wwPDB EM Validation Summary Report ⓘ

Mar 20, 2024 – 12:23 AM JST

PDB ID	:	6K61
EMDB ID	:	EMD-9918
Title	:	Cryo-EM structure of the tetrameric photosystem I from a heterocyst-forming cyanobacterium Anabaena sp. PCC7120
Authors	:	Zheng, L.; Li, Y.; Li, X.; Zhong, Q.; Li, N.; Zhang, K.; Zhang, Y.; Chu, H.; Ma, C.; Li, G.; Zhao, J.; Gao, N.
Deposited on	:	2019-05-31
Resolution	:	2.37 Å(reported)

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

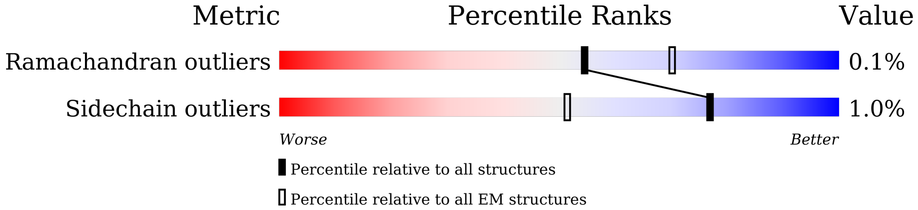
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance ⓘ

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

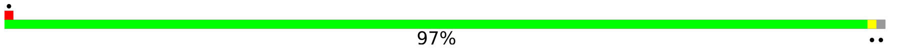
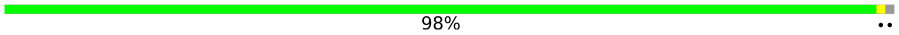
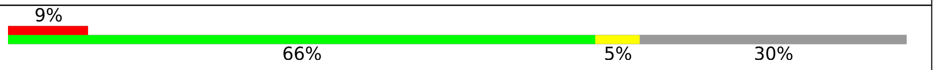
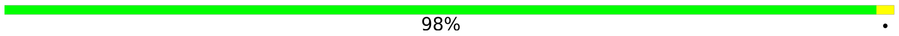
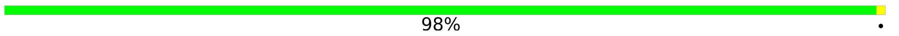
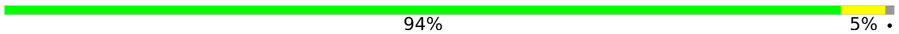
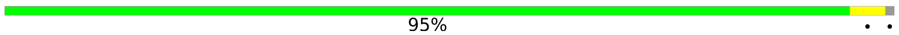
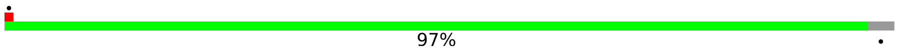
The reported resolution of this entry is 2.37 Å.

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)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	752	 • 97% ••
1	a	752	 98% ••
2	X	44	 68% • 30%
2	x	44	 9% 66% 5% 30%
3	B	741	 98% •
3	b	741	 98% •
4	C	81	 94% 5% •
4	c	81	 95% • •
5	D	139	 • 97% •

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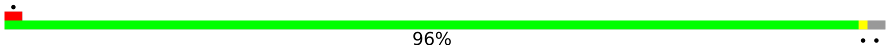
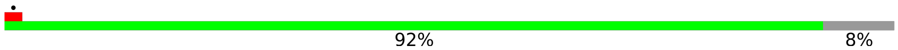
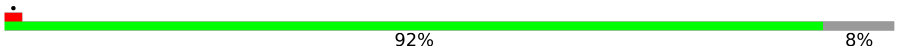
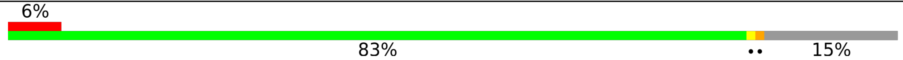
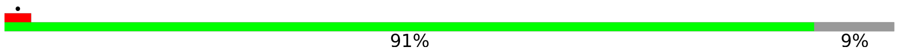
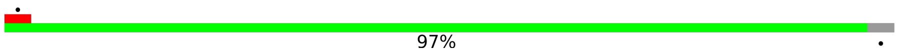
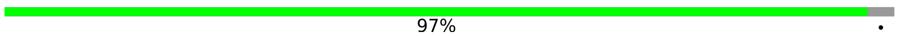
Mol	Chain	Length	Quality of chain
5	d	139	
6	E	70	
6	e	70	
7	F	164	
7	f	164	
8	J	49	
8	j	49	
9	K	86	
9	k	86	
10	I	46	
10	i	46	
11	L	172	
11	l	172	
12	M	32	
12	m	32	

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
13	CL0	A	801	X	-	-	-
13	CL0	a	801	X	-	-	-
14	CLA	A	802	X	-	-	-
14	CLA	A	803	X	-	-	-
14	CLA	A	804	X	-	-	-
14	CLA	A	805	X	-	-	-
14	CLA	A	806	X	-	-	-
14	CLA	A	807	X	-	-	-
14	CLA	A	808	X	-	-	-
14	CLA	A	809	X	-	-	-
14	CLA	A	810	X	-	-	-
14	CLA	A	811	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	A	812	X	-	-	-
14	CLA	A	813	X	-	-	-
14	CLA	A	814	X	-	-	-
14	CLA	A	815	X	-	-	-
14	CLA	A	816	X	-	-	-
14	CLA	A	817	X	-	-	-
14	CLA	A	818	X	-	-	-
14	CLA	A	819	X	-	-	-
14	CLA	A	820	X	-	-	-
14	CLA	A	821	X	-	-	-
14	CLA	A	822	X	-	-	-
14	CLA	A	823	X	-	-	-
14	CLA	A	824	X	-	-	-
14	CLA	A	825	X	-	-	-
14	CLA	A	826	X	-	-	-
14	CLA	A	827	X	-	-	-
14	CLA	A	828	X	-	-	-
14	CLA	A	829	X	-	-	-
14	CLA	A	830	X	-	-	-
14	CLA	A	831	X	-	-	-
14	CLA	A	832	X	-	-	-
14	CLA	A	833	X	-	-	-
14	CLA	A	834	X	-	-	-
14	CLA	A	835	X	-	-	-
14	CLA	A	836	X	-	-	-
14	CLA	A	837	X	-	-	-
14	CLA	A	838	X	-	-	-
14	CLA	A	840	X	-	-	-
14	CLA	A	841	X	-	-	-
14	CLA	A	842	X	-	-	-
14	CLA	A	843	X	-	-	-
14	CLA	B	801	X	-	-	-
14	CLA	B	802	X	-	-	-
14	CLA	B	804	X	-	-	-
14	CLA	B	805	X	-	-	-
14	CLA	B	806	X	-	-	-
14	CLA	B	807	X	-	-	-
14	CLA	B	808	X	-	-	-
14	CLA	B	809	X	-	-	-
14	CLA	B	810	X	-	-	-
14	CLA	B	811	X	-	-	-
14	CLA	B	812	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	B	813	X	-	-	-
14	CLA	B	814	X	-	-	-
14	CLA	B	815	X	-	-	-
14	CLA	B	816	X	-	-	-
14	CLA	B	817	X	-	-	-
14	CLA	B	818	X	-	-	-
14	CLA	B	819	X	-	-	-
14	CLA	B	820	X	-	-	-
14	CLA	B	821	X	-	-	-
14	CLA	B	822	X	-	-	-
14	CLA	B	823	X	-	-	-
14	CLA	B	824	X	-	-	-
14	CLA	B	825	X	-	-	-
14	CLA	B	826	X	-	-	-
14	CLA	B	827	X	-	-	-
14	CLA	B	828	X	-	-	-
14	CLA	B	829	X	-	-	-
14	CLA	B	830	X	-	-	-
14	CLA	B	831	X	-	-	-
14	CLA	B	832	X	-	-	-
14	CLA	B	833	X	-	-	-
14	CLA	B	834	X	-	-	-
14	CLA	B	835	X	-	-	-
14	CLA	B	836	X	-	-	-
14	CLA	B	837	X	-	-	-
14	CLA	B	838	X	-	-	-
14	CLA	B	839	X	-	-	-
14	CLA	B	840	X	-	-	-
14	CLA	B	841	X	-	-	-
14	CLA	B	842	X	-	-	-
14	CLA	B	843	X	-	-	-
14	CLA	F	202	X	-	-	-
14	CLA	F	204	X	-	-	-
14	CLA	J	101	X	-	-	-
14	CLA	J	102	X	-	-	-
14	CLA	K	101	X	-	-	-
14	CLA	K	102	X	-	-	-
14	CLA	L	1501	X	-	-	-
14	CLA	L	1503	X	-	-	-
14	CLA	X	1701	X	-	-	-
14	CLA	a	802	X	-	-	-
14	CLA	a	803	X	-	-	-

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

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	b	807	X	-	-	-
14	CLA	b	808	X	-	-	-
14	CLA	b	809	X	-	-	-
14	CLA	b	810	X	-	-	-
14	CLA	b	811	X	-	-	-
14	CLA	b	812	X	-	-	-
14	CLA	b	813	X	-	-	-
14	CLA	b	814	X	-	-	-
14	CLA	b	815	X	-	-	-
14	CLA	b	817	X	-	-	-
14	CLA	b	818	X	-	-	-
14	CLA	b	819	X	-	-	-
14	CLA	b	820	X	-	-	-
14	CLA	b	821	X	-	-	-
14	CLA	b	822	X	-	-	-
14	CLA	b	823	X	-	-	-
14	CLA	b	824	X	-	-	-
14	CLA	b	825	X	-	-	-
14	CLA	b	826	X	-	-	-
14	CLA	b	828	X	-	-	-
14	CLA	b	829	X	-	-	-
14	CLA	b	830	X	-	-	-
14	CLA	b	831	X	-	-	-
14	CLA	b	832	X	-	-	-
14	CLA	b	833	X	-	-	-
14	CLA	b	834	X	-	-	-
14	CLA	b	835	X	-	-	-
14	CLA	b	836	X	-	-	-
14	CLA	b	837	X	-	-	-
14	CLA	b	838	X	-	-	-
14	CLA	b	839	X	-	-	-
14	CLA	b	840	X	-	-	-
14	CLA	b	841	X	-	-	-
14	CLA	b	842	X	-	-	-
14	CLA	f	201	X	-	-	-
14	CLA	f	203	X	-	-	-
14	CLA	j	101	X	-	-	-
14	CLA	j	102	X	-	-	-
14	CLA	j	103	X	-	-	-
14	CLA	k	101	X	-	-	-
14	CLA	k	102	X	-	-	-
14	CLA	l	203	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	l	205	X	-	-	-
14	CLA	m	1201	X	-	-	-
14	CLA	x	1701	X	-	-	-

2 Entry composition ⓘ

There are 20 unique types of molecules in this entry. The entry contains 49283 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
			Total	C	N	O	S		
1	A	742	5823	3820	1003	979	21	0	0
1	a	742	5823	3820	1003	979	21	0	0

- Molecule 2 is a protein called Photosystem I 4.8 kDa protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	X	31	257	179	40	38	0	0
2	x	31	257	179	40	38	0	0

- Molecule 3 is a protein called Photosystem I P700 chlorophyll a apoprotein A2 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	B	740	5918	3905	991	1004	18	0	0
3	b	740	5918	3905	991	1004	18	0	0

- Molecule 4 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	C	80	598	367	103	117	11	0	0
4	c	80	598	367	103	117	11	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	135	Total	C	N	O	S	0	0
			1040	666	179	194	1		
5	d	136	Total	C	N	O	S	0	0
			1047	670	180	196	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
6	E	61	Total	C	N	O	0	0
			490	313	84	93		
6	e	61	Total	C	N	O	0	0
			490	313	84	93		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	141	Total	C	N	O	S	0	0
			1080	690	184	204	2		
7	f	141	Total	C	N	O	S	0	0
			1080	690	184	204	2		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
8	J	45	Total	C	N	O	0	0
			359	244	54	61		
8	j	45	Total	C	N	O	0	0
			359	244	54	61		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	73	Total	C	N	O	S	0	0
			537	357	89	90	1		
9	k	78	Total	C	N	O	S	0	0
			568	376	94	97	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
10	I	34	Total	C	N	O	0	0
			275	189	38	48		

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Mol	Chain	Residues	Atoms				AltConf	Trace
10	i	34	Total 275	C 189	N 38	O 48	0	0

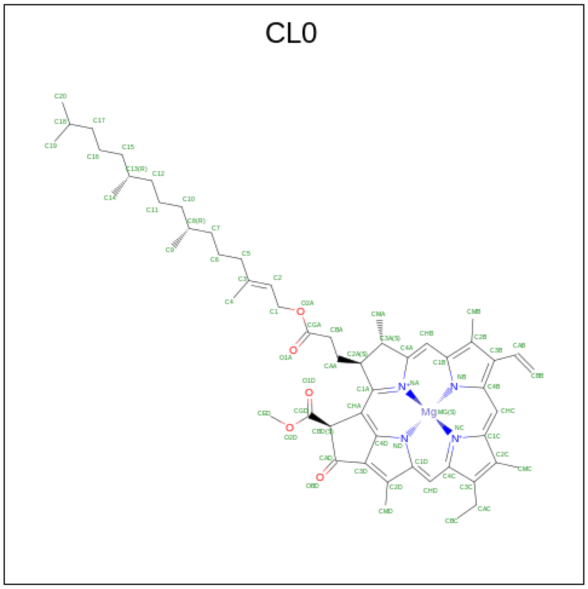
- Molecule 11 is a protein called Photosystem I reaction center subunit XI.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	155	Total 1163	C 763	N 197	O 202	S 1	0	0
11	l	155	Total 1163	C 763	N 197	O 202	S 1	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
12	M	31	Total 241	C 160	N 37	O 44	0	0
12	m	31	Total 241	C 160	N 37	O 44	0	0

- Molecule 13 is CHLOROPHYLL A ISOMER (three-letter code: CL0) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
13	A	1	Total 65	C 55	Mg 1	N 4	O 5	0

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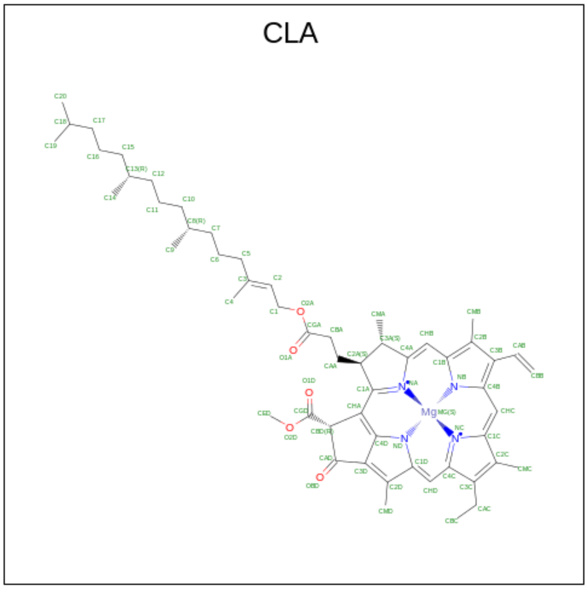
Mol	Chain	Residues	Atoms					AltConf
13	a	1	Total 65	C 55	Mg 1	N 4	O 5	0

- Molecule 14 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 54	C 44	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms	AltConf
14	A	1	Total C Mg N O 59 49 1 4 5	0
14	A	1	Total C Mg N O 60 50 1 4 5	0
14	A	1	Total C Mg N O 54 44 1 4 5	0
14	A	1	Total C Mg N O 45 35 1 4 5	0
14	A	1	Total C Mg N O 45 35 1 4 5	0
14	A	1	Total C Mg N O 59 49 1 4 5	0
14	A	1	Total C Mg N O 60 50 1 4 5	0
14	A	1	Total C Mg N O 65 55 1 4 5	0
14	A	1	Total C Mg N O 54 44 1 4 5	0
14	A	1	Total C Mg N O 65 55 1 4 5	0
14	A	1	Total C Mg N O 45 35 1 4 5	0
14	A	1	Total C Mg N O 54 44 1 4 5	0
14	A	1	Total C Mg N O 45 35 1 4 5	0
14	A	1	Total C Mg N O 65 55 1 4 5	0
14	A	1	Total C Mg N O 54 44 1 4 5	0
14	A	1	Total C Mg N O 65 55 1 4 5	0
14	A	1	Total C Mg N O 65 55 1 4 5	0
14	A	1	Total C Mg N O 65 55 1 4 5	0
14	A	1	Total C Mg N O 65 55 1 4 5	0
14	A	1	Total C Mg N O 54 44 1 4 5	0
14	A	1	Total C Mg N O 65 55 1 4 5	0

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Mol	Chain	Residues	Atoms	AltConf
14	A	1	Total C Mg N O 65 55 1 4 5	0
14	A	1	Total C Mg N O 65 55 1 4 5	0
14	A	1	Total C Mg N O 54 44 1 4 5	0
14	A	1	Total C Mg N O 45 35 1 4 5	0
14	A	1	Total C Mg N O 51 41 1 4 5	0
14	A	1	Total C Mg N O 65 55 1 4 5	0
14	A	1	Total C Mg N O 65 55 1 4 5	0
14	A	1	Total C Mg N O 59 49 1 4 5	0
14	A	1	Total C Mg N O 65 55 1 4 5	0
14	A	1	Total C Mg N O 65 55 1 4 5	0
14	A	1	Total C Mg N O 45 35 1 4 5	0
14	X	1	Total C Mg N O 49 39 1 4 5	0
14	B	1	Total C Mg N O 65 55 1 4 5	0
14	B	1	Total C Mg N O 65 55 1 4 5	0
14	B	1	Total C Mg N O 65 55 1 4 5	0
14	B	1	Total C Mg N O 65 55 1 4 5	0
14	B	1	Total C Mg N O 65 55 1 4 5	0
14	B	1	Total C Mg N O 55 45 1 4 5	0
14	B	1	Total C Mg N O 65 55 1 4 5	0
14	B	1	Total C Mg N O 65 55 1 4 5	0
14	B	1	Total C Mg N O 65 55 1 4 5	0

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Mol	Chain	Residues	Atoms	AltConf
14	B	1	Total C Mg N O 65 55 1 4 5	0
14	B	1	Total C Mg N O 65 55 1 4 5	0
14	B	1	Total C Mg N O 60 50 1 4 5	0
14	B	1	Total C Mg N O 54 44 1 4 5	0
14	B	1	Total C Mg N O 54 44 1 4 5	0
14	B	1	Total C Mg N O 65 55 1 4 5	0
14	B	1	Total C Mg N O 50 40 1 4 5	0
14	B	1	Total C Mg N O 49 39 1 4 5	0
14	B	1	Total C Mg N O 45 35 1 4 5	0
14	B	1	Total C Mg N O 65 55 1 4 5	0
14	B	1	Total C Mg N O 65 55 1 4 5	0
14	B	1	Total C Mg N O 65 55 1 4 5	0
14	B	1	Total C Mg N O 45 35 1 4 5	0
14	B	1	Total C Mg N O 45 35 1 4 5	0
14	B	1	Total C Mg N O 55 45 1 4 5	0
14	B	1	Total C Mg N O 65 55 1 4 5	0
14	B	1	Total C Mg N O 65 55 1 4 5	0
14	B	1	Total C Mg N O 65 55 1 4 5	0
14	B	1	Total C Mg N O 65 55 1 4 5	0
14	B	1	Total C Mg N O 65 55 1 4 5	0
14	B	1	Total C Mg N O 65 55 1 4 5	0

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Mol	Chain	Residues	Atoms	AltConf
14	B	1	Total C Mg N O 65 55 1 4 5	0
14	B	1	Total C Mg N O 54 44 1 4 5	0
14	B	1	Total C Mg N O 60 50 1 4 5	0
14	B	1	Total C Mg N O 58 48 1 4 5	0
14	B	1	Total C Mg N O 54 44 1 4 5	0
14	B	1	Total C Mg N O 45 35 1 4 5	0
14	B	1	Total C Mg N O 45 35 1 4 5	0
14	B	1	Total C Mg N O 60 50 1 4 5	0
14	B	1	Total C Mg N O 65 55 1 4 5	0
14	B	1	Total C Mg N O 47 37 1 4 5	0
14	B	1	Total C Mg N O 65 55 1 4 5	0
14	B	1	Total C Mg N O 65 55 1 4 5	0
14	F	1	Total C Mg N O 65 55 1 4 5	0
14	F	1	Total C Mg N O 45 35 1 4 5	0
14	J	1	Total C Mg N O 45 35 1 4 5	0
14	J	1	Total C Mg N O 37 31 1 4 1	0
14	K	1	Total C Mg N O 41 33 1 4 3	0
14	K	1	Total C Mg N O 49 39 1 4 5	0
14	L	1	Total C Mg N O 51 41 1 4 5	0
14	L	1	Total C Mg N O 60 50 1 4 5	0
14	L	1	Total C Mg N O 45 35 1 4 5	0

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Mol	Chain	Residues	Atoms	AltConf
14	a	1	Total C Mg N O 65 55 1 4 5	0
14	a	1	Total C Mg N O 54 44 1 4 5	0
14	a	1	Total C Mg N O 65 55 1 4 5	0
14	a	1	Total C Mg N O 65 55 1 4 5	0
14	a	1	Total C Mg N O 60 50 1 4 5	0
14	a	1	Total C Mg N O 65 55 1 4 5	0
14	a	1	Total C Mg N O 65 55 1 4 5	0
14	a	1	Total C Mg N O 45 35 1 4 5	0
14	a	1	Total C Mg N O 65 55 1 4 5	0
14	a	1	Total C Mg N O 59 49 1 4 5	0
14	a	1	Total C Mg N O 60 50 1 4 5	0
14	a	1	Total C Mg N O 54 44 1 4 5	0
14	a	1	Total C Mg N O 45 35 1 4 5	0
14	a	1	Total C Mg N O 45 35 1 4 5	0
14	a	1	Total C Mg N O 59 49 1 4 5	0
14	a	1	Total C Mg N O 60 50 1 4 5	0
14	a	1	Total C Mg N O 65 55 1 4 5	0
14	a	1	Total C Mg N O 54 44 1 4 5	0
14	a	1	Total C Mg N O 65 55 1 4 5	0
14	a	1	Total C Mg N O 45 35 1 4 5	0
14	a	1	Total C Mg N O 54 44 1 4 5	0

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Mol	Chain	Residues	Atoms	AltConf
14	a	1	Total C Mg N O 45 35 1 4 5	0
14	a	1	Total C Mg N O 65 55 1 4 5	0
14	a	1	Total C Mg N O 54 44 1 4 5	0
14	a	1	Total C Mg N O 65 55 1 4 5	0
14	a	1	Total C Mg N O 65 55 1 4 5	0
14	a	1	Total C Mg N O 65 55 1 4 5	0
14	a	1	Total C Mg N O 65 55 1 4 5	0
14	a	1	Total C Mg N O 54 44 1 4 5	0
14	a	1	Total C Mg N O 65 55 1 4 5	0
14	a	1	Total C Mg N O 65 55 1 4 5	0
14	a	1	Total C Mg N O 65 55 1 4 5	0
14	a	1	Total C Mg N O 54 44 1 4 5	0
14	a	1	Total C Mg N O 45 35 1 4 5	0
14	a	1	Total C Mg N O 51 41 1 4 5	0
14	a	1	Total C Mg N O 65 55 1 4 5	0
14	a	1	Total C Mg N O 65 55 1 4 5	0
14	a	1	Total C Mg N O 65 55 1 4 5	0
14	a	1	Total C Mg N O 65 55 1 4 5	0
14	a	1	Total C Mg N O 45 35 1 4 5	0
14	x	1	Total C Mg N O 49 39 1 4 5	0
14	b	1	Total C Mg N O 65 55 1 4 5	0

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Mol	Chain	Residues	Atoms	AltConf
14	b	1	Total C Mg N O 65 55 1 4 5	0
14	b	1	Total C Mg N O 65 55 1 4 5	0
14	b	1	Total C Mg N O 65 55 1 4 5	0
14	b	1	Total C Mg N O 65 55 1 4 5	0
14	b	1	Total C Mg N O 65 55 1 4 5	0
14	b	1	Total C Mg N O 65 55 1 4 5	0
14	b	1	Total C Mg N O 65 55 1 4 5	0
14	b	1	Total C Mg N O 65 55 1 4 5	0
14	b	1	Total C Mg N O 65 55 1 4 5	0
14	b	1	Total C Mg N O 65 55 1 4 5	0
14	b	1	Total C Mg N O 60 50 1 4 5	0
14	b	1	Total C Mg N O 54 44 1 4 5	0
14	b	1	Total C Mg N O 54 44 1 4 5	0
14	b	1	Total C Mg N O 65 55 1 4 5	0
14	b	1	Total C Mg N O 50 40 1 4 5	0
14	b	1	Total C Mg N O 49 39 1 4 5	0
14	b	1	Total C Mg N O 45 35 1 4 5	0
14	b	1	Total C Mg N O 65 55 1 4 5	0
14	b	1	Total C Mg N O 65 55 1 4 5	0
14	b	1	Total C Mg N O 65 55 1 4 5	0
14	b	1	Total C Mg N O 45 35 1 4 5	0

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Mol	Chain	Residues	Atoms	AltConf
14	b	1	Total C Mg N O 45 35 1 4 5	0
14	b	1	Total C Mg N O 55 45 1 4 5	0
14	b	1	Total C Mg N O 65 55 1 4 5	0
14	b	1	Total C Mg N O 65 55 1 4 5	0
14	b	1	Total C Mg N O 65 55 1 4 5	0
14	b	1	Total C Mg N O 65 55 1 4 5	0
14	b	1	Total C Mg N O 65 55 1 4 5	0
14	b	1	Total C Mg N O 65 55 1 4 5	0
14	b	1	Total C Mg N O 65 55 1 4 5	0
14	b	1	Total C Mg N O 54 44 1 4 5	0
14	b	1	Total C Mg N O 60 50 1 4 5	0
14	b	1	Total C Mg N O 65 55 1 4 5	0
14	b	1	Total C Mg N O 54 44 1 4 5	0
14	b	1	Total C Mg N O 45 35 1 4 5	0
14	b	1	Total C Mg N O 45 35 1 4 5	0
14	b	1	Total C Mg N O 60 50 1 4 5	0
14	b	1	Total C Mg N O 65 55 1 4 5	0
14	b	1	Total C Mg N O 47 37 1 4 5	0
14	b	1	Total C Mg N O 65 55 1 4 5	0
14	b	1	Total C Mg N O 65 55 1 4 5	0
14	f	1	Total C Mg N O 59 49 1 4 5	0

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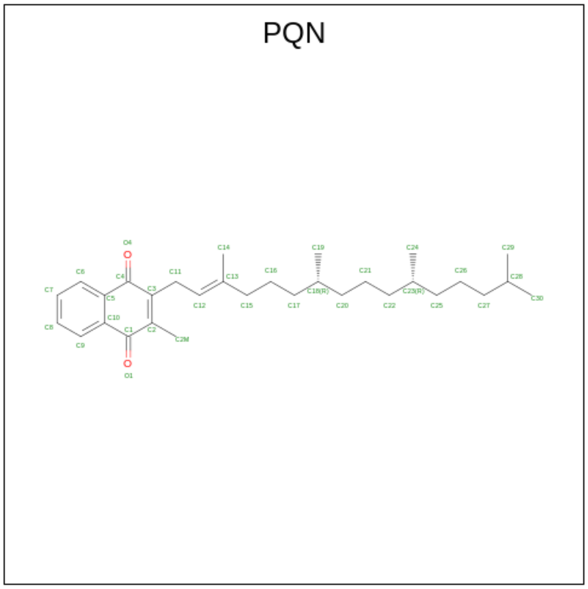
Mol	Chain	Residues	Atoms					AltConf
14	f	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	j	1	Total 58	C 48	Mg 1	N 4	O 5	0
14	j	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	j	1	Total 37	C 31	Mg 1	N 4	O 1	0
14	k	1	Total 41	C 33	Mg 1	N 4	O 3	0
14	k	1	Total 49	C 39	Mg 1	N 4	O 5	0
14	l	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	l	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	l	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	m	1	Total 55	C 45	Mg 1	N 4	O 5	0

- Molecule 15 is PHYLLOQUINONE (three-letter code: PQN) (formula: $C_{31}H_{46}O_2$) (labeled as "Ligand of Interest" by depositor).



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

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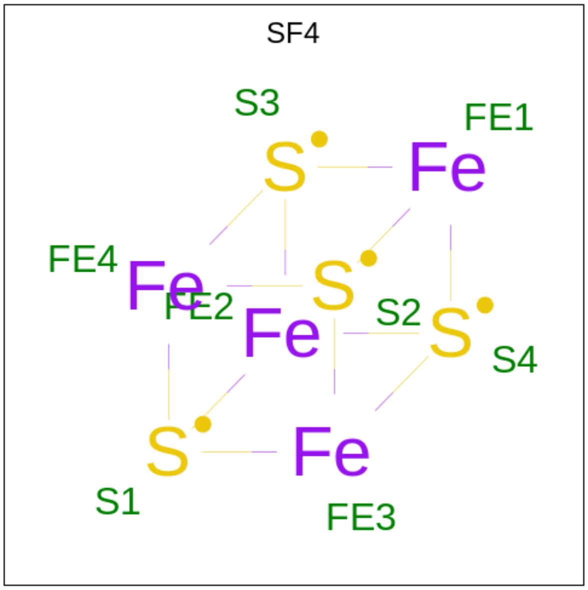
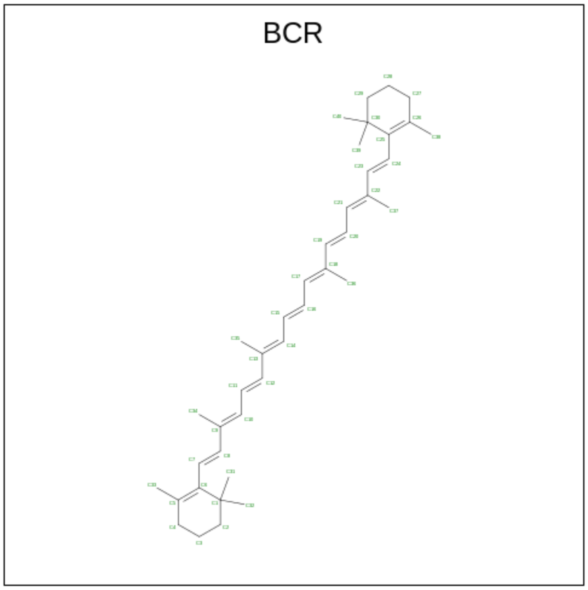
Mol	Chain	Residues	Atoms	AltConf
15	B	1	Total C O 33 31 2	0
15	a	1	Total C O 33 31 2	0
15	b	1	Total C O 33 31 2	0

- Molecule 16 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 17 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
17	A	1	Total C 40 40	0
17	A	1	Total C 40 40	0
17	A	1	Total C 40 40	0
17	A	1	Total C 40 40	0
17	A	1	Total C 40 40	0
17	A	1	Total C 40 40	0
17	B	1	Total C 40 40	0
17	B	1	Total C 40 40	0
17	B	1	Total C 40 40	0
17	B	1	Total C 40 40	0
17	B	1	Total C 40 40	0
17	B	1	Total C 40 40	0
17	F	1	Total C 40 40	0
17	F	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
17	J	1	Total C 40 40	0
17	J	1	Total C 40 40	0
17	J	1	Total C 40 40	0
17	K	1	Total C 40 40	0
17	I	1	Total C 40 40	0
17	I	1	Total C 40 40	0
17	L	1	Total C 40 40	0
17	M	1	Total C 40 40	0
17	a	1	Total C 40 40	0
17	a	1	Total C 40 40	0
17	a	1	Total C 40 40	0
17	a	1	Total C 40 40	0
17	a	1	Total C 40 40	0
17	a	1	Total C 40 40	0
17	b	1	Total C 40 40	0
17	b	1	Total C 40 40	0
17	b	1	Total C 40 40	0
17	b	1	Total C 40 40	0
17	b	1	Total C 40 40	0
17	b	1	Total C 40 40	0
17	f	1	Total C 40 40	0

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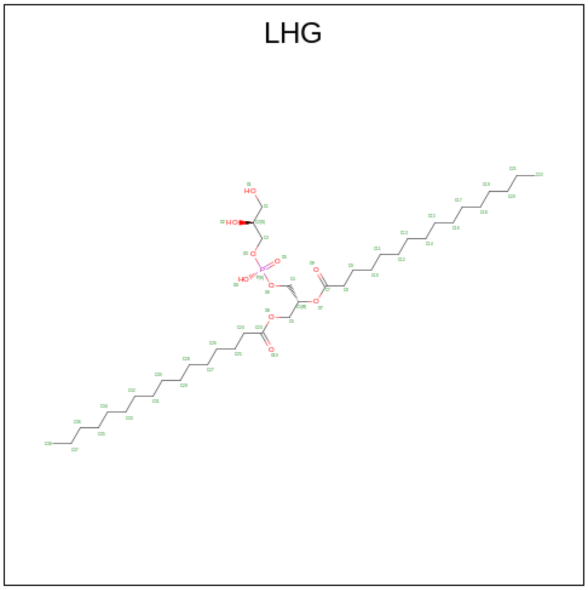
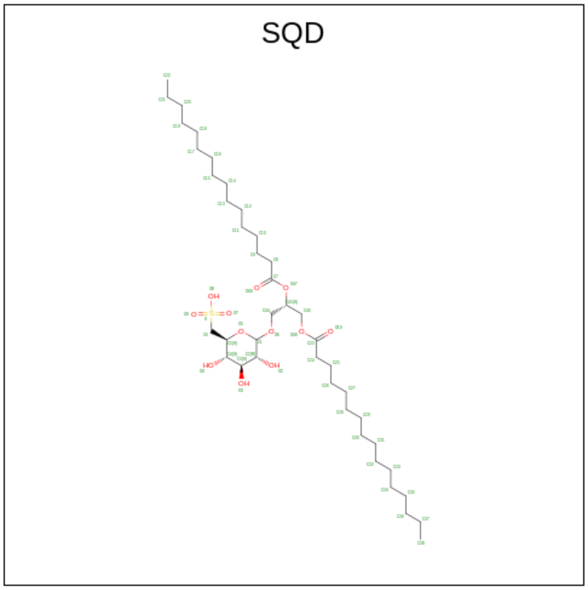
Mol	Chain	Residues	Atoms	AltConf
17	f	1	Total C 40 40	0
17	j	1	Total C 40 40	0
17	j	1	Total C 40 40	0
17	j	1	Total C 40 40	0
17	k	1	Total C 40 40	0
17	i	1	Total C 40 40	0
17	i	1	Total C 40 40	0
17	l	1	Total C 40 40	0
17	l	1	Total C 40 40	0
17	l	1	Total C 40 40	0
17	m	1	Total C 40 40	0

- Molecule 18 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$) (labeled as "Ligand of Interest" by depositor).



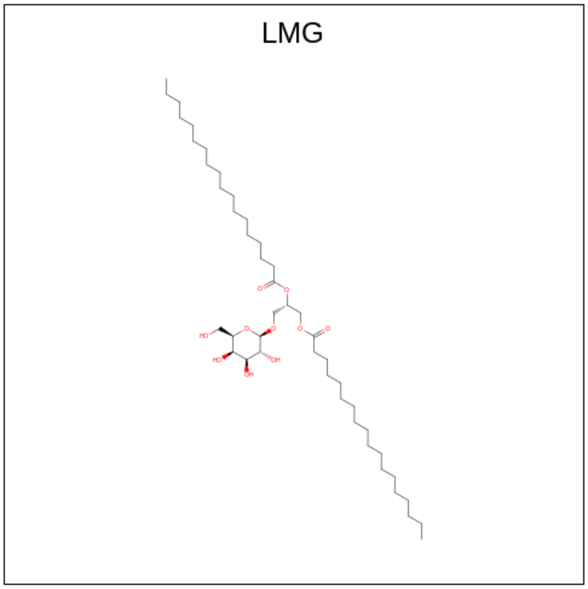
Mol	Chain	Residues	Atoms	AltConf
18	A	1	Total C O P 49 38 10 1	0
18	A	1	Total C O P 49 38 10 1	0
18	F	1	Total C O P 43 32 10 1	0
18	a	1	Total C O P 49 38 10 1	0
18	a	1	Total C O P 49 38 10 1	0
18	i	1	Total C O P 43 32 10 1	0

- Molecule 19 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: $C_{41}H_{78}O_{12}S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
19	X	1	Total C O S 54 41 12 1	0
19	x	1	Total C O S 54 41 12 1	0
19	b	1	Total C O S 54 41 12 1	0
19	l	1	Total C O S 54 41 12 1	0

- Molecule 20 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$) (labeled as "Ligand of Interest" by depositor).

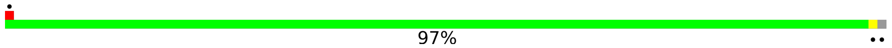


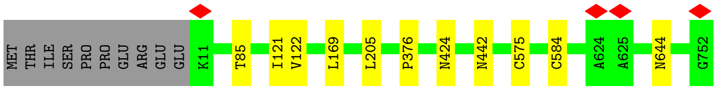
Mol	Chain	Residues	Atoms	AltConf
20	B	1	Total C O 35 25 10	0
20	B	1	Total C O 55 45 10	0
20	b	1	Total C O 55 45 10	0

3 Residue-property plots ⓘ

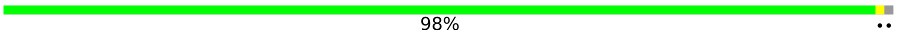
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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.

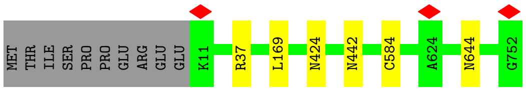
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

Chain A:




- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

Chain a:


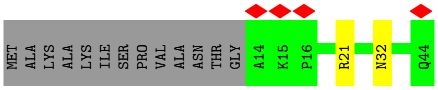


- Molecule 2: Photosystem I 4.8 kDa protein

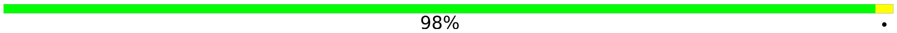
Chain X:

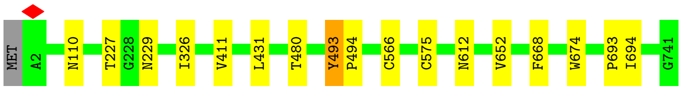

- Molecule 2: Photosystem I 4.8 kDa protein

Chain x:

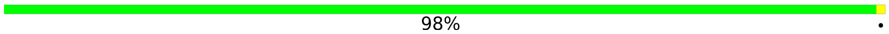
- Molecule 3: Photosystem I P700 chlorophyll a apoprotein A2 1

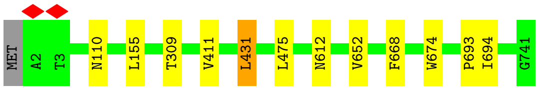
Chain B:




- Molecule 3: Photosystem I P700 chlorophyll a apoprotein A2 1

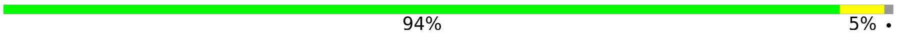
Chain b:

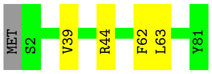




- Molecule 4: Photosystem I iron-sulfur center

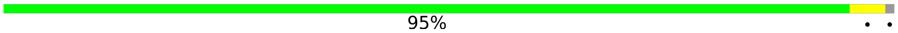
Chain C:

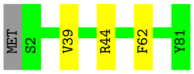




- Molecule 4: Photosystem I iron-sulfur center

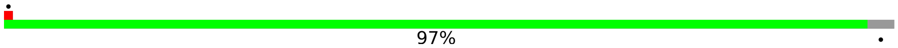
Chain c:

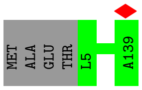




- Molecule 5: Photosystem I reaction center subunit II

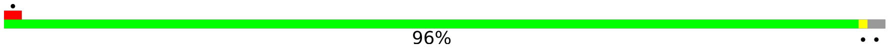
Chain D:

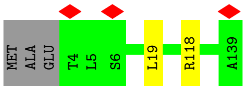




- Molecule 5: Photosystem I reaction center subunit II

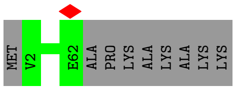
Chain d:





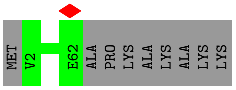
- Molecule 6: Photosystem I reaction center subunit IV

Chain E:



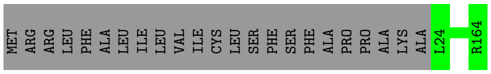
- Molecule 6: Photosystem I reaction center subunit IV

Chain e:



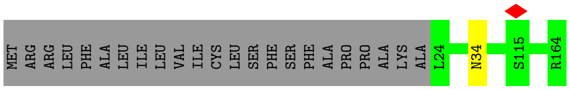
- Molecule 7: Photosystem I reaction center subunit III

Chain F:

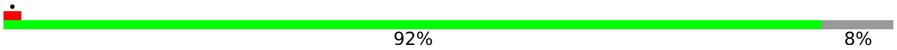



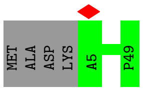
- Molecule 7: Photosystem I reaction center subunit III

Chain f:

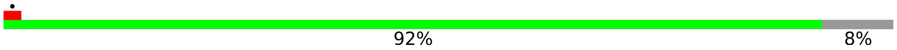



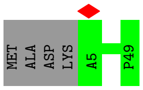
- Molecule 8: Photosystem I reaction center subunit IX

Chain J:




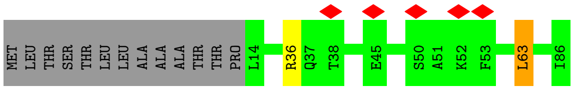
- Molecule 8: Photosystem I reaction center subunit IX

Chain j:




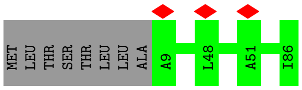
- Molecule 9: Photosystem I reaction center subunit PsaK 1

Chain K:

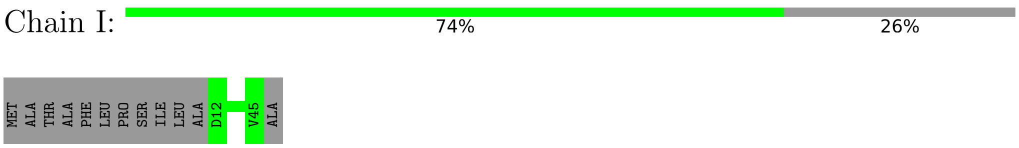



- Molecule 9: Photosystem I reaction center subunit PsaK 1

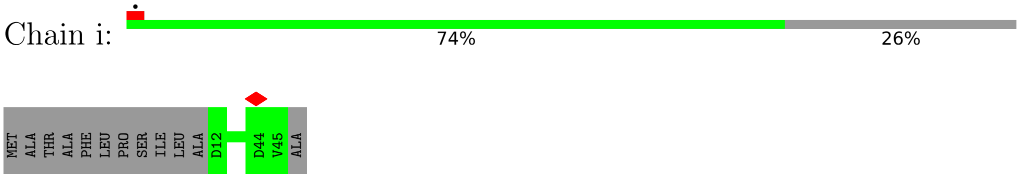
Chain k:

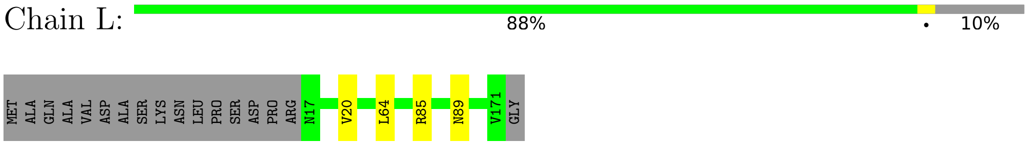
- Molecule 10: Photosystem I reaction center subunit VIII



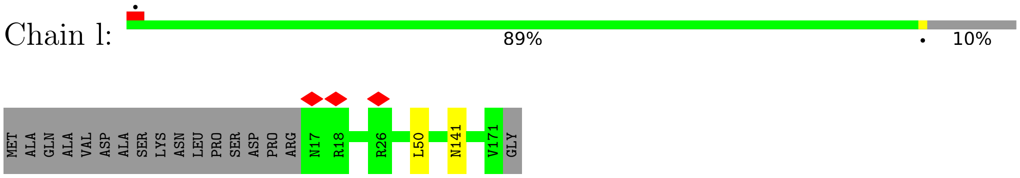
- Molecule 10: Photosystem I reaction center subunit VIII



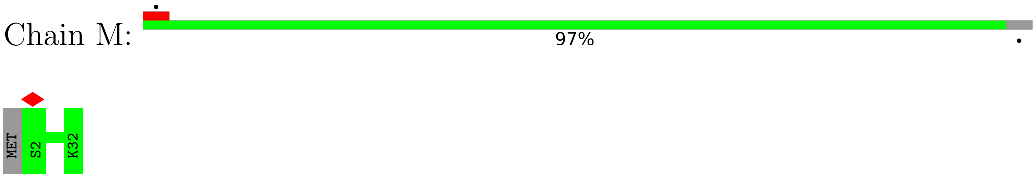
- Molecule 11: Photosystem I reaction center subunit XI



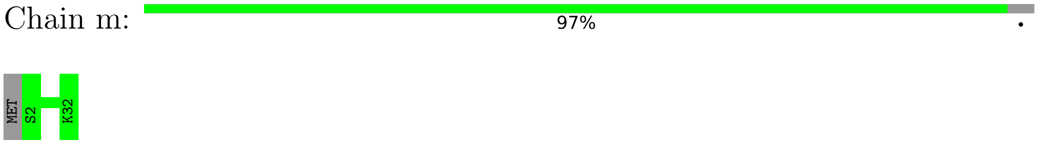
- Molecule 11: Photosystem I reaction center subunit XI



- Molecule 12: Photosystem I reaction center subunit XII



- Molecule 12: Photosystem I reaction center subunit XII



4 Experimental information ⓘ

Property	**Value**	**Source**
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	71600	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^{-}/\text{Å}^{2})$	58	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	0.173	Depositor
Minimum map value	-0.073	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.019	Depositor
Map size (Å)	420.80002, 420.80002, 420.80002	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.052, 1.052, 1.052	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CLA, LHG, LMG, CL0, PQN, SF4, SQD, BCR

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.49	1/6022 (0.0%)	0.59	3/8214 (0.0%)
1	a	0.50	0/6022	0.58	1/8214 (0.0%)
2	X	0.41	0/267	0.54	0/366
2	x	0.34	0/267	0.48	0/366
3	B	0.54	2/6142 (0.0%)	0.71	5/8396 (0.1%)
3	b	0.54	2/6142 (0.0%)	0.62	4/8396 (0.0%)
4	C	0.52	0/608	0.68	0/825
4	c	0.55	0/608	0.65	0/825
5	D	0.45	0/1064	0.62	0/1436
5	d	0.45	0/1071	0.62	1/1446 (0.1%)
6	E	0.43	0/499	0.48	0/677
6	e	0.41	0/499	0.46	0/677
7	F	0.38	0/1104	0.57	0/1500
7	f	0.40	0/1104	0.54	0/1500
8	J	0.38	0/371	0.52	0/509
8	j	0.36	0/371	0.51	0/509
9	K	0.35	0/551	0.67	1/750 (0.1%)
9	k	0.41	0/583	0.58	0/796
10	I	0.43	0/284	0.54	0/388
10	i	0.53	0/284	0.59	0/388
11	L	0.48	0/1198	0.64	1/1642 (0.1%)
11	l	0.50	0/1198	0.60	0/1642
12	M	0.44	0/245	0.57	0/334
12	m	0.46	0/245	0.59	0/334
All	All	0.49	5/36749 (0.0%)	0.61	16/50130 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
3	B	0	4
3	b	0	2
4	c	0	1
All	All	0	8

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	411	VAL	CB-CG1	-8.36	1.35	1.52
3	B	652	VAL	CB-CG2	-6.76	1.38	1.52
3	b	411	VAL	CB-CG1	-6.03	1.40	1.52
3	b	652	VAL	CB-CG2	-5.68	1.41	1.52
1	A	376	PRO	C-N	-5.04	1.22	1.34

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	493	TYR	C-N-CD	-20.83	74.77	120.60
3	B	493	TYR	C-N-CA	13.79	179.94	122.00
3	b	431	LEU	CA-CB-CG	7.55	132.66	115.30
5	d	19	LEU	CA-CB-CG	7.06	131.54	115.30
3	b	155	LEU	CA-CB-CG	6.75	130.83	115.30

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	121	ILE	Peptide
3	B	480	THR	Peptide
3	B	493	TYR	Peptide
3	B	674	TRP	Peptide
3	B	693	PRO	Peptide

5.2 Too-close contacts ⓘ

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	740/752 (98%)	709 (96%)	30 (4%)	1 (0%)	51	67
1	a	740/752 (98%)	710 (96%)	30 (4%)	0	100	100
2	X	29/44 (66%)	28 (97%)	1 (3%)	0	100	100
2	x	29/44 (66%)	28 (97%)	1 (3%)	0	100	100
3	B	738/741 (100%)	715 (97%)	21 (3%)	2 (0%)	41	53
3	b	738/741 (100%)	721 (98%)	16 (2%)	1 (0%)	51	67
4	C	78/81 (96%)	73 (94%)	3 (4%)	2 (3%)	5	4
4	c	78/81 (96%)	72 (92%)	6 (8%)	0	100	100
5	D	133/139 (96%)	130 (98%)	3 (2%)	0	100	100
5	d	134/139 (96%)	131 (98%)	3 (2%)	0	100	100
6	E	59/70 (84%)	57 (97%)	2 (3%)	0	100	100
6	e	59/70 (84%)	57 (97%)	2 (3%)	0	100	100
7	F	139/164 (85%)	131 (94%)	8 (6%)	0	100	100
7	f	139/164 (85%)	135 (97%)	4 (3%)	0	100	100
8	J	43/49 (88%)	43 (100%)	0	0	100	100
8	j	43/49 (88%)	43 (100%)	0	0	100	100
9	K	71/86 (83%)	69 (97%)	2 (3%)	0	100	100
9	k	76/86 (88%)	74 (97%)	2 (3%)	0	100	100
10	I	32/46 (70%)	31 (97%)	1 (3%)	0	100	100
10	i	32/46 (70%)	31 (97%)	1 (3%)	0	100	100
11	L	153/172 (89%)	152 (99%)	1 (1%)	0	100	100
11	l	153/172 (89%)	151 (99%)	2 (1%)	0	100	100
12	M	29/32 (91%)	28 (97%)	1 (3%)	0	100	100
12	m	29/32 (91%)	28 (97%)	1 (3%)	0	100	100
All	All	4494/4752 (95%)	4347 (97%)	141 (3%)	6 (0%)	54	67

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	122	VAL
3	B	494	PRO
3	B	694	ILE
3	b	694	ILE
4	C	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	A	595/605 (98%)	590 (99%)	5 (1%)	81	91
1	a	595/605 (98%)	590 (99%)	5 (1%)	81	91
2	X	25/34 (74%)	24 (96%)	1 (4%)	31	47
2	x	25/34 (74%)	23 (92%)	2 (8%)	12	17
3	B	600/602 (100%)	594 (99%)	6 (1%)	76	87
3	b	600/602 (100%)	596 (99%)	4 (1%)	84	92
4	C	67/69 (97%)	65 (97%)	2 (3%)	41	59
4	c	67/69 (97%)	65 (97%)	2 (3%)	41	59
5	D	107/110 (97%)	107 (100%)	0	100	100
5	d	108/110 (98%)	107 (99%)	1 (1%)	78	89
6	E	54/60 (90%)	54 (100%)	0	100	100
6	e	54/60 (90%)	54 (100%)	0	100	100
7	F	110/129 (85%)	110 (100%)	0	100	100
7	f	110/129 (85%)	109 (99%)	1 (1%)	78	89
8	J	39/42 (93%)	39 (100%)	0	100	100
8	j	39/42 (93%)	39 (100%)	0	100	100
9	K	54/64 (84%)	52 (96%)	2 (4%)	34	50
9	k	57/64 (89%)	57 (100%)	0	100	100
10	I	31/39 (80%)	31 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	i	31/39 (80%)	31 (100%)	0	100	100
11	L	118/131 (90%)	115 (98%)	3 (2%)	47	65
11	l	118/131 (90%)	116 (98%)	2 (2%)	60	76
12	M	26/27 (96%)	26 (100%)	0	100	100
12	m	26/27 (96%)	26 (100%)	0	100	100
All	All	3656/3824 (96%)	3620 (99%)	36 (1%)	77	87

5 of 36 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	b	431	LEU
11	l	141	ASN
3	b	612	ASN
5	d	118	ARG
4	C	39	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 69 such sidechains are listed below:

Mol	Chain	Res	Type
3	b	612	ASN
3	b	640	ASN
7	f	46	ASN
3	B	689	HIS
3	B	679	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

259 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$\|Z\| > 2$	Counts	RMSZ	#$\|Z\| > 2$
14	CLA	a	807	-	65,73,73	1.45	9 (13%)	76,113,113	1.54	10 (13%)
14	CLA	K	102	-	49,57,73	1.65	6 (12%)	55,93,113	1.69	8 (14%)
14	CLA	a	836	-	51,59,73	1.54	9 (17%)	59,96,113	1.71	11 (18%)
14	CLA	B	826	-	65,73,73	1.37	6 (9%)	76,113,113	1.60	10 (13%)
14	CLA	b	827	3	65,73,73	1.36	8 (12%)	76,113,113	1.55	12 (15%)
17	BCR	j	105	-	41,41,41	1.17	2 (4%)	56,56,56	1.32	7 (12%)
14	CLA	b	815	-	54,62,73	1.61	7 (12%)	62,99,113	1.70	10 (16%)
14	CLA	A	843	18	45,53,73	1.73	8 (17%)	52,89,113	1.73	9 (17%)
14	CLA	b	804	-	65,73,73	1.47	8 (12%)	76,113,113	1.53	10 (13%)
14	CLA	m	1201	3	55,63,73	1.53	9 (16%)	64,101,113	1.60	9 (14%)
14	CLA	b	831	-	65,73,73	1.31	9 (13%)	76,113,113	1.48	5 (6%)
17	BCR	i	102	-	41,41,41	1.20	3 (7%)	56,56,56	1.32	8 (14%)
14	CLA	A	835	1	54,62,73	1.61	8 (14%)	62,99,113	1.54	8 (12%)
14	CLA	a	827	-	65,73,73	1.36	6 (9%)	76,113,113	1.63	11 (14%)
14	CLA	B	823	3	45,53,73	1.68	9 (20%)	52,89,113	1.99	14 (26%)
14	CLA	a	830	1	54,62,73	1.53	9 (16%)	62,99,113	1.43	9 (14%)
14	CLA	A	821	-	65,73,73	1.56	7 (10%)	76,113,113	1.35	10 (13%)
14	CLA	A	841	1	65,73,73	1.44	9 (13%)	76,113,113	1.48	10 (13%)
14	CLA	F	204	-	45,53,73	1.74	7 (15%)	52,89,113	1.64	10 (19%)
14	CLA	a	832	1	65,73,73	1.36	7 (10%)	76,113,113	1.54	11 (14%)
17	BCR	B	848	-	41,41,41	1.09	3 (7%)	56,56,56	1.30	5 (8%)
17	BCR	a	847	-	41,41,41	1.12	2 (4%)	56,56,56	1.26	6 (10%)
14	CLA	a	837	1	65,73,73	1.38	10 (15%)	76,113,113	1.69	11 (14%)
14	CLA	j	102	-	45,53,73	1.72	7 (15%)	52,89,113	1.67	7 (13%)
14	CLA	B	838	-	45,53,73	1.83	8 (17%)	52,89,113	1.57	9 (17%)
14	CLA	b	813	-	60,68,73	1.58	9 (15%)	70,107,113	1.49	13 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
17	BCR	a	846	-	41,41,41	1.13	2 (4%)	56,56,56	1.45	9 (16%)
14	CLA	B	829	3	65,73,73	1.50	7 (10%)	76,113,113	1.69	10 (13%)
17	BCR	B	847	-	41,41,41	1.12	2 (4%)	56,56,56	1.34	9 (16%)
14	CLA	A	815	-	45,53,73	1.66	7 (15%)	52,89,113	1.92	6 (11%)
14	CLA	B	819	-	45,53,73	1.70	8 (17%)	52,89,113	1.62	9 (17%)
14	CLA	B	807	3	55,63,73	1.50	7 (12%)	64,101,113	1.61	8 (12%)
14	CLA	a	816	-	59,67,73	1.49	10 (16%)	68,105,113	1.57	11 (16%)
17	BCR	B	846	-	41,41,41	1.10	3 (7%)	56,56,56	1.33	9 (16%)
14	CLA	b	824	3	45,53,73	1.69	7 (15%)	52,89,113	1.68	7 (13%)
17	BCR	K	103	-	41,41,41	1.10	2 (4%)	56,56,56	1.32	8 (14%)
14	CLA	A	837	-	51,59,73	1.49	7 (13%)	59,96,113	1.89	10 (16%)
14	CLA	a	804	1	65,73,73	1.37	7 (10%)	76,113,113	1.67	14 (18%)
14	CLA	B	815	3	54,62,73	1.58	7 (12%)	62,99,113	1.57	9 (14%)
14	CLA	a	806	-	60,68,73	1.50	10 (16%)	70,107,113	1.49	9 (12%)
14	CLA	j	101	-	58,66,73	1.55	9 (15%)	67,104,113	1.59	10 (14%)
15	PQN	a	842	-	34,34,34	1.47	2 (5%)	42,45,45	1.27	5 (11%)
14	CLA	a	826	-	65,73,73	1.39	9 (13%)	76,113,113	1.59	8 (10%)
14	CLA	B	814	3	54,62,73	1.48	7 (12%)	62,99,113	1.81	11 (17%)
14	CLA	B	836	3	54,62,73	1.43	7 (12%)	62,99,113	1.83	12 (19%)
14	CLA	a	811	-	59,67,73	1.53	7 (11%)	68,105,113	1.50	8 (11%)
14	CLA	A	810	1	45,53,73	1.70	7 (15%)	52,89,113	1.73	7 (13%)
14	CLA	b	838	-	45,53,73	1.74	7 (15%)	52,89,113	1.60	6 (11%)
17	BCR	b	847	-	41,41,41	1.17	3 (7%)	56,56,56	1.41	10 (17%)
14	CLA	B	832	3	65,73,73	1.57	10 (15%)	76,113,113	1.76	11 (14%)
14	CLA	A	816	-	45,53,73	1.73	7 (15%)	52,89,113	1.72	8 (15%)
14	CLA	A	818	1	60,68,73	1.54	10 (16%)	70,107,113	1.46	7 (10%)
14	CLA	B	825	-	55,63,73	1.54	6 (10%)	64,101,113	1.64	7 (10%)
19	SQD	b	801	-	53,54,54	0.97	6 (11%)	62,65,65	1.73	11 (17%)
14	CLA	A	806	1	65,73,73	1.42	9 (13%)	76,113,113	1.58	10 (13%)
14	CLA	b	807	-	65,73,73	1.42	10 (15%)	76,113,113	1.91	12 (15%)
14	CLA	A	822	-	45,53,73	1.68	7 (15%)	52,89,113	1.69	8 (15%)
14	CLA	b	836	3	54,62,73	1.54	8 (14%)	62,99,113	1.78	13 (20%)
14	CLA	B	827	3	65,73,73	1.40	8 (12%)	76,113,113	1.72	13 (17%)
14	CLA	A	812	-	59,67,73	1.53	7 (11%)	68,105,113	1.47	7 (10%)
14	CLA	a	821	1	45,53,73	1.73	8 (17%)	52,89,113	1.80	11 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
17	BCR	B	849	-	41,41,41	1.21	6 (14%)	56,56,56	1.46	7 (12%)
14	CLA	A	813	-	60,68,73	1.52	9 (15%)	70,107,113	1.53	12 (17%)
14	CLA	B	812	-	65,73,73	1.39	8 (12%)	76,113,113	1.69	13 (17%)
14	CLA	B	805	-	65,73,73	1.36	8 (12%)	76,113,113	1.47	6 (7%)
14	CLA	b	803	-	65,73,73	1.44	10 (15%)	76,113,113	1.58	13 (17%)
14	CLA	b	832	3	65,73,73	1.51	9 (13%)	76,113,113	1.71	15 (19%)
17	BCR	k	103	-	41,41,41	1.06	2 (4%)	56,56,56	1.30	7 (12%)
14	CLA	j	103	-	38,45,73	1.86	9 (23%)	43,78,113	1.69	7 (16%)
17	BCR	A	850	-	41,41,41	1.15	3 (7%)	56,56,56	1.25	7 (12%)
14	CLA	b	837	-	45,53,73	1.70	7 (15%)	52,89,113	1.79	10 (19%)
14	CLA	a	815	-	45,53,73	1.73	7 (15%)	52,89,113	1.75	6 (11%)
17	BCR	J	103	-	41,41,41	1.13	3 (7%)	56,56,56	1.28	6 (10%)
14	CLA	a	819	-	54,62,73	1.58	7 (12%)	62,99,113	1.66	8 (12%)
14	CLA	L	1502	11	60,68,73	1.45	8 (13%)	70,107,113	1.67	10 (14%)
14	CLA	a	802	1	65,73,73	1.42	7 (10%)	76,113,113	1.53	8 (10%)
14	CLA	f	203	-	45,53,73	1.72	8 (17%)	52,89,113	1.69	6 (11%)
14	CLA	B	833	3	54,62,73	1.57	8 (14%)	62,99,113	1.51	7 (11%)
17	BCR	F	205	-	41,41,41	1.12	2 (4%)	56,56,56	1.28	7 (12%)
17	BCR	A	848	-	41,41,41	1.13	1 (2%)	56,56,56	1.46	9 (16%)
14	CLA	A	825	-	65,73,73	1.38	8 (12%)	76,113,113	1.55	9 (11%)
14	CLA	l	205	-	45,53,73	1.68	7 (15%)	52,89,113	1.92	9 (17%)
14	CLA	B	811	3	65,73,73	1.47	10 (15%)	76,113,113	1.86	14 (18%)
17	BCR	b	850	-	41,41,41	1.10	3 (7%)	56,56,56	1.10	3 (5%)
14	CLA	x	1701	2	49,57,73	1.66	8 (16%)	55,93,113	1.54	6 (10%)
17	BCR	f	202	-	41,41,41	1.20	3 (7%)	56,56,56	1.25	5 (8%)
14	CLA	B	834	-	60,68,73	1.43	7 (11%)	70,107,113	1.61	6 (8%)
14	CLA	A	830	1	65,73,73	1.57	9 (13%)	76,113,113	1.72	10 (13%)
17	BCR	A	847	-	41,41,41	1.09	3 (7%)	56,56,56	1.28	6 (10%)
14	CLA	a	810	-	65,73,73	1.45	9 (13%)	76,113,113	1.59	9 (11%)
14	CLA	A	819	-	65,73,73	1.44	7 (10%)	76,113,113	1.65	10 (13%)
17	BCR	A	849	-	41,41,41	1.17	3 (7%)	56,56,56	1.44	8 (14%)
17	BCR	a	848	-	41,41,41	1.16	2 (4%)	56,56,56	1.28	7 (12%)
14	CLA	A	805	1	65,73,73	1.36	7 (10%)	76,113,113	1.76	15 (19%)
14	CLA	a	818	-	65,73,73	1.36	7 (10%)	76,113,113	1.73	13 (17%)
14	CLA	b	811	-	65,73,73	1.42	11 (16%)	76,113,113	1.71	10 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
17	BCR	j	104	-	41,41,41	1.15	3 (7%)	56,56,56	1.33	7 (12%)
14	CLA	B	831	-	65,73,73	1.37	8 (12%)	76,113,113	1.48	6 (7%)
20	LMG	B	803	-	35,35,55	0.94	1 (2%)	43,43,63	1.24	4 (9%)
17	BCR	a	849	-	41,41,41	1.21	3 (7%)	56,56,56	1.29	4 (7%)
13	CL0	a	801	1	65,73,73	2.36	18 (27%)	76,113,113	2.61	22 (28%)
16	SF4	c	101	-	0,12,12	-	-	-		
14	CLA	A	802	-	65,73,73	1.47	9 (13%)	76,113,113	1.52	11 (14%)
14	CLA	b	821	3	65,73,73	1.35	9 (13%)	76,113,113	1.56	13 (17%)
14	CLA	J	101	-	45,53,73	1.73	8 (17%)	52,89,113	1.71	8 (15%)
14	CLA	B	806	-	65,73,73	1.46	8 (12%)	76,113,113	2.08	13 (17%)
14	CLA	A	836	1	45,53,73	1.68	7 (15%)	52,89,113	1.84	8 (15%)
14	CLA	a	812	-	60,68,73	1.54	9 (15%)	70,107,113	1.41	7 (10%)
15	PQN	b	844	-	34,34,34	1.41	2 (5%)	42,45,45	1.38	7 (16%)
14	CLA	a	823	1	45,53,73	1.64	6 (13%)	52,89,113	1.83	9 (17%)
14	CLA	B	804	-	65,73,73	1.39	7 (10%)	76,113,113	1.53	12 (15%)
14	CLA	b	841	3	47,55,73	1.65	9 (19%)	54,91,113	1.59	9 (16%)
14	CLA	B	813	-	60,68,73	1.52	9 (15%)	70,107,113	1.41	9 (12%)
14	CLA	L	1503	-	45,53,73	1.65	6 (13%)	52,89,113	1.88	9 (17%)
14	CLA	B	801	-	65,73,73	1.38	7 (10%)	76,113,113	1.71	11 (14%)
18	LHG	a	851	14	48,48,48	0.93	5 (10%)	51,54,54	0.98	2 (3%)
17	BCR	i	101	-	41,41,41	1.08	1 (2%)	56,56,56	1.43	9 (16%)
14	CLA	B	840	3	65,73,73	1.40	8 (12%)	76,113,113	1.60	12 (15%)
14	CLA	A	834	-	65,73,73	1.37	7 (10%)	76,113,113	1.69	14 (18%)
14	CLA	b	812	3	65,73,73	1.51	9 (13%)	76,113,113	1.65	10 (13%)
14	CLA	b	814	-	54,62,73	1.54	7 (12%)	62,99,113	1.66	9 (14%)
17	BCR	f	204	-	41,41,41	1.11	2 (4%)	56,56,56	1.31	8 (14%)
16	SF4	c	102	-	0,12,12	-	-	-		
14	CLA	a	813	-	54,62,73	1.55	7 (12%)	62,99,113	1.65	7 (11%)
14	CLA	A	823	1	54,62,73	1.52	7 (12%)	62,99,113	1.72	10 (16%)
14	CLA	J	102	-	38,45,73	1.87	7 (18%)	43,78,113	1.71	7 (16%)
14	CLA	B	837	-	45,53,73	1.68	7 (15%)	52,89,113	1.96	11 (21%)
14	CLA	a	834	1	54,62,73	1.59	9 (16%)	62,99,113	1.58	6 (9%)
14	CLA	A	817	-	59,67,73	1.56	8 (13%)	68,105,113	1.57	9 (13%)
14	CLA	B	810	3	65,73,73	1.31	7 (10%)	76,113,113	1.46	7 (9%)
14	CLA	a	825	-	54,62,73	1.54	7 (12%)	62,99,113	1.60	9 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\lvert Z\rvert > 2$	Counts	RMSZ	$\#\lvert Z\rvert > 2$
14	CLA	b	802	-	65,73,73	1.28	7 (10%)	76,113,113	1.67	7 (9%)
17	BCR	M	101	-	41,41,41	1.08	2 (4%)	56,56,56	1.32	9 (16%)
14	CLA	B	816	-	65,73,73	1.42	9 (13%)	76,113,113	1.48	8 (10%)
14	CLA	b	810	3	65,73,73	1.34	7 (10%)	76,113,113	1.57	9 (11%)
20	LMG	b	851	-	55,55,55	0.92	2 (3%)	63,63,63	1.49	11 (17%)
17	BCR	J	105	-	41,41,41	1.12	2 (4%)	56,56,56	1.33	9 (16%)
16	SF4	C	102	-	0,12,12	-	-	-		
14	CLA	a	803	-	54,62,73	1.56	6 (11%)	62,99,113	1.65	6 (9%)
14	CLA	b	842	-	65,73,73	1.44	6 (9%)	76,113,113	1.47	8 (10%)
14	CLA	b	818	-	49,57,73	1.62	9 (18%)	55,93,113	1.71	8 (14%)
14	CLA	B	817	-	50,58,73	1.57	7 (14%)	58,95,113	1.62	9 (15%)
14	CLA	A	804	-	54,62,73	1.55	8 (14%)	62,99,113	1.70	7 (11%)
17	BCR	F	203	-	41,41,41	1.17	2 (4%)	56,56,56	1.35	8 (14%)
16	SF4	a	843	-	0,12,12	-	-	-		
17	BCR	a	844	-	41,41,41	1.18	4 (9%)	56,56,56	1.32	8 (14%)
17	BCR	A	851	-	41,41,41	1.19	3 (7%)	56,56,56	1.22	4 (7%)
14	CLA	a	805	1	65,73,73	1.40	8 (12%)	76,113,113	1.53	8 (10%)
14	CLA	A	831	1	54,62,73	1.54	8 (14%)	62,99,113	1.62	10 (16%)
14	CLA	B	809	3	65,73,73	1.40	9 (13%)	76,113,113	1.59	10 (13%)
17	BCR	B	850	-	41,41,41	1.16	3 (7%)	56,56,56	1.19	3 (5%)
17	BCR	b	845	-	41,41,41	1.12	2 (4%)	56,56,56	1.17	3 (5%)
14	CLA	f	201	-	59,67,73	1.55	8 (13%)	68,105,113	1.35	7 (10%)
14	CLA	A	803	-	65,73,73	1.39	7 (10%)	76,113,113	1.62	8 (10%)
14	CLA	A	824	1	45,53,73	1.69	8 (17%)	52,89,113	1.70	8 (15%)
14	CLA	A	828	-	65,73,73	1.34	7 (10%)	76,113,113	1.64	11 (14%)
16	SF4	C	101	-	0,12,12	-	-	-		
18	LHG	i	103	-	42,42,48	0.64	0	45,48,54	1.26	6 (13%)
15	PQN	B	844	-	34,34,34	1.50	2 (5%)	42,45,45	1.26	4 (9%)
14	CLA	A	820	-	54,62,73	1.58	8 (14%)	62,99,113	1.61	10 (16%)
16	SF4	A	845	-	0,12,12	-	-	-		
14	CLA	A	814	1	54,62,73	1.55	7 (12%)	62,99,113	1.80	9 (14%)
14	CLA	b	809	3	65,73,73	1.37	8 (12%)	76,113,113	1.54	9 (11%)
14	CLA	a	817	-	60,68,73	1.56	10 (16%)	70,107,113	1.52	10 (14%)
13	CL0	A	801	-	65,73,73	2.35	18 (27%)	76,113,113	2.61	22 (28%)
14	CLA	b	829	-	65,73,73	1.42	8 (12%)	76,113,113	1.61	9 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	CLA	b	830	-	65,73,73	1.39	8 (12%)	76,113,113	1.49	10 (13%)
14	CLA	a	822	1	54,62,73	1.61	8 (14%)	62,99,113	1.47	12 (19%)
14	CLA	b	834	-	60,68,73	1.48	8 (13%)	70,107,113	1.54	8 (11%)
14	CLA	A	842	-	65,73,73	1.46	9 (13%)	76,113,113	1.66	10 (13%)
17	BCR	I	101	-	41,41,41	1.07	1 (2%)	56,56,56	1.30	8 (14%)
17	BCR	b	846	-	41,41,41	1.08	2 (4%)	56,56,56	1.26	7 (12%)
14	CLA	X	1701	2	49,57,73	1.63	8 (16%)	55,93,113	1.73	10 (18%)
14	CLA	A	809	1	65,73,73	1.42	6 (9%)	76,113,113	1.58	10 (13%)
14	CLA	a	829	-	65,73,73	1.50	9 (13%)	76,113,113	1.81	13 (17%)
18	LHG	F	201	-	42,42,48	0.73	1 (2%)	45,48,54	1.18	4 (8%)
20	LMG	B	851	-	55,55,55	0.91	2 (3%)	63,63,63	1.44	8 (12%)
17	BCR	m	1202	-	41,41,41	1.15	2 (4%)	56,56,56	1.31	10 (17%)
14	CLA	B	821	3	65,73,73	1.44	8 (12%)	76,113,113	1.36	7 (9%)
14	CLA	B	839	3	60,68,73	1.53	10 (16%)	70,107,113	1.45	11 (15%)
14	CLA	b	840	3	65,73,73	1.34	7 (10%)	76,113,113	1.61	10 (13%)
14	CLA	B	824	3	45,53,73	1.69	7 (15%)	52,89,113	1.74	8 (15%)
14	CLA	B	841	3	47,55,73	1.73	8 (17%)	54,91,113	1.57	8 (14%)
14	CLA	a	828	-	65,73,73	1.39	8 (12%)	76,113,113	1.53	8 (10%)
14	CLA	B	820	3	65,73,73	1.43	9 (13%)	76,113,113	1.54	7 (9%)
14	CLA	b	817	3	50,58,73	1.65	8 (16%)	58,95,113	1.69	8 (13%)
14	CLA	k	102	-	49,57,73	1.67	8 (16%)	55,93,113	1.74	10 (18%)
17	BCR	a	845	-	41,41,41	1.09	2 (4%)	56,56,56	1.28	3 (5%)
18	LHG	A	853	14	48,48,48	0.77	2 (4%)	51,54,54	1.21	6 (11%)
14	CLA	l	203	11	45,53,73	1.68	7 (15%)	52,89,113	1.93	11 (21%)
17	BCR	L	1504	-	41,41,41	1.07	3 (7%)	56,56,56	1.32	7 (12%)
14	CLA	a	820	-	65,73,73	1.45	7 (10%)	76,113,113	1.64	10 (13%)
17	BCR	l	207	-	41,41,41	1.11	2 (4%)	56,56,56	1.44	7 (12%)
14	CLA	B	843	3	65,73,73	1.39	9 (13%)	76,113,113	1.63	14 (18%)
14	CLA	a	814	-	45,53,73	1.69	7 (15%)	52,89,113	1.86	7 (13%)
14	CLA	a	824	-	65,73,73	1.39	6 (9%)	76,113,113	1.65	10 (13%)
14	CLA	b	823	3	45,53,73	1.72	9 (20%)	52,89,113	1.64	7 (13%)
19	SQD	l	202	-	53,54,54	0.97	6 (11%)	62,65,65	2.03	14 (22%)
14	CLA	B	802	1	65,73,73	1.40	9 (13%)	76,113,113	1.48	9 (11%)
17	BCR	b	848	-	41,41,41	1.15	2 (4%)	56,56,56	1.45	5 (8%)
14	CLA	b	816	-	65,73,73	1.45	8 (12%)	76,113,113	1.50	10 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
19	SQD	x	1702	-	53,54,54	0.97	5 (9%)	62,65,65	1.76	9 (14%)
14	CLA	A	838	1	65,73,73	1.35	7 (10%)	76,113,113	1.62	10 (13%)
14	CLA	b	833	-	54,62,73	1.61	10 (18%)	62,99,113	1.53	7 (11%)
14	CLA	b	820	-	65,73,73	1.44	10 (15%)	76,113,113	1.43	8 (10%)
14	CLA	A	829	-	65,73,73	1.36	8 (12%)	76,113,113	1.61	13 (17%)
17	BCR	l	206	-	41,41,41	1.09	1 (2%)	56,56,56	1.56	12 (21%)
14	CLA	L	1501	11	51,59,73	1.76	9 (17%)	59,96,113	1.60	10 (16%)
14	CLA	b	806	3	65,73,73	1.39	9 (13%)	76,113,113	1.54	8 (10%)
15	PQN	A	844	-	34,34,34	1.50	2 (5%)	42,45,45	1.08	4 (9%)
14	CLA	B	842	-	65,73,73	1.38	7 (10%)	76,113,113	1.49	9 (11%)
14	CLA	B	818	3	49,57,73	1.52	7 (14%)	55,93,113	1.69	9 (16%)
14	CLA	a	835	1	45,53,73	1.69	7 (15%)	52,89,113	1.73	7 (13%)
14	CLA	a	839	1	65,73,73	1.40	9 (13%)	76,113,113	1.49	8 (10%)
14	CLA	b	819	-	45,53,73	1.67	7 (15%)	52,89,113	1.80	8 (15%)
14	CLA	b	826	-	65,73,73	1.35	6 (9%)	76,113,113	1.56	10 (13%)
17	BCR	I	102	-	41,41,41	1.20	4 (9%)	56,56,56	1.46	8 (14%)
17	BCR	A	846	-	41,41,41	1.17	2 (4%)	56,56,56	1.27	7 (12%)
14	CLA	B	830	3	65,73,73	1.46	8 (12%)	76,113,113	1.54	11 (14%)
14	CLA	k	101	-	42,49,73	1.78	7 (16%)	48,83,113	1.62	5 (10%)
18	LHG	A	852	-	48,48,48	0.83	3 (6%)	51,54,54	1.33	7 (13%)
14	CLA	A	808	1	65,73,73	1.38	7 (10%)	76,113,113	1.57	10 (13%)
14	CLA	A	833	1	65,73,73	1.45	8 (12%)	76,113,113	1.46	9 (11%)
14	CLA	A	839	-	65,73,73	1.41	8 (12%)	76,113,113	1.51	10 (13%)
14	CLA	B	828	-	65,73,73	1.37	5 (7%)	76,113,113	1.74	19 (25%)
18	LHG	a	850	-	48,48,48	0.76	1 (2%)	51,54,54	1.33	6 (11%)
14	CLA	A	832	1	65,73,73	1.38	8 (12%)	76,113,113	1.62	7 (9%)
17	BCR	B	845	-	41,41,41	1.12	3 (7%)	56,56,56	1.25	6 (10%)
14	CLA	a	831	1	65,73,73	1.42	9 (13%)	76,113,113	1.57	11 (14%)
17	BCR	l	201	-	41,41,41	1.07	2 (4%)	56,56,56	1.30	8 (14%)
14	CLA	b	808	-	65,73,73	1.36	10 (15%)	76,113,113	1.76	11 (14%)
14	CLA	b	825	-	55,63,73	1.54	7 (12%)	64,101,113	1.57	7 (10%)
14	CLA	A	827	1	65,73,73	1.42	6 (9%)	76,113,113	1.52	7 (9%)
14	CLA	a	841	18	45,53,73	1.61	7 (15%)	52,89,113	4.16	9 (17%)
17	BCR	J	104	-	41,41,41	1.18	3 (7%)	56,56,56	1.39	9 (16%)
14	CLA	B	835	-	58,66,73	1.52	9 (15%)	67,104,113	1.51	7 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
14	CLA	l	204	11	60,68,73	1.46	8 (13%)	70,107,113	1.64	9 (12%)
17	BCR	b	849	-	41,41,41	1.21	4 (9%)	56,56,56	1.42	8 (14%)
14	CLA	a	840	1	65,73,73	1.47	9 (13%)	76,113,113	1.52	8 (10%)
14	CLA	b	805	-	65,73,73	1.43	7 (10%)	76,113,113	1.57	11 (14%)
14	CLA	a	809	1	45,53,73	1.68	7 (15%)	52,89,113	1.80	5 (9%)
14	CLA	K	101	-	42,49,73	1.77	7 (16%)	48,83,113	1.55	7 (14%)
14	CLA	b	843	3	65,73,73	1.47	9 (13%)	76,113,113	1.94	15 (19%)
17	BCR	j	106	-	41,41,41	1.15	2 (4%)	56,56,56	1.37	6 (10%)
14	CLA	B	808	-	65,73,73	1.51	10 (15%)	76,113,113	2.02	20 (26%)
14	CLA	A	840	-	59,67,73	1.50	9 (15%)	68,105,113	1.35	7 (10%)
14	CLA	B	822	-	65,73,73	1.43	7 (10%)	76,113,113	1.55	8 (10%)
14	CLA	a	838	-	65,73,73	1.43	8 (12%)	76,113,113	1.40	7 (9%)
14	CLA	b	835	3	65,73,73	1.48	8 (12%)	76,113,113	1.37	11 (14%)
14	CLA	b	839	-	60,68,73	1.56	9 (15%)	70,107,113	1.47	11 (15%)
14	CLA	A	807	-	60,68,73	1.51	8 (13%)	70,107,113	5.15	11 (15%)
19	SQD	X	1702	-	53,54,54	0.98	5 (9%)	62,65,65	1.74	12 (19%)
14	CLA	A	826	-	54,62,73	1.51	7 (12%)	62,99,113	1.68	12 (19%)
14	CLA	b	822	-	65,73,73	1.49	7 (10%)	76,113,113	1.64	9 (11%)
14	CLA	A	811	-	65,73,73	1.50	8 (12%)	76,113,113	1.66	12 (15%)
14	CLA	a	808	1	65,73,73	1.41	8 (12%)	76,113,113	1.59	10 (13%)
14	CLA	a	833	1	65,73,73	1.44	7 (10%)	76,113,113	1.83	17 (22%)
14	CLA	F	202	3	65,73,73	1.46	7 (10%)	76,113,113	1.52	9 (11%)
14	CLA	b	828	-	65,73,73	1.40	5 (7%)	76,113,113	1.74	14 (18%)

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
14	CLA	a	807	-	1/1/15/20	20/37/115/115	-
14	CLA	K	102	-	1/1/11/20	2/18/96/115	-
14	CLA	a	836	-	1/1/12/20	8/21/99/115	-
14	CLA	B	826	-	1/1/15/20	9/37/115/115	-
14	CLA	b	827	3	-	13/37/115/115	-
17	BCR	j	105	-	-	11/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	b	815	-	1/1/12/20	9/24/102/115	-
14	CLA	A	843	18	1/1/11/20	7/13/91/115	-
14	CLA	b	804	-	1/1/15/20	21/37/115/115	-
14	CLA	m	1201	3	1/1/13/20	9/25/103/115	-
14	CLA	b	831	-	1/1/15/20	12/37/115/115	-
17	BCR	i	102	-	-	12/29/63/63	0/2/2/2
14	CLA	A	835	1	1/1/12/20	8/24/102/115	-
14	CLA	a	827	-	1/1/15/20	9/37/115/115	-
14	CLA	B	823	3	1/1/11/20	7/13/91/115	-
14	CLA	a	830	1	1/1/12/20	7/24/102/115	-
14	CLA	A	821	-	1/1/15/20	12/37/115/115	-
14	CLA	A	841	1	1/1/15/20	21/37/115/115	-
14	CLA	F	204	-	1/1/11/20	1/13/91/115	-
14	CLA	a	832	1	1/1/15/20	8/37/115/115	-
17	BCR	B	848	-	-	12/29/63/63	0/2/2/2
17	BCR	a	847	-	-	17/29/63/63	0/2/2/2
14	CLA	a	837	1	1/1/15/20	16/37/115/115	-
14	CLA	j	102	-	1/1/11/20	9/13/91/115	-
14	CLA	B	838	-	1/1/11/20	6/13/91/115	-
14	CLA	b	813	-	1/1/14/20	16/31/109/115	-
17	BCR	a	846	-	-	15/29/63/63	0/2/2/2
14	CLA	B	829	3	1/1/15/20	10/37/115/115	-
17	BCR	B	847	-	-	13/29/63/63	0/2/2/2
14	CLA	A	815	-	1/1/11/20	3/13/91/115	-
14	CLA	B	819	-	1/1/11/20	1/13/91/115	-
14	CLA	B	807	3	1/1/13/20	6/25/103/115	-
14	CLA	a	816	-	1/1/13/20	9/30/108/115	-
17	BCR	B	846	-	-	9/29/63/63	0/2/2/2
14	CLA	b	824	3	1/1/11/20	2/13/91/115	-
17	BCR	K	103	-	-	12/29/63/63	0/2/2/2
14	CLA	A	837	-	1/1/12/20	11/21/99/115	-
14	CLA	a	804	1	1/1/15/20	17/37/115/115	-
14	CLA	B	815	3	1/1/12/20	5/24/102/115	-
14	CLA	a	806	-	1/1/14/20	8/31/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	j	101	-	1/1/13/20	10/29/107/115	-
15	PQN	a	842	-	-	5/23/43/43	0/2/2/2
14	CLA	a	826	-	-	7/37/115/115	-
14	CLA	B	814	3	1/1/12/20	9/24/102/115	-
14	CLA	B	836	3	1/1/12/20	11/24/102/115	-
14	CLA	a	811	-	1/1/13/20	11/30/108/115	-
14	CLA	A	810	1	1/1/11/20	3/13/91/115	-
14	CLA	b	838	-	1/1/11/20	5/13/91/115	-
17	BCR	b	847	-	-	10/29/63/63	0/2/2/2
14	CLA	B	832	3	1/1/15/20	9/37/115/115	-
14	CLA	A	816	-	1/1/11/20	0/13/91/115	-
14	CLA	A	818	1	1/1/14/20	8/31/109/115	-
14	CLA	B	825	-	1/1/13/20	11/25/103/115	-
19	SQD	b	801	-	-	22/49/69/69	0/1/1/1
14	CLA	A	806	1	1/1/15/20	14/37/115/115	-
14	CLA	b	807	-	1/1/15/20	12/37/115/115	-
14	CLA	A	822	-	1/1/11/20	6/13/91/115	-
14	CLA	b	836	3	1/1/12/20	8/24/102/115	-
14	CLA	B	827	3	1/1/15/20	7/37/115/115	-
14	CLA	A	812	-	1/1/13/20	7/30/108/115	-
14	CLA	a	821	1	1/1/11/20	4/13/91/115	-
17	BCR	B	849	-	-	12/29/63/63	0/2/2/2
14	CLA	A	813	-	1/1/14/20	14/31/109/115	-
14	CLA	B	812	-	1/1/15/20	13/37/115/115	-
14	CLA	B	805	-	1/1/15/20	12/37/115/115	-
14	CLA	b	803	-	1/1/15/20	9/37/115/115	-
14	CLA	b	832	3	1/1/15/20	11/37/115/115	-
17	BCR	k	103	-	-	7/29/63/63	0/2/2/2
14	CLA	j	103	-	1/1/8/20	0/2/76/115	-
17	BCR	A	850	-	-	13/29/63/63	0/2/2/2
14	CLA	b	837	-	1/1/11/20	2/13/91/115	-
14	CLA	a	815	-	1/1/11/20	0/13/91/115	-
17	BCR	J	103	-	-	12/29/63/63	0/2/2/2
14	CLA	a	819	-	1/1/12/20	9/24/102/115	-
14	CLA	L	1502	11	-	8/31/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	a	802	1	1/1/15/20	10/37/115/115	-
14	CLA	f	203	-	1/1/11/20	5/13/91/115	-
14	CLA	B	833	3	1/1/12/20	6/24/102/115	-
17	BCR	F	205	-	-	10/29/63/63	0/2/2/2
17	BCR	A	848	-	-	12/29/63/63	0/2/2/2
14	CLA	A	825	-	1/1/15/20	16/37/115/115	-
14	CLA	l	205	-	1/1/11/20	4/13/91/115	-
14	CLA	B	811	3	1/1/15/20	7/37/115/115	-
17	BCR	b	850	-	-	10/29/63/63	0/2/2/2
14	CLA	x	1701	2	1/1/11/20	7/18/96/115	-
17	BCR	f	202	-	-	16/29/63/63	0/2/2/2
14	CLA	B	834	-	1/1/14/20	16/31/109/115	-
14	CLA	A	830	1	1/1/15/20	9/37/115/115	-
17	BCR	A	847	-	-	10/29/63/63	0/2/2/2
14	CLA	a	810	-	1/1/15/20	7/37/115/115	-
14	CLA	A	819	-	1/1/15/20	12/37/115/115	-
17	BCR	A	849	-	-	15/29/63/63	0/2/2/2
17	BCR	a	848	-	-	9/29/63/63	0/2/2/2
14	CLA	A	805	1	1/1/15/20	16/37/115/115	-
14	CLA	a	818	-	1/1/15/20	13/37/115/115	-
14	CLA	b	811	-	1/1/15/20	7/37/115/115	-
17	BCR	j	104	-	-	14/29/63/63	0/2/2/2
14	CLA	B	831	-	1/1/15/20	11/37/115/115	-
20	LMG	B	803	-	-	12/30/50/70	0/1/1/1
17	BCR	a	849	-	-	15/29/63/63	0/2/2/2
13	CL0	a	801	1	3/3/20/25	4/37/135/135	-
16	SF4	c	101	-	-	-	0/6/5/5
14	CLA	A	802	-	1/1/15/20	8/37/115/115	-
14	CLA	b	821	3	1/1/15/20	9/37/115/115	-
14	CLA	J	101	-	1/1/11/20	8/13/91/115	-
14	CLA	B	806	-	1/1/15/20	12/37/115/115	-
14	CLA	A	836	1	1/1/11/20	3/13/91/115	-
14	CLA	a	812	-	1/1/14/20	15/31/109/115	-
15	PQN	b	844	-	-	5/23/43/43	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	a	823	1	1/1/11/20	4/13/91/115	-
14	CLA	B	804	-	1/1/15/20	15/37/115/115	-
14	CLA	b	841	3	1/1/11/20	7/16/94/115	-
14	CLA	B	813	-	1/1/14/20	13/31/109/115	-
14	CLA	L	1503	-	1/1/11/20	6/13/91/115	-
14	CLA	B	801	-	1/1/15/20	10/37/115/115	-
18	LHG	a	851	14	-	24/53/53/53	-
17	BCR	i	101	-	-	14/29/63/63	0/2/2/2
14	CLA	B	840	3	1/1/15/20	9/37/115/115	-
14	CLA	A	834	-	1/1/15/20	13/37/115/115	-
14	CLA	b	812	3	1/1/15/20	19/37/115/115	-
14	CLA	b	814	-	1/1/12/20	11/24/102/115	-
17	BCR	f	204	-	-	15/29/63/63	0/2/2/2
16	SF4	c	102	-	-	-	0/6/5/5
14	CLA	a	813	-	1/1/12/20	2/24/102/115	-
14	CLA	A	823	1	1/1/12/20	9/24/102/115	-
14	CLA	J	102	-	1/1/8/20	0/2/76/115	-
14	CLA	B	837	-	1/1/11/20	2/13/91/115	-
14	CLA	a	834	1	1/1/12/20	4/24/102/115	-
14	CLA	A	817	-	1/1/13/20	6/30/108/115	-
14	CLA	B	810	3	1/1/15/20	9/37/115/115	-
14	CLA	a	825	-	1/1/12/20	6/24/102/115	-
14	CLA	b	802	-	1/1/15/20	10/37/115/115	-
17	BCR	M	101	-	-	12/29/63/63	0/2/2/2
14	CLA	B	816	-	1/1/15/20	13/37/115/115	-
14	CLA	b	810	3	1/1/15/20	7/37/115/115	-
20	LMG	b	851	-	-	23/50/70/70	0/1/1/1
17	BCR	J	105	-	-	9/29/63/63	0/2/2/2
16	SF4	C	102	-	-	-	0/6/5/5
14	CLA	a	803	-	1/1/12/20	5/24/102/115	-
14	CLA	b	842	-	1/1/15/20	6/37/115/115	-
14	CLA	b	818	-	1/1/11/20	5/18/96/115	-
14	CLA	B	817	-	1/1/12/20	2/19/97/115	-
14	CLA	A	804	-	1/1/12/20	4/24/102/115	-
17	BCR	F	203	-	-	14/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	BCR	a	844	-	-	11/29/63/63	0/2/2/2
16	SF4	a	843	-	-	-	0/6/5/5
17	BCR	A	851	-	-	16/29/63/63	0/2/2/2
14	CLA	a	805	1	1/1/15/20	16/37/115/115	-
14	CLA	A	831	1	1/1/12/20	6/24/102/115	-
14	CLA	B	809	3	1/1/15/20	16/37/115/115	-
17	BCR	B	850	-	-	9/29/63/63	0/2/2/2
17	BCR	b	845	-	-	12/29/63/63	0/2/2/2
14	CLA	f	201	-	1/1/13/20	7/30/108/115	-
14	CLA	A	803	-	1/1/15/20	9/37/115/115	-
14	CLA	A	824	1	1/1/11/20	2/13/91/115	-
14	CLA	A	828	-	1/1/15/20	16/37/115/115	-
16	SF4	C	101	-	-	-	0/6/5/5
18	LHG	i	103	-	-	28/47/47/53	-
15	PQN	B	844	-	-	4/23/43/43	0/2/2/2
14	CLA	A	820	-	1/1/12/20	9/24/102/115	-
16	SF4	A	845	-	-	-	0/6/5/5
14	CLA	A	814	1	1/1/12/20	5/24/102/115	-
14	CLA	b	809	3	1/1/15/20	20/37/115/115	-
14	CLA	a	817	-	1/1/14/20	13/31/109/115	-
13	CL0	A	801	-	3/3/20/25	4/37/135/135	-
14	CLA	b	829	-	1/1/15/20	10/37/115/115	-
14	CLA	b	830	-	1/1/15/20	16/37/115/115	-
14	CLA	a	822	1	1/1/12/20	9/24/102/115	-
14	CLA	b	834	-	1/1/14/20	16/31/109/115	-
14	CLA	A	842	-	1/1/15/20	20/37/115/115	-
17	BCR	I	101	-	-	11/29/63/63	0/2/2/2
17	BCR	b	846	-	-	12/29/63/63	0/2/2/2
14	CLA	X	1701	2	1/1/11/20	9/18/96/115	-
14	CLA	A	809	1	1/1/15/20	12/37/115/115	-
14	CLA	a	829	-	1/1/15/20	11/37/115/115	-
18	LHG	F	201	-	-	27/47/47/53	-
20	LMG	B	851	-	-	28/50/70/70	0/1/1/1
17	BCR	m	1202	-	-	11/29/63/63	0/2/2/2
14	CLA	B	821	3	1/1/15/20	11/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	B	839	3	1/1/14/20	7/31/109/115	-
14	CLA	b	840	3	1/1/15/20	9/37/115/115	-
14	CLA	B	824	3	1/1/11/20	2/13/91/115	-
14	CLA	B	841	3	1/1/11/20	3/16/94/115	-
14	CLA	a	828	-	1/1/15/20	15/37/115/115	-
14	CLA	B	820	3	1/1/15/20	15/37/115/115	-
14	CLA	b	817	3	1/1/12/20	3/19/97/115	-
14	CLA	k	102	-	1/1/11/20	4/18/96/115	-
17	BCR	a	845	-	-	7/29/63/63	0/2/2/2
18	LHG	A	853	14	-	21/53/53/53	-
14	CLA	l	203	11	1/1/11/20	8/13/91/115	-
17	BCR	L	1504	-	-	13/29/63/63	0/2/2/2
14	CLA	a	820	-	1/1/15/20	16/37/115/115	-
17	BCR	l	207	-	-	6/29/63/63	0/2/2/2
14	CLA	B	843	3	1/1/15/20	15/37/115/115	-
14	CLA	a	814	-	1/1/11/20	6/13/91/115	-
14	CLA	a	824	-	1/1/15/20	13/37/115/115	-
14	CLA	b	823	3	1/1/11/20	6/13/91/115	-
19	SQD	l	202	-	-	25/49/69/69	0/1/1/1
14	CLA	B	802	1	1/1/15/20	12/37/115/115	-
17	BCR	b	848	-	-	15/29/63/63	0/2/2/2
14	CLA	b	816	-	-	16/37/115/115	-
19	SQD	x	1702	-	-	14/49/69/69	0/1/1/1
14	CLA	A	838	1	1/1/15/20	13/37/115/115	-
14	CLA	b	833	-	1/1/12/20	7/24/102/115	-
14	CLA	b	820	-	1/1/15/20	5/37/115/115	-
14	CLA	A	829	-	1/1/15/20	10/37/115/115	-
17	BCR	l	206	-	-	10/29/63/63	0/2/2/2
14	CLA	L	1501	11	1/1/12/20	5/21/99/115	-
14	CLA	b	806	3	1/1/15/20	9/37/115/115	-
15	PQN	A	844	-	-	5/23/43/43	0/2/2/2
14	CLA	B	842	-	1/1/15/20	5/37/115/115	-
14	CLA	B	818	3	1/1/11/20	5/18/96/115	-
14	CLA	a	835	1	1/1/11/20	7/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	a	839	1	1/1/15/20	5/37/115/115	-
14	CLA	b	819	-	1/1/11/20	2/13/91/115	-
14	CLA	b	826	-	1/1/15/20	8/37/115/115	-
17	BCR	I	102	-	-	11/29/63/63	0/2/2/2
17	BCR	A	846	-	-	10/29/63/63	0/2/2/2
14	CLA	B	830	3	1/1/15/20	12/37/115/115	-
14	CLA	k	101	-	1/1/9/20	2/7/81/115	-
18	LHG	A	852	-	-	21/53/53/53	-
14	CLA	A	808	1	1/1/15/20	21/37/115/115	-
14	CLA	A	833	1	1/1/15/20	10/37/115/115	-
14	CLA	B	828	-	1/1/15/20	12/37/115/115	-
14	CLA	A	839	-	-	16/37/115/115	-
18	LHG	a	850	-	-	17/53/53/53	-
14	CLA	A	832	1	1/1/15/20	18/37/115/115	-
17	BCR	B	845	-	-	12/29/63/63	0/2/2/2
14	CLA	a	831	1	1/1/15/20	15/37/115/115	-
17	BCR	l	201	-	-	9/29/63/63	0/2/2/2
14	CLA	b	808	-	1/1/15/20	13/37/115/115	-
14	CLA	b	825	-	1/1/13/20	13/25/103/115	-
14	CLA	A	827	1	1/1/15/20	14/37/115/115	-
14	CLA	a	841	18	1/1/11/20	8/13/91/115	-
17	BCR	J	104	-	-	13/29/63/63	0/2/2/2
14	CLA	B	835	-	1/1/13/20	12/29/107/115	-
14	CLA	l	204	11	-	9/31/109/115	-
17	BCR	b	849	-	-	8/29/63/63	0/2/2/2
14	CLA	a	840	1	1/1/15/20	6/37/115/115	-
14	CLA	b	805	-	1/1/15/20	18/37/115/115	-
14	CLA	a	809	1	1/1/11/20	7/13/91/115	-
14	CLA	K	101	-	1/1/9/20	5/7/81/115	-
14	CLA	b	843	3	-	12/37/115/115	-
17	BCR	j	106	-	-	15/29/63/63	0/2/2/2
14	CLA	B	808	-	1/1/15/20	17/37/115/115	-
14	CLA	A	840	-	1/1/13/20	7/30/108/115	-
14	CLA	B	822	-	1/1/15/20	10/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	a	838	-	1/1/15/20	11/37/115/115	-
14	CLA	b	835	3	1/1/15/20	15/37/115/115	-
14	CLA	b	839	-	1/1/14/20	8/31/109/115	-
14	CLA	A	807	-	1/1/14/20	17/31/109/115	-
19	SQD	X	1702	-	-	17/49/69/69	0/1/1/1
14	CLA	A	826	-	1/1/12/20	6/24/102/115	-
14	CLA	b	822	-	1/1/15/20	9/37/115/115	-
14	CLA	A	811	-	1/1/15/20	10/37/115/115	-
14	CLA	a	808	1	1/1/15/20	13/37/115/115	-
14	CLA	a	833	1	1/1/15/20	16/37/115/115	-
14	CLA	F	202	3	1/1/15/20	17/37/115/115	-
14	CLA	b	828	-	1/1/15/20	15/37/115/115	-

The worst 5 of 1676 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	a	801	CL0	MG-NA	9.30	2.28	2.06
13	A	801	CL0	MG-NA	9.30	2.28	2.06
14	A	821	CLA	C4B-NB	7.66	1.42	1.35
14	B	838	CLA	C4B-NB	7.58	1.42	1.35
14	A	811	CLA	C4B-NB	7.57	1.42	1.35

The worst 5 of 2279 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	807	CLA	O2D-CGD-CBD	25.81	157.13	111.27
14	A	807	CLA	O2D-CGD-O1D	-24.58	75.78	123.84
14	A	807	CLA	O1D-CGD-CBD	-21.05	81.42	124.48
14	a	841	CLA	O2A-CGA-O1A	-20.37	72.52	123.30
14	a	841	CLA	O2A-CGA-CBA	13.87	158.58	114.03

5 of 187 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
13	A	801	CL0	NC
13	A	801	CL0	NA
13	A	801	CL0	ND
13	a	801	CL0	NC
13	a	801	CL0	NA

5 of 2625 torsion outliers are listed below:

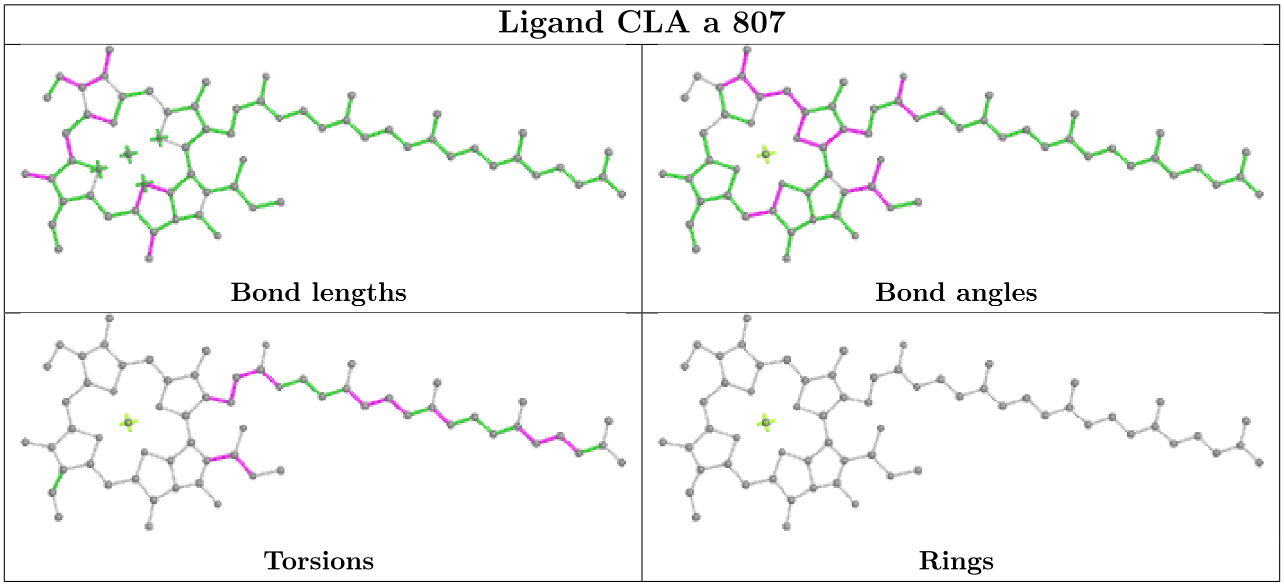
Mol	Chain	Res	Type	Atoms
14	A	804	CLA	C1A-C2A-CAA-CBA
14	A	804	CLA	C3A-C2A-CAA-CBA
14	A	805	CLA	CBA-CGA-O2A-C1
14	A	805	CLA	O1A-CGA-O2A-C1
14	A	805	CLA	CHA-CBD-CGD-O1D

There are no ring outliers.

No monomer is involved in short contacts.

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

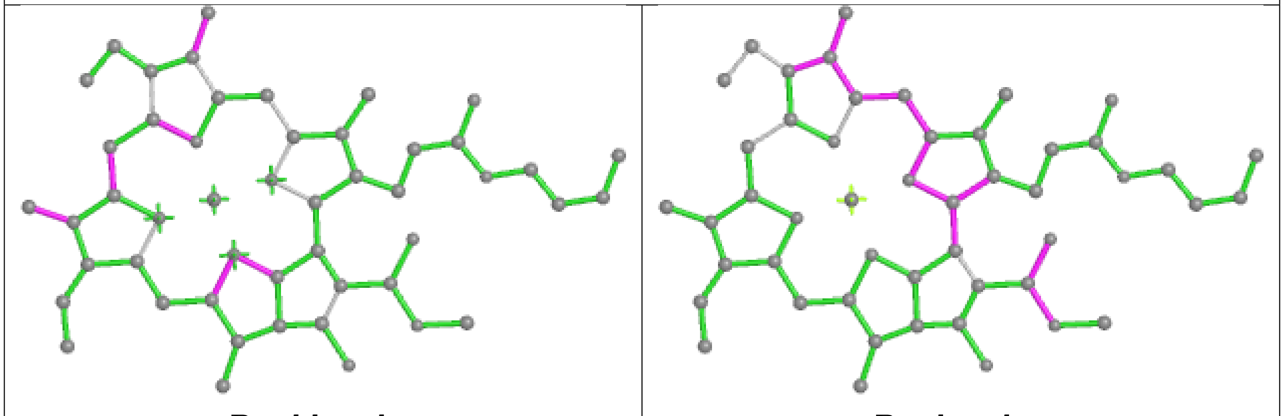
Ligand CLA a 807



Bond lengths **Bond angles**

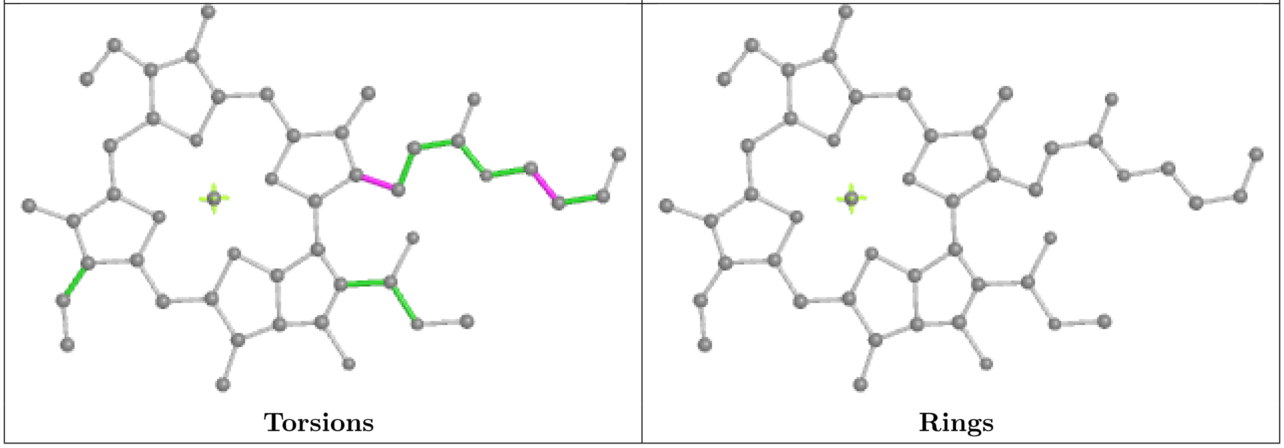
Torsions **Rings**

Ligand CLA K 102



Bond lengths

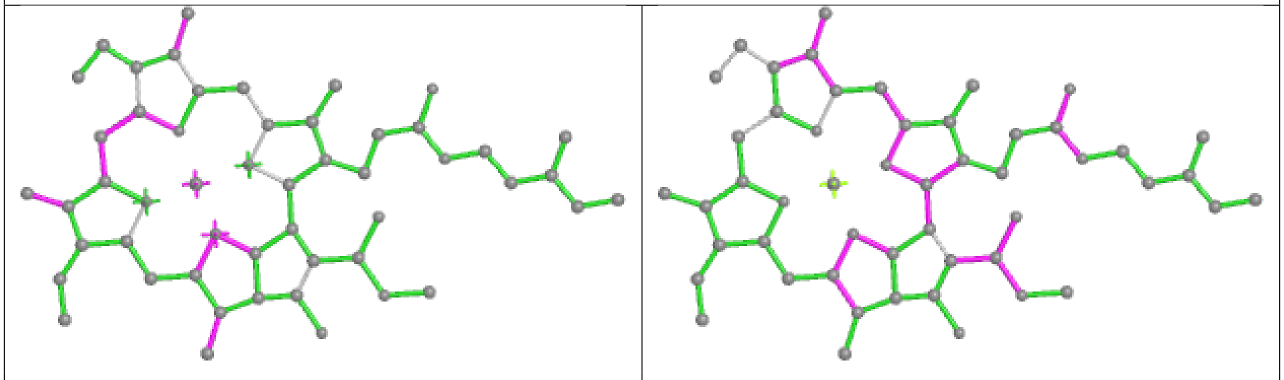
Bond angles



Torsions

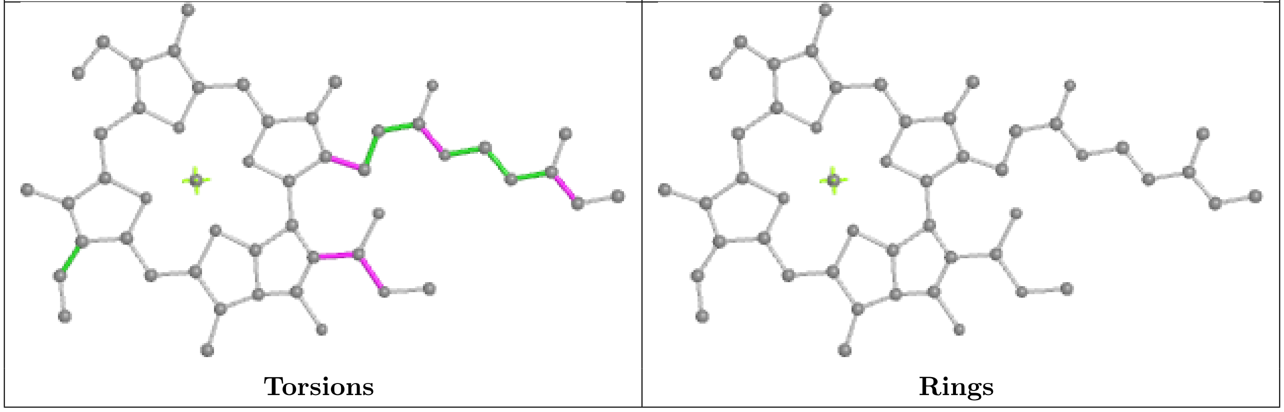
Rings

Ligand CLA a 836



Bond lengths

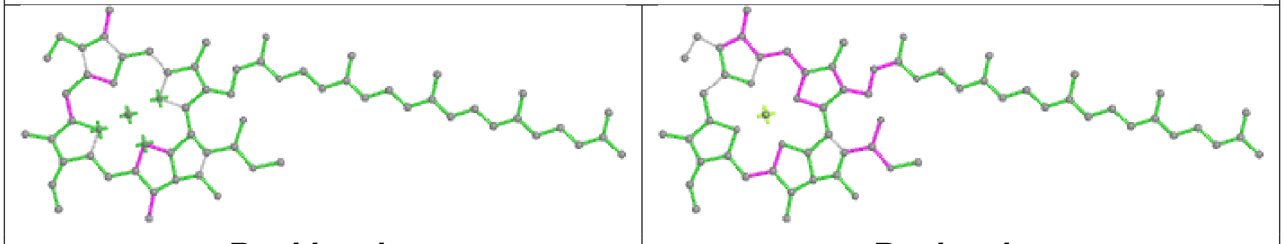
Bond angles



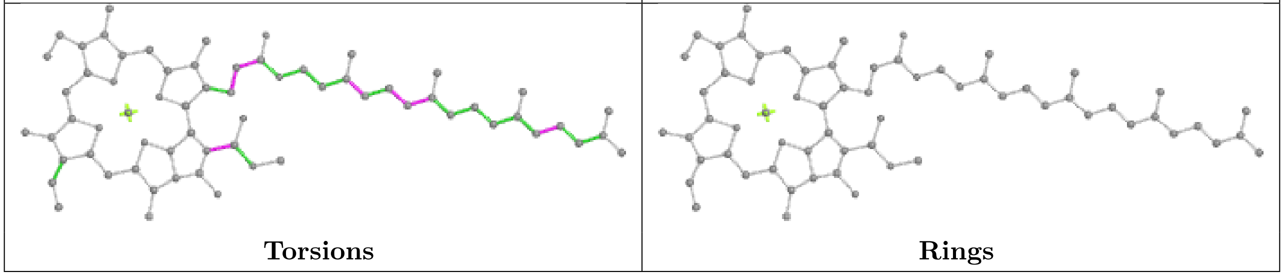
Torsions

Rings

Ligand CLA B 826



Bond lengths Bond angles



Torsions Rings

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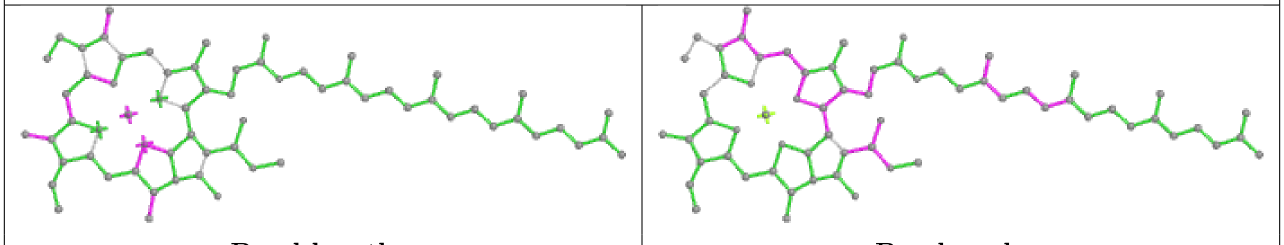
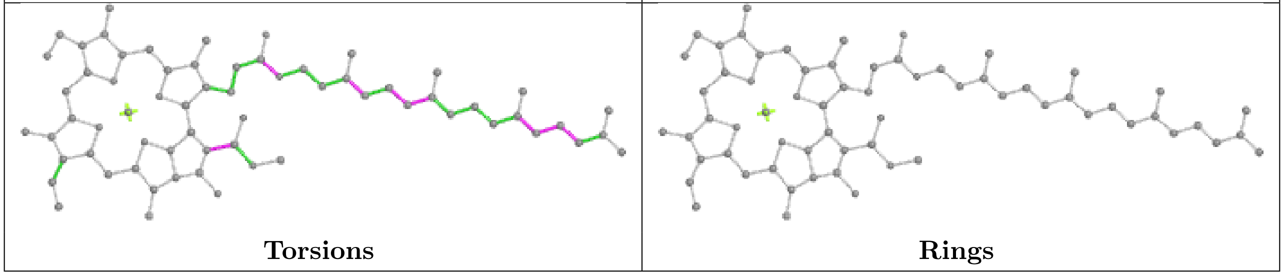
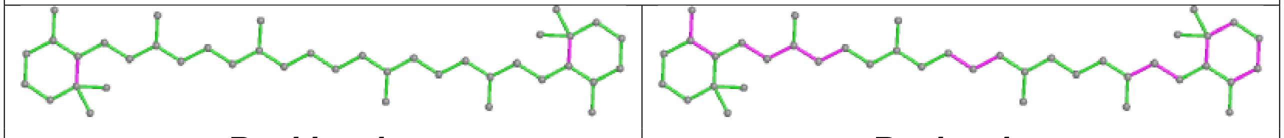


Bond lengths Bond angles

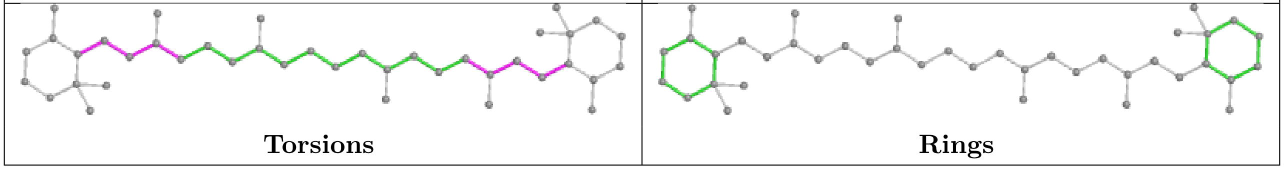


Torsions Rings

Ligand BCR j 105

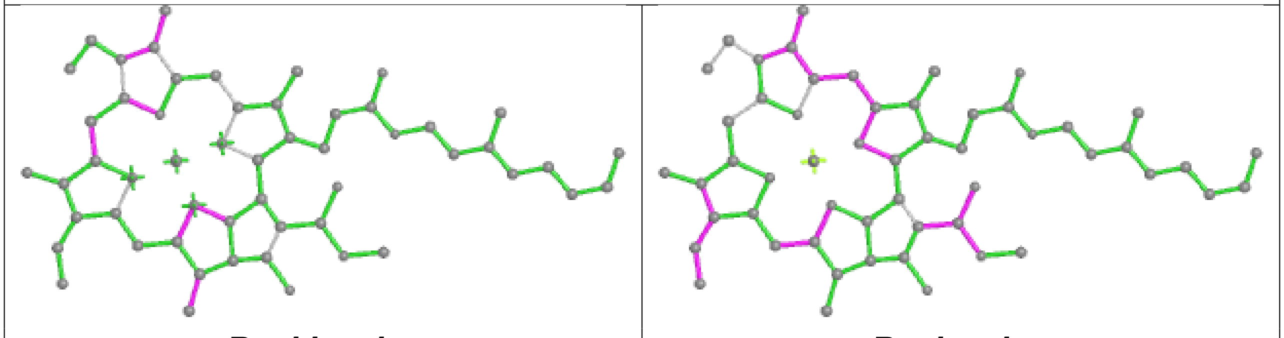


Bond lengths Bond angles



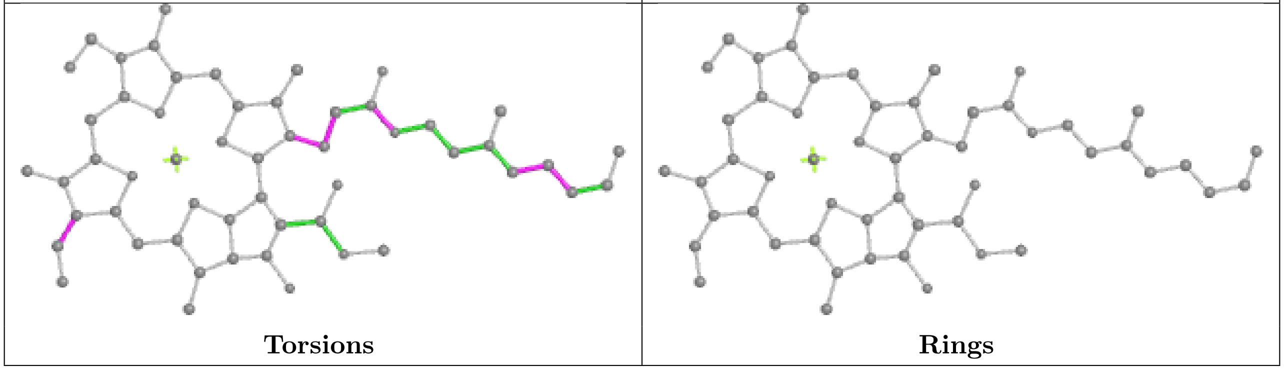
Torsions Rings

Ligand CLA b 815



Bond lengths

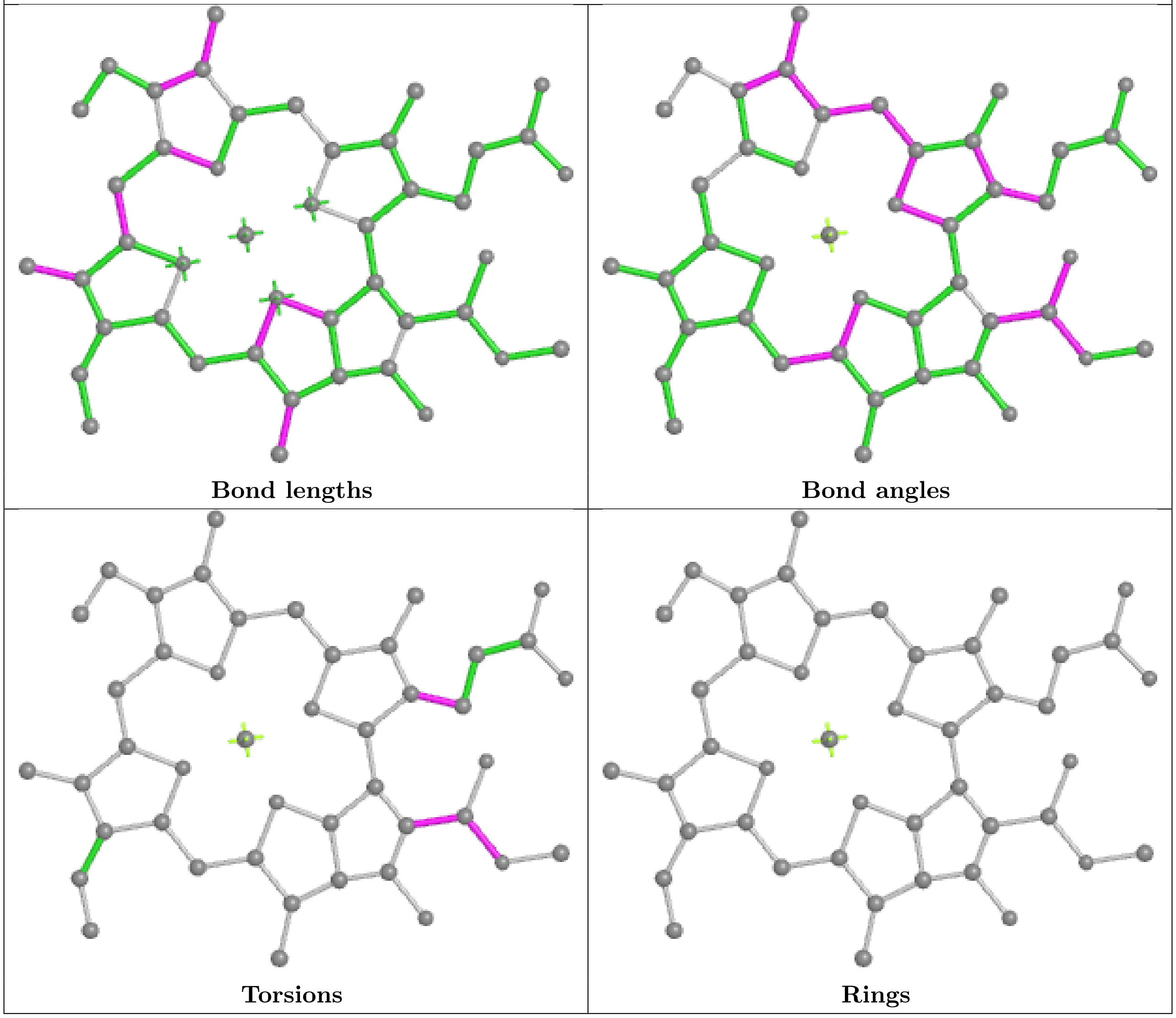
Bond angles



Torsions

Rings

Ligand CLA A 843



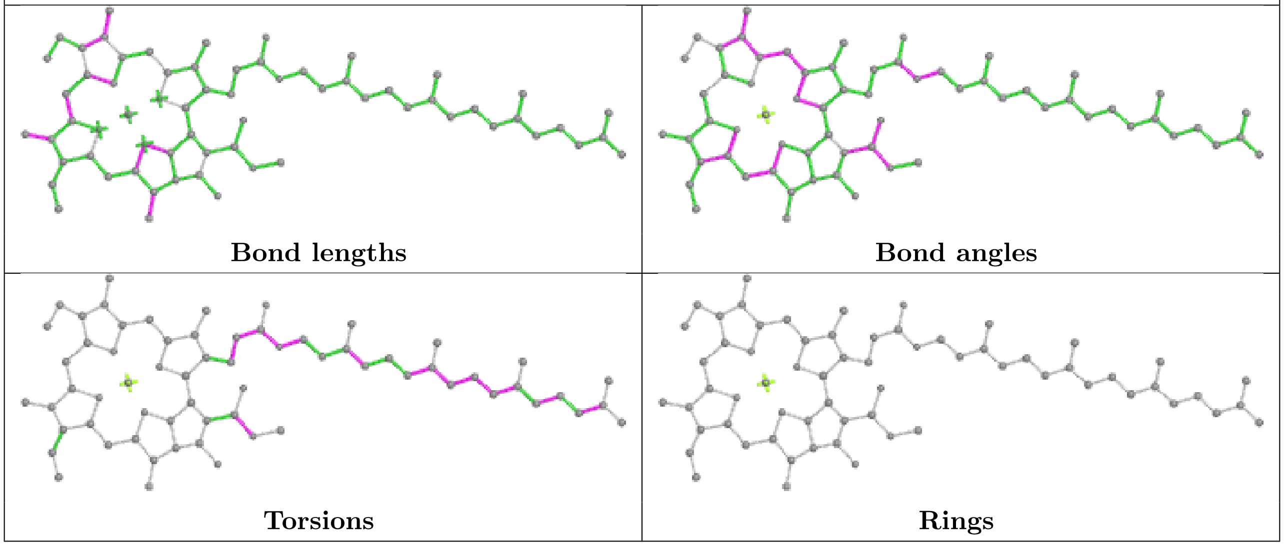
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA b 804



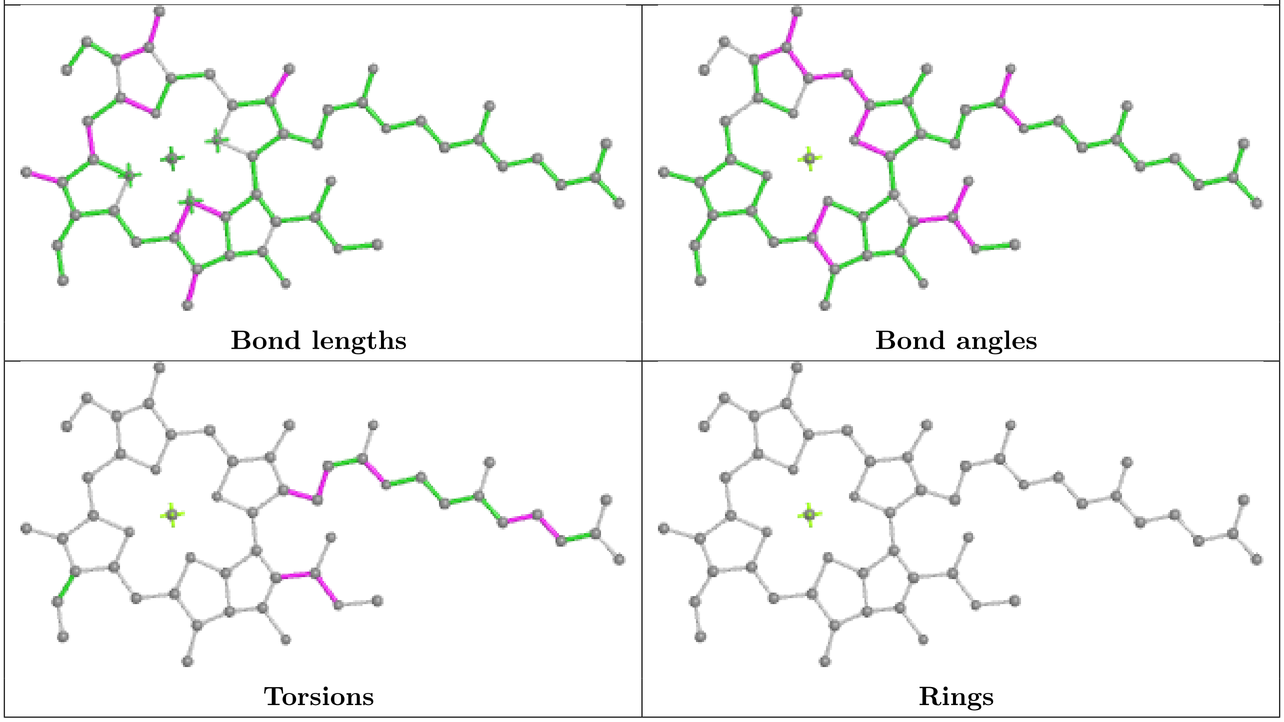
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA m 1201



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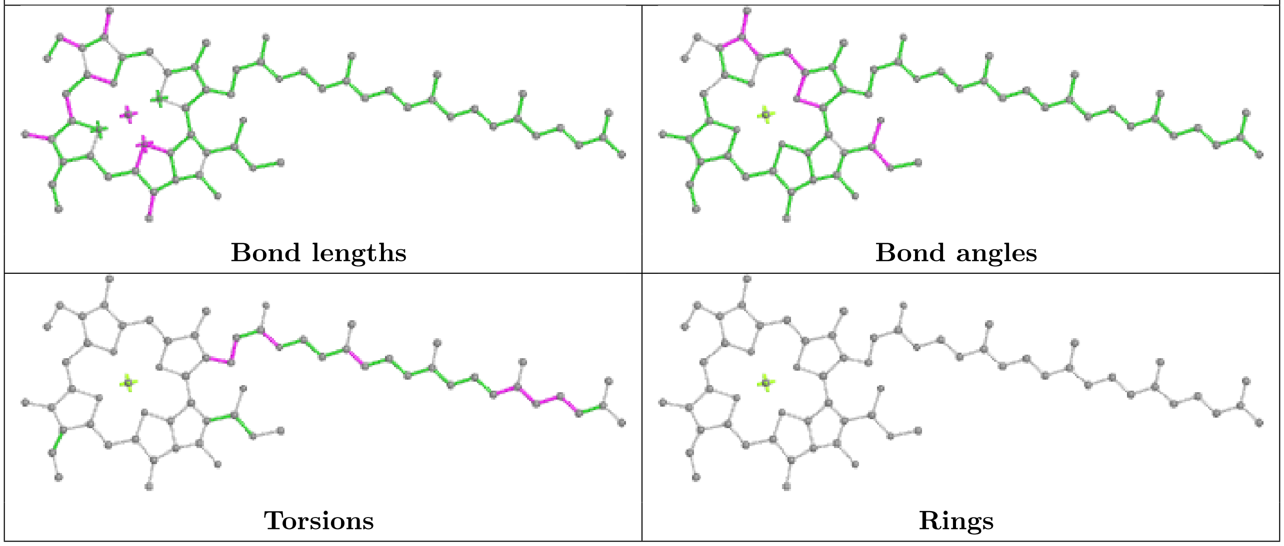
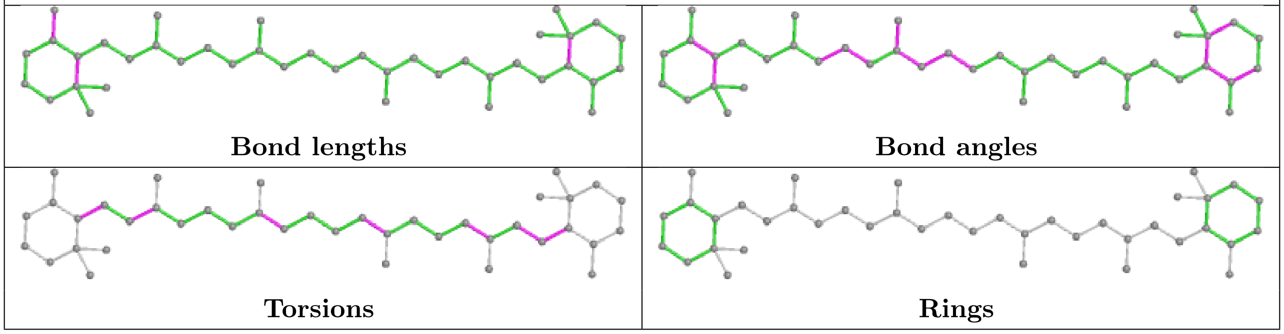


Ligand BCR i 102



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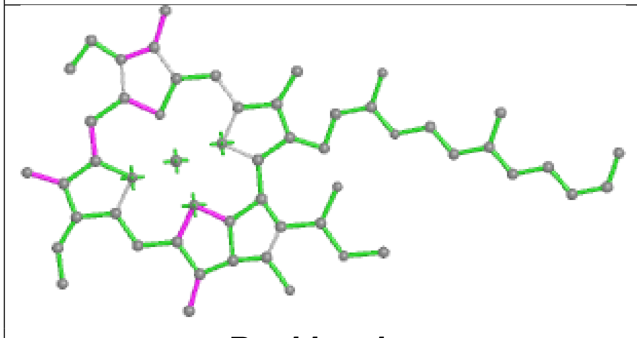
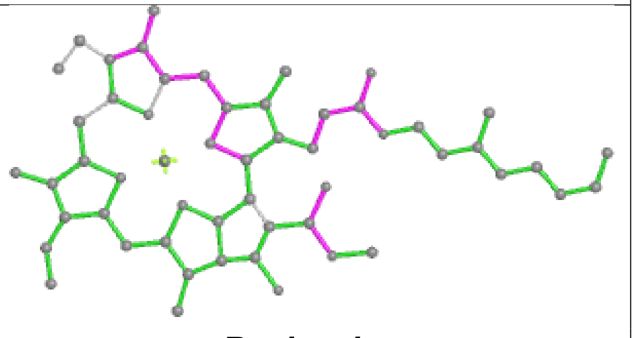
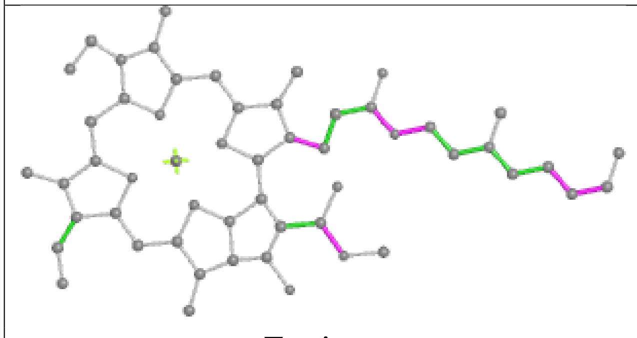


Bond lengths



Bond angles



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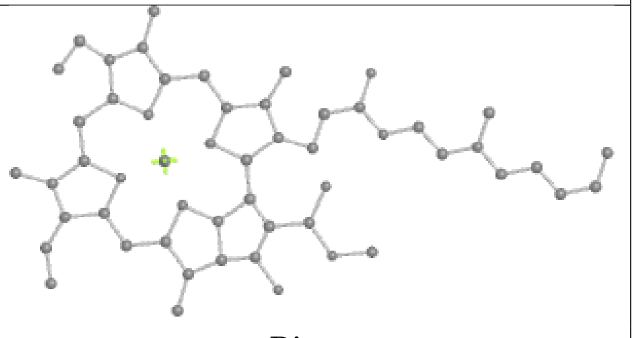
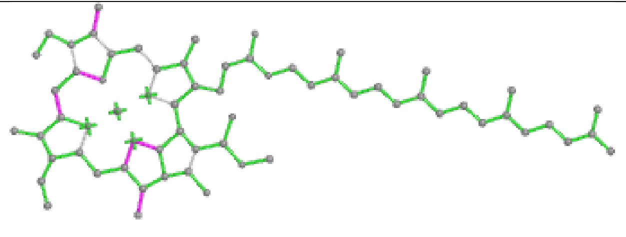


Rings

Ligand CLA a 827



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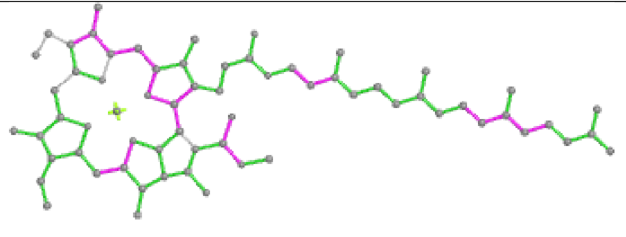

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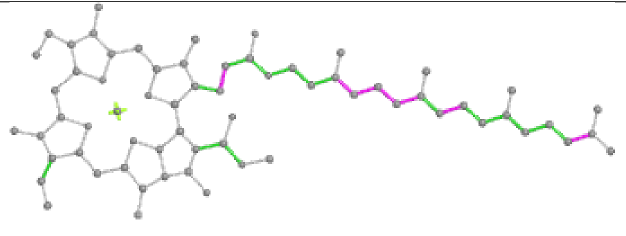

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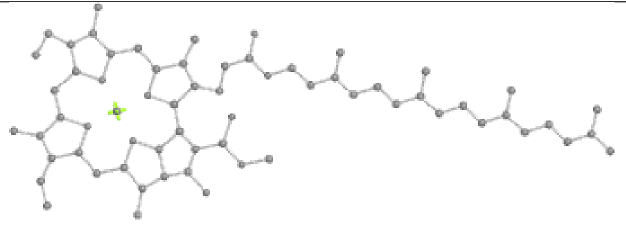

Rings

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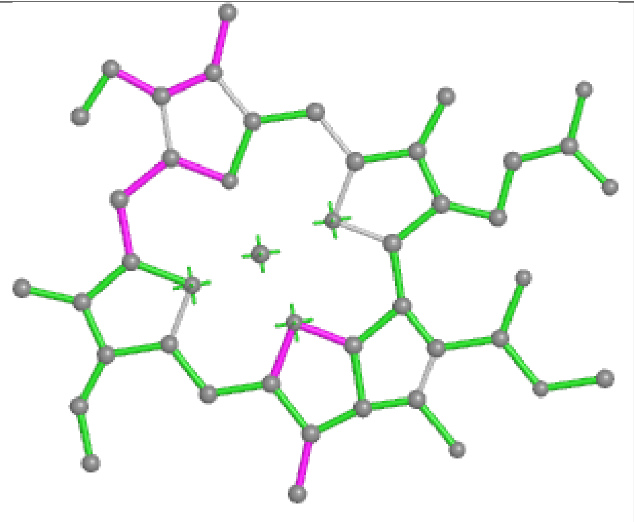
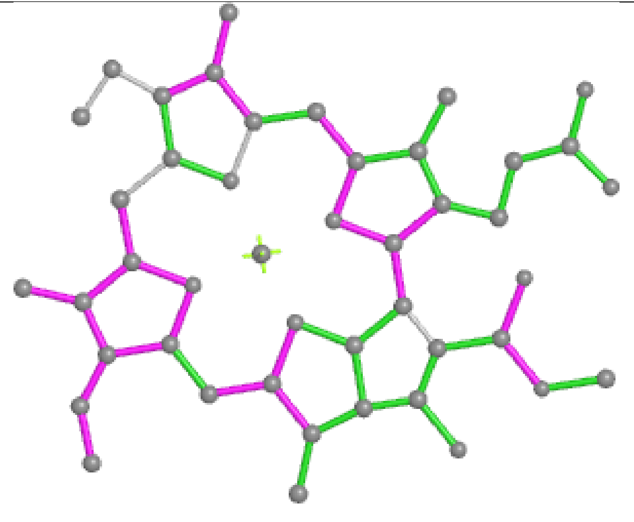
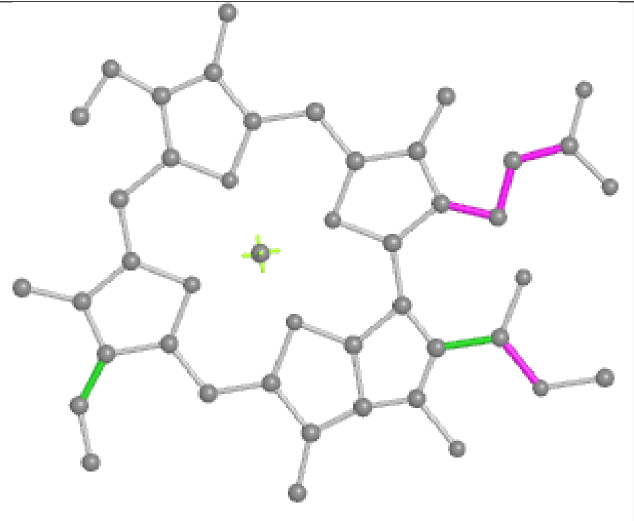
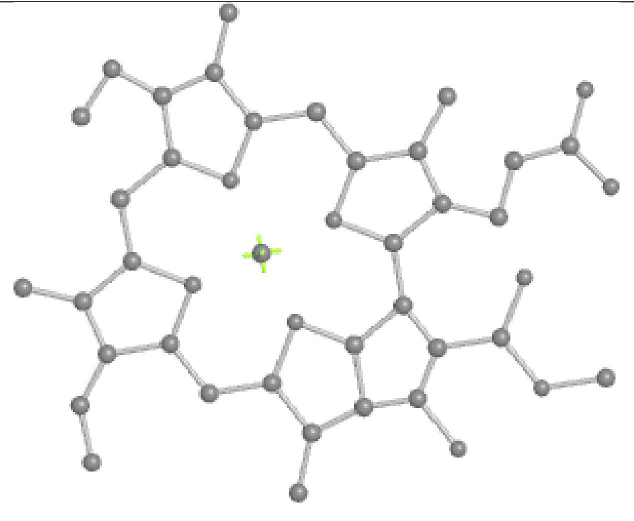
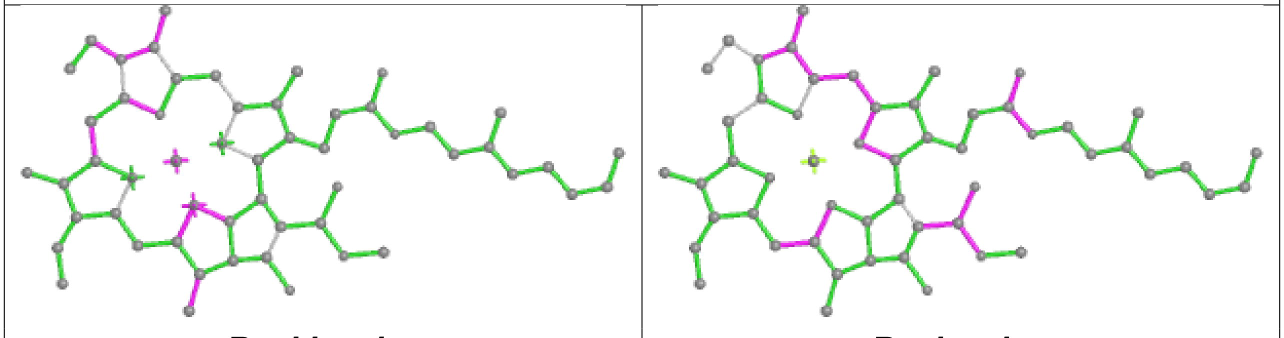
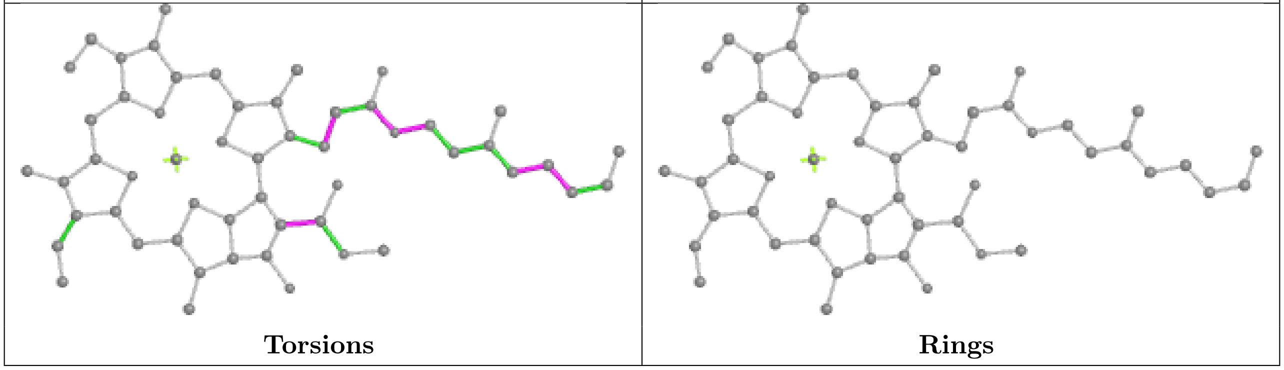
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA a 830



Bond lengths

Bond angles



Torsions

Rings

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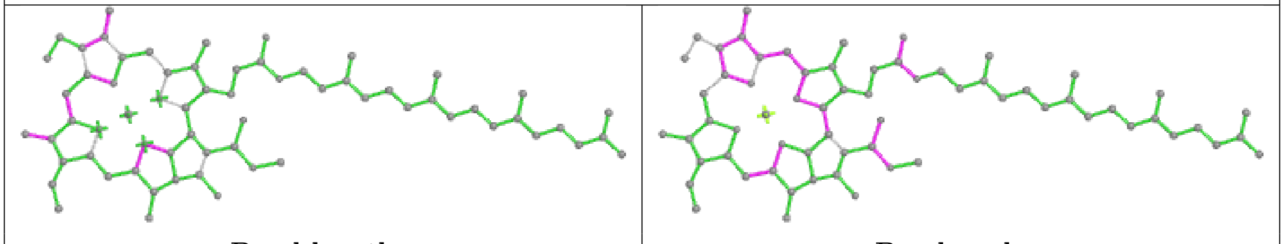
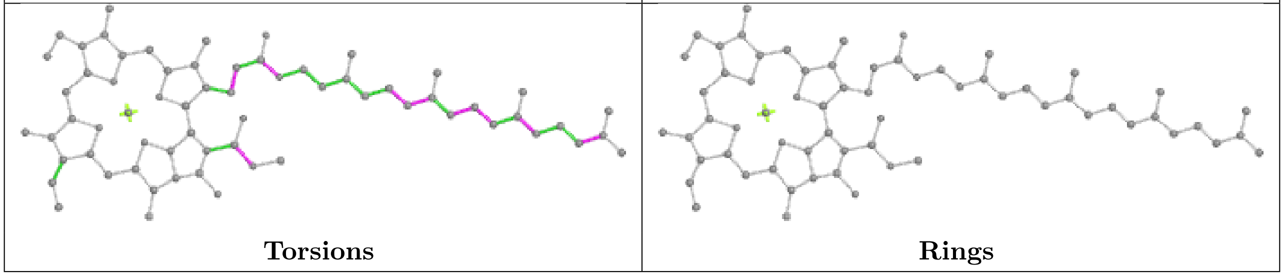


Bond lengths

Bond angles



Torsions

Rings

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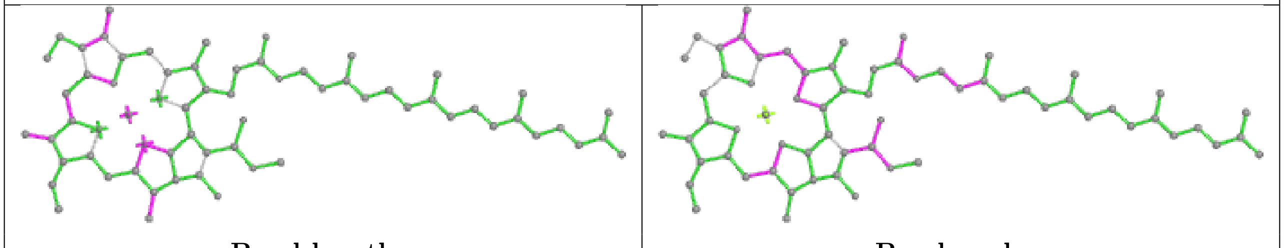
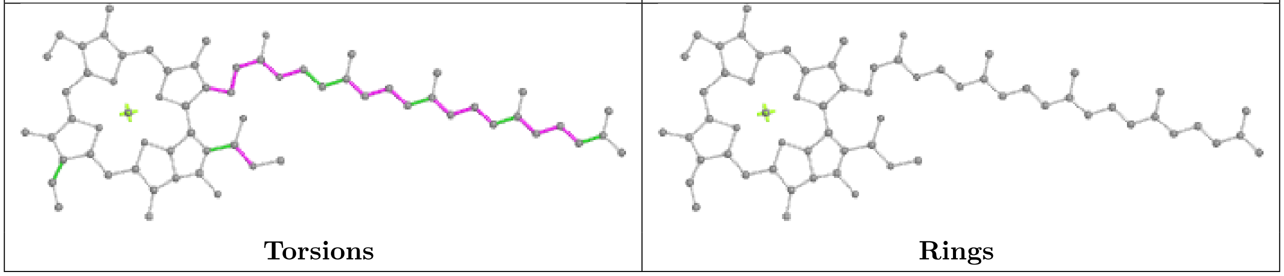


Bond lengths

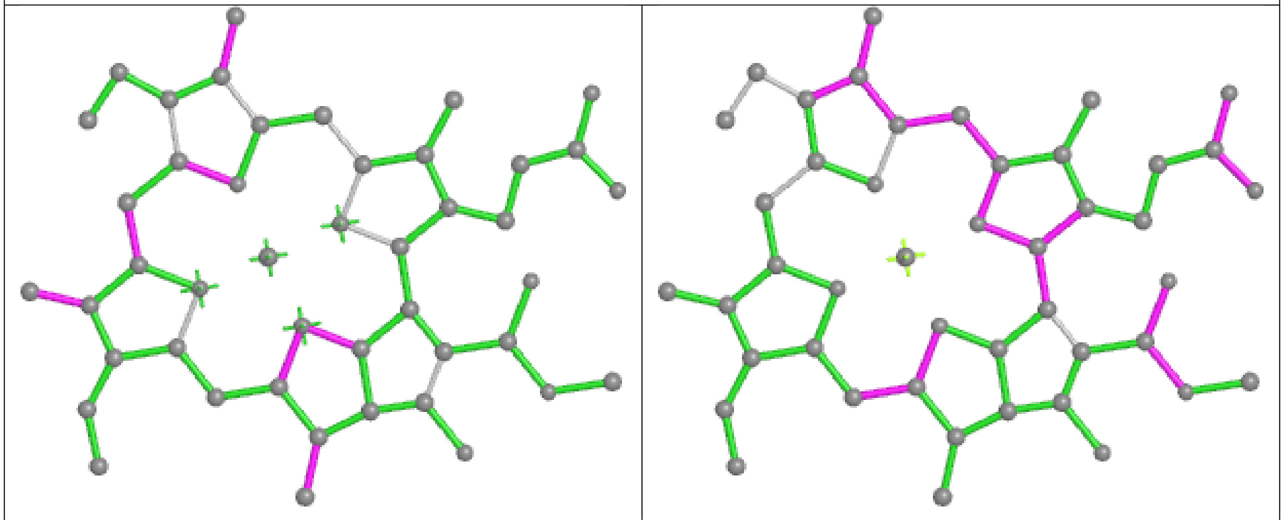
Bond angles



Torsions

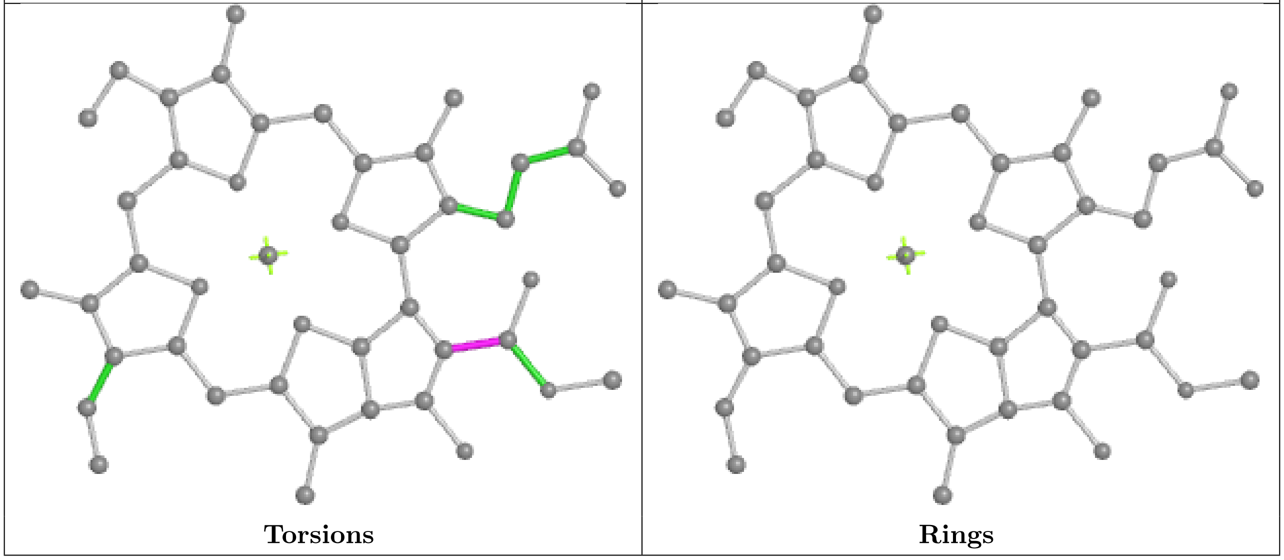
Rings

Ligand CLA F 204



Bond lengths

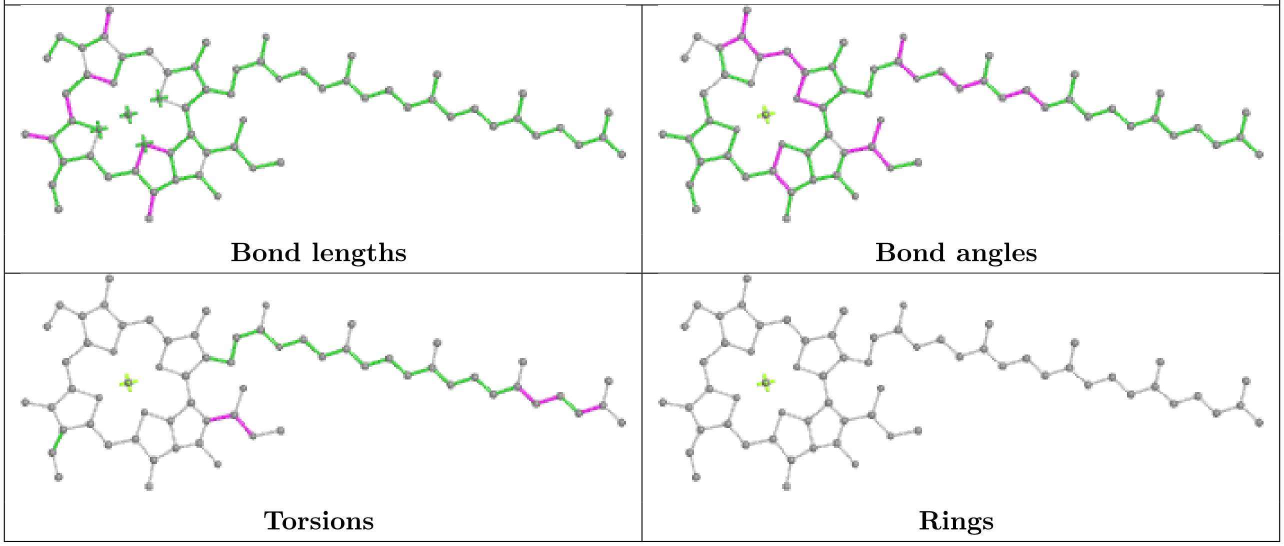
Bond angles



Torsions

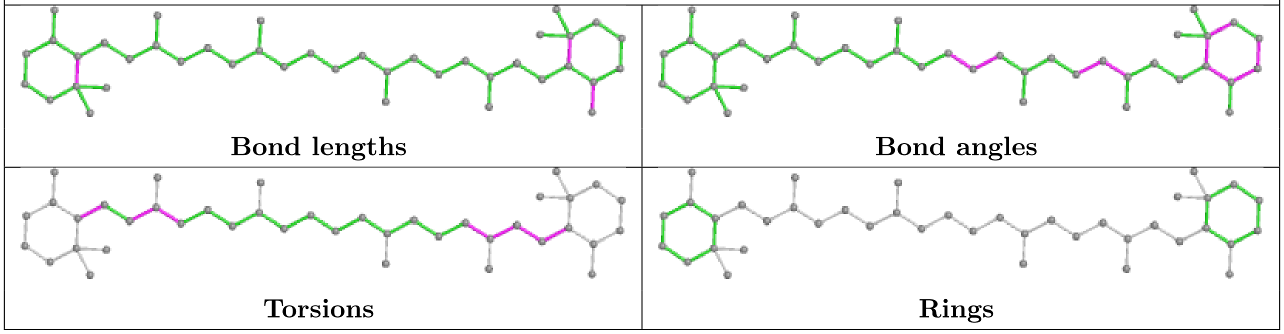
Rings

Ligand CLA a 832


Bond lengths Bond angles

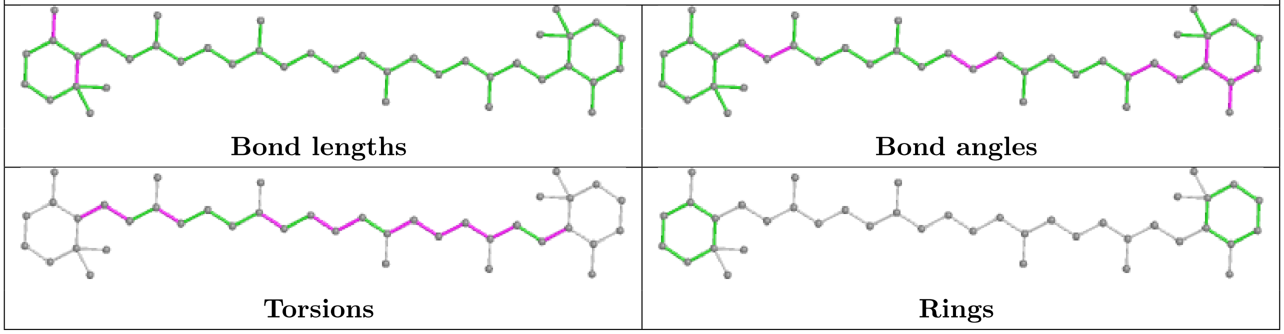
Torsions Rings

Ligand BCR B 848


Bond lengths Bond angles

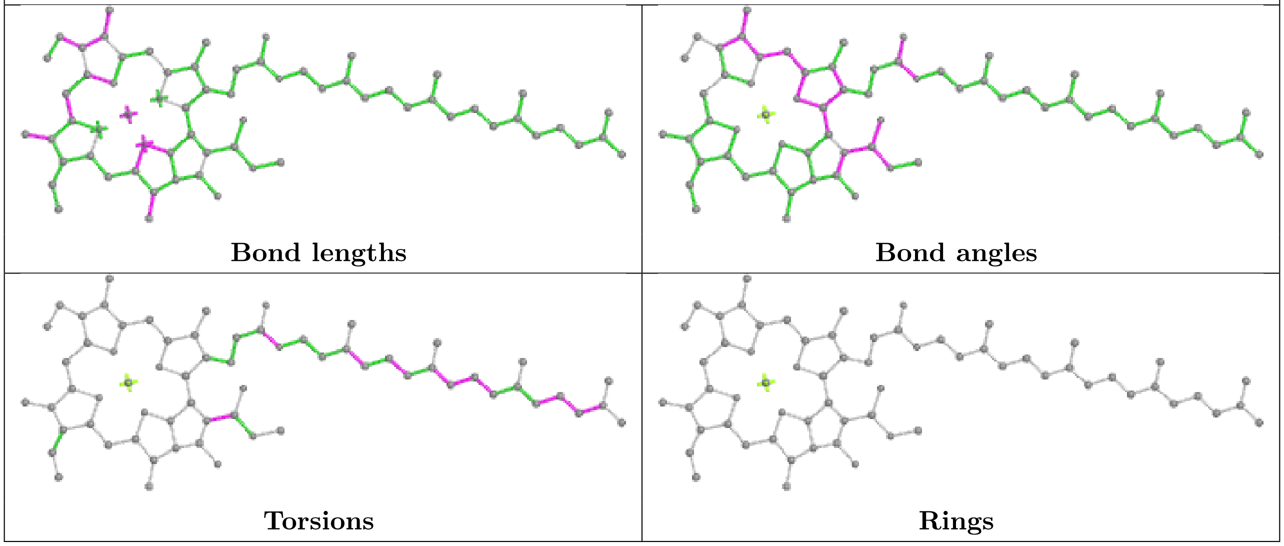
Torsions Rings

Ligand BCR a 847


Bond lengths Bond angles

Torsions Rings

Ligand CLA a 837



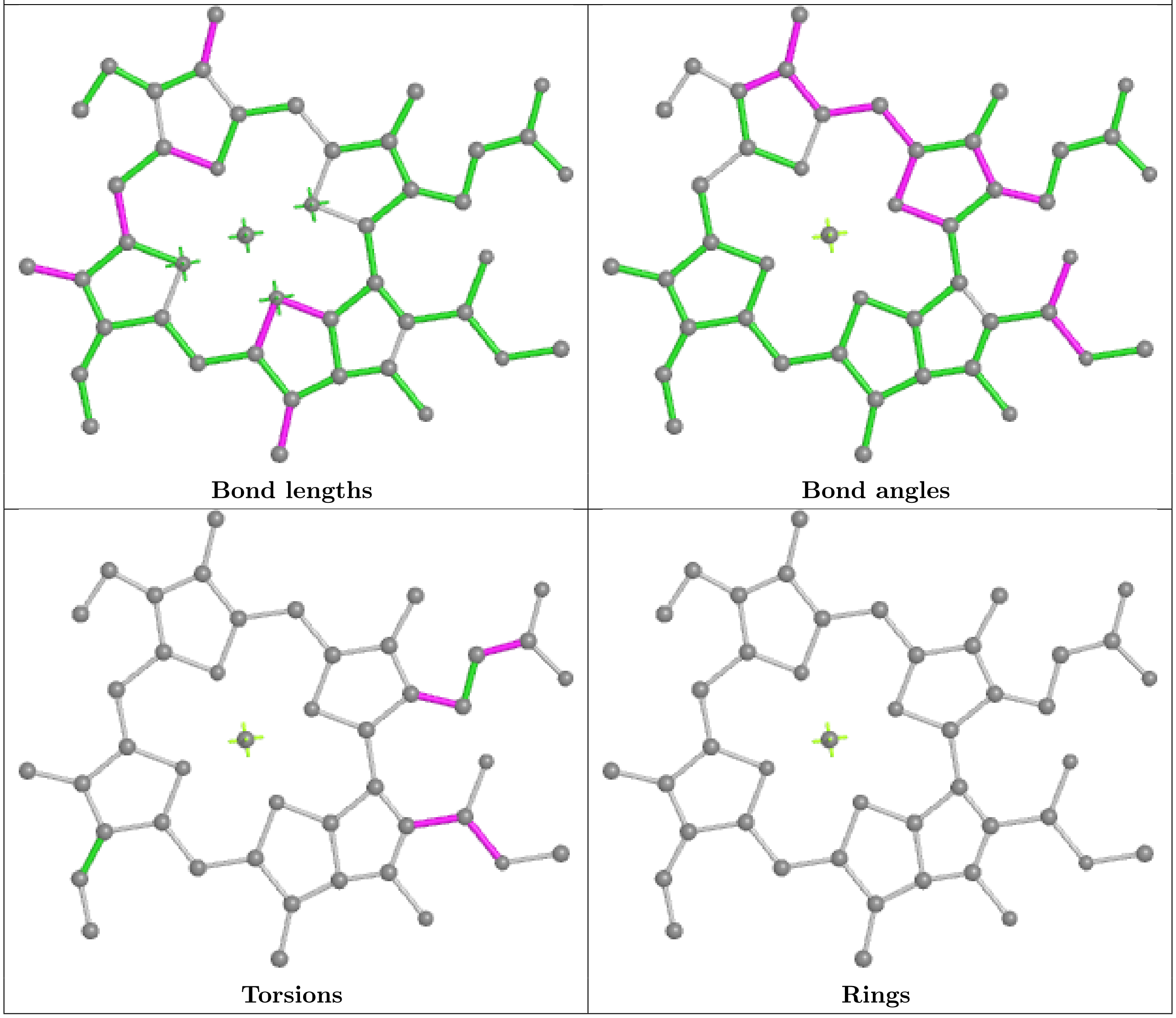
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA j 102



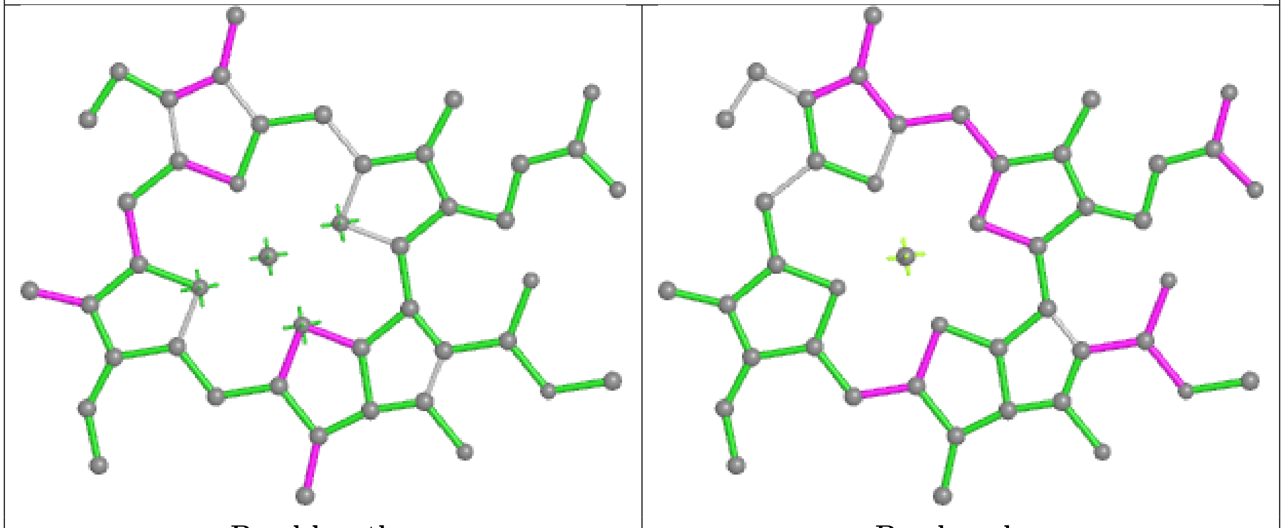
Bond lengths

Bond angles

Torsions

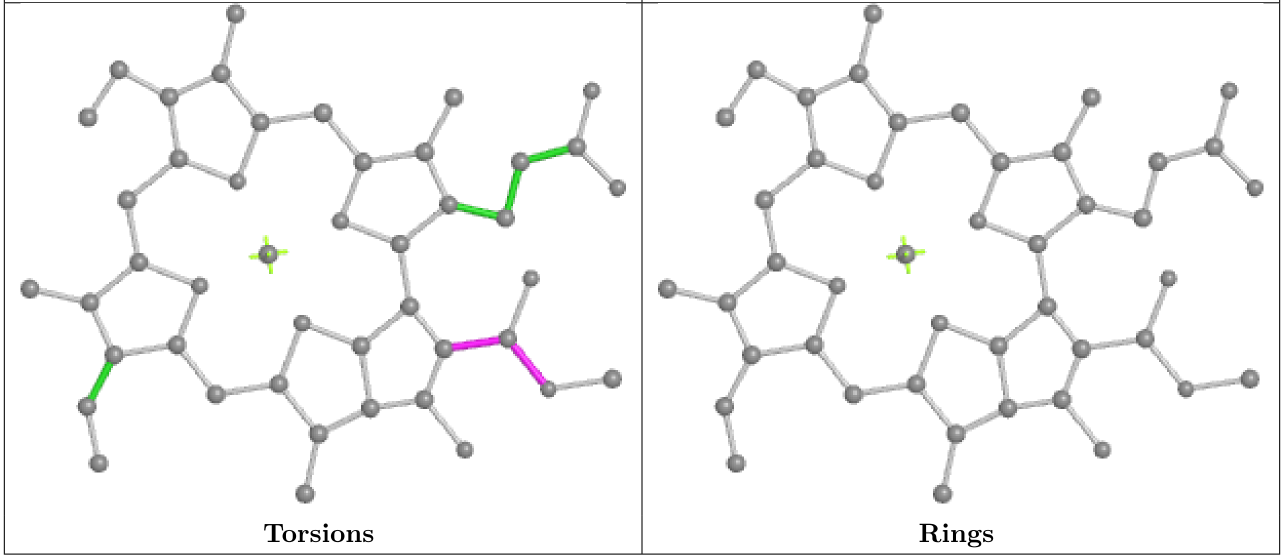
Rings

Ligand CLA B 838



Bond lengths

Bond angles



Torsions

Rings

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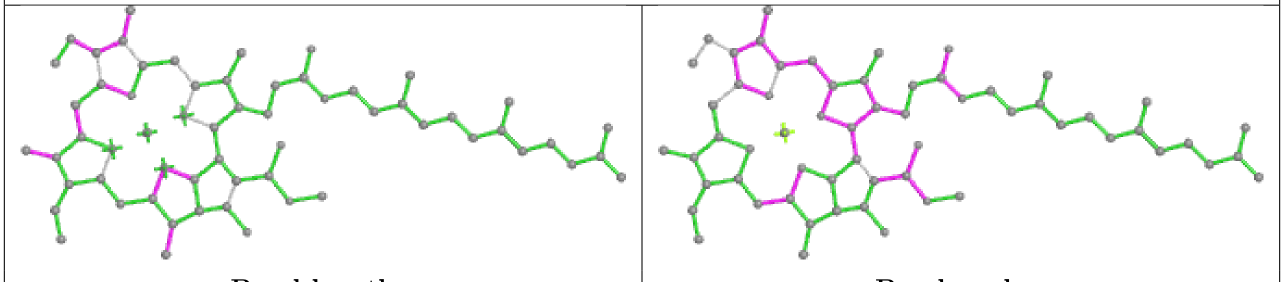
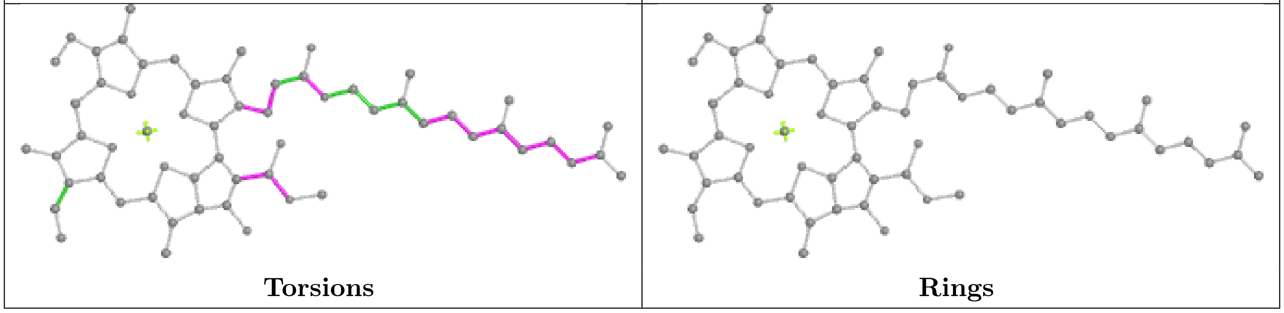


Bond lengths

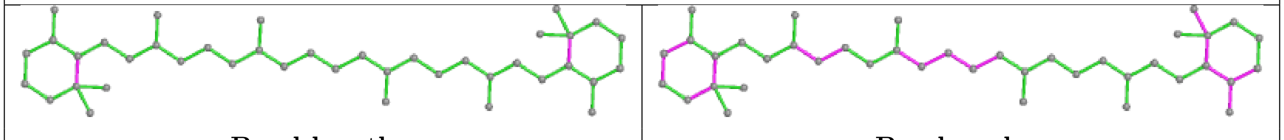
Bond angles



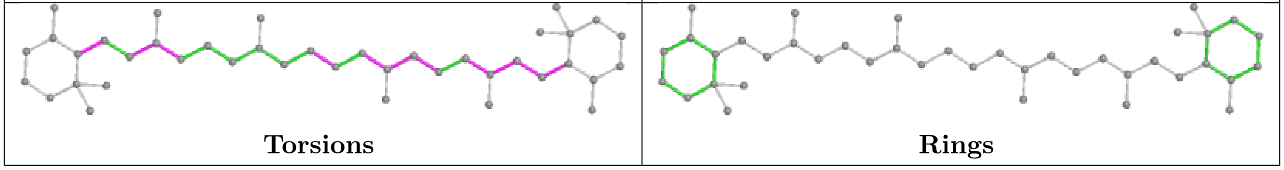
Torsions

Rings

Ligand BCR a 846

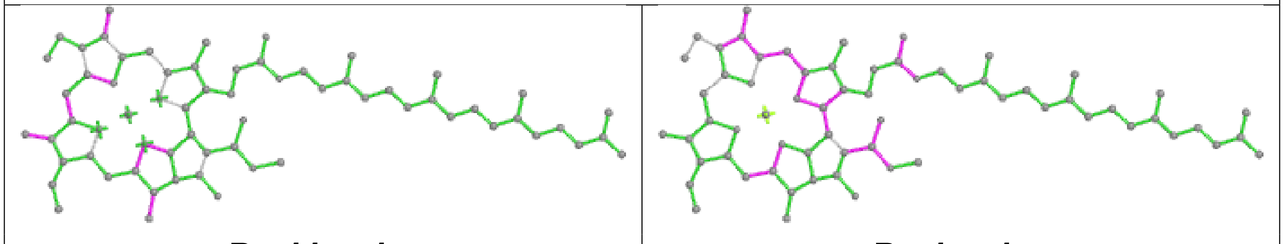


Bond lengths Bond angles

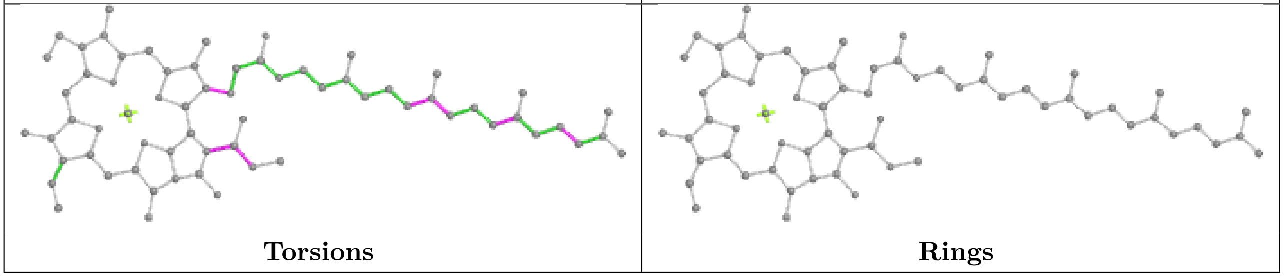


Torsions Rings

Ligand CLA B 829



Bond lengths Bond angles



Torsions Rings

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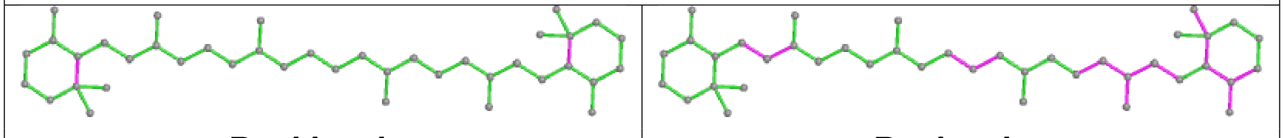
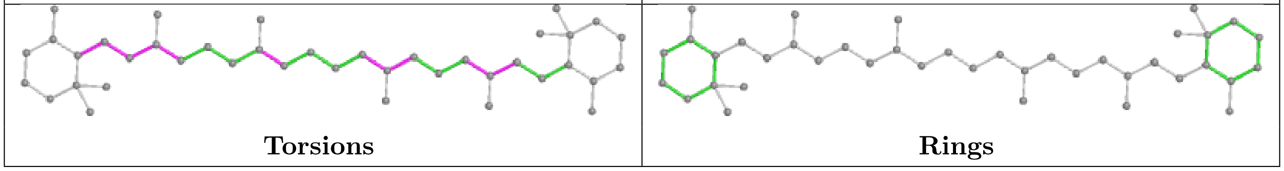
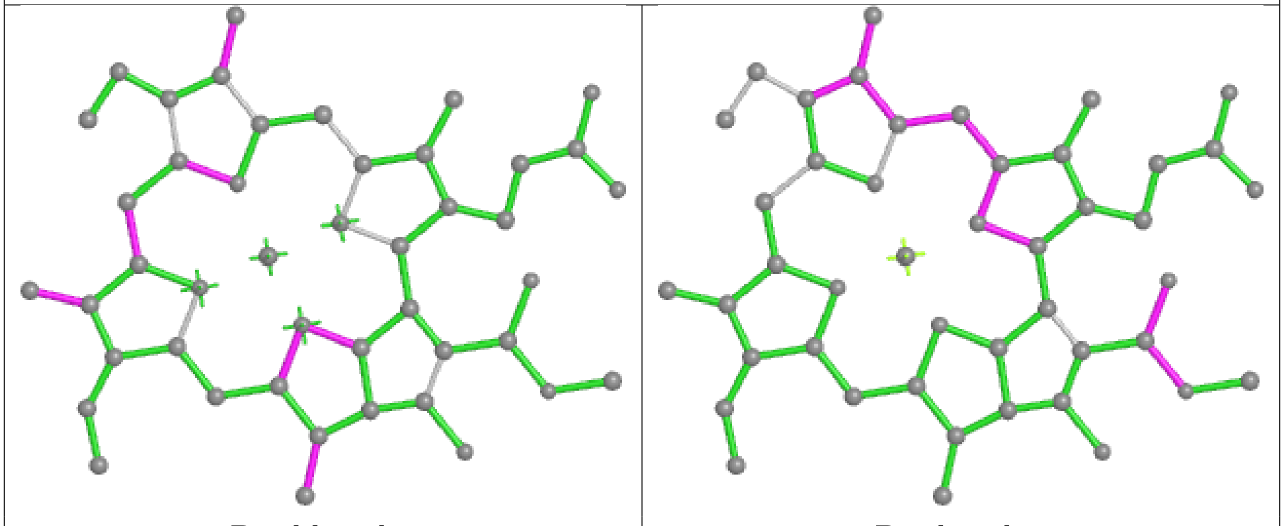


Bond lengths Bond angles

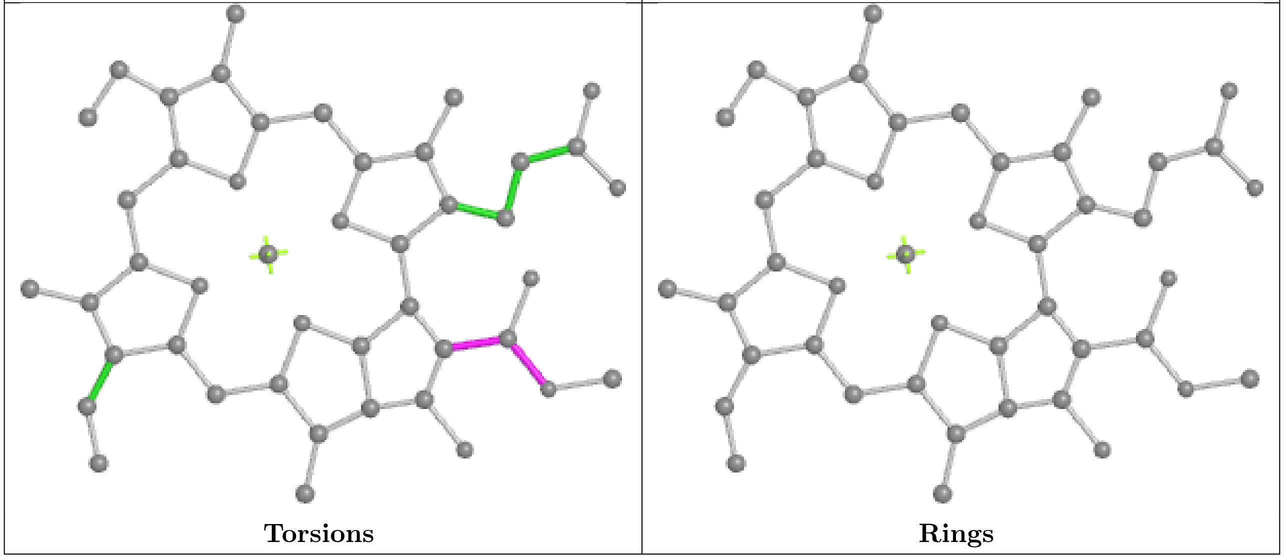


Torsions Rings

Ligand CLA A 815



Bond lengths **Bond angles**



Torsions **Rings**

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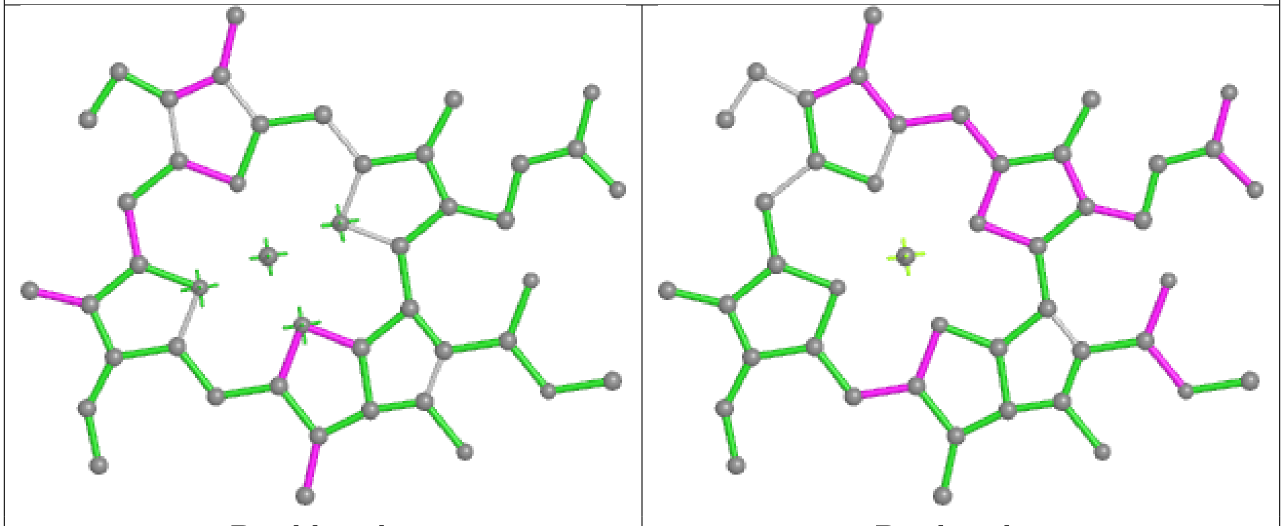
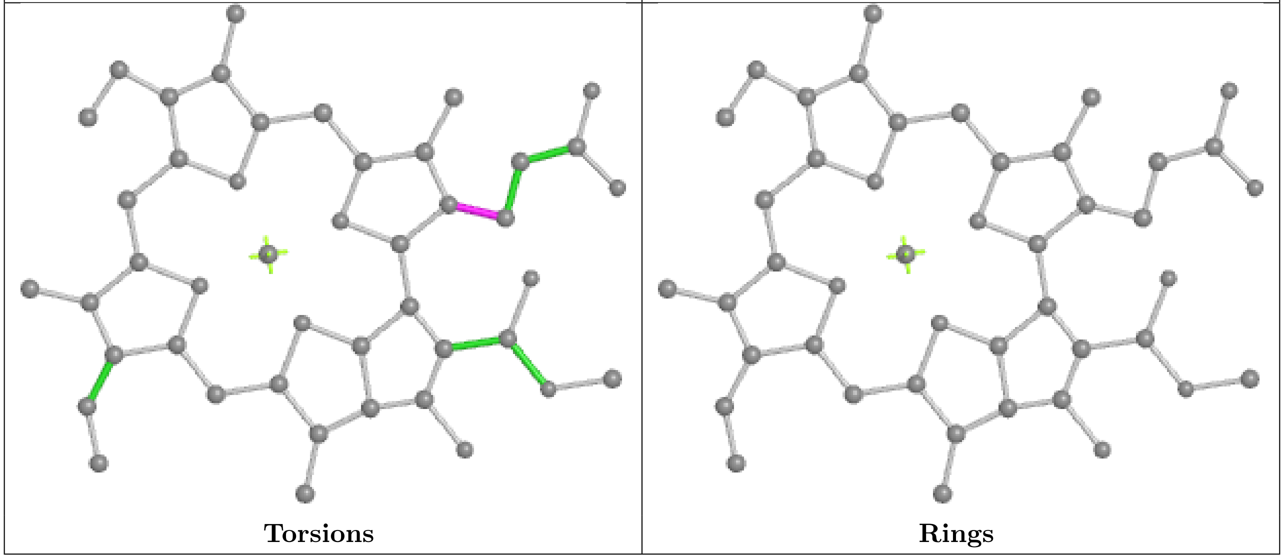
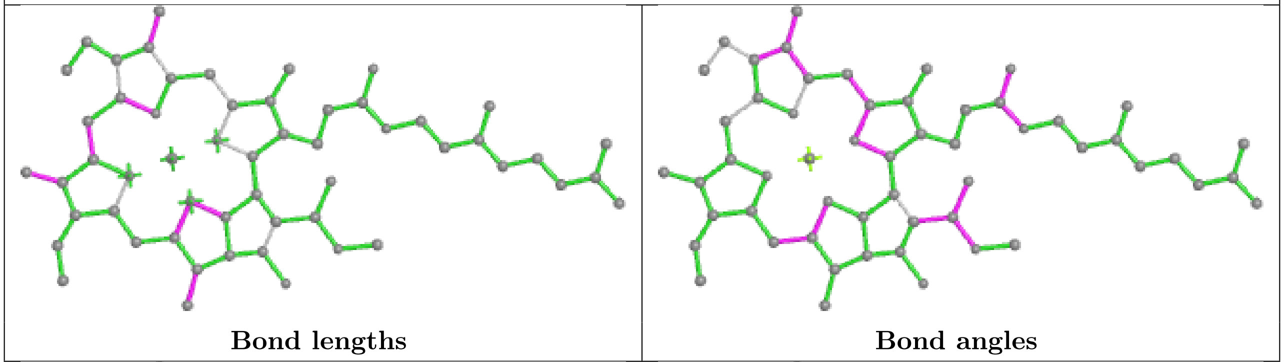


Bond lengths **Bond angles**

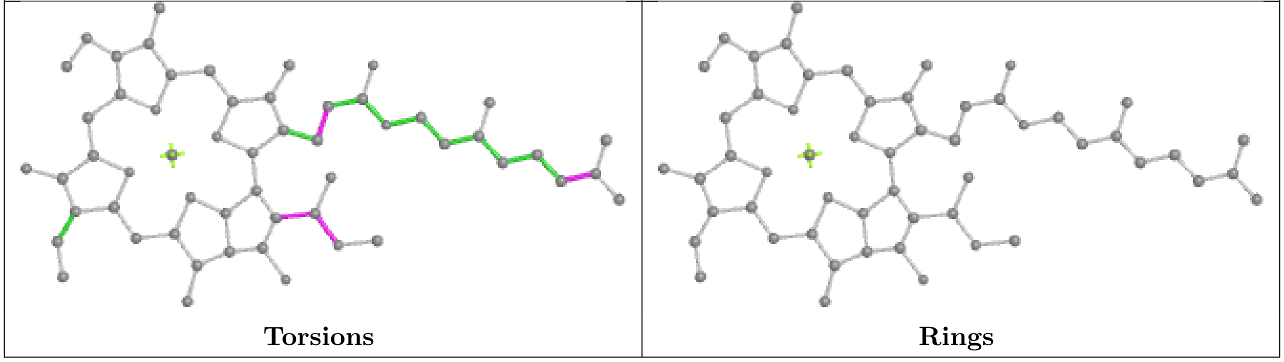


Torsions **Rings**

Ligand CLA B 807

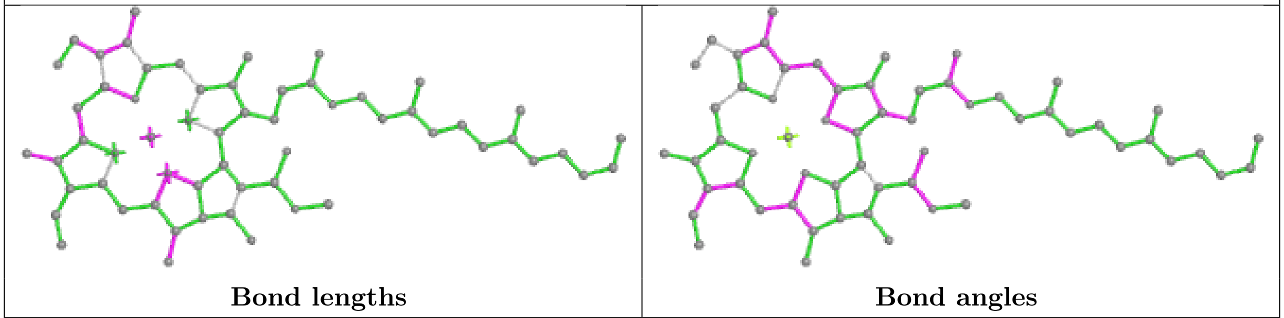


Bond lengths **Bond angles**

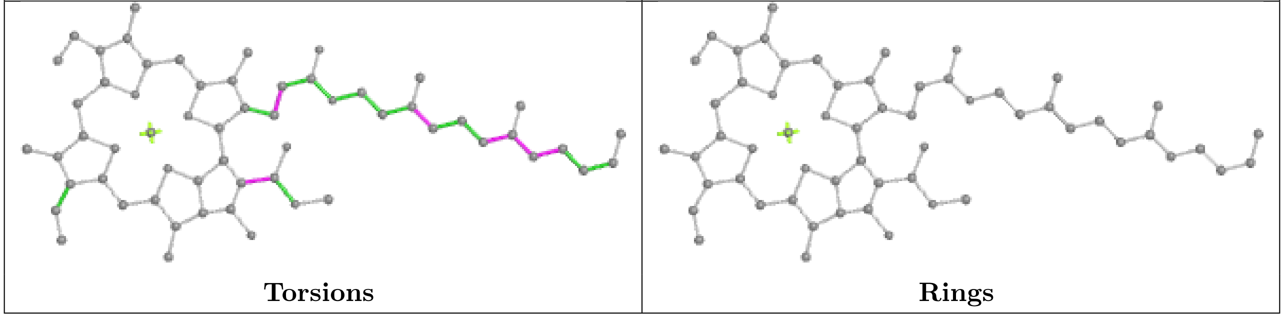


Torsions **Rings**

Ligand CLA a 816

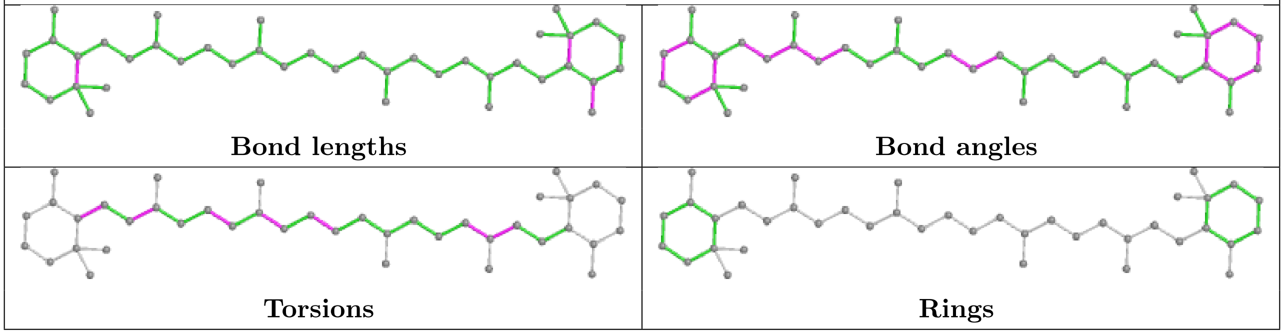


Bond lengths **Bond angles**

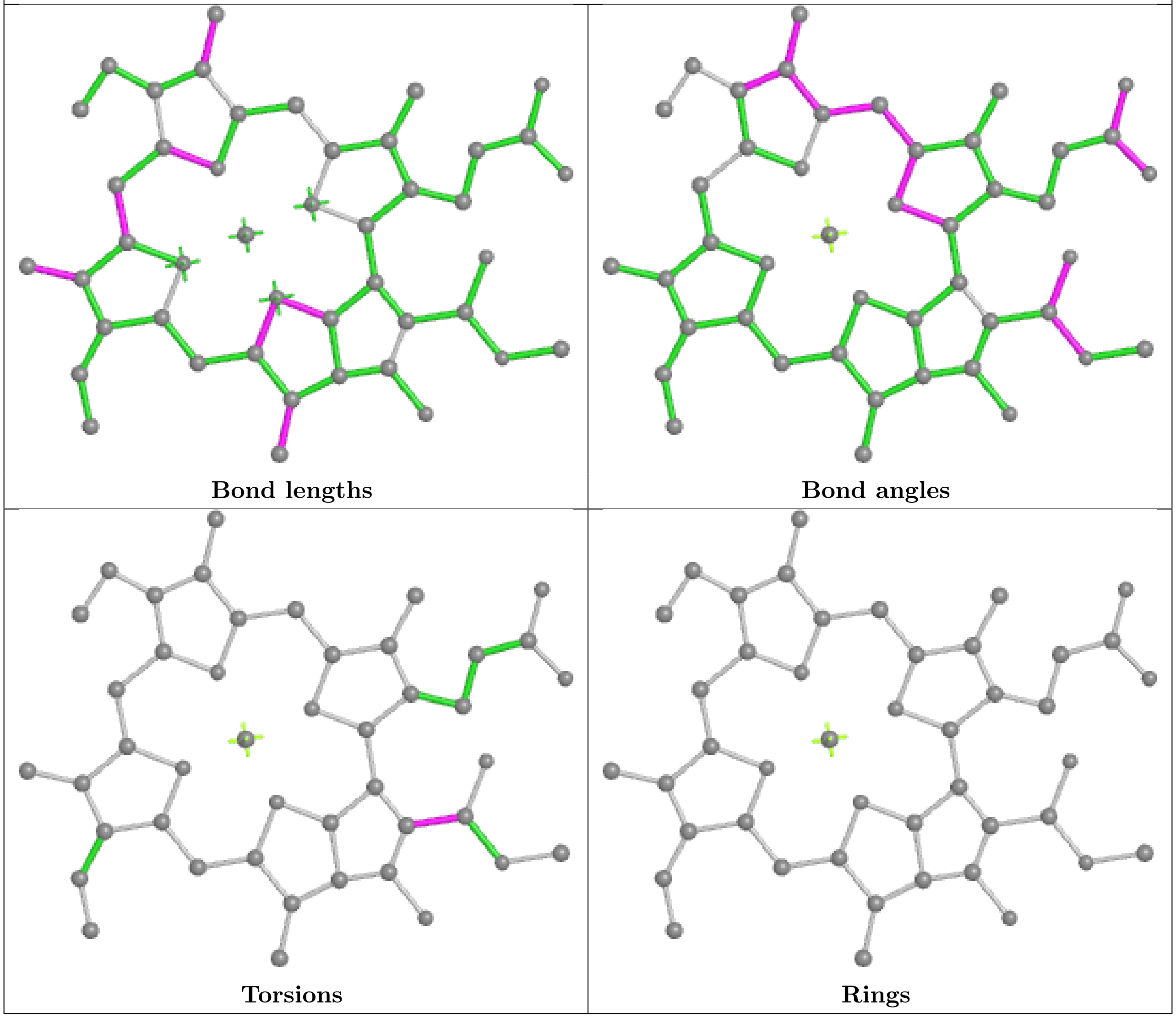


Torsions **Rings**

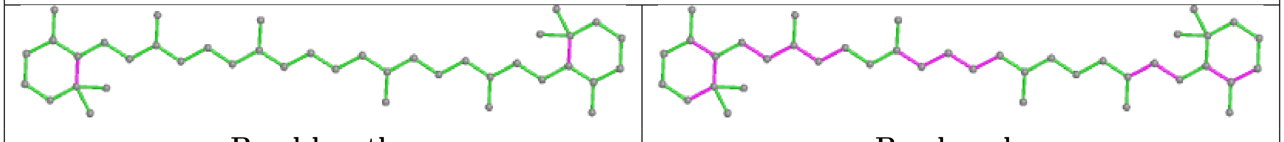
Ligand BCR B 846



Ligand CLA b 824

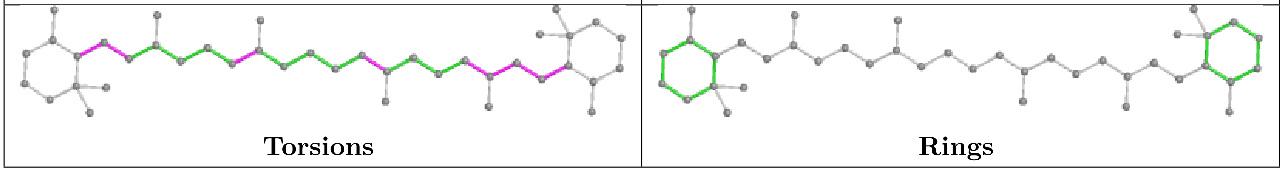


Ligand BCR K 103



Bond lengths

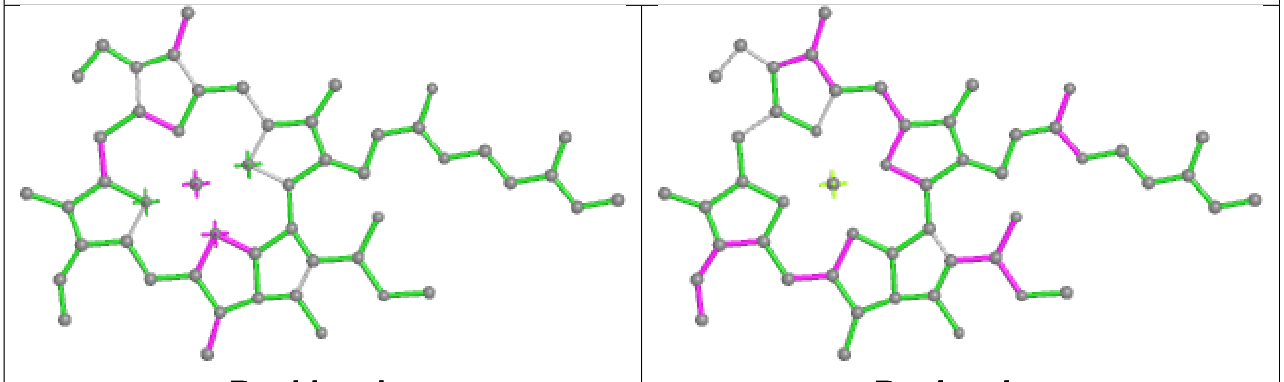
Bond angles



Torsions

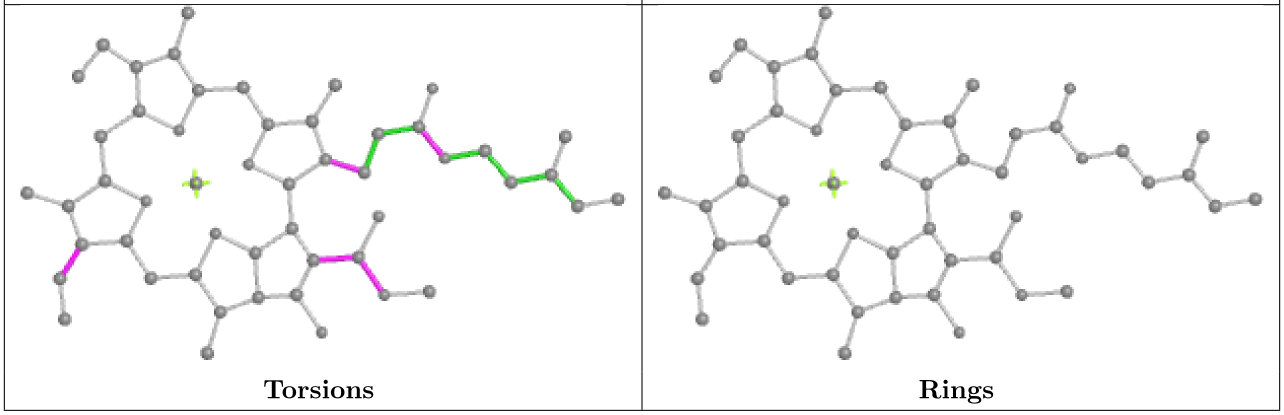
Rings

Ligand CLA A 837



Bond lengths

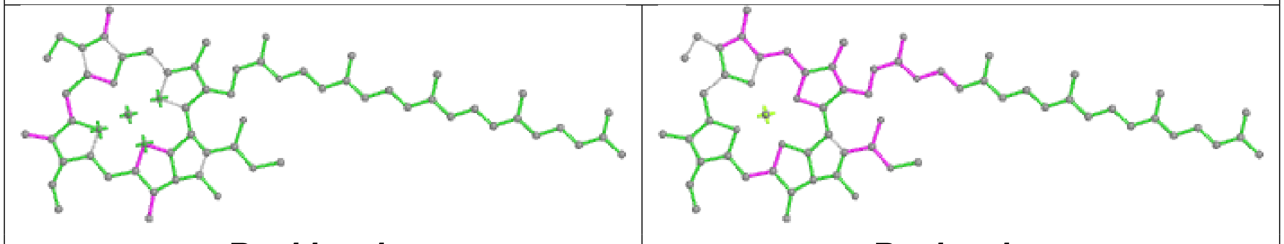
Bond angles



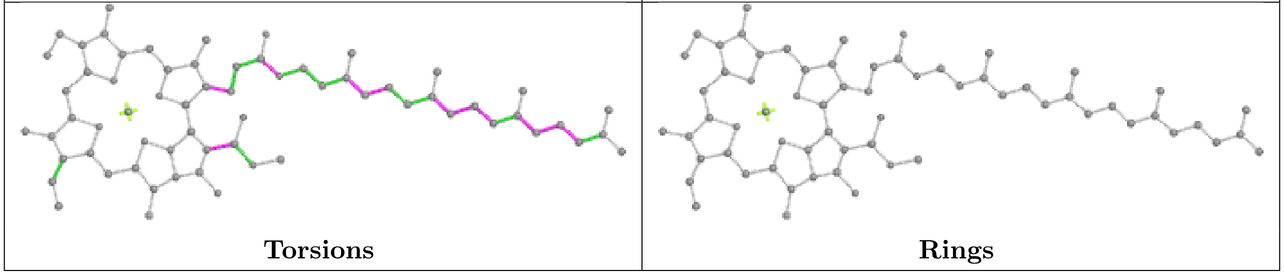
Torsions

Rings

Ligand CLA a 804

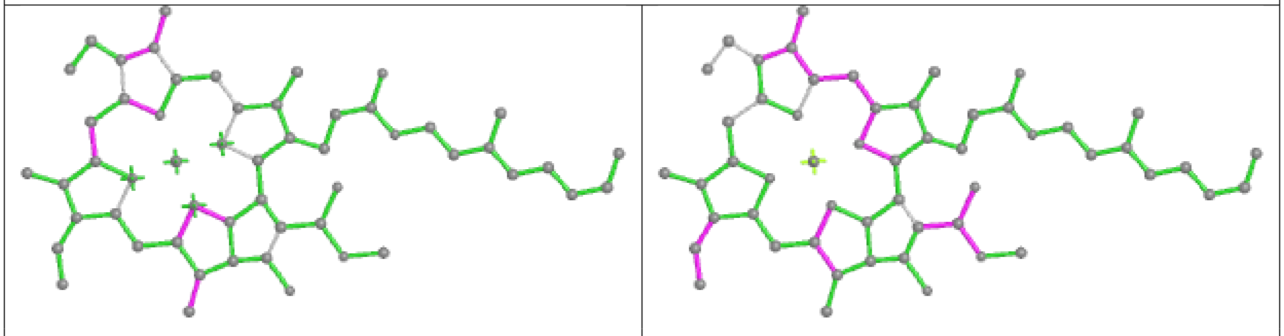


Bond lengths Bond angles

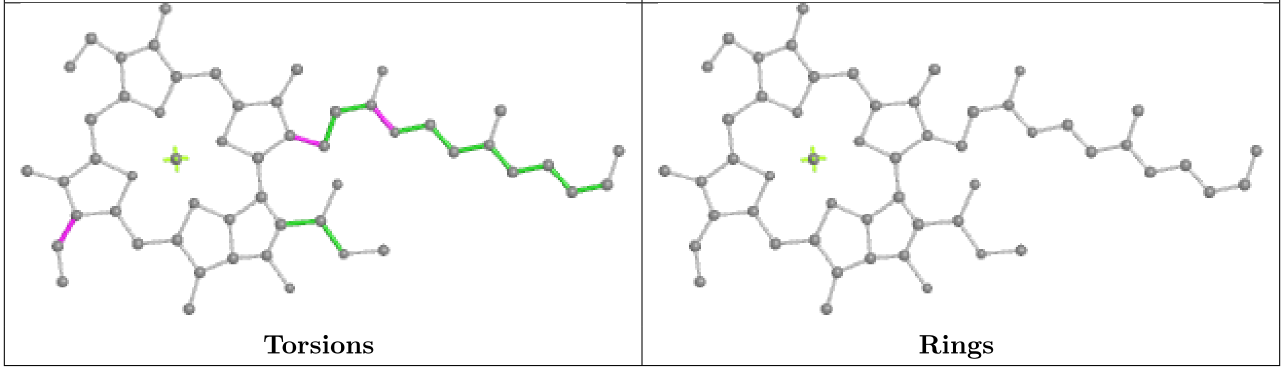


Torsions Rings

Ligand CLA B 815

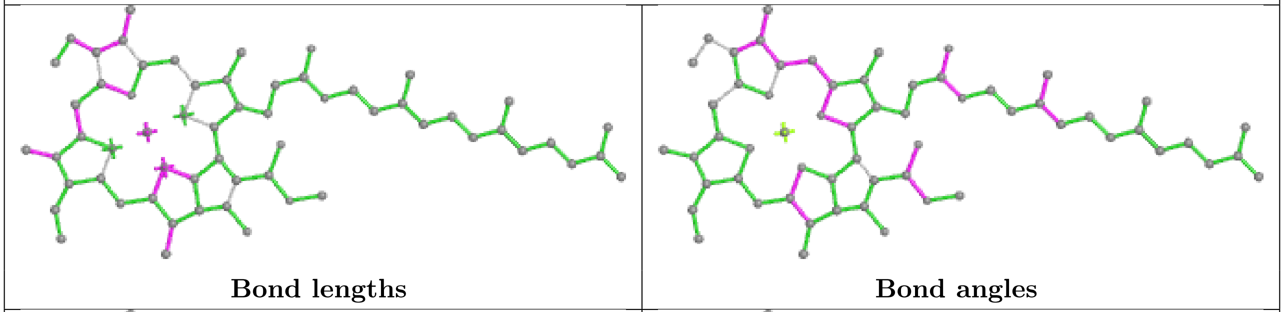


Bond lengths Bond angles



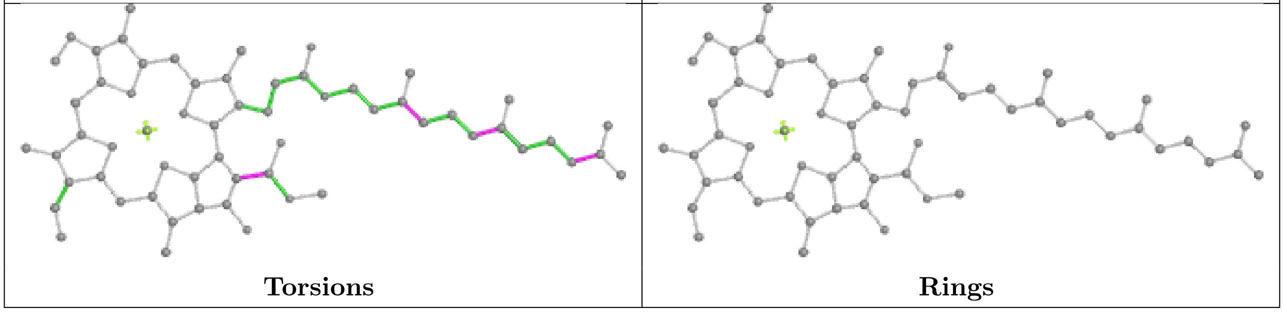
Torsions Rings

Ligand CLA a 806



Bond lengths

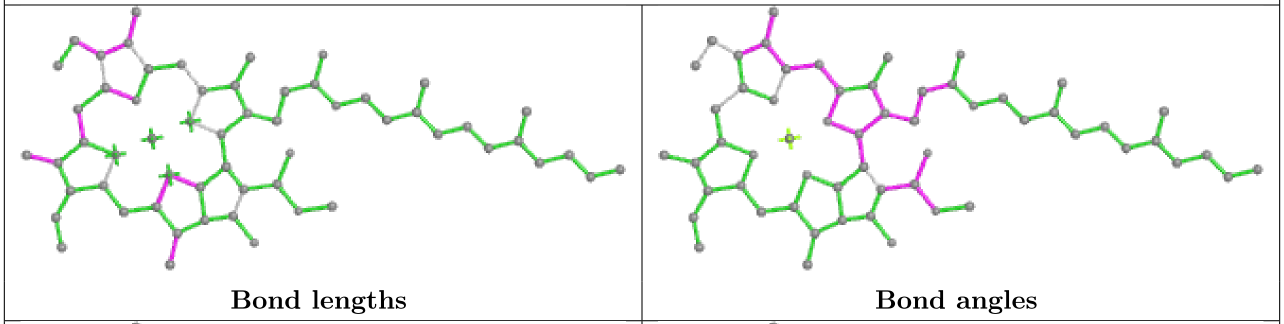
Bond angles



Torsions

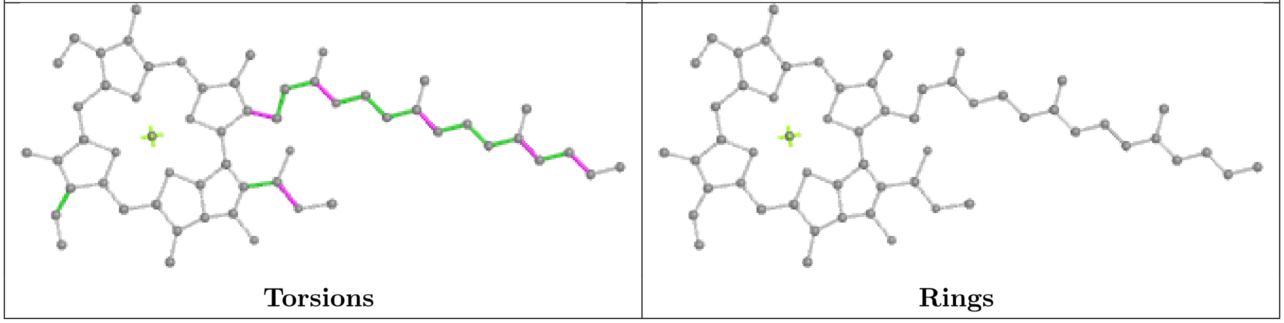
Rings

Ligand CLA j 101



Bond lengths

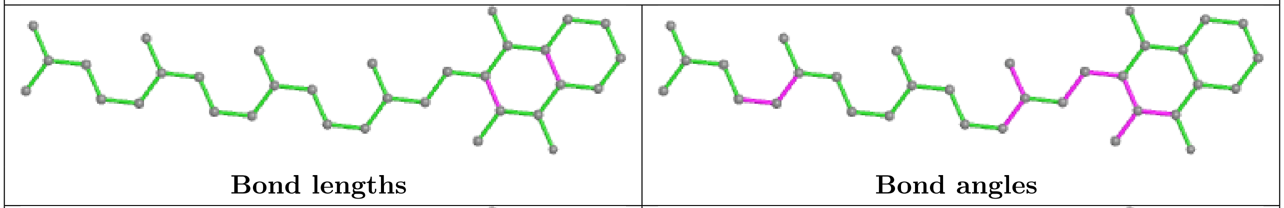
Bond angles



Torsions

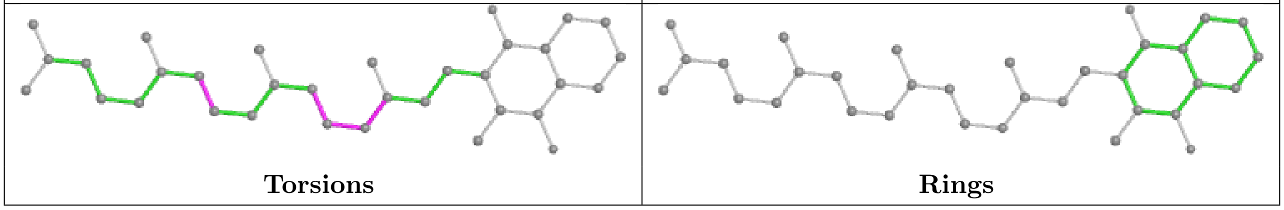
Rings

Ligand PQN a 842



Bond lengths

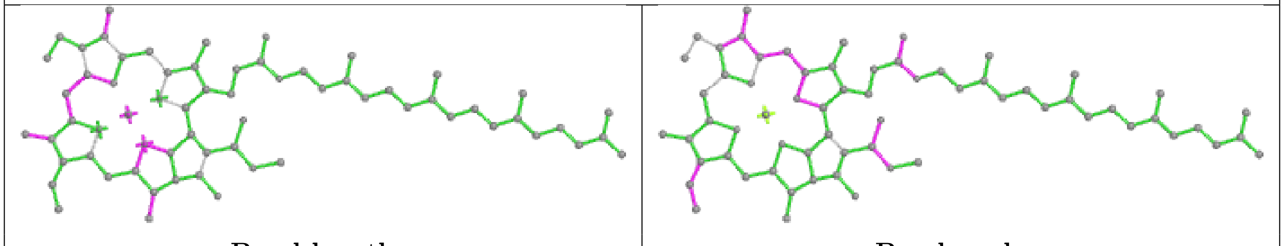
Bond angles



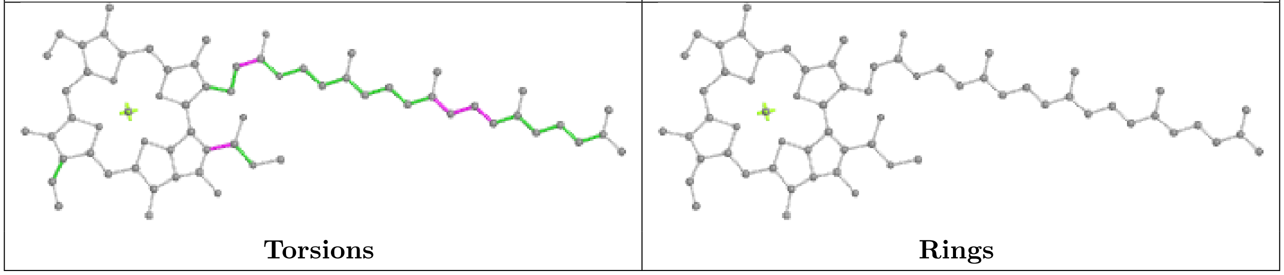
Torsions

Rings

Ligand CLA a 826

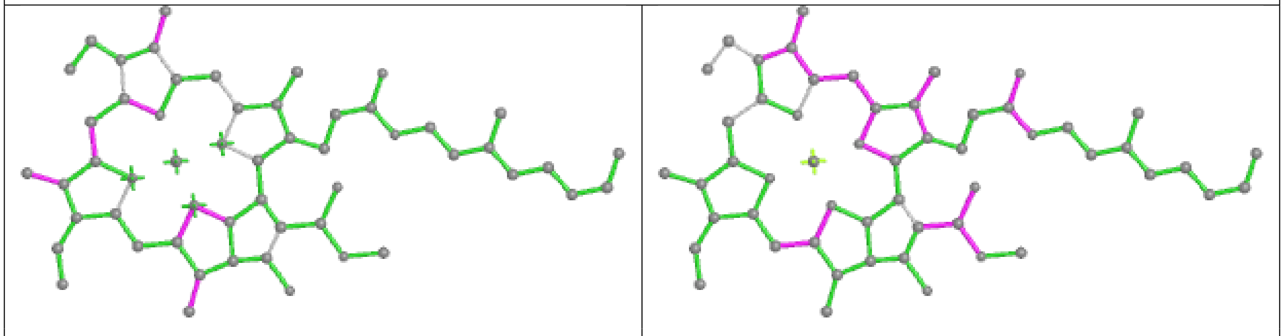


Bond lengths **Bond angles**

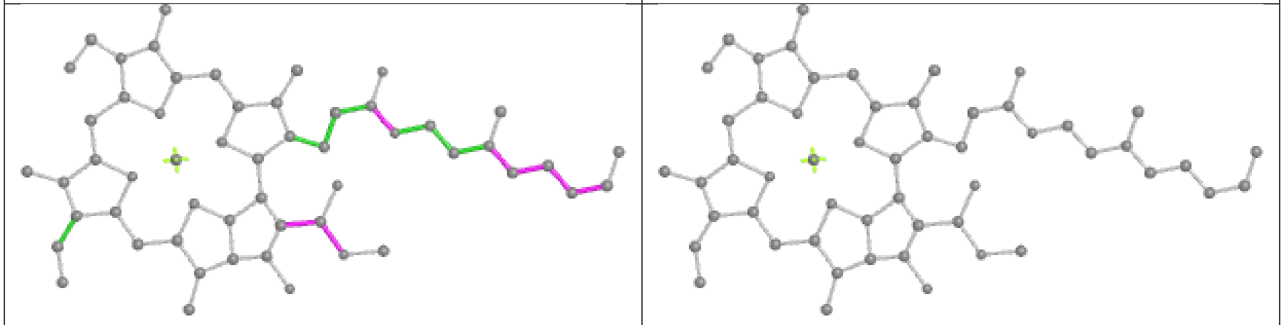


Torsions **Rings**

Ligand CLA B 814

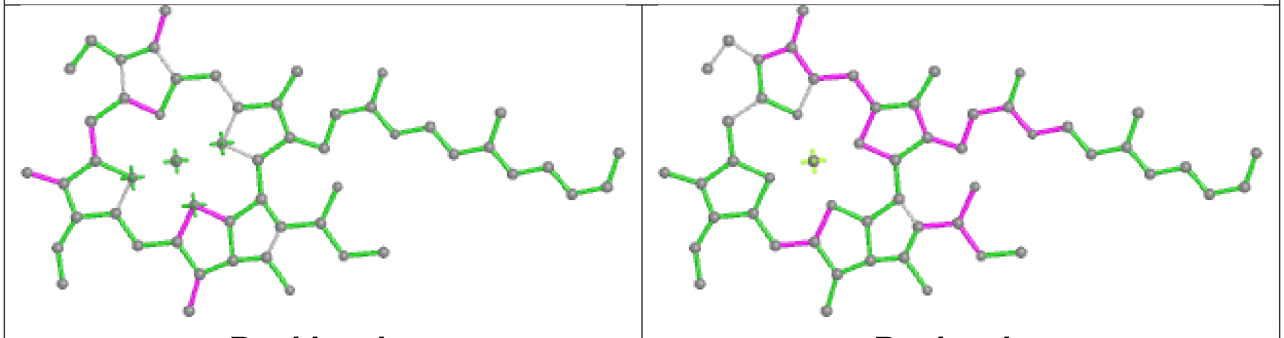


Bond lengths **Bond angles**



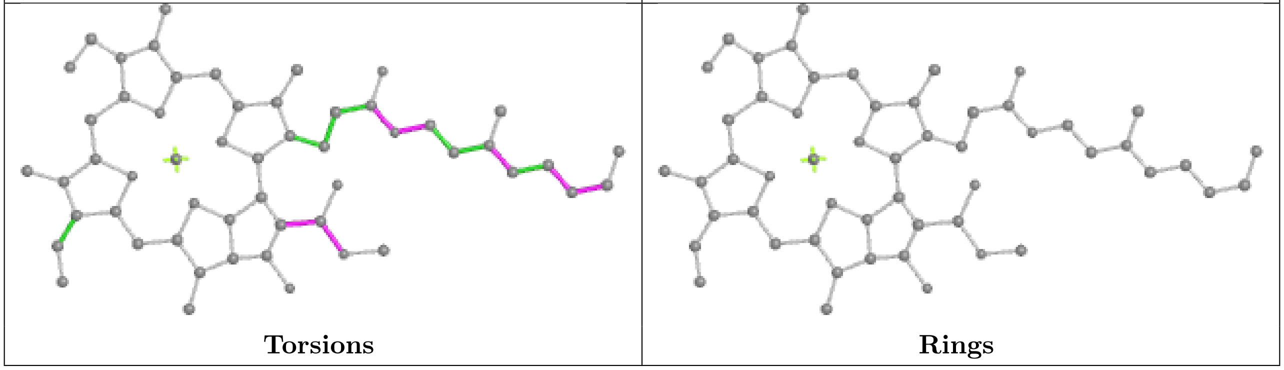
Torsions **Rings**

Ligand CLA B 836



Bond lengths

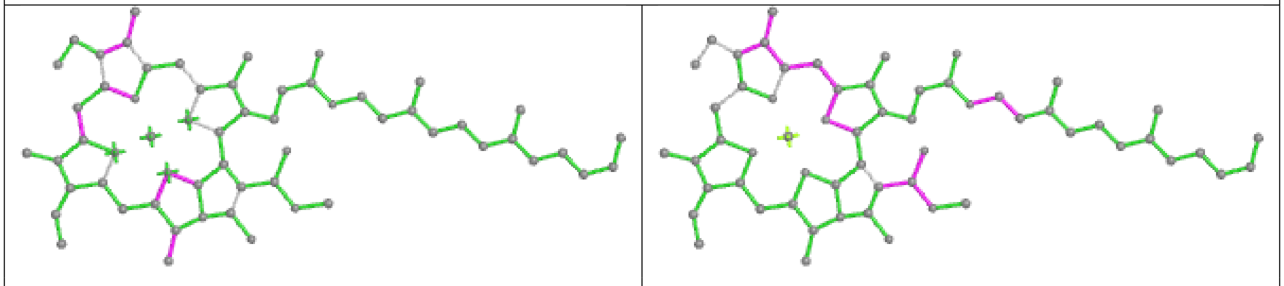
Bond angles



Torsions

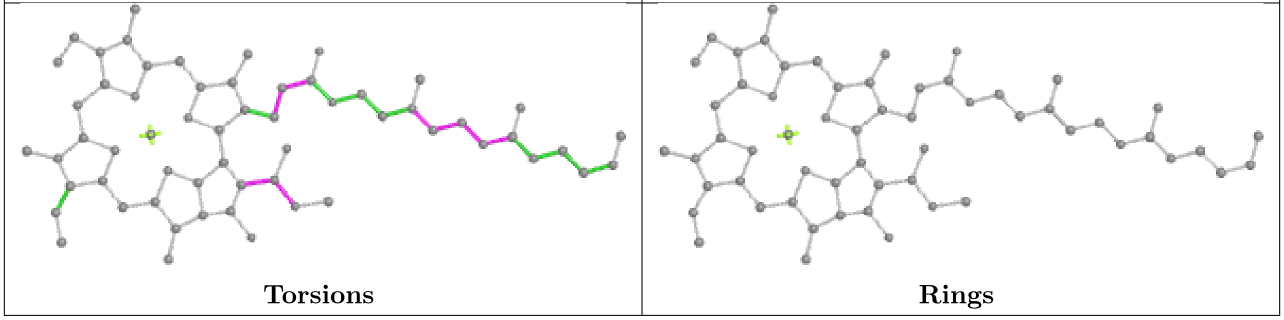
Rings

Ligand CLA a 811



Bond lengths

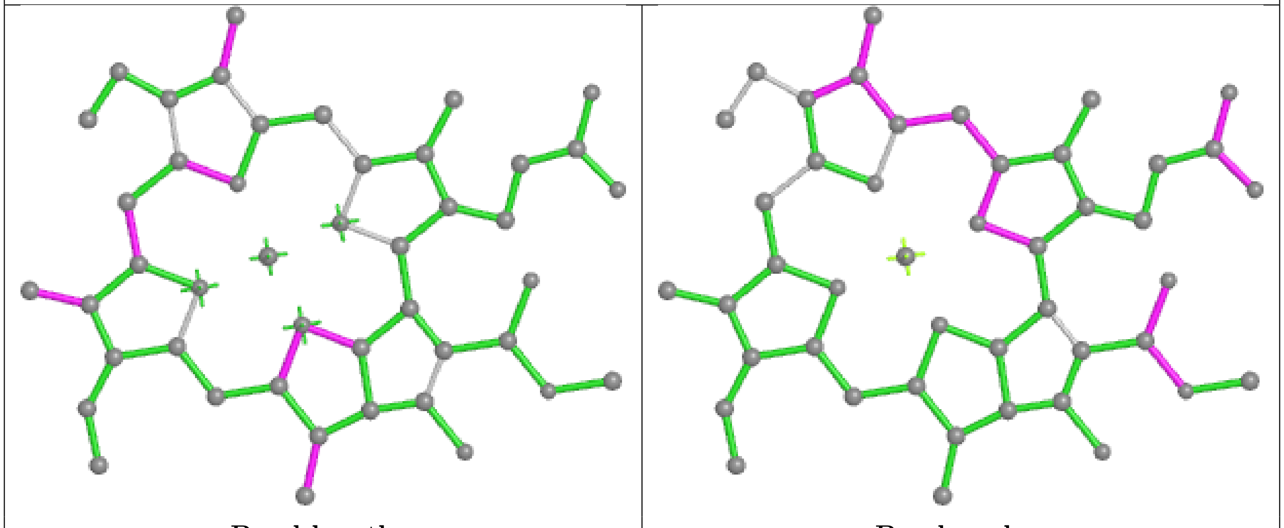
Bond angles



Torsions

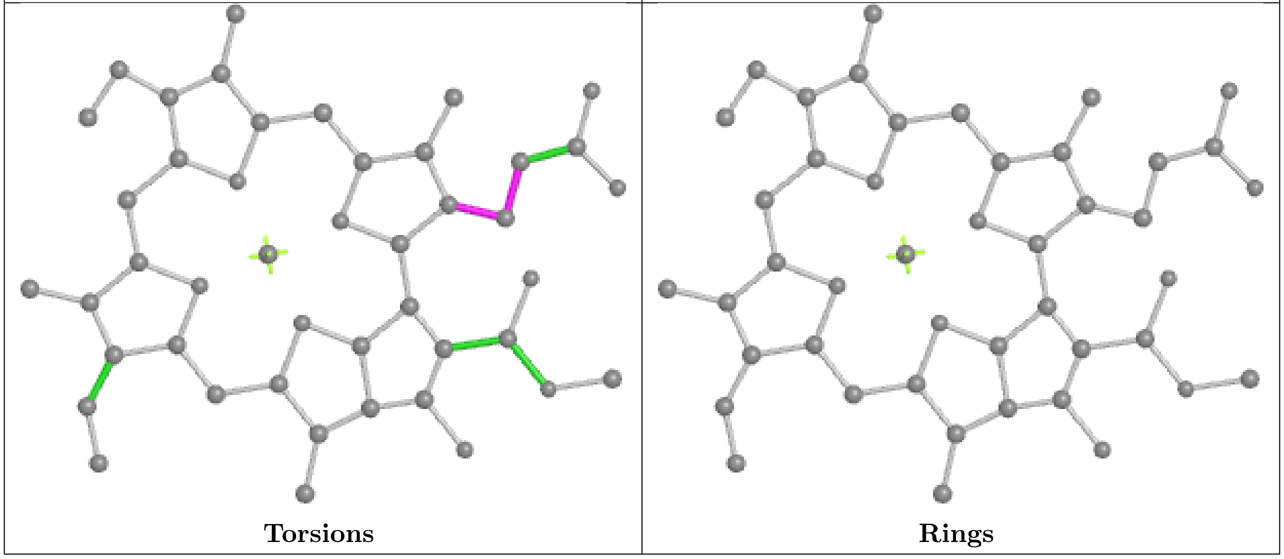
Rings

Ligand CLA A 810



Bond lengths

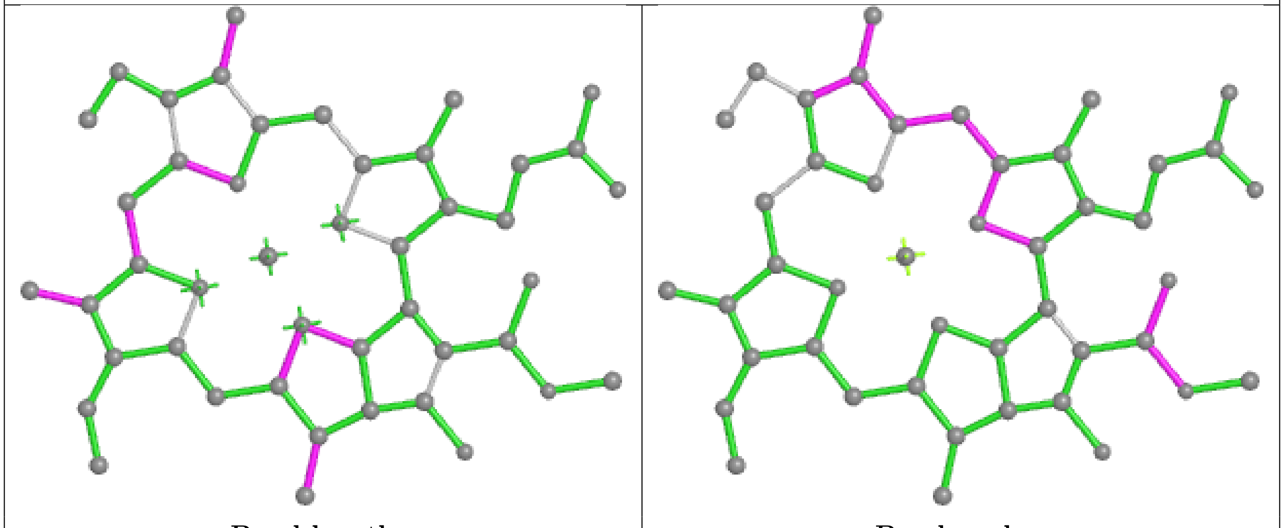
Bond angles



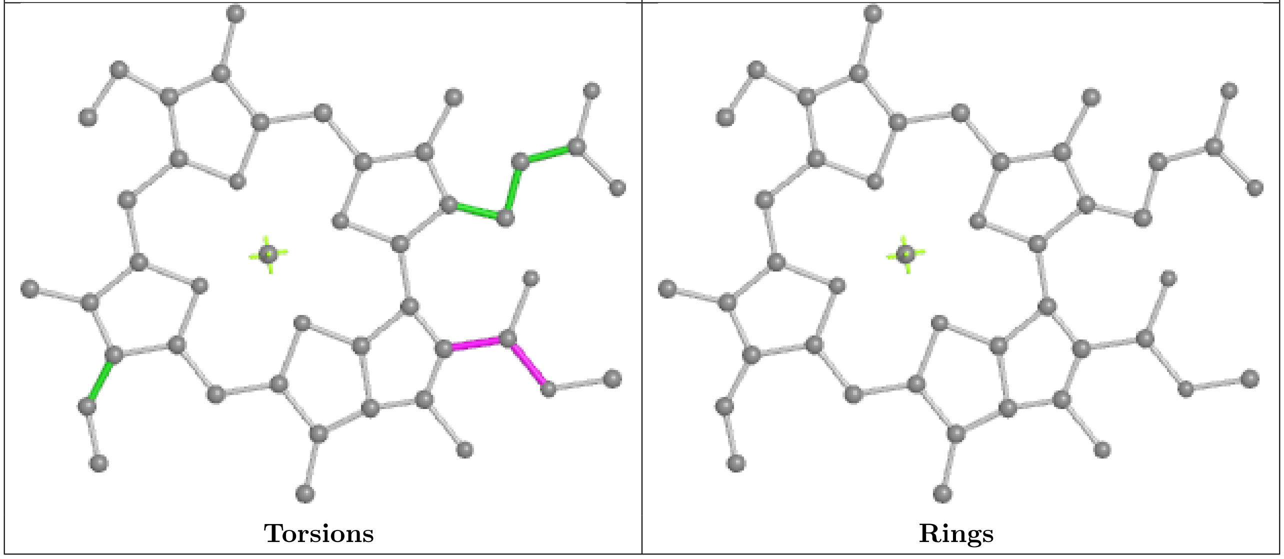
Torsions

Rings

Ligand CLA b 838

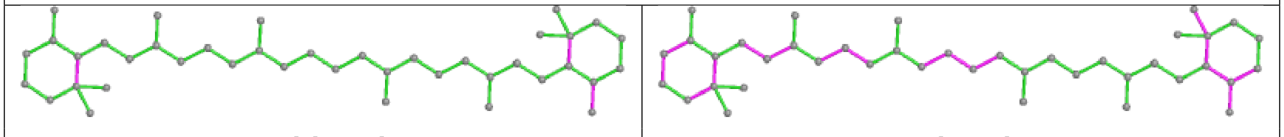


Bond lengths Bond angles

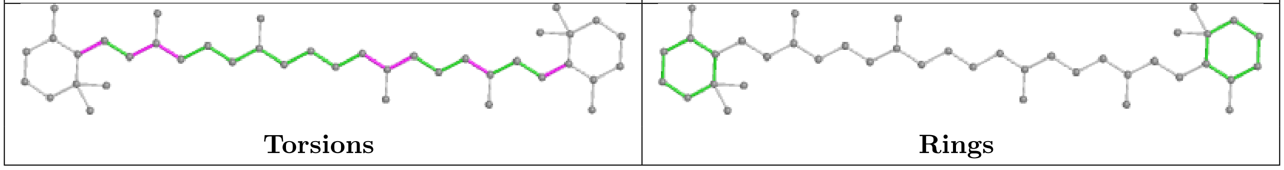


Torsions Rings

Ligand BCR b 847

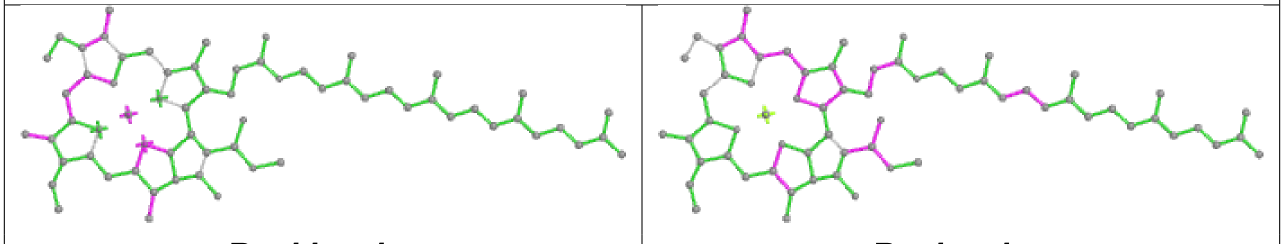


Bond lengths Bond angles



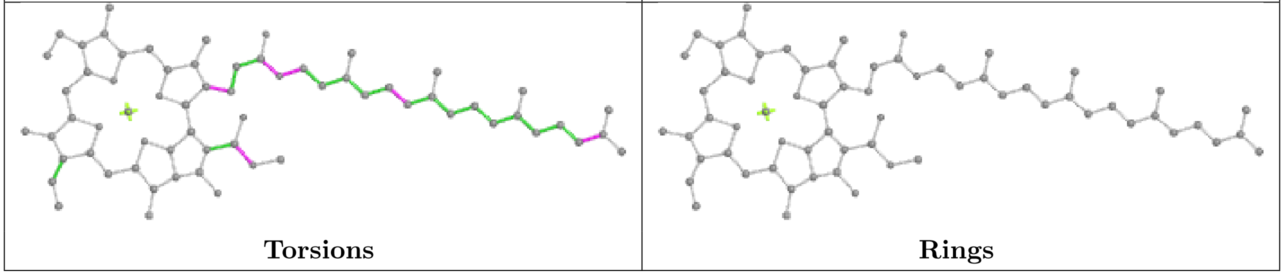
Torsions Rings

Ligand CLA B 832



Bond lengths

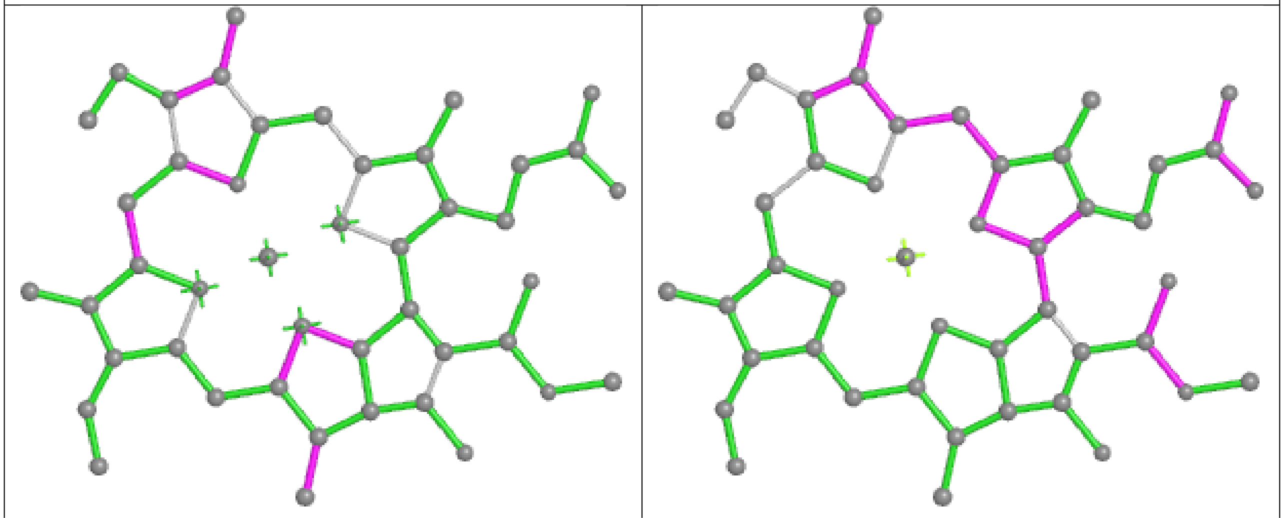
Bond angles



Torsions

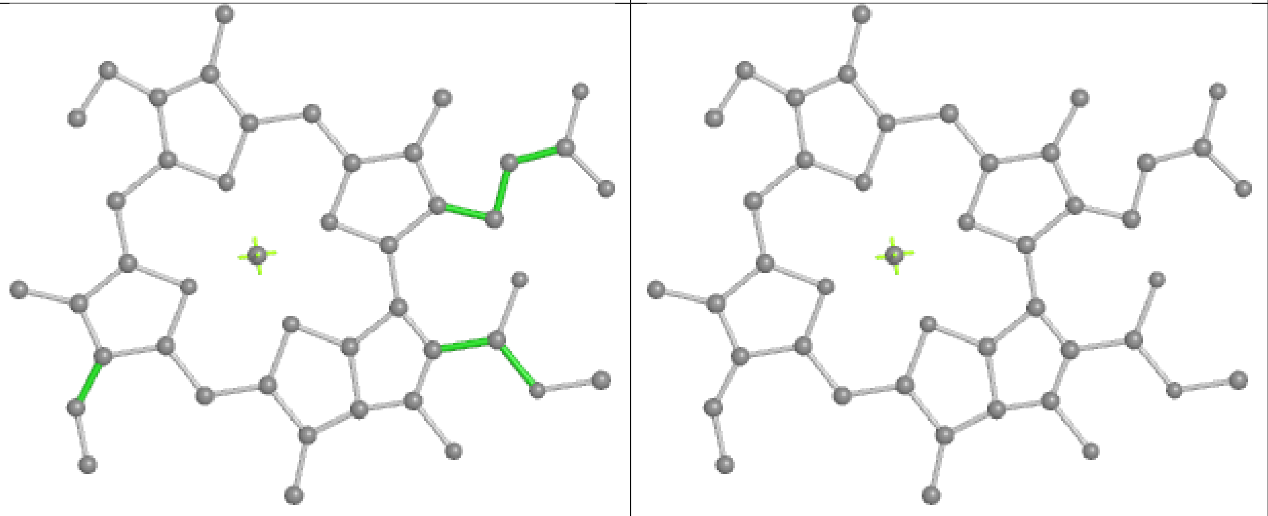
Rings

Ligand CLA A 816



Bond lengths

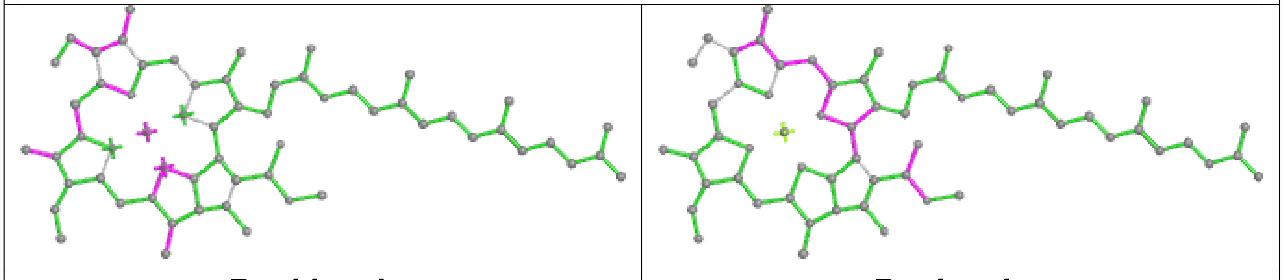
Bond angles



Torsions

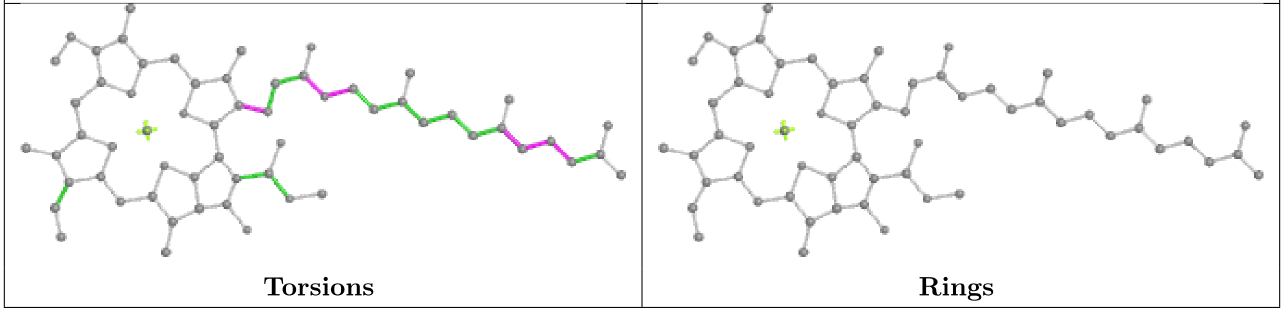
Rings

Ligand CLA A 818



Bond lengths

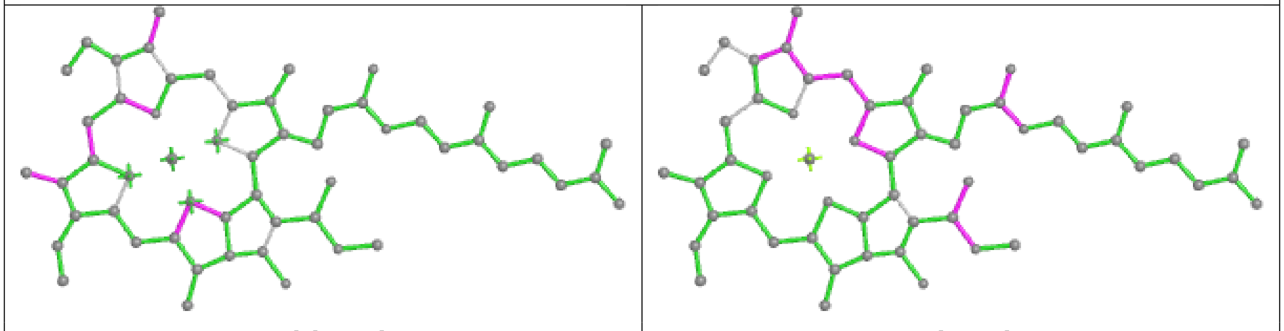
Bond angles



Torsions

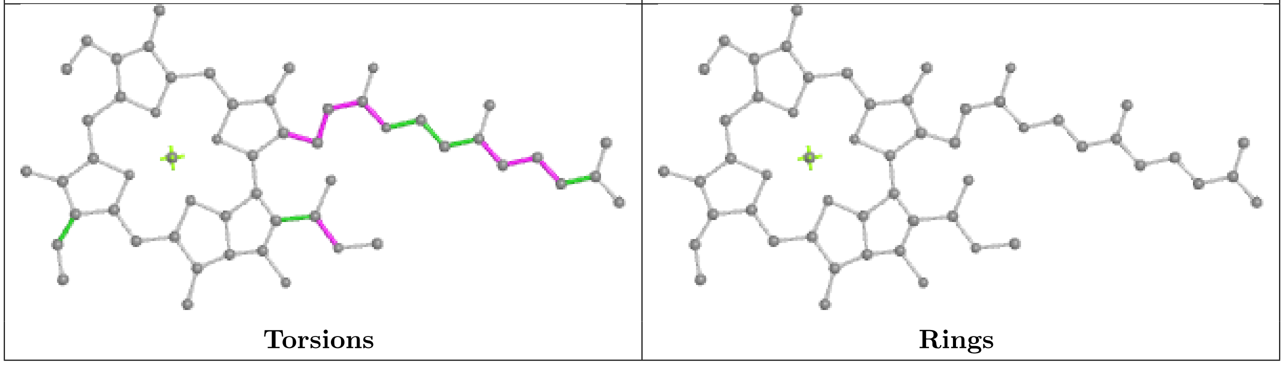
Rings

Ligand CLA B 825



Bond lengths

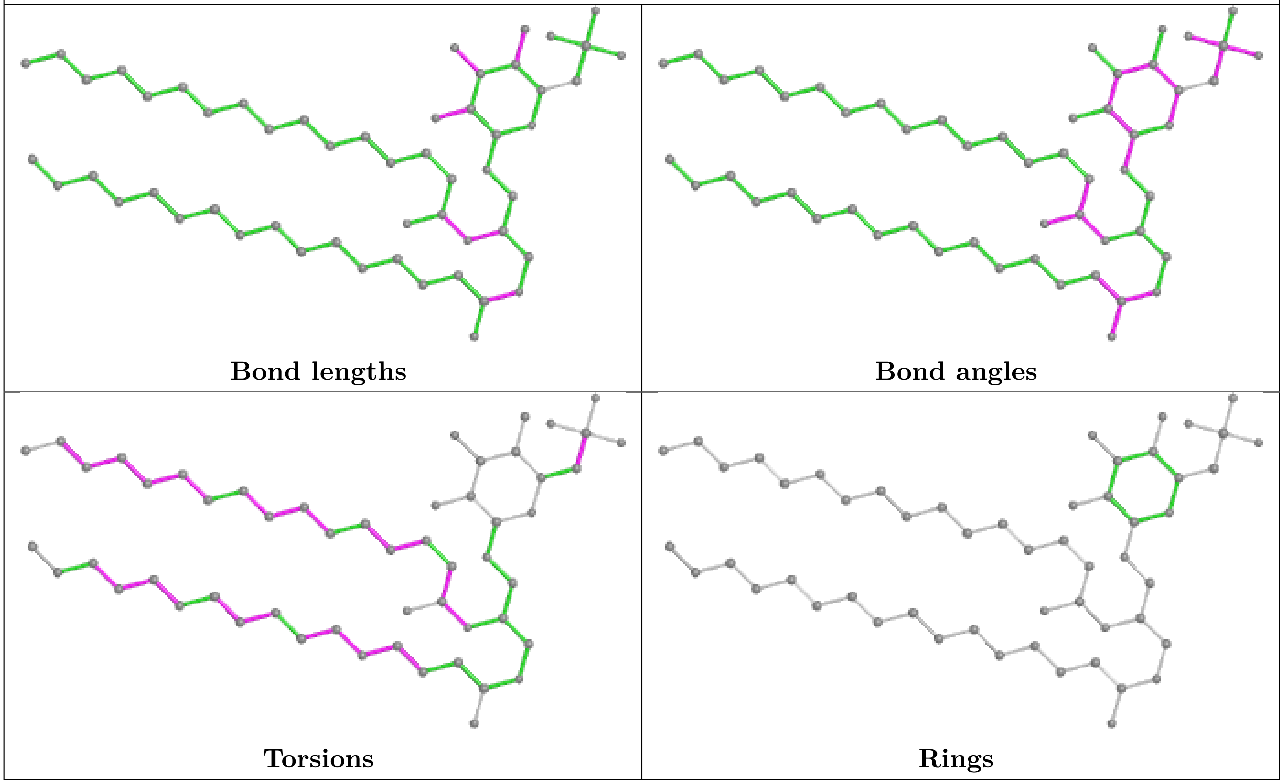
Bond angles



Torsions

Rings

Ligand SQD b 801



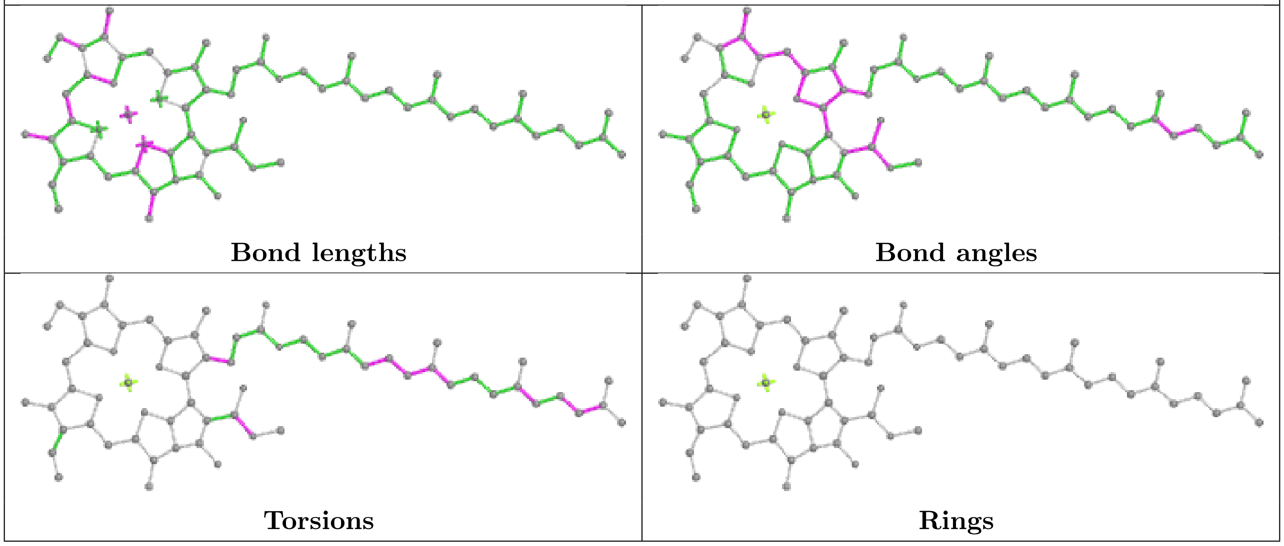
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA A 806



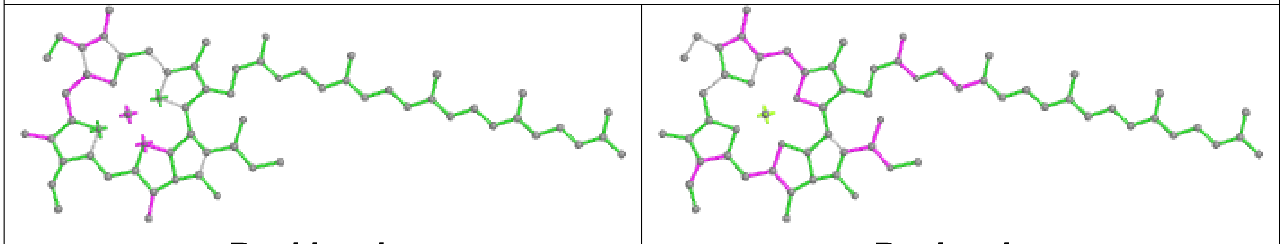
Bond lengths

Bond angles

Torsions

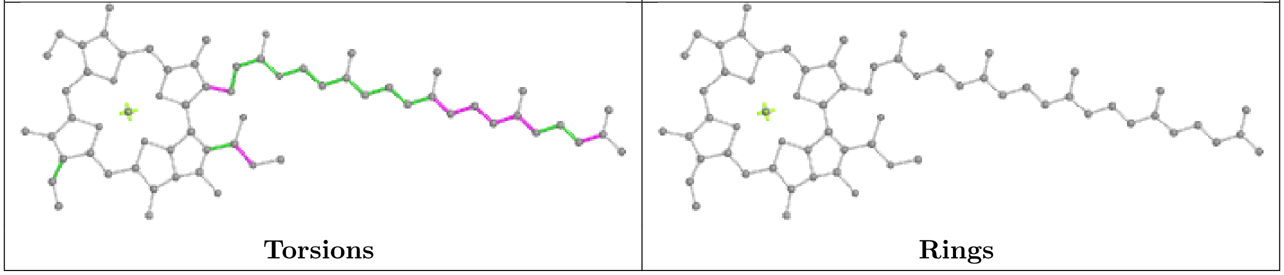
Rings

Ligand CLA b 807



Bond lengths

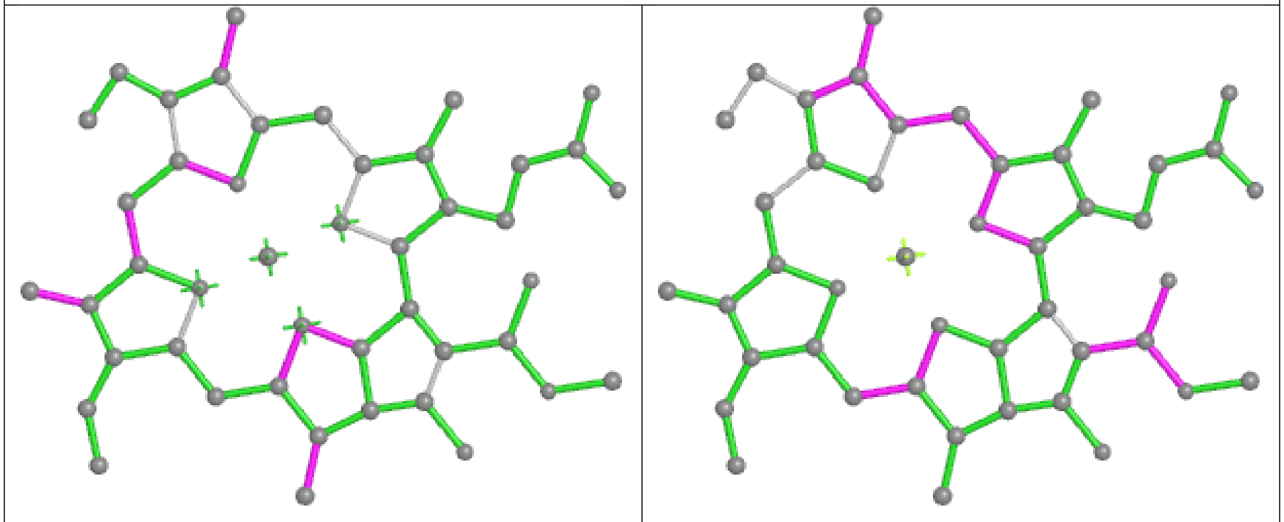
Bond angles



Torsions

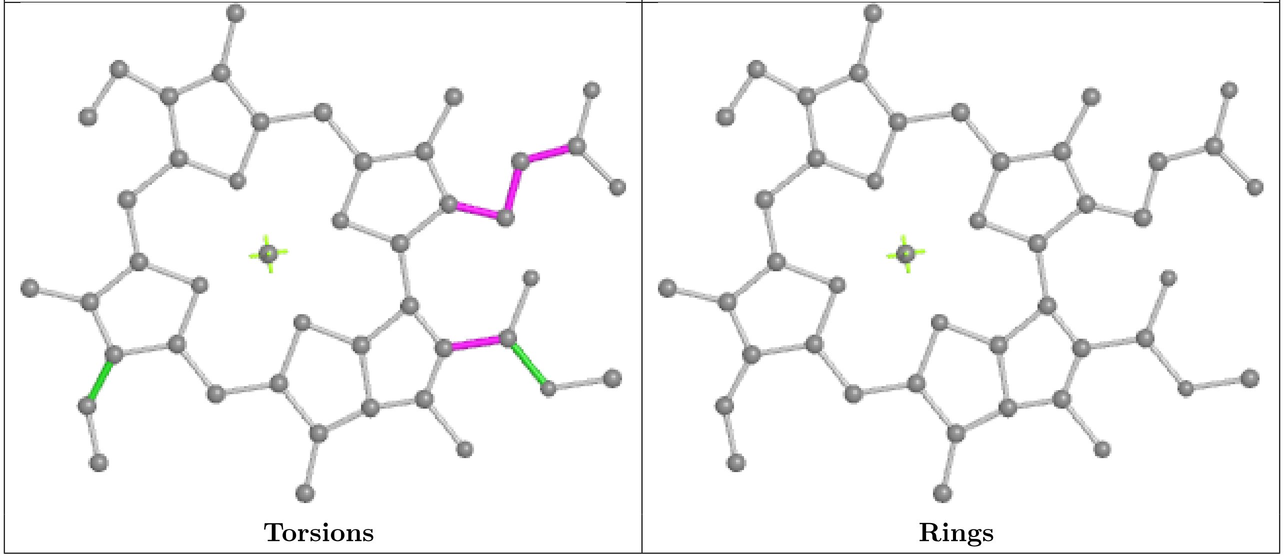
Rings

Ligand CLA A 822



Bond lengths

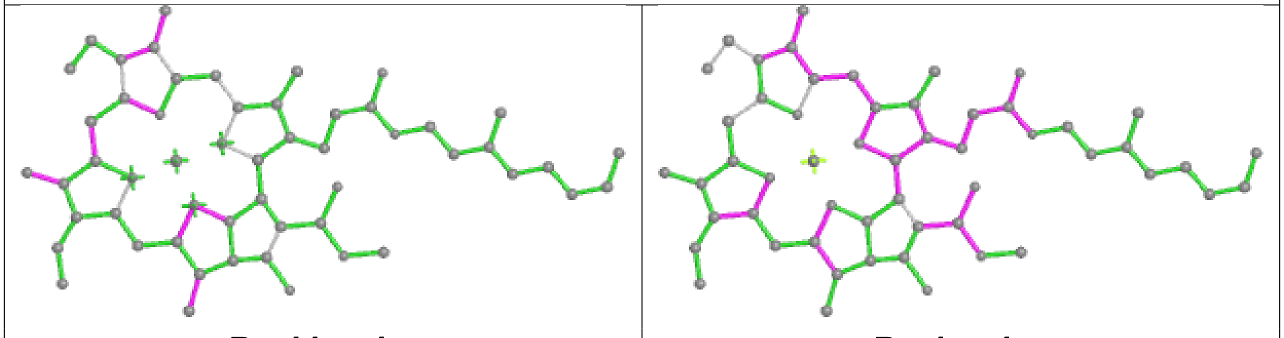
Bond angles



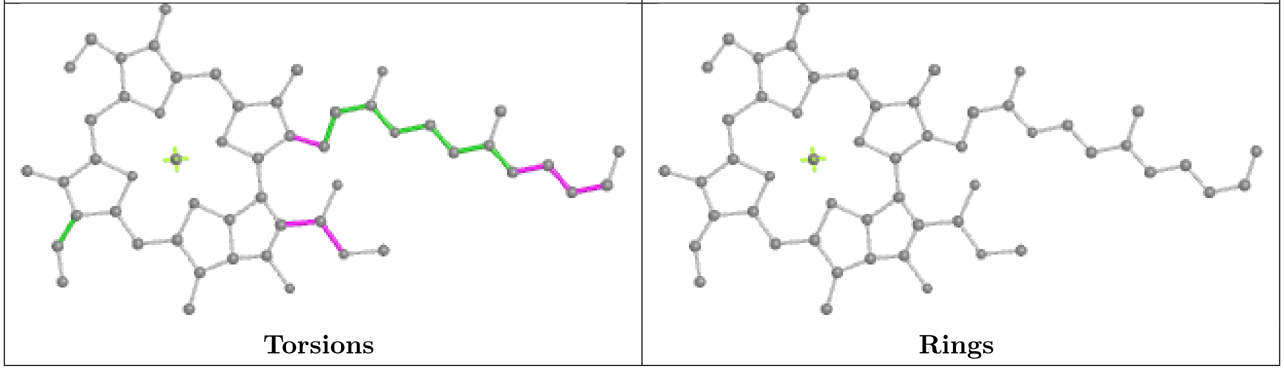
Torsions

Rings

Ligand CLA b 836

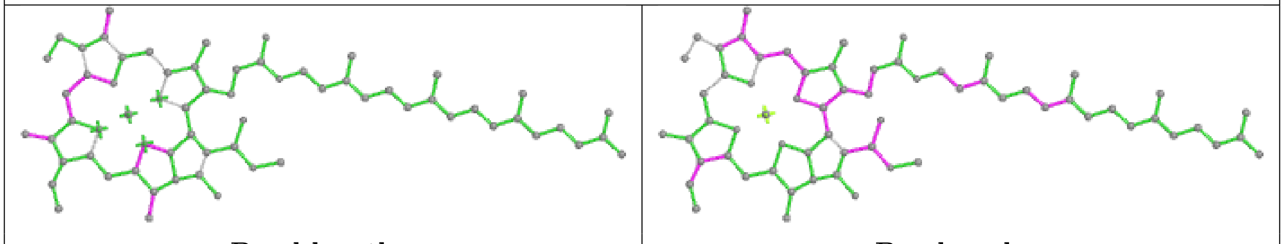


Bond lengths Bond angles

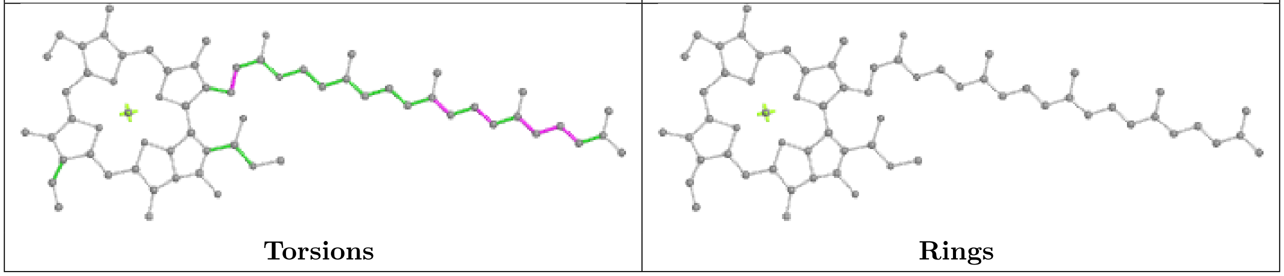


Torsions Rings

Ligand CLA B 827

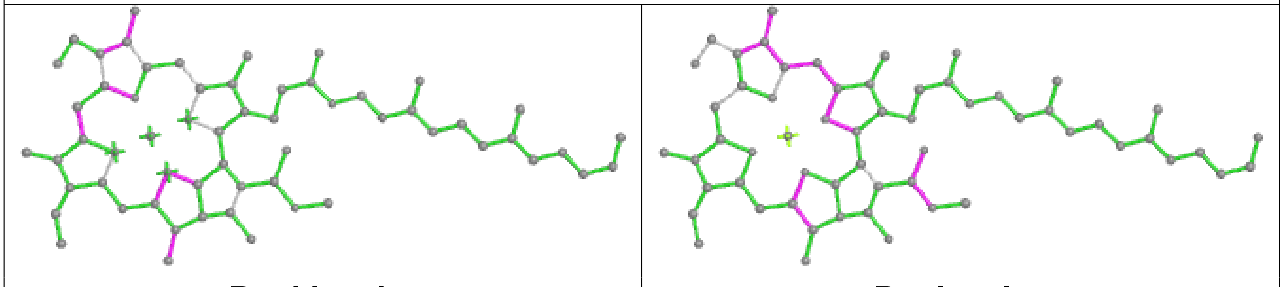


Bond lengths Bond angles

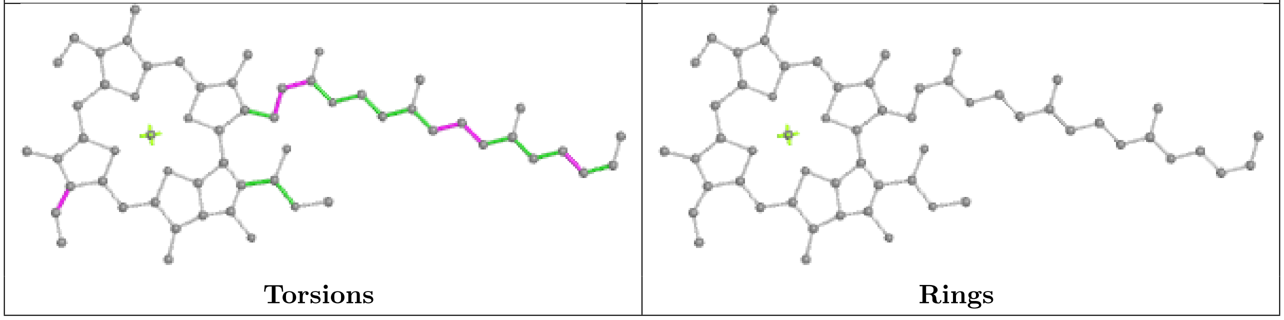


Torsions Rings

Ligand CLA A 812

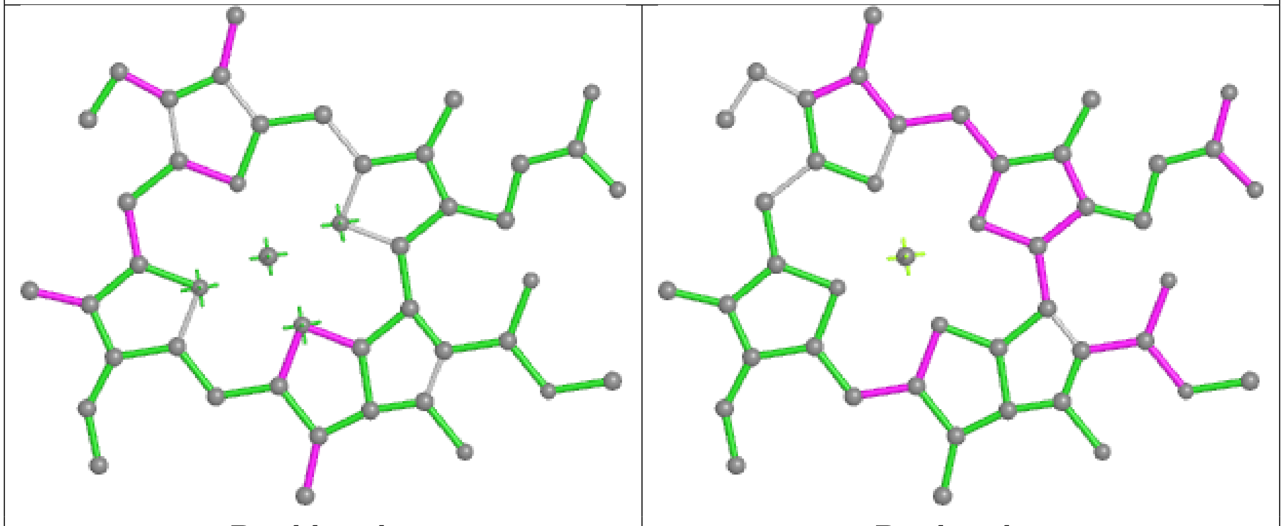


Bond lengths **Bond angles**

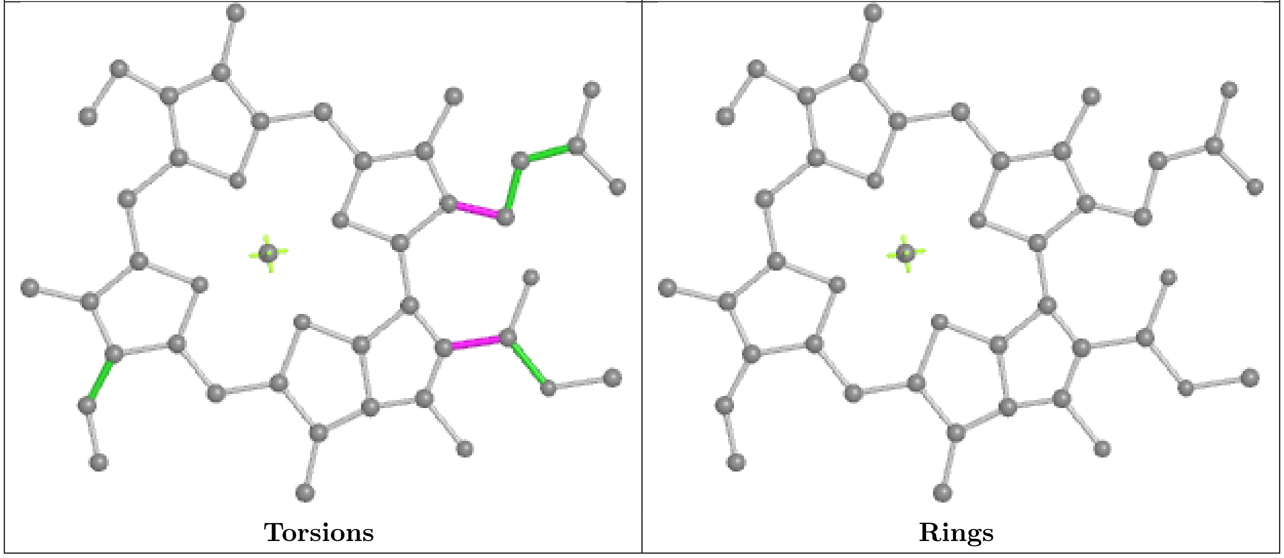


Torsions **Rings**

Ligand CLA a 821

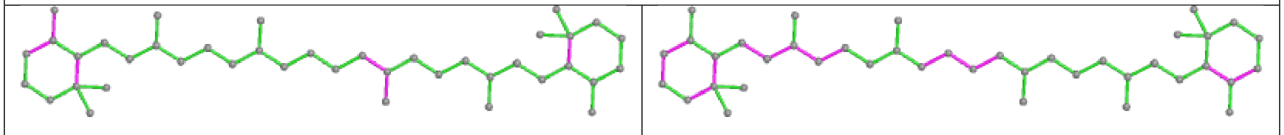


Bond lengths Bond angles

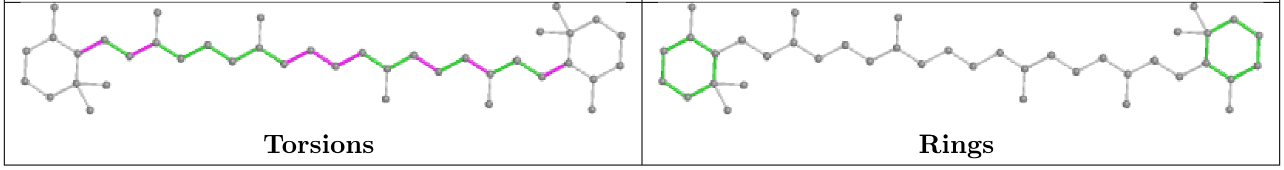


Torsions Rings

Ligand BCR B 849

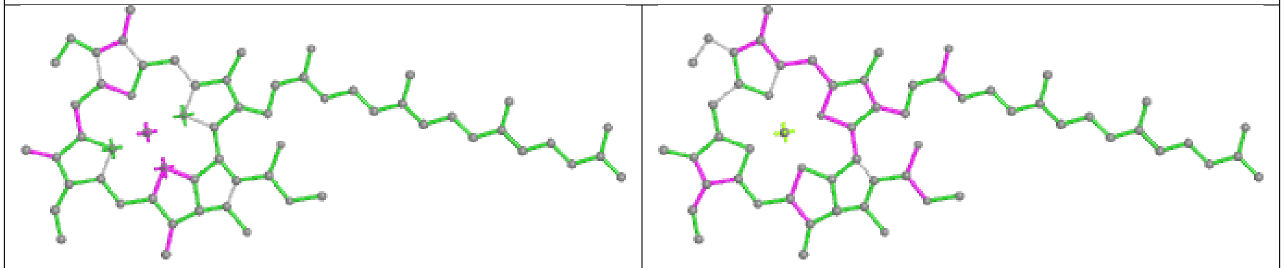


Bond lengths Bond angles



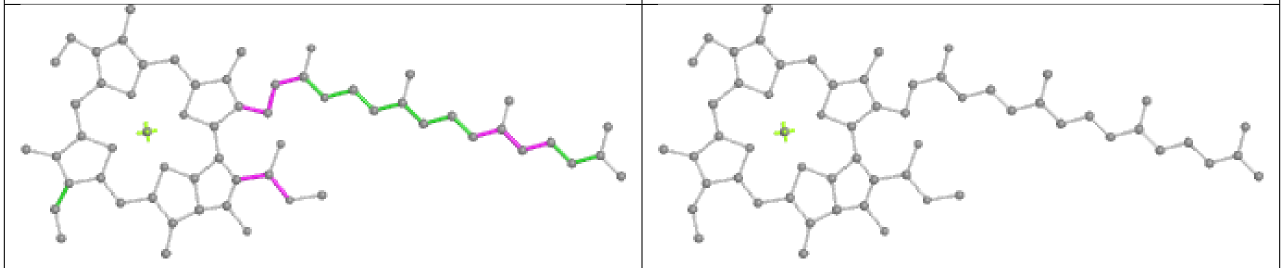
Torsions Rings

Ligand CLA A 813



Bond lengths

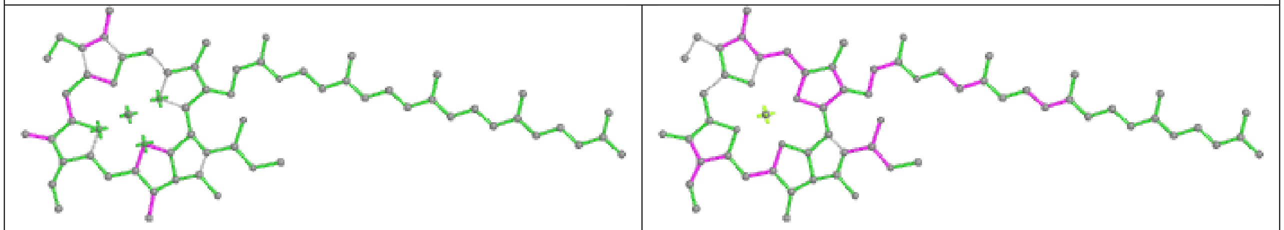
Bond angles



Torsions

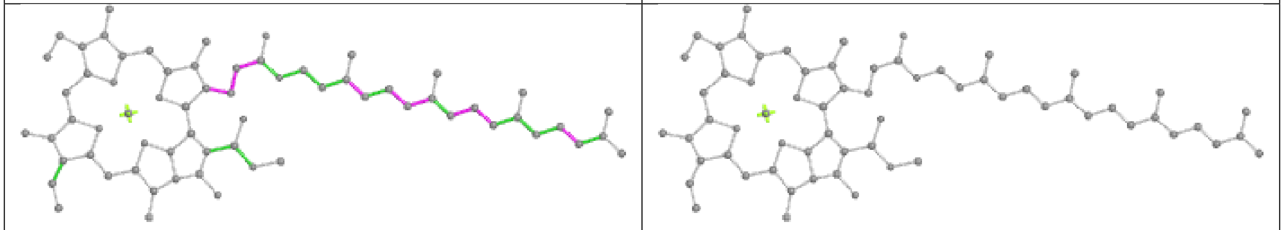
Rings

Ligand CLA B 812



Bond lengths

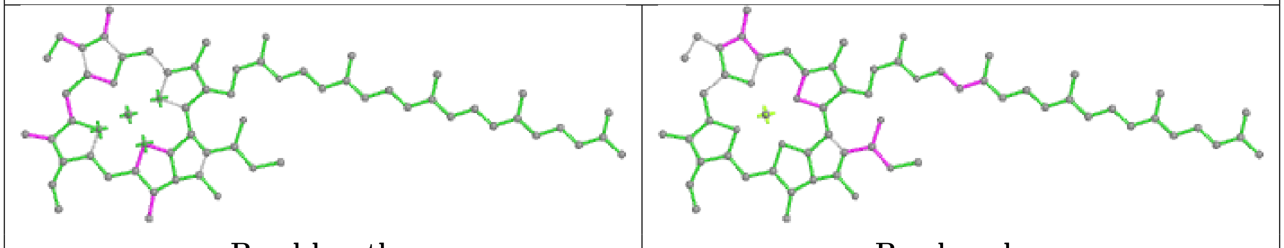
Bond angles



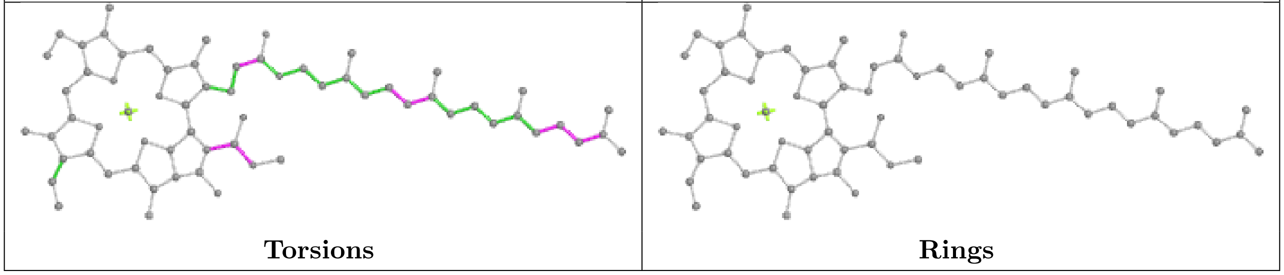
Torsions

Rings

Ligand CLA B 805

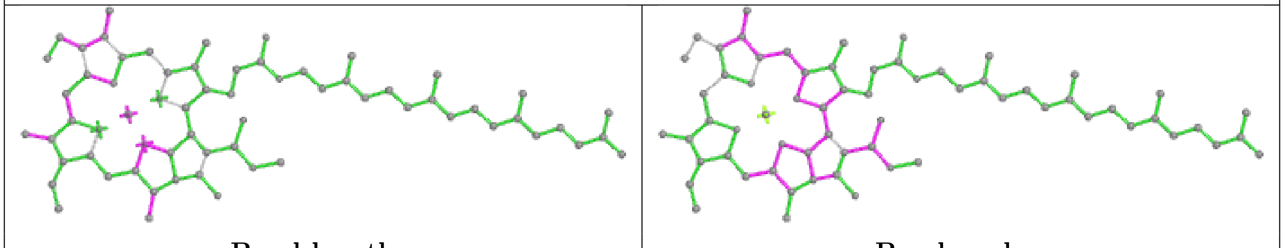


Bond lengths Bond angles

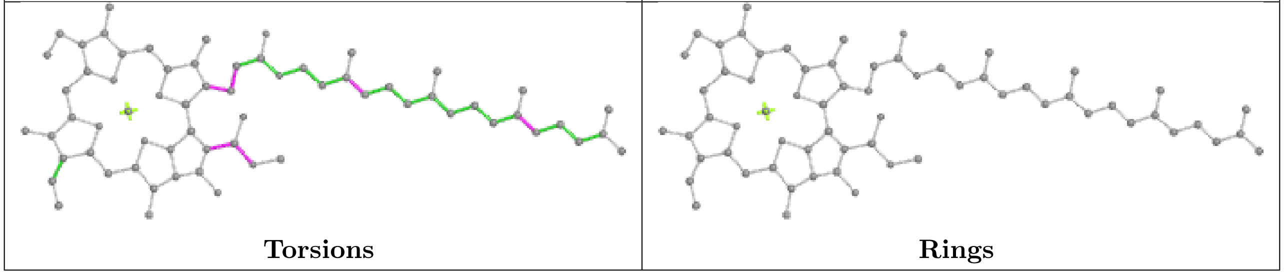


Torsions Rings

Ligand CLA b 803

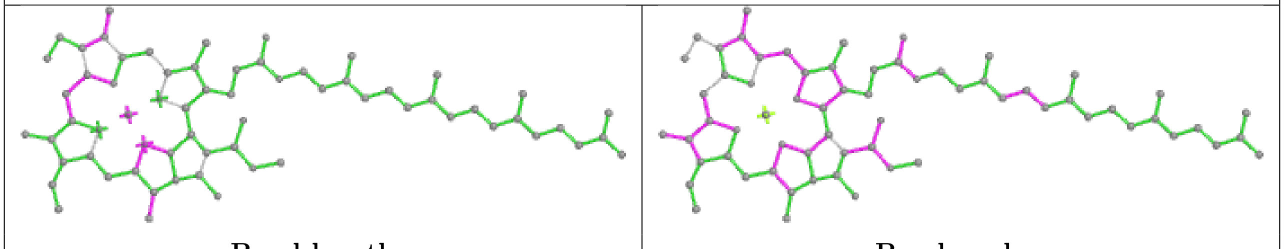


Bond lengths Bond angles

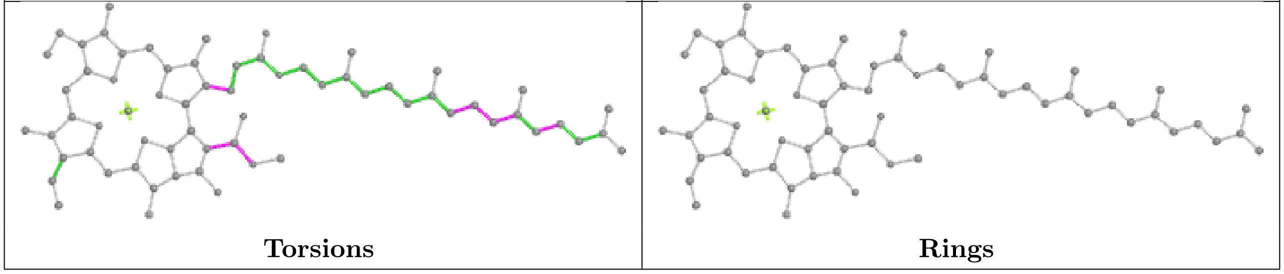


Torsions Rings

Ligand CLA b 832

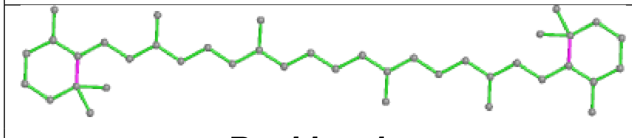


Bond lengths Bond angles

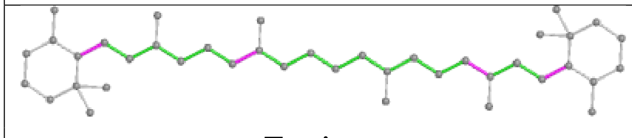


Torsions Rings

Ligand BCR k 103

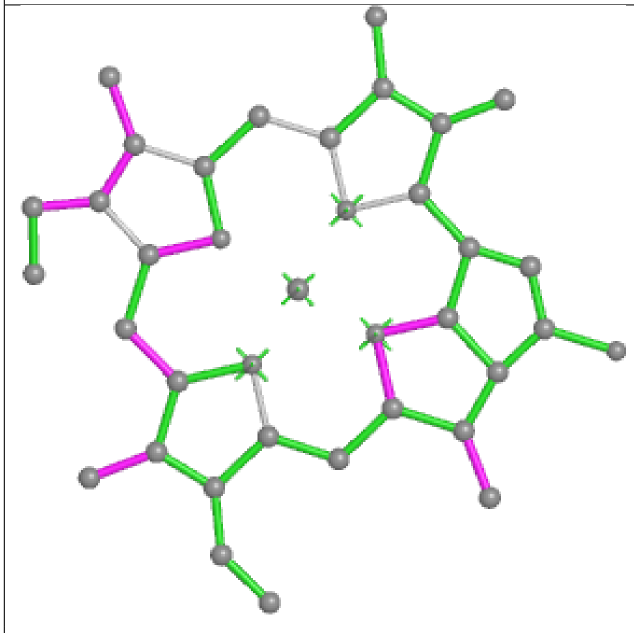


Bond lengths Bond angles

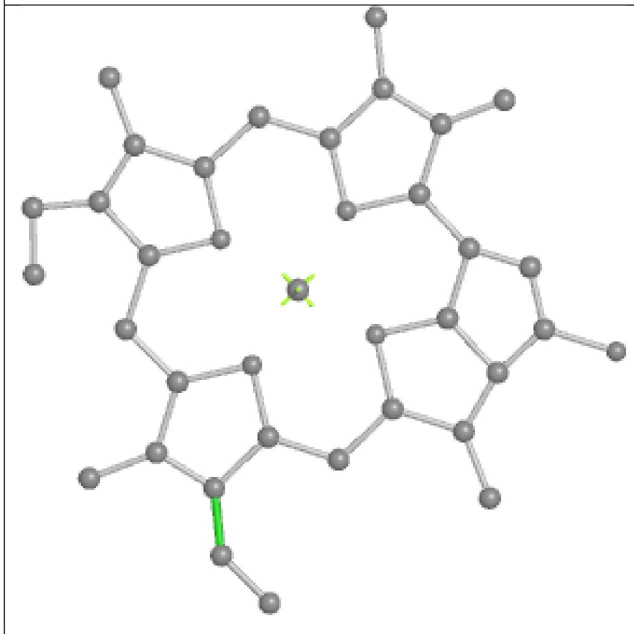


Torsions Rings

Ligand CLA j 103

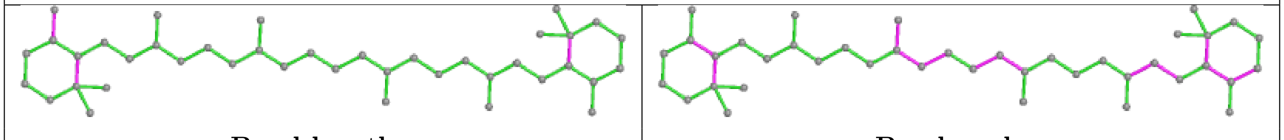


Bond lengths Bond angles

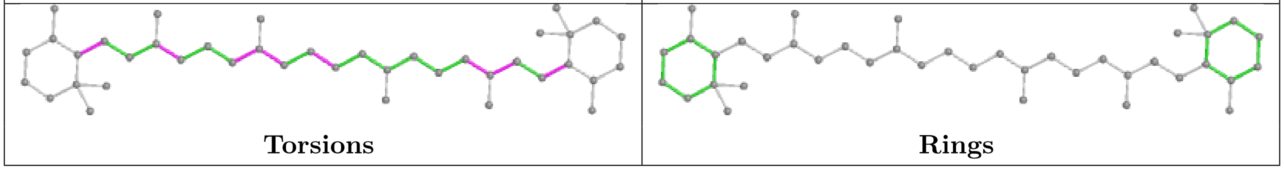


Torsions Rings

Ligand BCR A 850

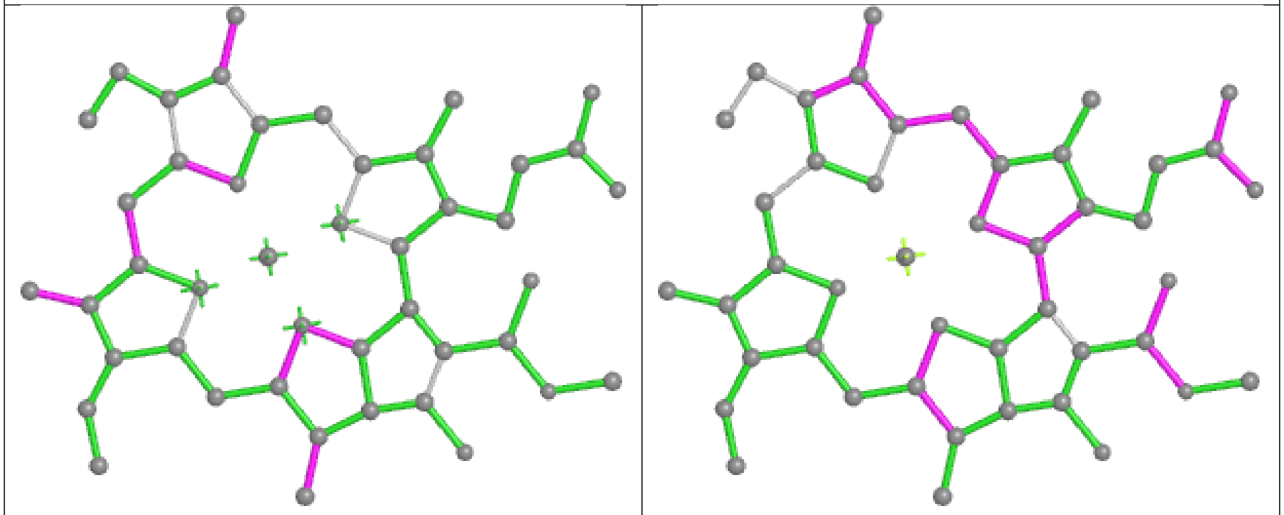


Bond lengths Bond angles

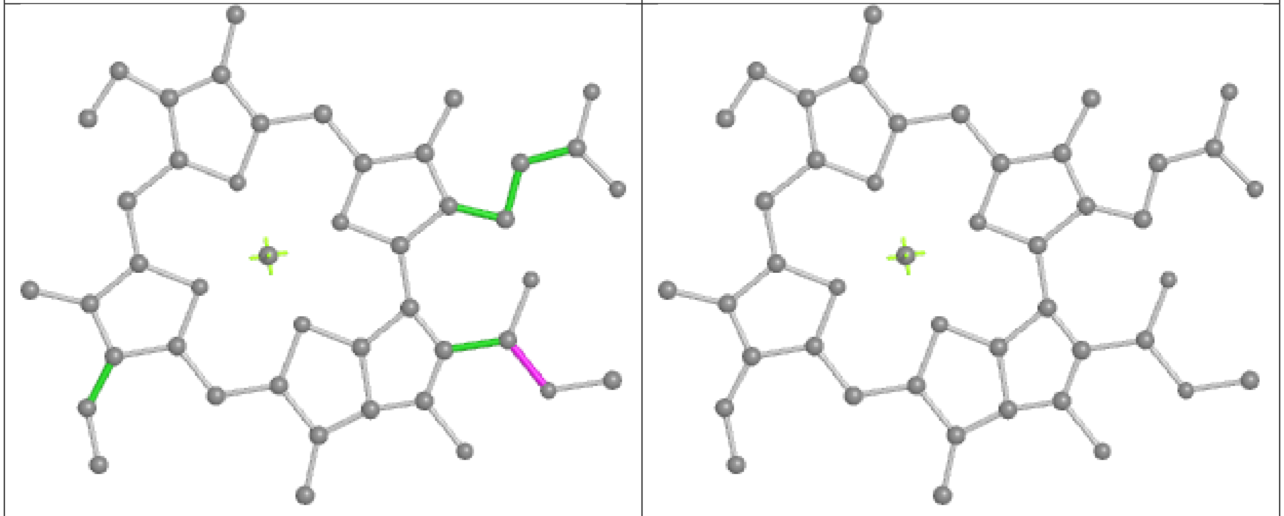


Torsions Rings

Ligand CLA b 837

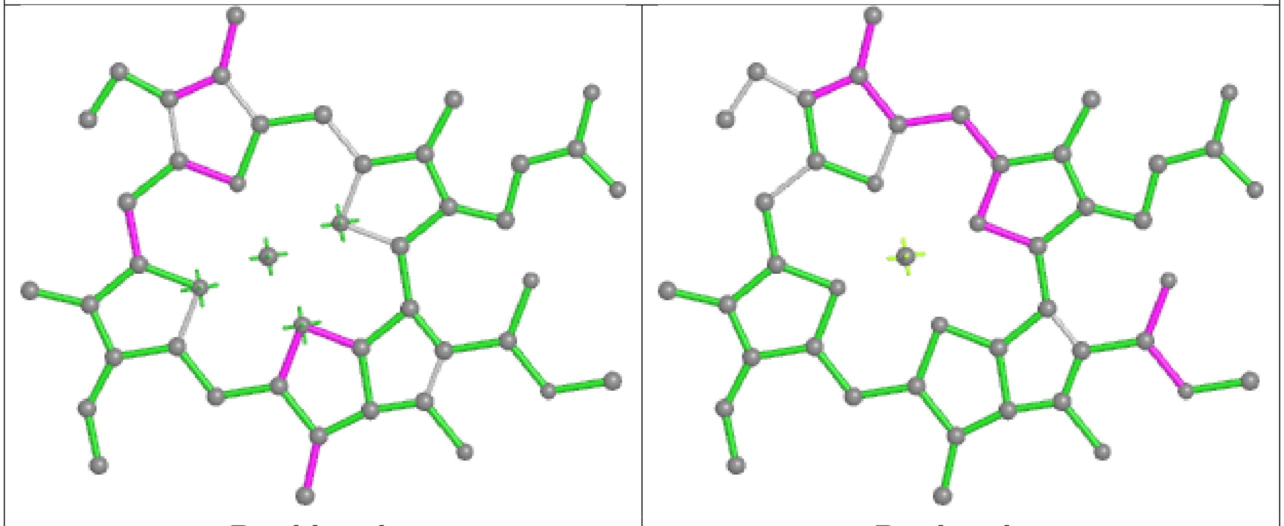


Bond lengths Bond angles

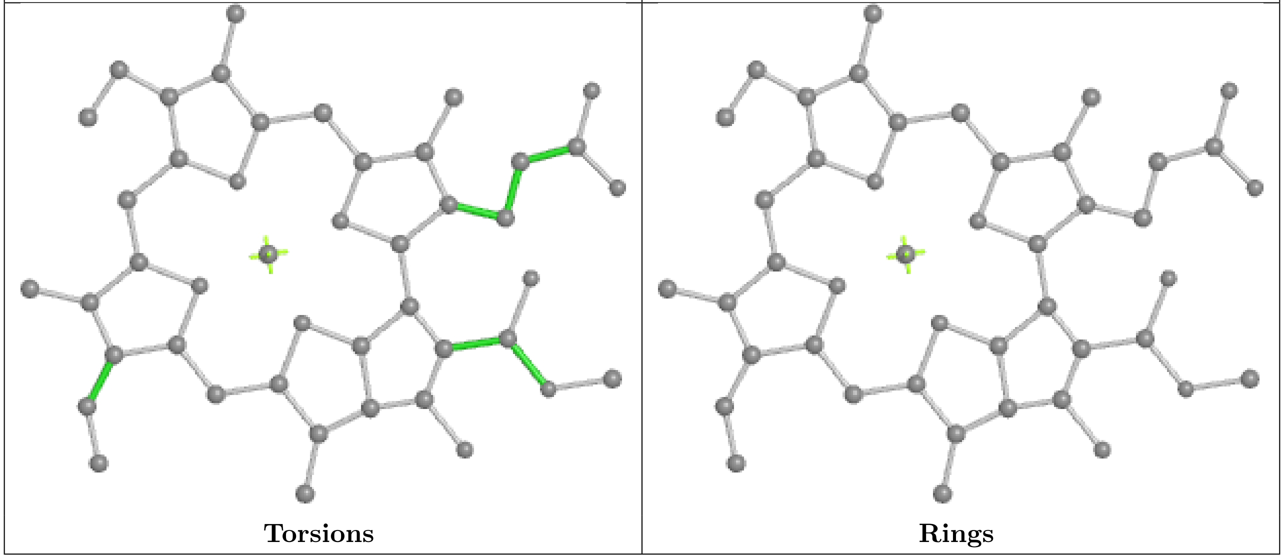


Torsions Rings

Ligand CLA a 815

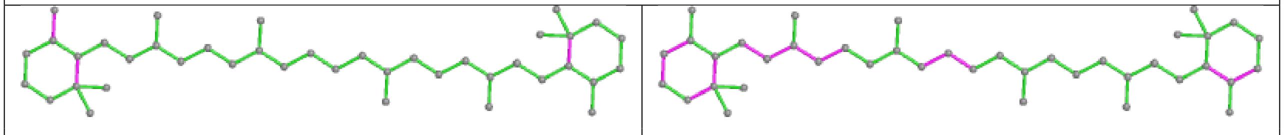


Bond lengths **Bond angles**

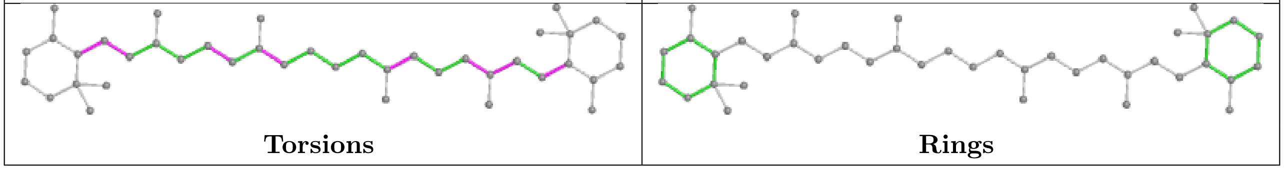


Torsions **Rings**

Ligand BCR J 103

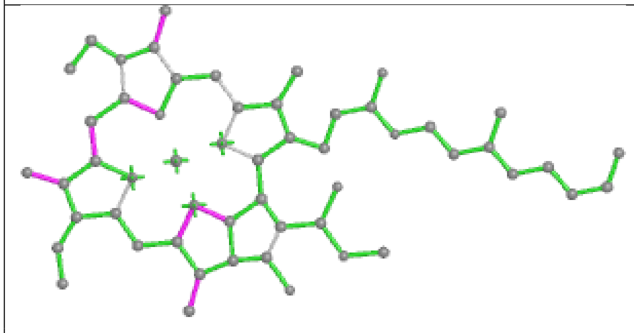
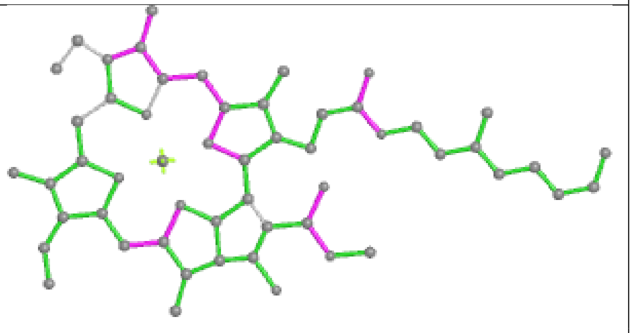
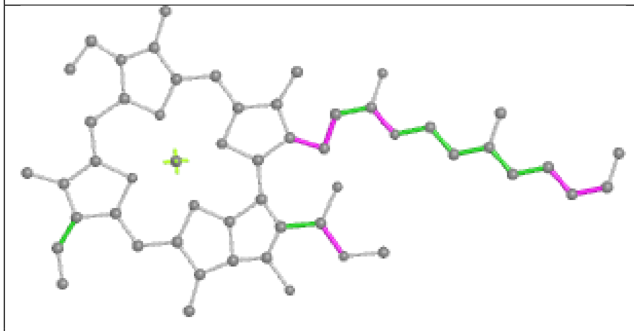
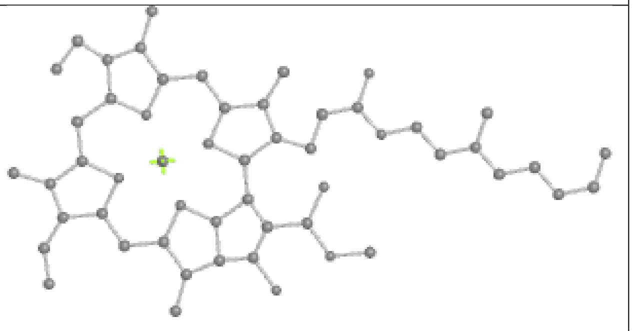


Bond lengths **Bond angles**

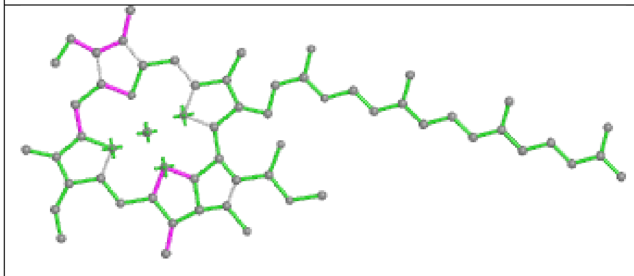
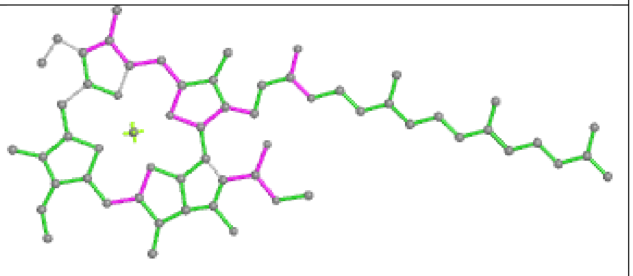
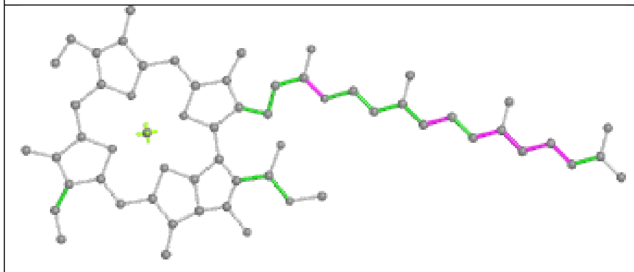
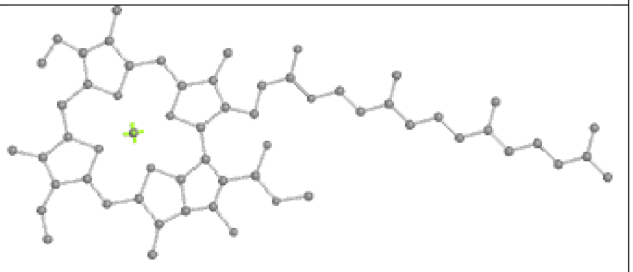


Torsions **Rings**

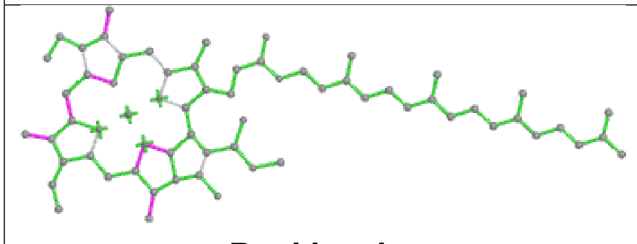
Ligand CLA a 819

 Bond lengths	 Bond angles
 Torsions	 Rings

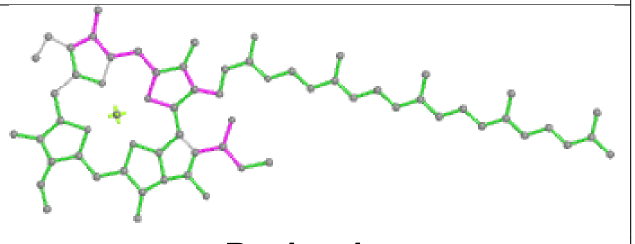
Ligand CLA L 1502

 Bond lengths	 Bond angles
 Torsions	 Rings

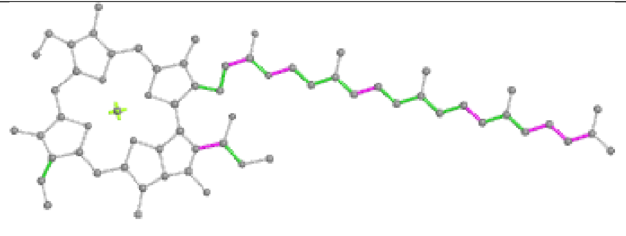
Ligand CLA a 802



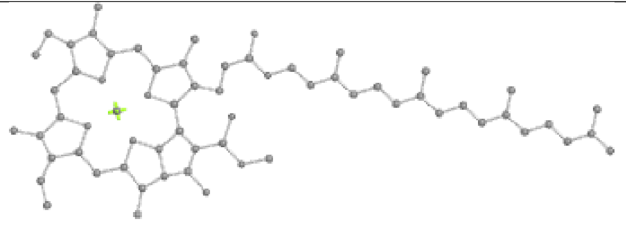
Bond lengths



Bond angles

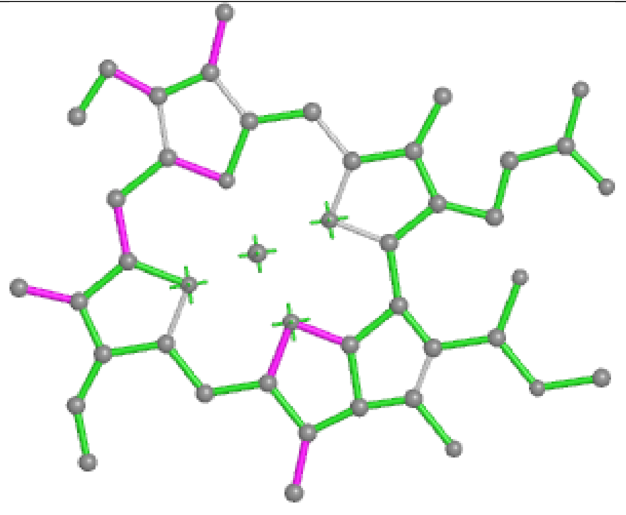


Torsions

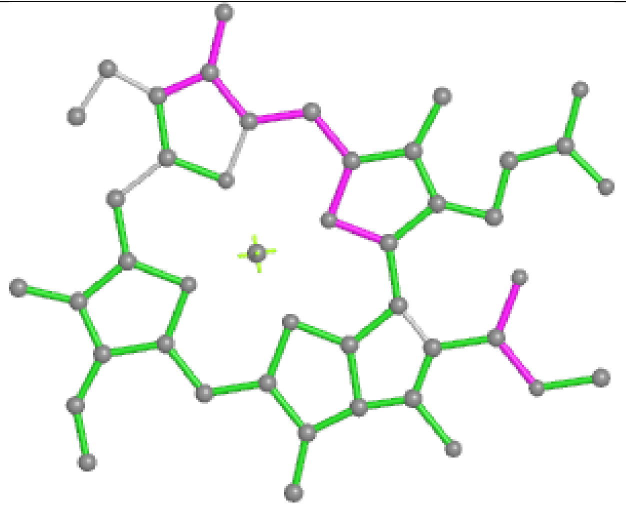


Rings

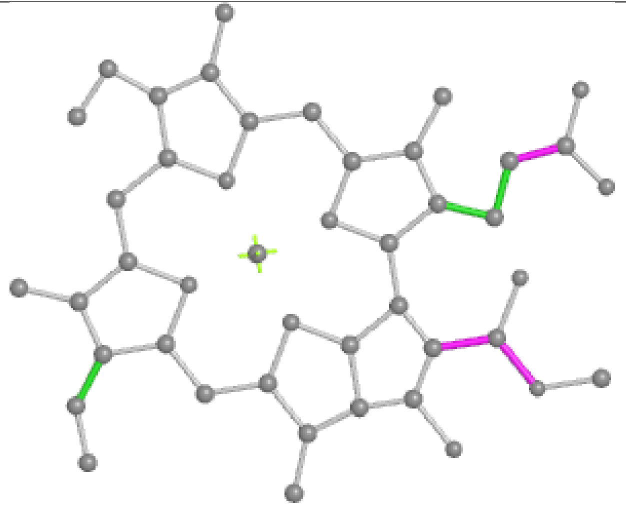
Ligand CLA f 203



Bond lengths



Bond angles



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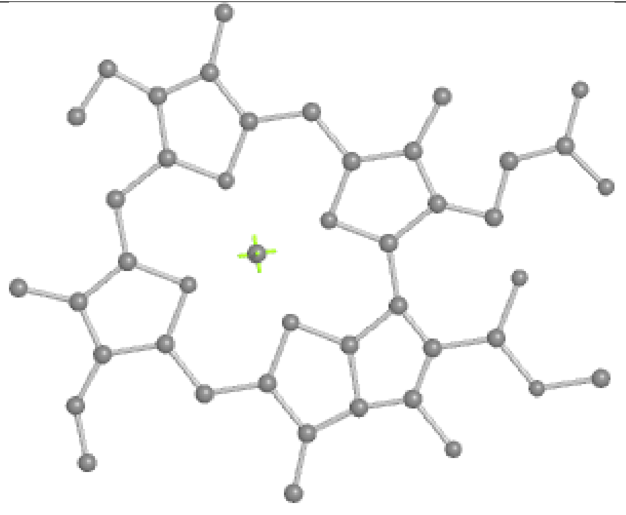
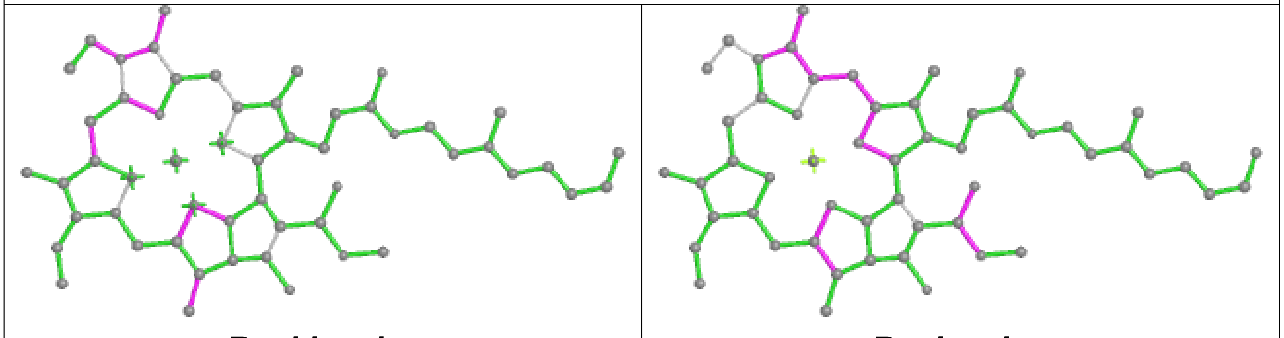
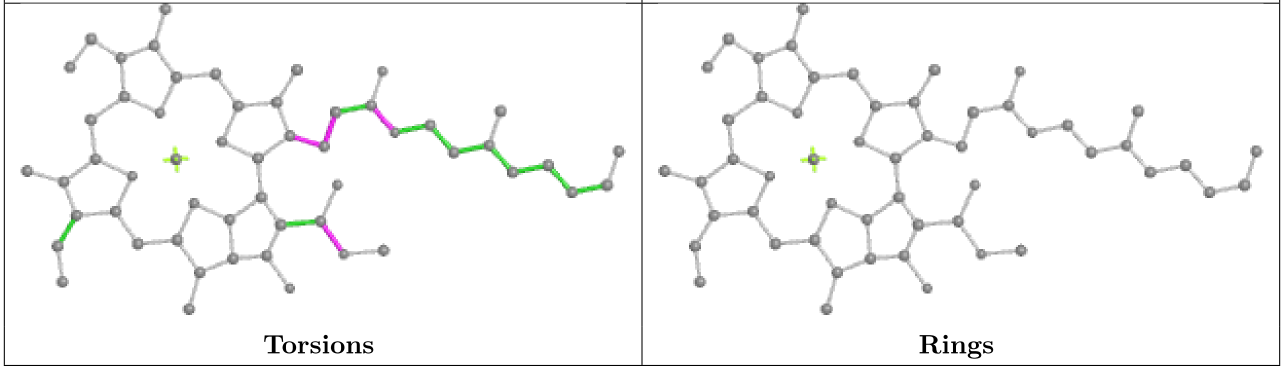


Rings

Ligand CLA B 833

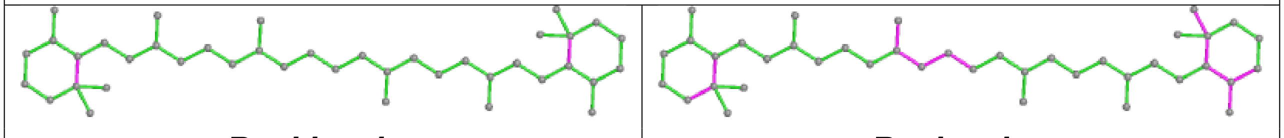

Bond lengths

Bond angles

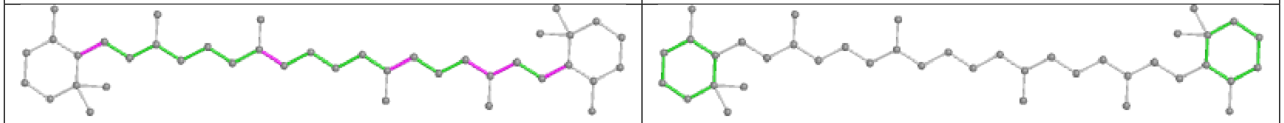

Torsions

Rings

Ligand BCR F 205

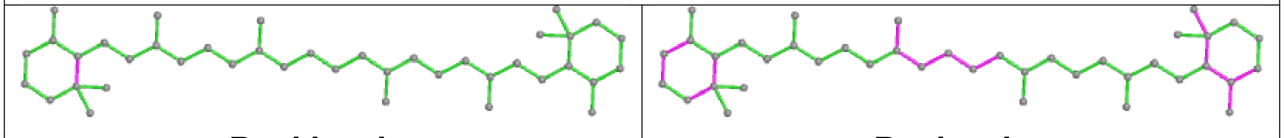

Bond lengths

Bond angles

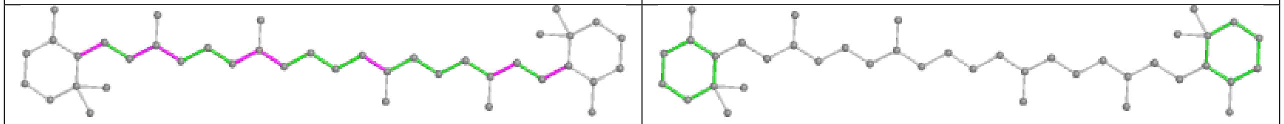

Torsions

Rings

Ligand BCR A 848

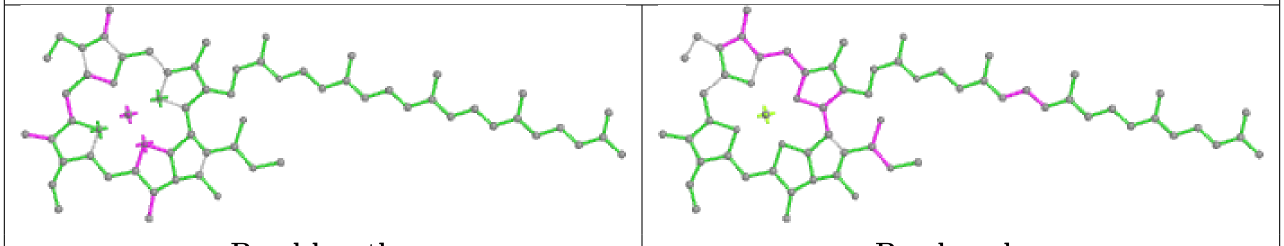

Bond lengths

Bond angles


Torsions

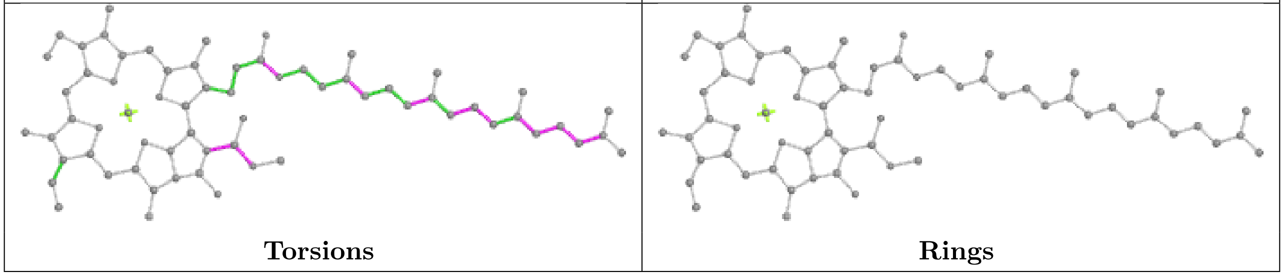
Rings

Ligand CLA A 825



Bond lengths

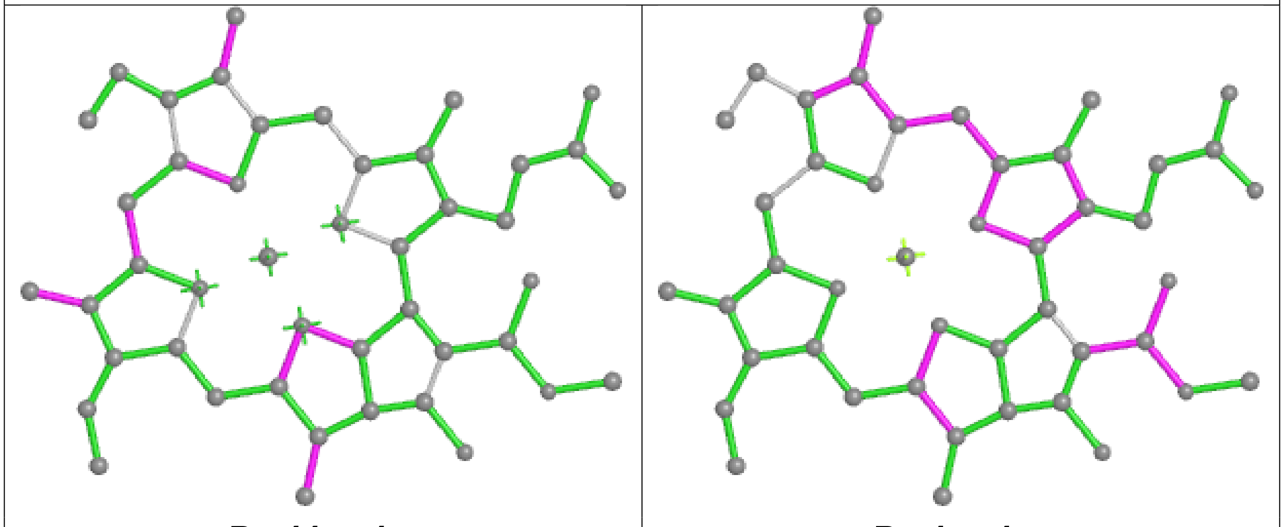
Bond angles



Torsions

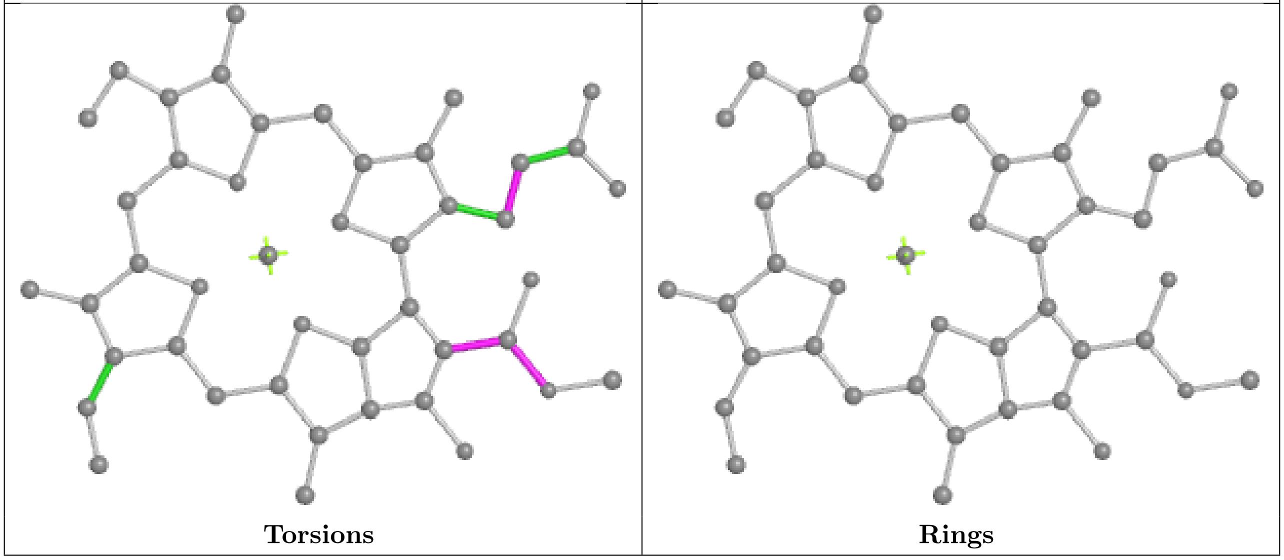
Rings

Ligand CLA l 205



Bond lengths

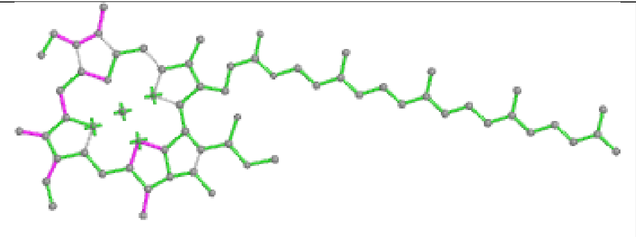
Bond angles



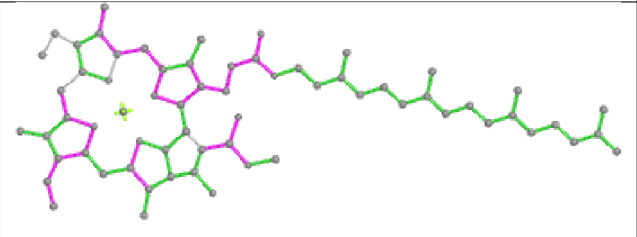
Torsions

Rings

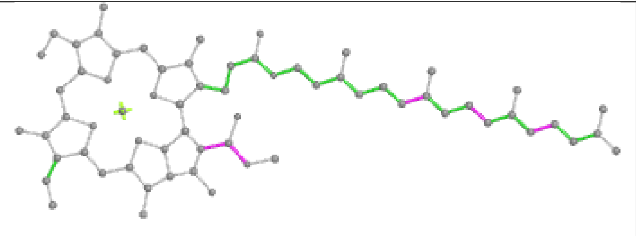
Ligand CLA B 811



Bond lengths



Bond angles



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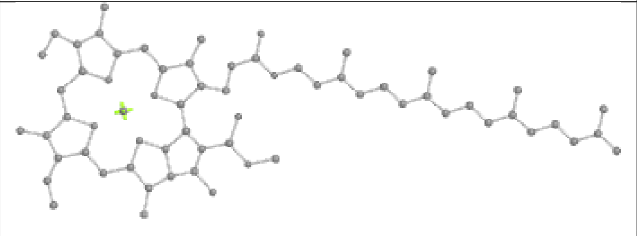
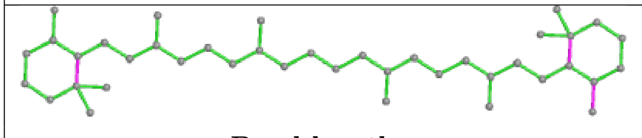


Rings

Ligand BCR b 850



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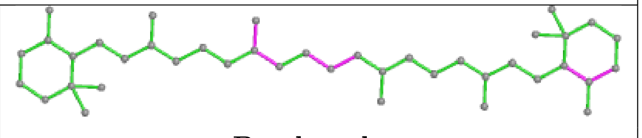
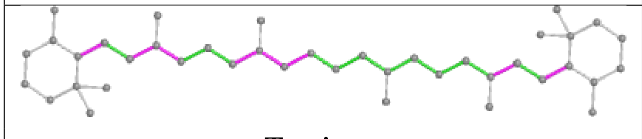


Bond angles



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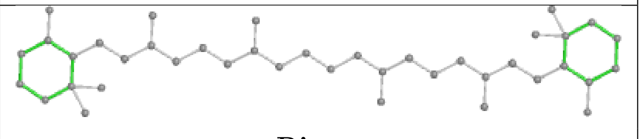
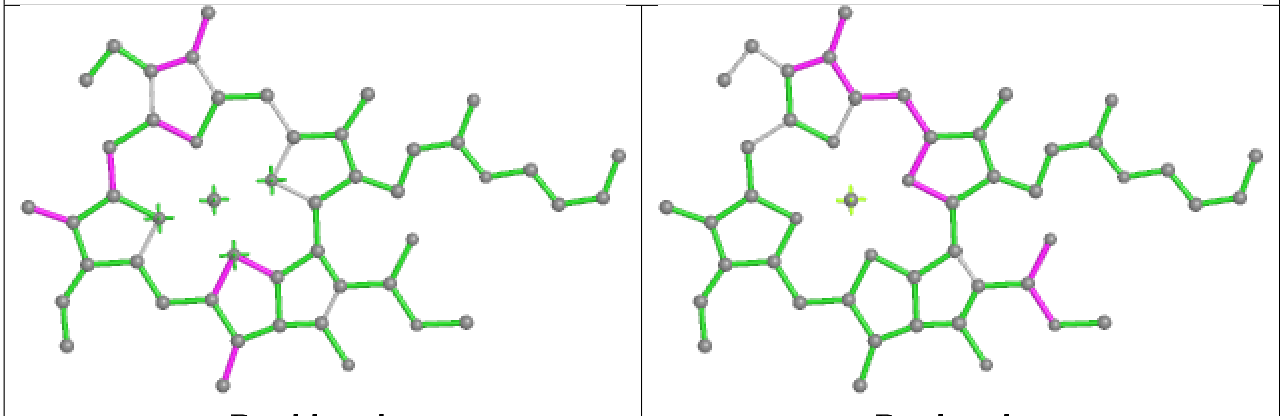


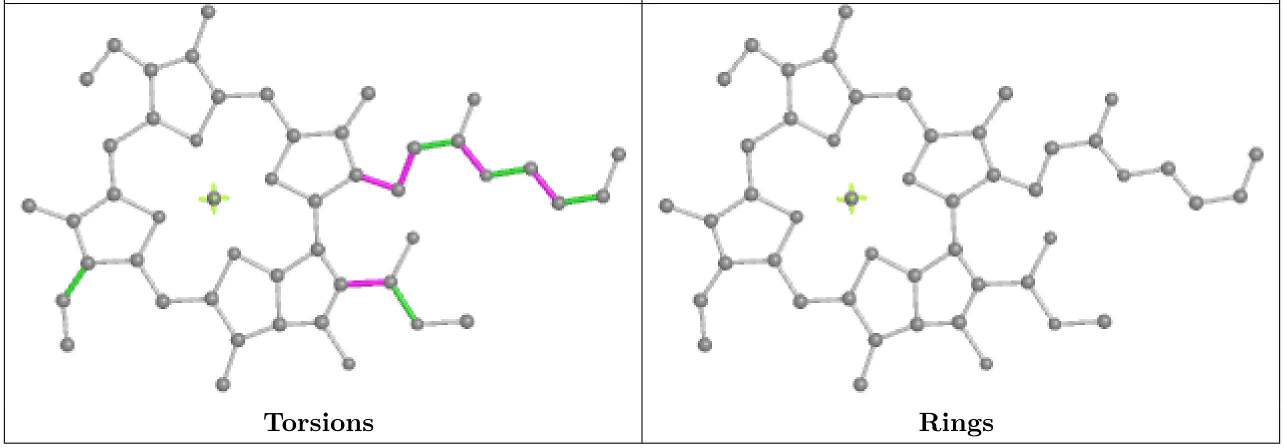
Rings

Ligand CLA x 1701



Bond lengths

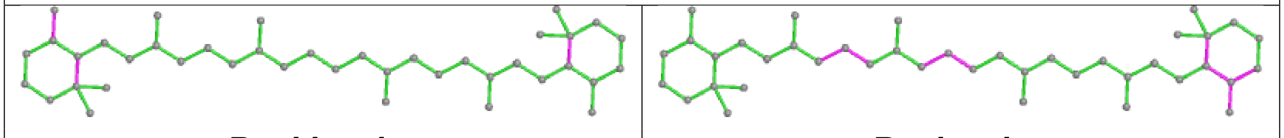
Bond angles



Torsions

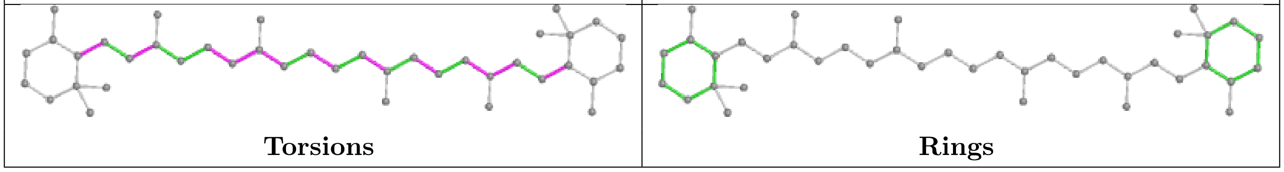
Rings

Ligand BCR f 202



Bond lengths

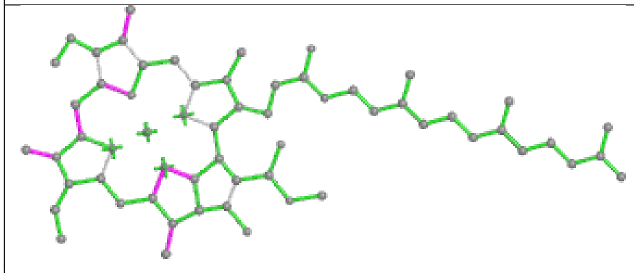
Bond angles



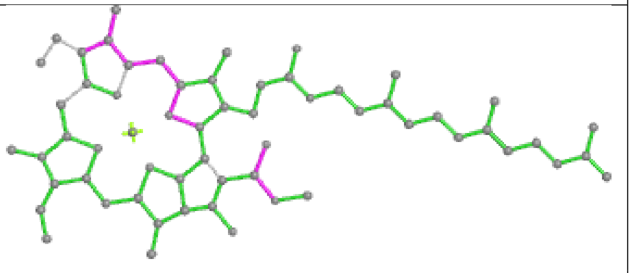
Torsions

Rings

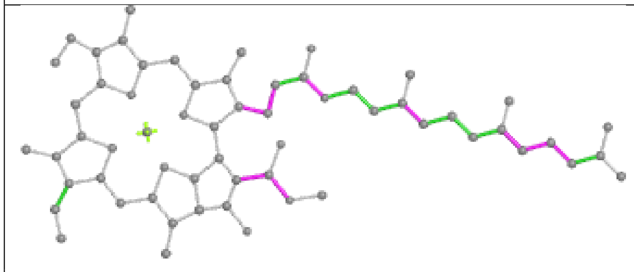
Ligand CLA B 834



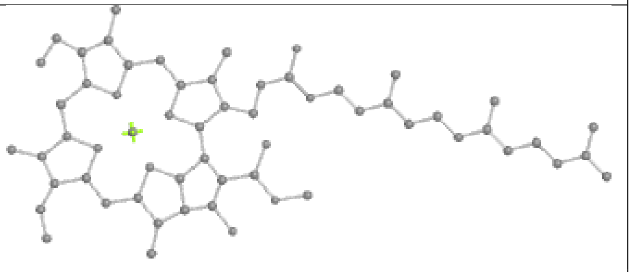
Bond lengths



Bond angles

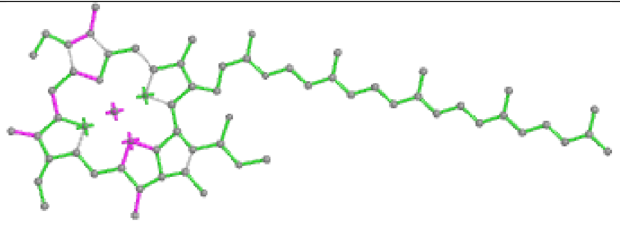


Torsions

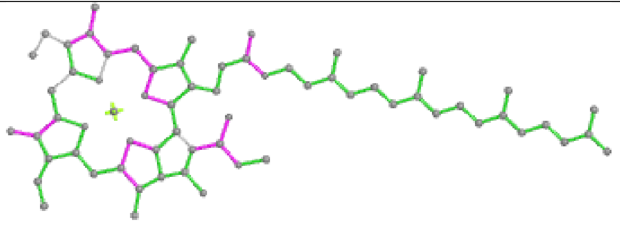


Rings

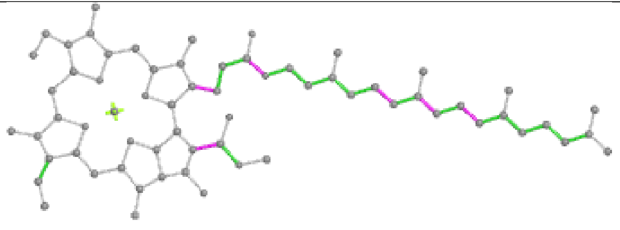
Ligand CLA A 830



Bond lengths



Bond angles



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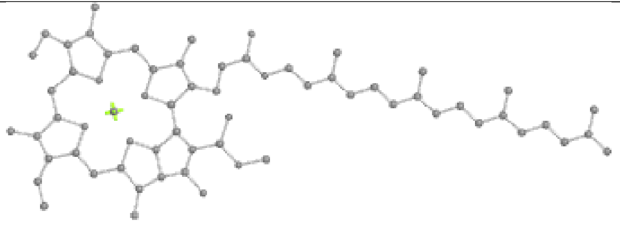
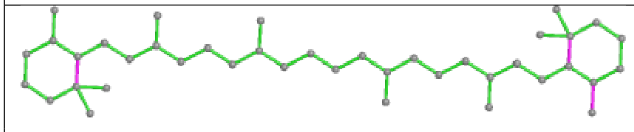
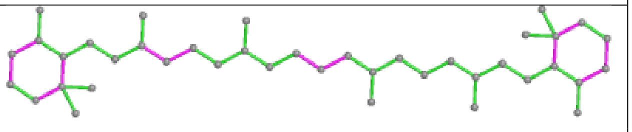


Rings

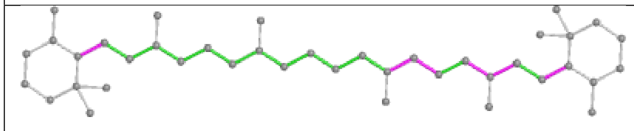
Ligand BCR A 847



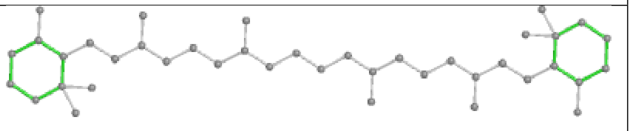
Bond lengths



Bond angles

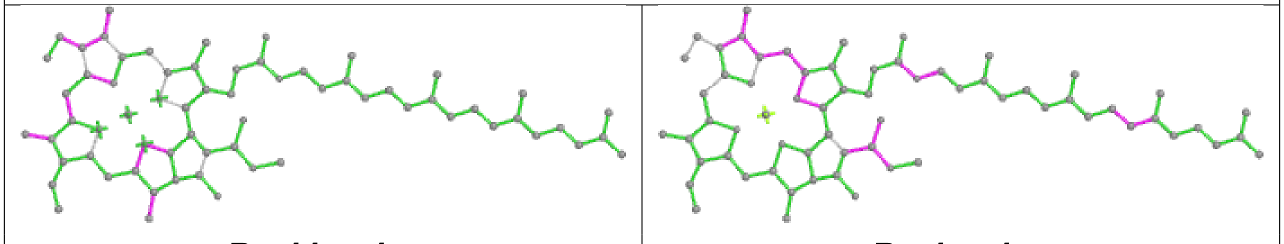


Torsions

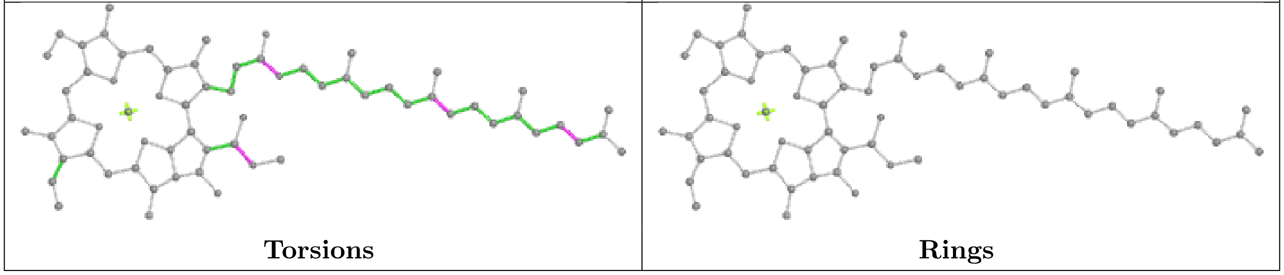


Rings

Ligand CLA a 810

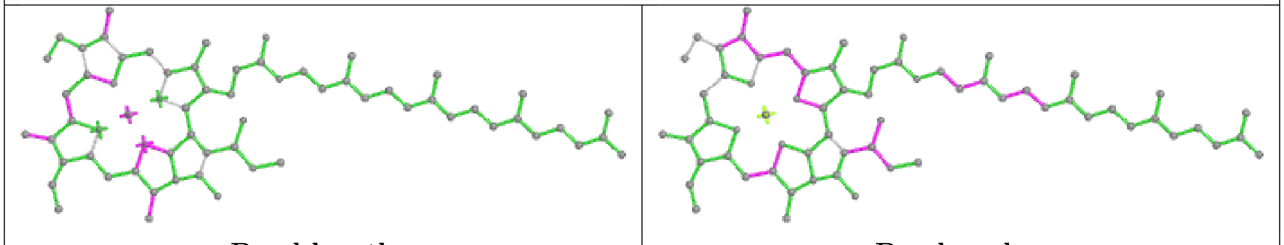


Bond lengths Bond angles

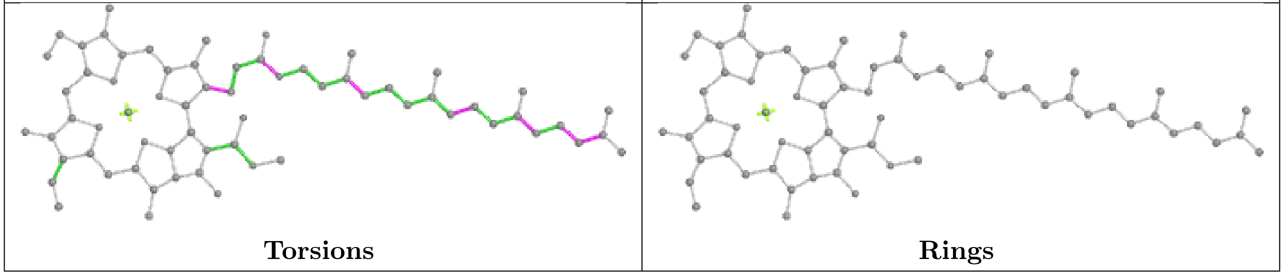


Torsions Rings

Ligand CLA A 819

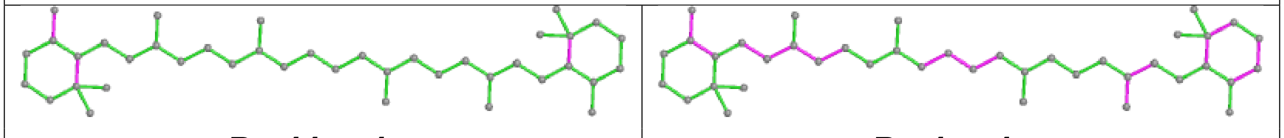


Bond lengths Bond angles

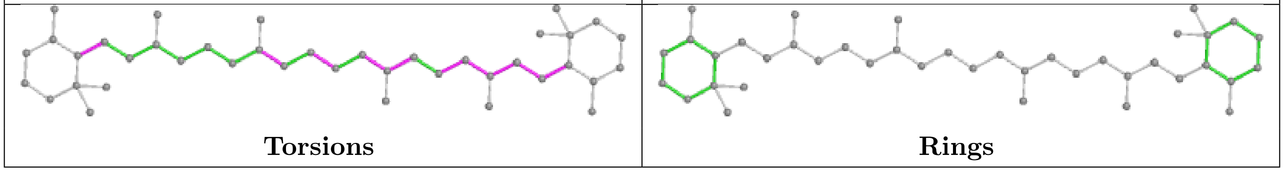


Torsions Rings

Ligand BCR A 849

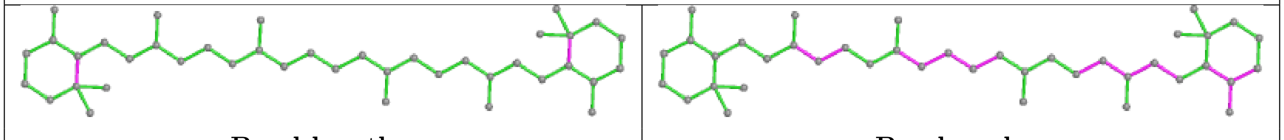


Bond lengths Bond angles



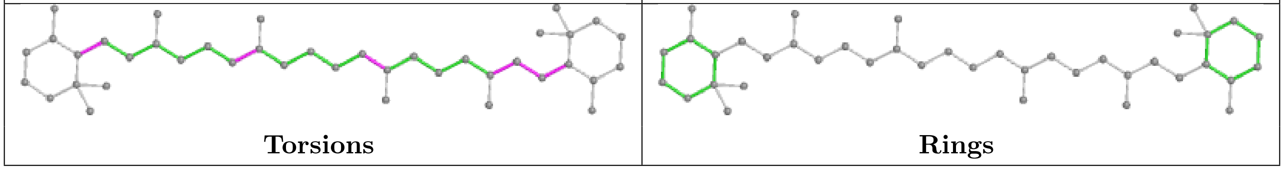
Torsions Rings

Ligand BCR a 848



Bond lengths

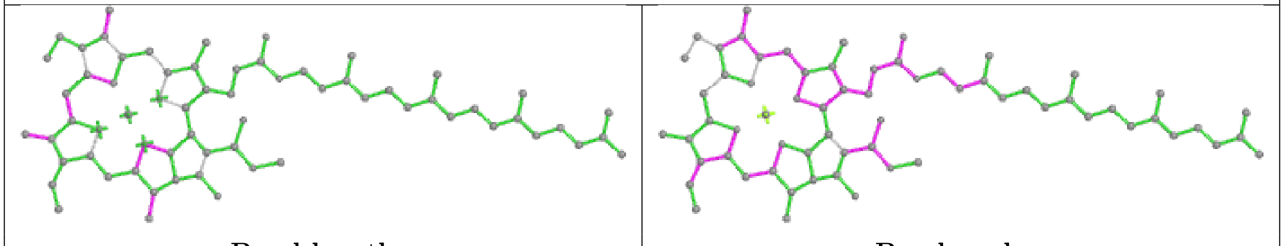
Bond angles



Torsions

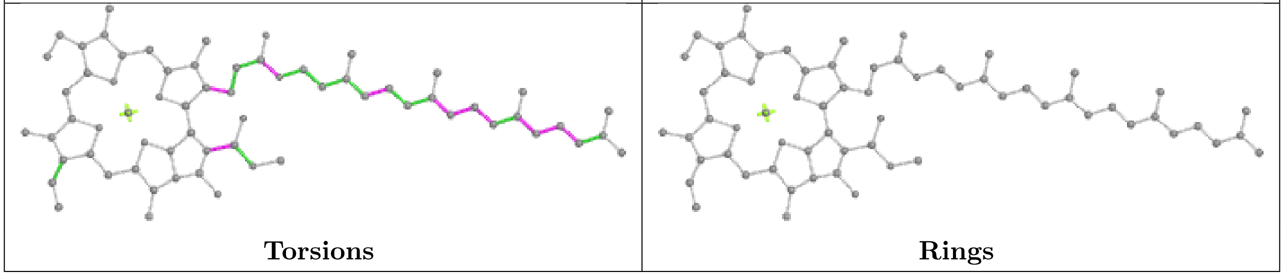
Rings

Ligand CLA A 805



Bond lengths

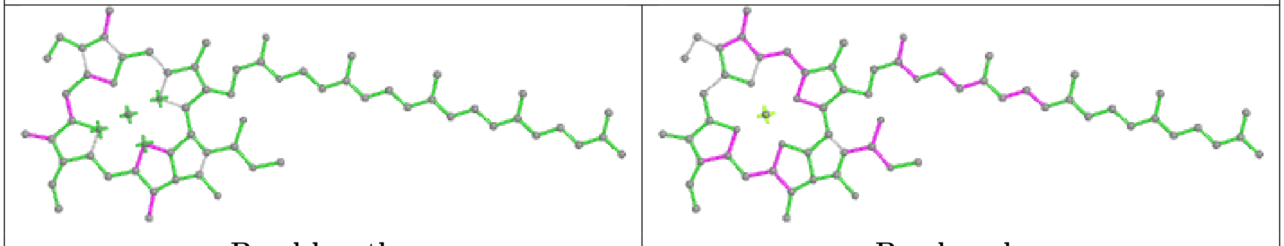
Bond angles



Torsions

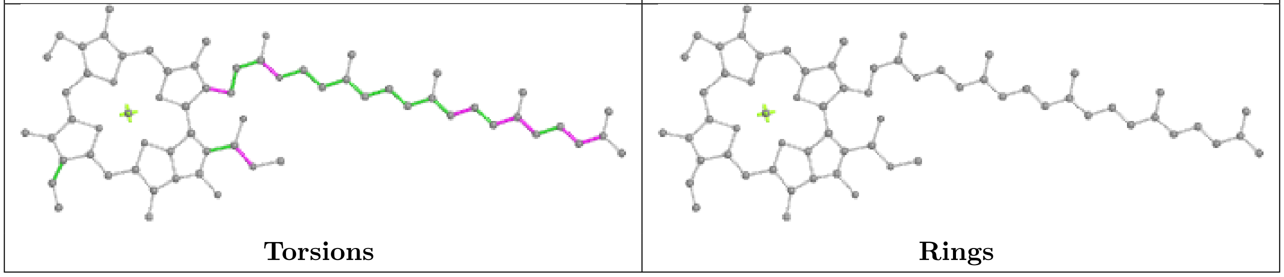
Rings

Ligand CLA a 818



Bond lengths

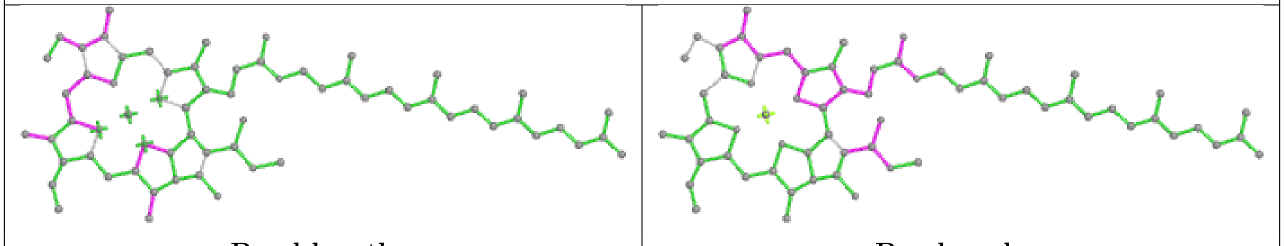
Bond angles



Torsions

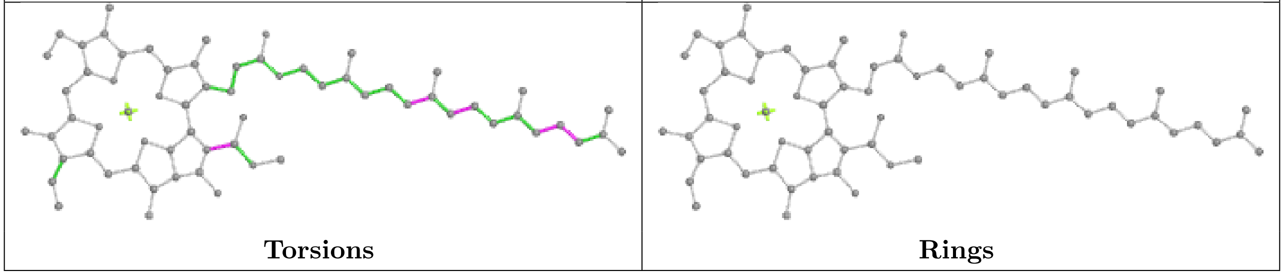
Rings

Ligand CLA b 811



Bond lengths

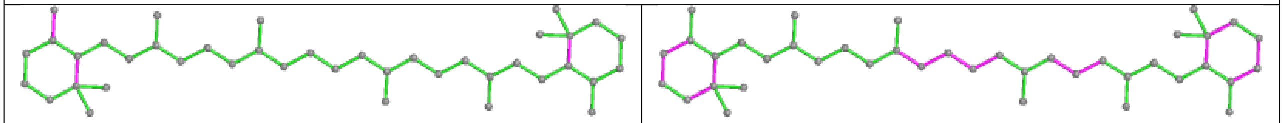
Bond angles



Torsions

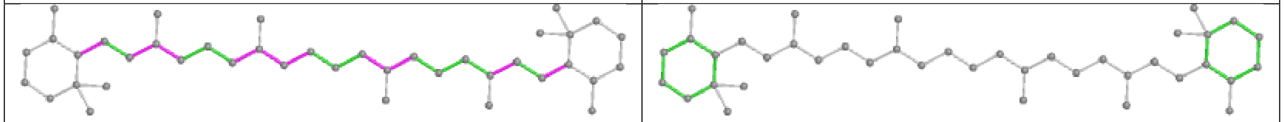
Rings

Ligand BCR j 104



Bond lengths

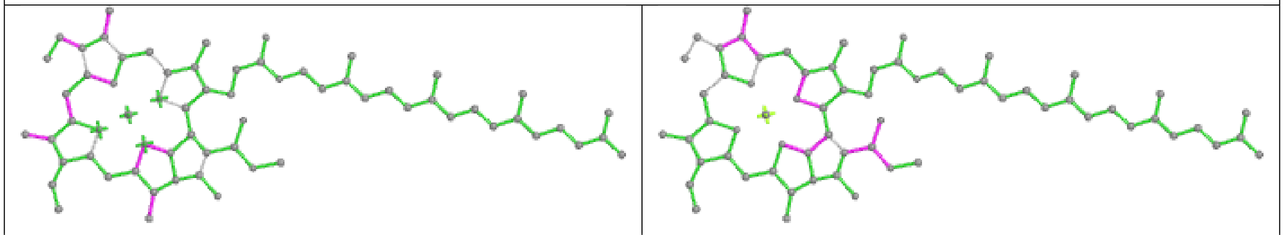
Bond angles



Torsions

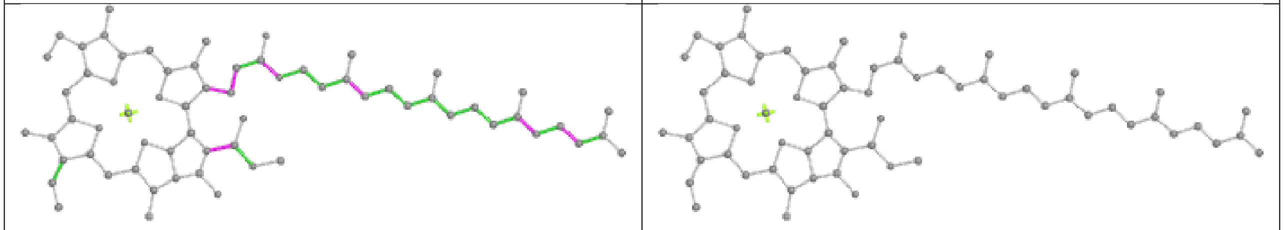
Rings

Ligand CLA B 831



Bond lengths

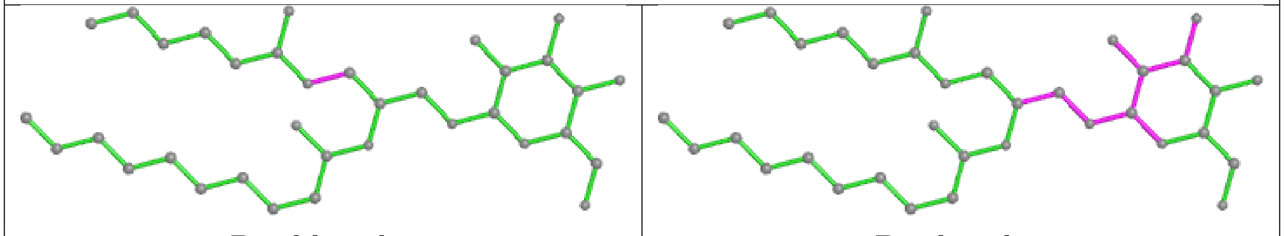
Bond angles



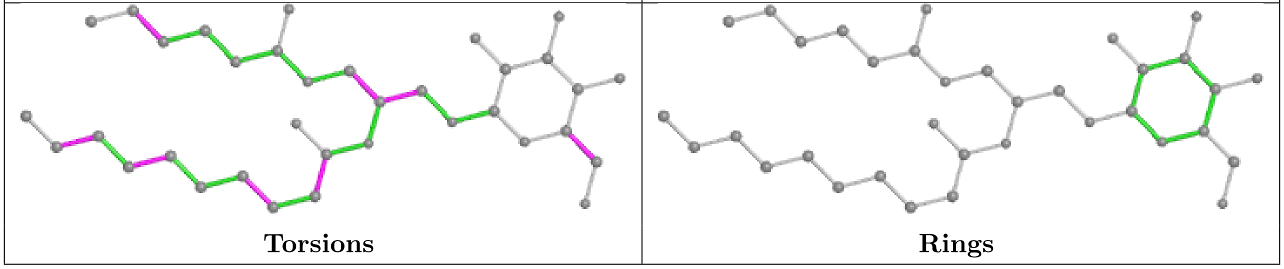
Torsions

Rings

Ligand LMG B 803

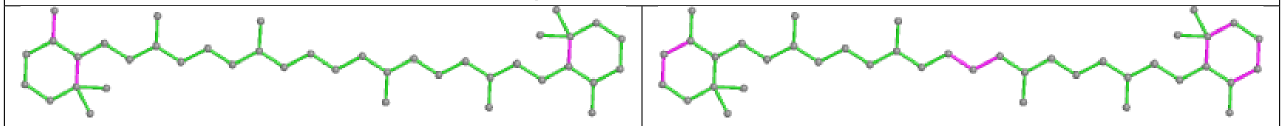


Bond lengths Bond angles

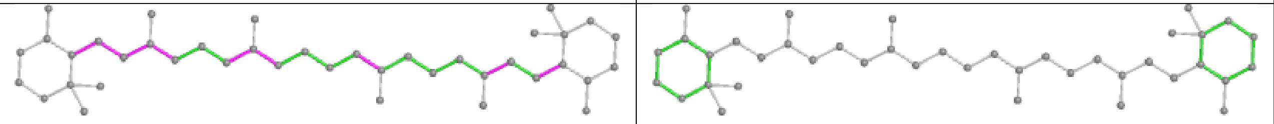


Torsions Rings

Ligand BCR a 849

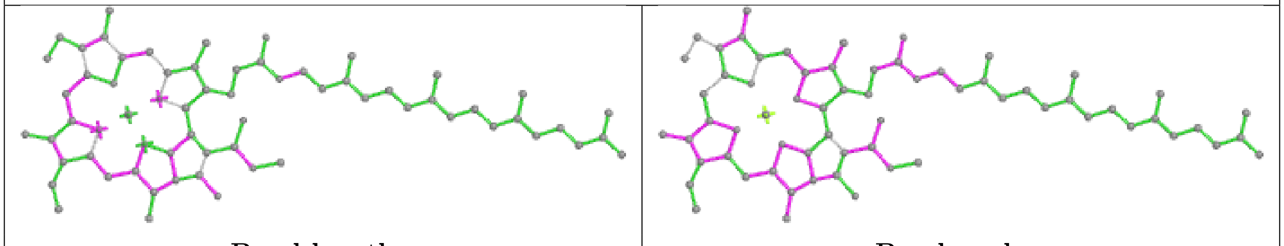


Bond lengths Bond angles

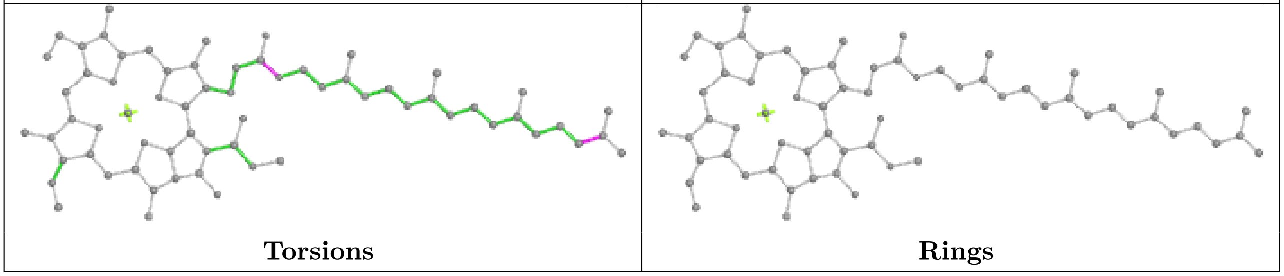


Torsions Rings

Ligand CL0 a 801

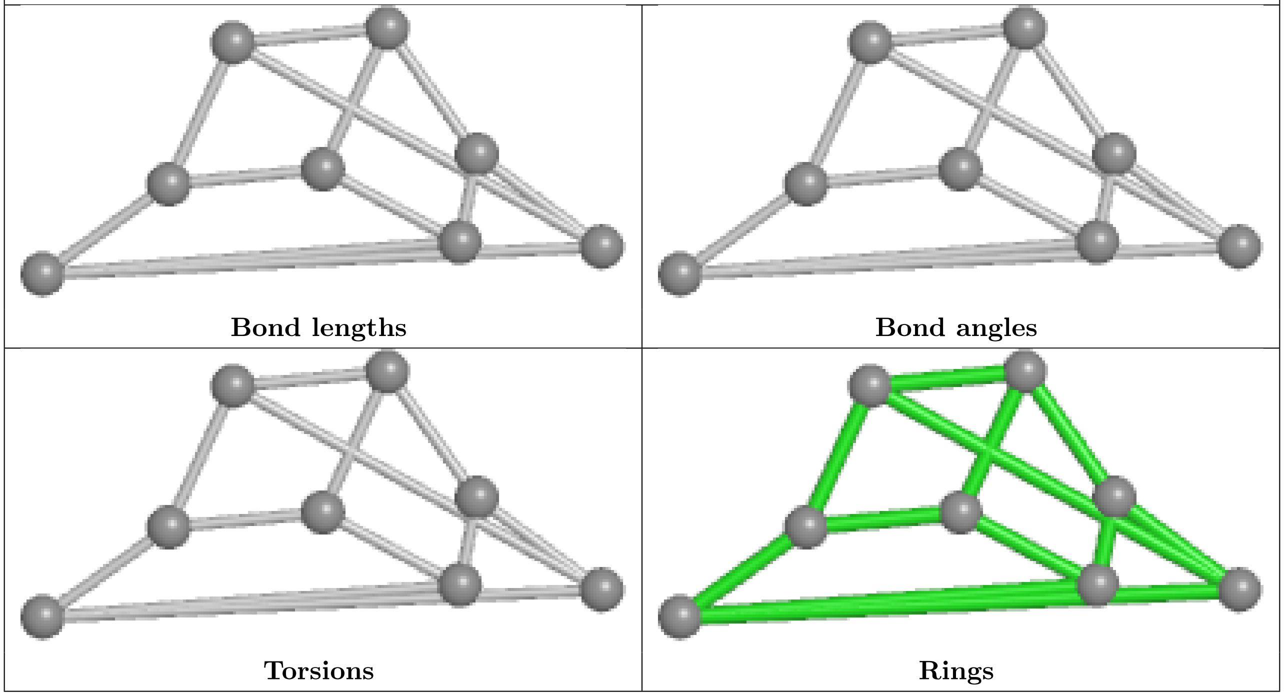


Bond lengths Bond angles



Torsions Rings

Ligand SF4 c 101



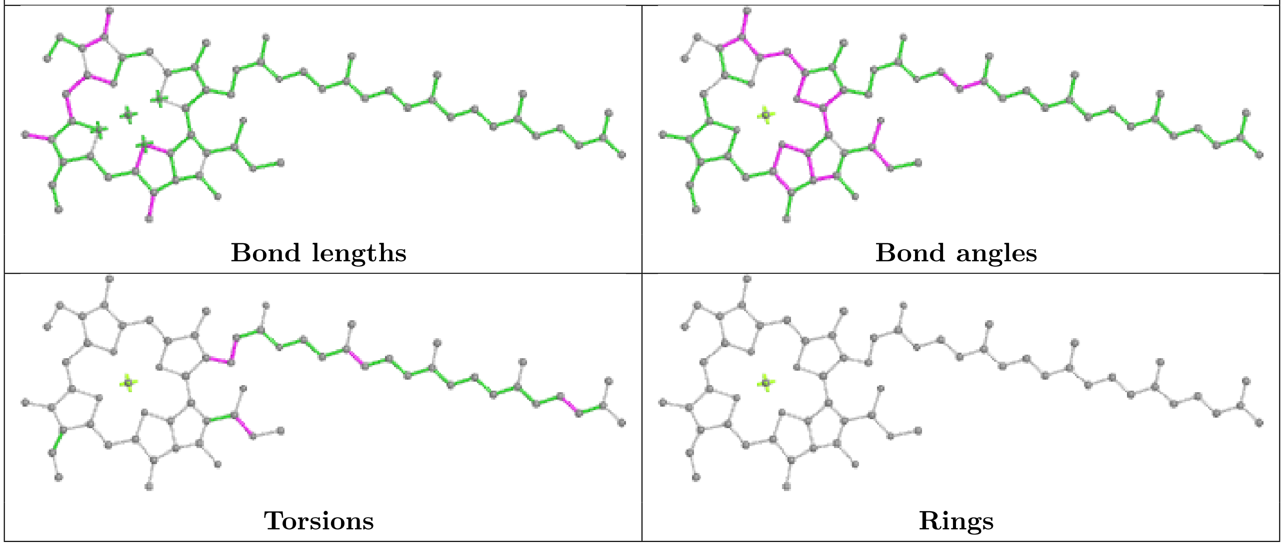
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA A 802



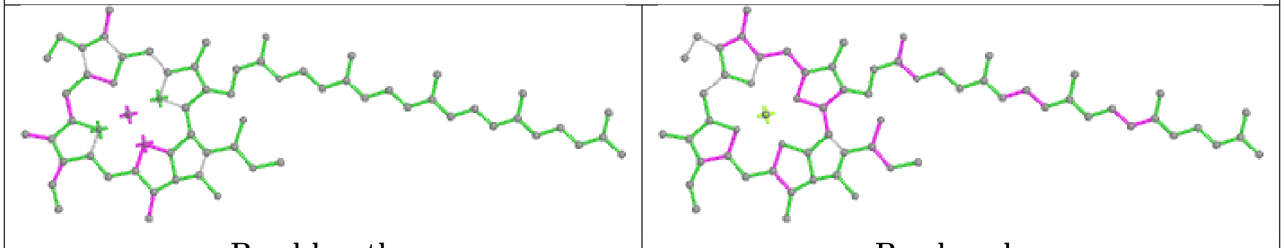
Bond lengths

Bond angles

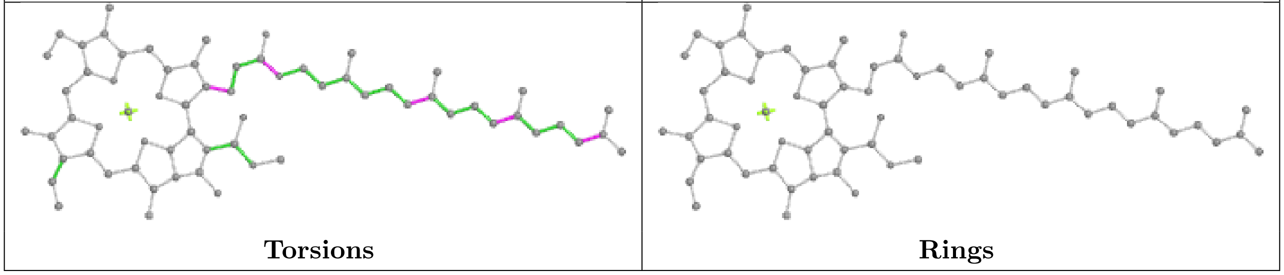
Torsions

Rings

Ligand CLA b 821

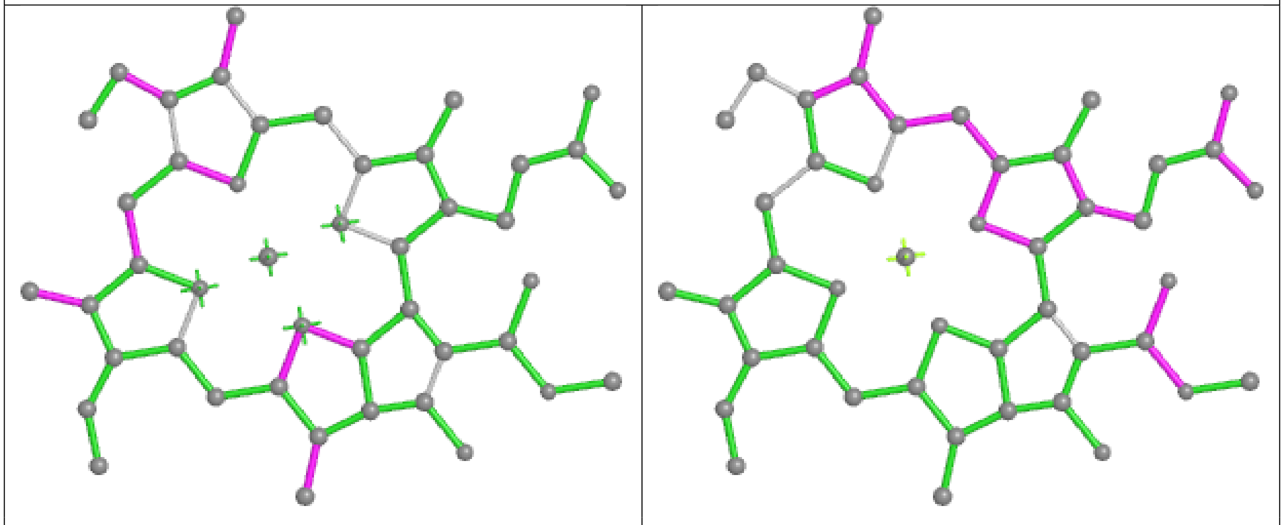


Bond lengths **Bond angles**

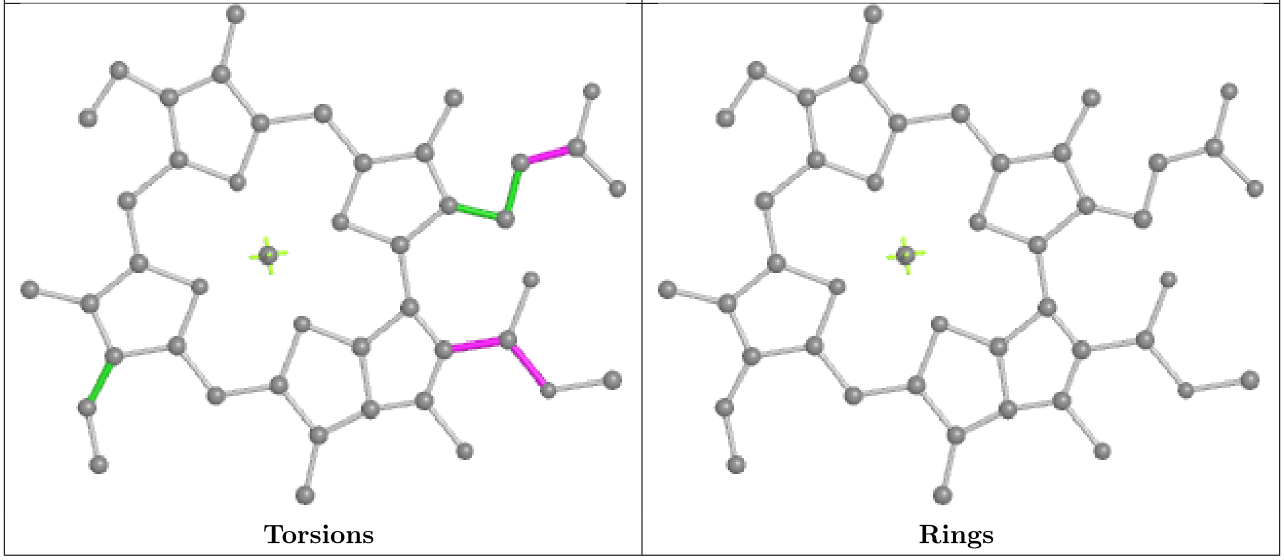


Torsions **Rings**

Ligand CLA J 101

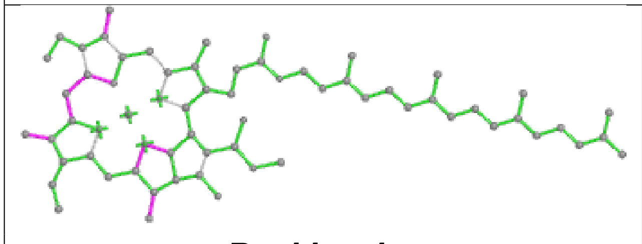


Bond lengths **Bond angles**

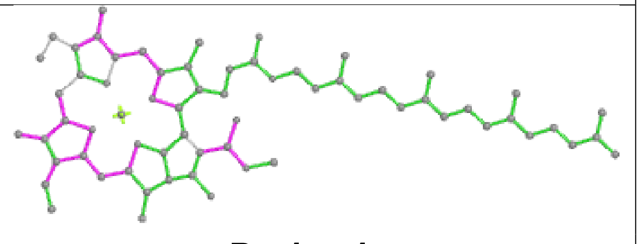


Torsions **Rings**

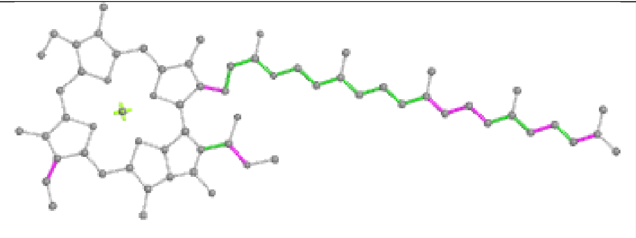
Ligand CLA B 806



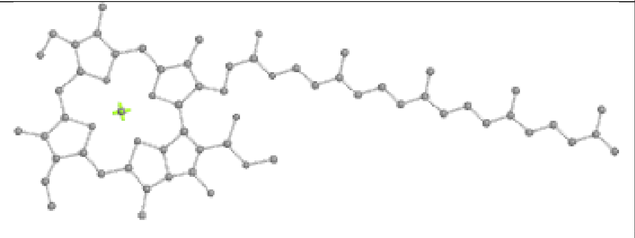
Bond lengths



Bond angles

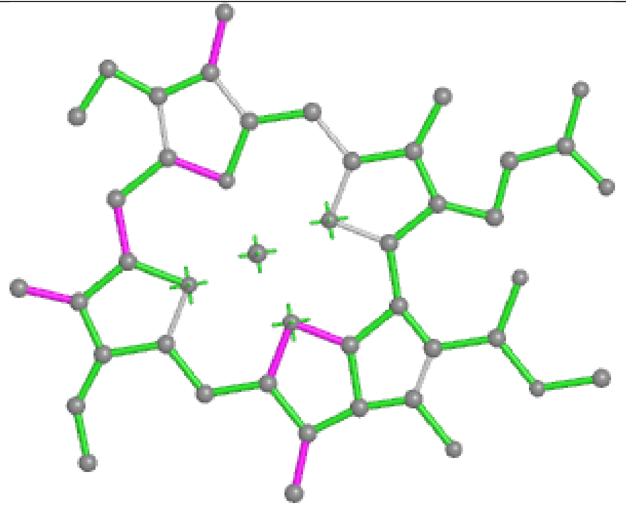


Torsions

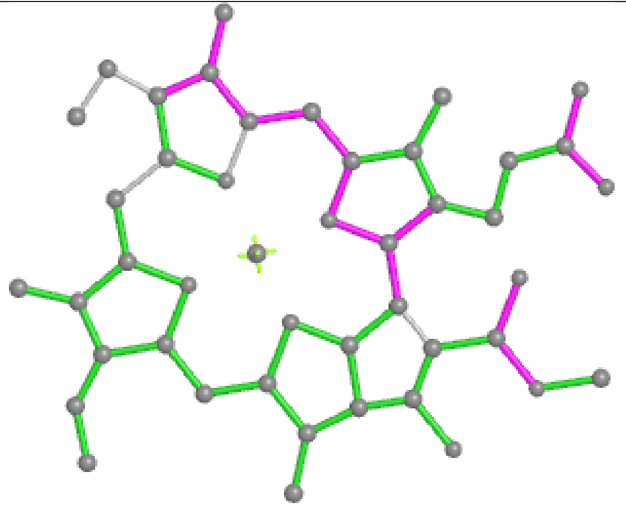


Rings

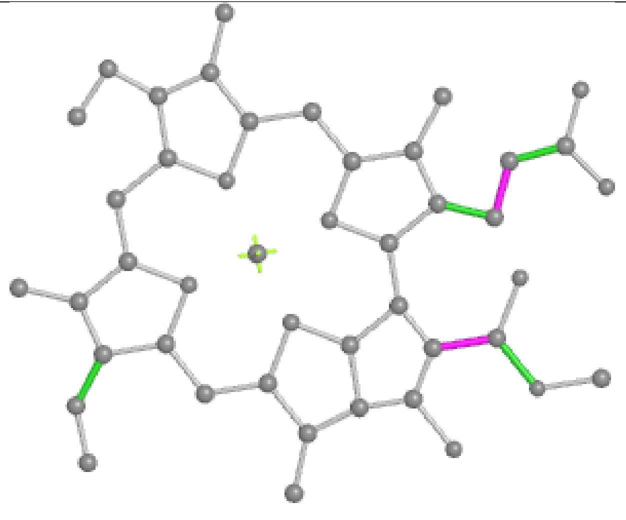
Ligand CLA A 836



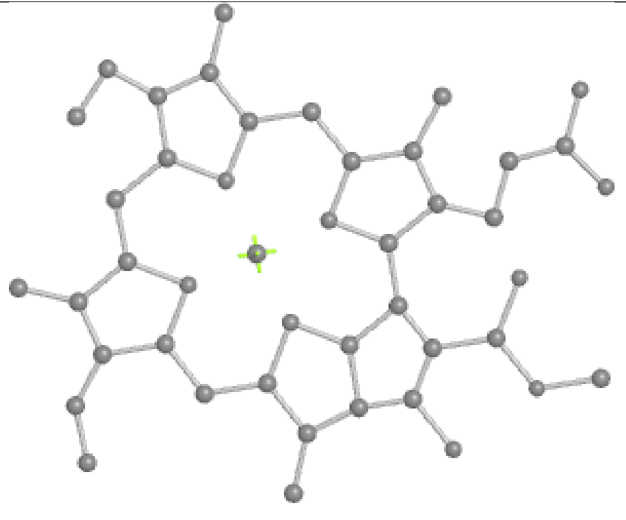
Bond lengths



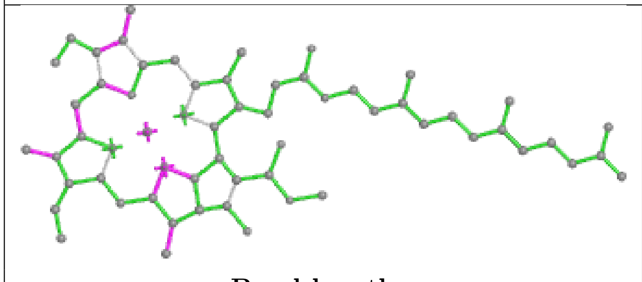
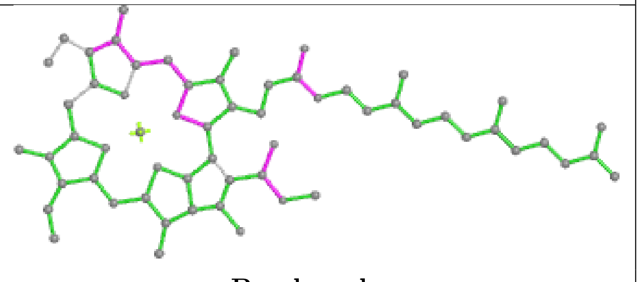
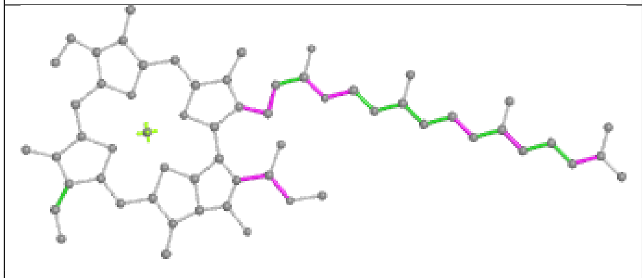
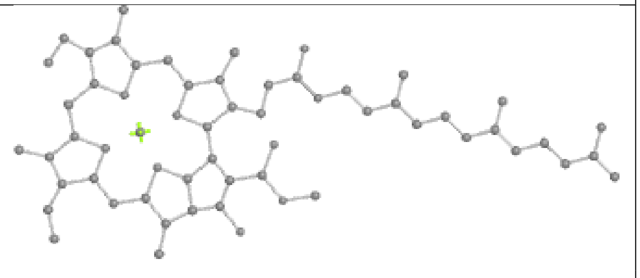
Bond angles

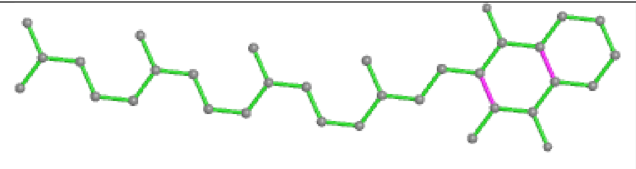
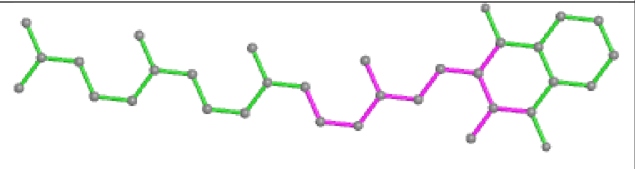
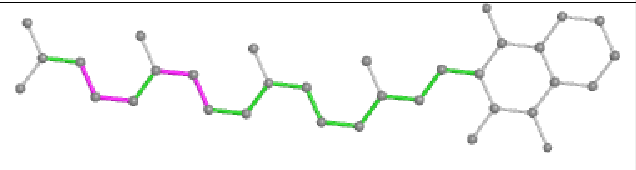
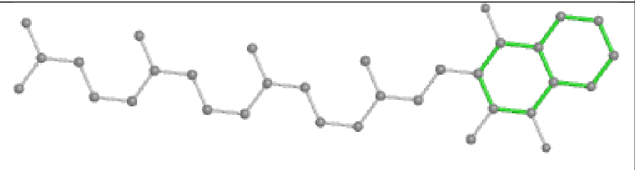


Torsions

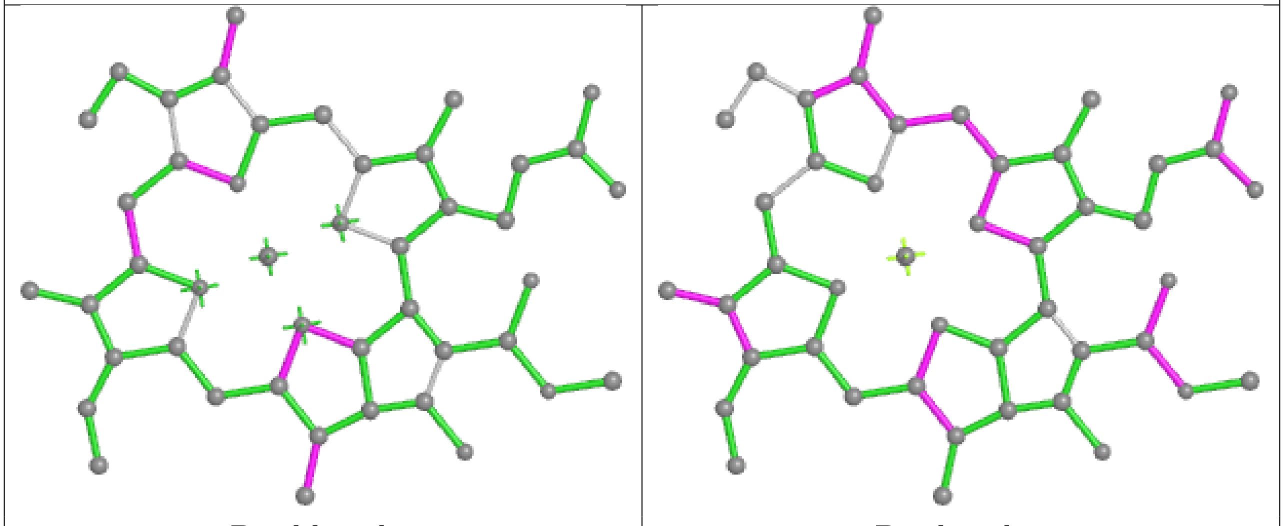


Rings

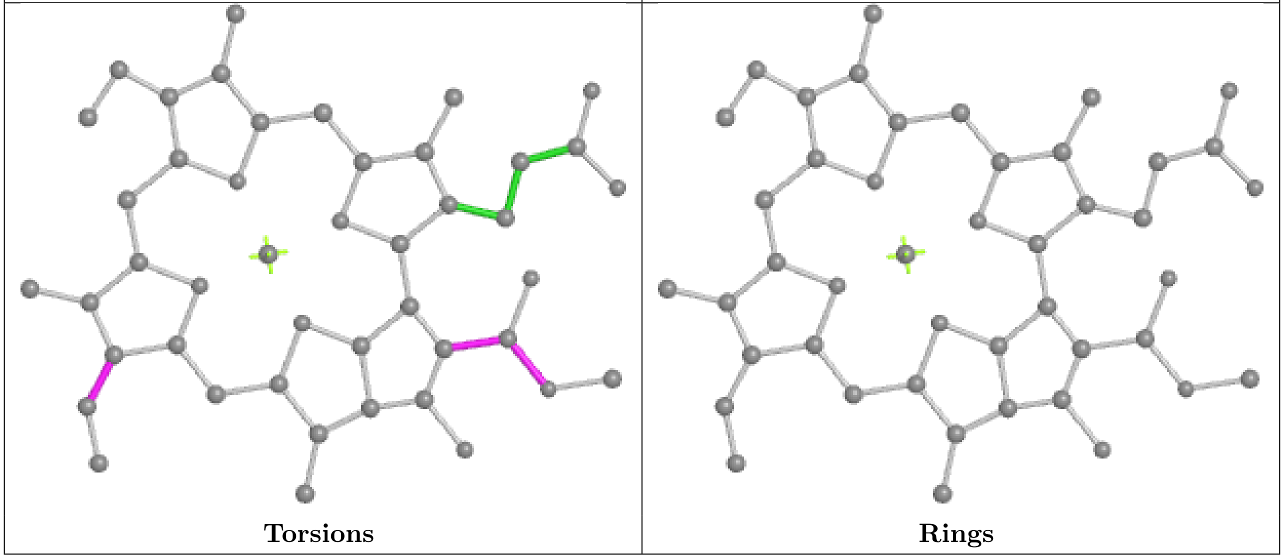
Ligand CLA a 812	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

Ligand PQN b 844	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

Ligand CLA a 823

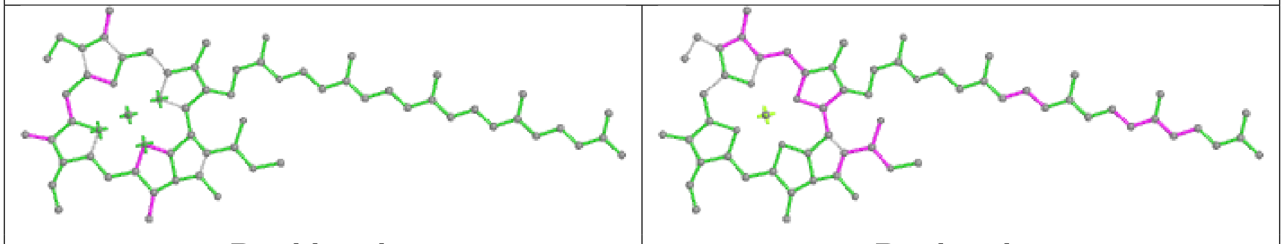


Bond lengths Bond angles

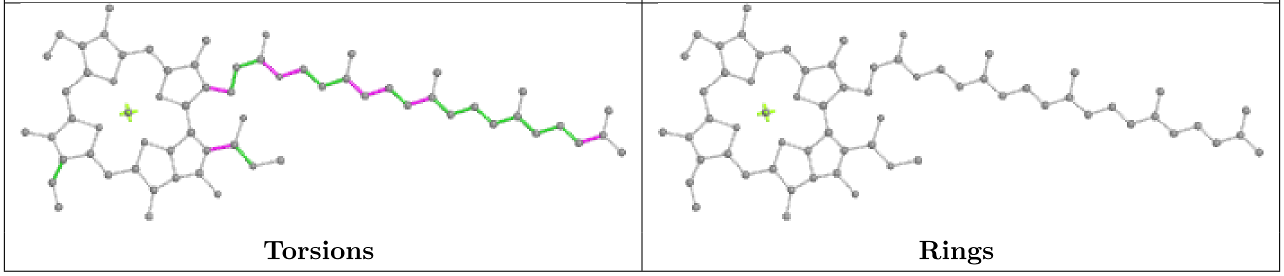


Torsions Rings

Ligand CLA B 804

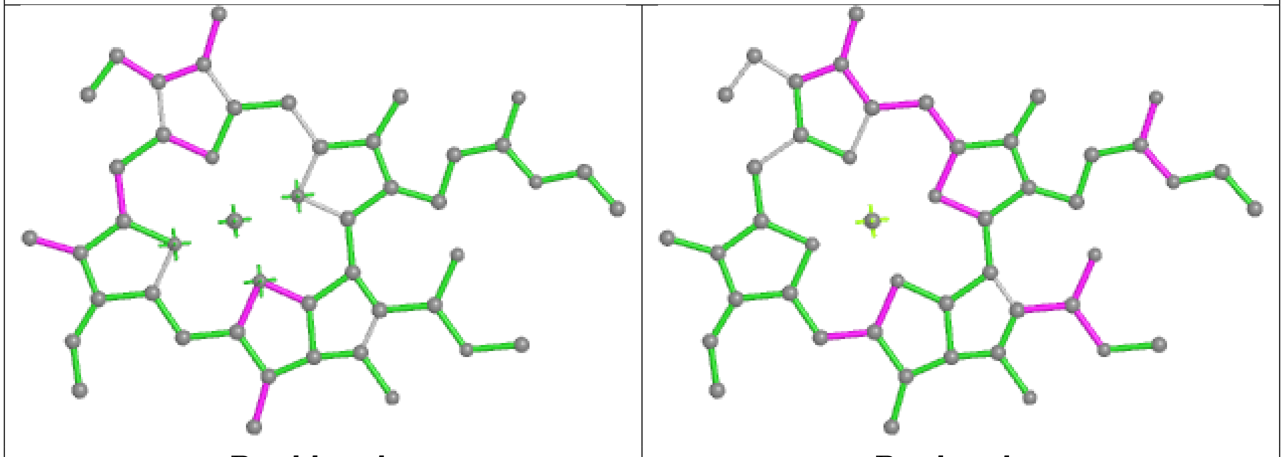


Bond lengths Bond angles



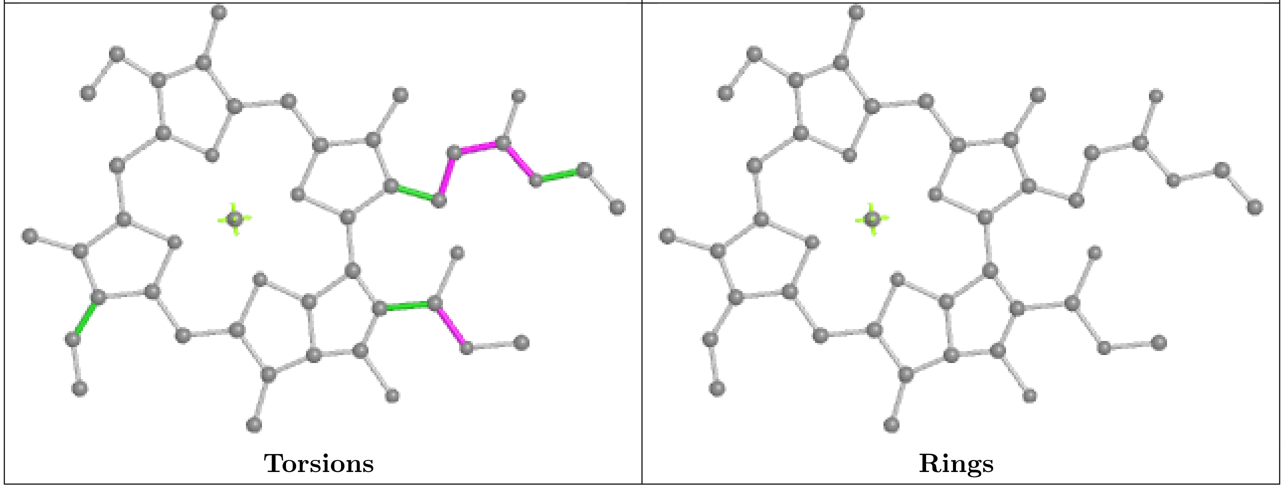
Torsions Rings

Ligand CLA b 841



Bond lengths

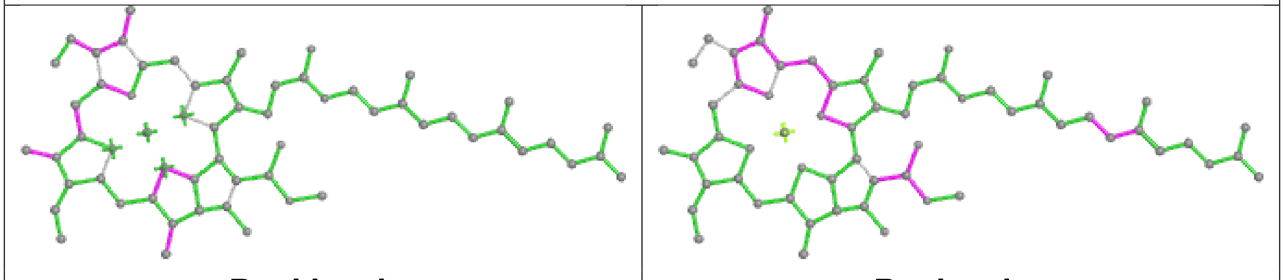
Bond angles



Torsions

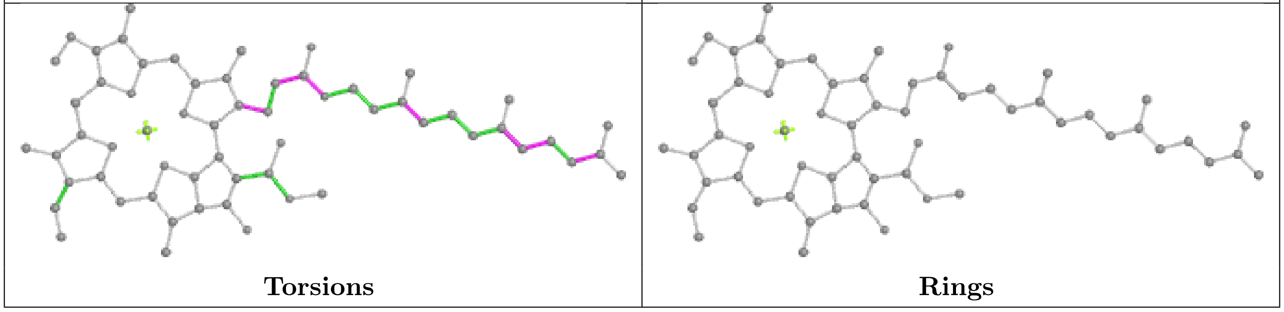
Rings

Ligand CLA B 813



Bond lengths

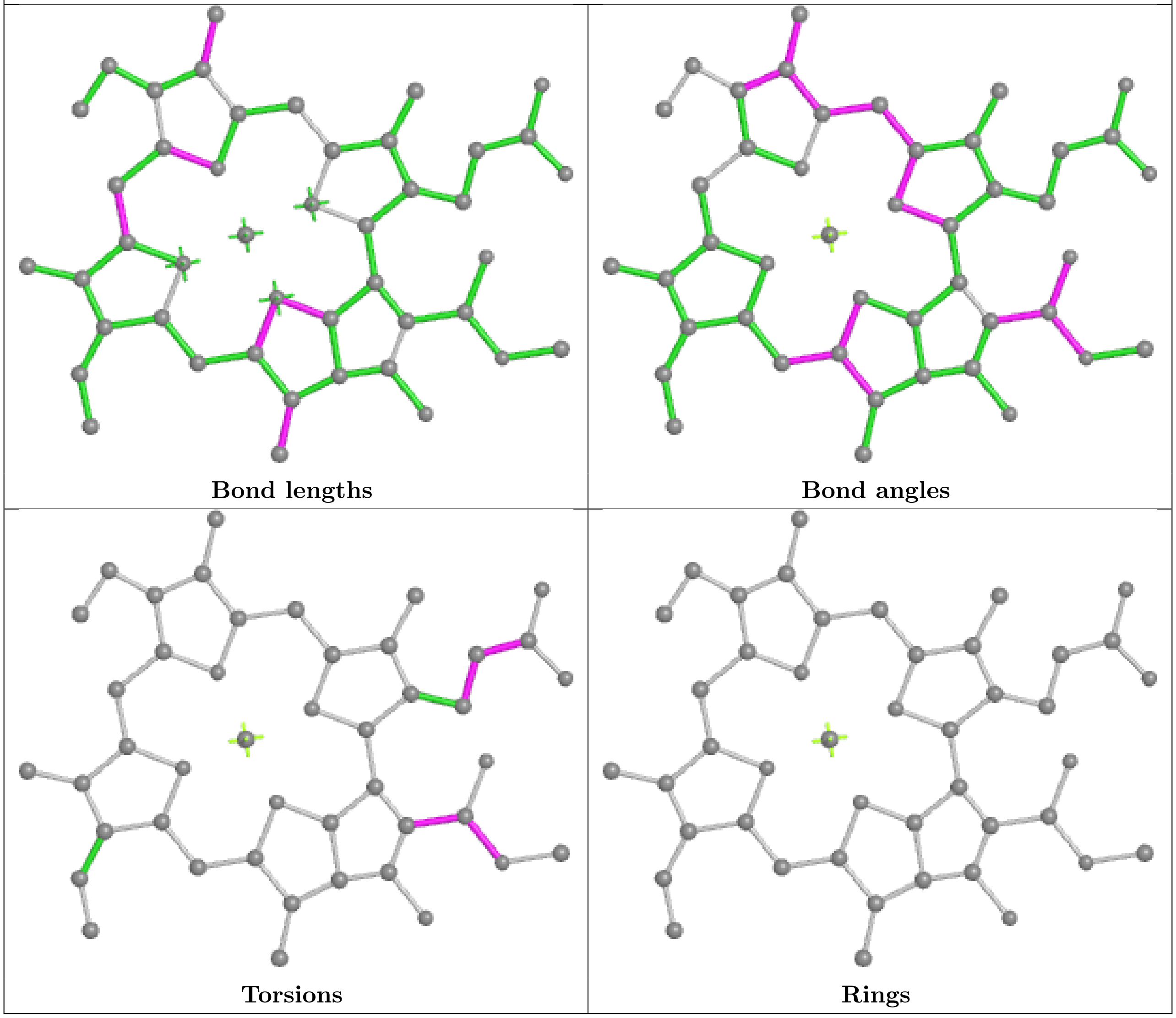
Bond angles



Torsions

Rings

Ligand CLA L 1503



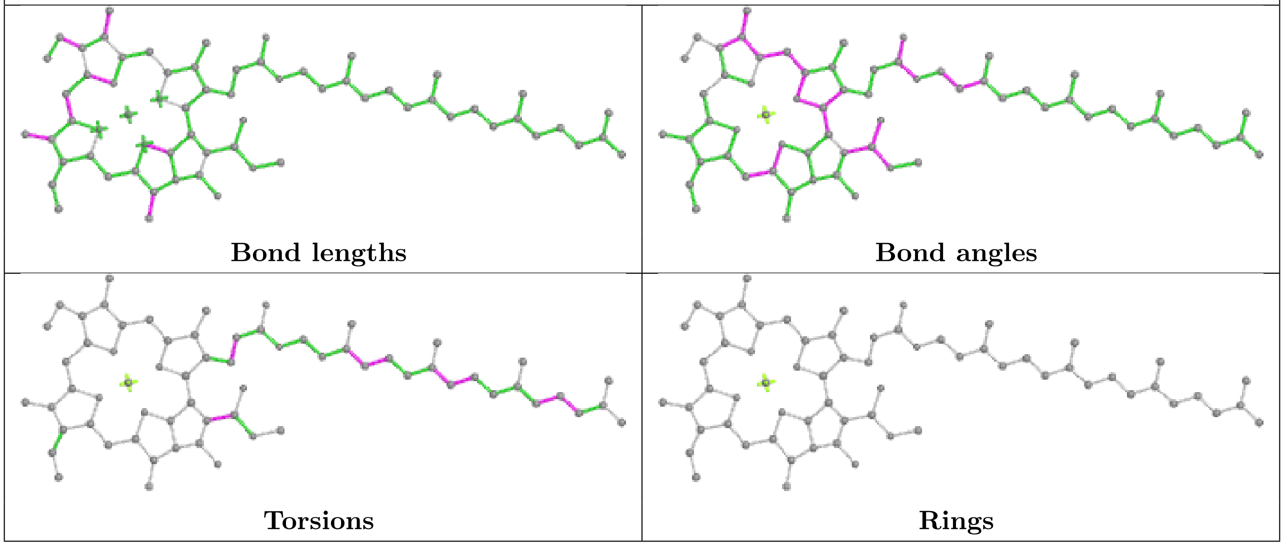
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA B 801



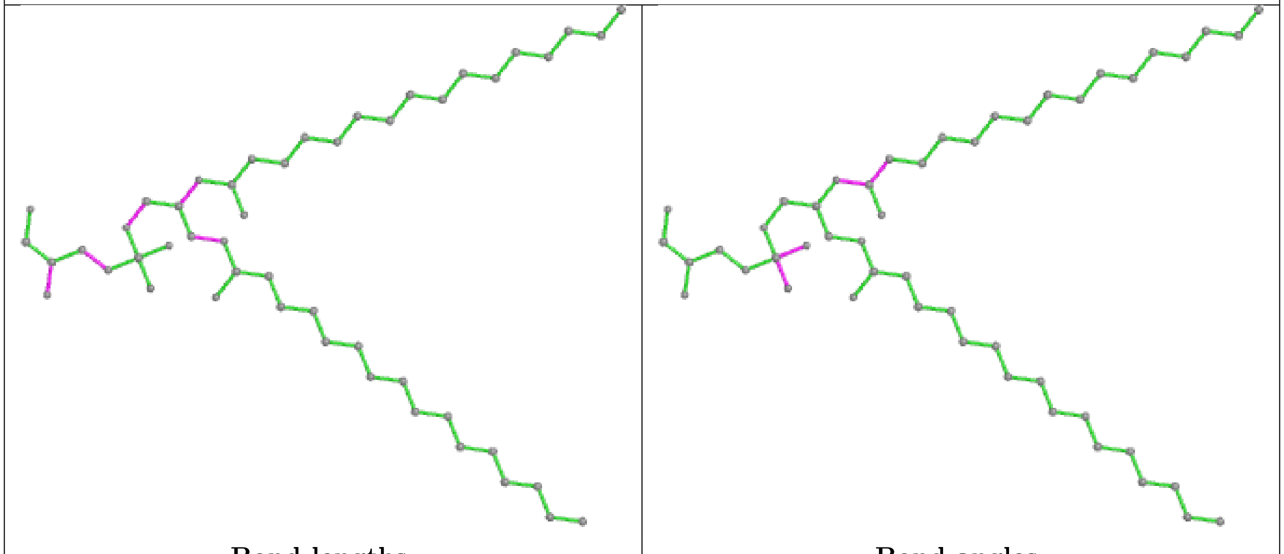
Bond lengths

Bond angles

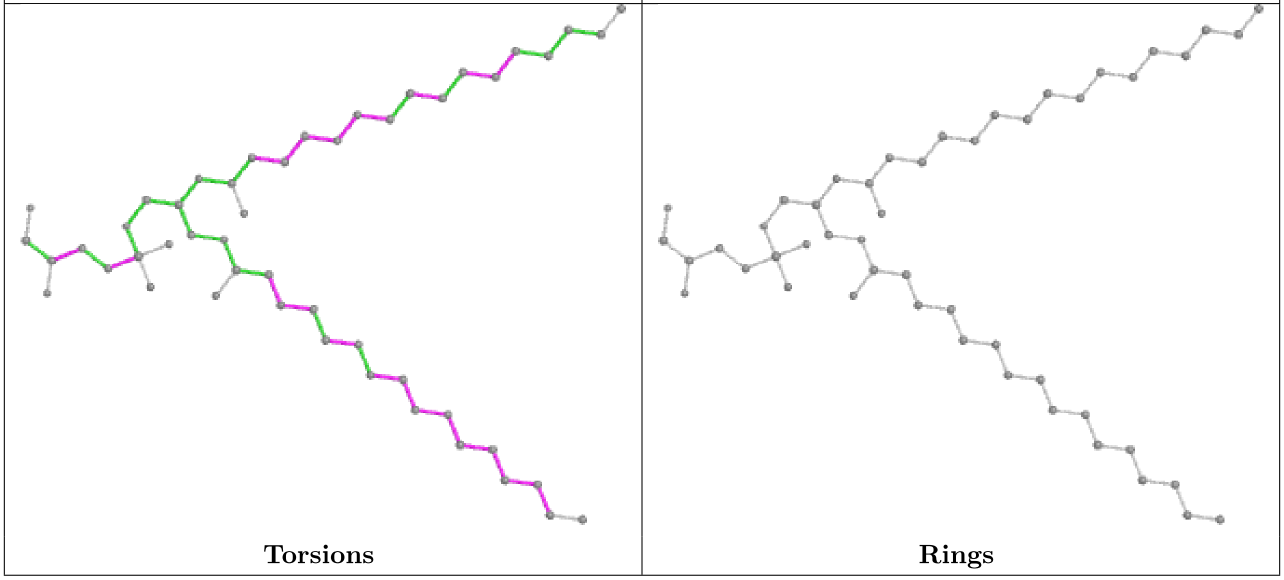
Torsions

Rings

Ligand LHG a 851

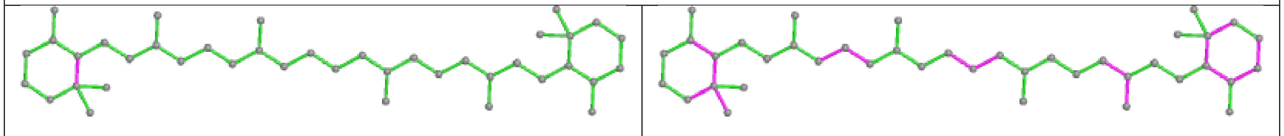


Bond lengths **Bond angles**

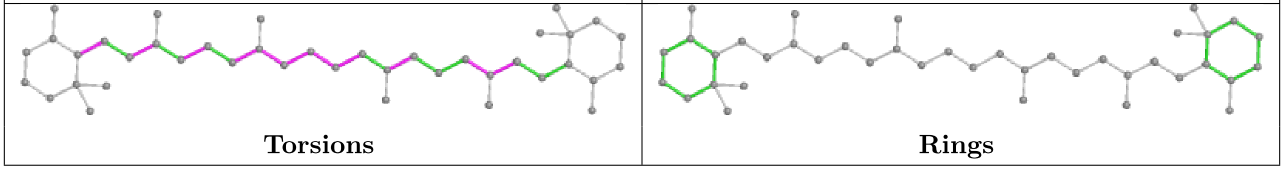


Torsions **Rings**

Ligand BCR i 101

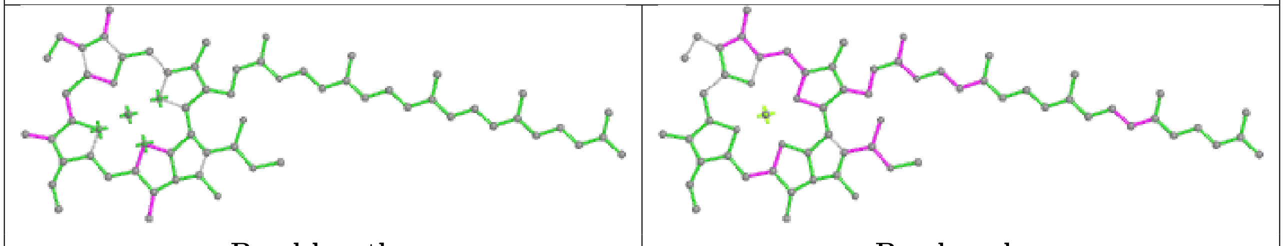


Bond lengths **Bond angles**

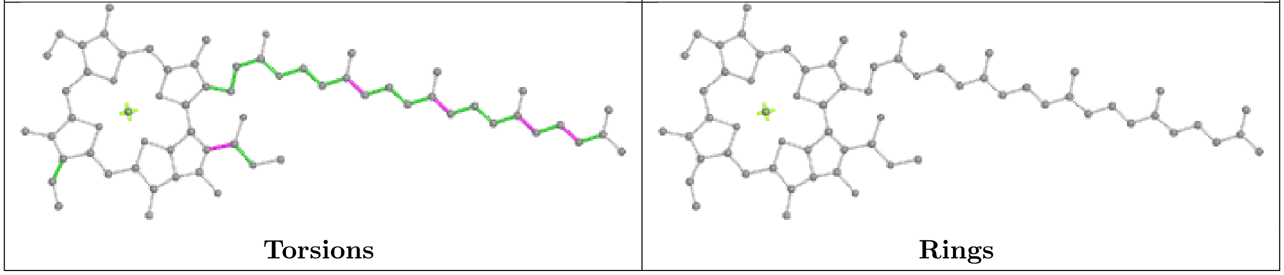


Torsions **Rings**

Ligand CLA B 840

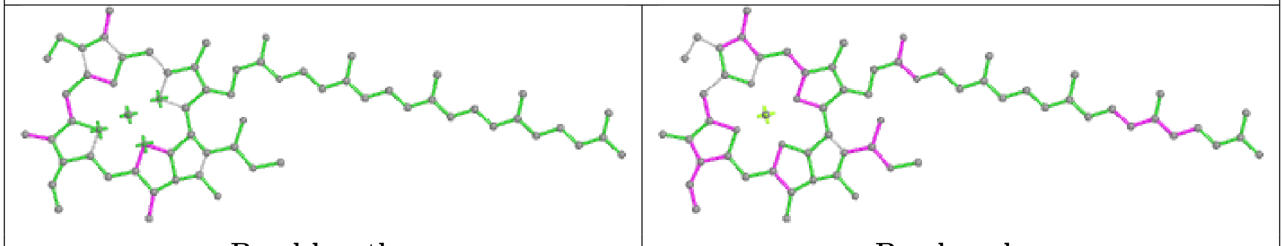


Bond lengths Bond angles

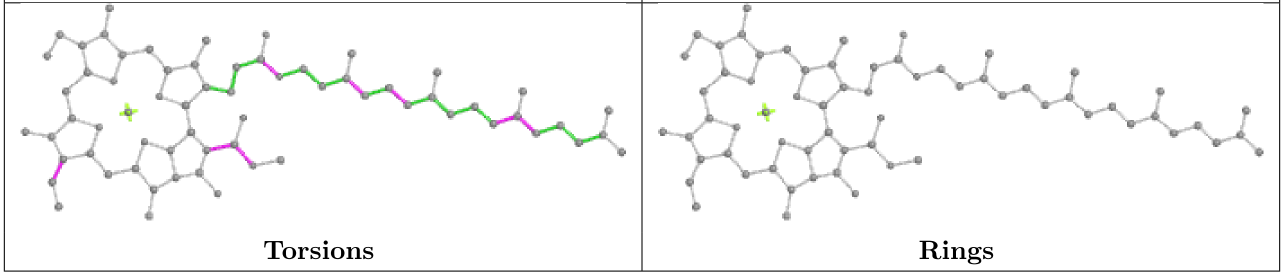


Torsions Rings

Ligand CLA A 834

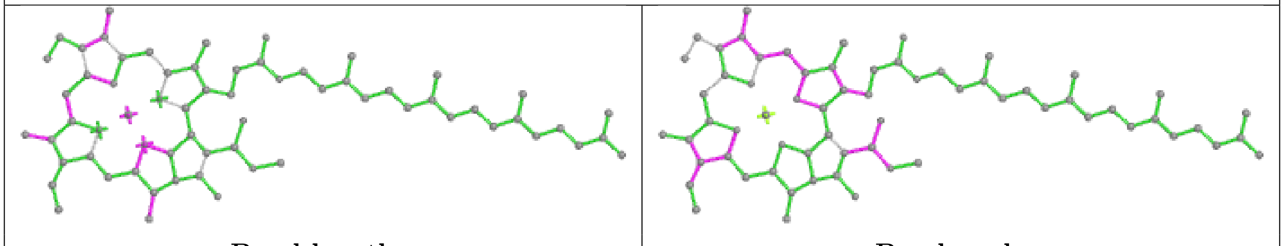


Bond lengths Bond angles

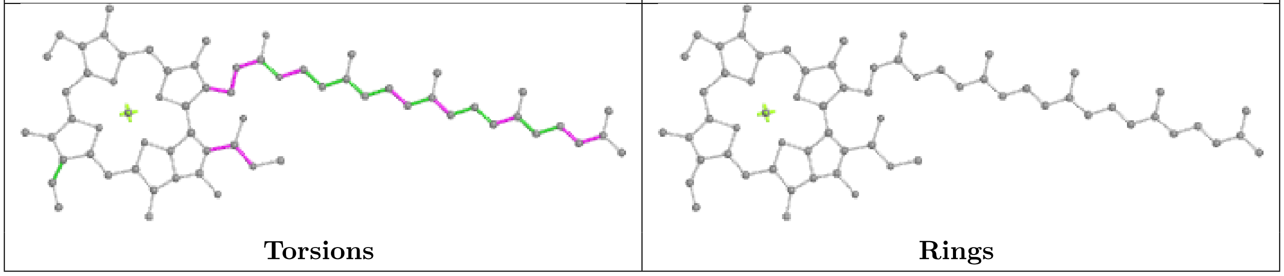


Torsions Rings

Ligand CLA b 812

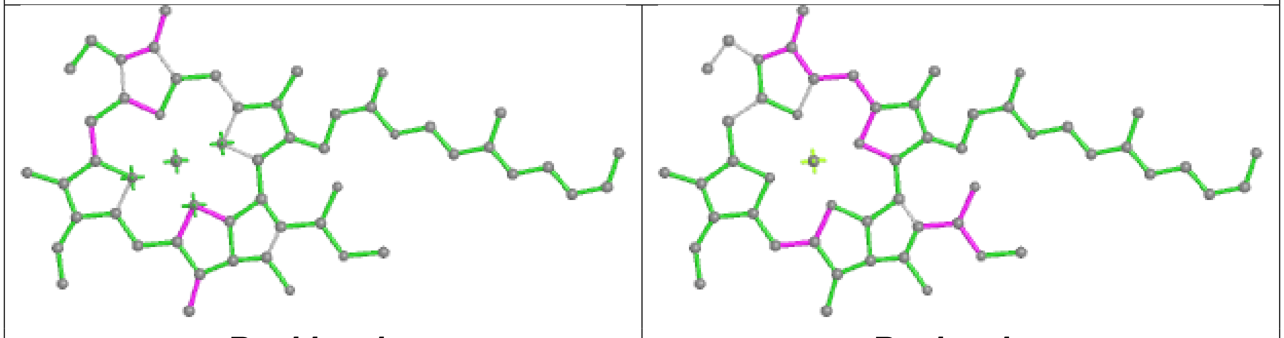


Bond lengths Bond angles



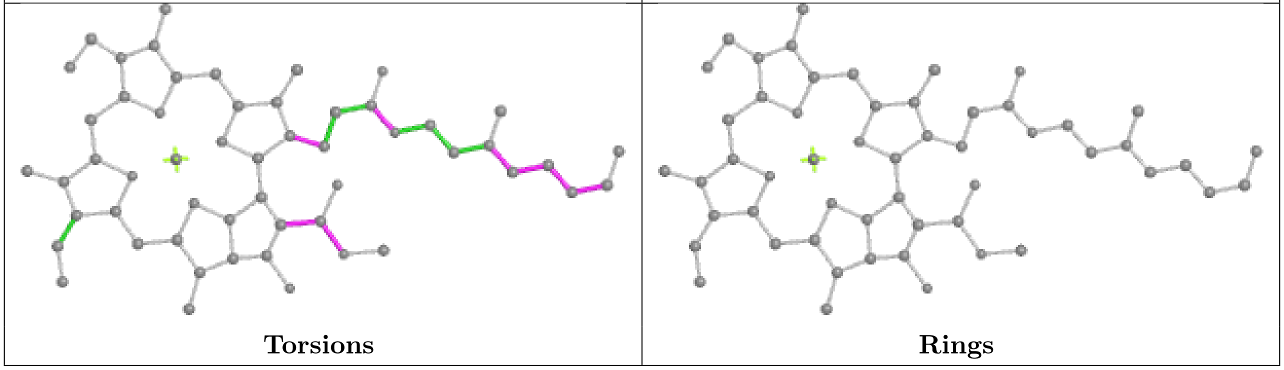
Torsions Rings

Ligand CLA b 814



Bond lengths

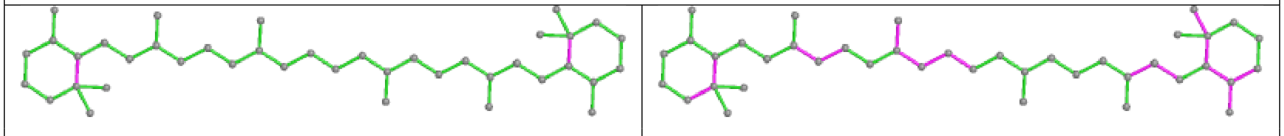
Bond angles



Torsions

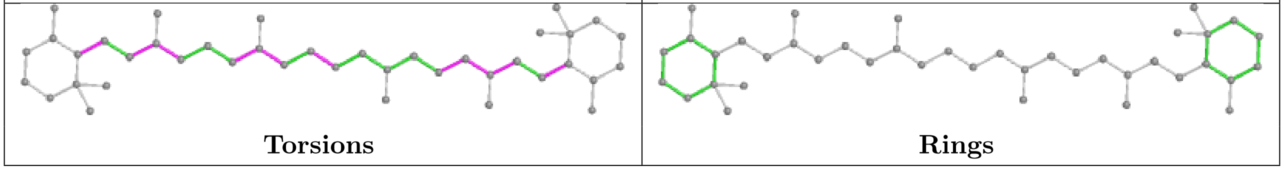
Rings

Ligand BCR f 204



Bond lengths

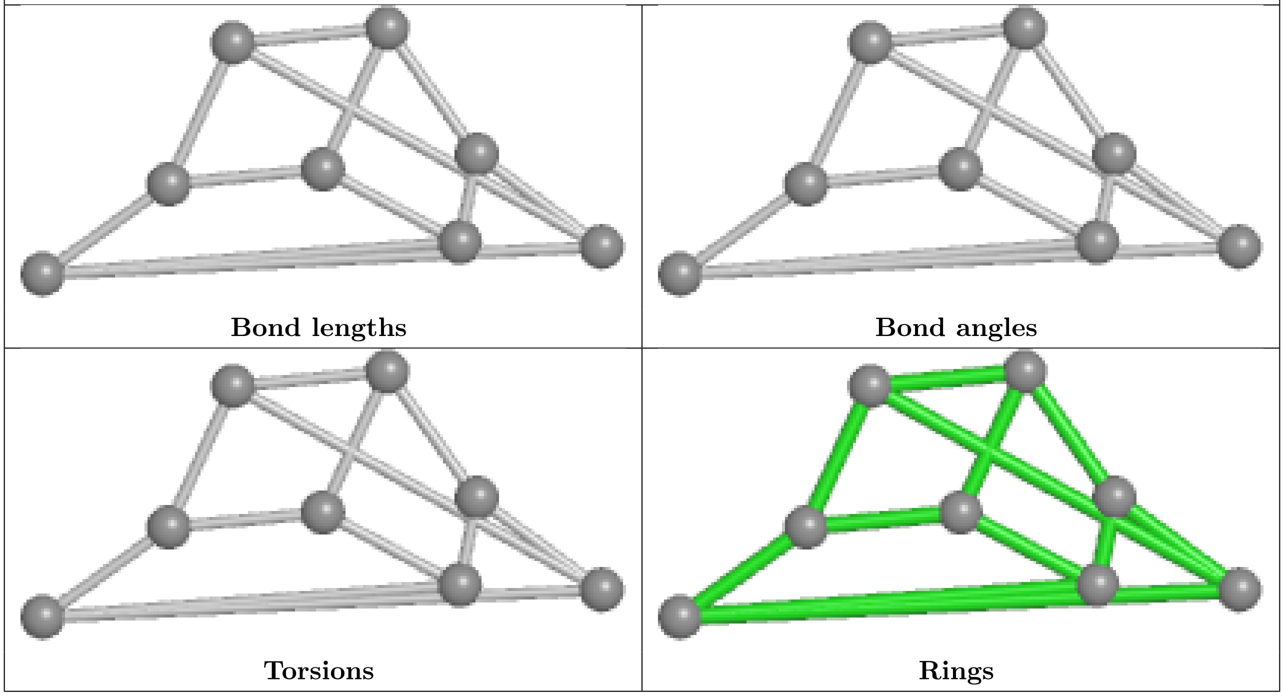
Bond angles



Torsions

Rings

Ligand SF4 c 102



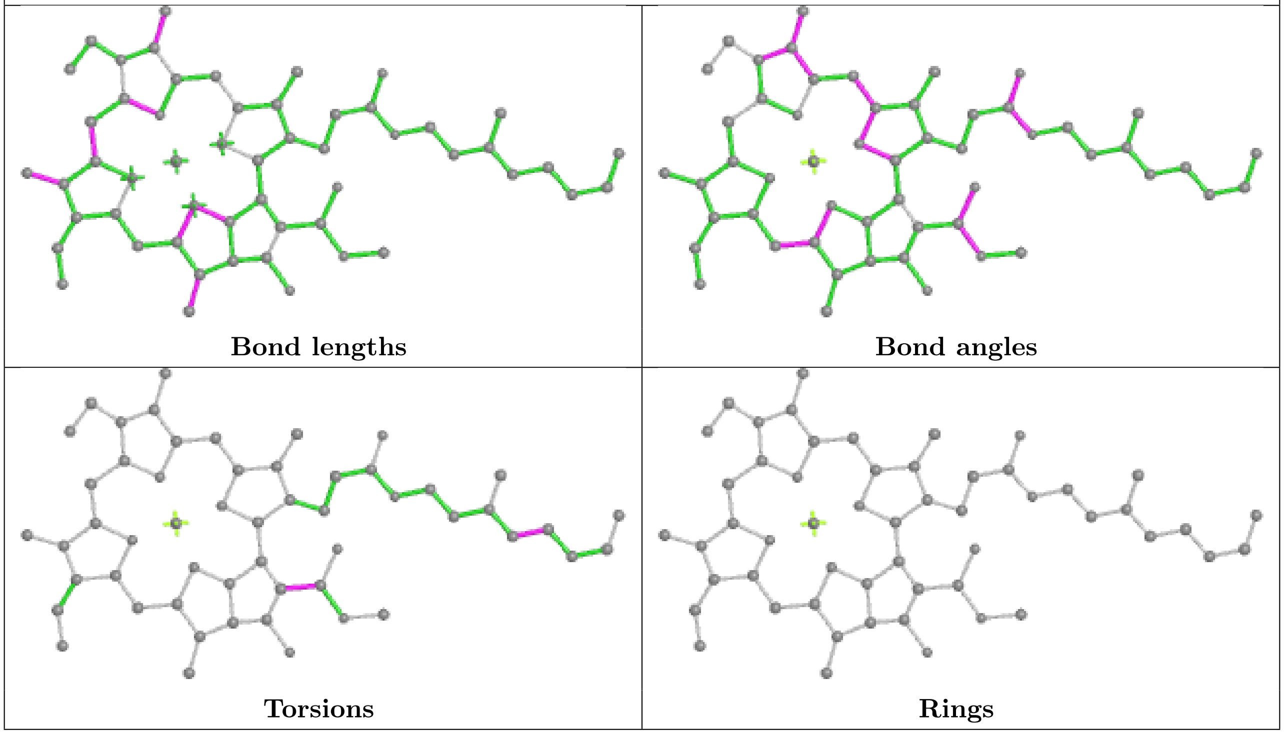
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA a 813



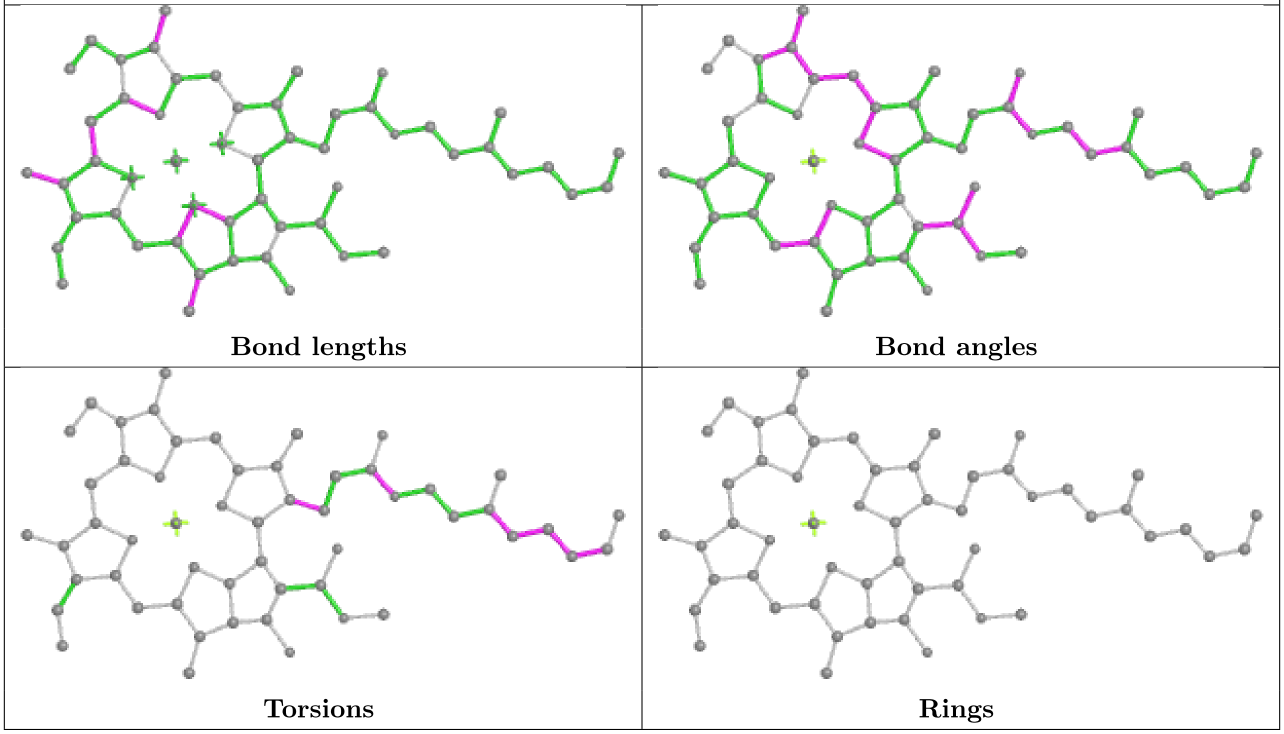
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA A 823



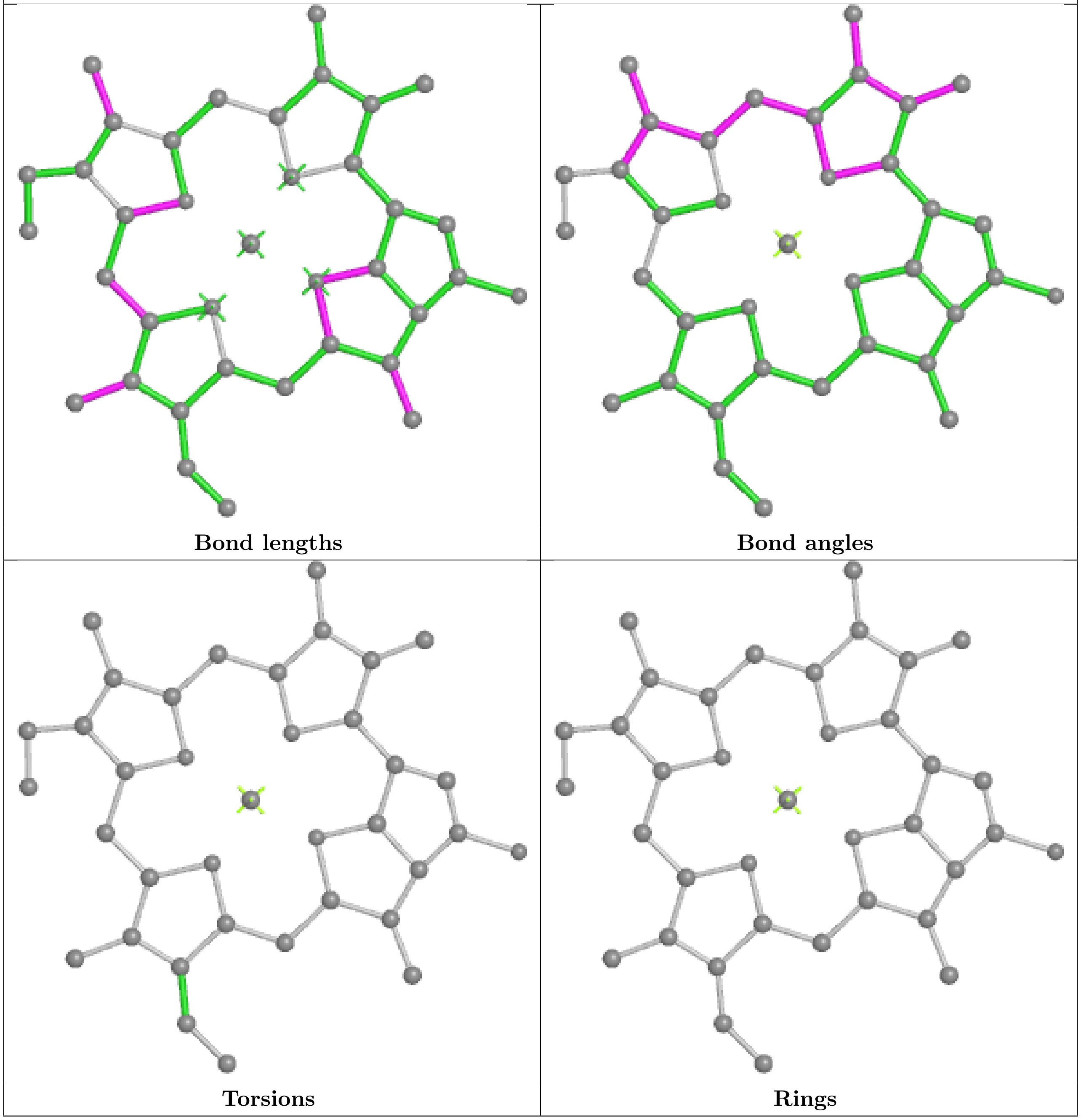
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA J 102



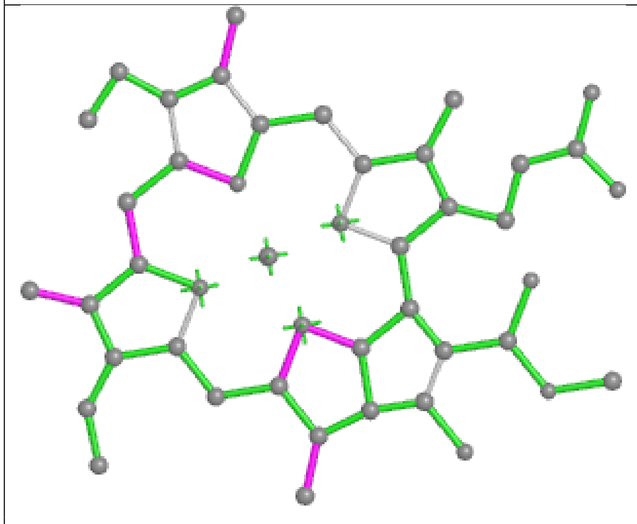
Bond lengths

Bond angles

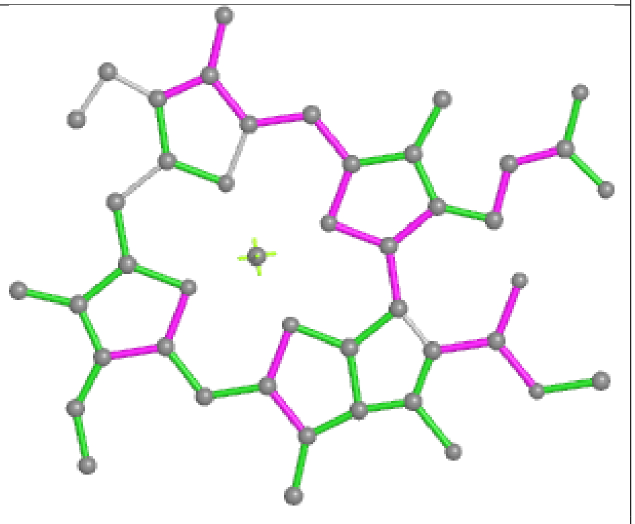
Torsions

Rings

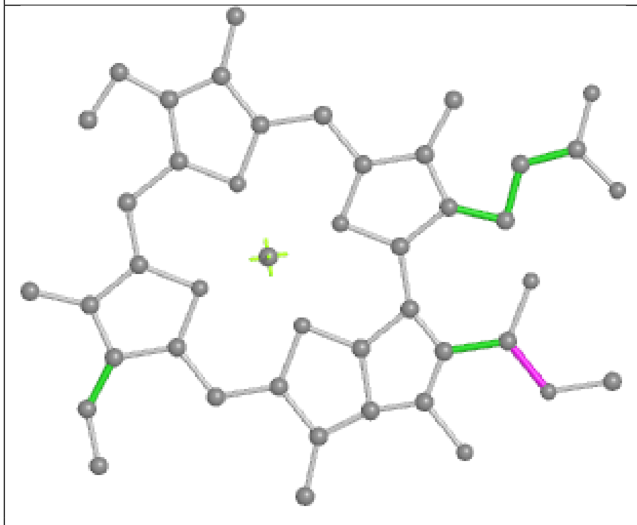
Ligand CLA B 837



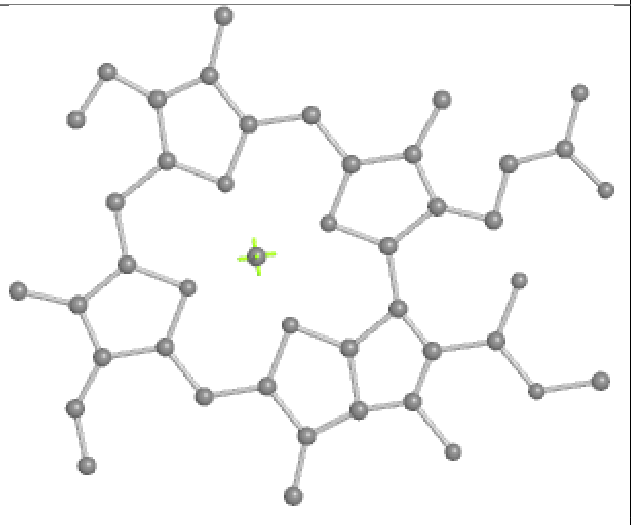
Bond lengths



Bond angles

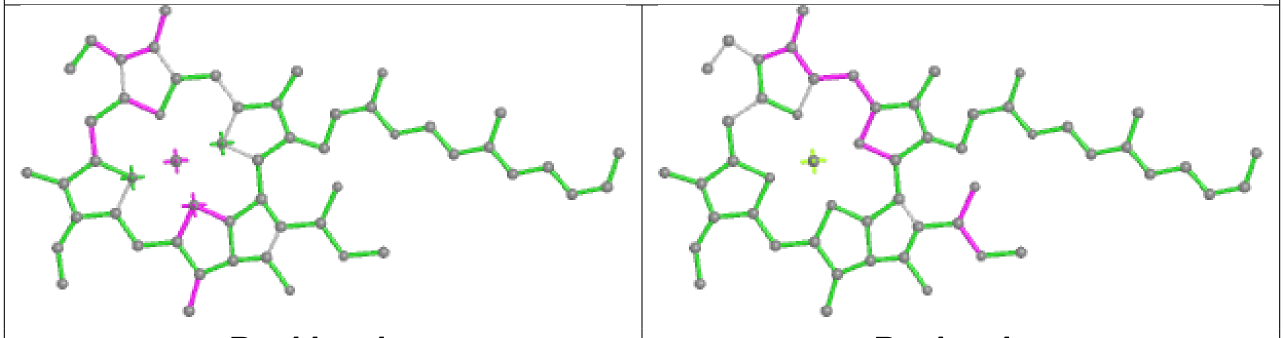


Torsions

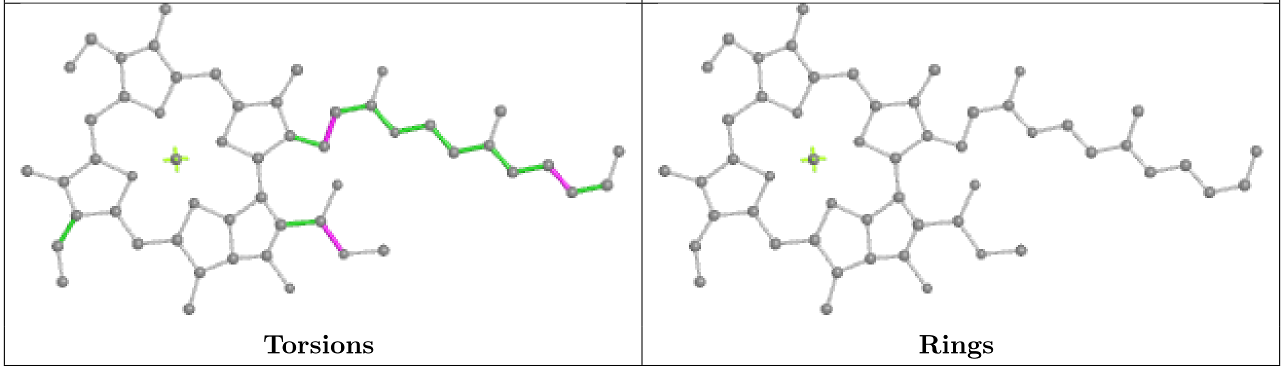


Rings

Ligand CLA a 834

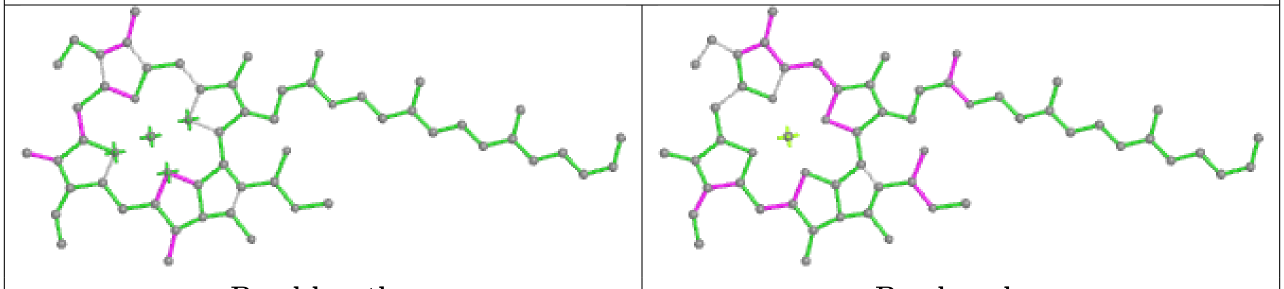


Bond lengths Bond angles

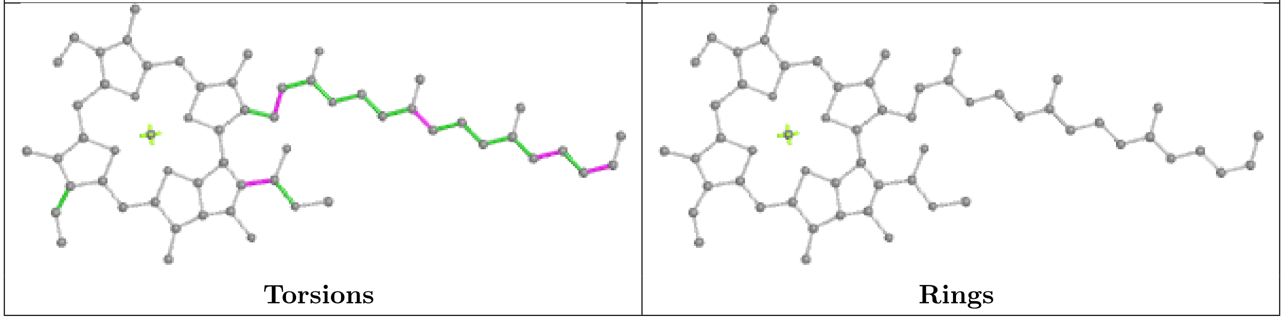


Torsions Rings

Ligand CLA A 817

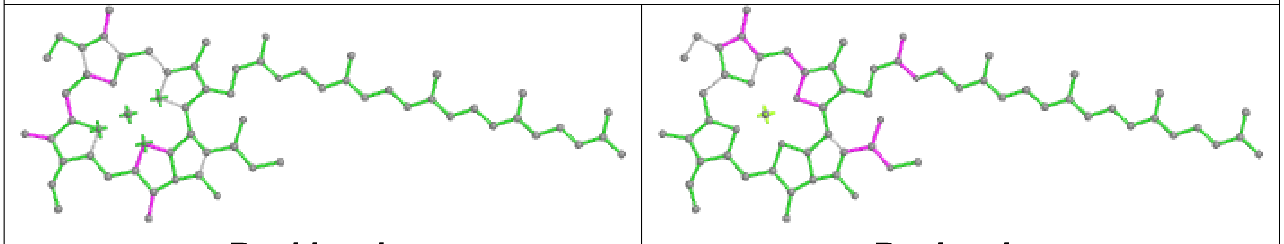


Bond lengths Bond angles

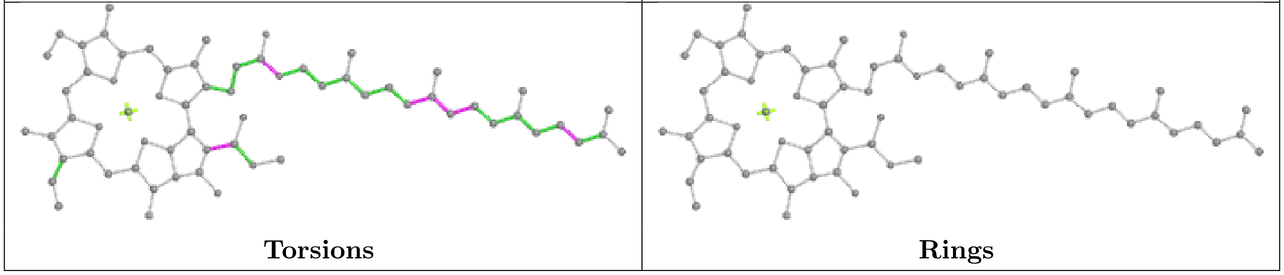


Torsions Rings

Ligand CLA B 810

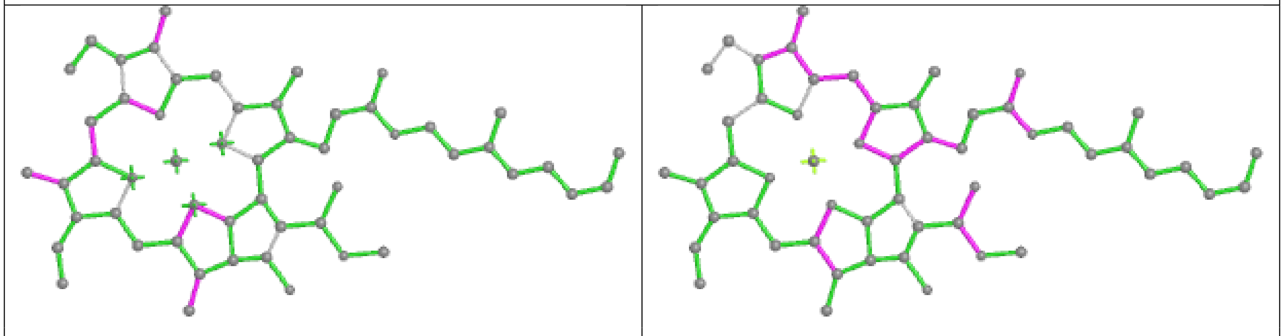


Bond lengths Bond angles

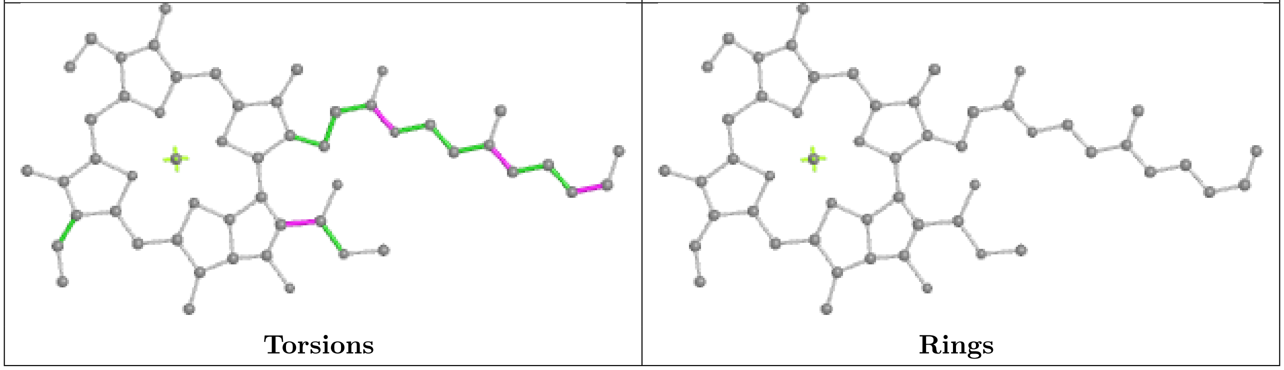


Torsions Rings

Ligand CLA a 825

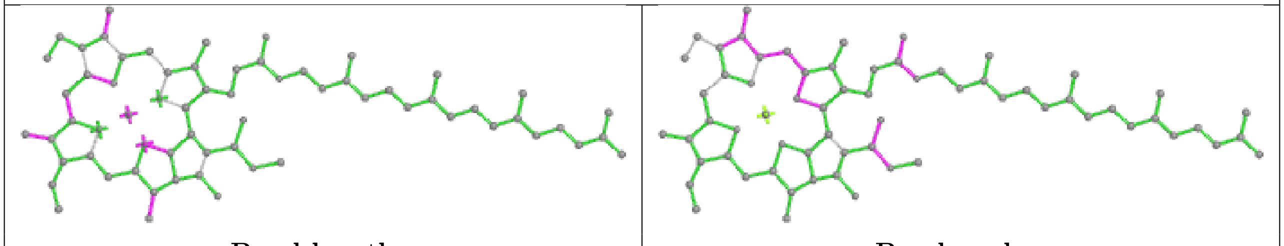


Bond lengths Bond angles

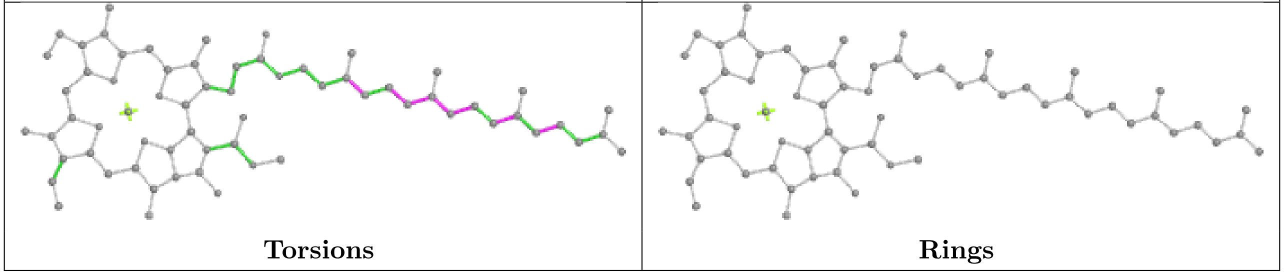


Torsions Rings

Ligand CLA b 802

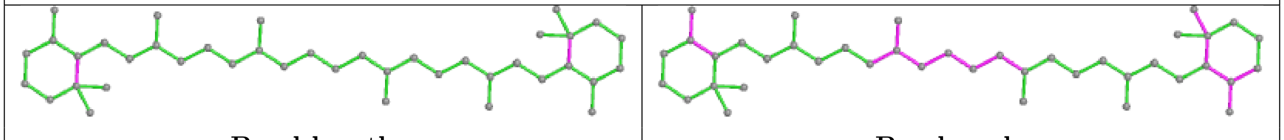


Bond lengths Bond angles

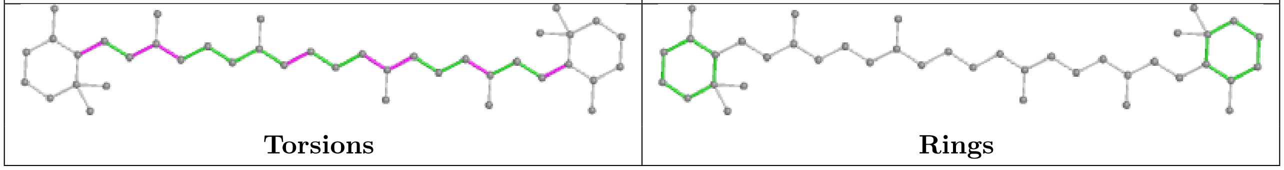


Torsions Rings

Ligand BCR M 101

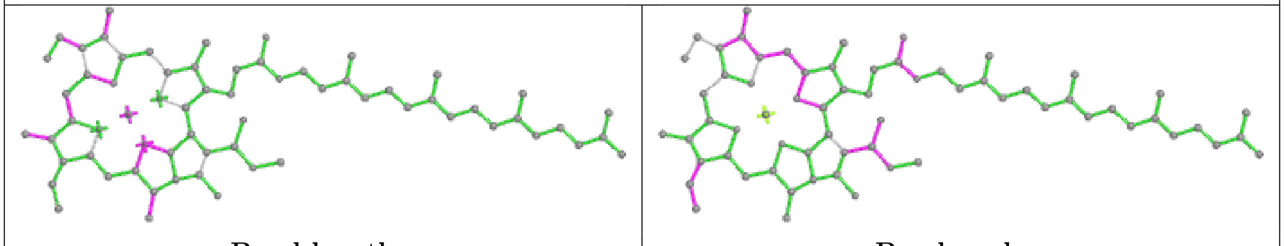


Bond lengths Bond angles

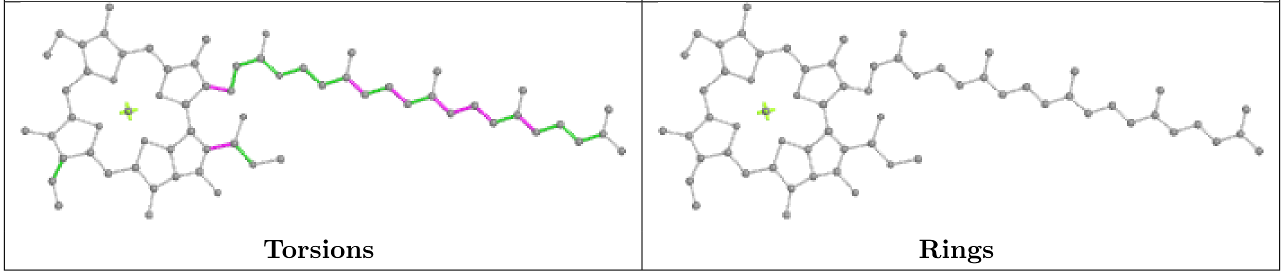


Torsions Rings

Ligand CLA B 816

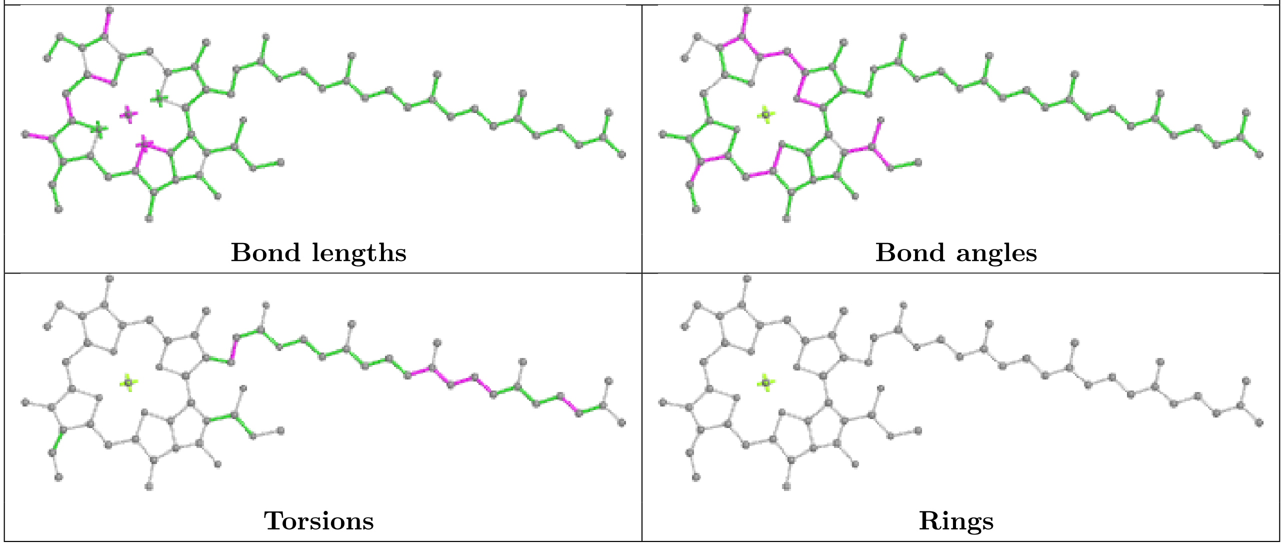


Bond lengths Bond angles

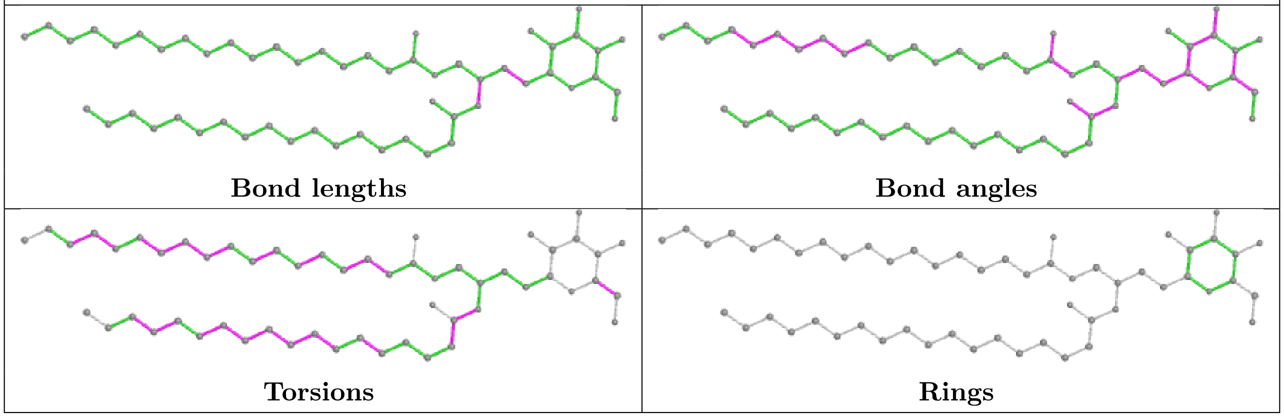


Torsions Rings

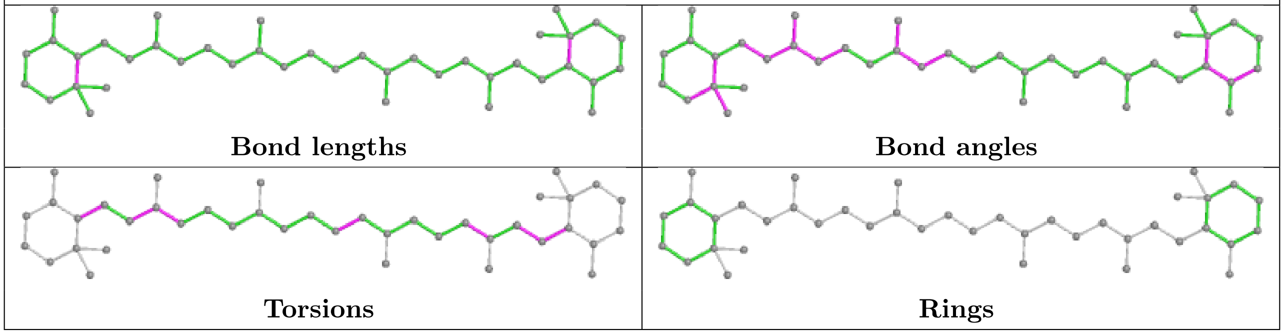
Ligand CLA b 810



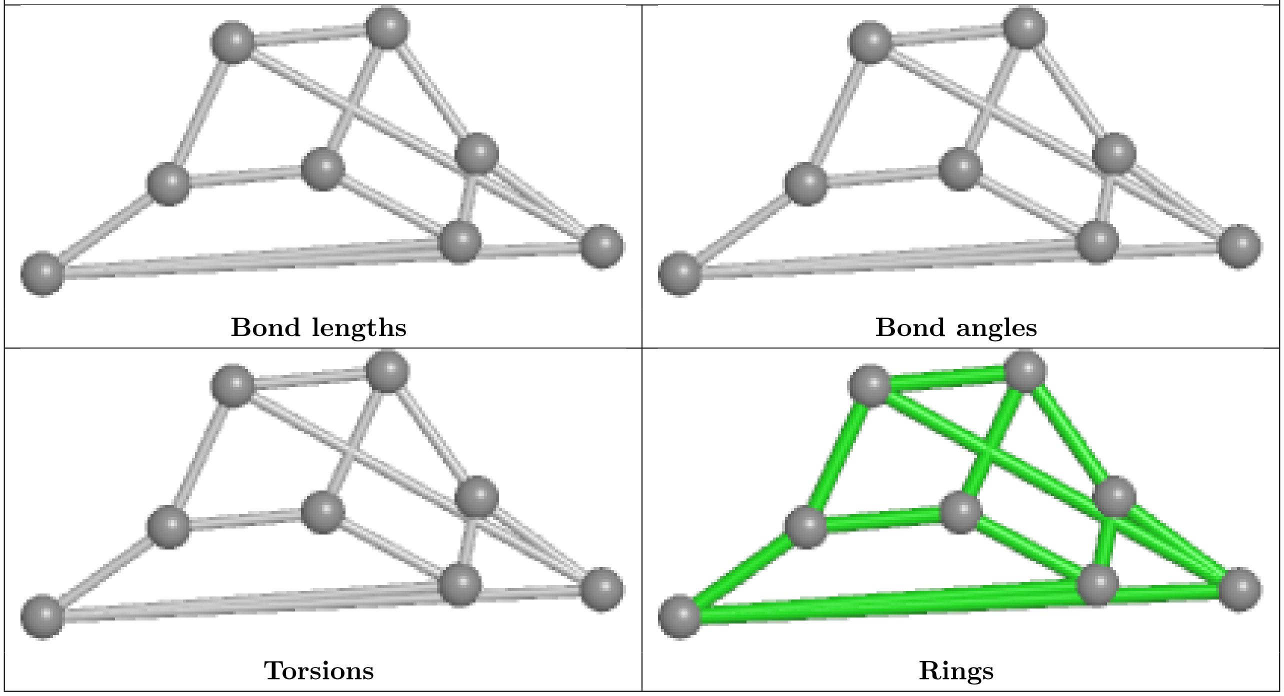
Ligand LMG b 851



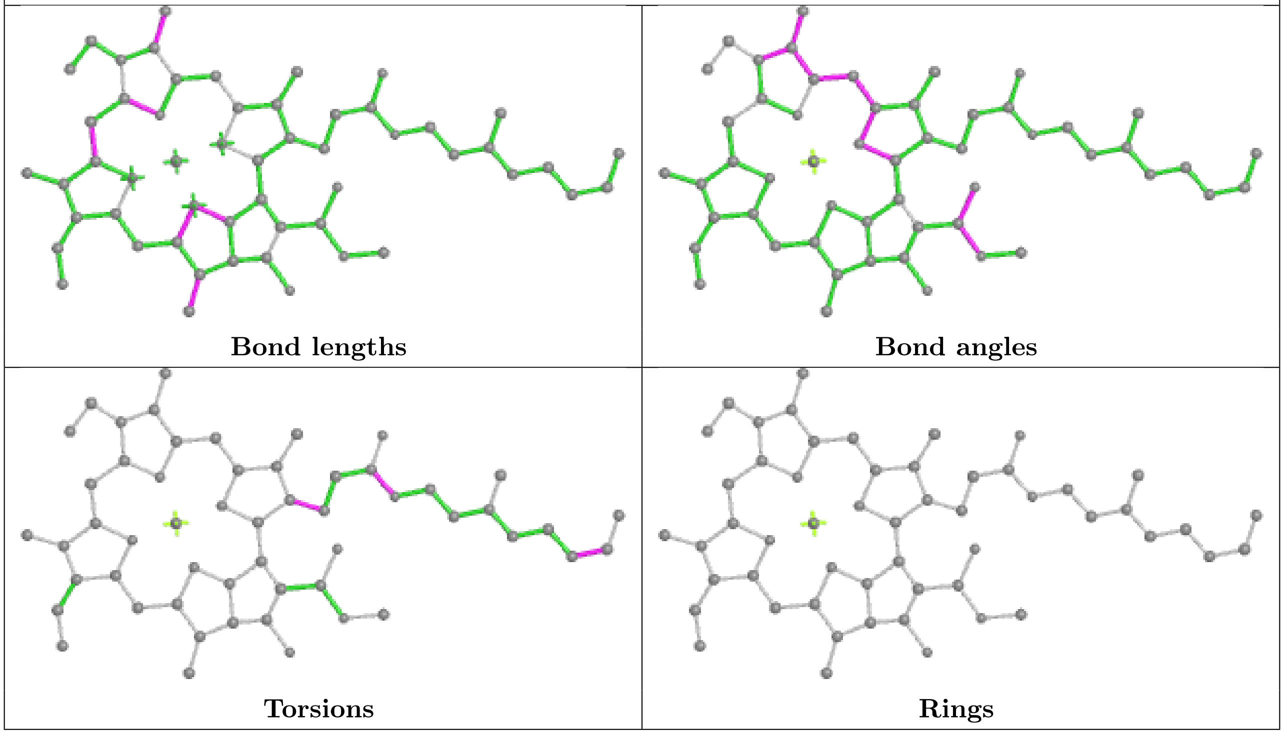
Ligand BCR J 105



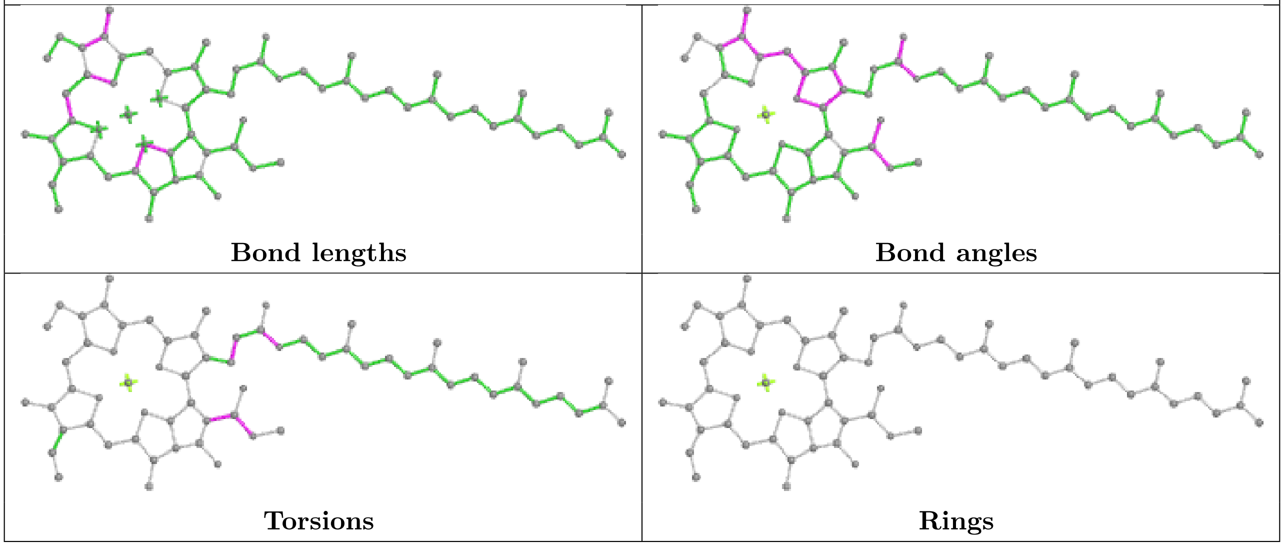
Ligand SF4 C 102



Ligand CLA a 803



Ligand CLA b 842



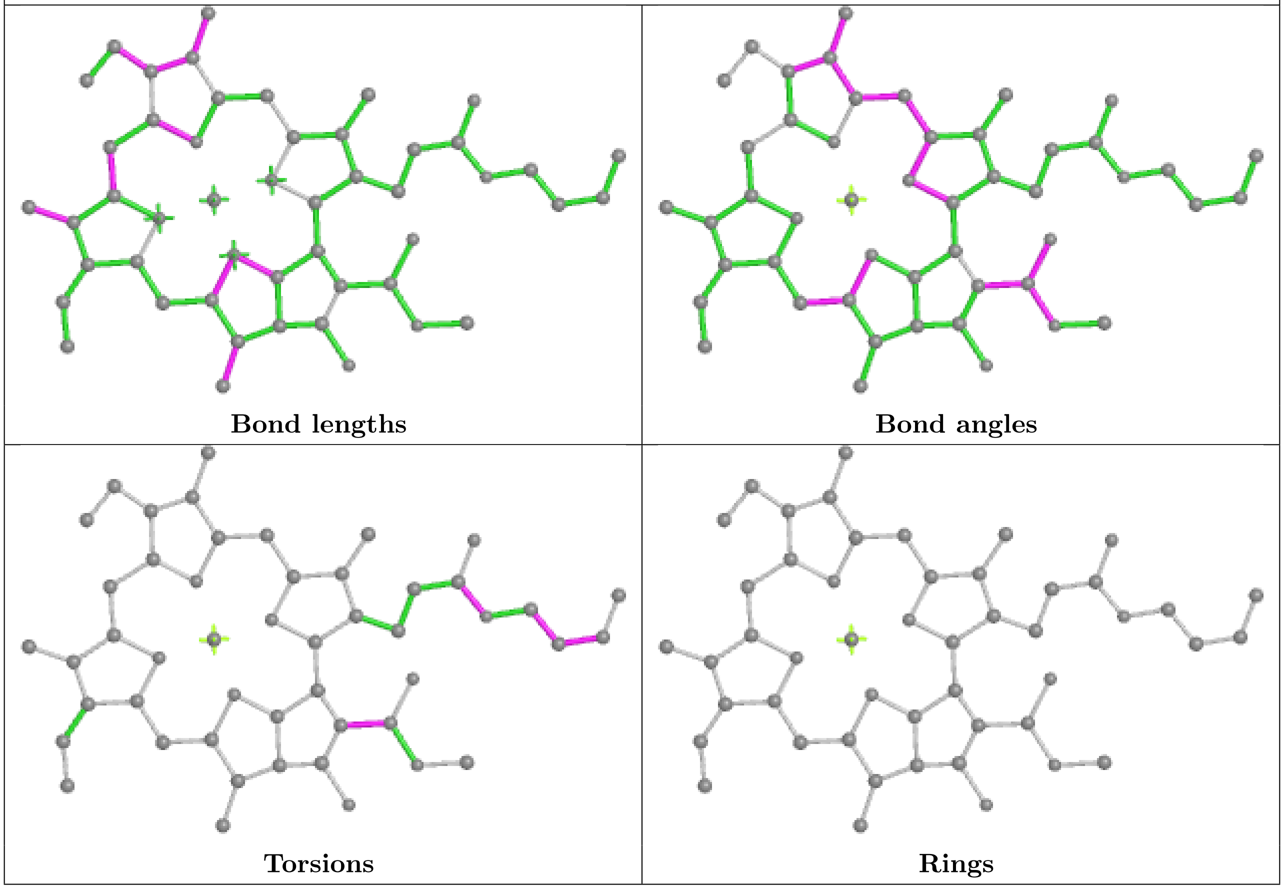
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA b 818



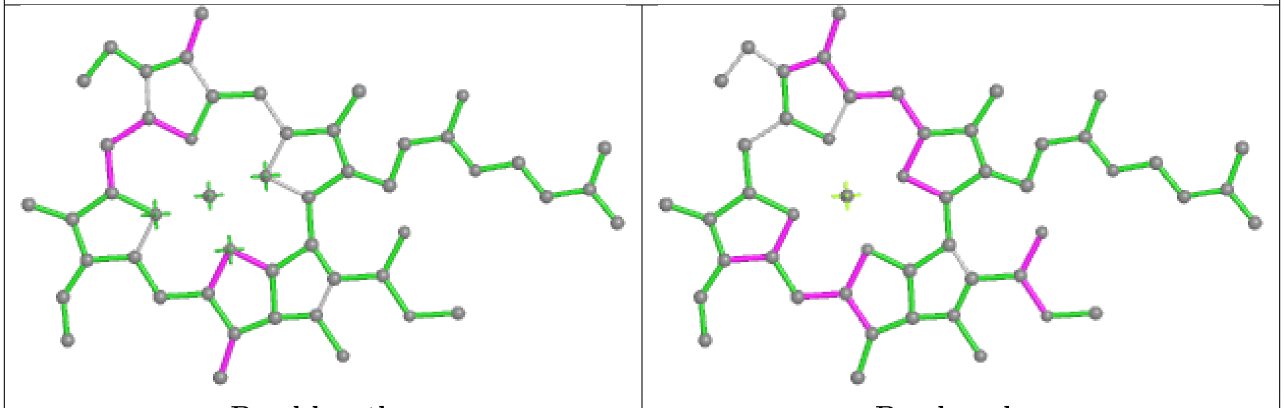
Bond lengths

Bond angles

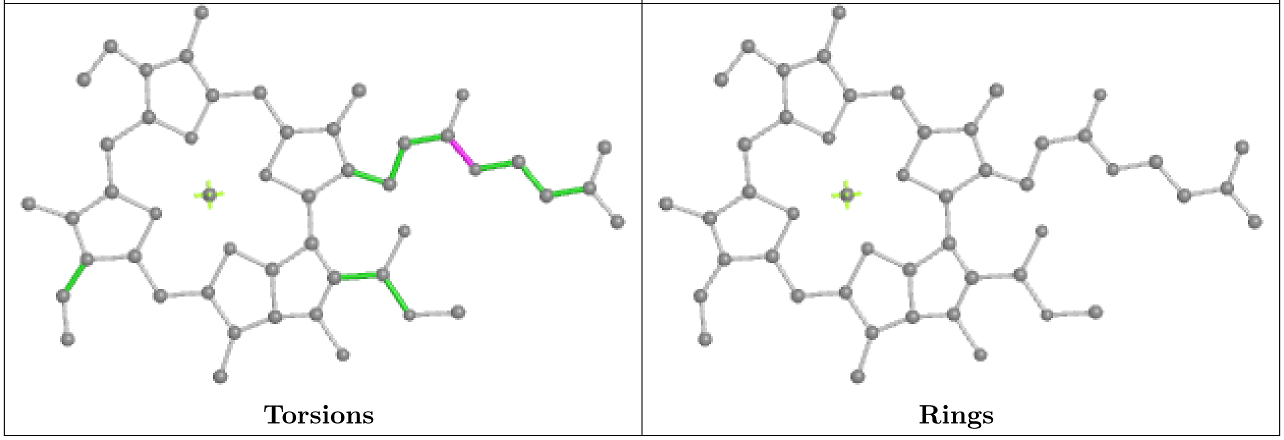
Torsions

Rings

Ligand CLA B 817

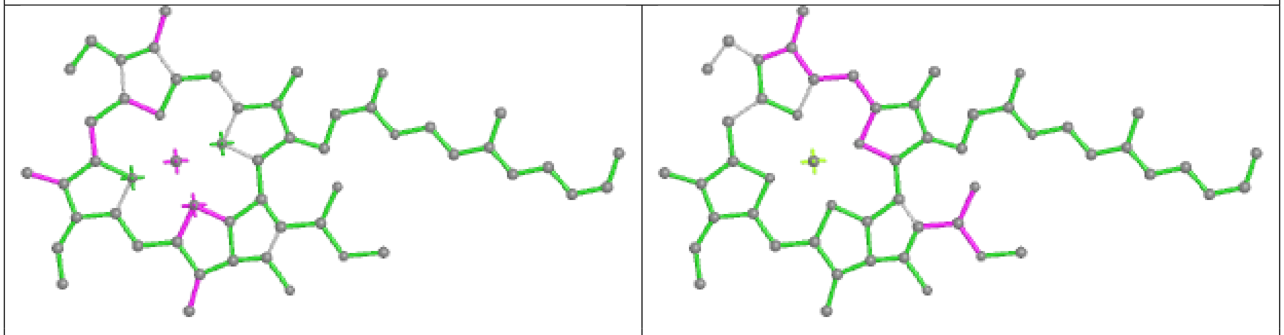


Bond lengths Bond angles

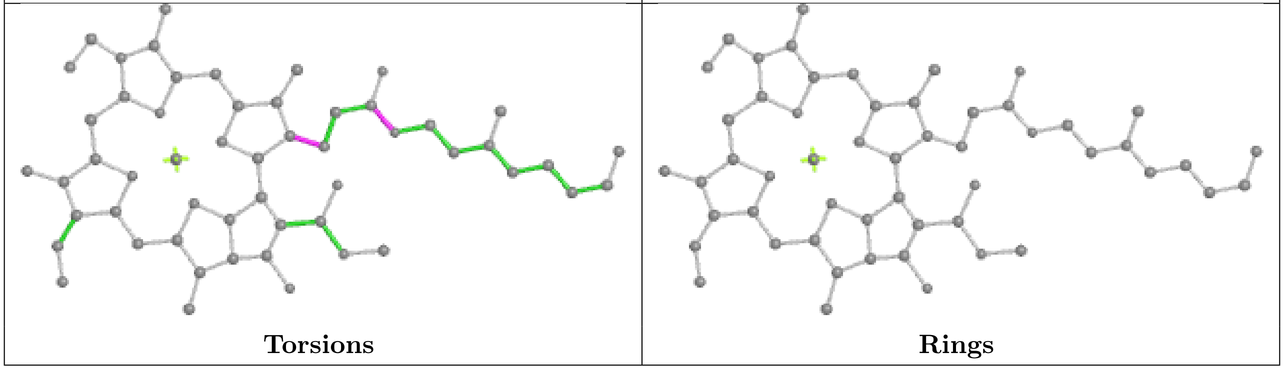


Torsions Rings

Ligand CLA A 804

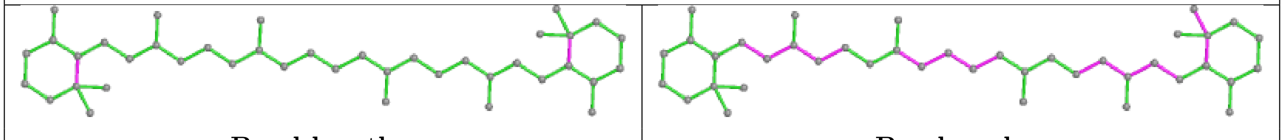


Bond lengths Bond angles

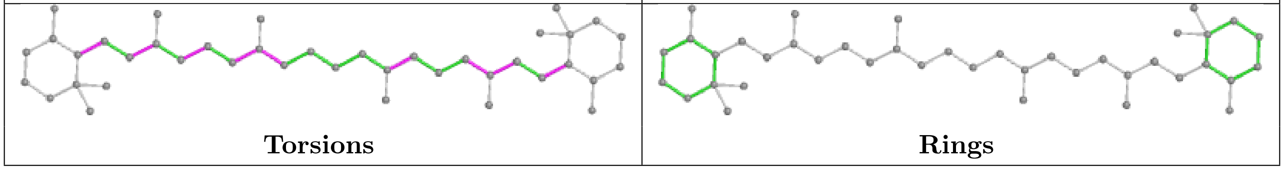


Torsions Rings

Ligand BCR F 203

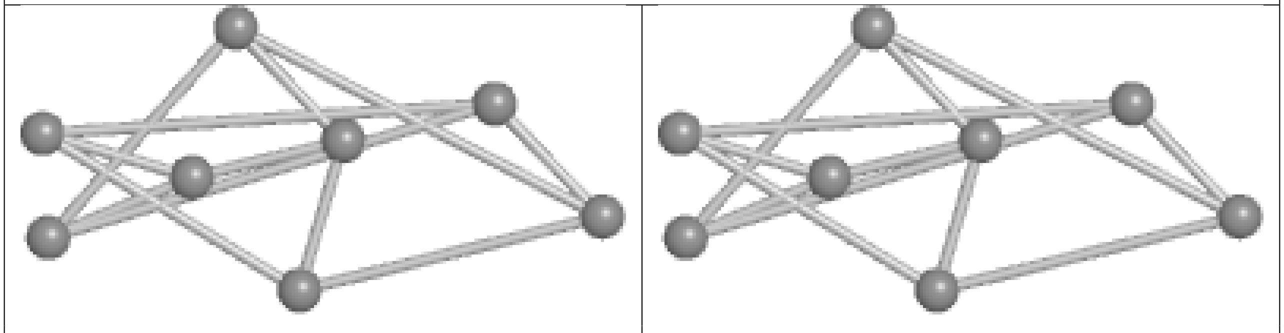


Bond lengths | Bond angles

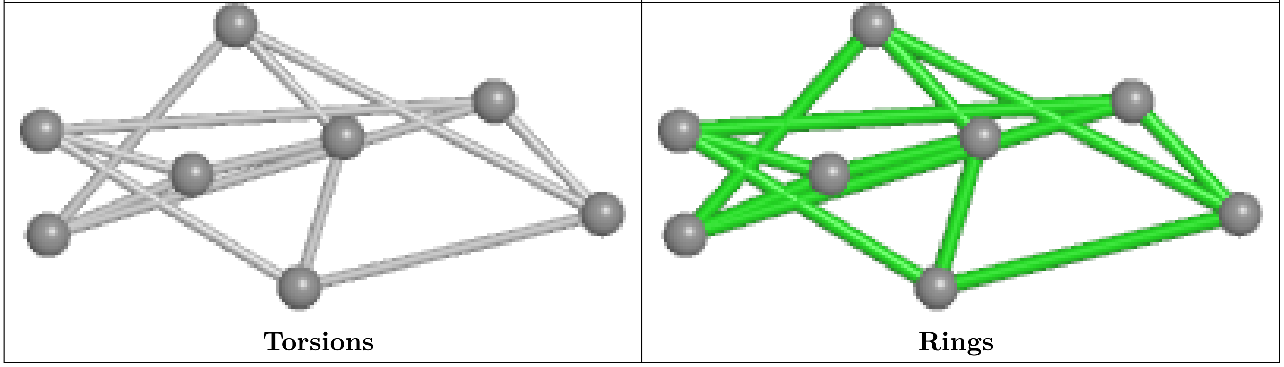


Torsions | Rings

Ligand SF4 a 843

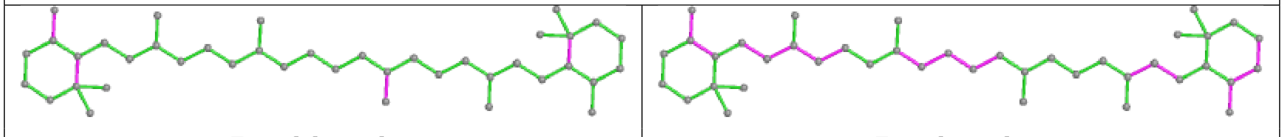


Bond lengths | Bond angles

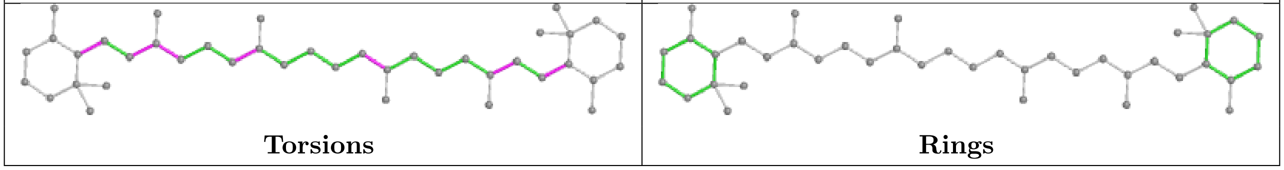


Torsions | Rings

Ligand BCR a 844

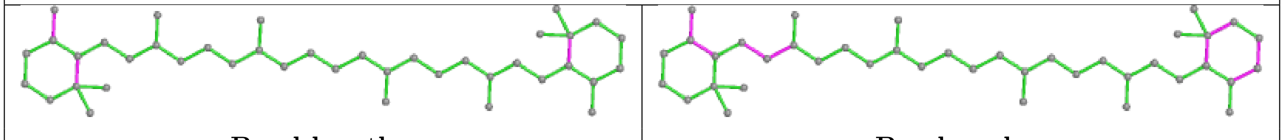


Bond lengths | Bond angles

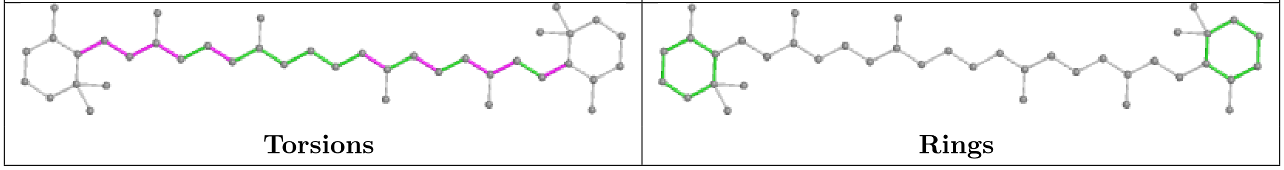


Torsions | Rings

Ligand BCR A 851

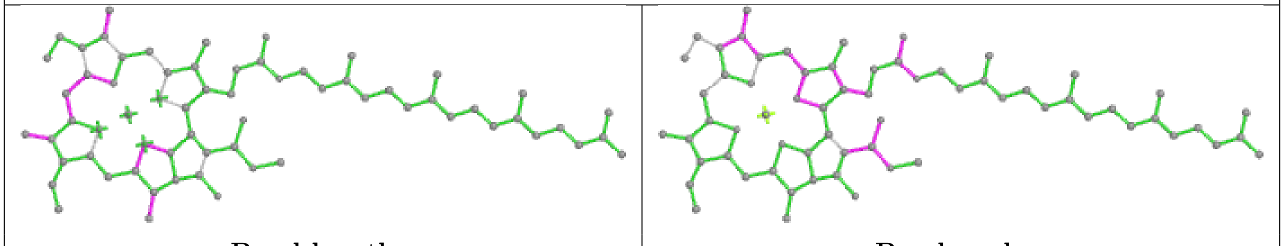


Bond lengths Bond angles

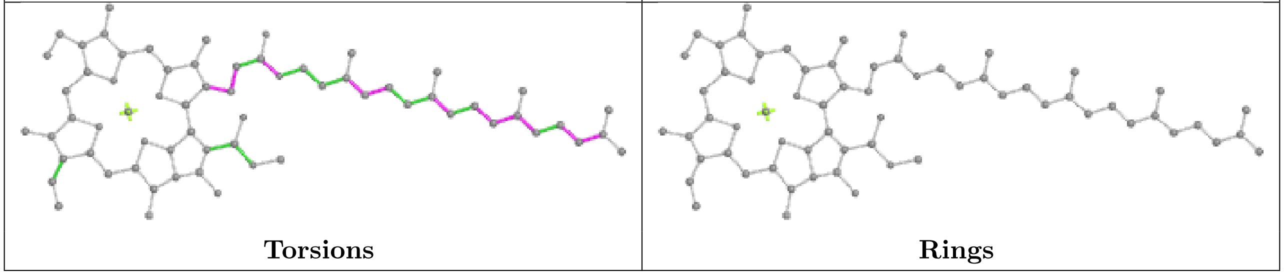


Torsions Rings

Ligand CLA a 805

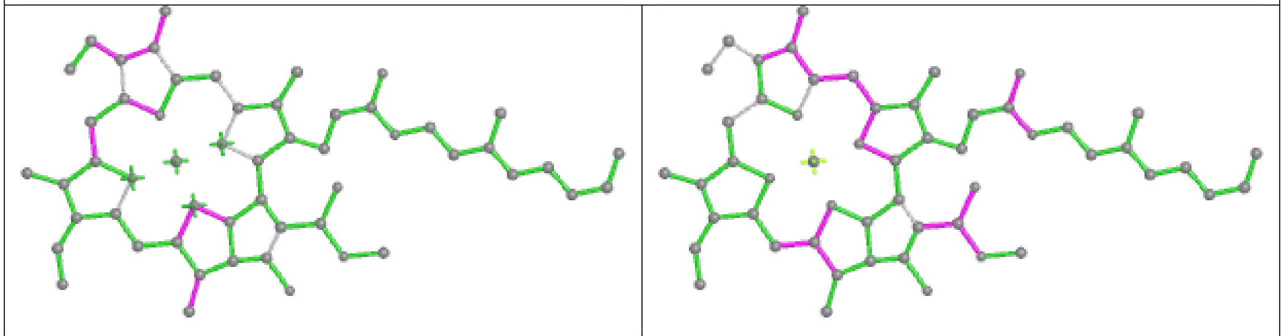


Bond lengths Bond angles

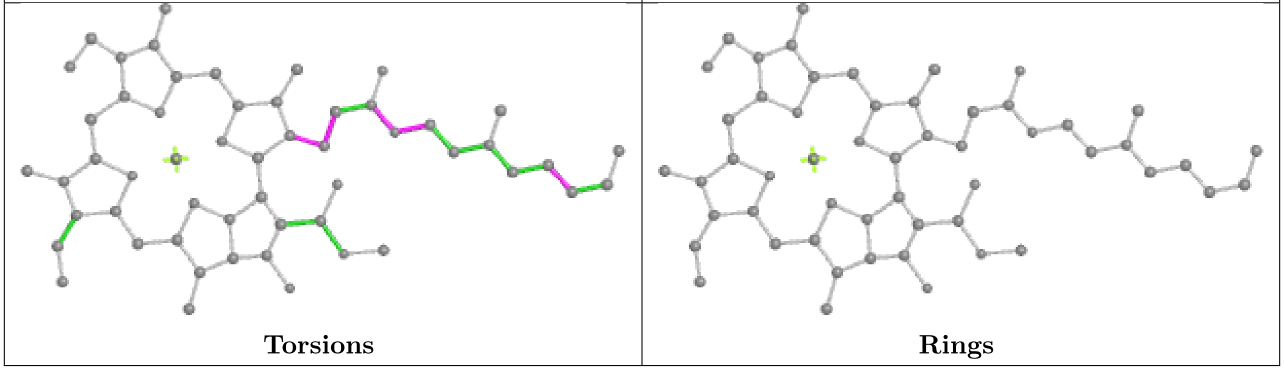


Torsions Rings

Ligand CLA A 831

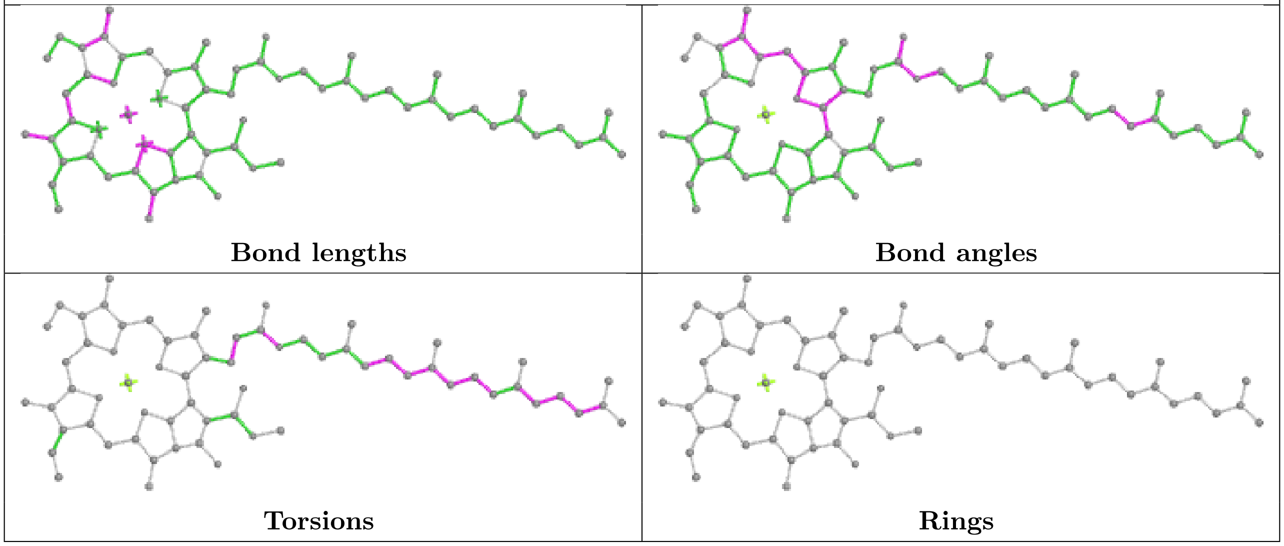


Bond lengths Bond angles

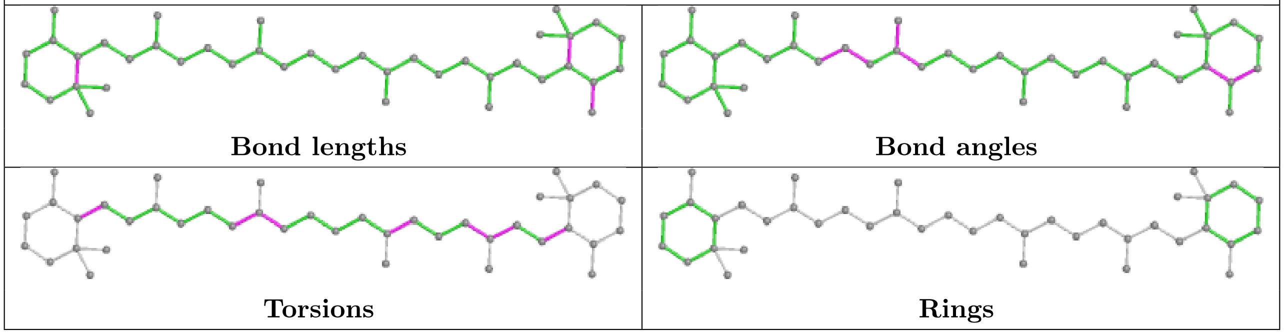


Torsions Rings

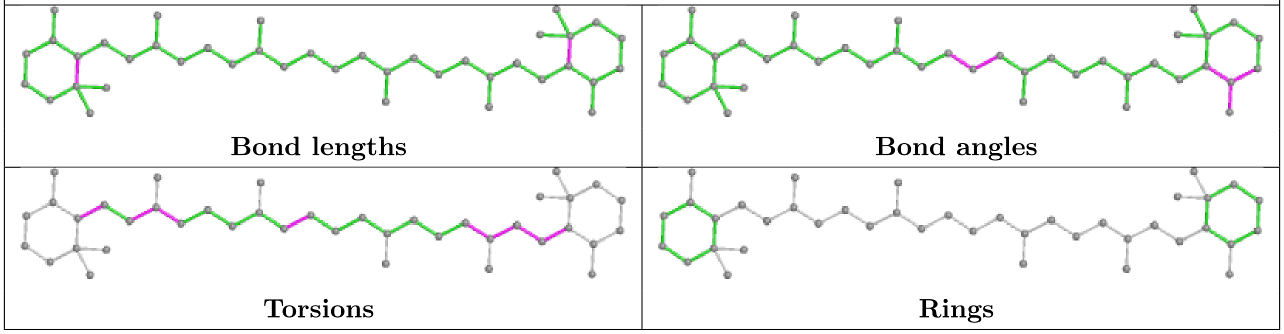
Ligand CLA B 809


Bond lengths
Bond angles
Torsions
Rings

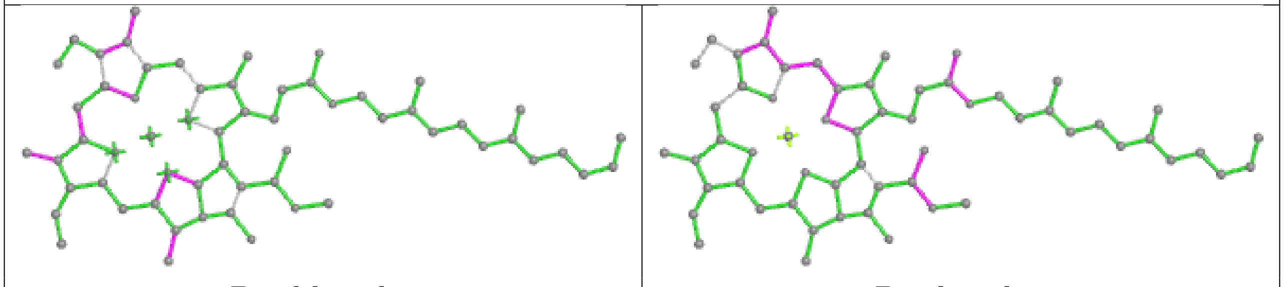
Ligand BCR B 850


Bond lengths
Bond angles
Torsions
Rings

Ligand BCR b 845

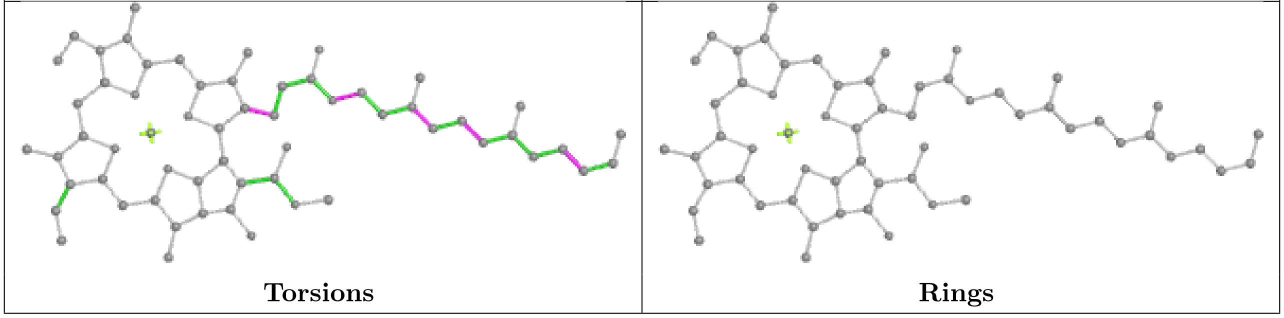

Bond lengths
Bond angles
Torsions
Rings

Ligand CLA f 201



Bond lengths

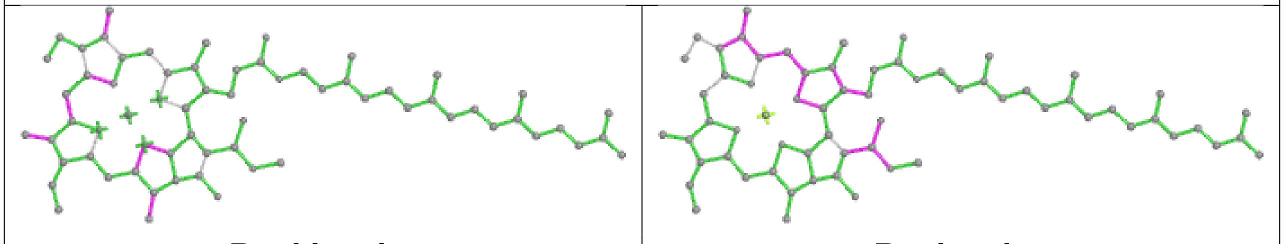
Bond angles



Torsions

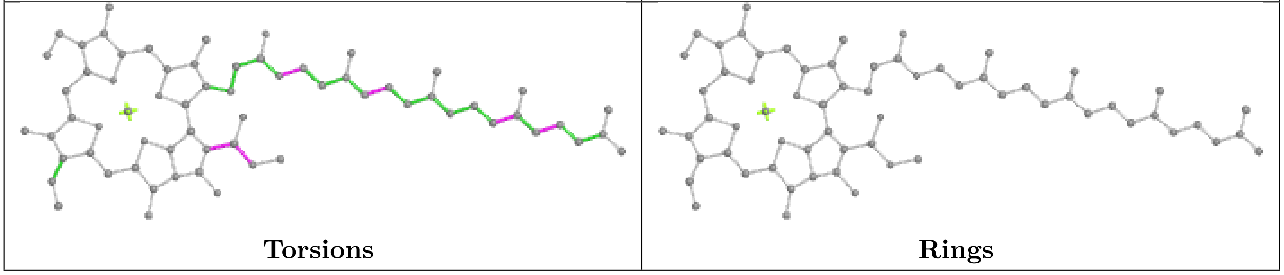
Rings

Ligand CLA A 803



Bond lengths

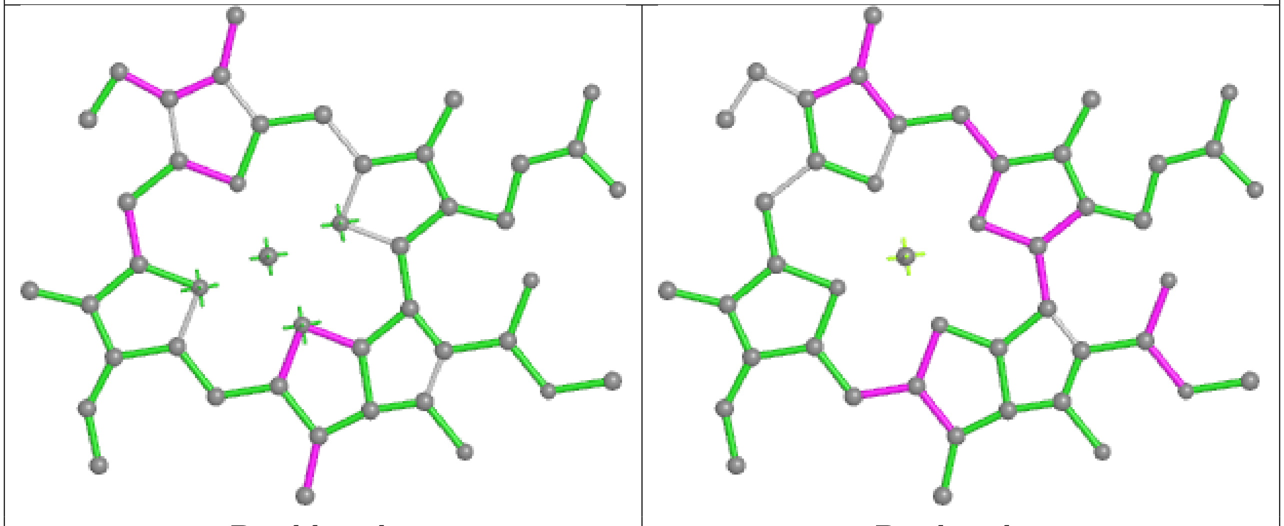
Bond angles



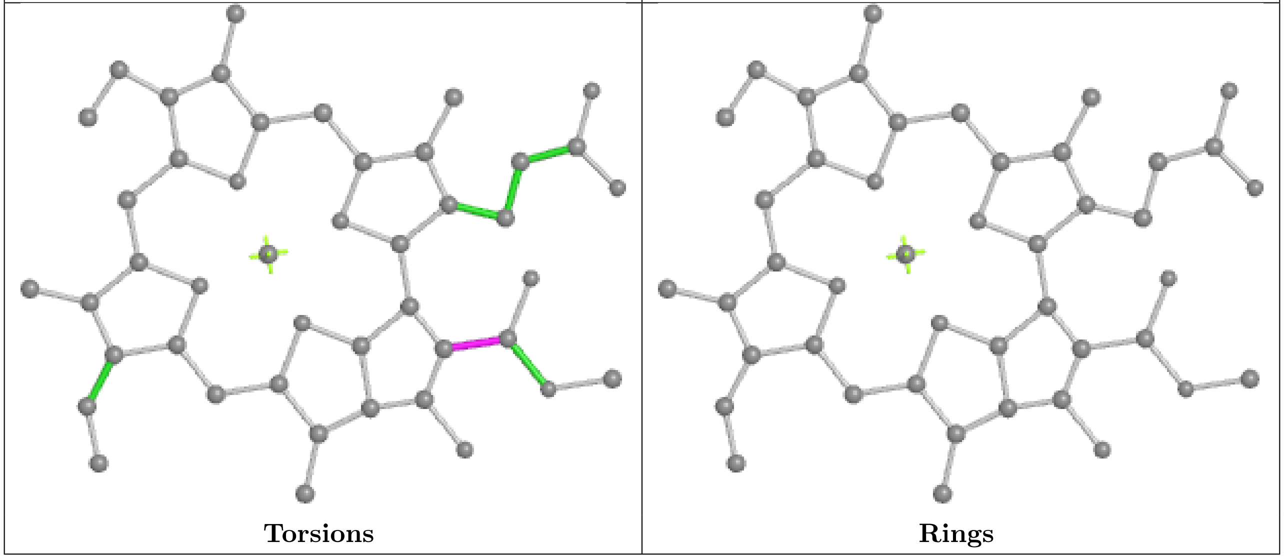
Torsions

Rings

Ligand CLA A 824

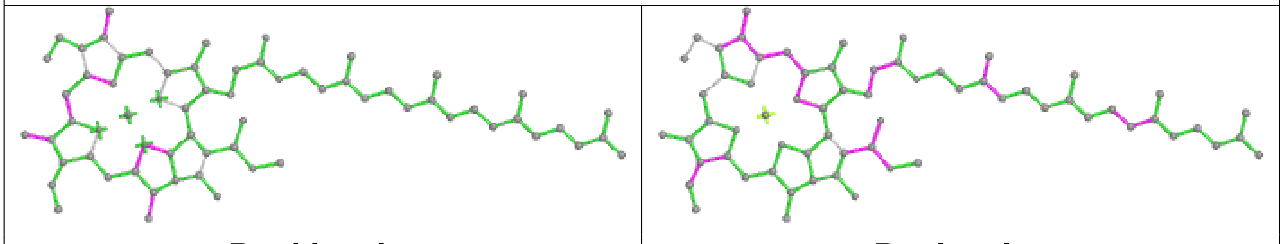


Bond lengths Bond angles

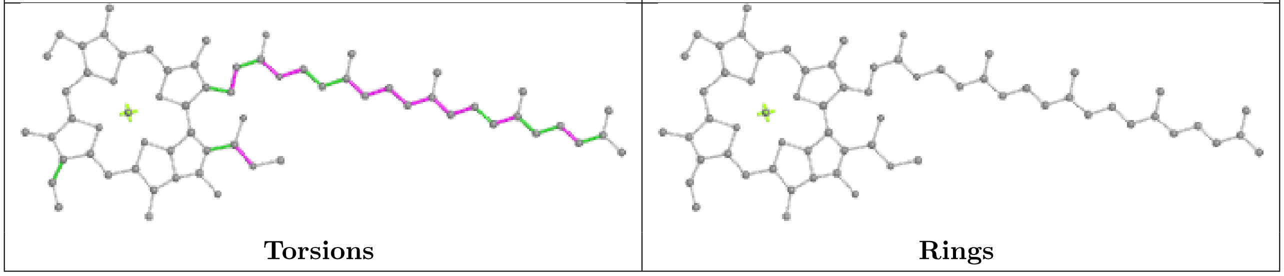


Torsions Rings

Ligand CLA A 828

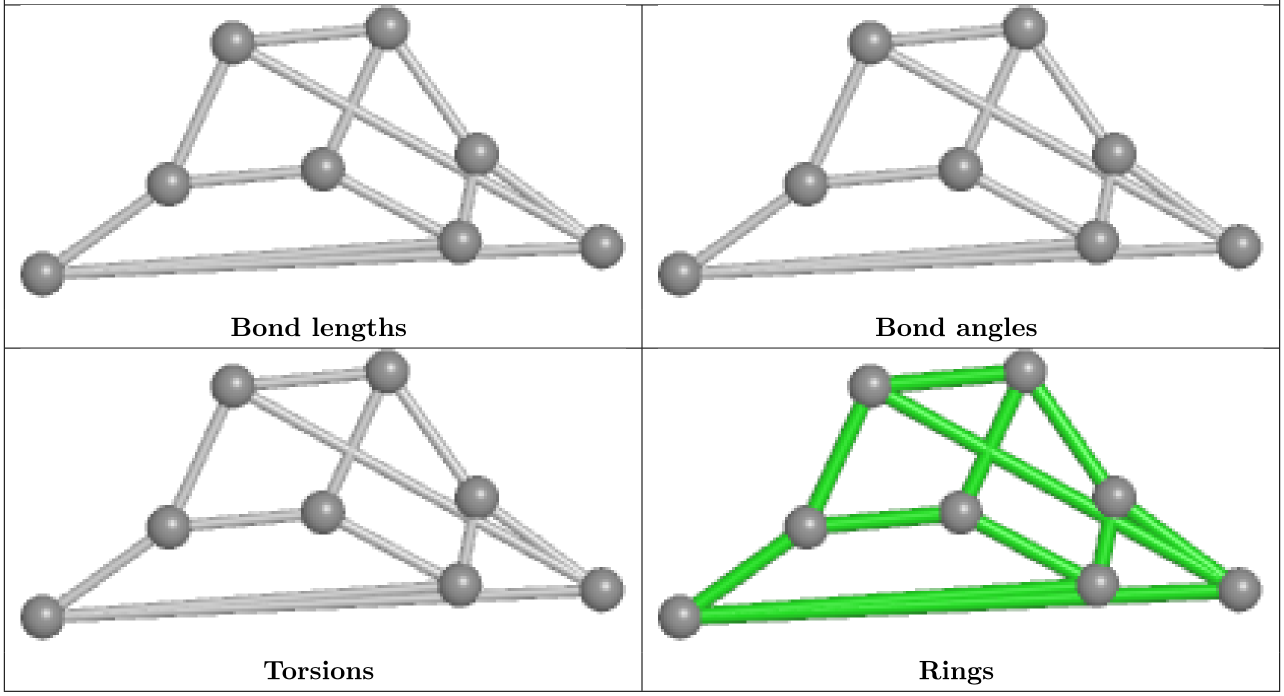


Bond lengths Bond angles

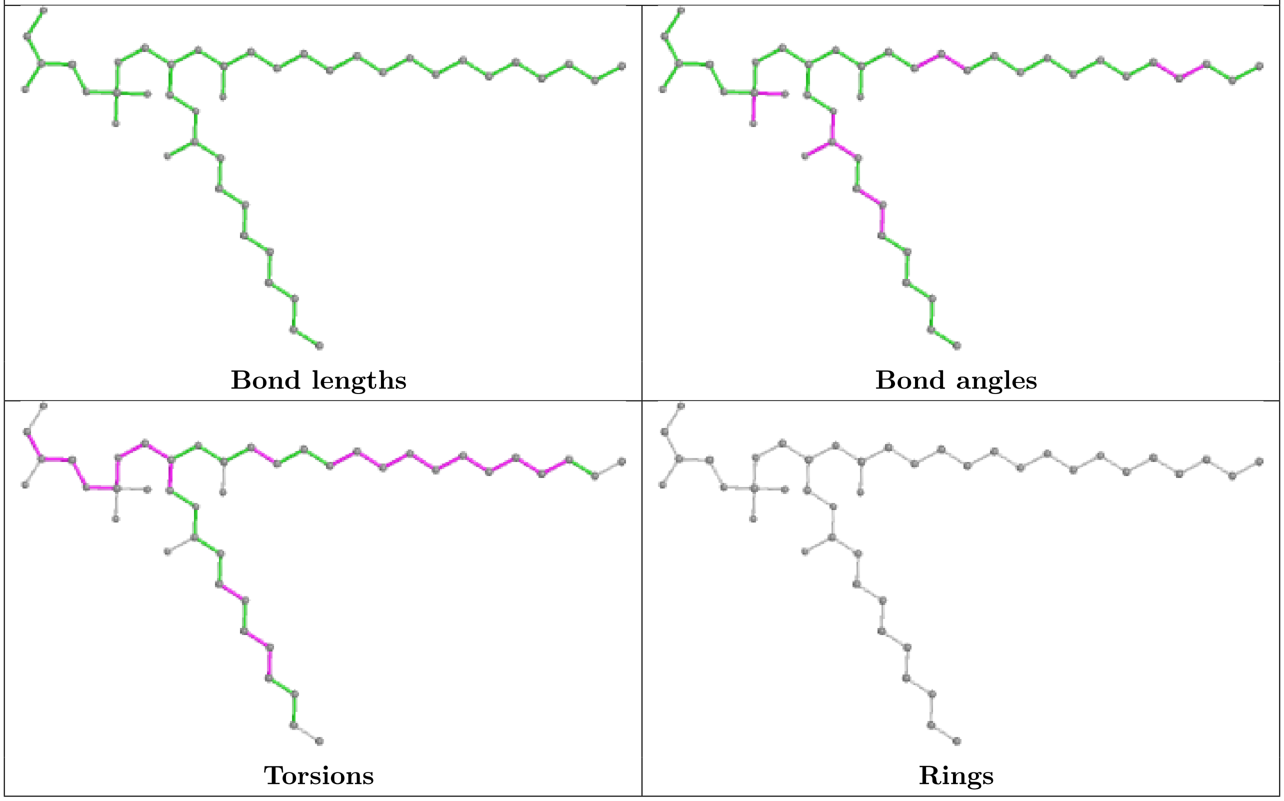


Torsions Rings

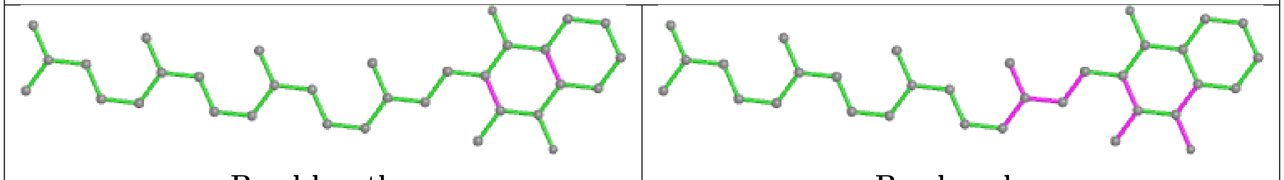
Ligand SF4 C 101



Ligand LHG i 103

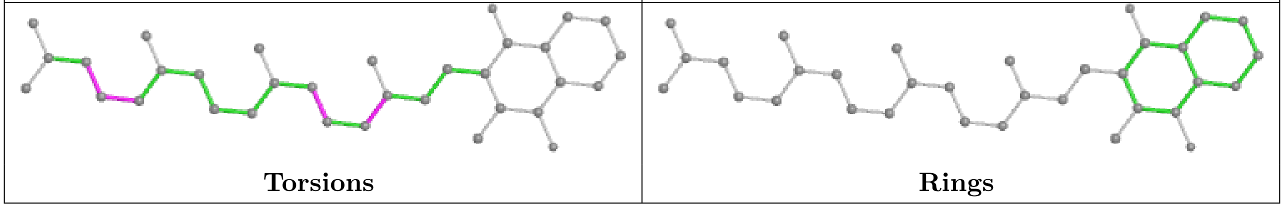


Ligand PQN B 844



Bond lengths

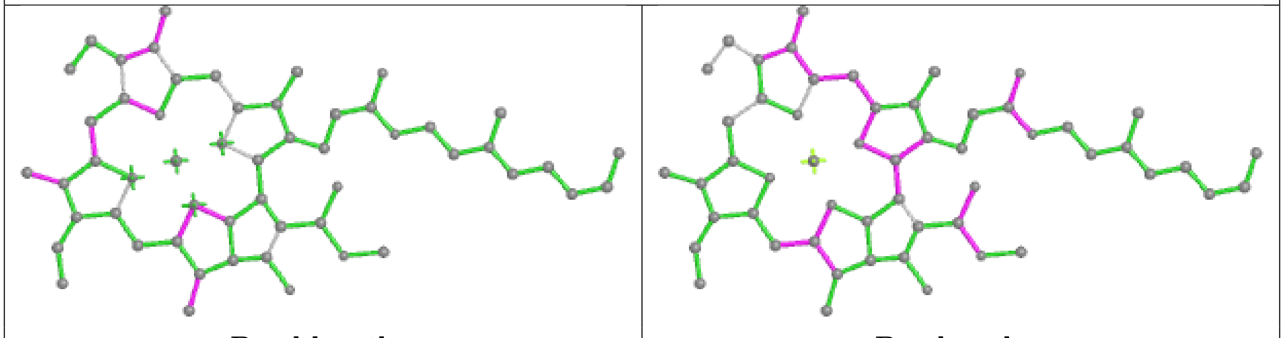
Bond angles



Torsions

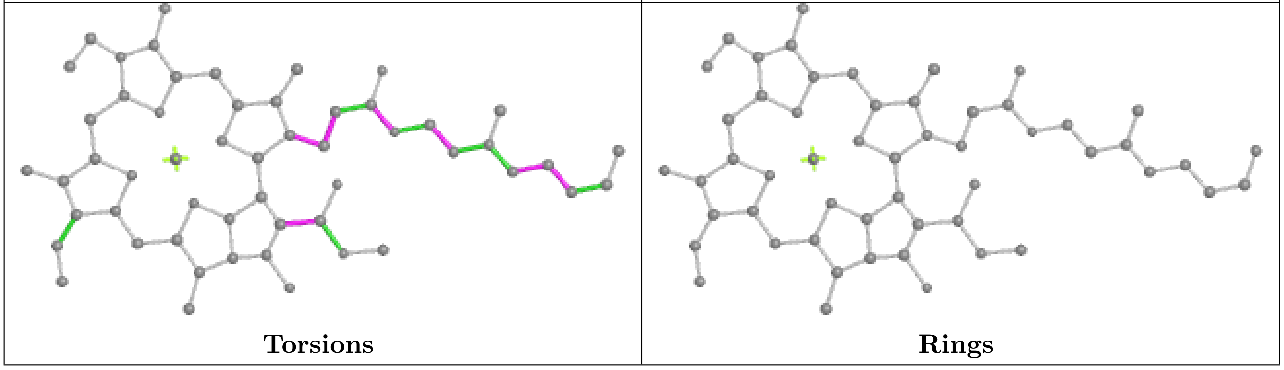
Rings

Ligand CLA A 820



Bond lengths

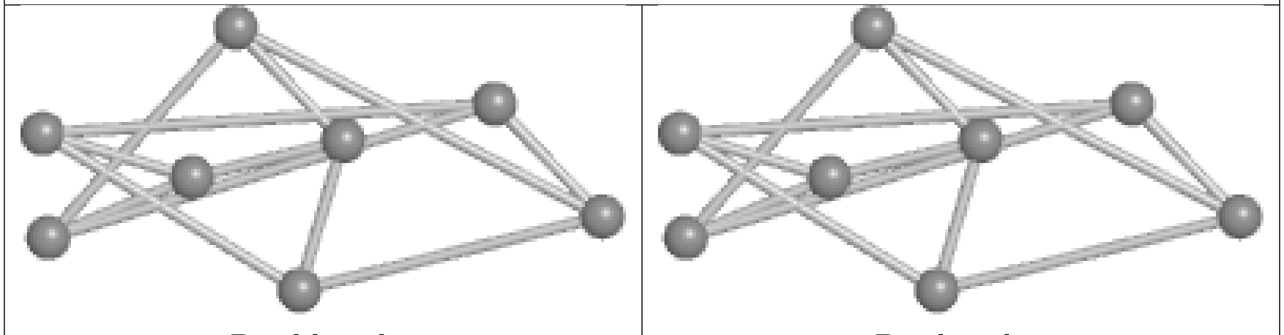
Bond angles



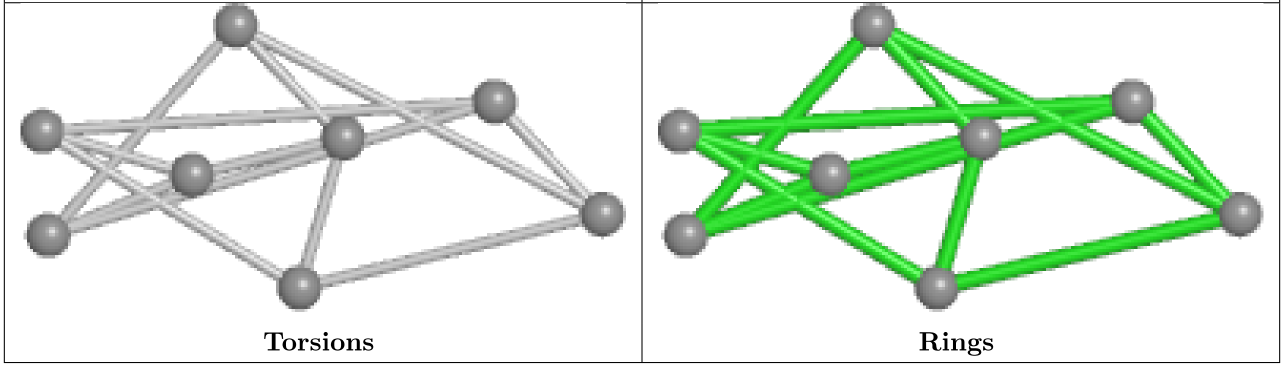
Torsions

Rings

Ligand SF4 A 845

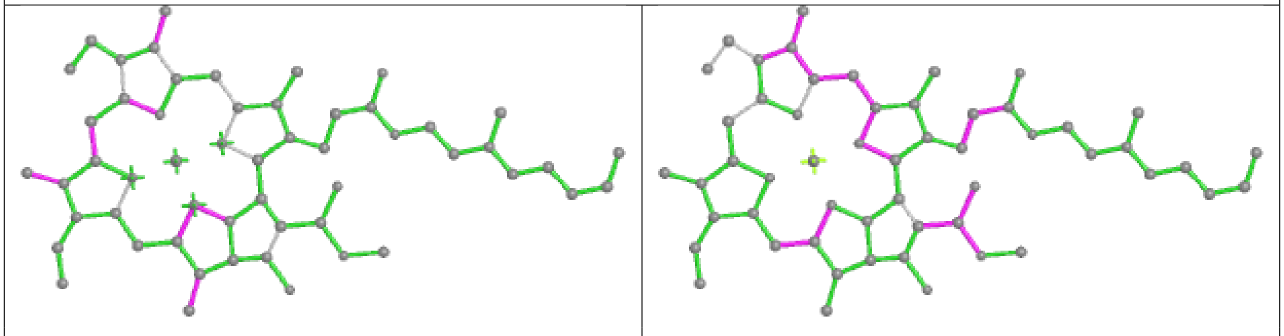


Bond lengths Bond angles

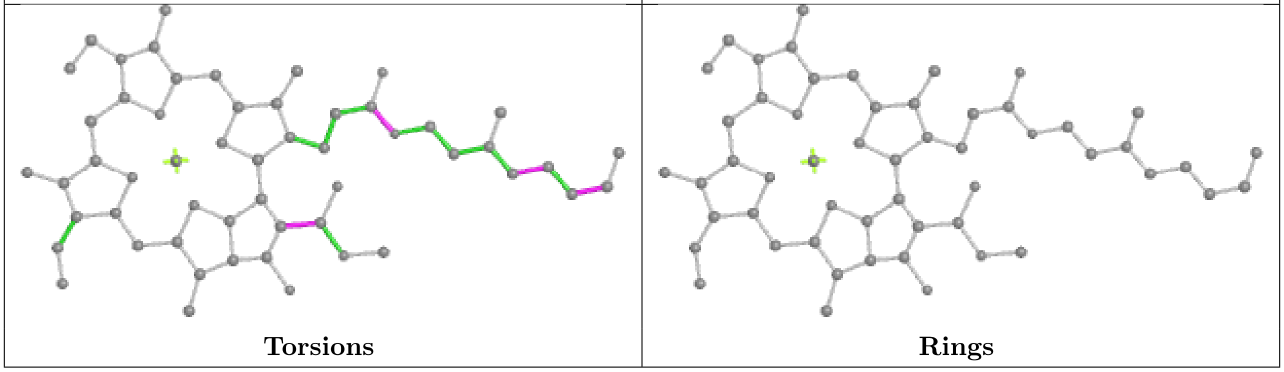


Torsions Rings

Ligand CLA A 814

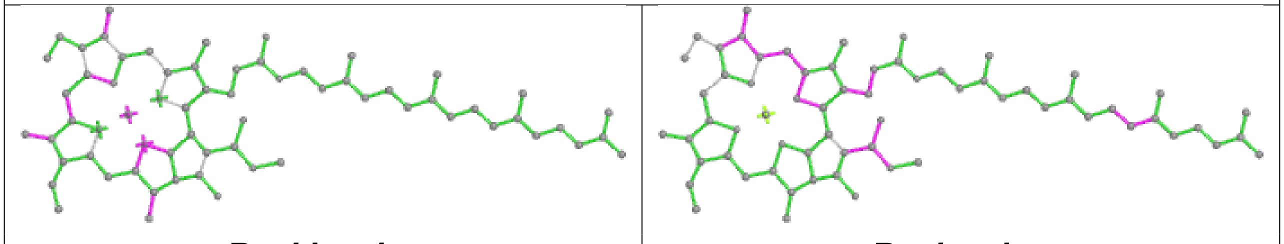


Bond lengths Bond angles



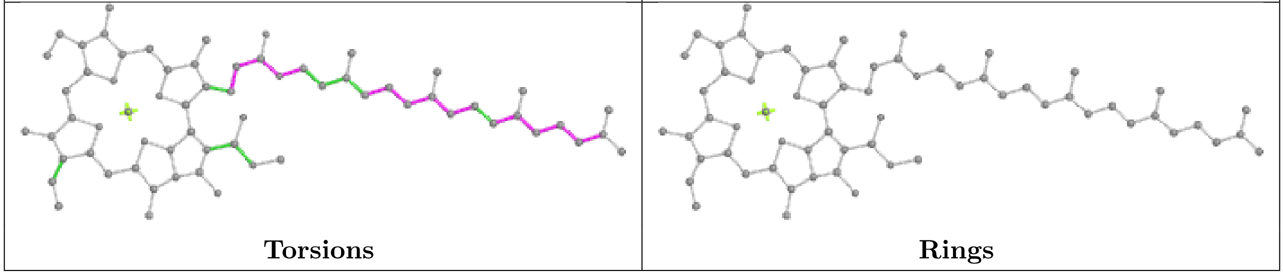
Torsions Rings

Ligand CLA b 809



Bond lengths

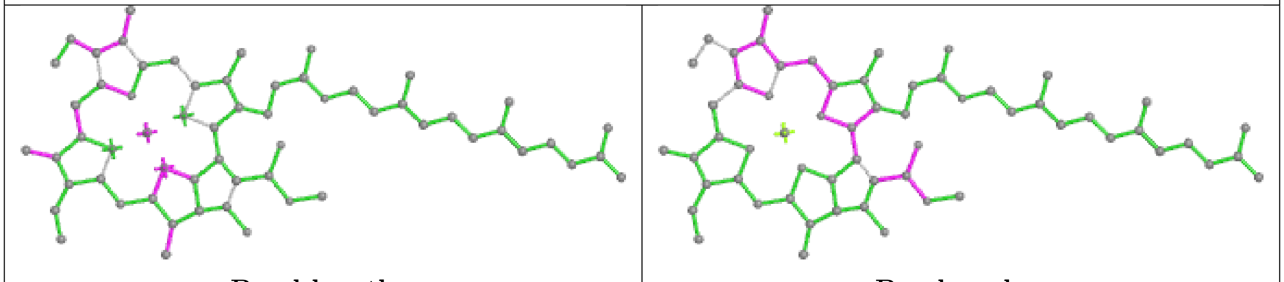
Bond angles



Torsions

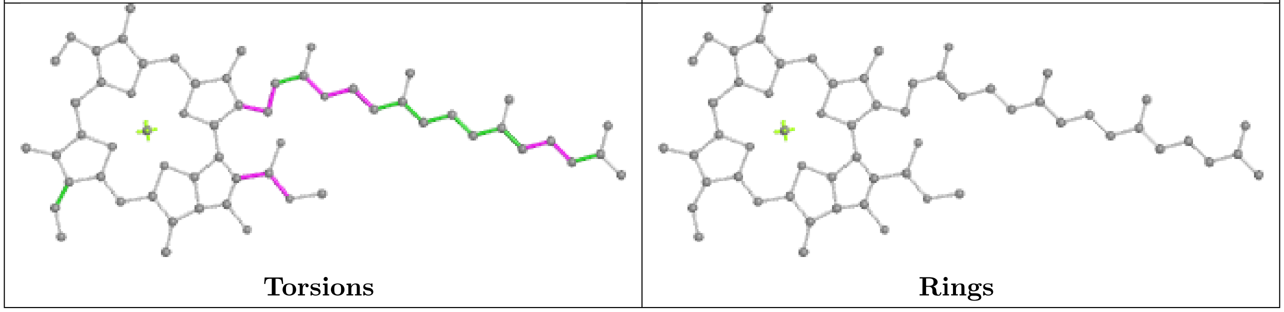
Rings

Ligand CLA a 817



Bond lengths

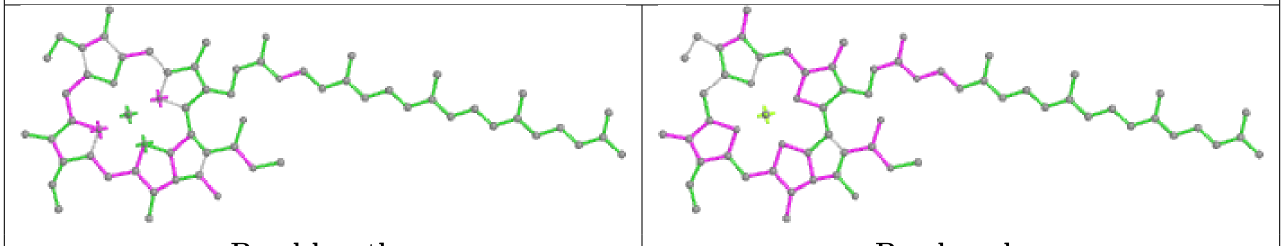
Bond angles



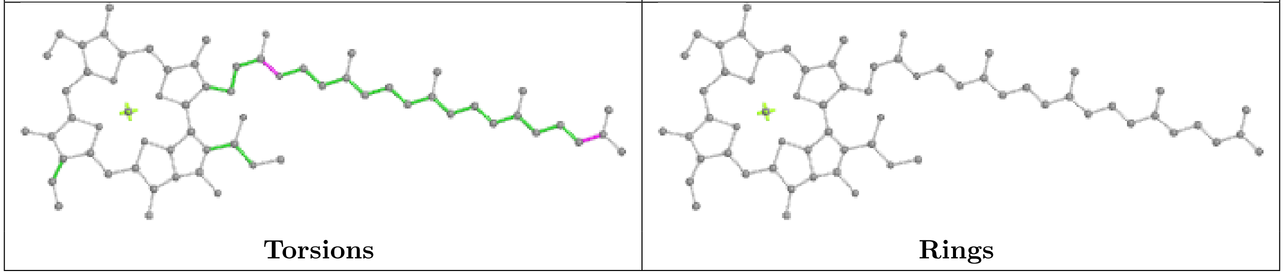
Torsions

Rings

Ligand CL0 A 801

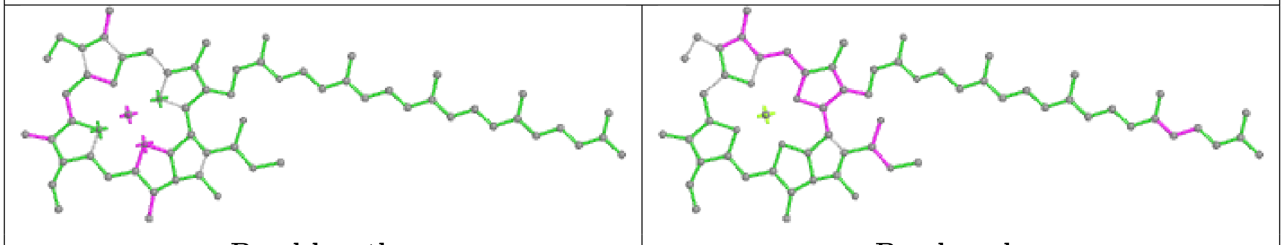


Bond lengths Bond angles

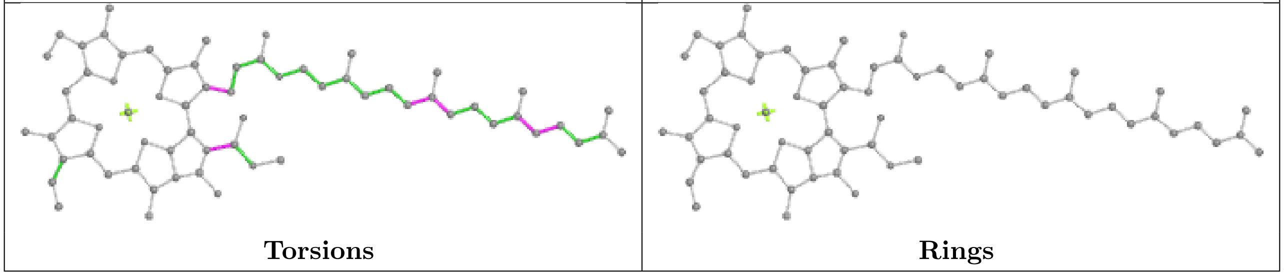


Torsions Rings

Ligand CLA b 829

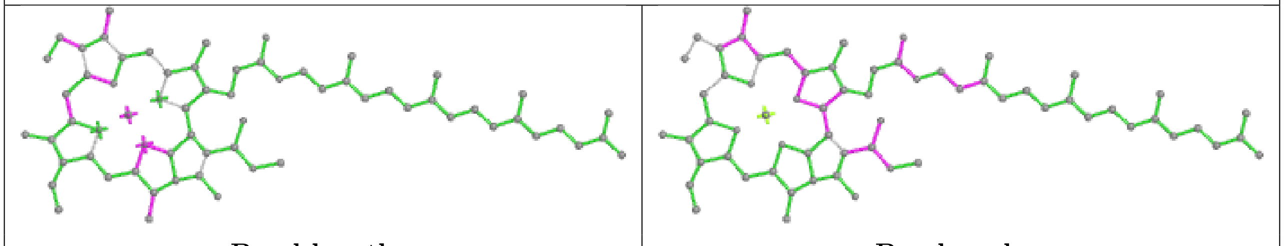


Bond lengths Bond angles

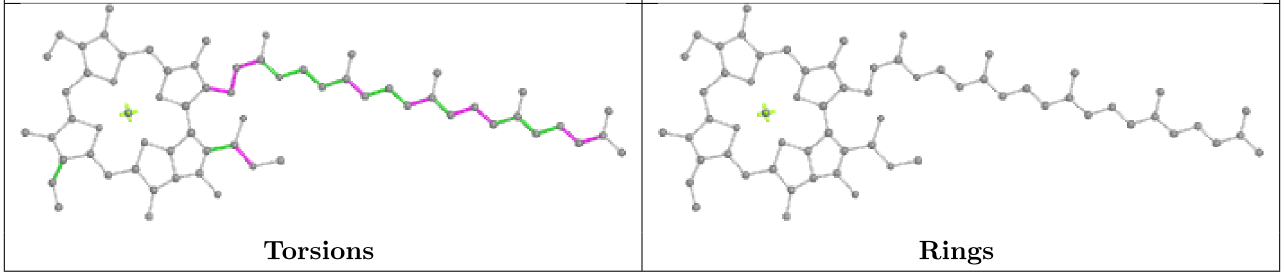


Torsions Rings

Ligand CLA b 830

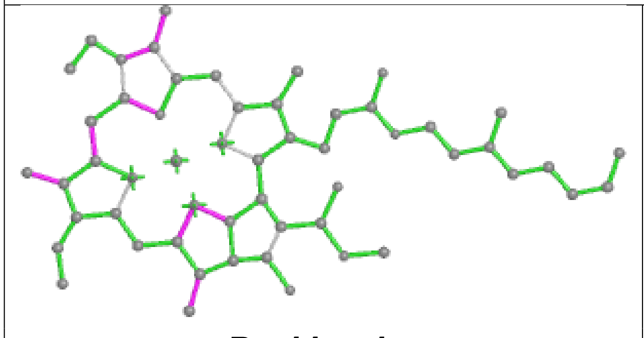


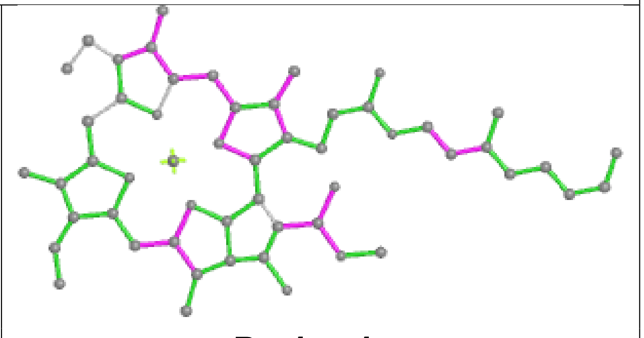
Bond lengths Bond angles

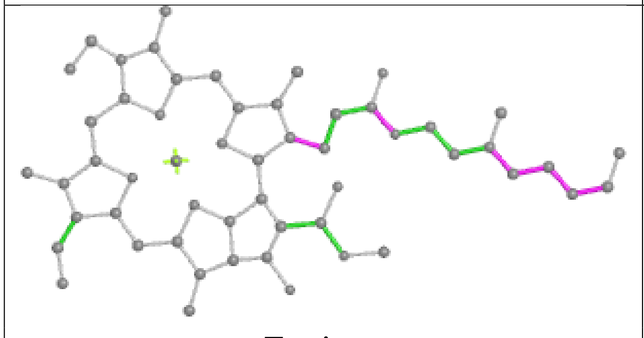


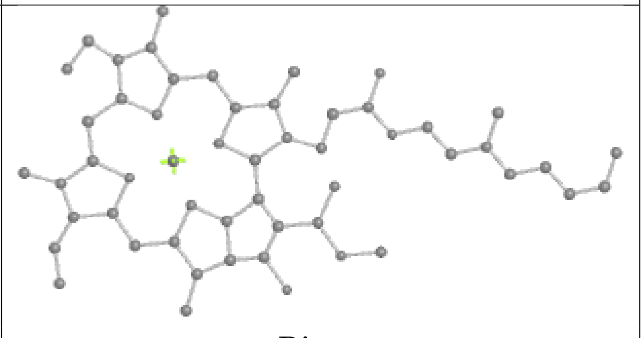
Torsions Rings

Ligand CLA a 822

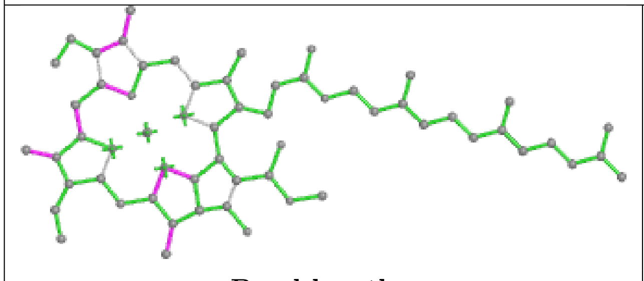

Bond lengths

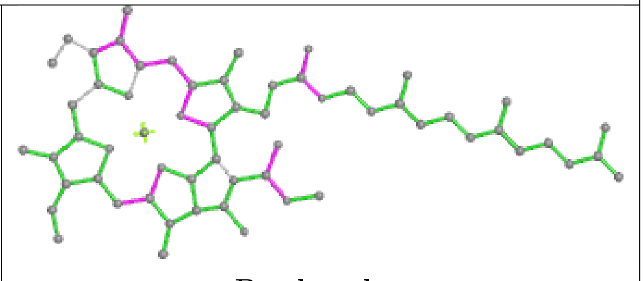

Bond angles

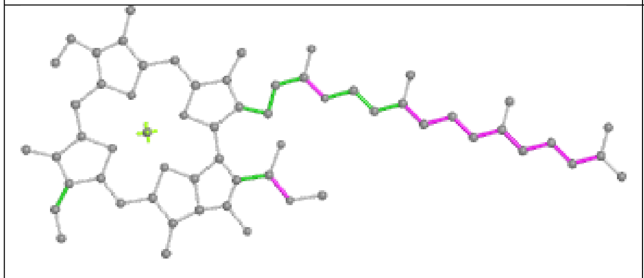

Torsions

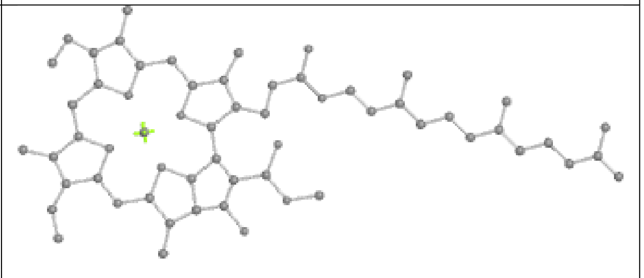

Rings

Ligand CLA b 834

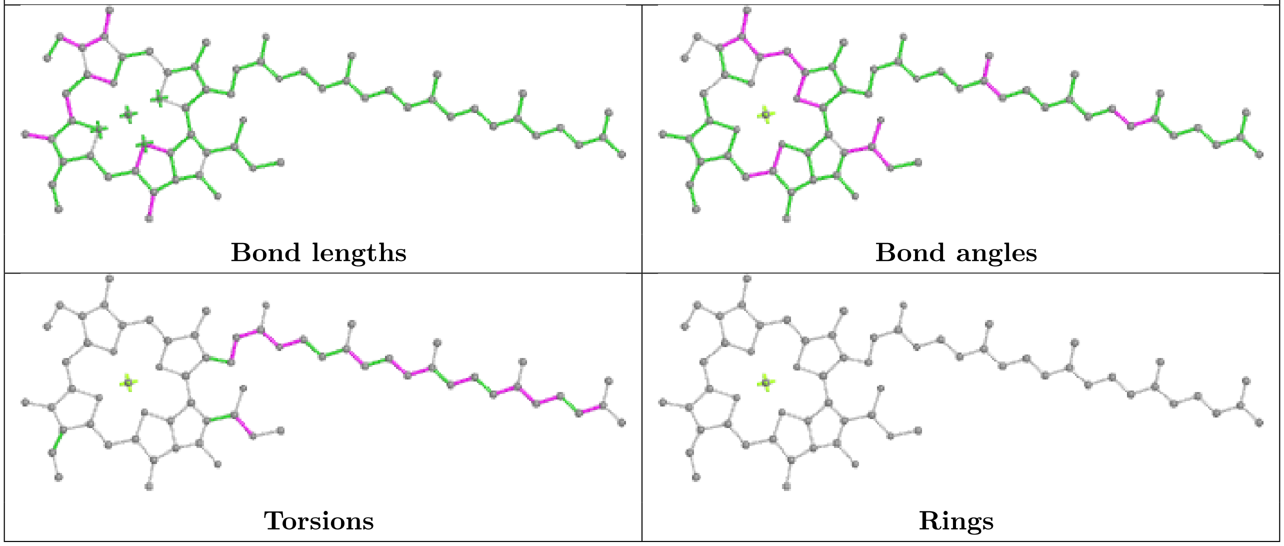

Bond lengths


Bond angles

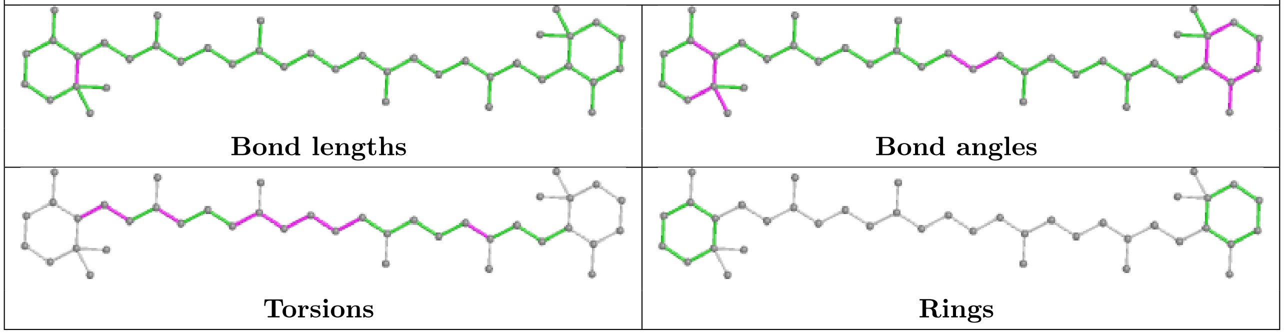

Torsions


Rings

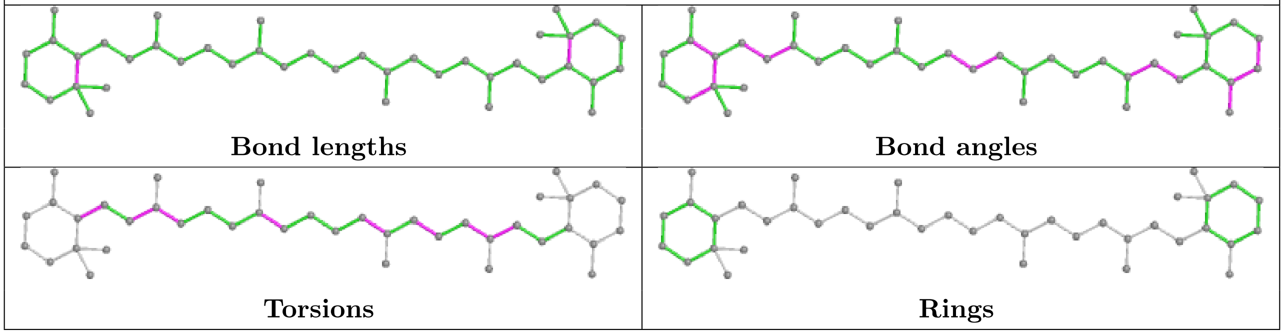
Ligand CLA A 842


Bond lengths
Bond angles
Torsions
Rings

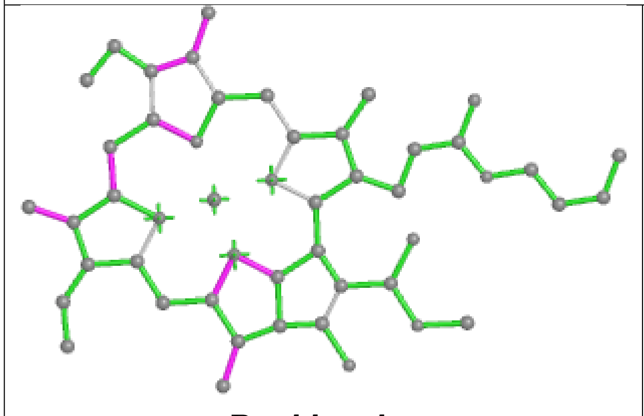
Ligand BCR I 101


Bond lengths
Bond angles
Torsions
Rings

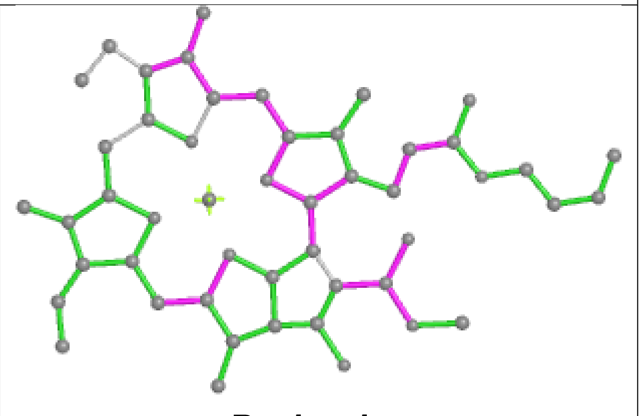
Ligand BCR b 846


Bond lengths
Bond angles
Torsions
Rings

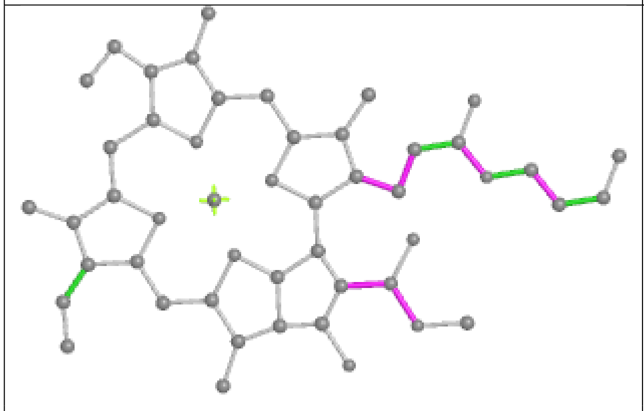
Ligand CLA X 1701



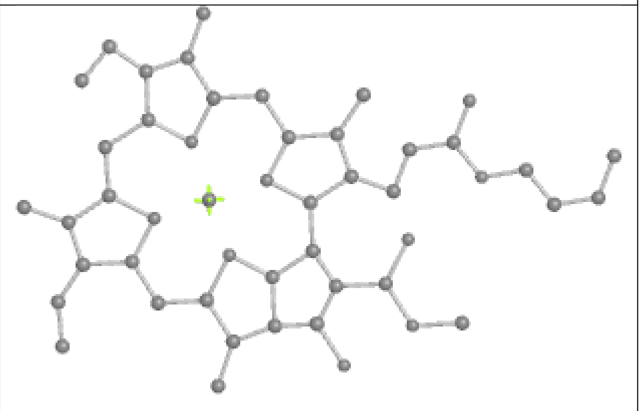
Bond lengths



Bond angles

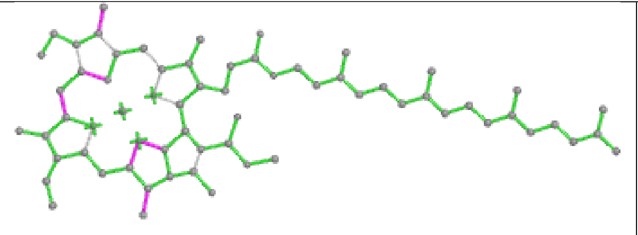


Torsions

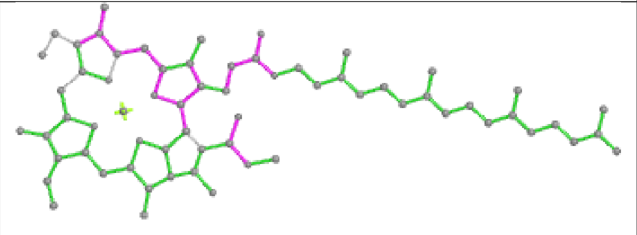


Rings

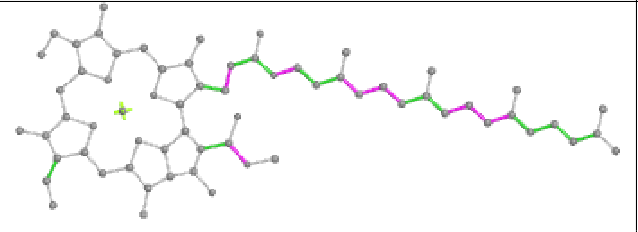
Ligand CLA A 809



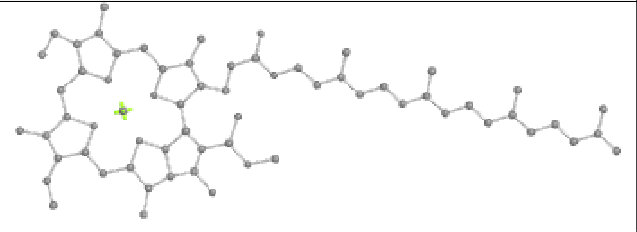
Bond lengths



Bond angles

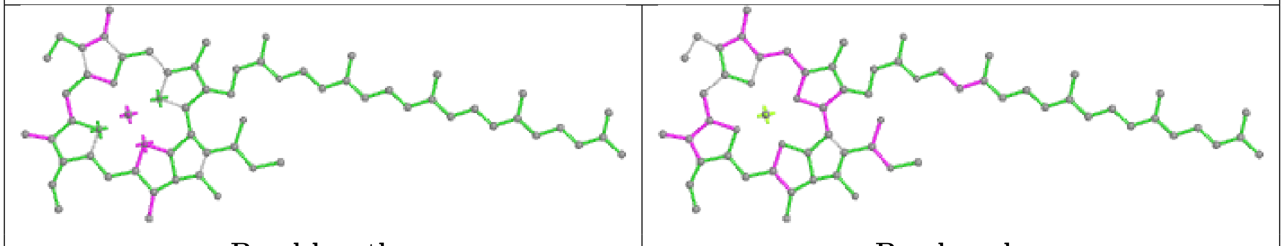


Torsions

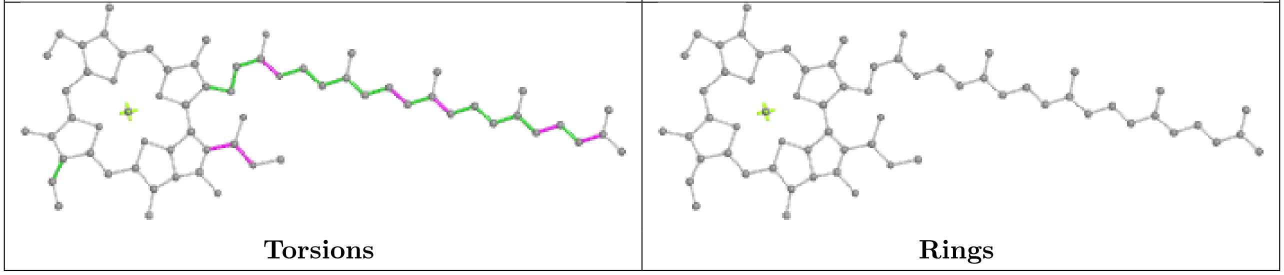


Rings

Ligand CLA a 829

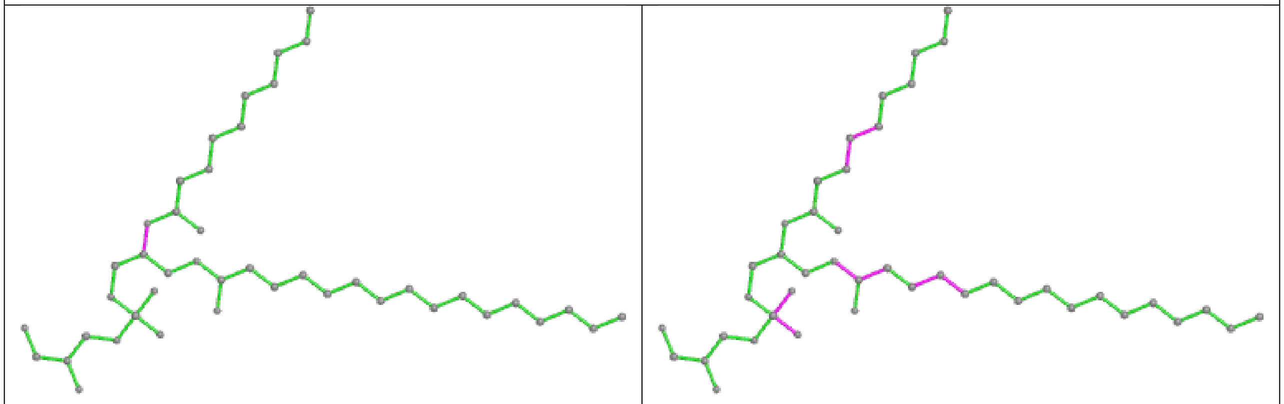


Bond lengths Bond angles

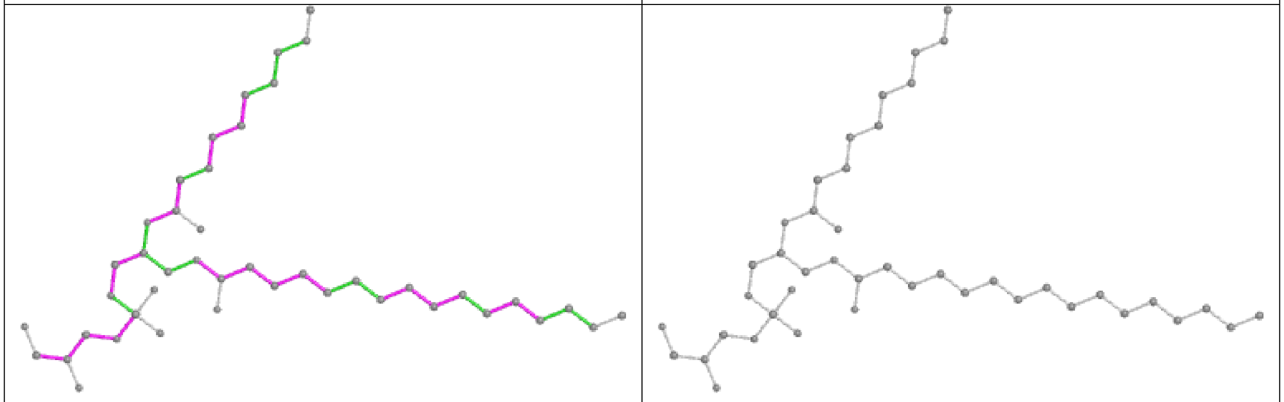


Torsions Rings

Ligand LHG F 201

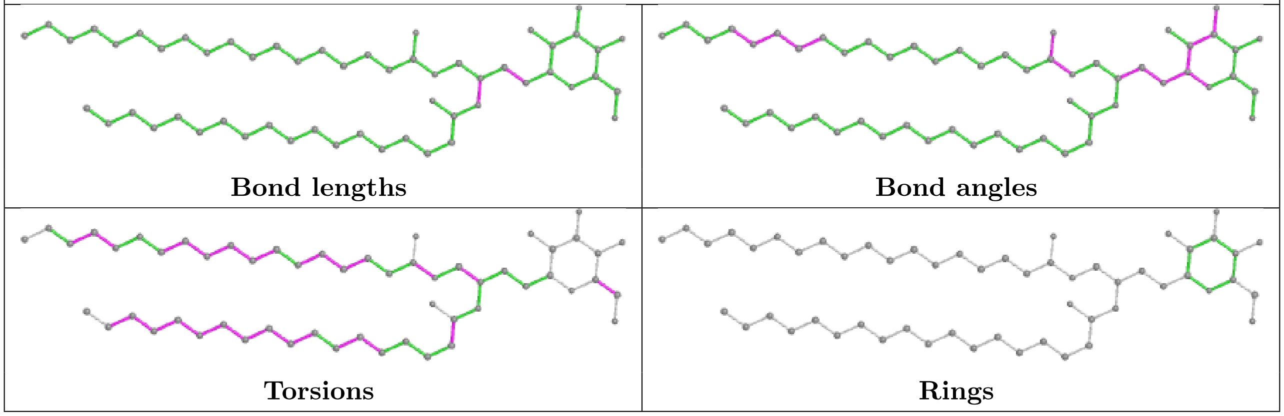


Bond lengths Bond angles

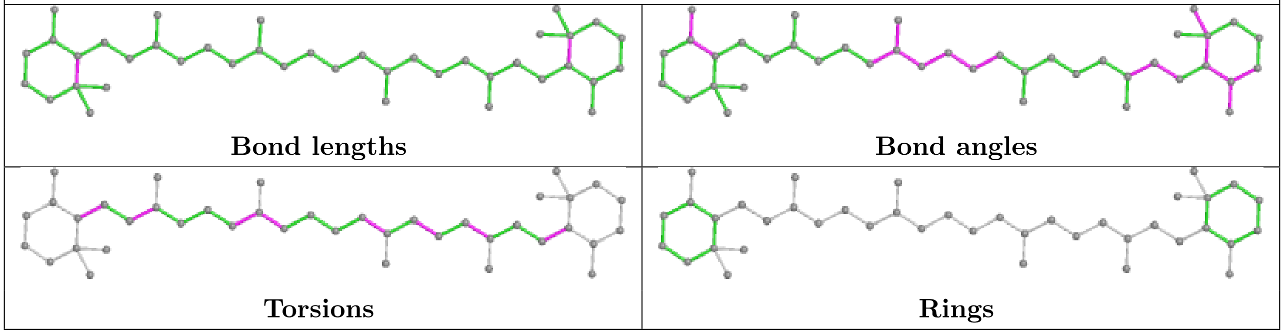


Torsions Rings

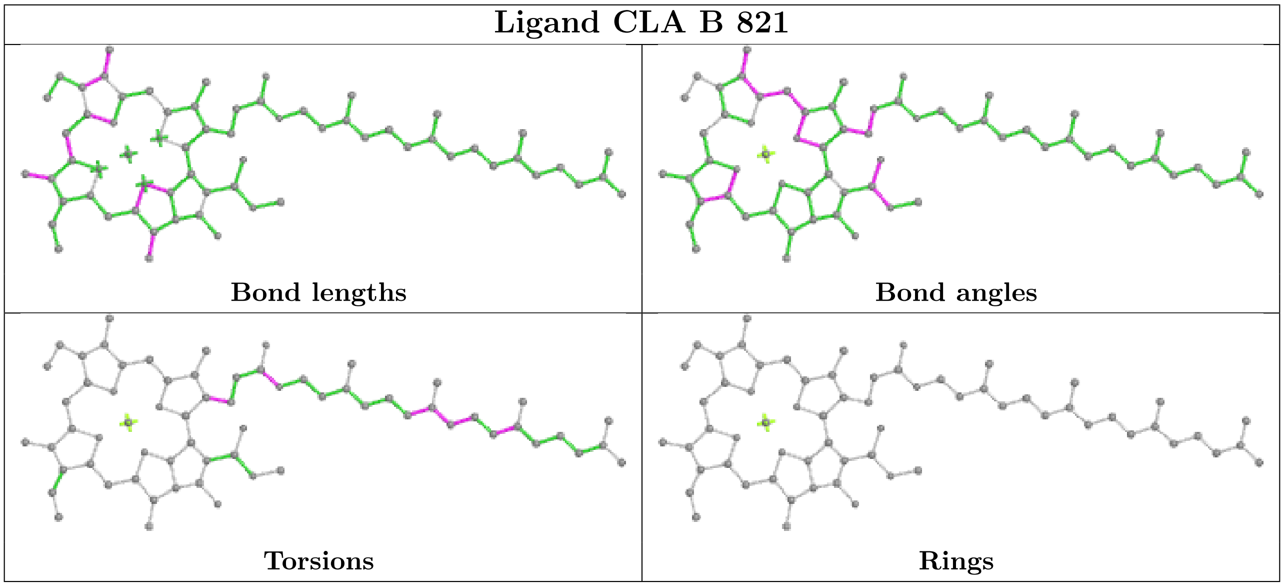
Ligand LMG B 851



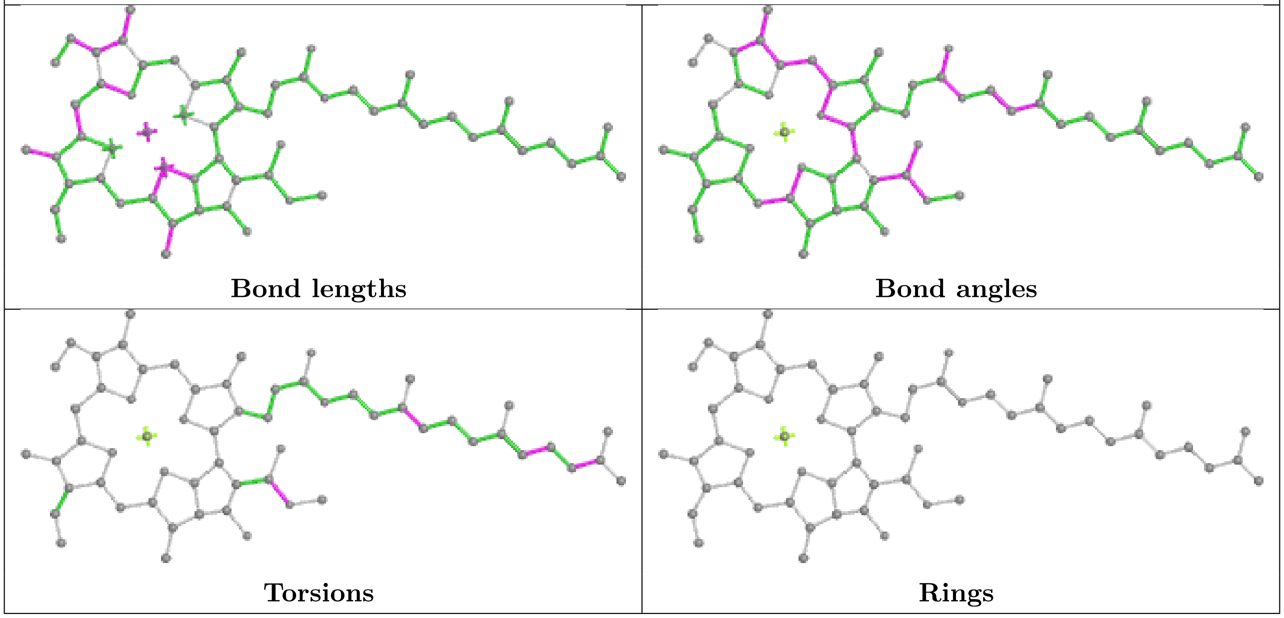
Ligand BCR m 1202



Ligand CLA B 821



Ligand CLA B 839



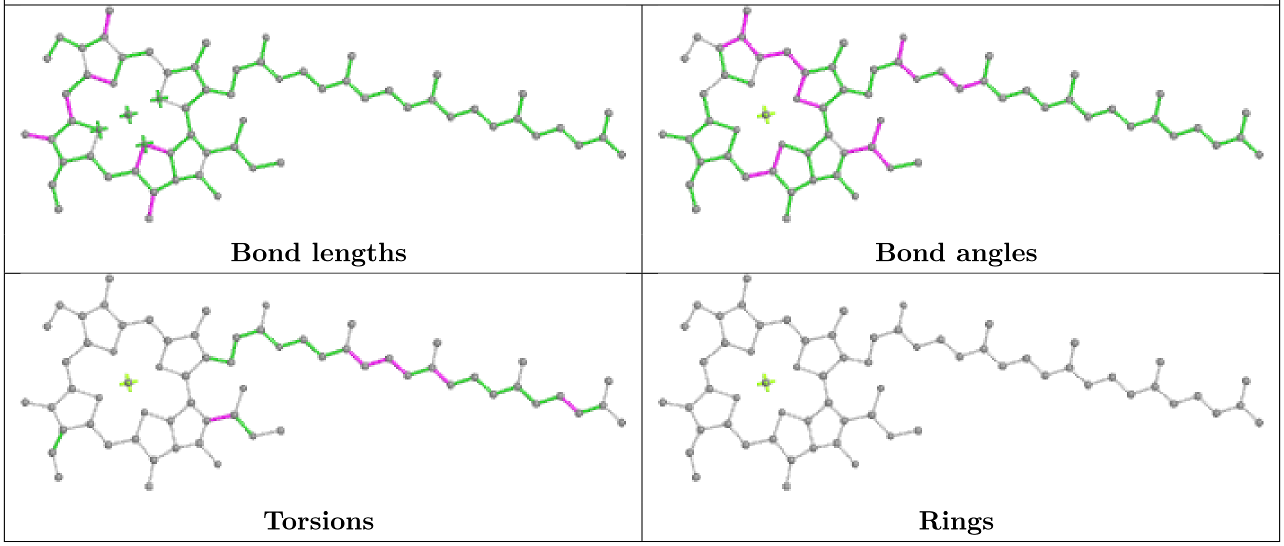
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA b 840



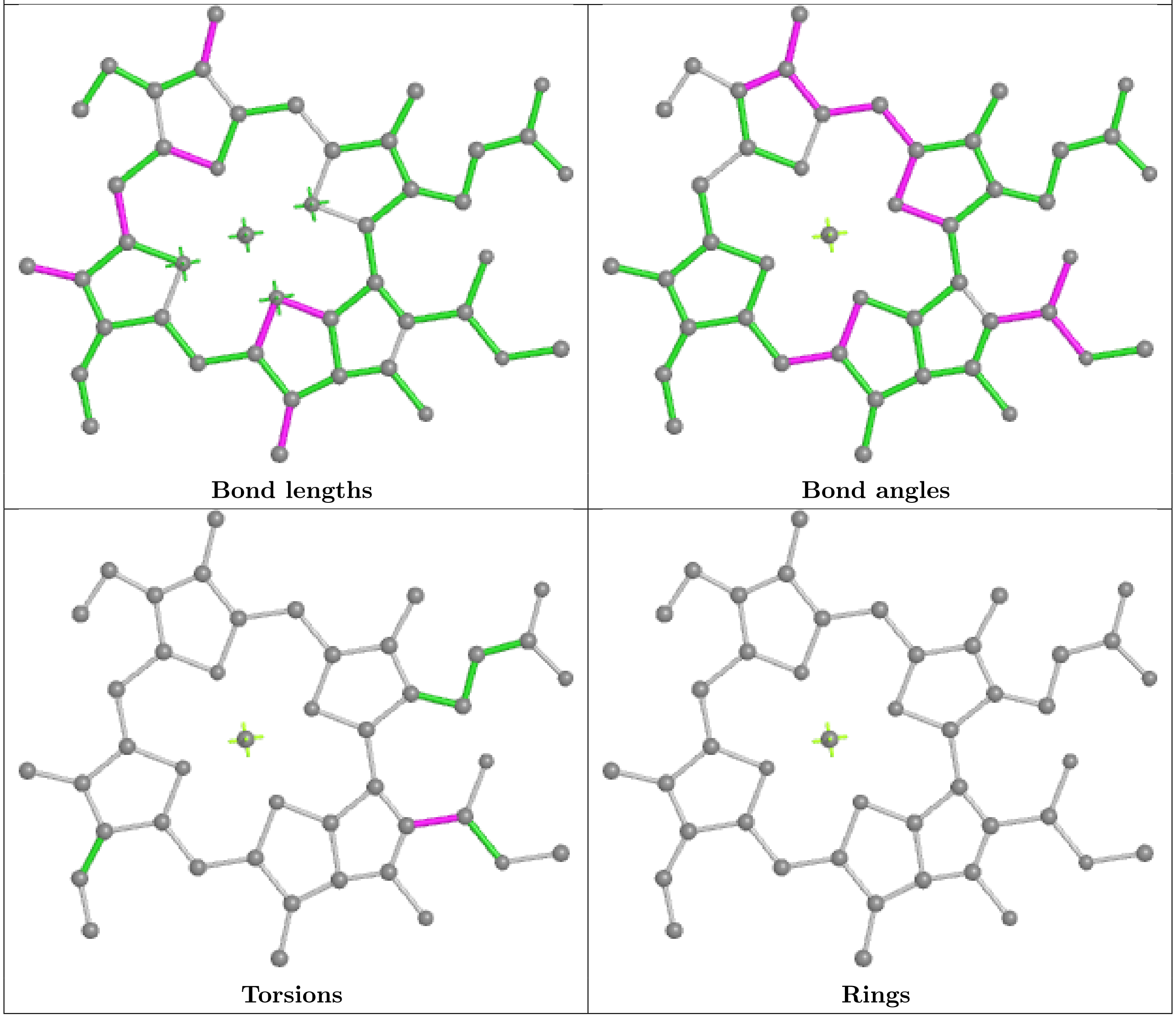
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA B 824



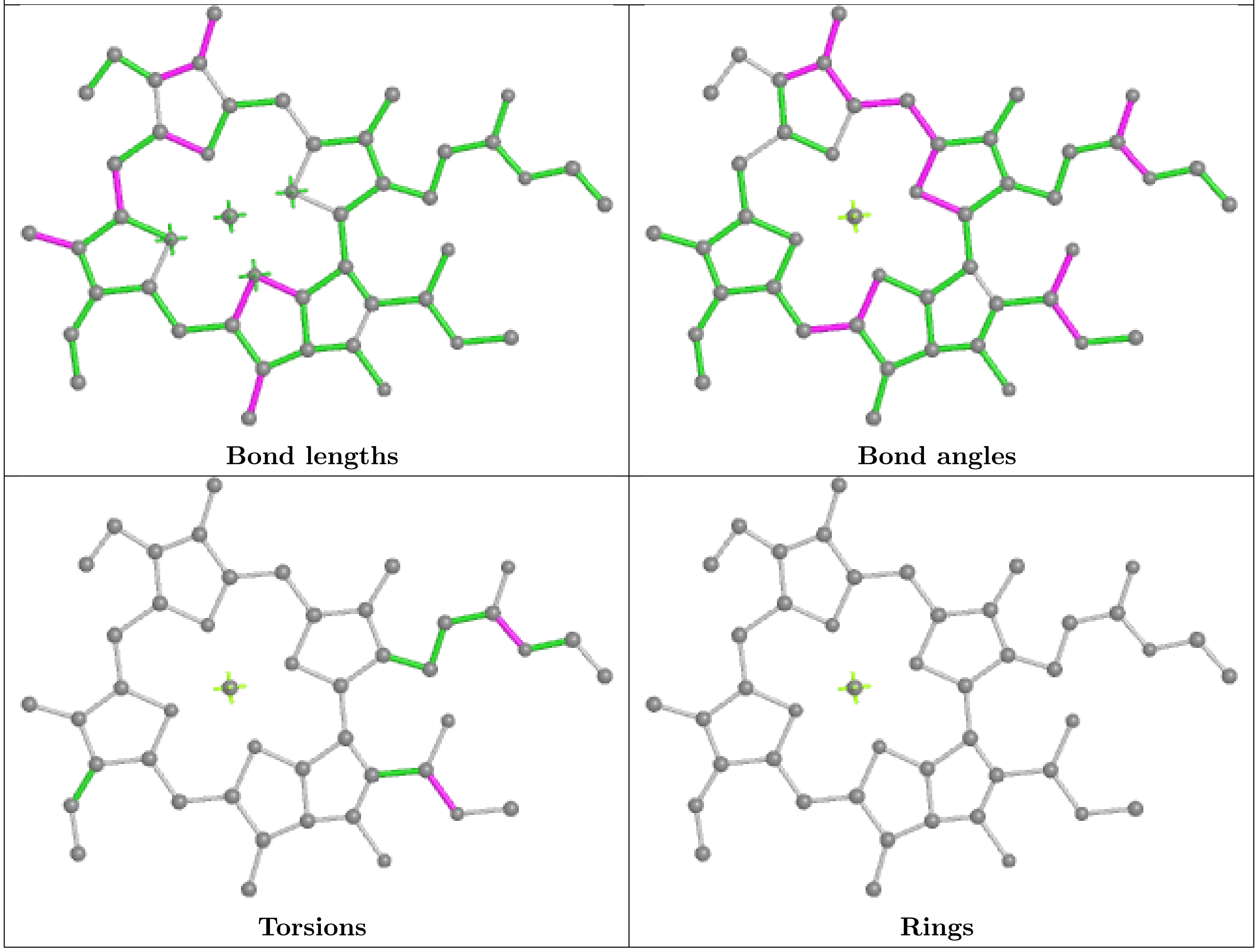
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA B 841



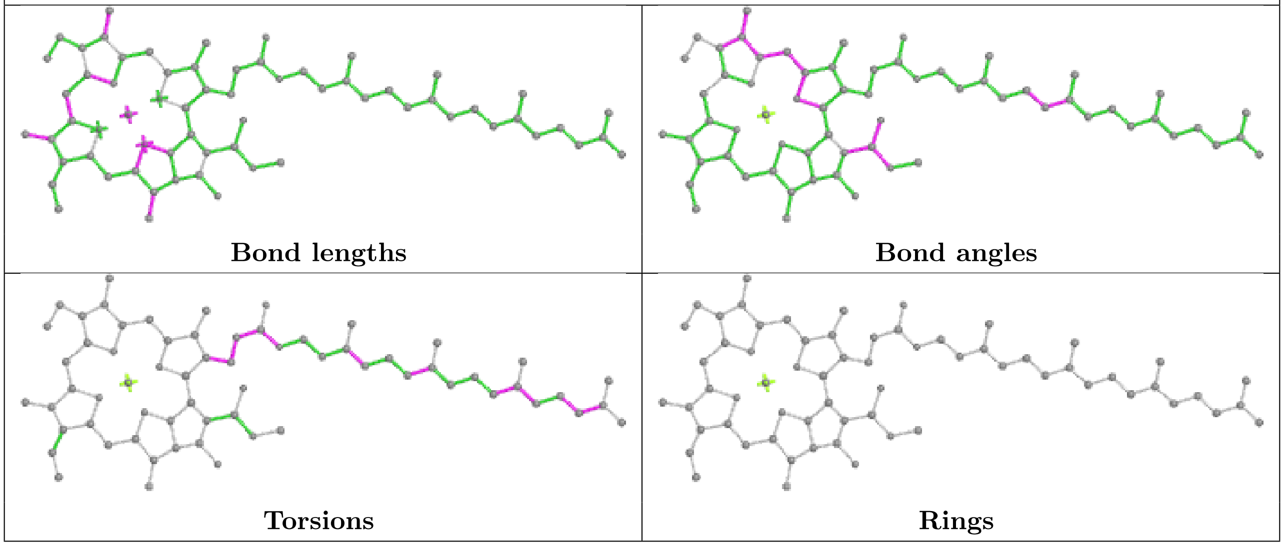
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA a 828



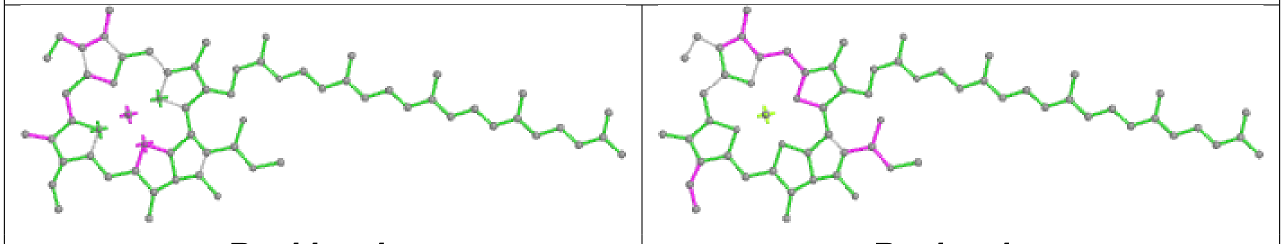
Bond lengths

Bond angles

Torsions

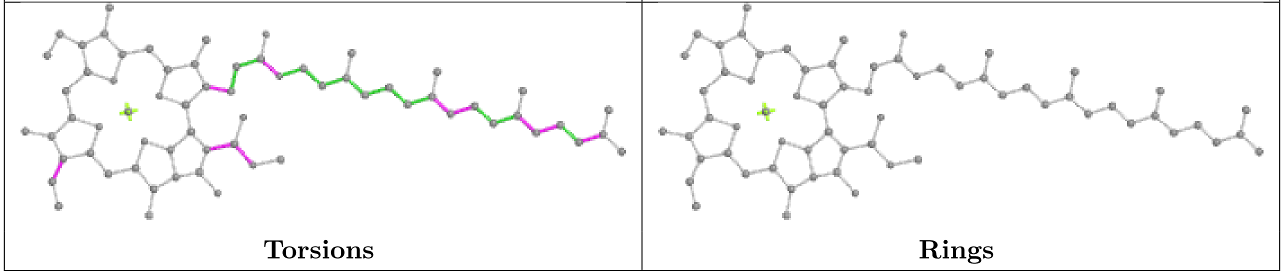
Rings

Ligand CLA B 820



Bond lengths

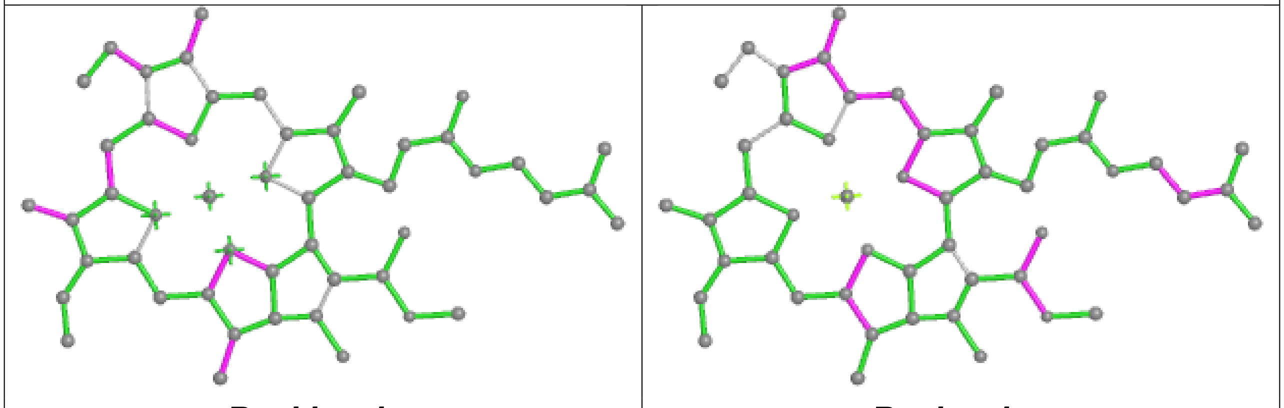
Bond angles



Torsions

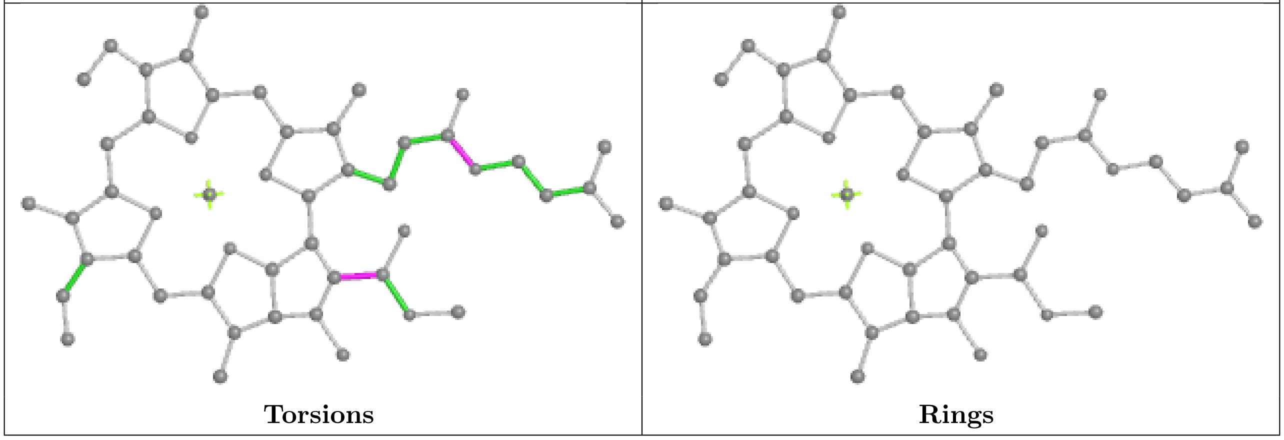
Rings

Ligand CLA b 817



Bond lengths

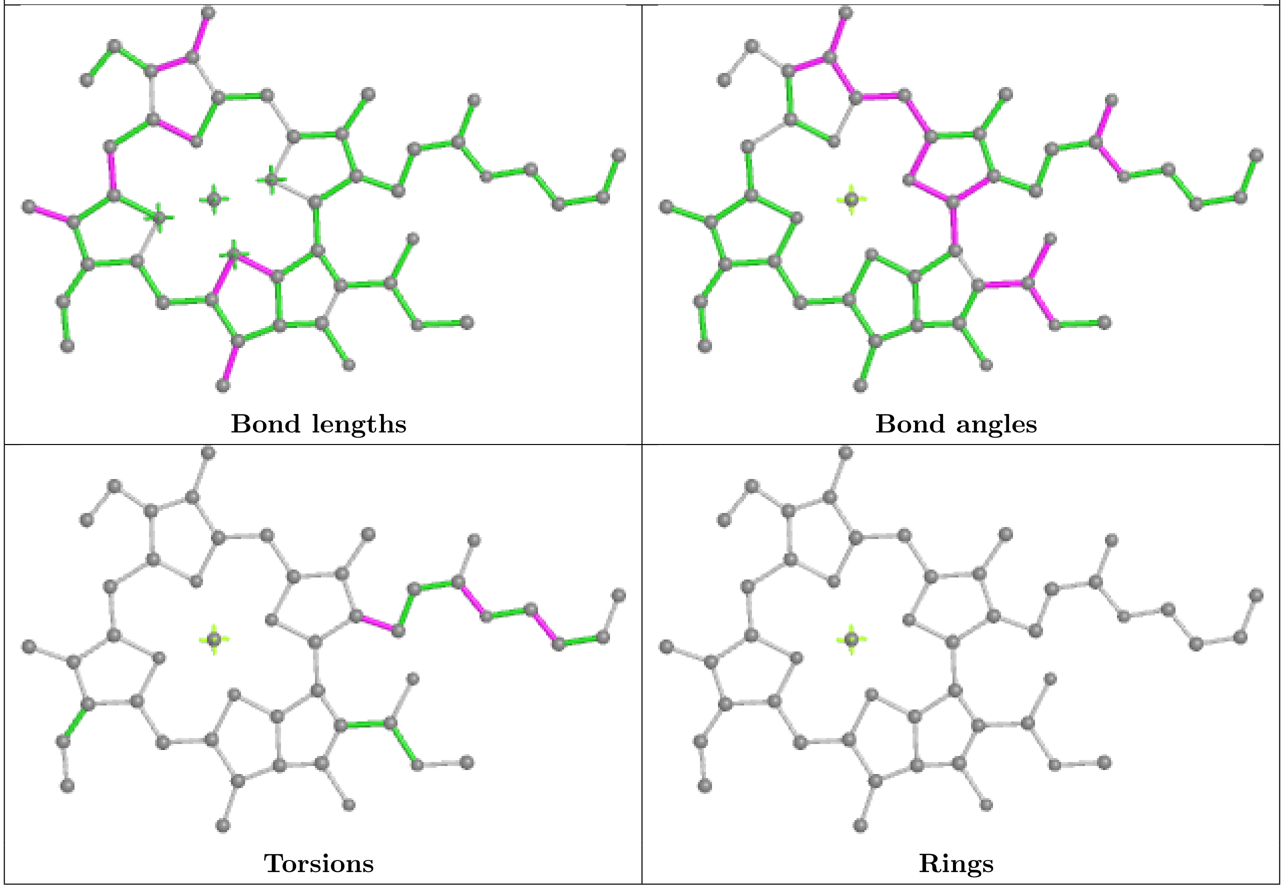
Bond angles



Torsions

Rings

Ligand CLA k 102



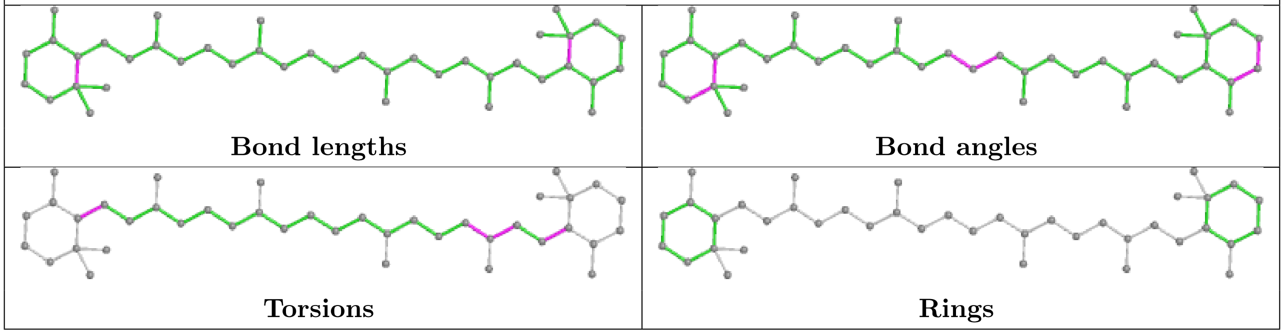
Bond lengths

Bond angles

Torsions

Rings

Ligand BCR a 845



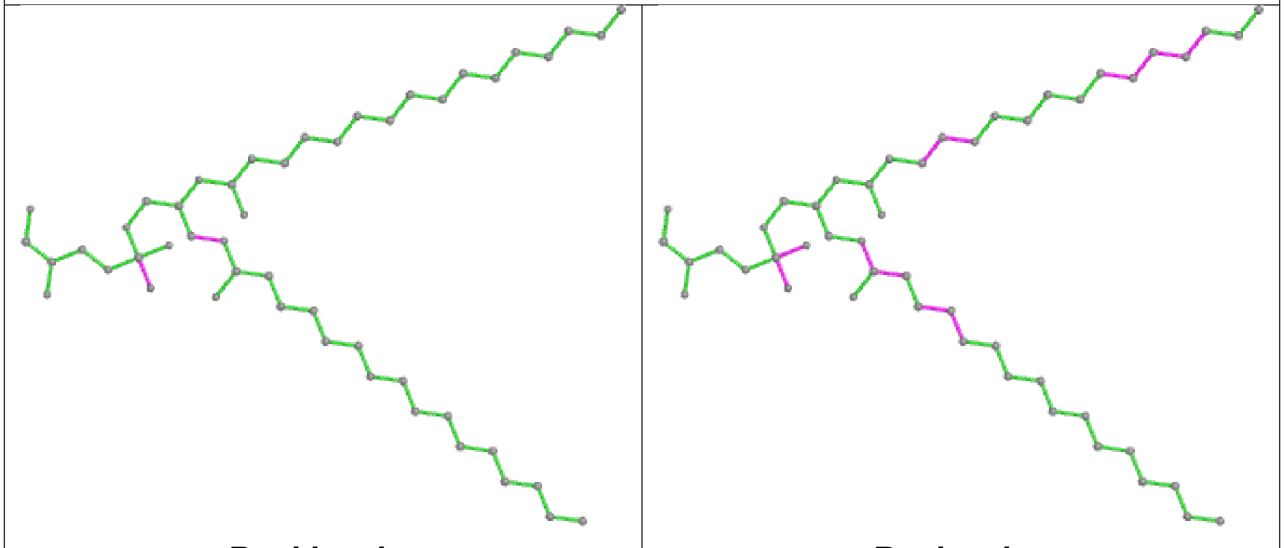
Bond lengths

Bond angles

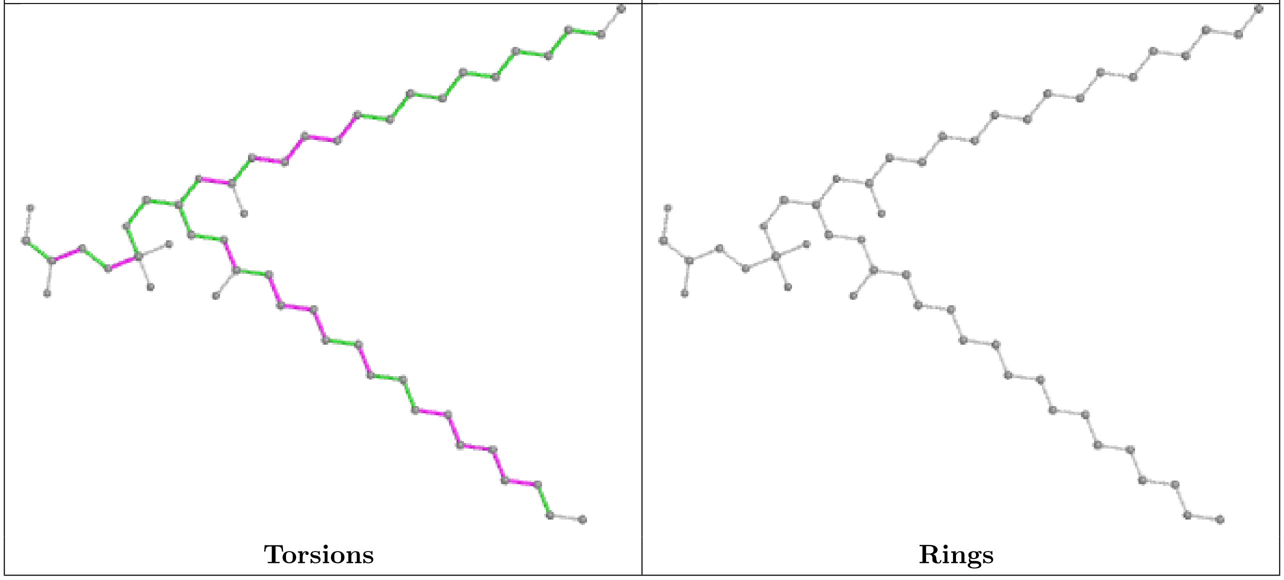
Torsions

Rings

Ligand LHG A 853

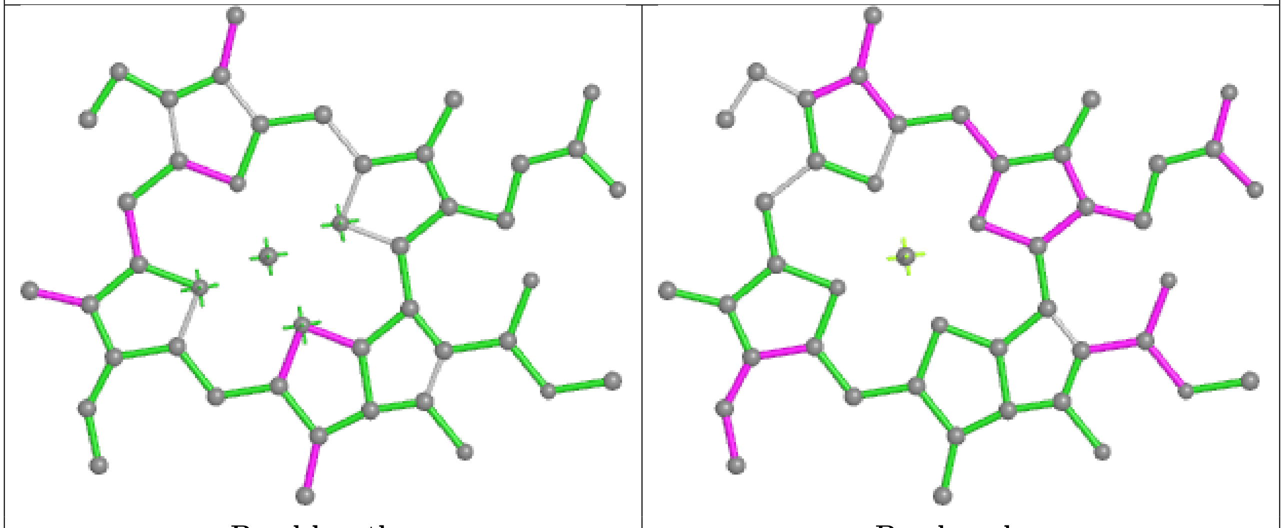


Bond lengths Bond angles



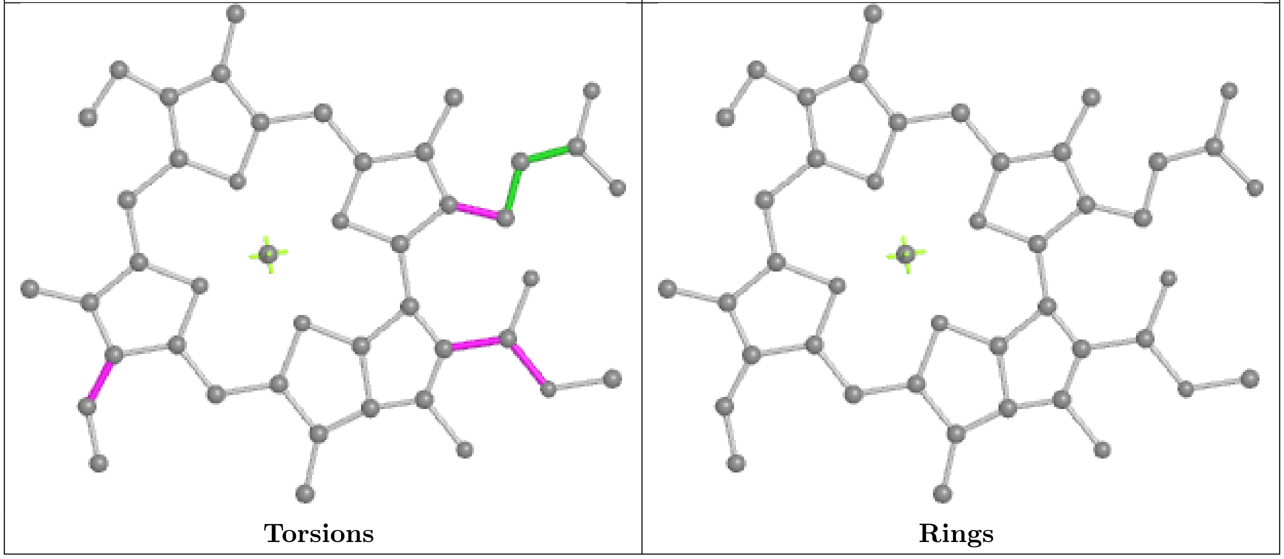
Torsions Rings

Ligand CLA l 203



Bond lengths

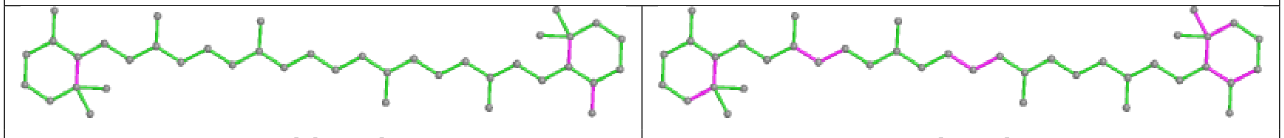
Bond angles



Torsions

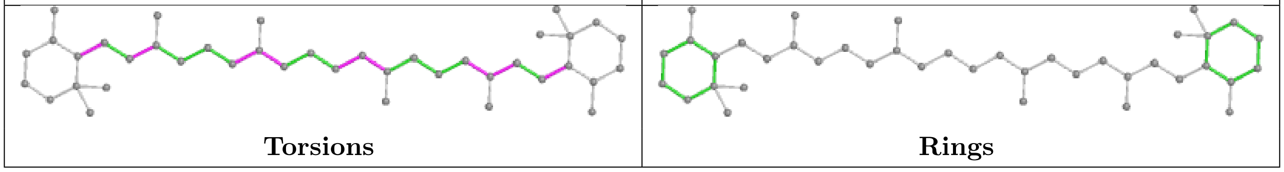
Rings

Ligand BCR L 1504



Bond lengths

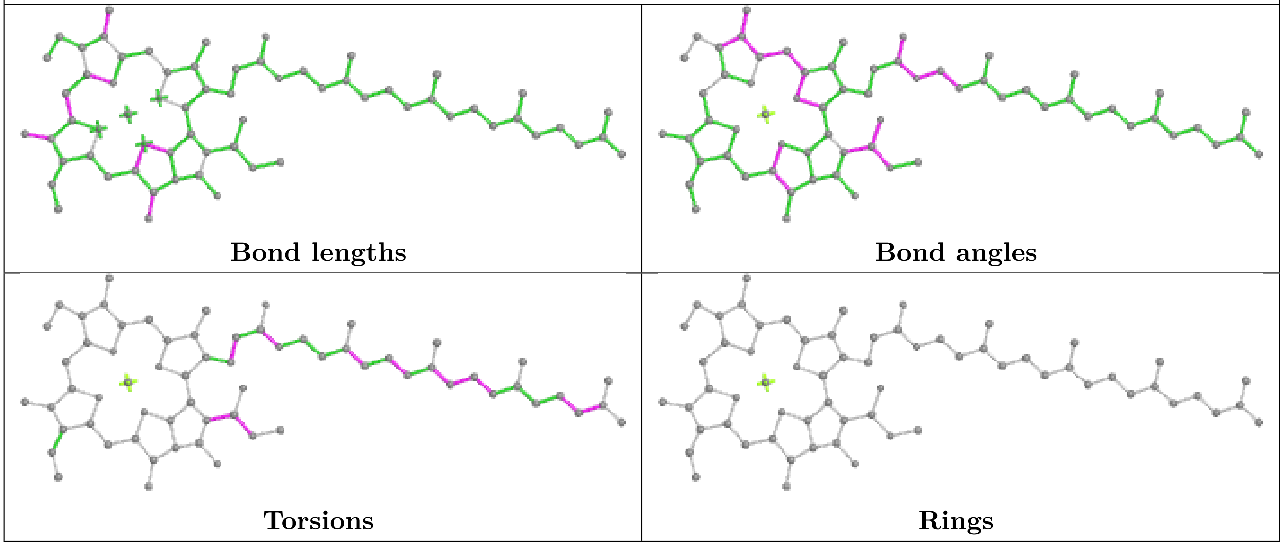
Bond angles



Torsions

Rings

Ligand CLA a 820



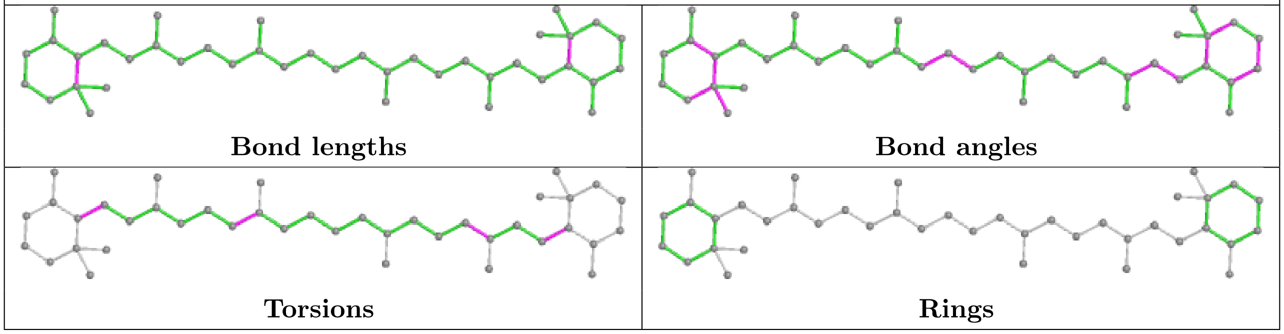
Bond lengths

Bond angles

Torsions

Rings

Ligand BCR l 207



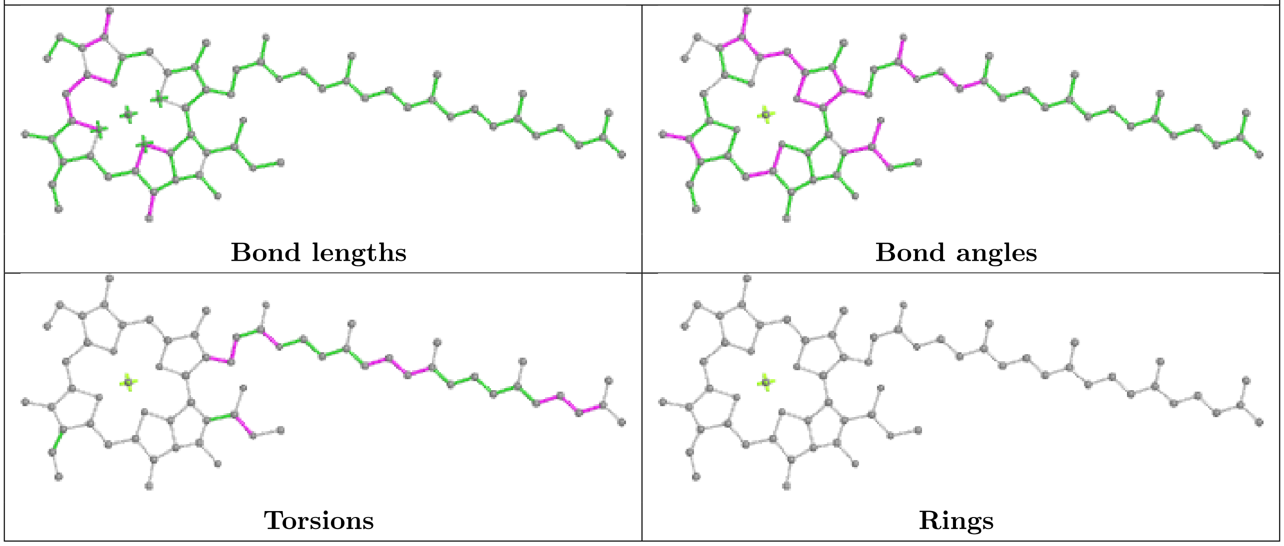
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA B 843



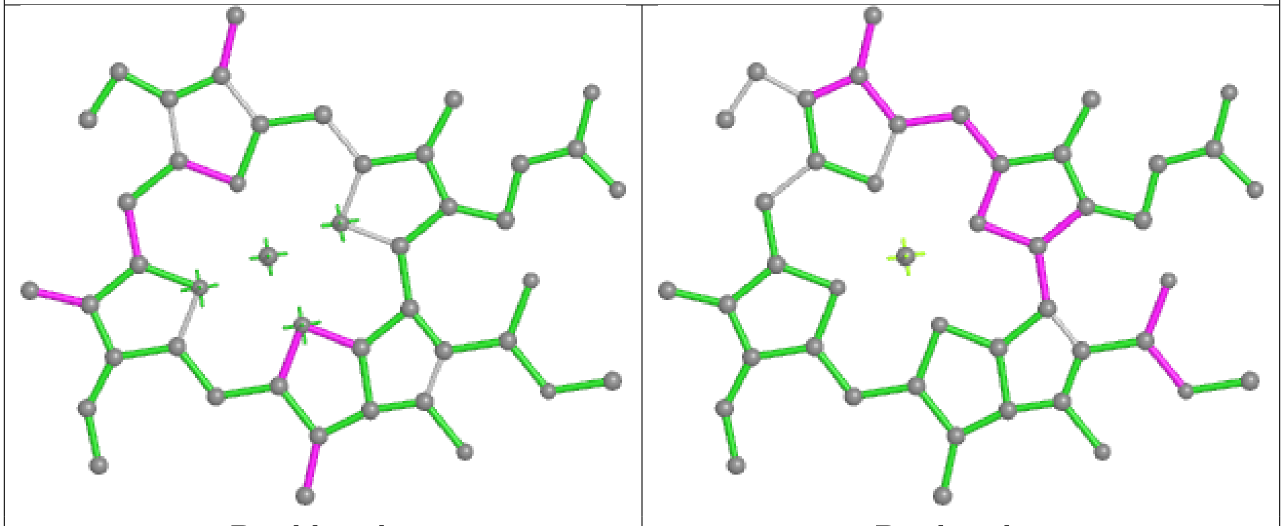
Bond lengths

Bond angles

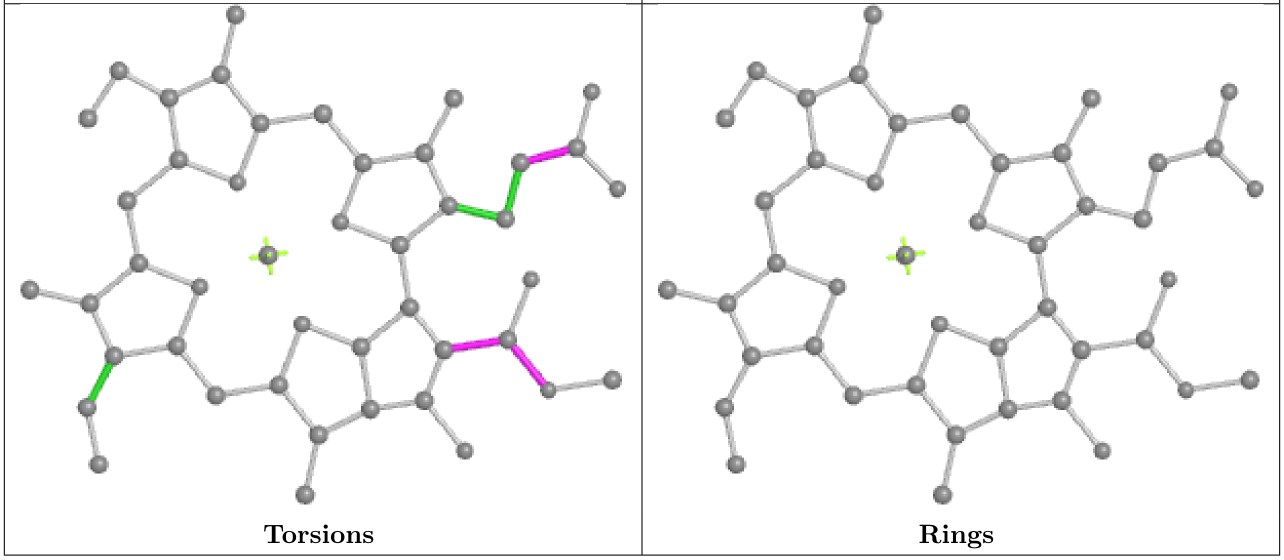
Torsions

Rings

Ligand CLA a 814

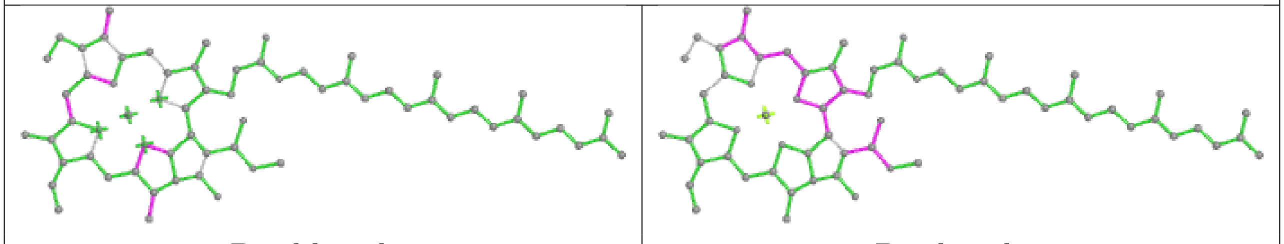


Bond lengths Bond angles

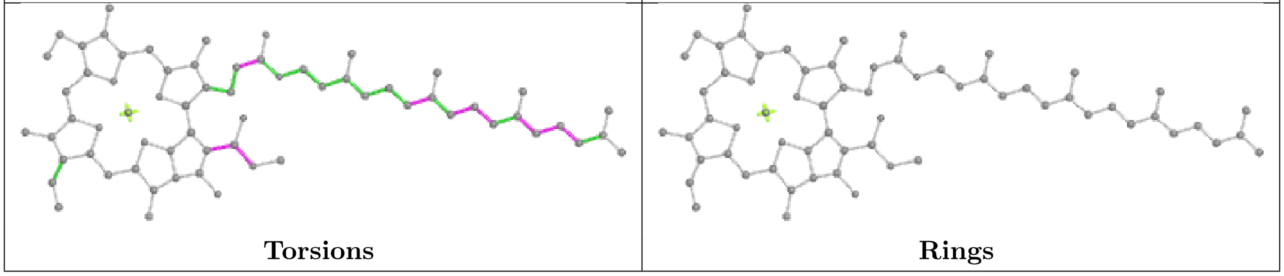


Torsions Rings

Ligand CLA a 824

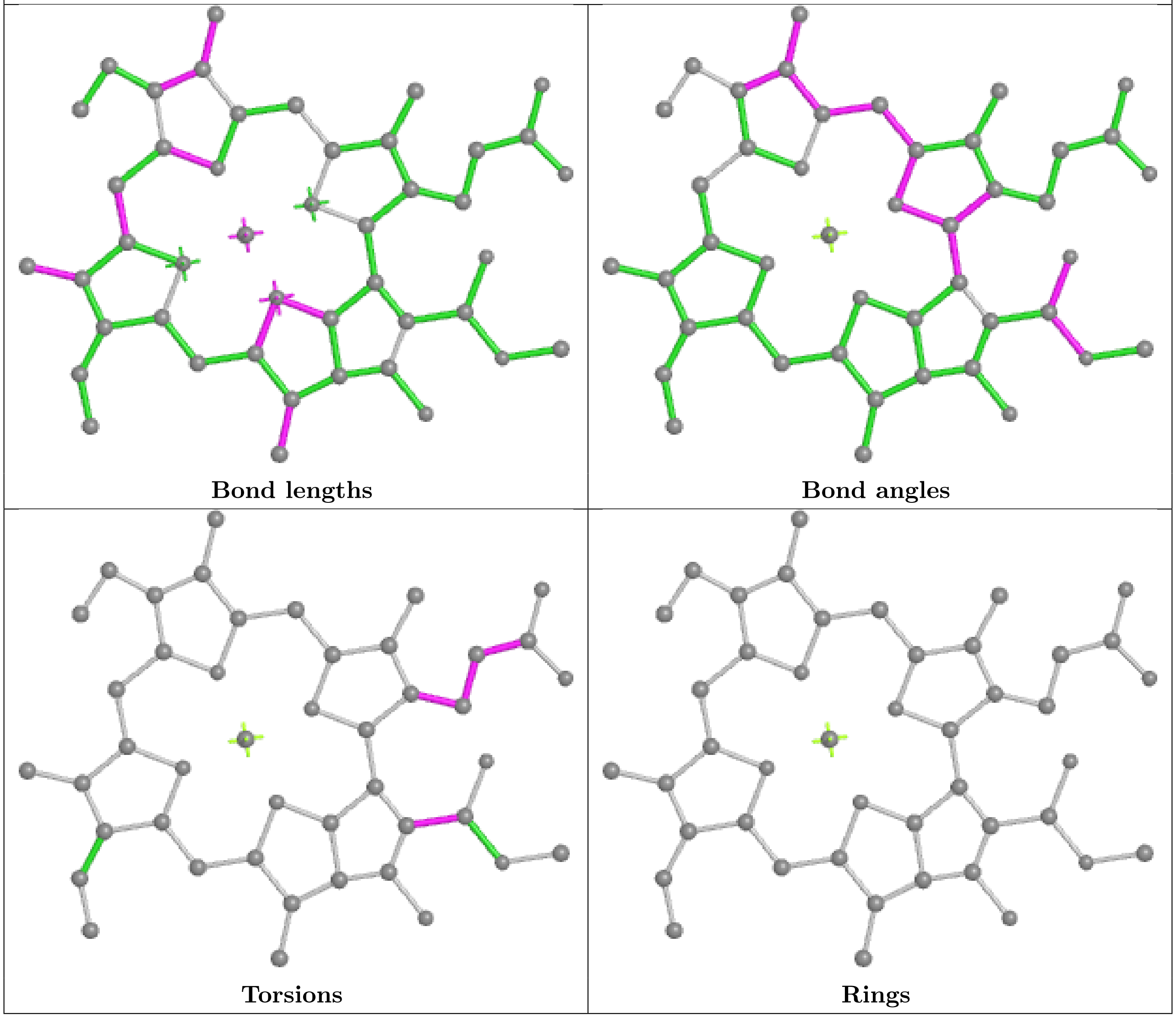


Bond lengths Bond angles

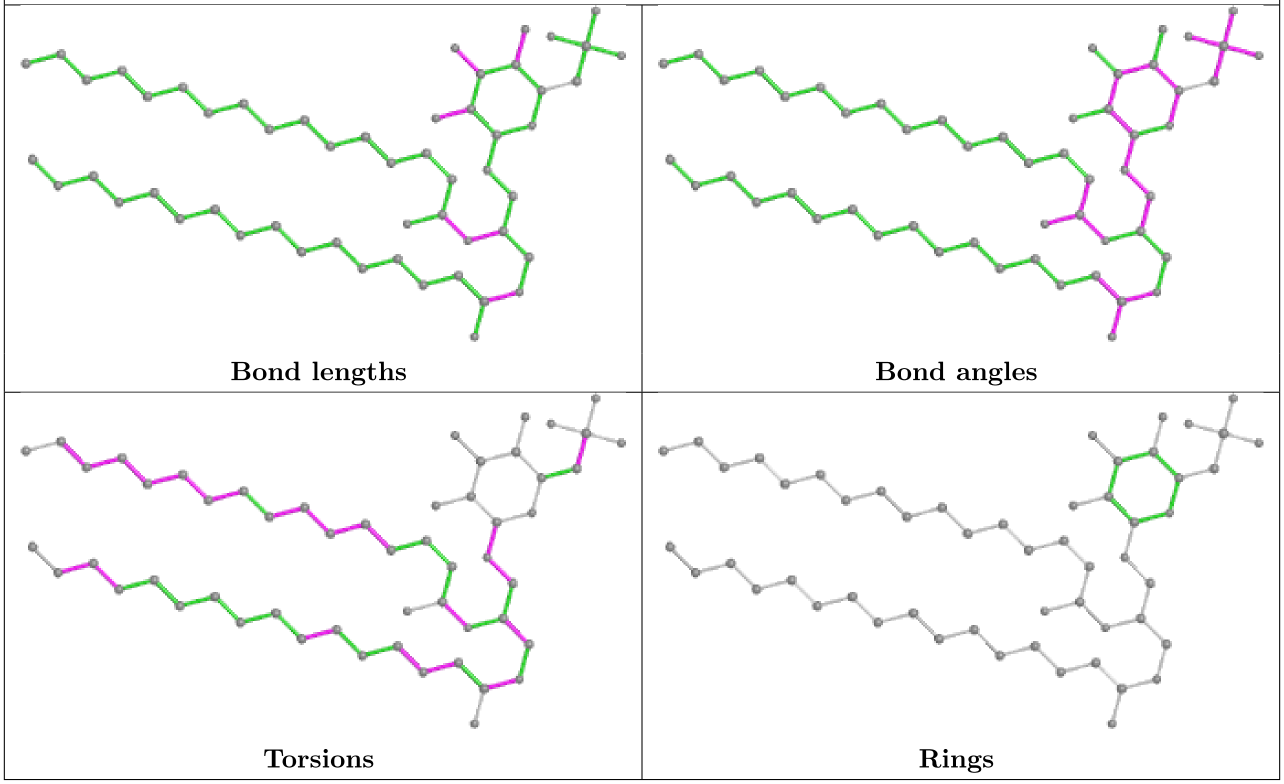


Torsions Rings

Ligand CLA b 823



Ligand SQD l 202



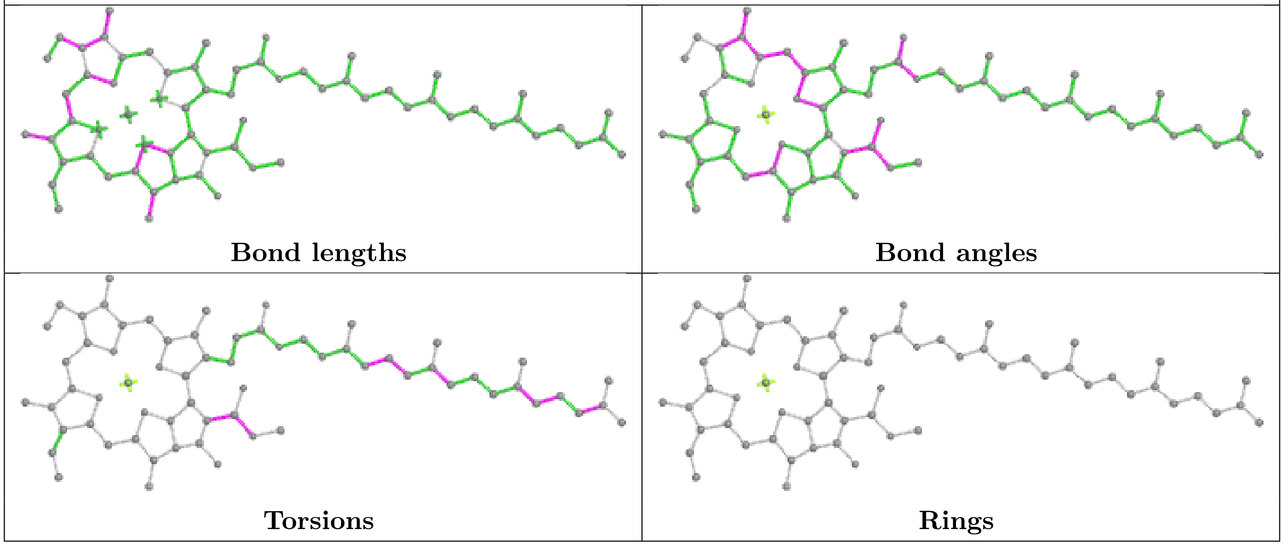
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA B 802



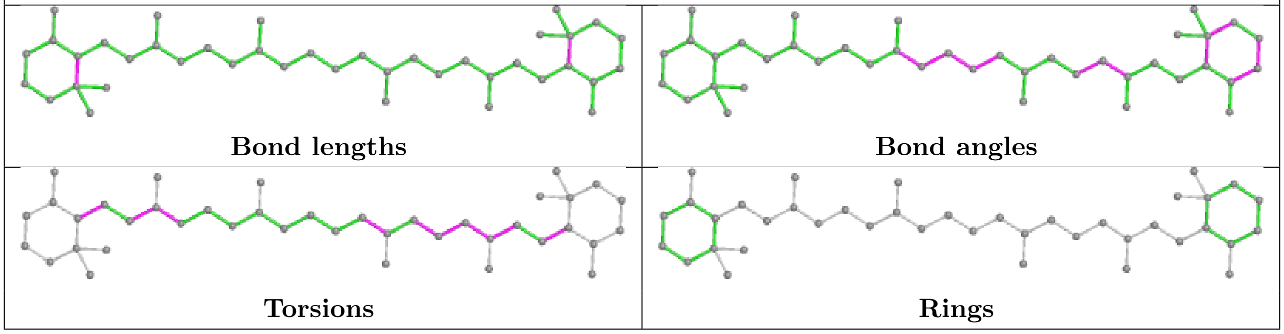
Bond lengths

Bond angles

Torsions

Rings

Ligand BCR b 848



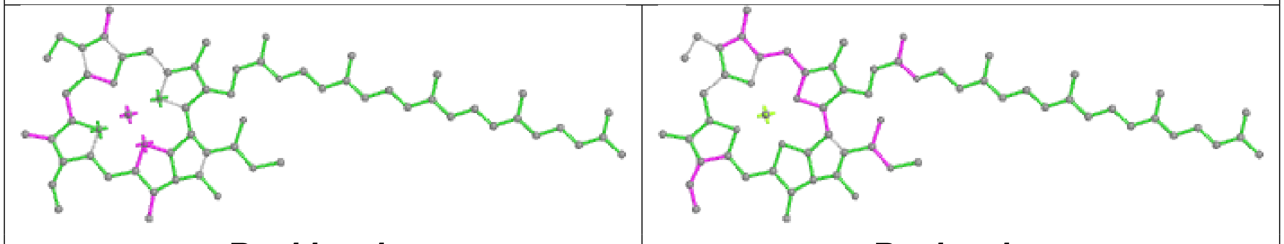
Bond lengths

Bond angles

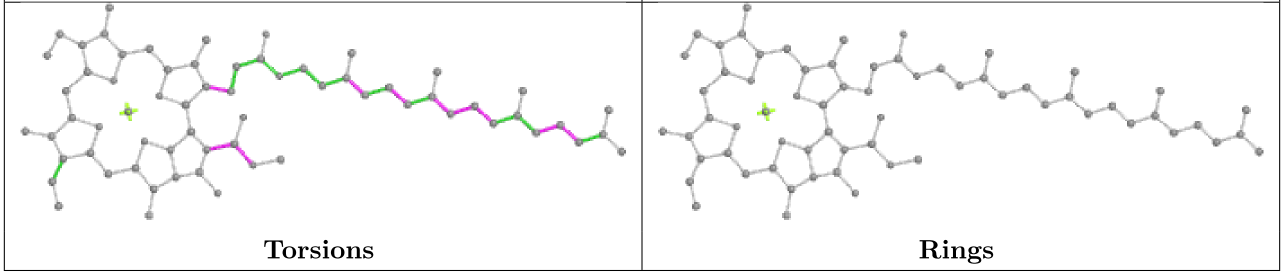
Torsions

Rings

Ligand CLA b 816

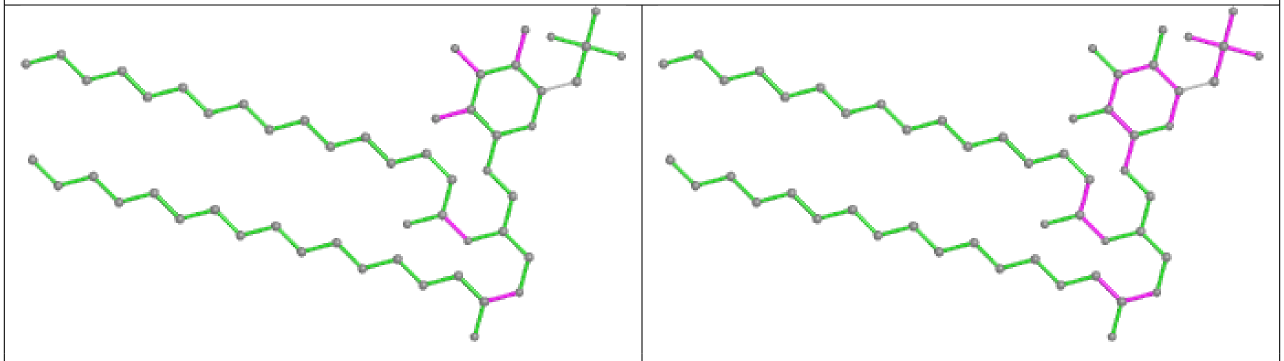


Bond lengths **Bond angles**

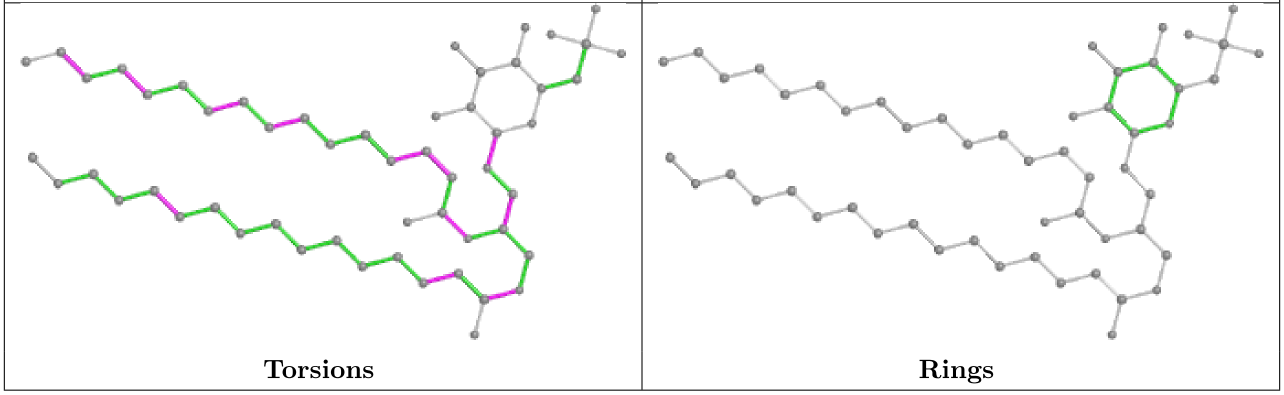


Torsions **Rings**

Ligand SQD x 1702

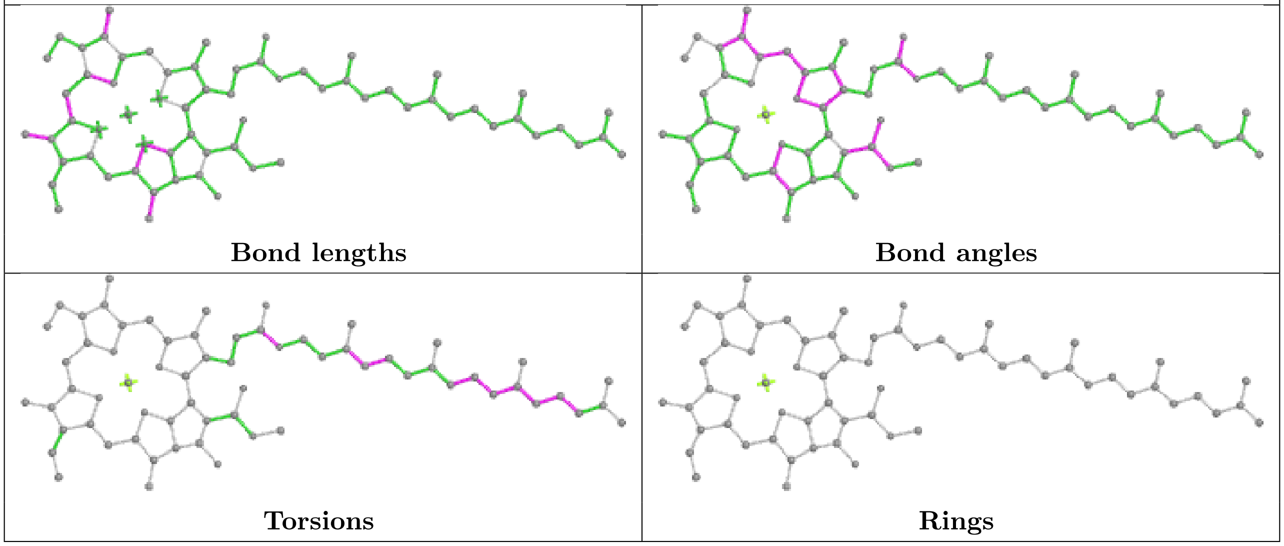


Bond lengths **Bond angles**



Torsions **Rings**

Ligand CLA A 838



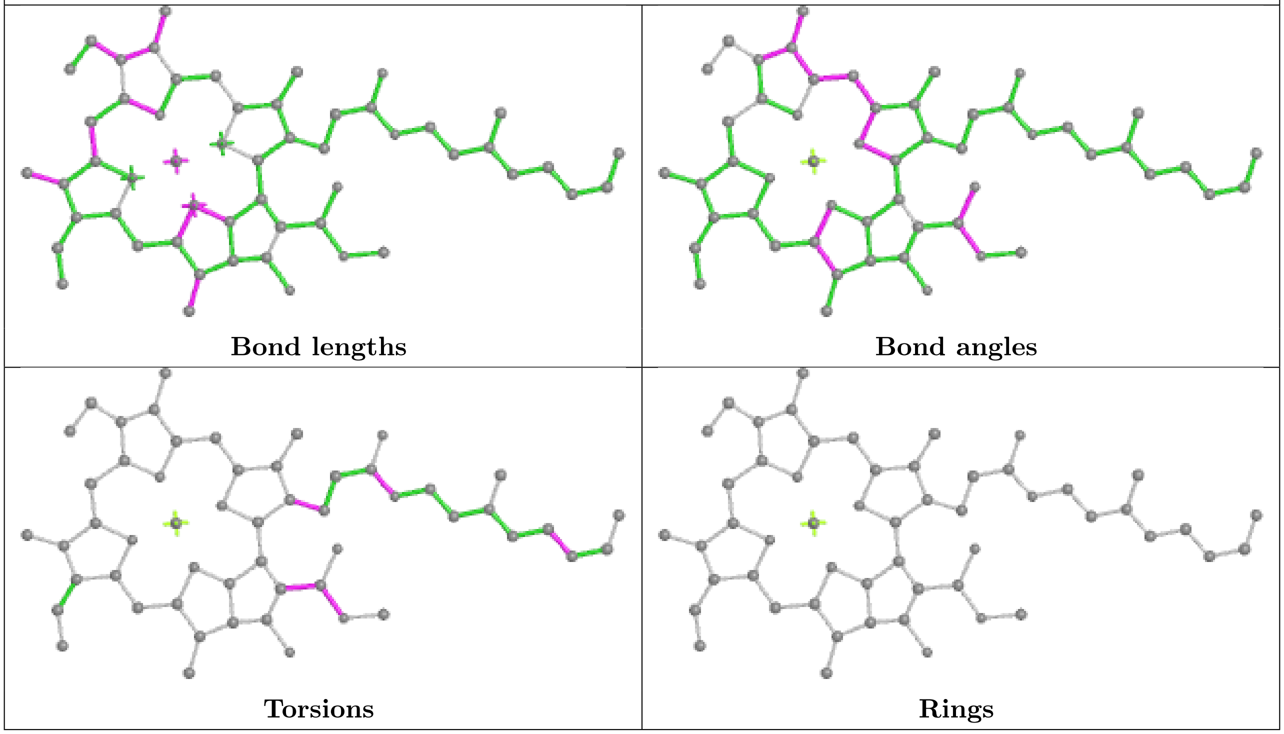
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA b 833



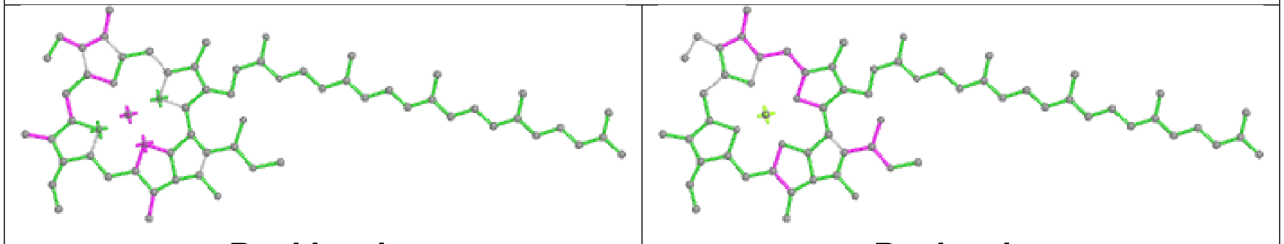
Bond lengths

Bond angles

Torsions

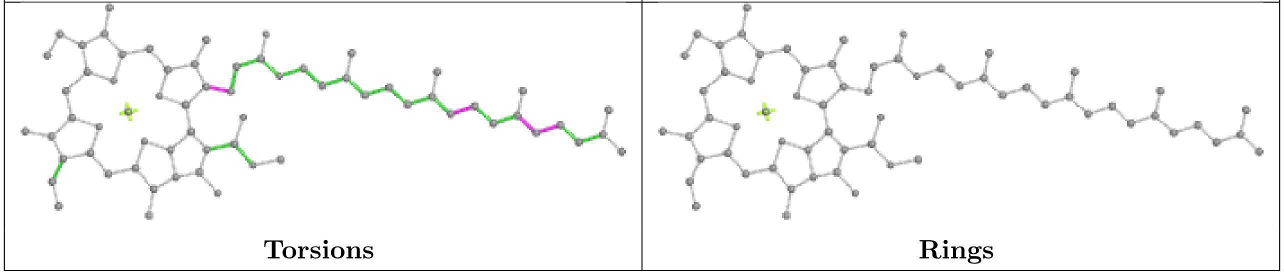
Rings

Ligand CLA b 820



Bond lengths

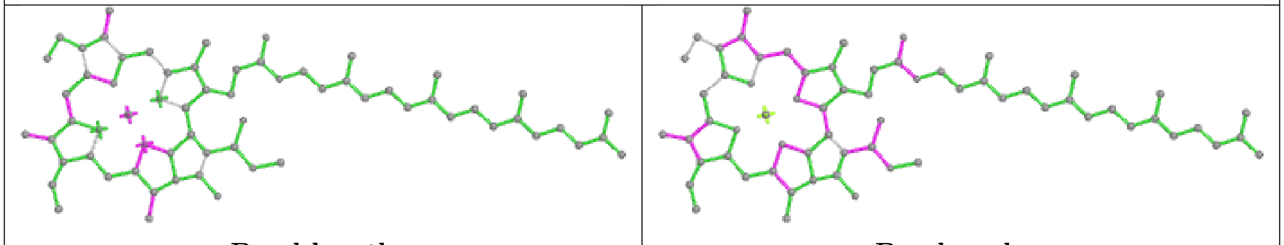
Bond angles



Torsions

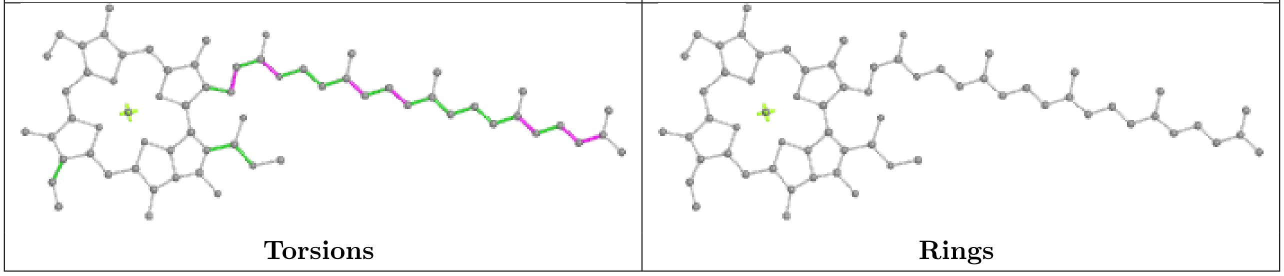
Rings

Ligand CLA A 829



Bond lengths

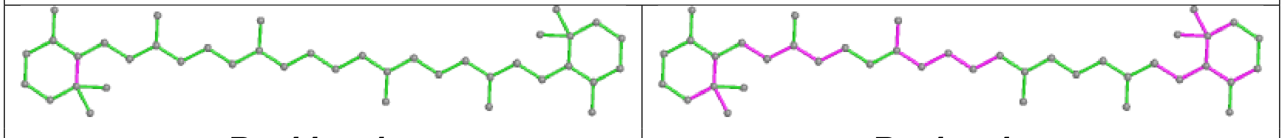
Bond angles



Torsions

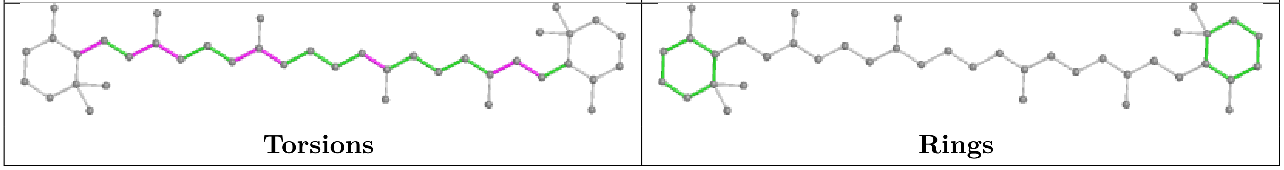
Rings

Ligand BCR l 206



Bond lengths

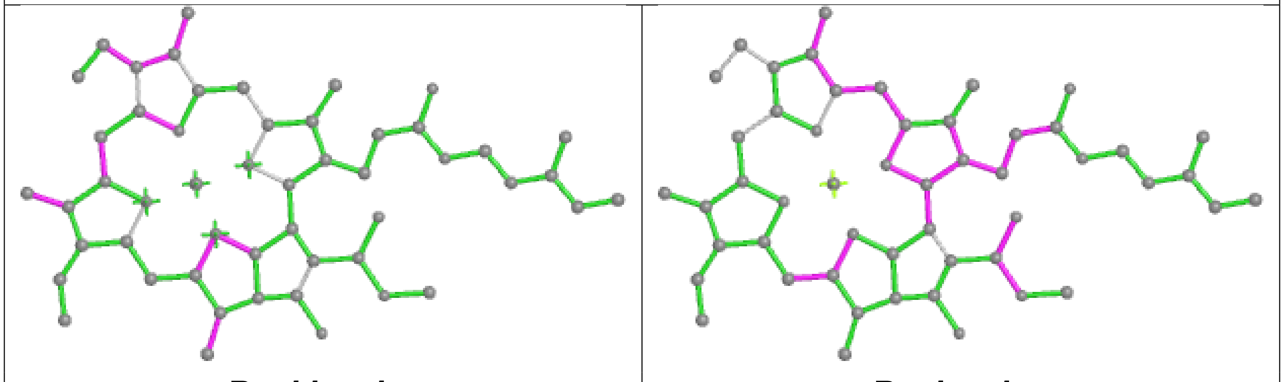
Bond angles



Torsions

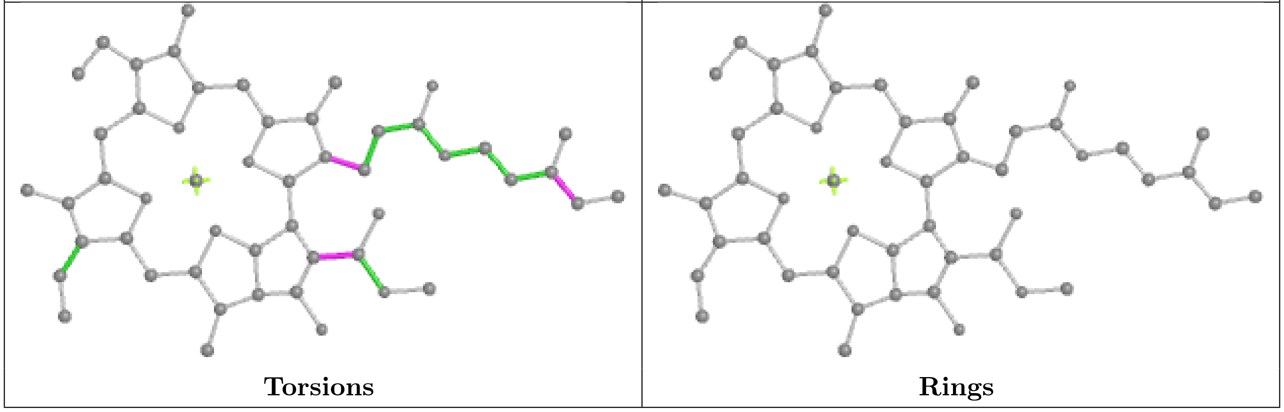
Rings

Ligand CLA L 1501



Bond lengths

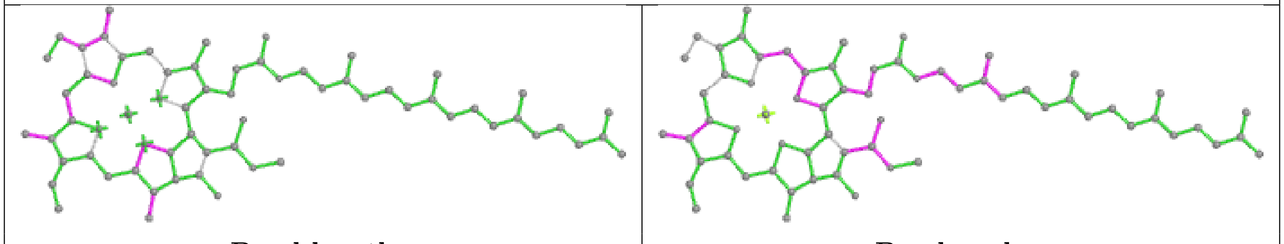
Bond angles



Torsions

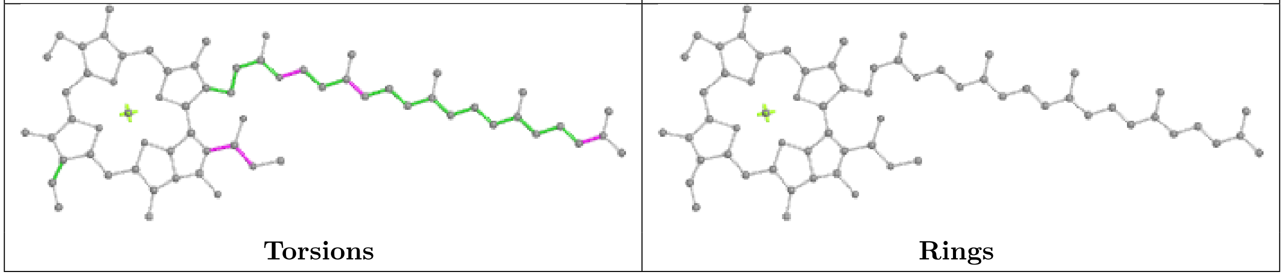
Rings

Ligand CLA b 806



Bond lengths

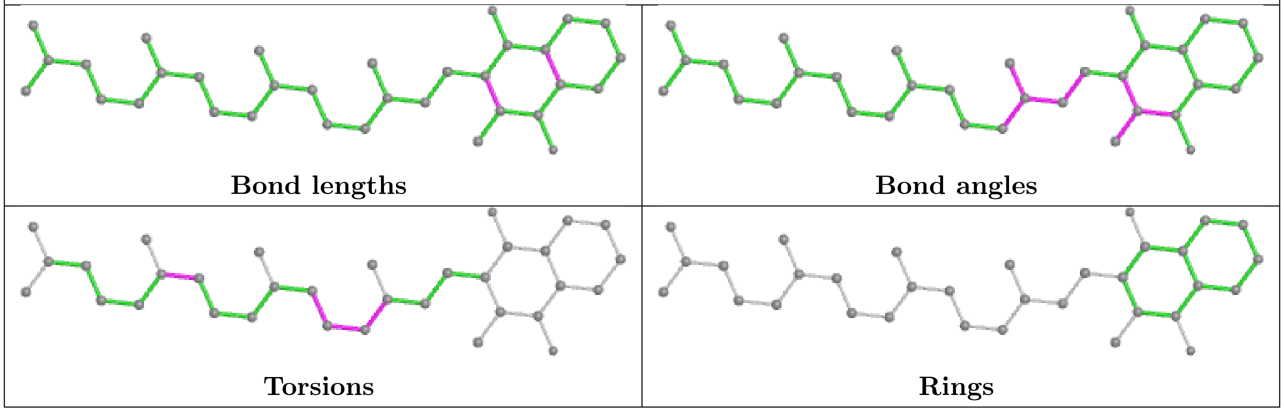
Bond angles



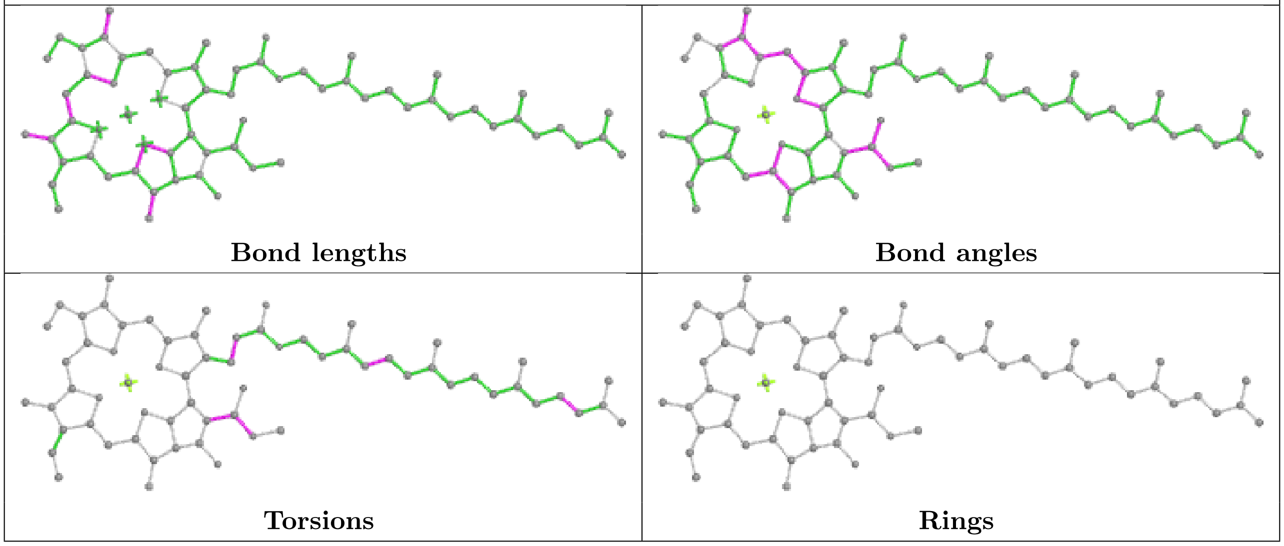
Torsions

Rings

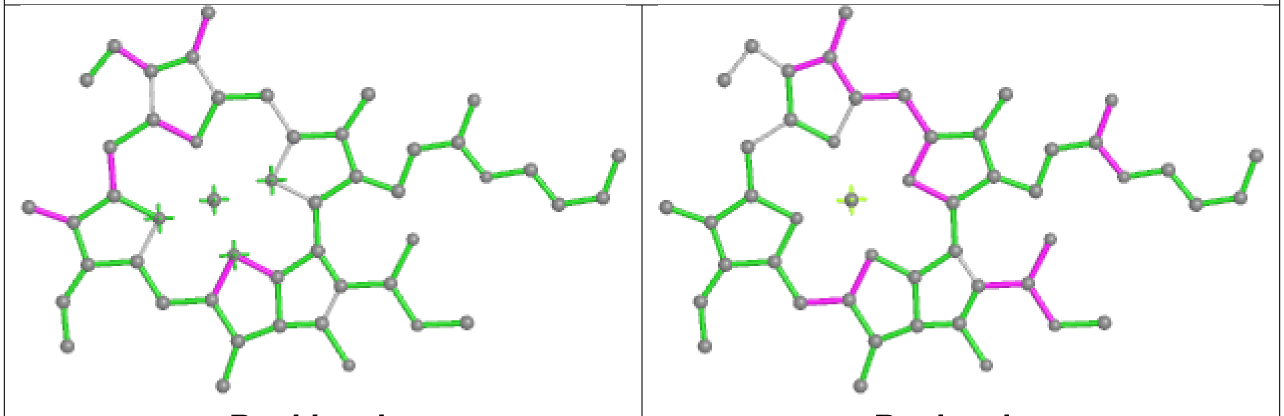
Ligand PQN A 844


Bond lengths
Bond angles
Torsions
Rings

Ligand CLA B 842

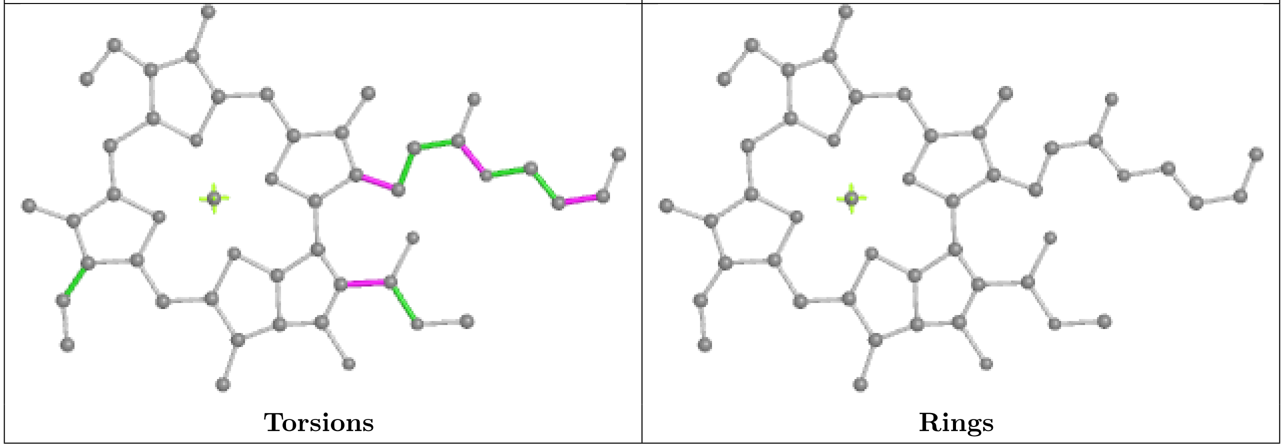

Bond lengths
Bond angles
Torsions
Rings

Ligand CLA B 818



Bond lengths

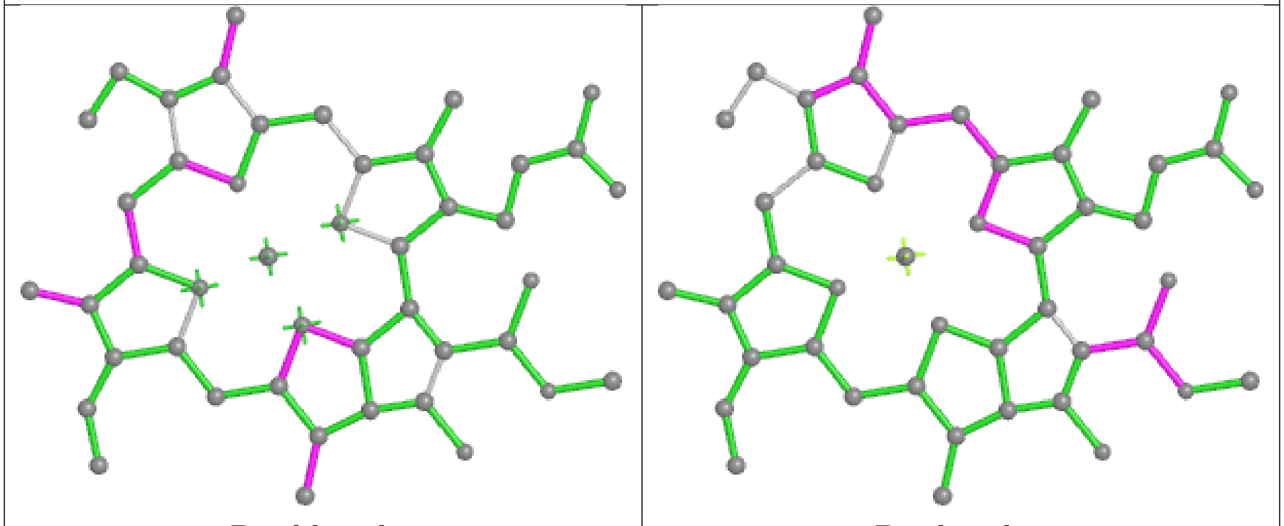
Bond angles



Torsions

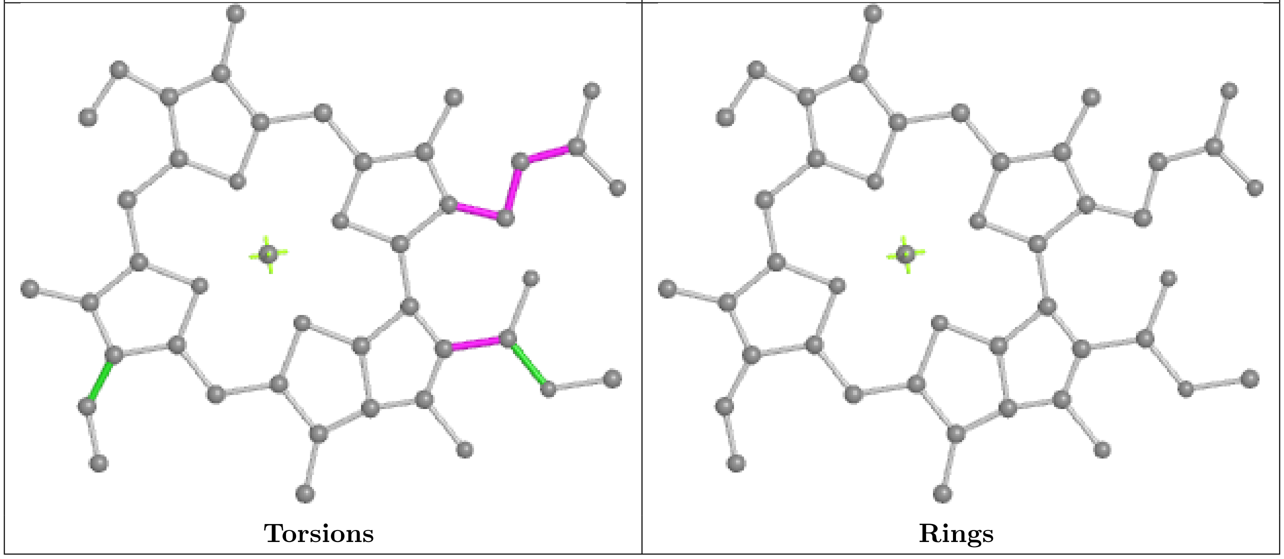
Rings

Ligand CLA a 835



Bond lengths

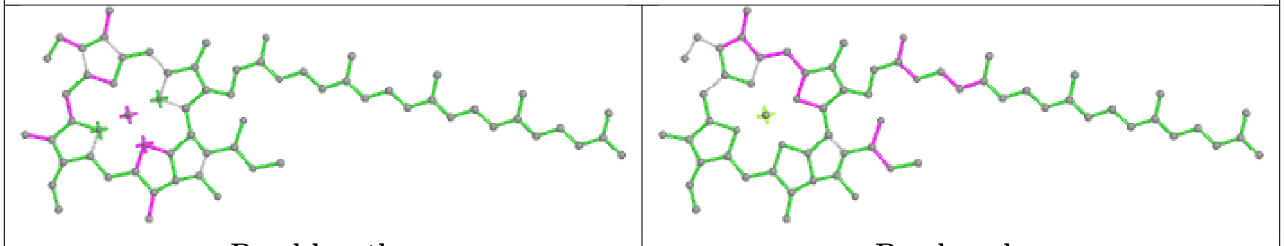
Bond angles



Torsions

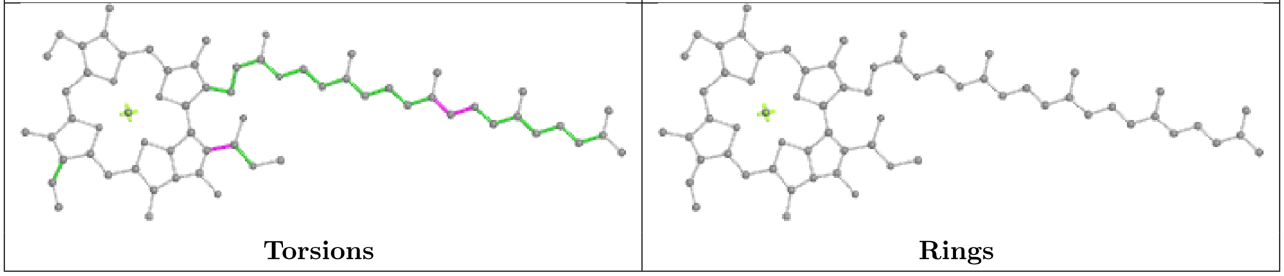
Rings

Ligand CLA a 839



Bond lengths

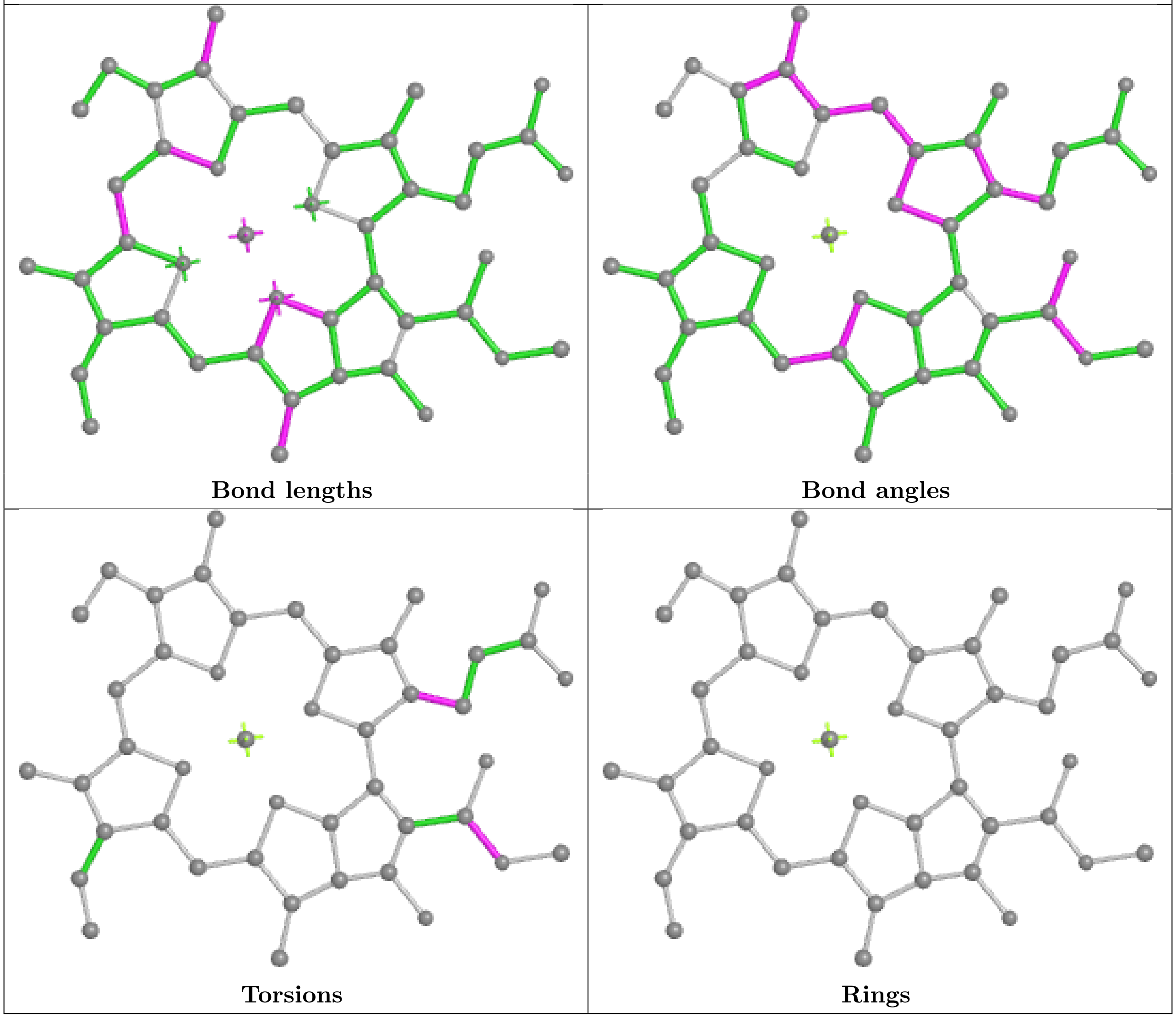
Bond angles



Torsions

Rings

Ligand CLA b 819



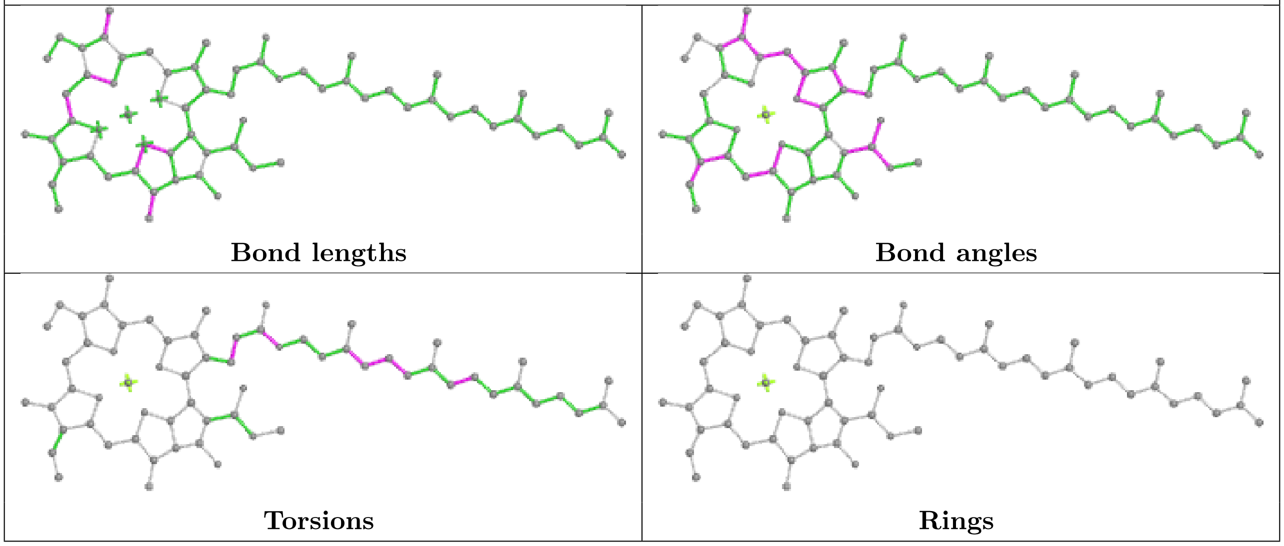
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA b 826



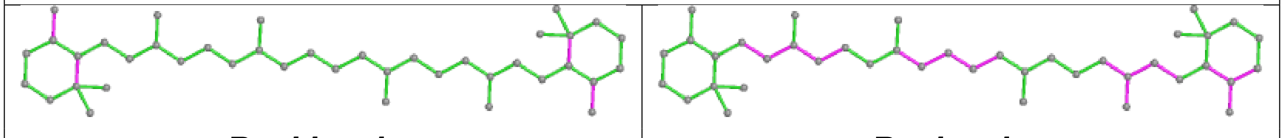
Bond lengths

Bond angles

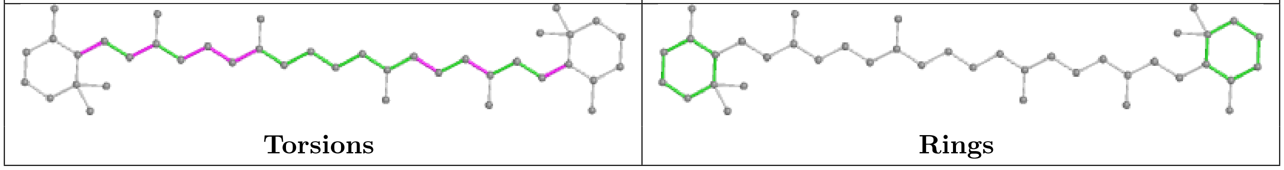
Torsions

Rings

Ligand BCR I 102

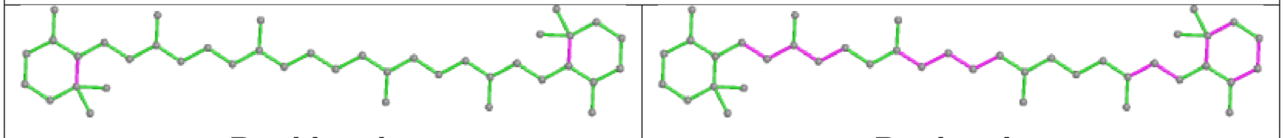


Bond lengths Bond angles

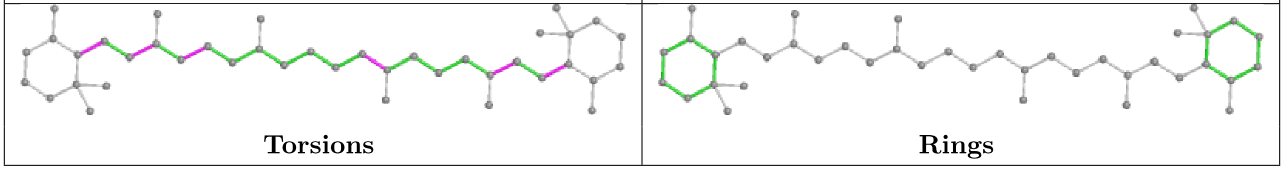


Torsions Rings

Ligand BCR A 846

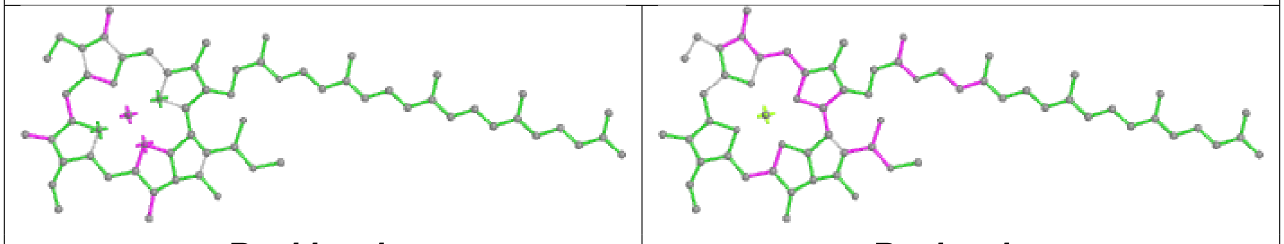


Bond lengths Bond angles

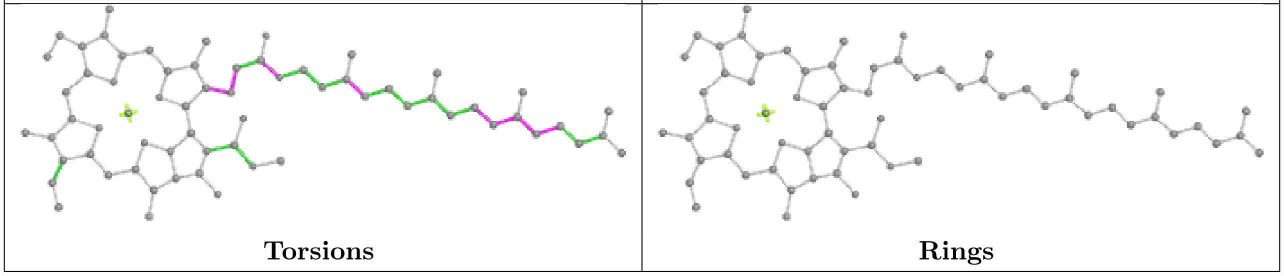


Torsions Rings

Ligand CLA B 830

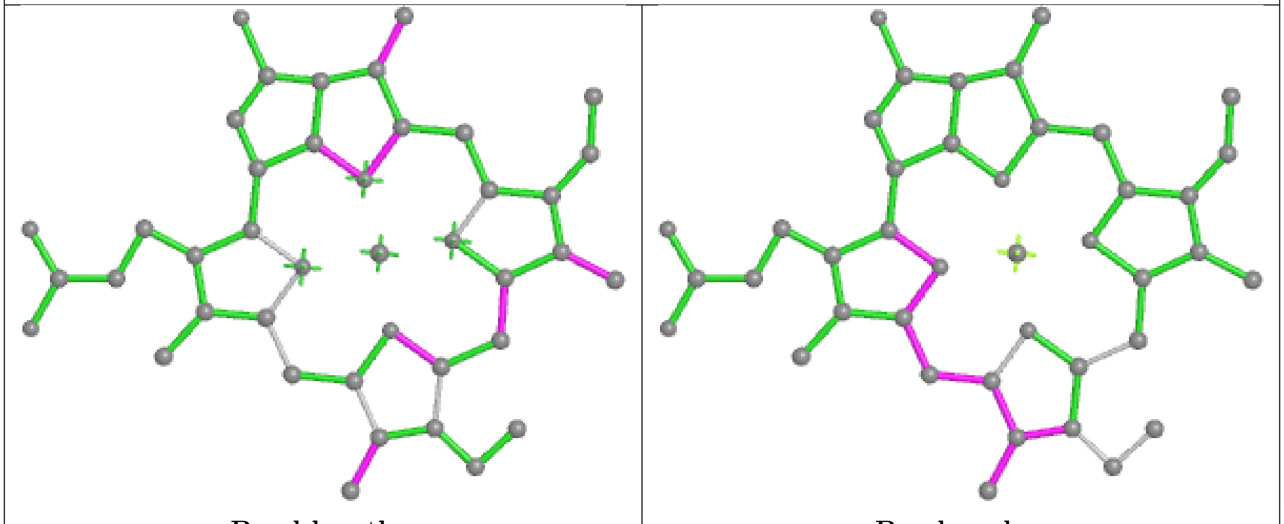


Bond lengths Bond angles

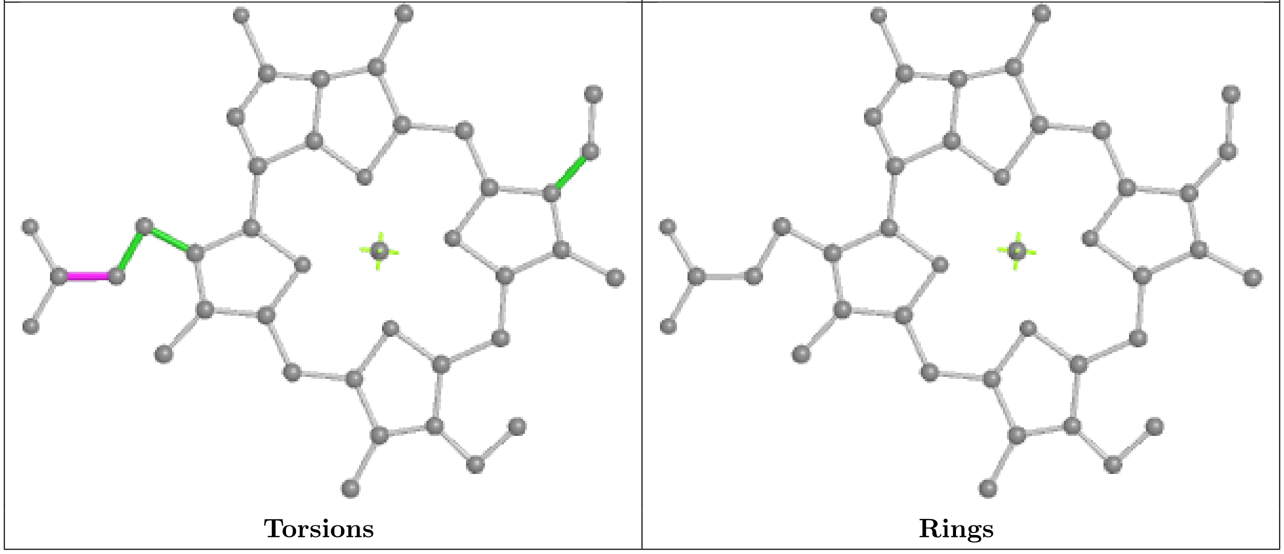


Torsions Rings

Ligand CLA k 101

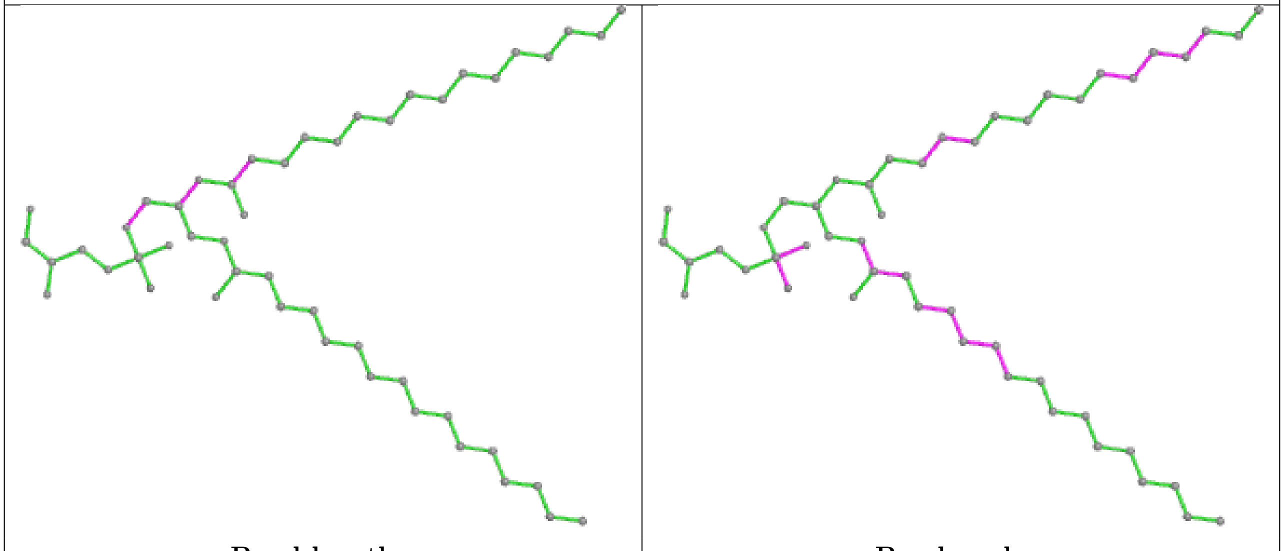


Bond lengths **Bond angles**



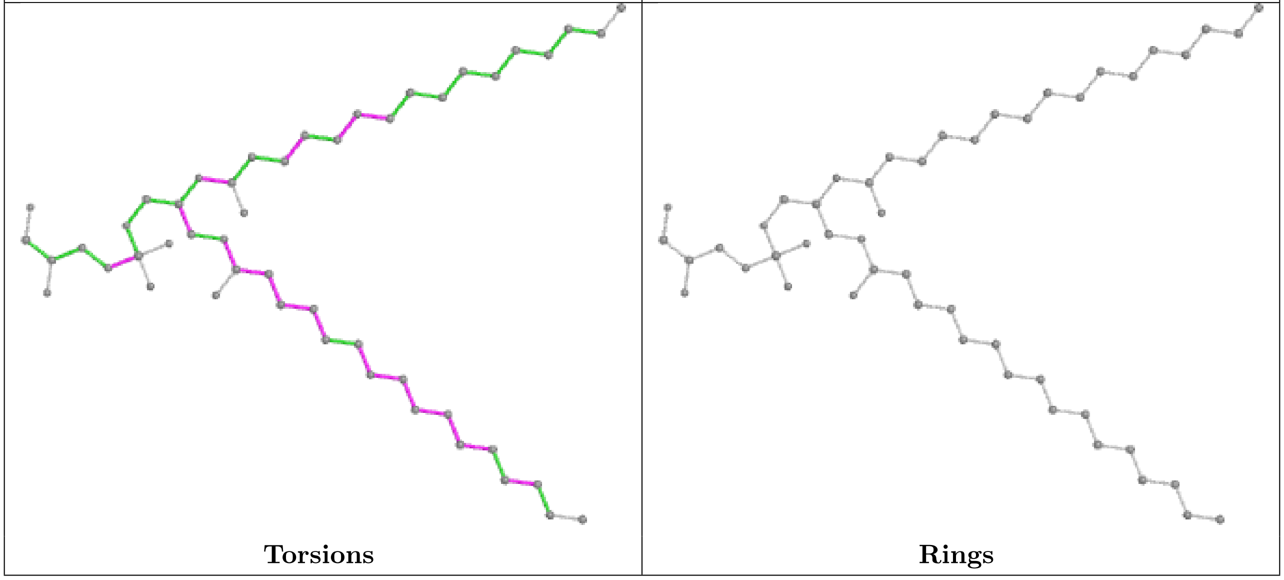
Torsions **Rings**

Ligand LHG A 852



Bond lengths

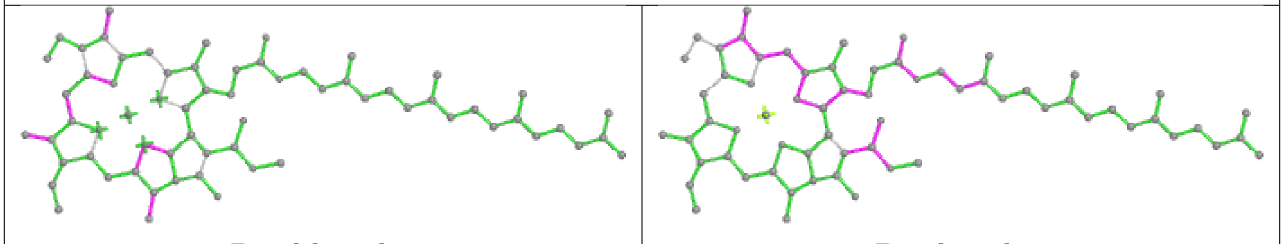
Bond angles



Torsions

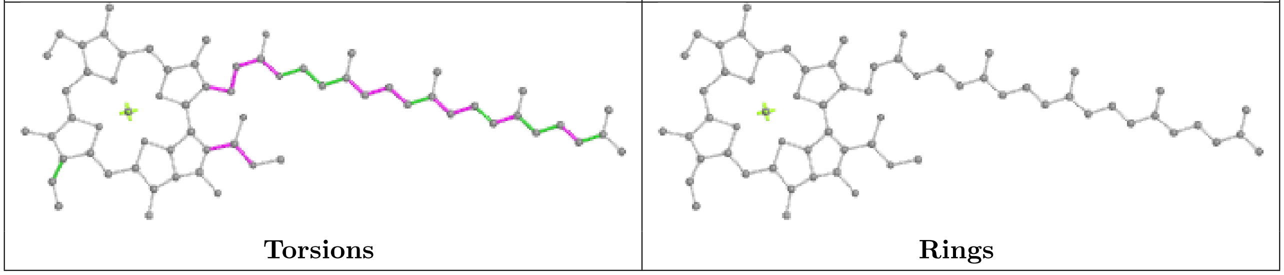
Rings

Ligand CLA A 808



Bond lengths

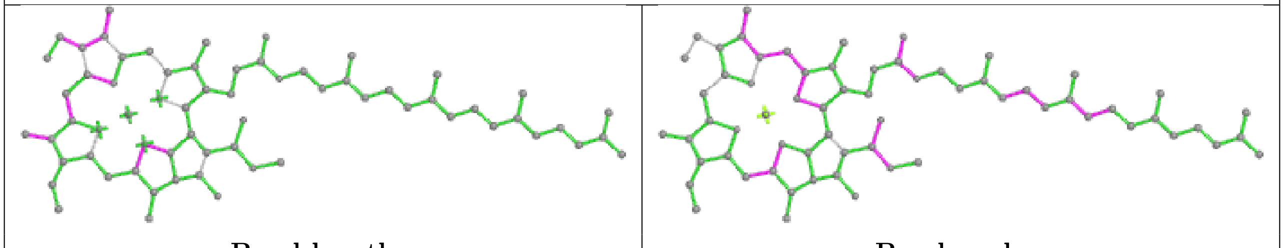
Bond angles



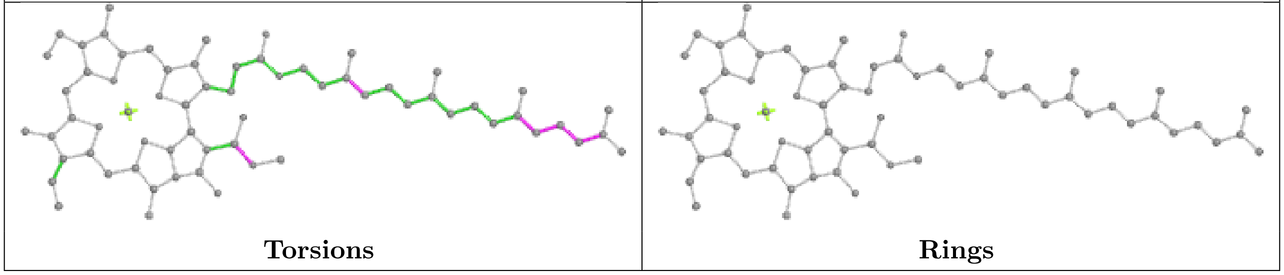
Torsions

Rings

Ligand CLA A 833

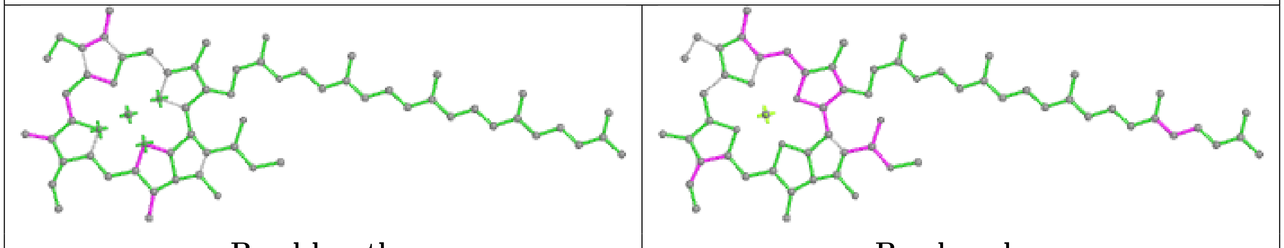


Bond lengths Bond angles

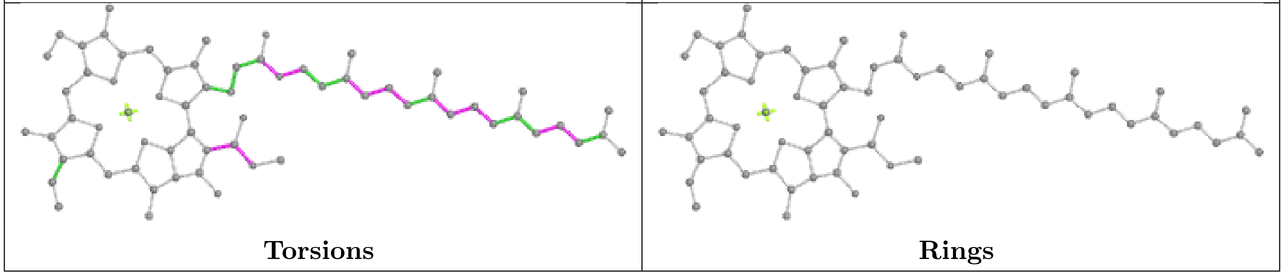


Torsions Rings

Ligand CLA A 839

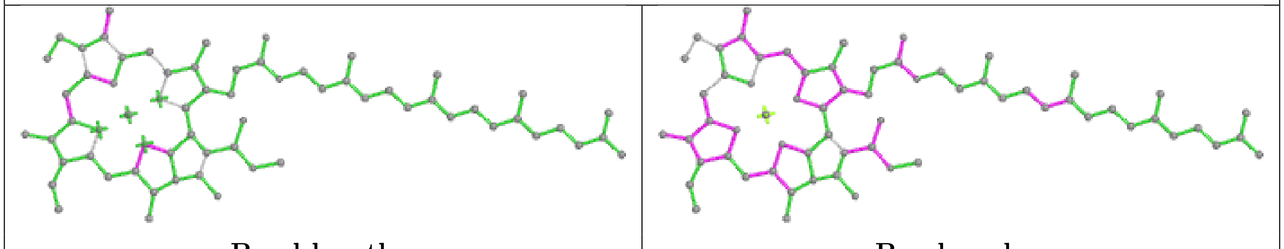


Bond lengths Bond angles

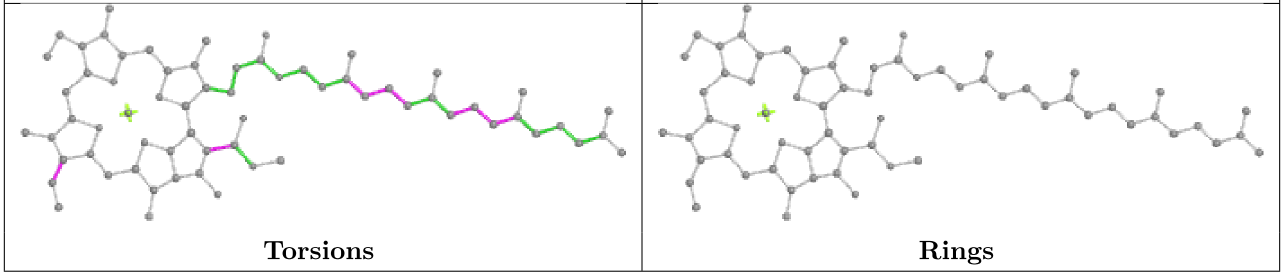


Torsions Rings

Ligand CLA B 828

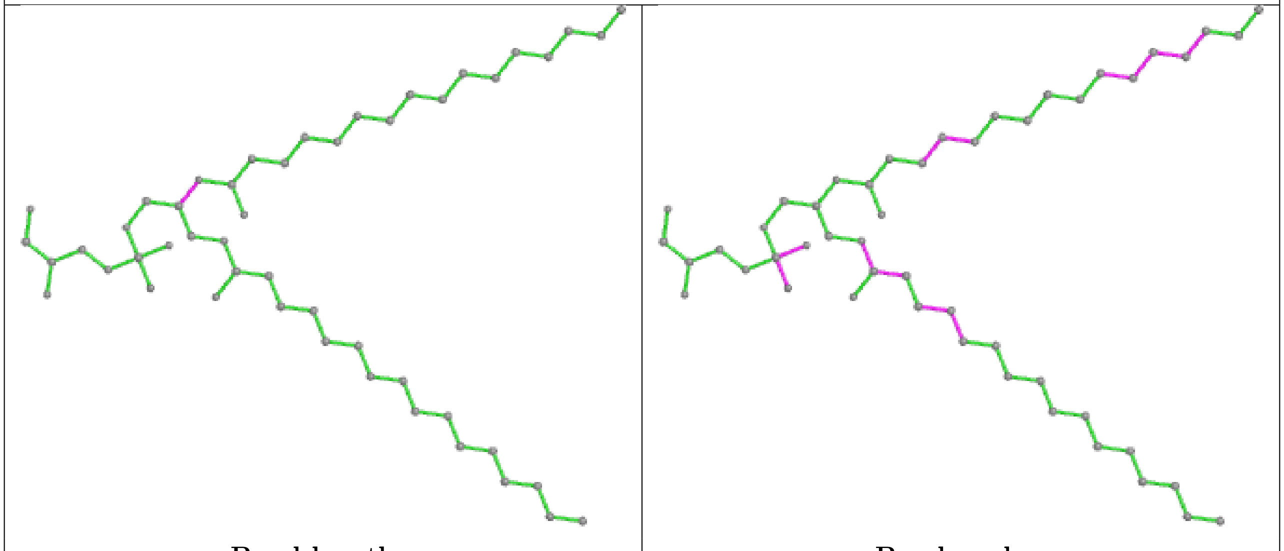


Bond lengths Bond angles

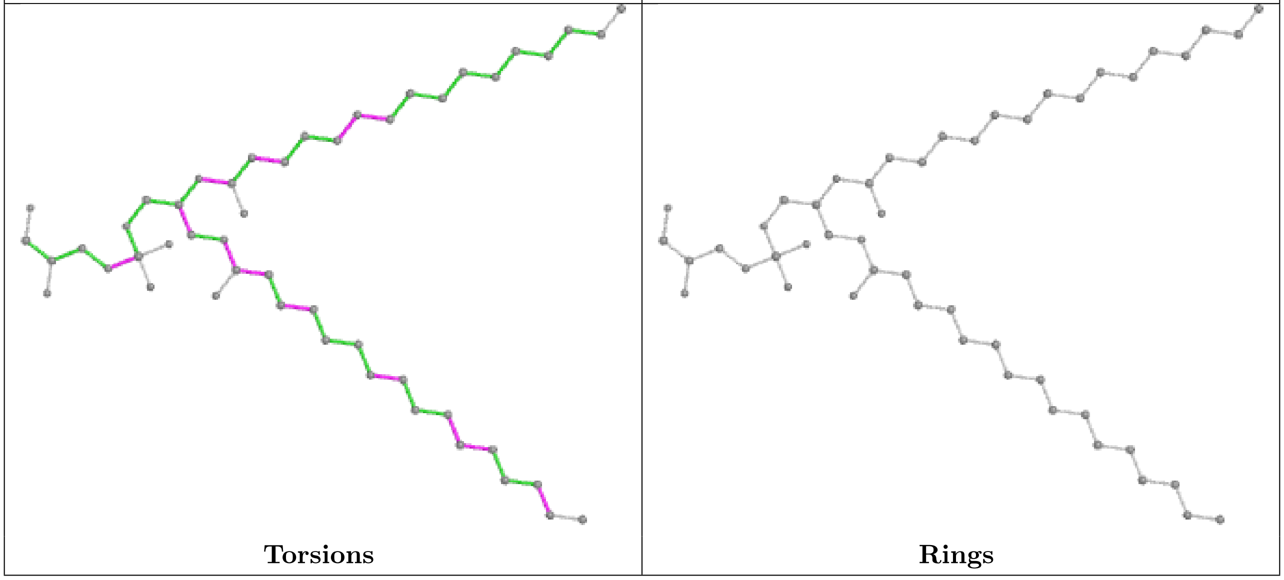


Torsions Rings

Ligand LHG a 850

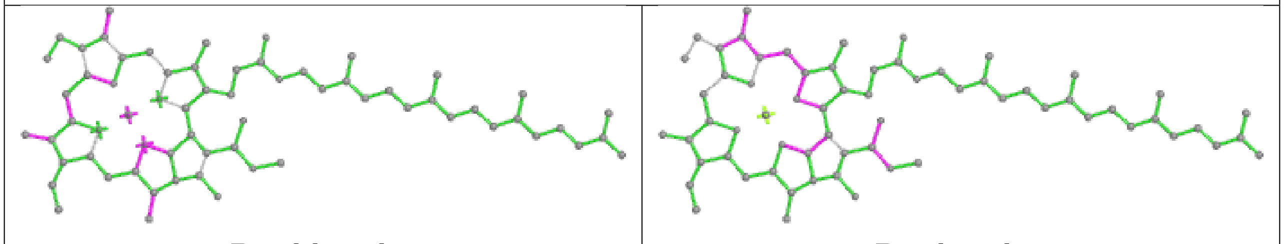


Bond lengths Bond angles

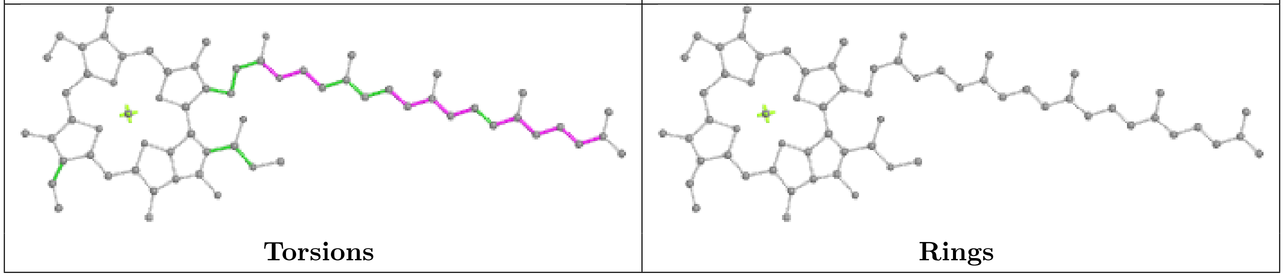


Torsions Rings

Ligand CLA A 832

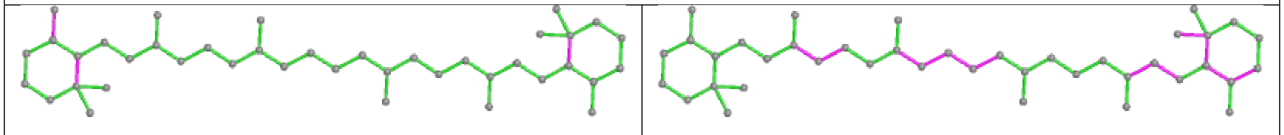


Bond lengths Bond angles



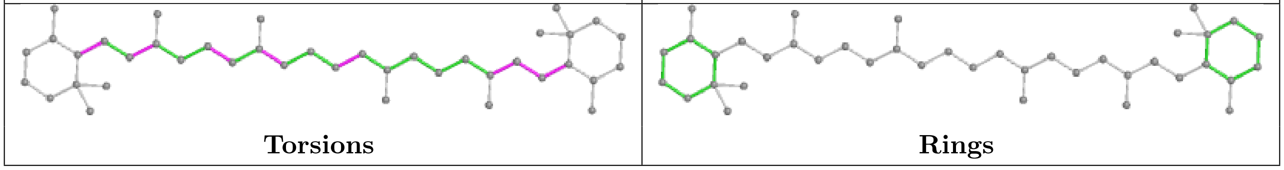
Torsions Rings

Ligand BCR B 845



Bond lengths

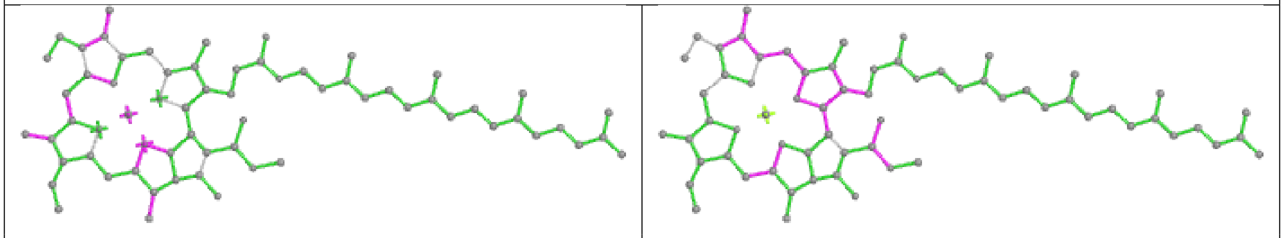
Bond angles



Torsions

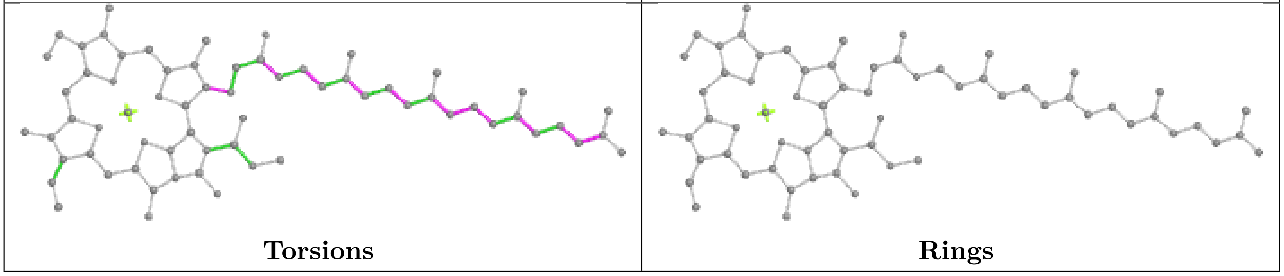
Rings

Ligand CLA a 831



Bond lengths

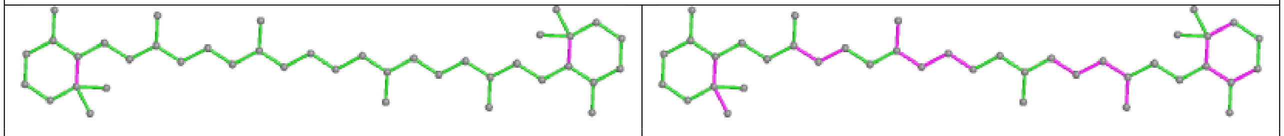
Bond angles



Torsions

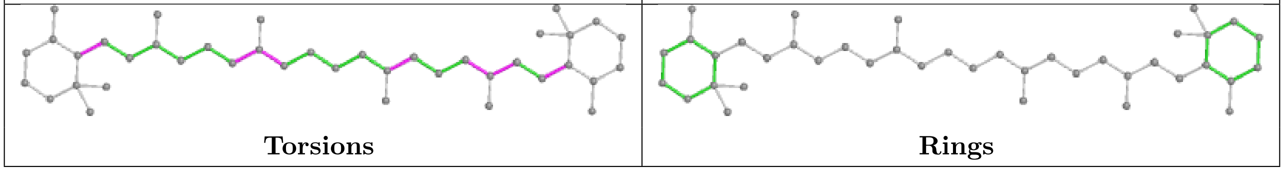
Rings

Ligand BCR l 201



Bond lengths

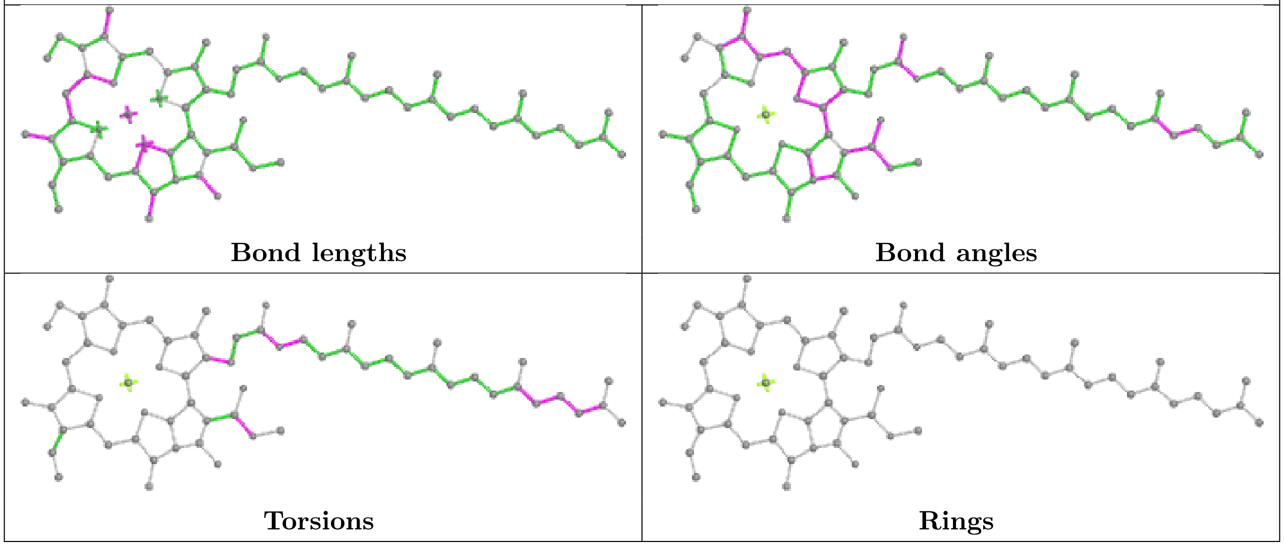
Bond angles



Torsions

Rings

Ligand CLA b 808



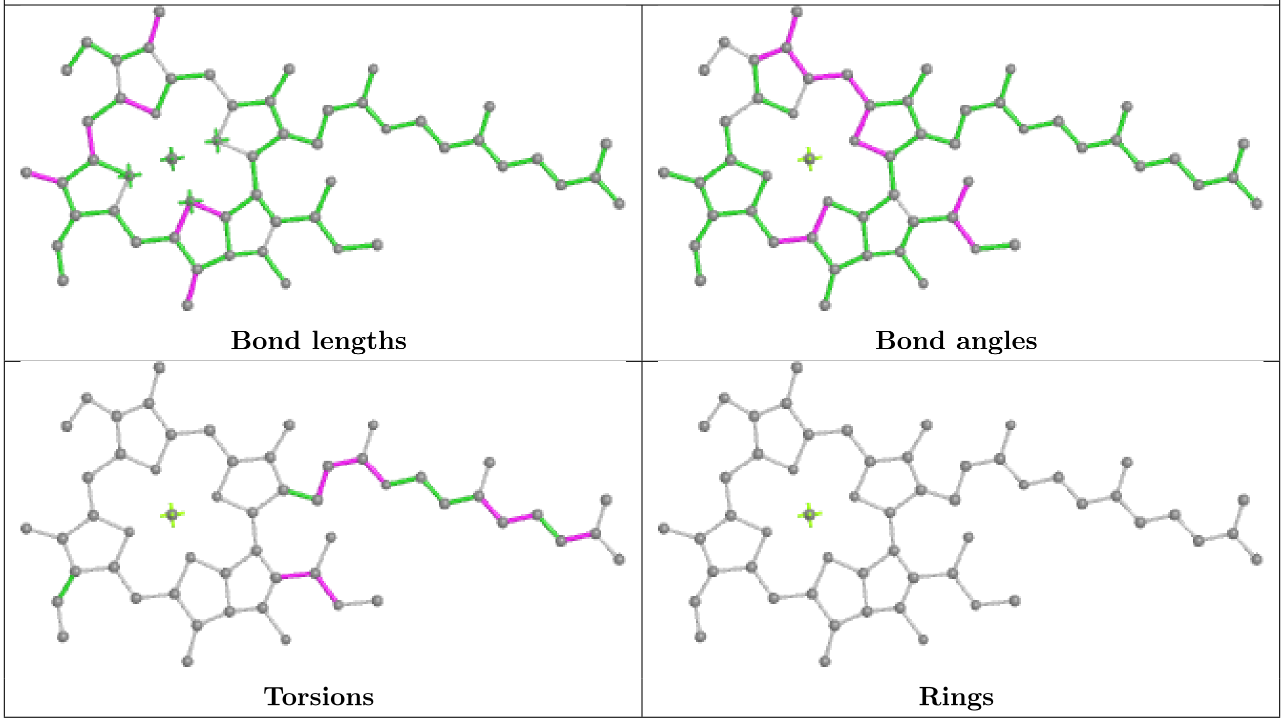
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA b 825



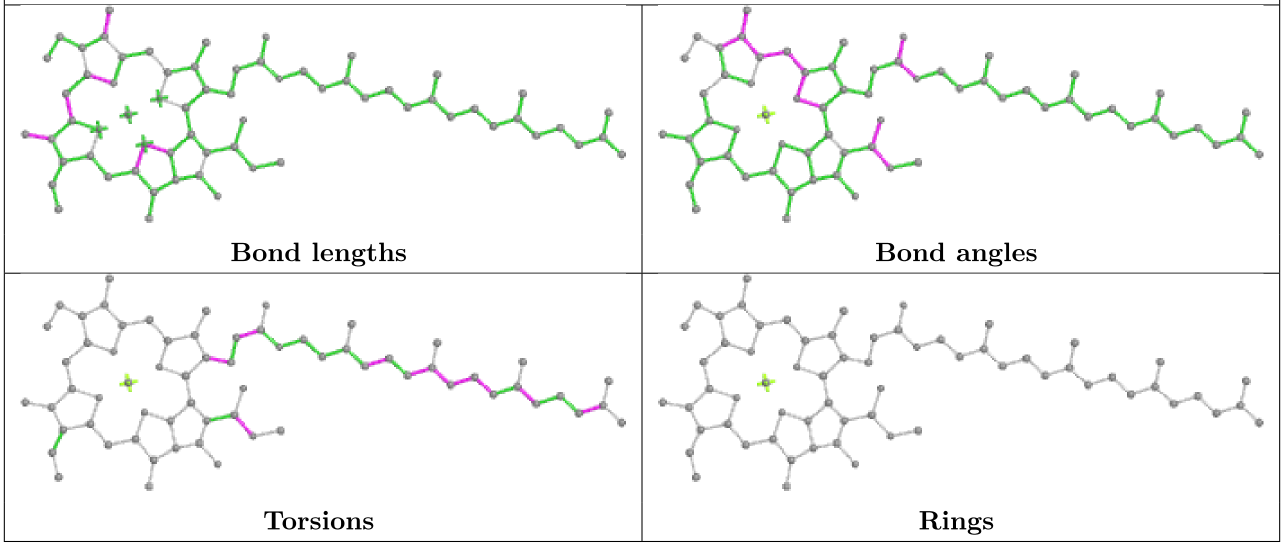
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA A 827



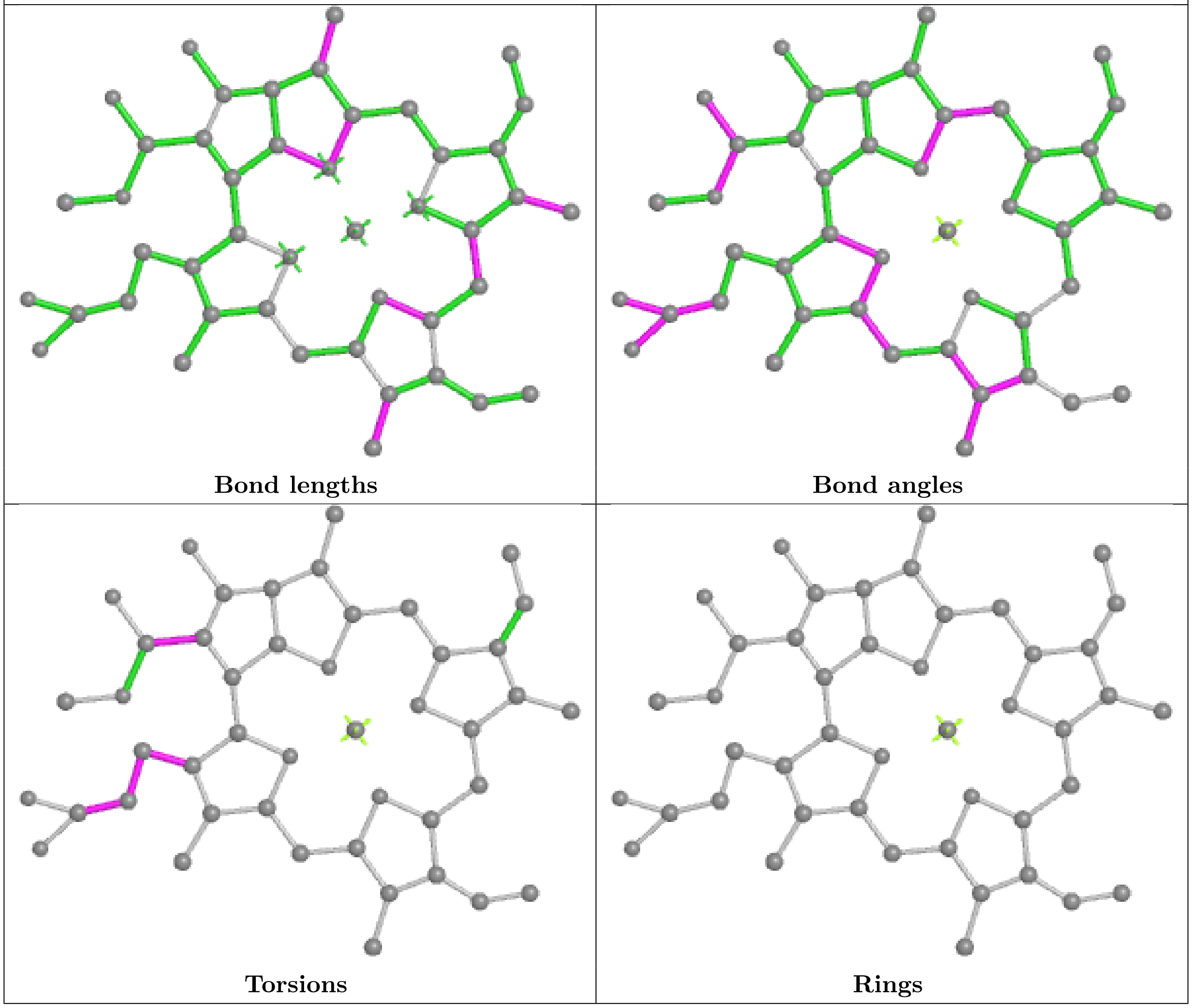
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA a 841



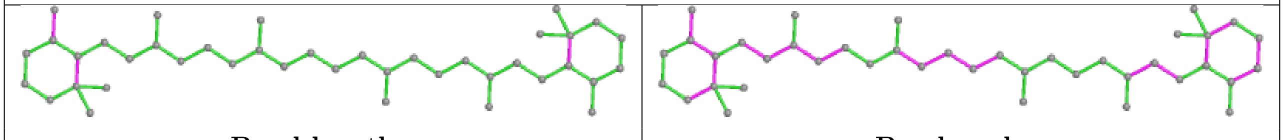
Bond lengths

Bond angles

Torsions

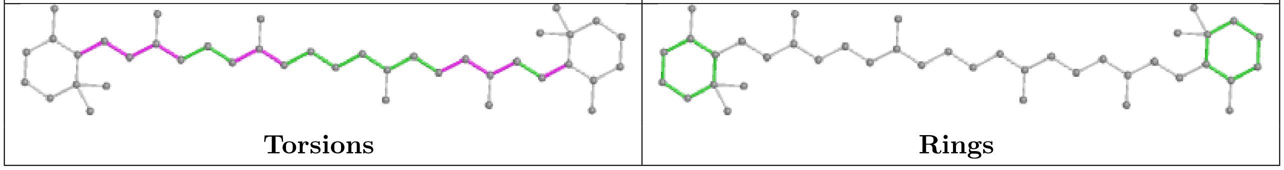
Rings

Ligand BCR J 104



Bond lengths

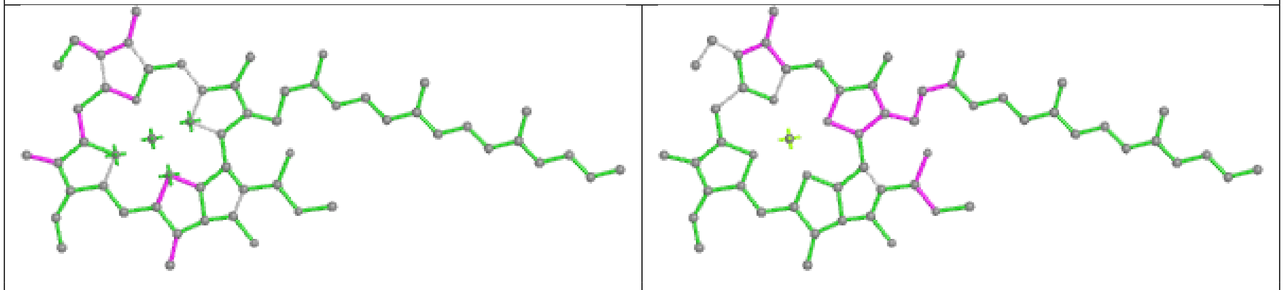
Bond angles



Torsions

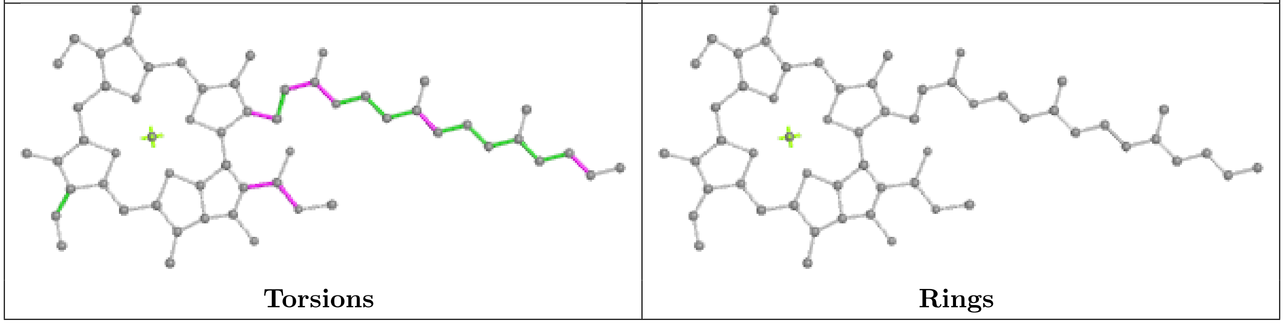
Rings

Ligand CLA B 835



Bond lengths

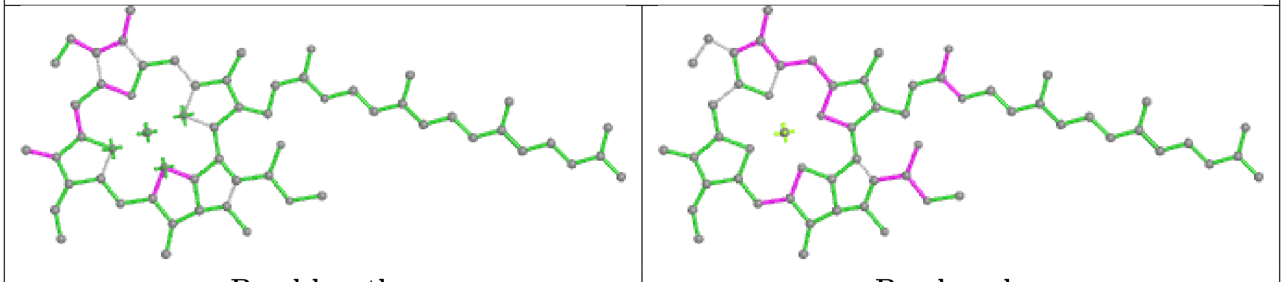
Bond angles



Torsions

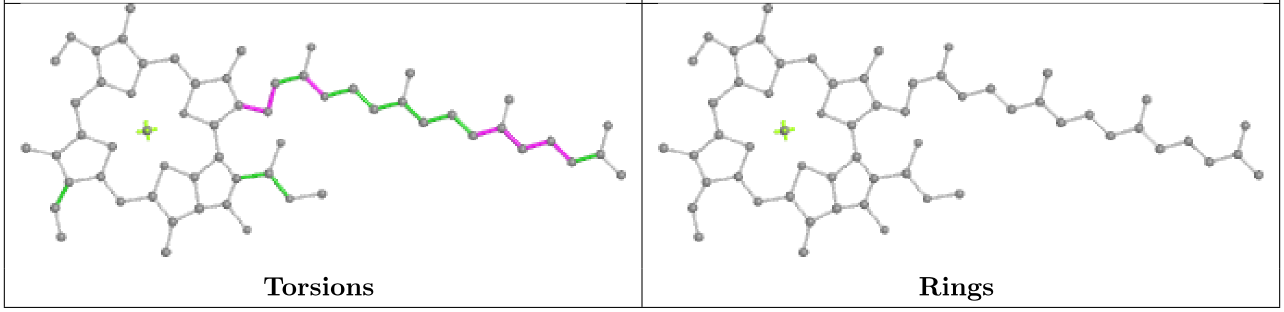
Rings

Ligand CLA l 204



Bond lengths

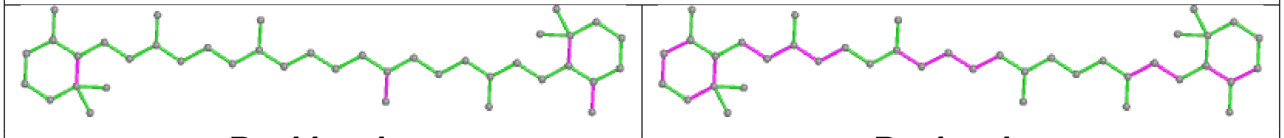
Bond angles



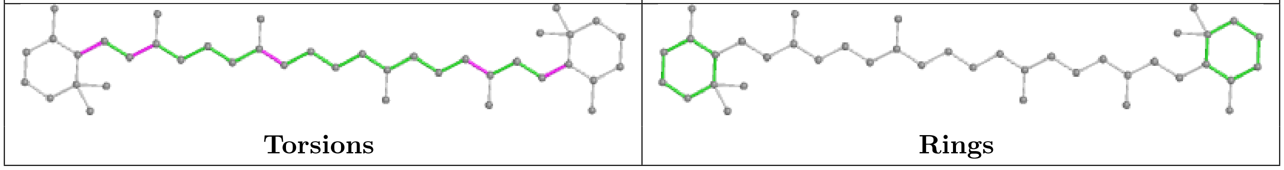
Torsions

Rings

Ligand BCR b 849

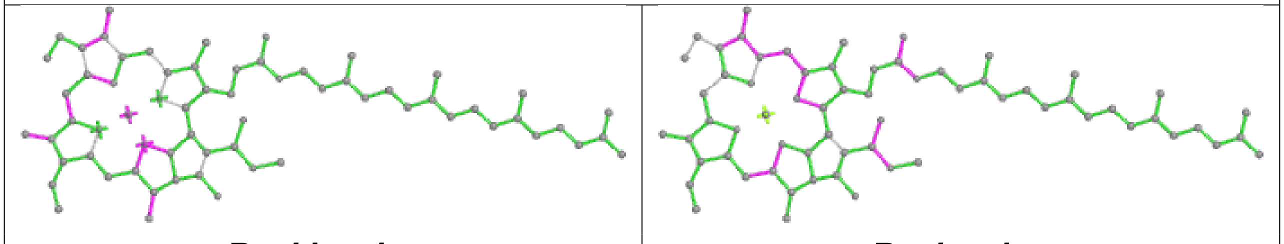


Bond lengths Bond angles

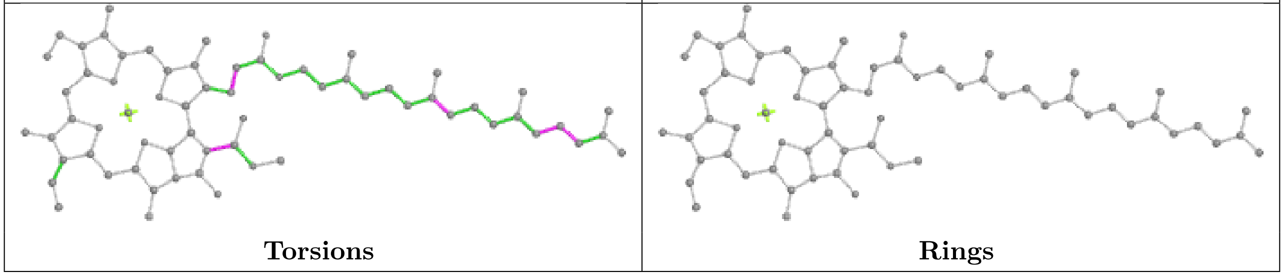


Torsions Rings

Ligand CLA a 840

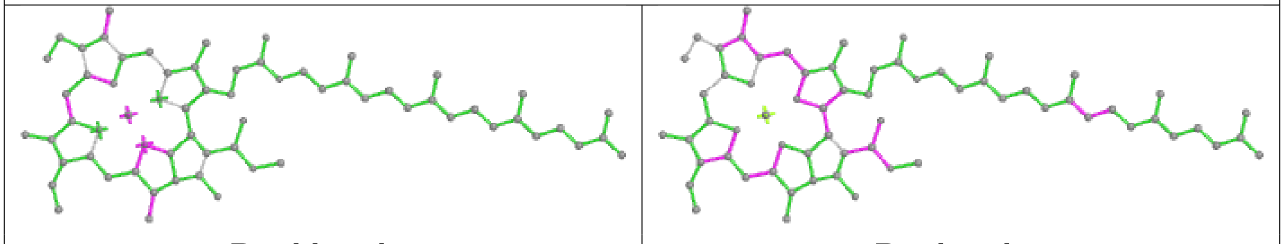


Bond lengths Bond angles

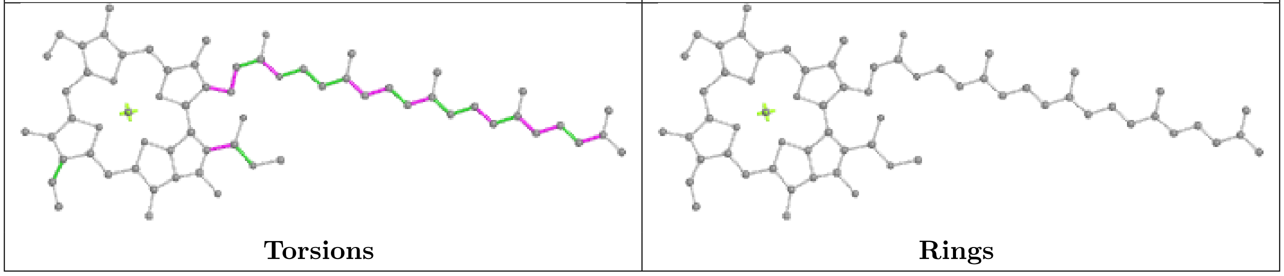


Torsions Rings

Ligand CLA b 805

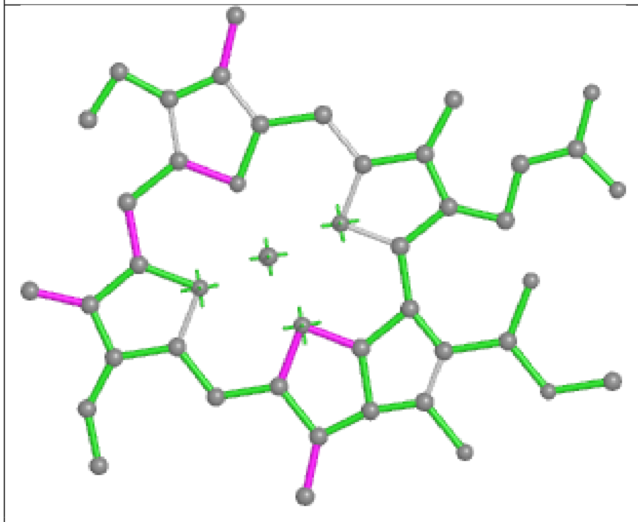


Bond lengths Bond angles

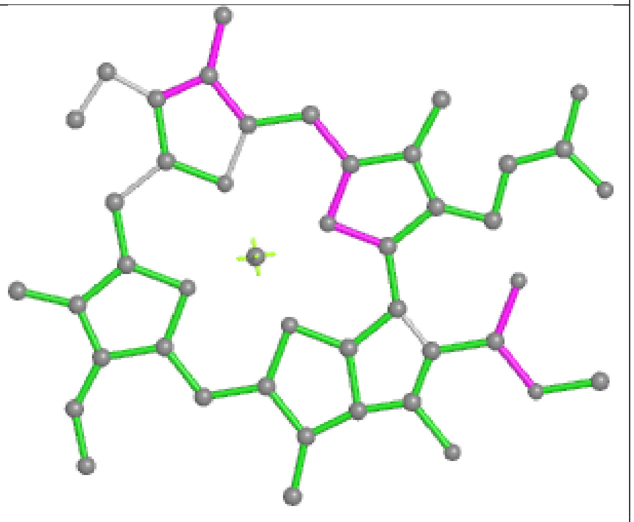


Torsions Rings

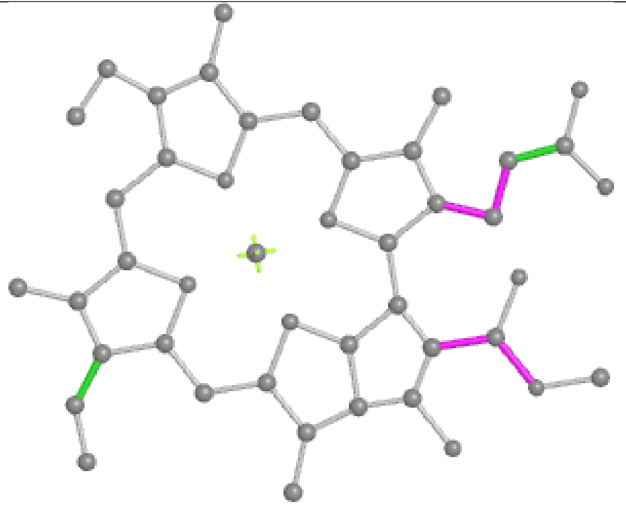
Ligand CLA a 809



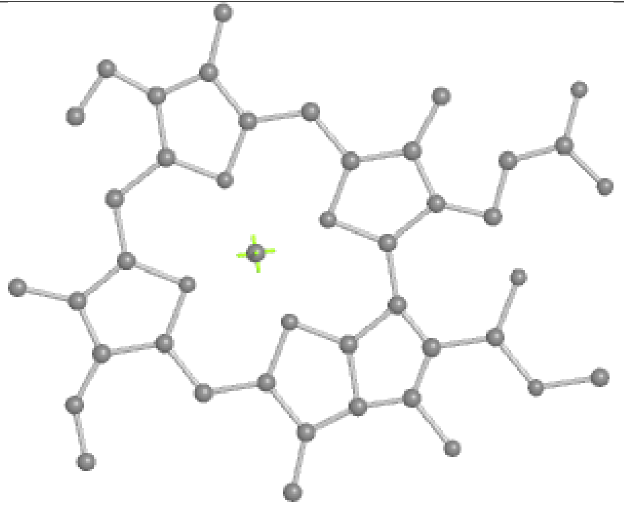
Bond lengths



Bond angles

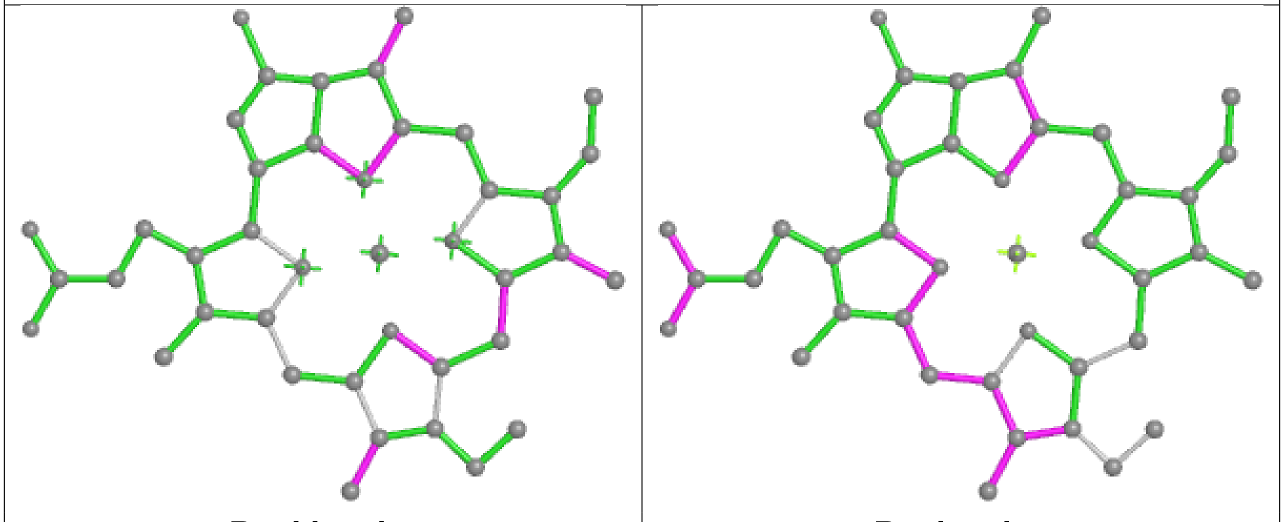


Torsions

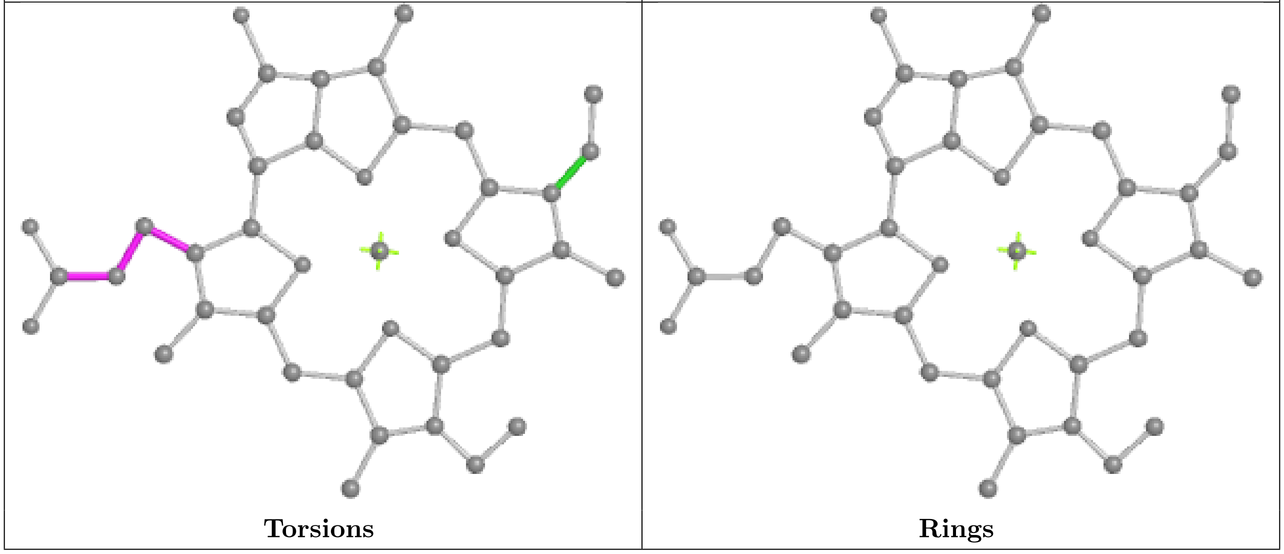


Rings

Ligand CLA K 101

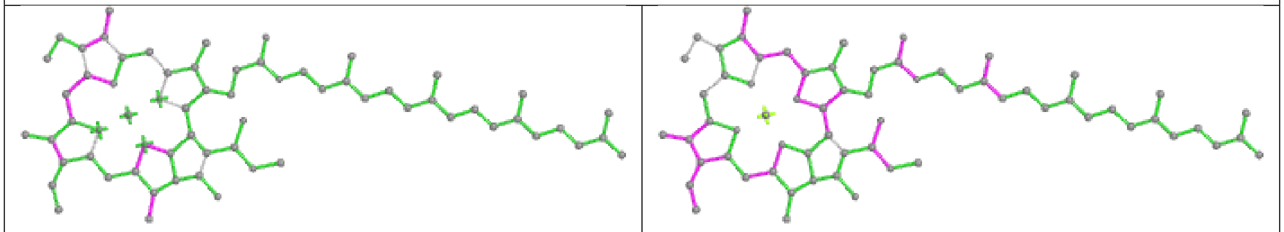


Bond lengths Bond angles

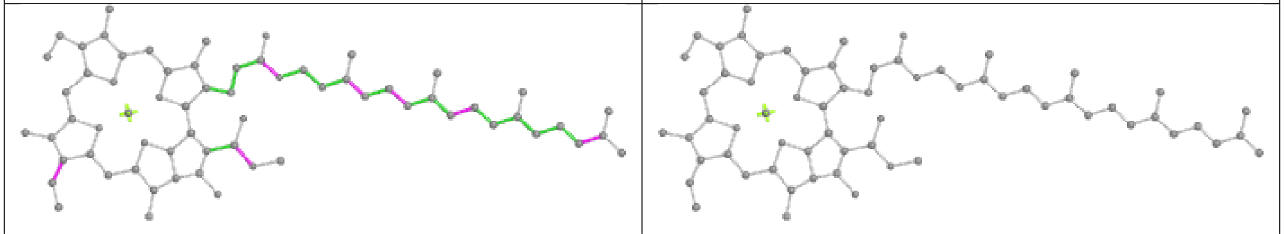


Torsions Rings

Ligand CLA b 843

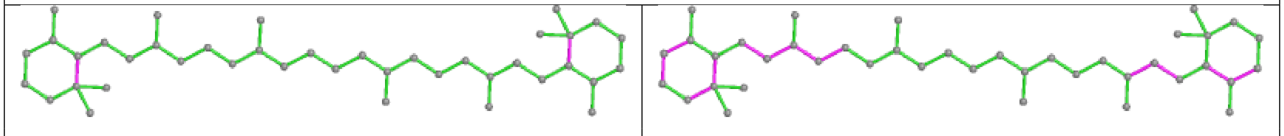


Bond lengths Bond angles

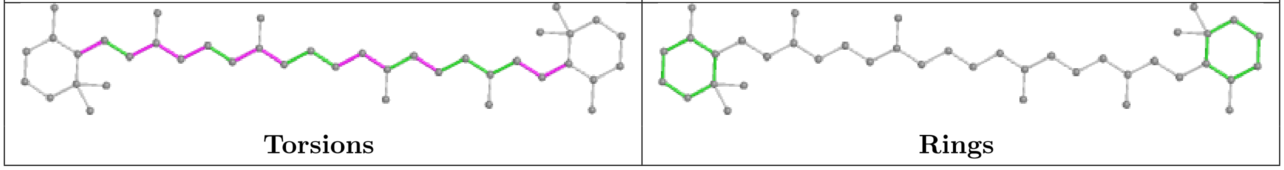


Torsions Rings

Ligand BCR j 106

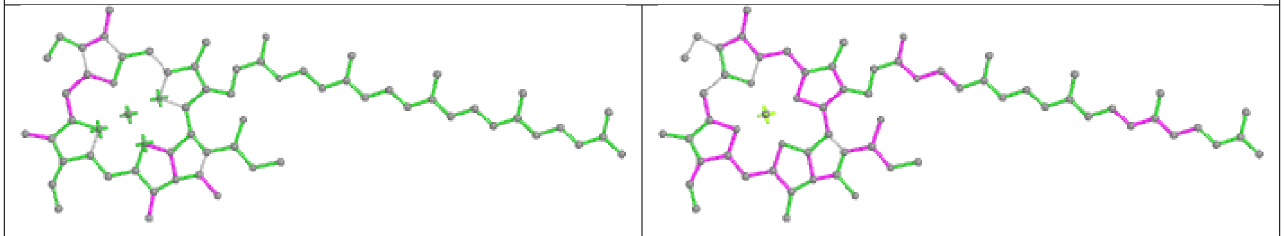


Bond lengths Bond angles

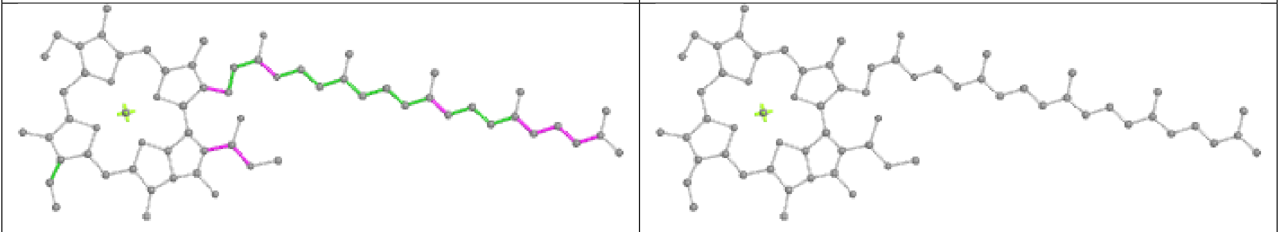


Torsions Rings

Ligand CLA B 808

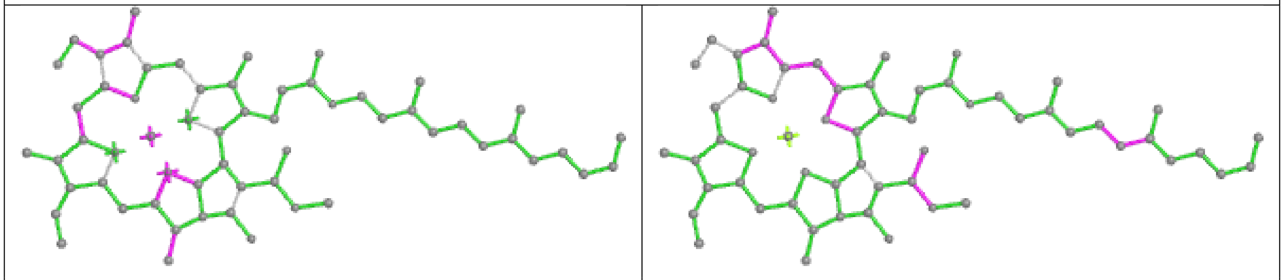


Bond lengths Bond angles

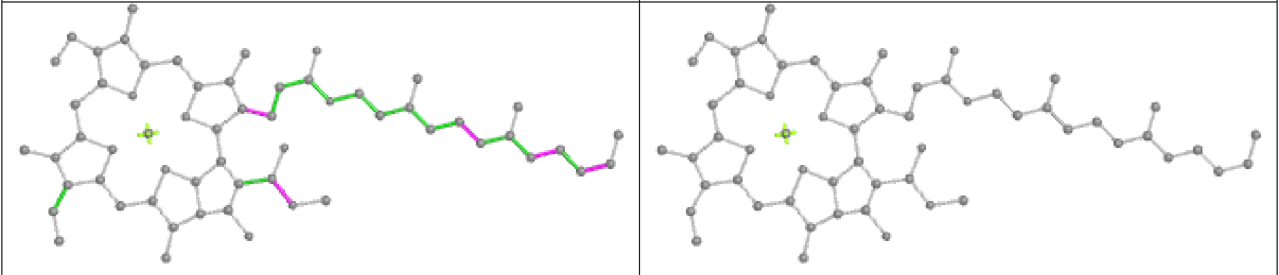


Torsions Rings

Ligand CLA A 840

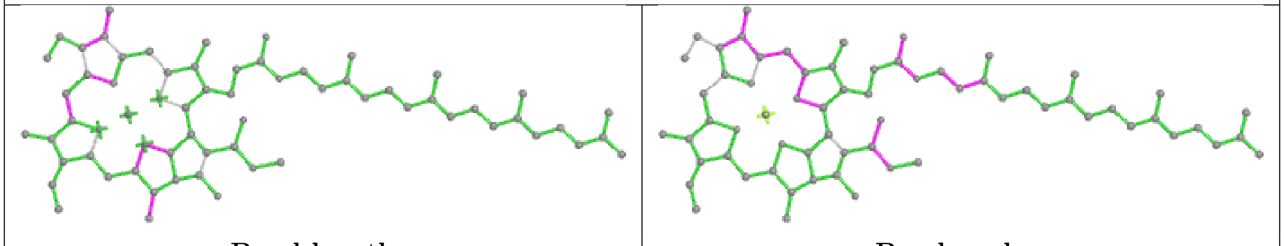


Bond lengths Bond angles



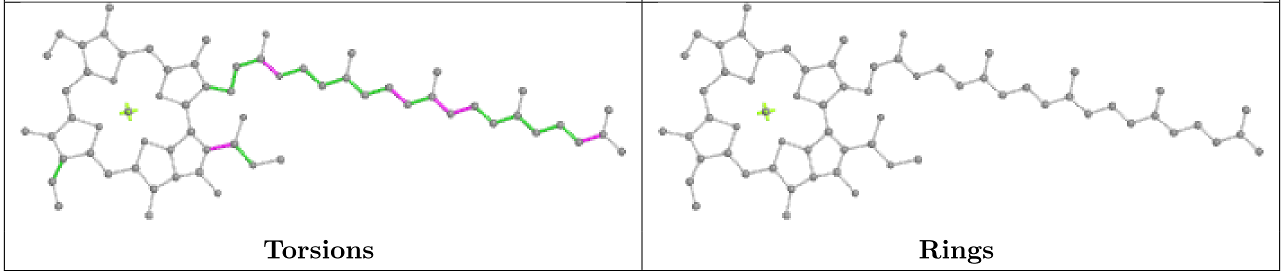
Torsions Rings

Ligand CLA B 822



Bond lengths

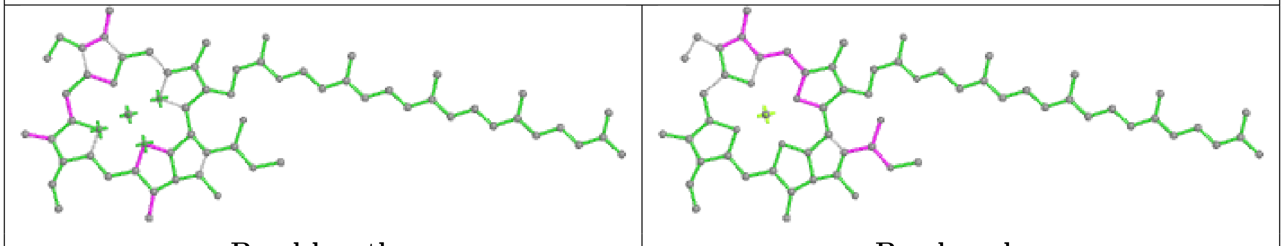
Bond angles



Torsions

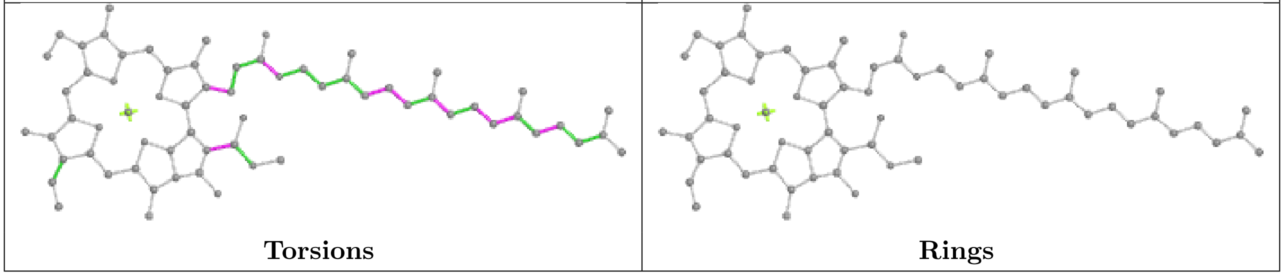
Rings

Ligand CLA a 838



Bond lengths

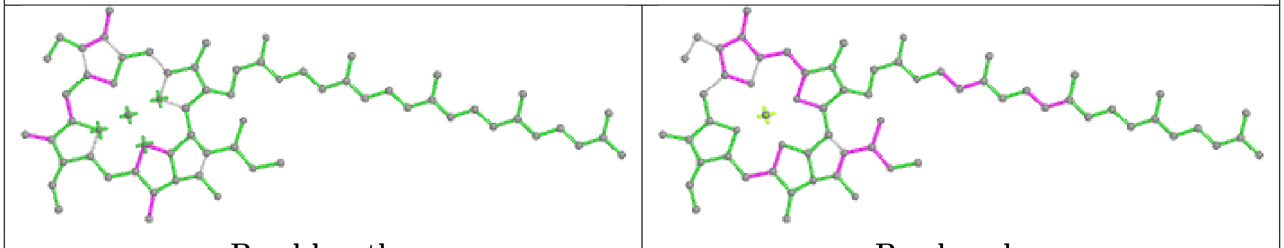
Bond angles



Torsions

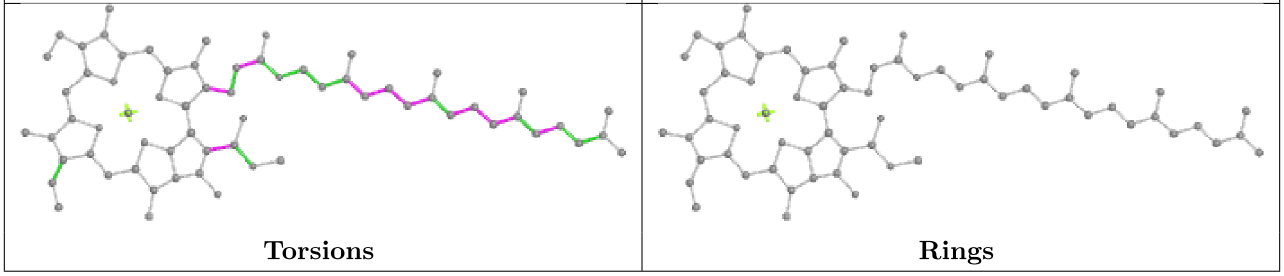
Rings

Ligand CLA b 835



Bond lengths

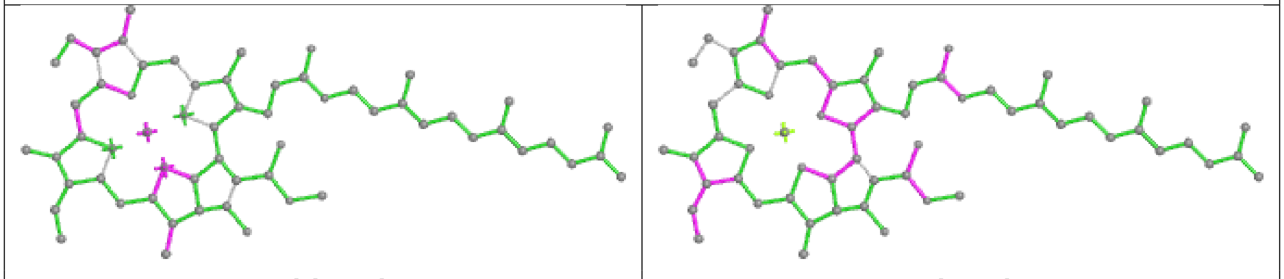
Bond angles



Torsions

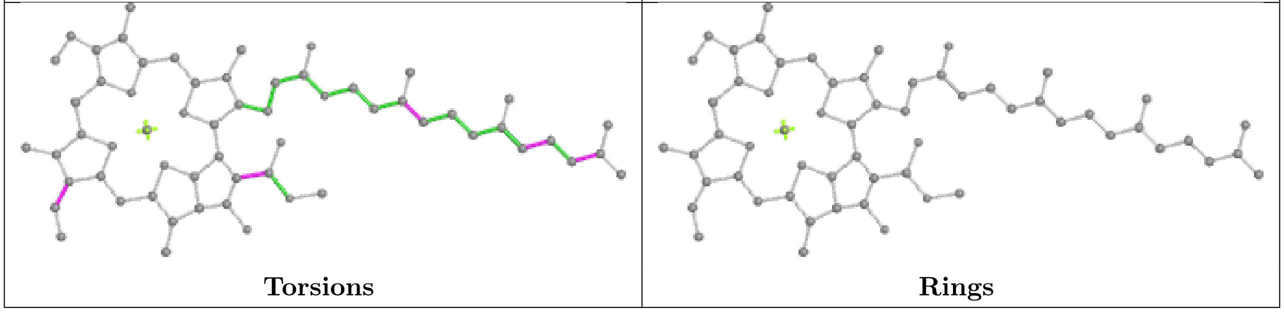
Rings

Ligand CLA b 839



Bond lengths

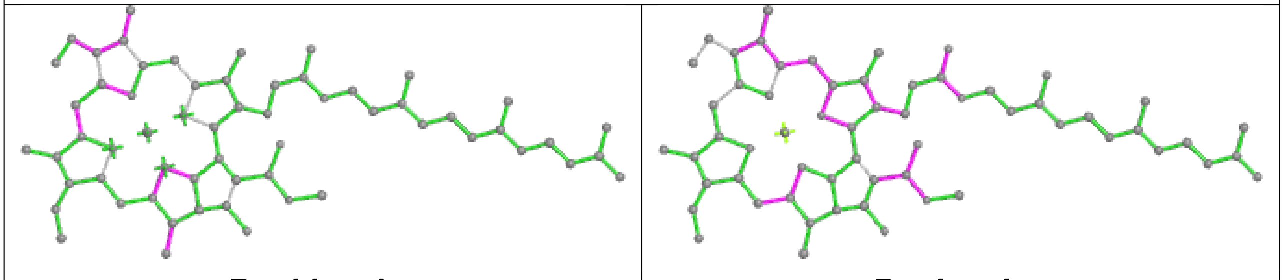
Bond angles



Torsions

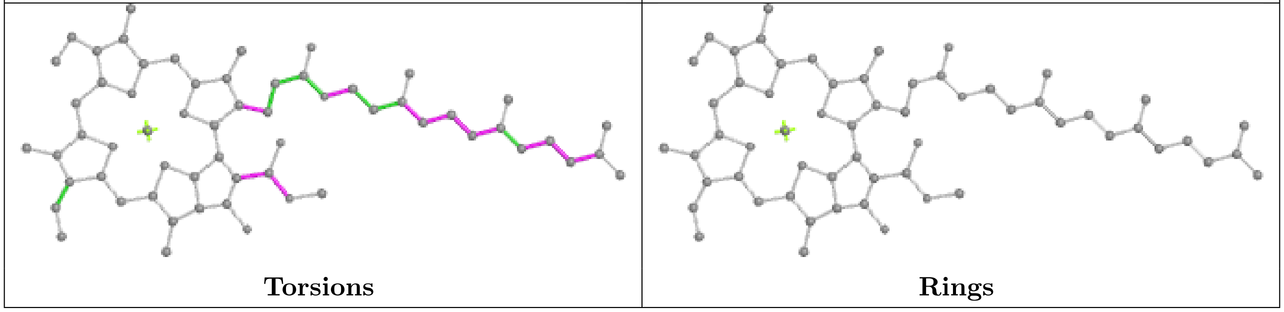
Rings

Ligand CLA A 807



Bond lengths

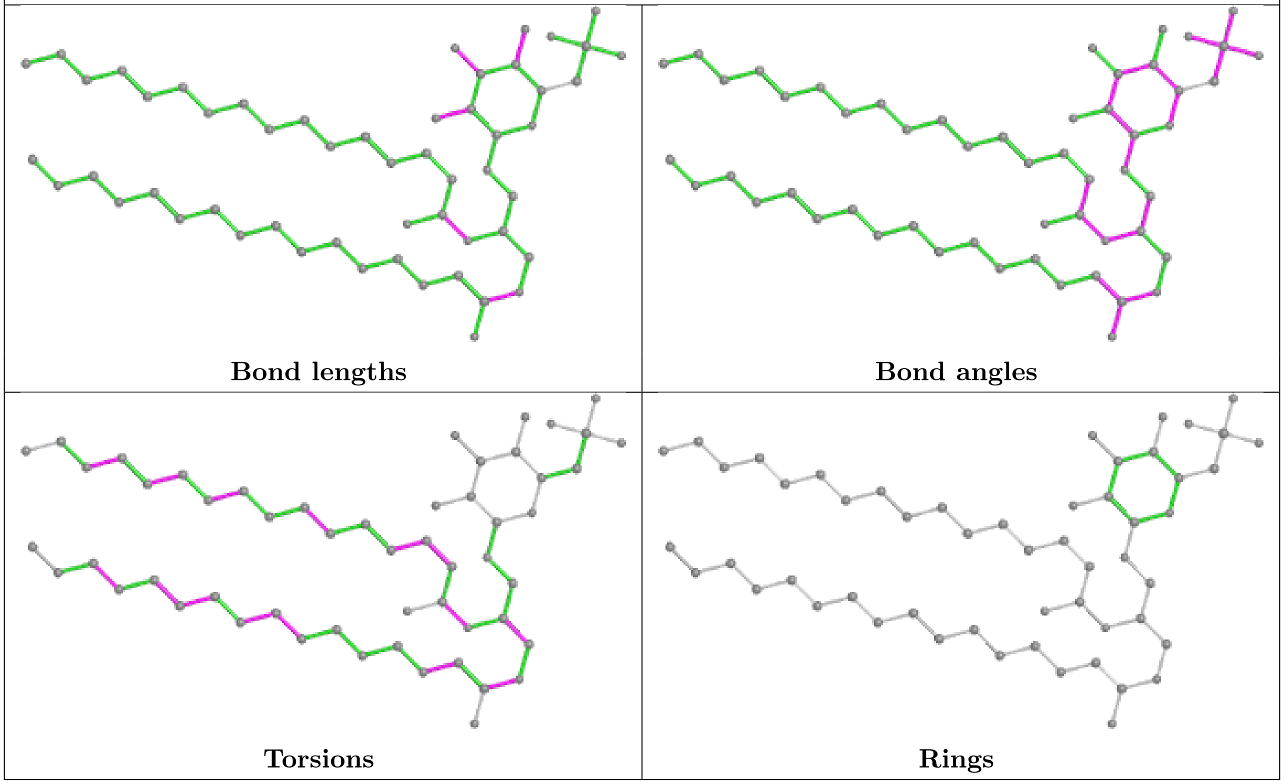
Bond angles



Torsions

Rings

Ligand SQD X 1702



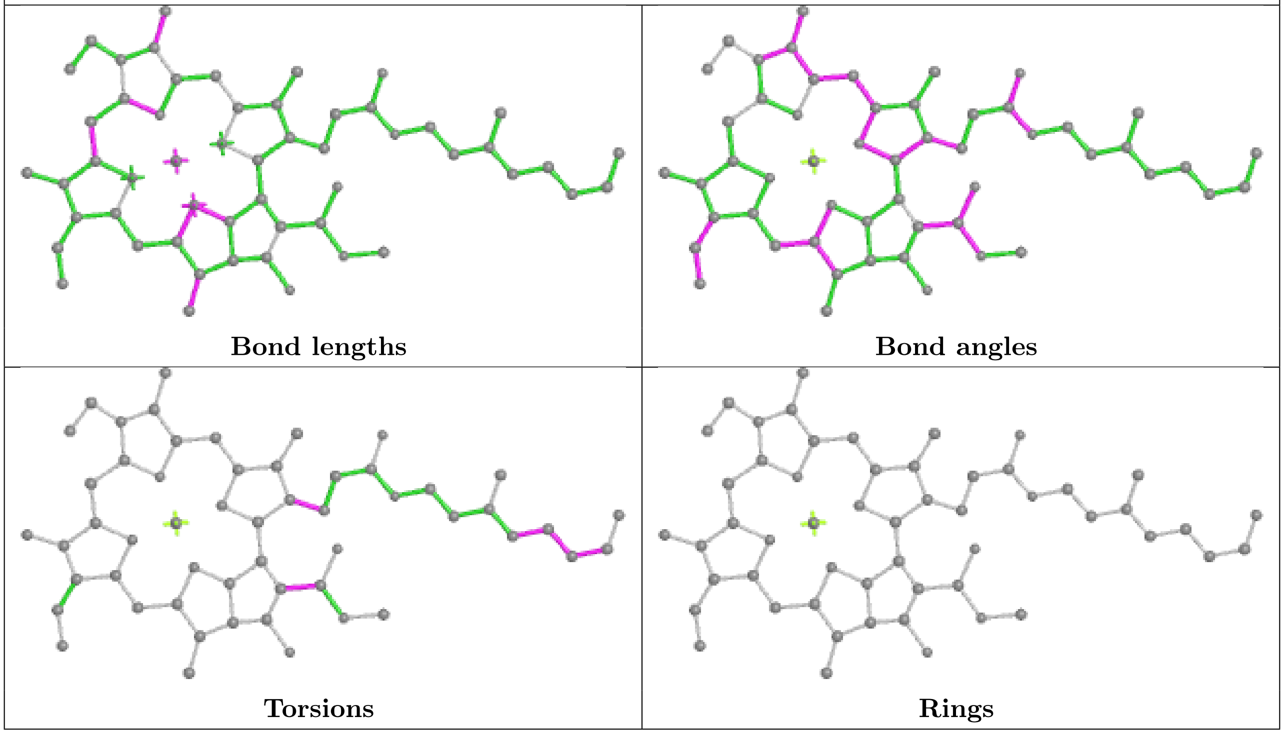
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA A 826



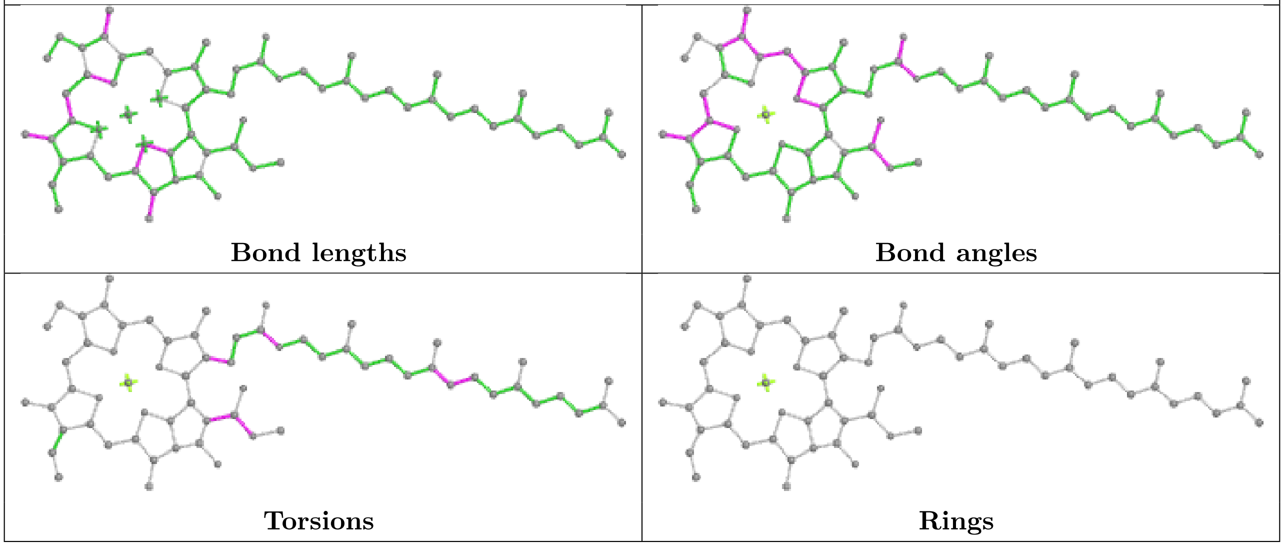
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA b 822



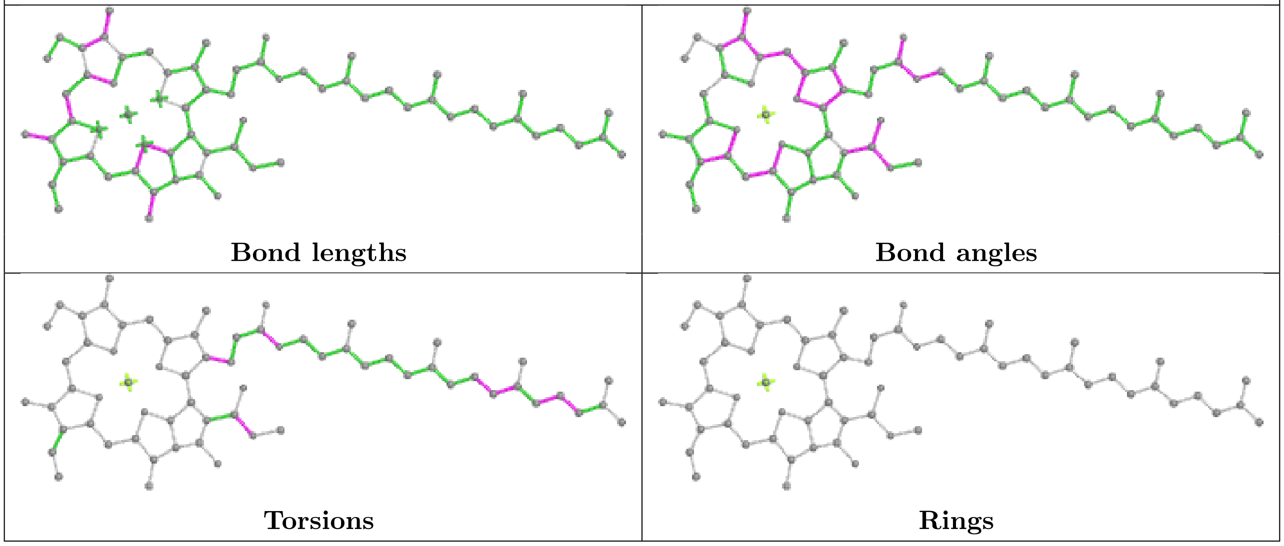
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA A 811



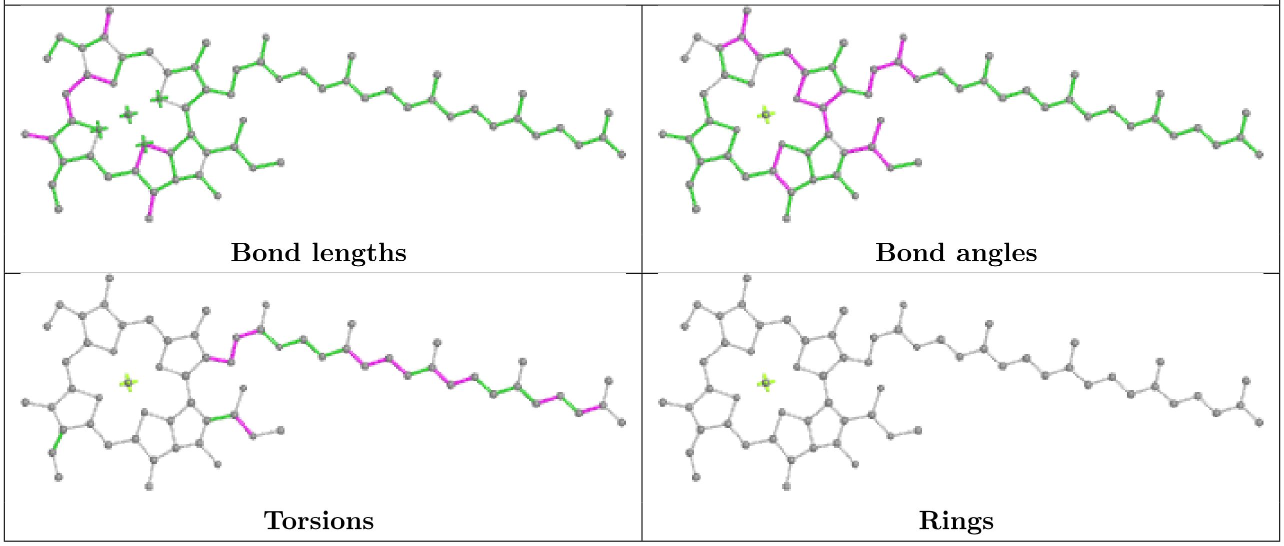
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA a 808



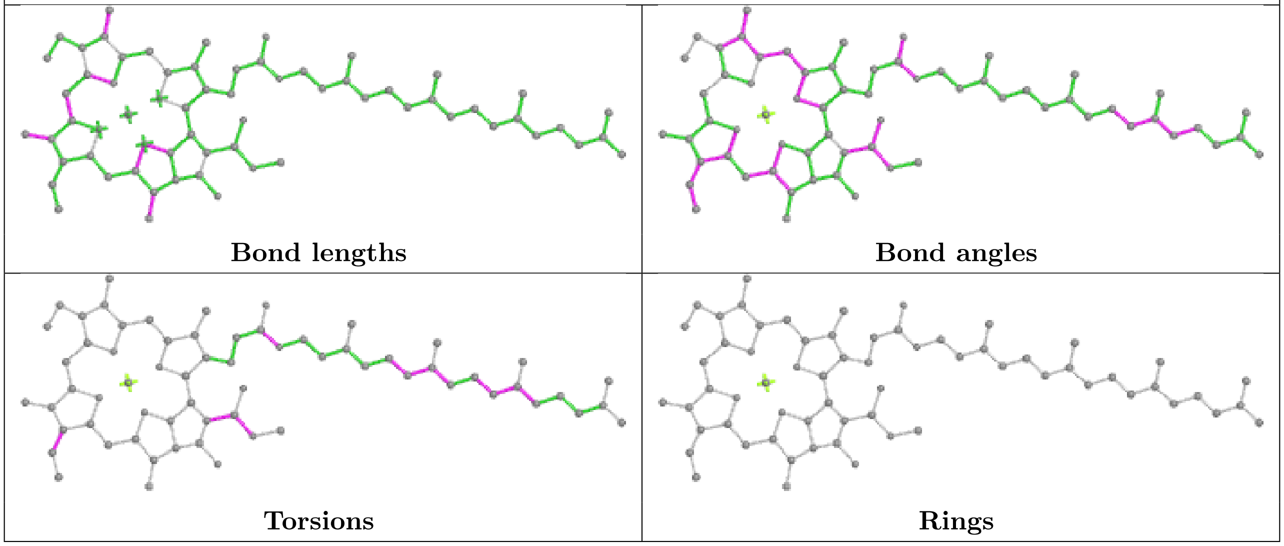
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA a 833



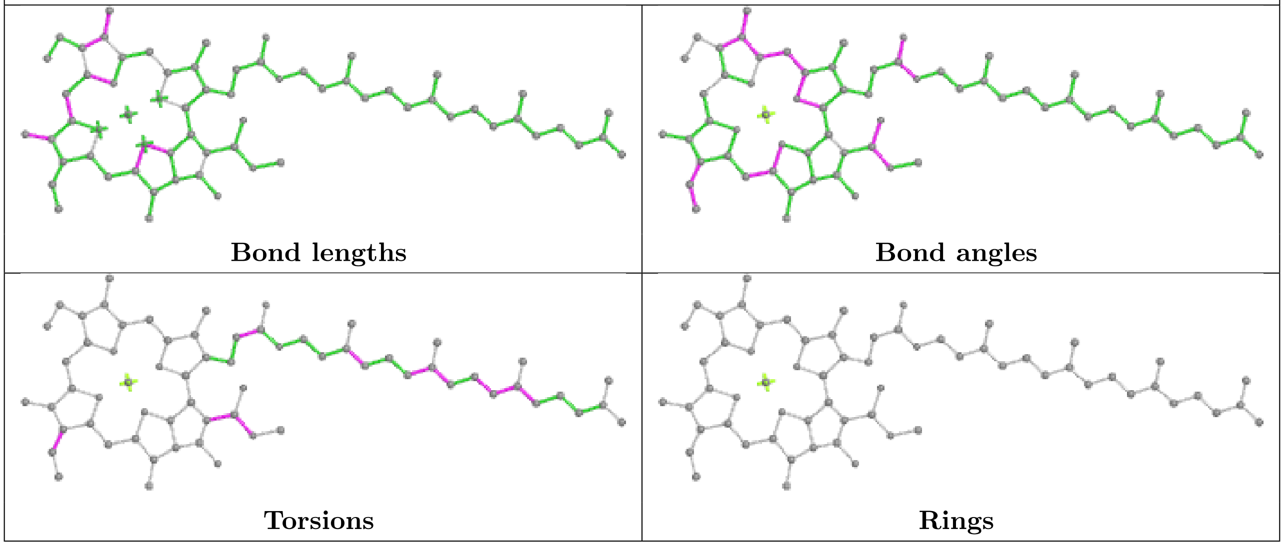
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA F 202



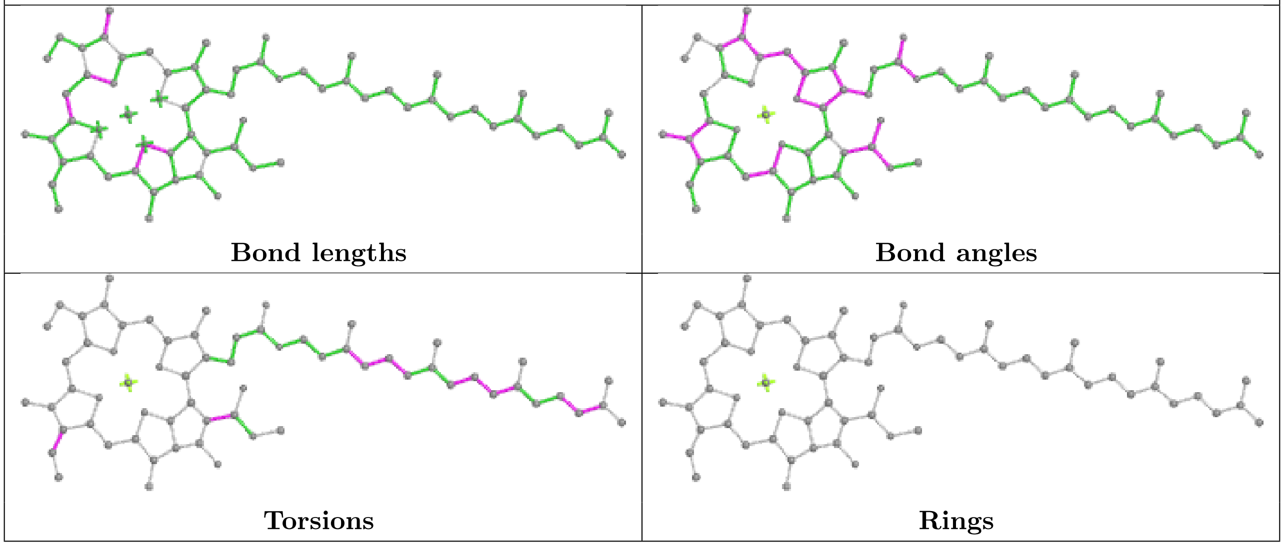
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA b 828



Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

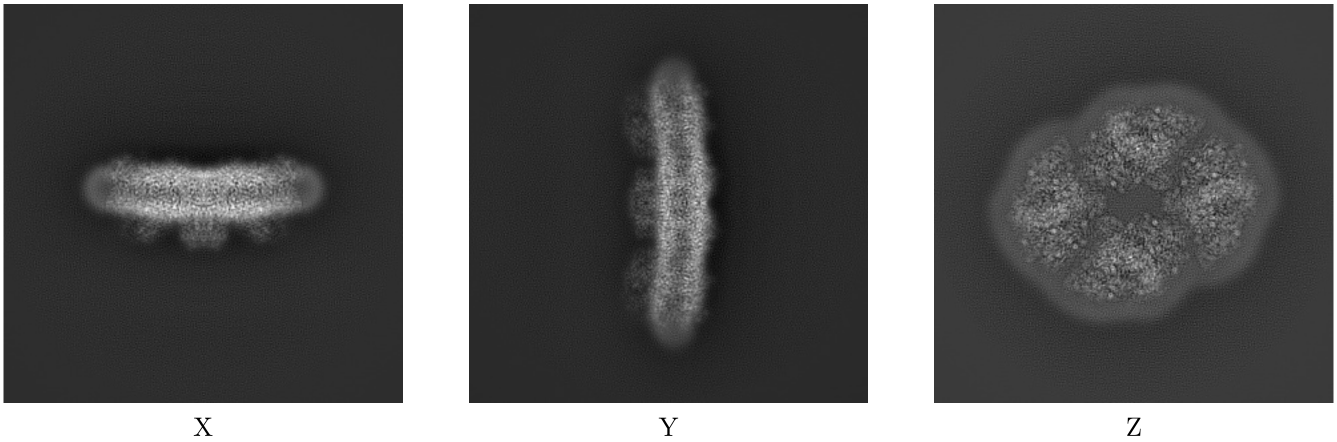
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-9918. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections (i)

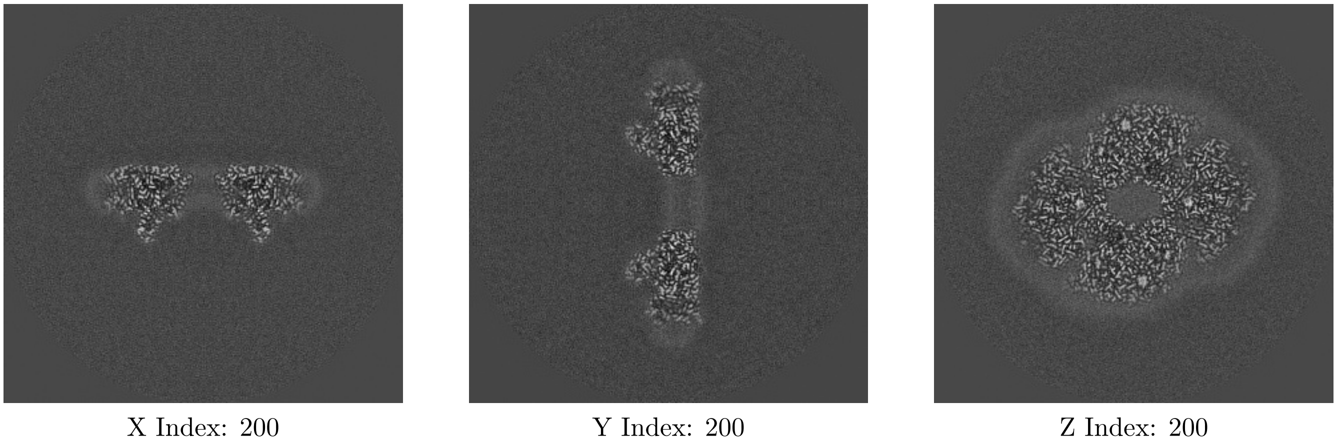
6.1.1 Primary map


X Y Z

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

6.2 Central slices (i)

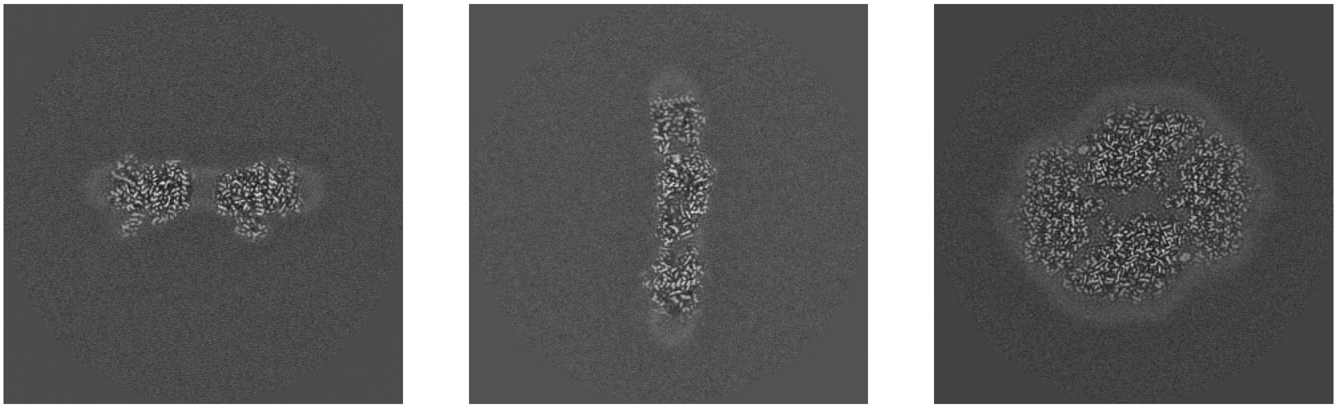
6.2.1 Primary map


X Index: 200 Y Index: 200 Z Index: 200

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

6.3 Largest variance slices ⓘ

6.3.1 Primary map

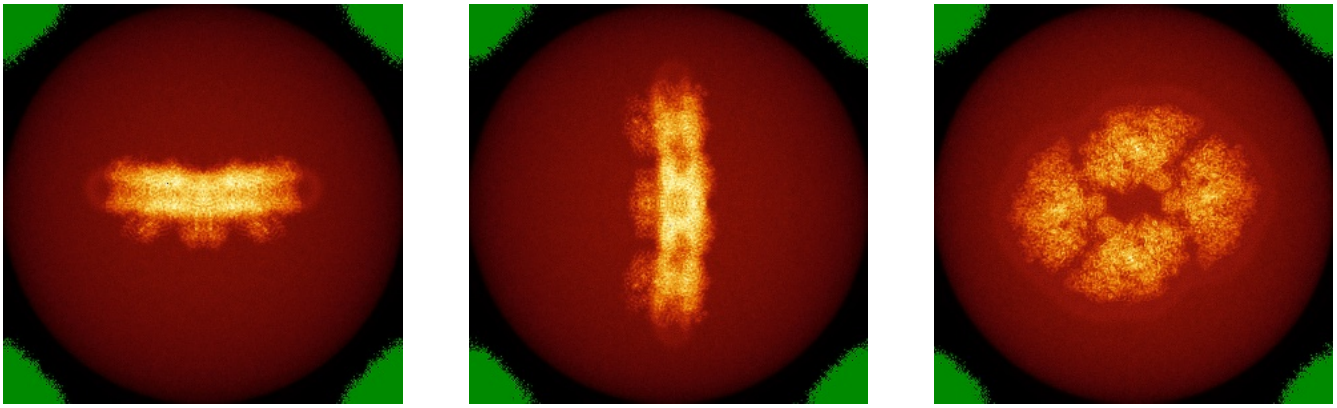


X Index: 219 Y Index: 171 Z Index: 223

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

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

6.4.1 Primary map

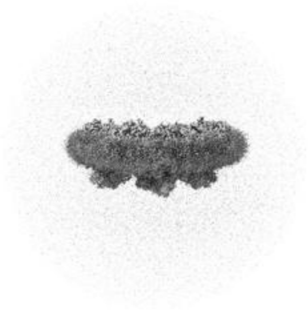


X Y Z

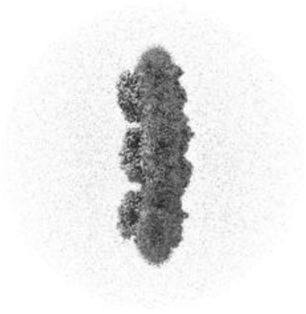
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views ⓘ

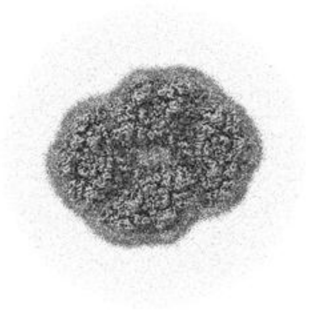
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.019. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

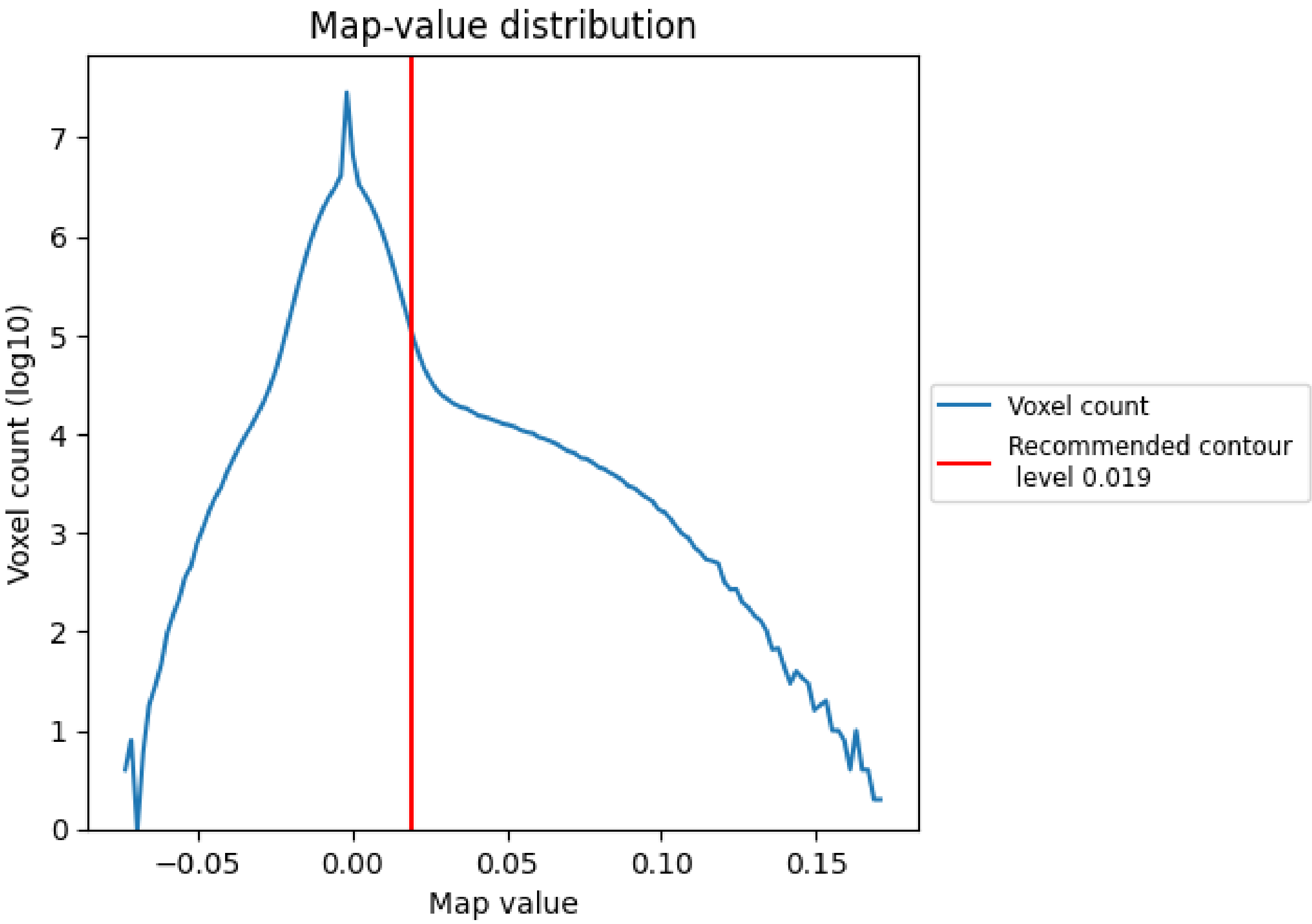
6.6 Mask visualisation ⓘ

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

7 Map analysis (i)

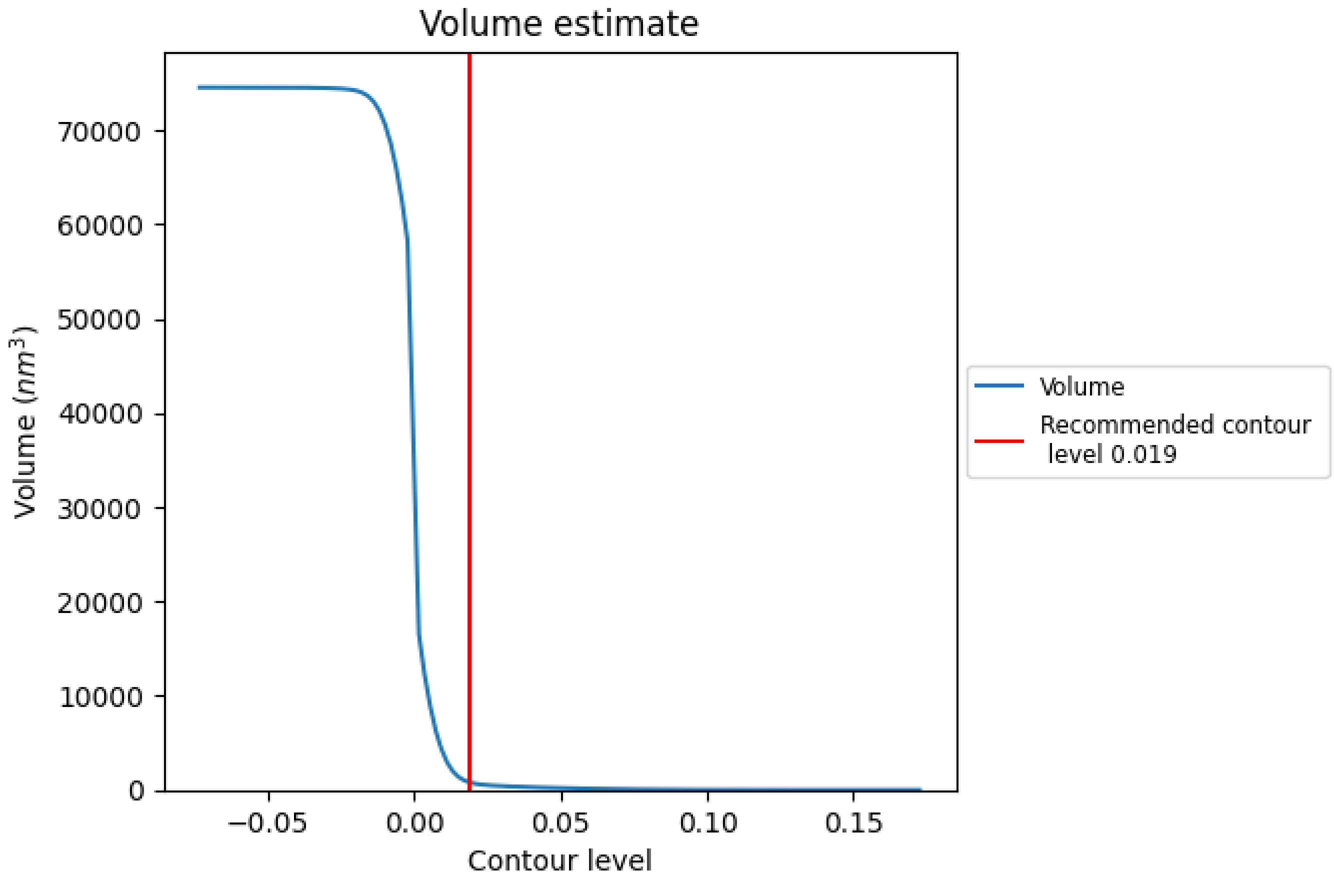
This section contains the results of statistical analysis of the map.

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.

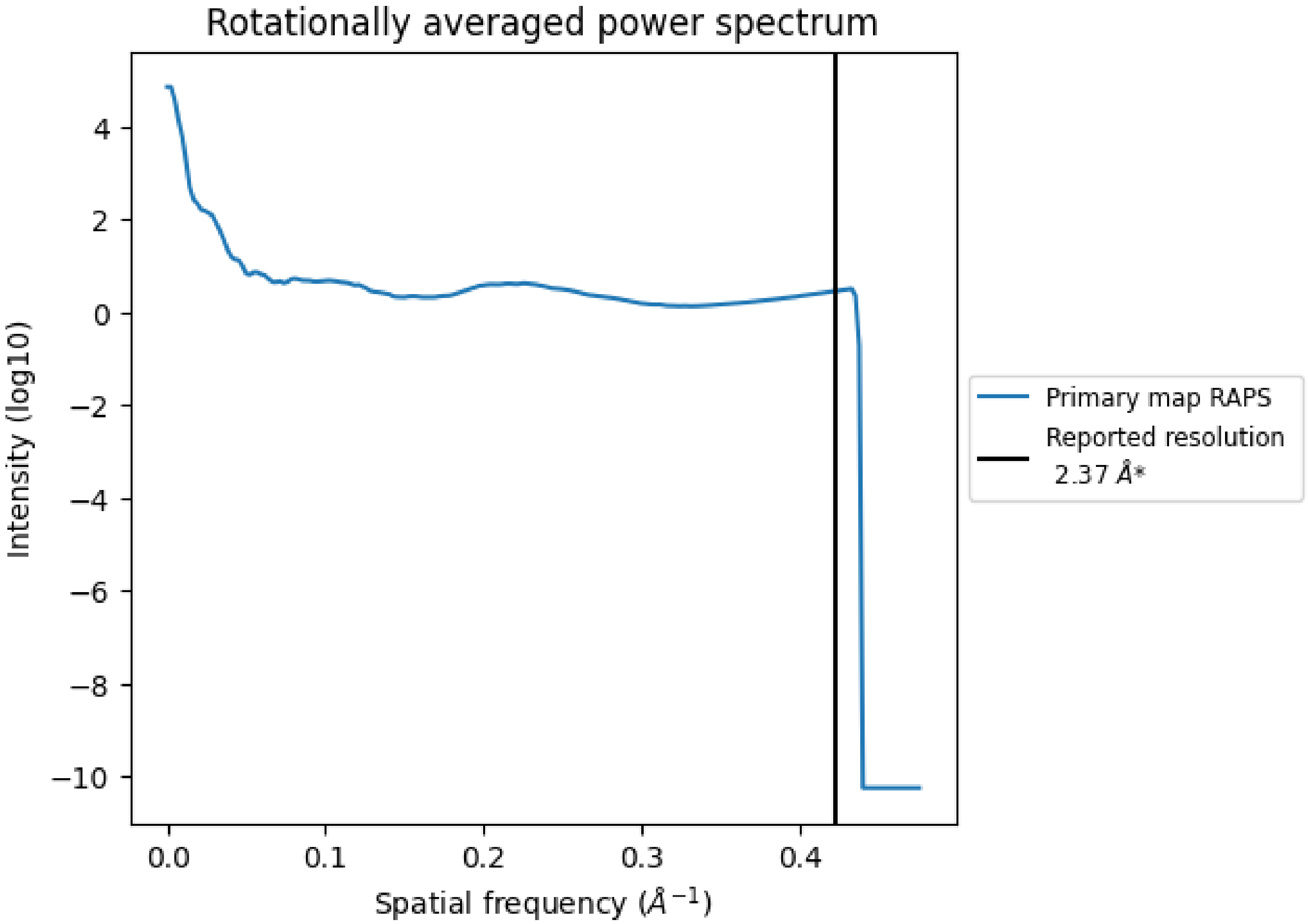
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 790 nm^3; this corresponds to an approximate mass of 714 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 0.422 Å^{-1}

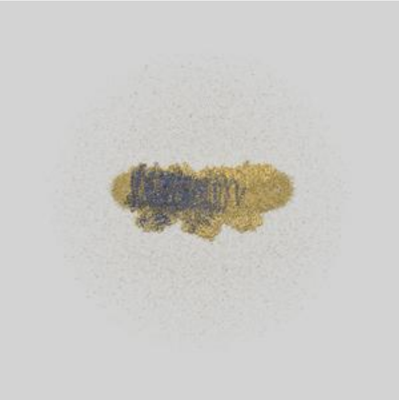
8 Fourier-Shell correlation ⓘ

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

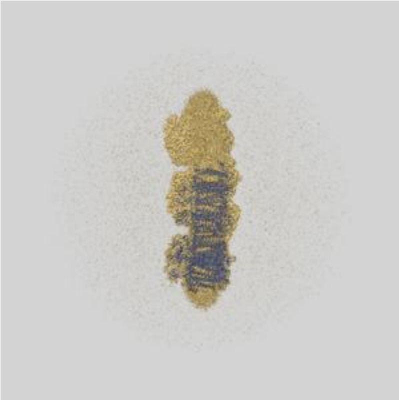
9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-9918 and PDB model 6K61. Per-residue inclusion information can be found in section 3 on page 28.

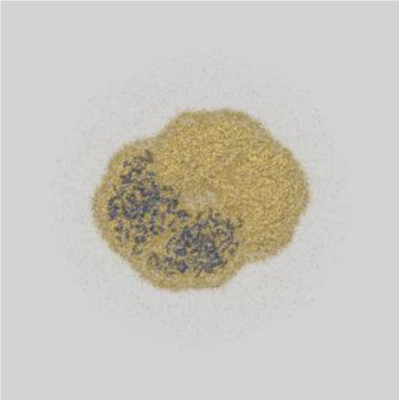
9.1 Map-model overlay ⓘ



X



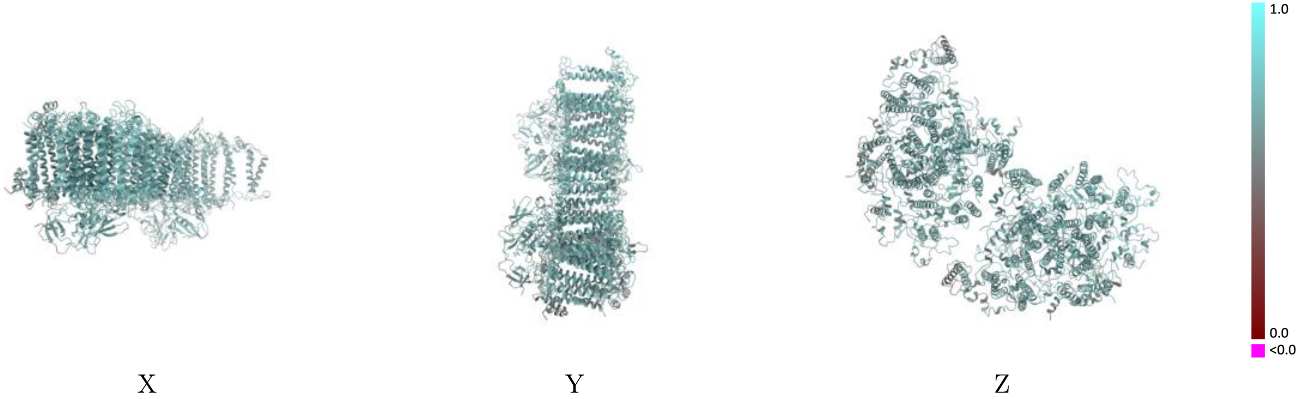
Y



Z

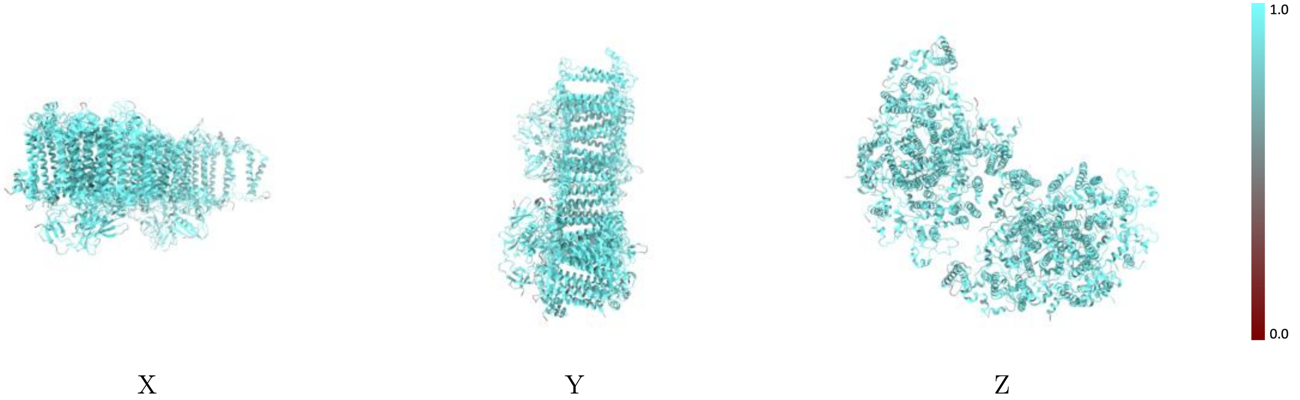
The images above show the 3D surface view of the map at the recommended contour level 0.019 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model ⓘ



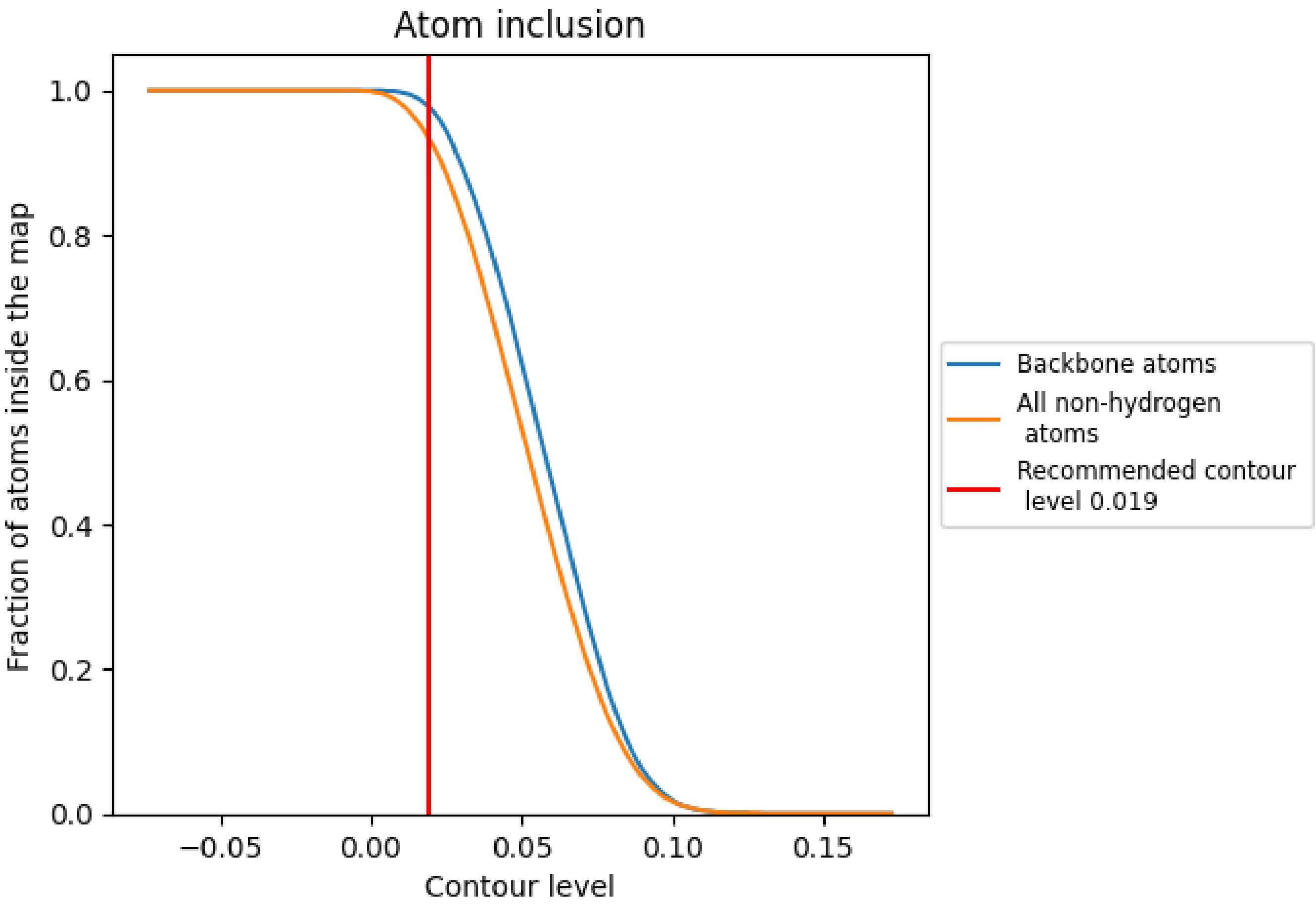
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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 (0.019).

9.4 Atom inclusion ⓘ



At the recommended contour level, 98% of all backbone atoms, 94% 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 (0.019) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9350	0.6500
A	0.9500	0.6610
B	0.9670	0.6840
C	0.9600	0.6560
D	0.9190	0.6340
E	0.8790	0.5980
F	0.8910	0.6090
I	0.9600	0.6630
J	0.9220	0.6240
K	0.7810	0.5180
L	0.9470	0.6660
M	0.9380	0.6720
X	0.8740	0.6140
a	0.9410	0.6510
b	0.9500	0.6590
c	0.9630	0.6480
d	0.9070	0.6180
e	0.8470	0.5610
f	0.8470	0.5680
i	0.9140	0.6670
j	0.8710	0.5820
k	0.7880	0.5380
l	0.9300	0.6700
m	0.9480	0.6580
x	0.7690	0.5330