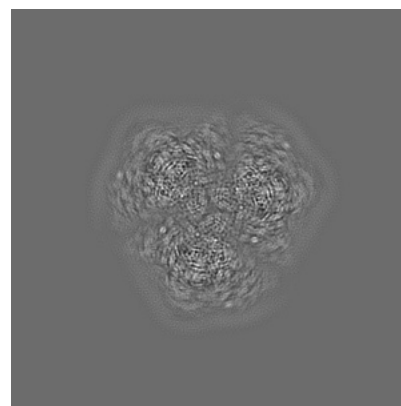
6.1.1 Primary map



X

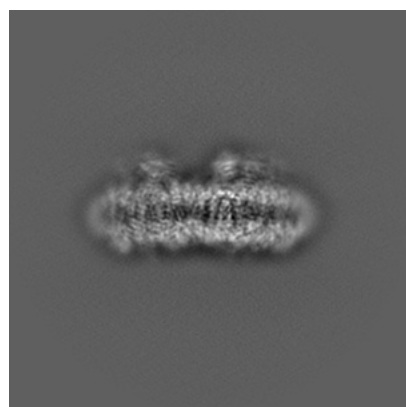


Y

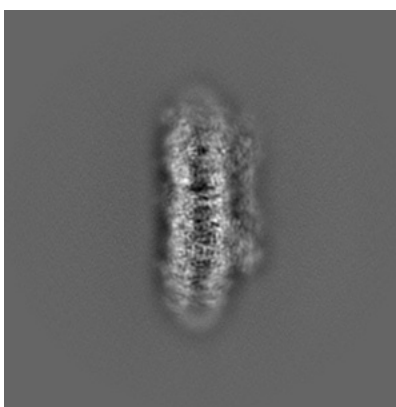


Z

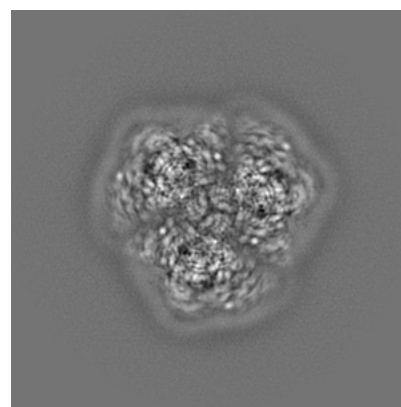
6.1.2 Raw map



X



Y

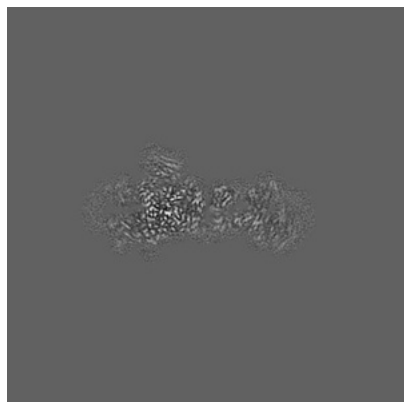


Z

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

6.2 Central slices [i](#)

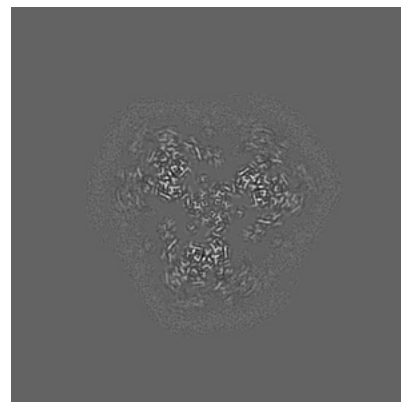
6.2.1 Primary map



X Index: 165

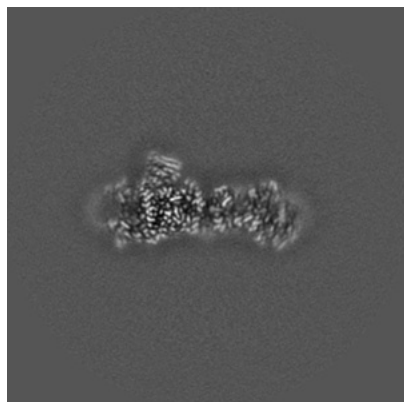


Y Index: 165

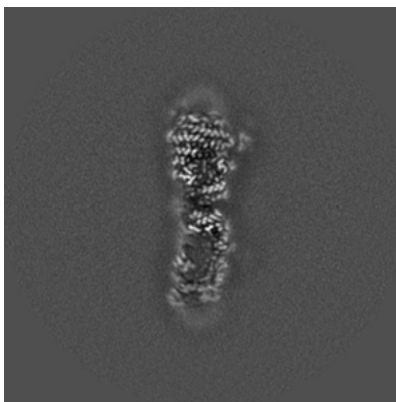


Z Index: 165

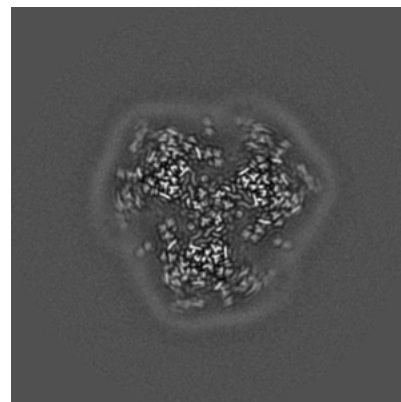
6.2.2 Raw map



X Index: 165



Y Index: 165

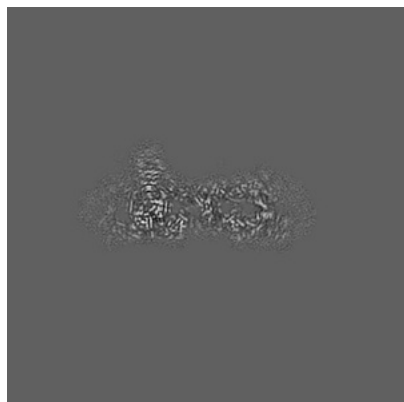


Z Index: 165

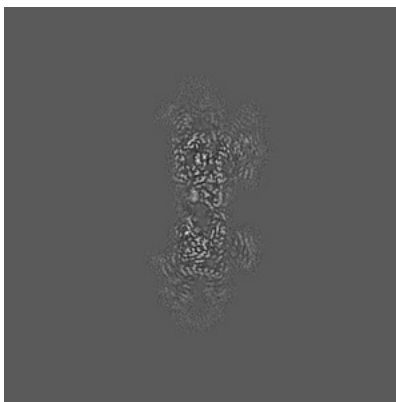
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

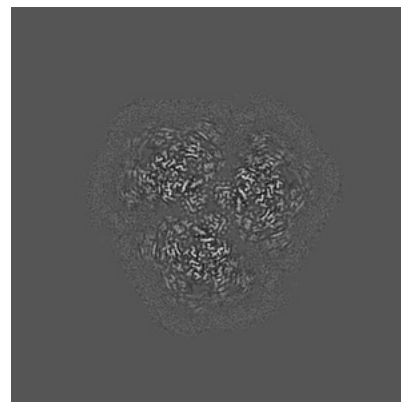
6.3.1 Primary map



X Index: 153

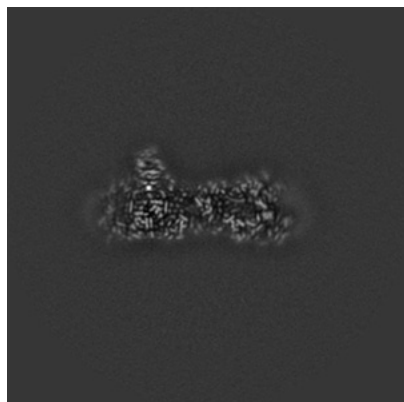


Y Index: 181

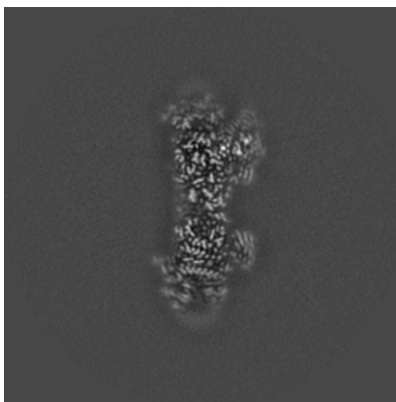


Z Index: 155

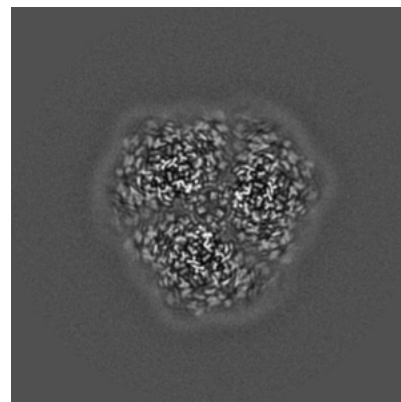
6.3.2 Raw map



X Index: 153



Y Index: 180

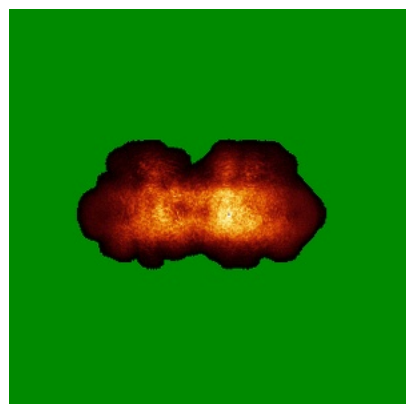


Z Index: 152

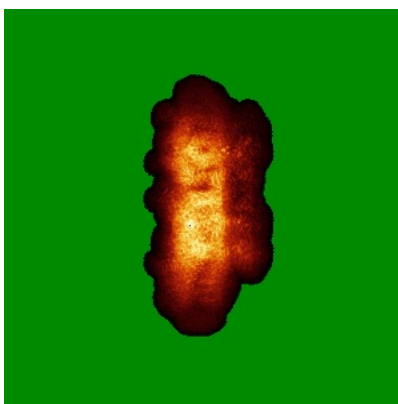
The images above show the largest variance slices of the map in three orthogonal directions.

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

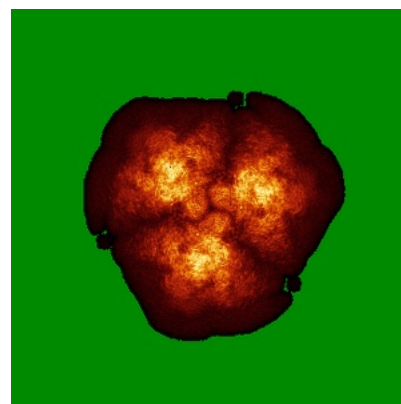
6.4.1 Primary map



X

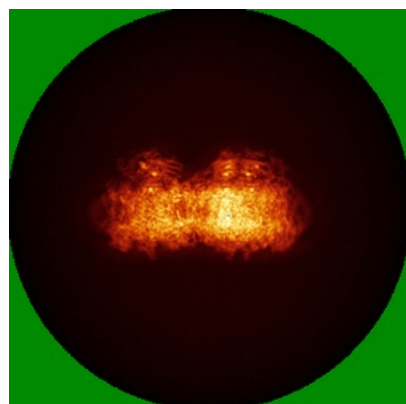


Y

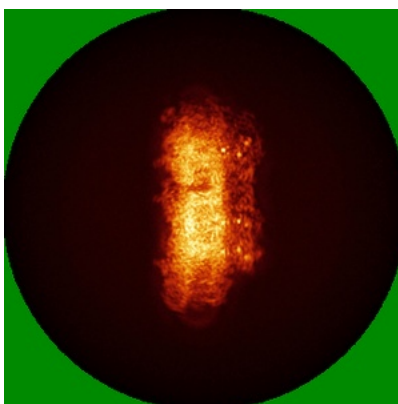


Z

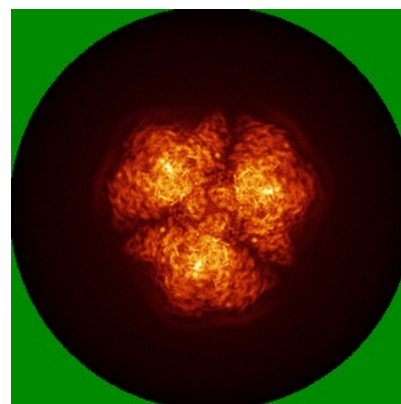
6.4.2 Raw map



X



Y

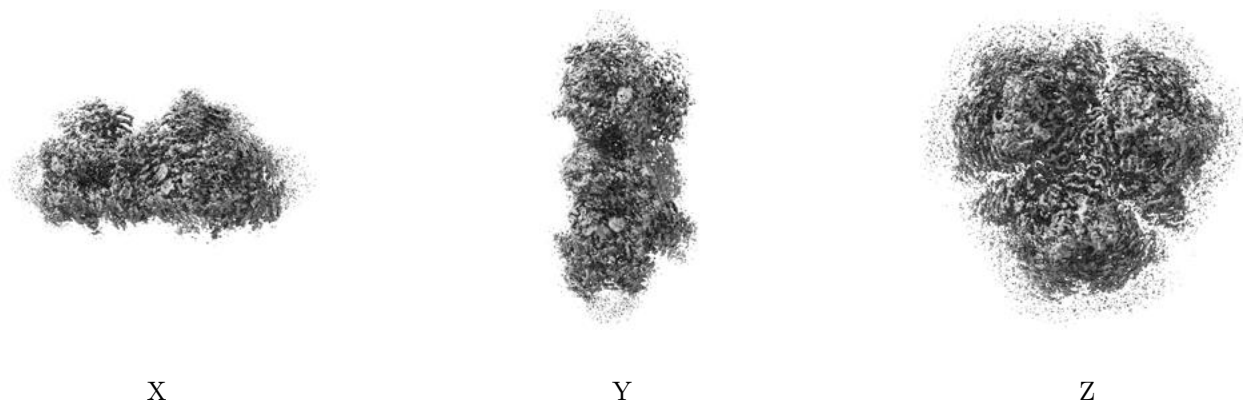


Z

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.

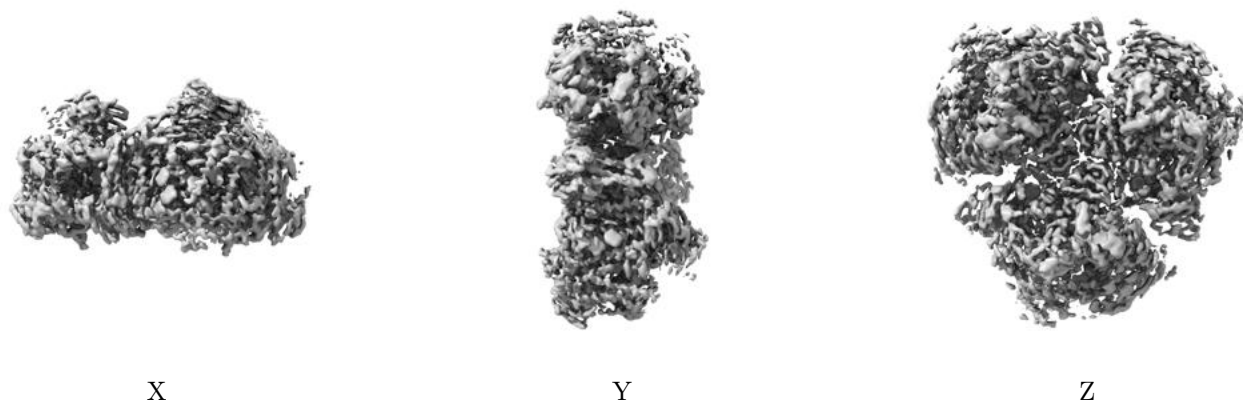
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.00637. 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.

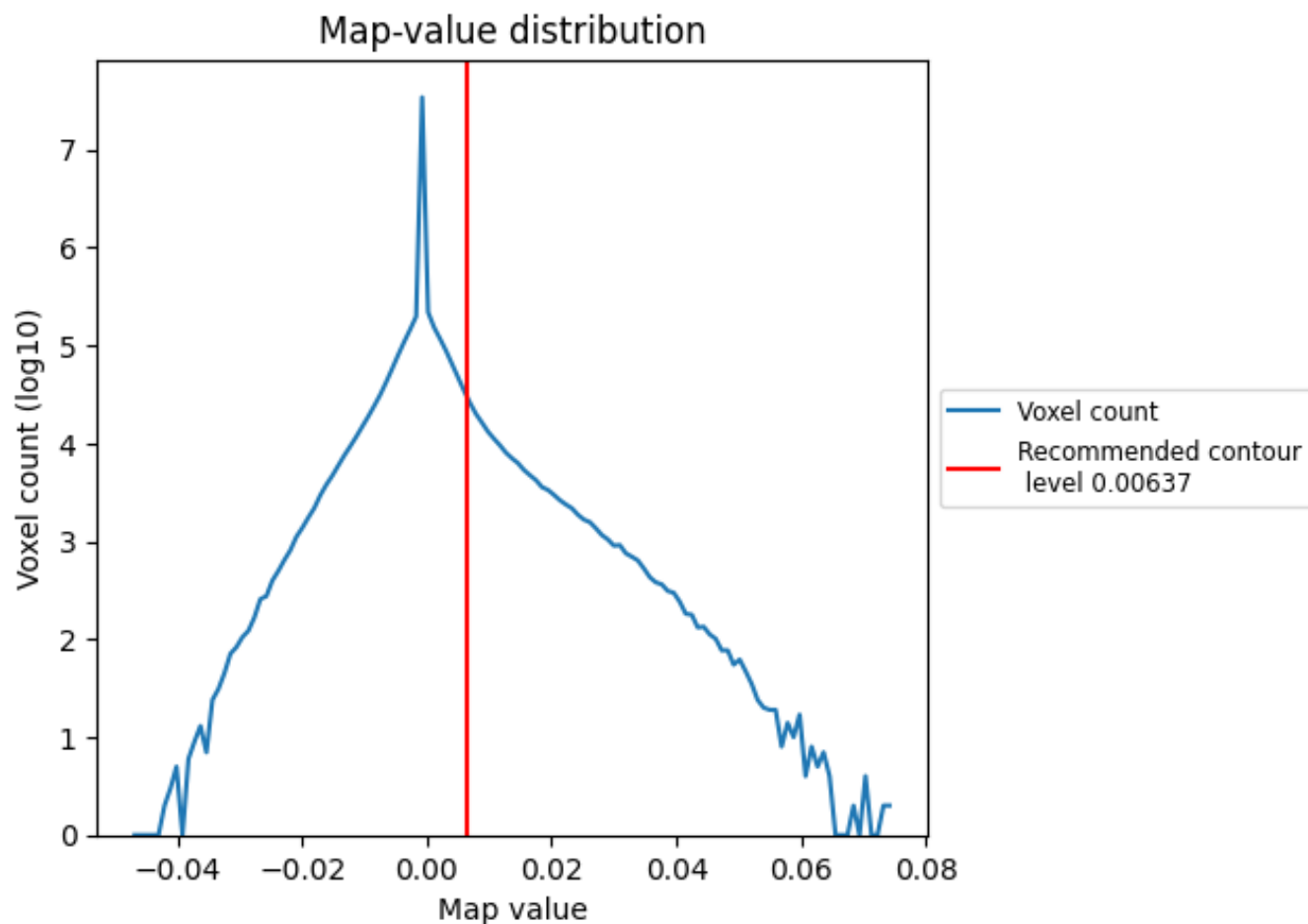
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

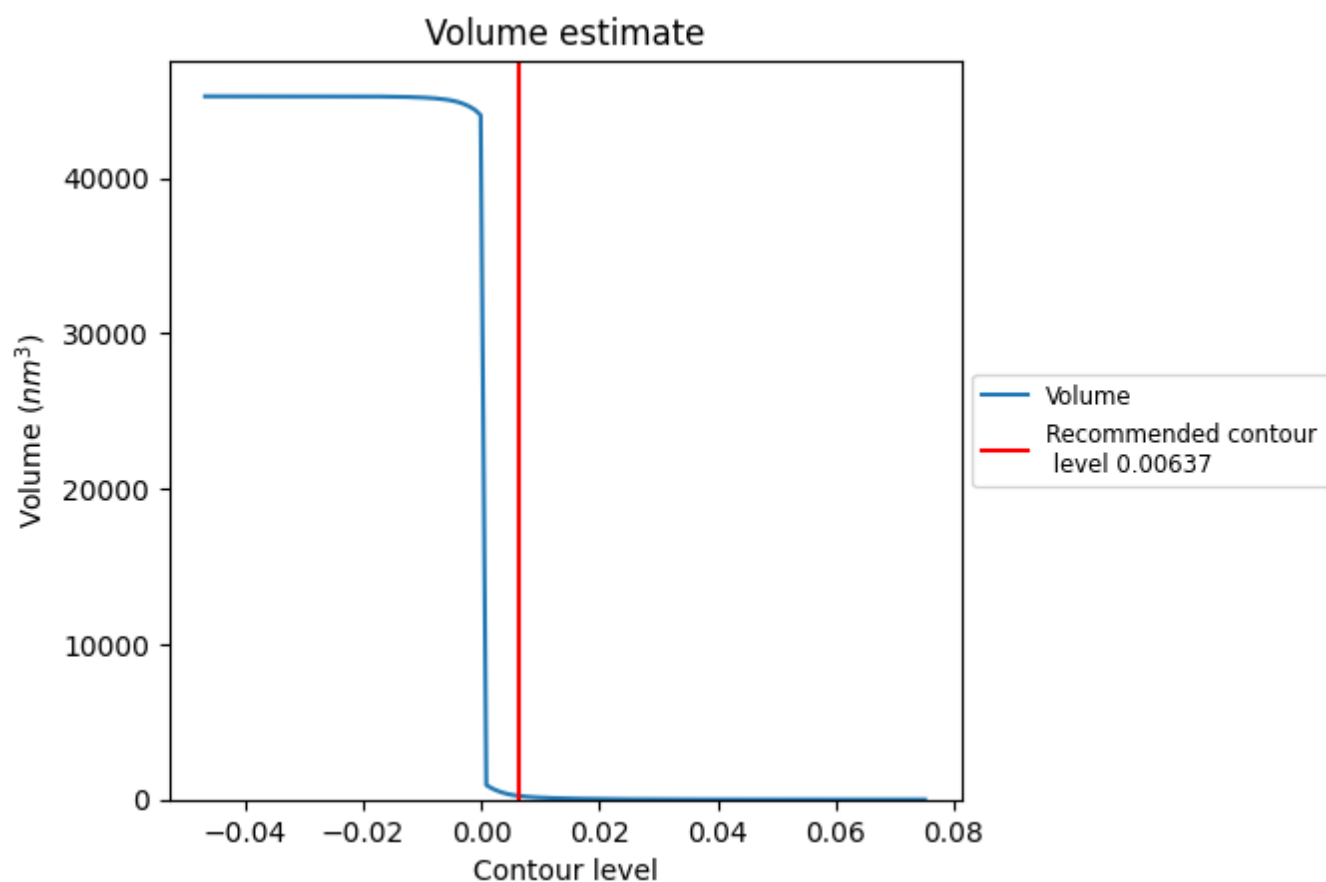
This section contains the results of statistical analysis of the map.

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.

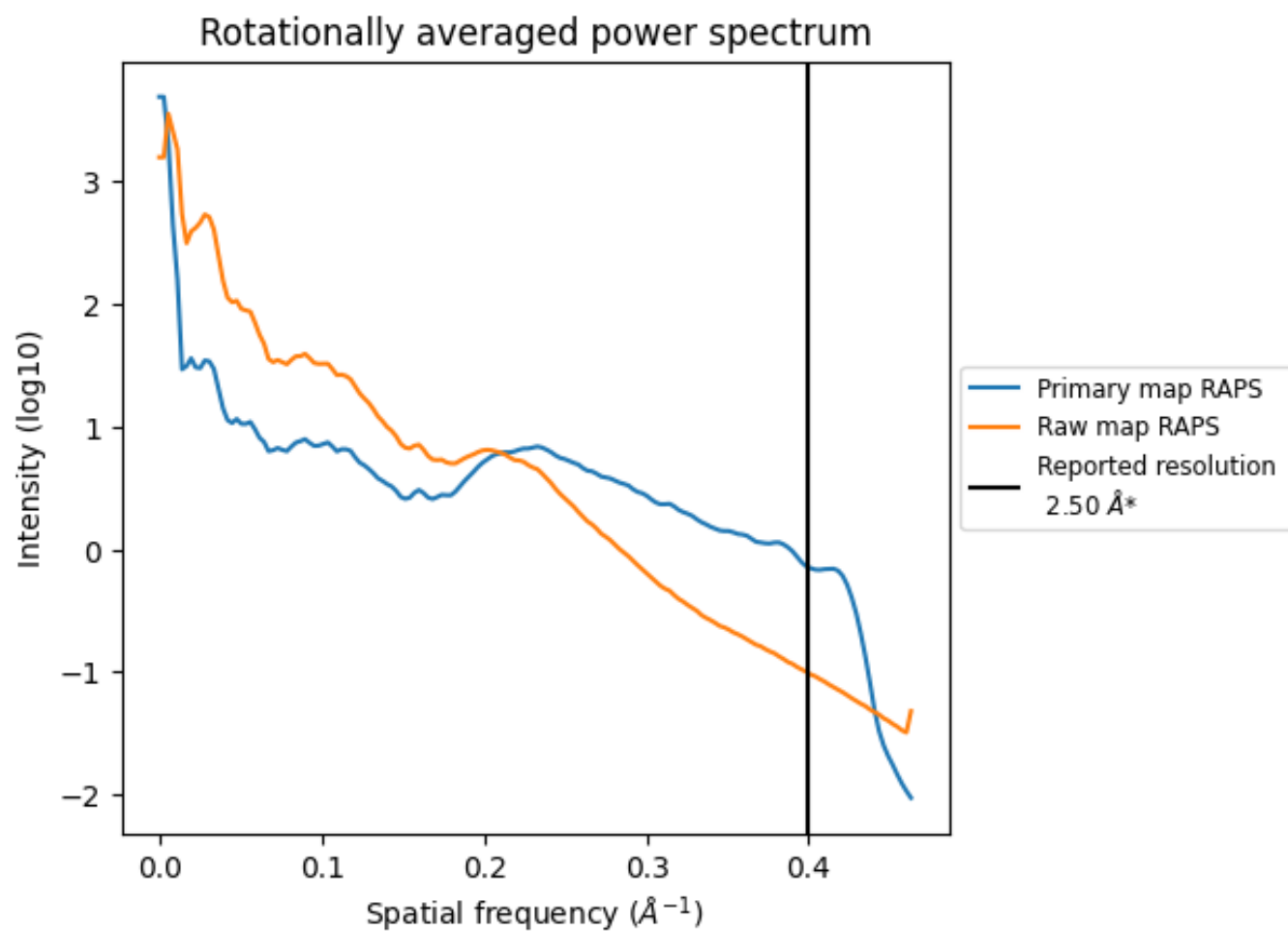
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 234 nm³; this corresponds to an approximate mass of 211 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 ⓘ

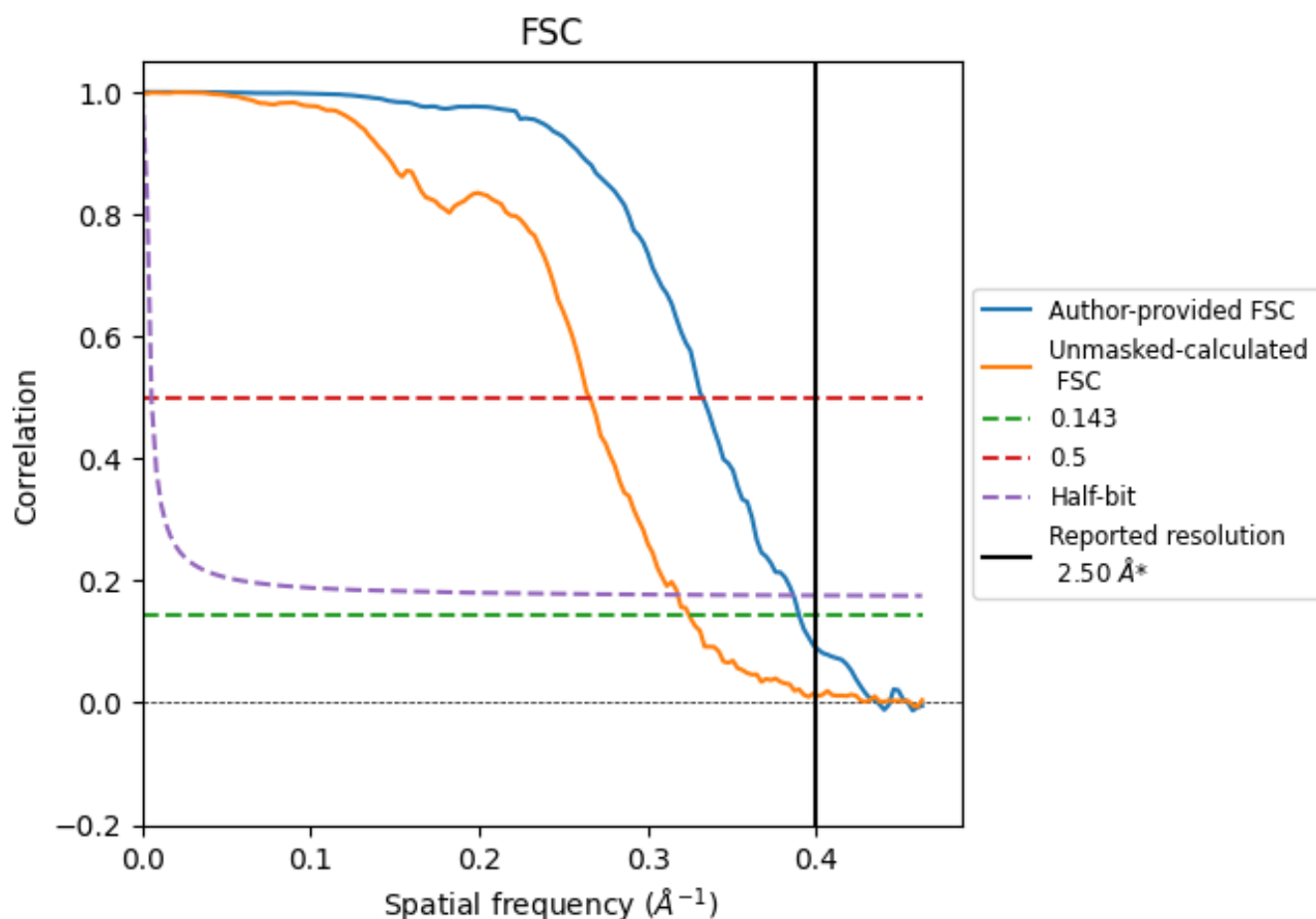


*Reported resolution corresponds to spatial frequency of 0.400 Å⁻¹

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 0.400 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

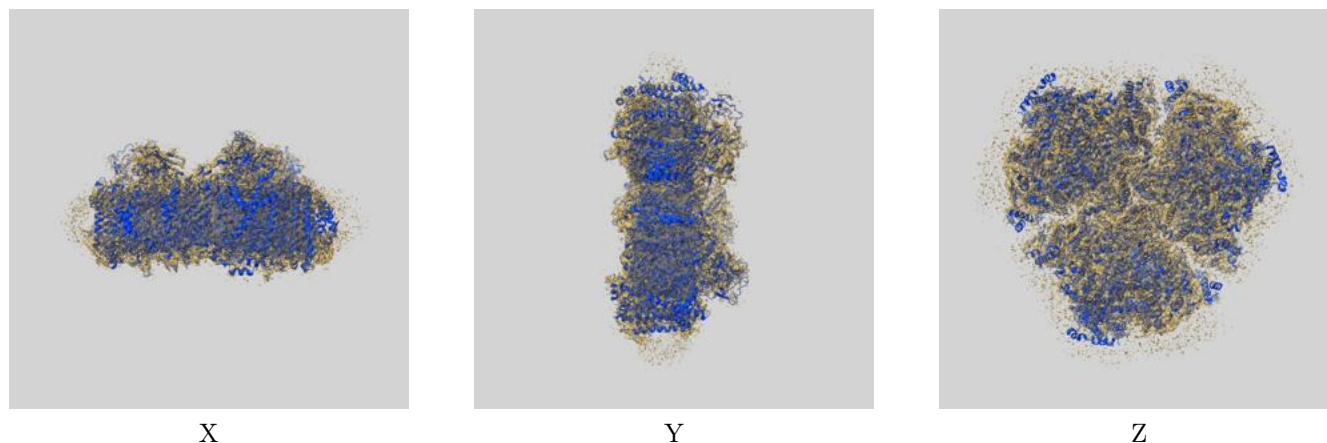
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.50	-	-
Author-provided FSC curve	2.56	3.01	2.59
Unmasked-calculated*	3.08	3.77	3.15

*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 3.08 differs from the reported value 2.5 by more than 10 %

9 Map-model fit [i](#)

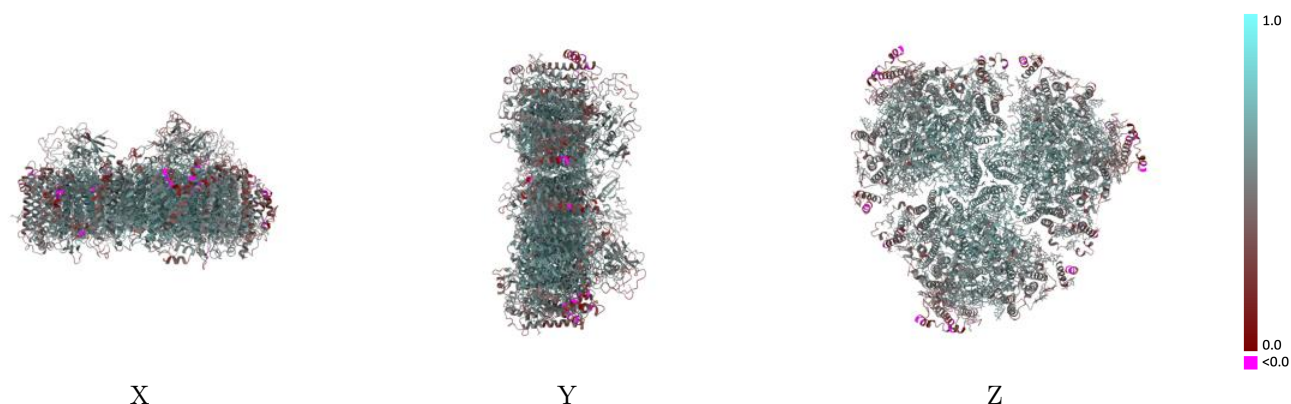
This section contains information regarding the fit between EMDB map EMD-30420 and PDB model 7COY. Per-residue inclusion information can be found in section [3](#) on page [30](#).

9.1 Map-model overlay [i](#)



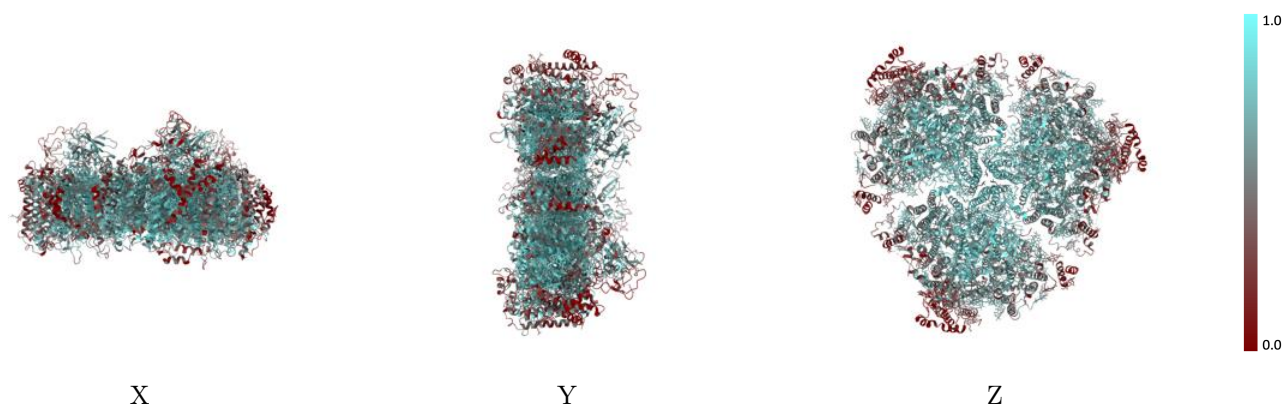
The images above show the 3D surface view of the map at the recommended contour level 0.00637 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



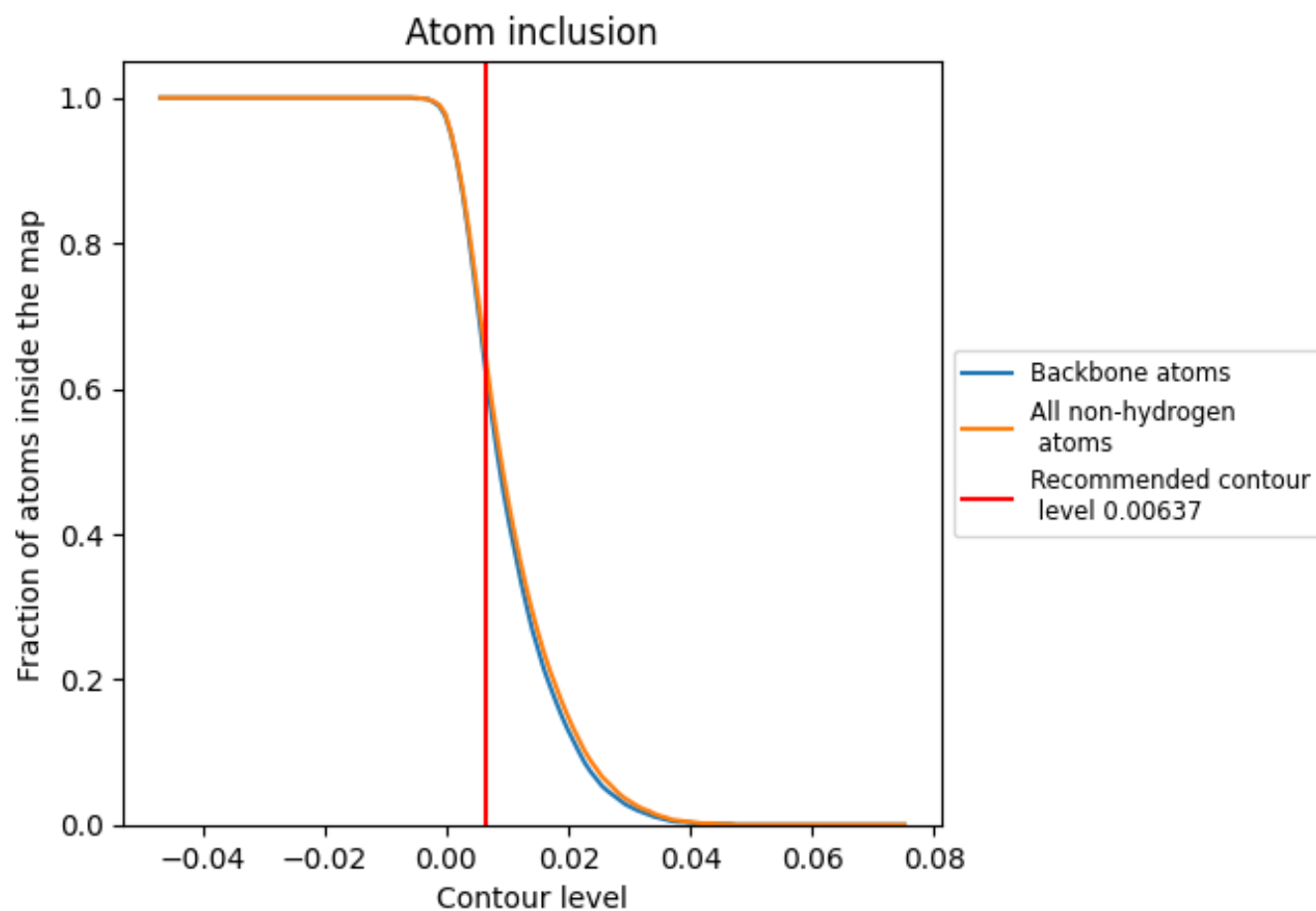
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.00637).

9.4 Atom inclusion [i](#)



At the recommended contour level, 63% of all backbone atoms, 65% 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 (0.00637) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6510	 0.5530
aA	 0.6990	 0.5750
aB	 0.6990	 0.5740
aC	 0.6750	 0.5290
aD	 0.5080	 0.4760
aE	 0.2160	 0.3930
aF	 0.2070	 0.3320
aI	 0.7970	 0.6330
aJ	 0.2620	 0.4220
aK	 0.0880	 0.2480
aL	 0.8270	 0.6390
aM	 0.5560	 0.5030
bA	 0.7030	 0.5760
bB	 0.6980	 0.5740
bC	 0.6780	 0.5310
bD	 0.5080	 0.4790
bE	 0.2070	 0.4020
bF	 0.1950	 0.3290
bI	 0.8040	 0.6290
bJ	 0.2590	 0.4280
bK	 0.0830	 0.2480
bL	 0.8320	 0.6390
bM	 0.5560	 0.5060
cA	 0.7070	 0.5790
cB	 0.6980	 0.5740
cC	 0.6900	 0.5280
cD	 0.5100	 0.4790
cE	 0.2000	 0.3950
cF	 0.1960	 0.3370
cI	 0.8170	 0.6330
cJ	 0.2650	 0.4260
cK	 0.0720	 0.2680
cL	 0.8340	 0.6370
cM	 0.5320	 0.4980

