wwPDB EM Validation Summary Report ⓘ

Nov 14, 2022 – 02:04 PM JST

PDB ID	:	6JEO
EMDB ID	:	EMD-9807
Title	:	Structure of PSI tetramer from Anabaena
Authors	:	Kato, K.; Nagao, R.; Shen, J.R.; Miyazaki, N.; Akita, F.
Deposited on	:	2019-02-06
Resolution	:	3.30 Å(reported)
Based on initial model	:	1JB0

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

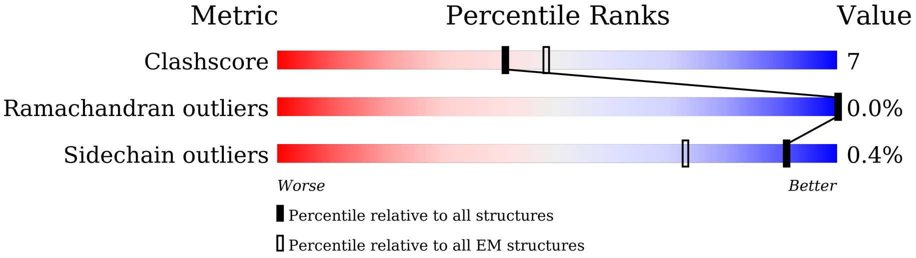
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

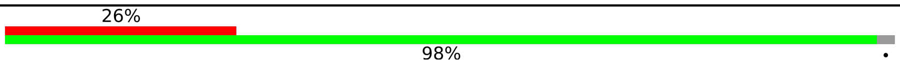
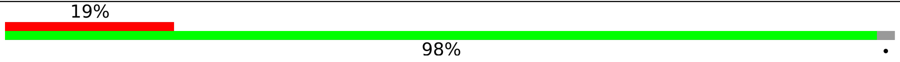
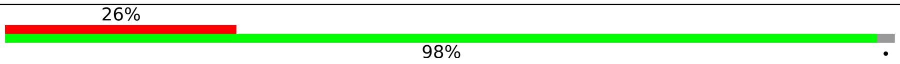
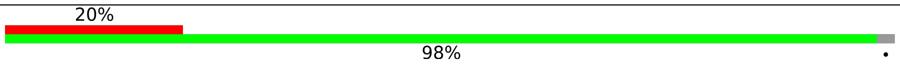
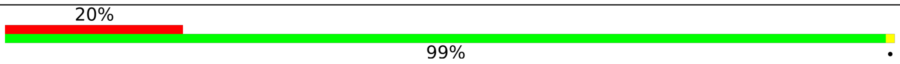
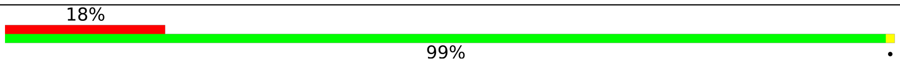
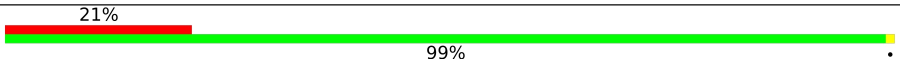
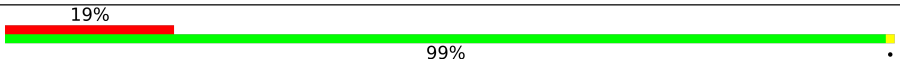
The reported resolution of this entry is 3.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



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

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

Mol	Chain	Length	Quality of chain
1	aA	752	
1	bA	752	
1	cA	752	
1	dA	752	
2	aB	741	
2	bB	741	
2	cB	741	
2	dB	741	

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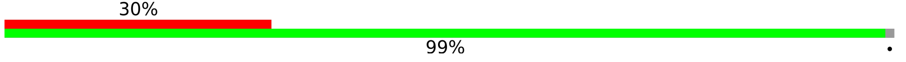
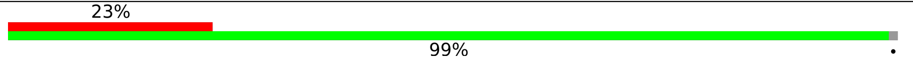
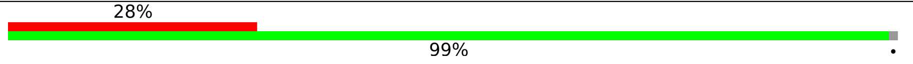
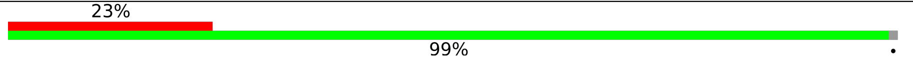
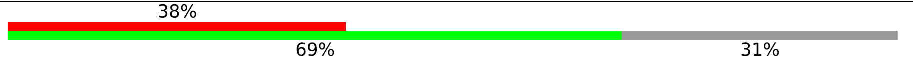
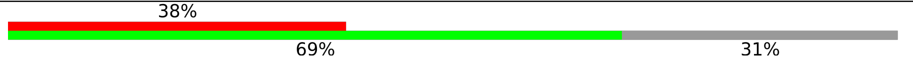
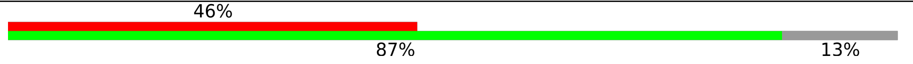
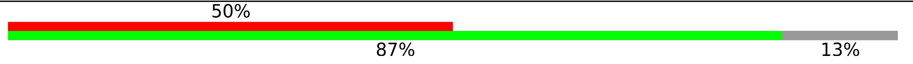
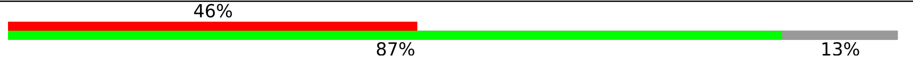
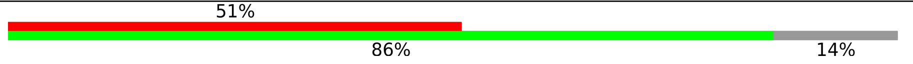
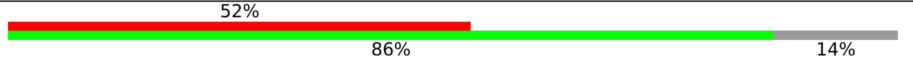
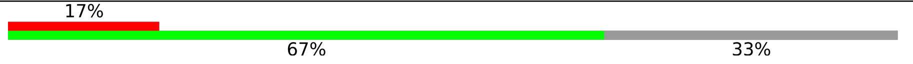
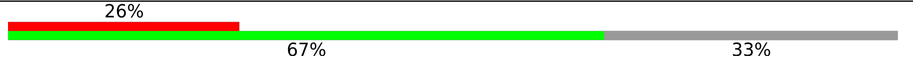
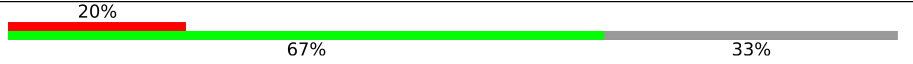
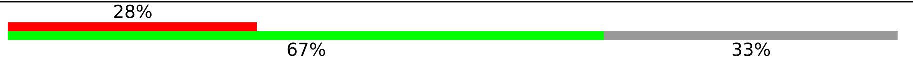
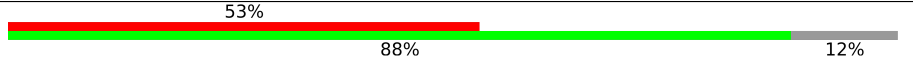
Mol	Chain	Length	Quality of chain
3	aC	81	
3	bC	81	
3	cC	81	
3	dC	81	
4	aD	139	
4	bD	139	
4	cD	139	
4	dD	139	
5	aE	70	
5	bE	70	
5	cE	70	
5	dE	70	
6	aF	164	
6	bF	164	
6	cF	164	
6	dF	164	
7	aI	46	
7	bI	46	
7	cI	46	
7	dI	46	
8	aJ	49	
8	bJ	49	
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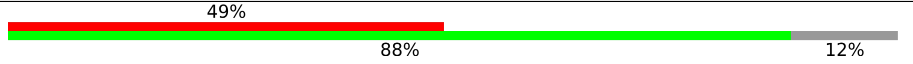
8	dJ	49	
9	aK	86	

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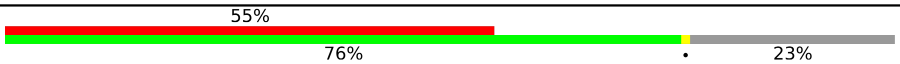
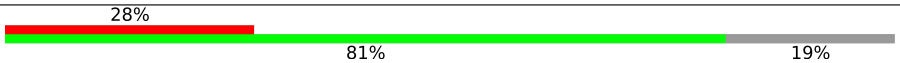
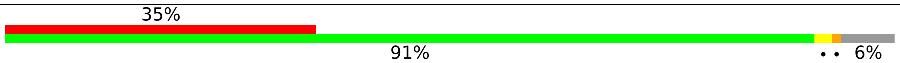
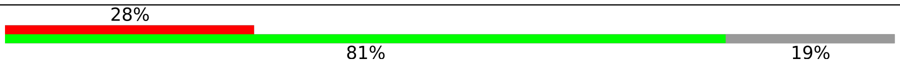
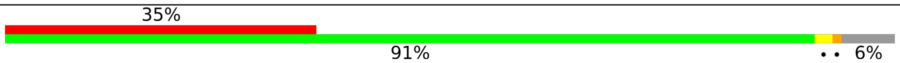
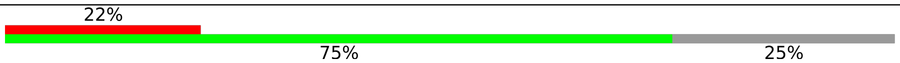
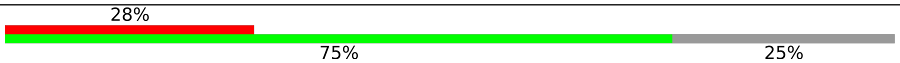
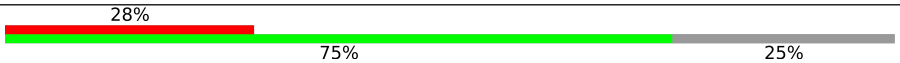
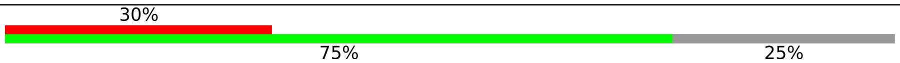
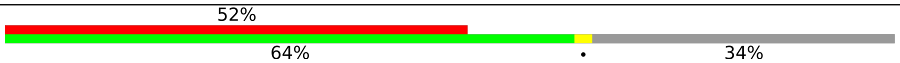
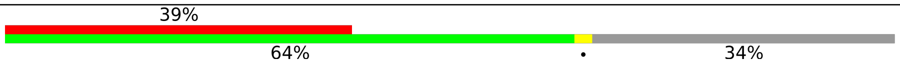
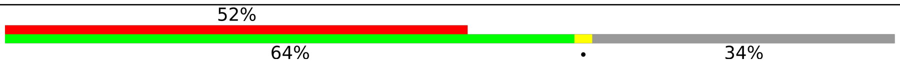
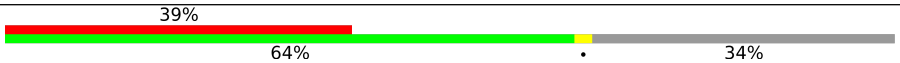
Mol	Chain	Length	Quality of chain
9	bK	86	
9	cK	86	
9	dK	86	
10	aL	172	
10	bL	172	
10	cL	172	
10	dL	172	
11	aM	40	
11	bM	40	
11	cM	40	
11	dM	40	
12	aX	44	
12	bX	44	
12	cX	44	
12	dX	44	

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	aA	801	X	-	-	-
13	CL0	bA	801	X	-	-	-
13	CL0	cA	801	X	-	-	-
13	CL0	dA	801	X	-	-	-
14	CLA	aA	802	X	-	-	-
14	CLA	aA	803	X	-	-	-
14	CLA	aA	804	X	-	-	-
14	CLA	aA	805	X	-	-	-
14	CLA	aA	806	X	-	-	-
14	CLA	aA	807	X	-	-	-
14	CLA	aA	808	X	-	-	-
14	CLA	aA	809	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	aA	810	X	-	-	-
14	CLA	aA	811	X	-	-	-
14	CLA	aA	812	X	-	-	-
14	CLA	aA	814	X	-	-	-
14	CLA	aA	815	X	-	-	-
14	CLA	aA	817	X	-	-	-
14	CLA	aA	818	X	-	-	-
14	CLA	aA	819	X	-	-	-
14	CLA	aA	820	X	-	-	-
14	CLA	aA	821	X	-	-	-
14	CLA	aA	822	X	-	-	-
14	CLA	aA	823	X	-	-	-
14	CLA	aA	824	X	-	-	-
14	CLA	aA	825	X	-	-	-
14	CLA	aA	826	X	-	-	-
14	CLA	aA	827	X	-	-	-
14	CLA	aA	828	X	-	-	-
14	CLA	aA	829	X	-	-	-
14	CLA	aA	830	X	-	-	-
14	CLA	aA	831	X	-	-	-
14	CLA	aA	832	X	-	-	-
14	CLA	aA	833	X	-	-	-
14	CLA	aA	834	X	-	-	-
14	CLA	aA	835	X	-	-	-
14	CLA	aA	836	X	-	-	-
14	CLA	aA	837	X	-	-	-
14	CLA	aA	838	X	-	-	-
14	CLA	aA	839	X	-	-	-
14	CLA	aA	840	X	-	-	-
14	CLA	aA	841	X	-	-	-
14	CLA	aA	842	X	-	-	-
14	CLA	aA	843	X	-	-	-
14	CLA	aB	801	X	-	-	-
14	CLA	aB	802	X	-	-	-
14	CLA	aB	803	X	-	-	-
14	CLA	aB	804	X	-	-	-
14	CLA	aB	805	X	-	-	-
14	CLA	aB	806	X	-	-	-
14	CLA	aB	807	X	-	-	-
14	CLA	aB	808	X	-	-	-
14	CLA	aB	809	X	-	-	-
14	CLA	aB	810	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	aB	811	X	-	-	-
14	CLA	aB	812	X	-	-	-
14	CLA	aB	813	X	-	-	-
14	CLA	aB	814	X	-	-	-
14	CLA	aB	815	X	-	-	-
14	CLA	aB	816	X	-	-	-
14	CLA	aB	817	X	-	-	-
14	CLA	aB	818	X	-	-	-
14	CLA	aB	819	X	-	-	-
14	CLA	aB	820	X	-	-	-
14	CLA	aB	821	X	-	-	-
14	CLA	aB	822	X	-	-	-
14	CLA	aB	823	X	-	-	-
14	CLA	aB	825	X	-	-	-
14	CLA	aB	826	X	-	-	-
14	CLA	aB	827	X	-	-	-
14	CLA	aB	828	X	-	-	-
14	CLA	aB	829	X	-	-	-
14	CLA	aB	830	X	-	-	-
14	CLA	aB	831	X	-	-	-
14	CLA	aB	832	X	-	-	-
14	CLA	aB	833	X	-	-	-
14	CLA	aB	834	X	-	-	-
14	CLA	aB	835	X	-	-	-
14	CLA	aB	837	X	-	-	-
14	CLA	aB	838	X	-	-	-
14	CLA	aB	840	X	-	-	-
14	CLA	aB	841	X	-	-	-
14	CLA	aF	201	X	-	-	-
14	CLA	aF	203	X	-	-	-
14	CLA	aJ	101	X	-	-	-
14	CLA	aJ	102	X	-	-	-
14	CLA	aK	101	X	-	-	-
14	CLA	aK	102	X	-	-	-
14	CLA	aL	202	X	-	-	-
14	CLA	aL	203	X	-	-	-
14	CLA	aL	204	X	-	-	-
14	CLA	aX	101	X	-	-	-
14	CLA	bA	802	X	-	-	-
14	CLA	bA	803	X	-	-	-
14	CLA	bA	804	X	-	-	-
14	CLA	bA	805	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	bA	806	X	-	-	-
14	CLA	bA	807	X	-	-	-
14	CLA	bA	808	X	-	-	-
14	CLA	bA	809	X	-	-	-
14	CLA	bA	810	X	-	-	-
14	CLA	bA	811	X	-	-	-
14	CLA	bA	812	X	-	-	-
14	CLA	bA	814	X	-	-	-
14	CLA	bA	815	X	-	-	-
14	CLA	bA	817	X	-	-	-
14	CLA	bA	818	X	-	-	-
14	CLA	bA	819	X	-	-	-
14	CLA	bA	820	X	-	-	-
14	CLA	bA	821	X	-	-	-
14	CLA	bA	822	X	-	-	-
14	CLA	bA	823	X	-	-	-
14	CLA	bA	824	X	-	-	-
14	CLA	bA	825	X	-	-	-
14	CLA	bA	826	X	-	-	-
14	CLA	bA	827	X	-	-	-
14	CLA	bA	828	X	-	-	-
14	CLA	bA	829	X	-	-	-
14	CLA	bA	830	X	-	-	-
14	CLA	bA	831	X	-	-	-
14	CLA	bA	832	X	-	-	-
14	CLA	bA	833	X	-	-	-
14	CLA	bA	834	X	-	-	-
14	CLA	bA	835	X	-	-	-
14	CLA	bA	836	X	-	-	-
14	CLA	bA	837	X	-	-	-
14	CLA	bA	838	X	-	-	-
14	CLA	bA	839	X	-	-	-
14	CLA	bA	840	X	-	-	-
14	CLA	bA	841	X	-	-	-
14	CLA	bA	842	X	-	-	-
14	CLA	bB	801	X	-	-	-
14	CLA	bB	802	X	-	-	-
14	CLA	bB	803	X	-	-	-
14	CLA	bB	804	X	-	-	-
14	CLA	bB	805	X	-	-	-
14	CLA	bB	806	X	-	-	-
14	CLA	bB	807	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	bB	808	X	-	-	-
14	CLA	bB	809	X	-	-	-
14	CLA	bB	810	X	-	-	-
14	CLA	bB	811	X	-	-	-
14	CLA	bB	812	X	-	-	-
14	CLA	bB	813	X	-	-	-
14	CLA	bB	814	X	-	-	-
14	CLA	bB	815	X	-	-	-
14	CLA	bB	816	X	-	-	-
14	CLA	bB	817	X	-	-	-
14	CLA	bB	818	X	-	-	-
14	CLA	bB	819	X	-	-	-
14	CLA	bB	820	X	-	-	-
14	CLA	bB	821	X	-	-	-
14	CLA	bB	822	X	-	-	-
14	CLA	bB	823	X	-	-	-
14	CLA	bB	824	X	-	-	-
14	CLA	bB	826	X	-	-	-
14	CLA	bB	827	X	-	-	-
14	CLA	bB	828	X	-	-	-
14	CLA	bB	829	X	-	-	-
14	CLA	bB	830	X	-	-	-
14	CLA	bB	831	X	-	-	-
14	CLA	bB	832	X	-	-	-
14	CLA	bB	833	X	-	-	-
14	CLA	bB	834	X	-	-	-
14	CLA	bB	835	X	-	-	-
14	CLA	bB	836	X	-	-	-
14	CLA	bB	838	X	-	-	-
14	CLA	bB	839	X	-	-	-
14	CLA	bB	841	X	-	-	-
14	CLA	bB	842	X	-	-	-
14	CLA	bF	201	X	-	-	-
14	CLA	bF	203	X	-	-	-
14	CLA	bJ	101	X	-	-	-
14	CLA	bJ	102	X	-	-	-
14	CLA	bK	101	X	-	-	-
14	CLA	bK	103	X	-	-	-
14	CLA	bL	201	X	-	-	-
14	CLA	bL	202	X	-	-	-
14	CLA	bL	204	X	-	-	-
14	CLA	bL	205	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	bL	206	X	-	-	-
14	CLA	bX	101	X	-	-	-
14	CLA	cA	802	X	-	-	-
14	CLA	cA	803	X	-	-	-
14	CLA	cA	804	X	-	-	-
14	CLA	cA	805	X	-	-	-
14	CLA	cA	806	X	-	-	-
14	CLA	cA	807	X	-	-	-
14	CLA	cA	808	X	-	-	-
14	CLA	cA	809	X	-	-	-
14	CLA	cA	810	X	-	-	-
14	CLA	cA	811	X	-	-	-
14	CLA	cA	812	X	-	-	-
14	CLA	cA	814	X	-	-	-
14	CLA	cA	815	X	-	-	-
14	CLA	cA	817	X	-	-	-
14	CLA	cA	818	X	-	-	-
14	CLA	cA	819	X	-	-	-
14	CLA	cA	820	X	-	-	-
14	CLA	cA	821	X	-	-	-
14	CLA	cA	822	X	-	-	-
14	CLA	cA	823	X	-	-	-
14	CLA	cA	824	X	-	-	-
14	CLA	cA	825	X	-	-	-
14	CLA	cA	826	X	-	-	-
14	CLA	cA	827	X	-	-	-
14	CLA	cA	828	X	-	-	-
14	CLA	cA	829	X	-	-	-
14	CLA	cA	830	X	-	-	-
14	CLA	cA	831	X	-	-	-
14	CLA	cA	832	X	-	-	-
14	CLA	cA	833	X	-	-	-
14	CLA	cA	834	X	-	-	-
14	CLA	cA	835	X	-	-	-
14	CLA	cA	836	X	-	-	-
14	CLA	cA	837	X	-	-	-
14	CLA	cA	838	X	-	-	-
14	CLA	cA	839	X	-	-	-
14	CLA	cA	840	X	-	-	-
14	CLA	cA	841	X	-	-	-
14	CLA	cA	842	X	-	-	-
14	CLA	cA	843	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	cB	801	X	-	-	-
14	CLA	cB	802	X	-	-	-
14	CLA	cB	803	X	-	-	-
14	CLA	cB	804	X	-	-	-
14	CLA	cB	805	X	-	-	-
14	CLA	cB	806	X	-	-	-
14	CLA	cB	807	X	-	-	-
14	CLA	cB	808	X	-	-	-
14	CLA	cB	809	X	-	-	-
14	CLA	cB	810	X	-	-	-
14	CLA	cB	811	X	-	-	-
14	CLA	cB	812	X	-	-	-
14	CLA	cB	813	X	-	-	-
14	CLA	cB	814	X	-	-	-
14	CLA	cB	815	X	-	-	-
14	CLA	cB	816	X	-	-	-
14	CLA	cB	817	X	-	-	-
14	CLA	cB	818	X	-	-	-
14	CLA	cB	819	X	-	-	-
14	CLA	cB	820	X	-	-	-
14	CLA	cB	821	X	-	-	-
14	CLA	cB	822	X	-	-	-
14	CLA	cB	823	X	-	-	-
14	CLA	cB	825	X	-	-	-
14	CLA	cB	826	X	-	-	-
14	CLA	cB	827	X	-	-	-
14	CLA	cB	828	X	-	-	-
14	CLA	cB	829	X	-	-	-
14	CLA	cB	830	X	-	-	-
14	CLA	cB	831	X	-	-	-
14	CLA	cB	832	X	-	-	-
14	CLA	cB	833	X	-	-	-
14	CLA	cB	834	X	-	-	-
14	CLA	cB	835	X	-	-	-
14	CLA	cB	837	X	-	-	-
14	CLA	cB	838	X	-	-	-
14	CLA	cB	840	X	-	-	-
14	CLA	cB	841	X	-	-	-
14	CLA	cF	201	X	-	-	-
14	CLA	cF	203	X	-	-	-
14	CLA	cJ	101	X	-	-	-
14	CLA	cJ	102	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	cK	101	X	-	-	-
14	CLA	cK	102	X	-	-	-
14	CLA	cL	202	X	-	-	-
14	CLA	cL	203	X	-	-	-
14	CLA	cL	204	X	-	-	-
14	CLA	cX	101	X	-	-	-
14	CLA	dA	802	X	-	-	-
14	CLA	dA	803	X	-	-	-
14	CLA	dA	804	X	-	-	-
14	CLA	dA	805	X	-	-	-
14	CLA	dA	806	X	-	-	-
14	CLA	dA	807	X	-	-	-
14	CLA	dA	808	X	-	-	-
14	CLA	dA	809	X	-	-	-
14	CLA	dA	810	X	-	-	-
14	CLA	dA	811	X	-	-	-
14	CLA	dA	812	X	-	-	-
14	CLA	dA	814	X	-	-	-
14	CLA	dA	815	X	-	-	-
14	CLA	dA	817	X	-	-	-
14	CLA	dA	818	X	-	-	-
14	CLA	dA	819	X	-	-	-
14	CLA	dA	820	X	-	-	-
14	CLA	dA	821	X	-	-	-
14	CLA	dA	822	X	-	-	-
14	CLA	dA	823	X	-	-	-
14	CLA	dA	824	X	-	-	-
14	CLA	dA	825	X	-	-	-
14	CLA	dA	826	X	-	-	-
14	CLA	dA	827	X	-	-	-
14	CLA	dA	828	X	-	-	-
14	CLA	dA	829	X	-	-	-
14	CLA	dA	830	X	-	-	-
14	CLA	dA	831	X	-	-	-
14	CLA	dA	832	X	-	-	-
14	CLA	dA	833	X	-	-	-
14	CLA	dA	834	X	-	-	-
14	CLA	dA	835	X	-	-	-
14	CLA	dA	836	X	-	-	-
14	CLA	dA	837	X	-	-	-
14	CLA	dA	838	X	-	-	-
14	CLA	dA	839	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	dA	840	X	-	-	-
14	CLA	dA	841	X	-	-	-
14	CLA	dA	842	X	-	-	-
14	CLA	dB	801	X	-	-	-
14	CLA	dB	802	X	-	-	-
14	CLA	dB	803	X	-	-	-
14	CLA	dB	804	X	-	-	-
14	CLA	dB	805	X	-	-	-
14	CLA	dB	806	X	-	-	-
14	CLA	dB	807	X	-	-	-
14	CLA	dB	808	X	-	-	-
14	CLA	dB	809	X	-	-	-
14	CLA	dB	810	X	-	-	-
14	CLA	dB	811	X	-	-	-
14	CLA	dB	812	X	-	-	-
14	CLA	dB	813	X	-	-	-
14	CLA	dB	814	X	-	-	-
14	CLA	dB	815	X	-	-	-
14	CLA	dB	816	X	-	-	-
14	CLA	dB	817	X	-	-	-
14	CLA	dB	818	X	-	-	-
14	CLA	dB	819	X	-	-	-
14	CLA	dB	820	X	-	-	-
14	CLA	dB	821	X	-	-	-
14	CLA	dB	822	X	-	-	-
14	CLA	dB	823	X	-	-	-
14	CLA	dB	824	X	-	-	-
14	CLA	dB	826	X	-	-	-
14	CLA	dB	827	X	-	-	-
14	CLA	dB	828	X	-	-	-
14	CLA	dB	829	X	-	-	-
14	CLA	dB	830	X	-	-	-
14	CLA	dB	831	X	-	-	-
14	CLA	dB	832	X	-	-	-
14	CLA	dB	833	X	-	-	-
14	CLA	dB	834	X	-	-	-
14	CLA	dB	835	X	-	-	-
14	CLA	dB	836	X	-	-	-
14	CLA	dB	838	X	-	-	-
14	CLA	dB	839	X	-	-	-
14	CLA	dB	841	X	-	-	-
14	CLA	dB	842	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	dF	201	X	-	-	-
14	CLA	dF	203	X	-	-	-
14	CLA	dJ	101	X	-	-	-
14	CLA	dJ	102	X	-	-	-
14	CLA	dK	101	X	-	-	-
14	CLA	dK	103	X	-	-	-
14	CLA	dL	201	X	-	-	-
14	CLA	dL	202	X	-	-	-
14	CLA	dL	204	X	-	-	-
14	CLA	dL	205	X	-	-	-
14	CLA	dL	206	X	-	-	-
14	CLA	dX	101	X	-	-	-

2 Entry composition ⓘ

There are 19 unique types of molecules in this entry. The entry contains 94576 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	aA	739	Total	C	N	O	S	0	0
			5801	3806	998	976	21		
1	bA	739	Total	C	N	O	S	0	0
			5801	3806	998	976	21		
1	cA	739	Total	C	N	O	S	0	0
			5801	3806	998	976	21		
1	dA	739	Total	C	N	O	S	0	0
			5801	3806	998	976	21		

- Molecule 2 is a protein called Photosystem I P700 chlorophyll a apoprotein A2 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	aB	739	Total	C	N	O	S	0	0
			5919	3906	990	1005	18		
2	bB	739	Total	C	N	O	S	0	0
			5919	3906	990	1005	18		
2	cB	739	Total	C	N	O	S	0	0
			5919	3906	990	1005	18		
2	dB	739	Total	C	N	O	S	0	0
			5919	3906	990	1005	18		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	aC	80	Total	C	N	O	S	0	0
			599	367	103	118	11		
3	bC	80	Total	C	N	O	S	0	0
			599	367	103	118	11		
3	cC	80	Total	C	N	O	S	0	0
			599	367	103	118	11		
3	dC	80	Total	C	N	O	S	0	0
			599	367	103	118	11		

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

Mol	Chain	Residues	Atoms	AltConf	Trace
4	aD	73	Total C N O S 581 378 97 105 1	0	0
4	bD	96	Total C N O S 740 479 122 138 1	0	0
4	cD	73	Total C N O S 581 378 97 105 1	0	0
4	dD	96	Total C N O S 740 479 122 138 1	0	0

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

Mol	Chain	Residues	Atoms	AltConf	Trace
5	aE	61	Total C N O 490 313 84 93	0	0
5	bE	61	Total C N O 490 313 84 93	0	0
5	cE	61	Total C N O 490 313 84 93	0	0
5	dE	61	Total C N O 490 313 84 93	0	0

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

Mol	Chain	Residues	Atoms	AltConf	Trace
6	aF	140	Total C N O S 1072 684 183 203 2	0	0
6	bF	141	Total C N O S 1080 690 184 204 2	0	0
6	cF	140	Total C N O S 1072 684 183 203 2	0	0
6	dF	141	Total C N O S 1080 690 184 204 2	0	0

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

Mol	Chain	Residues	Atoms	AltConf	Trace
7	aI	31	Total C N O 253 177 35 41	0	0
7	bI	31	Total C N O 253 177 35 41	0	0
7	cI	31	Total C N O 253 177 35 41	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
7	dI	31	253	177	35	41	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
8	aJ	43	347	236	52	59	0	0
8	bJ	43	347	236	52	59	0	0
8	cJ	43	347	236	52	59	0	0
8	dJ	43	347	236	52	59	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	aK	66	480	322	78	79	1	0	0
9	bK	66	480	322	78	79	1	0	0
9	cK	66	480	322	78	79	1	0	0
9	dK	66	480	322	78	79	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	aL	140	1037	684	172	180	1	0	0
10	bL	161	1210	792	206	211	1	0	0
10	cL	140	1037	684	172	180	1	0	0
10	dL	161	1210	792	206	211	1	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
11	aM	30	Total 235	C 157	N 36	O 42	0	0
11	bM	30	Total 235	C 157	N 36	O 42	0	0
11	cM	30	Total 235	C 157	N 36	O 42	0	0
11	dM	30	Total 235	C 157	N 36	O 42	0	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
aM	1	MET	-	see sequence details	UNP Q8YNB0
aM	2	PRO	-	see sequence details	UNP Q8YNB0
aM	3	THR	-	see sequence details	UNP Q8YNB0
aM	4	LEU	-	see sequence details	UNP Q8YNB0
aM	5	TYR	-	see sequence details	UNP Q8YNB0
aM	6	LEU	-	see sequence details	UNP Q8YNB0
aM	7	ALA	-	see sequence details	UNP Q8YNB0
aM	8	GLN	-	see sequence details	UNP Q8YNB0
aM	9	VAL	-	see sequence details	UNP Q8YNB0
bM	1	MET	-	see sequence details	UNP Q8YNB0
bM	2	PRO	-	see sequence details	UNP Q8YNB0
bM	3	THR	-	see sequence details	UNP Q8YNB0
bM	4	LEU	-	see sequence details	UNP Q8YNB0
bM	5	TYR	-	see sequence details	UNP Q8YNB0
bM	6	LEU	-	see sequence details	UNP Q8YNB0
bM	7	ALA	-	see sequence details	UNP Q8YNB0
bM	8	GLN	-	see sequence details	UNP Q8YNB0
bM	9	VAL	-	see sequence details	UNP Q8YNB0
cM	1	MET	-	see sequence details	UNP Q8YNB0
cM	2	PRO	-	see sequence details	UNP Q8YNB0
cM	3	THR	-	see sequence details	UNP Q8YNB0
cM	4	LEU	-	see sequence details	UNP Q8YNB0
cM	5	TYR	-	see sequence details	UNP Q8YNB0
cM	6	LEU	-	see sequence details	UNP Q8YNB0
cM	7	ALA	-	see sequence details	UNP Q8YNB0
cM	8	GLN	-	see sequence details	UNP Q8YNB0
cM	9	VAL	-	see sequence details	UNP Q8YNB0
dM	1	MET	-	see sequence details	UNP Q8YNB0
dM	2	PRO	-	see sequence details	UNP Q8YNB0
dM	3	THR	-	see sequence details	UNP Q8YNB0
dM	4	LEU	-	see sequence details	UNP Q8YNB0

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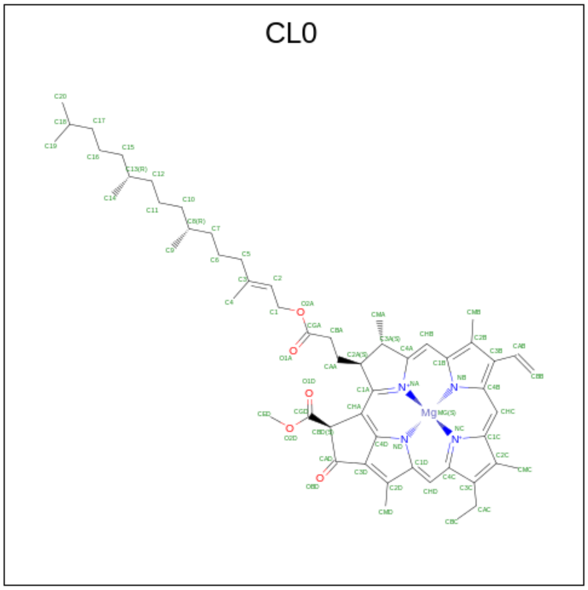
Chain	Residue	Modelled	Actual	Comment	Reference
dM	5	TYR	-	see sequence details	UNP Q8YNB0
dM	6	LEU	-	see sequence details	UNP Q8YNB0
dM	7	ALA	-	see sequence details	UNP Q8YNB0
dM	8	GLN	-	see sequence details	UNP Q8YNB0
dM	9	VAL	-	see sequence details	UNP Q8YNB0

- Molecule 12 is a protein called Photosystem I 4.8 kDa protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	aX	29	Total 243	C 170	N 37	O 36	0	0
12	bX	29	Total 243	C 170	N 37	O 36	0	0
12	cX	29	Total 243	C 170	N 37	O 36	0	0
12	dX	29	Total 243	C 170	N 37	O 36	0	0

- Molecule 13 is CHLOROPHYLL A ISOMER (three-letter code: CL0) (formula: $C_{55}H_{72}MgN_4O_5$).



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

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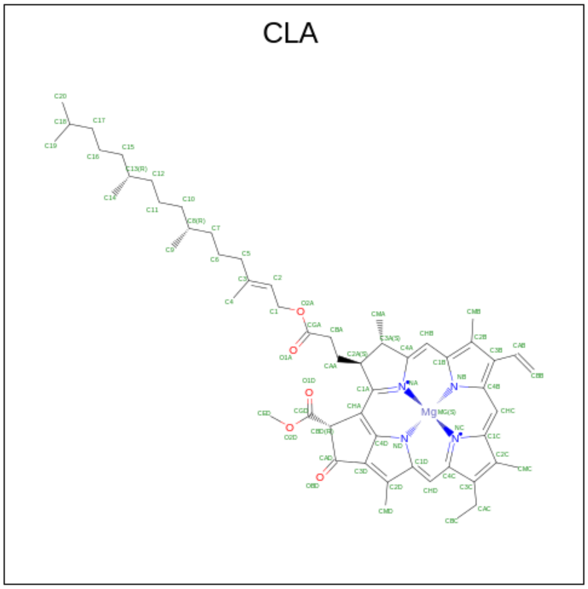
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
13	dA	1	65	55	1	4	5	0

- Molecule 14 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
14	aA	1	2332	1912	42	168	210	0
14	aA	1	2332	1912	42	168	210	0
14	aA	1	2332	1912	42	168	210	0
14	aA	1	2332	1912	42	168	210	0
14	aA	1	2332	1912	42	168	210	0
14	aA	1	2332	1912	42	168	210	0
14	aA	1	2332	1912	42	168	210	0
14	aA	1	2332	1912	42	168	210	0
14	aA	1	2332	1912	42	168	210	0
14	aA	1	2332	1912	42	168	210	0

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Mol	Chain	Residues	Atoms	AltConf
14	aA	1	Total C Mg N O 2332 1912 42 168 210	0
14	aA	1	Total C Mg N O 2332 1912 42 168 210	0
14	aA	1	Total C Mg N O 2332 1912 42 168 210	0
14	aA	1	Total C Mg N O 2332 1912 42 168 210	0
14	aA	1	Total C Mg N O 2332 1912 42 168 210	0
14	aA	1	Total C Mg N O 2332 1912 42 168 210	0
14	aA	1	Total C Mg N O 2332 1912 42 168 210	0
14	aA	1	Total C Mg N O 2332 1912 42 168 210	0
14	aA	1	Total C Mg N O 2332 1912 42 168 210	0
14	aA	1	Total C Mg N O 2332 1912 42 168 210	0
14	aA	1	Total C Mg N O 2332 1912 42 168 210	0
14	aA	1	Total C Mg N O 2332 1912 42 168 210	0
14	aA	1	Total C Mg N O 2332 1912 42 168 210	0
14	aA	1	Total C Mg N O 2332 1912 42 168 210	0
14	aA	1	Total C Mg N O 2332 1912 42 168 210	0
14	aA	1	Total C Mg N O 2332 1912 42 168 210	0
14	aA	1	Total C Mg N O 2332 1912 42 168 210	0
14	aA	1	Total C Mg N O 2332 1912 42 168 210	0
14	aA	1	Total C Mg N O 2332 1912 42 168 210	0
14	aA	1	Total C Mg N O 2332 1912 42 168 210	0
14	aA	1	Total C Mg N O 2332 1912 42 168 210	0

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Mol	Chain	Residues	Atoms					AltConf
14	aA	1	Total 2332	C 1912	Mg 42	N 168	O 210	0
14	aA	1	Total 2332	C 1912	Mg 42	N 168	O 210	0
14	aA	1	Total 2332	C 1912	Mg 42	N 168	O 210	0
14	aA	1	Total 2332	C 1912	Mg 42	N 168	O 210	0
14	aA	1	Total 2332	C 1912	Mg 42	N 168	O 210	0
14	aA	1	Total 2332	C 1912	Mg 42	N 168	O 210	0
14	aA	1	Total 2332	C 1912	Mg 42	N 168	O 210	0
14	aA	1	Total 2332	C 1912	Mg 42	N 168	O 210	0
14	aA	1	Total 2332	C 1912	Mg 42	N 168	O 210	0
14	aA	1	Total 2332	C 1912	Mg 42	N 168	O 210	0
14	aA	1	Total 2332	C 1912	Mg 42	N 168	O 210	0
14	aB	1	Total 2340	C 1930	Mg 41	N 164	O 205	0
14	aB	1	Total 2340	C 1930	Mg 41	N 164	O 205	0
14	aB	1	Total 2340	C 1930	Mg 41	N 164	O 205	0
14	aB	1	Total 2340	C 1930	Mg 41	N 164	O 205	0
14	aB	1	Total 2340	C 1930	Mg 41	N 164	O 205	0
14	aB	1	Total 2340	C 1930	Mg 41	N 164	O 205	0
14	aB	1	Total 2340	C 1930	Mg 41	N 164	O 205	0
14	aB	1	Total 2340	C 1930	Mg 41	N 164	O 205	0
14	aB	1	Total 2340	C 1930	Mg 41	N 164	O 205	0
14	aB	1	Total 2340	C 1930	Mg 41	N 164	O 205	0

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Mol	Chain	Residues	Atoms					AltConf
14	aB	1	Total 2340	C 1930	Mg 41	N 164	O 205	0
14	aB	1	Total 2340	C 1930	Mg 41	N 164	O 205	0
14	aB	1	Total 2340	C 1930	Mg 41	N 164	O 205	0
14	aB	1	Total 2340	C 1930	Mg 41	N 164	O 205	0
14	aB	1	Total 2340	C 1930	Mg 41	N 164	O 205	0
14	aB	1	Total 2340	C 1930	Mg 41	N 164	O 205	0
14	aB	1	Total 2340	C 1930	Mg 41	N 164	O 205	0
14	aB	1	Total 2340	C 1930	Mg 41	N 164	O 205	0
14	aB	1	Total 2340	C 1930	Mg 41	N 164	O 205	0
14	aB	1	Total 2340	C 1930	Mg 41	N 164	O 205	0
14	aB	1	Total 2340	C 1930	Mg 41	N 164	O 205	0
14	aB	1	Total 2340	C 1930	Mg 41	N 164	O 205	0
14	aB	1	Total 2340	C 1930	Mg 41	N 164	O 205	0
14	aB	1	Total 2340	C 1930	Mg 41	N 164	O 205	0
14	aB	1	Total 2340	C 1930	Mg 41	N 164	O 205	0
14	aB	1	Total 2340	C 1930	Mg 41	N 164	O 205	0
14	aB	1	Total 2340	C 1930	Mg 41	N 164	O 205	0
14	aB	1	Total 2340	C 1930	Mg 41	N 164	O 205	0
14	aB	1	Total 2340	C 1930	Mg 41	N 164	O 205	0
14	aB	1	Total 2340	C 1930	Mg 41	N 164	O 205	0
14	aB	1	Total 2340	C 1930	Mg 41	N 164	O 205	0

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Mol	Chain	Residues	Atoms	AltConf
14	aB	1	Total C Mg N O 2340 1930 41 164 205	0
14	aB	1	Total C Mg N O 2340 1930 41 164 205	0
14	aB	1	Total C Mg N O 2340 1930 41 164 205	0
14	aB	1	Total C Mg N O 2340 1930 41 164 205	0
14	aB	1	Total C Mg N O 2340 1930 41 164 205	0
14	aB	1	Total C Mg N O 2340 1930 41 164 205	0
14	aB	1	Total C Mg N O 2340 1930 41 164 205	0
14	aB	1	Total C Mg N O 2340 1930 41 164 205	0
14	aB	1	Total C Mg N O 2340 1930 41 164 205	0
14	aB	1	Total C Mg N O 2340 1930 41 164 205	0
14	aF	1	Total C Mg N O 96 76 2 8 10	0
14	aF	1	Total C Mg N O 96 76 2 8 10	0
14	aJ	1	Total C Mg N O 82 66 2 8 6	0
14	aJ	1	Total C Mg N O 82 66 2 8 6	0
14	aK	1	Total C Mg N O 86 68 2 8 8	0
14	aK	1	Total C Mg N O 86 68 2 8 8	0
14	aL	1	Total C Mg N O 182 152 3 12 15	0
14	aL	1	Total C Mg N O 182 152 3 12 15	0
14	aL	1	Total C Mg N O 182 152 3 12 15	0
14	aX	1	Total C Mg N O 45 35 1 4 5	0
14	bA	1	Total C Mg N O 2280 1870 41 164 205	0

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Mol	Chain	Residues	Atoms	AltConf
14	bA	1	Total C Mg N O 2280 1870 41 164 205	0
14	bA	1	Total C Mg N O 2280 1870 41 164 205	0
14	bA	1	Total C Mg N O 2280 1870 41 164 205	0
14	bA	1	Total C Mg N O 2280 1870 41 164 205	0
14	bA	1	Total C Mg N O 2280 1870 41 164 205	0
14	bA	1	Total C Mg N O 2280 1870 41 164 205	0
14	bA	1	Total C Mg N O 2280 1870 41 164 205	0
14	bA	1	Total C Mg N O 2280 1870 41 164 205	0
14	bA	1	Total C Mg N O 2280 1870 41 164 205	0
14	bA	1	Total C Mg N O 2280 1870 41 164 205	0
14	bA	1	Total C Mg N O 2280 1870 41 164 205	0
14	bA	1	Total C Mg N O 2280 1870 41 164 205	0
14	bA	1	Total C Mg N O 2280 1870 41 164 205	0
14	bA	1	Total C Mg N O 2280 1870 41 164 205	0
14	bA	1	Total C Mg N O 2280 1870 41 164 205	0
14	bA	1	Total C Mg N O 2280 1870 41 164 205	0
14	bA	1	Total C Mg N O 2280 1870 41 164 205	0
14	bA	1	Total C Mg N O 2280 1870 41 164 205	0
14	bA	1	Total C Mg N O 2280 1870 41 164 205	0
14	bA	1	Total C Mg N O 2280 1870 41 164 205	0
14	bA	1	Total C Mg N O 2280 1870 41 164 205	0

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Mol	Chain	Residues	Atoms					AltConf
14	bA	1	Total 2280	C 1870	Mg 41	N 164	O 205	0
14	bA	1	Total 2280	C 1870	Mg 41	N 164	O 205	0
14	bA	1	Total 2280	C 1870	Mg 41	N 164	O 205	0
14	bA	1	Total 2280	C 1870	Mg 41	N 164	O 205	0
14	bA	1	Total 2280	C 1870	Mg 41	N 164	O 205	0
14	bA	1	Total 2280	C 1870	Mg 41	N 164	O 205	0
14	bA	1	Total 2280	C 1870	Mg 41	N 164	O 205	0
14	bA	1	Total 2280	C 1870	Mg 41	N 164	O 205	0
14	bA	1	Total 2280	C 1870	Mg 41	N 164	O 205	0
14	bA	1	Total 2280	C 1870	Mg 41	N 164	O 205	0
14	bA	1	Total 2280	C 1870	Mg 41	N 164	O 205	0
14	bA	1	Total 2280	C 1870	Mg 41	N 164	O 205	0
14	bA	1	Total 2280	C 1870	Mg 41	N 164	O 205	0
14	bA	1	Total 2280	C 1870	Mg 41	N 164	O 205	0
14	bA	1	Total 2280	C 1870	Mg 41	N 164	O 205	0
14	bA	1	Total 2280	C 1870	Mg 41	N 164	O 205	0
14	bA	1	Total 2280	C 1870	Mg 41	N 164	O 205	0
14	bA	1	Total 2280	C 1870	Mg 41	N 164	O 205	0
14	bA	1	Total 2280	C 1870	Mg 41	N 164	O 205	0
14	bB	1	Total 2405	C 1985	Mg 42	N 168	O 210	0
14	bB	1	Total 2405	C 1985	Mg 42	N 168	O 210	0

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Mol	Chain	Residues	Atoms	AltConf
14	bB	1	Total C Mg N O 2405 1985 42 168 210	0
14	bB	1	Total C Mg N O 2405 1985 42 168 210	0
14	bB	1	Total C Mg N O 2405 1985 42 168 210	0
14	bB	1	Total C Mg N O 2405 1985 42 168 210	0
14	bB	1	Total C Mg N O 2405 1985 42 168 210	0
14	bB	1	Total C Mg N O 2405 1985 42 168 210	0
14	bB	1	Total C Mg N O 2405 1985 42 168 210	0
14	bB	1	Total C Mg N O 2405 1985 42 168 210	0
14	bB	1	Total C Mg N O 2405 1985 42 168 210	0
14	bB	1	Total C Mg N O 2405 1985 42 168 210	0
14	bB	1	Total C Mg N O 2405 1985 42 168 210	0
14	bB	1	Total C Mg N O 2405 1985 42 168 210	0
14	bB	1	Total C Mg N O 2405 1985 42 168 210	0
14	bB	1	Total C Mg N O 2405 1985 42 168 210	0
14	bB	1	Total C Mg N O 2405 1985 42 168 210	0
14	bB	1	Total C Mg N O 2405 1985 42 168 210	0
14	bB	1	Total C Mg N O 2405 1985 42 168 210	0
14	bB	1	Total C Mg N O 2405 1985 42 168 210	0
14	bB	1	Total C Mg N O 2405 1985 42 168 210	0
14	bB	1	Total C Mg N O 2405 1985 42 168 210	0
14	bB	1	Total C Mg N O 2405 1985 42 168 210	0

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Mol	Chain	Residues	Atoms	AltConf
14	bB	1	Total C Mg N O 2405 1985 42 168 210	0
14	bB	1	Total C Mg N O 2405 1985 42 168 210	0
14	bB	1	Total C Mg N O 2405 1985 42 168 210	0
14	bB	1	Total C Mg N O 2405 1985 42 168 210	0
14	bB	1	Total C Mg N O 2405 1985 42 168 210	0
14	bB	1	Total C Mg N O 2405 1985 42 168 210	0
14	bB	1	Total C Mg N O 2405 1985 42 168 210	0
14	bB	1	Total C Mg N O 2405 1985 42 168 210	0
14	bB	1	Total C Mg N O 2405 1985 42 168 210	0
14	bB	1	Total C Mg N O 2405 1985 42 168 210	0
14	bB	1	Total C Mg N O 2405 1985 42 168 210	0
14	bB	1	Total C Mg N O 2405 1985 42 168 210	0
14	bB	1	Total C Mg N O 2405 1985 42 168 210	0
14	bB	1	Total C Mg N O 2405 1985 42 168 210	0
14	bB	1	Total C Mg N O 2405 1985 42 168 210	0
14	bB	1	Total C Mg N O 2405 1985 42 168 210	0
14	bB	1	Total C Mg N O 2405 1985 42 168 210	0
14	bB	1	Total C Mg N O 2405 1985 42 168 210	0
14	bB	1	Total C Mg N O 2405 1985 42 168 210	0
14	bF	1	Total C Mg N O 96 76 2 8 10	0
14	bF	1	Total C Mg N O 96 76 2 8 10	0

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Mol	Chain	Residues	Atoms	AltConf
14	bJ	1	Total C Mg N O 82 66 2 8 6	0
14	bJ	1	Total C Mg N O 82 66 2 8 6	0
14	bK	1	Total C Mg N O 86 68 2 8 8	0
14	bK	1	Total C Mg N O 86 68 2 8 8	0
14	bL	1	Total C Mg N O 299 249 5 20 25	0
14	bL	1	Total C Mg N O 299 249 5 20 25	0
14	bL	1	Total C Mg N O 299 249 5 20 25	0
14	bL	1	Total C Mg N O 299 249 5 20 25	0
14	bL	1	Total C Mg N O 299 249 5 20 25	0
14	bX	1	Total C Mg N O 45 35 1 4 5	0
14	cA	1	Total C Mg N O 2332 1912 42 168 210	0
14	cA	1	Total C Mg N O 2332 1912 42 168 210	0
14	cA	1	Total C Mg N O 2332 1912 42 168 210	0
14	cA	1	Total C Mg N O 2332 1912 42 168 210	0
14	cA	1	Total C Mg N O 2332 1912 42 168 210	0
14	cA	1	Total C Mg N O 2332 1912 42 168 210	0
14	cA	1	Total C Mg N O 2332 1912 42 168 210	0
14	cA	1	Total C Mg N O 2332 1912 42 168 210	0
14	cA	1	Total C Mg N O 2332 1912 42 168 210	0
14	cA	1	Total C Mg N O 2332 1912 42 168 210	0
14	cA	1	Total C Mg N O 2332 1912 42 168 210	0

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Mol	Chain	Residues	Atoms					AltConf
14	cA	1	Total 2332	C 1912	Mg 42	N 168	O 210	0
14	cA	1	Total 2332	C 1912	Mg 42	N 168	O 210	0
14	cA	1	Total 2332	C 1912	Mg 42	N 168	O 210	0
14	cA	1	Total 2332	C 1912	Mg 42	N 168	O 210	0
14	cA	1	Total 2332	C 1912	Mg 42	N 168	O 210	0
14	cA	1	Total 2332	C 1912	Mg 42	N 168	O 210	0
14	cA	1	Total 2332	C 1912	Mg 42	N 168	O 210	0
14	cA	1	Total 2332	C 1912	Mg 42	N 168	O 210	0
14	cA	1	Total 2332	C 1912	Mg 42	N 168	O 210	0
14	cA	1	Total 2332	C 1912	Mg 42	N 168	O 210	0
14	cA	1	Total 2332	C 1912	Mg 42	N 168	O 210	0
14	cA	1	Total 2332	C 1912	Mg 42	N 168	O 210	0
14	cA	1	Total 2332	C 1912	Mg 42	N 168	O 210	0
14	cA	1	Total 2332	C 1912	Mg 42	N 168	O 210	0
14	cA	1	Total 2332	C 1912	Mg 42	N 168	O 210	0
14	cA	1	Total 2332	C 1912	Mg 42	N 168	O 210	0
14	cA	1	Total 2332	C 1912	Mg 42	N 168	O 210	0
14	cA	1	Total 2332	C 1912	Mg 42	N 168	O 210	0
14	cA	1	Total 2332	C 1912	Mg 42	N 168	O 210	0
14	cA	1	Total 2332	C 1912	Mg 42	N 168	O 210	0
14	cA	1	Total 2332	C 1912	Mg 42	N 168	O 210	0

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Mol	Chain	Residues	Atoms					AltConf
14	cA	1	Total 2332	C 1912	Mg 42	N 168	O 210	0
14	cA	1	Total 2332	C 1912	Mg 42	N 168	O 210	0
14	cA	1	Total 2332	C 1912	Mg 42	N 168	O 210	0
14	cA	1	Total 2332	C 1912	Mg 42	N 168	O 210	0
14	cA	1	Total 2332	C 1912	Mg 42	N 168	O 210	0
14	cA	1	Total 2332	C 1912	Mg 42	N 168	O 210	0
14	cA	1	Total 2332	C 1912	Mg 42	N 168	O 210	0
14	cA	1	Total 2332	C 1912	Mg 42	N 168	O 210	0
14	cA	1	Total 2332	C 1912	Mg 42	N 168	O 210	0
14	cA	1	Total 2332	C 1912	Mg 42	N 168	O 210	0
14	cB	1	Total 2340	C 1930	Mg 41	N 164	O 205	0
14	cB	1	Total 2340	C 1930	Mg 41	N 164	O 205	0
14	cB	1	Total 2340	C 1930	Mg 41	N 164	O 205	0
14	cB	1	Total 2340	C 1930	Mg 41	N 164	O 205	0
14	cB	1	Total 2340	C 1930	Mg 41	N 164	O 205	0
14	cB	1	Total 2340	C 1930	Mg 41	N 164	O 205	0
14	cB	1	Total 2340	C 1930	Mg 41	N 164	O 205	0
14	cB	1	Total 2340	C 1930	Mg 41	N 164	O 205	0
14	cB	1	Total 2340	C 1930	Mg 41	N 164	O 205	0
14	cB	1	Total 2340	C 1930	Mg 41	N 164	O 205	0
14	cB	1	Total 2340	C 1930	Mg 41	N 164	O 205	0

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Mol	Chain	Residues	Atoms					AltConf
14	cB	1	Total 2340	C 1930	Mg 41	N 164	O 205	0
14	cB	1	Total 2340	C 1930	Mg 41	N 164	O 205	0
14	cB	1	Total 2340	C 1930	Mg 41	N 164	O 205	0
14	cB	1	Total 2340	C 1930	Mg 41	N 164	O 205	0
14	cB	1	Total 2340	C 1930	Mg 41	N 164	O 205	0
14	cB	1	Total 2340	C 1930	Mg 41	N 164	O 205	0
14	cB	1	Total 2340	C 1930	Mg 41	N 164	O 205	0
14	cB	1	Total 2340	C 1930	Mg 41	N 164	O 205	0
14	cB	1	Total 2340	C 1930	Mg 41	N 164	O 205	0
14	cB	1	Total 2340	C 1930	Mg 41	N 164	O 205	0
14	cB	1	Total 2340	C 1930	Mg 41	N 164	O 205	0
14	cB	1	Total 2340	C 1930	Mg 41	N 164	O 205	0
14	cB	1	Total 2340	C 1930	Mg 41	N 164	O 205	0
14	cB	1	Total 2340	C 1930	Mg 41	N 164	O 205	0
14	cB	1	Total 2340	C 1930	Mg 41	N 164	O 205	0
14	cB	1	Total 2340	C 1930	Mg 41	N 164	O 205	0
14	cB	1	Total 2340	C 1930	Mg 41	N 164	O 205	0
14	cB	1	Total 2340	C 1930	Mg 41	N 164	O 205	0
14	cB	1	Total 2340	C 1930	Mg 41	N 164	O 205	0
14	cB	1	Total 2340	C 1930	Mg 41	N 164	O 205	0
14	cB	1	Total 2340	C 1930	Mg 41	N 164	O 205	0

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Mol	Chain	Residues	Atoms	AltConf
14	cB	1	Total C Mg N O 2340 1930 41 164 205	0
14	cB	1	Total C Mg N O 2340 1930 41 164 205	0
14	cB	1	Total C Mg N O 2340 1930 41 164 205	0
14	cB	1	Total C Mg N O 2340 1930 41 164 205	0
14	cB	1	Total C Mg N O 2340 1930 41 164 205	0
14	cB	1	Total C Mg N O 2340 1930 41 164 205	0
14	cB	1	Total C Mg N O 2340 1930 41 164 205	0
14	cB	1	Total C Mg N O 2340 1930 41 164 205	0
14	cB	1	Total C Mg N O 2340 1930 41 164 205	0
14	cF	1	Total C Mg N O 96 76 2 8 10	0
14	cF	1	Total C Mg N O 96 76 2 8 10	0
14	cJ	1	Total C Mg N O 82 66 2 8 6	0
14	cJ	1	Total C Mg N O 82 66 2 8 6	0
14	cK	1	Total C Mg N O 86 68 2 8 8	0
14	cK	1	Total C Mg N O 86 68 2 8 8	0
14	cL	1	Total C Mg N O 182 152 3 12 15	0
14	cL	1	Total C Mg N O 182 152 3 12 15	0
14	cL	1	Total C Mg N O 182 152 3 12 15	0
14	cX	1	Total C Mg N O 45 35 1 4 5	0
14	dA	1	Total C Mg N O 2280 1870 41 164 205	0
14	dA	1	Total C Mg N O 2280 1870 41 164 205	0

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Mol	Chain	Residues	Atoms					AltConf
14	dA	1	Total 2280	C 1870	Mg 41	N 164	O 205	0
14	dA	1	Total 2280	C 1870	Mg 41	N 164	O 205	0
14	dA	1	Total 2280	C 1870	Mg 41	N 164	O 205	0
14	dA	1	Total 2280	C 1870	Mg 41	N 164	O 205	0
14	dA	1	Total 2280	C 1870	Mg 41	N 164	O 205	0
14	dA	1	Total 2280	C 1870	Mg 41	N 164	O 205	0
14	dA	1	Total 2280	C 1870	Mg 41	N 164	O 205	0
14	dA	1	Total 2280	C 1870	Mg 41	N 164	O 205	0
14	dA	1	Total 2280	C 1870	Mg 41	N 164	O 205	0
14	dA	1	Total 2280	C 1870	Mg 41	N 164	O 205	0
14	dA	1	Total 2280	C 1870	Mg 41	N 164	O 205	0
14	dA	1	Total 2280	C 1870	Mg 41	N 164	O 205	0
14	dA	1	Total 2280	C 1870	Mg 41	N 164	O 205	0
14	dA	1	Total 2280	C 1870	Mg 41	N 164	O 205	0
14	dA	1	Total 2280	C 1870	Mg 41	N 164	O 205	0
14	dA	1	Total 2280	C 1870	Mg 41	N 164	O 205	0
14	dA	1	Total 2280	C 1870	Mg 41	N 164	O 205	0
14	dA	1	Total 2280	C 1870	Mg 41	N 164	O 205	0
14	dA	1	Total 2280	C 1870	Mg 41	N 164	O 205	0
14	dA	1	Total 2280	C 1870	Mg 41	N 164	O 205	0
14	dA	1	Total 2280	C 1870	Mg 41	N 164	O 205	0

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Mol	Chain	Residues	Atoms					AltConf
14	dA	1	Total 2280	C 1870	Mg 41	N 164	O 205	0
14	dA	1	Total 2280	C 1870	Mg 41	N 164	O 205	0
14	dA	1	Total 2280	C 1870	Mg 41	N 164	O 205	0
14	dA	1	Total 2280	C 1870	Mg 41	N 164	O 205	0
14	dA	1	Total 2280	C 1870	Mg 41	N 164	O 205	0
14	dA	1	Total 2280	C 1870	Mg 41	N 164	O 205	0
14	dA	1	Total 2280	C 1870	Mg 41	N 164	O 205	0
14	dA	1	Total 2280	C 1870	Mg 41	N 164	O 205	0
14	dA	1	Total 2280	C 1870	Mg 41	N 164	O 205	0
14	dA	1	Total 2280	C 1870	Mg 41	N 164	O 205	0
14	dA	1	Total 2280	C 1870	Mg 41	N 164	O 205	0
14	dA	1	Total 2280	C 1870	Mg 41	N 164	O 205	0
14	dA	1	Total 2280	C 1870	Mg 41	N 164	O 205	0
14	dA	1	Total 2280	C 1870	Mg 41	N 164	O 205	0
14	dA	1	Total 2280	C 1870	Mg 41	N 164	O 205	0
14	dA	1	Total 2280	C 1870	Mg 41	N 164	O 205	0
14	dA	1	Total 2280	C 1870	Mg 41	N 164	O 205	0
14	dA	1	Total 2280	C 1870	Mg 41	N 164	O 205	0
14	dB	1	Total 2405	C 1985	Mg 42	N 168	O 210	0
14	dB	1	Total 2405	C 1985	Mg 42	N 168	O 210	0
14	dB	1	Total 2405	C 1985	Mg 42	N 168	O 210	0

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Mol	Chain	Residues	Atoms	AltConf
14	dB	1	Total C Mg N O 2405 1985 42 168 210	0
14	dB	1	Total C Mg N O 2405 1985 42 168 210	0
14	dB	1	Total C Mg N O 2405 1985 42 168 210	0
14	dB	1	Total C Mg N O 2405 1985 42 168 210	0
14	dB	1	Total C Mg N O 2405 1985 42 168 210	0
14	dB	1	Total C Mg N O 2405 1985 42 168 210	0
14	dB	1	Total C Mg N O 2405 1985 42 168 210	0
14	dB	1	Total C Mg N O 2405 1985 42 168 210	0
14	dB	1	Total C Mg N O 2405 1985 42 168 210	0
14	dB	1	Total C Mg N O 2405 1985 42 168 210	0
14	dB	1	Total C Mg N O 2405 1985 42 168 210	0
14	dB	1	Total C Mg N O 2405 1985 42 168 210	0
14	dB	1	Total C Mg N O 2405 1985 42 168 210	0
14	dB	1	Total C Mg N O 2405 1985 42 168 210	0
14	dB	1	Total C Mg N O 2405 1985 42 168 210	0
14	dB	1	Total C Mg N O 2405 1985 42 168 210	0
14	dB	1	Total C Mg N O 2405 1985 42 168 210	0
14	dB	1	Total C Mg N O 2405 1985 42 168 210	0
14	dB	1	Total C Mg N O 2405 1985 42 168 210	0
14	dB	1	Total C Mg N O 2405 1985 42 168 210	0
14	dB	1	Total C Mg N O 2405 1985 42 168 210	0

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Mol	Chain	Residues	Atoms	AltConf
14	dB	1	Total C Mg N O 2405 1985 42 168 210	0
14	dB	1	Total C Mg N O 2405 1985 42 168 210	0
14	dB	1	Total C Mg N O 2405 1985 42 168 210	0
14	dB	1	Total C Mg N O 2405 1985 42 168 210	0
14	dB	1	Total C Mg N O 2405 1985 42 168 210	0
14	dB	1	Total C Mg N O 2405 1985 42 168 210	0
14	dB	1	Total C Mg N O 2405 1985 42 168 210	0
14	dB	1	Total C Mg N O 2405 1985 42 168 210	0
14	dB	1	Total C Mg N O 2405 1985 42 168 210	0
14	dB	1	Total C Mg N O 2405 1985 42 168 210	0
14	dB	1	Total C Mg N O 2405 1985 42 168 210	0
14	dB	1	Total C Mg N O 2405 1985 42 168 210	0
14	dB	1	Total C Mg N O 2405 1985 42 168 210	0
14	dB	1	Total C Mg N O 2405 1985 42 168 210	0
14	dB	1	Total C Mg N O 2405 1985 42 168 210	0
14	dB	1	Total C Mg N O 2405 1985 42 168 210	0
14	dB	1	Total C Mg N O 2405 1985 42 168 210	0
14	dB	1	Total C Mg N O 2405 1985 42 168 210	0
14	dF	1	Total C Mg N O 96 76 2 8 10	0
14	dF	1	Total C Mg N O 96 76 2 8 10	0
14	dJ	1	Total C Mg N O 82 66 2 8 6	0

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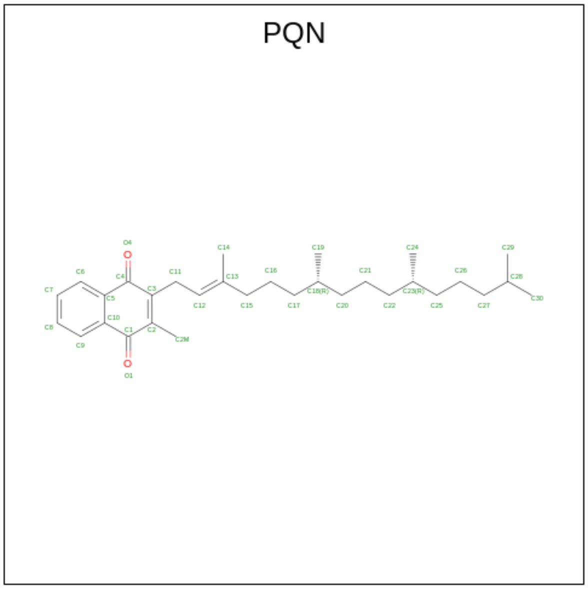
Mol	Chain	Residues	Atoms	AltConf
14	dJ	1	Total C Mg N O 82 66 2 8 6	0
14	dK	1	Total C Mg N O 86 68 2 8 8	0
14	dK	1	Total C Mg N O 86 68 2 8 8	0
14	dL	1	Total C Mg N O 299 249 5 20 25	0
14	dL	1	Total C Mg N O 299 249 5 20 25	0
14	dL	1	Total C Mg N O 299 249 5 20 25	0
14	dL	1	Total C Mg N O 299 249 5 20 25	0
14	dL	1	Total C Mg N O 299 249 5 20 25	0
14	dX	1	Total C Mg N O 45 35 1 4 5	0

- Molecule 15 is PHYLLOQUINONE (three-letter code: PQN) (formula: $C_{31}H_{46}O_2$).



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

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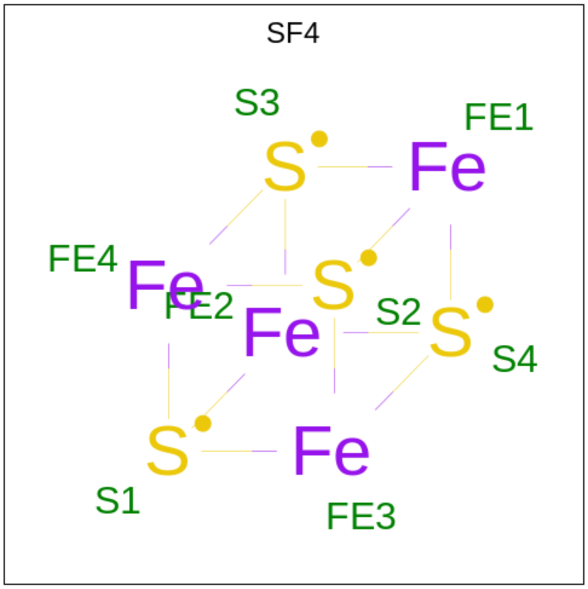
Mol	Chain	Residues	Atoms	AltConf
15	bA	1	Total C O 33 31 2	0
15	bB	1	Total C O 33 31 2	0
15	cA	1	Total C O 33 31 2	0
15	cB	1	Total C O 33 31 2	0
15	dA	1	Total C O 33 31 2	0
15	dB	1	Total C O 33 31 2	0

- Molecule 16 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms	AltConf
16	aA	1	Total Fe S 8 4 4	0
16	aC	1	Total Fe S 16 8 8	0
16	aC	1	Total Fe S 16 8 8	0
16	bA	1	Total Fe S 8 4 4	0
16	bC	1	Total Fe S 16 8 8	0

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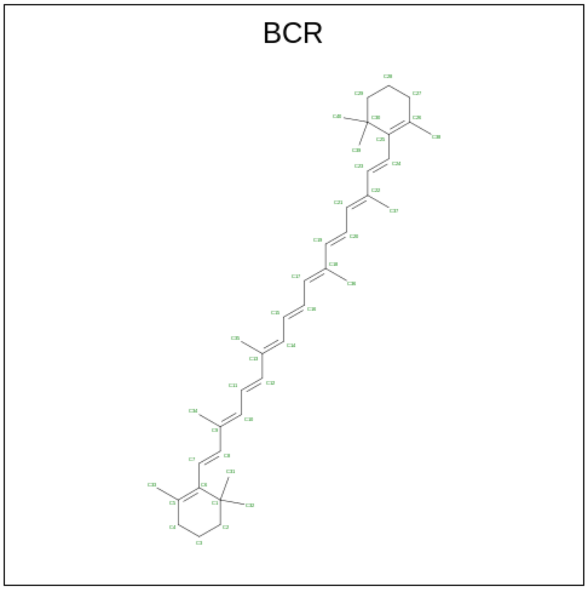
Mol	Chain	Residues	Atoms	AltConf
16	bC	1	Total Fe S 16 8 8	0
16	cA	1	Total Fe S 8 4 4	0
16	cC	1	Total Fe S 16 8 8	0
16	cC	1	Total Fe S 16 8 8	0
16	dA	1	Total Fe S 8 4 4	0
16	dC	1	Total Fe S 16 8 8	0
16	dC	1	Total Fe S 16 8 8	0

- Molecule 17 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms	AltConf
17	aA	1	Total C 240 240	0
17	aA	1	Total C 240 240	0
17	aA	1	Total C 240 240	0
17	aA	1	Total C 240 240	0

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Mol	Chain	Residues	Atoms	AltConf
17	aA	1	Total C 240 240	0
17	aA	1	Total C 240 240	0
17	aB	1	Total C 280 280	0
17	aB	1	Total C 280 280	0
17	aB	1	Total C 280 280	0
17	aB	1	Total C 280 280	0
17	aB	1	Total C 280 280	0
17	aB	1	Total C 280 280	0
17	aB	1	Total C 280 280	0
17	aF	1	Total C 80 80	0
17	aF	1	Total C 80 80	0
17	aI	1	Total C 40 40	0
17	aJ	1	Total C 80 80	0
17	aJ	1	Total C 80 80	0
17	aL	1	Total C 120 120	0
17	aL	1	Total C 120 120	0
17	aL	1	Total C 120 120	0
17	aM	1	Total C 40 40	0
17	bA	1	Total C 200 200	0
17	bA	1	Total C 200 200	0
17	bA	1	Total C 200 200	0

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Mol	Chain	Residues	Atoms	AltConf
17	bA	1	Total C 200 200	0
17	bA	1	Total C 200 200	0
17	bB	1	Total C 280 280	0
17	bB	1	Total C 280 280	0
17	bB	1	Total C 280 280	0
17	bB	1	Total C 280 280	0
17	bB	1	Total C 280 280	0
17	bB	1	Total C 280 280	0
17	bB	1	Total C 280 280	0
17	bF	1	Total C 80 80	0
17	bF	1	Total C 80 80	0
17	bI	1	Total C 40 40	0
17	bJ	1	Total C 80 80	0
17	bJ	1	Total C 80 80	0
17	bK	1	Total C 40 40	0
17	bL	1	Total C 120 120	0
17	bL	1	Total C 120 120	0
17	bL	1	Total C 120 120	0
17	bM	1	Total C 40 40	0
17	cA	1	Total C 240 240	0
17	cA	1	Total C 240 240	0

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Mol	Chain	Residues	Atoms	AltConf
17	cA	1	Total C 240 240	0
17	cA	1	Total C 240 240	0
17	cA	1	Total C 240 240	0
17	cA	1	Total C 240 240	0
17	cB	1	Total C 280 280	0
17	cB	1	Total C 280 280	0
17	cB	1	Total C 280 280	0
17	cB	1	Total C 280 280	0
17	cB	1	Total C 280 280	0
17	cB	1	Total C 280 280	0
17	cB	1	Total C 280 280	0
17	cF	1	Total C 80 80	0
17	cF	1	Total C 80 80	0
17	cI	1	Total C 40 40	0
17	cJ	1	Total C 80 80	0
17	cJ	1	Total C 80 80	0
17	cL	1	Total C 120 120	0
17	cL	1	Total C 120 120	0
17	cL	1	Total C 120 120	0
17	cM	1	Total C 40 40	0
17	dA	1	Total C 200 200	0

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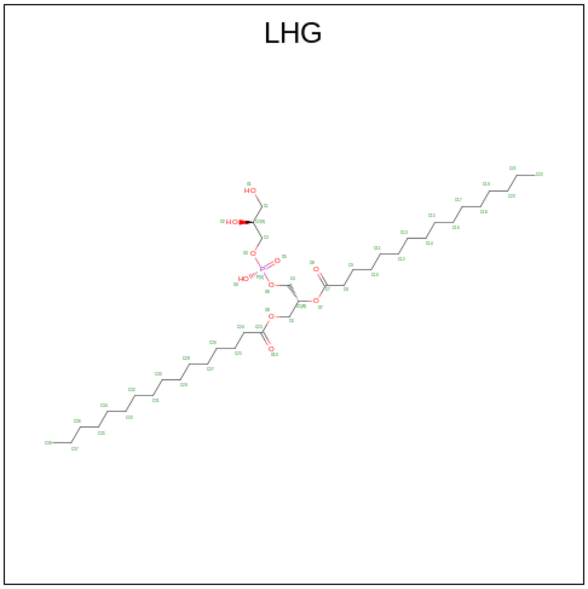
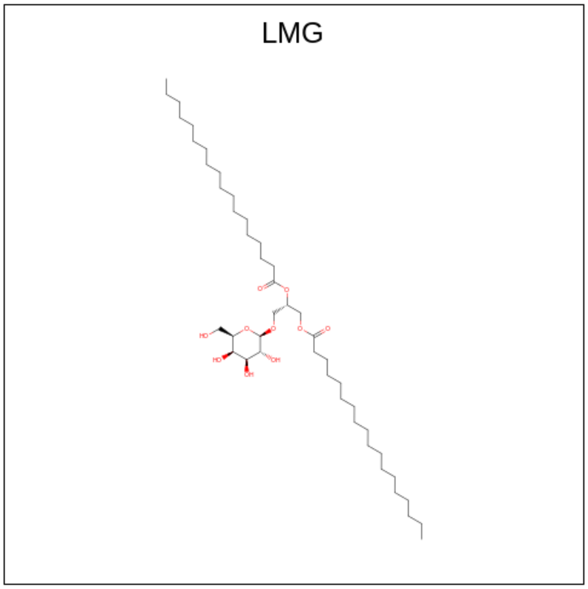
Mol	Chain	Residues	Atoms	AltConf
17	dA	1	Total C 200 200	0
17	dA	1	Total C 200 200	0
17	dA	1	Total C 200 200	0
17	dA	1	Total C 200 200	0
17	dB	1	Total C 280 280	0
17	dB	1	Total C 280 280	0
17	dB	1	Total C 280 280	0
17	dB	1	Total C 280 280	0
17	dB	1	Total C 280 280	0
17	dB	1	Total C 280 280	0
17	dB	1	Total C 280 280	0
17	dF	1	Total C 80 80	0
17	dF	1	Total C 80 80	0
17	dI	1	Total C 40 40	0
17	dJ	1	Total C 80 80	0
17	dJ	1	Total C 80 80	0
17	dK	1	Total C 40 40	0
17	dL	1	Total C 120 120	0
17	dL	1	Total C 120 120	0
17	dL	1	Total C 120 120	0
17	dM	1	Total C 40 40	0

- Molecule 18 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
18	aA	1	76	54	20	2	0
18	aA	1	76	54	20	2	0
18	aB	1	23	12	10	1	0
18	bA	1	76	54	20	2	0
18	bA	1	76	54	20	2	0
18	bB	1	23	12	10	1	0
18	cA	1	76	54	20	2	0
18	cA	1	76	54	20	2	0
18	cB	1	23	12	10	1	0
18	dA	1	76	54	20	2	0
18	dA	1	76	54	20	2	0
18	dB	1	23	12	10	1	0

- Molecule 19 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



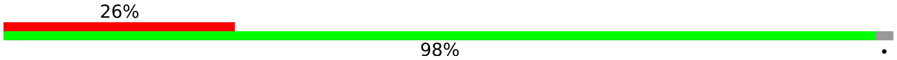
Mol	Chain	Residues	Atoms	AltConf
19	aB	1	Total C O 55 45 10	0
19	bB	1	Total C O 55 45 10	0
19	cB	1	Total C O 55 45 10	0
19	dB	1	Total C O 55 45 10	0

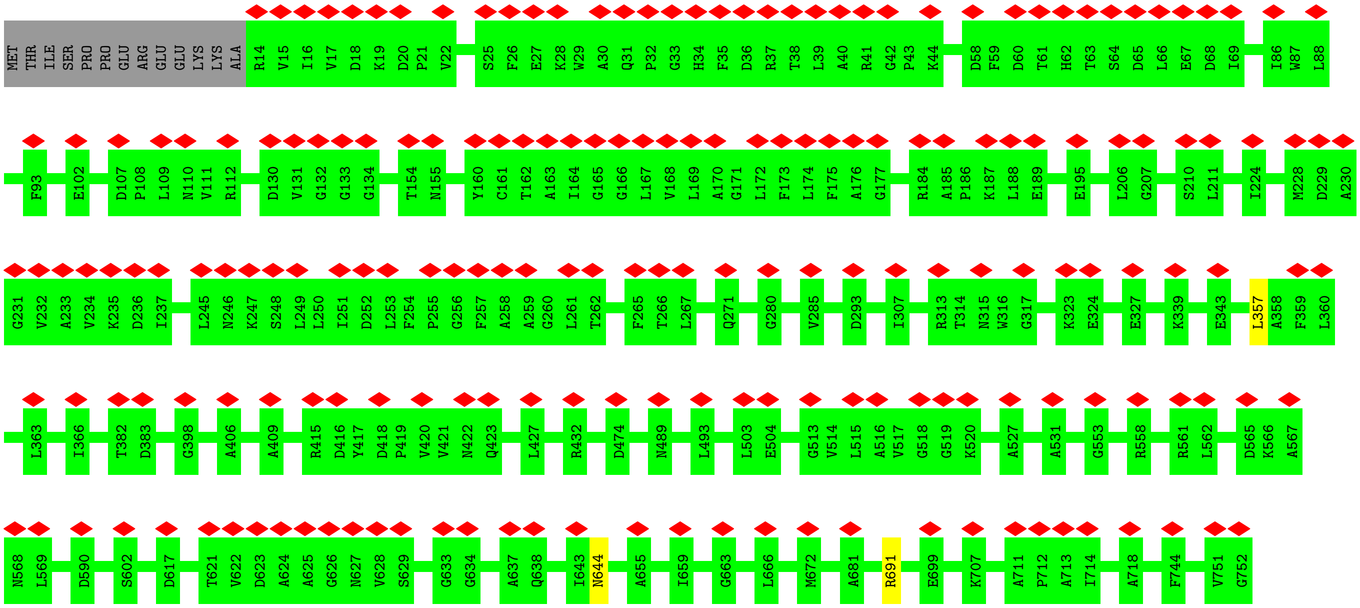
3 Residue-property plots ⓘ

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

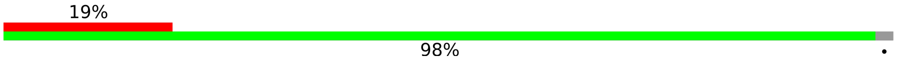
Chain aA:

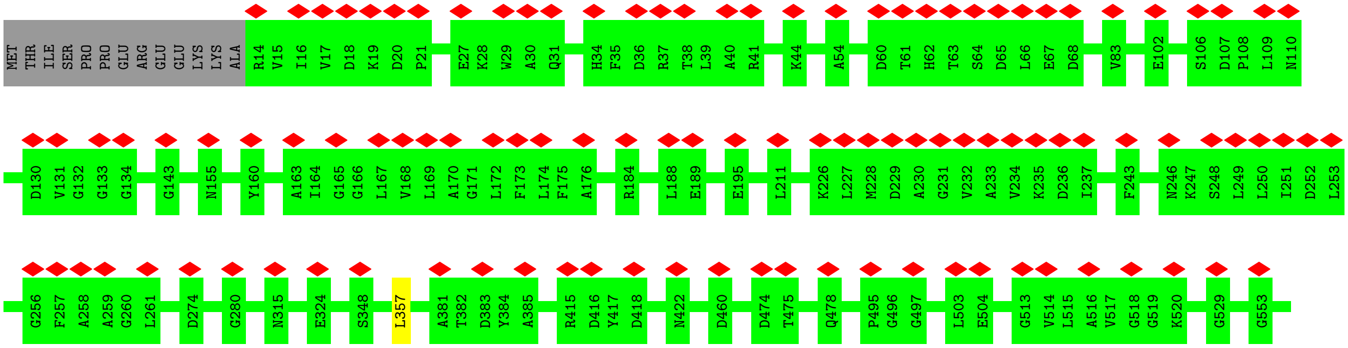


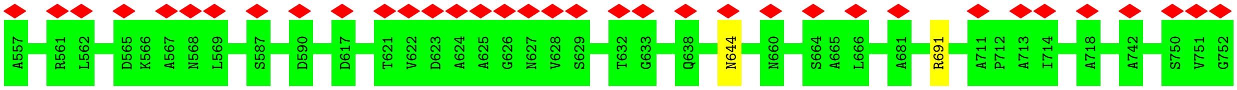


- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

Chain bA:

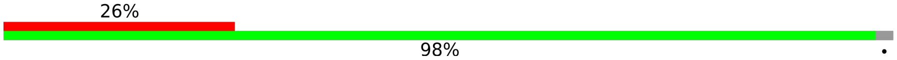


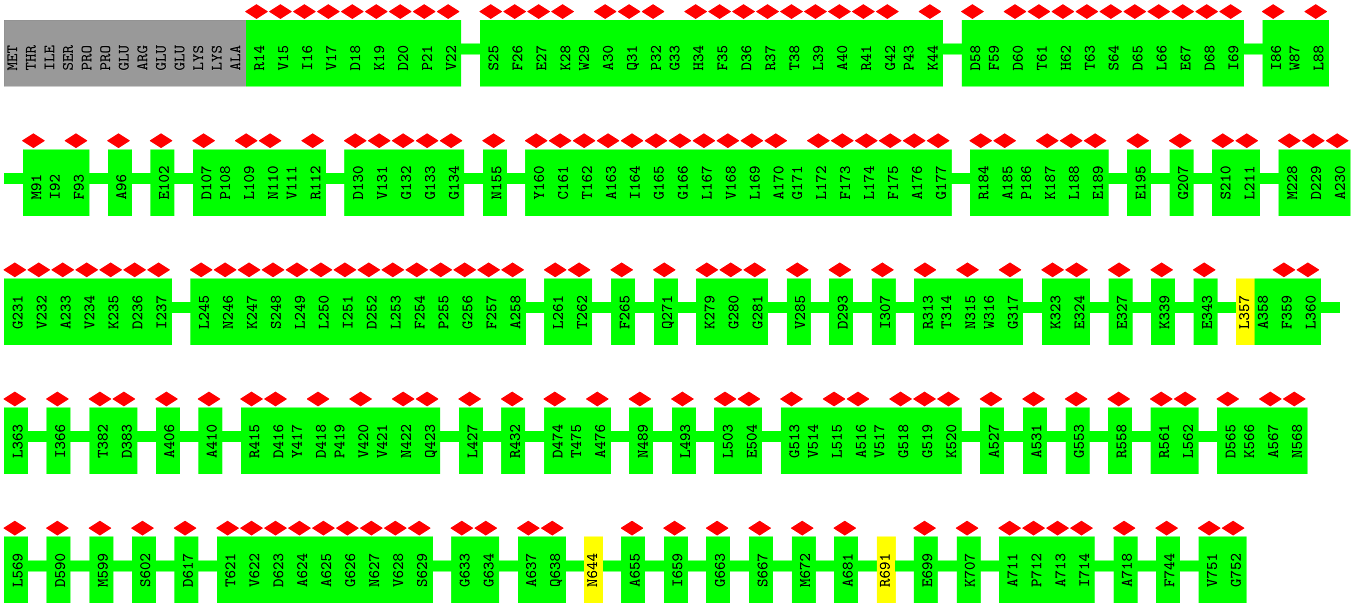




- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

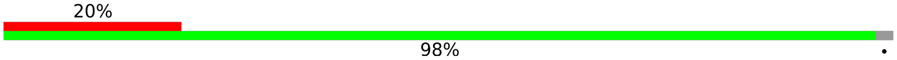
Chain cA:

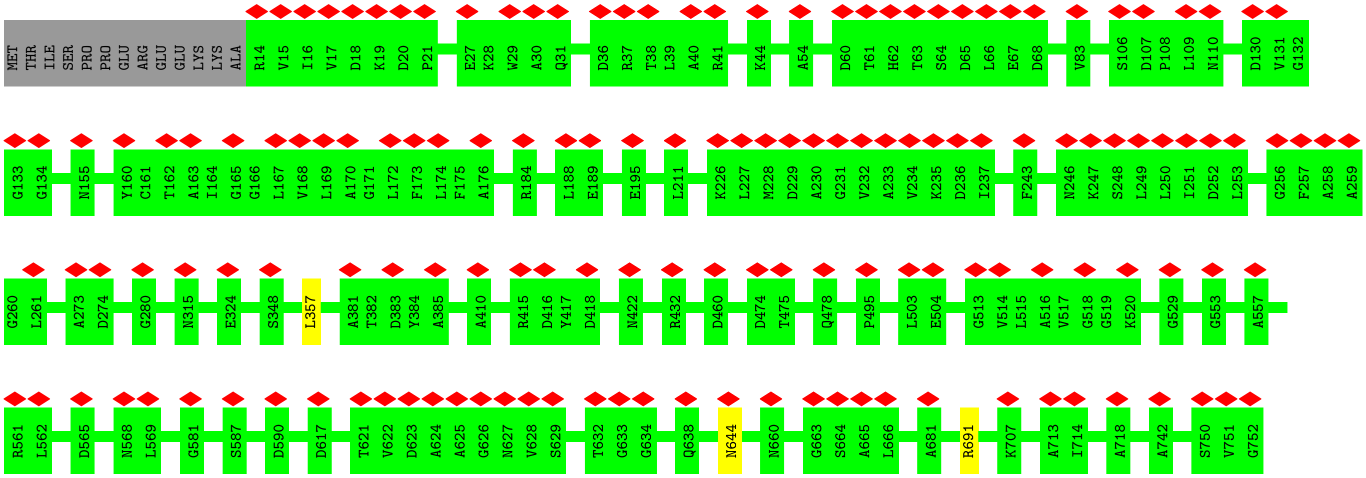




- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

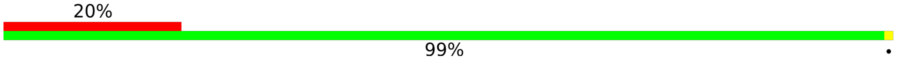
Chain dA:

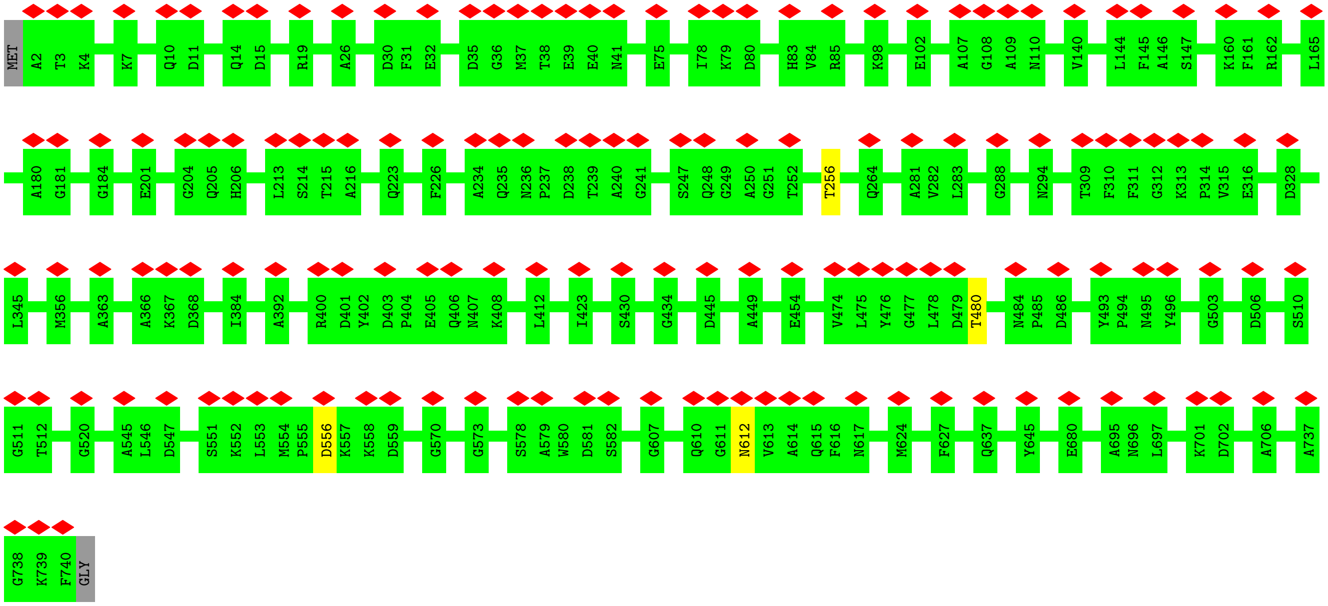




- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2 1

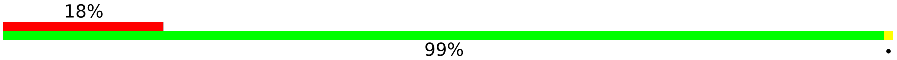
Chain aB:

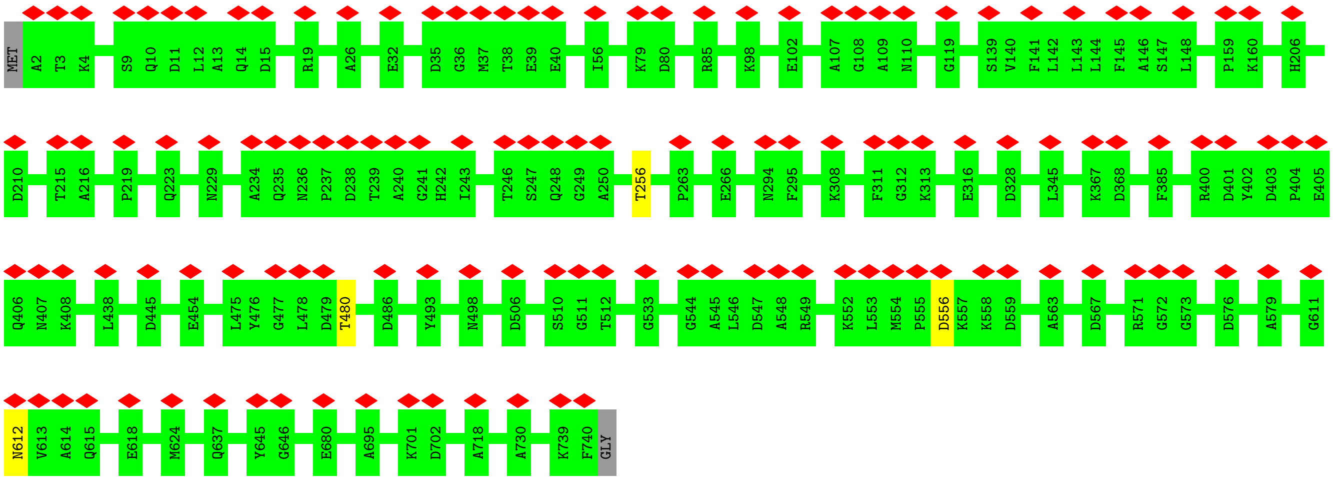




- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2 1

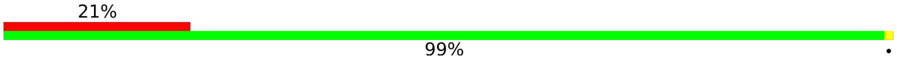
Chain bB:

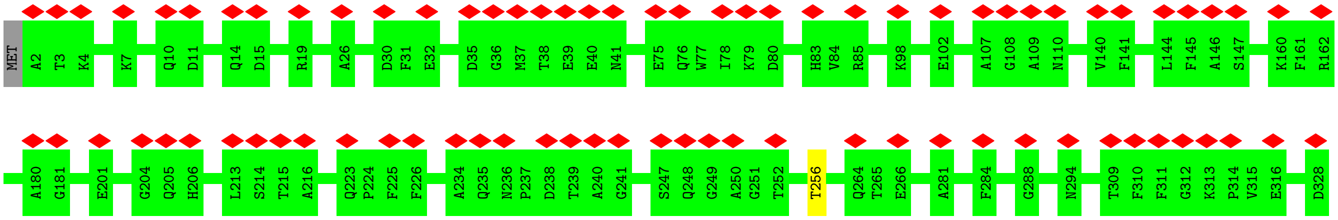


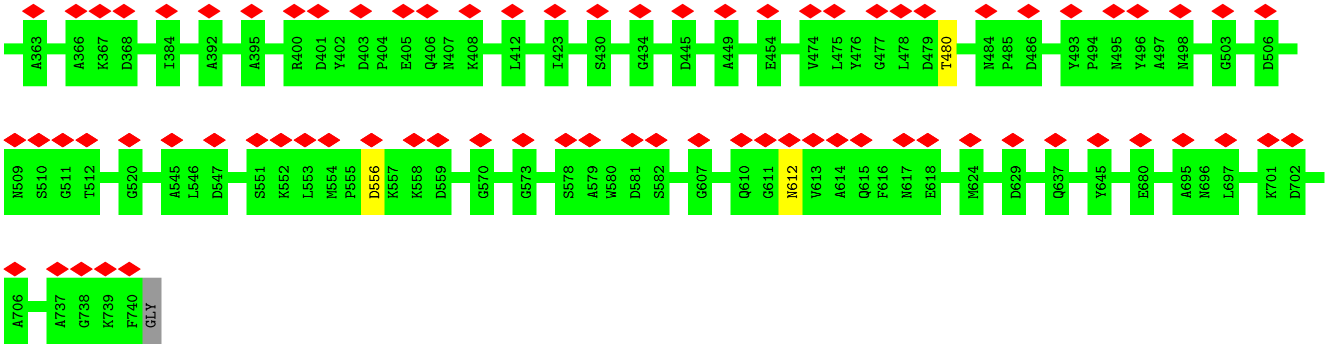


- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2 1

Chain cB:

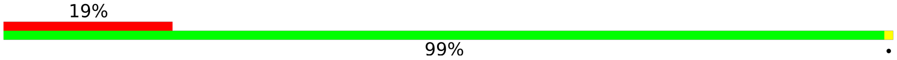


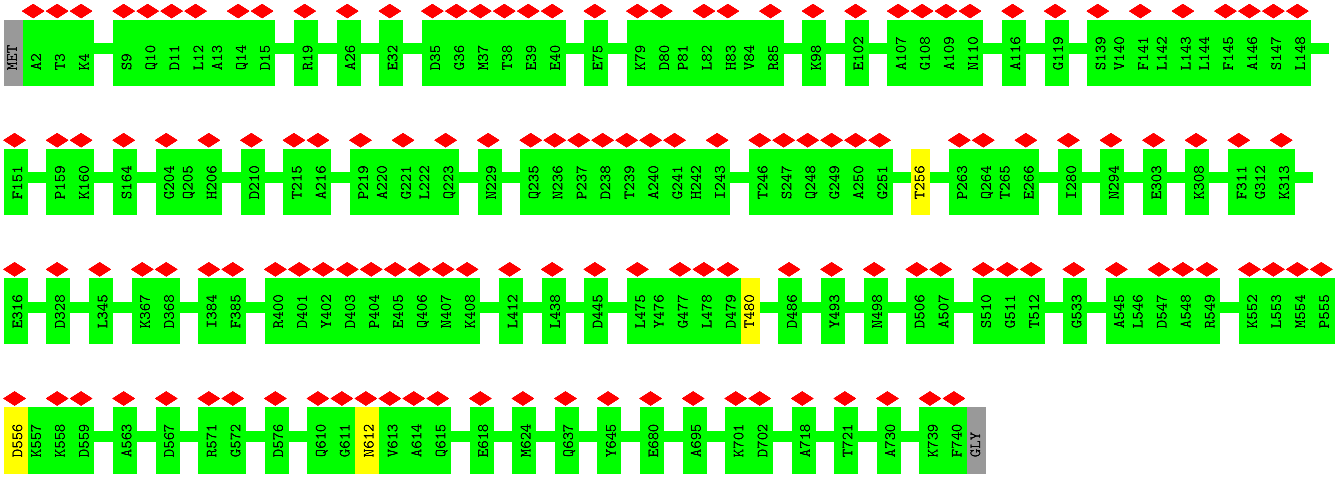




- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2 1

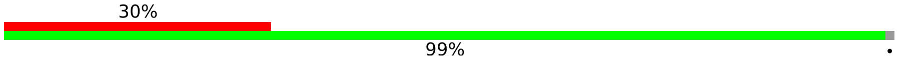
Chain dB:

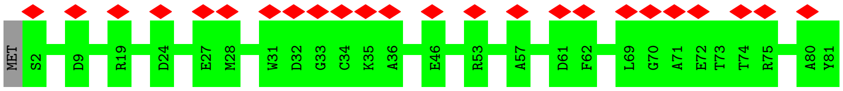




- Molecule 3: Photosystem I iron-sulfur center

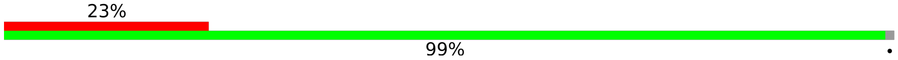
Chain aC:

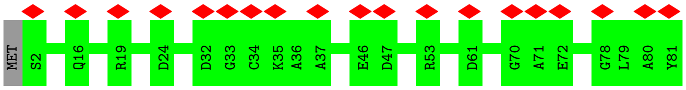




- Molecule 3: Photosystem I iron-sulfur center

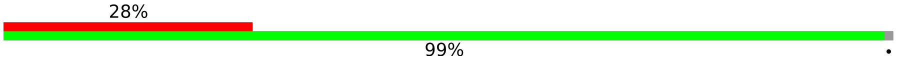
Chain bC:

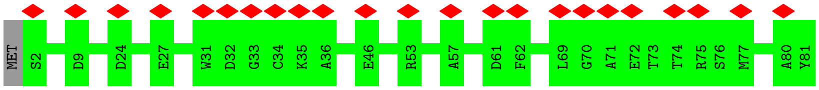




- Molecule 3: Photosystem I iron-sulfur center

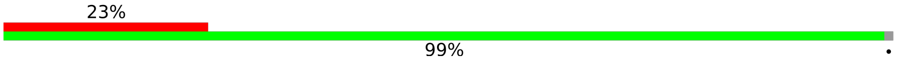
Chain cC:

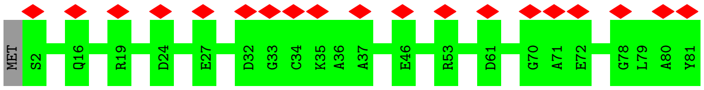




- Molecule 3: Photosystem I iron-sulfur center

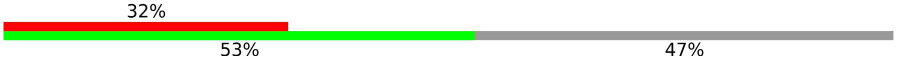
Chain dC:

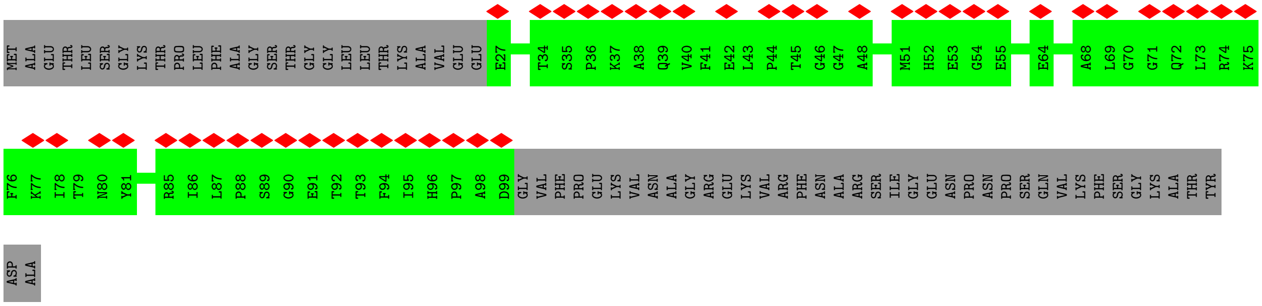




- Molecule 4: Photosystem I reaction center subunit II

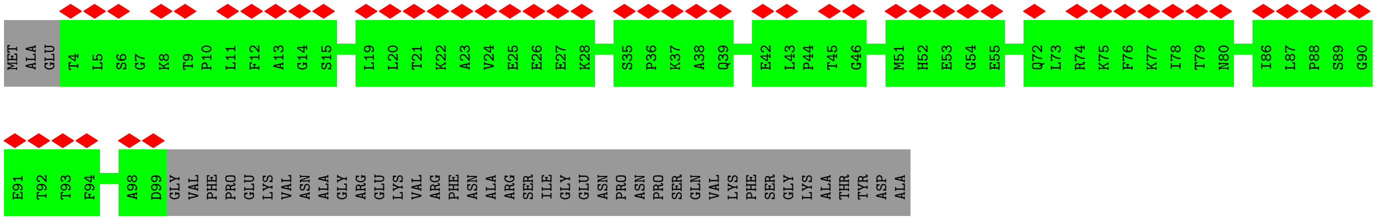
Chain aD:





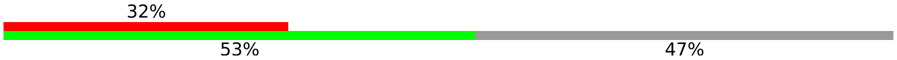
- Molecule 4: Photosystem I reaction center subunit II

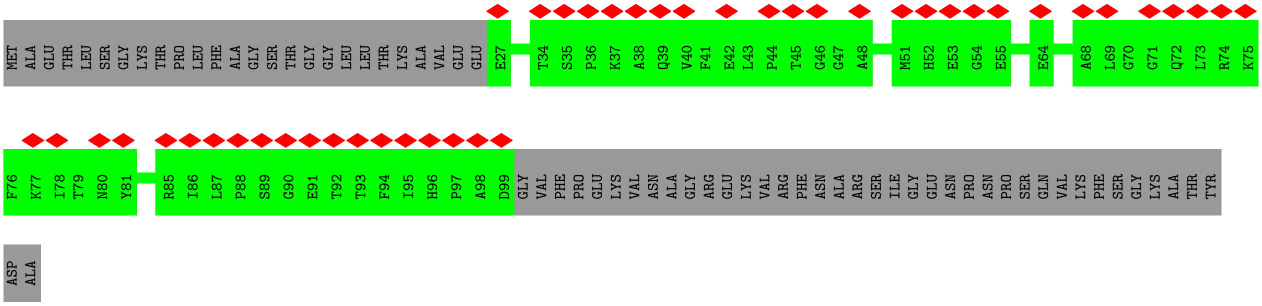
Chain bD:



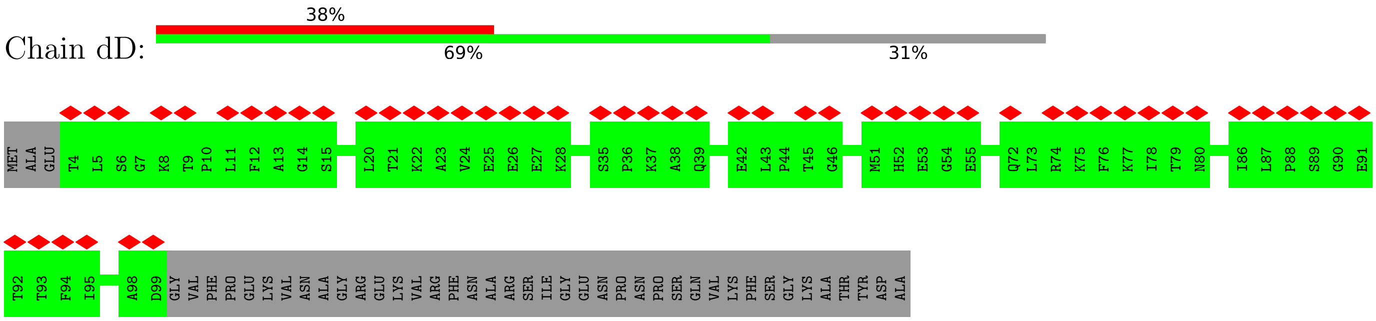
- Molecule 4: Photosystem I reaction center subunit II

Chain cD:

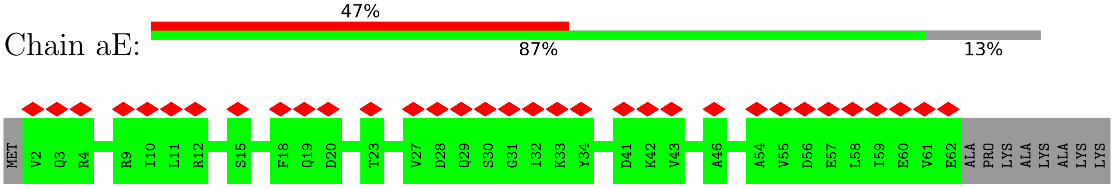




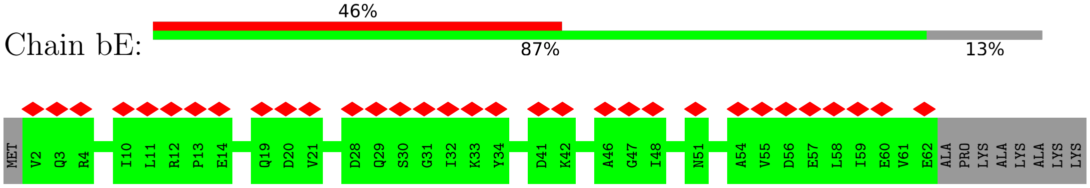
- Molecule 4: Photosystem I reaction center subunit II



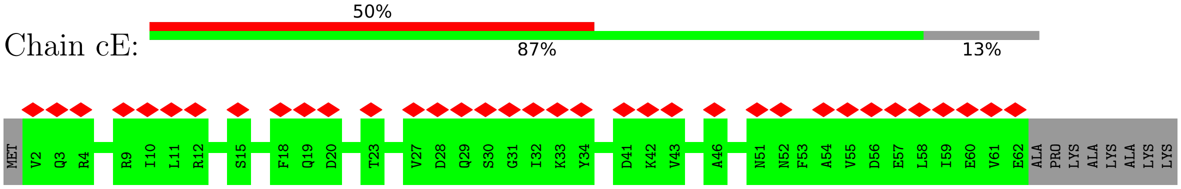
- Molecule 5: Photosystem I reaction center subunit IV



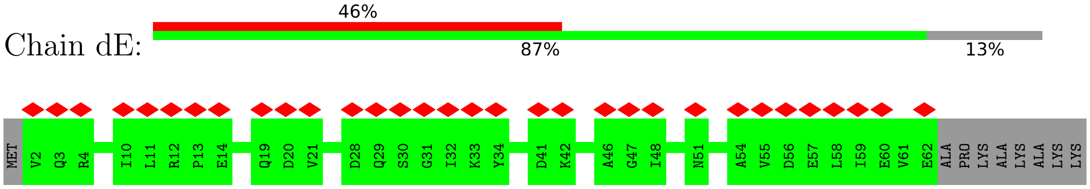
- Molecule 5: Photosystem I reaction center subunit IV



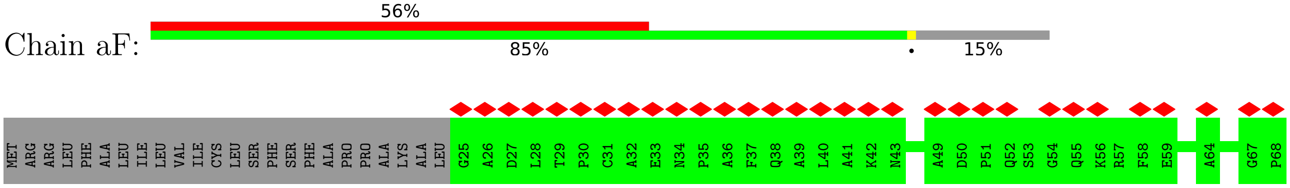
- Molecule 5: Photosystem I reaction center subunit IV

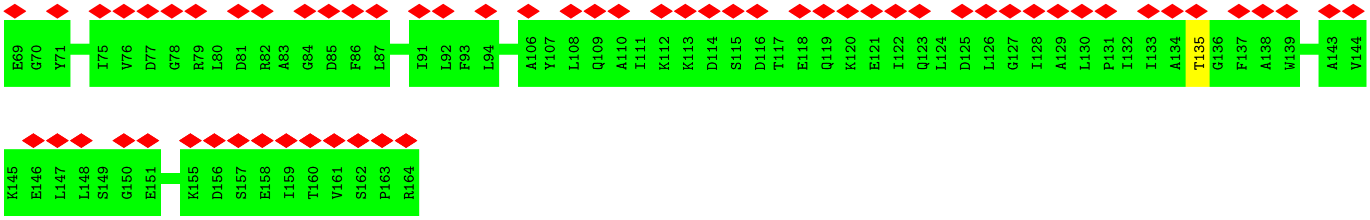


- Molecule 5: Photosystem I reaction center subunit IV



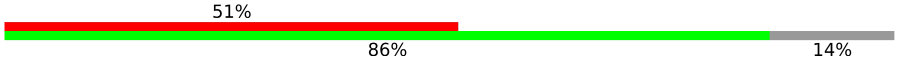
- Molecule 6: Photosystem I reaction center subunit III

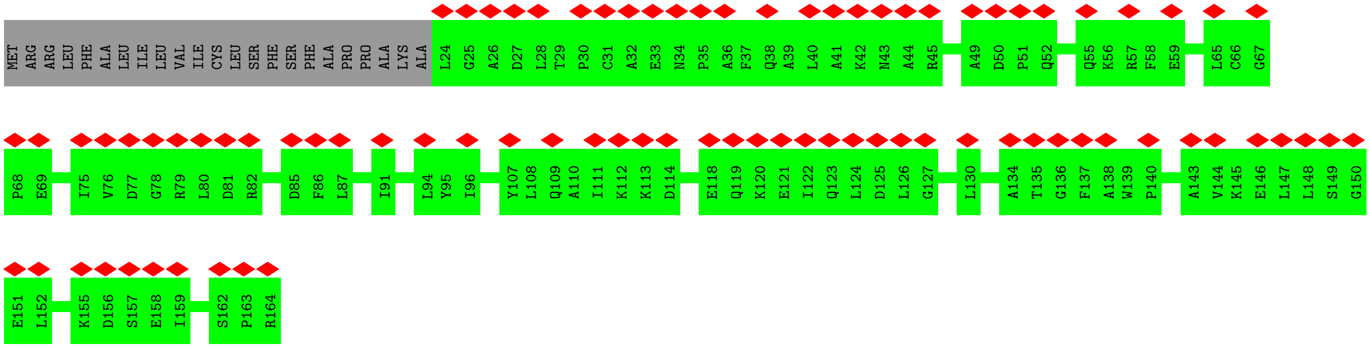




- Molecule 6: Photosystem I reaction center subunit III

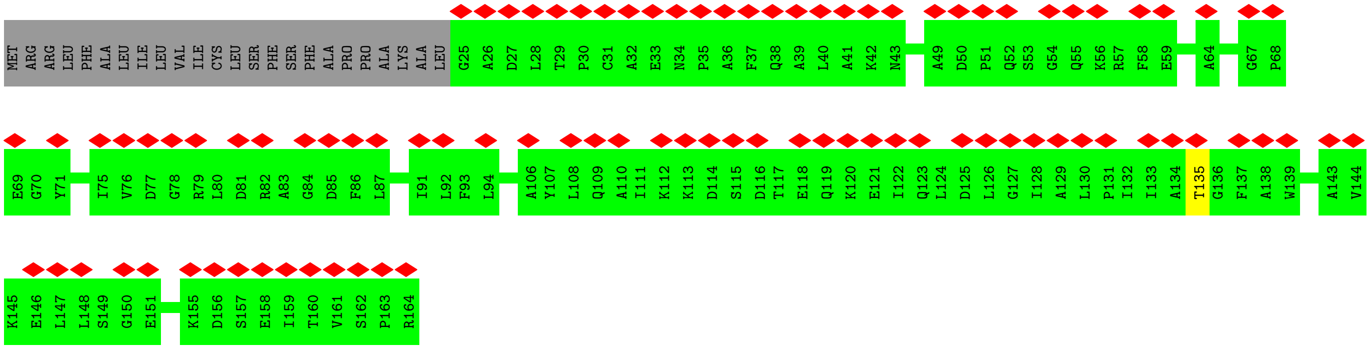
Chain bF:





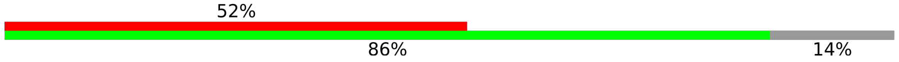
- Molecule 6: Photosystem I reaction center subunit III

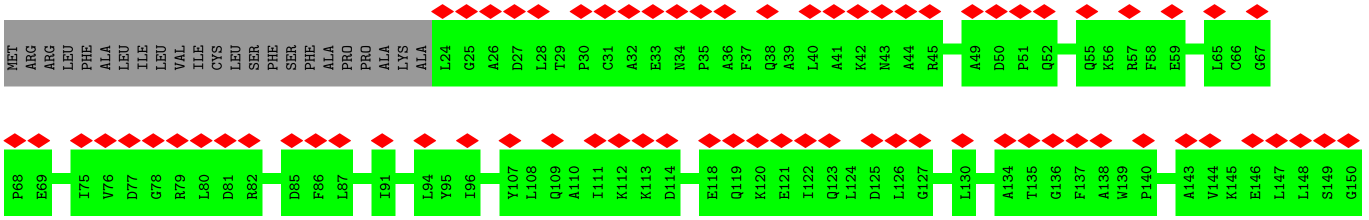
Chain cF:

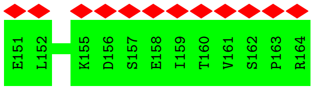


- Molecule 6: Photosystem I reaction center subunit III

Chain dF:

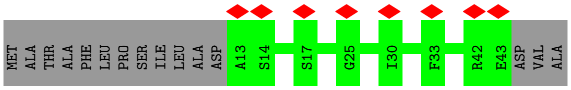






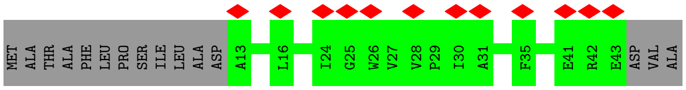
- Molecule 7: Photosystem I reaction center subunit VIII

Chain aI:



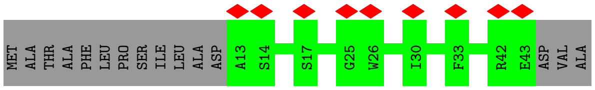
- Molecule 7: Photosystem I reaction center subunit VIII

Chain bI:



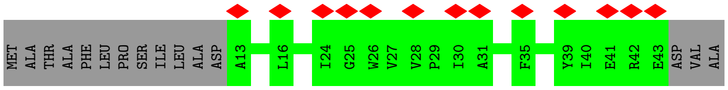
- Molecule 7: Photosystem I reaction center subunit VIII

Chain cI:



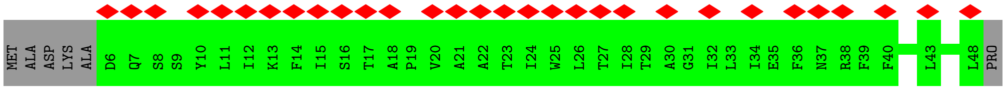
- Molecule 7: Photosystem I reaction center subunit VIII

Chain dI:



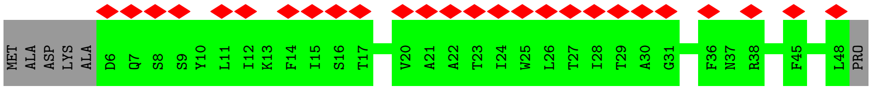
- Molecule 8: Photosystem I reaction center subunit IX

Chain aJ:



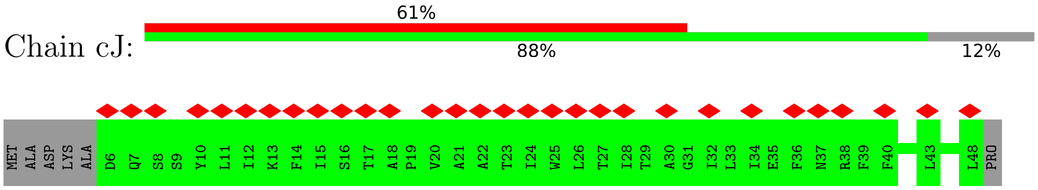
- Molecule 8: Photosystem I reaction center subunit IX

Chain bJ:



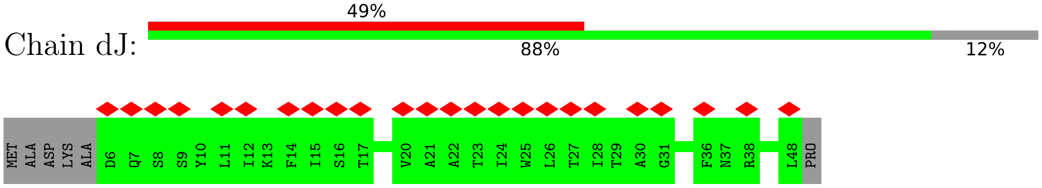
- Molecule 8: Photosystem I reaction center subunit IX

Chain cJ:



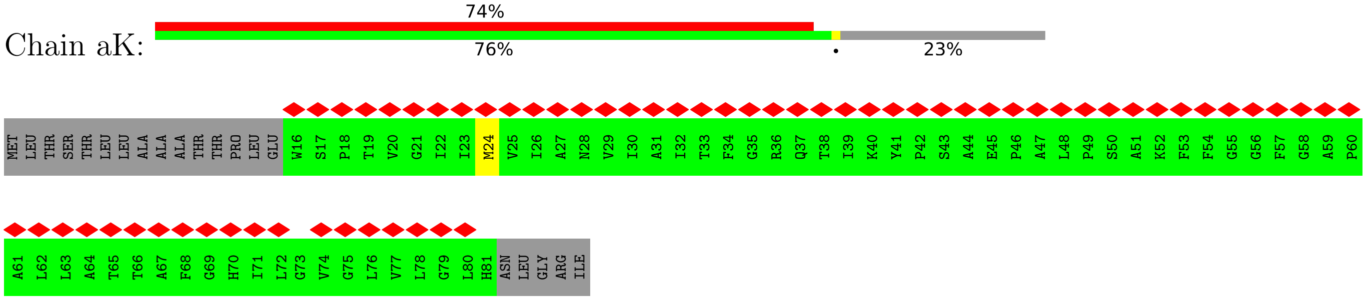
- Molecule 8: Photosystem I reaction center subunit IX

Chain dJ:



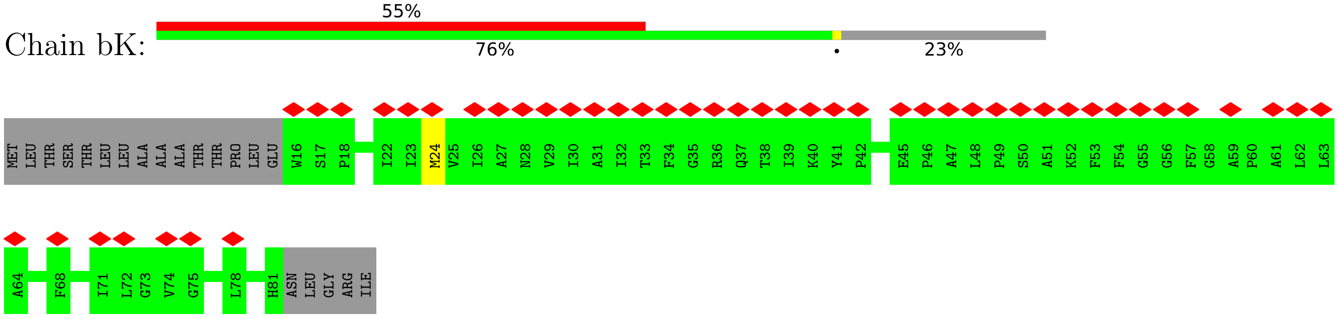
- Molecule 9: Photosystem I reaction center subunit PsaK 1

Chain aK:



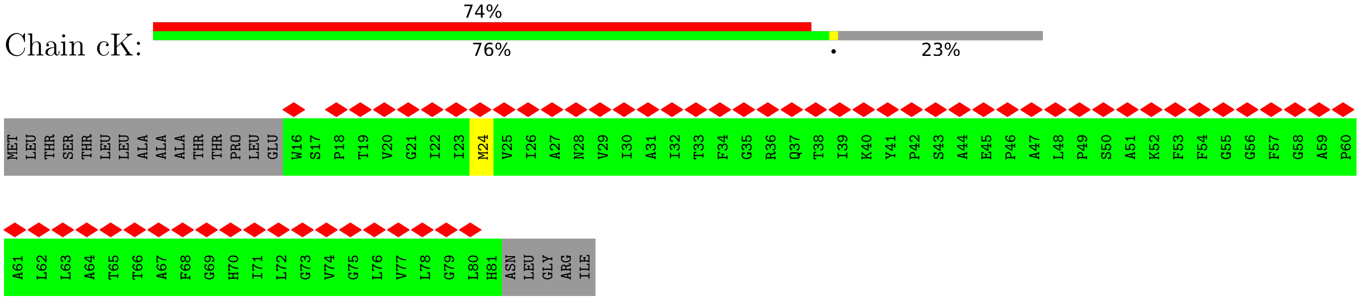
- Molecule 9: Photosystem I reaction center subunit PsaK 1

Chain bK:



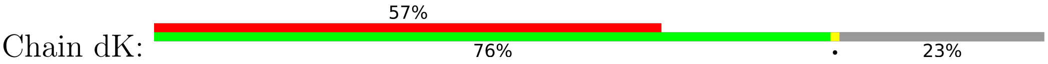
- Molecule 9: Photosystem I reaction center subunit PsaK 1

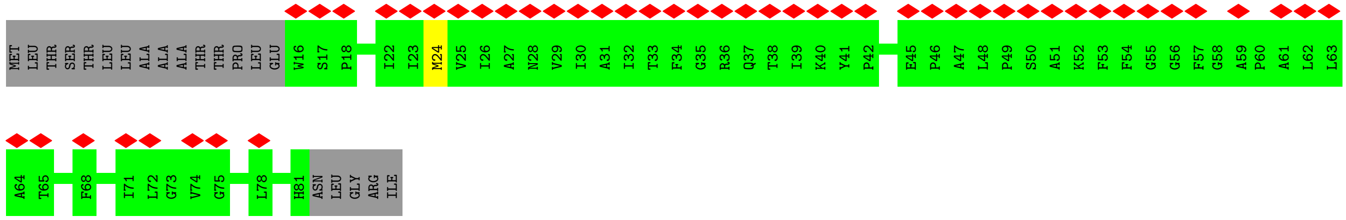
Chain cK:



- Molecule 9: Photosystem I reaction center subunit PsaK 1

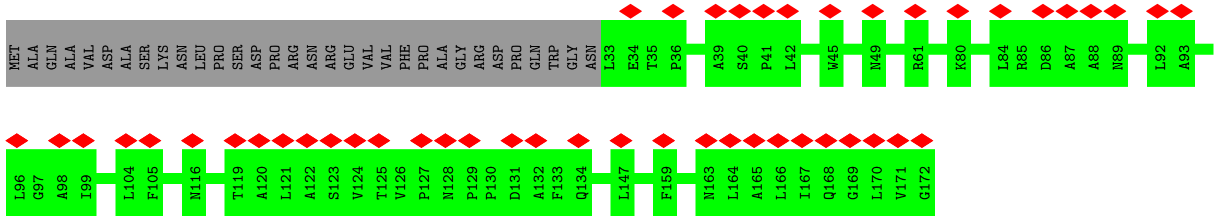
Chain dK:





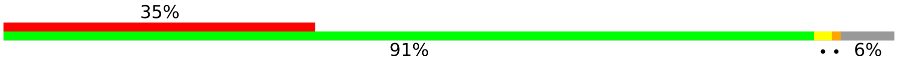
- Molecule 10: Photosystem I reaction center subunit XI

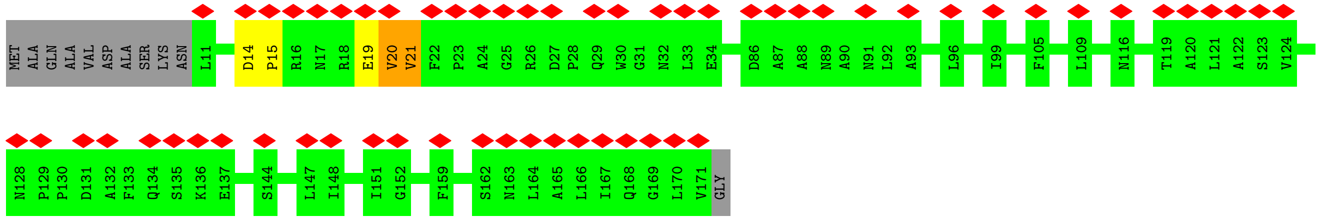
Chain aL:



- Molecule 10: Photosystem I reaction center subunit XI

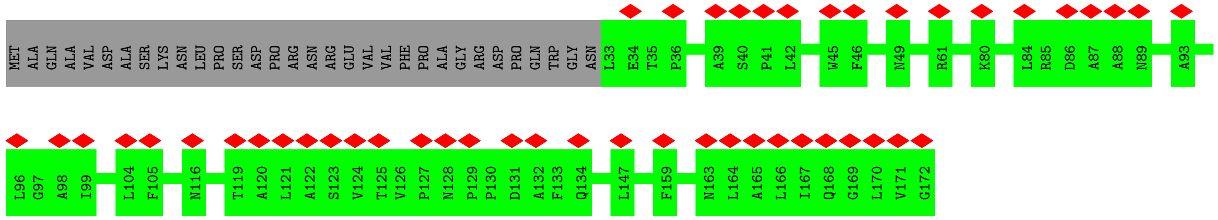
Chain bL:





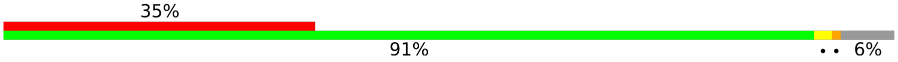
- Molecule 10: Photosystem I reaction center subunit XI

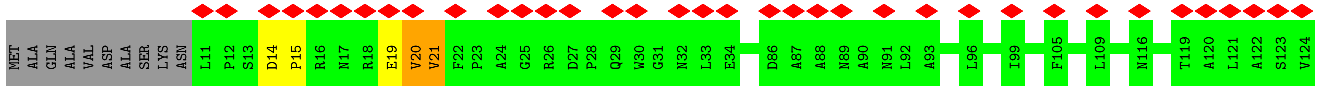
Chain cL:

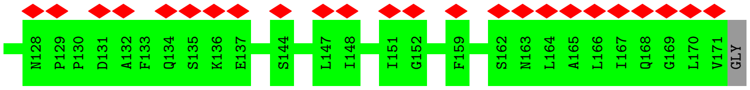


- Molecule 10: Photosystem I reaction center subunit XI

Chain dL:

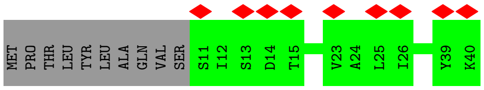






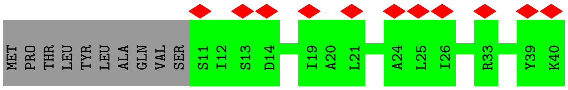
- Molecule 11: Photosystem I reaction center subunit XII

Chain aM:



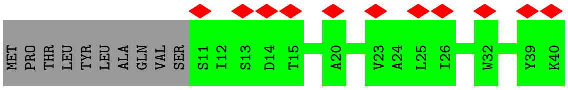
- Molecule 11: Photosystem I reaction center subunit XII

Chain bM:



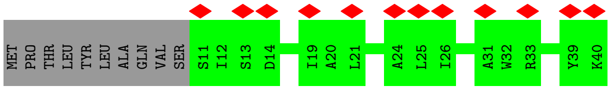
- Molecule 11: Photosystem I reaction center subunit XII

Chain cM:



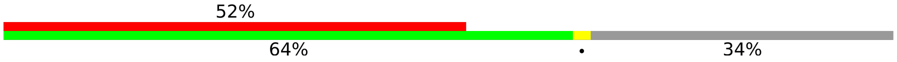
- Molecule 11: Photosystem I reaction center subunit XII

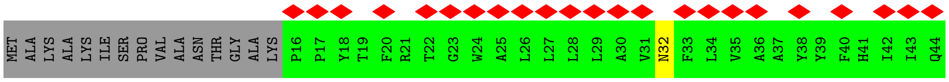
Chain dM:



- Molecule 12: Photosystem I 4.8 kDa protein

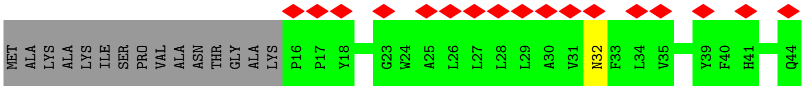
Chain aX:



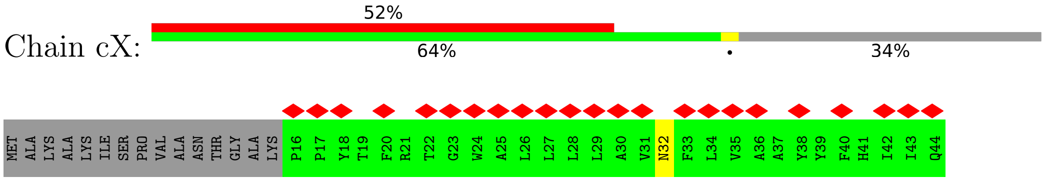


- Molecule 12: Photosystem I 4.8 kDa protein

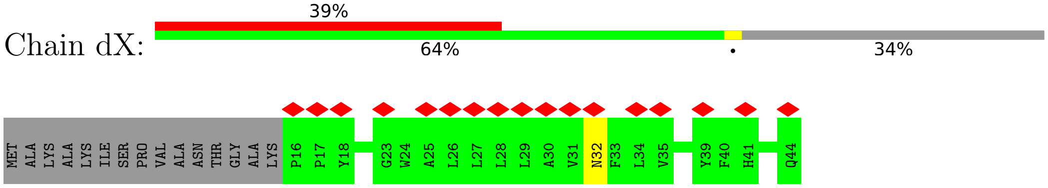
Chain bX:



- Molecule 12: Photosystem I 4.8 kDa protein



- Molecule 12: Photosystem I 4.8 kDa protein



4 Experimental information ⓘ

Property	**Value**	**Source**
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	111400	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 $(e^-/\text{Å}^2)$	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.260	Depositor
Minimum map value	-0.129	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.06	Depositor
Map size (Å)	492.8, 492.8, 492.8	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.12, 1.12, 1.12	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	aA	0.40	0/6000	0.52	1/8187 (0.0%)
1	bA	0.40	0/6000	0.52	1/8187 (0.0%)
1	cA	0.40	0/6000	0.52	1/8187 (0.0%)
1	dA	0.40	0/6000	0.52	1/8187 (0.0%)
2	aB	0.44	0/6143	0.55	1/8398 (0.0%)
2	bB	0.44	0/6143	0.55	1/8398 (0.0%)
2	cB	0.44	0/6143	0.55	1/8398 (0.0%)
2	dB	0.44	0/6143	0.55	1/8398 (0.0%)
3	aC	0.37	0/609	0.54	0/826
3	bC	0.37	0/609	0.54	0/826
3	cC	0.37	0/609	0.54	0/826
3	dC	0.37	0/609	0.54	0/826
4	aD	0.33	0/596	0.53	0/806
4	bD	0.36	0/757	0.58	0/1024
4	cD	0.33	0/596	0.53	0/806
4	dD	0.36	0/757	0.58	0/1024
5	aE	0.41	0/499	0.50	0/677
5	bE	0.41	0/499	0.50	0/677
5	cE	0.41	0/499	0.50	0/677
5	dE	0.41	0/499	0.50	0/677
6	aF	0.33	0/1096	0.55	0/1489
6	bF	0.37	0/1104	0.61	0/1500
6	cF	0.33	0/1096	0.55	0/1489
6	dF	0.37	0/1104	0.61	0/1500
7	aI	0.40	0/262	0.59	0/358
7	bI	0.40	0/262	0.59	0/358
7	cI	0.40	0/262	0.59	0/358
7	dI	0.39	0/262	0.59	0/358
8	aJ	0.33	0/358	0.51	0/490
8	bJ	0.34	0/358	0.51	0/490
8	cJ	0.34	0/358	0.51	0/490
8	dJ	0.33	0/358	0.51	0/490

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
9	aK	0.34	0/494	0.70	0/675
9	bK	0.34	0/494	0.70	0/675
9	cK	0.34	0/494	0.70	0/675
9	dK	0.34	0/494	0.70	0/675
10	aL	0.38	0/1067	0.58	0/1462
10	bL	0.41	0/1247	0.67	1/1710 (0.1%)
10	cL	0.38	0/1067	0.58	0/1462
10	dL	0.41	0/1247	0.68	1/1710 (0.1%)
11	aM	0.32	0/239	0.50	0/326
11	bM	0.32	0/239	0.50	0/326
11	cM	0.32	0/239	0.50	0/326
11	dM	0.32	0/239	0.50	0/326
12	aX	0.37	0/253	0.44	0/347
12	bX	0.37	0/253	0.44	0/347
12	cX	0.37	0/253	0.44	0/347
12	dX	0.37	0/253	0.45	0/347
All	All	0.41	0/71162	0.55	10/97118 (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
2	aB	0	1
2	bB	0	1
2	cB	0	1
2	dB	0	1
6	aF	0	1
6	cF	0	1
10	bL	0	3
10	dL	0	3
All	All	0	12

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	dL	21	VAL	CG1-CB-CG2	-9.94	95.00	110.90
10	bL	21	VAL	CG1-CB-CG2	-9.93	95.01	110.90
2	bB	556	ASP	CB-CG-OD1	5.99	123.69	118.30
2	cB	556	ASP	CB-CG-OD1	5.92	123.63	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	aB	556	ASP	CB-CG-OD1	5.92	123.63	118.30

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	aB	480	THR	Peptide
6	aF	135	THR	Peptide
2	bB	480	THR	Peptide
10	bL	14	ASP	Peptide
10	bL	19	GLU	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	aA	5801	0	5667	0	0
1	bA	5801	0	5667	0	0
1	cA	5801	0	5667	0	0
1	dA	5801	0	5667	0	0
2	aB	5919	0	5675	0	0
2	bB	5919	0	5675	0	0
2	cB	5919	0	5675	0	0
2	dB	5919	0	5675	0	0
3	aC	599	0	577	0	0
3	bC	599	0	577	0	0
3	cC	599	0	577	0	0
3	dC	599	0	577	0	0
4	aD	581	0	584	0	0
4	bD	740	0	751	0	0
4	cD	581	0	584	0	0
4	dD	740	0	751	0	0
5	aE	490	0	484	0	0
5	bE	490	0	484	0	0
5	cE	490	0	484	0	0
5	dE	490	0	484	0	0
6	aF	1072	0	1065	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	bF	1080	0	1076	0	0
6	cF	1072	0	1065	0	0
6	dF	1080	0	1076	0	0
7	aI	253	0	255	0	0
7	bI	253	0	255	0	0
7	cI	253	0	255	0	0
7	dI	253	0	255	0	0
8	aJ	347	0	352	0	0
8	bJ	347	0	352	0	0
8	cJ	347	0	352	0	0
8	dJ	347	0	352	0	0
9	aK	480	0	501	0	0
9	bK	480	0	501	0	0
9	cK	480	0	501	0	0
9	dK	480	0	501	0	0
10	aL	1037	0	1051	0	0
10	bL	1210	0	1213	0	0
10	cL	1037	0	1051	0	0
10	dL	1210	0	1213	0	0
11	aM	235	0	251	0	0
11	bM	235	0	251	0	0
11	cM	235	0	251	0	0
11	dM	235	0	251	0	0
12	aX	243	0	244	0	0
12	bX	243	0	244	0	0
12	cX	243	0	244	0	0
12	dX	243	0	244	0	0
13	aA	65	0	72	0	0
13	bA	65	0	72	0	0
13	cA	65	0	72	0	0
13	dA	65	0	72	0	0
14	aA	2332	0	2197	0	0
14	aB	2340	0	2282	0	0
14	aF	96	0	74	0	0
14	aJ	82	0	58	0	0
14	aK	86	0	62	0	0
14	aL	182	0	187	0	0
14	aX	45	0	33	0	0
14	bA	2280	0	2154	0	0
14	bB	2405	0	2354	0	0
14	bF	96	0	74	0	0
14	bJ	82	0	58	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	bK	86	0	62	0	0
14	bL	299	0	301	0	0
14	bX	45	0	33	0	0
14	cA	2332	0	2197	0	0
14	cB	2340	0	2282	0	0
14	cF	96	0	74	0	0
14	cJ	82	0	58	0	0
14	cK	86	0	62	0	0
14	cL	182	0	187	0	0
14	cX	45	0	33	0	0
14	dA	2280	0	2154	0	0
14	dB	2405	0	2354	0	0
14	dF	96	0	74	0	0
14	dJ	82	0	58	0	0
14	dK	86	0	62	0	0
14	dL	299	0	301	0	0
14	dX	45	0	33	0	0
15	aA	33	0	46	0	0
15	aB	33	0	46	0	0
15	bA	33	0	46	0	0
15	bB	33	0	46	0	0
15	cA	33	0	46	0	0
15	cB	33	0	46	0	0
15	dA	33	0	46	0	0
15	dB	33	0	46	0	0
16	aA	8	0	0	0	0
16	aC	16	0	0	0	0
16	bA	8	0	0	0	0
16	bC	16	0	0	0	0
16	cA	8	0	0	0	0
16	cC	16	0	0	0	0
16	dA	8	0	0	0	0
16	dC	16	0	0	0	0
17	aA	240	0	336	0	0
17	aB	280	0	392	0	0
17	aF	80	0	112	0	0
17	aI	40	0	56	0	0
17	aJ	80	0	112	0	0
17	aL	120	0	168	0	0
17	aM	40	0	56	0	0
17	bA	200	0	280	0	0
17	bB	280	0	392	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	bF	80	0	112	0	0
17	bI	40	0	56	0	0
17	bJ	80	0	112	0	0
17	bK	40	0	56	0	0
17	bL	120	0	168	0	0
17	bM	40	0	56	0	0
17	cA	240	0	336	0	0
17	cB	280	0	392	0	0
17	cF	80	0	112	0	0
17	cI	40	0	56	0	0
17	cJ	80	0	112	0	0
17	cL	120	0	168	0	0
17	cM	40	0	56	0	0
17	dA	200	0	280	0	0
17	dB	280	0	392	0	0
17	dF	80	0	112	0	0
17	dI	40	0	56	0	0
17	dJ	80	0	112	0	0
17	dK	40	0	56	0	0
17	dL	120	0	168	0	0
17	dM	40	0	56	0	0
18	aA	76	0	98	0	0
18	aB	23	0	16	0	0
18	bA	76	0	98	0	0
18	bB	23	0	16	0	0
18	cA	76	0	98	0	0
18	cB	23	0	16	0	0
18	dA	76	0	98	0	0
18	dB	23	0	16	0	0
19	aB	55	0	86	0	0
19	bB	55	0	86	0	0
19	cB	55	0	86	0	0
19	dB	55	0	86	0	0
All	All	94576	0	93746	0	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

There are no clashes within the asymmetric unit.

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	aA	737/752 (98%)	704 (96%)	33 (4%)	0	100	100
1	bA	737/752 (98%)	703 (95%)	34 (5%)	0	100	100
1	cA	737/752 (98%)	704 (96%)	33 (4%)	0	100	100
1	dA	737/752 (98%)	703 (95%)	34 (5%)	0	100	100
2	aB	737/741 (100%)	707 (96%)	30 (4%)	0	100	100
2	bB	737/741 (100%)	707 (96%)	30 (4%)	0	100	100
2	cB	737/741 (100%)	707 (96%)	30 (4%)	0	100	100
2	dB	737/741 (100%)	707 (96%)	30 (4%)	0	100	100
3	aC	78/81 (96%)	74 (95%)	4 (5%)	0	100	100
3	bC	78/81 (96%)	74 (95%)	4 (5%)	0	100	100
3	cC	78/81 (96%)	74 (95%)	4 (5%)	0	100	100
3	dC	78/81 (96%)	74 (95%)	4 (5%)	0	100	100
4	aD	71/139 (51%)	69 (97%)	2 (3%)	0	100	100
4	bD	94/139 (68%)	89 (95%)	5 (5%)	0	100	100
4	cD	71/139 (51%)	69 (97%)	2 (3%)	0	100	100
4	dD	94/139 (68%)	89 (95%)	5 (5%)	0	100	100
5	aE	59/70 (84%)	53 (90%)	6 (10%)	0	100	100
5	bE	59/70 (84%)	53 (90%)	6 (10%)	0	100	100
5	cE	59/70 (84%)	53 (90%)	6 (10%)	0	100	100
5	dE	59/70 (84%)	53 (90%)	6 (10%)	0	100	100
6	aF	138/164 (84%)	129 (94%)	9 (6%)	0	100	100
6	bF	139/164 (85%)	131 (94%)	8 (6%)	0	100	100
6	cF	138/164 (84%)	130 (94%)	8 (6%)	0	100	100
6	dF	139/164 (85%)	131 (94%)	8 (6%)	0	100	100
7	aI	29/46 (63%)	28 (97%)	1 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	bI	29/46 (63%)	28 (97%)	1 (3%)	0	100	100
7	cI	29/46 (63%)	28 (97%)	1 (3%)	0	100	100
7	dI	29/46 (63%)	28 (97%)	1 (3%)	0	100	100
8	aJ	41/49 (84%)	41 (100%)	0	0	100	100
8	bJ	41/49 (84%)	41 (100%)	0	0	100	100
8	cJ	41/49 (84%)	41 (100%)	0	0	100	100
8	dJ	41/49 (84%)	41 (100%)	0	0	100	100
9	aK	64/86 (74%)	55 (86%)	9 (14%)	0	100	100
9	bK	64/86 (74%)	55 (86%)	9 (14%)	0	100	100
9	cK	64/86 (74%)	55 (86%)	9 (14%)	0	100	100
9	dK	64/86 (74%)	55 (86%)	9 (14%)	0	100	100
10	aL	138/172 (80%)	134 (97%)	4 (3%)	0	100	100
10	bL	159/172 (92%)	145 (91%)	12 (8%)	2 (1%)	12	40
10	cL	138/172 (80%)	134 (97%)	4 (3%)	0	100	100
10	dL	159/172 (92%)	144 (91%)	13 (8%)	2 (1%)	12	40
11	aM	28/40 (70%)	28 (100%)	0	0	100	100
11	bM	28/40 (70%)	28 (100%)	0	0	100	100
11	cM	28/40 (70%)	28 (100%)	0	0	100	100
11	dM	28/40 (70%)	28 (100%)	0	0	100	100
12	aX	27/44 (61%)	27 (100%)	0	0	100	100
12	bX	27/44 (61%)	27 (100%)	0	0	100	100
12	cX	27/44 (61%)	27 (100%)	0	0	100	100
12	dX	27/44 (61%)	27 (100%)	0	0	100	100
All	All	8678/9536 (91%)	8260 (95%)	414 (5%)	4 (0%)	100	100

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	bL	15	PRO
10	dL	15	PRO
10	dL	21	VAL
10	bL	21	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	aA	593/605 (98%)	591 (100%)	2 (0%)	92	96
1	bA	593/605 (98%)	591 (100%)	2 (0%)	92	96
1	cA	593/605 (98%)	591 (100%)	2 (0%)	92	96
1	dA	593/605 (98%)	591 (100%)	2 (0%)	92	96
2	aB	601/602 (100%)	599 (100%)	2 (0%)	92	96
2	bB	601/602 (100%)	599 (100%)	2 (0%)	92	96
2	cB	601/602 (100%)	599 (100%)	2 (0%)	92	96
2	dB	601/602 (100%)	599 (100%)	2 (0%)	92	96
3	aC	68/69 (99%)	68 (100%)	0	100	100
3	bC	68/69 (99%)	68 (100%)	0	100	100
3	cC	68/69 (99%)	68 (100%)	0	100	100
3	dC	68/69 (99%)	68 (100%)	0	100	100
4	aD	59/110 (54%)	59 (100%)	0	100	100
4	bD	76/110 (69%)	76 (100%)	0	100	100
4	cD	59/110 (54%)	59 (100%)	0	100	100
4	dD	76/110 (69%)	76 (100%)	0	100	100
5	aE	54/60 (90%)	54 (100%)	0	100	100
5	bE	54/60 (90%)	54 (100%)	0	100	100
5	cE	54/60 (90%)	54 (100%)	0	100	100
5	dE	54/60 (90%)	54 (100%)	0	100	100
6	aF	109/129 (84%)	109 (100%)	0	100	100
6	bF	110/129 (85%)	110 (100%)	0	100	100
6	cF	109/129 (84%)	109 (100%)	0	100	100
6	dF	110/129 (85%)	110 (100%)	0	100	100
7	aI	28/39 (72%)	28 (100%)	0	100	100
7	bI	28/39 (72%)	28 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	cI	28/39 (72%)	28 (100%)	0	100	100
7	dI	28/39 (72%)	28 (100%)	0	100	100
8	aJ	38/42 (90%)	38 (100%)	0	100	100
8	bJ	38/42 (90%)	38 (100%)	0	100	100
8	cJ	38/42 (90%)	38 (100%)	0	100	100
8	dJ	38/42 (90%)	38 (100%)	0	100	100
9	aK	48/64 (75%)	47 (98%)	1 (2%)	53	75
9	bK	48/64 (75%)	47 (98%)	1 (2%)	53	75
9	cK	48/64 (75%)	47 (98%)	1 (2%)	53	75
9	dK	48/64 (75%)	47 (98%)	1 (2%)	53	75
10	aL	105/131 (80%)	105 (100%)	0	100	100
10	bL	124/131 (95%)	123 (99%)	1 (1%)	81	89
10	cL	105/131 (80%)	105 (100%)	0	100	100
10	dL	124/131 (95%)	123 (99%)	1 (1%)	81	89
11	aM	25/34 (74%)	25 (100%)	0	100	100
11	bM	25/34 (74%)	25 (100%)	0	100	100
11	cM	25/34 (74%)	25 (100%)	0	100	100
11	dM	25/34 (74%)	25 (100%)	0	100	100
12	aX	24/34 (71%)	23 (96%)	1 (4%)	30	60
12	bX	24/34 (71%)	23 (96%)	1 (4%)	30	60
12	cX	24/34 (71%)	23 (96%)	1 (4%)	30	60
12	dX	24/34 (71%)	23 (96%)	1 (4%)	30	60
All	All	7082/7676 (92%)	7056 (100%)	26 (0%)	91	95

5 of 26 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	cA	691	ARG
9	cK	24	MET
10	dL	20	VAL
2	cB	612	ASN
12	cX	32	ASN

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

Mol	Chain	Res	Type
2	dB	114	ASN
2	dB	354	GLN
2	dB	640	ASN
2	bB	407	ASN
2	bB	262	HIS

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 ⓘ

504 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	cB	804	-	65,73,73	1.39	9 (13%)	76,113,113	1.80	12 (15%)
14	CLA	bA	819	1	65,73,73	1.44	9 (13%)	76,113,113	1.55	9 (11%)
14	CLA	bA	828	1	65,73,73	1.42	8 (12%)	76,113,113	1.59	10 (13%)
14	CLA	cB	838	2	65,73,73	1.43	7 (10%)	76,113,113	1.61	9 (11%)
14	CLA	dB	814	2	65,73,73	1.43	10 (15%)	76,113,113	1.52	9 (11%)
14	CLA	dB	834	2	58,66,73	1.55	8 (13%)	67,104,113	1.48	9 (13%)
14	CLA	dA	838	1	65,73,73	1.47	9 (13%)	76,113,113	1.52	9 (11%)
17	BCR	aB	845	-	41,41,41	1.17	3 (7%)	56,56,56	1.17	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
14	CLA	cA	840	1	65,73,73	1.46	10 (15%)	76,113,113	1.49	7 (9%)
17	BCR	bK	102	-	41,41,41	1.20	3 (7%)	56,56,56	1.42	10 (17%)
14	CLA	aB	804	-	65,73,73	1.39	9 (13%)	76,113,113	1.80	12 (15%)
14	CLA	cA	816	-	49,57,73	1.69	6 (12%)	55,93,113	1.65	7 (12%)
14	CLA	aB	830	2	45,53,73	1.77	9 (20%)	52,89,113	1.59	6 (11%)
16	SF4	cC	102	3	0,12,12	-	-	-		
18	LHG	bB	851	-	22,22,48	0.89	1 (4%)	25,28,54	1.20	1 (4%)
14	CLA	cA	832	1	65,73,73	1.45	10 (15%)	76,113,113	1.48	10 (13%)
14	CLA	bA	838	1	65,73,73	1.47	9 (13%)	76,113,113	1.51	9 (11%)
15	PQN	bB	843	-	34,34,34	1.53	2 (5%)	42,45,45	1.20	4 (9%)
14	CLA	cA	842	-	65,73,73	1.49	10 (15%)	76,113,113	1.45	7 (9%)
14	CLA	bB	814	2	65,73,73	1.43	10 (15%)	76,113,113	1.52	9 (11%)
14	CLA	aA	802	-	45,53,73	1.68	8 (17%)	52,89,113	1.84	6 (11%)
14	CLA	dK	103	-	45,53,73	1.73	8 (17%)	52,89,113	1.66	6 (11%)
14	CLA	cA	815	1	45,53,73	1.78	8 (17%)	52,89,113	1.72	6 (11%)
14	CLA	aA	810	1	45,53,73	1.70	6 (13%)	52,89,113	1.65	6 (11%)
14	CLA	dA	840	1	65,73,73	1.46	10 (15%)	76,113,113	1.50	7 (9%)
17	BCR	bL	208	-	41,41,41	1.12	2 (4%)	56,56,56	1.38	10 (17%)
14	CLA	aA	820	1	61,69,73	1.52	8 (13%)	71,108,113	1.50	7 (9%)
17	BCR	dA	845	-	41,41,41	1.14	3 (7%)	56,56,56	1.29	8 (14%)
17	BCR	bB	849	-	41,41,41	1.21	2 (4%)	56,56,56	1.17	4 (7%)
17	BCR	aL	201	-	41,41,41	1.23	3 (7%)	56,56,56	1.26	5 (8%)
18	LHG	aA	853	14	26,26,48	0.86	1 (3%)	29,32,54	1.31	3 (10%)
14	CLA	cK	101	9	42,49,73	1.74	7 (16%)	48,83,113	1.68	6 (12%)
17	BCR	dA	847	-	41,41,41	1.17	2 (4%)	56,56,56	1.22	3 (5%)
14	CLA	aA	829	1	65,73,73	1.47	10 (15%)	76,113,113	1.38	7 (9%)
14	CLA	dB	812	2	45,53,73	1.71	8 (17%)	52,89,113	1.68	7 (13%)
14	CLA	bA	807	1	51,59,73	1.63	7 (13%)	59,96,113	1.61	6 (10%)
14	CLA	bB	824	2	45,53,73	1.77	8 (17%)	52,89,113	1.57	8 (15%)
14	CLA	aB	802	2	65,73,73	1.47	9 (13%)	76,113,113	1.35	5 (6%)
14	CLA	bB	817	2	55,63,73	1.63	9 (16%)	64,101,113	1.47	9 (14%)
14	CLA	dA	814	1	45,53,73	1.74	7 (15%)	52,89,113	1.67	8 (15%)
17	BCR	aJ	103	-	41,41,41	1.16	3 (7%)	56,56,56	1.25	6 (10%)
13	CL0	cA	801	1	65,73,73	2.03	18 (27%)	76,113,113	2.76	26 (34%)
18	LHG	dB	851	-	22,22,48	0.90	1 (4%)	25,28,54	1.20	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$\lvert Z\rvert > 2$	Counts	RMSZ	#$\lvert Z\rvert > 2$
14	CLA	aF	201	-	51,59,73	1.64	7 (13%)	59,96,113	1.61	7 (11%)
14	CLA	aA	841	1	65,73,73	1.46	9 (13%)	76,113,113	1.43	7 (9%)
14	CLA	cB	825	-	46,54,73	1.66	10 (21%)	53,90,113	1.69	8 (15%)
14	CLA	cA	817	1	54,62,73	1.61	8 (14%)	62,99,113	1.54	8 (12%)
17	BCR	bB	846	-	41,41,41	1.16	2 (4%)	56,56,56	1.17	3 (5%)
17	BCR	dA	849	-	41,41,41	1.15	2 (4%)	56,56,56	1.24	6 (10%)
14	CLA	aA	805	1	45,53,73	1.82	10 (22%)	52,89,113	1.72	9 (17%)
14	CLA	bB	829	2	65,73,73	1.43	10 (15%)	76,113,113	1.46	8 (10%)
13	CL0	dA	801	1	65,73,73	2.03	17 (26%)	76,113,113	2.79	28 (36%)
14	CLA	bJ	101	-	45,53,73	1.76	7 (15%)	52,89,113	1.63	6 (11%)
14	CLA	aB	819	-	65,73,73	1.42	8 (12%)	76,113,113	1.54	6 (7%)
14	CLA	cA	833	1	65,73,73	1.44	8 (12%)	76,113,113	1.53	10 (13%)
14	CLA	cB	832	2	65,73,73	1.53	8 (12%)	76,113,113	1.42	8 (10%)
14	CLA	dB	809	2	65,73,73	1.45	12 (18%)	76,113,113	1.60	9 (11%)
14	CLA	dB	816	2	45,53,73	1.73	7 (15%)	52,89,113	1.74	7 (13%)
13	CL0	bA	801	1	65,73,73	2.03	17 (26%)	76,113,113	2.79	28 (36%)
17	BCR	cB	845	-	41,41,41	1.17	2 (4%)	56,56,56	1.16	3 (5%)
14	CLA	aB	814	2	56,64,73	1.54	7 (12%)	65,102,113	1.53	6 (9%)
14	CLA	aB	834	2	45,53,73	1.71	7 (15%)	52,89,113	1.88	7 (13%)
14	CLA	bA	806	1	65,73,73	1.46	10 (15%)	76,113,113	1.47	9 (11%)
14	CLA	dA	827	14,1	65,73,73	1.42	8 (12%)	76,113,113	1.53	8 (10%)
17	BCR	cJ	103	-	41,41,41	1.15	2 (4%)	56,56,56	1.25	6 (10%)
14	CLA	dB	842	2	65,73,73	1.47	9 (13%)	76,113,113	1.51	7 (9%)
16	SF4	dC	102	3	0,12,12	-	-	-		
14	CLA	bL	201	2,10	65,73,73	1.45	10 (15%)	76,113,113	1.36	7 (9%)
18	LHG	aA	852	-	48,48,48	0.65	1 (2%)	51,54,54	1.29	5 (9%)
18	LHG	dA	851	14	26,26,48	0.87	1 (3%)	29,32,54	1.31	3 (10%)
14	CLA	dA	818	1	54,62,73	1.56	9 (16%)	62,99,113	1.62	7 (11%)
17	BCR	bB	848	-	41,41,41	1.16	2 (4%)	56,56,56	1.32	5 (8%)
14	CLA	aB	839	2	47,55,73	1.66	7 (14%)	54,91,113	1.74	8 (14%)
15	PQN	dA	843	-	34,34,34	1.50	2 (5%)	42,45,45	1.27	6 (14%)
14	CLA	cA	813	1	45,53,73	1.73	9 (20%)	52,89,113	1.69	12 (23%)
14	CLA	cB	809	2	65,73,73	1.46	12 (18%)	76,113,113	1.60	9 (11%)
17	BCR	dL	207	-	41,41,41	1.17	3 (7%)	56,56,56	1.43	7 (12%)
14	CLA	cL	203	10	65,73,73	1.45	10 (15%)	76,113,113	1.55	9 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	CLA	dX	101	12	45,53,73	1.75	9 (20%)	52,89,113	1.64	6 (11%)
14	CLA	bA	826	-	55,63,73	1.57	8 (14%)	64,101,113	1.56	8 (12%)
14	CLA	dL	206	-	65,73,73	1.45	10 (15%)	76,113,113	1.38	7 (9%)
14	CLA	cB	827	2	65,73,73	1.40	7 (10%)	76,113,113	1.55	9 (11%)
14	CLA	bB	842	2	65,73,73	1.47	10 (15%)	76,113,113	1.51	7 (9%)
14	CLA	aB	821	2	45,53,73	1.71	8 (17%)	52,89,113	1.67	7 (13%)
14	CLA	aB	809	2	65,73,73	1.45	11 (16%)	76,113,113	1.61	9 (11%)
14	CLA	aK	102	-	45,53,73	1.72	8 (17%)	52,89,113	1.66	6 (11%)
14	CLA	dJ	101	-	45,53,73	1.76	7 (15%)	52,89,113	1.64	6 (11%)
14	CLA	bB	819	2	60,68,73	1.53	10 (16%)	70,107,113	1.48	7 (10%)
17	BCR	aL	205	-	41,41,41	1.18	2 (4%)	56,56,56	1.36	7 (12%)
14	CLA	cA	804	14,1	45,53,73	1.80	9 (20%)	52,89,113	1.79	8 (15%)
14	CLA	bX	101	12	45,53,73	1.75	8 (17%)	52,89,113	1.64	6 (11%)
14	CLA	dA	817	1	54,62,73	1.60	8 (14%)	62,99,113	1.54	8 (12%)
17	BCR	bA	848	-	41,41,41	1.21	2 (4%)	56,56,56	1.22	6 (10%)
14	CLA	dB	806	2	65,73,73	1.37	8 (12%)	76,113,113	1.58	8 (10%)
17	BCR	dA	846	-	41,41,41	1.10	2 (4%)	56,56,56	1.32	8 (14%)
14	CLA	dB	833	2	65,73,73	1.53	8 (12%)	76,113,113	1.41	8 (10%)
14	CLA	aB	836	-	45,53,73	1.82	9 (20%)	52,89,113	1.56	7 (13%)
17	BCR	bJ	103	-	41,41,41	1.15	3 (7%)	56,56,56	1.25	7 (12%)
14	CLA	dA	826	-	55,63,73	1.57	8 (14%)	64,101,113	1.56	8 (12%)
14	CLA	cB	824	2	54,62,73	1.65	10 (18%)	62,99,113	1.45	8 (12%)
14	CLA	dA	829	1	65,73,73	1.48	10 (15%)	76,113,113	1.38	7 (9%)
14	CLA	dA	804	14,1	45,53,73	1.80	8 (17%)	52,89,113	1.78	8 (15%)
14	CLA	dA	836	1	45,53,73	1.72	7 (15%)	52,89,113	1.82	8 (15%)
14	CLA	aB	813	2	65,73,73	1.43	10 (15%)	76,113,113	1.52	9 (11%)
17	BCR	bA	846	-	41,41,41	1.10	2 (4%)	56,56,56	1.32	8 (14%)
18	LHG	cB	850	-	22,22,48	0.89	1 (4%)	25,28,54	1.20	1 (4%)
14	CLA	dB	831	2	45,53,73	1.76	9 (20%)	52,89,113	1.59	6 (11%)
14	CLA	bA	834	1	65,73,73	1.46	8 (12%)	76,113,113	1.43	7 (9%)
14	CLA	bA	829	1	65,73,73	1.47	10 (15%)	76,113,113	1.38	7 (9%)
14	CLA	cB	822	-	55,63,73	1.55	8 (14%)	64,101,113	1.60	6 (9%)
14	CLA	aA	837	1	51,59,73	1.57	8 (15%)	59,96,113	1.70	8 (13%)
14	CLA	bA	825	-	65,73,73	1.40	8 (12%)	76,113,113	1.56	10 (13%)
14	CLA	dF	203	-	45,53,73	1.71	8 (17%)	52,89,113	1.68	7 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	CLA	bB	841	-	65,73,73	1.47	10 (15%)	76,113,113	1.33	7 (9%)
14	CLA	aK	101	9	42,49,73	1.74	6 (14%)	48,83,113	1.68	6 (12%)
14	CLA	bB	808	2	65,73,73	1.50	7 (10%)	76,113,113	1.49	9 (11%)
16	SF4	dA	844	2,1	0,12,12	-	-	-		
17	BCR	aB	843	-	41,41,41	1.13	2 (4%)	56,56,56	1.31	6 (10%)
14	CLA	aB	822	-	55,63,73	1.57	8 (14%)	64,101,113	1.61	6 (9%)
14	CLA	bJ	102	-	38,45,73	1.85	7 (18%)	43,78,113	1.70	7 (16%)
18	LHG	cA	853	14	26,26,48	0.87	1 (3%)	29,32,54	1.31	3 (10%)
14	CLA	cK	102	-	45,53,73	1.73	7 (15%)	52,89,113	1.66	6 (11%)
14	CLA	cB	802	2	65,73,73	1.46	9 (13%)	76,113,113	1.36	6 (7%)
17	BCR	bA	847	-	41,41,41	1.17	3 (7%)	56,56,56	1.22	3 (5%)
17	BCR	dJ	104	-	41,41,41	1.13	3 (7%)	56,56,56	1.21	4 (7%)
17	BCR	dB	845	-	41,41,41	1.11	2 (4%)	56,56,56	1.15	5 (8%)
14	CLA	dA	816	-	49,57,73	1.69	6 (12%)	55,93,113	1.65	7 (12%)
14	CLA	aB	837	2	60,68,73	1.51	8 (13%)	70,107,113	1.48	9 (12%)
14	CLA	cB	821	2	45,53,73	1.72	9 (20%)	52,89,113	1.67	7 (13%)
17	BCR	dB	844	-	41,41,41	1.13	2 (4%)	56,56,56	1.32	6 (10%)
14	CLA	bL	205	10	65,73,73	1.44	9 (13%)	76,113,113	1.55	9 (11%)
14	CLA	dA	842	-	65,73,73	1.49	10 (15%)	76,113,113	1.45	7 (9%)
15	PQN	aA	844	-	34,34,34	1.52	2 (5%)	42,45,45	1.26	5 (11%)
17	BCR	dB	847	-	41,41,41	1.06	2 (4%)	56,56,56	1.26	4 (7%)
14	CLA	cA	838	1	65,73,73	1.46	9 (13%)	76,113,113	1.51	9 (11%)
17	BCR	aB	844	-	41,41,41	1.10	2 (4%)	56,56,56	1.15	5 (8%)
14	CLA	aL	203	10	65,73,73	1.45	10 (15%)	76,113,113	1.54	9 (11%)
14	CLA	cA	834	1	65,73,73	1.45	9 (13%)	76,113,113	1.44	7 (9%)
14	CLA	cB	805	2	54,62,73	1.57	7 (12%)	62,99,113	1.61	7 (11%)
14	CLA	dA	808	1	45,53,73	1.74	9 (20%)	52,89,113	1.67	8 (15%)
17	BCR	cM	101	-	41,41,41	1.14	2 (4%)	56,56,56	1.28	6 (10%)
14	CLA	bA	841	1	65,73,73	1.46	9 (13%)	76,113,113	1.44	7 (9%)
14	CLA	aA	809	1	45,53,73	1.71	8 (17%)	52,89,113	1.73	8 (15%)
14	CLA	aA	842	-	65,73,73	1.49	10 (15%)	76,113,113	1.46	7 (9%)
14	CLA	dB	825	2	54,62,73	1.65	10 (18%)	62,99,113	1.44	8 (12%)
14	CLA	aJ	102	-	38,45,73	1.85	7 (18%)	43,78,113	1.70	7 (16%)
14	CLA	bA	808	1	45,53,73	1.73	9 (20%)	52,89,113	1.67	8 (15%)
14	CLA	cA	823	1	51,59,73	1.66	8 (15%)	59,96,113	1.54	8 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
14	CLA	dB	811	2	65,73,73	1.45	10 (15%)	76,113,113	1.37	8 (10%)
17	BCR	aF	202	-	41,41,41	1.17	2 (4%)	56,56,56	1.29	5 (8%)
16	SF4	cA	845	2,1	0,12,12	-	-	-		
14	CLA	bF	201	-	51,59,73	1.64	7 (13%)	59,96,113	1.61	7 (11%)
17	BCR	dB	849	-	41,41,41	1.21	2 (4%)	56,56,56	1.16	4 (7%)
14	CLA	bL	202	10,18	52,60,73	1.62	8 (15%)	60,97,113	2.13	12 (20%)
17	BCR	cB	847	-	41,41,41	1.17	2 (4%)	56,56,56	1.32	5 (8%)
14	CLA	dB	837	-	45,53,73	1.81	8 (17%)	52,89,113	1.57	7 (13%)
13	CL0	aA	801	1	65,73,73	2.04	18 (27%)	76,113,113	2.77	25 (32%)
17	BCR	bL	203	-	41,41,41	1.23	3 (7%)	56,56,56	1.25	5 (8%)
17	BCR	dM	101	-	41,41,41	1.13	2 (4%)	56,56,56	1.28	6 (10%)
18	LHG	bA	851	14	26,26,48	0.87	1 (3%)	29,32,54	1.31	3 (10%)
14	CLA	aA	817	1	54,62,73	1.60	8 (14%)	62,99,113	1.54	8 (12%)
14	CLA	aA	836	1	45,53,73	1.72	7 (15%)	52,89,113	1.81	8 (15%)
14	CLA	cA	809	1	45,53,73	1.71	8 (17%)	52,89,113	1.72	8 (15%)
17	BCR	aA	850	-	41,41,41	1.20	2 (4%)	56,56,56	1.21	5 (8%)
17	BCR	dF	204	-	41,41,41	1.12	2 (4%)	56,56,56	1.30	8 (14%)
14	CLA	bB	832	2	49,57,73	1.69	7 (14%)	55,93,113	1.71	9 (16%)
15	PQN	cA	844	-	34,34,34	1.52	2 (5%)	42,45,45	1.27	5 (11%)
14	CLA	bA	818	1	54,62,73	1.57	9 (16%)	62,99,113	1.63	7 (11%)
14	CLA	aB	810	2	65,73,73	1.48	10 (15%)	76,113,113	1.47	6 (7%)
14	CLA	cB	830	2	45,53,73	1.77	10 (22%)	52,89,113	1.60	6 (11%)
17	BCR	bB	845	-	41,41,41	1.10	2 (4%)	56,56,56	1.15	5 (8%)
14	CLA	cB	835	-	45,53,73	1.79	8 (17%)	52,89,113	1.71	8 (15%)
17	BCR	bB	847	-	41,41,41	1.06	2 (4%)	56,56,56	1.26	4 (7%)
17	BCR	cF	204	-	41,41,41	1.10	2 (4%)	56,56,56	1.29	8 (14%)
14	CLA	dA	803	1	45,53,73	1.75	8 (17%)	52,89,113	1.69	9 (17%)
14	CLA	cB	831	2	49,57,73	1.69	7 (14%)	55,93,113	1.70	9 (16%)
14	CLA	dB	828	2	65,73,73	1.40	7 (10%)	76,113,113	1.55	9 (11%)
17	BCR	bF	204	-	41,41,41	1.12	2 (4%)	56,56,56	1.29	8 (14%)
14	CLA	bA	835	1	54,62,73	1.65	10 (18%)	62,99,113	1.54	8 (12%)
17	BCR	cA	851	-	41,41,41	1.15	2 (4%)	56,56,56	1.25	6 (10%)
14	CLA	cB	839	2	47,55,73	1.66	7 (14%)	54,91,113	1.74	8 (14%)
16	SF4	bC	101	3	0,12,12	-	-	-		
17	BCR	cA	849	-	41,41,41	1.17	2 (4%)	56,56,56	1.22	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
19	LMG	bB	850	-	55,55,55	0.79	2 (3%)	63,63,63	1.46	9 (14%)
14	CLA	cF	201	-	51,59,73	1.65	7 (13%)	59,96,113	1.61	7 (11%)
14	CLA	dA	819	1	65,73,73	1.44	9 (13%)	76,113,113	1.56	9 (11%)
14	CLA	bB	827	2	65,73,73	1.45	10 (15%)	76,113,113	1.45	8 (10%)
14	CLA	aA	813	1	45,53,73	1.73	9 (20%)	52,89,113	1.69	11 (21%)
14	CLA	dL	204	10	52,60,73	1.66	9 (17%)	60,97,113	1.63	9 (15%)
14	CLA	cA	824	1	47,55,73	1.71	8 (17%)	54,91,113	1.64	8 (14%)
14	CLA	aB	826	2	65,73,73	1.45	10 (15%)	76,113,113	1.45	8 (10%)
14	CLA	bB	834	2	58,66,73	1.56	8 (13%)	67,104,113	1.48	10 (14%)
14	CLA	bA	832	1	65,73,73	1.45	10 (15%)	76,113,113	1.49	10 (13%)
14	CLA	aB	811	2	45,53,73	1.72	8 (17%)	52,89,113	1.68	7 (13%)
14	CLA	dB	839	2	65,73,73	1.43	7 (10%)	76,113,113	1.62	9 (11%)
17	BCR	aB	851	-	41,41,41	1.18	2 (4%)	56,56,56	1.38	8 (14%)
17	BCR	dB	848	-	41,41,41	1.17	2 (4%)	56,56,56	1.32	5 (8%)
14	CLA	aA	843	18	52,60,73	1.62	8 (15%)	60,97,113	2.13	11 (18%)
17	BCR	bF	202	-	41,41,41	1.16	2 (4%)	56,56,56	1.29	5 (8%)
14	CLA	cB	841	2	65,73,73	1.46	9 (13%)	76,113,113	1.52	7 (9%)
14	CLA	aL	204	-	52,60,73	1.61	8 (15%)	60,97,113	1.56	9 (15%)
14	CLA	bB	839	2	65,73,73	1.43	7 (10%)	76,113,113	1.61	9 (11%)
14	CLA	bA	816	-	49,57,73	1.69	6 (12%)	55,93,113	1.65	7 (12%)
14	CLA	cL	204	-	52,60,73	1.60	8 (15%)	60,97,113	1.56	8 (13%)
14	CLA	cB	808	2	65,73,73	1.48	7 (10%)	76,113,113	1.49	9 (11%)
14	CLA	cB	812	2	45,53,73	1.76	9 (20%)	52,89,113	1.64	7 (13%)
14	CLA	dB	819	2	60,68,73	1.53	10 (16%)	70,107,113	1.47	7 (10%)
14	CLA	aA	840	1	65,73,73	1.46	10 (15%)	76,113,113	1.50	7 (9%)
17	BCR	cL	201	-	41,41,41	1.24	3 (7%)	56,56,56	1.25	5 (8%)
14	CLA	bB	806	2	65,73,73	1.38	8 (12%)	76,113,113	1.57	8 (10%)
17	BCR	dJ	103	-	41,41,41	1.15	2 (4%)	56,56,56	1.26	7 (12%)
14	CLA	aA	804	14,1	45,53,73	1.81	9 (20%)	52,89,113	1.78	8 (15%)
14	CLA	bL	204	10	52,60,73	1.65	9 (17%)	60,97,113	1.63	9 (15%)
17	BCR	dB	852	-	41,41,41	1.18	2 (4%)	56,56,56	1.38	8 (14%)
14	CLA	cB	828	2	65,73,73	1.43	10 (15%)	76,113,113	1.46	8 (10%)
14	CLA	bB	801	-	65,73,73	1.45	10 (15%)	76,113,113	1.42	7 (9%)
14	CLA	cA	831	1	50,58,73	1.63	10 (20%)	58,95,113	1.66	8 (13%)
14	CLA	dB	830	2	65,73,73	1.46	10 (15%)	76,113,113	1.70	9 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$\|Z\| > 2$	Counts	RMSZ	#$\|Z\| > 2$
14	CLA	dB	838	2	60,68,73	1.52	9 (15%)	70,107,113	1.49	9 (12%)
14	CLA	dB	827	2	65,73,73	1.46	9 (13%)	76,113,113	1.44	8 (10%)
17	BCR	bA	849	-	41,41,41	1.16	2 (4%)	56,56,56	1.24	6 (10%)
14	CLA	aA	803	1	45,53,73	1.76	8 (17%)	52,89,113	1.70	9 (17%)
14	CLA	dA	832	1	65,73,73	1.46	10 (15%)	76,113,113	1.49	10 (13%)
14	CLA	cA	821	14	65,73,73	1.44	10 (15%)	76,113,113	1.52	7 (9%)
14	CLA	dB	803	-	65,73,73	1.44	9 (13%)	76,113,113	1.40	6 (7%)
14	CLA	aB	828	2	65,73,73	1.44	10 (15%)	76,113,113	1.46	8 (10%)
14	CLA	dA	839	1	65,73,73	1.48	8 (12%)	76,113,113	1.49	8 (10%)
17	BCR	bB	852	-	41,41,41	1.19	2 (4%)	56,56,56	1.37	8 (14%)
14	CLA	bB	810	2	65,73,73	1.48	10 (15%)	76,113,113	1.47	6 (7%)
14	CLA	bB	812	2	45,53,73	1.71	8 (17%)	52,89,113	1.68	7 (13%)
14	CLA	cB	823	2	45,53,73	1.76	8 (17%)	52,89,113	1.57	8 (15%)
17	BCR	cL	206	-	41,41,41	1.07	1 (2%)	56,56,56	1.33	7 (12%)
14	CLA	dA	806	1	65,73,73	1.47	10 (15%)	76,113,113	1.46	9 (11%)
14	CLA	cA	805	1	45,53,73	1.83	10 (22%)	52,89,113	1.72	9 (17%)
14	CLA	cA	843	18	52,60,73	1.62	8 (15%)	60,97,113	2.12	11 (18%)
17	BCR	cB	848	-	41,41,41	1.22	2 (4%)	56,56,56	1.16	4 (7%)
17	BCR	cI	101	-	41,41,41	1.14	2 (4%)	56,56,56	1.33	7 (12%)
14	CLA	bA	839	1	65,73,73	1.48	9 (13%)	76,113,113	1.49	8 (10%)
17	BCR	aJ	104	-	41,41,41	1.13	3 (7%)	56,56,56	1.21	4 (7%)
14	CLA	dB	840	2	47,55,73	1.66	7 (14%)	54,91,113	1.74	8 (14%)
14	CLA	bA	817	1	54,62,73	1.61	8 (14%)	62,99,113	1.54	8 (12%)
14	CLA	cB	803	-	65,73,73	1.44	8 (12%)	76,113,113	1.41	6 (7%)
14	CLA	cB	836	-	45,53,73	1.82	9 (20%)	52,89,113	1.57	7 (13%)
14	CLA	bA	830	1	65,73,73	1.49	9 (13%)	76,113,113	1.52	7 (9%)
14	CLA	dA	841	1	65,73,73	1.47	9 (13%)	76,113,113	1.42	6 (7%)
14	CLA	bB	807	2	65,73,73	1.44	8 (12%)	76,113,113	1.46	6 (7%)
14	CLA	bA	815	1	45,53,73	1.77	8 (17%)	52,89,113	1.71	6 (11%)
14	CLA	bB	826	-	46,54,73	1.66	9 (19%)	53,90,113	1.70	8 (15%)
14	CLA	dA	834	1	65,73,73	1.46	8 (12%)	76,113,113	1.44	7 (9%)
14	CLA	bB	811	2	65,73,73	1.46	10 (15%)	76,113,113	1.37	7 (9%)
17	BCR	aA	851	-	41,41,41	1.15	2 (4%)	56,56,56	1.24	6 (10%)
14	CLA	cL	202	10	65,73,73	1.47	7 (10%)	76,113,113	1.39	9 (11%)
14	CLA	dA	831	1	50,58,73	1.62	10 (20%)	58,95,113	1.66	8 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
14	CLA	cB	811	2	45,53,73	1.72	8 (17%)	52,89,113	1.67	7 (13%)
19	LMG	aB	849	-	55,55,55	0.79	2 (3%)	63,63,63	1.46	9 (14%)
14	CLA	aA	814	1	45,53,73	1.73	7 (15%)	52,89,113	1.67	8 (15%)
14	CLA	aA	834	1	65,73,73	1.46	8 (12%)	76,113,113	1.43	7 (9%)
14	CLA	cA	835	1	54,62,73	1.65	9 (16%)	62,99,113	1.54	8 (12%)
14	CLA	dL	201	2,10	65,73,73	1.45	10 (15%)	76,113,113	1.36	8 (10%)
14	CLA	aB	838	2	65,73,73	1.43	7 (10%)	76,113,113	1.61	9 (11%)
16	SF4	bC	102	3	0,12,12	-	-	-		
14	CLA	bB	836	-	45,53,73	1.79	8 (17%)	52,89,113	1.71	9 (17%)
14	CLA	aJ	101	-	45,53,73	1.75	7 (15%)	52,89,113	1.64	6 (11%)
17	BCR	aL	206	-	41,41,41	1.08	1 (2%)	56,56,56	1.32	7 (12%)
14	CLA	aB	803	-	65,73,73	1.43	8 (12%)	76,113,113	1.40	6 (7%)
14	CLA	cB	816	2	55,63,73	1.64	9 (16%)	64,101,113	1.47	9 (14%)
14	CLA	dB	832	2	49,57,73	1.69	7 (14%)	55,93,113	1.71	9 (16%)
14	CLA	cB	807	2	65,73,73	1.45	8 (12%)	76,113,113	1.47	6 (7%)
14	CLA	bA	820	1	61,69,73	1.52	9 (14%)	71,108,113	1.50	8 (11%)
14	CLA	cB	801	-	65,73,73	1.45	10 (15%)	76,113,113	1.42	7 (9%)
14	CLA	bA	813	1	45,53,73	1.73	9 (20%)	52,89,113	1.69	11 (21%)
14	CLA	dB	818	2	59,67,73	1.54	9 (15%)	68,105,113	1.54	9 (13%)
14	CLA	bB	816	2	45,53,73	1.73	7 (15%)	52,89,113	1.73	7 (13%)
14	CLA	aA	821	14	65,73,73	1.44	10 (15%)	76,113,113	1.52	7 (9%)
14	CLA	bB	830	2	65,73,73	1.47	10 (15%)	76,113,113	1.69	9 (11%)
14	CLA	aA	839	1	65,73,73	1.48	9 (13%)	76,113,113	1.49	8 (10%)
14	CLA	cB	806	2	65,73,73	1.38	8 (12%)	76,113,113	1.58	8 (10%)
14	CLA	dB	826	-	46,54,73	1.66	10 (21%)	53,90,113	1.70	8 (15%)
14	CLA	bB	809	2	65,73,73	1.46	12 (18%)	76,113,113	1.61	9 (11%)
17	BCR	cJ	104	-	41,41,41	1.14	3 (7%)	56,56,56	1.21	4 (7%)
14	CLA	dB	824	2	45,53,73	1.77	8 (17%)	52,89,113	1.58	8 (15%)
14	CLA	dB	822	2	45,53,73	1.72	9 (20%)	52,89,113	1.67	7 (13%)
14	CLA	aA	828	1	65,73,73	1.42	7 (10%)	76,113,113	1.59	9 (11%)
14	CLA	dA	812	1	54,62,73	1.61	9 (16%)	62,99,113	1.56	6 (9%)
14	CLA	dF	201	-	51,59,73	1.65	7 (13%)	59,96,113	1.62	8 (13%)
17	BCR	aM	101	-	41,41,41	1.14	2 (4%)	56,56,56	1.28	6 (10%)
14	CLA	dK	101	9	42,49,73	1.74	7 (16%)	48,83,113	1.67	6 (12%)
17	BCR	dI	101	-	41,41,41	1.14	2 (4%)	56,56,56	1.33	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
14	CLA	aB	840	-	65,73,73	1.47	10 (15%)	76,113,113	1.33	7 (9%)
14	CLA	bA	804	14,1	45,53,73	1.81	9 (20%)	52,89,113	1.77	8 (15%)
14	CLA	dB	810	2	65,73,73	1.48	10 (15%)	76,113,113	1.47	6 (7%)
14	CLA	aB	816	2	55,63,73	1.64	9 (16%)	64,101,113	1.47	9 (14%)
14	CLA	dJ	102	-	38,45,73	1.85	8 (21%)	43,78,113	1.70	7 (16%)
14	CLA	aA	838	1	65,73,73	1.46	9 (13%)	76,113,113	1.51	9 (11%)
14	CLA	bB	815	2	56,64,73	1.54	7 (12%)	65,102,113	1.53	6 (9%)
16	SF4	cC	101	3	0,12,12	-	-	-		
14	CLA	cA	812	1	54,62,73	1.61	9 (16%)	62,99,113	1.56	6 (9%)
14	CLA	aB	827	2	65,73,73	1.40	7 (10%)	76,113,113	1.55	9 (11%)
15	PQN	cB	842	-	34,34,34	1.52	2 (5%)	42,45,45	1.23	5 (11%)
14	CLA	cB	813	2	65,73,73	1.44	10 (15%)	76,113,113	1.52	9 (11%)
14	CLA	cA	818	1	54,62,73	1.56	9 (16%)	62,99,113	1.63	7 (11%)
14	CLA	bB	802	2	65,73,73	1.46	9 (13%)	76,113,113	1.35	6 (7%)
14	CLA	cF	203	-	45,53,73	1.74	8 (17%)	52,89,113	1.65	6 (11%)
14	CLA	aA	807	1	51,59,73	1.65	8 (15%)	59,96,113	1.61	6 (10%)
17	BCR	bB	844	-	41,41,41	1.14	2 (4%)	56,56,56	1.31	6 (10%)
14	CLA	dA	824	1	47,55,73	1.70	8 (17%)	54,91,113	1.65	8 (14%)
14	CLA	dB	821	2	47,55,73	1.67	8 (17%)	54,91,113	1.58	6 (11%)
14	CLA	cA	819	1	65,73,73	1.44	9 (13%)	76,113,113	1.56	9 (11%)
14	CLA	cB	819	-	65,73,73	1.42	8 (12%)	76,113,113	1.53	6 (7%)
14	CLA	dA	815	1	45,53,73	1.76	7 (15%)	52,89,113	1.72	6 (11%)
17	BCR	bM	101	-	41,41,41	1.14	2 (4%)	56,56,56	1.27	6 (10%)
17	BCR	aB	848	-	41,41,41	1.22	2 (4%)	56,56,56	1.16	4 (7%)
14	CLA	dB	841	-	65,73,73	1.47	10 (15%)	76,113,113	1.33	7 (9%)
17	BCR	bA	845	-	41,41,41	1.13	3 (7%)	56,56,56	1.29	8 (14%)
17	BCR	cB	843	-	41,41,41	1.13	2 (4%)	56,56,56	1.31	6 (10%)
17	BCR	dL	208	-	41,41,41	1.12	2 (4%)	56,56,56	1.38	10 (17%)
14	CLA	bB	813	2	45,53,73	1.76	9 (20%)	52,89,113	1.64	7 (13%)
14	CLA	bB	833	2	65,73,73	1.53	8 (12%)	76,113,113	1.41	8 (10%)
14	CLA	bB	803	-	65,73,73	1.43	9 (13%)	76,113,113	1.41	6 (7%)
15	PQN	aB	842	-	34,34,34	1.52	2 (5%)	42,45,45	1.23	5 (11%)
14	CLA	aA	811	14,1	65,73,73	1.48	9 (13%)	76,113,113	1.41	8 (10%)
15	PQN	bA	843	-	34,34,34	1.51	2 (5%)	42,45,45	1.27	6 (14%)
14	CLA	bA	814	1	45,53,73	1.74	7 (15%)	52,89,113	1.66	8 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
14	CLA	bB	825	2	54,62,73	1.65	10 (18%)	62,99,113	1.43	8 (12%)
14	CLA	aB	825	-	46,54,73	1.67	10 (21%)	53,90,113	1.69	8 (15%)
18	LHG	cA	852	-	48,48,48	0.65	1 (2%)	51,54,54	1.29	5 (9%)
14	CLA	dA	830	1	65,73,73	1.50	9 (13%)	76,113,113	1.52	7 (9%)
14	CLA	dA	833	1	65,73,73	1.44	9 (13%)	76,113,113	1.53	10 (13%)
14	CLA	bA	802	-	45,53,73	1.68	8 (17%)	52,89,113	1.83	6 (11%)
14	CLA	cX	101	12	45,53,73	1.76	8 (17%)	52,89,113	1.65	6 (11%)
17	BCR	cB	846	-	41,41,41	1.06	2 (4%)	56,56,56	1.26	4 (7%)
14	CLA	cA	811	14,1	65,73,73	1.47	9 (13%)	76,113,113	1.41	8 (10%)
14	CLA	bA	827	14,1	65,73,73	1.42	7 (10%)	76,113,113	1.52	8 (10%)
14	CLA	bB	840	2	47,55,73	1.65	7 (14%)	54,91,113	1.74	8 (14%)
17	BCR	cA	850	-	41,41,41	1.21	2 (4%)	56,56,56	1.22	5 (8%)
14	CLA	dB	807	2	65,73,73	1.44	8 (12%)	76,113,113	1.46	6 (7%)
16	SF4	dC	101	3	0,12,12	-	-	-		
14	CLA	dB	815	2	56,64,73	1.53	7 (12%)	65,102,113	1.54	6 (9%)
14	CLA	cA	810	1	45,53,73	1.72	6 (13%)	52,89,113	1.66	6 (11%)
14	CLA	aA	822	1	49,57,73	1.65	9 (18%)	55,93,113	1.64	6 (10%)
14	CLA	cB	829	2	65,73,73	1.46	10 (15%)	76,113,113	1.69	9 (11%)
14	CLA	dA	825	-	65,73,73	1.40	8 (12%)	76,113,113	1.56	10 (13%)
14	CLA	dB	835	2	45,53,73	1.71	7 (15%)	52,89,113	1.88	7 (13%)
14	CLA	aA	816	-	49,57,73	1.69	6 (12%)	55,93,113	1.65	7 (12%)
14	CLA	cB	834	2	45,53,73	1.72	7 (15%)	52,89,113	1.87	7 (13%)
17	BCR	aB	846	-	41,41,41	1.05	2 (4%)	56,56,56	1.26	4 (7%)
14	CLA	dB	808	2	65,73,73	1.48	8 (12%)	76,113,113	1.50	9 (11%)
14	CLA	bA	805	1	45,53,73	1.82	10 (22%)	52,89,113	1.72	9 (17%)
14	CLA	aB	829	2	65,73,73	1.47	10 (15%)	76,113,113	1.69	9 (11%)
14	CLA	aB	824	2	54,62,73	1.65	10 (18%)	62,99,113	1.45	8 (12%)
14	CLA	cA	807	1	51,59,73	1.64	7 (13%)	59,96,113	1.62	6 (10%)
14	CLA	bA	811	14,1	65,73,73	1.47	9 (13%)	76,113,113	1.40	8 (10%)
14	CLA	cA	820	1	61,69,73	1.51	8 (13%)	71,108,113	1.50	7 (9%)
14	CLA	aA	831	1	50,58,73	1.62	10 (20%)	58,95,113	1.66	8 (13%)
14	CLA	bB	804	-	65,73,73	1.40	9 (13%)	76,113,113	1.79	12 (15%)
14	CLA	bA	837	1	51,59,73	1.57	8 (15%)	59,96,113	1.70	8 (13%)
17	BCR	cF	202	-	41,41,41	1.16	2 (4%)	56,56,56	1.30	5 (8%)
14	CLA	dB	823	-	55,63,73	1.56	9 (16%)	64,101,113	1.60	6 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\lvert Z\rvert > 2$	Counts	RMSZ	$\#\lvert Z\rvert > 2$
14	CLA	cA	806	1	65,73,73	1.46	10 (15%)	76,113,113	1.46	9 (11%)
14	CLA	aB	841	2	65,73,73	1.46	10 (15%)	76,113,113	1.51	7 (9%)
14	CLA	cA	841	1	65,73,73	1.47	9 (13%)	76,113,113	1.44	7 (9%)
17	BCR	aA	848	-	41,41,41	1.10	2 (4%)	56,56,56	1.32	8 (14%)
14	CLA	cA	827	14,1	65,73,73	1.42	7 (10%)	76,113,113	1.53	8 (10%)
17	BCR	aI	101	-	41,41,41	1.14	2 (4%)	56,56,56	1.33	7 (12%)
14	CLA	dA	813	1	45,53,73	1.73	8 (17%)	52,89,113	1.68	11 (21%)
16	SF4	bA	844	2,1	0,12,12	-	-	-		
14	CLA	cA	837	1	51,59,73	1.56	8 (15%)	59,96,113	1.69	8 (13%)
14	CLA	bB	818	2	59,67,73	1.54	9 (15%)	68,105,113	1.53	9 (13%)
14	CLA	dA	809	1	45,53,73	1.73	8 (17%)	52,89,113	1.73	8 (15%)
17	BCR	dF	202	-	41,41,41	1.16	2 (4%)	56,56,56	1.29	5 (8%)
14	CLA	bA	840	1	65,73,73	1.46	10 (15%)	76,113,113	1.50	7 (9%)
14	CLA	bA	824	1	47,55,73	1.70	7 (14%)	54,91,113	1.65	8 (14%)
14	CLA	bA	833	1	65,73,73	1.44	9 (13%)	76,113,113	1.53	10 (13%)
14	CLA	aB	818	2	60,68,73	1.54	10 (16%)	70,107,113	1.47	7 (10%)
14	CLA	cB	826	2	65,73,73	1.46	9 (13%)	76,113,113	1.44	8 (10%)
17	BCR	aA	846	-	41,41,41	1.20	3 (7%)	56,56,56	1.42	11 (19%)
17	BCR	cB	851	-	41,41,41	1.18	2 (4%)	56,56,56	1.38	8 (14%)
14	CLA	bA	809	1	45,53,73	1.71	8 (17%)	52,89,113	1.72	8 (15%)
14	CLA	bA	842	-	65,73,73	1.49	10 (15%)	76,113,113	1.46	7 (9%)
14	CLA	cB	810	2	65,73,73	1.48	10 (15%)	76,113,113	1.48	6 (7%)
14	CLA	cB	814	2	56,64,73	1.54	8 (14%)	65,102,113	1.54	6 (9%)
14	CLA	dB	836	-	45,53,73	1.81	8 (17%)	52,89,113	1.72	9 (17%)
14	CLA	aB	807	2	65,73,73	1.45	8 (12%)	76,113,113	1.47	6 (7%)
17	BCR	aF	204	-	41,41,41	1.11	2 (4%)	56,56,56	1.29	9 (16%)
14	CLA	aB	823	2	45,53,73	1.77	8 (17%)	52,89,113	1.57	8 (15%)
14	CLA	bA	831	1	50,58,73	1.63	10 (20%)	58,95,113	1.66	8 (13%)
14	CLA	aA	825	-	65,73,73	1.40	8 (12%)	76,113,113	1.55	9 (11%)
14	CLA	aB	808	2	65,73,73	1.49	8 (12%)	76,113,113	1.49	9 (11%)
14	CLA	aB	812	2	45,53,73	1.76	9 (20%)	52,89,113	1.63	7 (13%)
17	BCR	cA	848	-	41,41,41	1.10	2 (4%)	56,56,56	1.33	8 (14%)
16	SF4	aC	102	3	0,12,12	-	-	-		
14	CLA	cA	802	-	45,53,73	1.68	8 (17%)	52,89,113	1.83	6 (11%)
14	CLA	bB	837	-	45,53,73	1.81	8 (17%)	52,89,113	1.57	7 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
14	CLA	bB	828	2	65,73,73	1.41	7 (10%)	76,113,113	1.55	9 (11%)
14	CLA	cB	820	2	47,55,73	1.67	8 (17%)	54,91,113	1.58	6 (11%)
17	BCR	aA	847	-	41,41,41	1.13	3 (7%)	56,56,56	1.29	8 (14%)
14	CLA	dB	802	2	65,73,73	1.46	9 (13%)	76,113,113	1.35	6 (7%)
17	BCR	dL	203	-	41,41,41	1.24	3 (7%)	56,56,56	1.25	5 (8%)
17	BCR	cB	844	-	41,41,41	1.10	2 (4%)	56,56,56	1.15	5 (8%)
14	CLA	aF	203	-	45,53,73	1.72	8 (17%)	52,89,113	1.65	6 (11%)
14	CLA	aA	812	1	54,62,73	1.61	8 (14%)	62,99,113	1.55	6 (9%)
16	SF4	aC	101	3	0,12,12	-	-	-		
19	LMG	cB	849	-	55,55,55	0.79	2 (3%)	63,63,63	1.46	9 (14%)
14	CLA	cA	822	1	49,57,73	1.65	9 (18%)	55,93,113	1.64	7 (12%)
14	CLA	aA	824	1	47,55,73	1.71	8 (17%)	54,91,113	1.65	8 (14%)
17	BCR	aB	847	-	41,41,41	1.17	2 (4%)	56,56,56	1.31	5 (8%)
14	CLA	dA	822	1	49,57,73	1.65	9 (18%)	55,93,113	1.63	7 (12%)
17	BCR	cA	847	-	41,41,41	1.13	3 (7%)	56,56,56	1.29	8 (14%)
14	CLA	aX	101	12	45,53,73	1.75	8 (17%)	52,89,113	1.65	6 (11%)
14	CLA	aB	835	-	45,53,73	1.80	8 (17%)	52,89,113	1.71	9 (17%)
14	CLA	aA	808	1	45,53,73	1.73	9 (20%)	52,89,113	1.66	8 (15%)
14	CLA	bA	822	1	49,57,73	1.65	9 (18%)	55,93,113	1.64	7 (12%)
14	CLA	bB	835	2	45,53,73	1.71	7 (15%)	52,89,113	1.88	7 (13%)
14	CLA	bA	803	1	45,53,73	1.75	8 (17%)	52,89,113	1.70	9 (17%)
17	BCR	aA	849	-	41,41,41	1.17	2 (4%)	56,56,56	1.22	3 (5%)
14	CLA	dA	828	1	65,73,73	1.42	8 (12%)	76,113,113	1.60	10 (13%)
14	CLA	dB	817	2	55,63,73	1.63	9 (16%)	64,101,113	1.47	9 (14%)
14	CLA	dA	802	-	45,53,73	1.69	8 (17%)	52,89,113	1.83	6 (11%)
14	CLA	dL	202	10,18	52,60,73	1.62	8 (15%)	60,97,113	2.12	11 (18%)
14	CLA	bF	203	-	45,53,73	1.72	8 (17%)	52,89,113	1.68	7 (13%)
14	CLA	cA	814	1	45,53,73	1.73	8 (17%)	52,89,113	1.66	9 (17%)
14	CLA	bA	823	1	51,59,73	1.66	8 (15%)	59,96,113	1.54	8 (13%)
17	BCR	cA	846	-	41,41,41	1.20	3 (7%)	56,56,56	1.42	11 (19%)
14	CLA	dA	823	1	51,59,73	1.66	9 (17%)	59,96,113	1.55	8 (13%)
14	CLA	cB	840	-	65,73,73	1.47	10 (15%)	76,113,113	1.34	7 (9%)
14	CLA	aA	818	1	54,62,73	1.56	9 (16%)	62,99,113	1.61	7 (11%)
14	CLA	cB	833	2	58,66,73	1.54	8 (13%)	67,104,113	1.48	10 (14%)
14	CLA	aB	832	2	65,73,73	1.53	8 (12%)	76,113,113	1.41	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\lvert Z\rvert > 2$	Counts	RMSZ	$\#\lvert Z\rvert > 2$
14	CLA	cA	829	1	65,73,73	1.48	10 (15%)	76,113,113	1.39	8 (10%)
14	CLA	bB	823	-	55,63,73	1.56	9 (16%)	64,101,113	1.60	6 (9%)
14	CLA	aL	202	10	65,73,73	1.47	7 (10%)	76,113,113	1.38	9 (11%)
14	CLA	dA	835	1	54,62,73	1.64	9 (16%)	62,99,113	1.56	8 (12%)
14	CLA	aA	823	1	51,59,73	1.65	8 (15%)	59,96,113	1.55	8 (13%)
14	CLA	aB	806	2	65,73,73	1.39	8 (12%)	76,113,113	1.57	8 (10%)
14	CLA	aA	826	-	55,63,73	1.57	8 (14%)	64,101,113	1.56	8 (12%)
14	CLA	cB	815	2	45,53,73	1.73	7 (15%)	52,89,113	1.73	7 (13%)
14	CLA	bL	206	-	65,73,73	1.46	10 (15%)	76,113,113	1.37	7 (9%)
14	CLA	aA	833	1	65,73,73	1.45	9 (13%)	76,113,113	1.53	10 (13%)
14	CLA	dA	837	1	51,59,73	1.57	8 (15%)	59,96,113	1.70	8 (13%)
14	CLA	dB	805	2	54,62,73	1.56	7 (12%)	62,99,113	1.61	8 (12%)
14	CLA	bA	836	1	45,53,73	1.72	7 (15%)	52,89,113	1.81	8 (15%)
14	CLA	aA	819	1	65,73,73	1.44	9 (13%)	76,113,113	1.55	9 (11%)
14	CLA	aA	835	1	54,62,73	1.66	9 (16%)	62,99,113	1.55	8 (12%)
14	CLA	cA	836	1	45,53,73	1.72	7 (15%)	52,89,113	1.82	8 (15%)
14	CLA	aB	815	2	45,53,73	1.74	7 (15%)	52,89,113	1.74	7 (13%)
14	CLA	cA	839	1	65,73,73	1.48	8 (12%)	76,113,113	1.49	8 (10%)
14	CLA	dA	811	14,1	65,73,73	1.48	9 (13%)	76,113,113	1.41	8 (10%)
14	CLA	aB	833	2	58,66,73	1.56	8 (13%)	67,104,113	1.49	10 (14%)
14	CLA	cA	830	1	65,73,73	1.49	10 (15%)	76,113,113	1.53	7 (9%)
14	CLA	dA	810	1	45,53,73	1.71	6 (13%)	52,89,113	1.65	6 (11%)
14	CLA	bK	101	9	42,49,73	1.73	7 (16%)	48,83,113	1.67	6 (12%)
14	CLA	dB	820	-	65,73,73	1.43	8 (12%)	76,113,113	1.53	6 (7%)
17	BCR	bI	101	-	41,41,41	1.14	2 (4%)	56,56,56	1.33	7 (12%)
14	CLA	cJ	101	-	45,53,73	1.75	7 (15%)	52,89,113	1.64	6 (11%)
14	CLA	cA	826	-	55,63,73	1.56	8 (14%)	64,101,113	1.55	8 (12%)
14	CLA	cJ	102	-	38,45,73	1.86	8 (21%)	43,78,113	1.70	7 (16%)
17	BCR	cL	205	-	41,41,41	1.18	2 (4%)	56,56,56	1.37	9 (16%)
14	CLA	bB	838	2	60,68,73	1.52	8 (13%)	70,107,113	1.49	9 (12%)
17	BCR	dA	848	-	41,41,41	1.21	2 (4%)	56,56,56	1.22	6 (10%)
14	CLA	cA	808	1	45,53,73	1.73	9 (20%)	52,89,113	1.68	8 (15%)
14	CLA	bA	810	1	45,53,73	1.71	6 (13%)	52,89,113	1.66	6 (11%)
17	BCR	dK	102	-	41,41,41	1.19	3 (7%)	56,56,56	1.42	10 (17%)
14	CLA	bB	831	2	45,53,73	1.77	9 (20%)	52,89,113	1.60	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\lvert Z\rvert > 2$	Counts	RMSZ	$\#\lvert Z\rvert > 2$
14	CLA	dB	813	2	45,53,73	1.76	9 (20%)	52,89,113	1.63	7 (13%)
18	LHG	aB	850	-	22,22,48	0.89	1 (4%)	25,28,54	1.20	1 (4%)
14	CLA	cB	817	2	59,67,73	1.54	9 (15%)	68,105,113	1.52	9 (13%)
14	CLA	dB	829	2	65,73,73	1.43	10 (15%)	76,113,113	1.45	8 (10%)
14	CLA	bB	820	-	65,73,73	1.42	8 (12%)	76,113,113	1.53	6 (7%)
14	CLA	dB	804	-	65,73,73	1.39	9 (13%)	76,113,113	1.80	12 (15%)
14	CLA	aB	817	2	59,67,73	1.53	9 (15%)	68,105,113	1.54	9 (13%)
14	CLA	dL	205	10	65,73,73	1.43	9 (13%)	76,113,113	1.55	9 (11%)
17	BCR	bJ	104	-	41,41,41	1.13	3 (7%)	56,56,56	1.21	5 (8%)
14	CLA	cB	837	2	60,68,73	1.51	9 (15%)	70,107,113	1.48	9 (12%)
14	CLA	bA	812	1	54,62,73	1.61	8 (14%)	62,99,113	1.56	6 (9%)
14	CLA	aA	827	14,1	65,73,73	1.42	8 (12%)	76,113,113	1.53	8 (10%)
14	CLA	cA	828	1	65,73,73	1.42	7 (10%)	76,113,113	1.59	9 (11%)
14	CLA	dA	805	1	45,53,73	1.84	10 (22%)	52,89,113	1.72	9 (17%)
14	CLA	bB	821	2	47,55,73	1.67	8 (17%)	54,91,113	1.59	6 (11%)
15	PQN	dB	843	-	34,34,34	1.52	2 (5%)	42,45,45	1.27	4 (9%)
14	CLA	dA	820	1	61,69,73	1.52	9 (14%)	71,108,113	1.49	7 (9%)
18	LHG	dA	850	-	48,48,48	0.65	1 (2%)	51,54,54	1.29	5 (9%)
14	CLA	bB	822	2	45,53,73	1.72	8 (17%)	52,89,113	1.67	7 (13%)
14	CLA	bB	805	2	54,62,73	1.57	7 (12%)	62,99,113	1.61	7 (11%)
14	CLA	aA	832	1	65,73,73	1.44	10 (15%)	76,113,113	1.49	10 (13%)
14	CLA	aB	805	2	54,62,73	1.57	7 (12%)	62,99,113	1.61	7 (11%)
14	CLA	aB	831	2	49,57,73	1.69	7 (14%)	55,93,113	1.70	9 (16%)
18	LHG	bA	850	-	48,48,48	0.65	1 (2%)	51,54,54	1.29	5 (9%)
14	CLA	dA	807	1	51,59,73	1.65	8 (15%)	59,96,113	1.61	6 (10%)
14	CLA	cA	803	1	45,53,73	1.75	8 (17%)	52,89,113	1.70	9 (17%)
17	BCR	dB	846	-	41,41,41	1.16	2 (4%)	56,56,56	1.17	3 (5%)
14	CLA	aA	806	1	65,73,73	1.47	10 (15%)	76,113,113	1.46	9 (11%)
16	SF4	aA	845	2,1	0,12,12	-	-	-		
14	CLA	aB	820	2	47,55,73	1.67	8 (17%)	54,91,113	1.58	6 (11%)
17	BCR	bL	207	-	41,41,41	1.18	3 (7%)	56,56,56	1.42	7 (12%)
14	CLA	cB	818	2	60,68,73	1.54	10 (16%)	70,107,113	1.47	7 (10%)
14	CLA	dA	821	14	65,73,73	1.44	10 (15%)	76,113,113	1.52	7 (9%)
14	CLA	cA	825	-	65,73,73	1.39	8 (12%)	76,113,113	1.55	10 (13%)
14	CLA	bK	103	-	45,53,73	1.72	8 (17%)	52,89,113	1.66	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	CLA	dB	801	-	65,73,73	1.46	10 (15%)	76,113,113	1.42	7 (9%)
14	CLA	aA	830	1	65,73,73	1.50	10 (15%)	76,113,113	1.53	7 (9%)
14	CLA	aA	815	1	45,53,73	1.77	8 (17%)	52,89,113	1.70	6 (11%)
19	LMG	dB	850	-	55,55,55	0.79	2 (3%)	63,63,63	1.46	9 (14%)
14	CLA	bA	821	14	65,73,73	1.44	10 (15%)	76,113,113	1.52	7 (9%)
14	CLA	aB	801	-	65,73,73	1.46	10 (15%)	76,113,113	1.42	7 (9%)

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	cB	804	-	1/1/15/20	13/37/115/115	-
14	CLA	bA	819	1	1/1/15/20	19/37/115/115	-
14	CLA	bA	828	1	1/1/15/20	6/37/115/115	-
14	CLA	cB	838	2	1/1/15/20	8/37/115/115	-
14	CLA	dB	814	2	1/1/15/20	13/37/115/115	-
14	CLA	dB	834	2	1/1/13/20	11/29/107/115	-
14	CLA	dA	838	1	1/1/15/20	14/37/115/115	-
17	BCR	aB	845	-	-	12/29/63/63	0/2/2/2
14	CLA	cA	840	1	1/1/15/20	12/37/115/115	-
17	BCR	bK	102	-	-	6/29/63/63	0/2/2/2
14	CLA	aB	804	-	1/1/15/20	13/37/115/115	-
14	CLA	cA	816	-	-	8/18/96/115	-
14	CLA	aB	830	2	1/1/11/20	6/13/91/115	-
18	LHG	bB	851	-	-	11/26/26/53	-
16	SF4	cC	102	3	-	-	0/6/5/5
14	CLA	cA	832	1	1/1/15/20	12/37/115/115	-
14	CLA	bA	838	1	1/1/15/20	14/37/115/115	-
15	PQN	bB	843	-	-	7/23/43/43	0/2/2/2
14	CLA	cA	842	-	1/1/15/20	12/37/115/115	-
14	CLA	bB	814	2	1/1/15/20	13/37/115/115	-
14	CLA	aA	802	-	1/1/11/20	3/13/91/115	-
14	CLA	dK	103	-	1/1/11/20	3/13/91/115	-
14	CLA	cA	815	1	1/1/11/20	4/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	aA	810	1	1/1/11/20	5/13/91/115	-
14	CLA	dA	840	1	1/1/15/20	12/37/115/115	-
17	BCR	bL	208	-	-	15/29/63/63	0/2/2/2
14	CLA	aA	820	1	1/1/14/20	11/33/111/115	-
17	BCR	dA	845	-	-	7/29/63/63	0/2/2/2
17	BCR	bB	849	-	-	7/29/63/63	0/2/2/2
17	BCR	aL	201	-	-	13/29/63/63	0/2/2/2
18	LHG	aA	853	14	-	10/31/31/53	-
14	CLA	cK	101	9	1/1/9/20	3/7/81/115	-
17	BCR	dA	847	-	-	18/29/63/63	0/2/2/2
14	CLA	aA	829	1	1/1/15/20	14/37/115/115	-
14	CLA	dB	812	2	1/1/11/20	4/13/91/115	-
14	CLA	bA	807	1	1/1/12/20	2/21/99/115	-
14	CLA	bB	824	2	1/1/11/20	6/13/91/115	-
14	CLA	aB	802	2	1/1/15/20	12/37/115/115	-
14	CLA	bB	817	2	1/1/13/20	8/25/103/115	-
14	CLA	dA	814	1	1/1/11/20	5/13/91/115	-
17	BCR	aJ	103	-	-	15/29/63/63	0/2/2/2
13	CL0	cA	801	1	3/3/20/25	20/37/135/135	-
18	LHG	dB	851	-	-	11/26/26/53	-
14	CLA	aF	201	-	1/1/12/20	5/21/99/115	-
14	CLA	aA	841	1	1/1/15/20	12/37/115/115	-
14	CLA	cB	825	-	1/1/11/20	6/15/93/115	-
14	CLA	cA	817	1	1/1/12/20	9/24/102/115	-
17	BCR	bB	846	-	-	12/29/63/63	0/2/2/2
17	BCR	dA	849	-	-	20/29/63/63	0/2/2/2
14	CLA	aA	805	1	1/1/11/20	5/13/91/115	-
14	CLA	bB	829	2	1/1/15/20	9/37/115/115	-
13	CL0	dA	801	1	2/2/20/25	11/37/135/135	-
14	CLA	bJ	101	-	1/1/11/20	10/13/91/115	-
14	CLA	aB	819	-	1/1/15/20	9/37/115/115	-
14	CLA	cA	833	1	1/1/15/20	9/37/115/115	-
14	CLA	cB	832	2	1/1/15/20	15/37/115/115	-
14	CLA	dB	809	2	1/1/15/20	9/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	dB	816	2	1/1/11/20	5/13/91/115	-
13	CL0	bA	801	1	2/2/20/25	12/37/135/135	-
17	BCR	cB	845	-	-	12/29/63/63	0/2/2/2
14	CLA	aB	814	2	1/1/13/20	2/27/105/115	-
14	CLA	aB	834	2	1/1/11/20	4/13/91/115	-
14	CLA	bA	806	1	1/1/15/20	10/37/115/115	-
14	CLA	dA	827	14,1	1/1/15/20	12/37/115/115	-
17	BCR	cJ	103	-	-	15/29/63/63	0/2/2/2
14	CLA	dB	842	2	1/1/15/20	20/37/115/115	-
16	SF4	dC	102	3	-	-	0/6/5/5
14	CLA	bL	201	2,10	1/1/15/20	6/37/115/115	-
18	LHG	aA	852	-	-	18/53/53/53	-
18	LHG	dA	851	14	-	10/31/31/53	-
14	CLA	dA	818	1	1/1/12/20	7/24/102/115	-
17	BCR	bB	848	-	-	10/29/63/63	0/2/2/2
14	CLA	aB	839	2	-	1/16/94/115	-
15	PQN	dA	843	-	-	5/23/43/43	0/2/2/2
14	CLA	cA	813	1	-	6/13/91/115	-
14	CLA	cB	809	2	1/1/15/20	9/37/115/115	-
17	BCR	dL	207	-	-	9/29/63/63	0/2/2/2
14	CLA	cL	203	10	1/1/15/20	12/37/115/115	-
14	CLA	dX	101	12	1/1/11/20	7/13/91/115	-
14	CLA	bA	826	-	1/1/13/20	5/25/103/115	-
14	CLA	dL	206	-	1/1/15/20	20/37/115/115	-
14	CLA	cB	827	2	1/1/15/20	13/37/115/115	-
14	CLA	bB	842	2	1/1/15/20	20/37/115/115	-
14	CLA	aB	821	2	1/1/11/20	5/13/91/115	-
14	CLA	aB	809	2	1/1/15/20	9/37/115/115	-
14	CLA	aK	102	-	1/1/11/20	3/13/91/115	-
14	CLA	dJ	101	-	1/1/11/20	10/13/91/115	-
14	CLA	bB	819	2	1/1/14/20	8/31/109/115	-
17	BCR	aL	205	-	-	9/29/63/63	0/2/2/2
14	CLA	cA	804	14,1	1/1/11/20	4/13/91/115	-
14	CLA	bX	101	12	1/1/11/20	7/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	dA	817	1	1/1/12/20	9/24/102/115	-
17	BCR	bA	848	-	-	9/29/63/63	0/2/2/2
14	CLA	dB	806	2	1/1/15/20	15/37/115/115	-
17	BCR	dA	846	-	-	8/29/63/63	0/2/2/2
14	CLA	dB	833	2	1/1/15/20	15/37/115/115	-
14	CLA	aB	836	-	-	6/13/91/115	-
17	BCR	bJ	103	-	-	15/29/63/63	0/2/2/2
14	CLA	dA	826	-	1/1/13/20	5/25/103/115	-
14	CLA	dA	829	1	1/1/15/20	14/37/115/115	-
14	CLA	cB	824	2	-	6/24/102/115	-
14	CLA	dA	804	14,1	1/1/11/20	4/13/91/115	-
14	CLA	dA	836	1	1/1/11/20	7/13/91/115	-
14	CLA	aB	813	2	1/1/15/20	13/37/115/115	-
17	BCR	bA	846	-	-	8/29/63/63	0/2/2/2
18	LHG	cB	850	-	-	11/26/26/53	-
14	CLA	dB	831	2	1/1/11/20	6/13/91/115	-
14	CLA	bA	834	1	1/1/15/20	9/37/115/115	-
14	CLA	bA	829	1	1/1/15/20	14/37/115/115	-
14	CLA	cB	822	-	1/1/13/20	12/25/103/115	-
14	CLA	aA	837	1	1/1/12/20	7/21/99/115	-
14	CLA	bA	825	-	1/1/15/20	13/37/115/115	-
14	CLA	dF	203	-	1/1/11/20	3/13/91/115	-
14	CLA	bB	841	-	1/1/15/20	3/37/115/115	-
14	CLA	aK	101	9	1/1/9/20	3/7/81/115	-
14	CLA	bB	808	2	1/1/15/20	8/37/115/115	-
16	SF4	dA	844	2,1	-	-	0/6/5/5
17	BCR	aB	843	-	-	10/29/63/63	0/2/2/2
14	CLA	aB	822	-	1/1/13/20	13/25/103/115	-
14	CLA	bJ	102	-	1/1/8/20	0/2/76/115	-
18	LHG	cA	853	14	-	10/31/31/53	-
14	CLA	cK	102	-	1/1/11/20	3/13/91/115	-
14	CLA	cB	802	2	1/1/15/20	13/37/115/115	-
17	BCR	bA	847	-	-	18/29/63/63	0/2/2/2
17	BCR	dJ	104	-	-	9/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	BCR	dB	845	-	-	9/29/63/63	0/2/2/2
14	CLA	dA	816	-	-	8/18/96/115	-
14	CLA	aB	837	2	1/1/14/20	8/31/109/115	-
14	CLA	cB	821	2	1/1/11/20	5/13/91/115	-
17	BCR	dB	844	-	-	10/29/63/63	0/2/2/2
14	CLA	bL	205	10	1/1/15/20	10/37/115/115	-
14	CLA	dA	842	-	1/1/15/20	12/37/115/115	-
15	PQN	aA	844	-	-	8/23/43/43	0/2/2/2
17	BCR	dB	847	-	-	17/29/63/63	0/2/2/2
14	CLA	cA	838	1	1/1/15/20	14/37/115/115	-
17	BCR	aB	844	-	-	9/29/63/63	0/2/2/2
14	CLA	aL	203	10	1/1/15/20	12/37/115/115	-
14	CLA	cA	834	1	1/1/15/20	9/37/115/115	-
14	CLA	cB	805	2	1/1/12/20	7/24/102/115	-
14	CLA	dA	808	1	1/1/11/20	4/13/91/115	-
17	BCR	cM	101	-	-	9/29/63/63	0/2/2/2
14	CLA	bA	841	1	1/1/15/20	12/37/115/115	-
14	CLA	aA	809	1	1/1/11/20	5/13/91/115	-
14	CLA	aA	842	-	1/1/15/20	12/37/115/115	-
14	CLA	dB	825	2	-	6/24/102/115	-
14	CLA	aJ	102	-	1/1/8/20	0/2/76/115	-
14	CLA	bA	808	1	1/1/11/20	4/13/91/115	-
14	CLA	cA	823	1	1/1/12/20	12/21/99/115	-
14	CLA	dB	811	2	1/1/15/20	6/37/115/115	-
17	BCR	aF	202	-	-	11/29/63/63	0/2/2/2
16	SF4	cA	845	2,1	-	-	0/6/5/5
14	CLA	bF	201	-	1/1/12/20	5/21/99/115	-
17	BCR	dB	849	-	-	7/29/63/63	0/2/2/2
14	CLA	bL	202	10,18	1/1/12/20	13/22/100/115	-
17	BCR	cB	847	-	-	9/29/63/63	0/2/2/2
14	CLA	dB	837	-	-	6/13/91/115	-
13	CL0	aA	801	1	3/3/20/25	17/37/135/135	-
17	BCR	bL	203	-	-	13/29/63/63	0/2/2/2
17	BCR	dM	101	-	-	9/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	LHG	bA	851	14	-	10/31/31/53	-
14	CLA	aA	817	1	1/1/12/20	9/24/102/115	-
14	CLA	aA	836	1	1/1/11/20	7/13/91/115	-
14	CLA	cA	809	1	1/1/11/20	5/13/91/115	-
17	BCR	aA	850	-	-	9/29/63/63	0/2/2/2
17	BCR	dF	204	-	-	13/29/63/63	0/2/2/2
14	CLA	bB	832	2	1/1/11/20	11/18/96/115	-
15	PQN	cA	844	-	-	8/23/43/43	0/2/2/2
14	CLA	bA	818	1	1/1/12/20	7/24/102/115	-
14	CLA	aB	810	2	1/1/15/20	9/37/115/115	-
14	CLA	cB	830	2	1/1/11/20	6/13/91/115	-
17	BCR	bB	845	-	-	9/29/63/63	0/2/2/2
14	CLA	cB	835	-	1/1/11/20	2/13/91/115	-
17	BCR	bB	847	-	-	17/29/63/63	0/2/2/2
17	BCR	cF	204	-	-	14/29/63/63	0/2/2/2
14	CLA	dA	803	1	1/1/11/20	6/13/91/115	-
14	CLA	cB	831	2	1/1/11/20	11/18/96/115	-
14	CLA	dB	828	2	1/1/15/20	13/37/115/115	-
17	BCR	bF	204	-	-	13/29/63/63	0/2/2/2
14	CLA	bA	835	1	1/1/12/20	5/24/102/115	-
17	BCR	cA	851	-	-	20/29/63/63	0/2/2/2
14	CLA	cB	839	2	-	1/16/94/115	-
16	SF4	bC	101	3	-	-	0/6/5/5
17	BCR	cA	849	-	-	18/29/63/63	0/2/2/2
19	LMG	bB	850	-	-	23/50/70/70	0/1/1/1
14	CLA	cF	201	-	1/1/12/20	5/21/99/115	-
14	CLA	dA	819	1	1/1/15/20	19/37/115/115	-
14	CLA	bB	827	2	1/1/15/20	20/37/115/115	-
14	CLA	aA	813	1	-	6/13/91/115	-
14	CLA	dL	204	10	1/1/12/20	8/22/100/115	-
14	CLA	cA	824	1	1/1/11/20	5/16/94/115	-
14	CLA	aB	826	2	1/1/15/20	20/37/115/115	-
14	CLA	bB	834	2	1/1/13/20	11/29/107/115	-
14	CLA	bA	832	1	1/1/15/20	11/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	aB	811	2	1/1/11/20	4/13/91/115	-
14	CLA	dB	839	2	1/1/15/20	8/37/115/115	-
17	BCR	aB	851	-	-	8/29/63/63	0/2/2/2
17	BCR	dB	848	-	-	10/29/63/63	0/2/2/2
14	CLA	aA	843	18	1/1/12/20	13/22/100/115	-
17	BCR	bF	202	-	-	11/29/63/63	0/2/2/2
14	CLA	cB	841	2	1/1/15/20	20/37/115/115	-
14	CLA	aL	204	-	1/1/12/20	8/22/100/115	-
14	CLA	bB	839	2	1/1/15/20	8/37/115/115	-
14	CLA	cL	204	-	1/1/12/20	7/22/100/115	-
14	CLA	bA	816	-	-	8/18/96/115	-
14	CLA	cB	808	2	1/1/15/20	8/37/115/115	-
14	CLA	cB	812	2	1/1/11/20	6/13/91/115	-
14	CLA	dB	819	2	1/1/14/20	8/31/109/115	-
14	CLA	aA	840	1	1/1/15/20	12/37/115/115	-
17	BCR	cL	201	-	-	13/29/63/63	0/2/2/2
14	CLA	bB	806	2	1/1/15/20	15/37/115/115	-
17	BCR	dJ	103	-	-	15/29/63/63	0/2/2/2
14	CLA	aA	804	14,1	1/1/11/20	4/13/91/115	-
14	CLA	bL	204	10	1/1/12/20	8/22/100/115	-
17	BCR	dB	852	-	-	8/29/63/63	0/2/2/2
14	CLA	cB	828	2	1/1/15/20	9/37/115/115	-
14	CLA	bB	801	-	1/1/15/20	14/37/115/115	-
14	CLA	cA	831	1	1/1/12/20	2/19/97/115	-
14	CLA	dB	830	2	1/1/15/20	13/37/115/115	-
14	CLA	dB	838	2	1/1/14/20	8/31/109/115	-
14	CLA	dB	827	2	1/1/15/20	20/37/115/115	-
17	BCR	bA	849	-	-	20/29/63/63	0/2/2/2
14	CLA	aA	803	1	1/1/11/20	6/13/91/115	-
14	CLA	dA	832	1	1/1/15/20	11/37/115/115	-
14	CLA	cA	821	14	1/1/15/20	14/37/115/115	-
14	CLA	dB	803	-	1/1/15/20	18/37/115/115	-
14	CLA	aB	828	2	1/1/15/20	9/37/115/115	-
14	CLA	dA	839	1	1/1/15/20	10/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	BCR	bB	852	-	-	8/29/63/63	0/2/2/2
14	CLA	bB	810	2	1/1/15/20	9/37/115/115	-
14	CLA	bB	812	2	1/1/11/20	4/13/91/115	-
14	CLA	cB	823	2	1/1/11/20	6/13/91/115	-
17	BCR	cL	206	-	-	11/29/63/63	0/2/2/2
14	CLA	dA	806	1	1/1/15/20	10/37/115/115	-
14	CLA	cA	805	1	1/1/11/20	5/13/91/115	-
14	CLA	cA	843	18	1/1/12/20	13/22/100/115	-
17	BCR	cB	848	-	-	7/29/63/63	0/2/2/2
17	BCR	cI	101	-	-	14/29/63/63	0/2/2/2
14	CLA	bA	839	1	1/1/15/20	10/37/115/115	-
17	BCR	aJ	104	-	-	9/29/63/63	0/2/2/2
14	CLA	dB	840	2	-	1/16/94/115	-
14	CLA	bA	817	1	1/1/12/20	9/24/102/115	-
14	CLA	cB	803	-	1/1/15/20	18/37/115/115	-
14	CLA	cB	836	-	-	6/13/91/115	-
14	CLA	bA	830	1	1/1/15/20	12/37/115/115	-
14	CLA	dA	841	1	1/1/15/20	12/37/115/115	-
14	CLA	bB	807	2	1/1/15/20	20/37/115/115	-
14	CLA	bA	815	1	1/1/11/20	4/13/91/115	-
14	CLA	bB	826	-	1/1/11/20	6/15/93/115	-
14	CLA	dA	834	1	1/1/15/20	9/37/115/115	-
14	CLA	bB	811	2	1/1/15/20	6/37/115/115	-
17	BCR	aA	851	-	-	20/29/63/63	0/2/2/2
14	CLA	cL	202	10	1/1/15/20	10/37/115/115	-
14	CLA	dA	831	1	1/1/12/20	2/19/97/115	-
14	CLA	cB	811	2	1/1/11/20	4/13/91/115	-
19	LMG	aB	849	-	-	23/50/70/70	0/1/1/1
14	CLA	aA	814	1	1/1/11/20	5/13/91/115	-
14	CLA	aA	834	1	1/1/15/20	9/37/115/115	-
14	CLA	cA	835	1	1/1/12/20	5/24/102/115	-
14	CLA	dL	201	2,10	1/1/15/20	6/37/115/115	-
14	CLA	aB	838	2	1/1/15/20	8/37/115/115	-
16	SF4	bC	102	3	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	bB	836	-	1/1/11/20	2/13/91/115	-
14	CLA	aJ	101	-	1/1/11/20	10/13/91/115	-
17	BCR	aL	206	-	-	11/29/63/63	0/2/2/2
14	CLA	aB	803	-	1/1/15/20	18/37/115/115	-
14	CLA	cB	816	2	1/1/13/20	8/25/103/115	-
14	CLA	dB	832	2	1/1/11/20	11/18/96/115	-
14	CLA	cB	807	2	1/1/15/20	20/37/115/115	-
14	CLA	bA	820	1	1/1/14/20	11/33/111/115	-
14	CLA	cB	801	-	1/1/15/20	14/37/115/115	-
14	CLA	dB	818	2	1/1/13/20	9/30/108/115	-
14	CLA	bA	813	1	-	6/13/91/115	-
14	CLA	bB	816	2	1/1/11/20	5/13/91/115	-
14	CLA	aA	821	14	1/1/15/20	14/37/115/115	-
14	CLA	bB	830	2	1/1/15/20	13/37/115/115	-
14	CLA	aA	839	1	1/1/15/20	10/37/115/115	-
14	CLA	cB	806	2	1/1/15/20	15/37/115/115	-
14	CLA	dB	826	-	1/1/11/20	6/15/93/115	-
14	CLA	bB	809	2	1/1/15/20	9/37/115/115	-
17	BCR	cJ	104	-	-	9/29/63/63	0/2/2/2
14	CLA	dB	824	2	1/1/11/20	6/13/91/115	-
14	CLA	dB	822	2	1/1/11/20	5/13/91/115	-
14	CLA	aA	828	1	1/1/15/20	6/37/115/115	-
14	CLA	dA	812	1	1/1/12/20	11/24/102/115	-
14	CLA	dF	201	-	1/1/12/20	5/21/99/115	-
17	BCR	aM	101	-	-	9/29/63/63	0/2/2/2
14	CLA	dK	101	9	1/1/9/20	3/7/81/115	-
17	BCR	dI	101	-	-	14/29/63/63	0/2/2/2
14	CLA	aB	840	-	1/1/15/20	2/37/115/115	-
14	CLA	bA	804	14,1	1/1/11/20	4/13/91/115	-
14	CLA	dB	810	2	1/1/15/20	9/37/115/115	-
14	CLA	aB	816	2	1/1/13/20	8/25/103/115	-
14	CLA	dJ	102	-	1/1/8/20	0/2/76/115	-
14	CLA	aA	838	1	1/1/15/20	14/37/115/115	-
14	CLA	bB	815	2	1/1/13/20	2/27/105/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	SF4	cC	101	3	-	-	0/6/5/5
14	CLA	cA	812	1	1/1/12/20	11/24/102/115	-
14	CLA	aB	827	2	1/1/15/20	13/37/115/115	-
15	PQN	cB	842	-	-	9/23/43/43	0/2/2/2
14	CLA	cB	813	2	1/1/15/20	13/37/115/115	-
14	CLA	cA	818	1	1/1/12/20	7/24/102/115	-
14	CLA	bB	802	2	1/1/15/20	12/37/115/115	-
14	CLA	cF	203	-	1/1/11/20	4/13/91/115	-
14	CLA	aA	807	1	1/1/12/20	2/21/99/115	-
17	BCR	bB	844	-	-	10/29/63/63	0/2/2/2
14	CLA	dA	824	1	1/1/11/20	5/16/94/115	-
14	CLA	dB	821	2	1/1/11/20	8/16/94/115	-
14	CLA	cA	819	1	1/1/15/20	19/37/115/115	-
14	CLA	cB	819	-	1/1/15/20	9/37/115/115	-
14	CLA	dA	815	1	1/1/11/20	4/13/91/115	-
17	BCR	bM	101	-	-	9/29/63/63	0/2/2/2
17	BCR	aB	848	-	-	7/29/63/63	0/2/2/2
14	CLA	dB	841	-	1/1/15/20	2/37/115/115	-
17	BCR	bA	845	-	-	7/29/63/63	0/2/2/2
17	BCR	cB	843	-	-	10/29/63/63	0/2/2/2
17	BCR	dL	208	-	-	15/29/63/63	0/2/2/2
14	CLA	bB	813	2	1/1/11/20	6/13/91/115	-
14	CLA	bB	833	2	1/1/15/20	15/37/115/115	-
14	CLA	bB	803	-	1/1/15/20	18/37/115/115	-
15	PQN	aB	842	-	-	9/23/43/43	0/2/2/2
14	CLA	aA	811	14,1	1/1/15/20	11/37/115/115	-
15	PQN	bA	843	-	-	5/23/43/43	0/2/2/2
14	CLA	bA	814	1	1/1/11/20	5/13/91/115	-
14	CLA	bB	825	2	-	6/24/102/115	-
14	CLA	aB	825	-	1/1/11/20	6/15/93/115	-
18	LHG	cA	852	-	-	18/53/53/53	-
14	CLA	dA	830	1	1/1/15/20	12/37/115/115	-
14	CLA	dA	833	1	1/1/15/20	9/37/115/115	-
14	CLA	bA	802	-	1/1/11/20	3/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	cX	101	12	1/1/11/20	7/13/91/115	-
17	BCR	cB	846	-	-	17/29/63/63	0/2/2/2
14	CLA	cA	811	14,1	1/1/15/20	11/37/115/115	-
14	CLA	bA	827	14,1	1/1/15/20	12/37/115/115	-
14	CLA	bB	840	2	-	1/16/94/115	-
17	BCR	cA	850	-	-	9/29/63/63	0/2/2/2
14	CLA	dB	807	2	1/1/15/20	20/37/115/115	-
16	SF4	dC	101	3	-	-	0/6/5/5
14	CLA	dB	815	2	1/1/13/20	2/27/105/115	-
14	CLA	cA	810	1	1/1/11/20	5/13/91/115	-
14	CLA	aA	822	1	1/1/11/20	11/18/96/115	-
14	CLA	cB	829	2	1/1/15/20	13/37/115/115	-
14	CLA	dA	825	-	1/1/15/20	13/37/115/115	-
14	CLA	dB	835	2	1/1/11/20	4/13/91/115	-
14	CLA	aA	816	-	-	8/18/96/115	-
14	CLA	cB	834	2	1/1/11/20	4/13/91/115	-
17	BCR	aB	846	-	-	17/29/63/63	0/2/2/2
14	CLA	dB	808	2	1/1/15/20	8/37/115/115	-
14	CLA	bA	805	1	1/1/11/20	5/13/91/115	-
14	CLA	aB	829	2	1/1/15/20	13/37/115/115	-
14	CLA	aB	824	2	-	6/24/102/115	-
14	CLA	cA	807	1	1/1/12/20	2/21/99/115	-
14	CLA	bA	811	14,1	1/1/15/20	11/37/115/115	-
14	CLA	cA	820	1	1/1/14/20	11/33/111/115	-
14	CLA	aA	831	1	1/1/12/20	2/19/97/115	-
14	CLA	bB	804	-	1/1/15/20	13/37/115/115	-
14	CLA	bA	837	1	1/1/12/20	7/21/99/115	-
17	BCR	cF	202	-	-	11/29/63/63	0/2/2/2
14	CLA	dB	823	-	1/1/13/20	12/25/103/115	-
14	CLA	cA	806	1	1/1/15/20	10/37/115/115	-
14	CLA	aB	841	2	1/1/15/20	20/37/115/115	-
14	CLA	cA	841	1	1/1/15/20	12/37/115/115	-
17	BCR	aA	848	-	-	8/29/63/63	0/2/2/2
14	CLA	cA	827	14,1	1/1/15/20	12/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	BCR	aI	101	-	-	14/29/63/63	0/2/2/2
14	CLA	dA	813	1	-	6/13/91/115	-
16	SF4	bA	844	2,1	-	-	0/6/5/5
14	CLA	cA	837	1	1/1/12/20	7/21/99/115	-
14	CLA	bB	818	2	1/1/13/20	9/30/108/115	-
14	CLA	dA	809	1	1/1/11/20	5/13/91/115	-
17	BCR	dF	202	-	-	11/29/63/63	0/2/2/2
14	CLA	bA	840	1	1/1/15/20	12/37/115/115	-
14	CLA	bA	824	1	1/1/11/20	5/16/94/115	-
14	CLA	bA	833	1	1/1/15/20	9/37/115/115	-
14	CLA	aB	818	2	1/1/14/20	8/31/109/115	-
14	CLA	cB	826	2	1/1/15/20	20/37/115/115	-
17	BCR	aA	846	-	-	6/29/63/63	0/2/2/2
17	BCR	cB	851	-	-	8/29/63/63	0/2/2/2
14	CLA	bA	809	1	1/1/11/20	5/13/91/115	-
14	CLA	bA	842	-	1/1/15/20	12/37/115/115	-
14	CLA	cB	810	2	1/1/15/20	9/37/115/115	-
14	CLA	cB	814	2	1/1/13/20	2/27/105/115	-
14	CLA	dB	836	-	1/1/11/20	2/13/91/115	-
14	CLA	aB	807	2	1/1/15/20	20/37/115/115	-
17	BCR	aF	204	-	-	14/29/63/63	0/2/2/2
14	CLA	aB	823	2	1/1/11/20	6/13/91/115	-
14	CLA	bA	831	1	1/1/12/20	2/19/97/115	-
14	CLA	aA	825	-	1/1/15/20	13/37/115/115	-
14	CLA	aB	808	2	1/1/15/20	8/37/115/115	-
14	CLA	aB	812	2	1/1/11/20	6/13/91/115	-
17	BCR	cA	848	-	-	8/29/63/63	0/2/2/2
16	SF4	aC	102	3	-	-	0/6/5/5
14	CLA	cA	802	-	1/1/11/20	3/13/91/115	-
14	CLA	bB	837	-	-	6/13/91/115	-
14	CLA	bB	828	2	1/1/15/20	13/37/115/115	-
14	CLA	cB	820	2	1/1/11/20	8/16/94/115	-
17	BCR	aA	847	-	-	7/29/63/63	0/2/2/2
14	CLA	dB	802	2	1/1/15/20	12/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	BCR	dL	203	-	-	13/29/63/63	0/2/2/2
17	BCR	cB	844	-	-	9/29/63/63	0/2/2/2
14	CLA	aF	203	-	1/1/11/20	4/13/91/115	-
14	CLA	aA	812	1	1/1/12/20	11/24/102/115	-
16	SF4	aC	101	3	-	-	0/6/5/5
19	LMG	cB	849	-	-	23/50/70/70	0/1/1/1
14	CLA	cA	822	1	1/1/11/20	11/18/96/115	-
14	CLA	aA	824	1	1/1/11/20	5/16/94/115	-
17	BCR	aB	847	-	-	9/29/63/63	0/2/2/2
14	CLA	dA	822	1	1/1/11/20	11/18/96/115	-
17	BCR	cA	847	-	-	7/29/63/63	0/2/2/2
14	CLA	aX	101	12	1/1/11/20	7/13/91/115	-
14	CLA	aB	835	-	1/1/11/20	2/13/91/115	-
14	CLA	aA	808	1	1/1/11/20	4/13/91/115	-
14	CLA	bA	822	1	1/1/11/20	11/18/96/115	-
14	CLA	bB	835	2	1/1/11/20	4/13/91/115	-
14	CLA	bA	803	1	1/1/11/20	6/13/91/115	-
17	BCR	aA	849	-	-	18/29/63/63	0/2/2/2
14	CLA	dA	828	1	1/1/15/20	6/37/115/115	-
14	CLA	dB	817	2	1/1/13/20	8/25/103/115	-
14	CLA	dA	802	-	1/1/11/20	3/13/91/115	-
14	CLA	dL	202	10,18	1/1/12/20	13/22/100/115	-
14	CLA	bF	203	-	1/1/11/20	3/13/91/115	-
14	CLA	cA	814	1	1/1/11/20	5/13/91/115	-
14	CLA	bA	823	1	1/1/12/20	12/21/99/115	-
17	BCR	cA	846	-	-	6/29/63/63	0/2/2/2
14	CLA	dA	823	1	1/1/12/20	12/21/99/115	-
14	CLA	cB	840	-	1/1/15/20	3/37/115/115	-
14	CLA	aA	818	1	1/1/12/20	7/24/102/115	-
14	CLA	cB	833	2	1/1/13/20	11/29/107/115	-
14	CLA	aB	832	2	1/1/15/20	15/37/115/115	-
14	CLA	cA	829	1	1/1/15/20	14/37/115/115	-
14	CLA	bB	823	-	1/1/13/20	13/25/103/115	-
14	CLA	aL	202	10	1/1/15/20	10/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	dA	835	1	1/1/12/20	5/24/102/115	-
14	CLA	aA	823	1	1/1/12/20	12/21/99/115	-
14	CLA	aB	806	2	1/1/15/20	15/37/115/115	-
14	CLA	aA	826	-	1/1/13/20	5/25/103/115	-
14	CLA	cB	815	2	1/1/11/20	5/13/91/115	-
14	CLA	bL	206	-	1/1/15/20	20/37/115/115	-
14	CLA	aA	833	1	1/1/15/20	9/37/115/115	-
14	CLA	dA	837	1	1/1/12/20	7/21/99/115	-
14	CLA	dB	805	2	1/1/12/20	7/24/102/115	-
14	CLA	bA	836	1	1/1/11/20	7/13/91/115	-
14	CLA	aA	819	1	1/1/15/20	19/37/115/115	-
14	CLA	aA	835	1	1/1/12/20	5/24/102/115	-
14	CLA	cA	836	1	1/1/11/20	7/13/91/115	-
14	CLA	aB	815	2	1/1/11/20	5/13/91/115	-
14	CLA	cA	839	1	1/1/15/20	10/37/115/115	-
14	CLA	dA	811	14,1	1/1/15/20	11/37/115/115	-
14	CLA	aB	833	2	1/1/13/20	11/29/107/115	-
14	CLA	cA	830	1	1/1/15/20	12/37/115/115	-
14	CLA	dA	810	1	1/1/11/20	5/13/91/115	-
14	CLA	bK	101	9	1/1/9/20	3/7/81/115	-
14	CLA	dB	820	-	1/1/15/20	9/37/115/115	-
17	BCR	bI	101	-	-	14/29/63/63	0/2/2/2
14	CLA	cJ	101	-	1/1/11/20	10/13/91/115	-
14	CLA	cA	826	-	1/1/13/20	5/25/103/115	-
14	CLA	cJ	102	-	1/1/8/20	0/2/76/115	-
17	BCR	cL	205	-	-	9/29/63/63	0/2/2/2
14	CLA	bB	838	2	1/1/14/20	8/31/109/115	-
17	BCR	dA	848	-	-	9/29/63/63	0/2/2/2
14	CLA	cA	808	1	1/1/11/20	4/13/91/115	-
14	CLA	bA	810	1	1/1/11/20	5/13/91/115	-
17	BCR	dK	102	-	-	6/29/63/63	0/2/2/2
14	CLA	bB	831	2	1/1/11/20	6/13/91/115	-
14	CLA	dB	813	2	1/1/11/20	6/13/91/115	-
18	LHG	aB	850	-	-	11/26/26/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	cB	817	2	1/1/13/20	9/30/108/115	-
14	CLA	dB	829	2	1/1/15/20	9/37/115/115	-
14	CLA	bB	820	-	1/1/15/20	9/37/115/115	-
14	CLA	dB	804	-	1/1/15/20	13/37/115/115	-
14	CLA	aB	817	2	1/1/13/20	9/30/108/115	-
14	CLA	dL	205	10	1/1/15/20	10/37/115/115	-
17	BCR	bJ	104	-	-	9/29/63/63	0/2/2/2
14	CLA	cB	837	2	1/1/14/20	8/31/109/115	-
14	CLA	bA	812	1	1/1/12/20	11/24/102/115	-
14	CLA	aA	827	14,1	1/1/15/20	12/37/115/115	-
14	CLA	cA	828	1	1/1/15/20	6/37/115/115	-
14	CLA	dA	805	1	1/1/11/20	5/13/91/115	-
14	CLA	bB	821	2	1/1/11/20	8/16/94/115	-
15	PQN	dB	843	-	-	5/23/43/43	0/2/2/2
14	CLA	dA	820	1	1/1/14/20	11/33/111/115	-
18	LHG	dA	850	-	-	18/53/53/53	-
14	CLA	bB	822	2	1/1/11/20	5/13/91/115	-
14	CLA	bB	805	2	1/1/12/20	7/24/102/115	-
14	CLA	aA	832	1	1/1/15/20	11/37/115/115	-
14	CLA	aB	805	2	1/1/12/20	7/24/102/115	-
14	CLA	aB	831	2	1/1/11/20	11/18/96/115	-
18	LHG	bA	850	-	-	18/53/53/53	-
14	CLA	dA	807	1	1/1/12/20	2/21/99/115	-
14	CLA	cA	803	1	1/1/11/20	6/13/91/115	-
17	BCR	dB	846	-	-	12/29/63/63	0/2/2/2
14	CLA	aA	806	1	1/1/15/20	10/37/115/115	-
16	SF4	aA	845	2,1	-	-	0/6/5/5
14	CLA	aB	820	2	1/1/11/20	8/16/94/115	-
17	BCR	bL	207	-	-	9/29/63/63	0/2/2/2
14	CLA	cB	818	2	1/1/14/20	8/31/109/115	-
14	CLA	dA	821	14	1/1/15/20	14/37/115/115	-
14	CLA	cA	825	-	1/1/15/20	13/37/115/115	-
14	CLA	bK	103	-	1/1/11/20	3/13/91/115	-
14	CLA	dB	801	-	1/1/15/20	14/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	aA	830	1	1/1/15/20	12/37/115/115	-
14	CLA	aA	815	1	1/1/11/20	4/13/91/115	-
19	LMG	dB	850	-	-	23/50/70/70	0/1/1/1
14	CLA	bA	821	14	1/1/15/20	14/37/115/115	-
14	CLA	aB	801	-	1/1/15/20	14/37/115/115	-

The worst 5 of 3502 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	bB	808	CLA	C4B-NB	7.89	1.42	1.35
14	bB	833	CLA	C4B-NB	7.83	1.42	1.35
14	dB	833	CLA	C4B-NB	7.81	1.42	1.35
14	aB	832	CLA	C4B-NB	7.80	1.42	1.35
14	cB	832	CLA	C4B-NB	7.78	1.42	1.35

The worst 5 of 3665 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	aB	804	CLA	C4A-NA-C1A	9.40	110.93	106.71
14	dB	804	CLA	C4A-NA-C1A	9.36	110.91	106.71
14	bB	804	CLA	C4A-NA-C1A	9.30	110.89	106.71
14	cB	804	CLA	C4A-NA-C1A	9.28	110.88	106.71
13	aA	801	CL0	C1D-ND-C4D	-8.96	99.97	106.33

5 of 366 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
13	aA	801	CL0	NC
13	aA	801	CL0	ND
13	aA	801	CL0	NA
13	bA	801	CL0	ND
13	bA	801	CL0	NC

5 of 4615 torsion outliers are listed below:

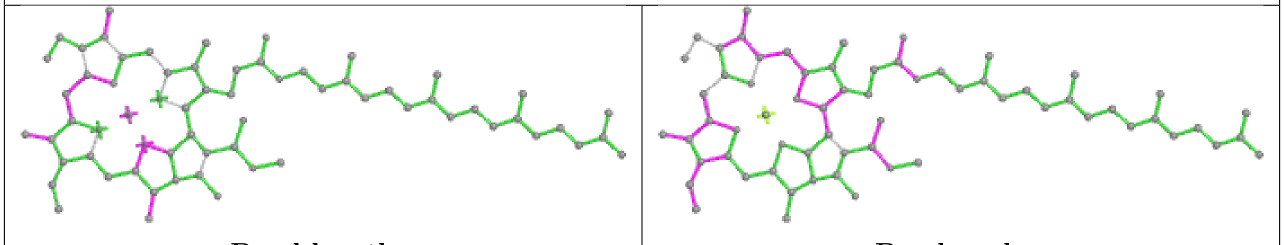
Mol	Chain	Res	Type	Atoms
14	aA	803	CLA	CHA-CBD-CGD-O1D
14	aA	803	CLA	CHA-CBD-CGD-O2D
14	aA	805	CLA	C1A-C2A-CAA-CBA
14	aA	805	CLA	C3A-C2A-CAA-CBA
14	aA	806	CLA	C1A-C2A-CAA-CBA

There are no ring outliers.

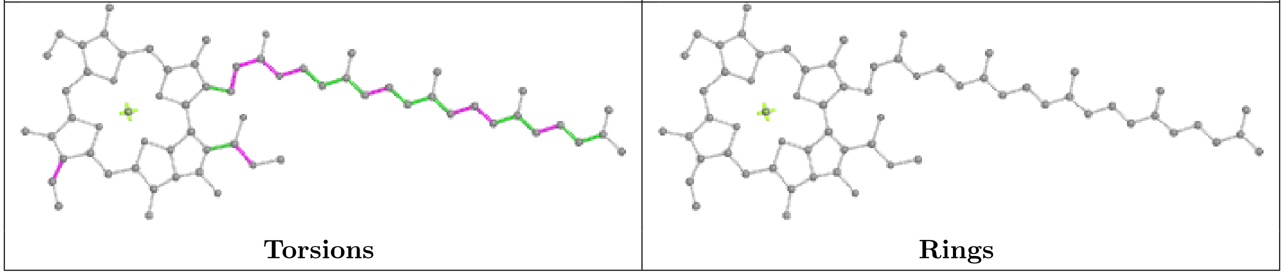
No monomer is involved in short contacts.

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 cB 804

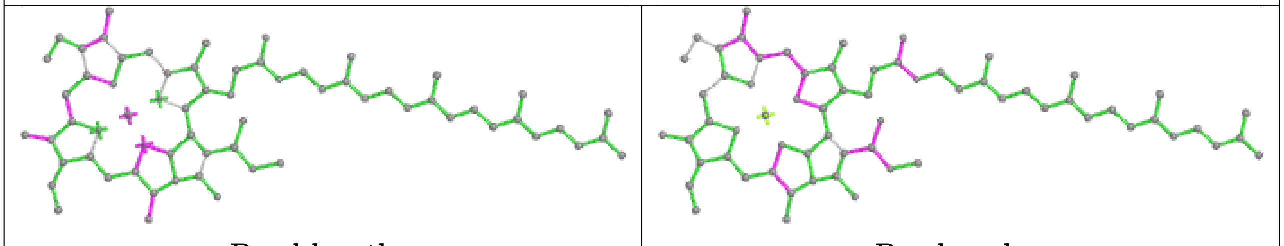


Bond lengths **Bond angles**

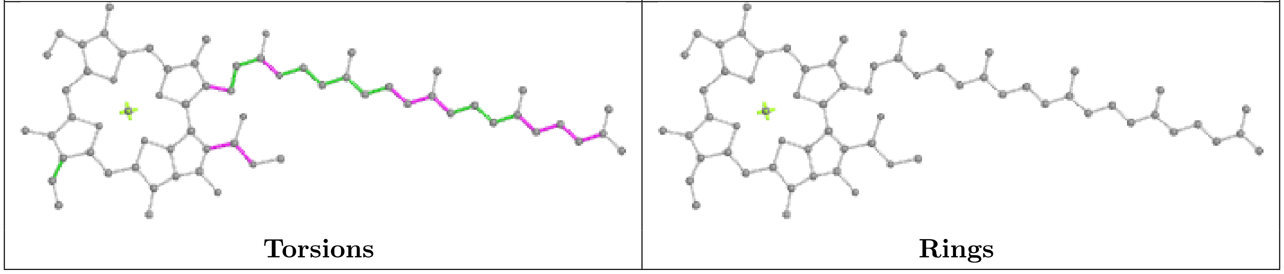


Torsions **Rings**

Ligand CLA bA 819

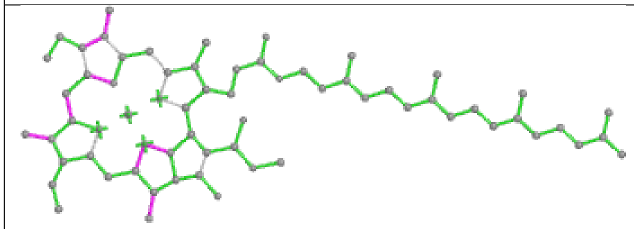


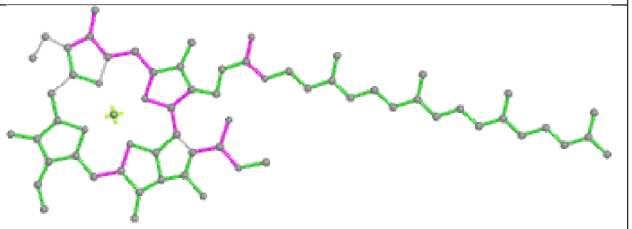
Bond lengths **Bond angles**

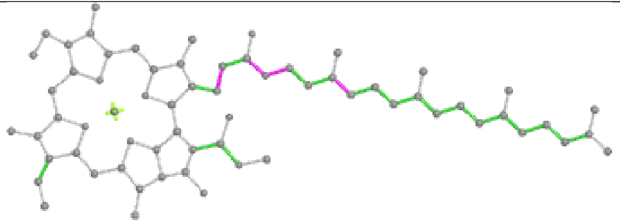


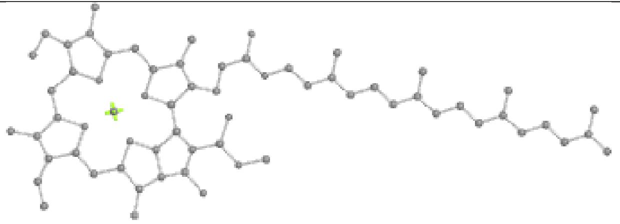
Torsions **Rings**

Ligand CLA bA 828

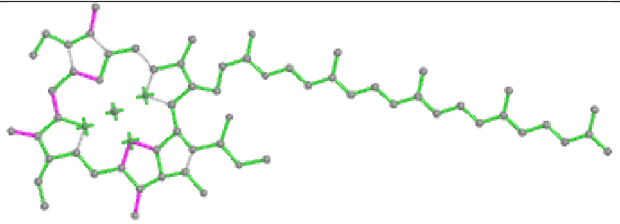

Bond lengths

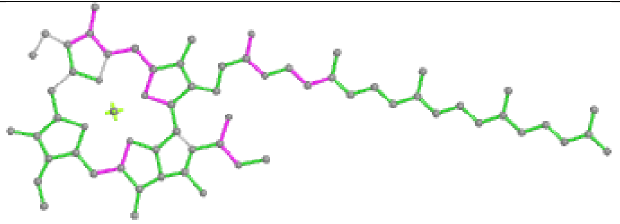

Bond angles


Torsions


Rings

Ligand CLA cB 838


Bond lengths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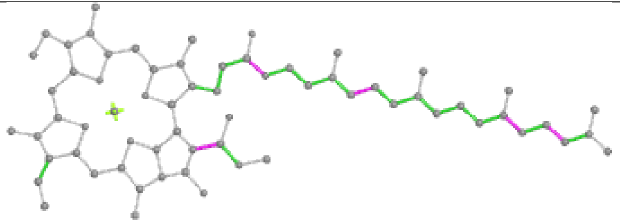
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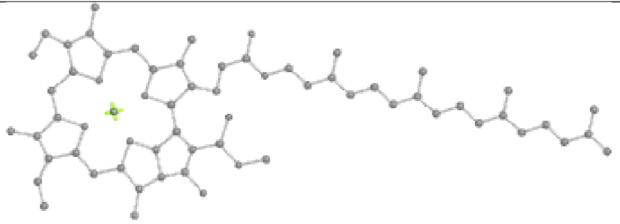
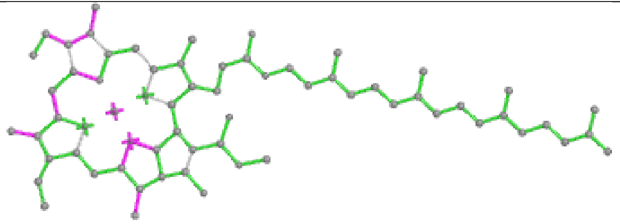
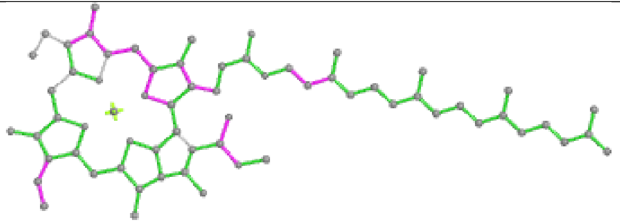

Rings

Ligand CLA dB 814


Bond lengths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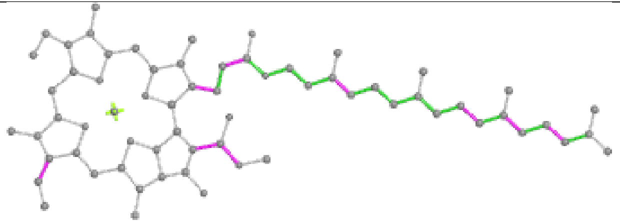
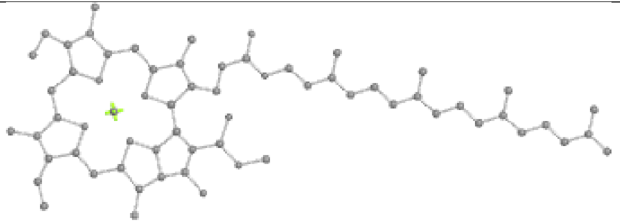
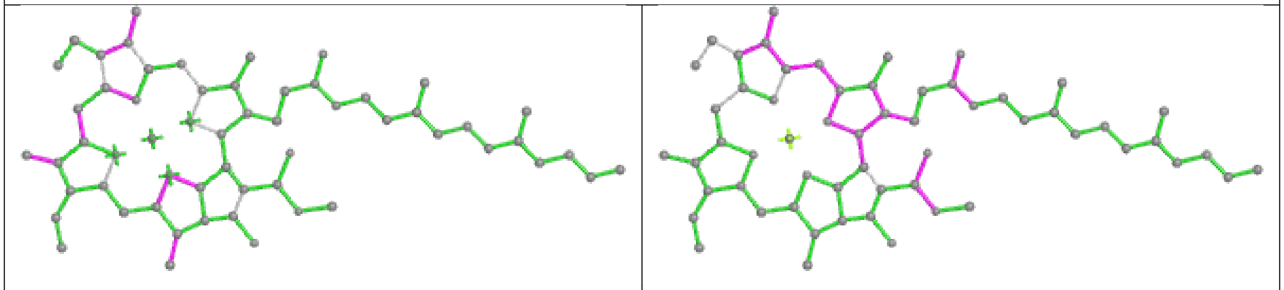

Torsions

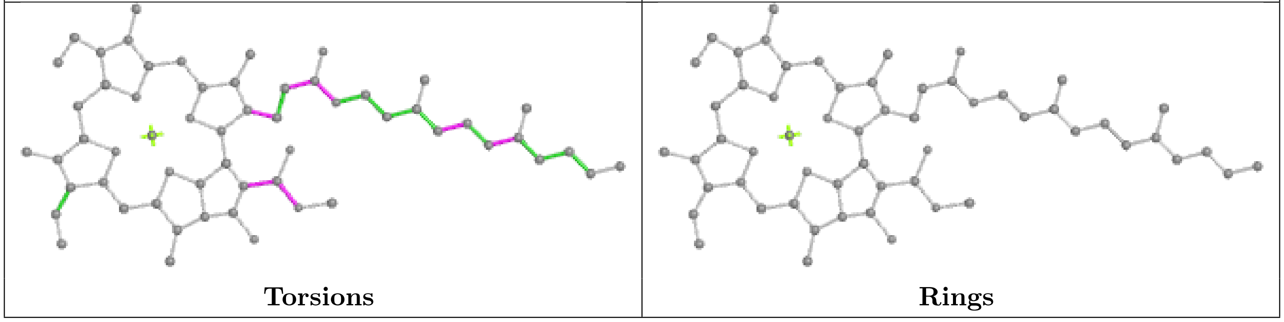

Rings

Ligand CLA dB 834



Bond lengths

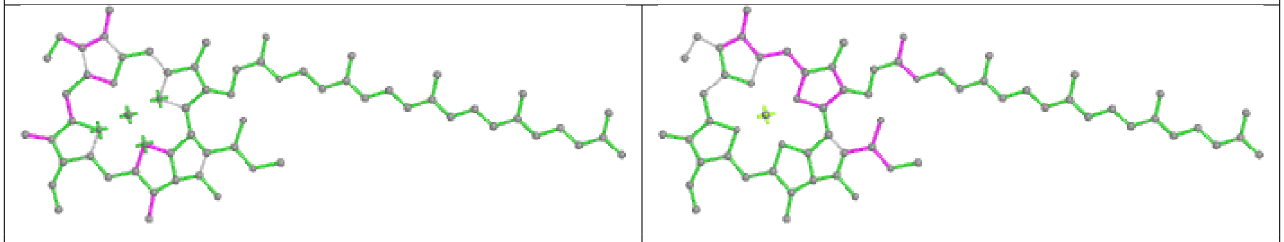
Bond angles



Torsions

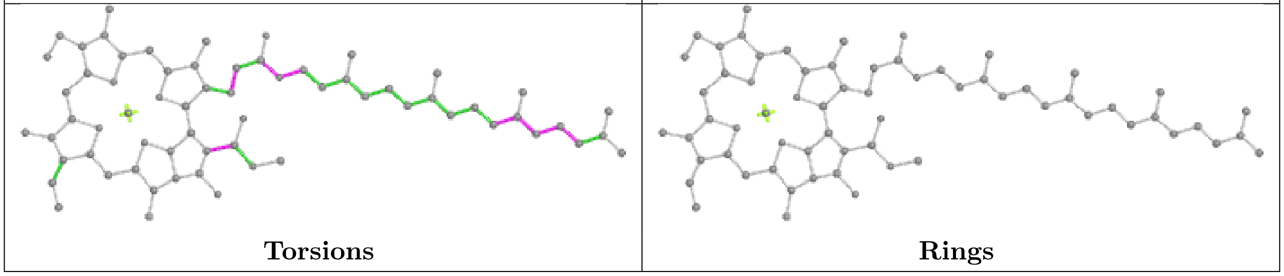
Rings

Ligand CLA dA 838



Bond lengths

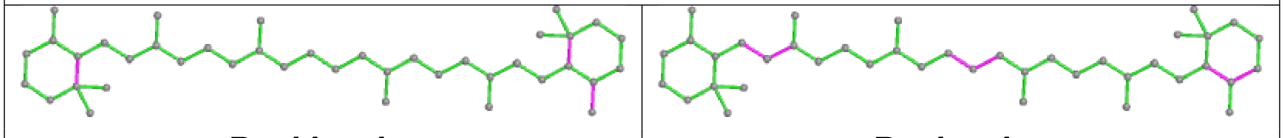
Bond angles



Torsions

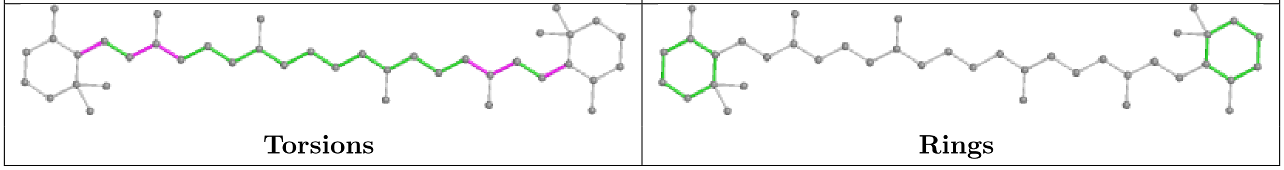
Rings

Ligand BCR aB 845



Bond lengths

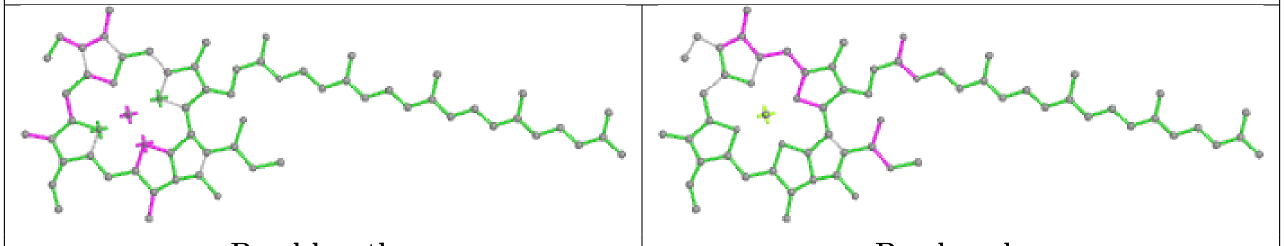
Bond angles



Torsions

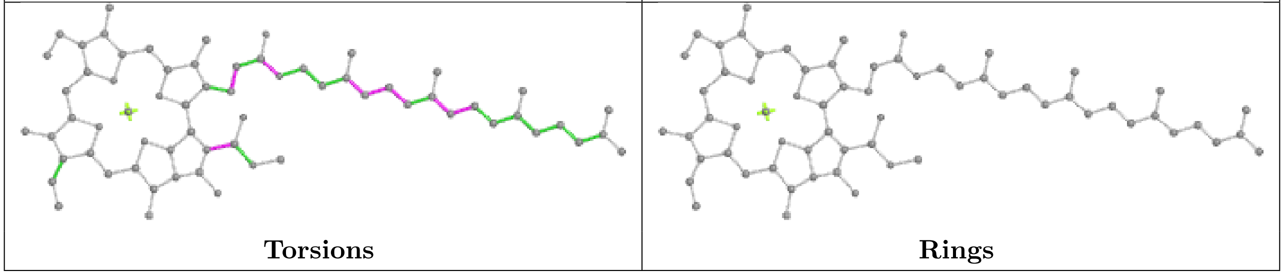
Rings

Ligand CLA cA 840



Bond lengths

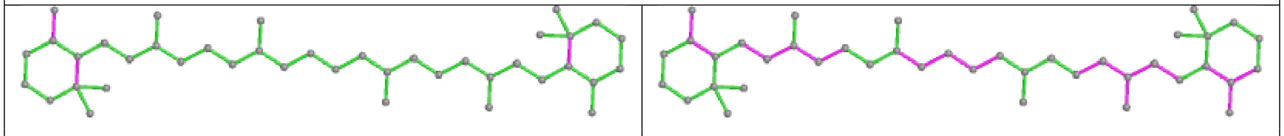
Bond angles



Torsions

Rings

Ligand BCR bK 102



Bond lengths

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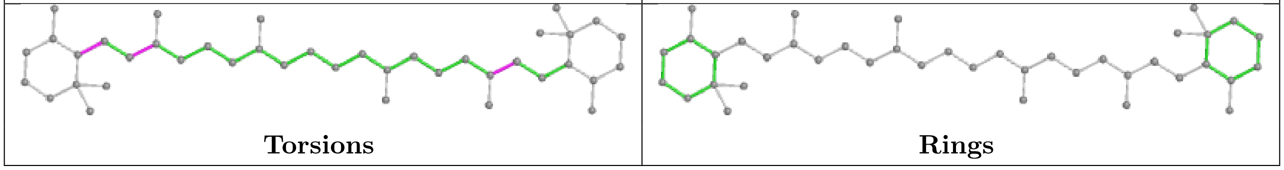
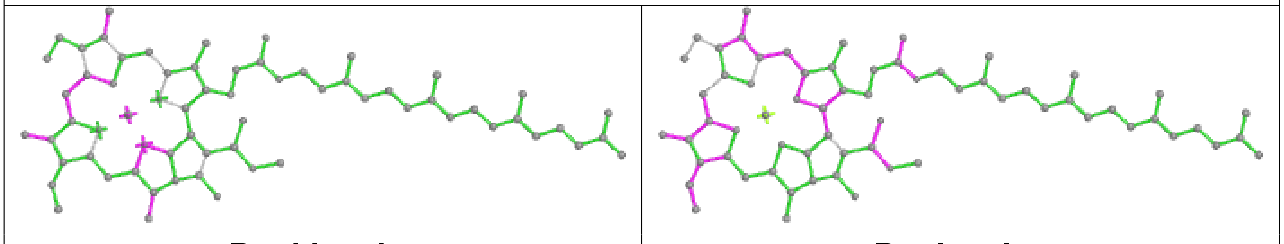


Torsions

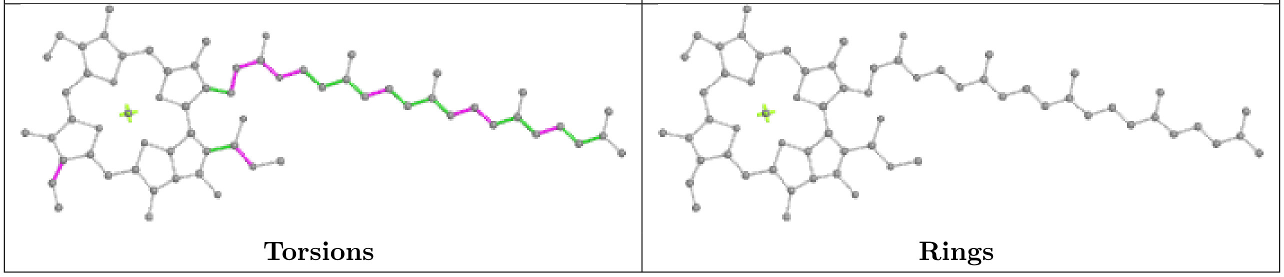
Rings

Ligand CLA aB 804



Bond lengths

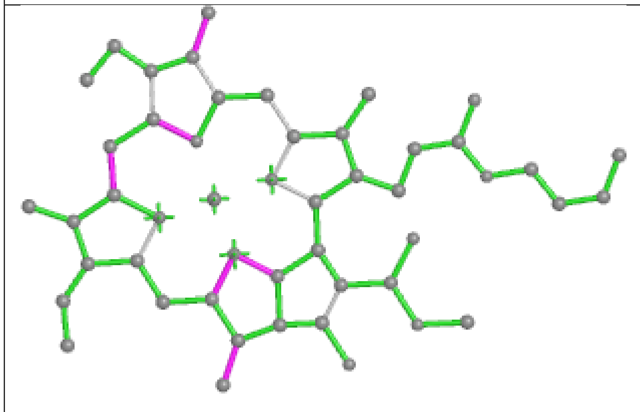
Bond angles



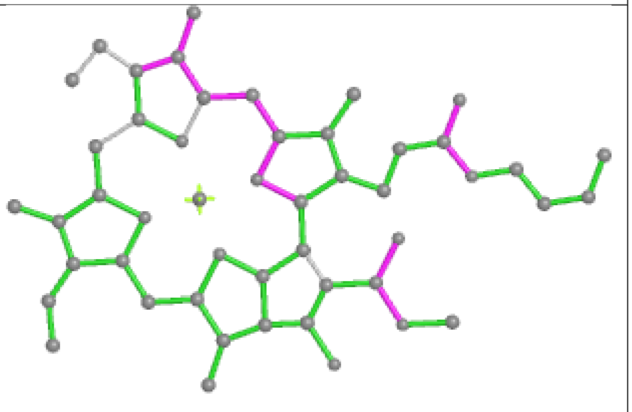
Torsions

Rings

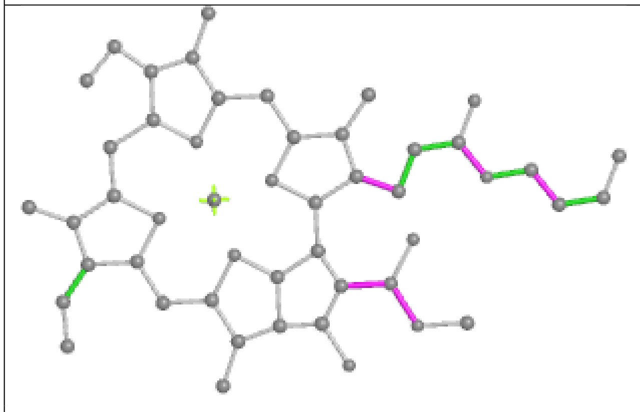
Ligand CLA cA 816



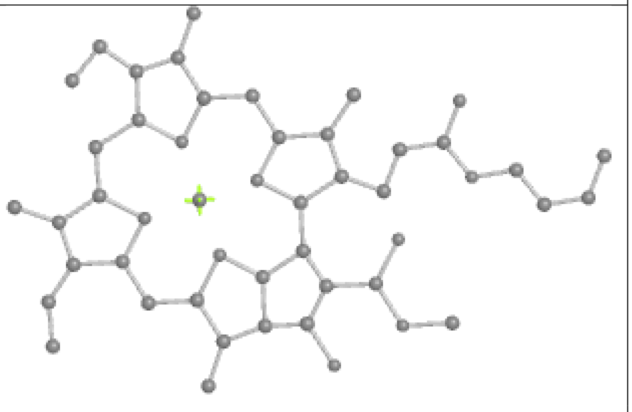
Bond lengths



Bond angles

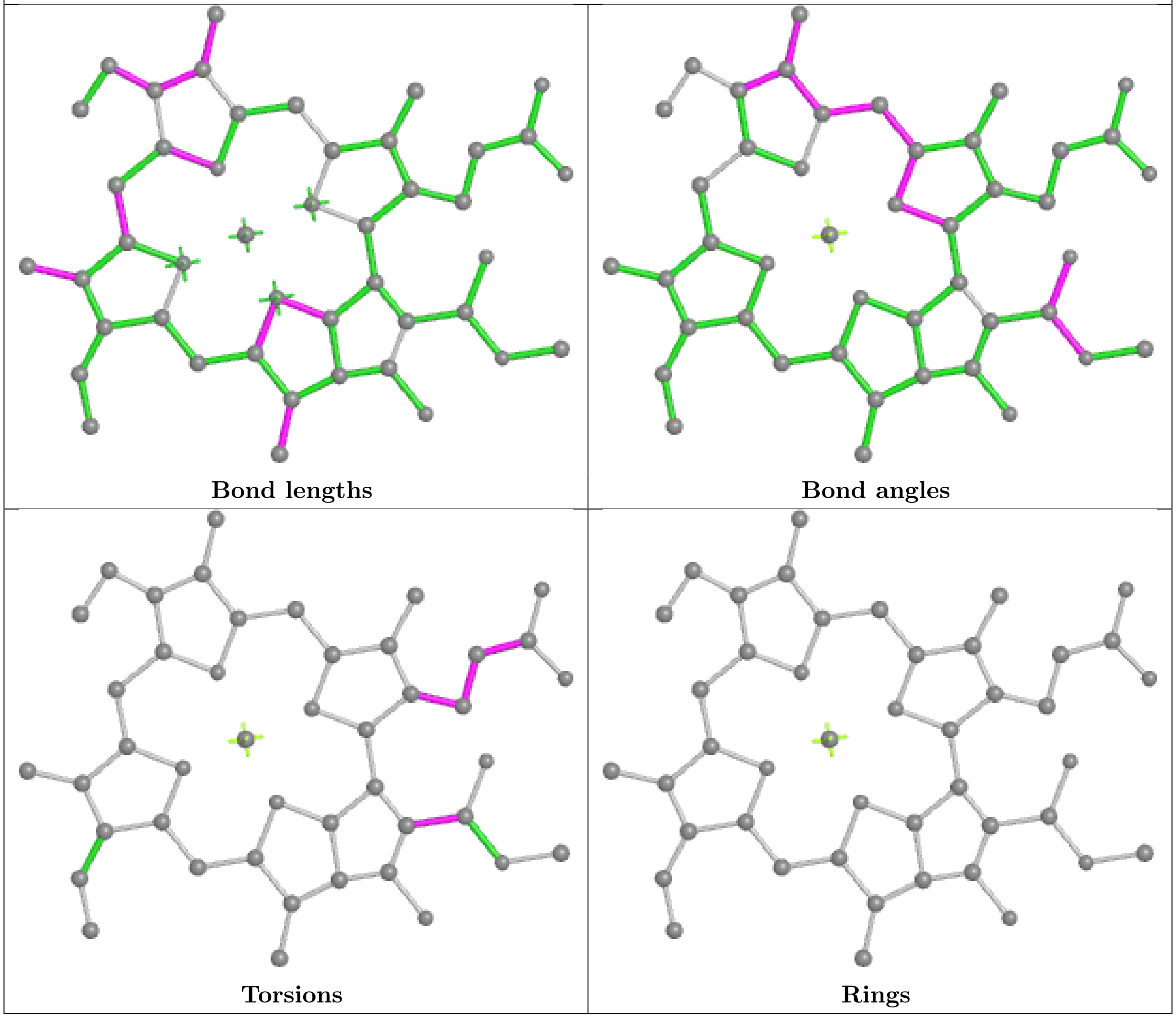


Torsions



Rings

Ligand CLA aB 830



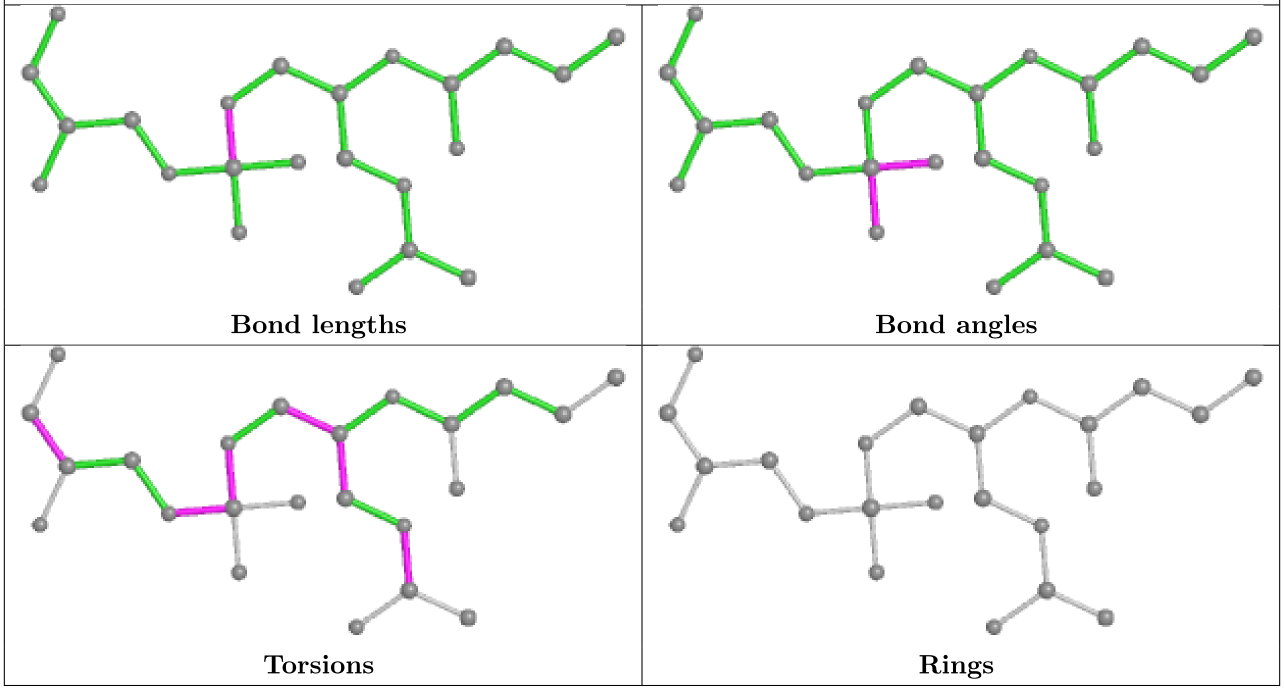
Bond lengths

Bond angles

Torsions

Rings

Ligand LHG bB 851



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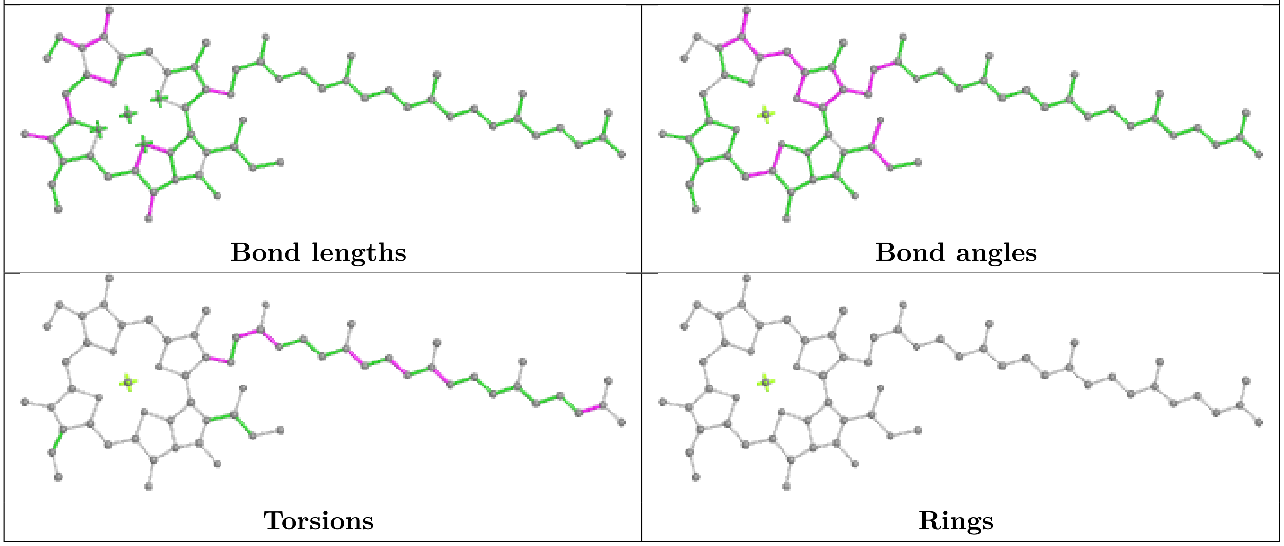
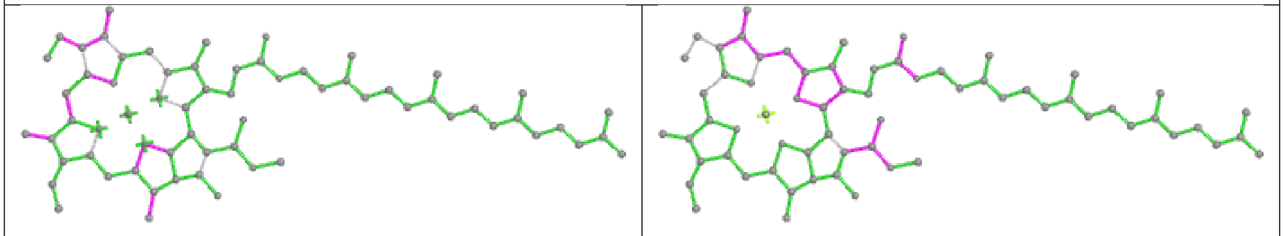
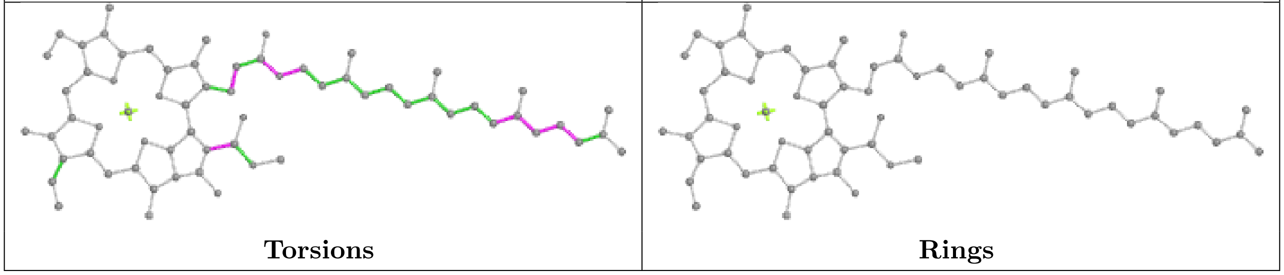


Ligand CLA bA 838

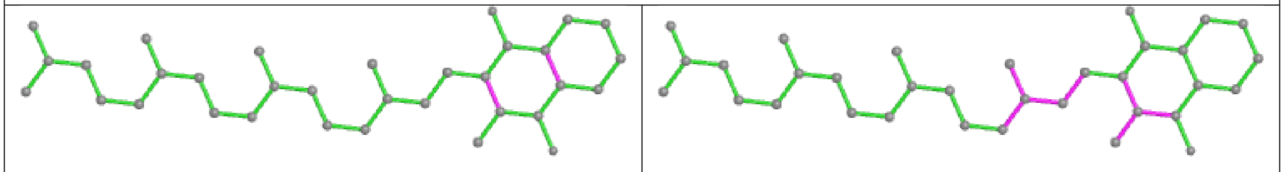


Bond lengths Bond angles

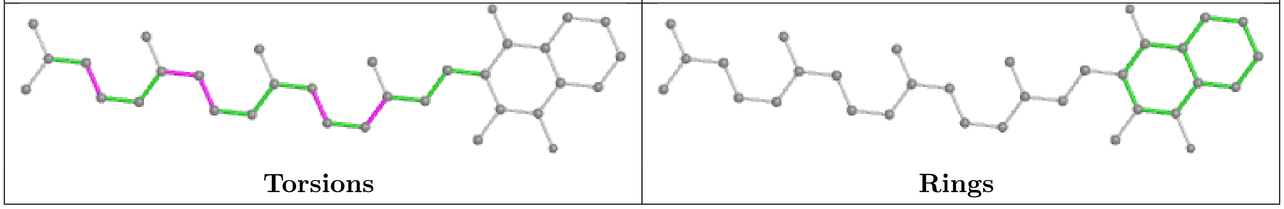


Torsions Rings

Ligand PQN bB 843

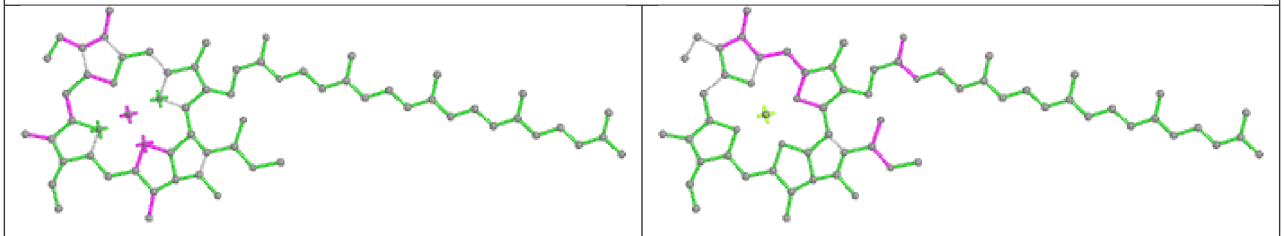


Bond lengths Bond angles

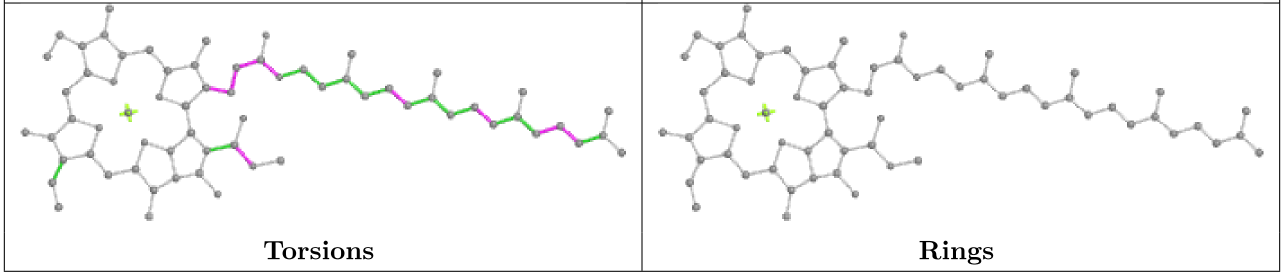


Torsions Rings

Ligand CLA cA 842

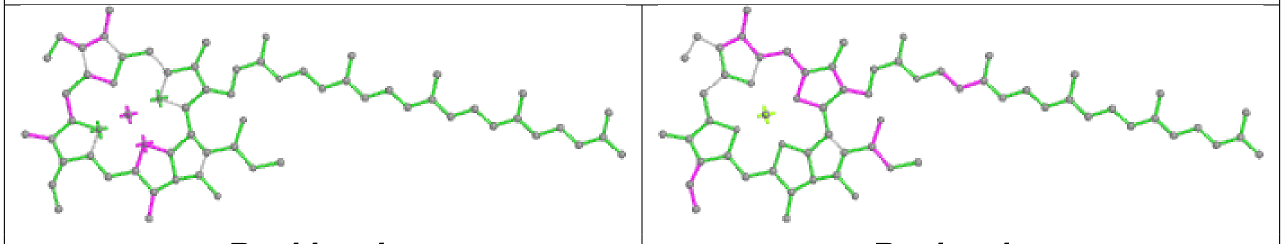


Bond lengths Bond angles

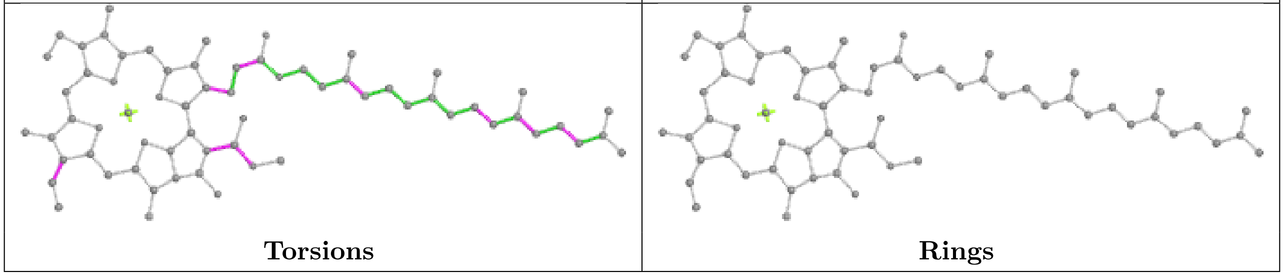


Torsions Rings

Ligand CLA bB 814

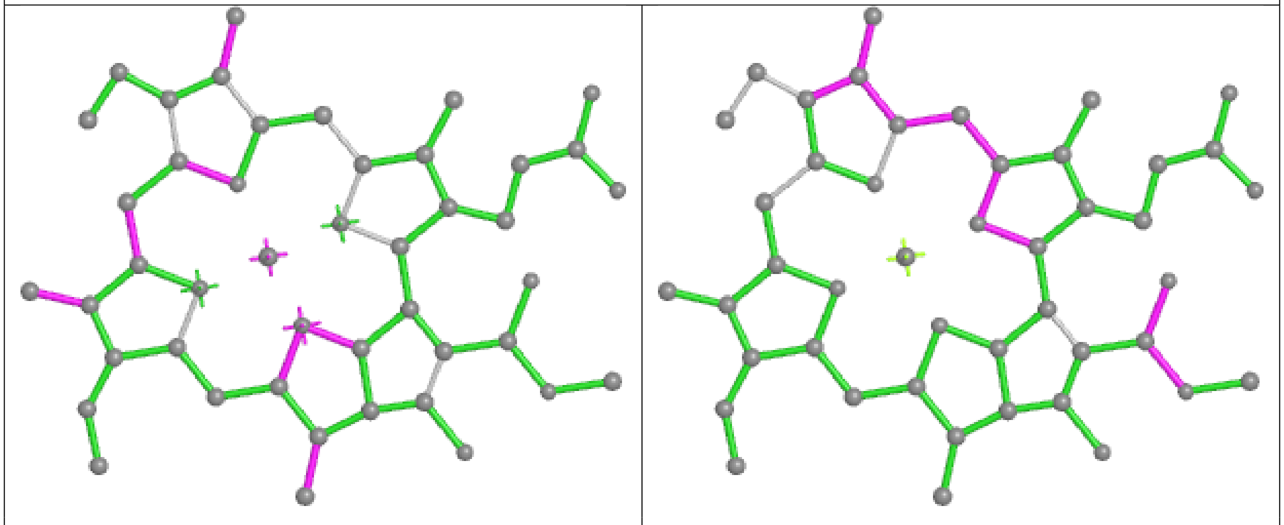


Bond lengths Bond angles

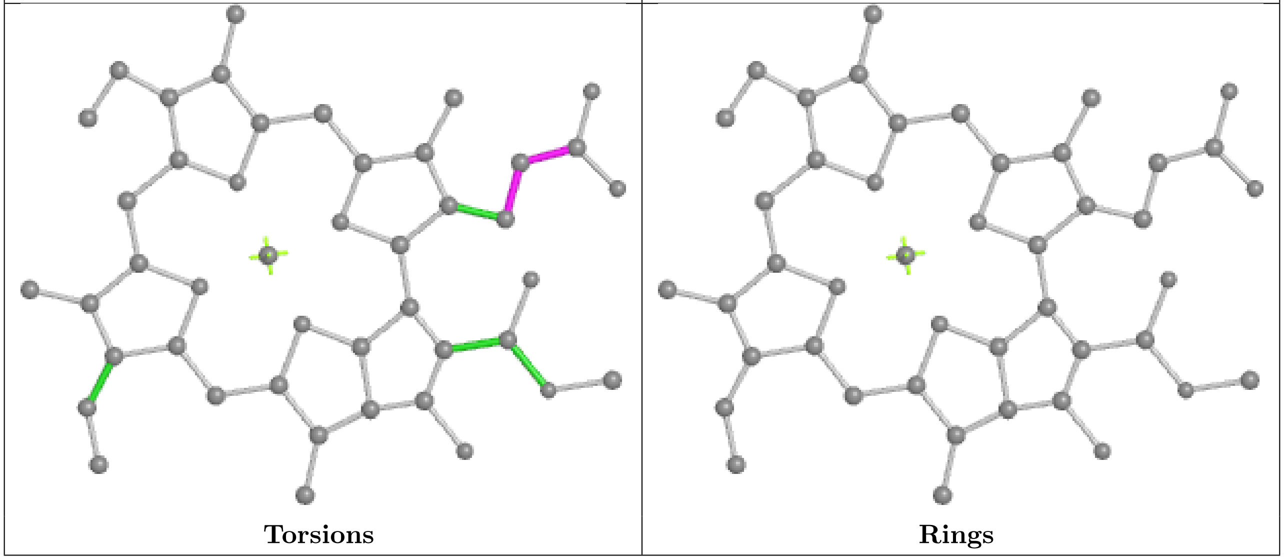


Torsions Rings

Ligand CLA aA 802

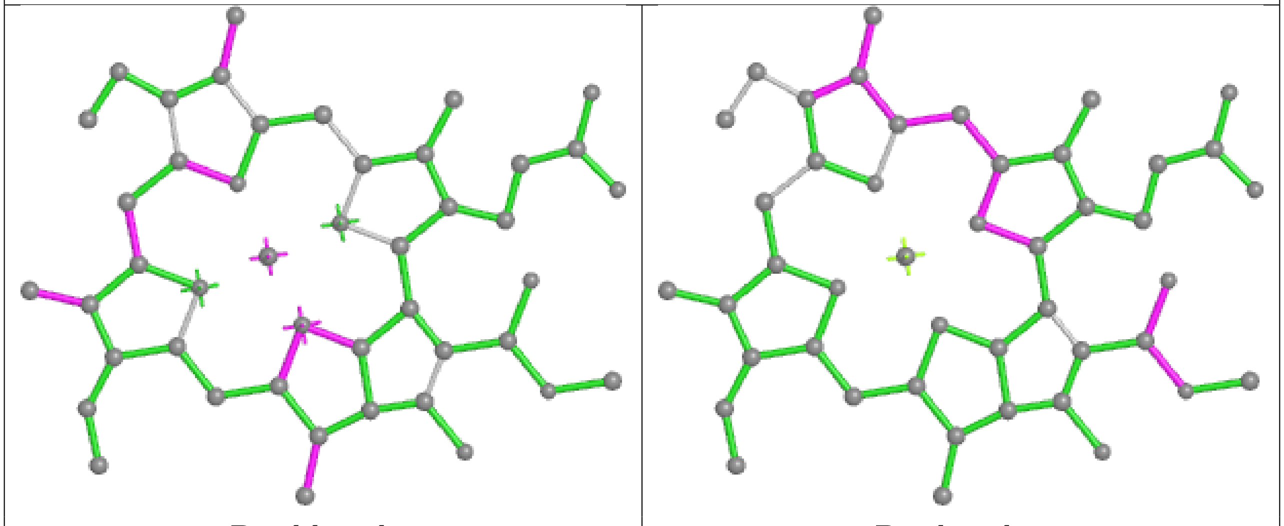


Bond lengths Bond angles

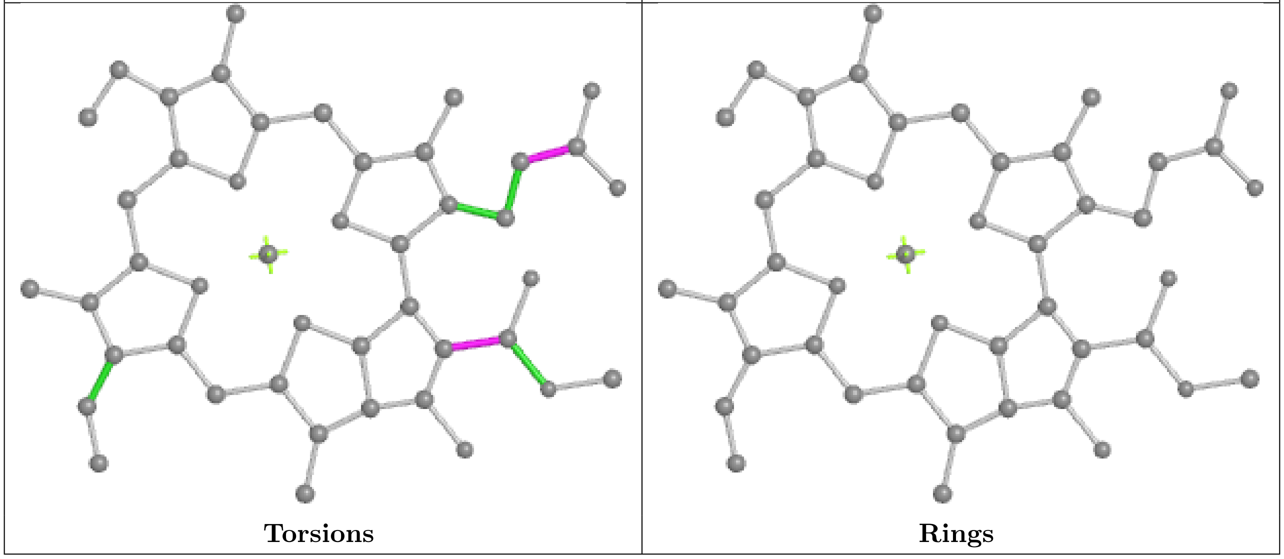


Torsions Rings

Ligand CLA dK 103

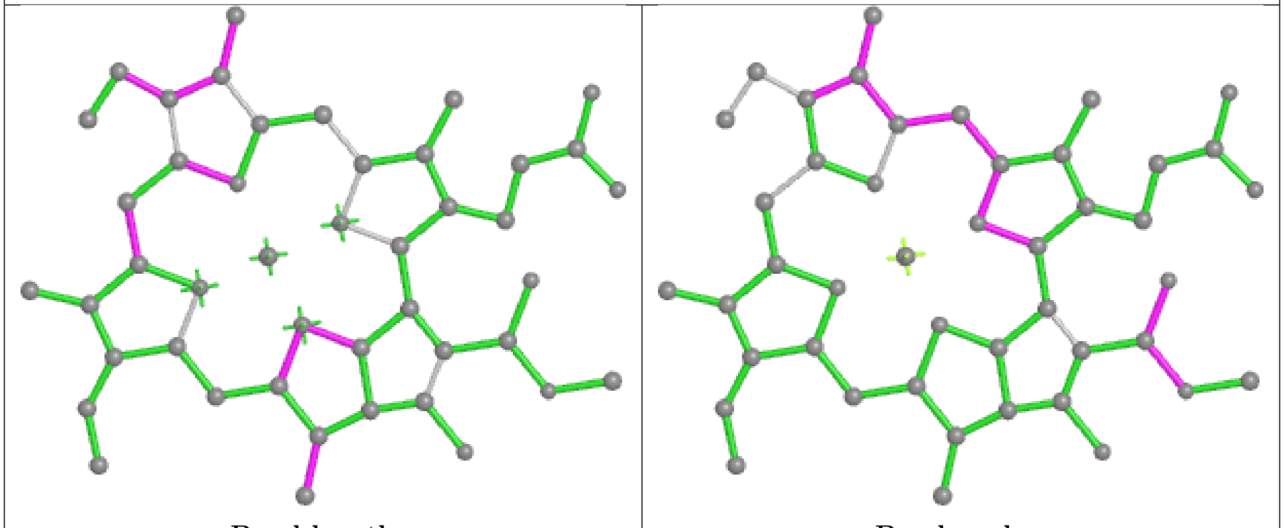


Bond lengths **Bond angles**



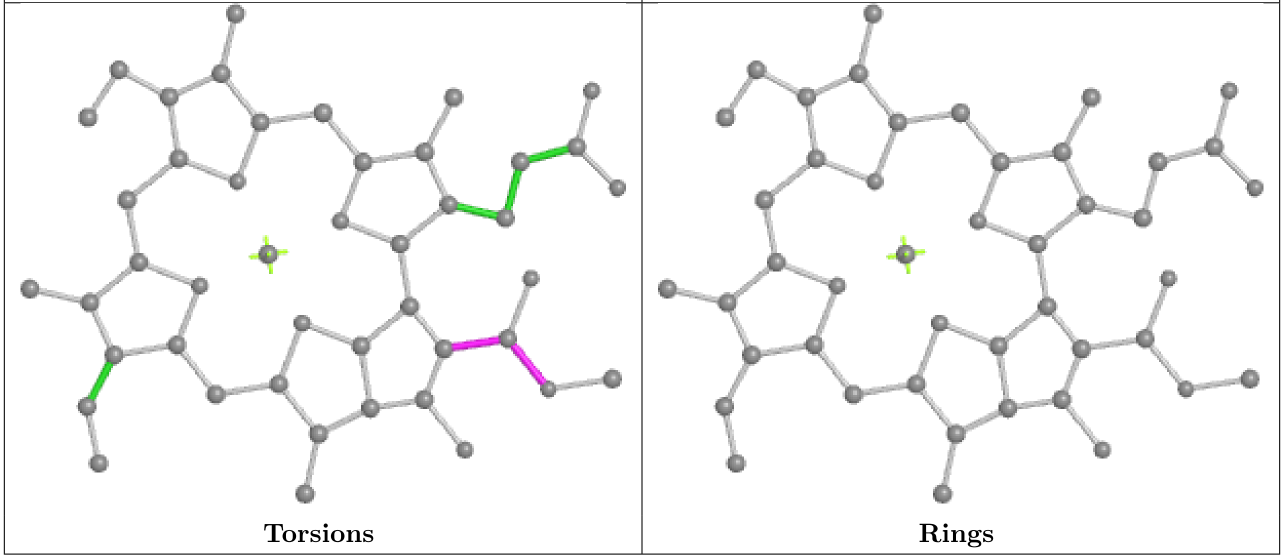
Torsions **Rings**

Ligand CLA cA 815



Bond lengths

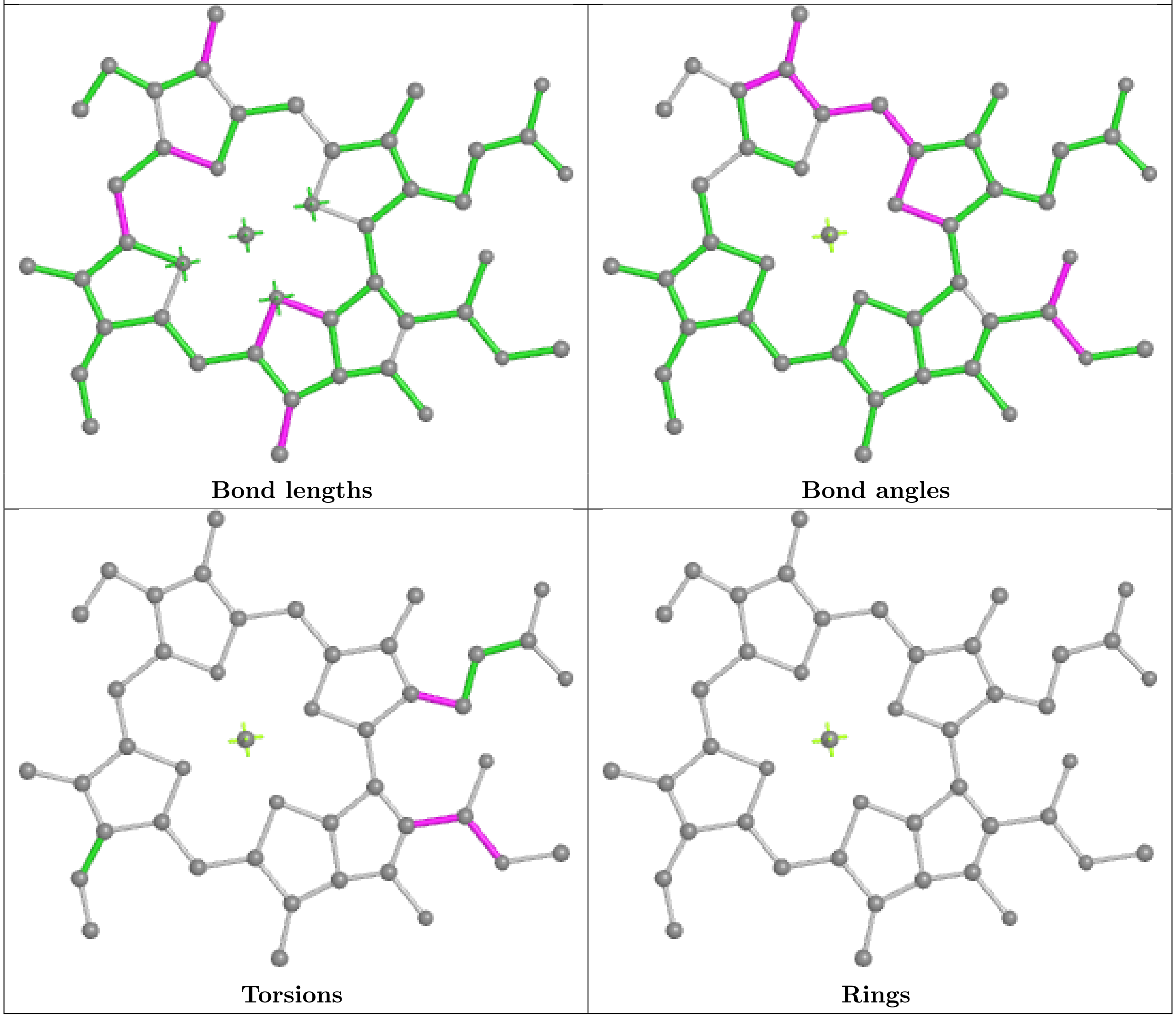
Bond angles



Torsions

Rings

Ligand CLA aA 810



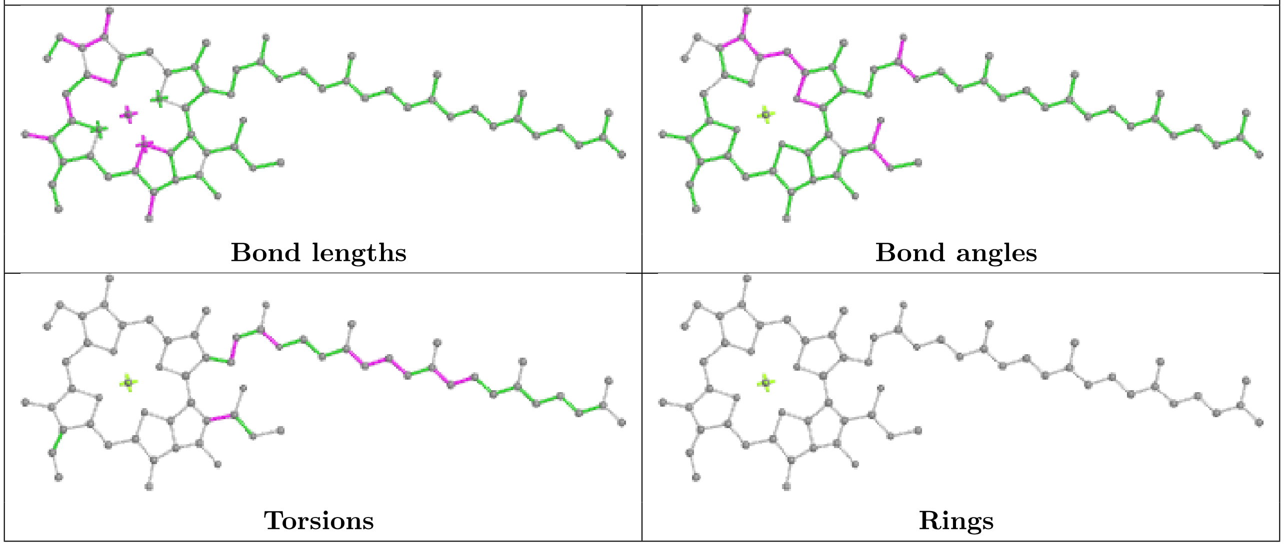
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA dA 840



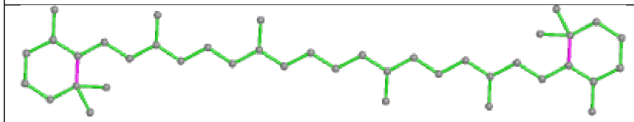
Bond lengths

Bond angles

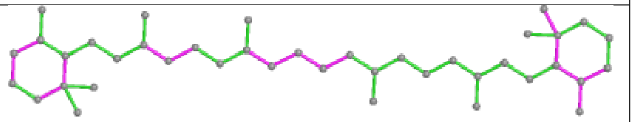
Torsions

Rings

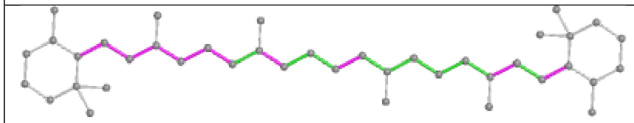
Ligand BCR bL 208



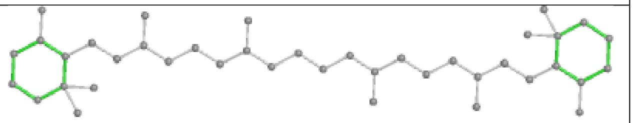
Bond lengths



Bond angles

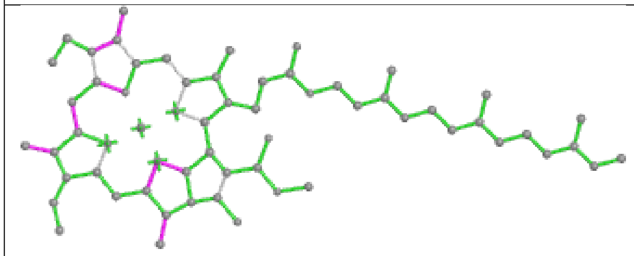


Torsions

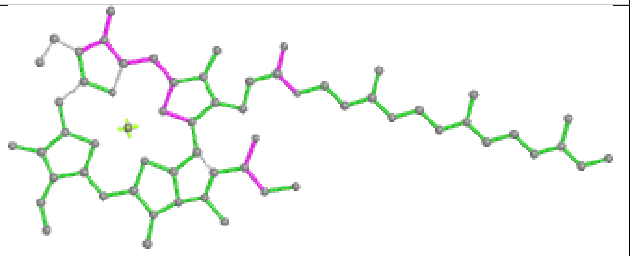


Rings

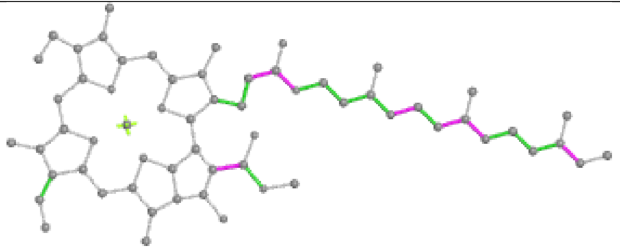
Ligand CLA aA 820



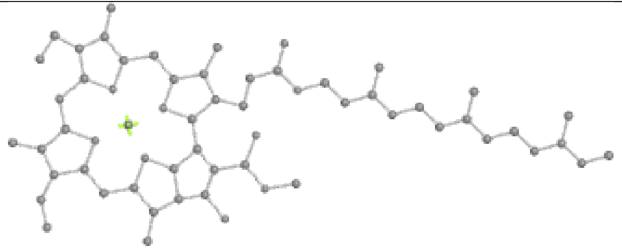
Bond lengths



Bond angles

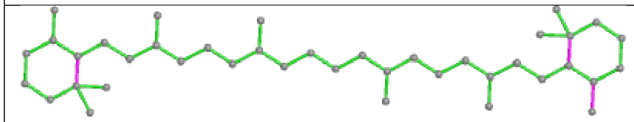


Torsions

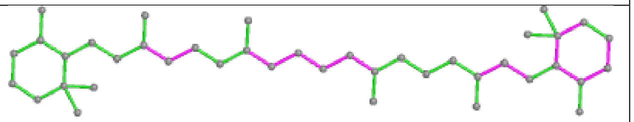


Rings

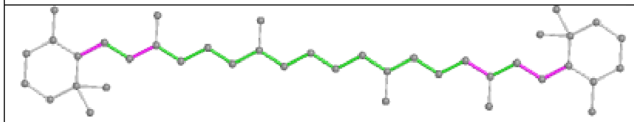
Ligand BCR dA 845



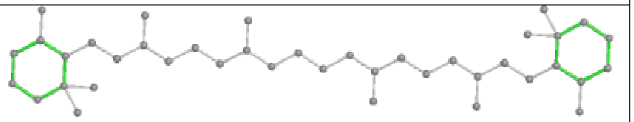
Bond lengths



Bond angles

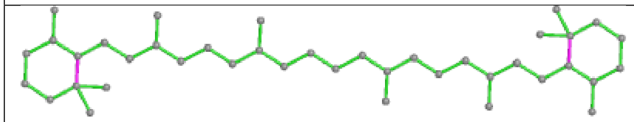


Torsions

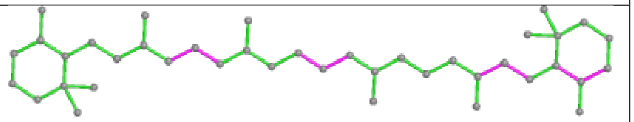


Rings

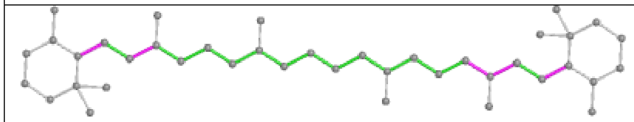
Ligand BCR bB 849



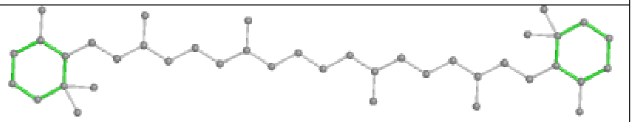
Bond lengths



Bond angles

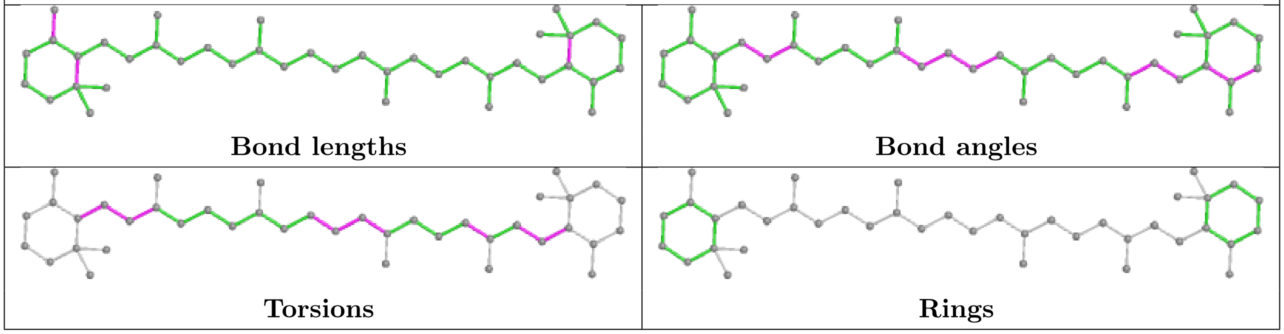


Torsions



Rings

Ligand BCR aL 201



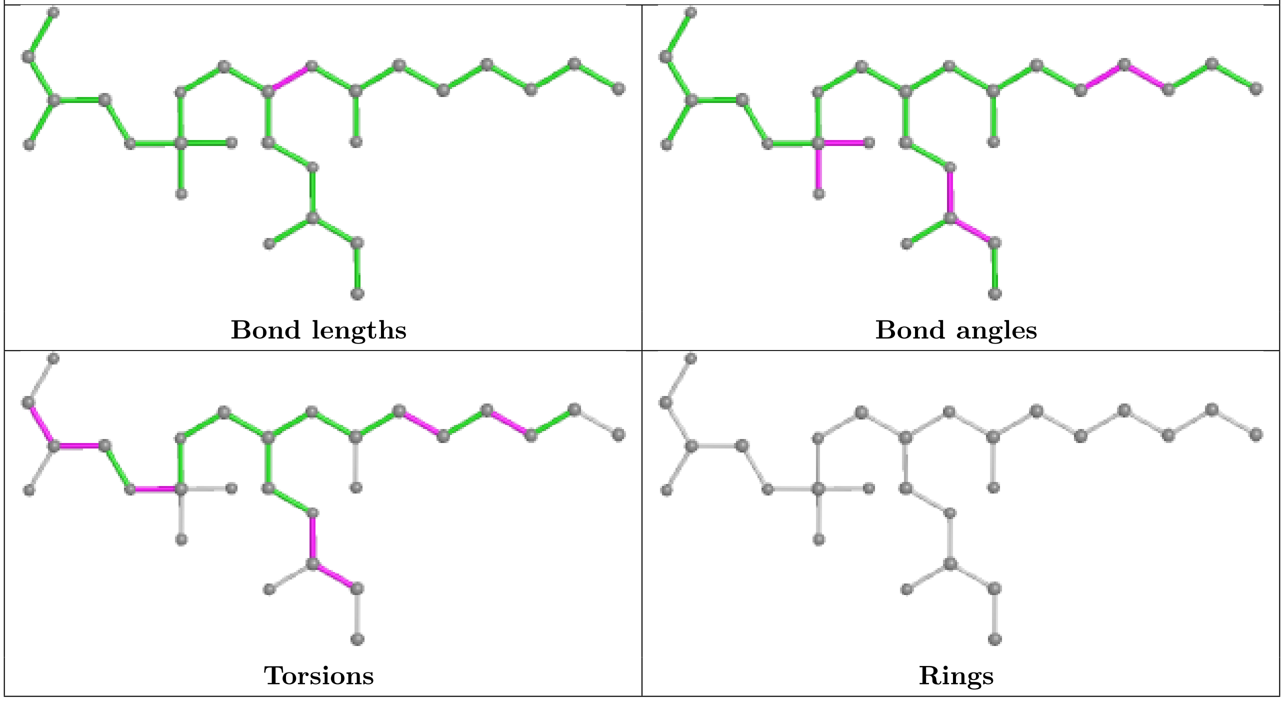
Bond lengths

Bond angles

Torsions

Rings

Ligand LHG aA 853



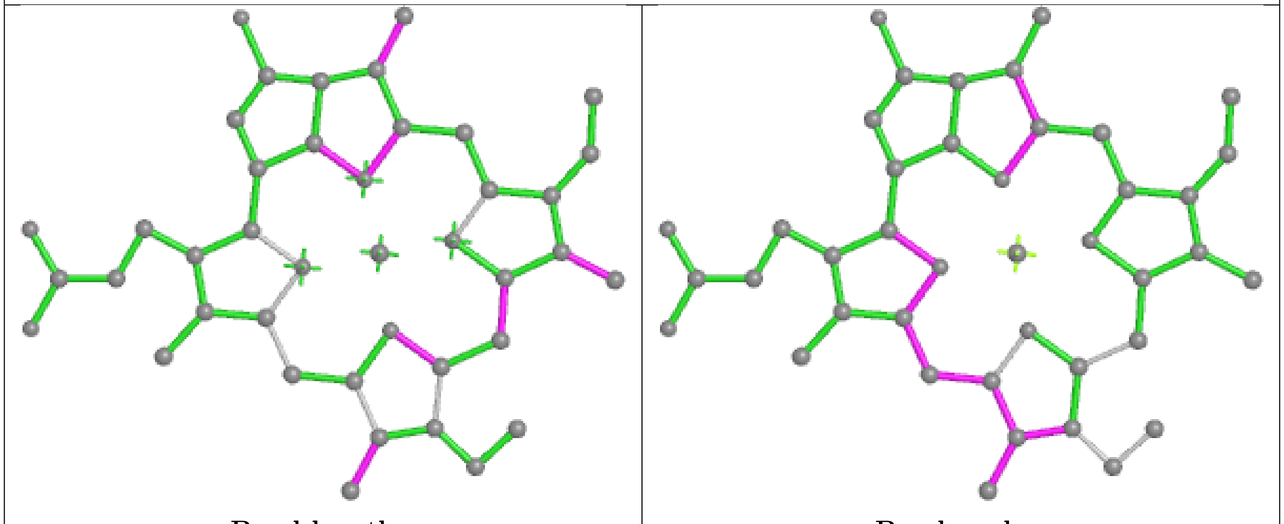
Bond lengths

Bond angles

Torsions

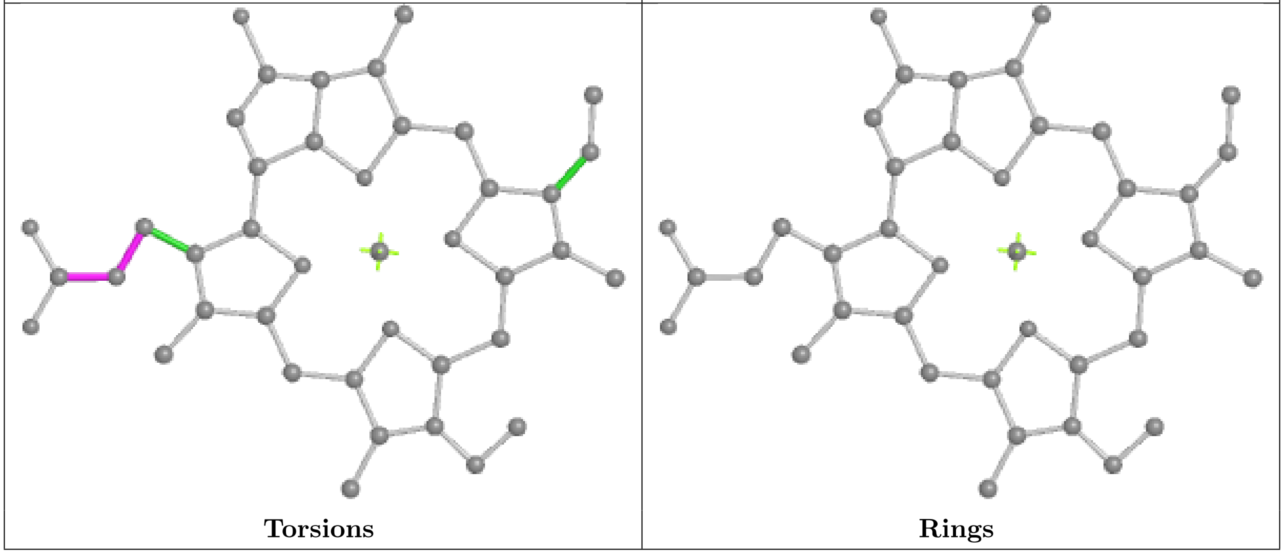
Rings

Ligand CLA cK 101



Bond lengths

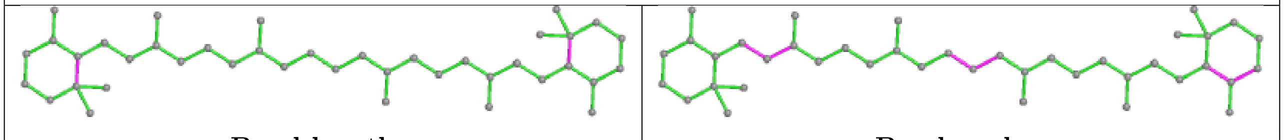
Bond angles



Torsions

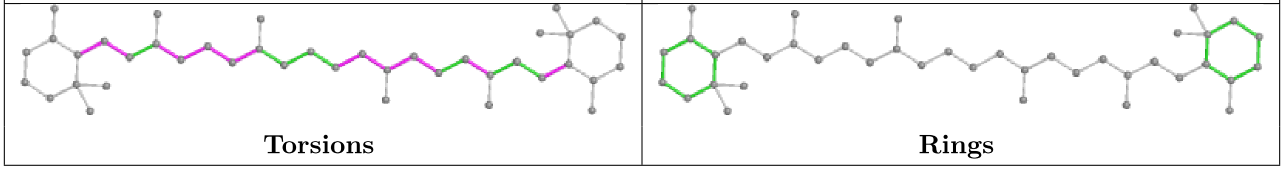
Rings

Ligand BCR dA 847



Bond lengths

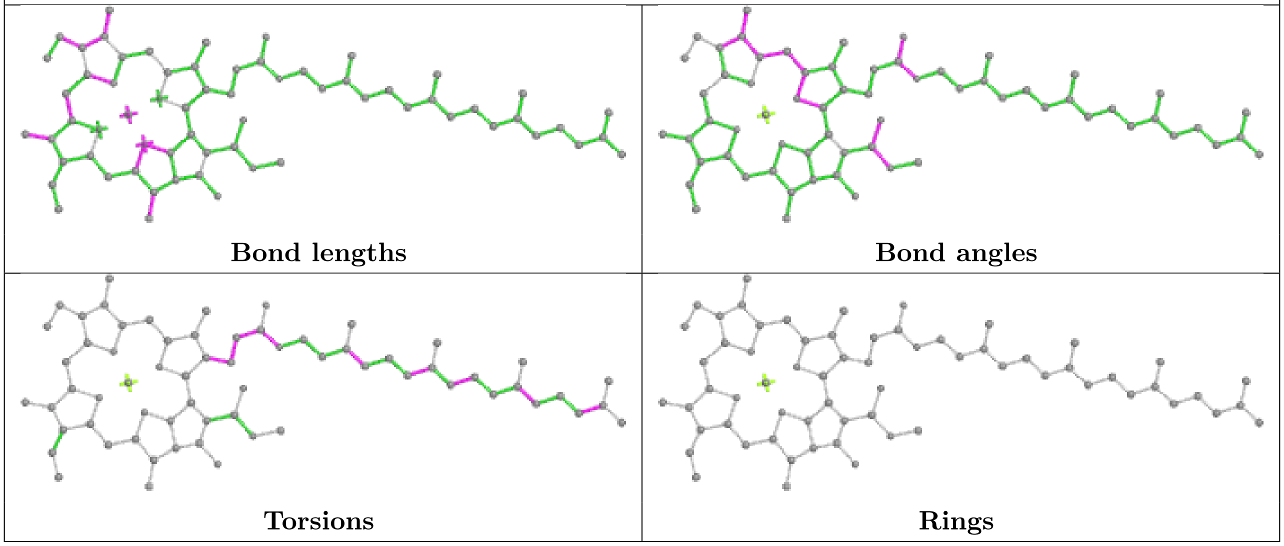
Bond angles



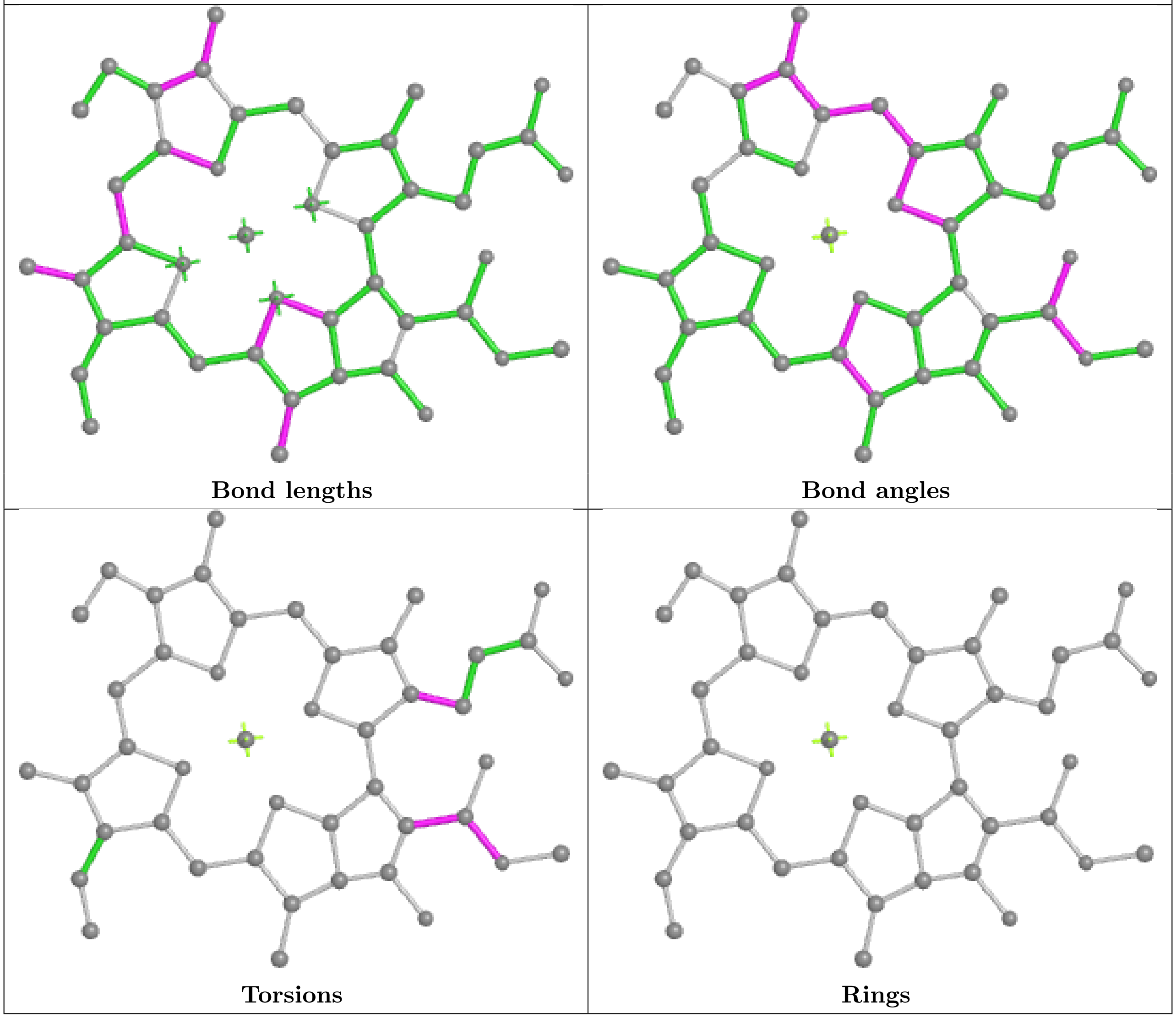
Torsions

Rings

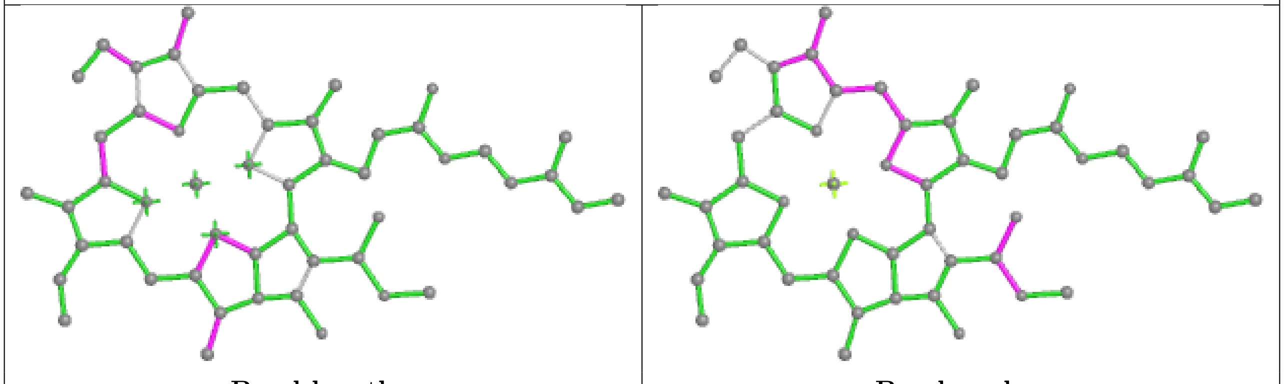
Ligand CLA aA 829



Ligand CLA dB 812

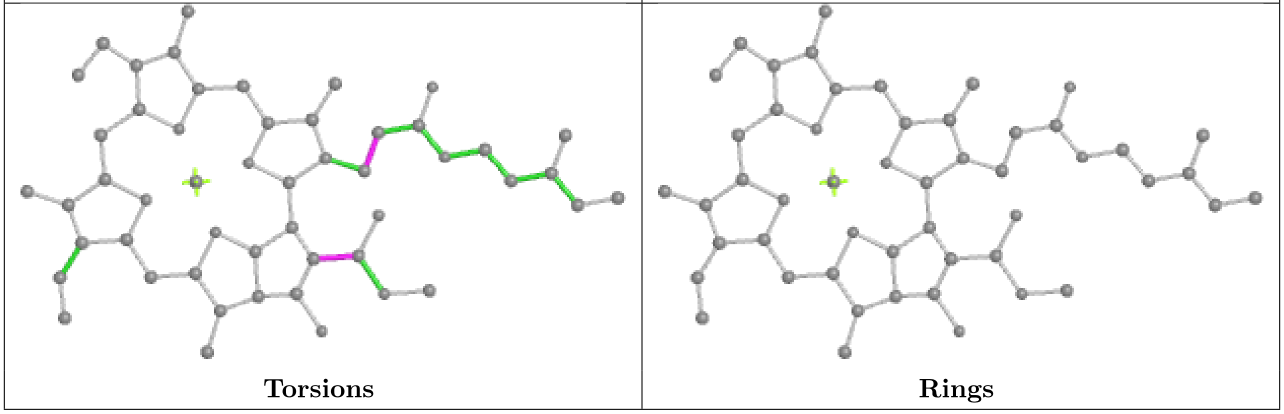


Ligand CLA bA 807



Bond lengths

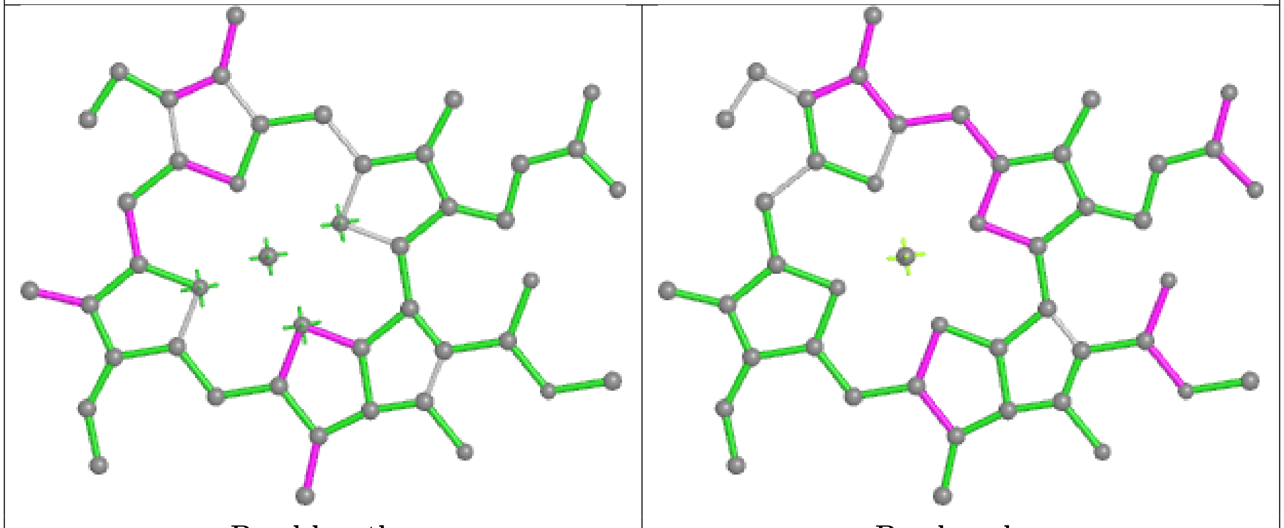
Bond angles



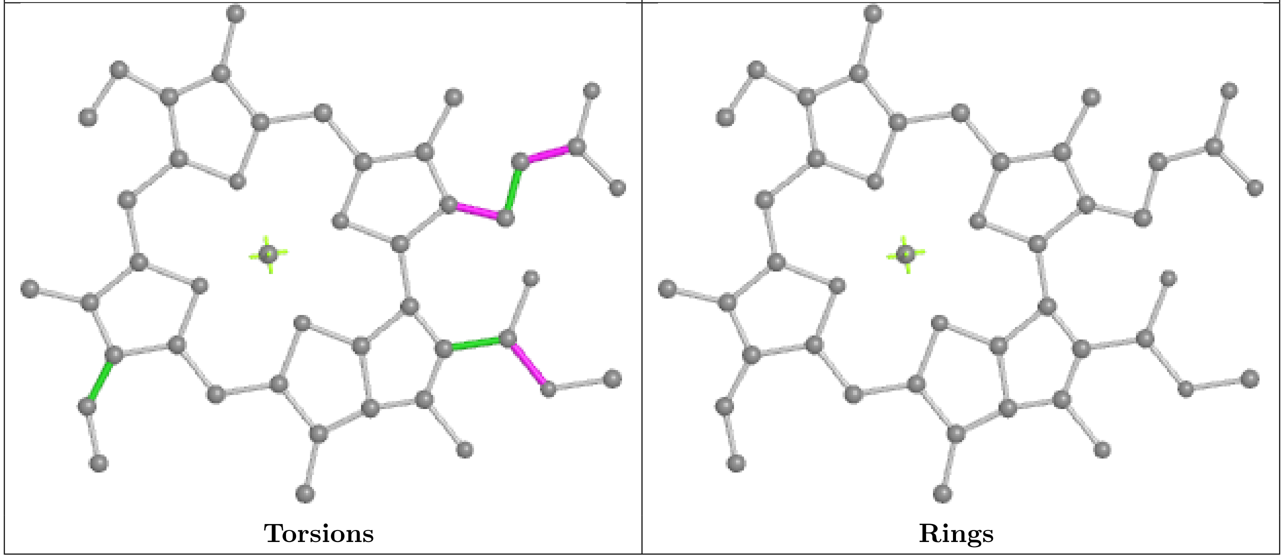
Torsions

Rings

Ligand CLA bB 824

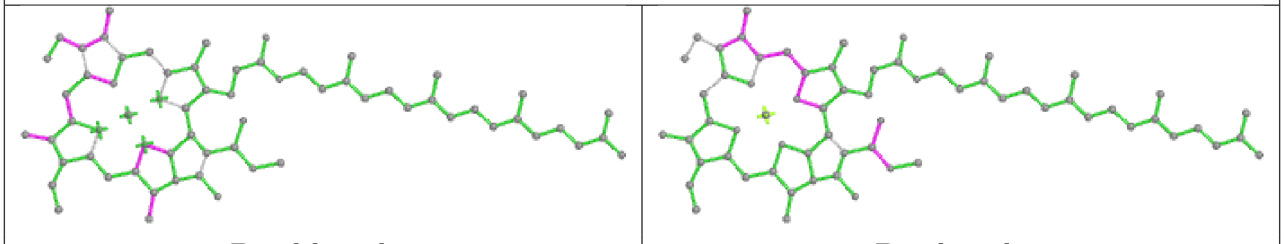


Bond lengths Bond angles

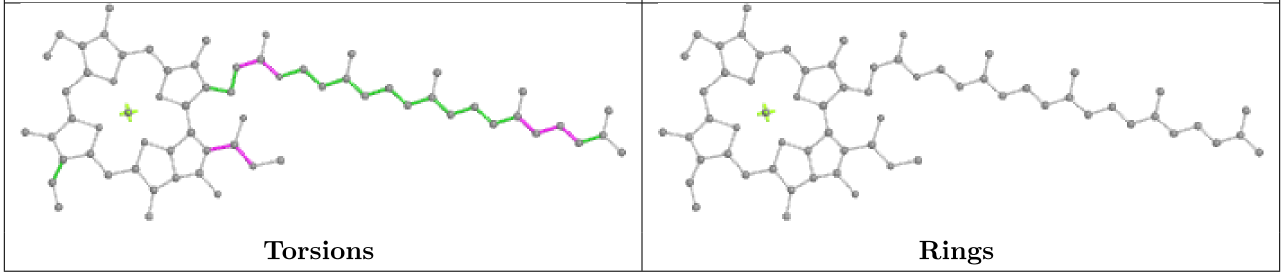


Torsions Rings

Ligand CLA aB 802

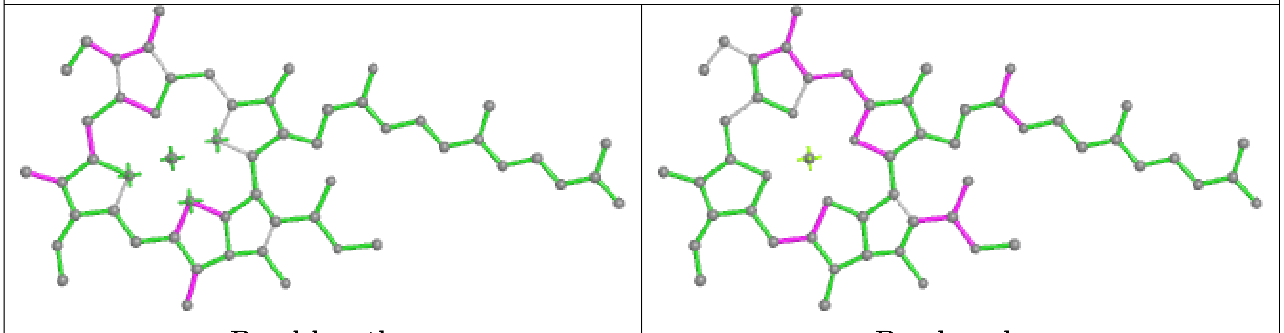


Bond lengths Bond angles



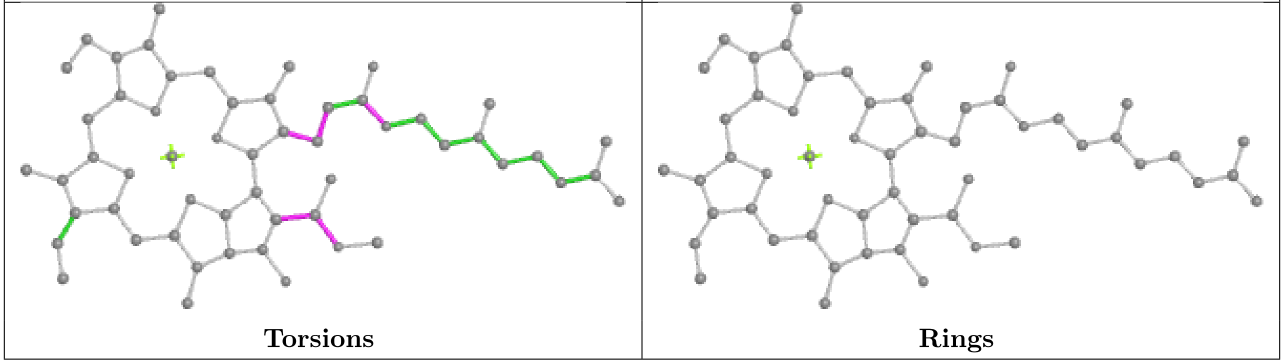
Torsions Rings

Ligand CLA bB 817



Bond lengths

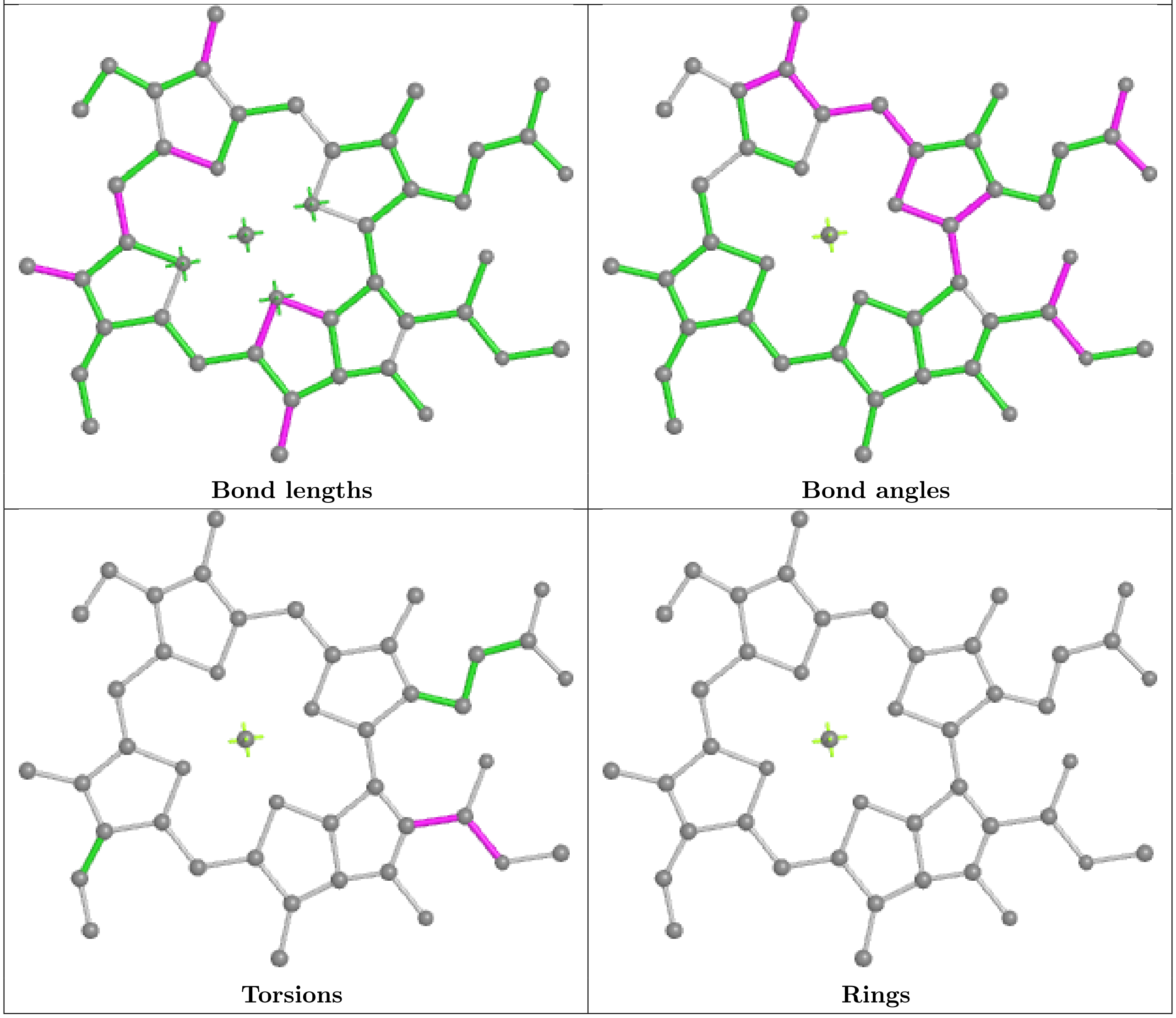
Bond angles



Torsions

Rings

Ligand CLA dA 814



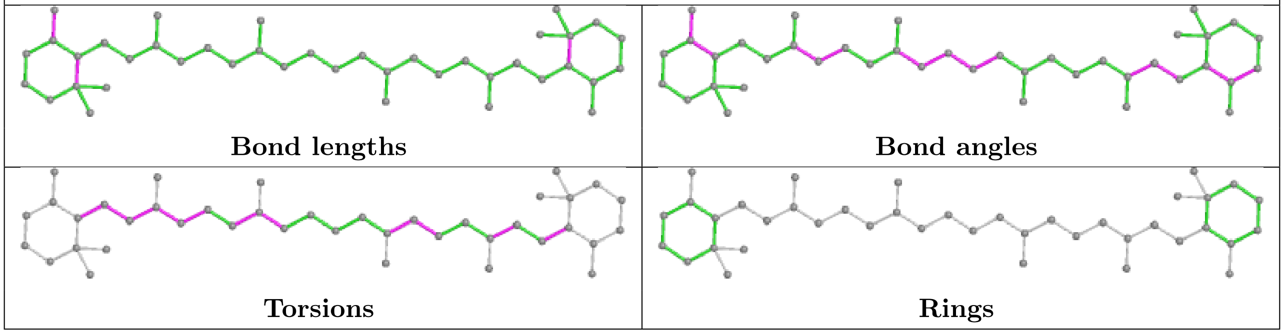
Bond lengths

Bond angles

Torsions

Rings

Ligand BCR aJ 103



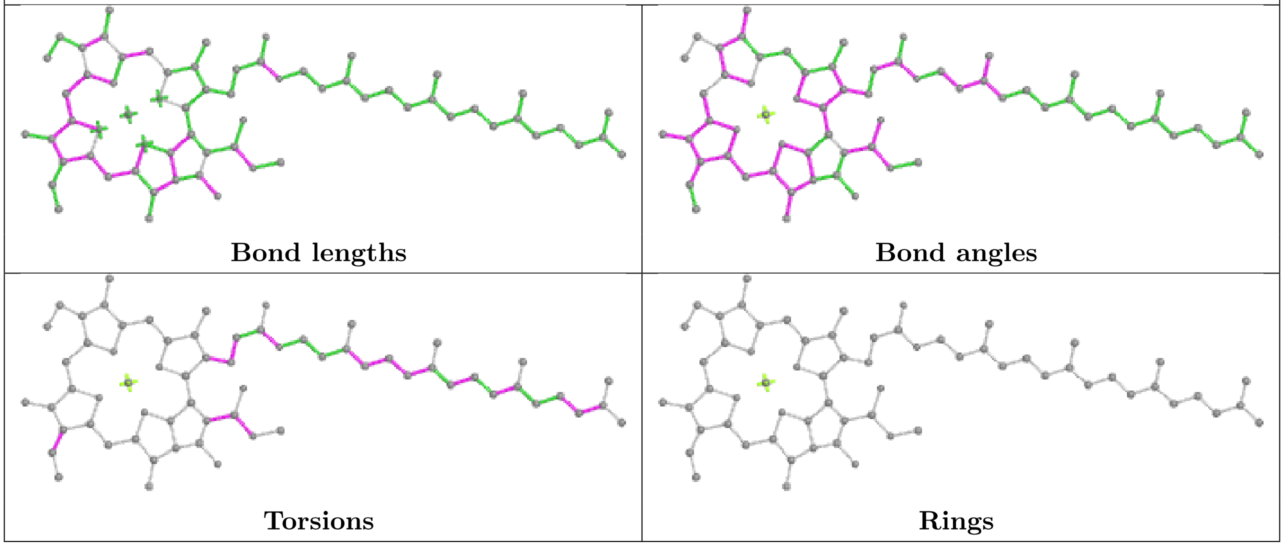
Bond lengths

Bond angles

Torsions

Rings

Ligand CL0 cA 801



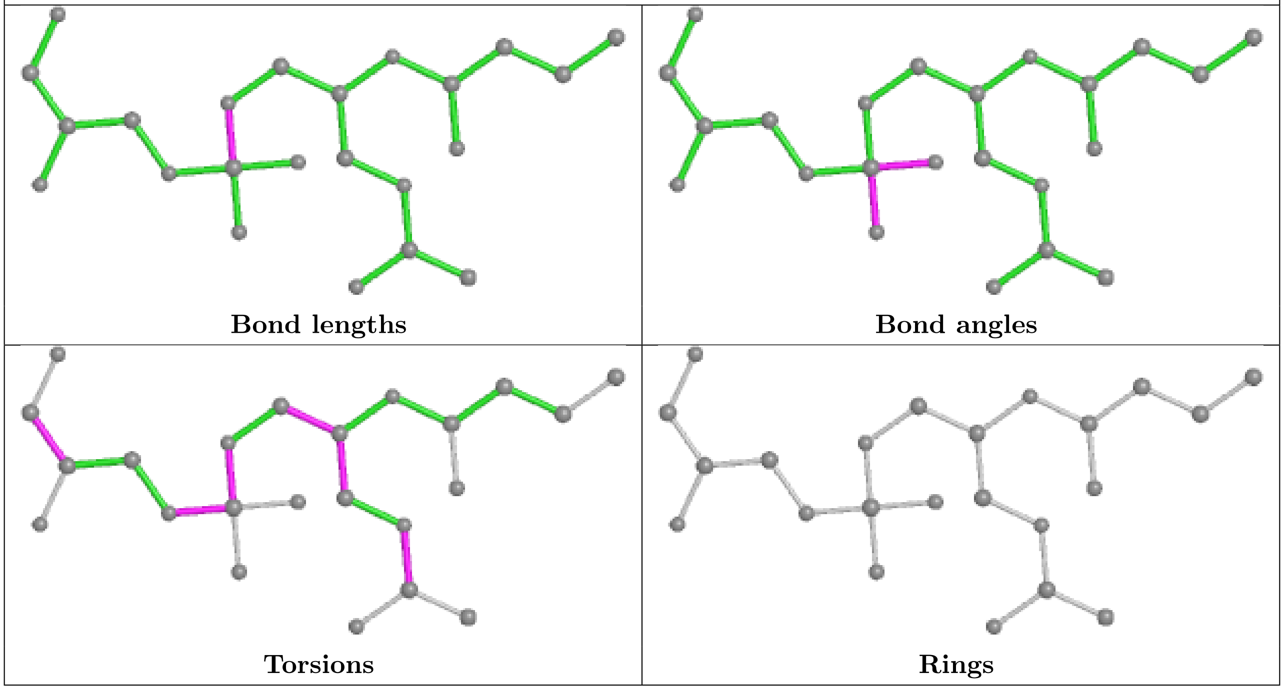
Bond lengths

Bond angles

Torsions

Rings

Ligand LHG dB 851



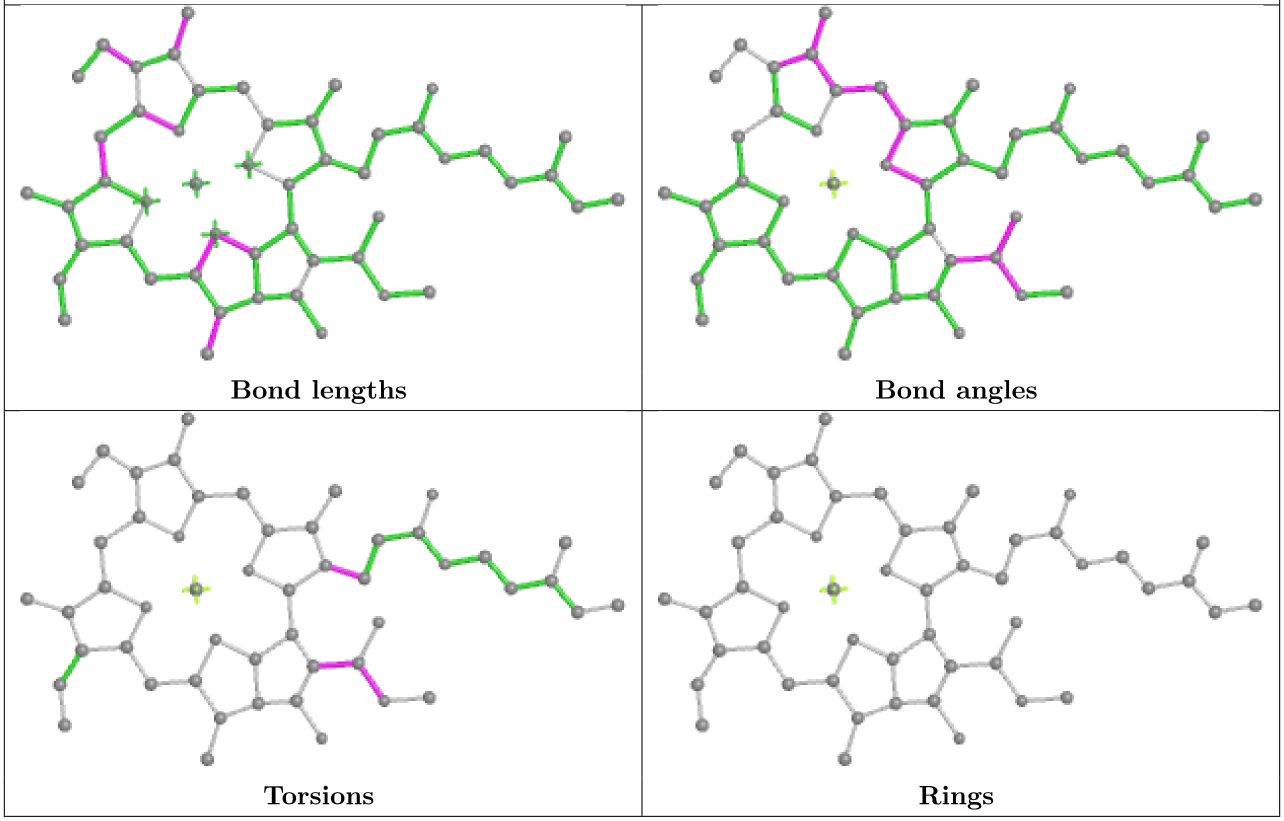
Bond lengths

Bond angles

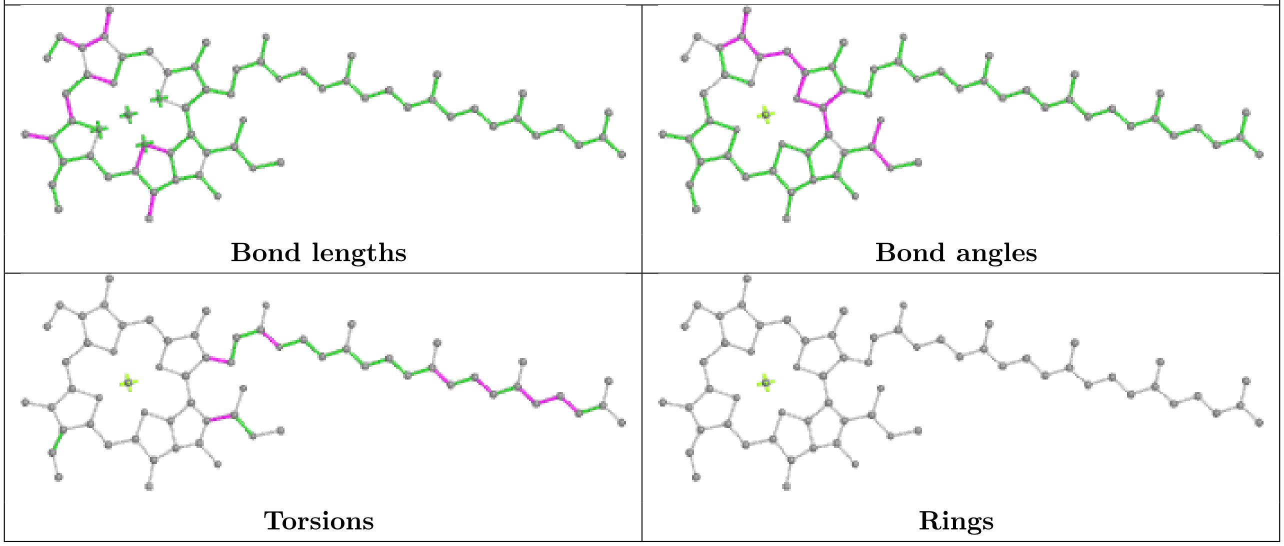
Torsions

Rings

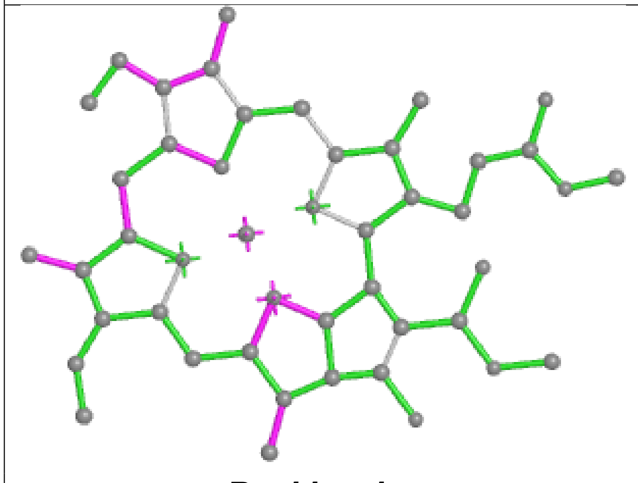
Ligand CLA aF 201



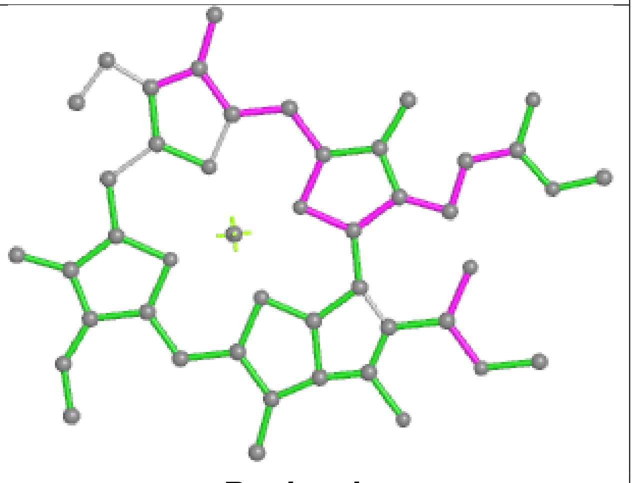
Ligand CLA aA 841



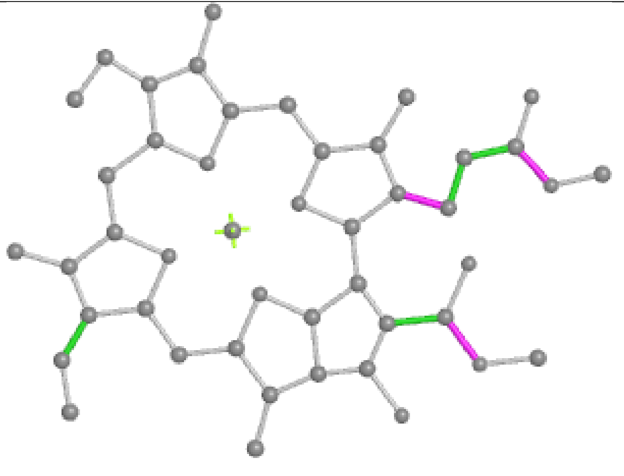
Ligand CLA cB 825



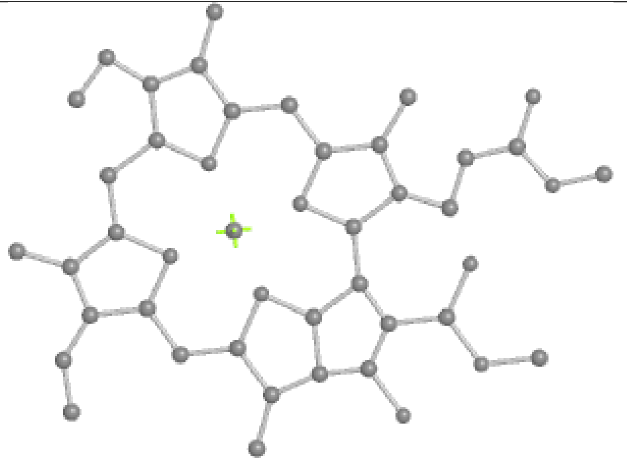
Bond lengths



Bond angles

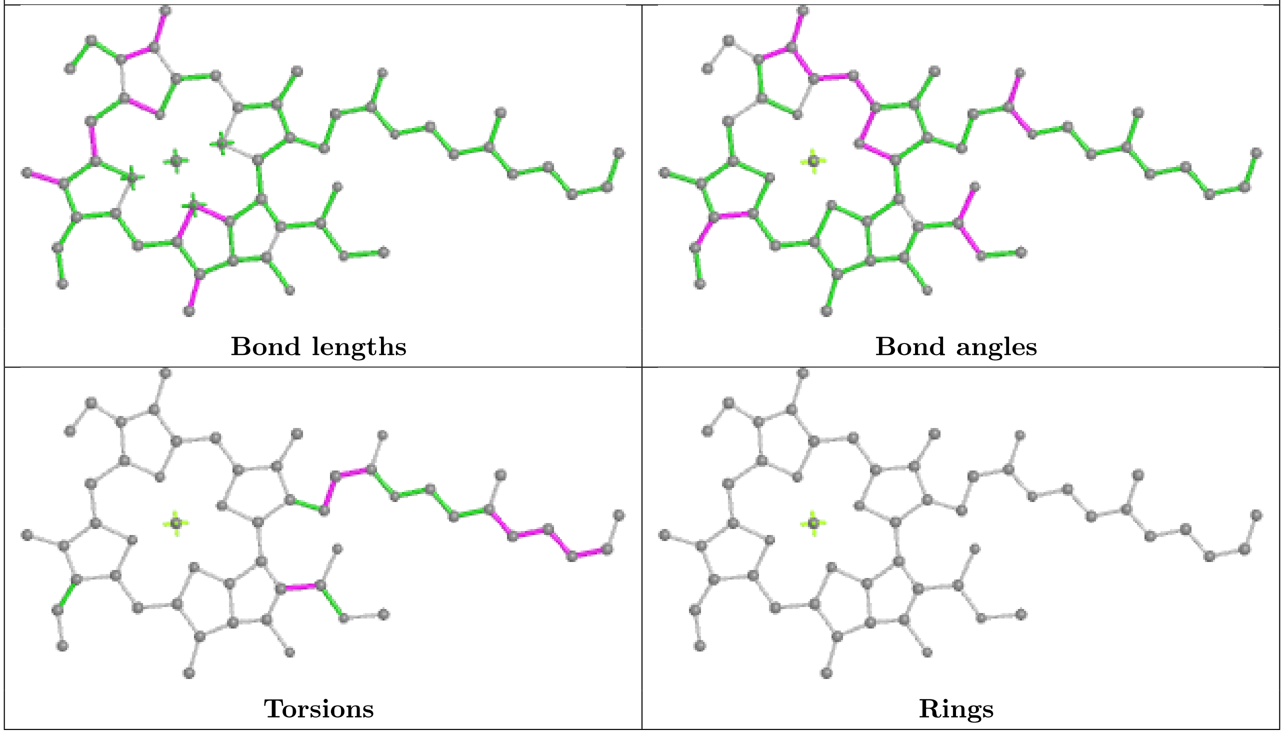


Torsions

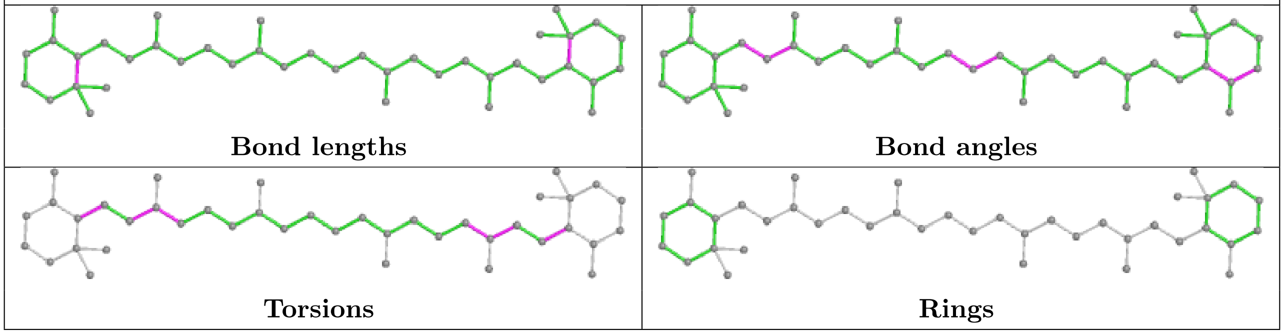


Rings

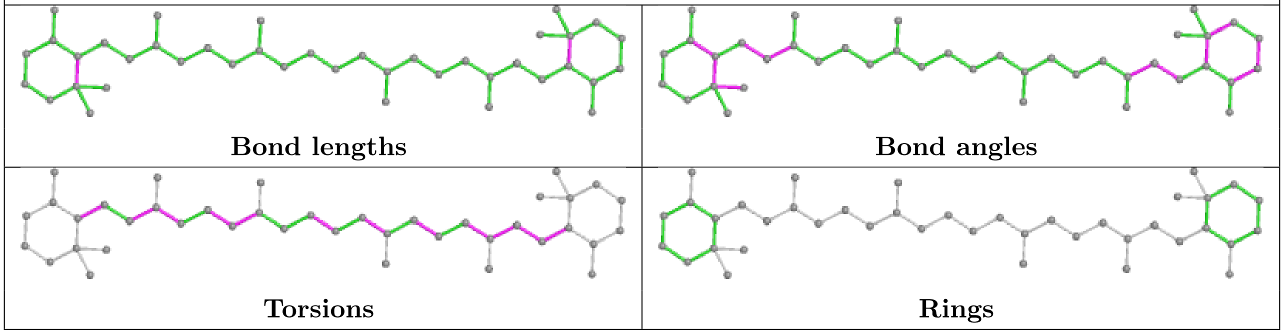
Ligand CLA cA 817


Bond lengths
Bond angles
Torsions
Rings

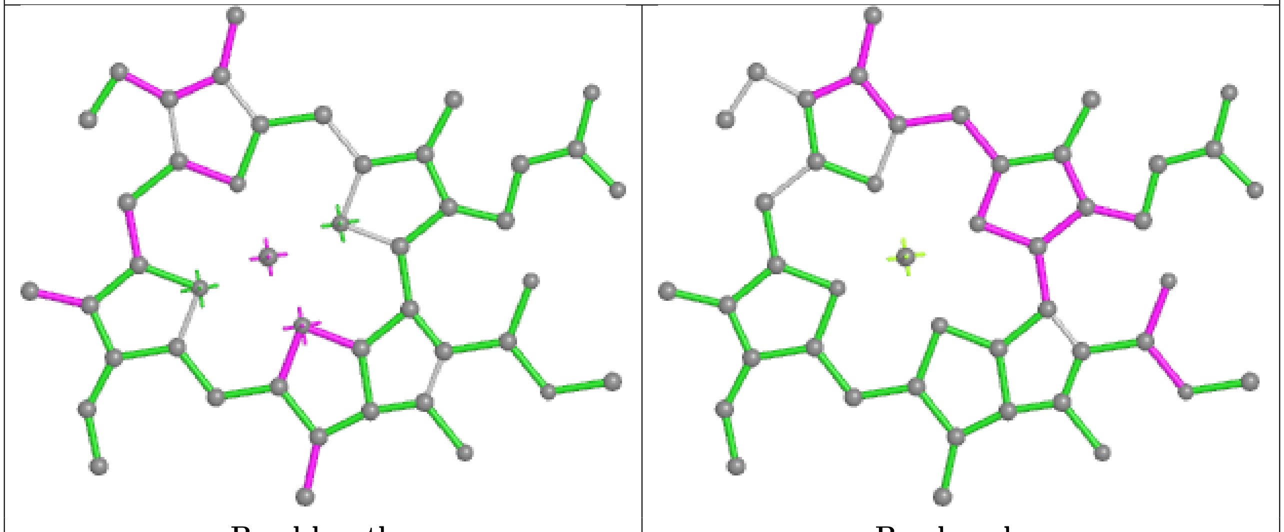
Ligand BCR bB 846


Bond lengths
Bond angles
Torsions
Rings

Ligand BCR dA 849

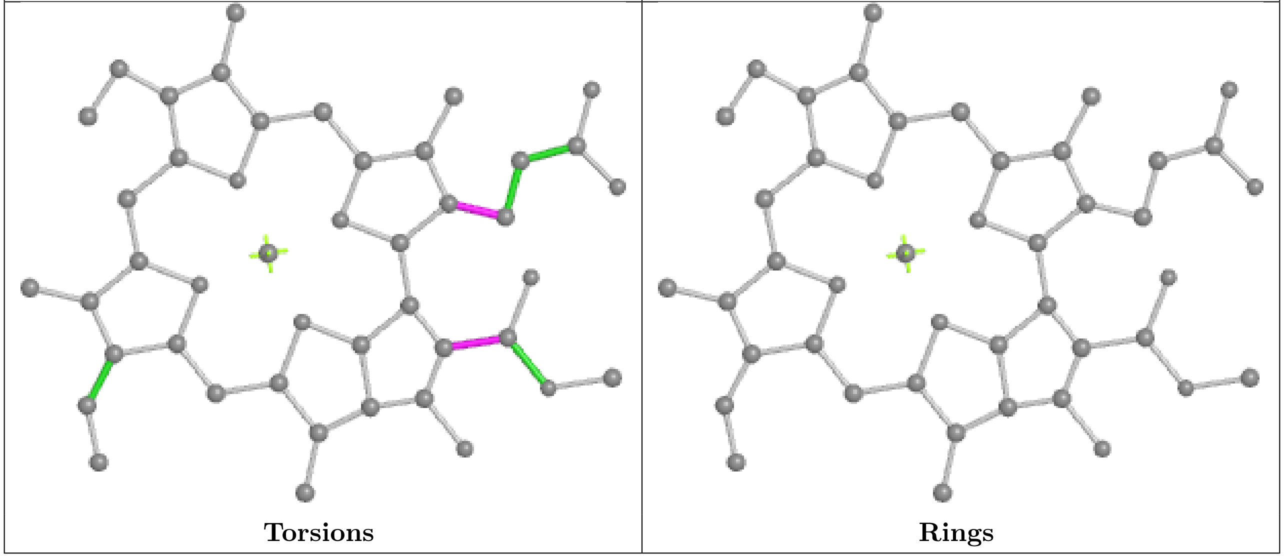

Bond lengths
Bond angles
Torsions
Rings

Ligand CLA aA 805



Bond lengths

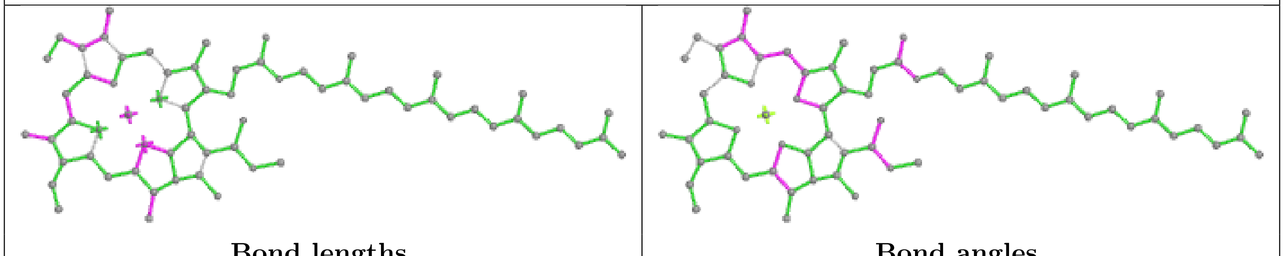
Bond angles



Torsions

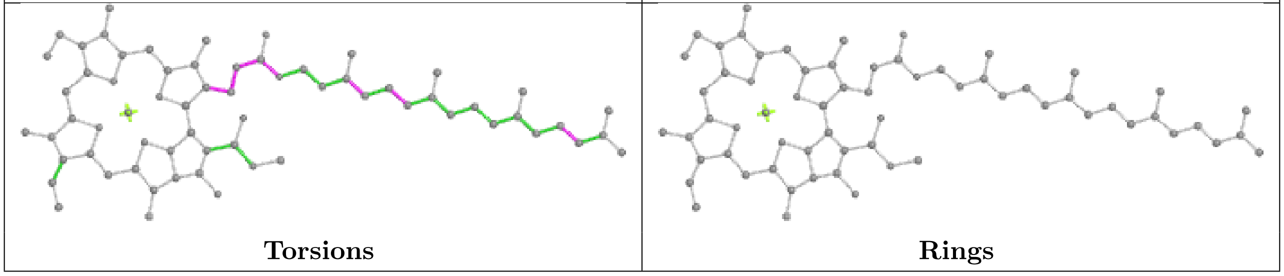
Rings

Ligand CLA bB 829



Bond lengths

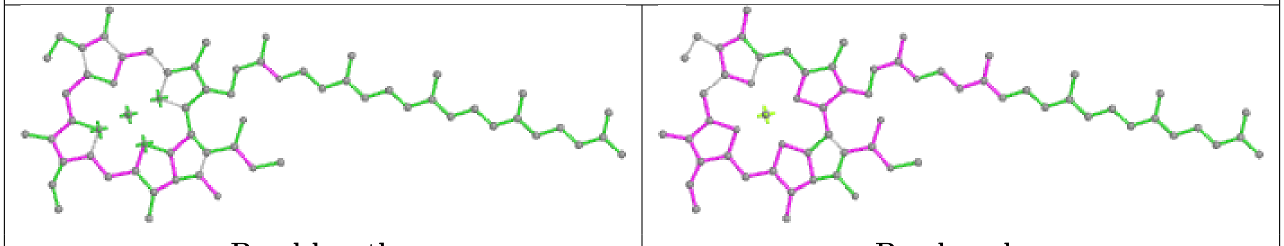
Bond angles



Torsions

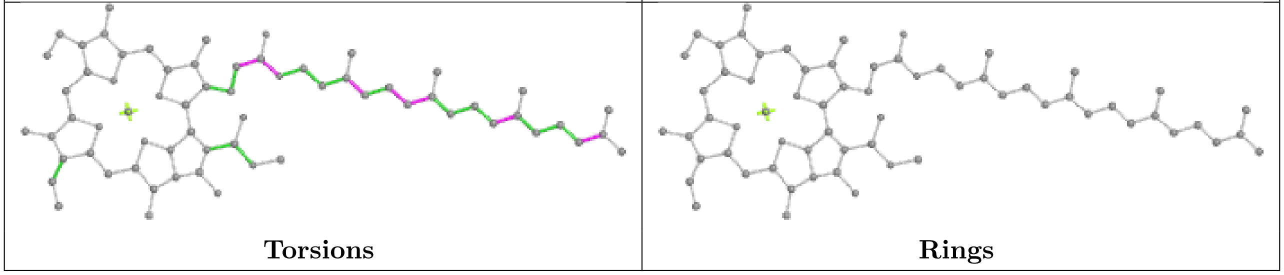
Rings

Ligand CL0 dA 801



Bond lengths

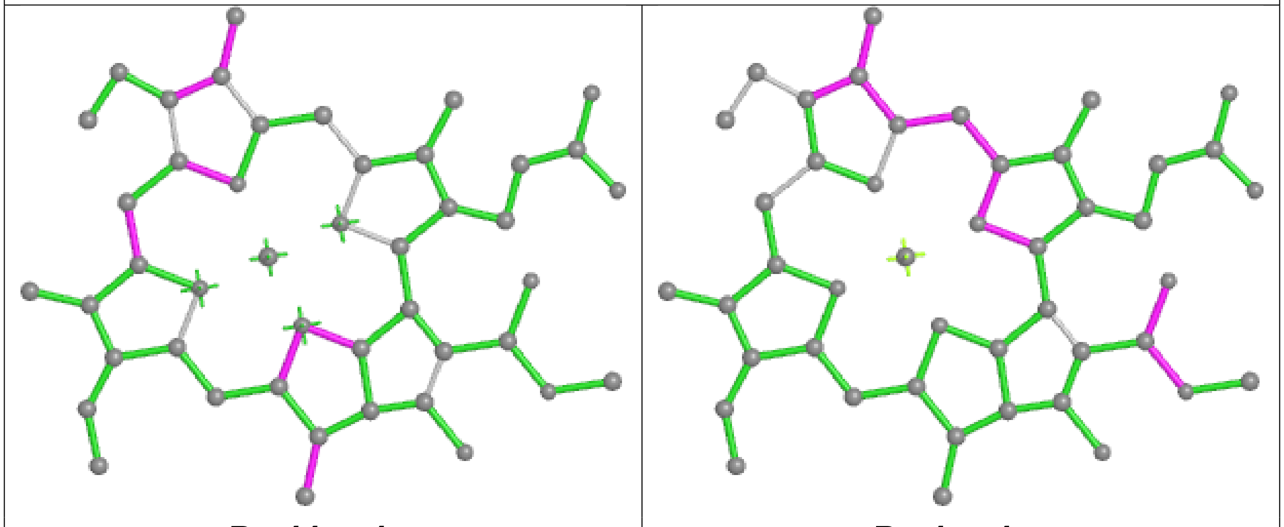
Bond angles



Torsions

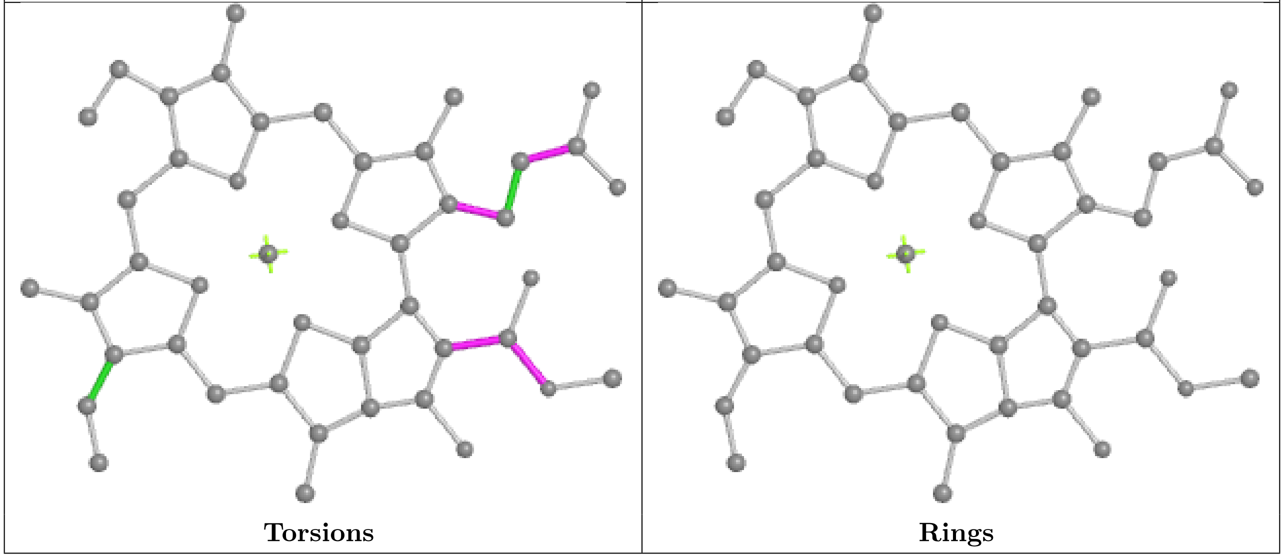
Rings

Ligand CLA bJ 101



Bond lengths

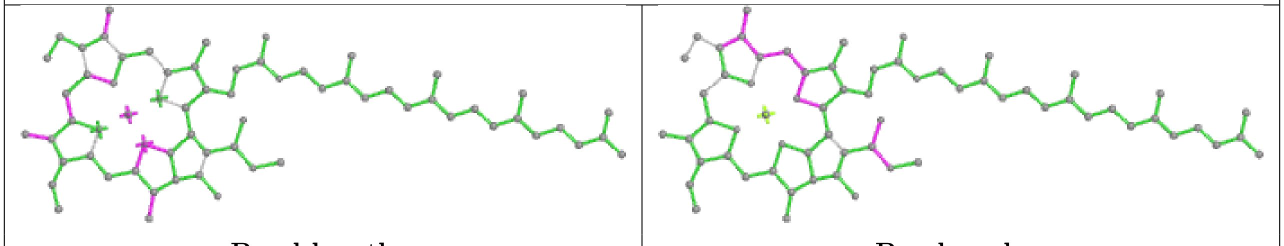
Bond angles



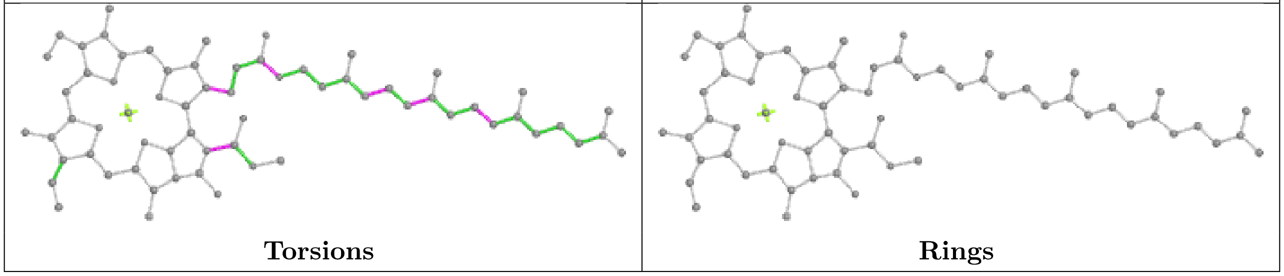
Torsions

Rings

Ligand CLA aB 819

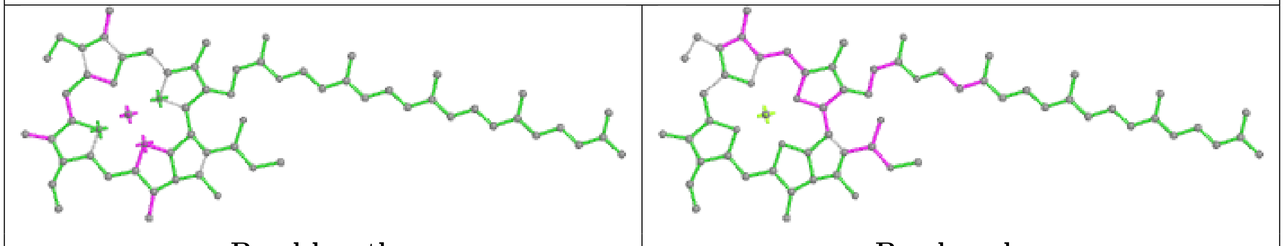


Bond lengths Bond angles

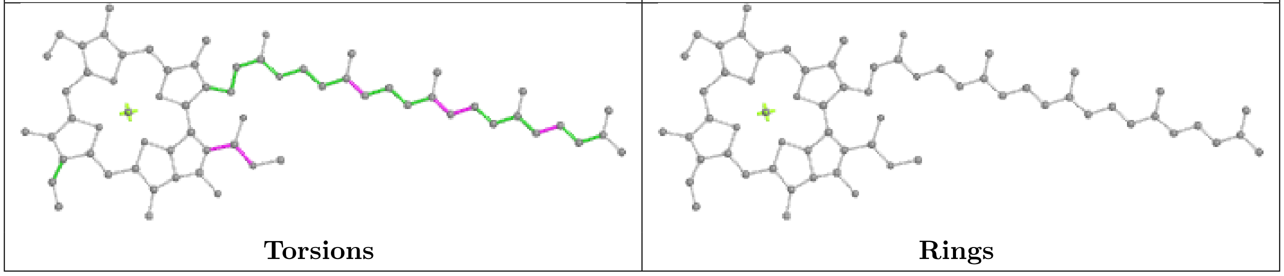


Torsions Rings

Ligand CLA cA 833

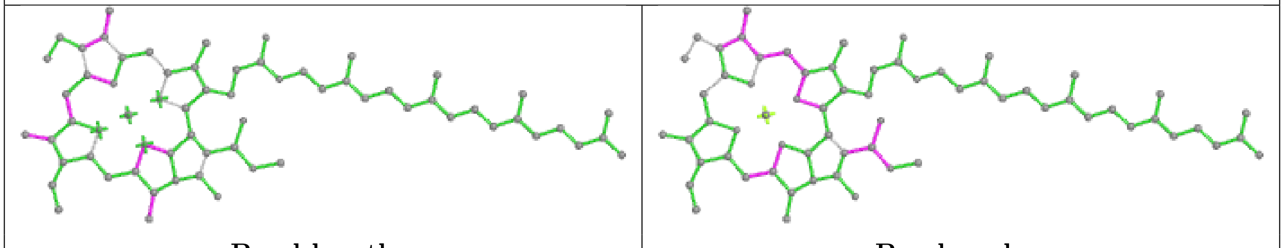


Bond lengths Bond angles

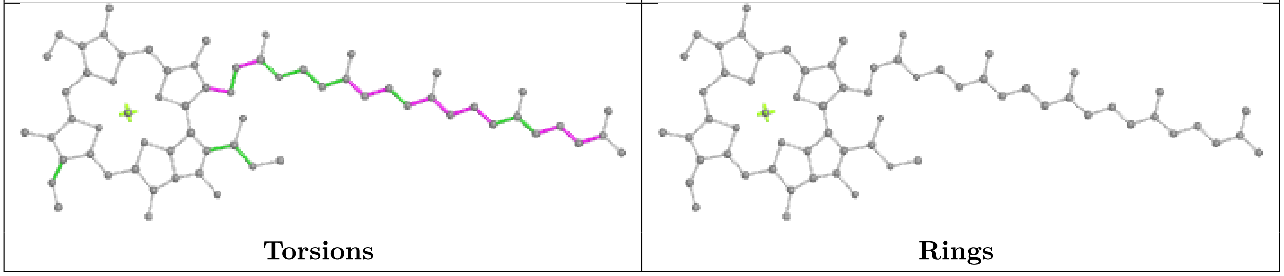


Torsions Rings

Ligand CLA cB 832

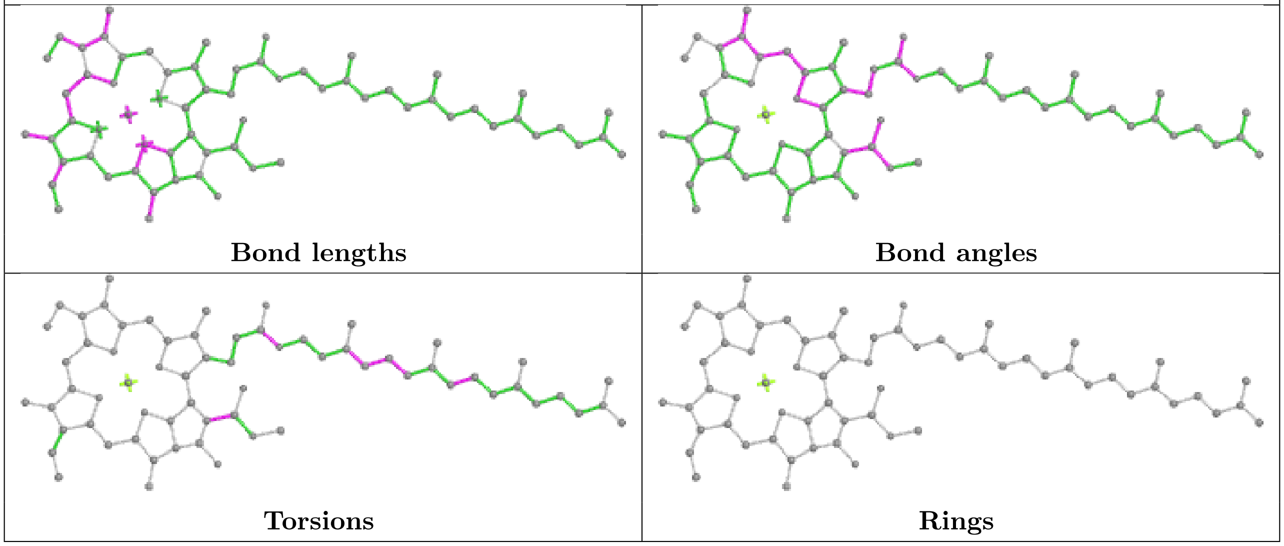


Bond lengths Bond angles



Torsions Rings

Ligand CLA dB 809



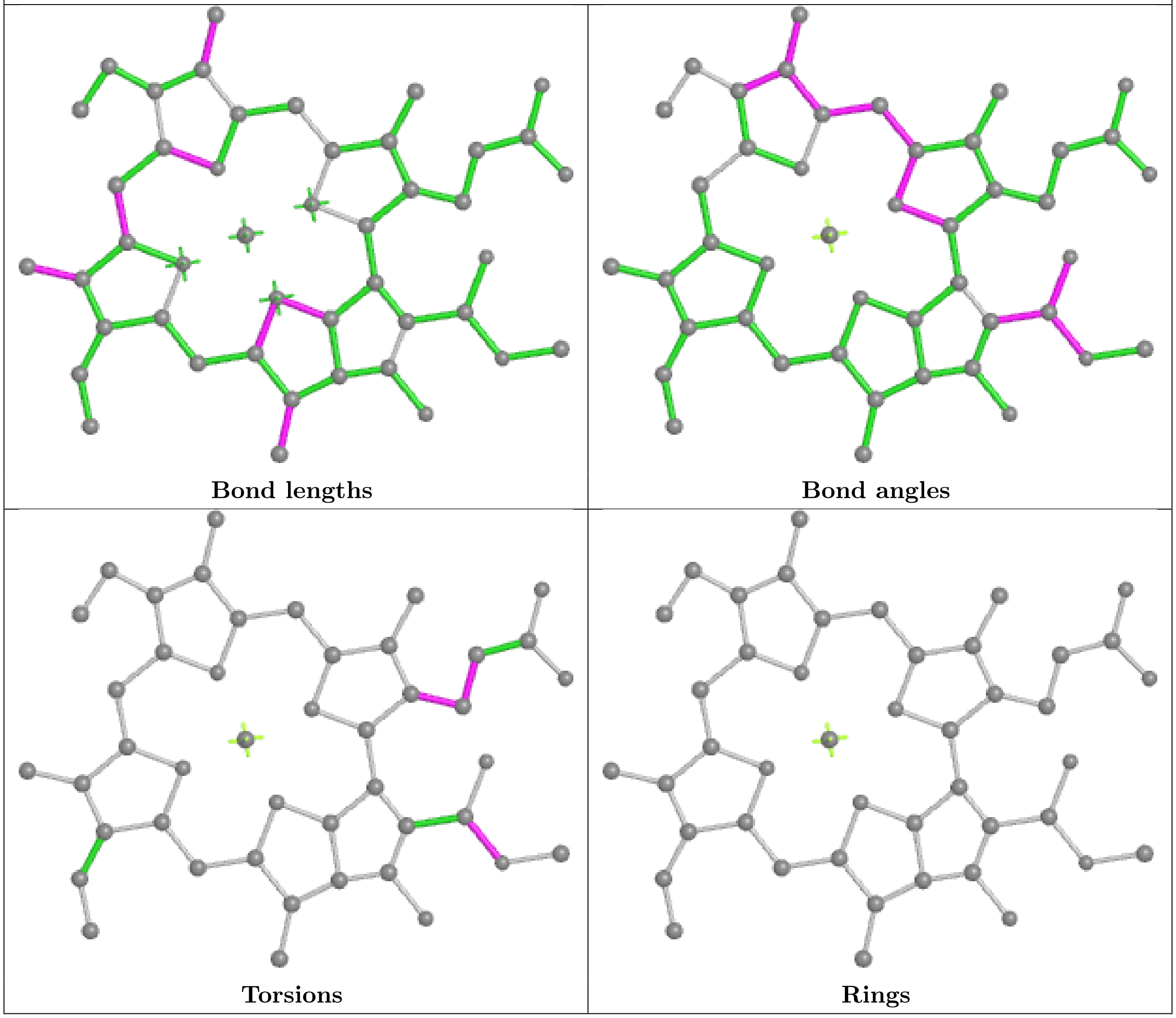
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA dB 816



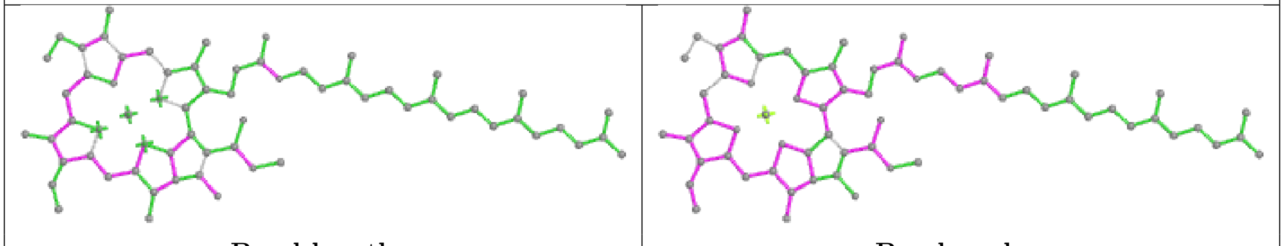
Bond lengths

Bond angles

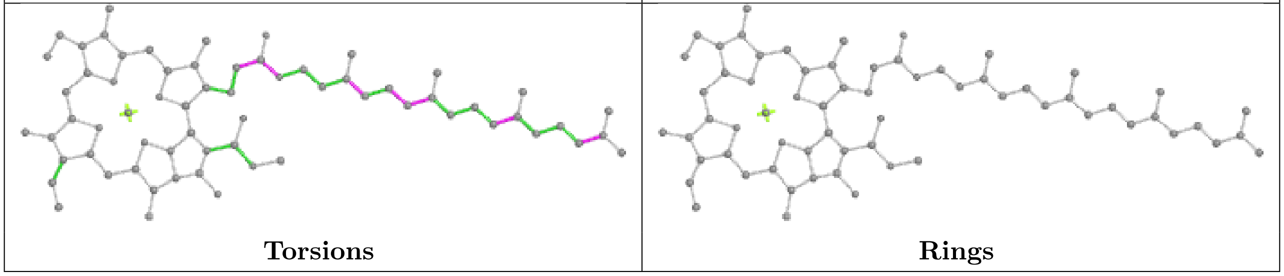
Torsions

Rings

Ligand CL0 bA 801

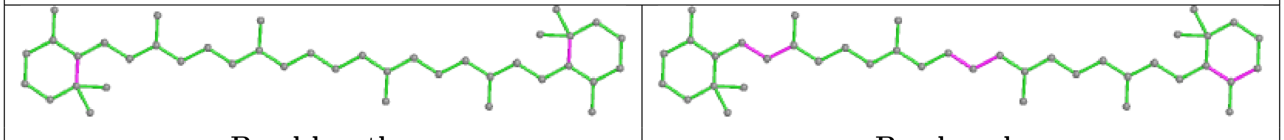


Bond lengths **Bond angles**

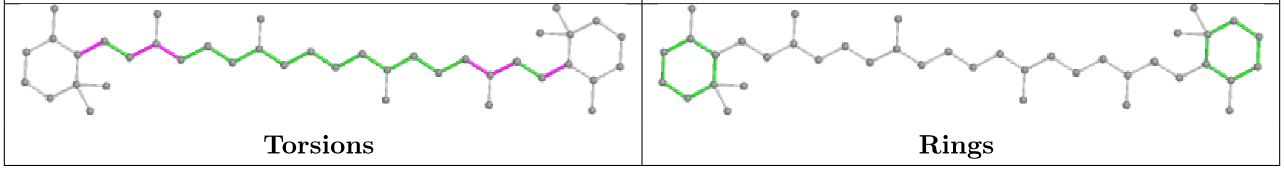


Torsions **Rings**

Ligand BCR cB 845

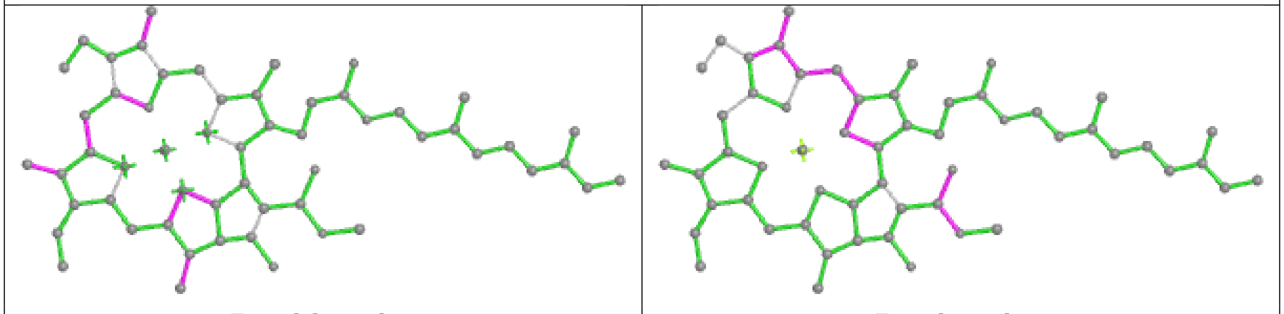


Bond lengths **Bond angles**

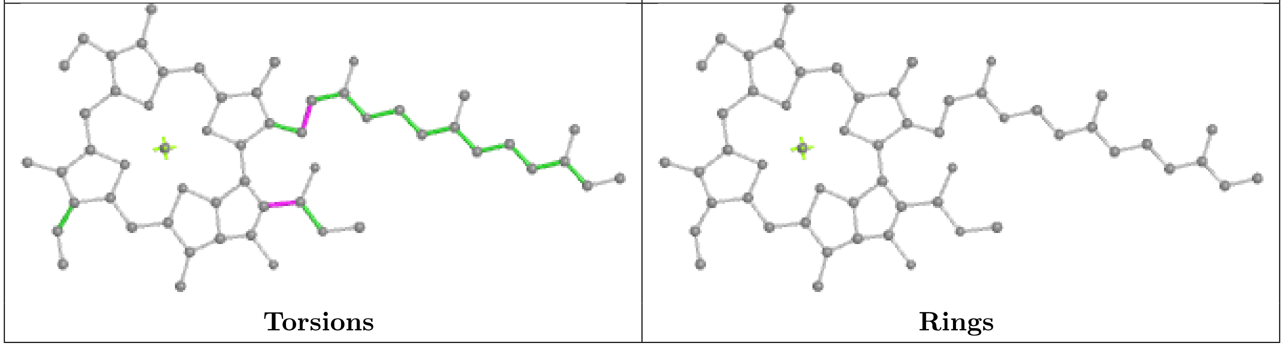


Torsions **Rings**

Ligand CLA aB 814

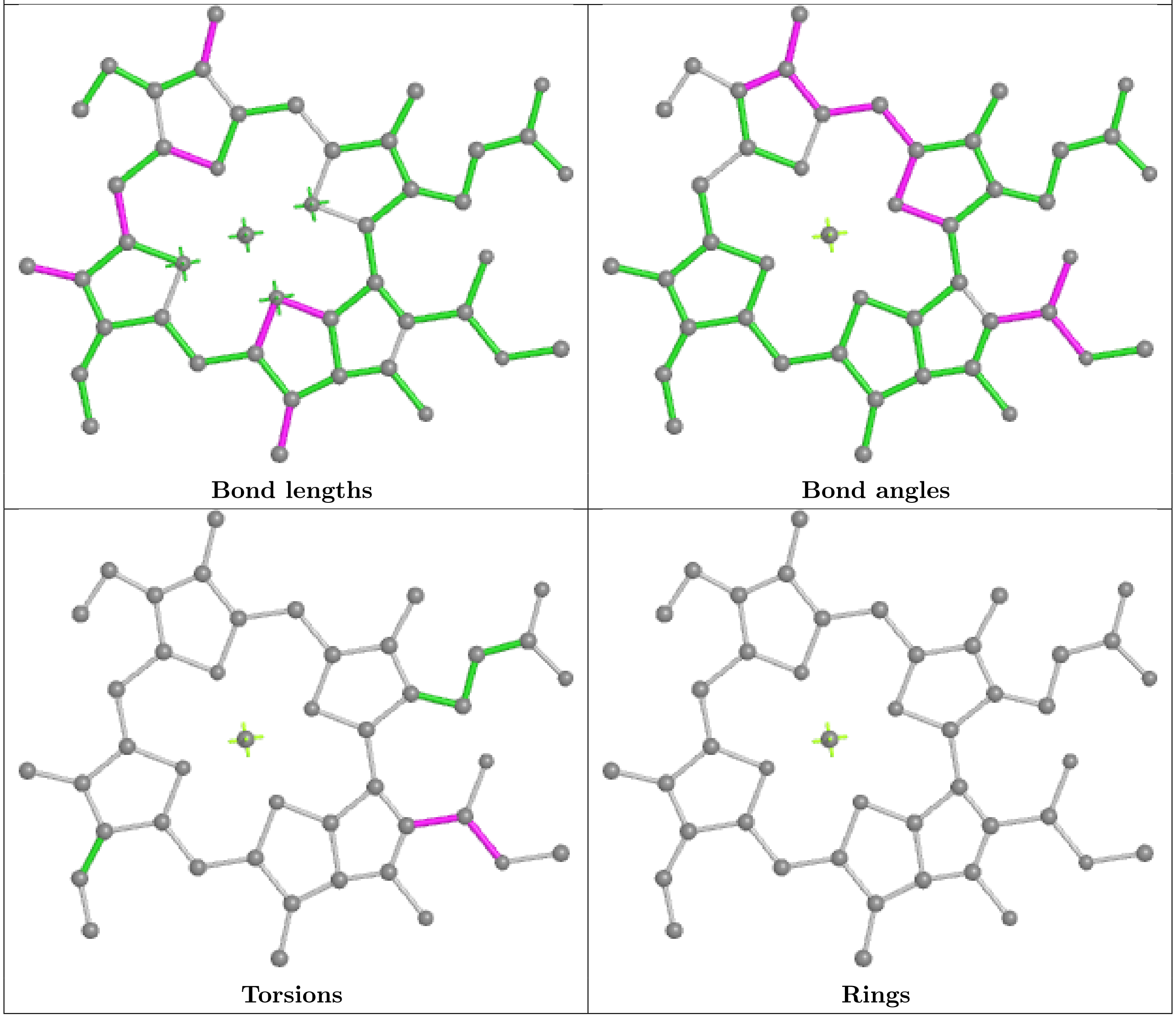


Bond lengths **Bond angles**

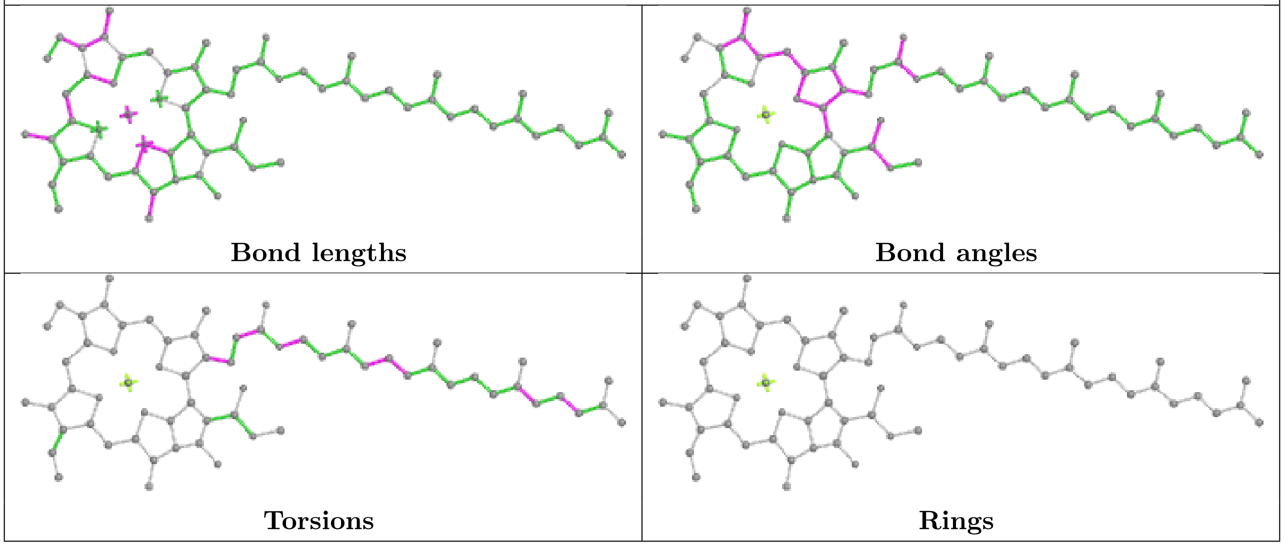


Torsions **Rings**

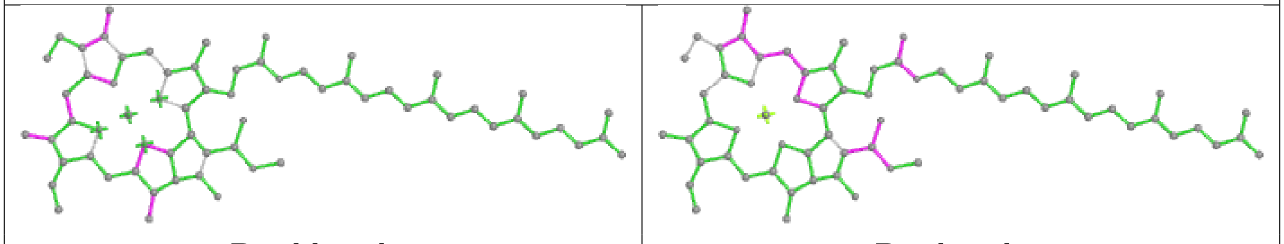
Ligand CLA aB 834



Ligand CLA bA 806

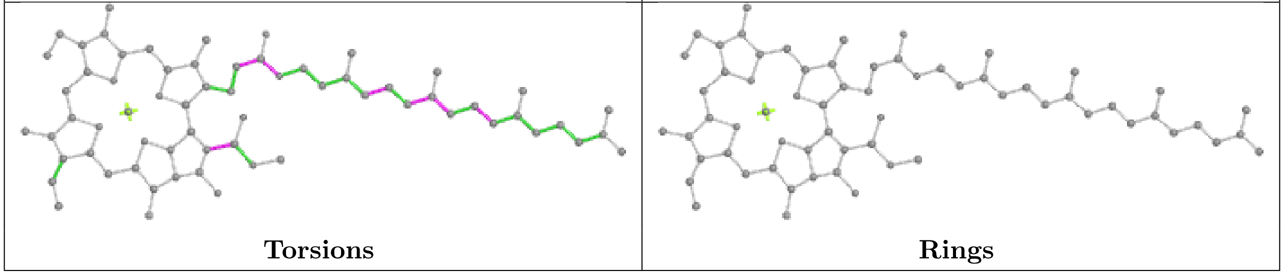


Ligand CLA dA 827



Bond lengths

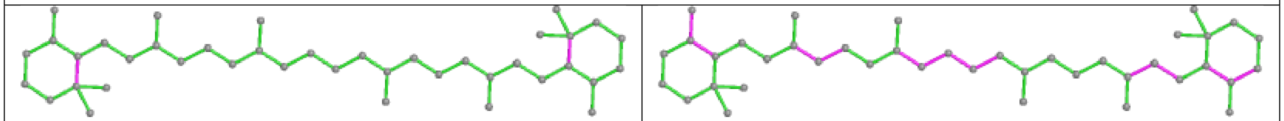
Bond angles



Torsions

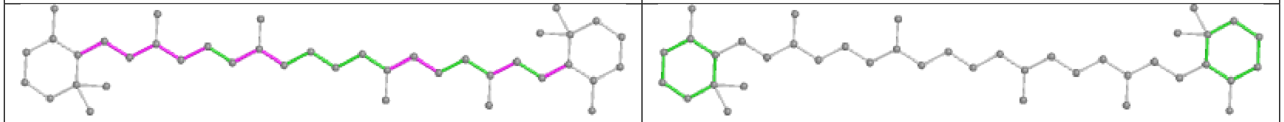
Rings

Ligand BCR cJ 103



Bond lengths

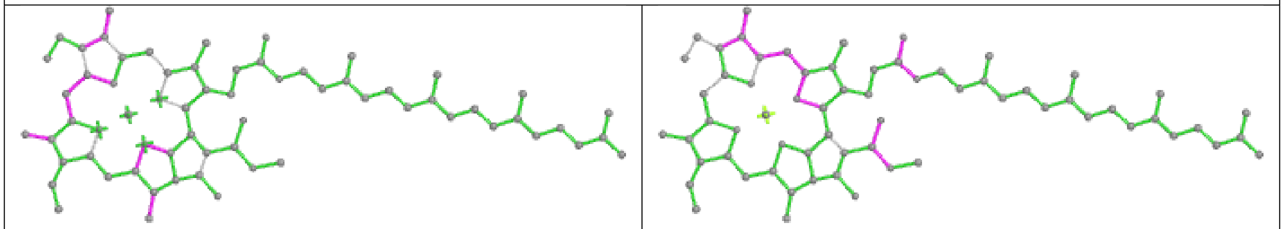
Bond angles



Torsions

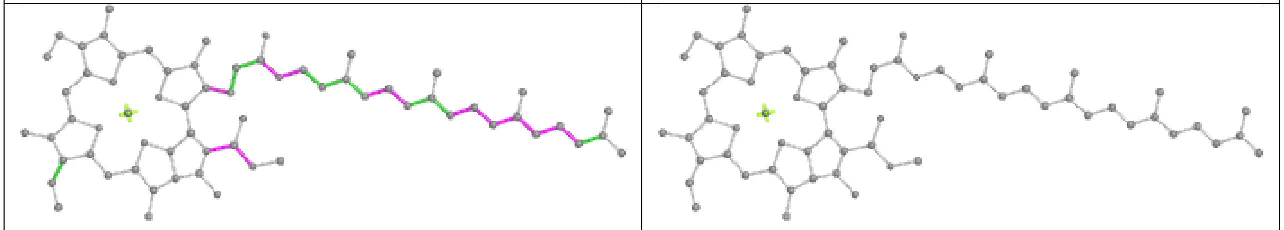
Rings

Ligand CLA dB 842



Bond lengths

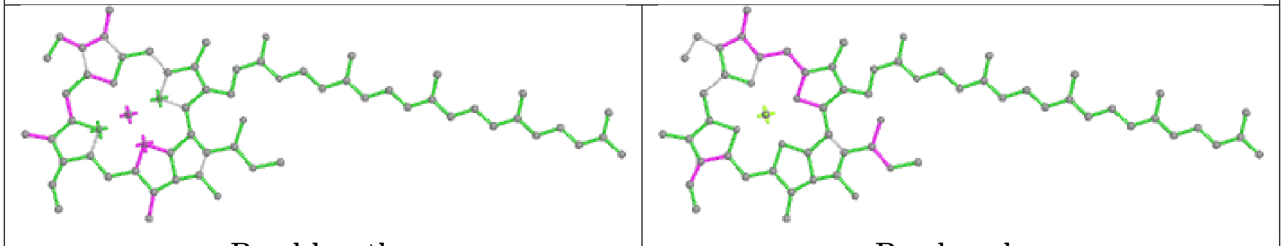
Bond angles



Torsions

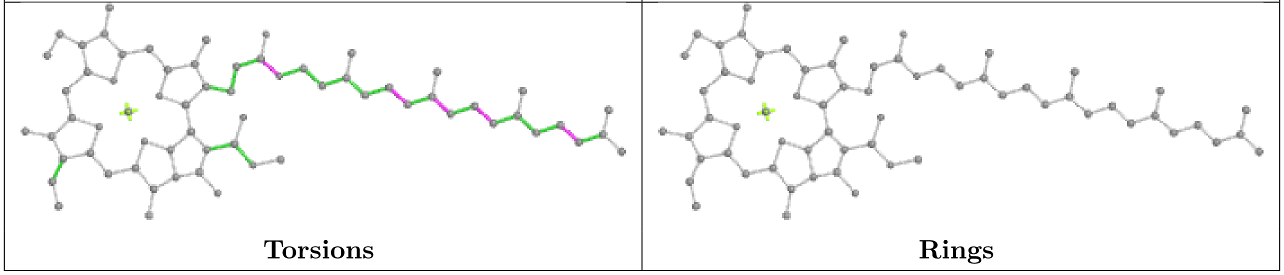
Rings

Ligand CLA bL 201



Bond lengths

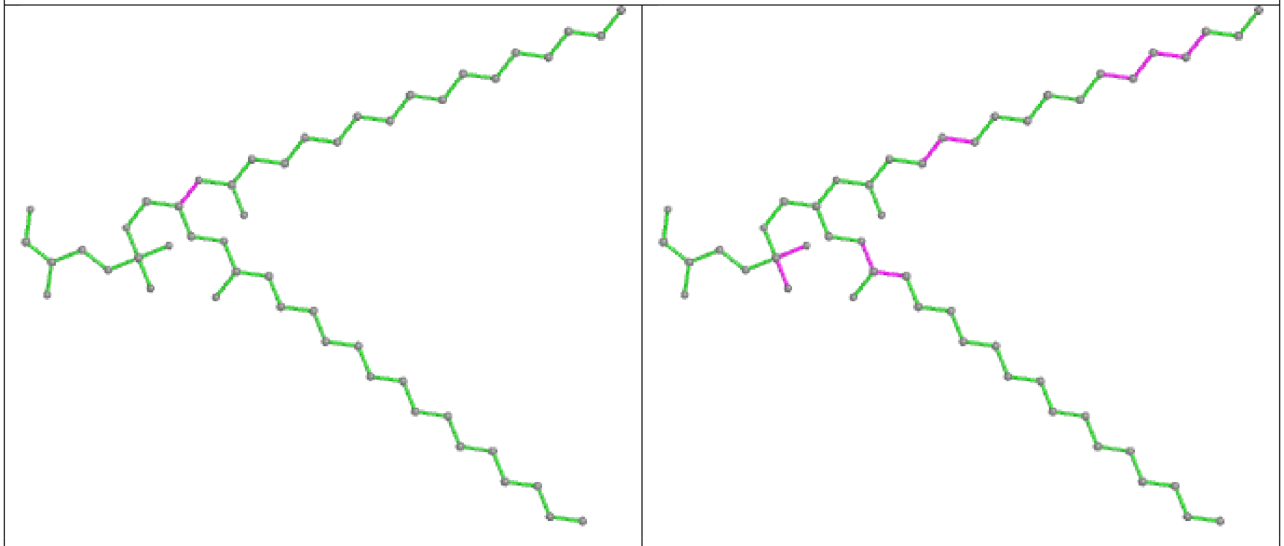
Bond angles



Torsions

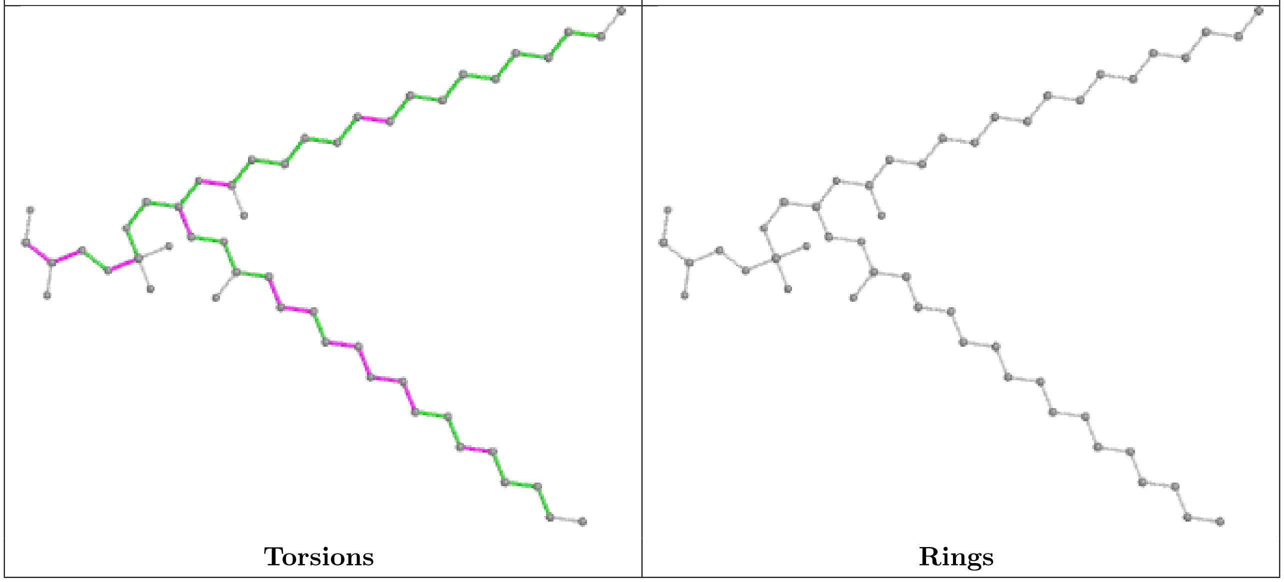
Rings

Ligand LHG aA 852



Bond lengths

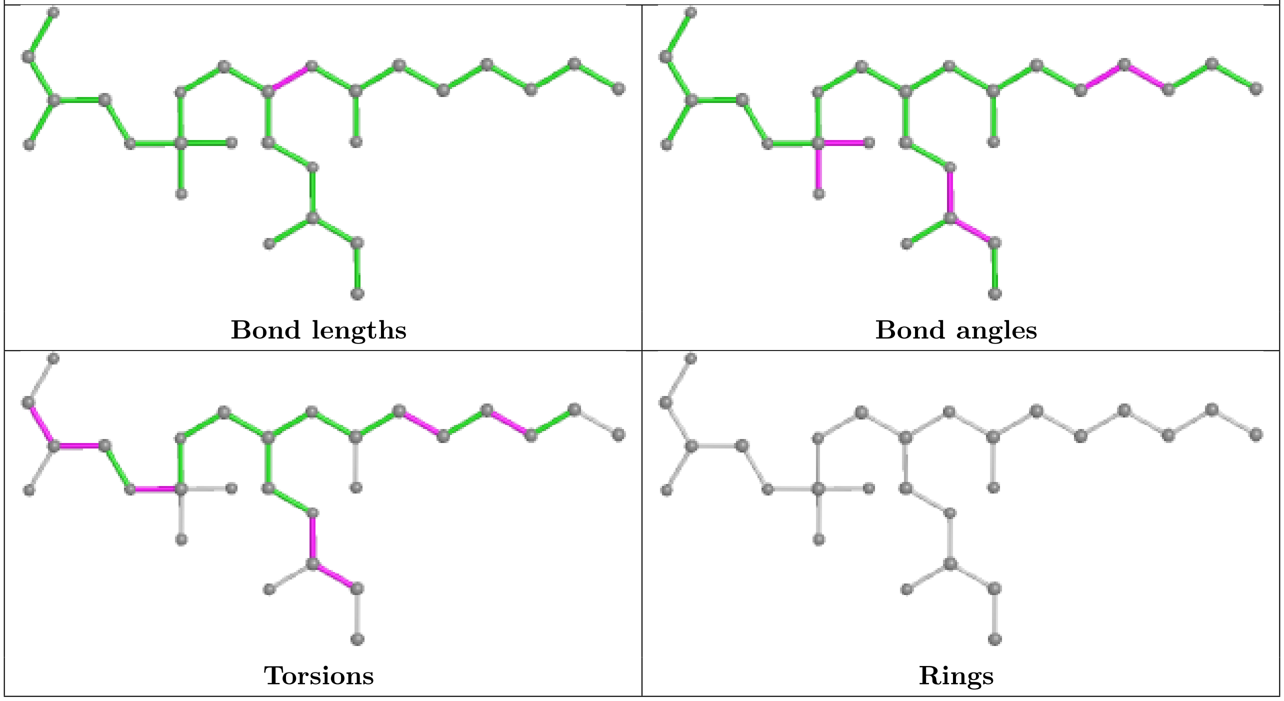
Bond angles



Torsions

Rings

Ligand LHG dA 851



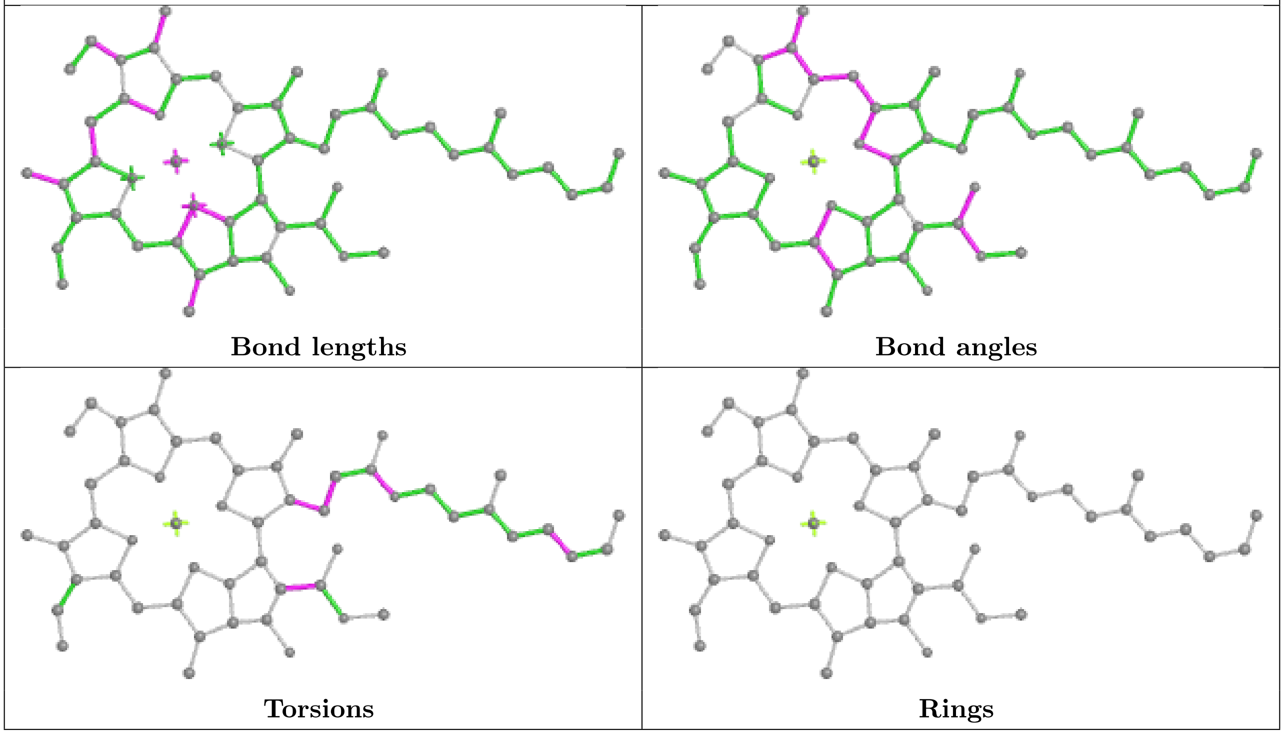
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA dA 818



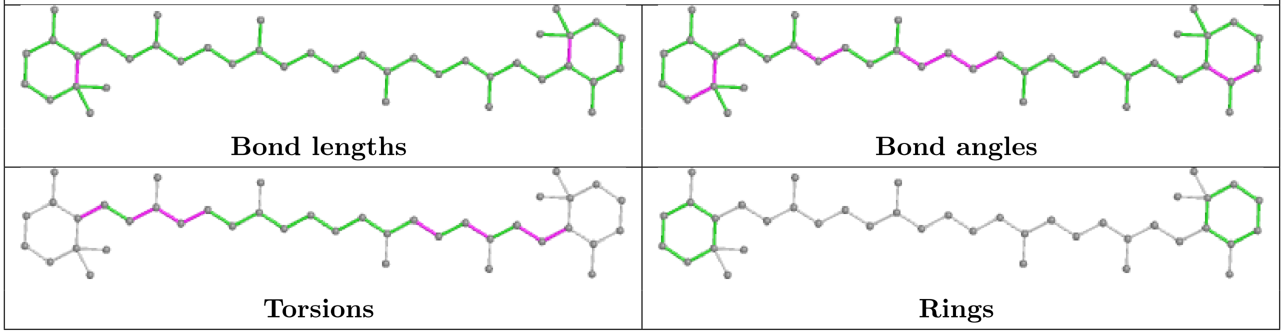
Bond lengths

Bond angles

Torsions

Rings

Ligand BCR bB 848



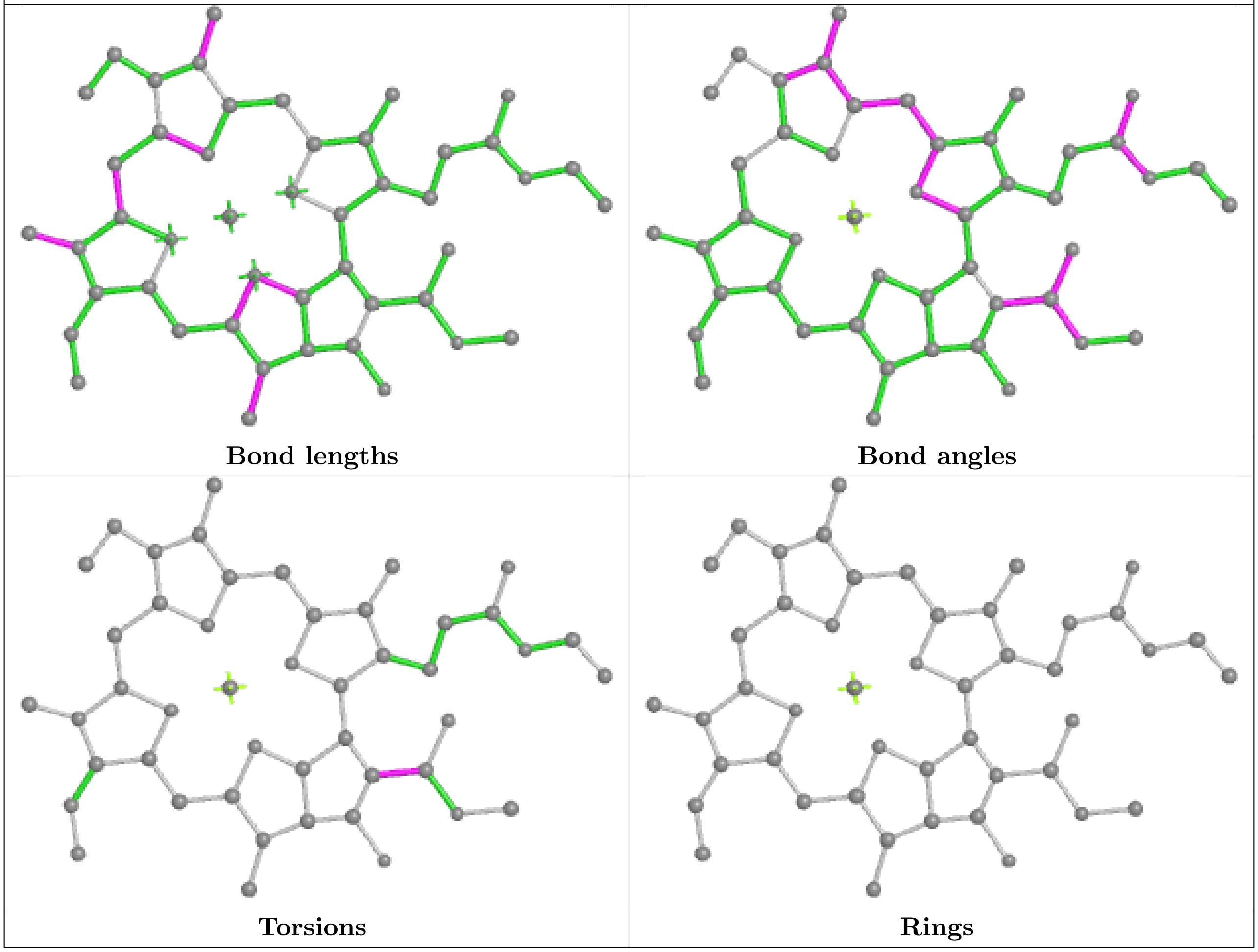
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA aB 839



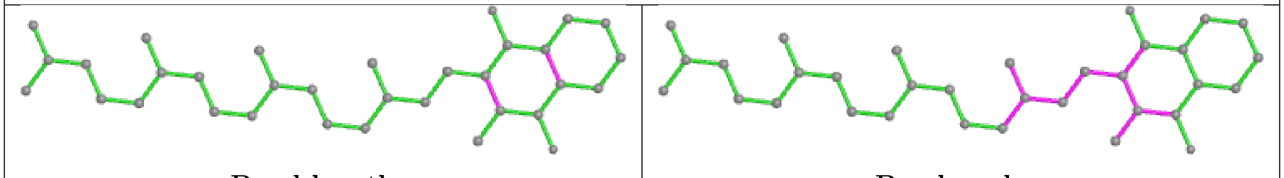
Bond lengths

Bond angles

Torsions

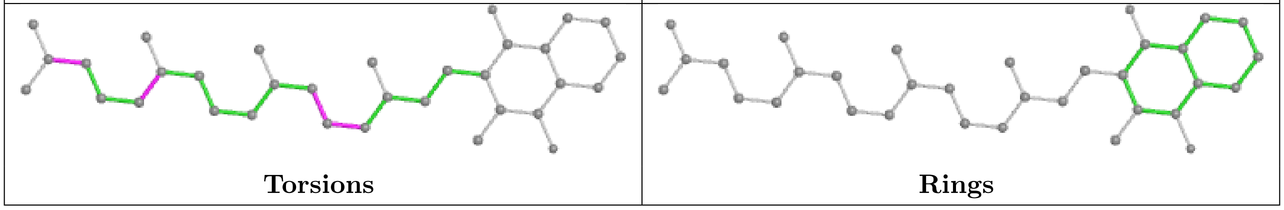
Rings

Ligand PQN dA 843



Bond lengths

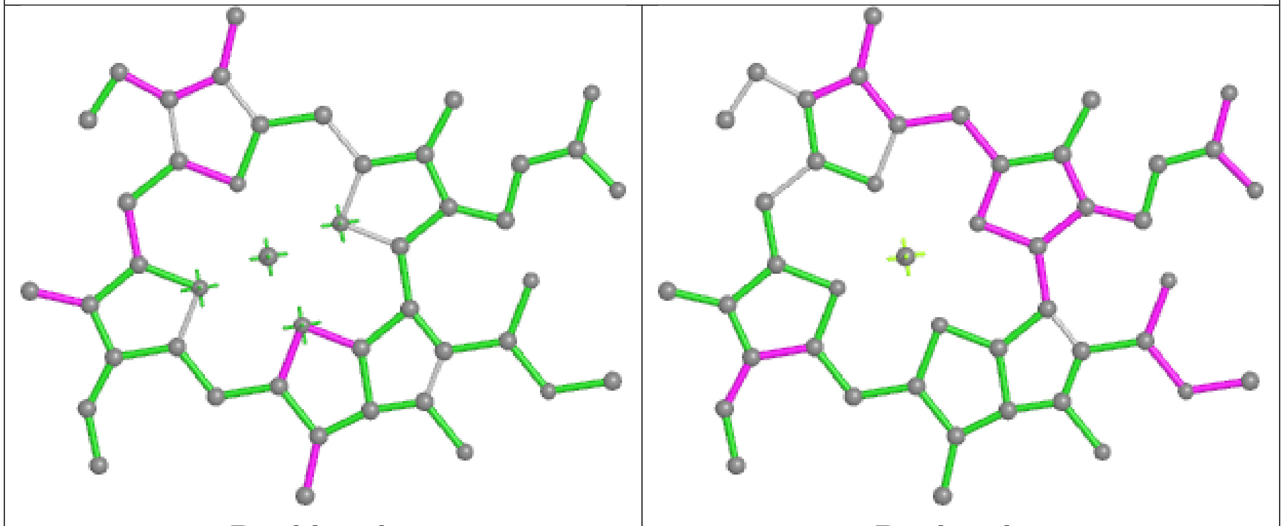
Bond angles



Torsions

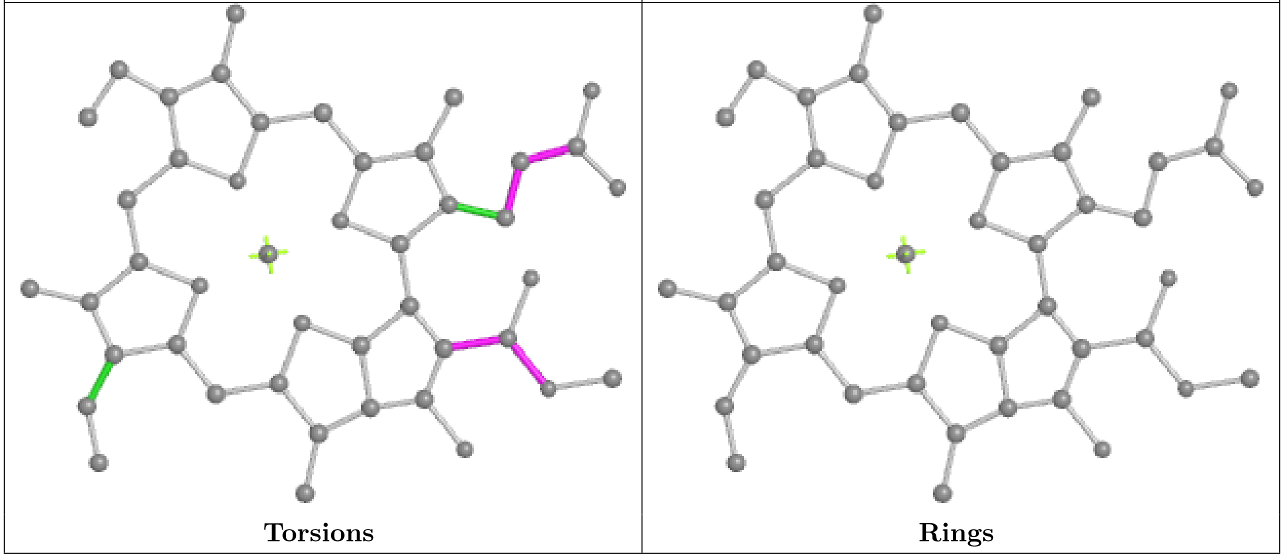
Rings

Ligand CLA cA 813



Bond lengths

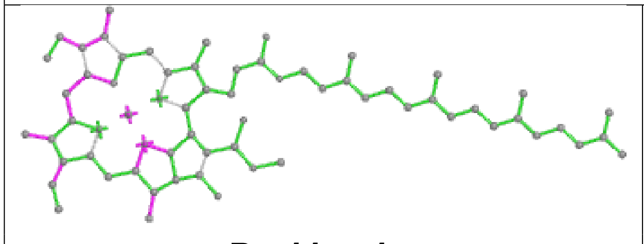
Bond angles



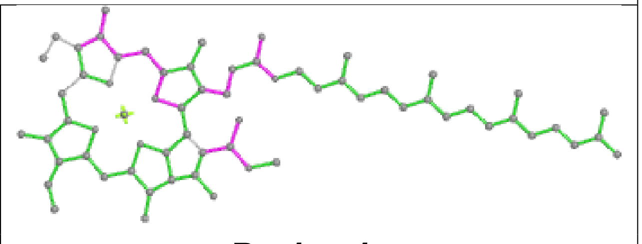
Torsions

Rings

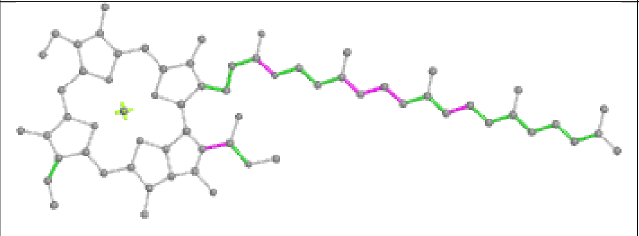
Ligand CLA cB 809



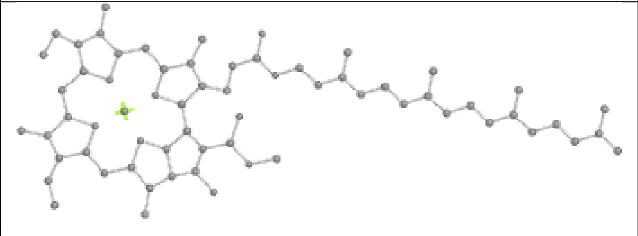
Bond lengths



Bond angles

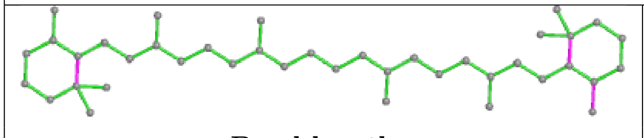


Torsions

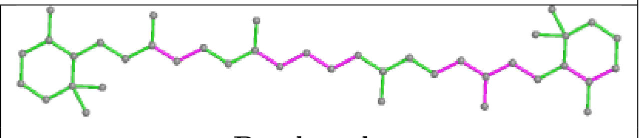


Rings

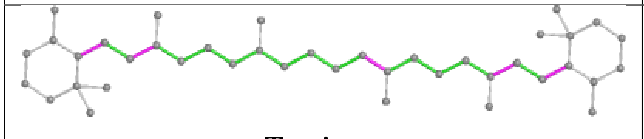
Ligand BCR dL 207



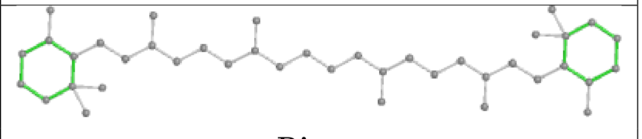
Bond lengths



Bond angles

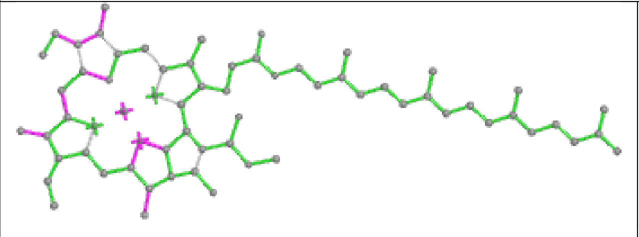


Torsions

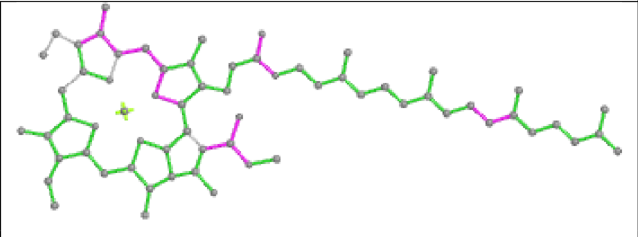


Rings

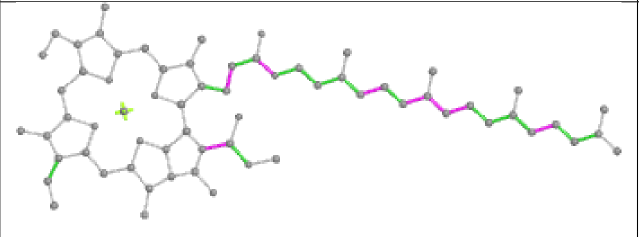
Ligand CLA cL 203



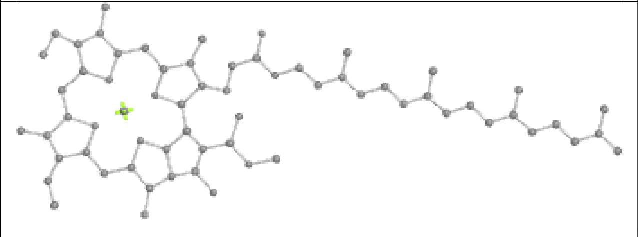
Bond lengths



Bond angles

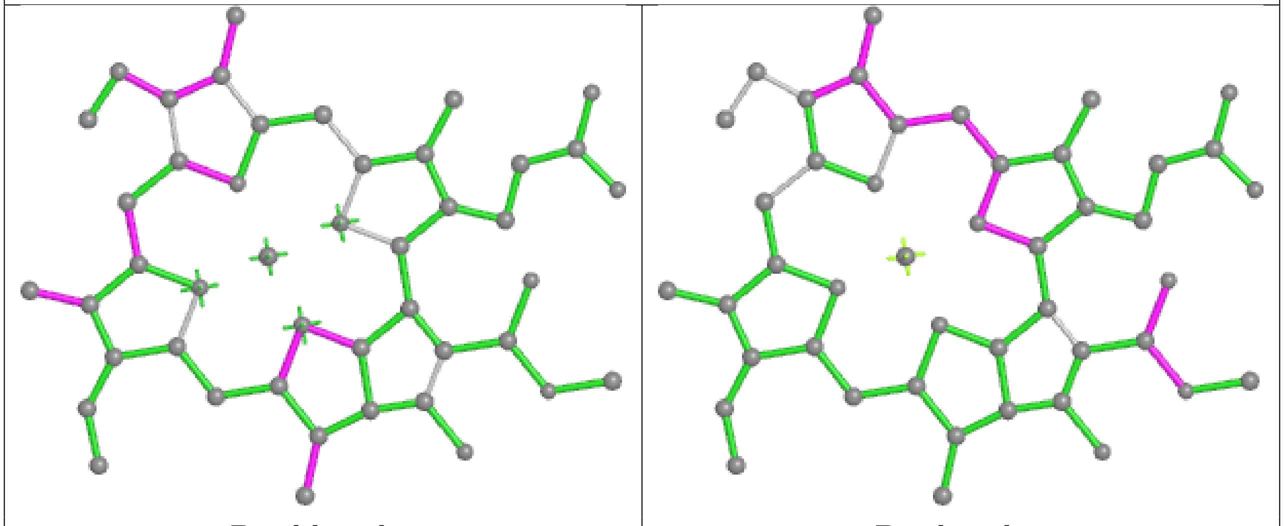


Torsions

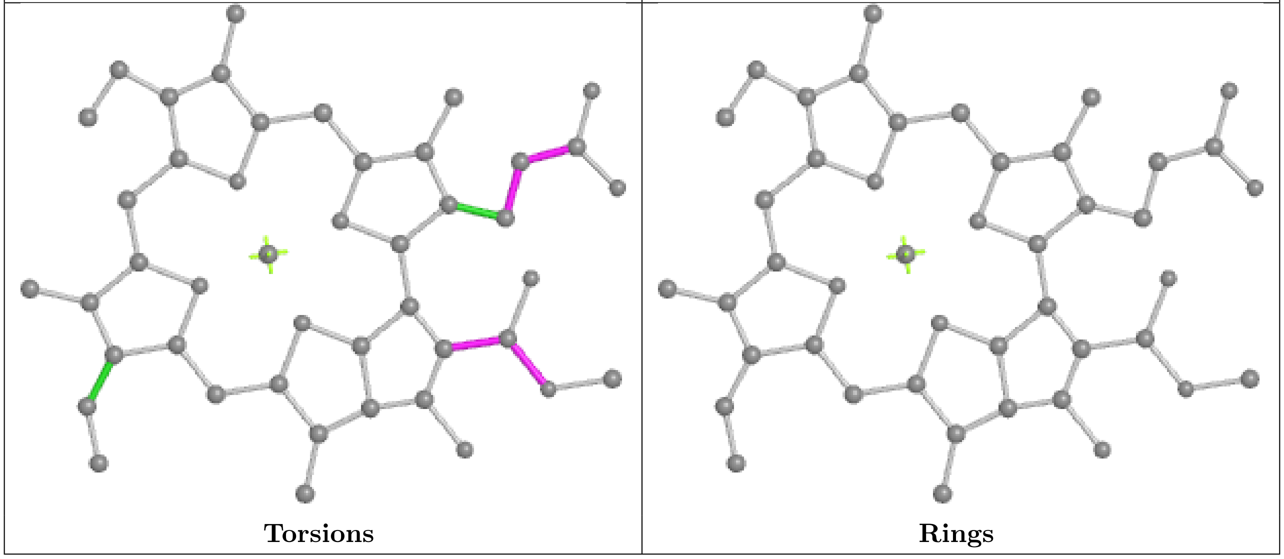


Rings

Ligand CLA dX 101

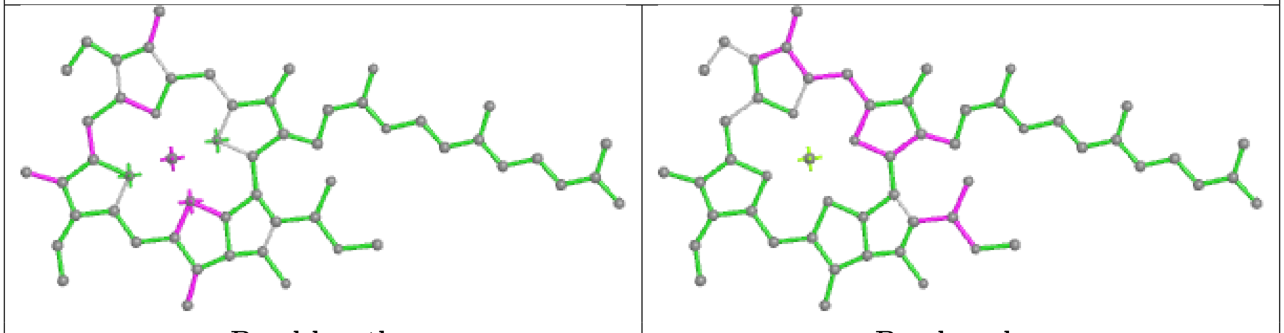


Bond lengths **Bond angles**

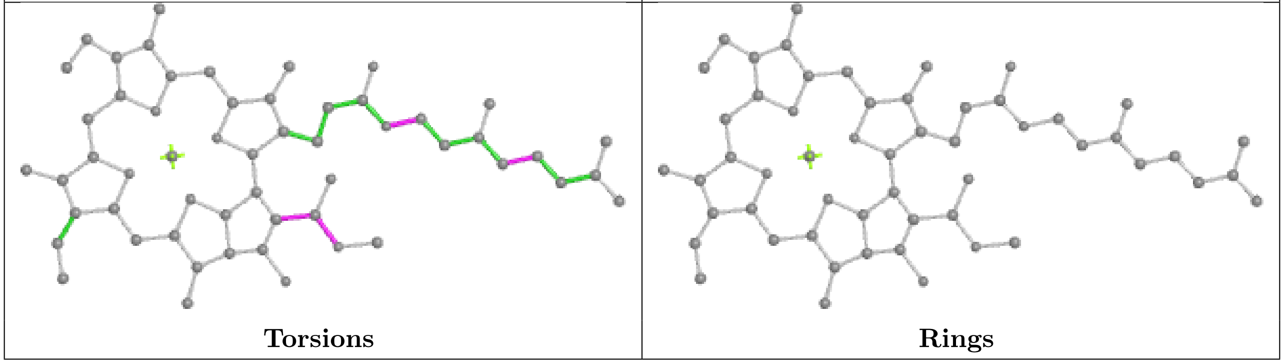


Torsions **Rings**

Ligand CLA bA 826

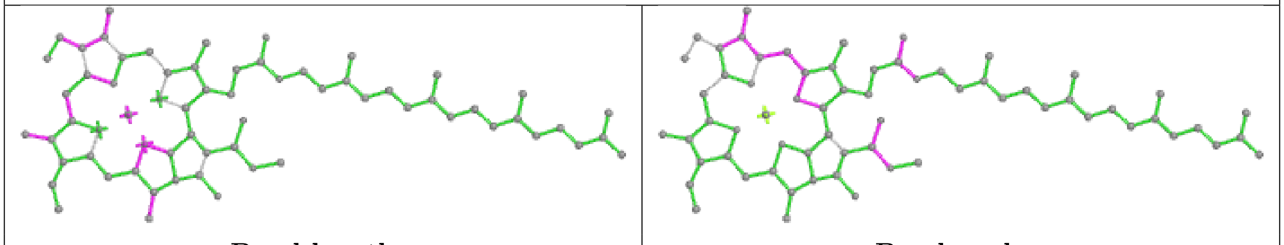


Bond lengths **Bond angles**

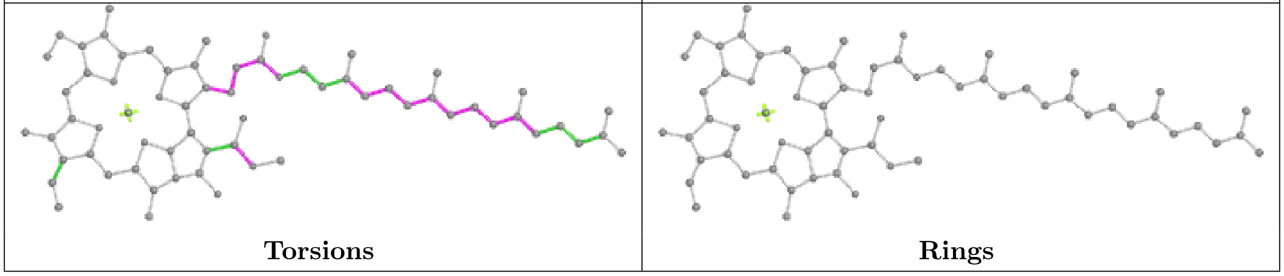


Torsions **Rings**

Ligand CLA dL 206

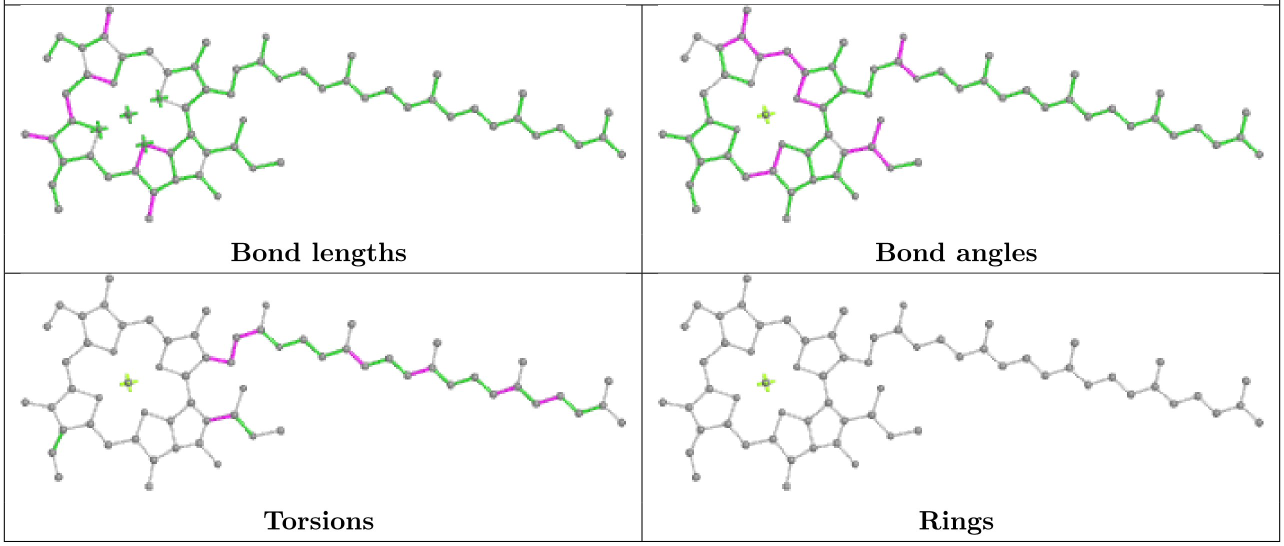


Bond lengths **Bond angles**



Torsions **Rings**

Ligand CLA cB 827



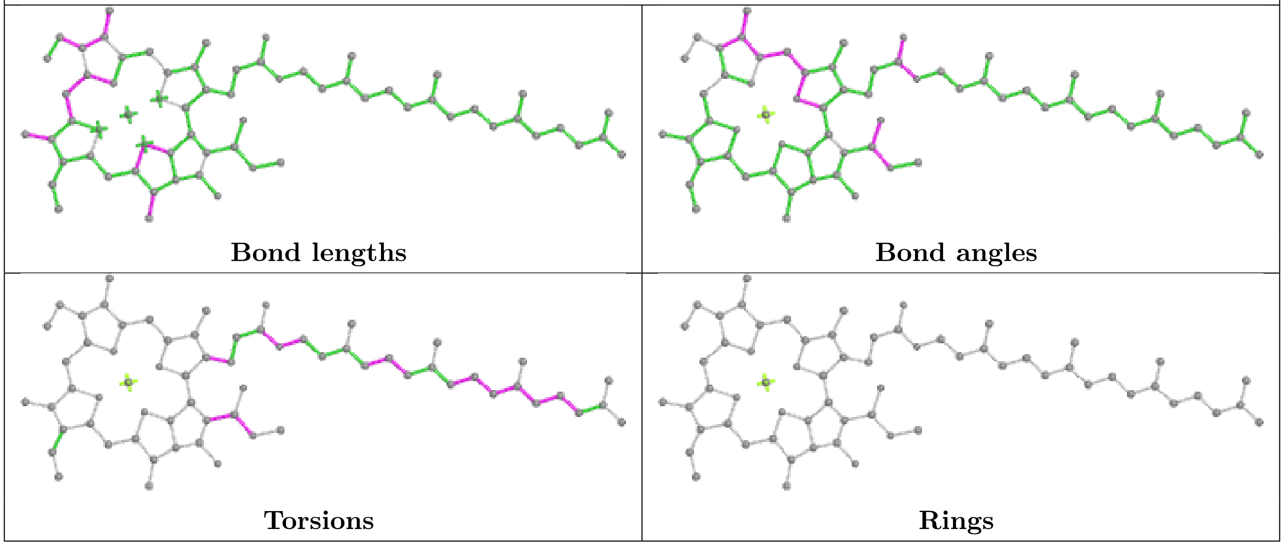
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA bB 842



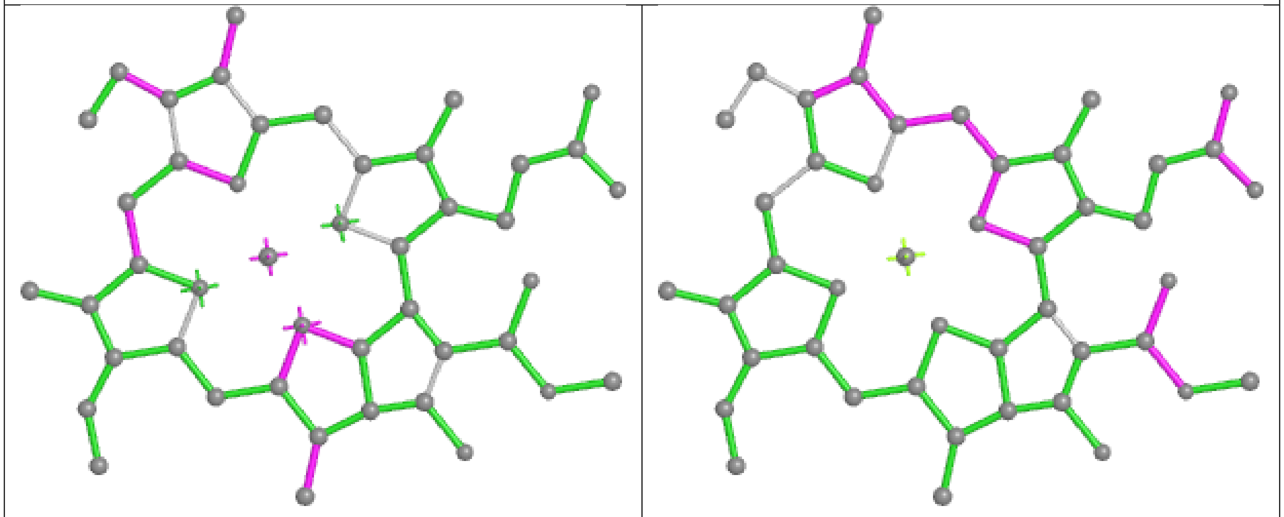
Bond lengths

Bond angles

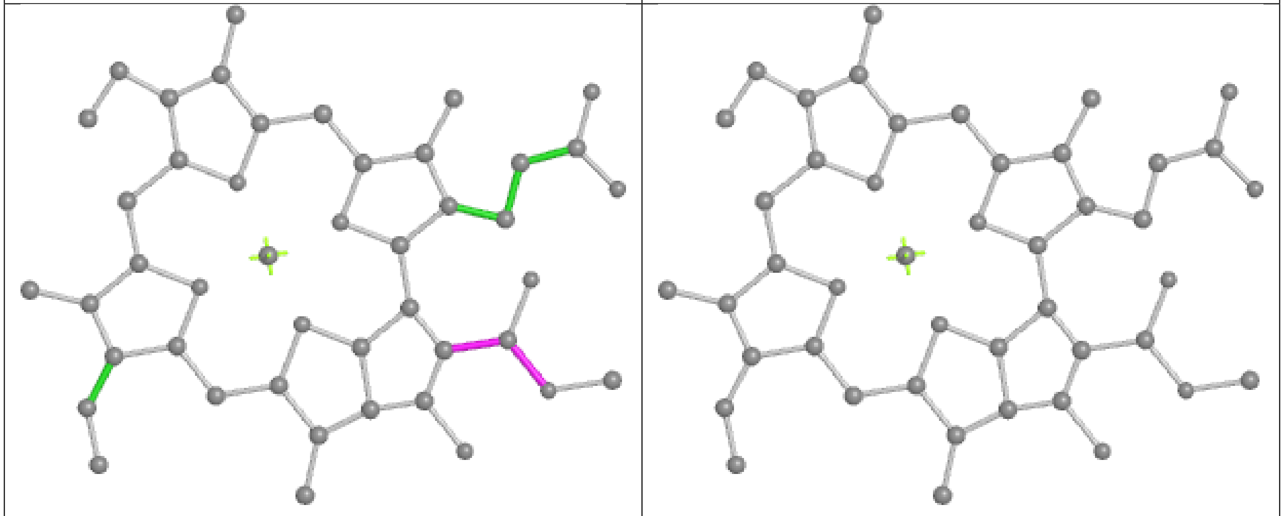
Torsions

Rings

Ligand CLA aB 821

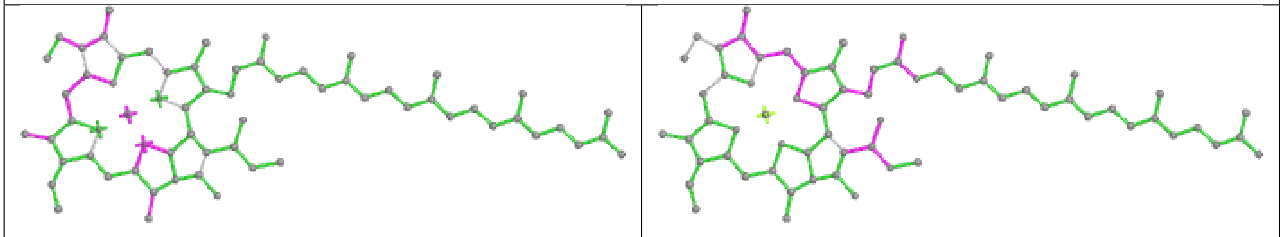


Bond lengths **Bond angles**

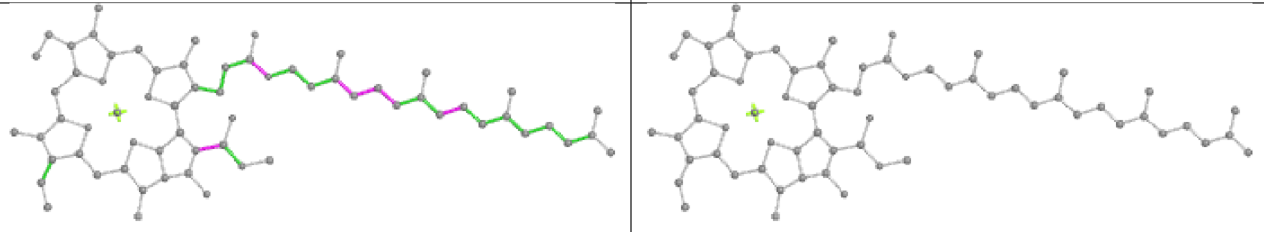


Torsions **Rings**

Ligand CLA aB 809

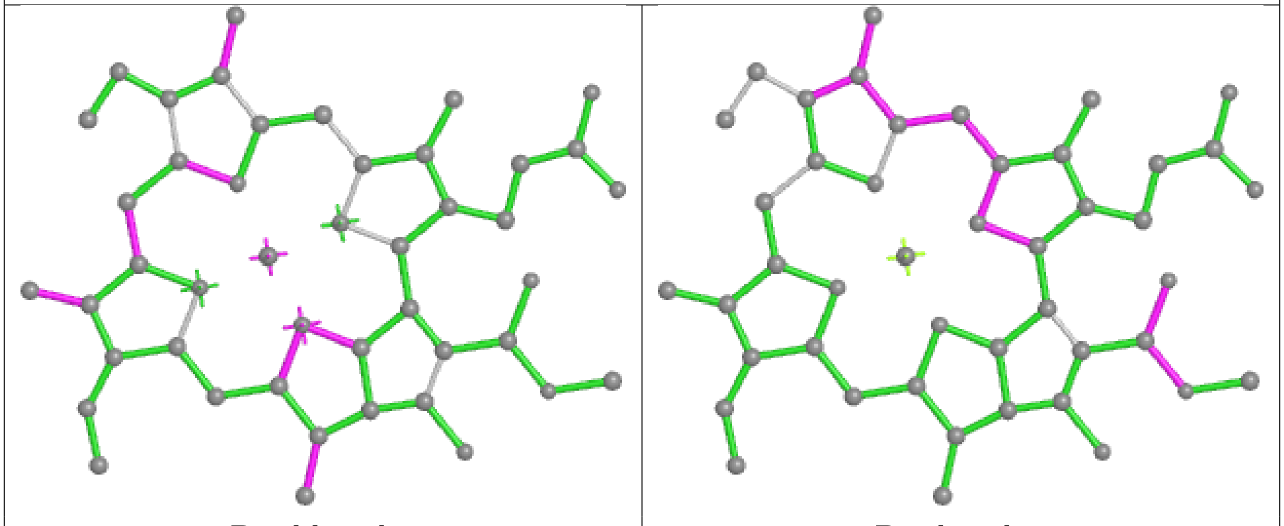


Bond lengths **Bond angles**

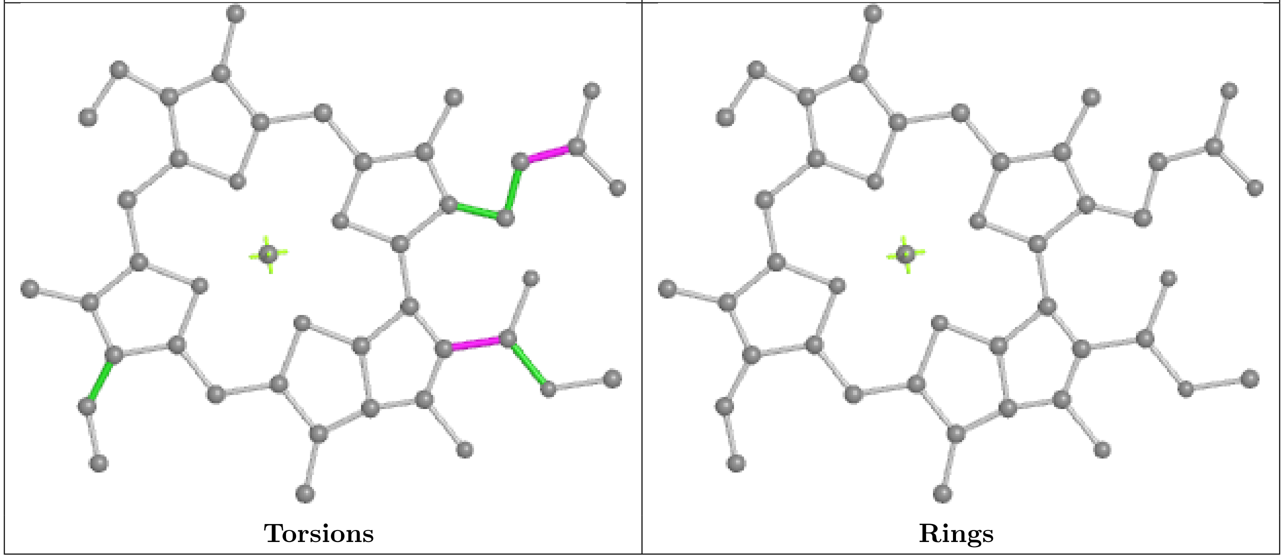


Torsions **Rings**

Ligand CLA aK 102

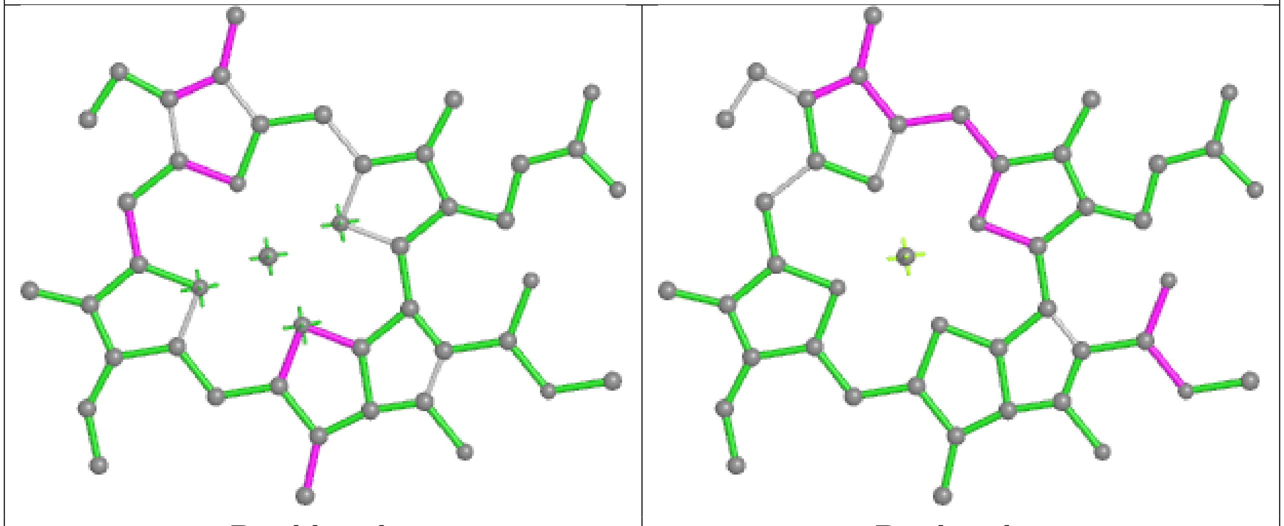


Bond lengths Bond angles

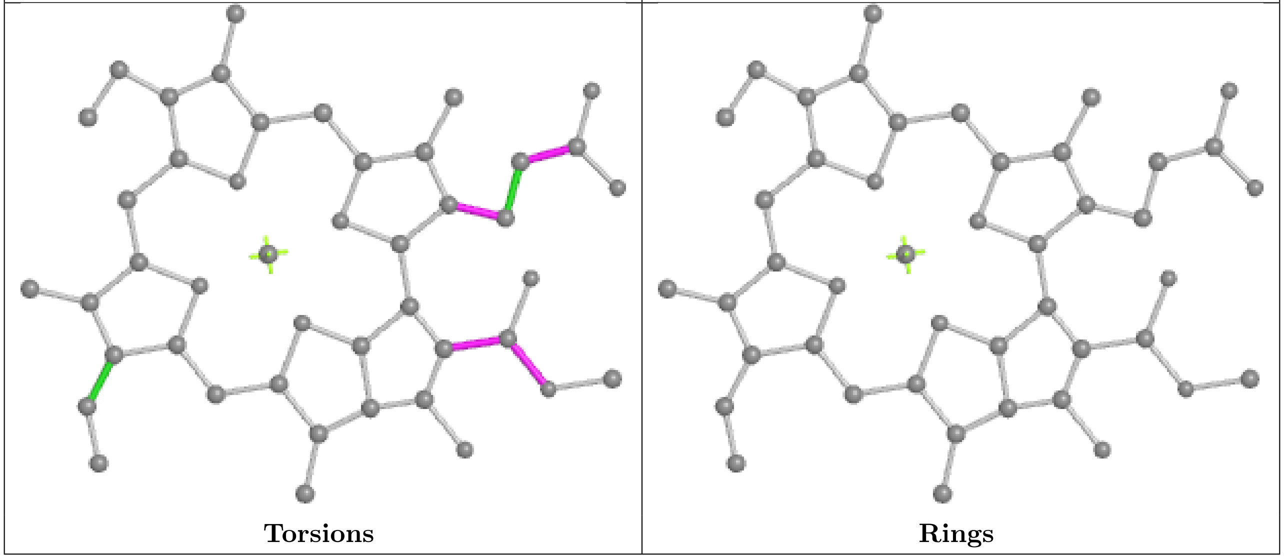


Torsions Rings

Ligand CLA dJ 101

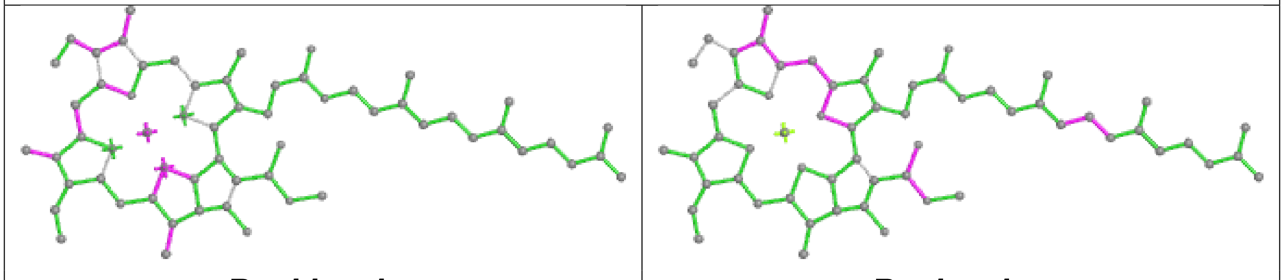

Bond lengths

Bond angles

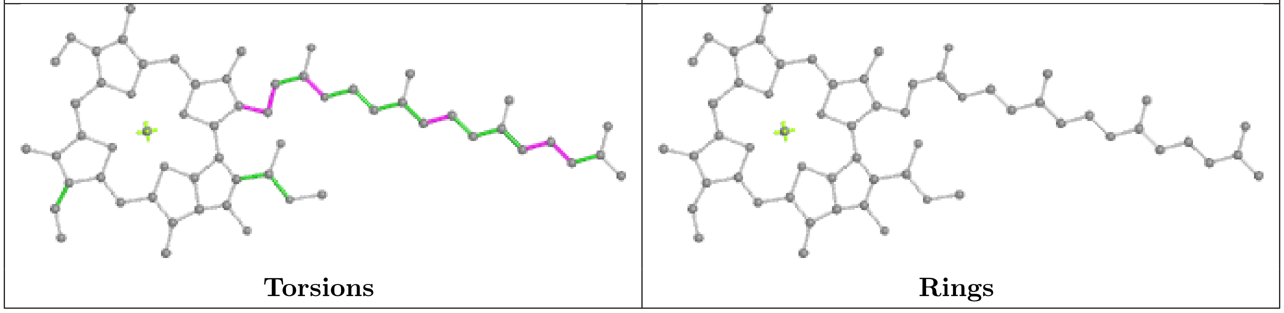

Torsions

Rings

Ligand CLA bB 819

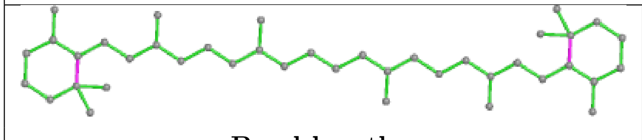

Bond lengths

Bond angles

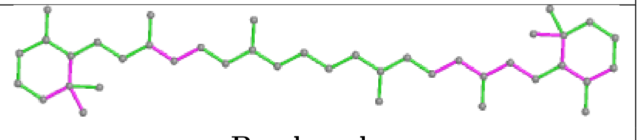

Torsions

Rings

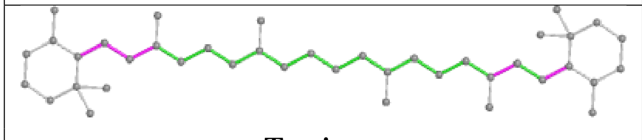
Ligand BCR aL 205



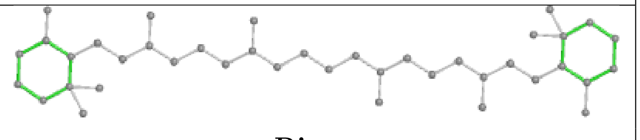
Bond lengths



Bond angles

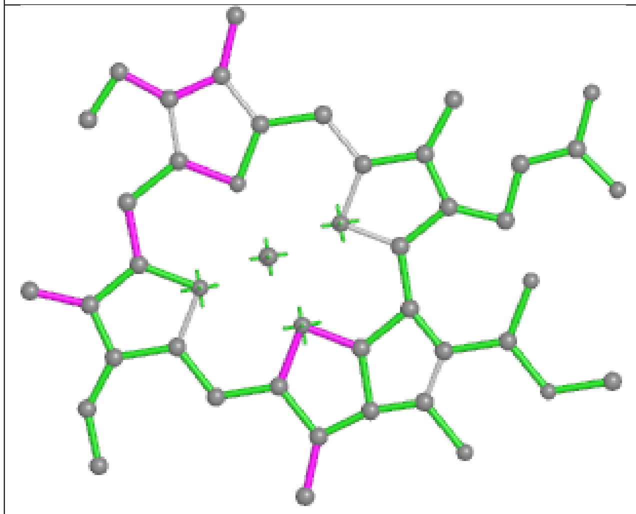


Torsions

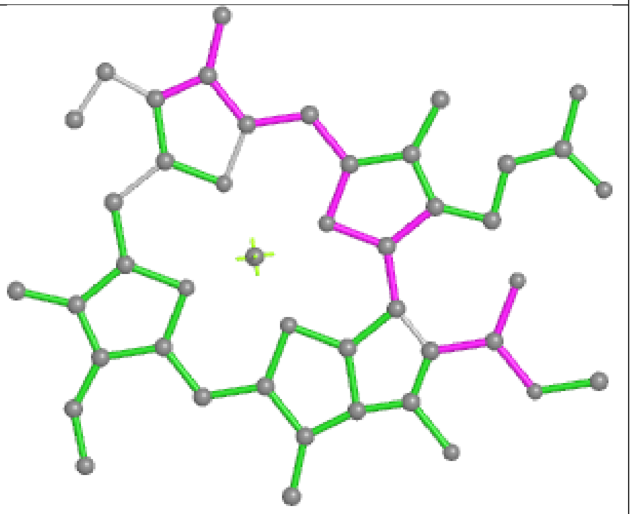


Rings

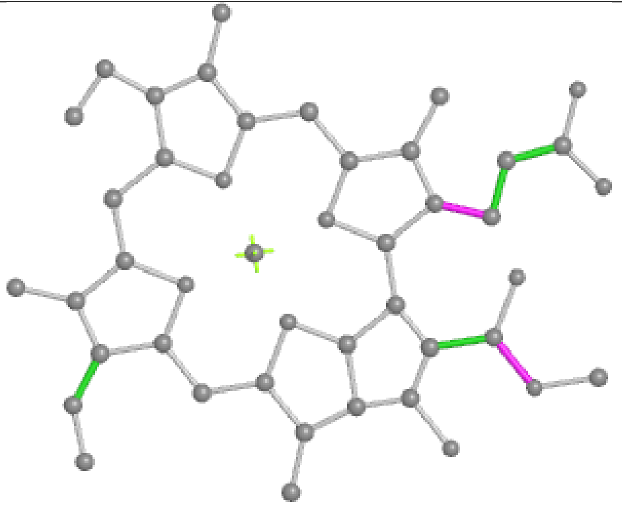
Ligand CLA cA 804



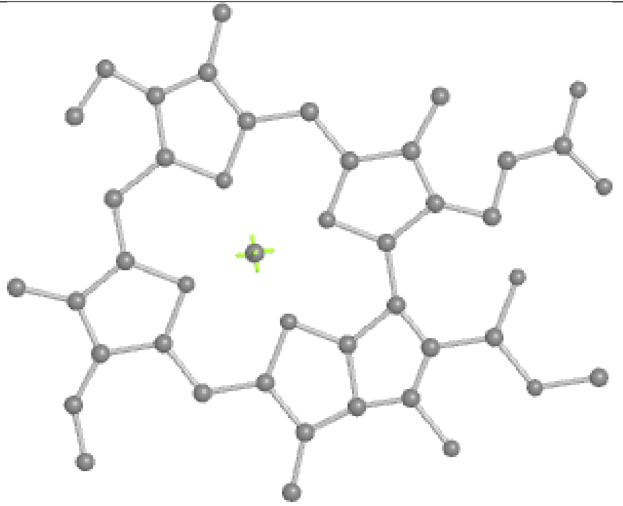
Bond lengths



Bond angles

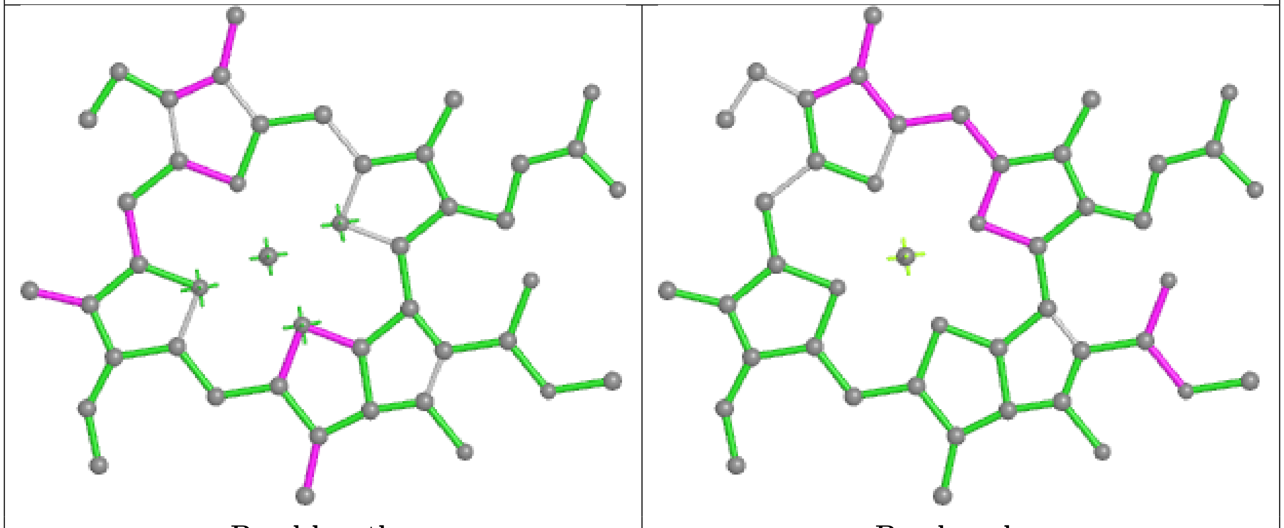


Torsions



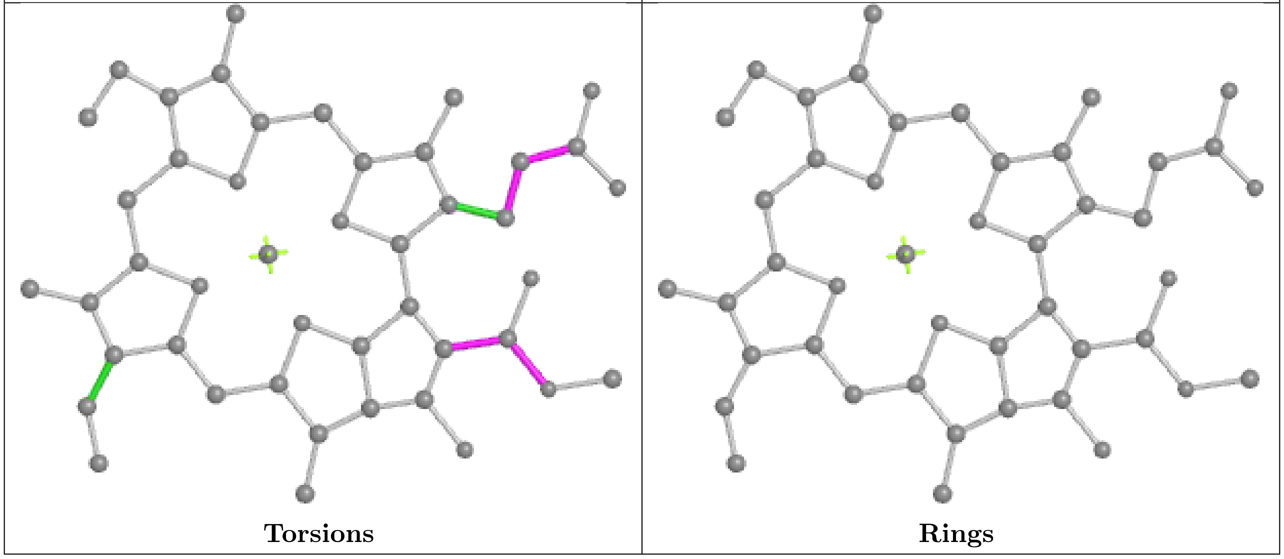
Rings

Ligand CLA bX 101



Bond lengths

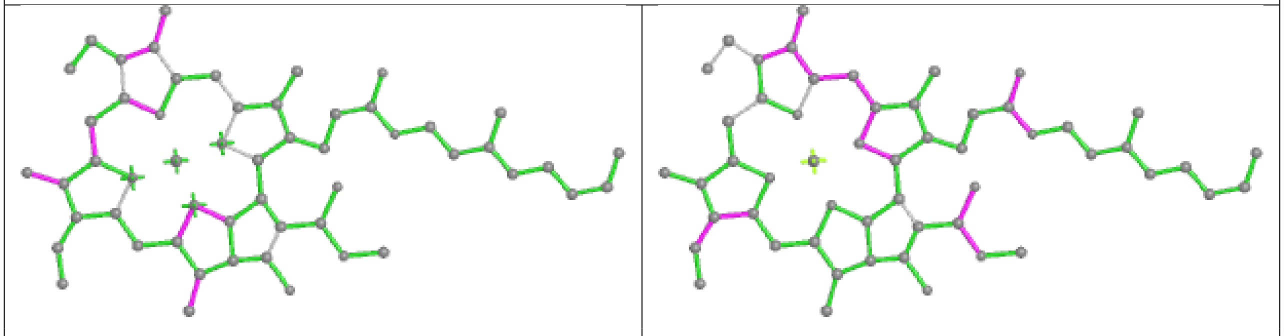
Bond angles



Torsions

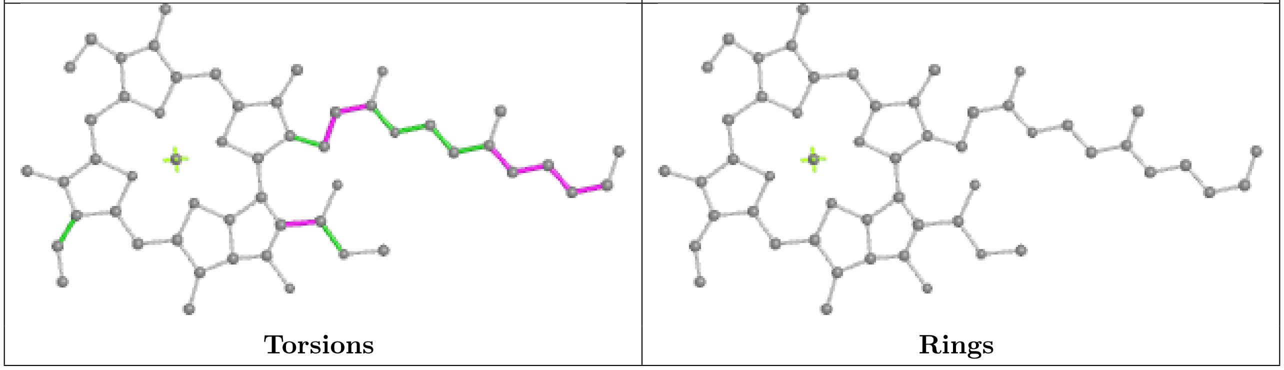
Rings

Ligand CLA dA 817



Bond lengths

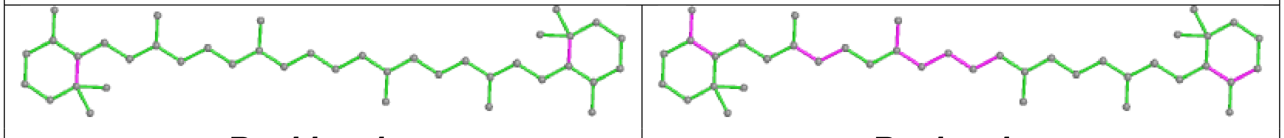
Bond angles



Torsions

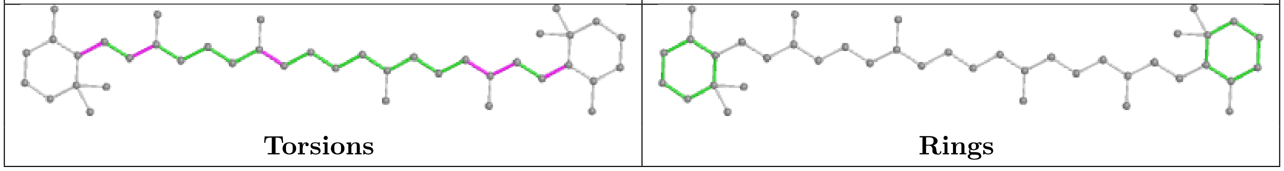
Rings

Ligand BCR bA 848



Bond lengths

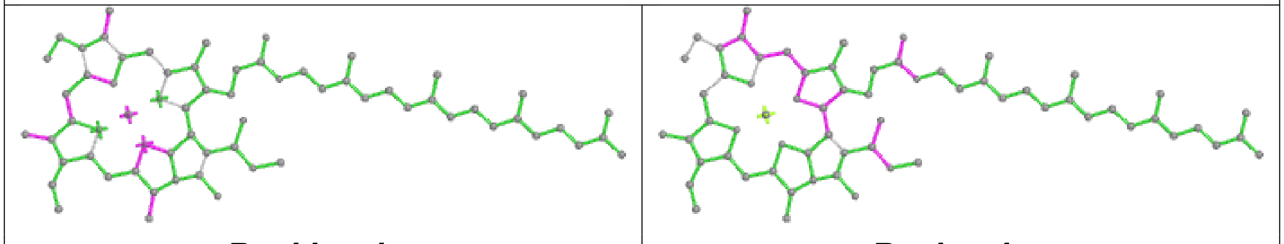
Bond angles



Torsions

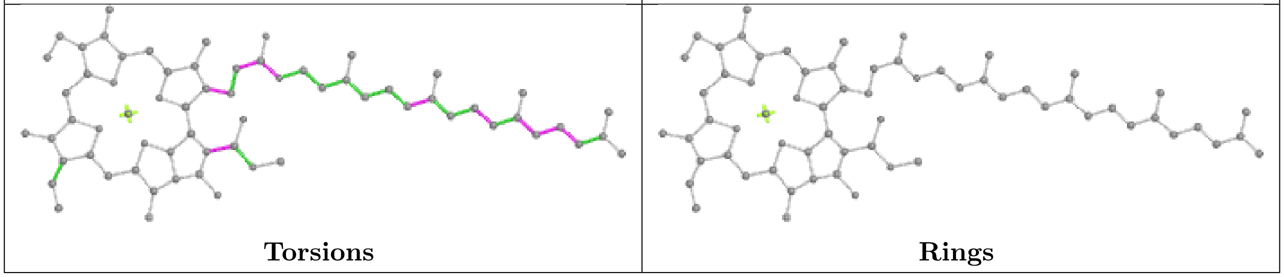
Rings

Ligand CLA dB 806



Bond lengths

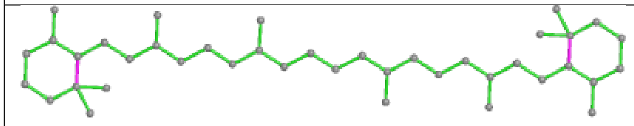
Bond angles



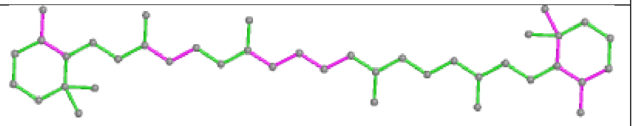
Torsions

Rings

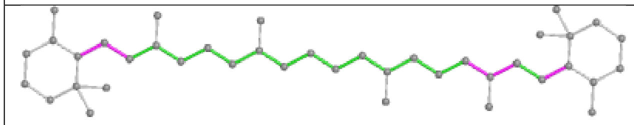
Ligand BCR dA 846



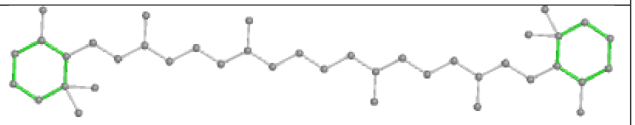
Bond lengths



Bond angles

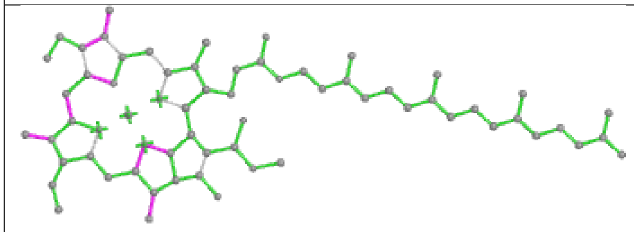


Torsions

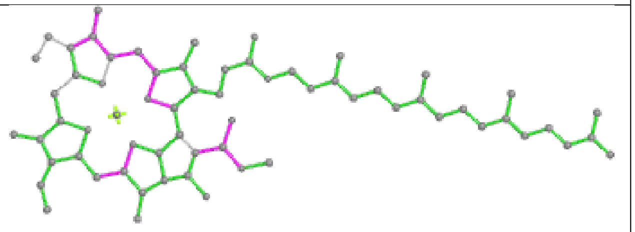


Rings

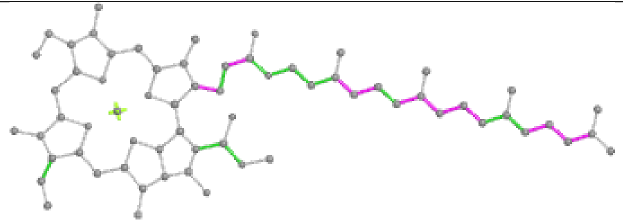
Ligand CLA dB 833



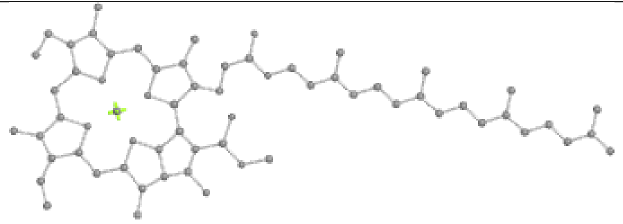
Bond lengths



Bond angles

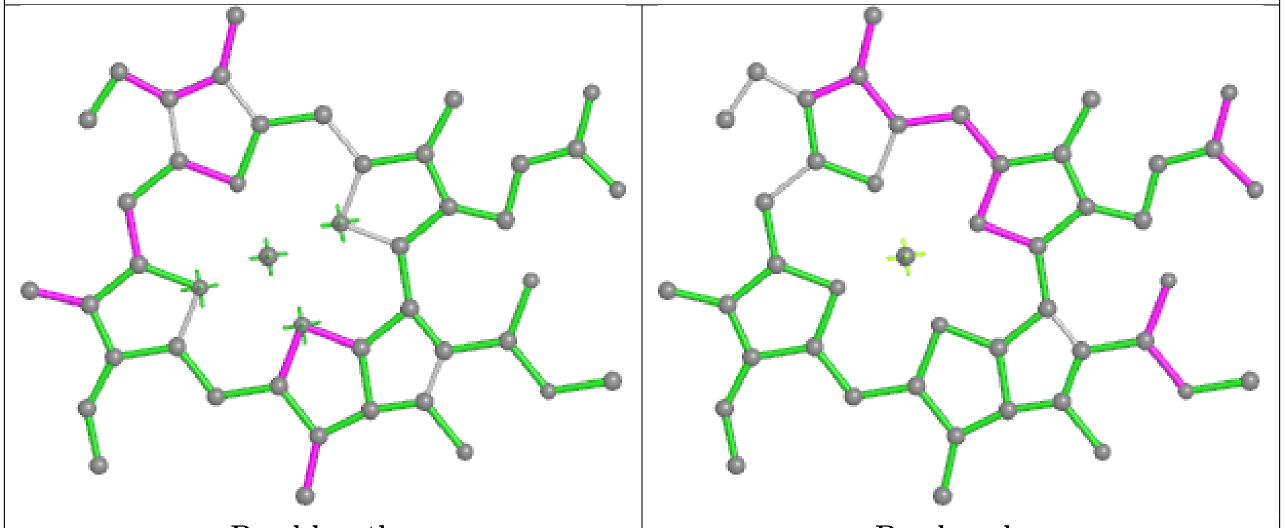


Torsions



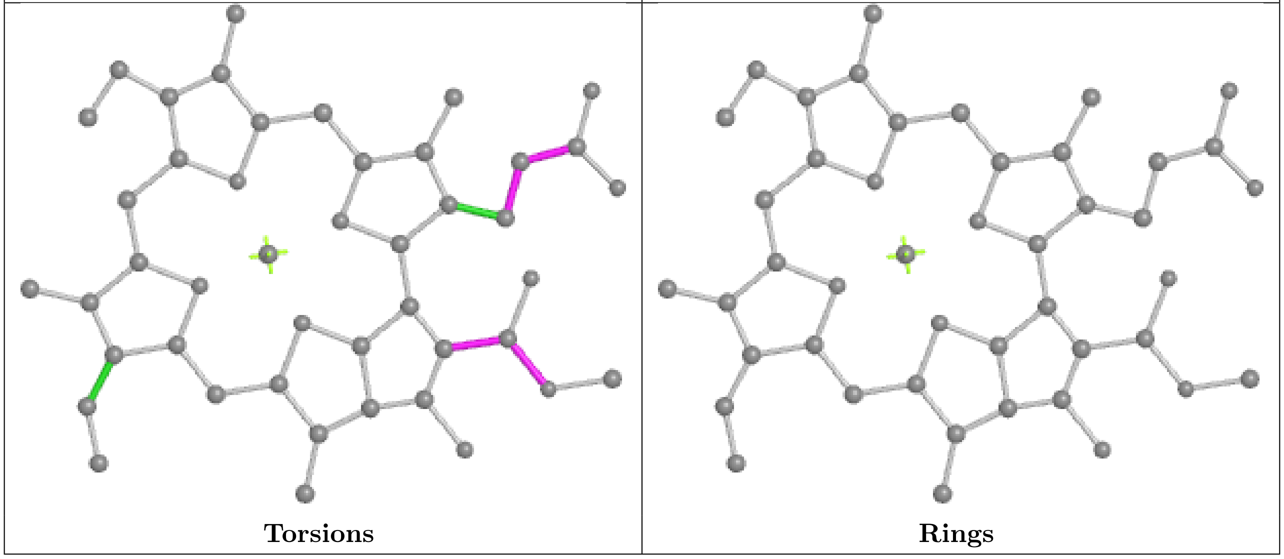
Rings

Ligand CLA aB 836



Bond lengths

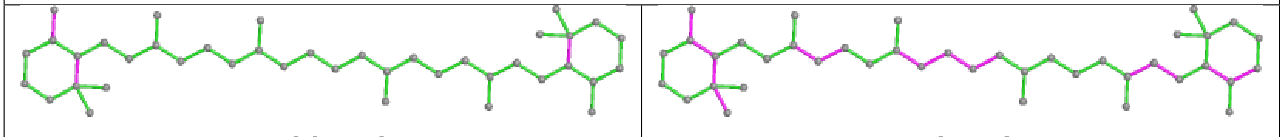
Bond angles



Torsions

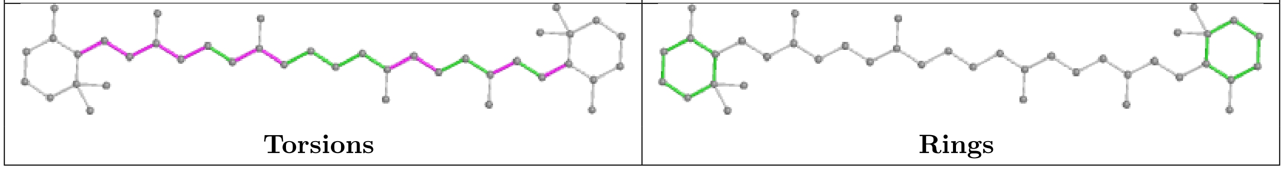
Rings

Ligand BCR bJ 103



Bond lengths

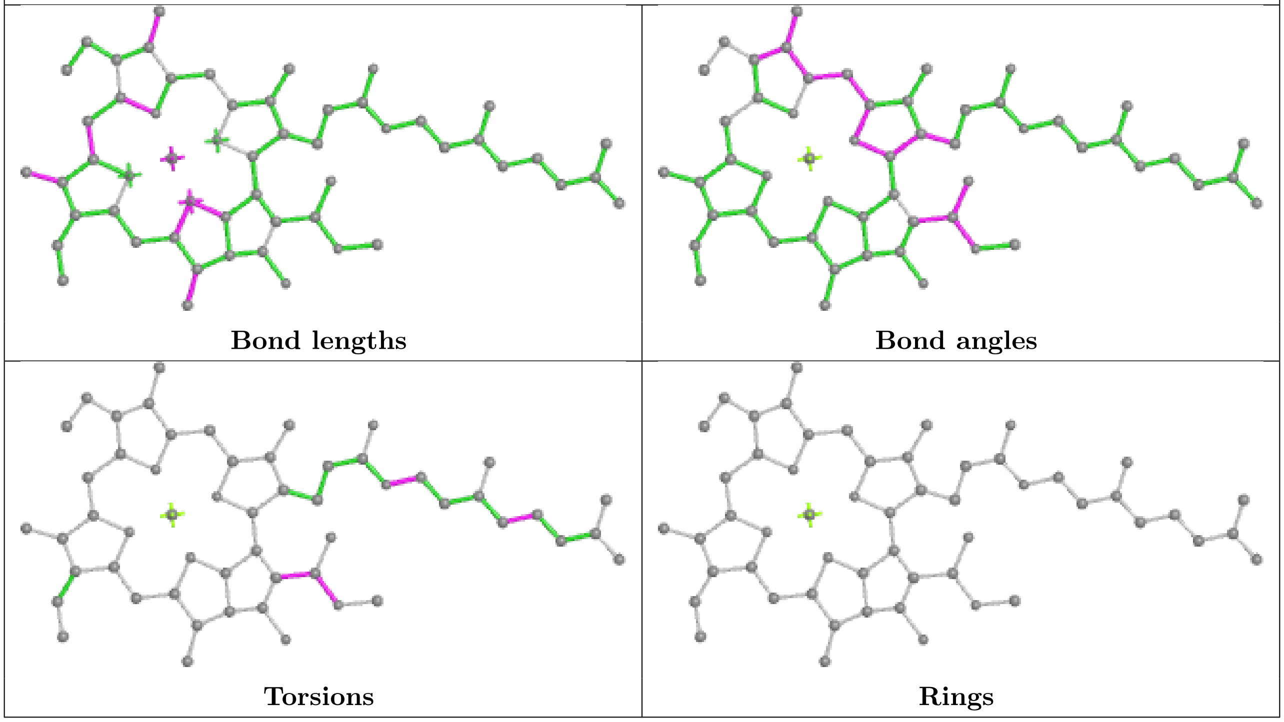
Bond angles



Torsions

Rings

Ligand CLA dA 826



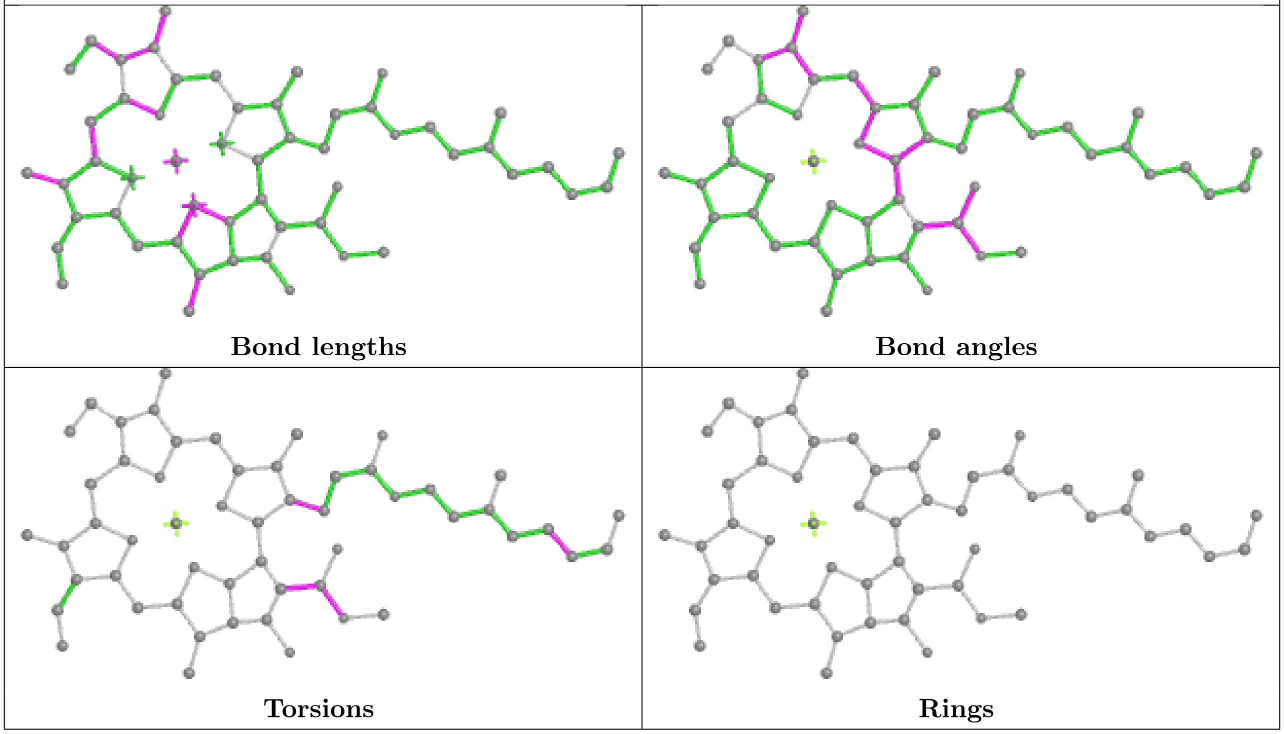
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA cB 824



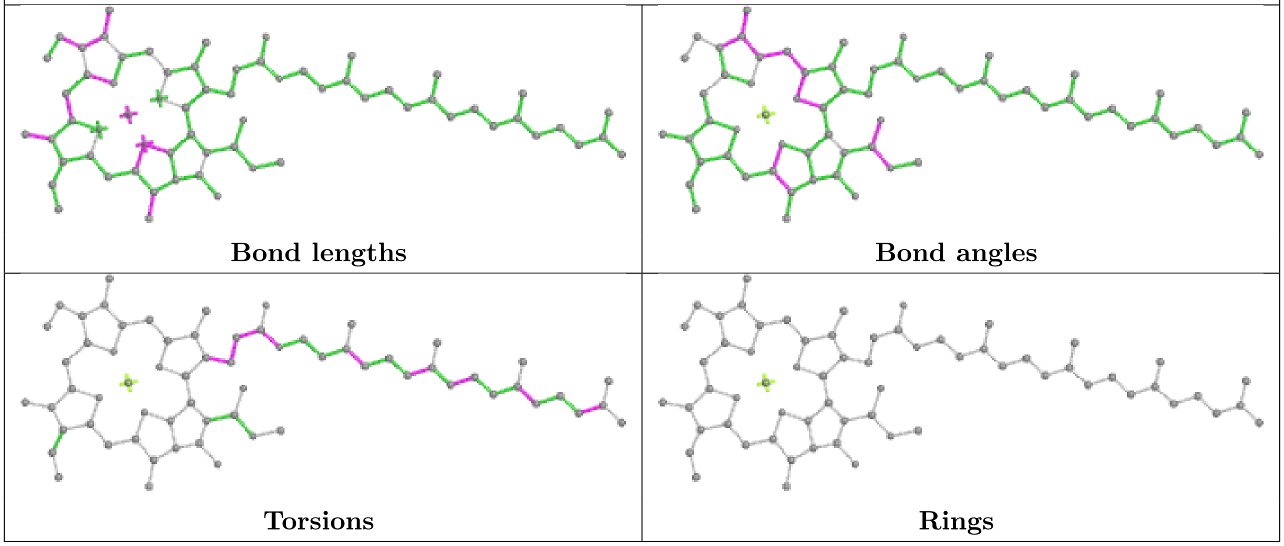
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA dA 829



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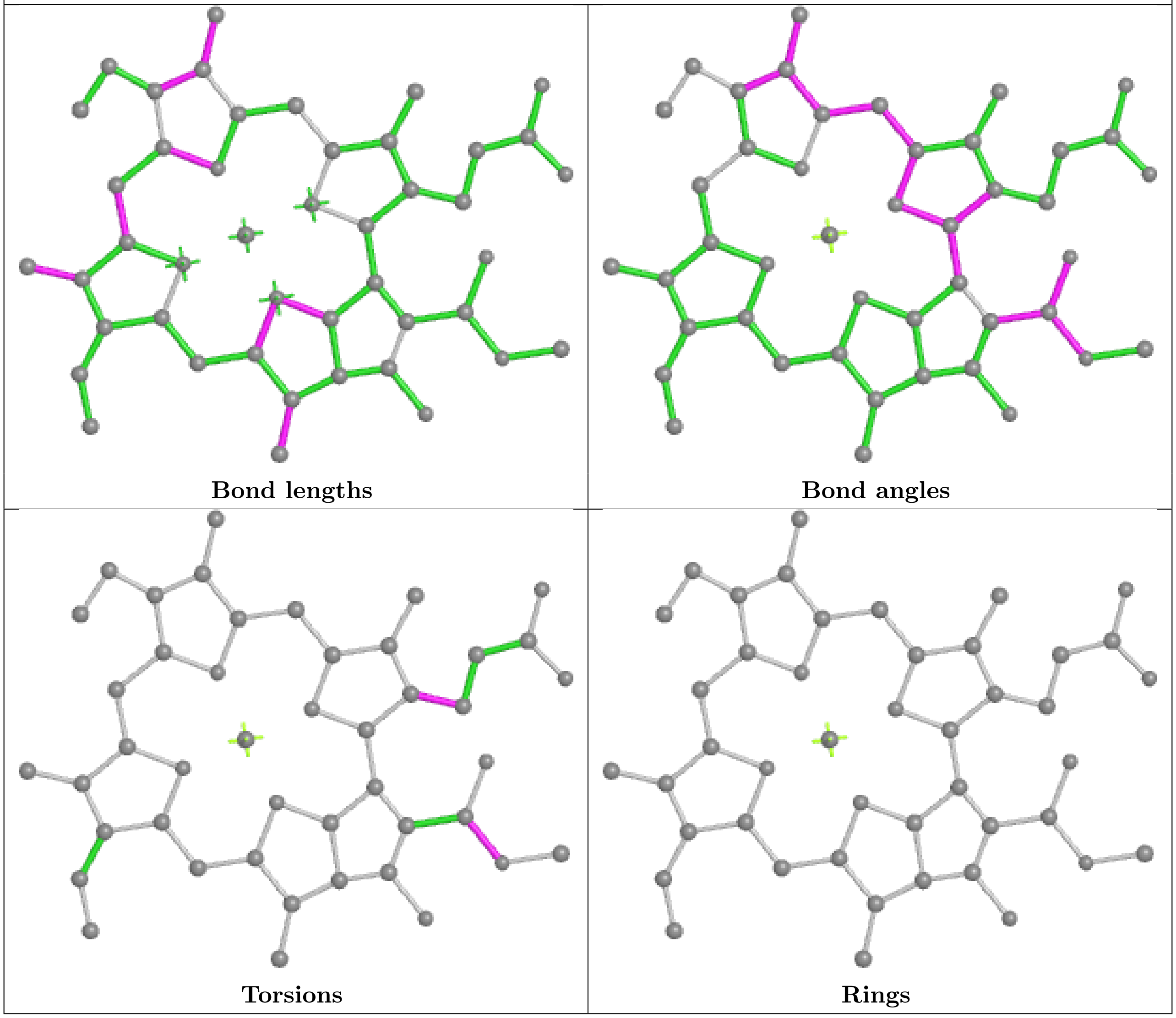

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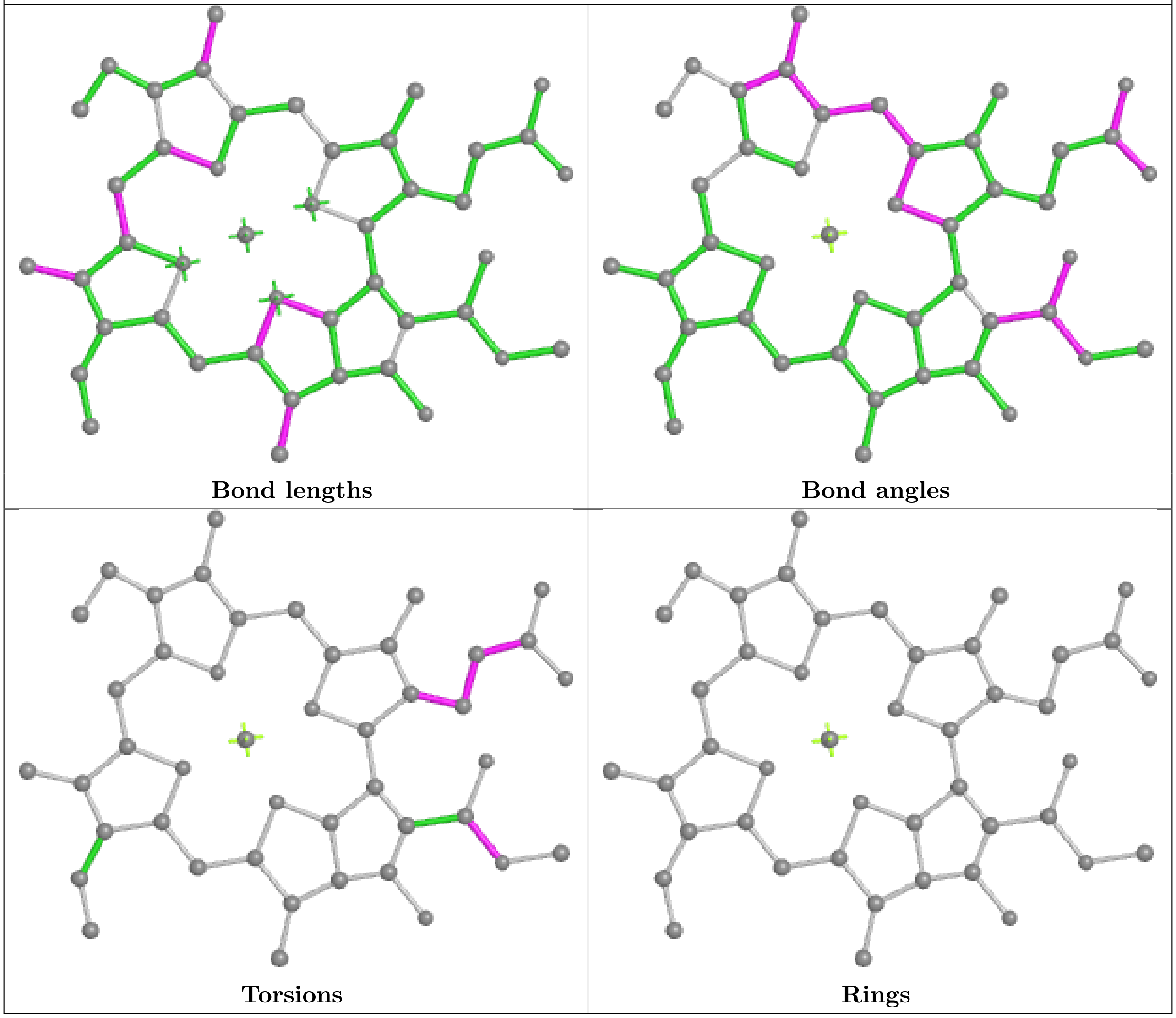
Bond lengths
Bond angles
Torsions
Rings

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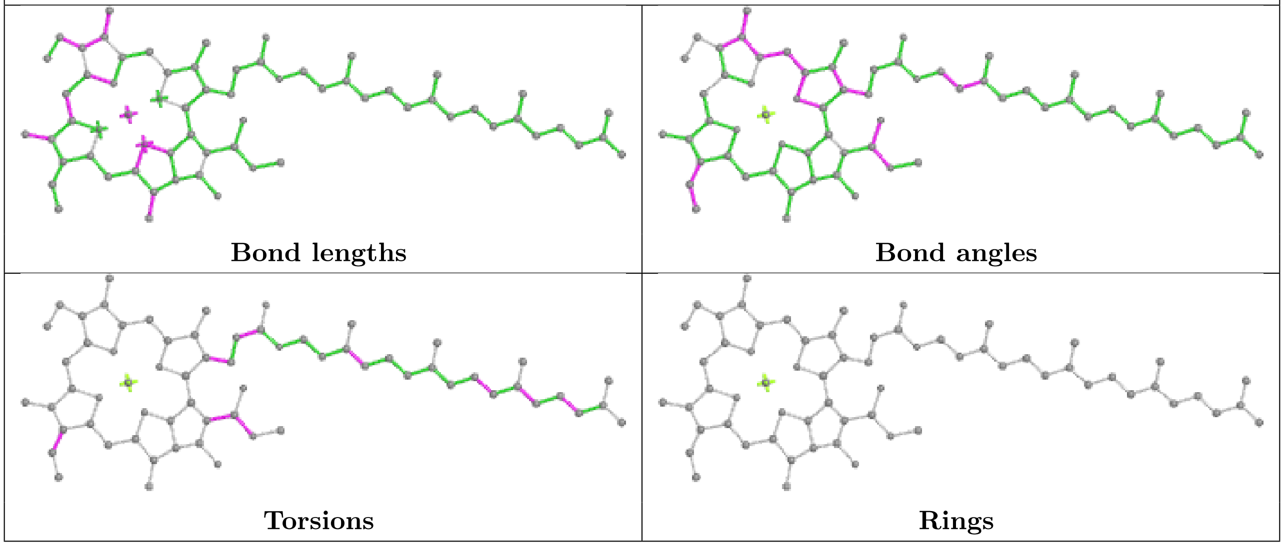
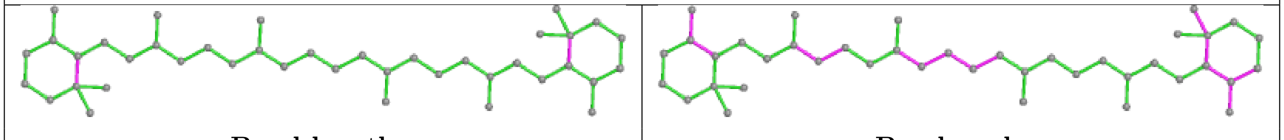
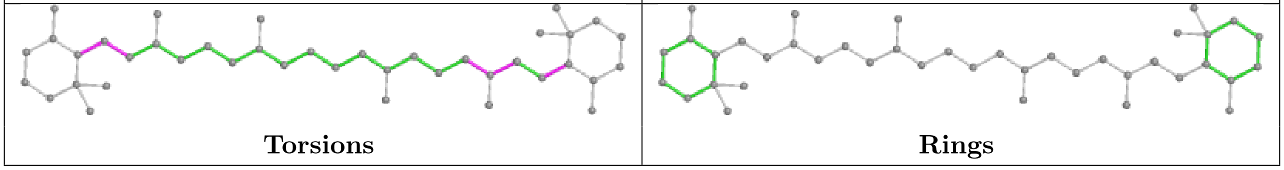

Bond lengths
Bond angles
Torsions
Rings

Ligand BCR bA 846

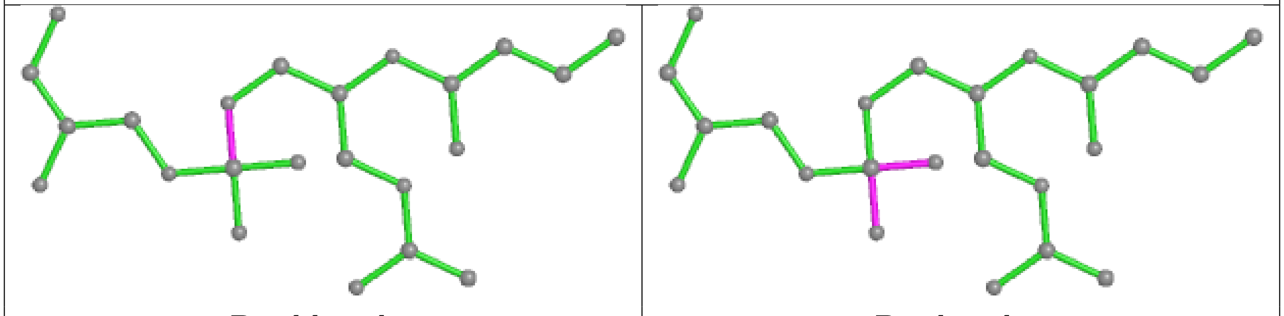


Bond lengths Bond angles

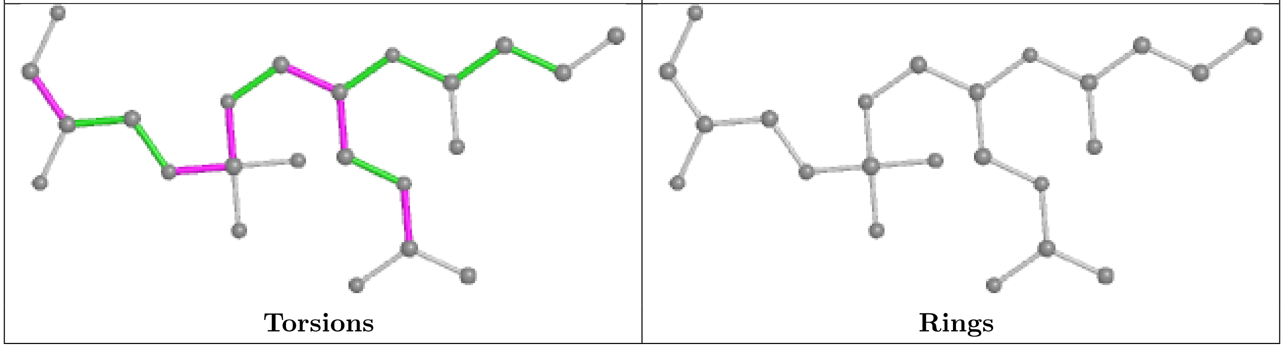


Torsions Rings

Ligand LHG cB 850



Bond lengths Bond angles



Torsions Rings

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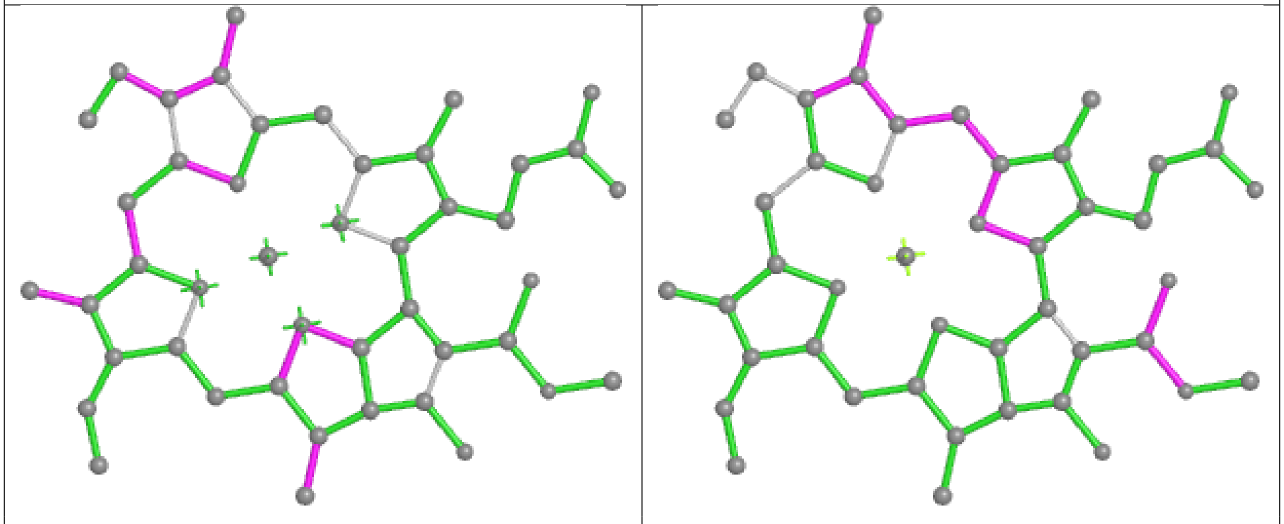
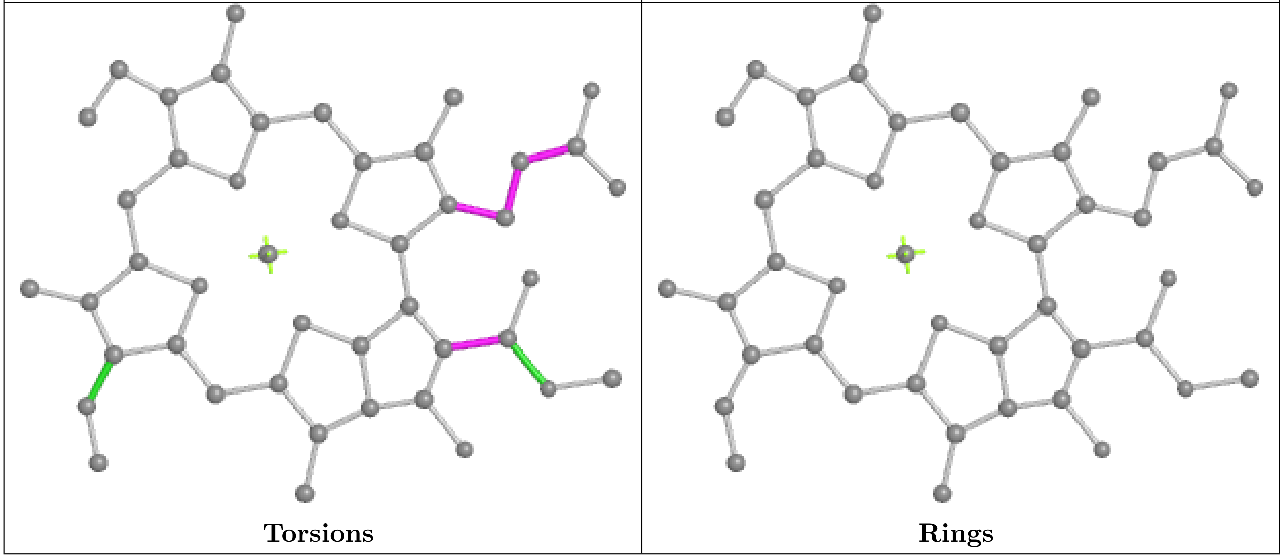
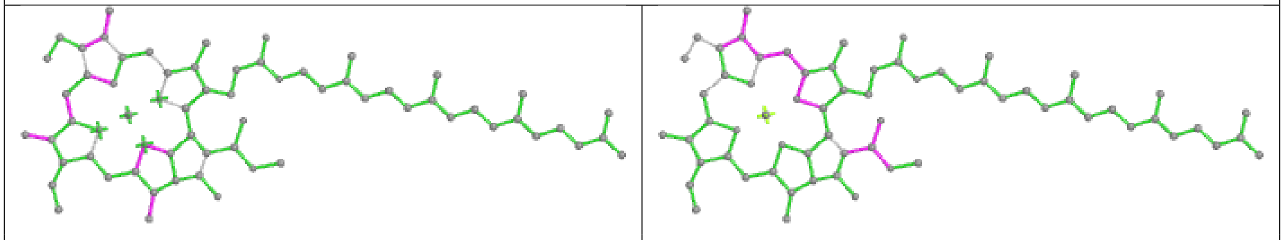


Bond lengths **Bond angles**

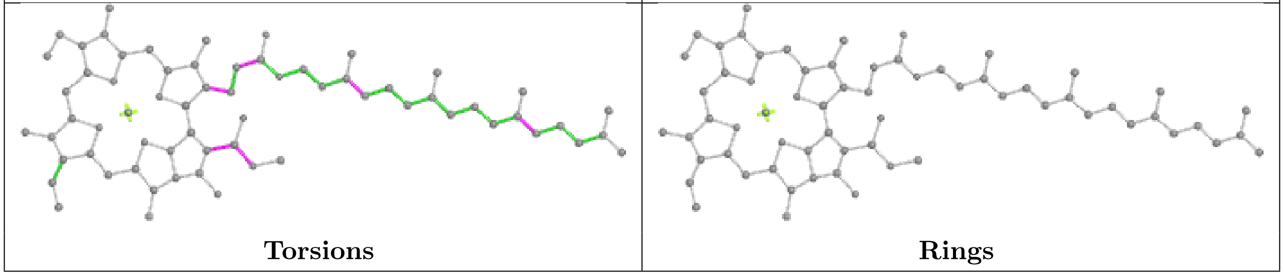


Torsions **Rings**

Ligand CLA bA 834



Bond lengths **Bond angles**



Torsions **Rings**

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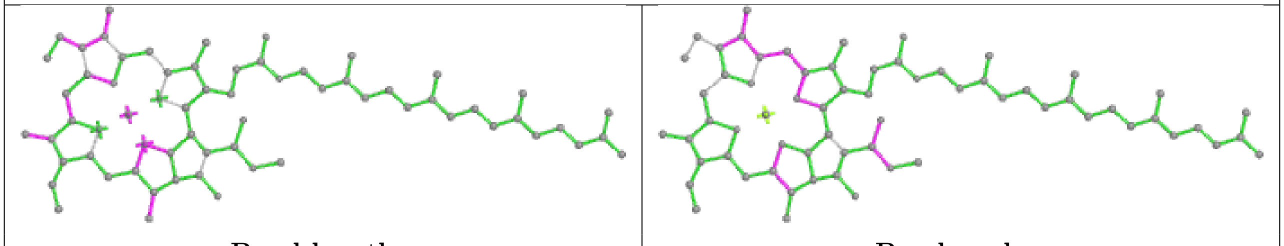
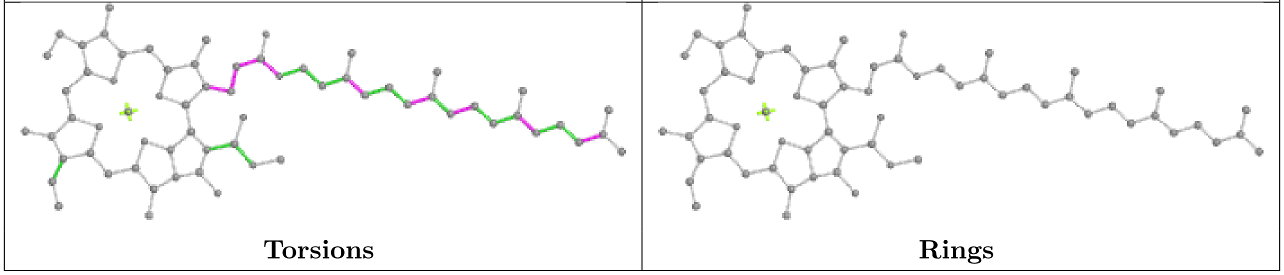
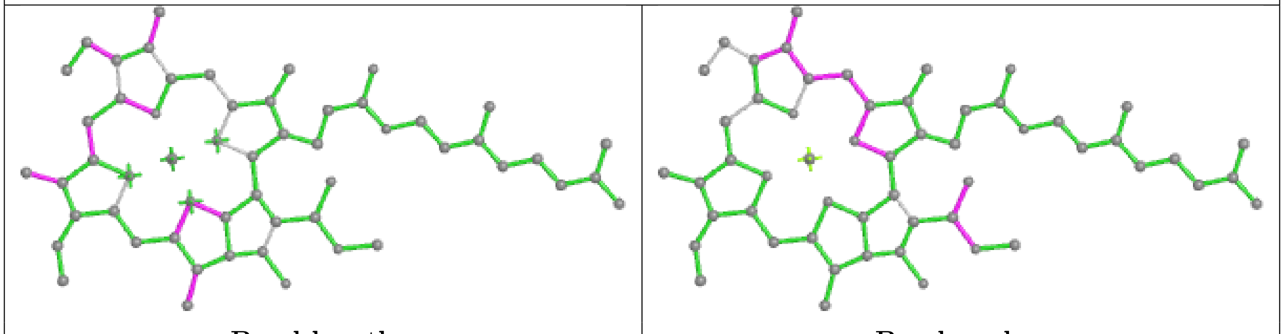
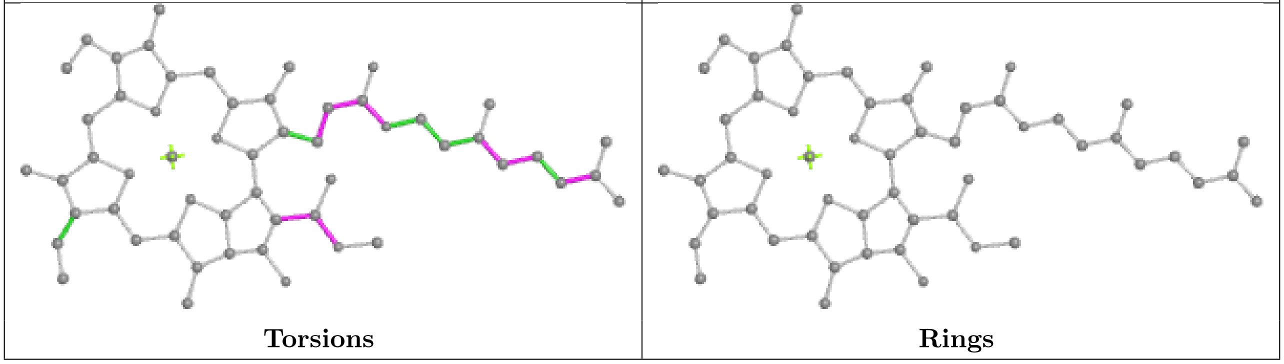

Bond lengths Bond angles

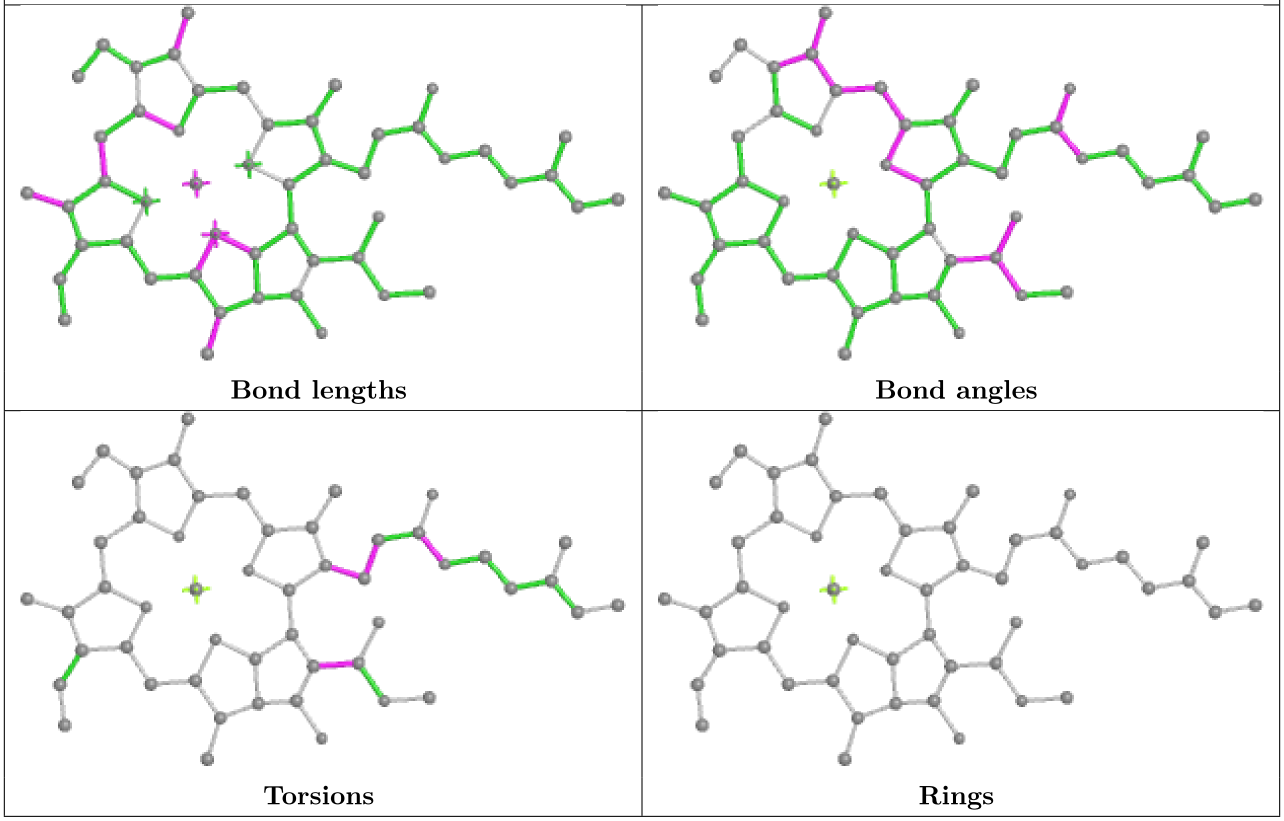

Torsions Rings

Ligand CLA cB 822


Bond lengths Bond angles


Torsions Rings

Ligand CLA aA 837



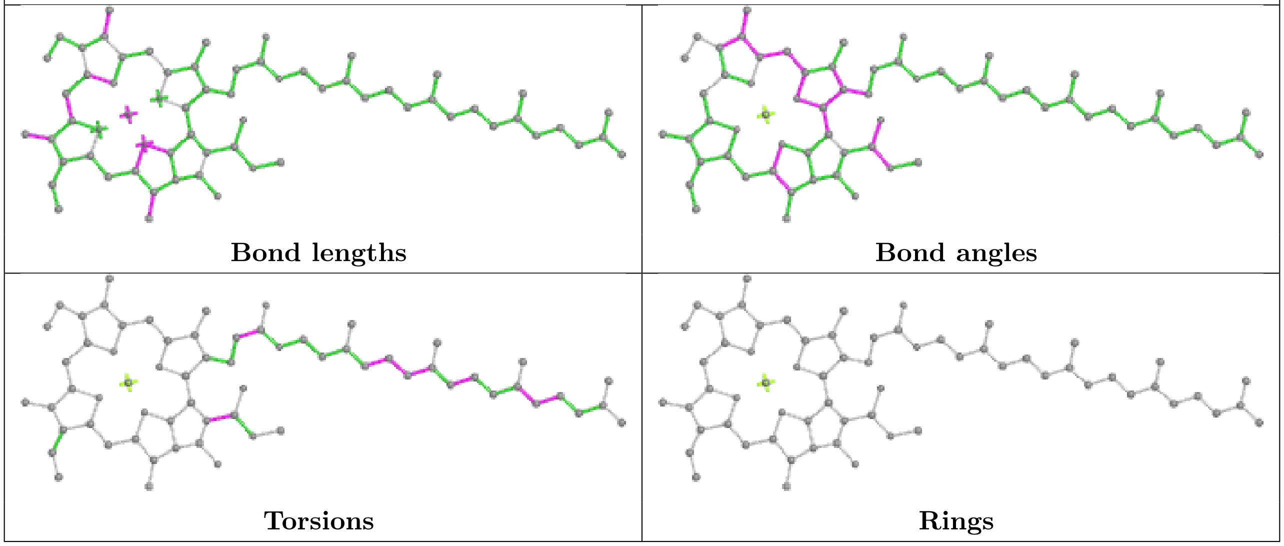
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA bA 825



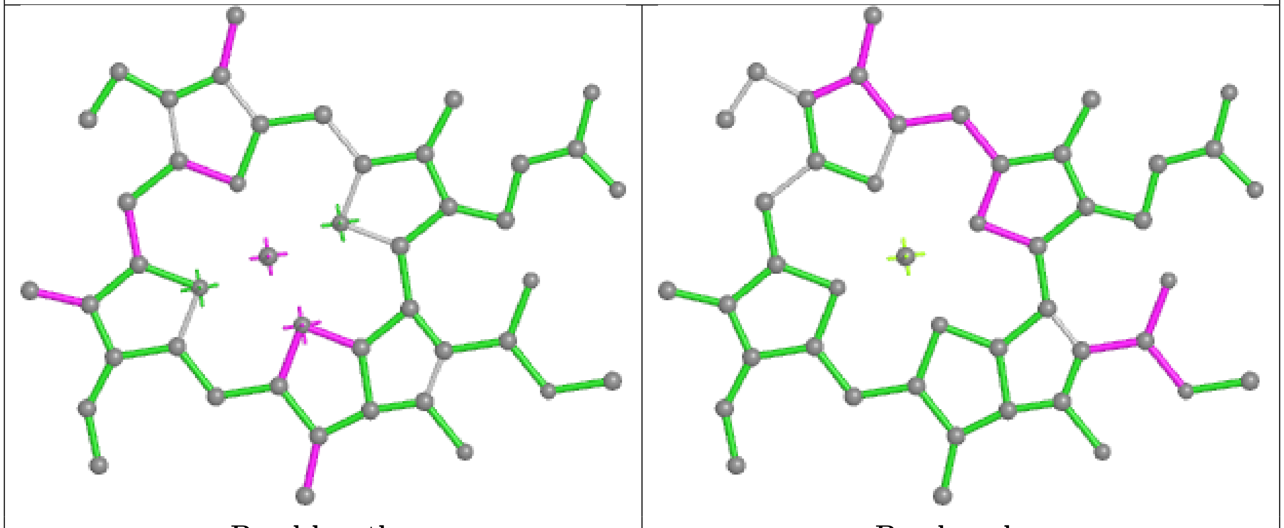
Bond lengths

Bond angles

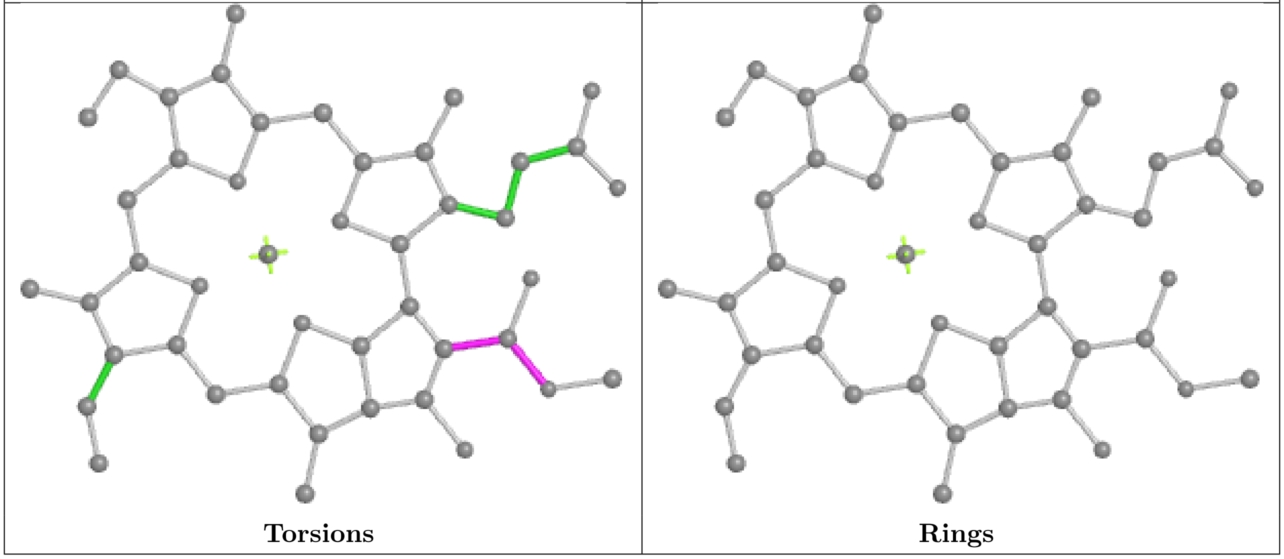
Torsions

Rings

Ligand CLA dF 203

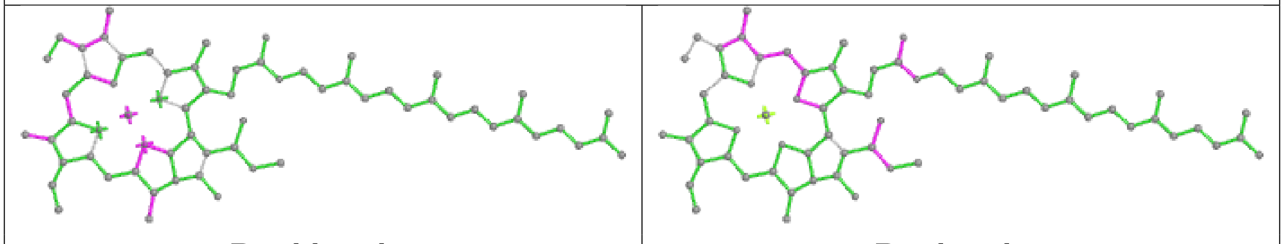


Bond lengths **Bond angles**

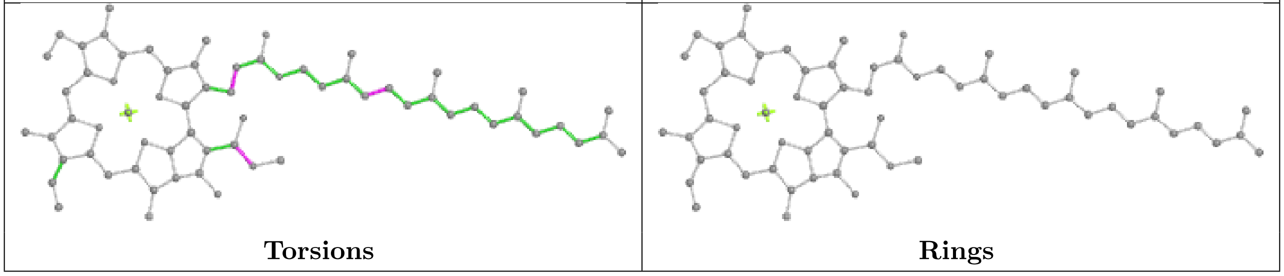


Torsions **Rings**

Ligand CLA bB 841

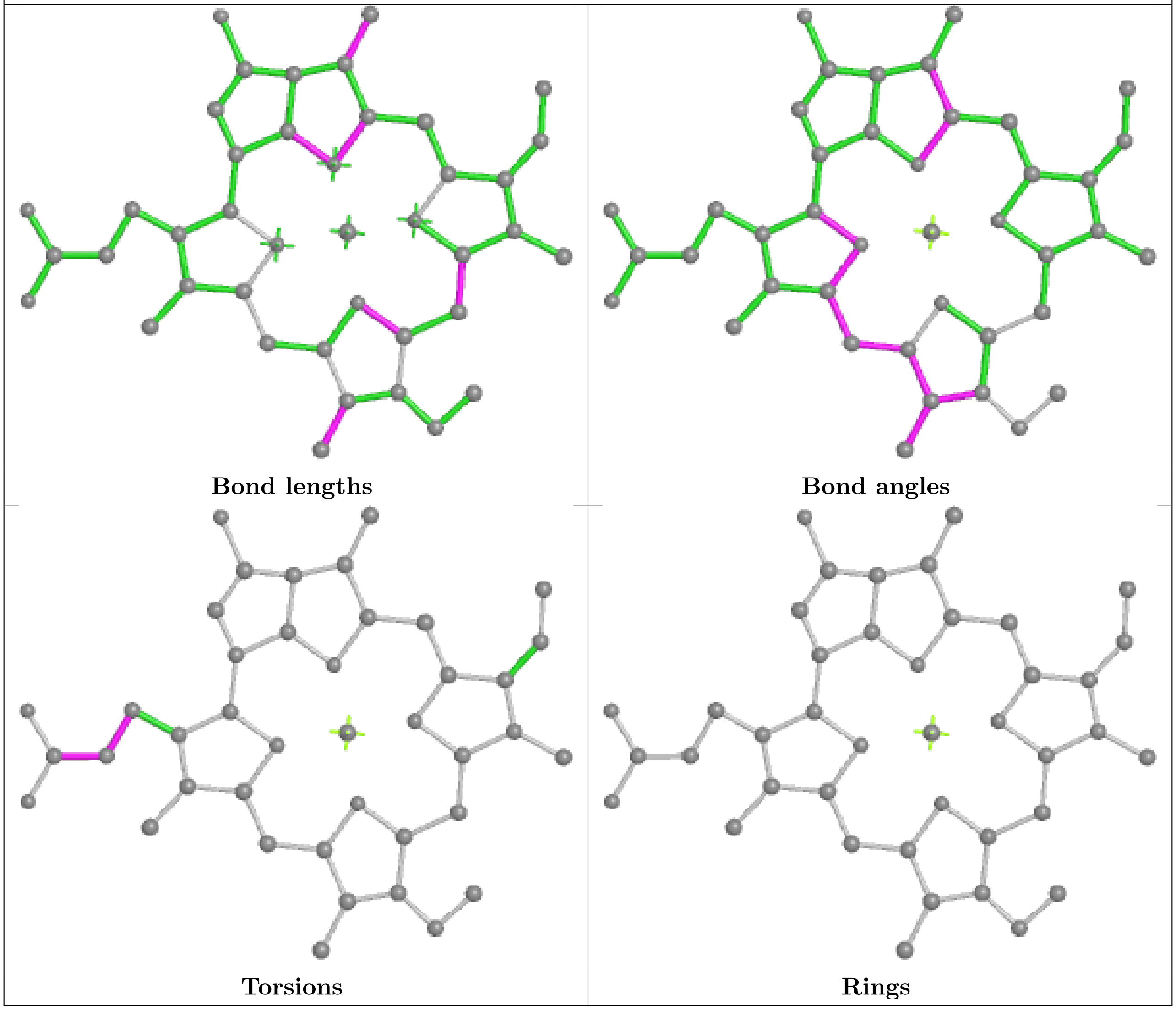


Bond lengths **Bond angles**



Torsions **Rings**

Ligand CLA aK 101



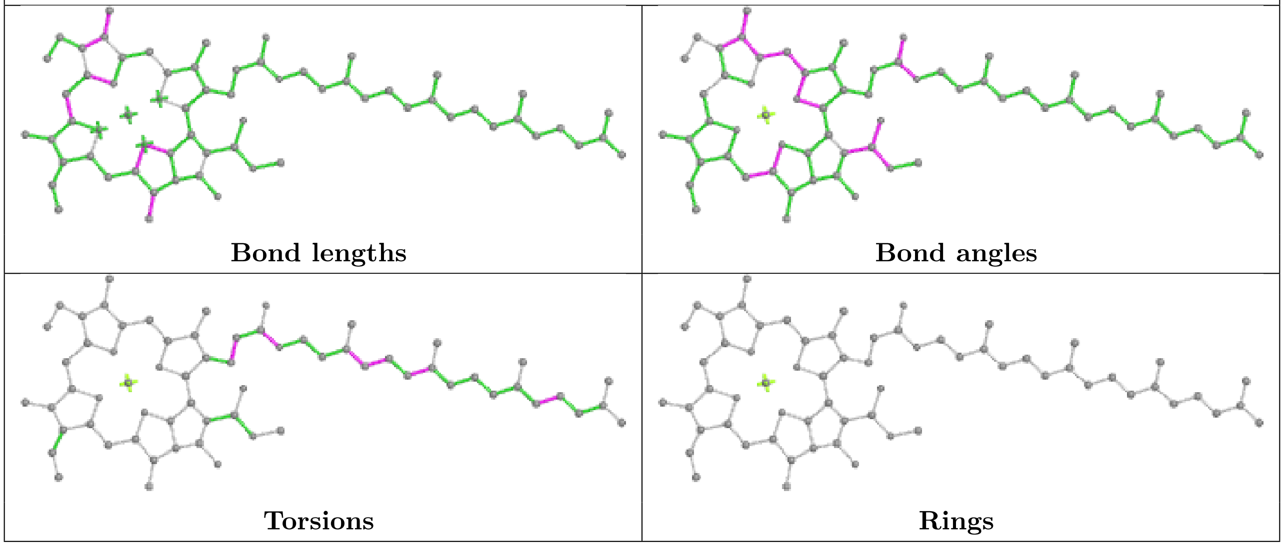
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA bB 808



Bond lengths

Bond angles

Torsions

Rings

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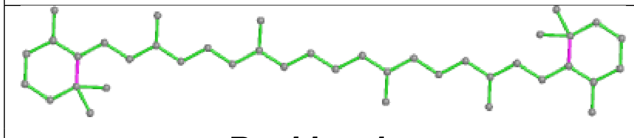
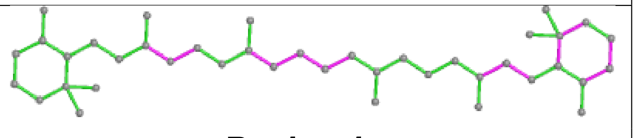
<tr><td>
Bond lengths</td><td>
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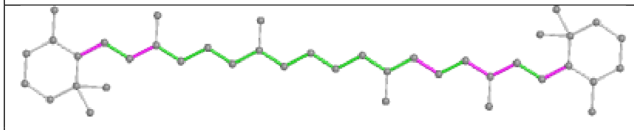
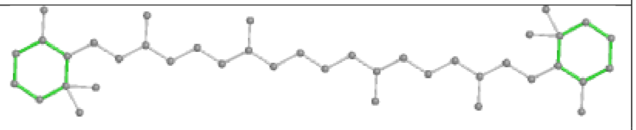
<tr><td>
Torsions</td><td>
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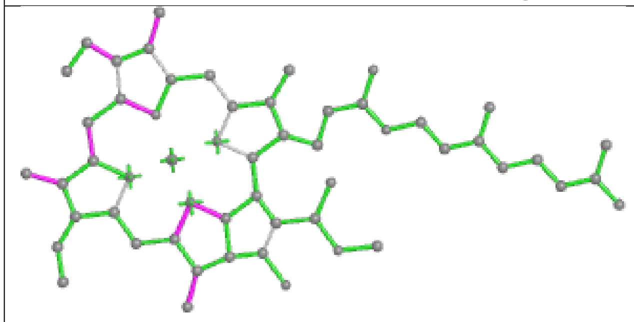
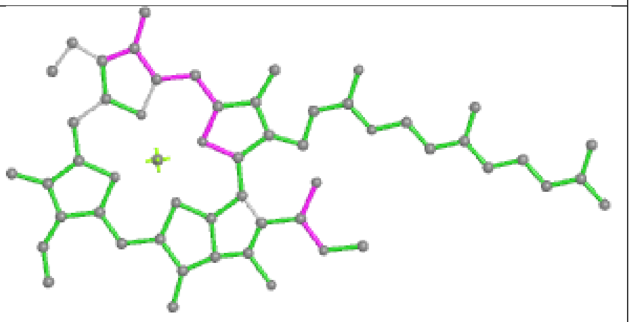
<tr><td>
Bond lengths</td><td>
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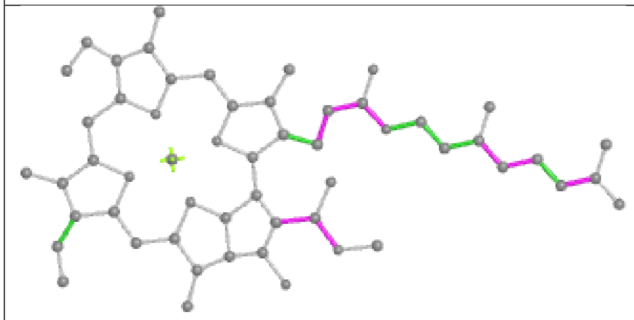
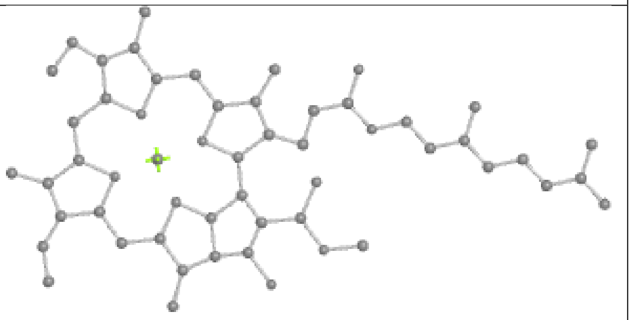
<tr><td>
Torsions</td><td>
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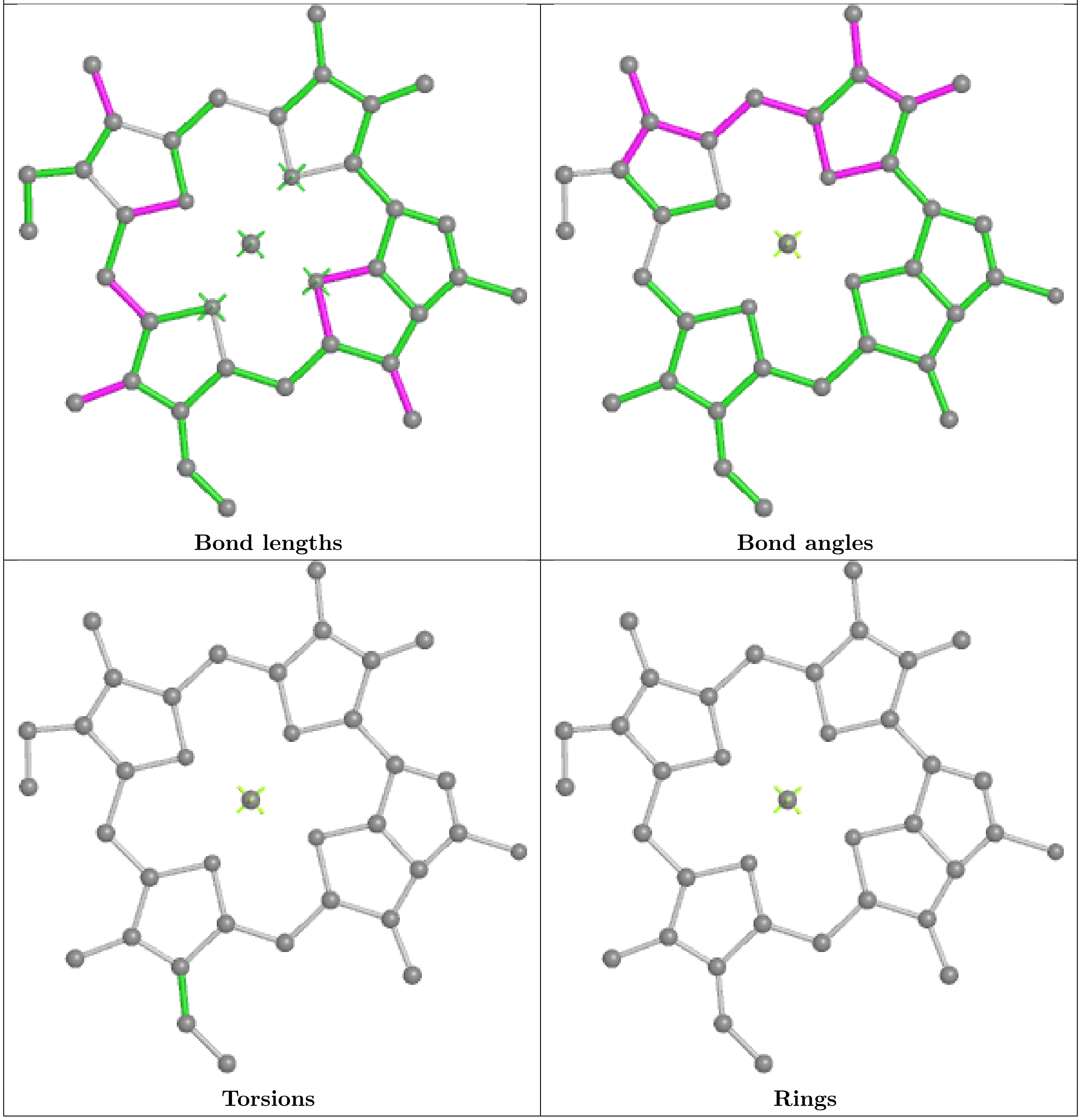
Ligand CLA bJ 102



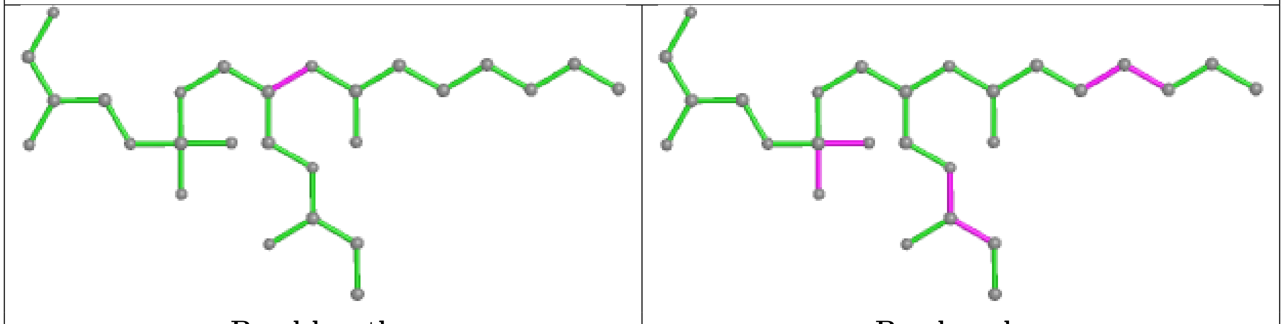
Bond lengths

Bond angles

Torsions

Rings

Ligand LHG cA 853



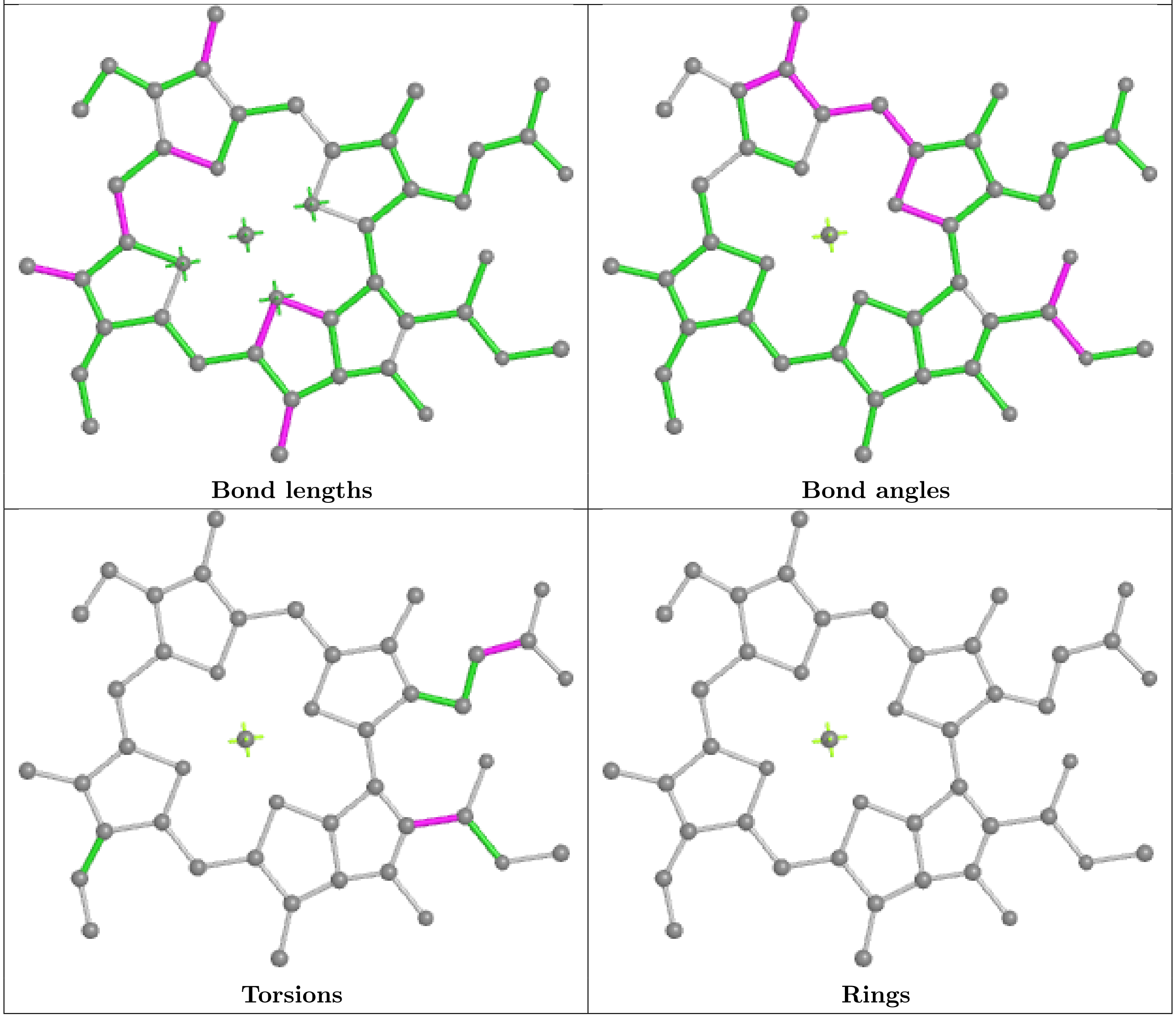
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA cK 102


Bond lengths

Bond angles

Torsions

Rings

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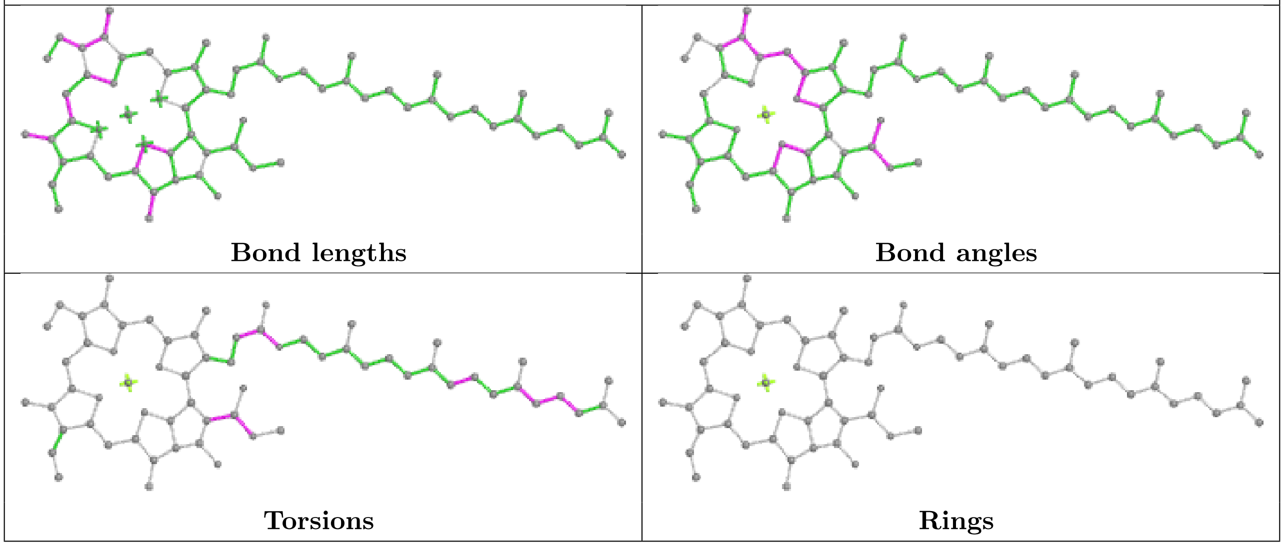
Bond lengths

Bond angles

Torsions

Rings

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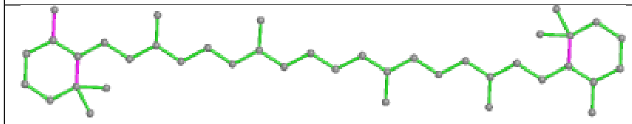
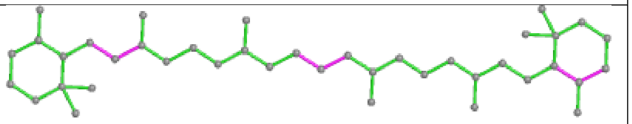
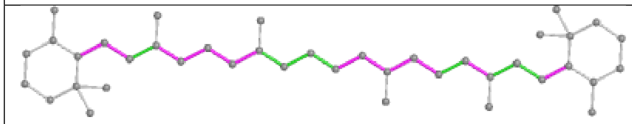
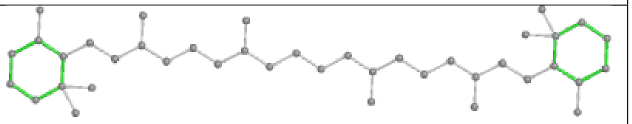
 Bond lengths	 Bond angles
 Torsions	 Rings

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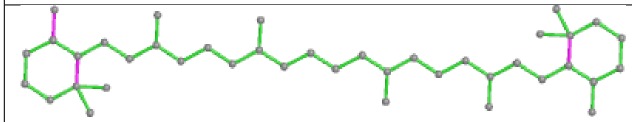
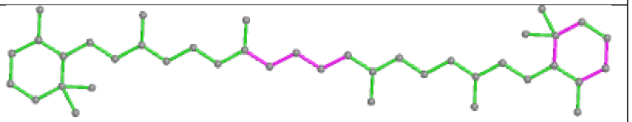
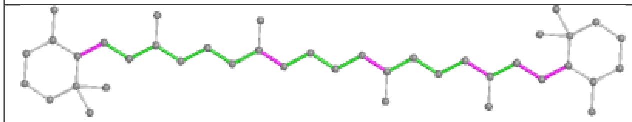
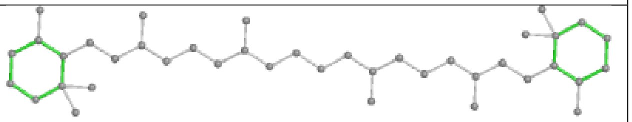
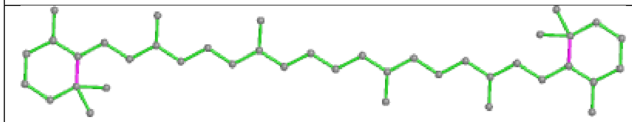
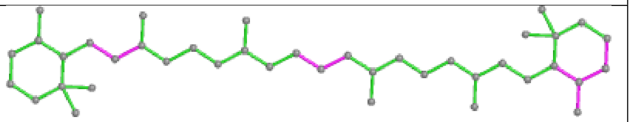
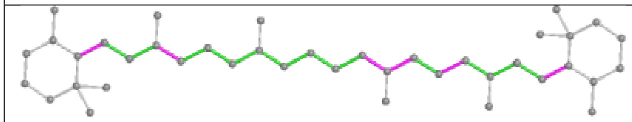
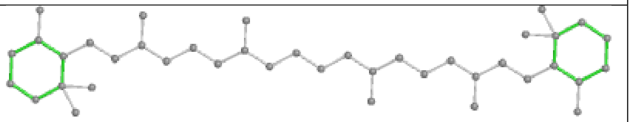
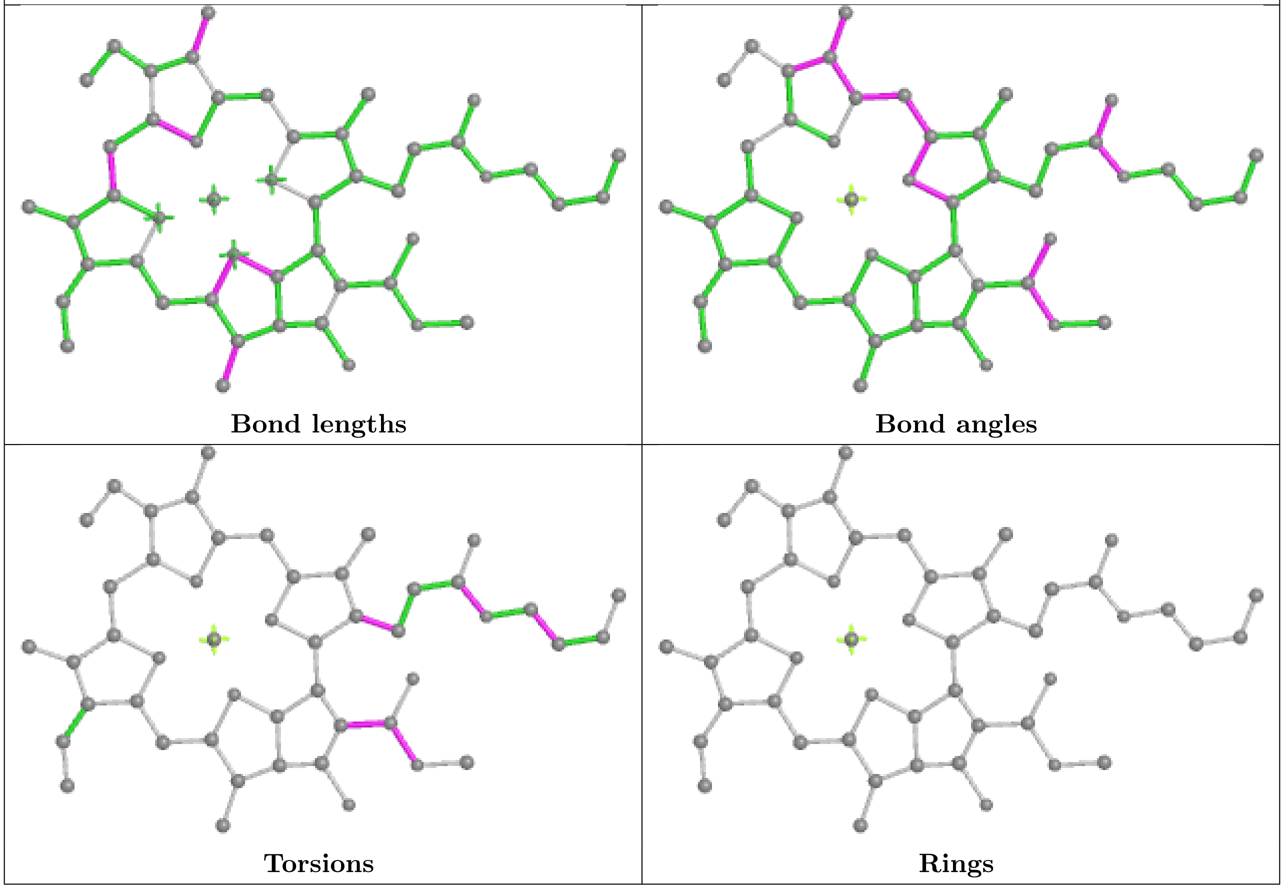
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR dB 845

 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA dA 816



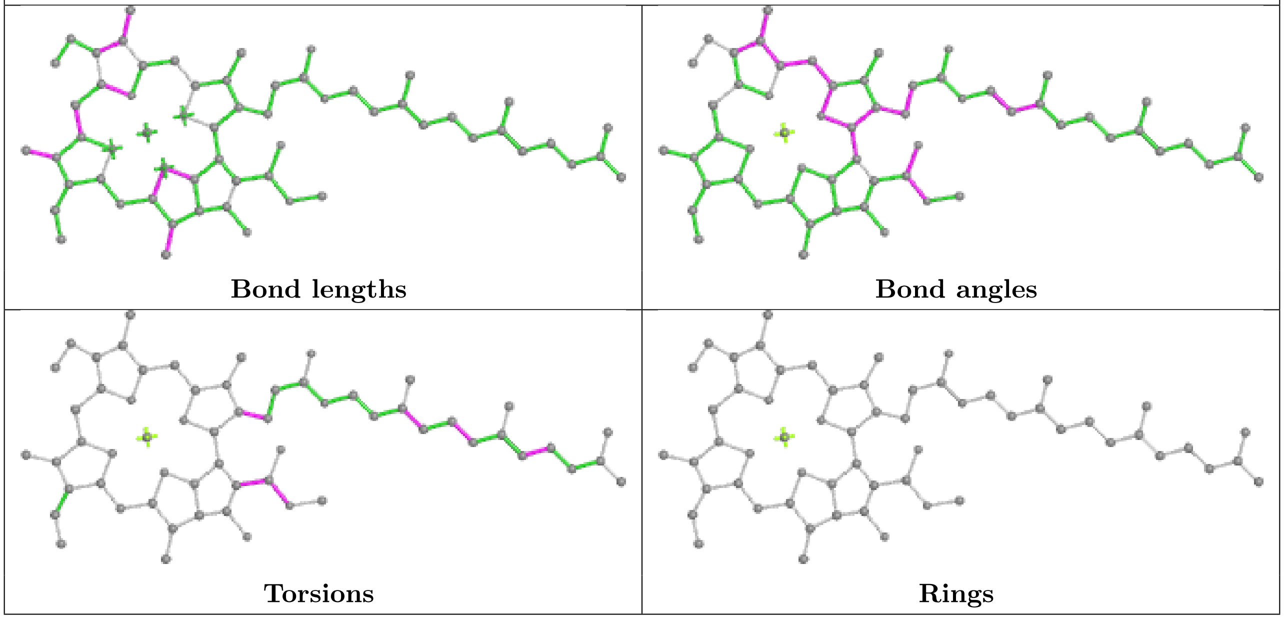
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA aB 837



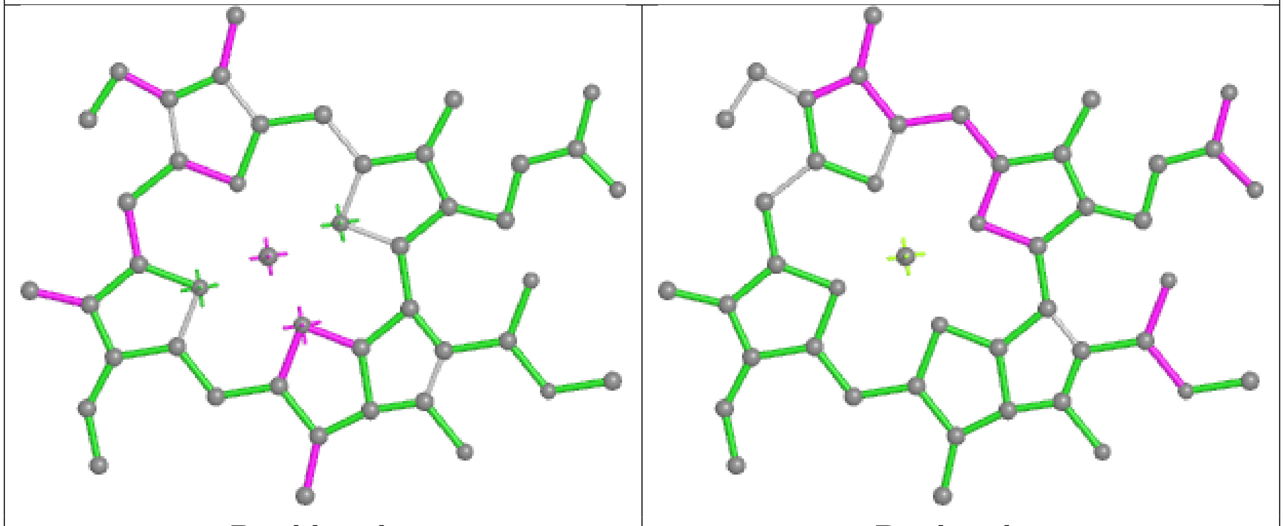
Bond lengths

Bond angles

Torsions

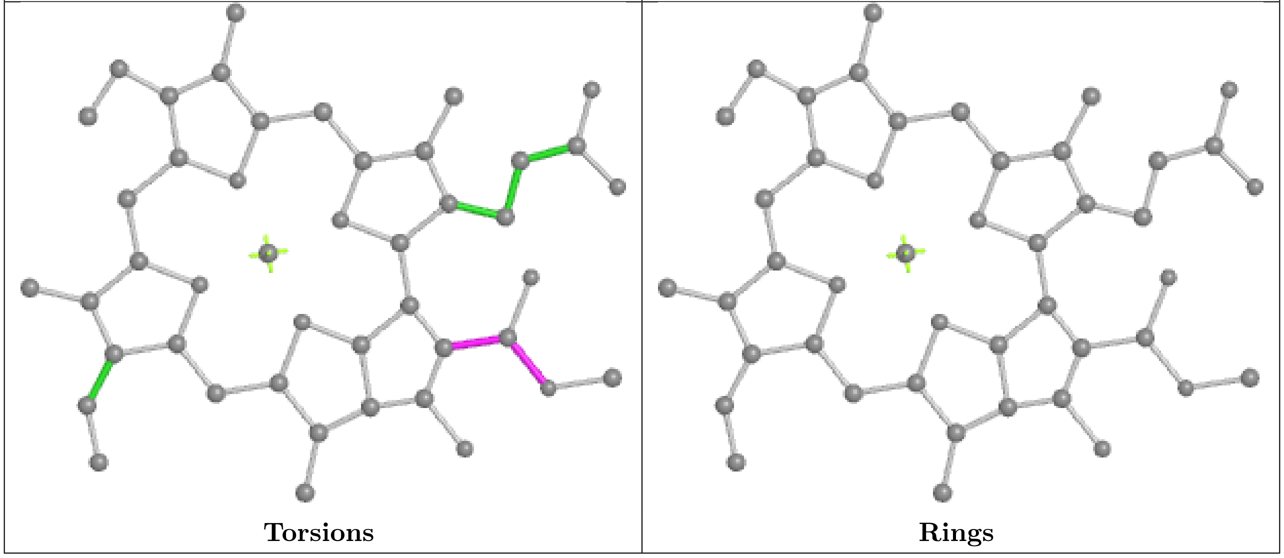
Rings

Ligand CLA cB 821



Bond lengths

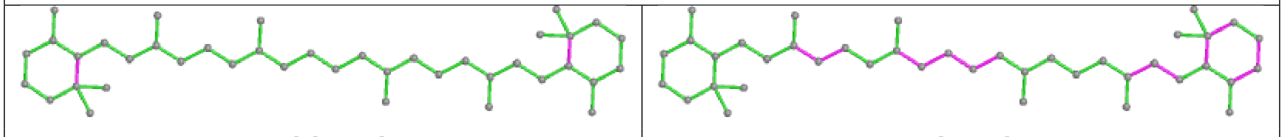
Bond angles



Torsions

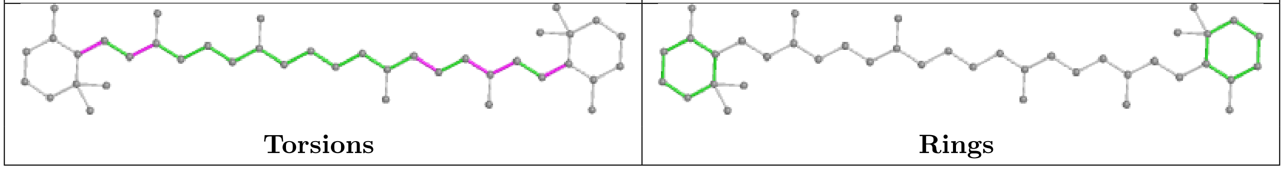
Rings

Ligand BCR dB 844



Bond lengths

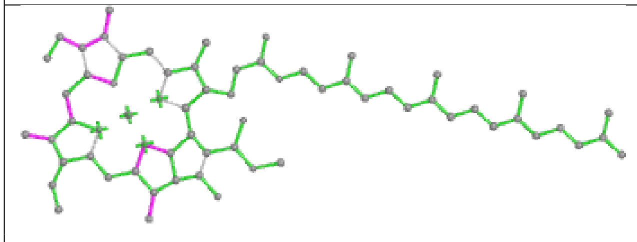
Bond angles



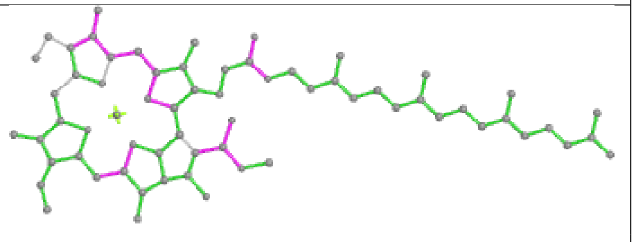
Torsions

Rings

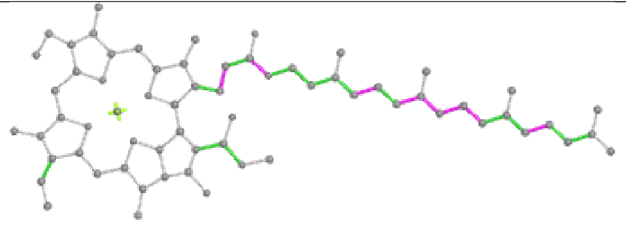
Ligand CLA bL 205



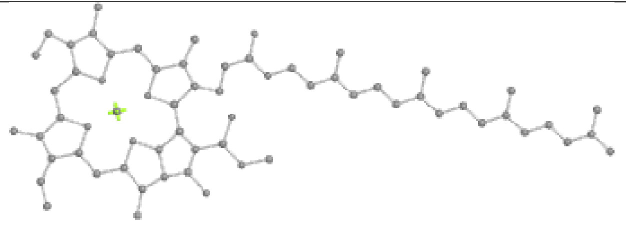
Bond lengths



Bond angles

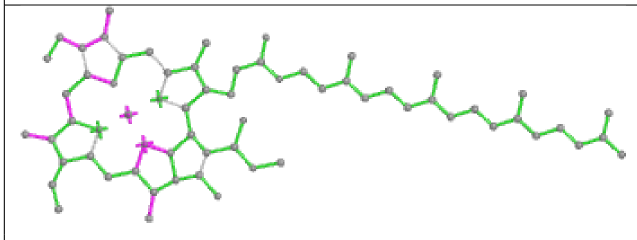


Torsions

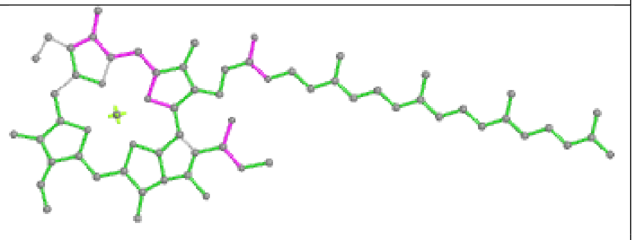


Rings

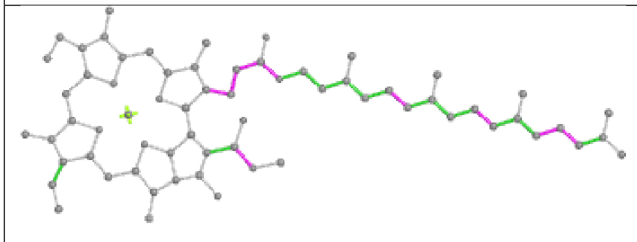
Ligand CLA dA 842



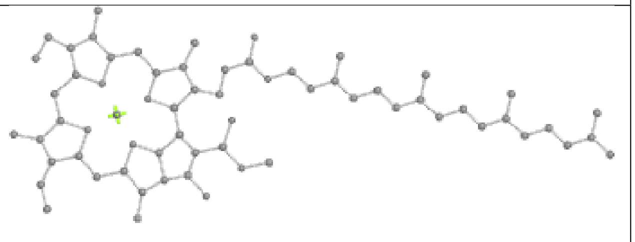
Bond lengths



Bond angles

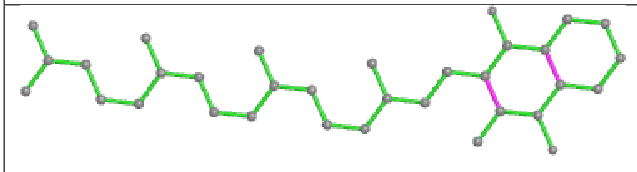


Torsions

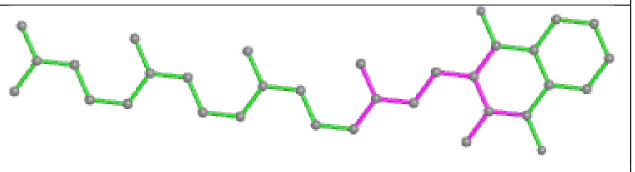


Rings

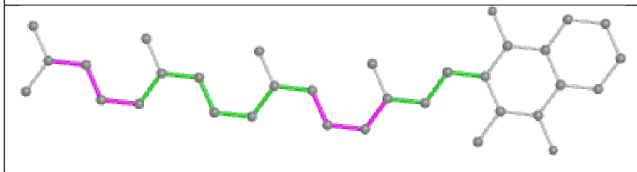
Ligand PQN aA 844



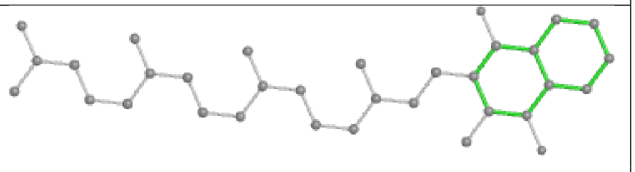
Bond lengths



Bond angles

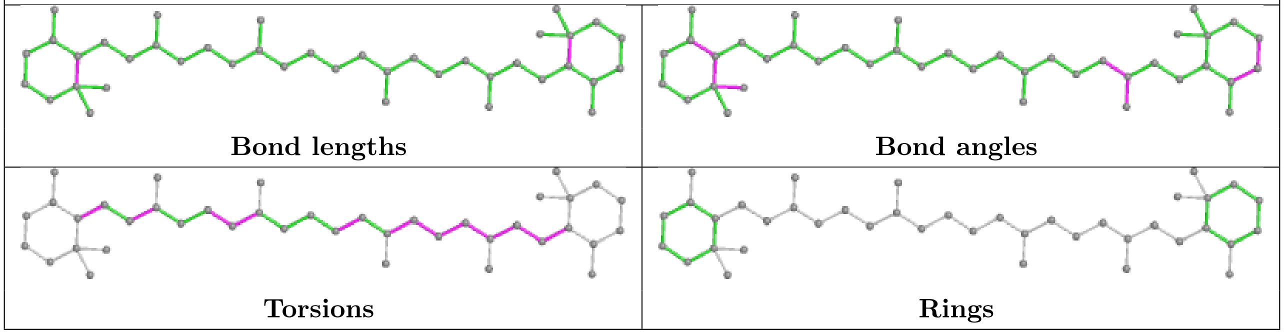


Torsions

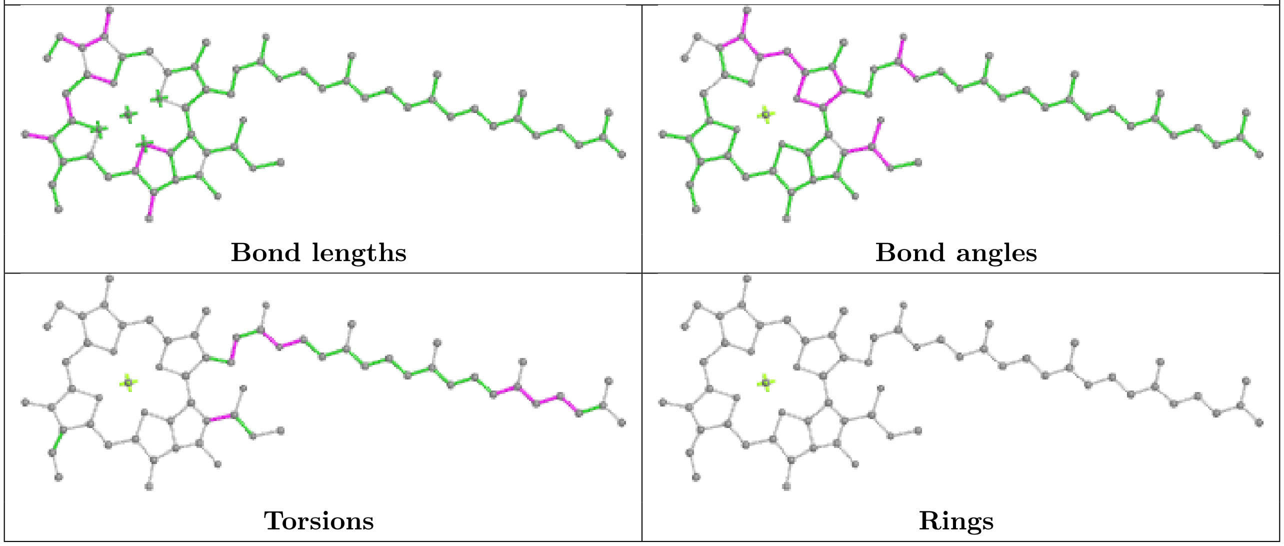


Rings

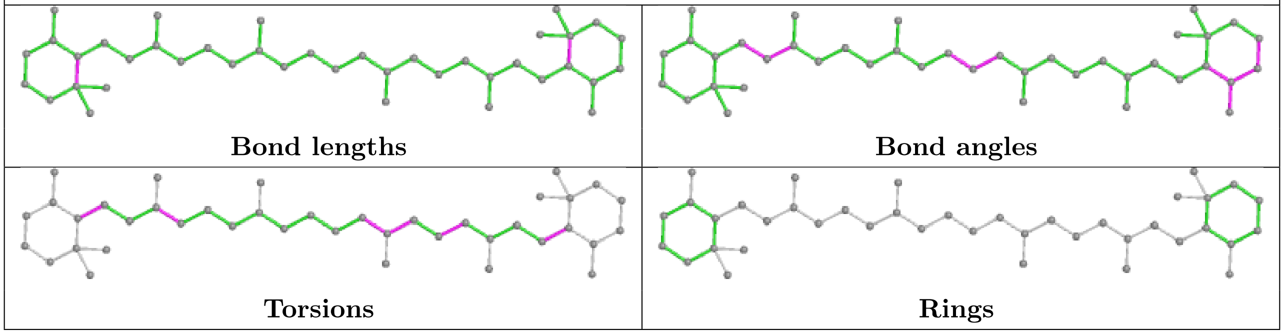
Ligand BCR dB 847


Bond lengths
Bond angles
Torsions
Rings

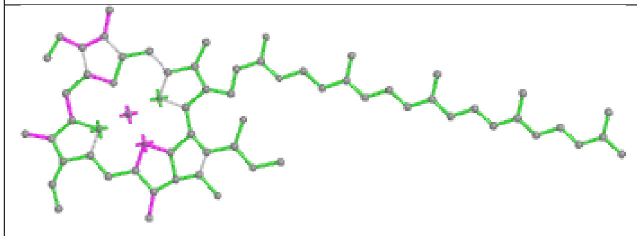
Ligand CLA cA 838

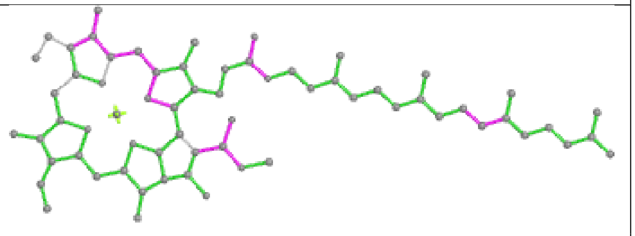

Bond lengths
Bond angles
Torsions
Rings

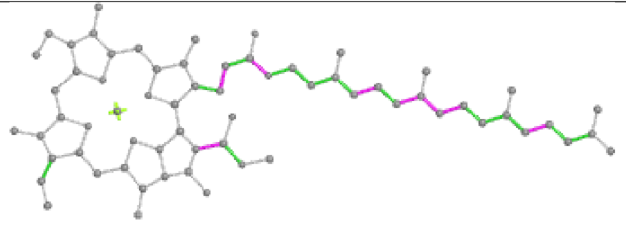
Ligand BCR aB 844

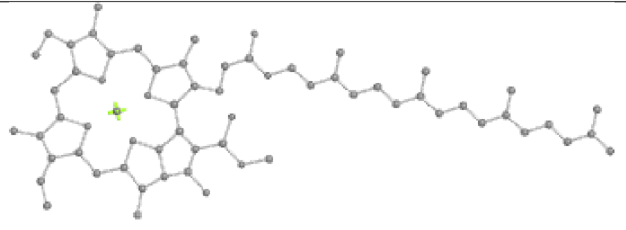

Bond lengths
Bond angles
Torsions
Rings

Ligand CLA aL 203

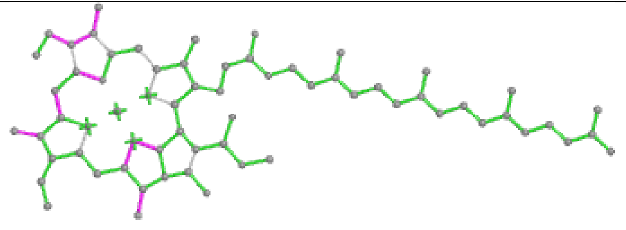

Bond lengths

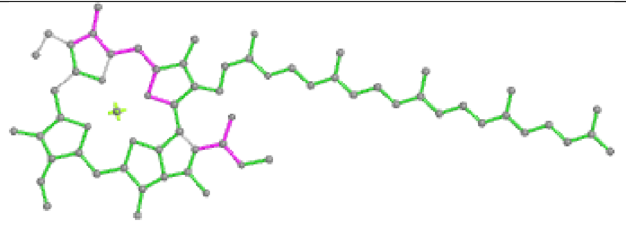

Bond angles

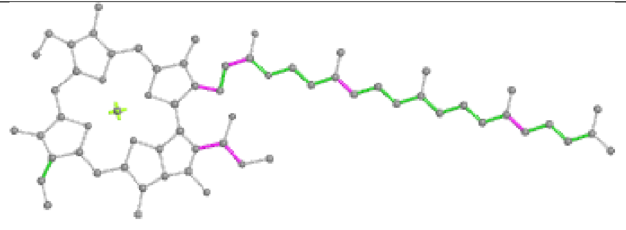

Torsions

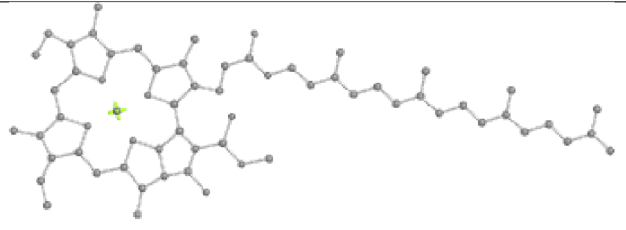

Rings

Ligand CLA cA 834

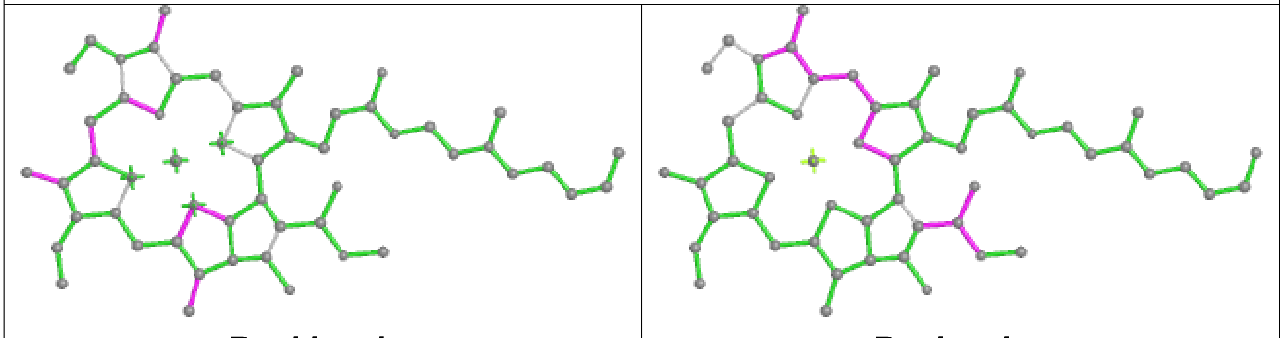

Bond lengths


Bond angles


Torsions

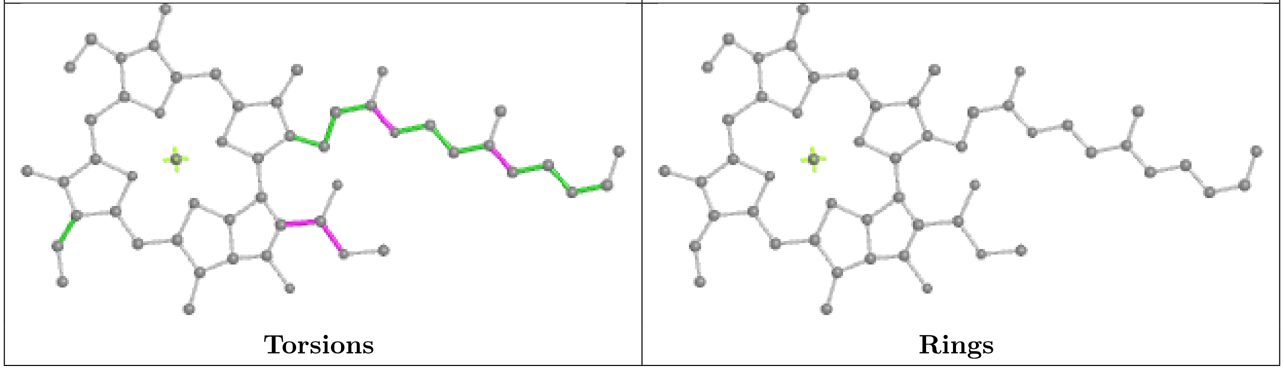

Rings

Ligand CLA cB 805



Bond lengths

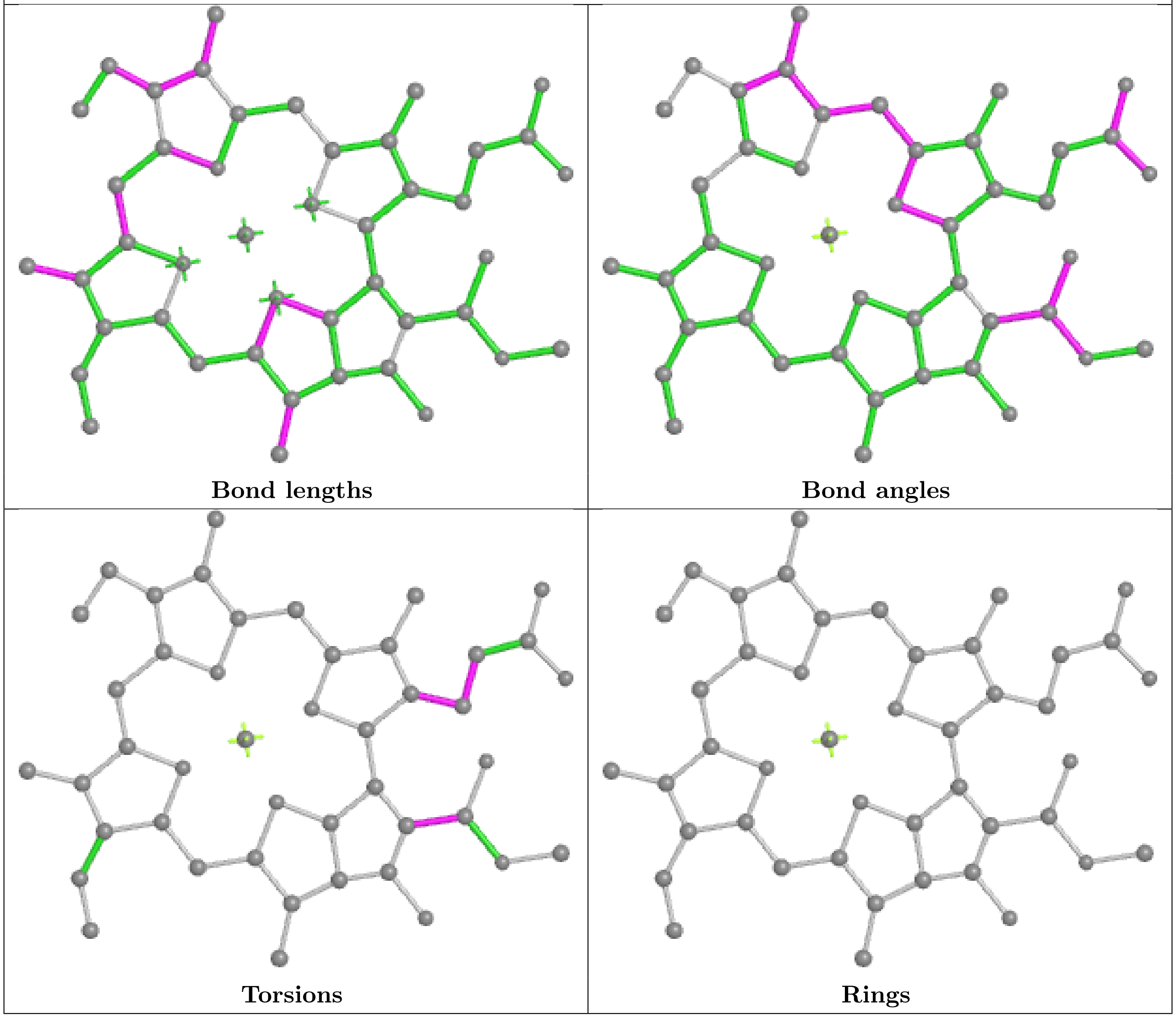
Bond angles



Torsions

Rings

Ligand CLA dA 808



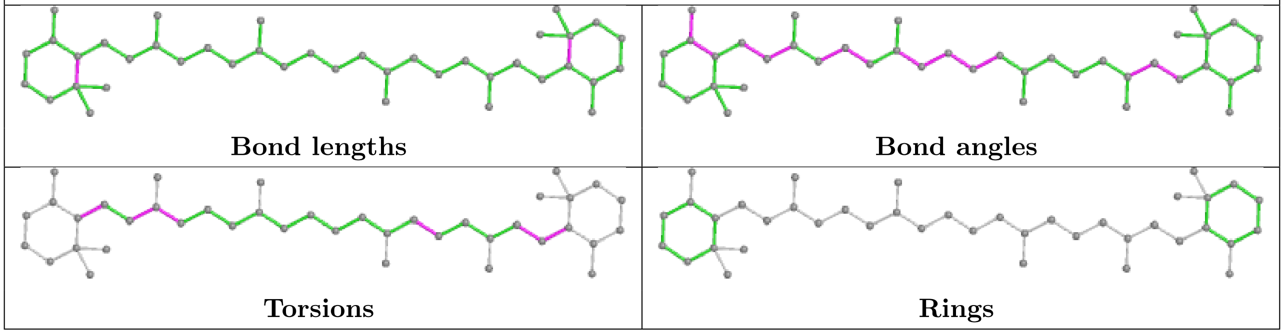
Bond lengths

Bond angles

Torsions

Rings

Ligand BCR cM 101



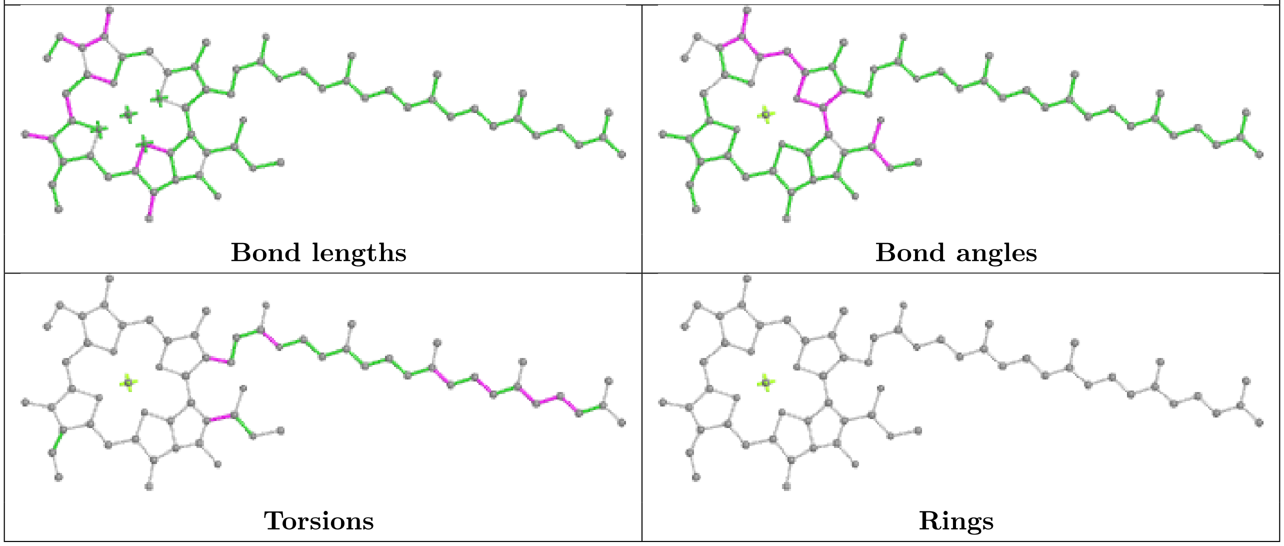
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA bA 841



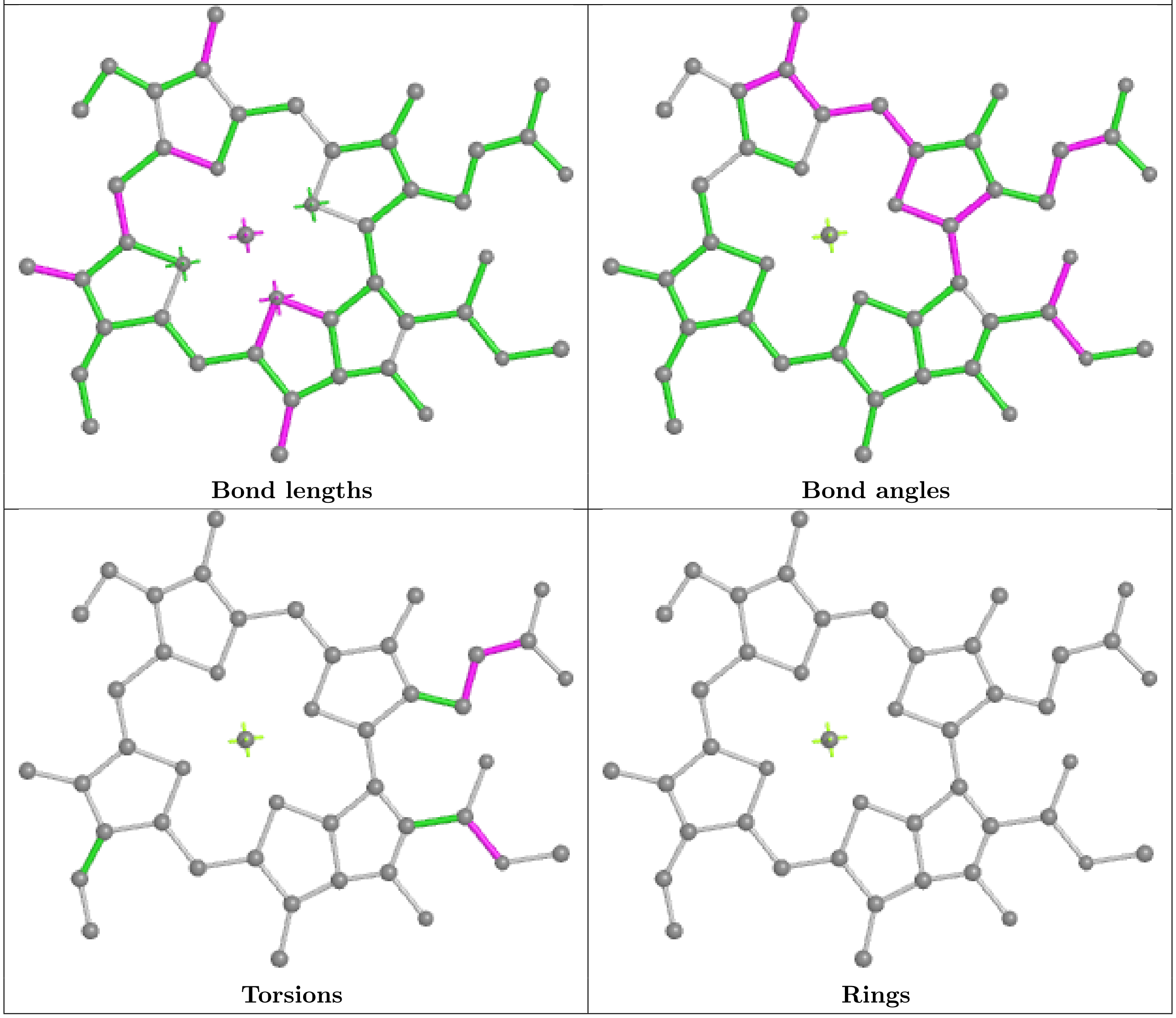
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA aA 809



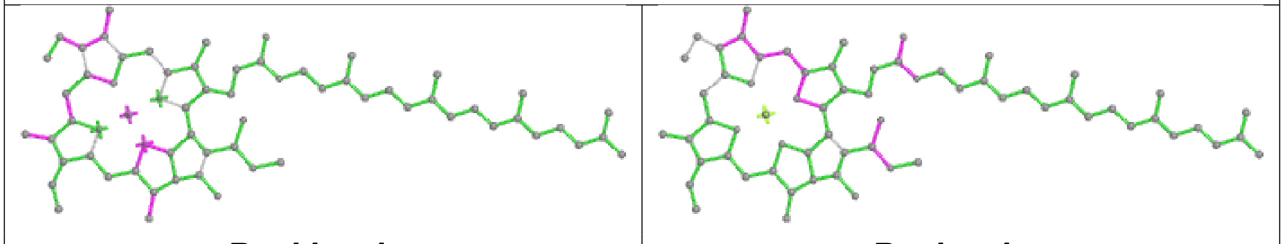
Bond lengths

Bond angles

Torsions

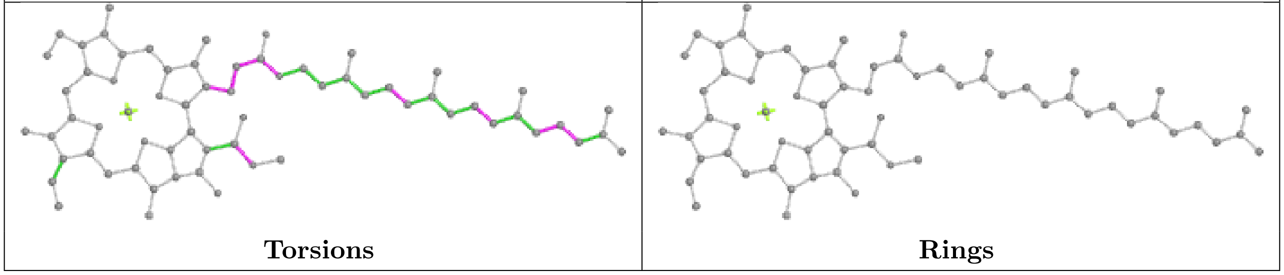
Rings

Ligand CLA aA 842



Bond lengths

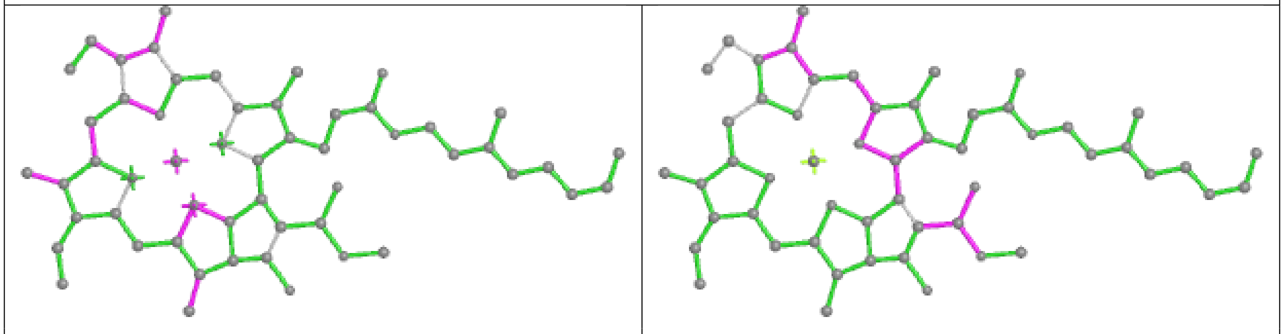
Bond angles



Torsions

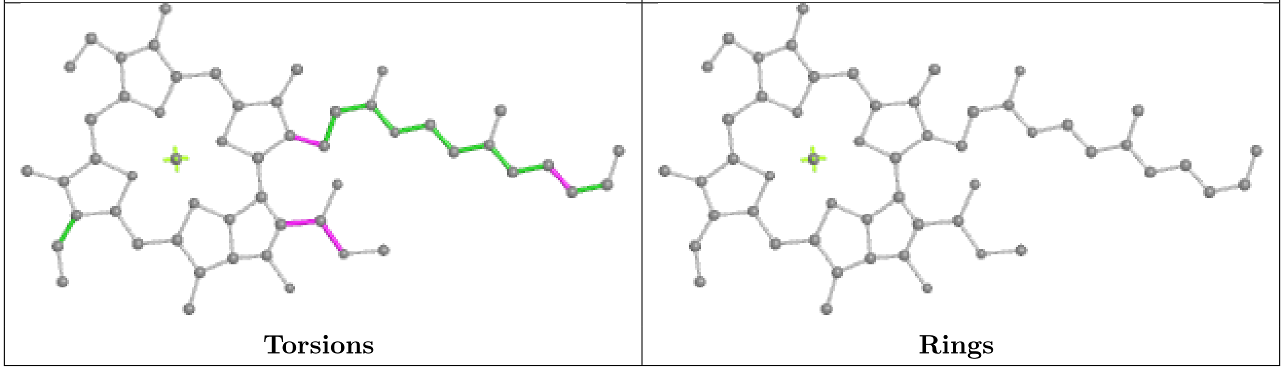
Rings

Ligand CLA dB 825



Bond lengths

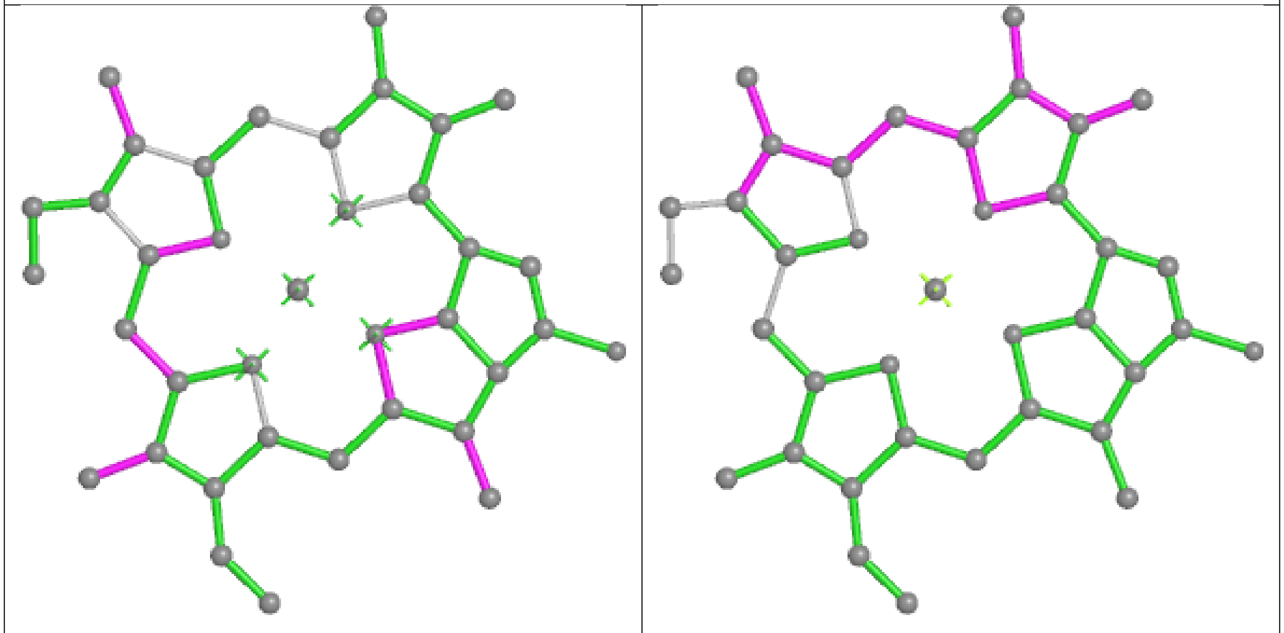
Bond angles



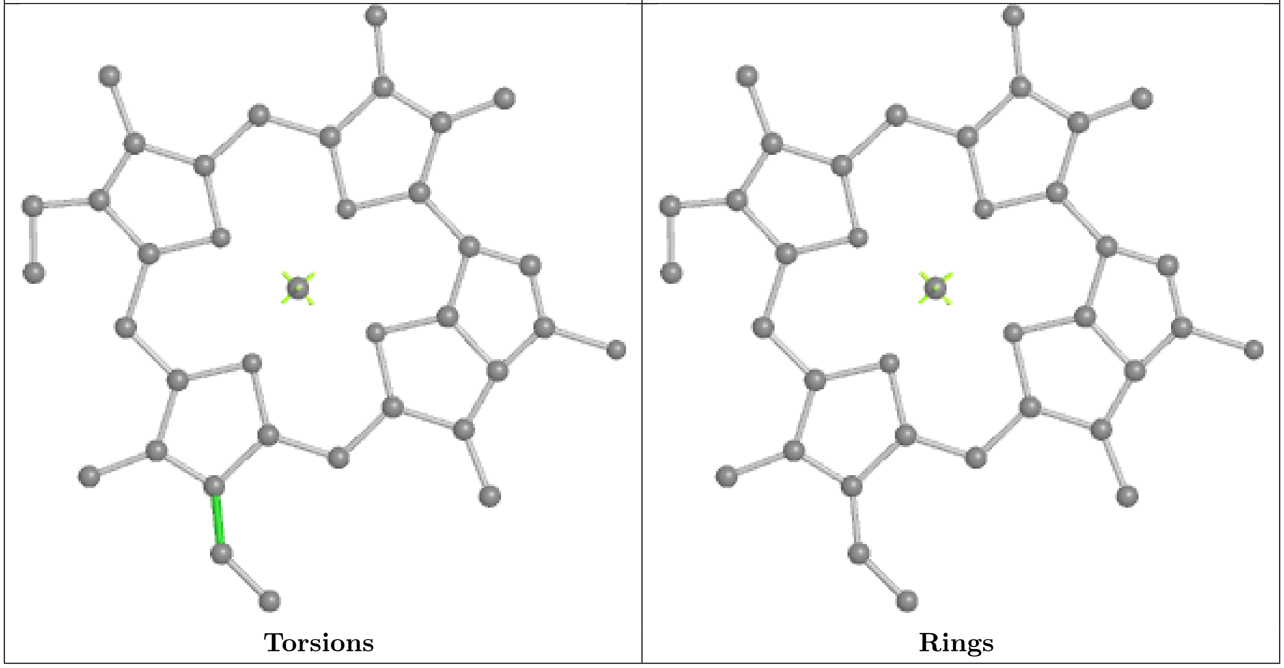
Torsions

Rings

Ligand CLA aJ 102

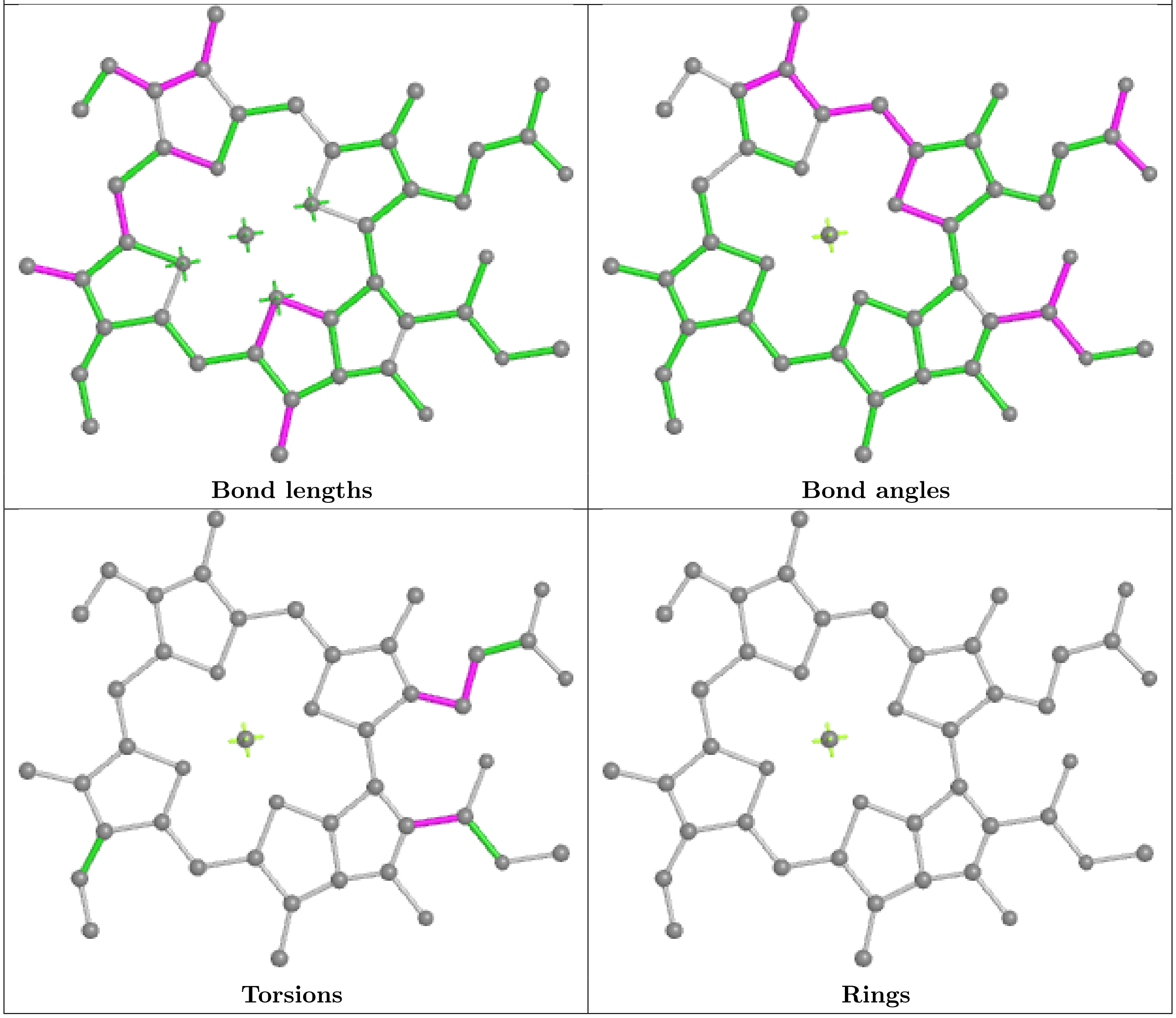


Bond lengths **Bond angles**



Torsions **Rings**

Ligand CLA bA 808



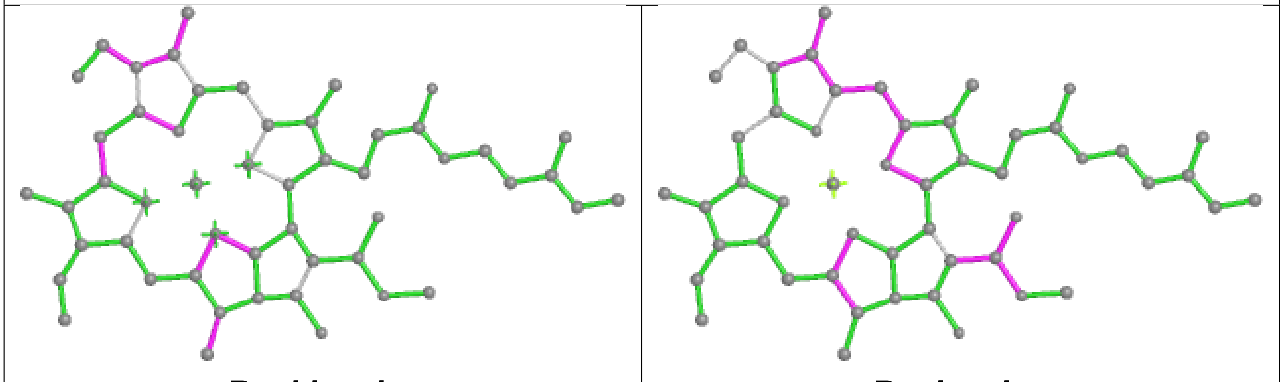
Bond lengths

Bond angles

Torsions

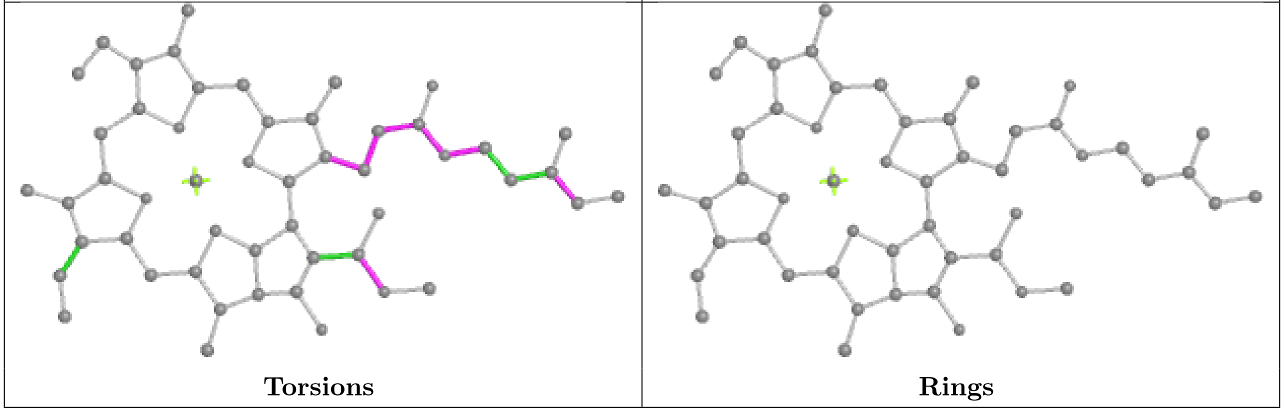
Rings

Ligand CLA cA 823



Bond lengths

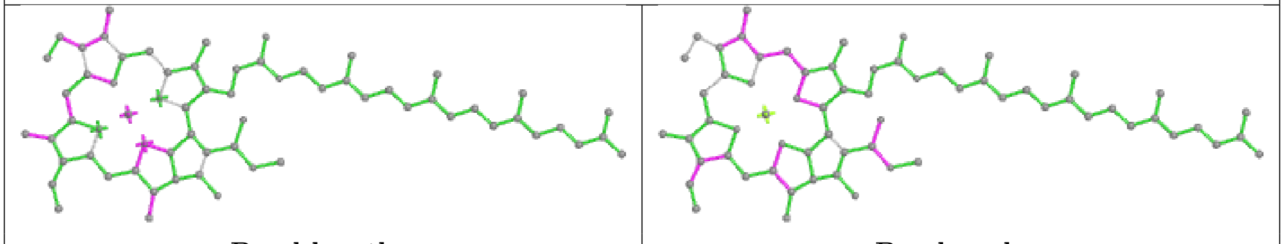
Bond angles



Torsions

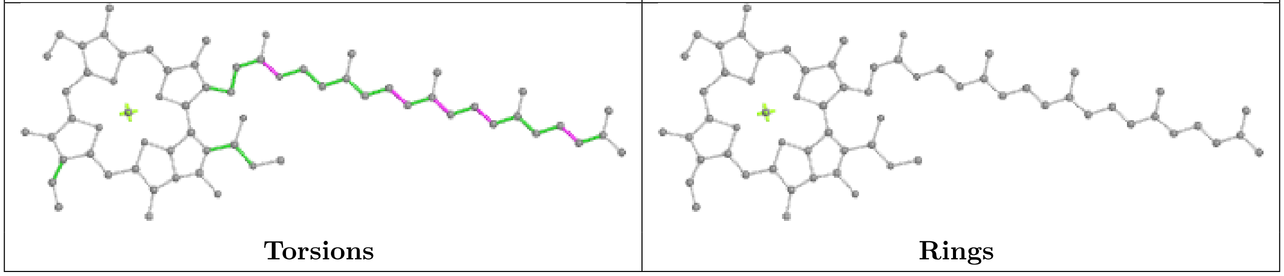
Rings

Ligand CLA dB 811



Bond lengths

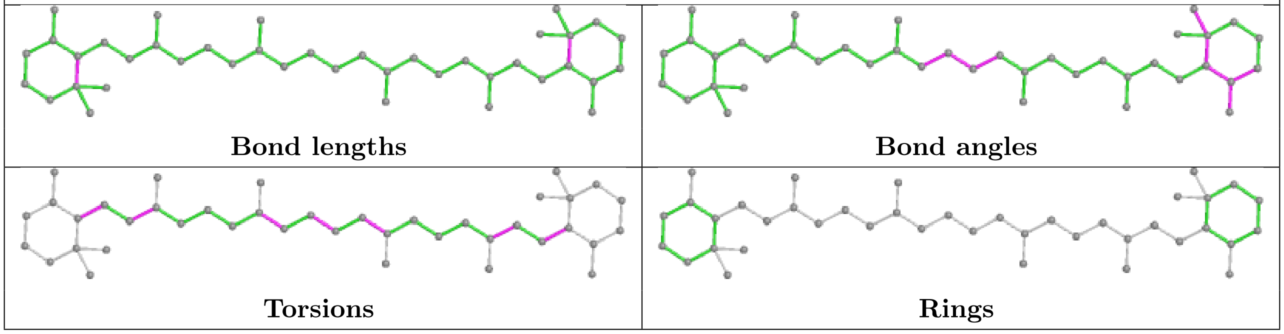
Bond angles



Torsions

Rings

Ligand BCR aF 202



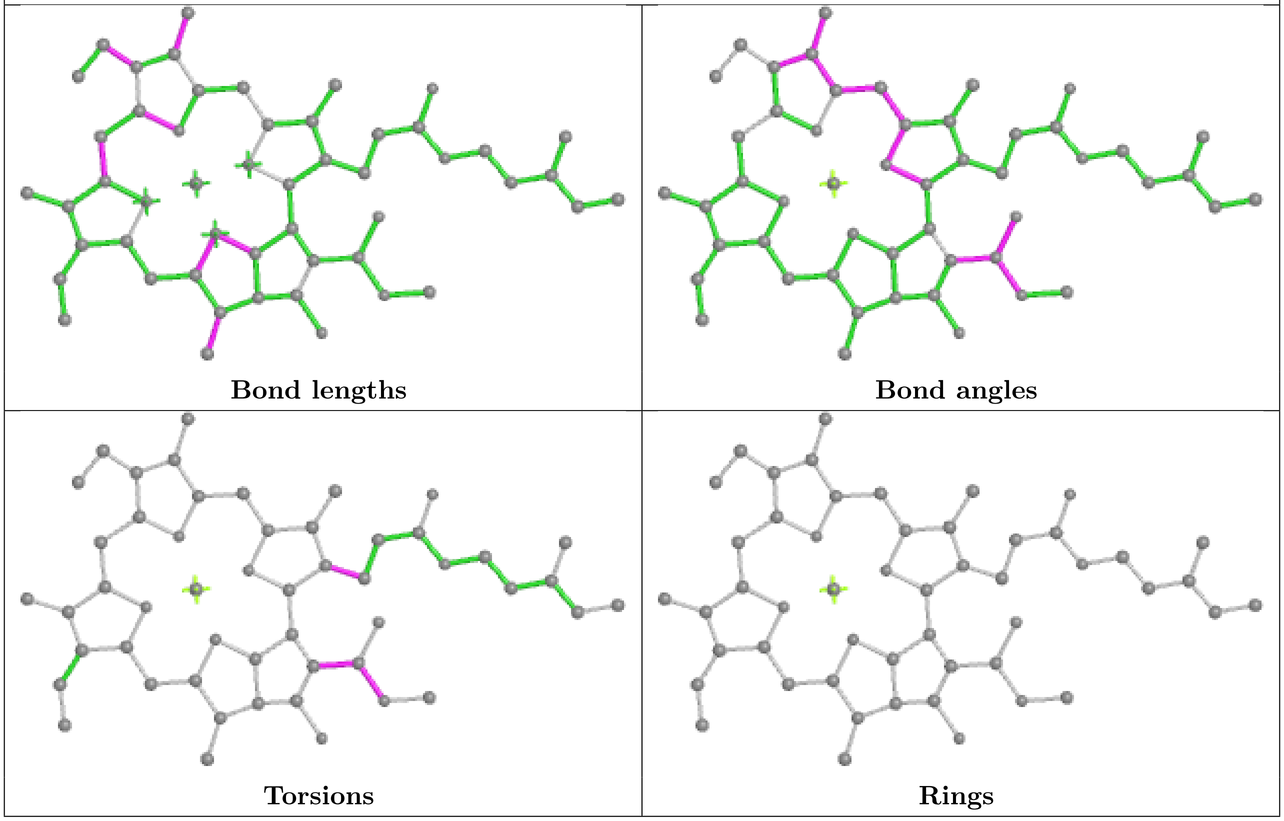
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA bF 201



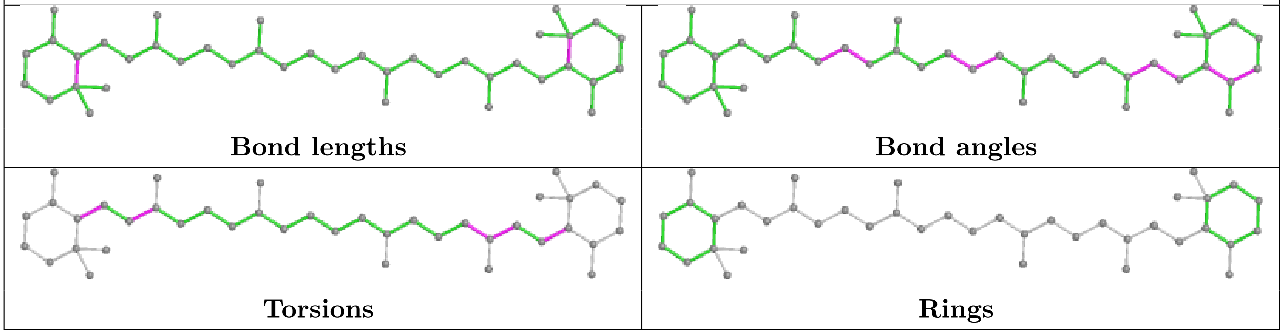
Bond lengths

Bond angles

Torsions

Rings

Ligand BCR dB 849



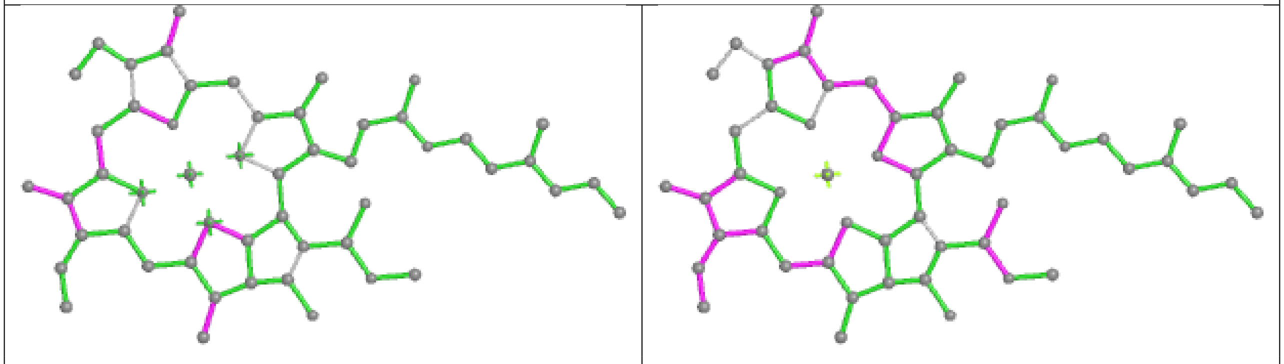
Bond lengths

Bond angles

Torsions

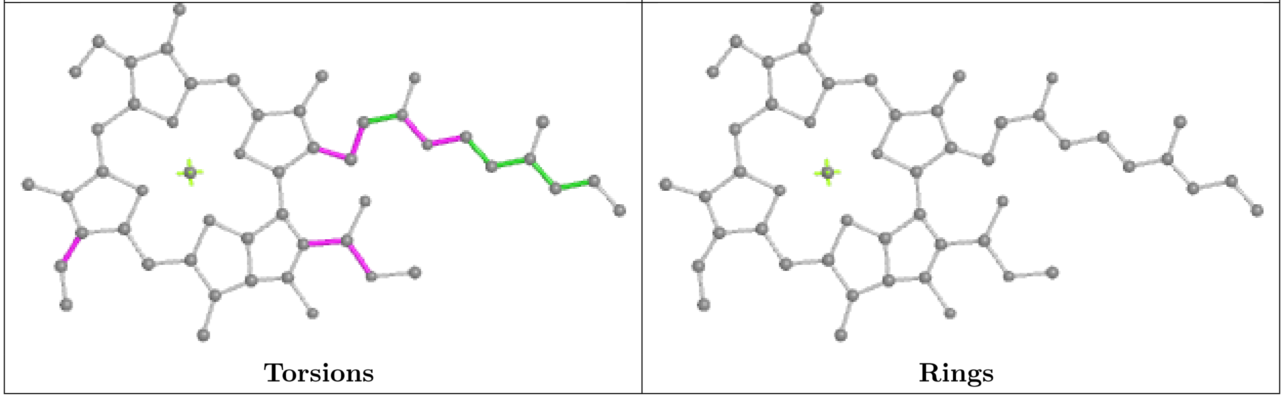
Rings

Ligand CLA bL 202



Bond lengths

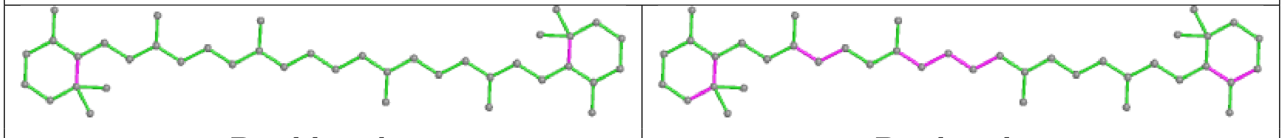
Bond angles



Torsions

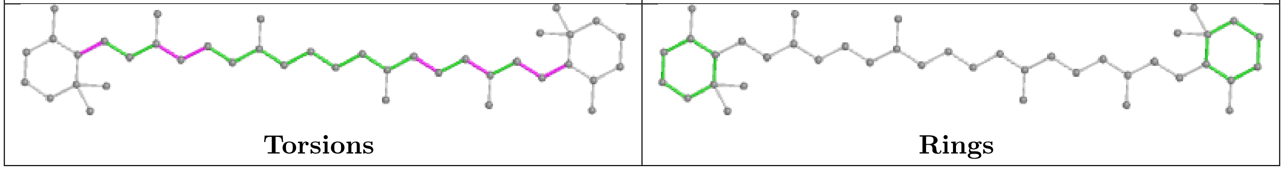
Rings

Ligand BCR cB 847



Bond lengths

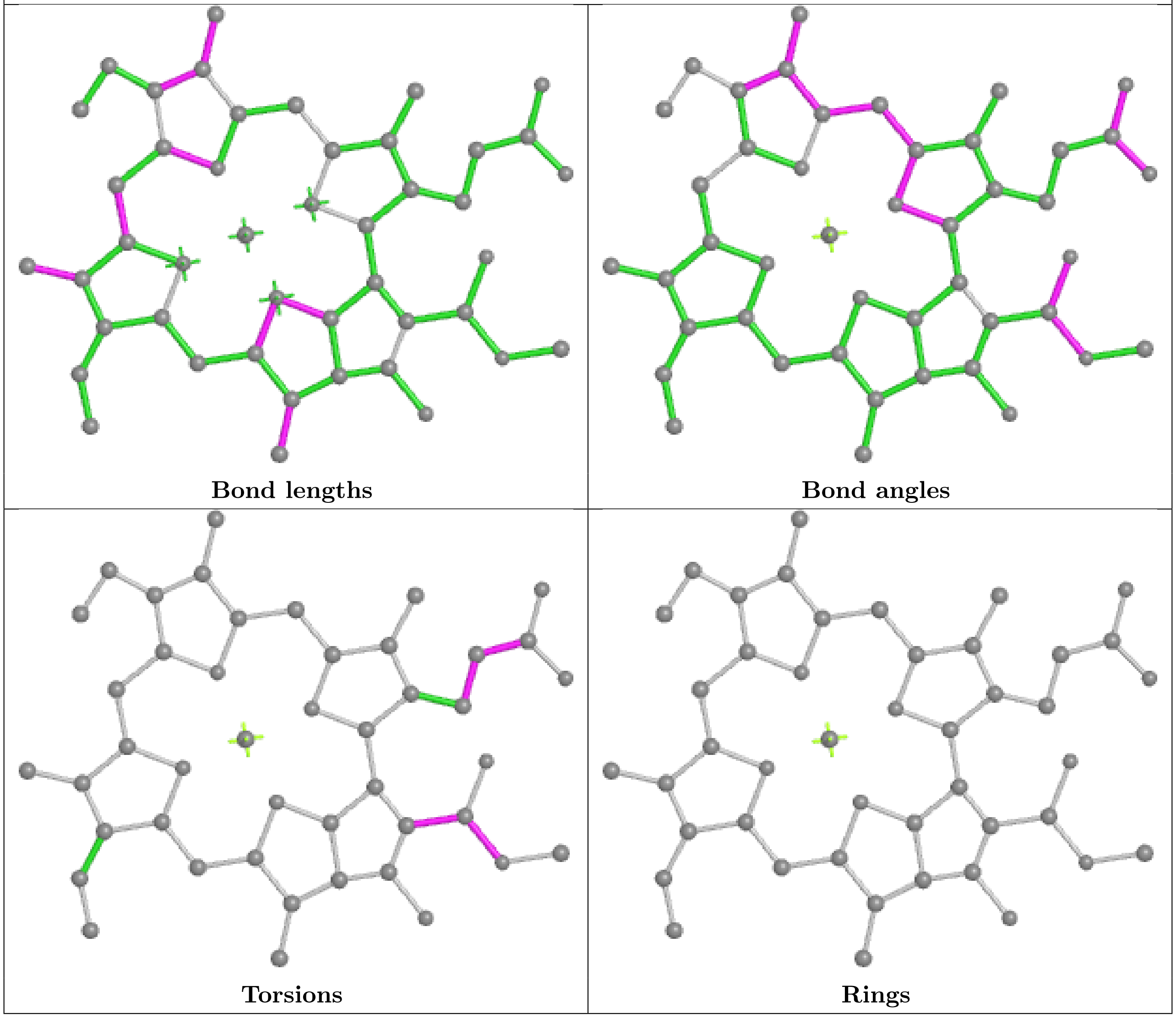
Bond angles



Torsions

Rings

Ligand CLA dB 837



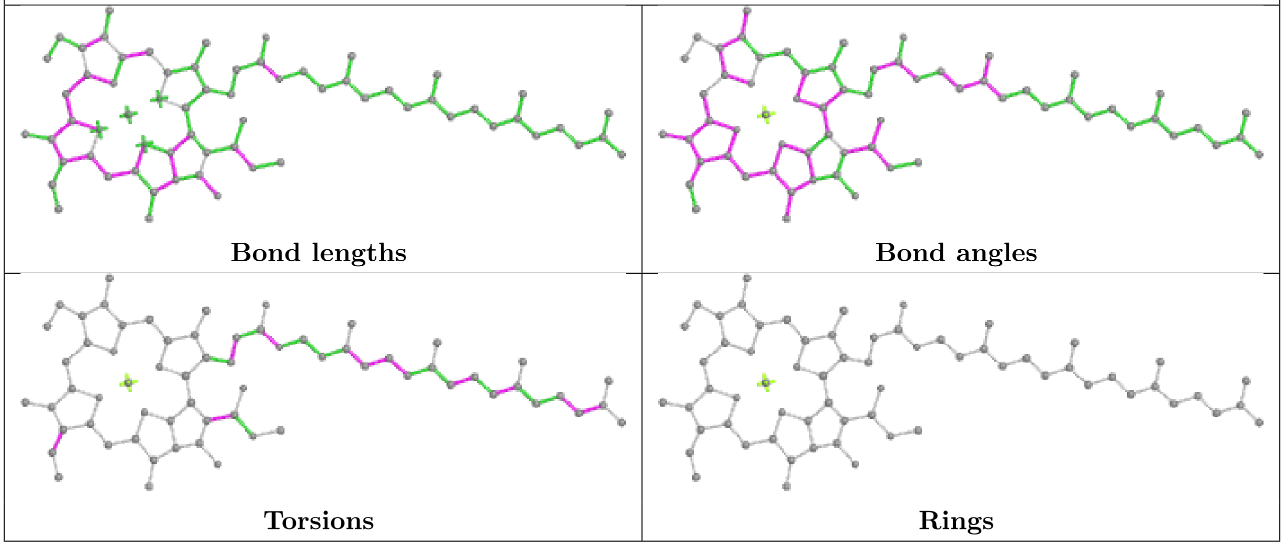
Bond lengths

Bond angles

Torsions

Rings

Ligand CL0 aA 801



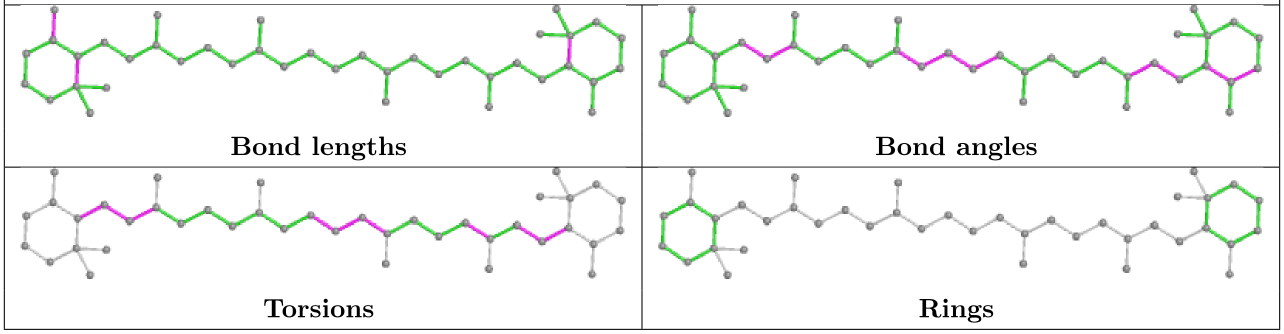
Bond lengths

Bond angles

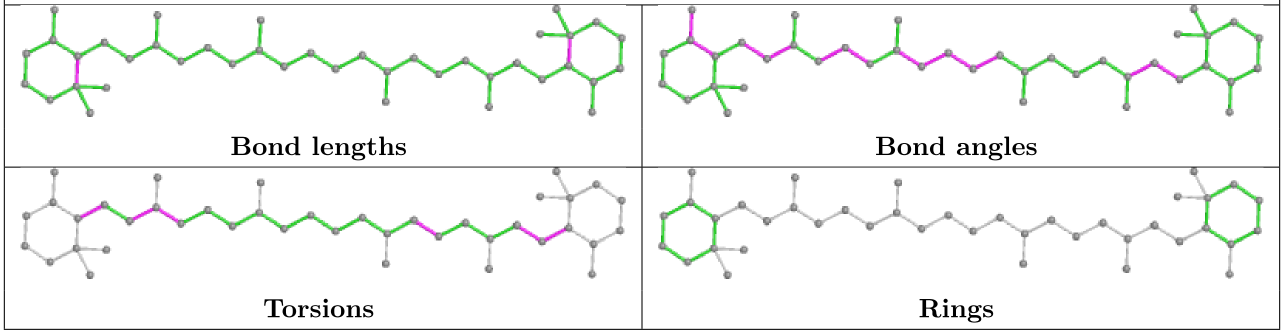
Torsions

Rings

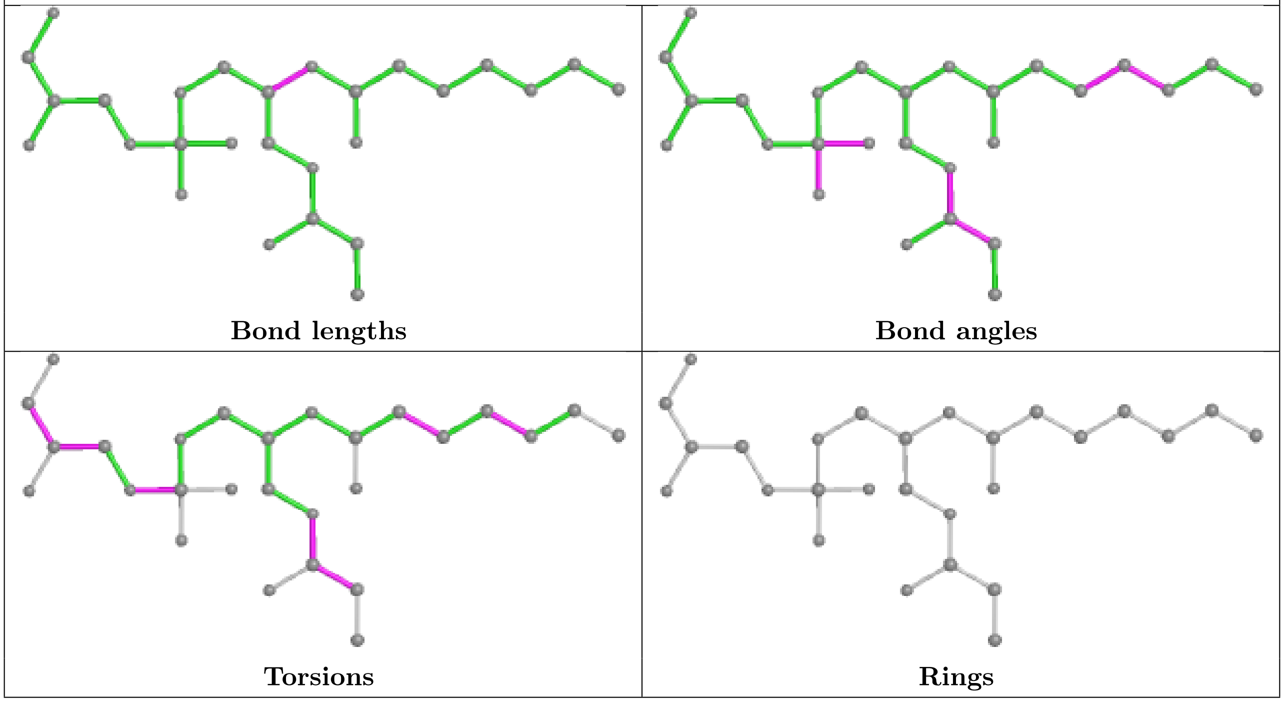
Ligand BCR bL 203


Bond lengths
Bond angles
Torsions
Rings

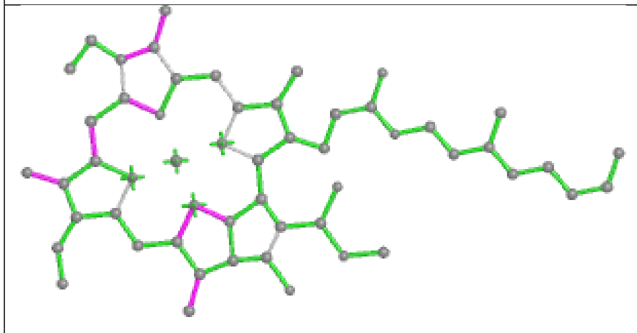
Ligand BCR dM 101


Bond lengths
Bond angles
Torsions
Rings

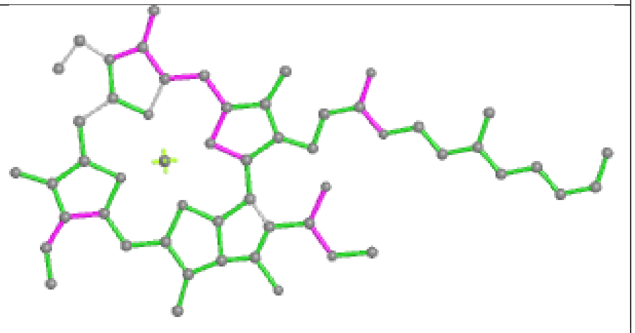
Ligand LHG bA 851


Bond lengths
Bond angles
Torsions
Rings

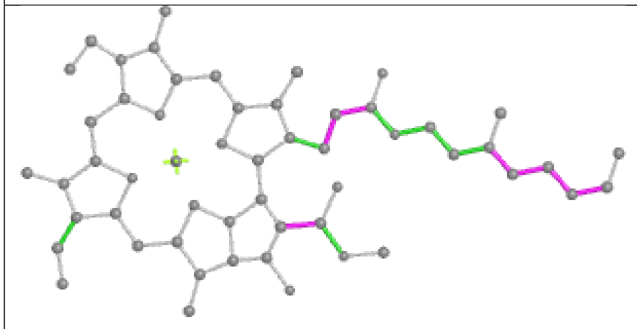
Ligand CLA aA 817



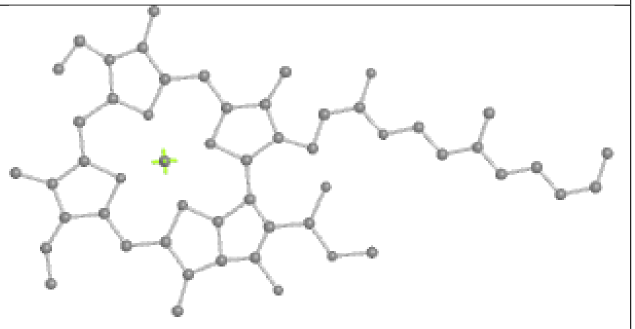
Bond lengths



Bond angles

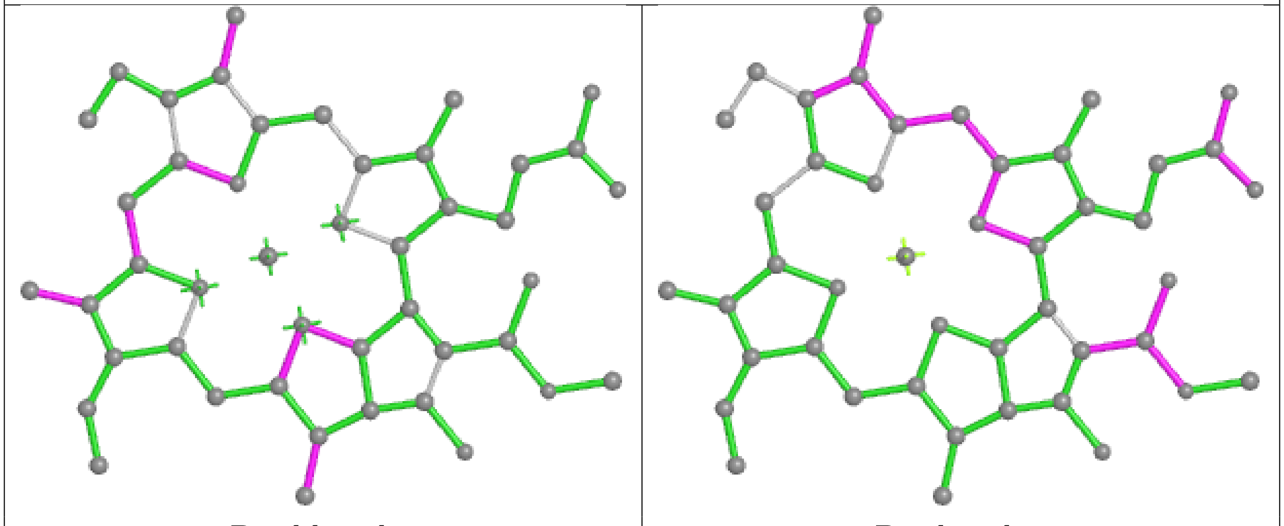


Torsions



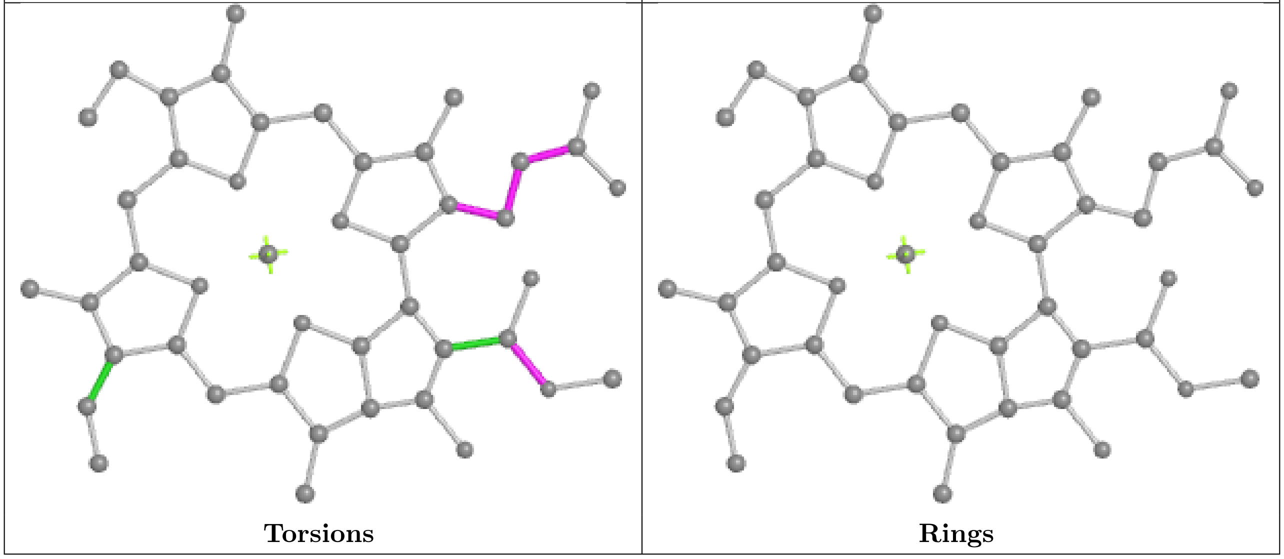
Rings

Ligand CLA aA 836



Bond lengths

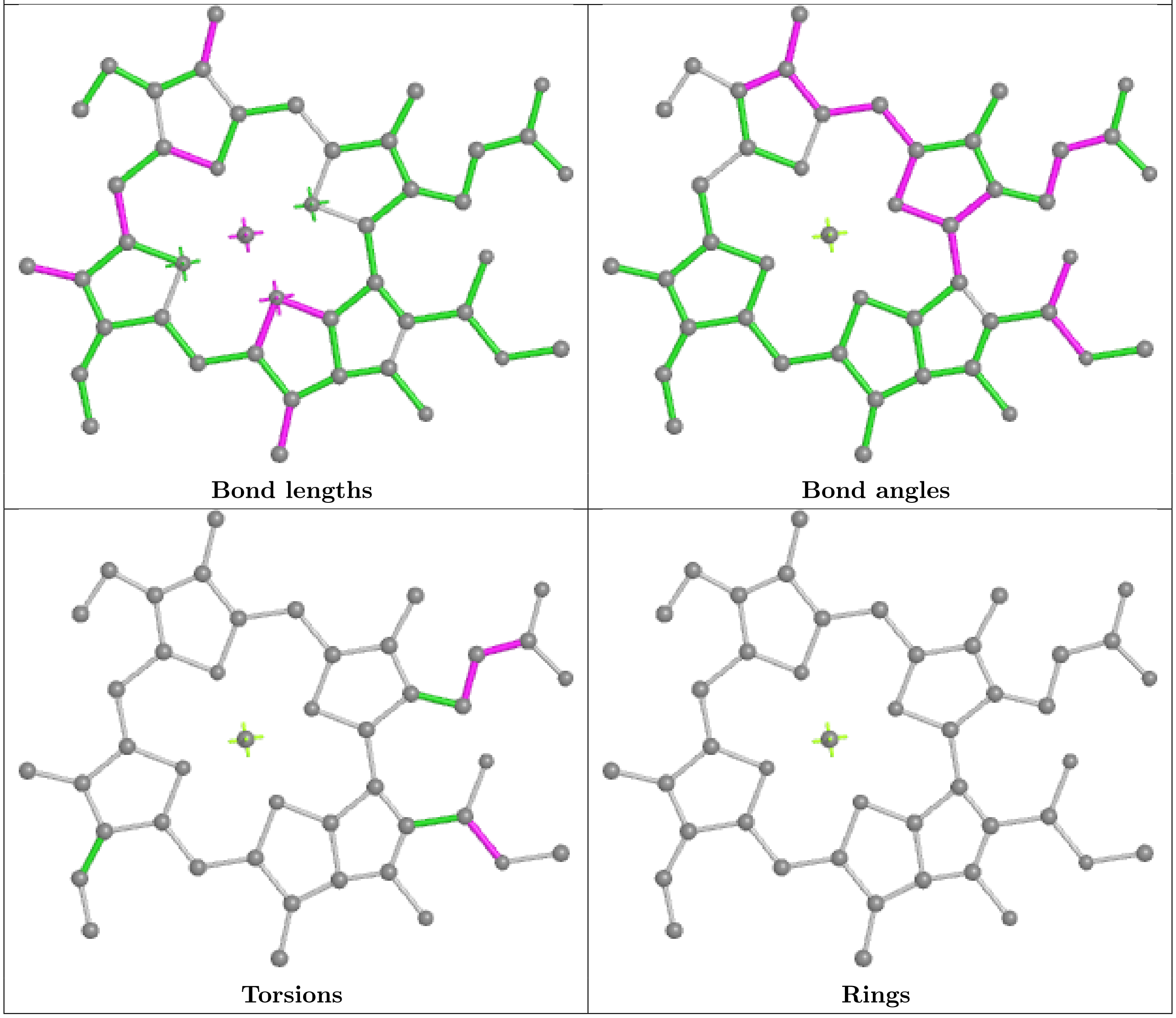
Bond angles



Torsions

Rings

Ligand CLA cA 809



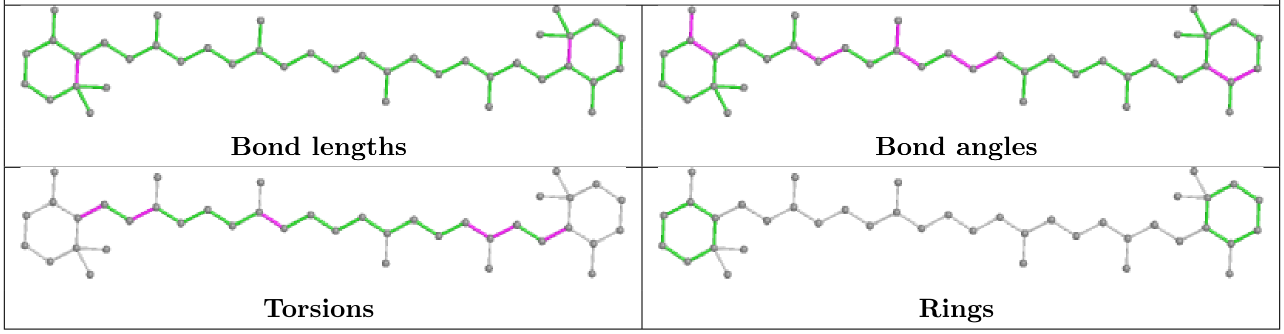
Bond lengths

Bond angles

Torsions

Rings

Ligand BCR aA 850



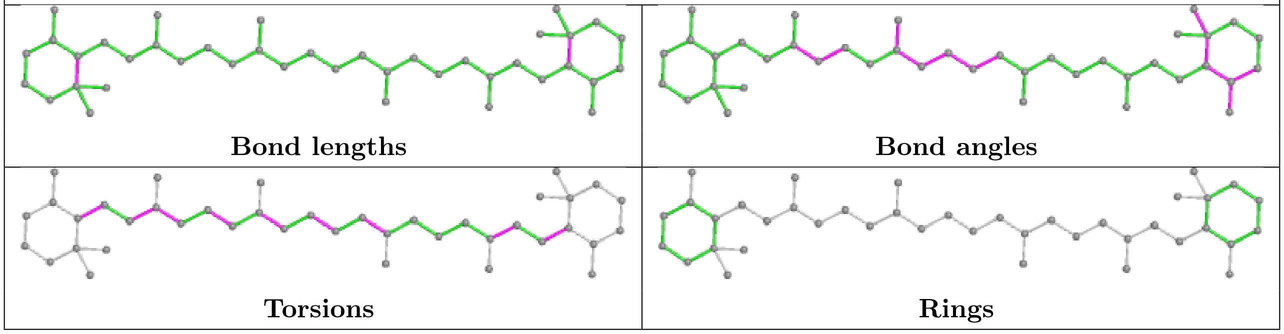
Bond lengths

Bond angles

Torsions

Rings

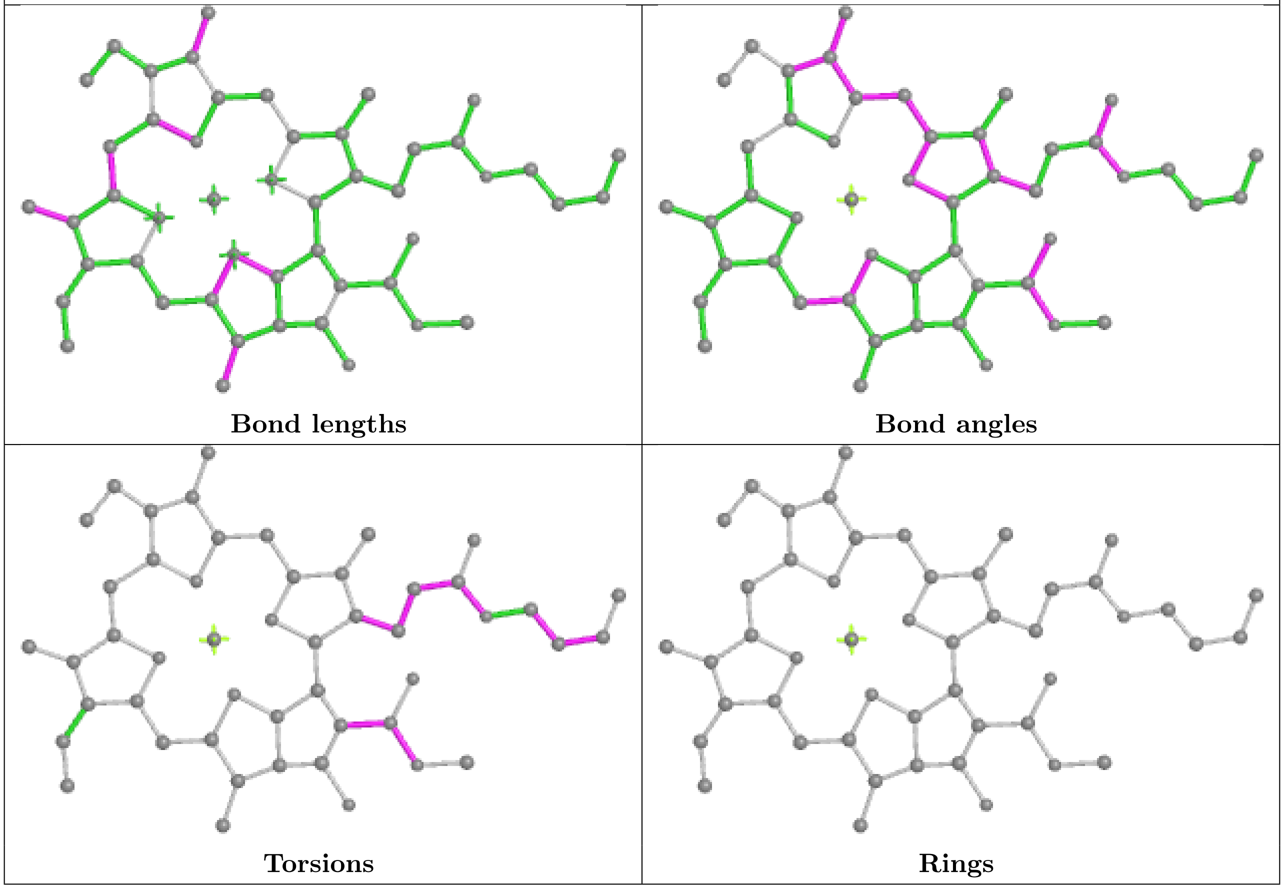
Ligand BCR dF 204



Bond lengths Bond angles

Torsions Rings

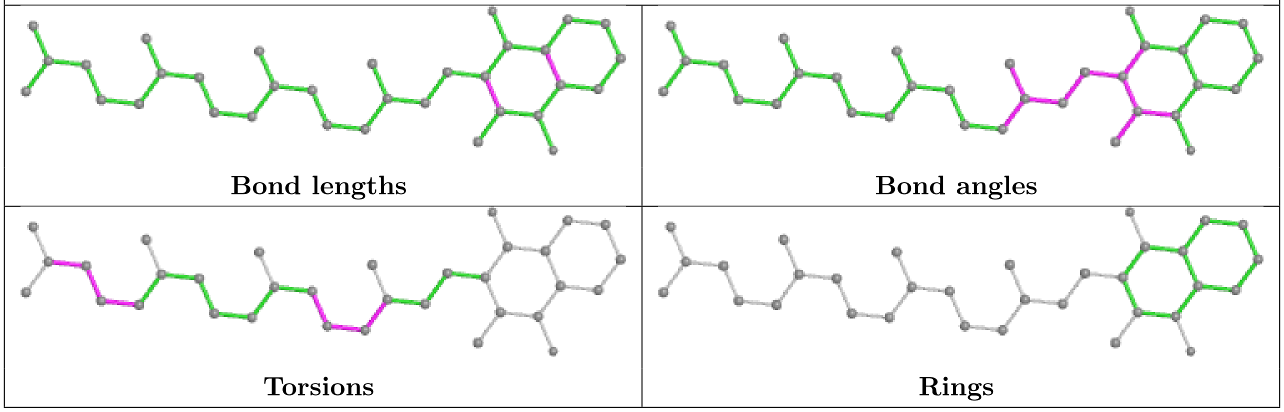
Ligand CLA bB 832



Bond lengths Bond angles

Torsions Rings

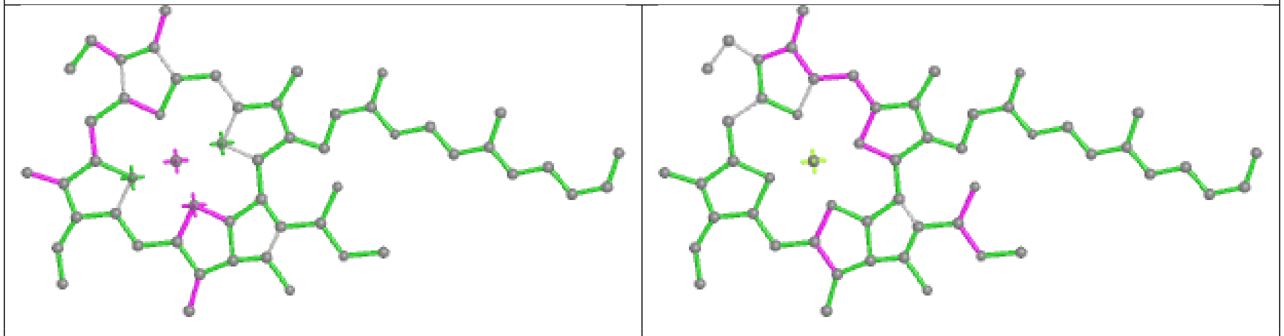
Ligand PQN cA 844



Bond lengths Bond angles

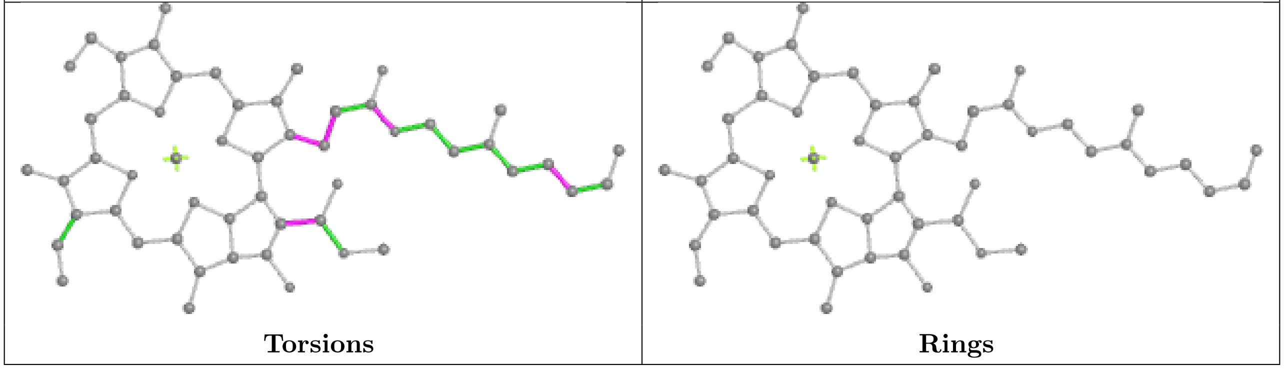
Torsions Rings

Ligand CLA bA 818



Bond lengths

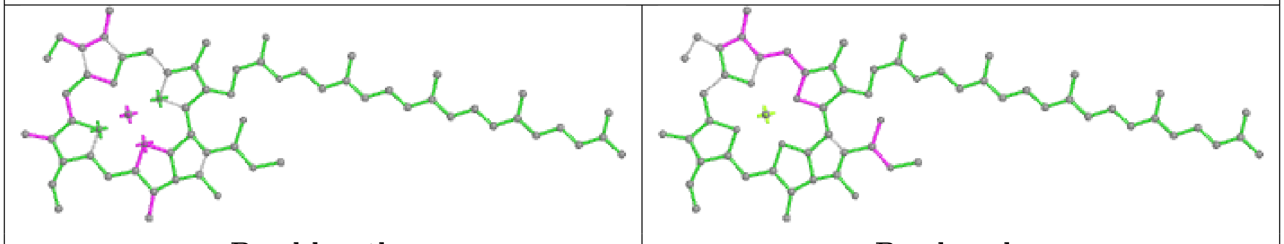
Bond angles



Torsions

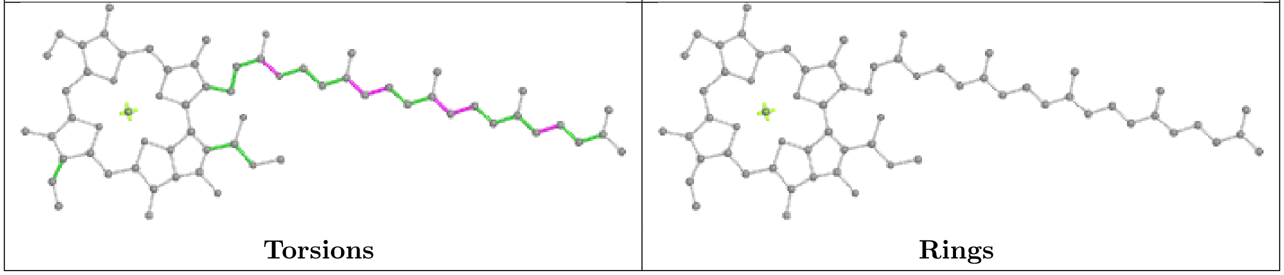
Rings

Ligand CLA aB 810



Bond lengths

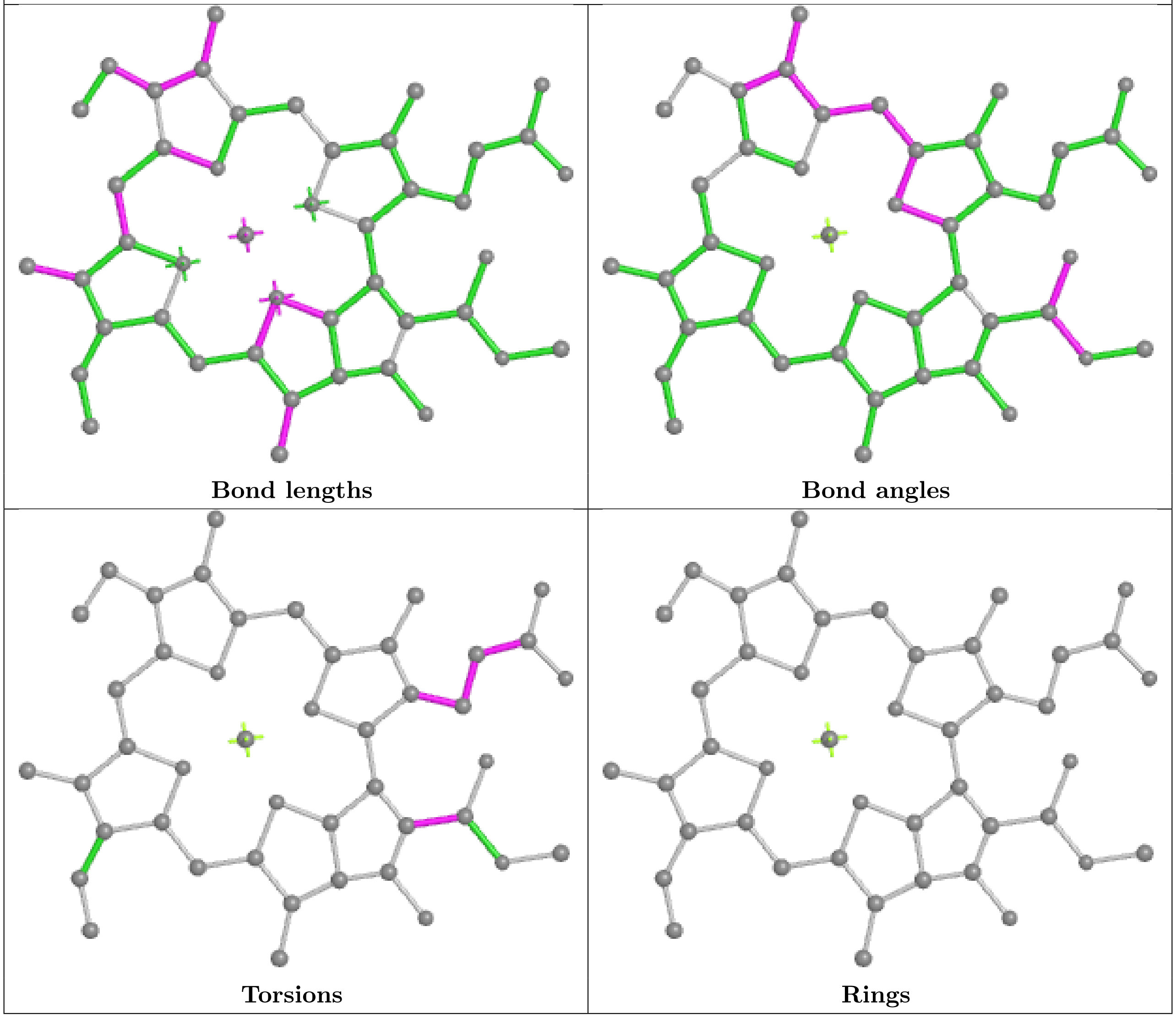
Bond angles



Torsions

Rings

Ligand CLA cB 830



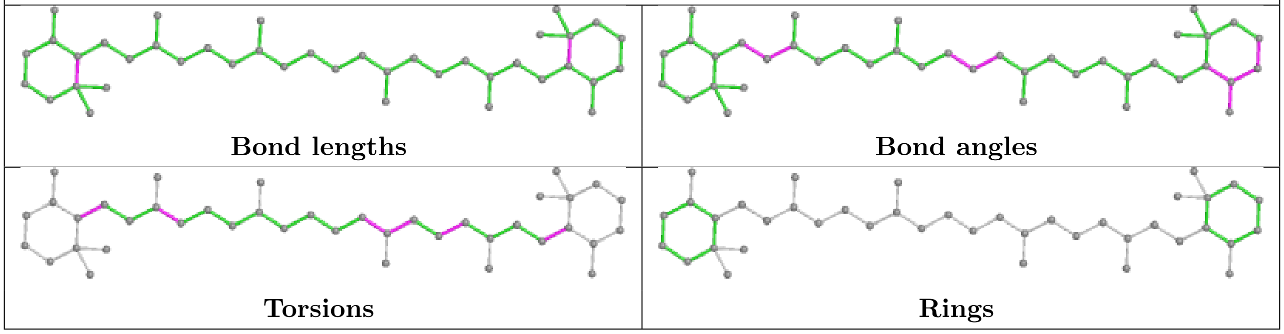
Bond lengths

Bond angles

Torsions

Rings

Ligand BCR bB 845



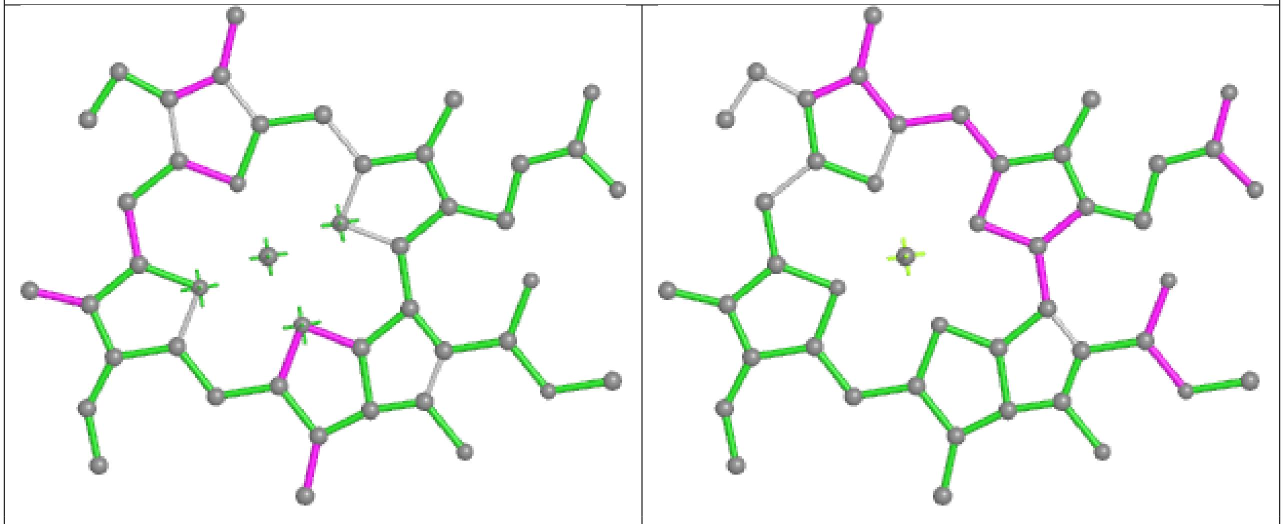
Bond lengths

Bond angles

Torsions

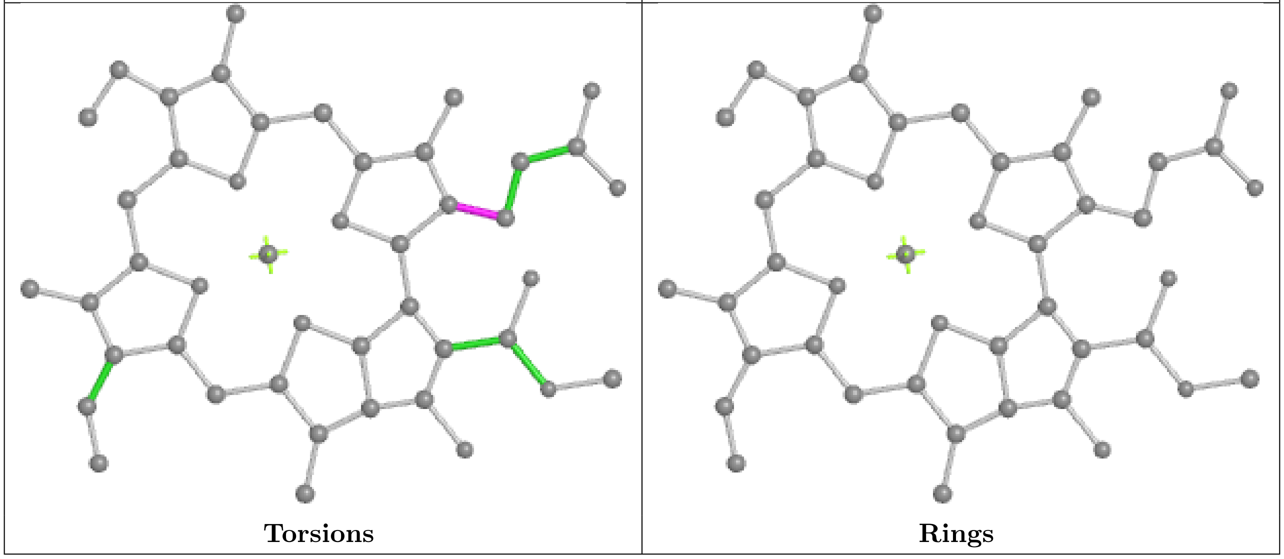
Rings

Ligand CLA cB 835



Bond lengths

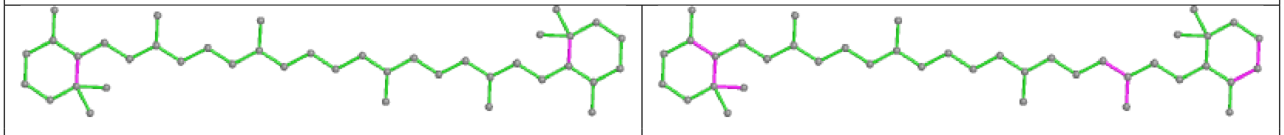
Bond angles



Torsions

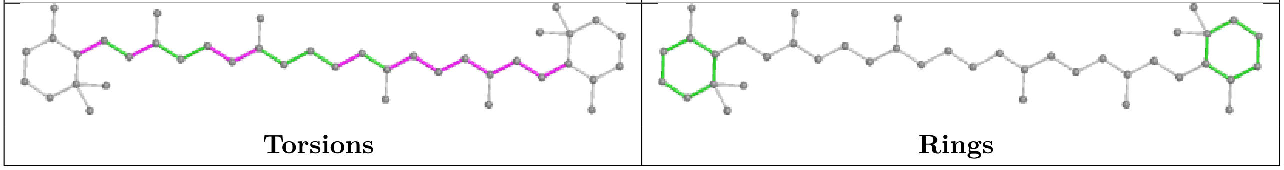
Rings

Ligand BCR bB 847



Bond lengths

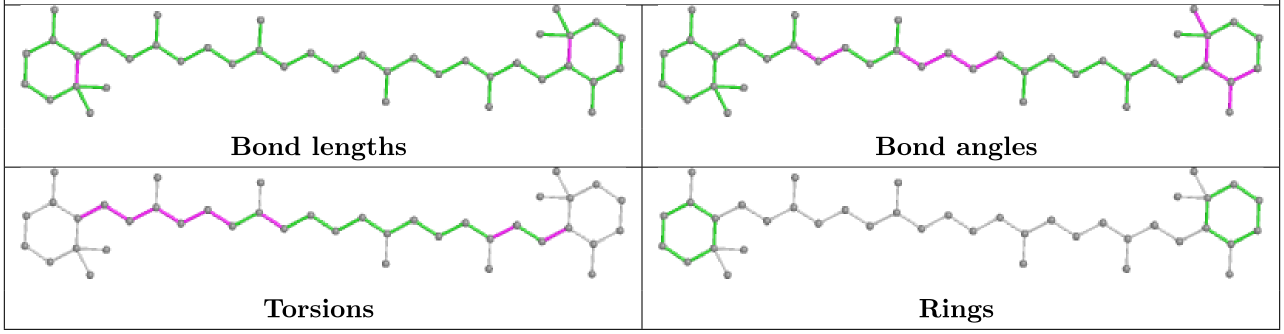
Bond angles



Torsions

Rings

Ligand BCR cF 204



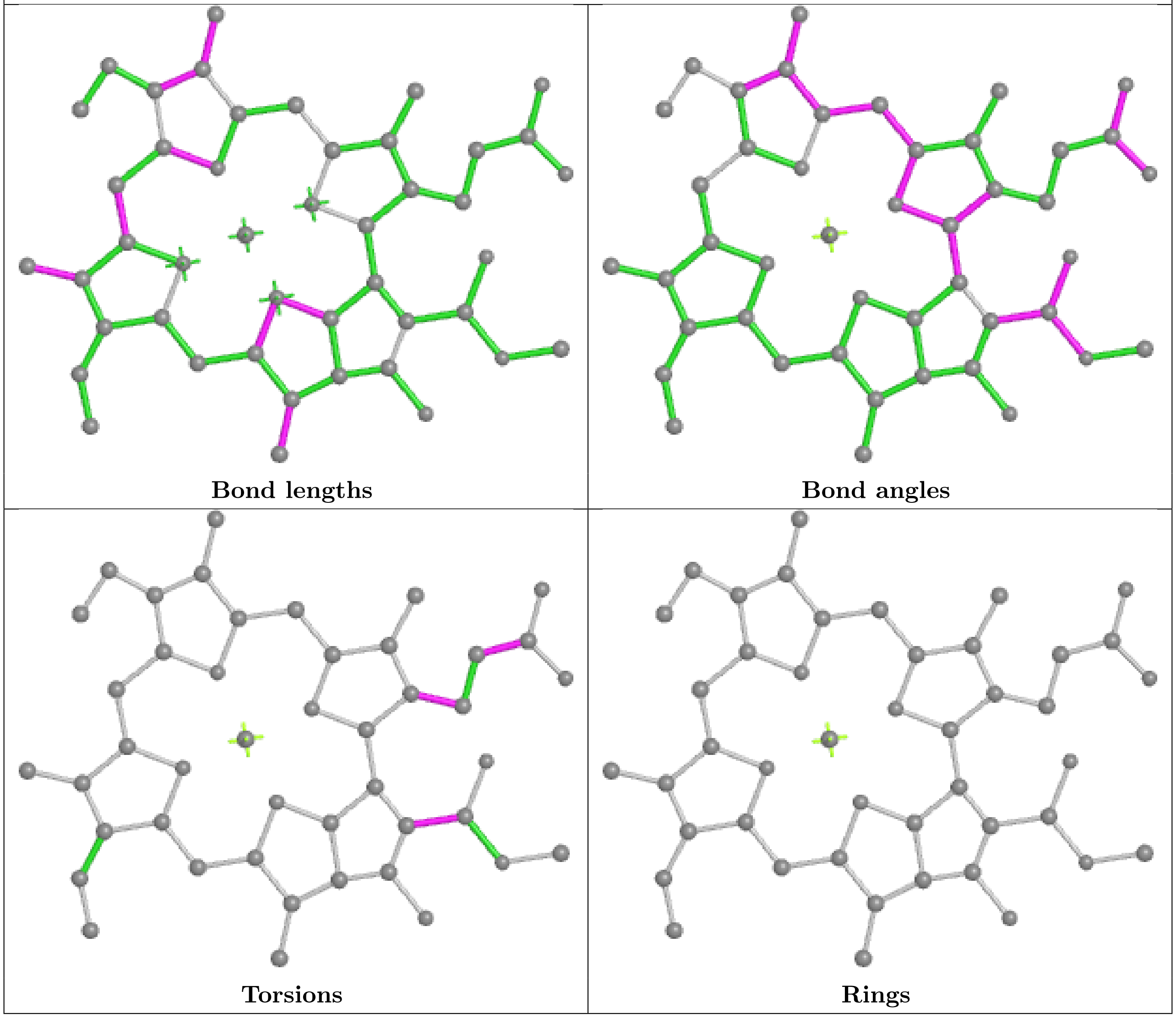
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA dA 803



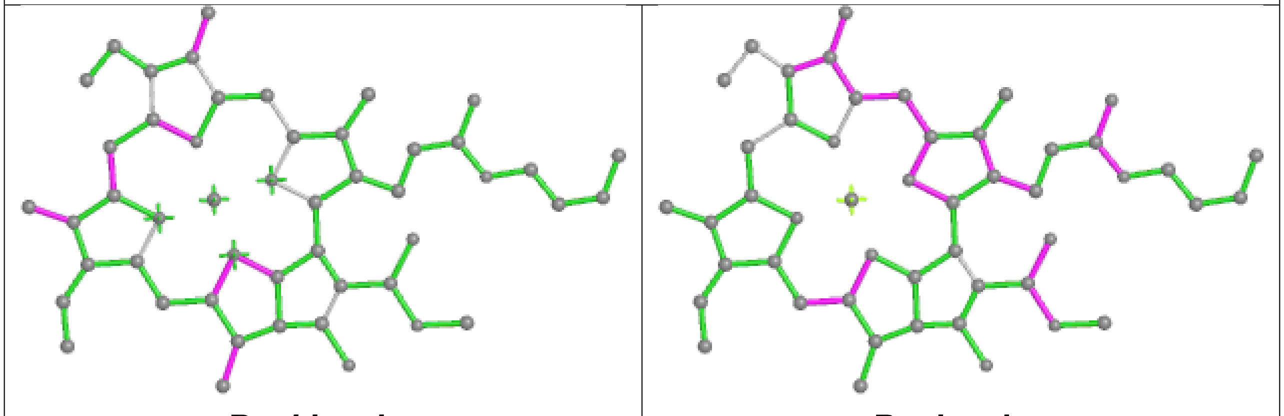
Bond lengths

Bond angles

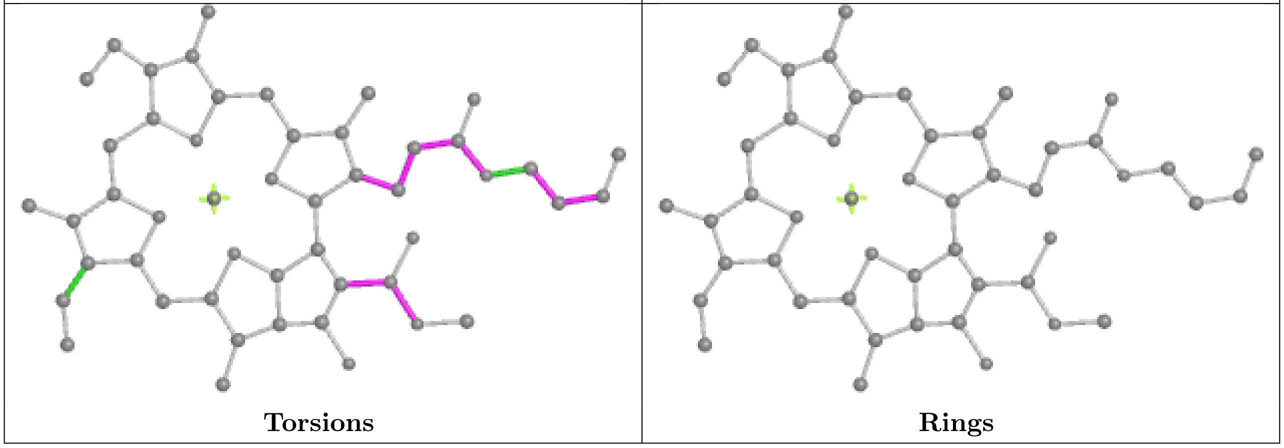
Torsions

Rings

Ligand CLA cB 831

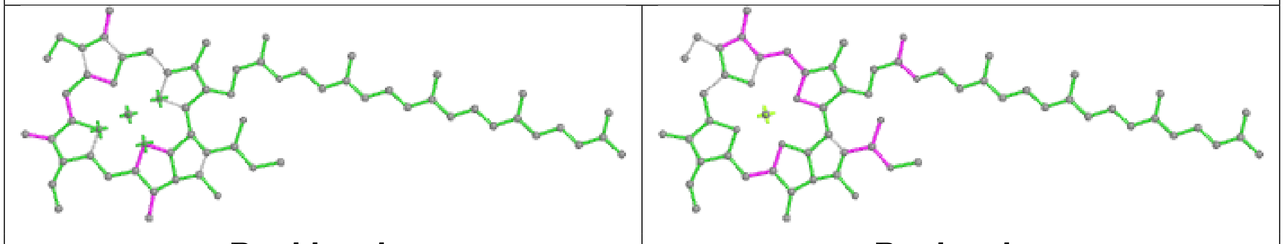


Bond lengths Bond angles

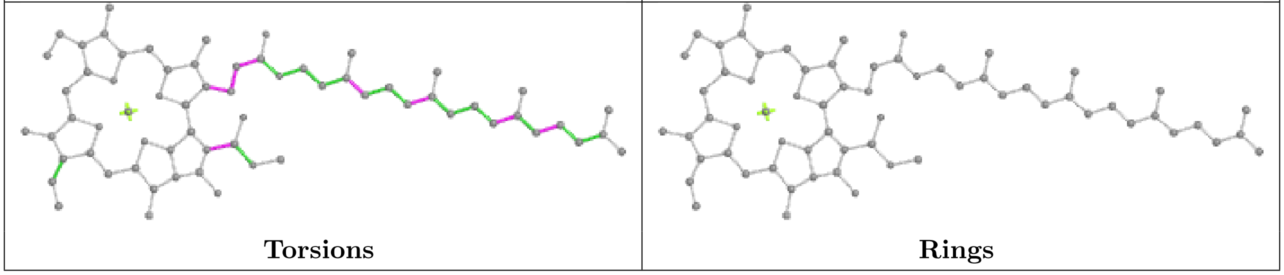


Torsions Rings

Ligand CLA dB 828

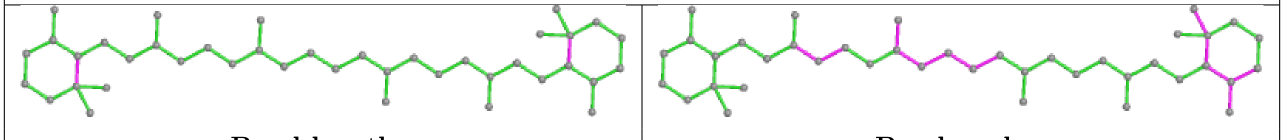


Bond lengths Bond angles



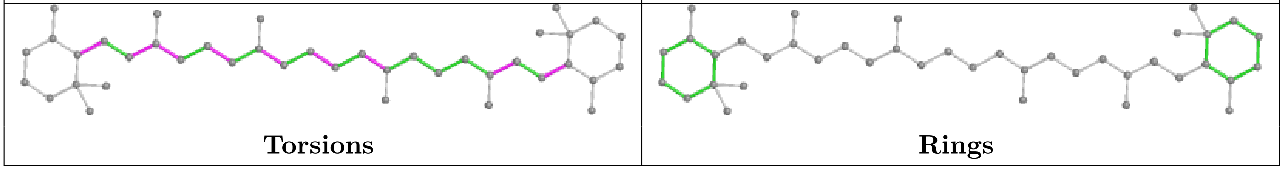
Torsions Rings

Ligand BCR bF 204



Bond lengths

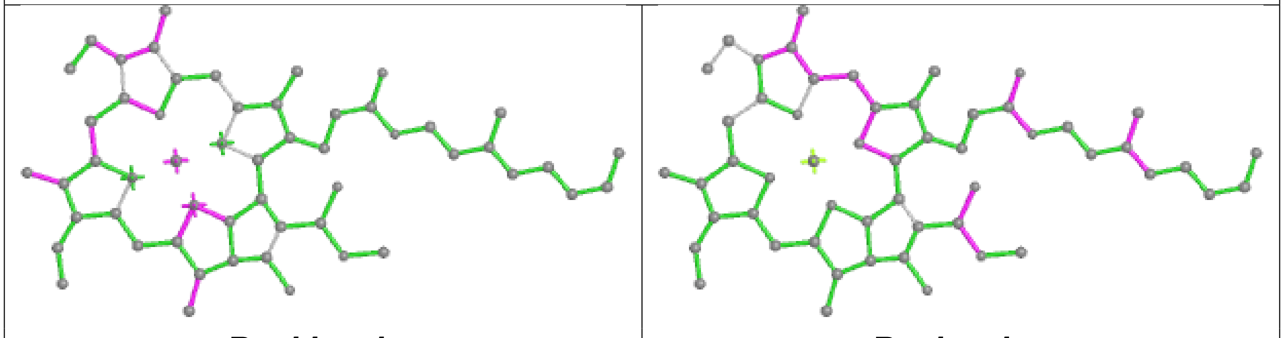
Bond angles



Torsions

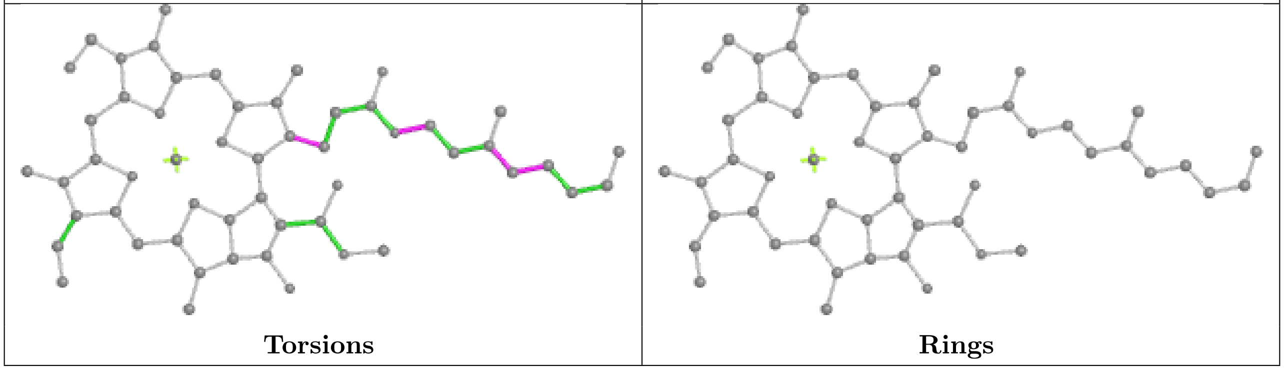
Rings

Ligand CLA bA 835



Bond lengths

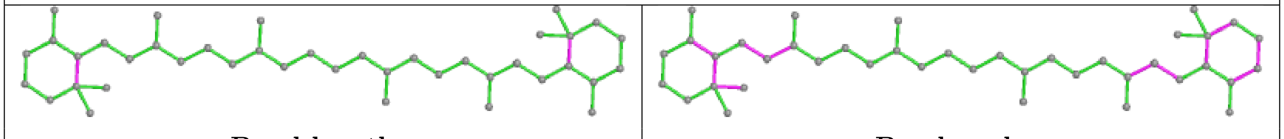
Bond angles



Torsions

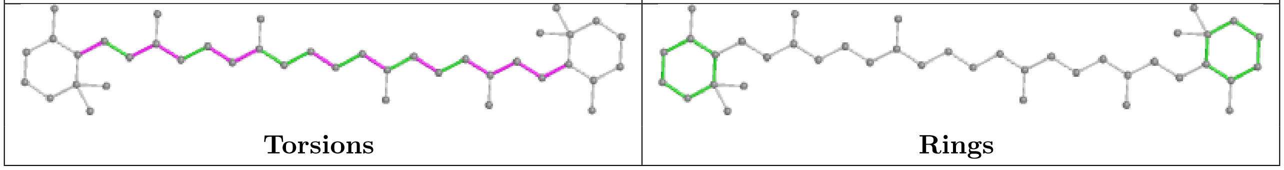
Rings

Ligand BCR cA 851



Bond lengths

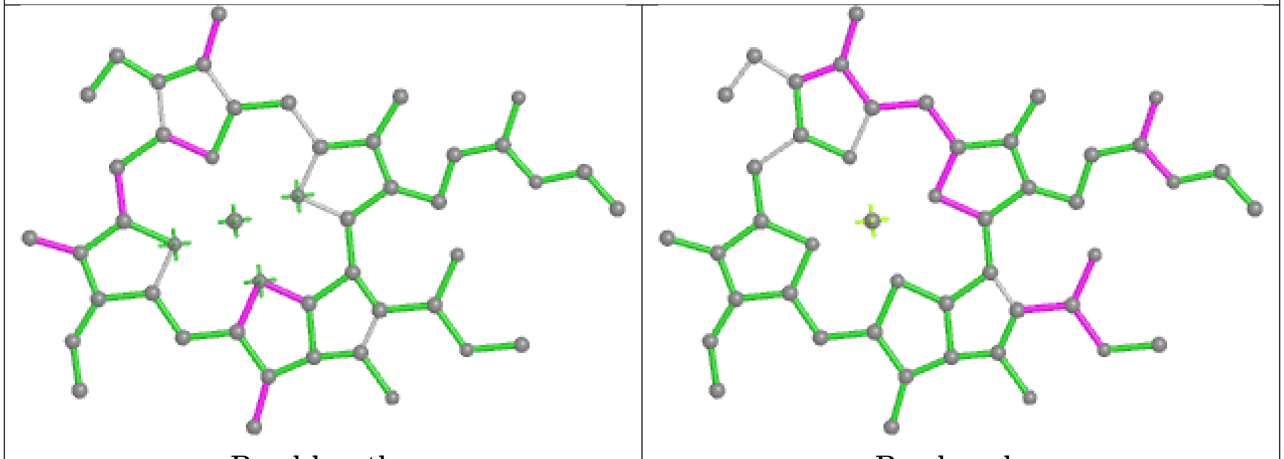
Bond angles



Torsions

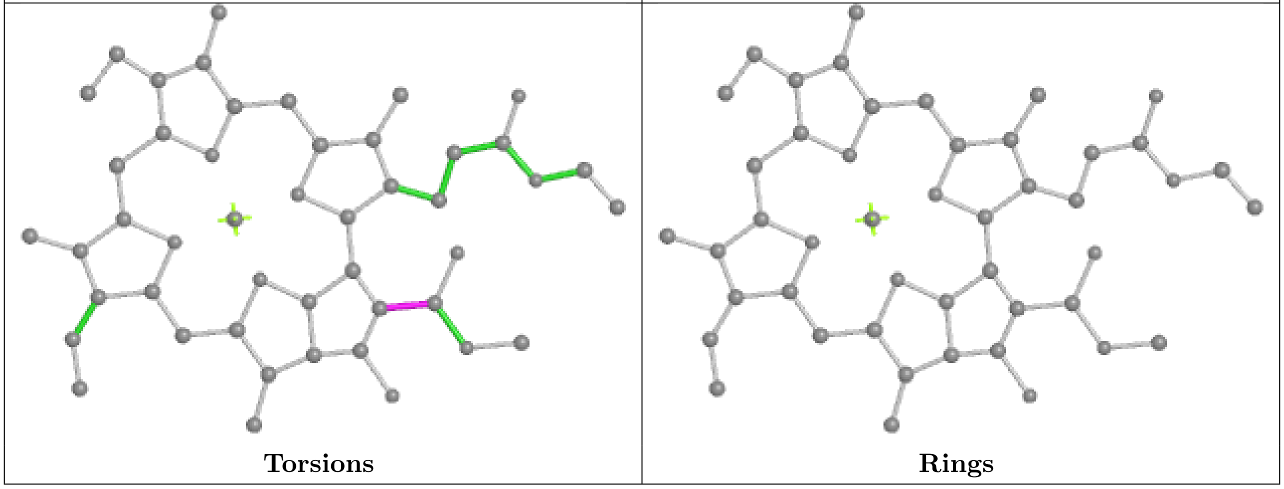
Rings

Ligand CLA cB 839



Bond lengths

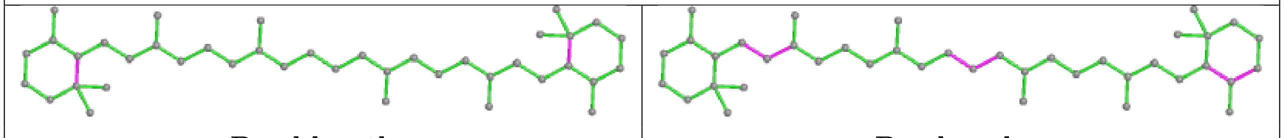
Bond angles



Torsions

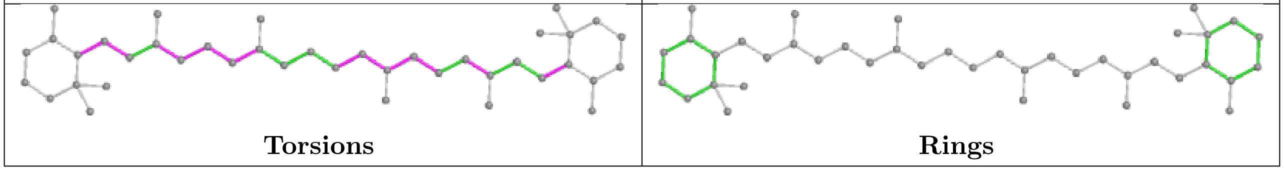
Rings

Ligand BCR cA 849



Bond lengths

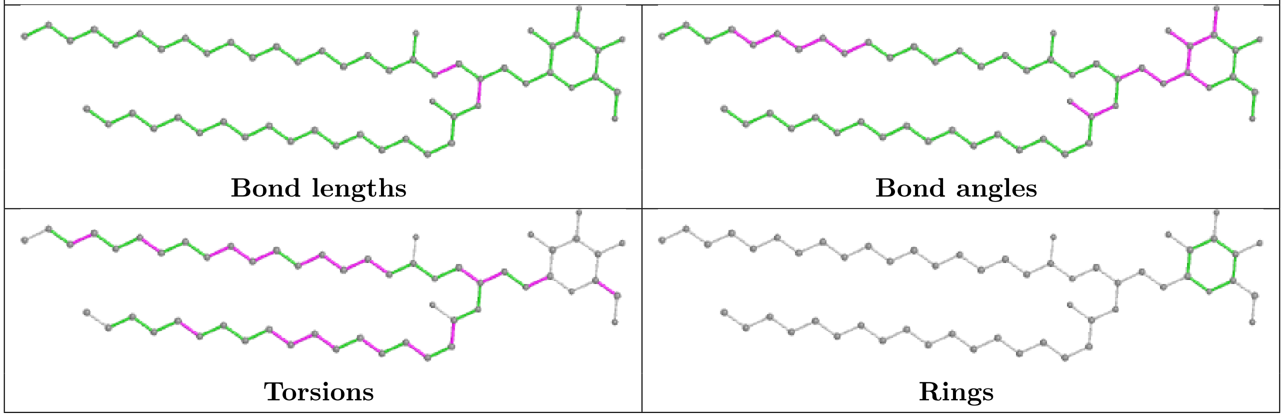
Bond angles



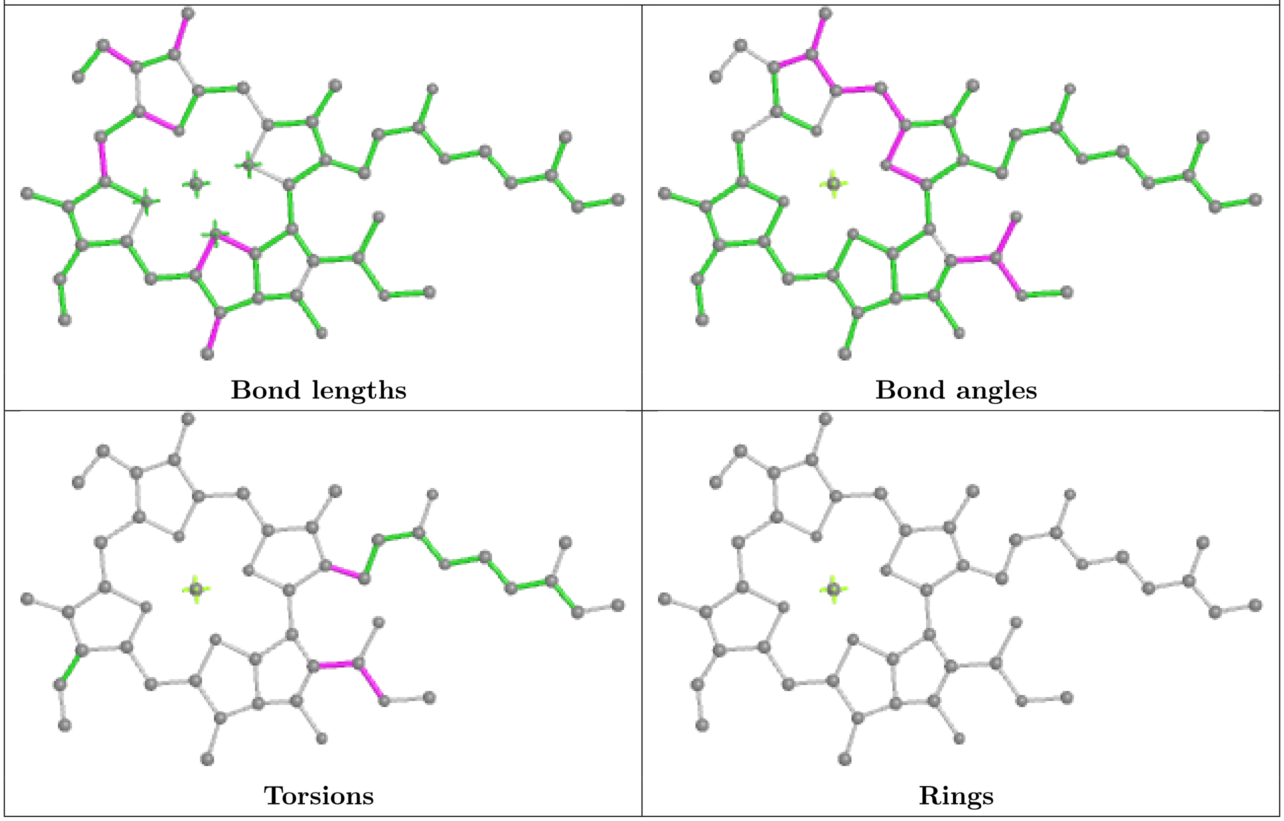
Torsions

Rings

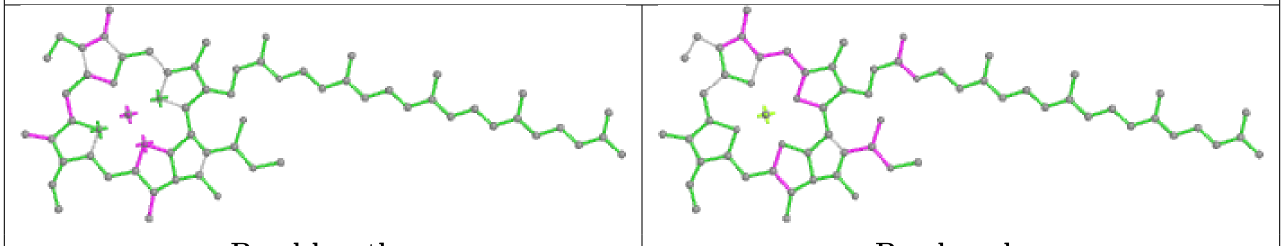
Ligand LMG bB 850



Ligand CLA cF 201

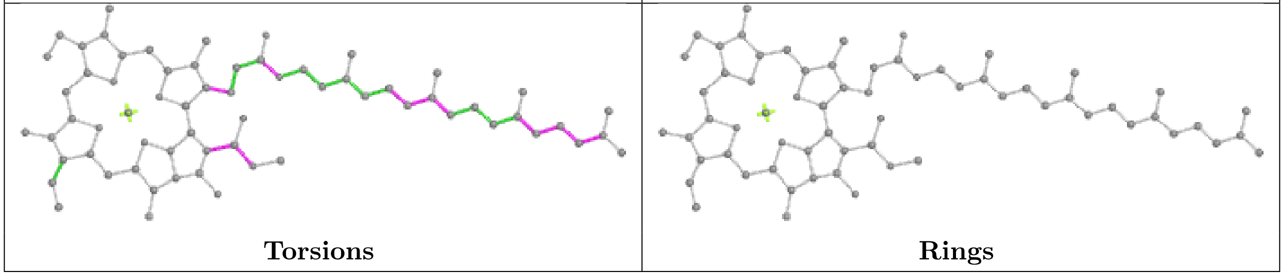


Ligand CLA dA 819



Bond lengths

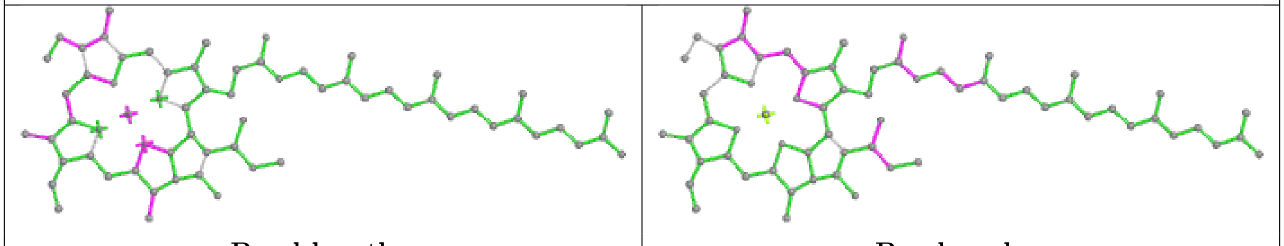
Bond angles



Torsions

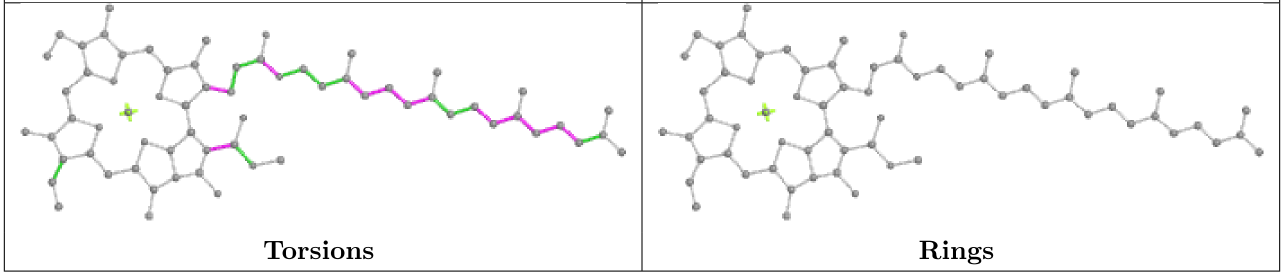
Rings

Ligand CLA bB 827



Bond lengths

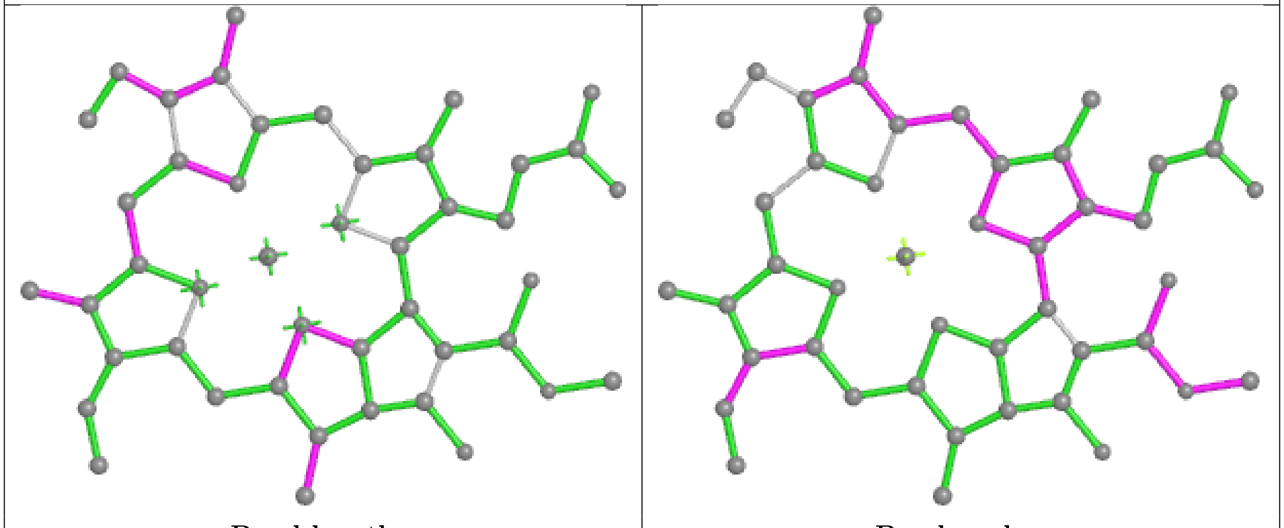
Bond angles



Torsions

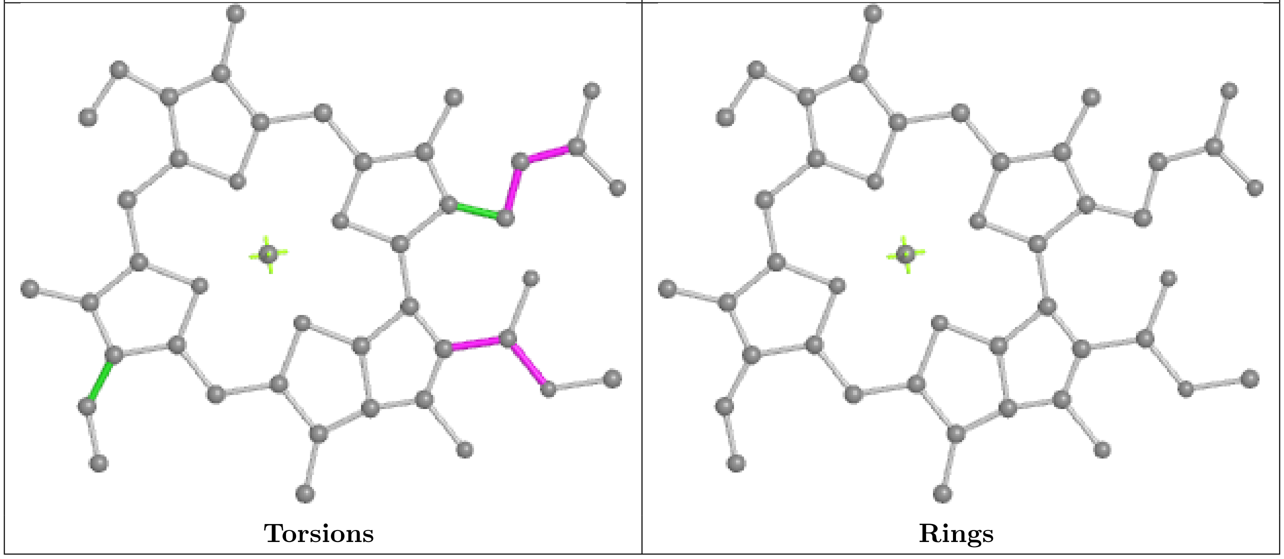
Rings

Ligand CLA aA 813



Bond lengths

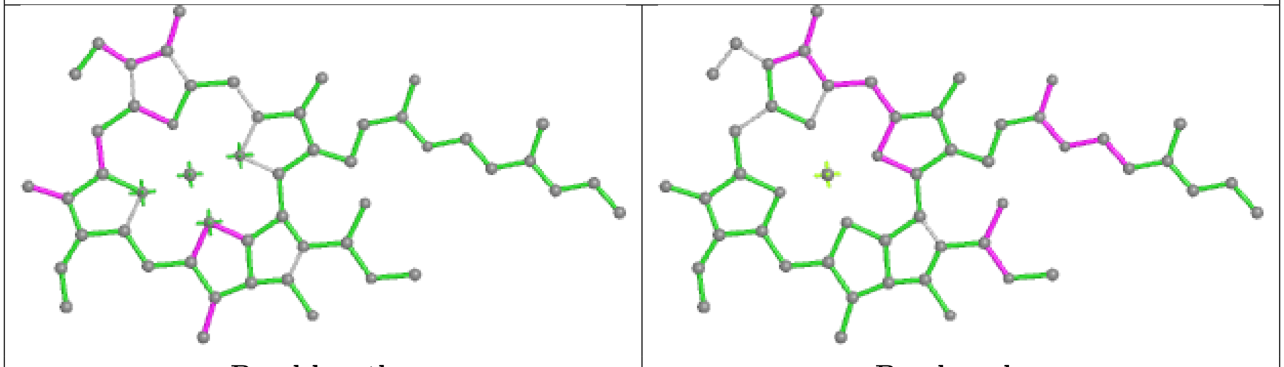
Bond angles



Torsions

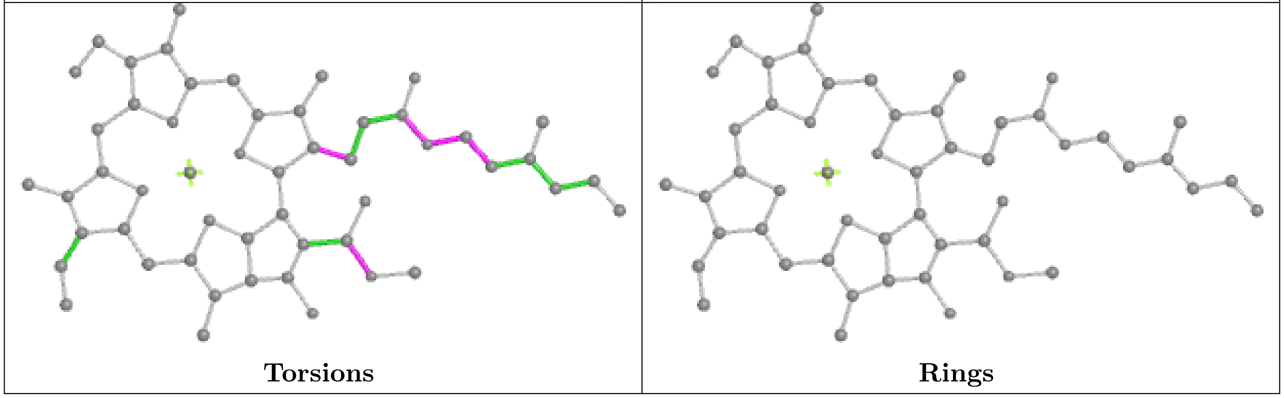
Rings

Ligand CLA dL 204



Bond lengths

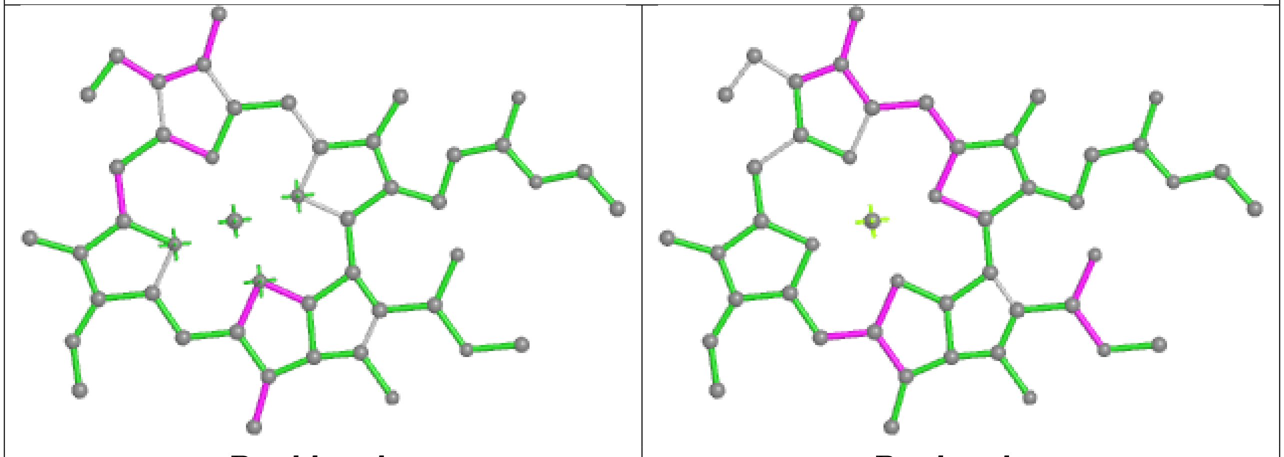
Bond angles



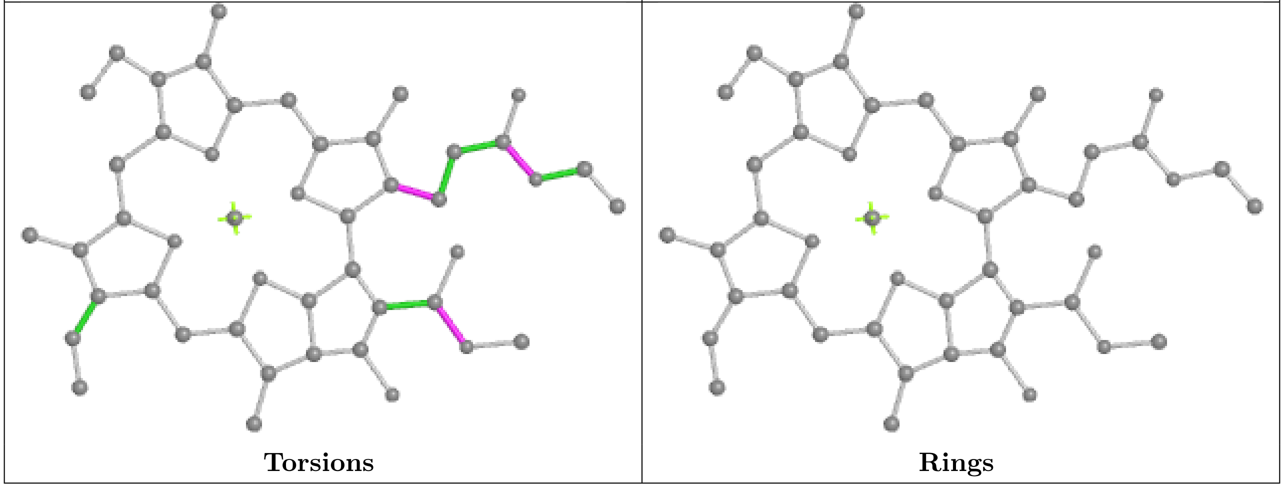
Torsions

Rings

Ligand CLA cA 824

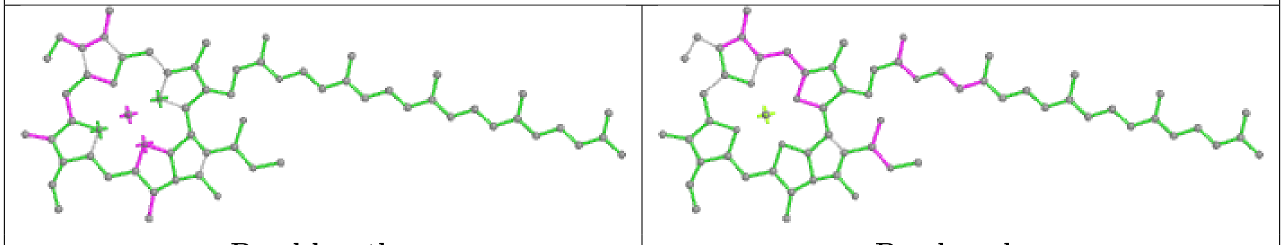


Bond lengths Bond angles

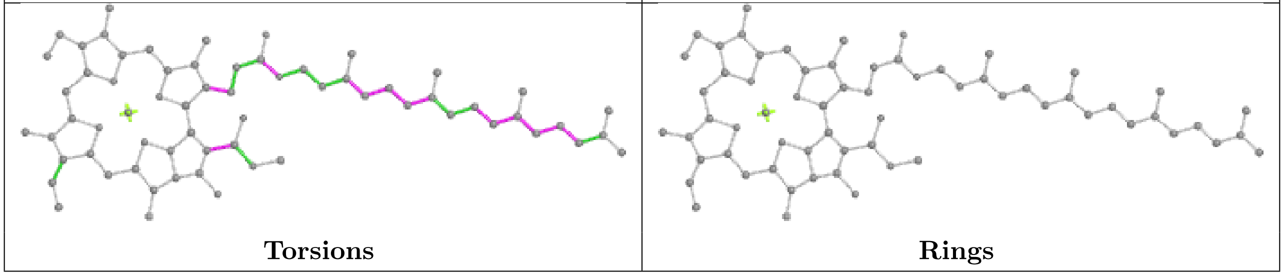


Torsions Rings

Ligand CLA aB 826

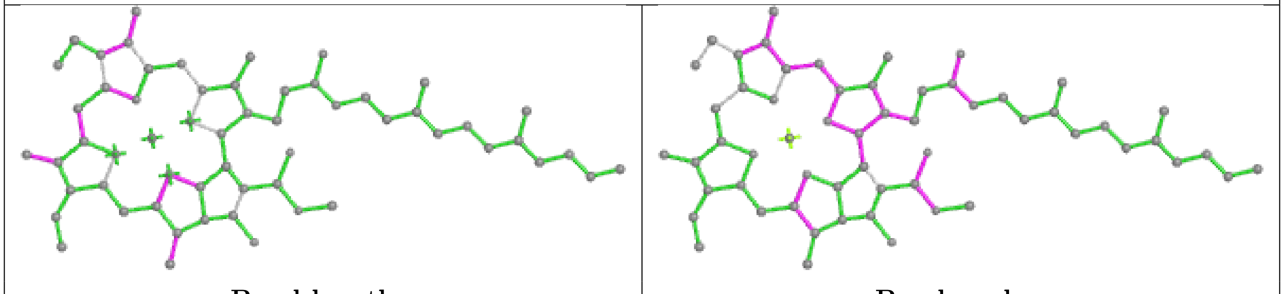


Bond lengths Bond angles



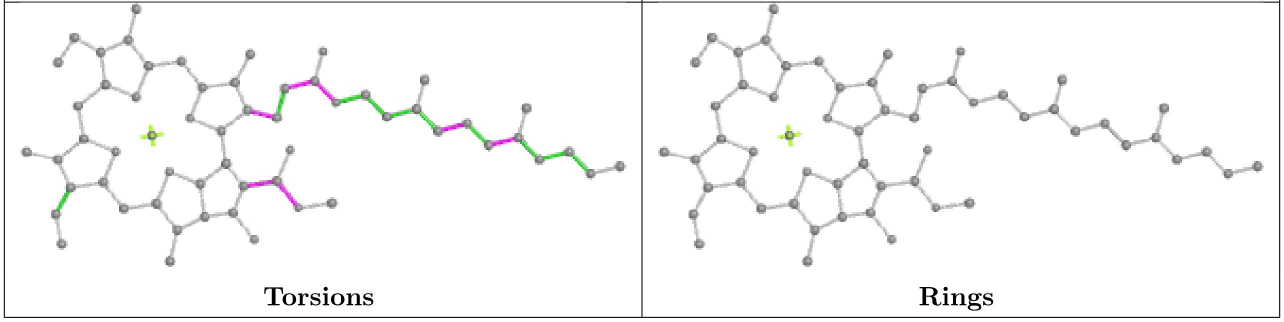
Torsions Rings

Ligand CLA bB 834



Bond lengths

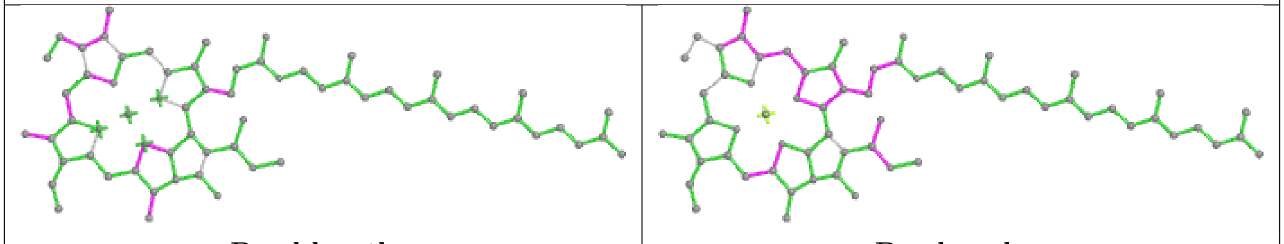
Bond angles



Torsions

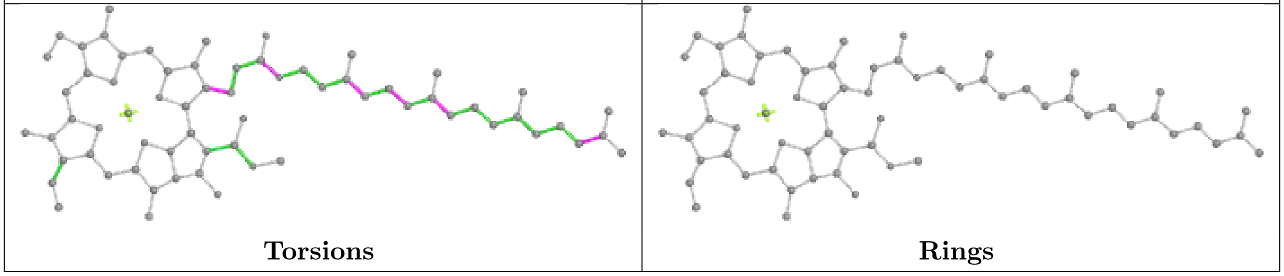
Rings

Ligand CLA bA 832



Bond lengths

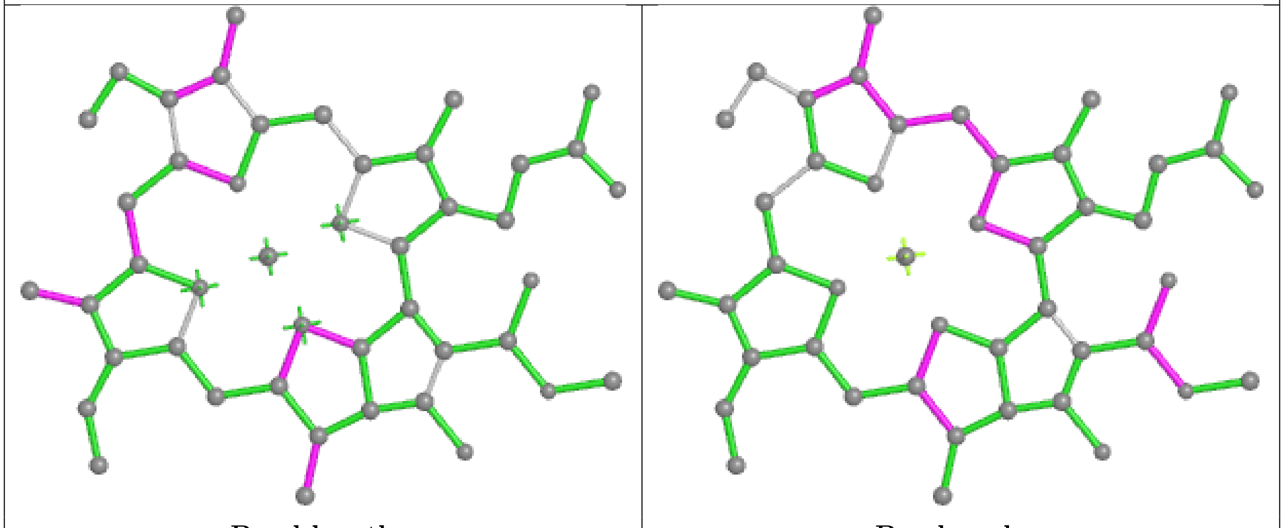
Bond angles



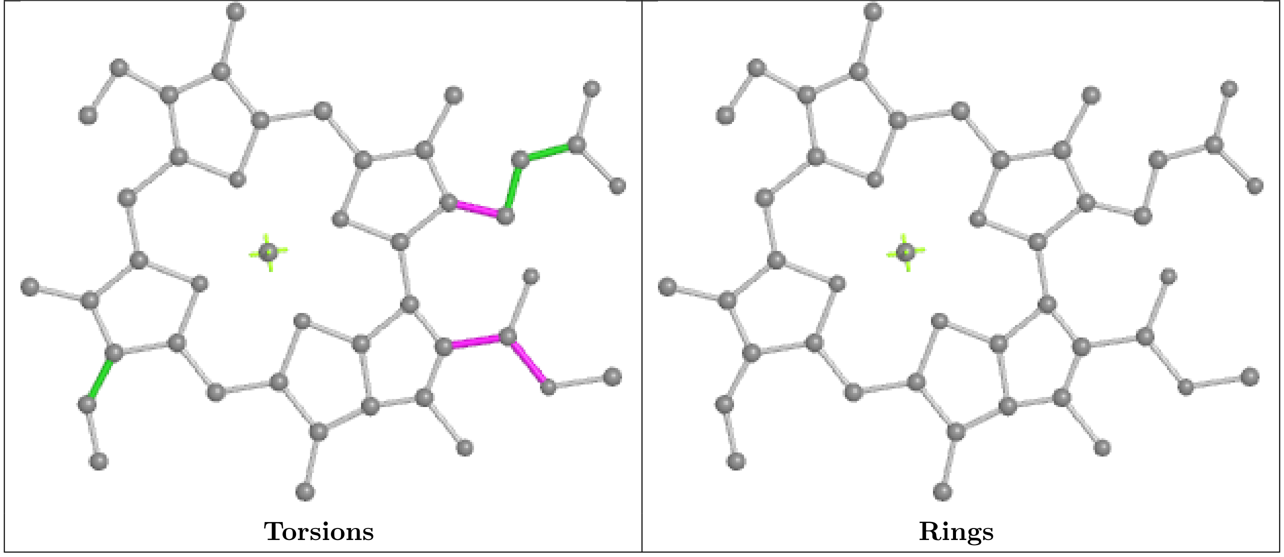
Torsions

Rings

Ligand CLA aB 811

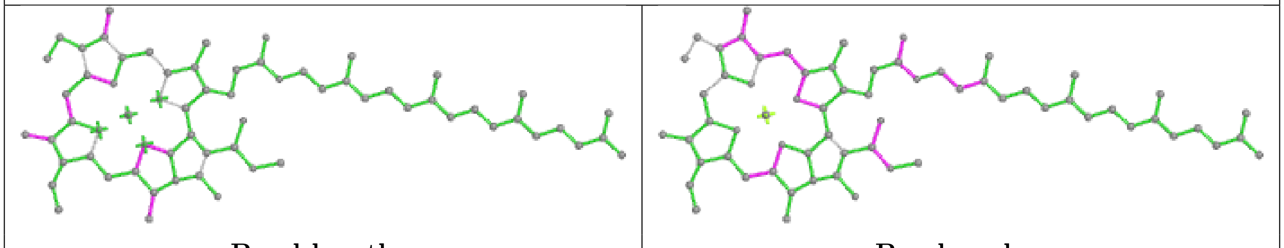


Bond lengths Bond angles

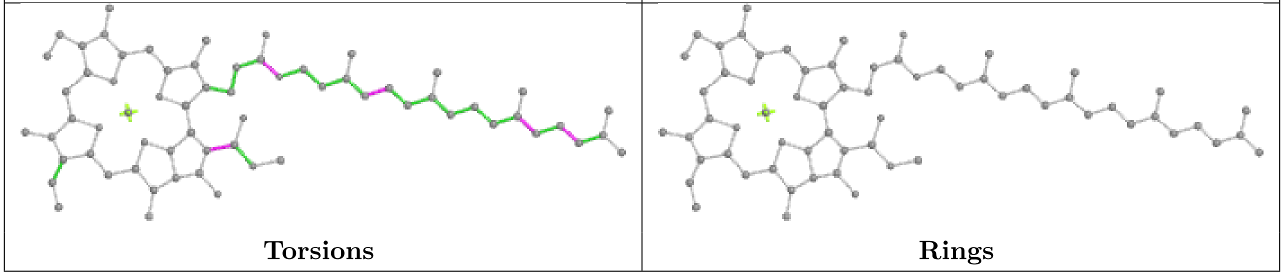


Torsions Rings

Ligand CLA dB 839

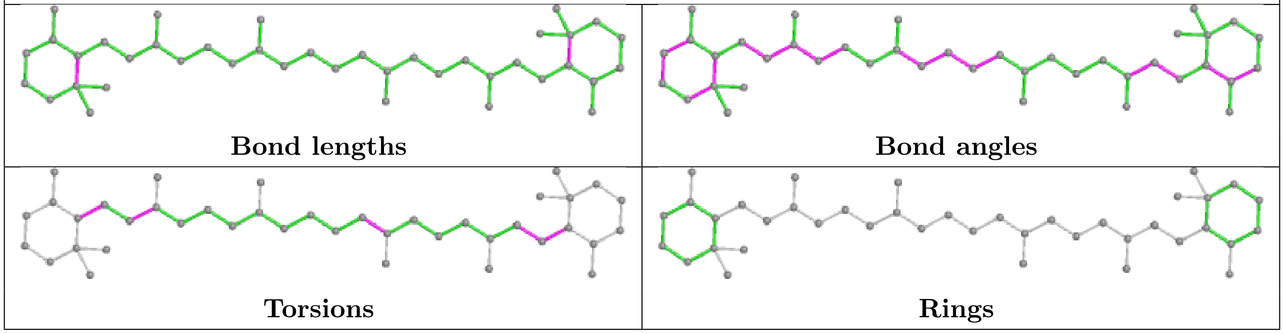


Bond lengths Bond angles



Torsions Rings

Ligand BCR aB 851



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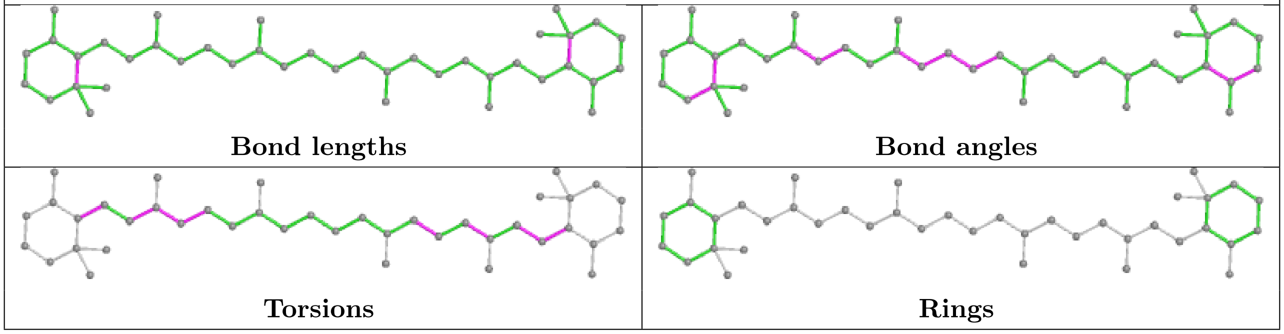
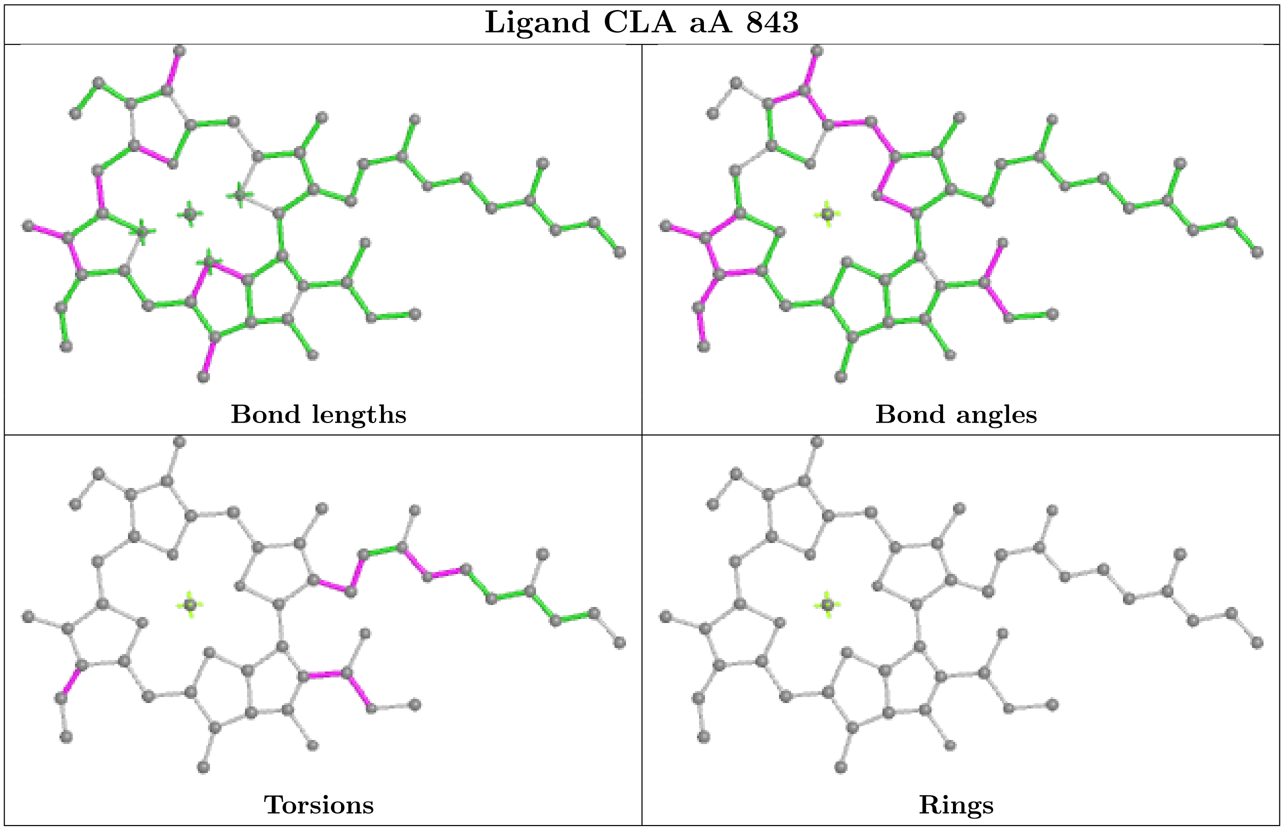
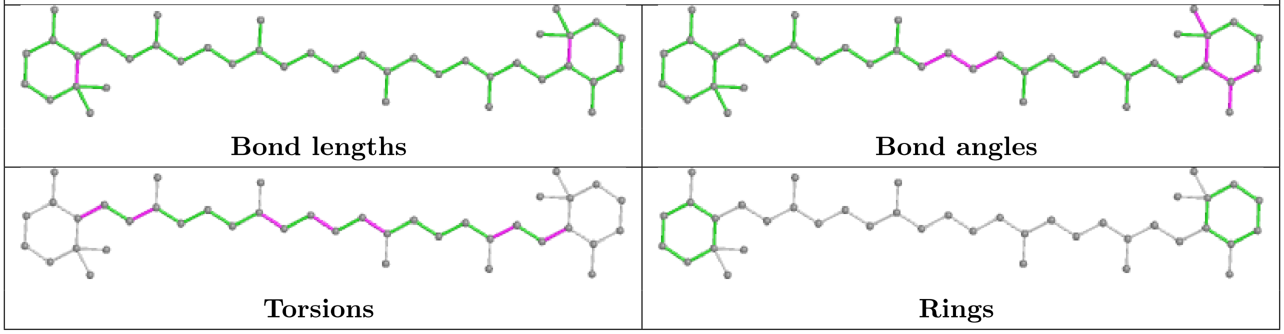


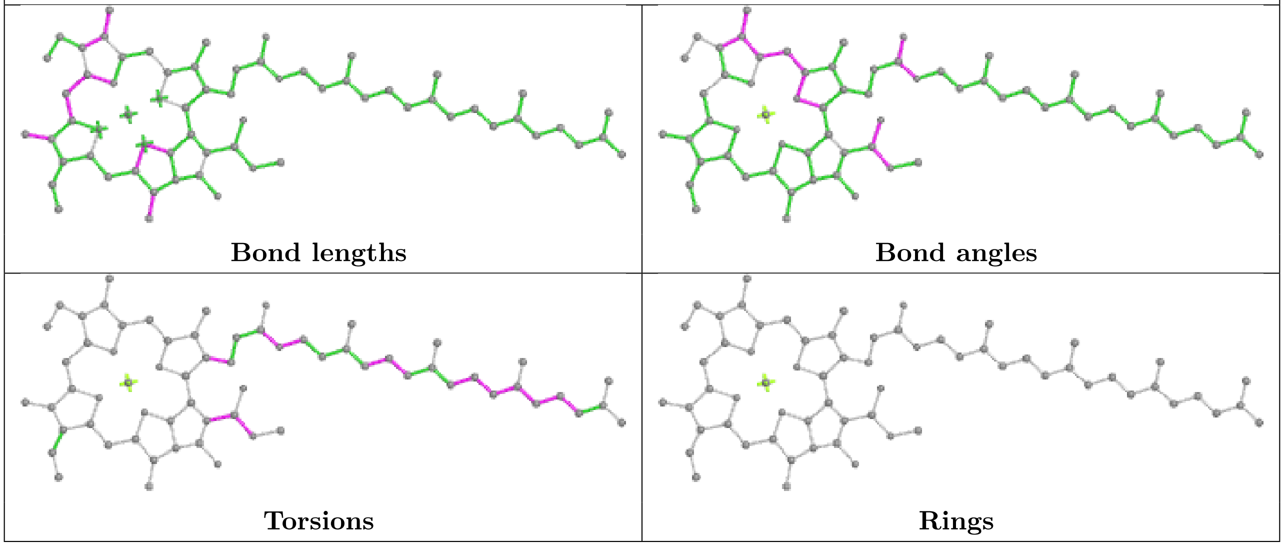
Ligand CLA aA 843



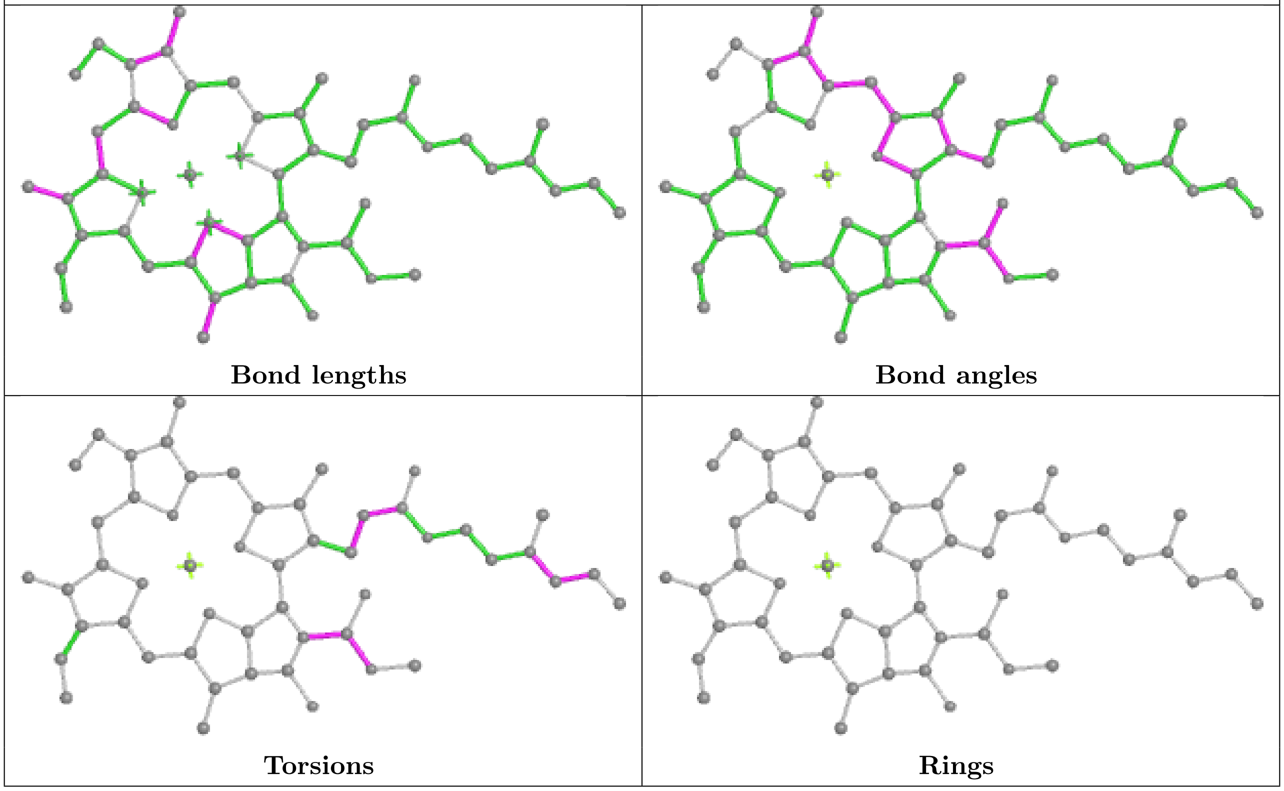
Ligand BCR bF 202



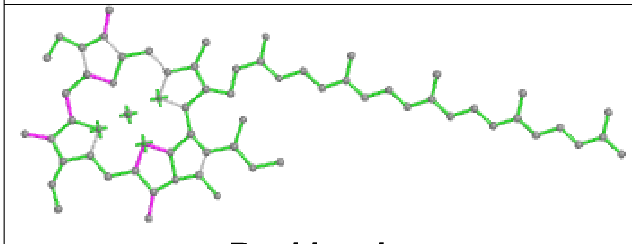
Ligand CLA cB 841



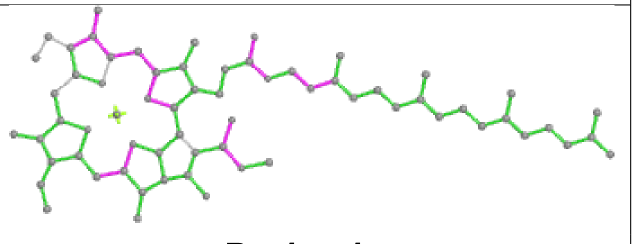
Ligand CLA aL 204



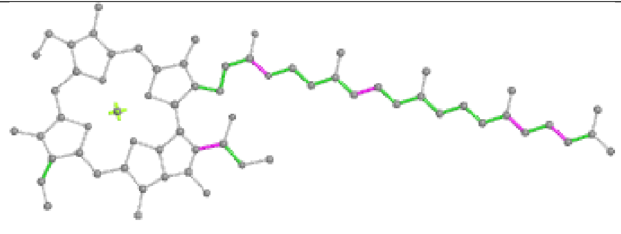
Ligand CLA bB 839



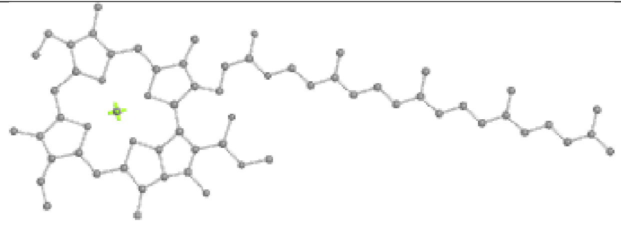
Bond lengths



Bond angles

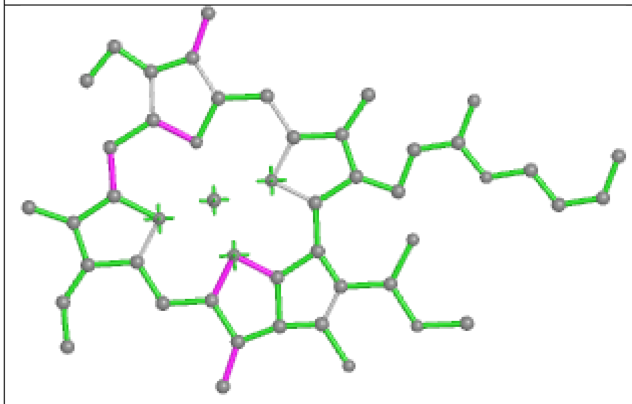


Torsions

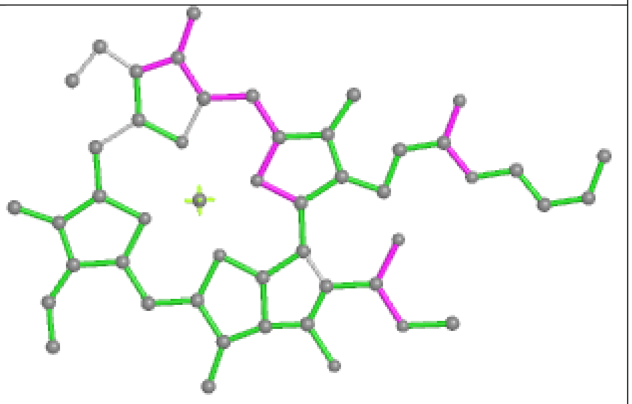


Rings

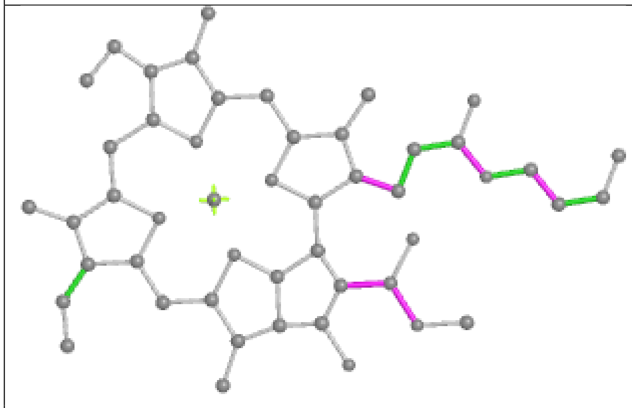
Ligand CLA bA 816



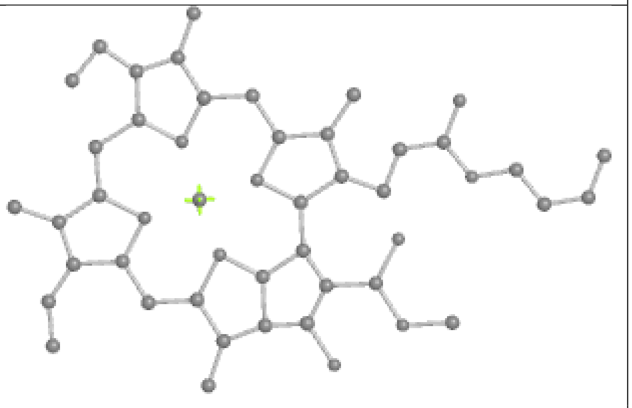
Bond lengths



Bond angles

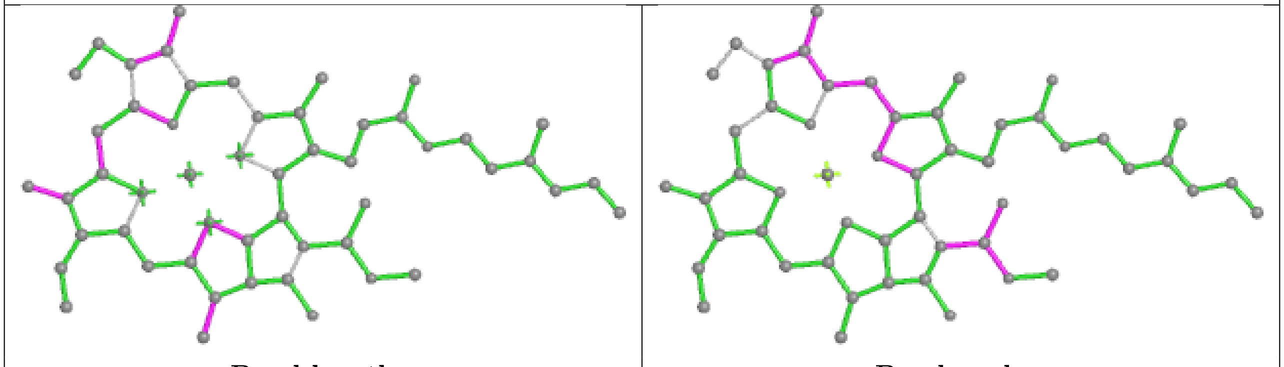


Torsions



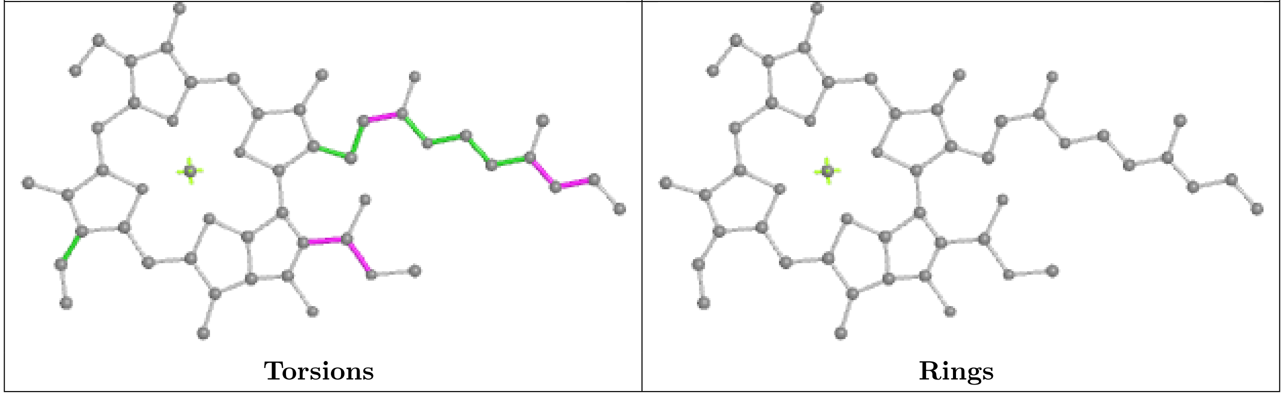
Rings

Ligand CLA cL 204



Bond lengths

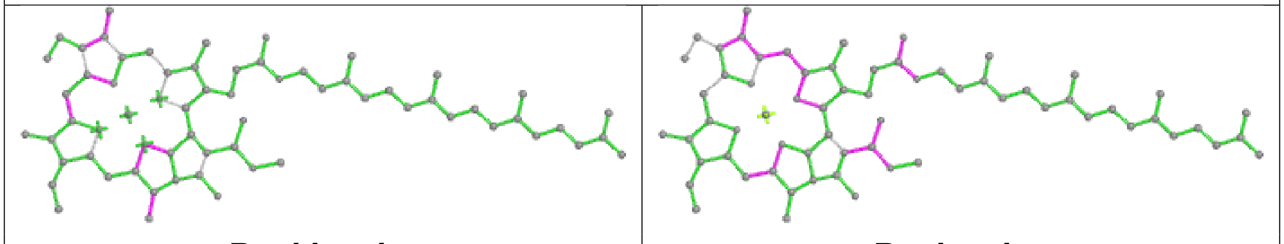
Bond angles



Torsions

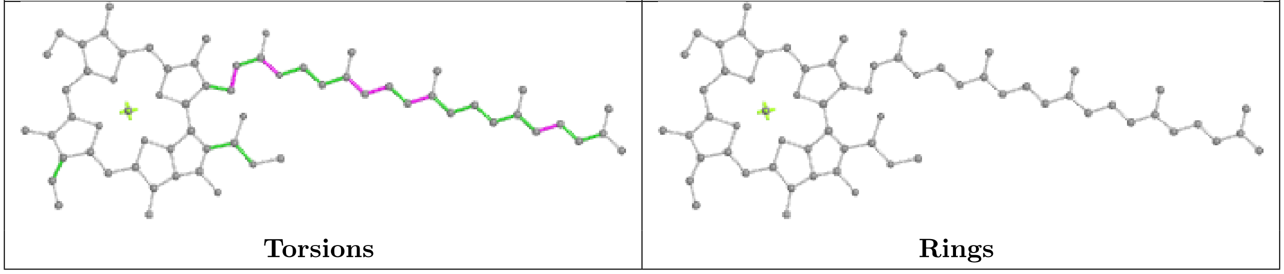
Rings

Ligand CLA cB 808



Bond lengths

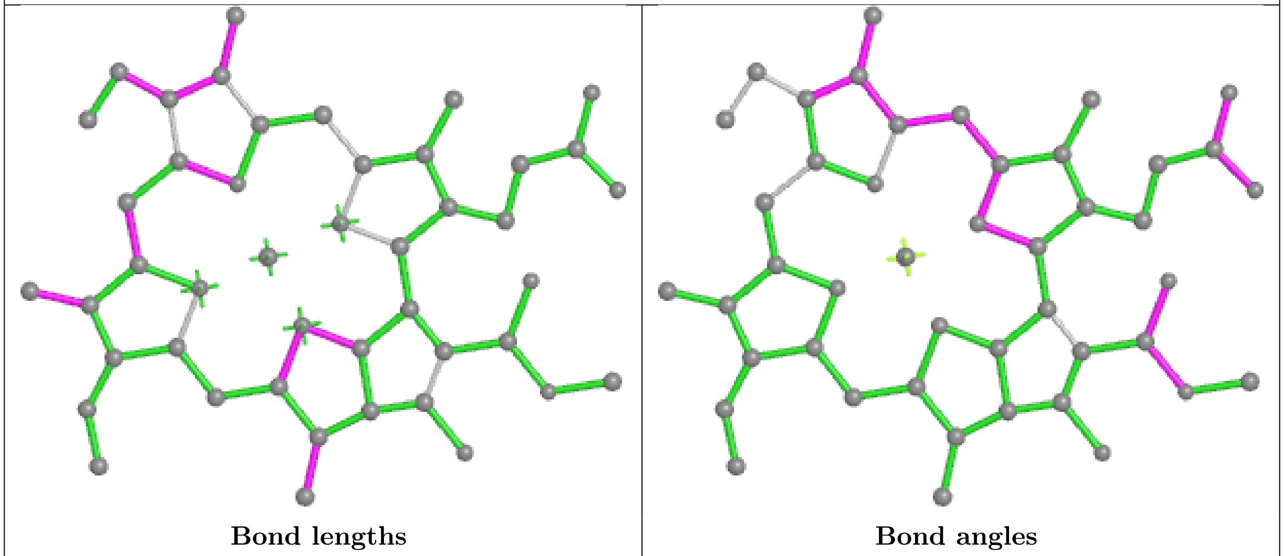
Bond angles



Torsions

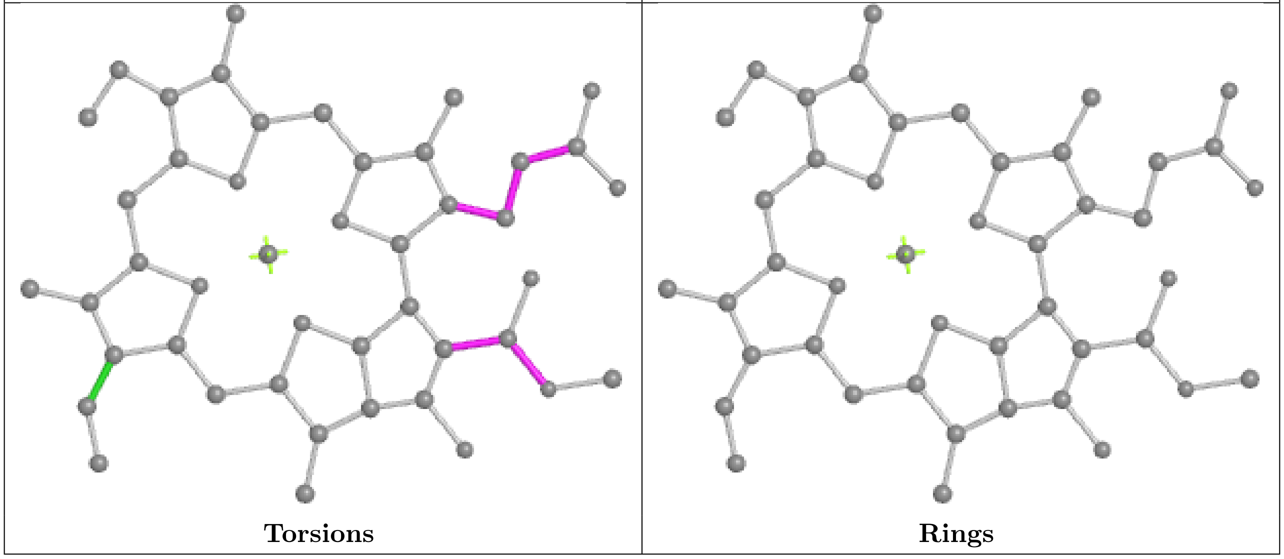
Rings

Ligand CLA cB 812



Bond lengths

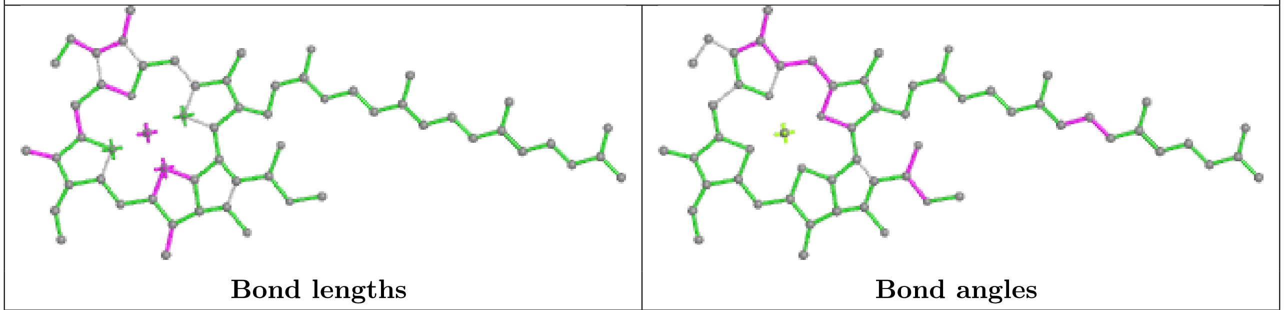
Bond angles



Torsions

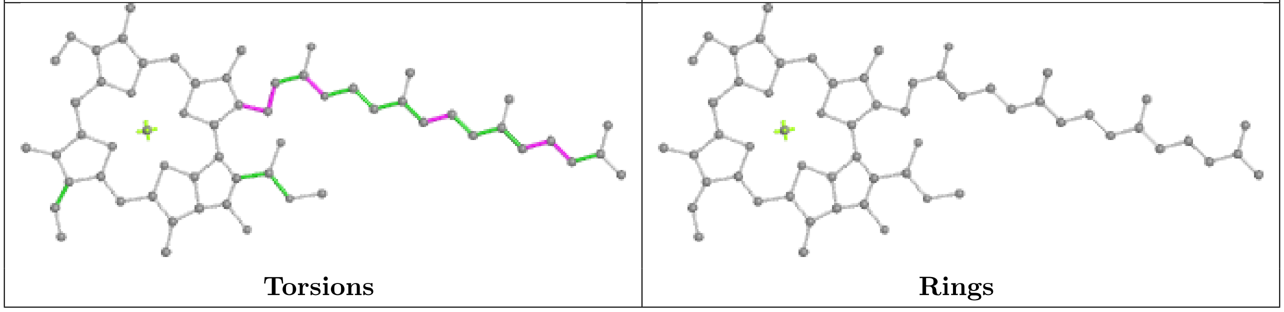
Rings

Ligand CLA dB 819



Bond lengths

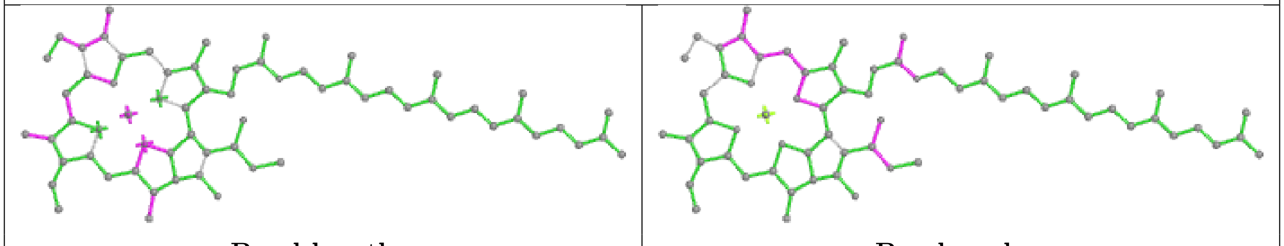
Bond angles



Torsions

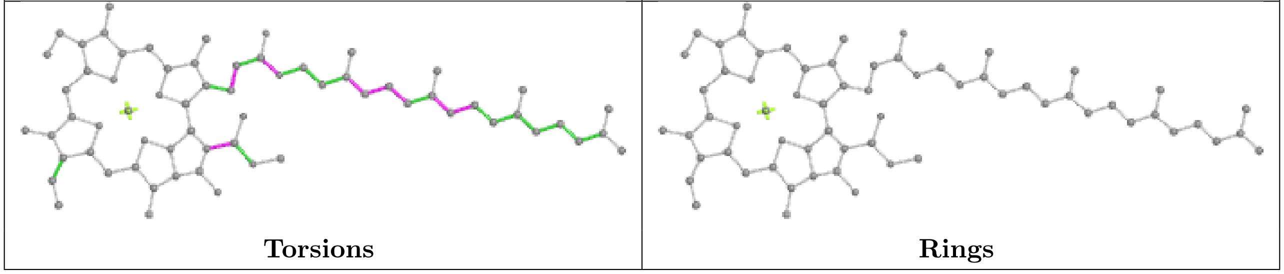
Rings

Ligand CLA aA 840



Bond lengths

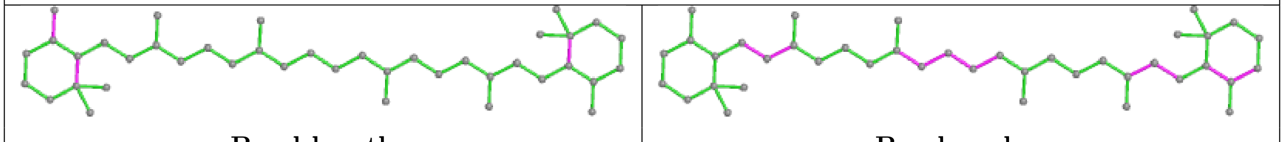
Bond angles



Torsions

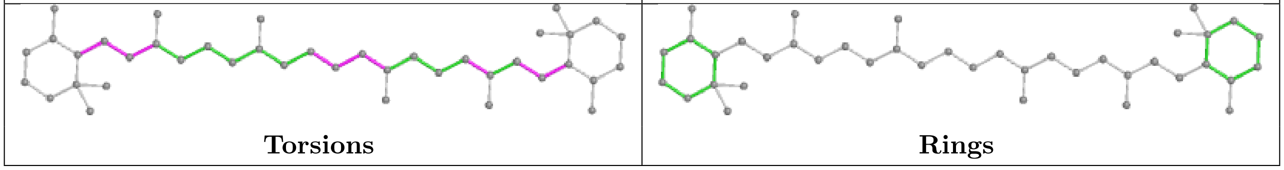
Rings

Ligand BCR cL 201



Bond lengths

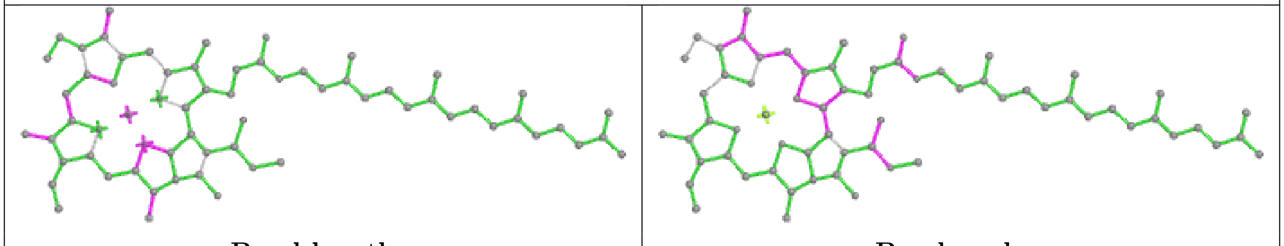
Bond angles



Torsions

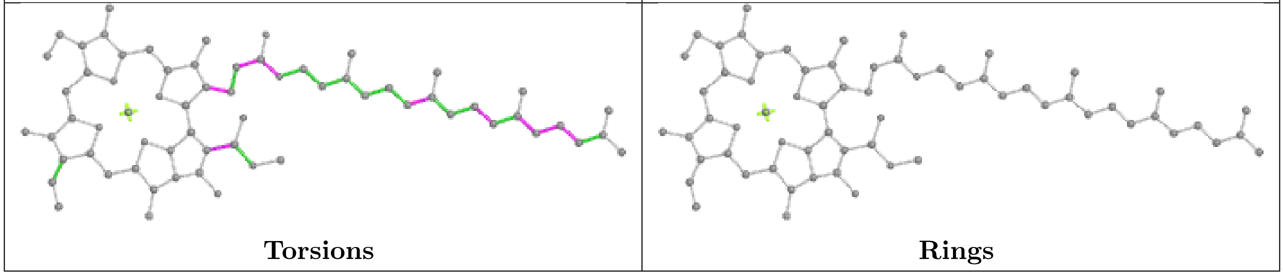
Rings

Ligand CLA bB 806



Bond lengths

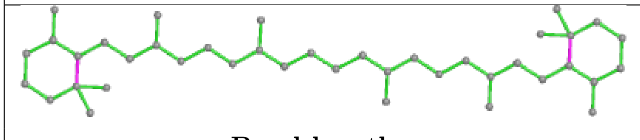
Bond angles



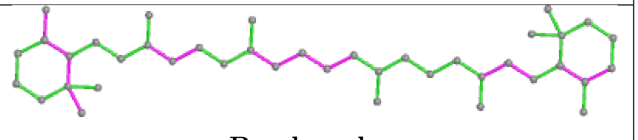
Torsions

Rings

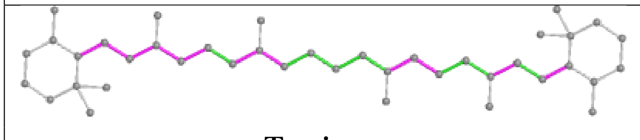
Ligand BCR dJ 103



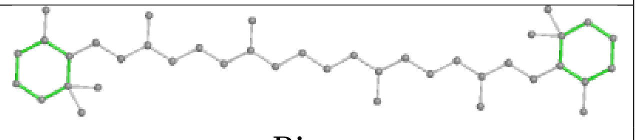
Bond lengths



Bond angles

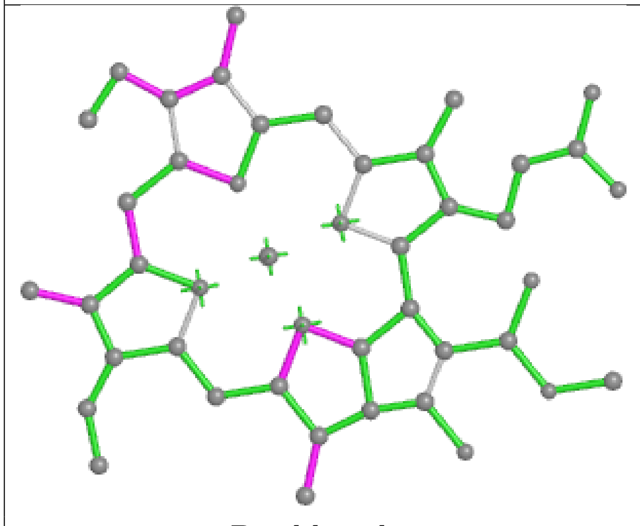


Torsions

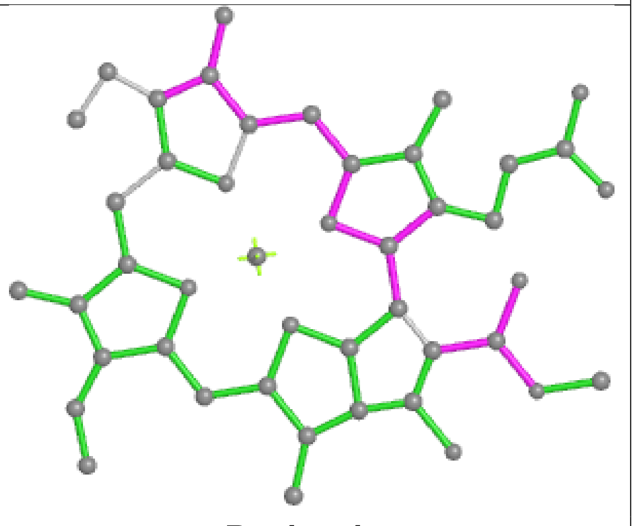


Rings

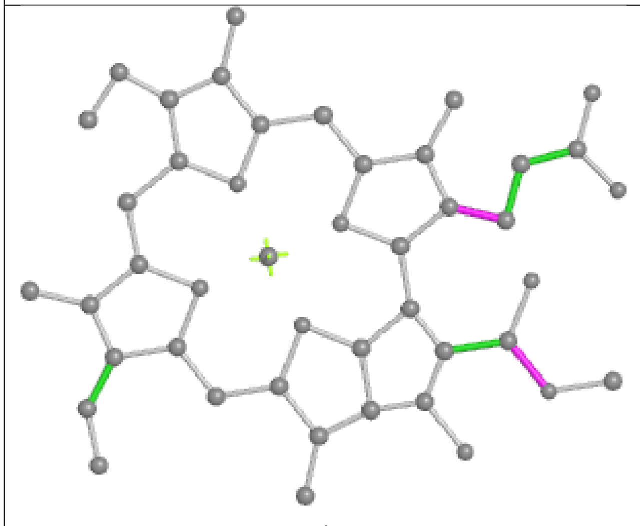
Ligand CLA aA 804



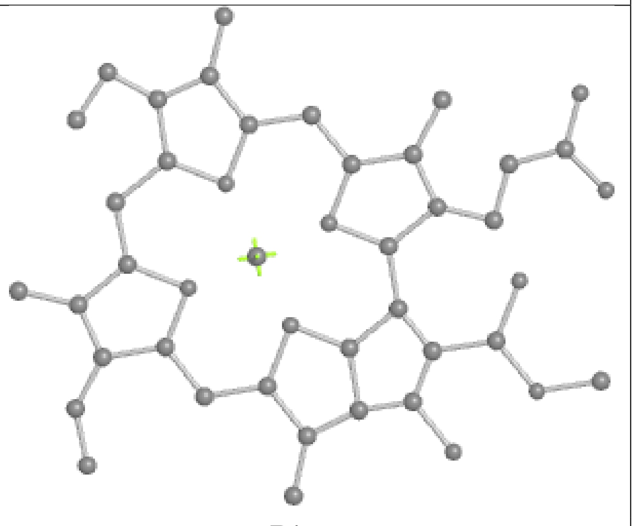
Bond lengths



Bond angles

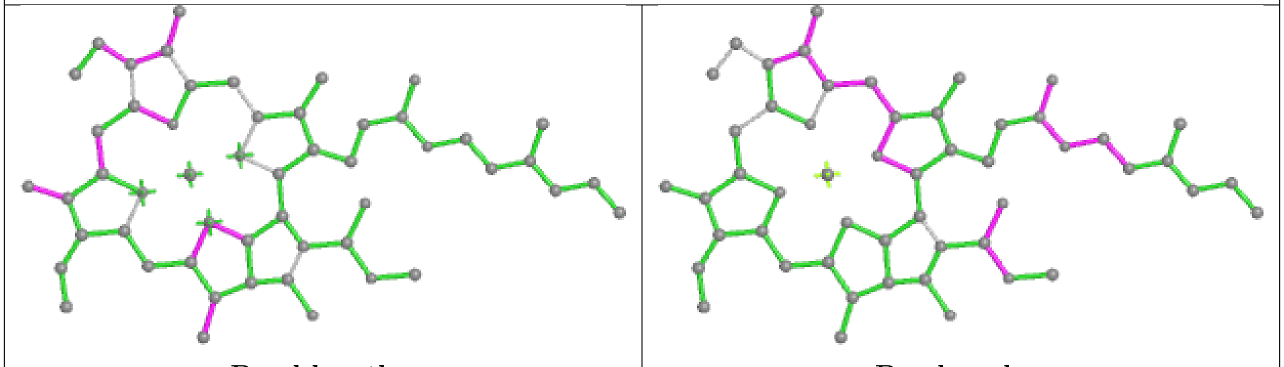


Torsions

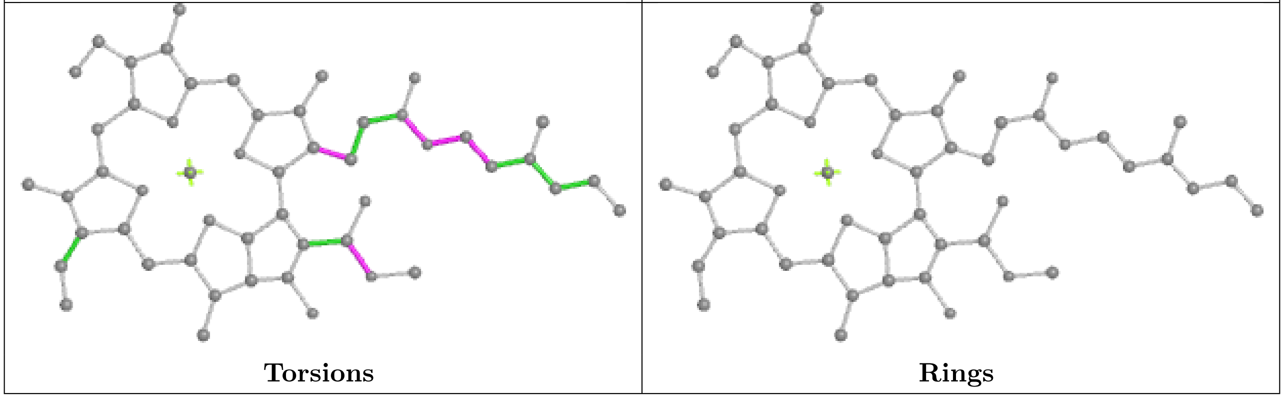


Rings

Ligand CLA bL 204

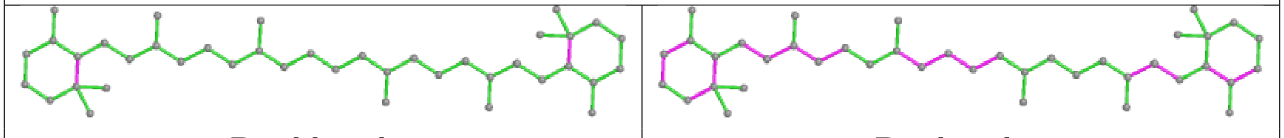


Bond lengths Bond angles

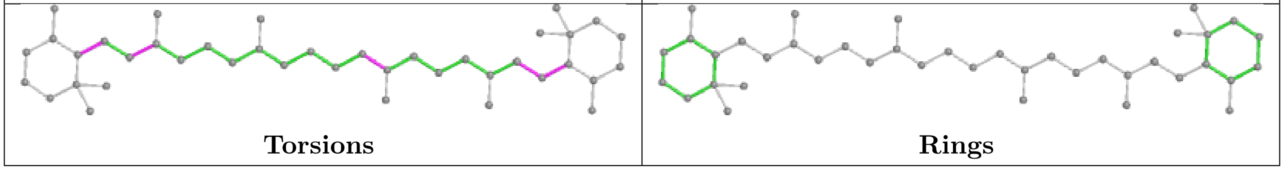


Torsions Rings

Ligand BCR dB 852

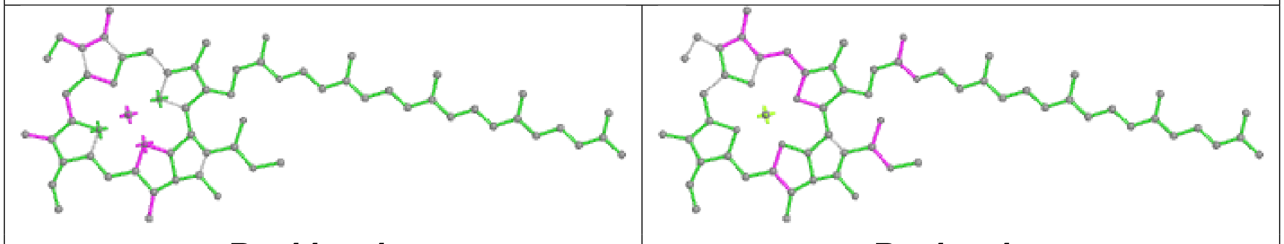


Bond lengths Bond angles

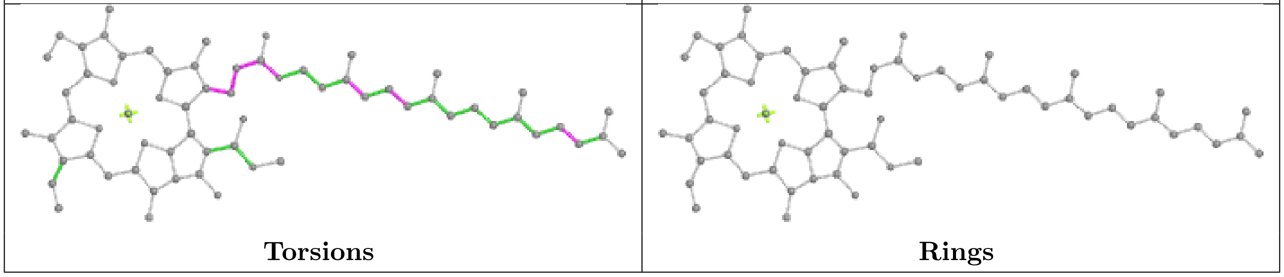


Torsions Rings

Ligand CLA cB 828

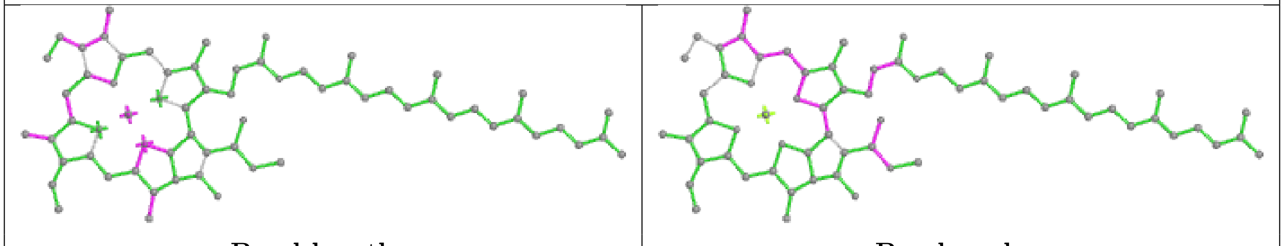


Bond lengths Bond angles



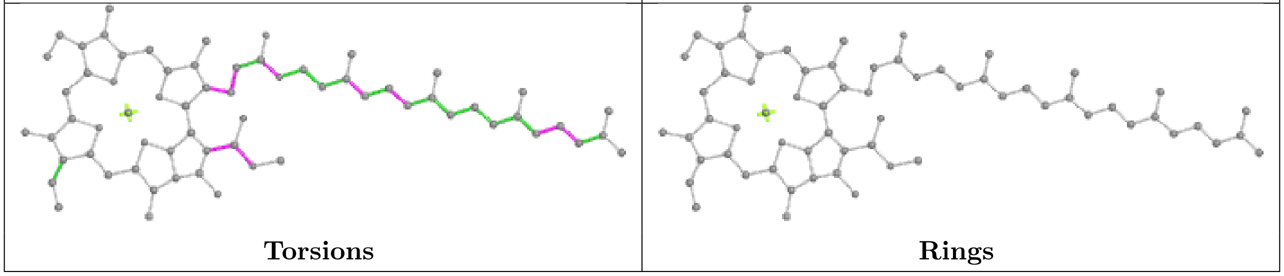
Torsions Rings

Ligand CLA bB 801



Bond lengths

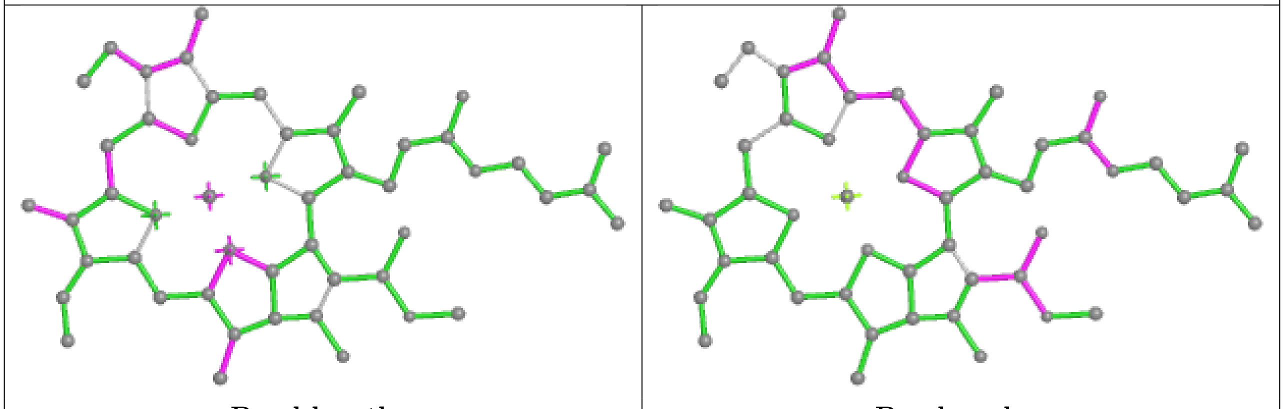
Bond angles



Torsions

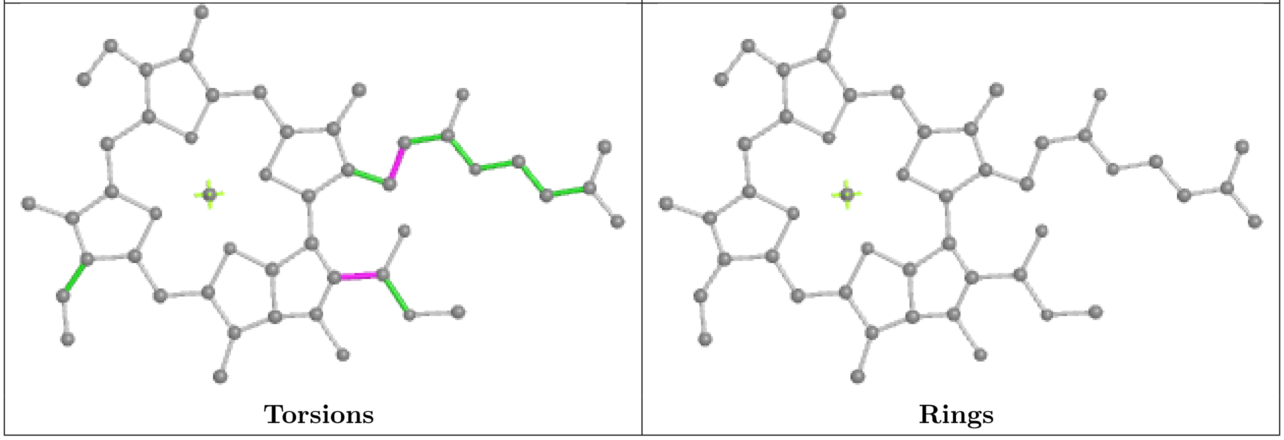
Rings

Ligand CLA cA 831



Bond lengths

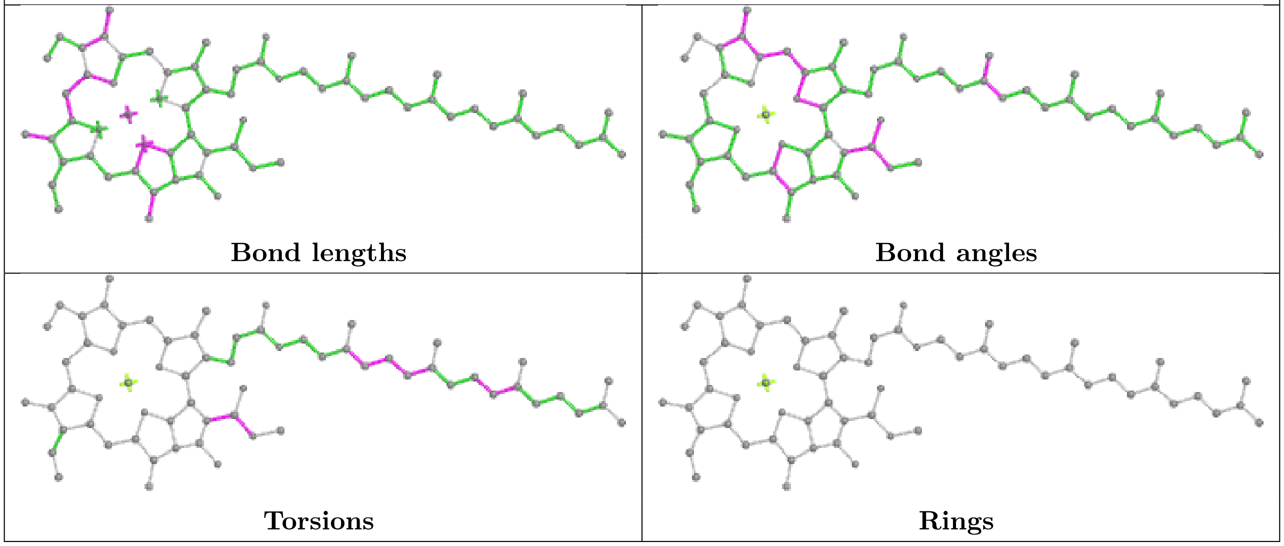
Bond angles



Torsions

Rings

Ligand CLA dB 830



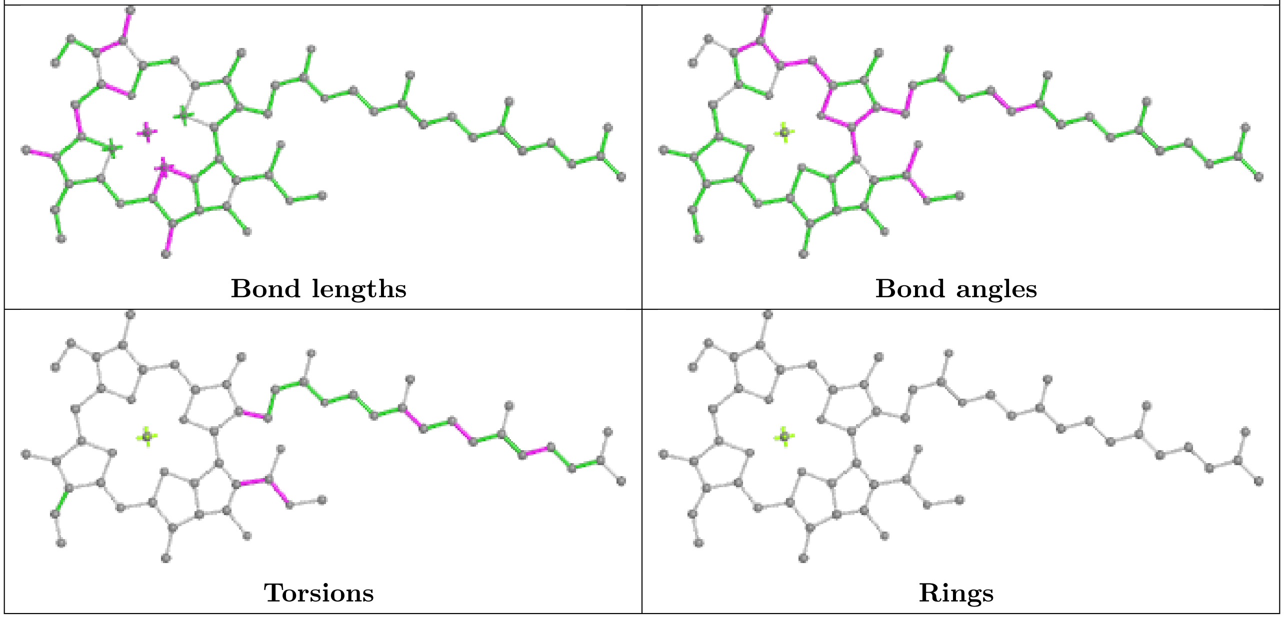
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA dB 838



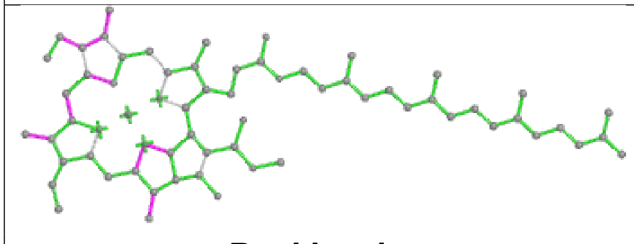
Bond lengths

Bond angles

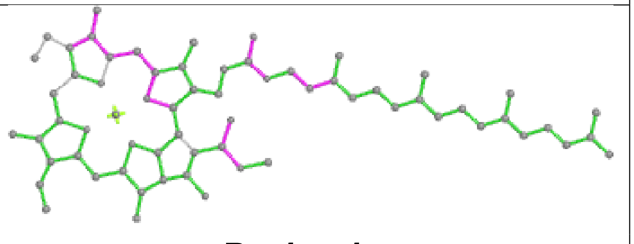
Torsions

Rings

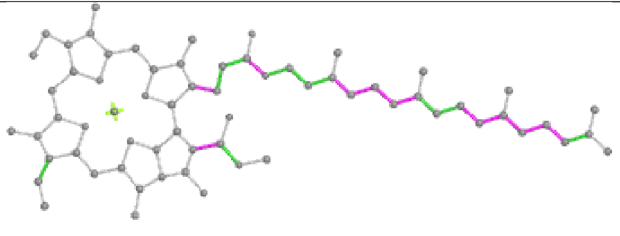
Ligand CLA dB 827



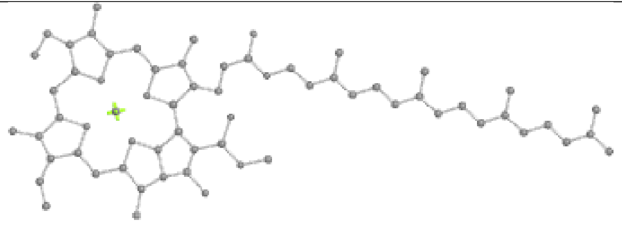
Bond lengths



Bond angles

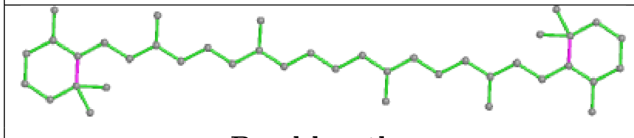


Torsions

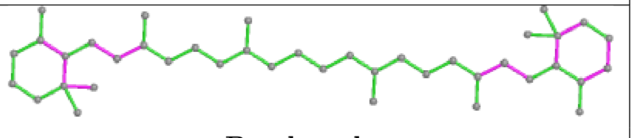


Rings

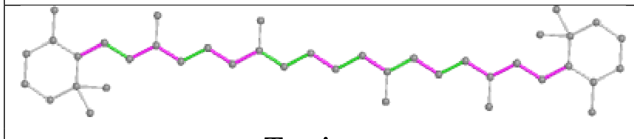
Ligand BCR bA 849



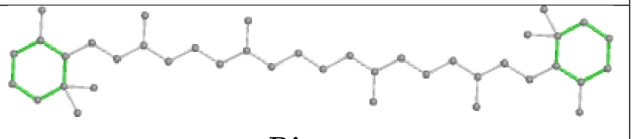
Bond lengths



Bond angles

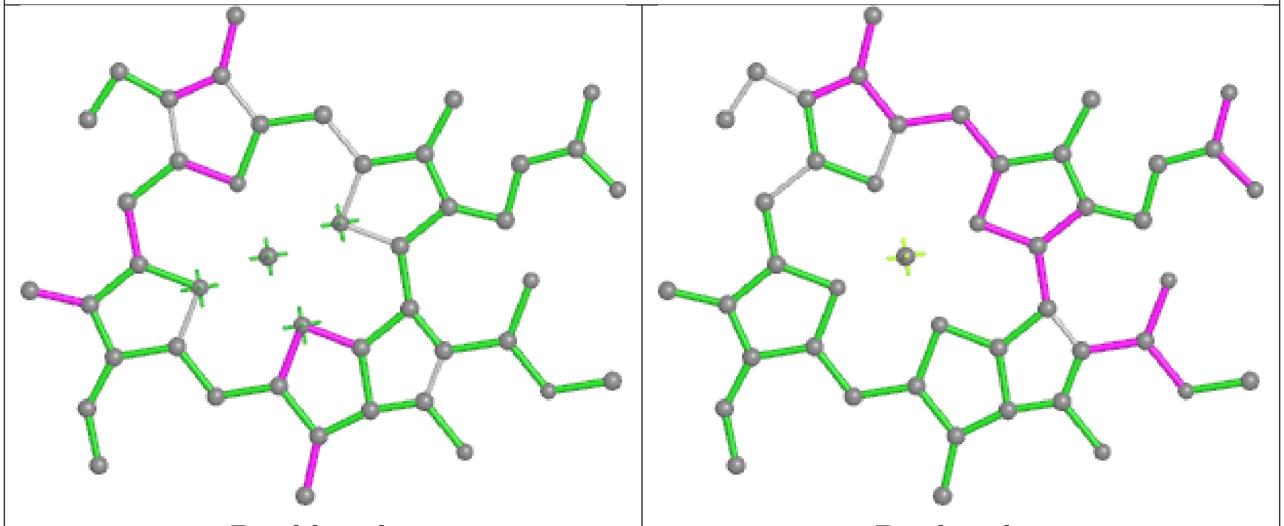


Torsions



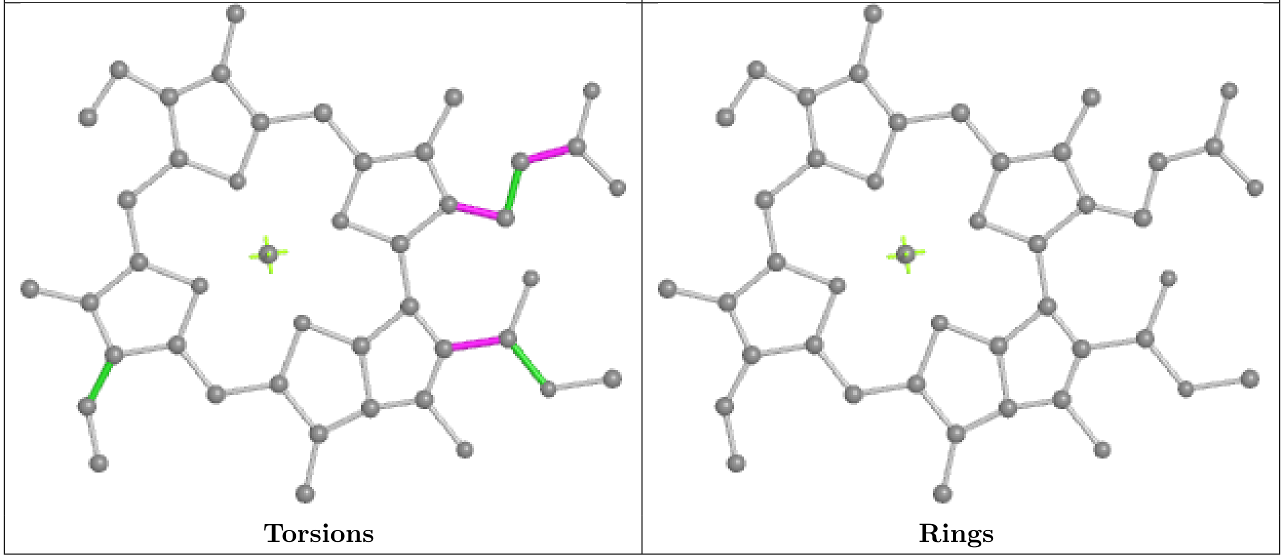
Rings

Ligand CLA aA 803



Bond lengths

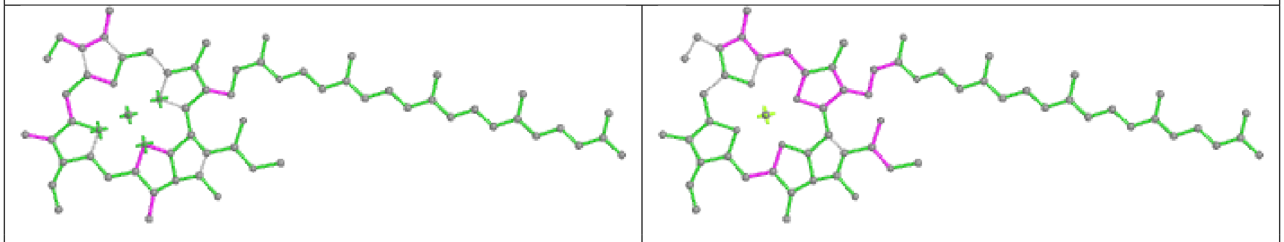
Bond angles



Torsions

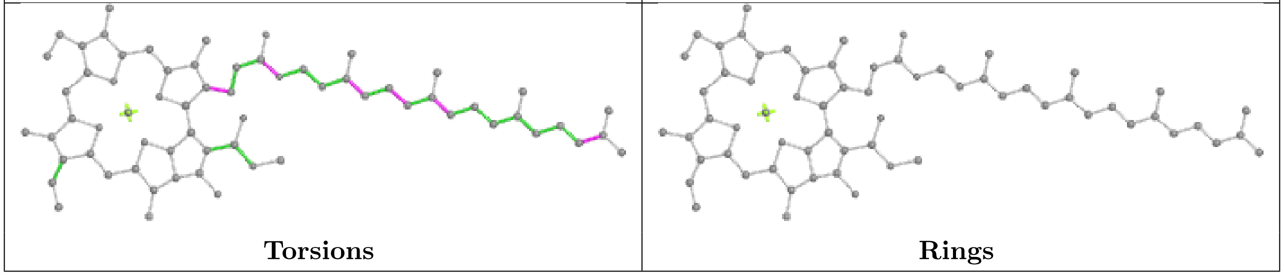
Rings

Ligand CLA dA 832



Bond lengths

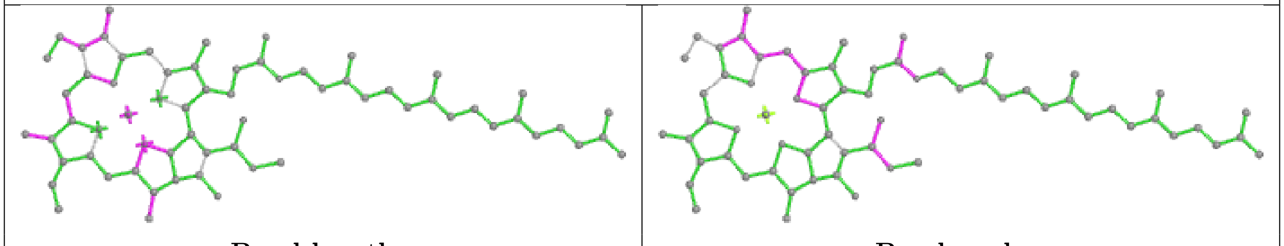
Bond angles



Torsions

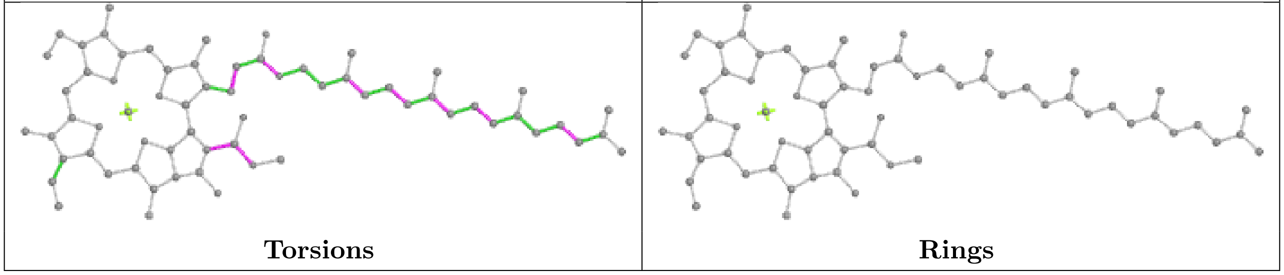
Rings

Ligand CLA cA 821



Bond lengths

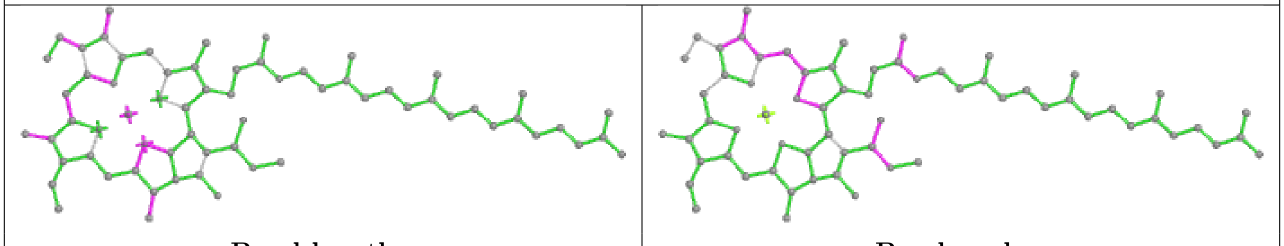
Bond angles



Torsions

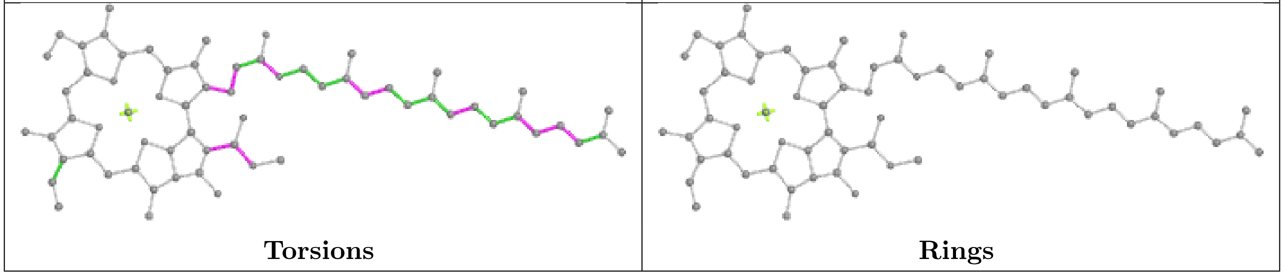
Rings

Ligand CLA dB 803



Bond lengths

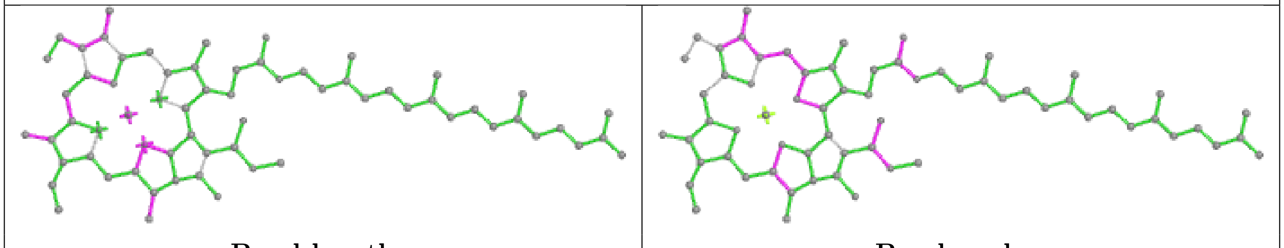
Bond angles



Torsions

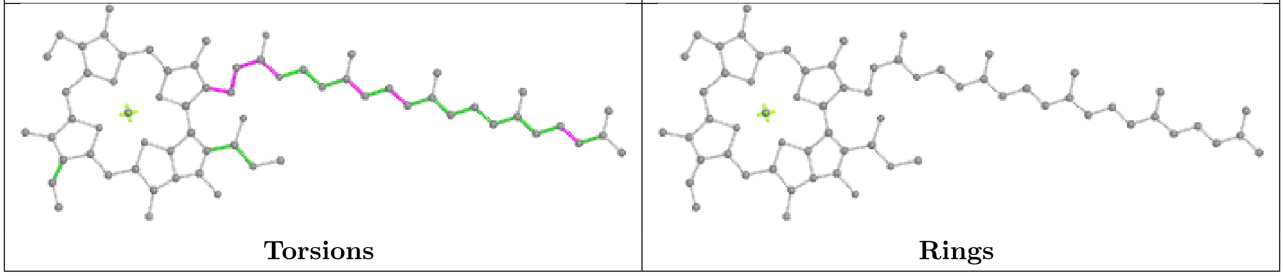
Rings

Ligand CLA aB 828



Bond lengths

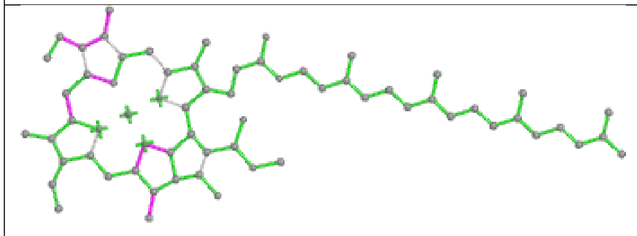
Bond angles



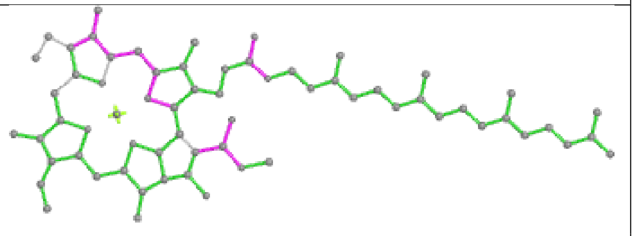
Torsions

Rings

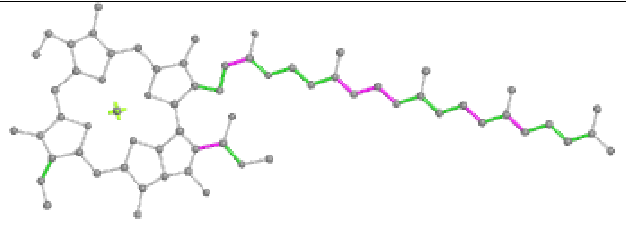
Ligand CLA dA 839



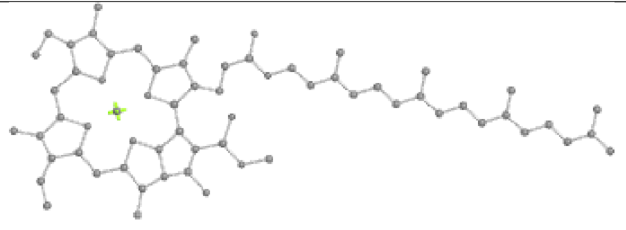
Bond lengths



Bond angles

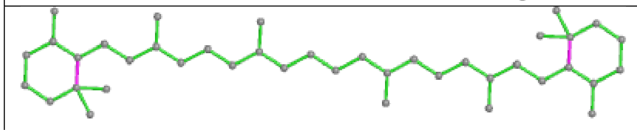


Torsions

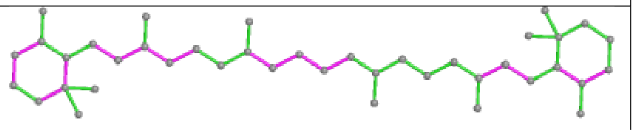


Rings

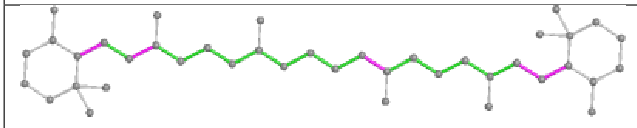
Ligand BCR bB 852



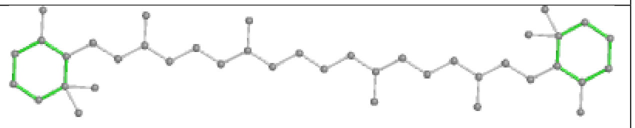
Bond lengths



Bond angles

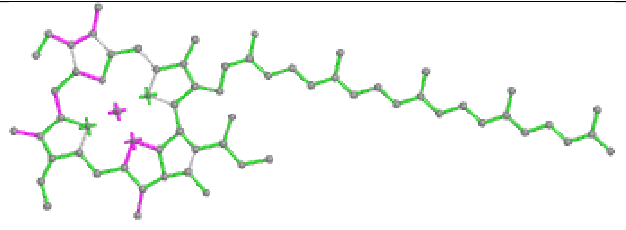


Torsions

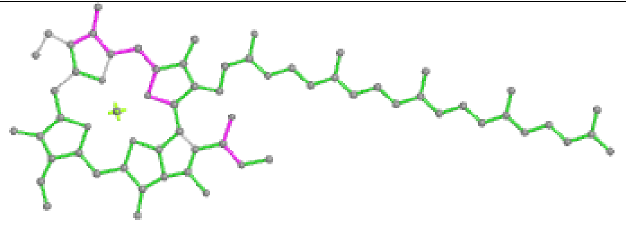


Rings

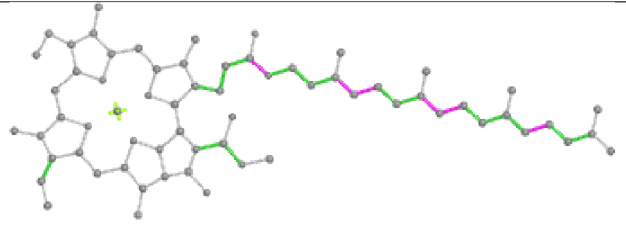
Ligand CLA bB 810



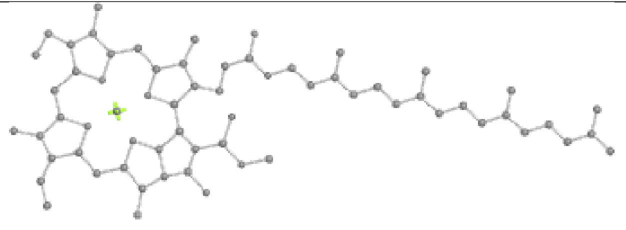
Bond lengths



Bond angles

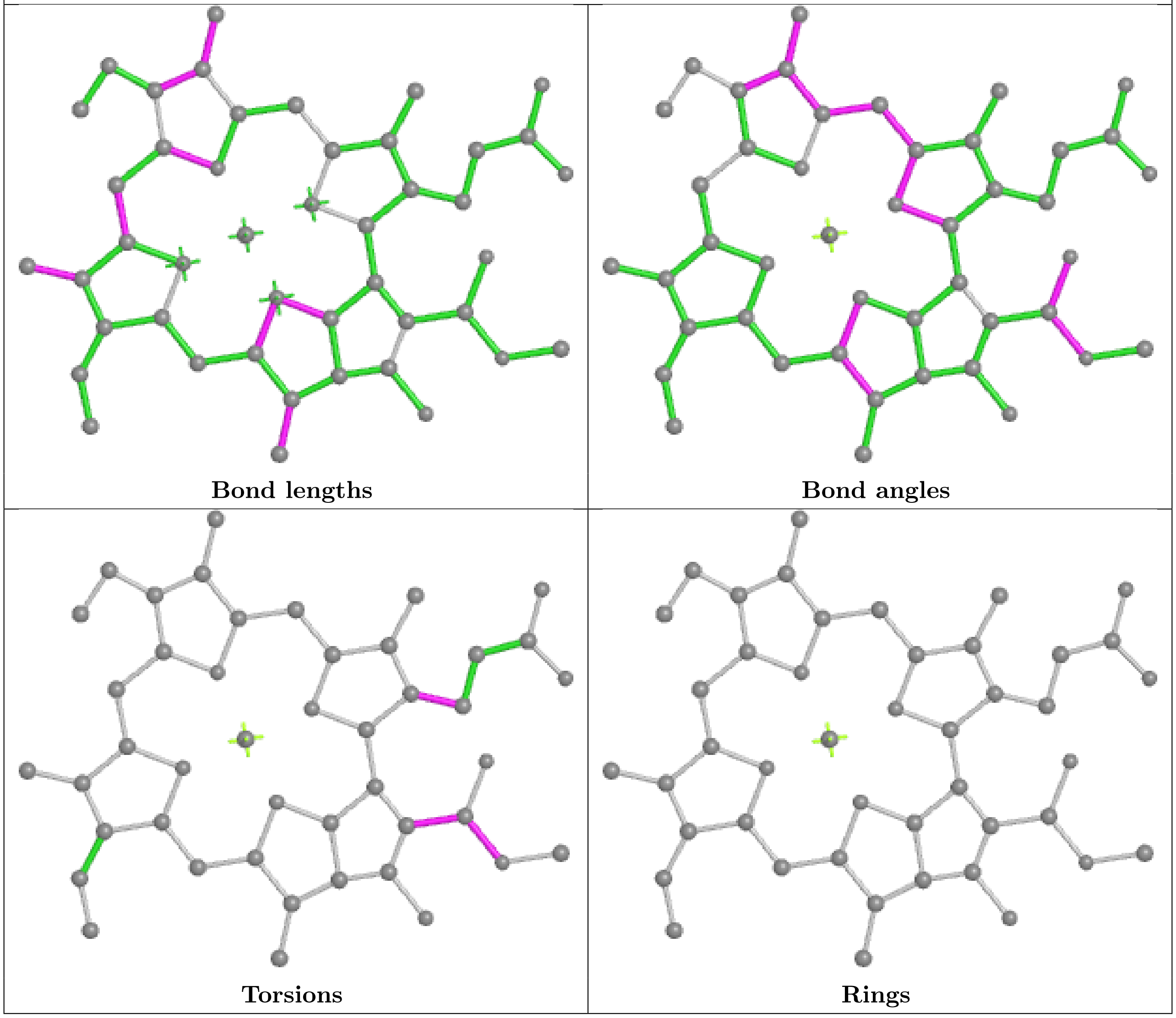


Torsions



Rings

Ligand CLA bB 812



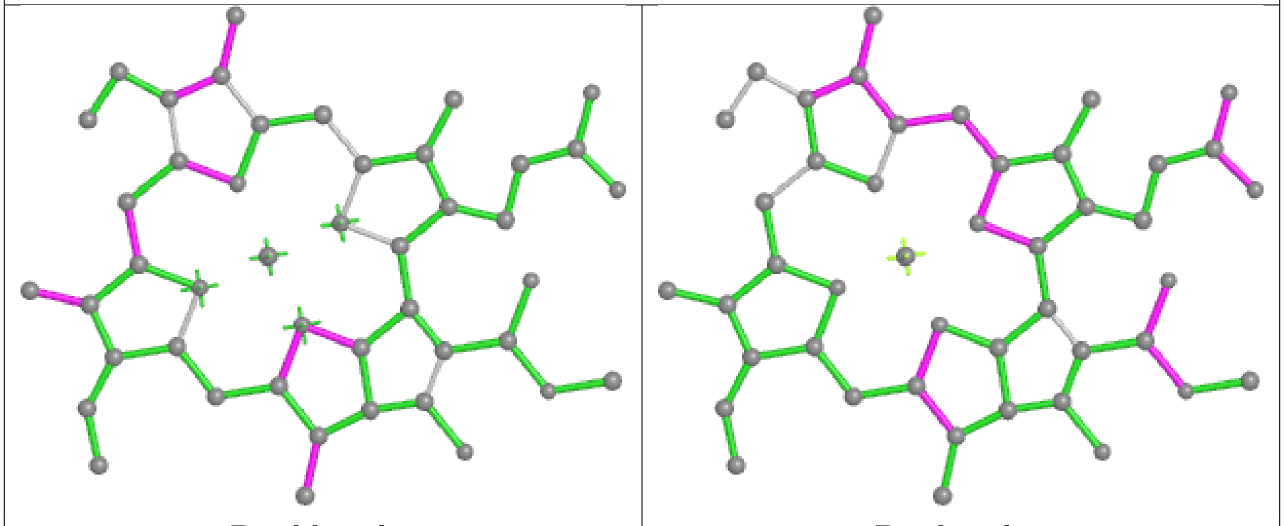
Bond lengths

Bond angles

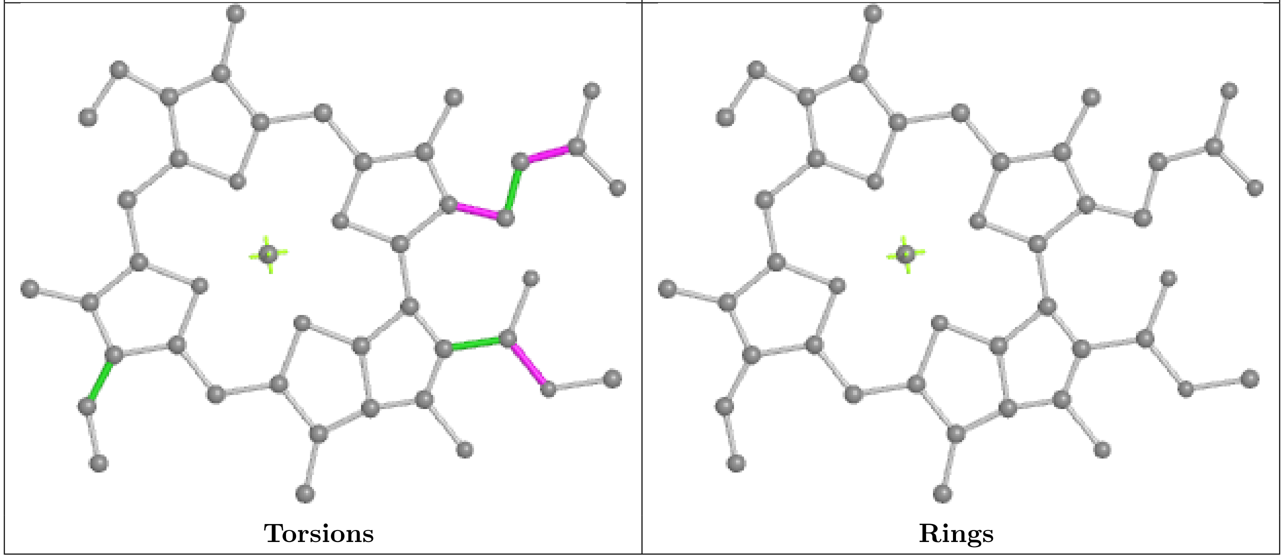
Torsions

Rings

Ligand CLA cB 823

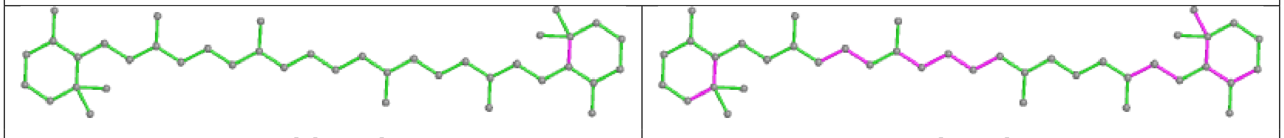


Bond lengths Bond angles

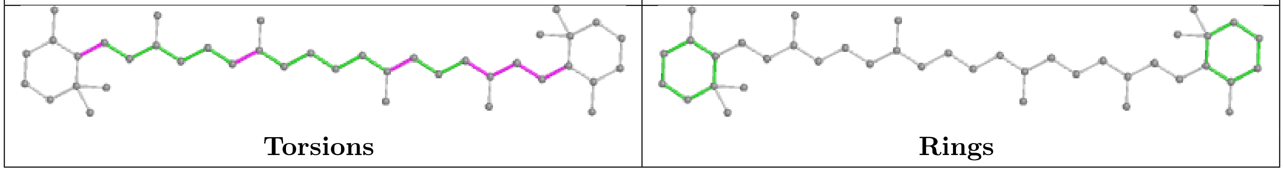


Torsions Rings

Ligand BCR cL 206

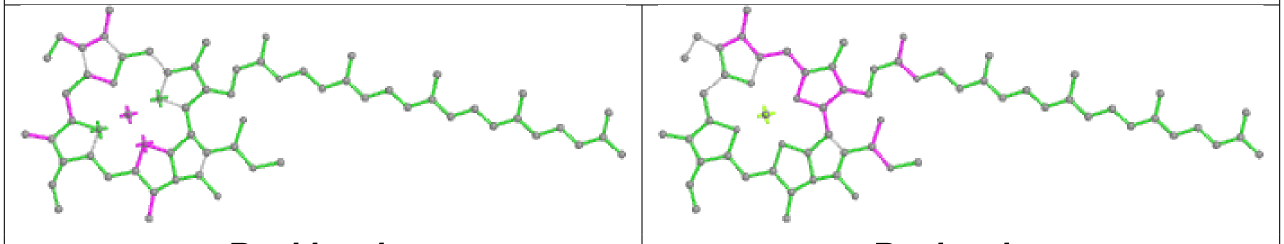


Bond lengths Bond angles



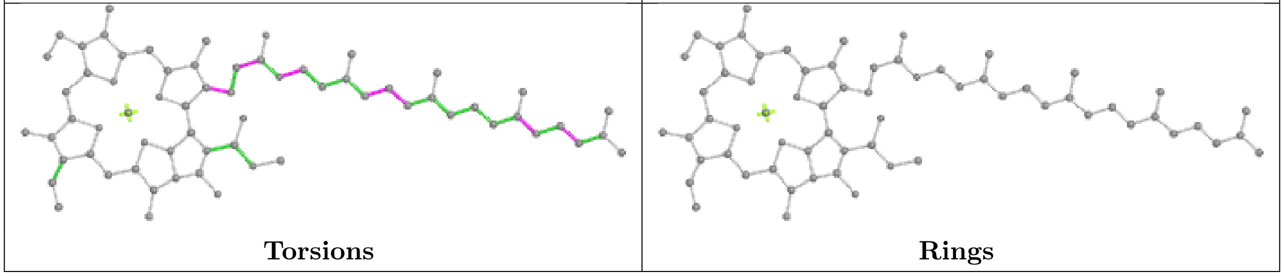
Torsions Rings

Ligand CLA dA 806



Bond lengths

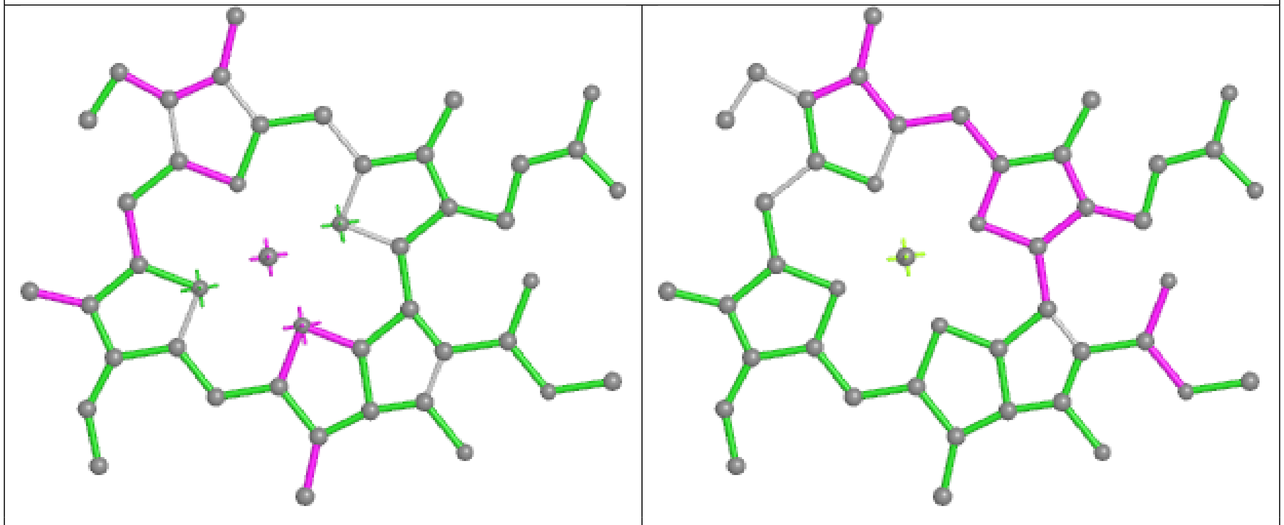
Bond angles



Torsions

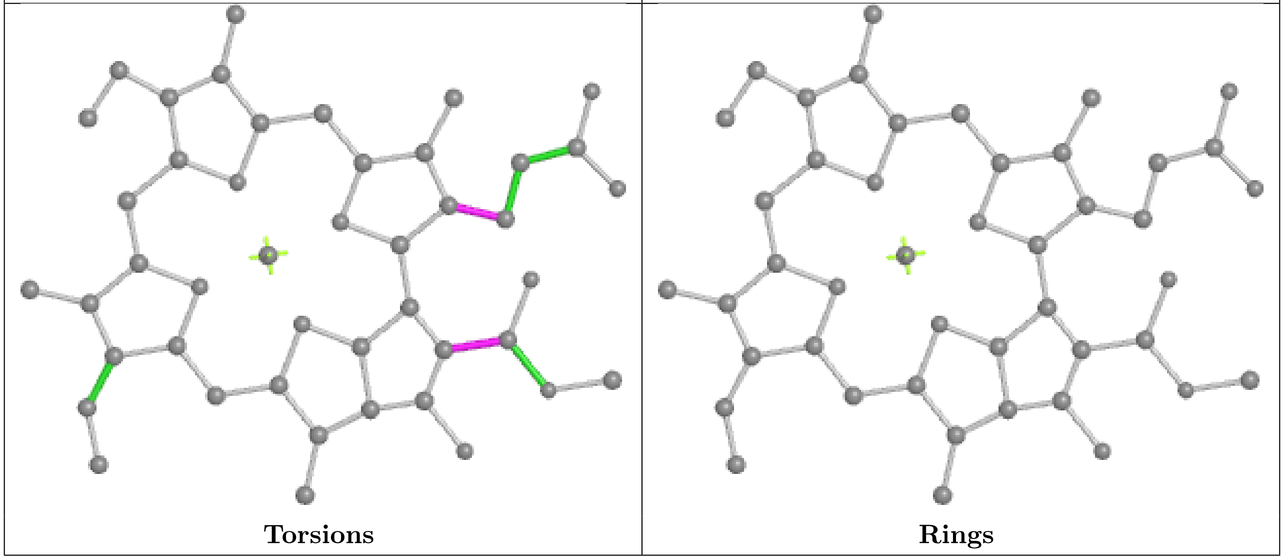
Rings

Ligand CLA cA 805



Bond lengths

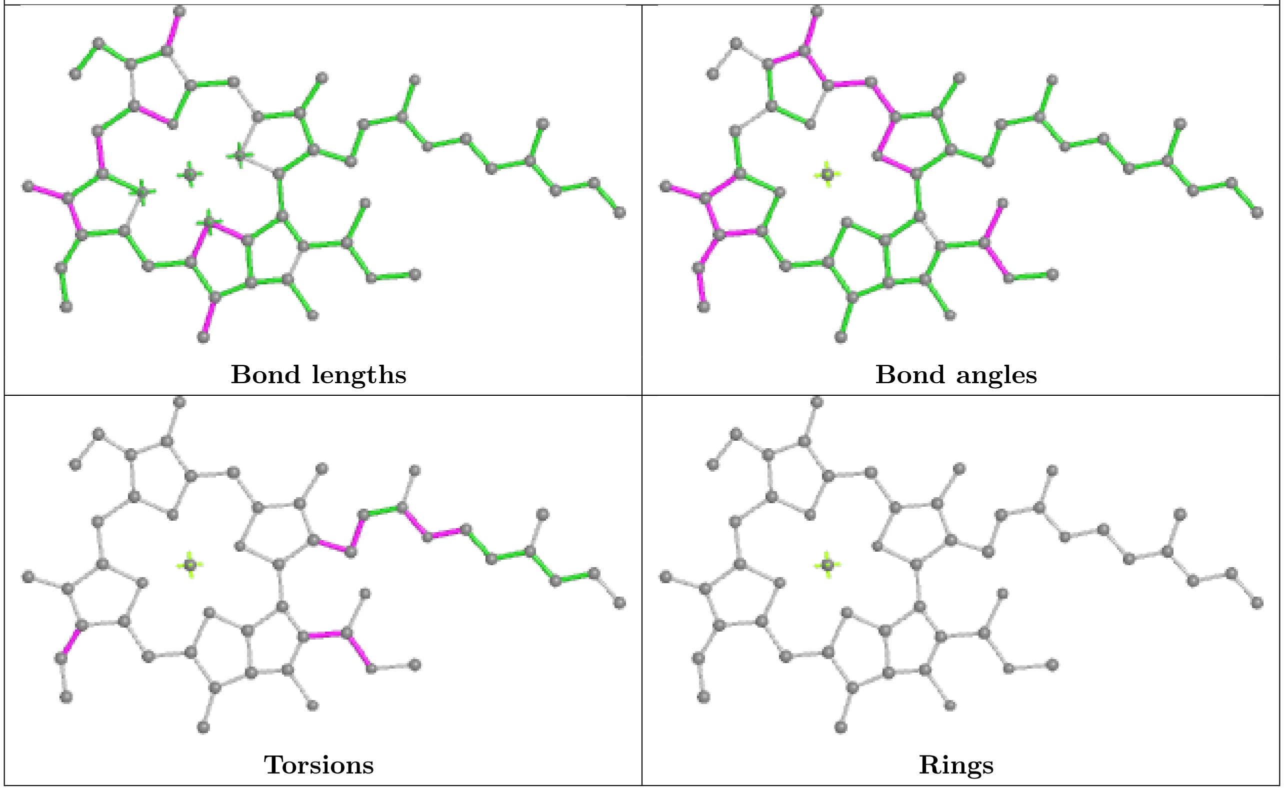
Bond angles



Torsions

Rings

Ligand CLA cA 843



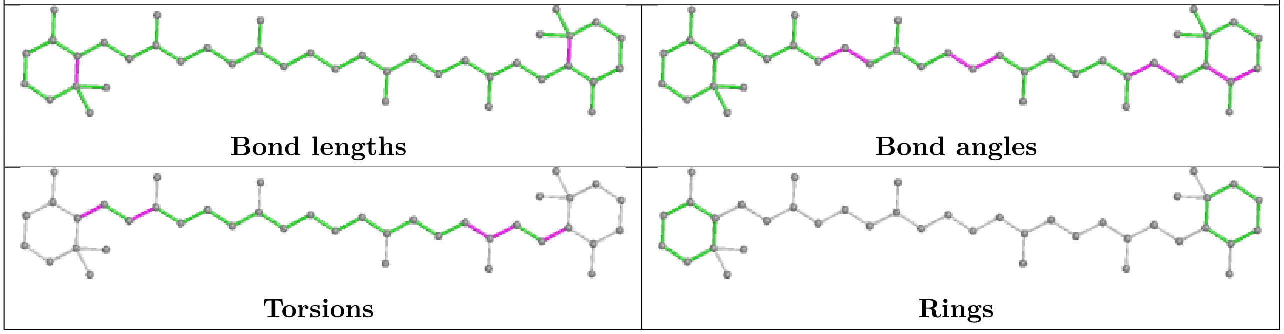
Bond lengths

Bond angles

Torsions

Rings

Ligand BCR cB 848



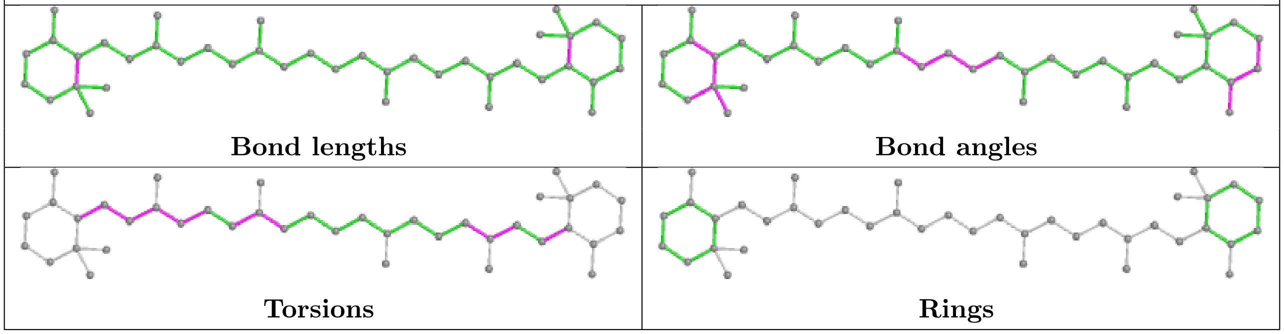
Bond lengths

Bond angles

Torsions

Rings

Ligand BCR cI 101

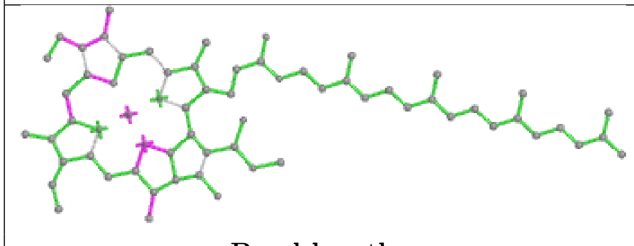
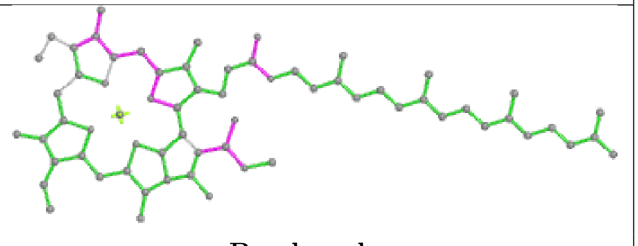
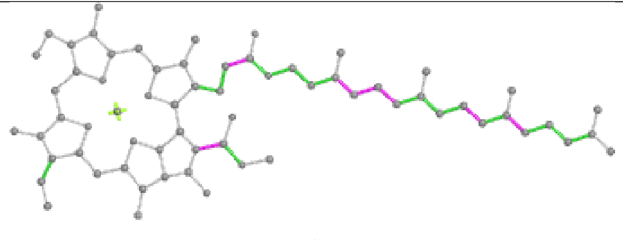
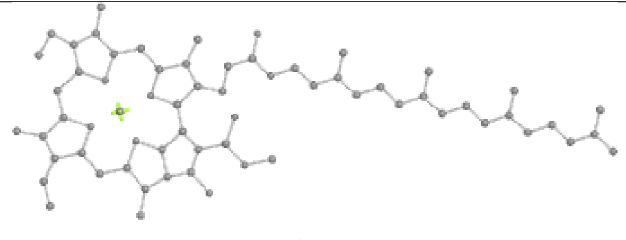


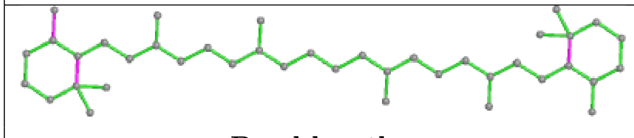
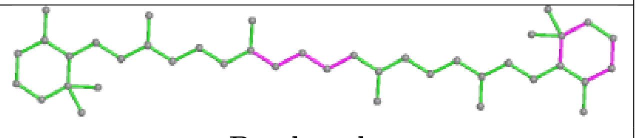
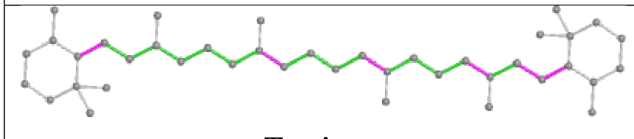
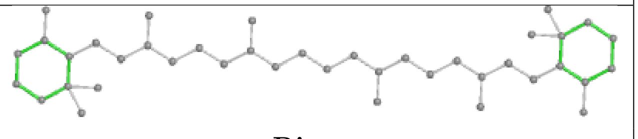
Bond lengths

Bond angles

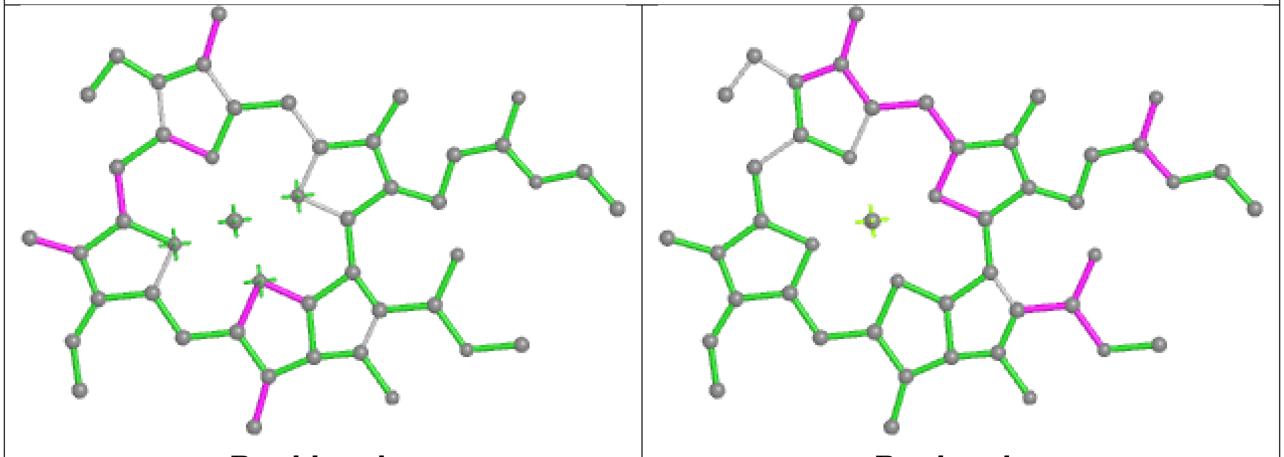
Torsions

Rings

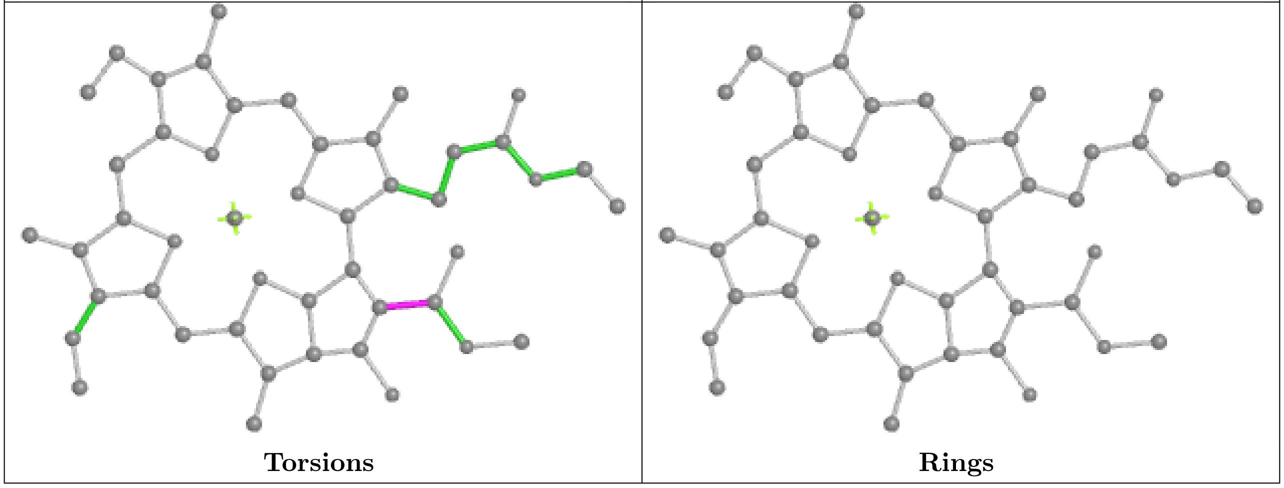
Ligand CLA bA 839	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR aJ 104	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA dB 840

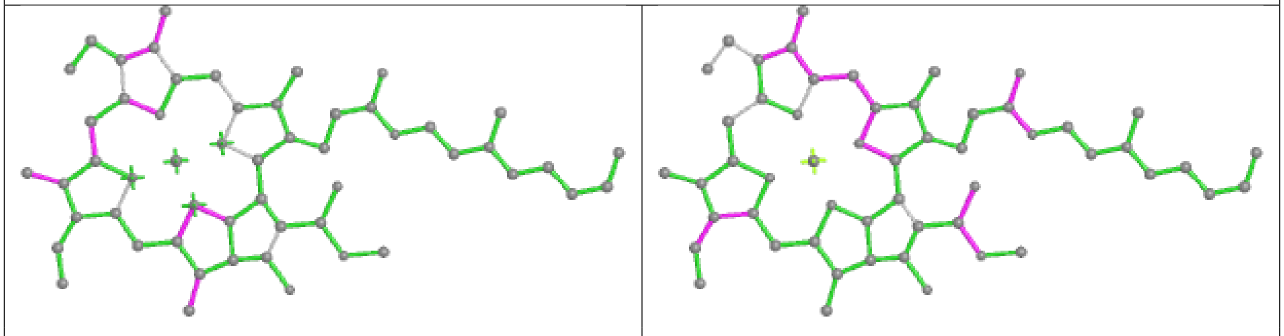


Bond lengths **Bond angles**

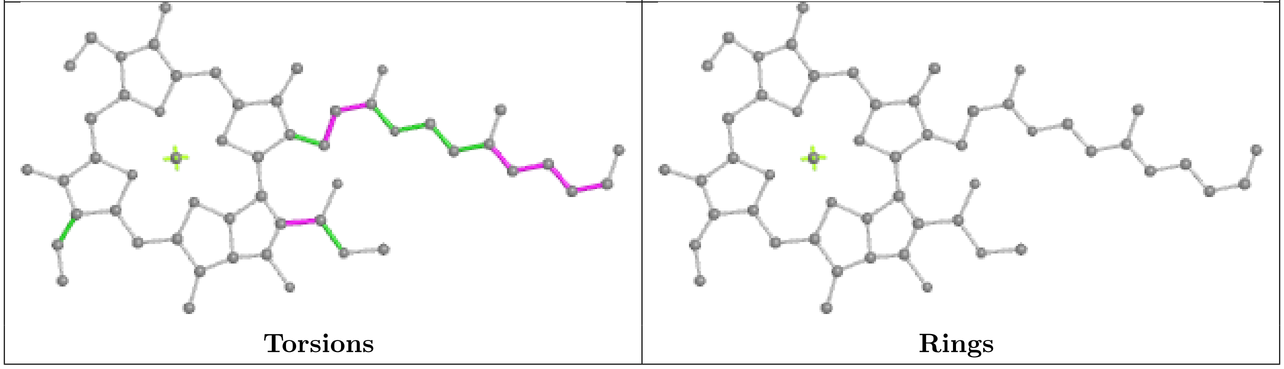


Torsions **Rings**

Ligand CLA bA 817

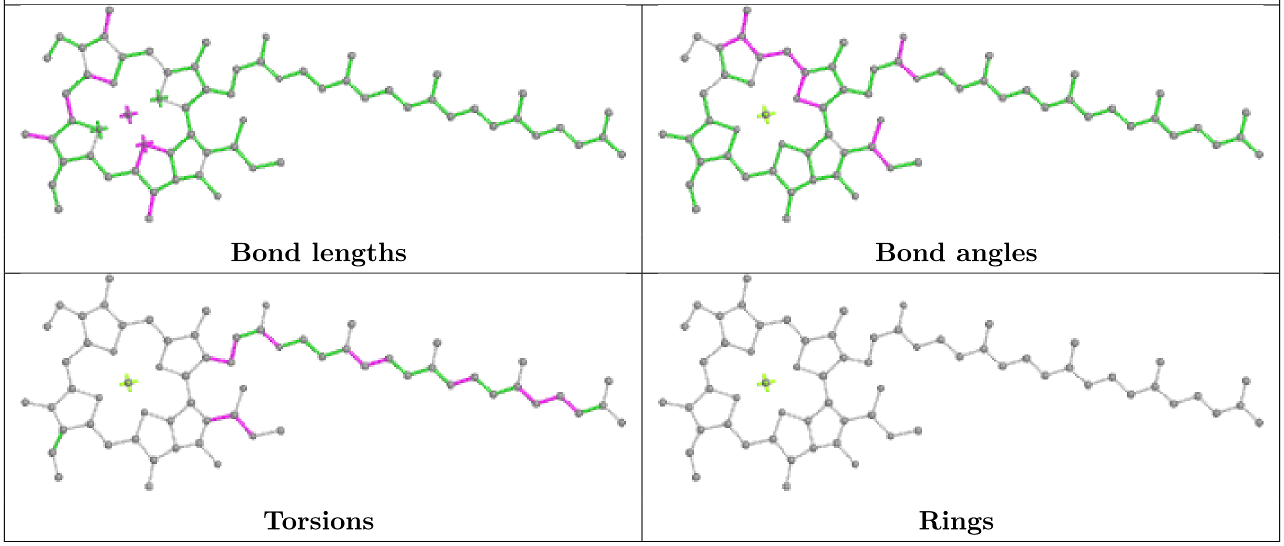


Bond lengths **Bond angles**



Torsions **Rings**

Ligand CLA cB 803



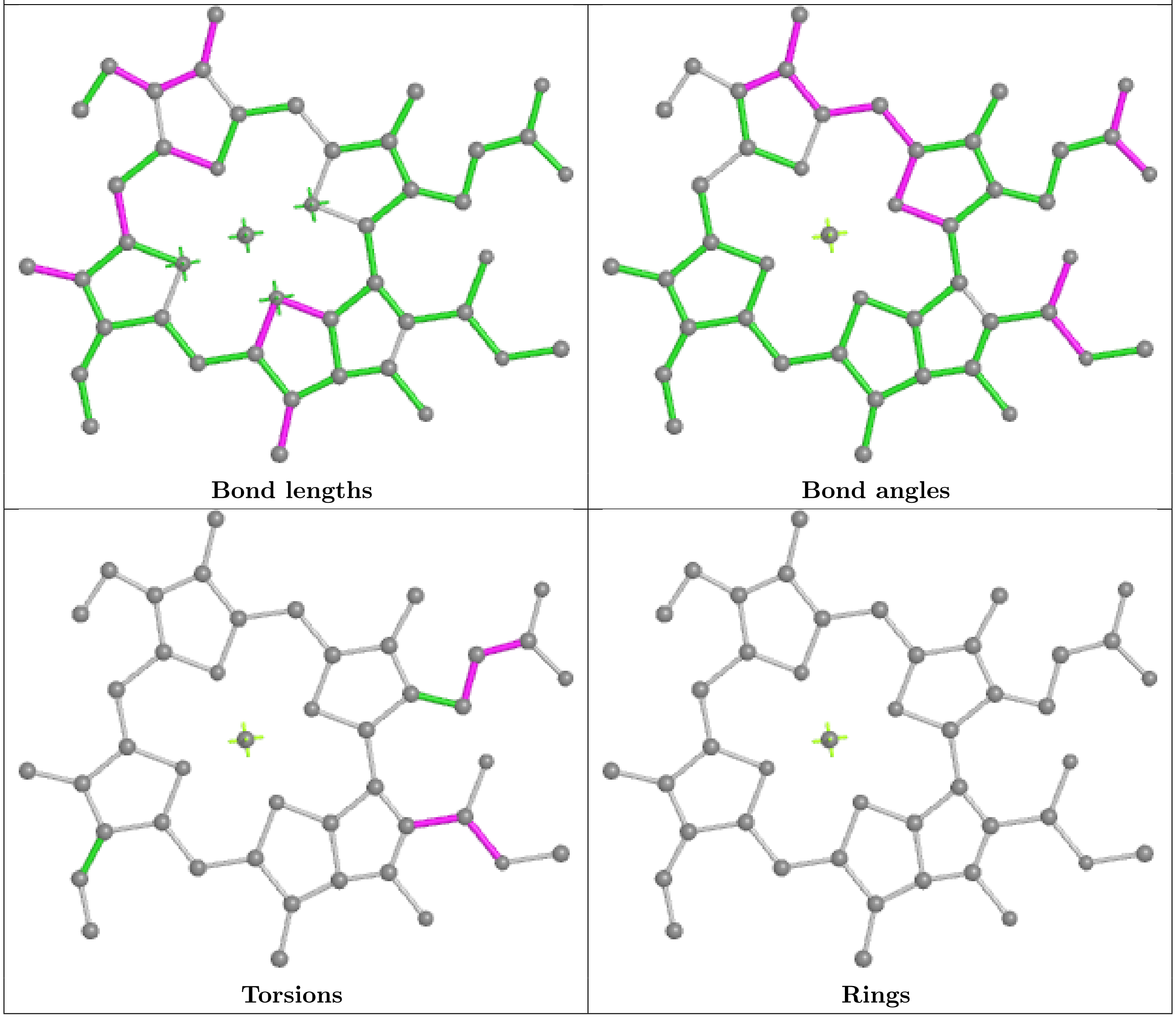
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA cB 836



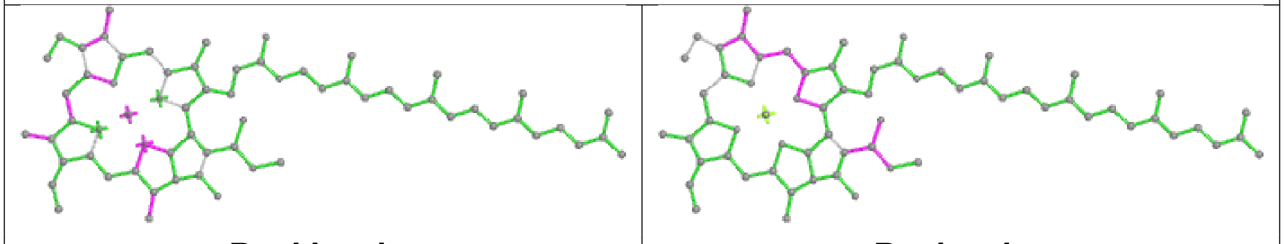
Bond lengths

Bond angles

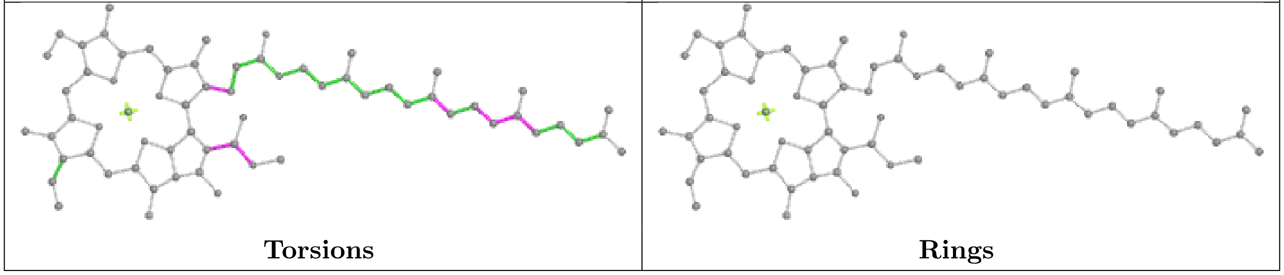
Torsions

Rings

Ligand CLA bA 830

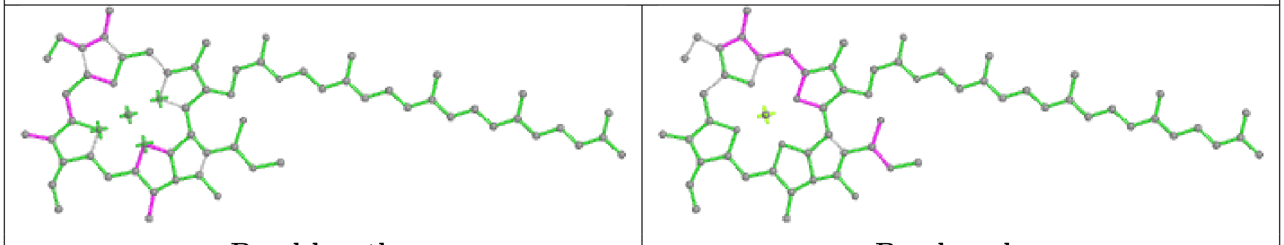


Bond lengths Bond angles

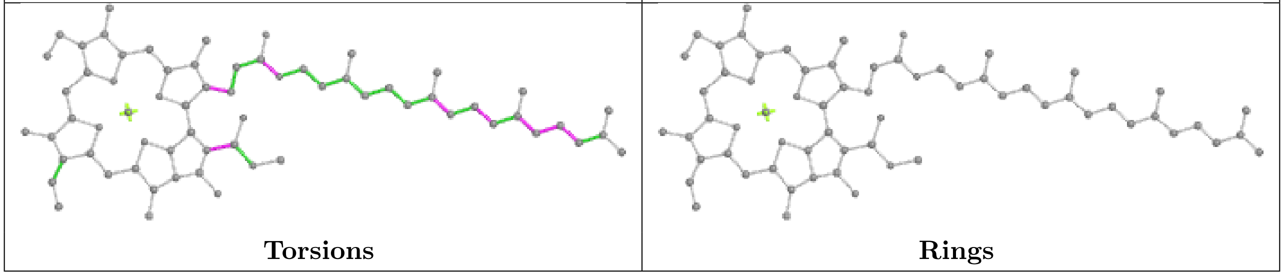


Torsions Rings

Ligand CLA dA 841

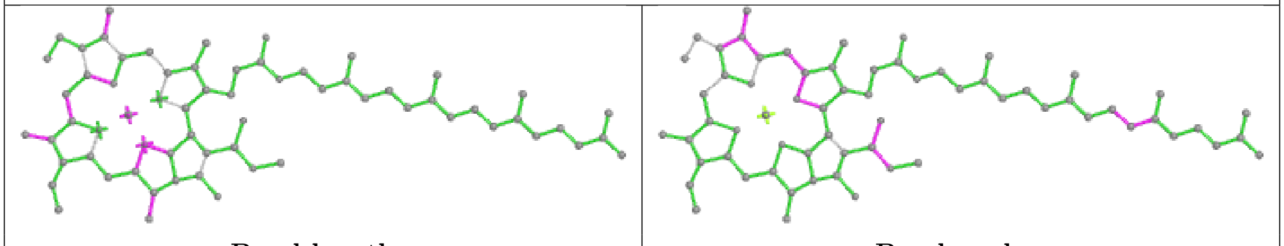


Bond lengths Bond angles

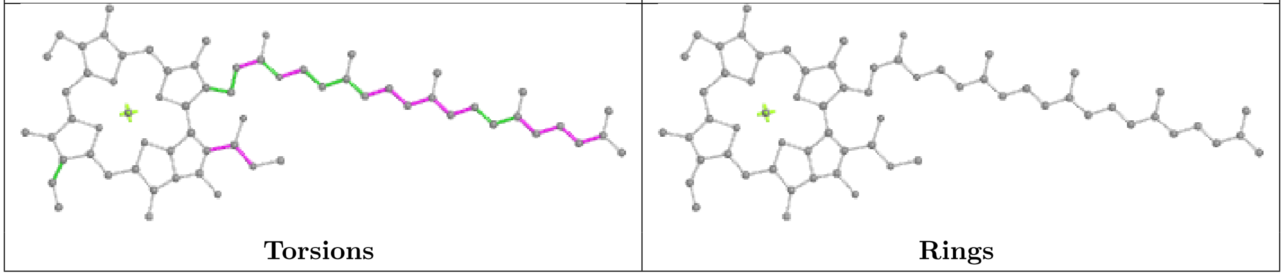


Torsions Rings

Ligand CLA bB 807

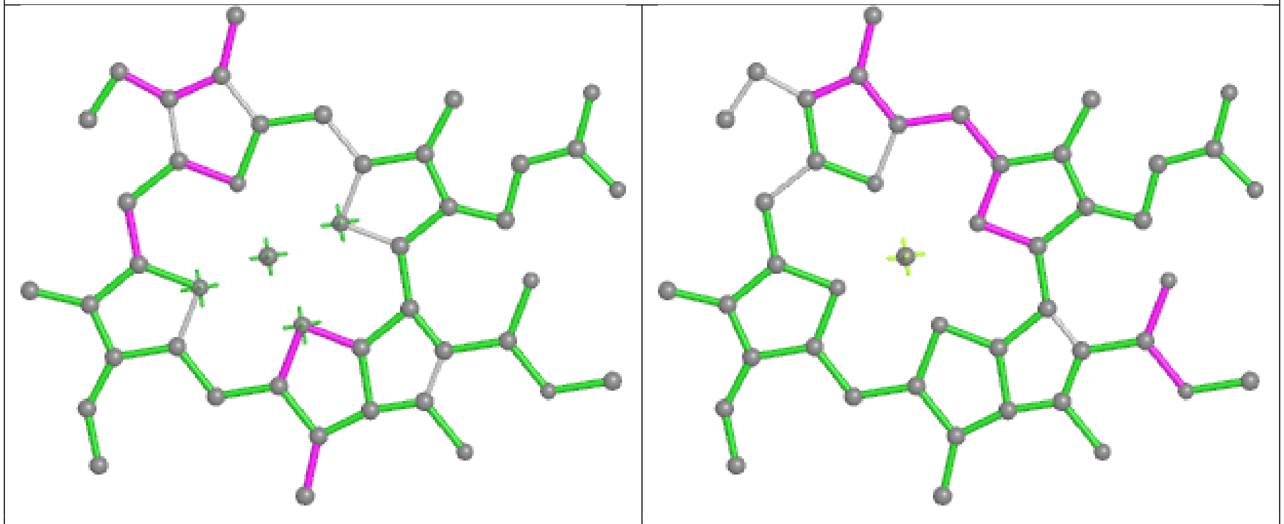


Bond lengths Bond angles



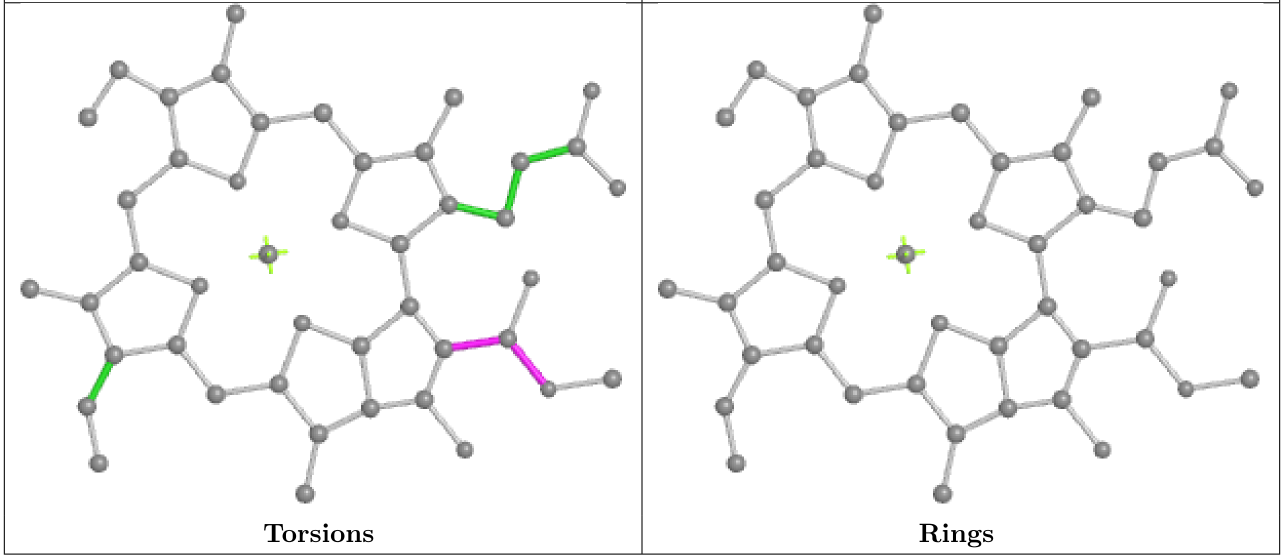
Torsions Rings

Ligand CLA bA 815



Bond lengths

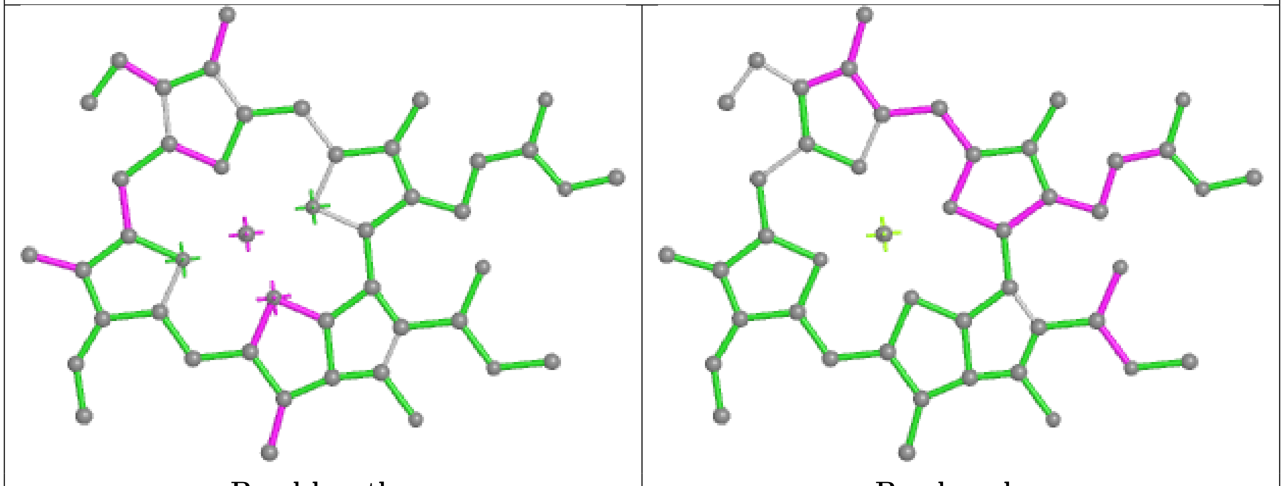
Bond angles



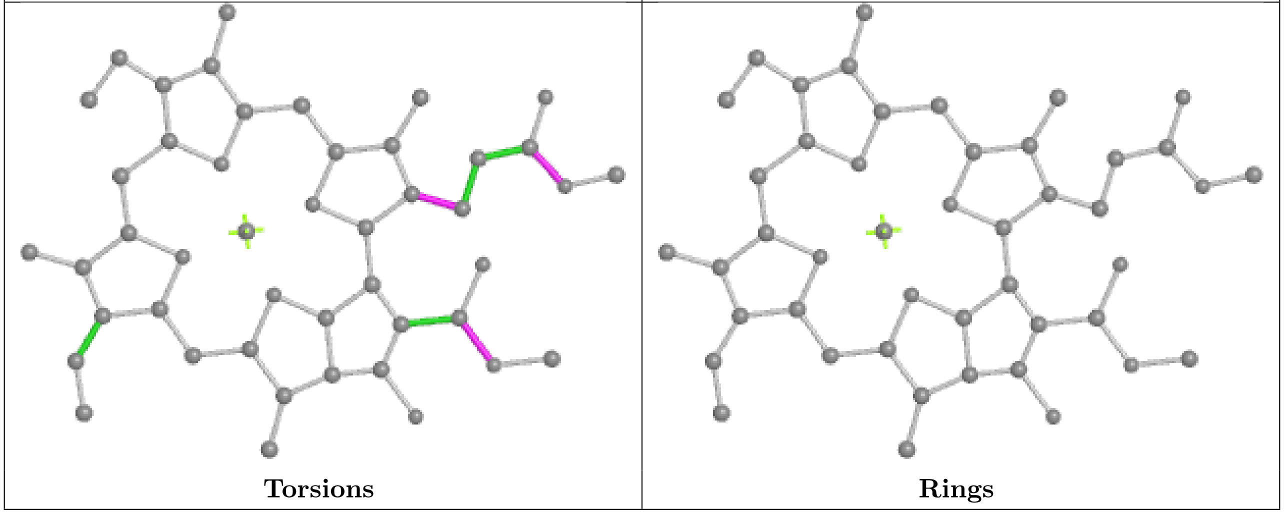
Torsions

Rings

Ligand CLA bB 826

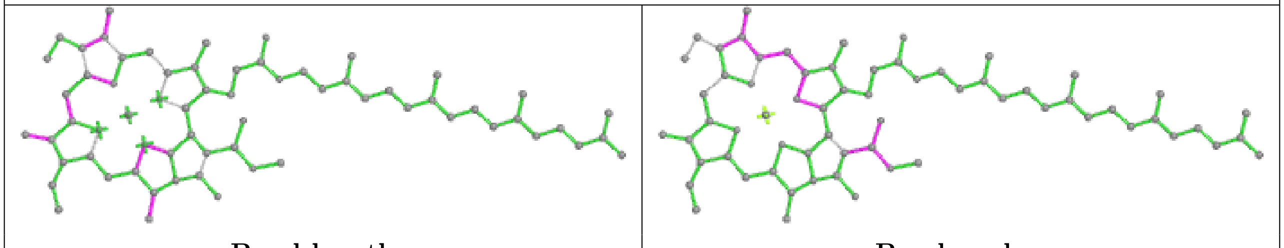


Bond lengths Bond angles

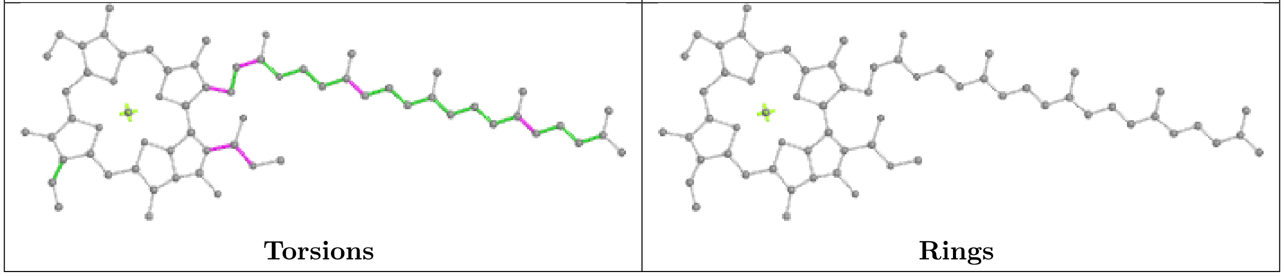


Torsions Rings

Ligand CLA dA 834

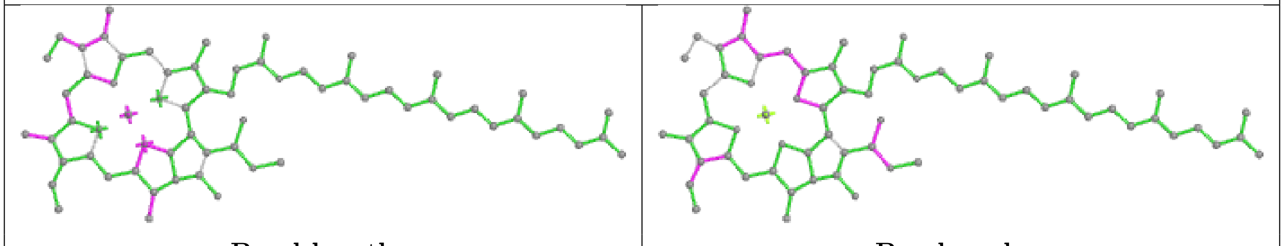


Bond lengths Bond angles

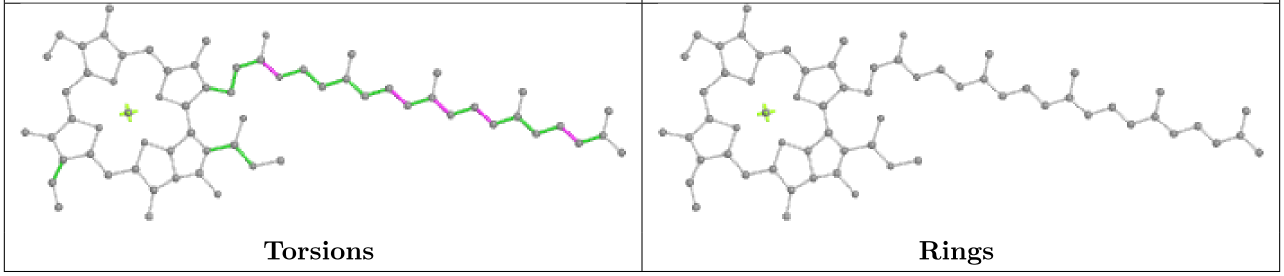


Torsions Rings

Ligand CLA bB 811

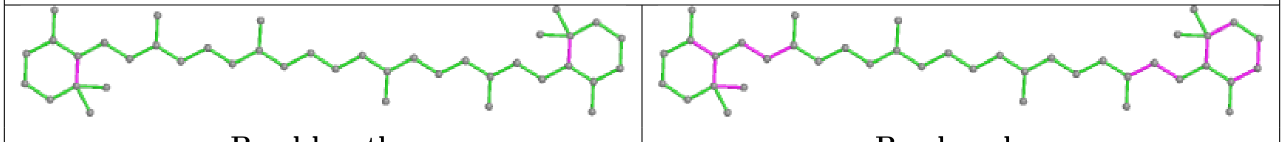


Bond lengths Bond angles

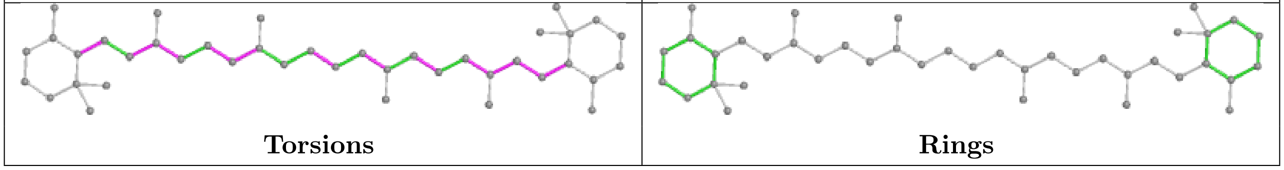


Torsions Rings

Ligand BCR aA 851

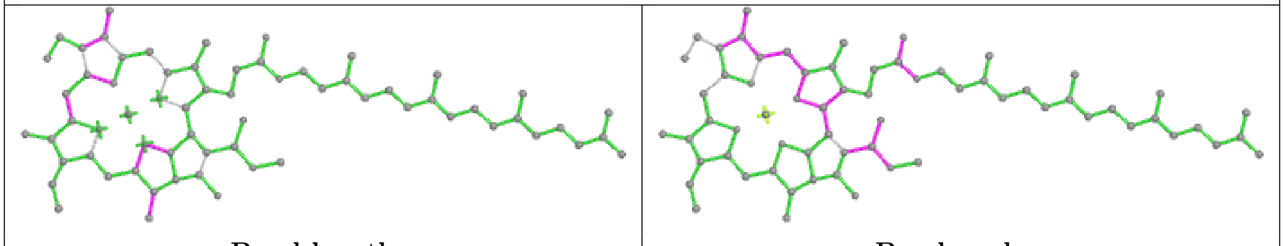


Bond lengths Bond angles

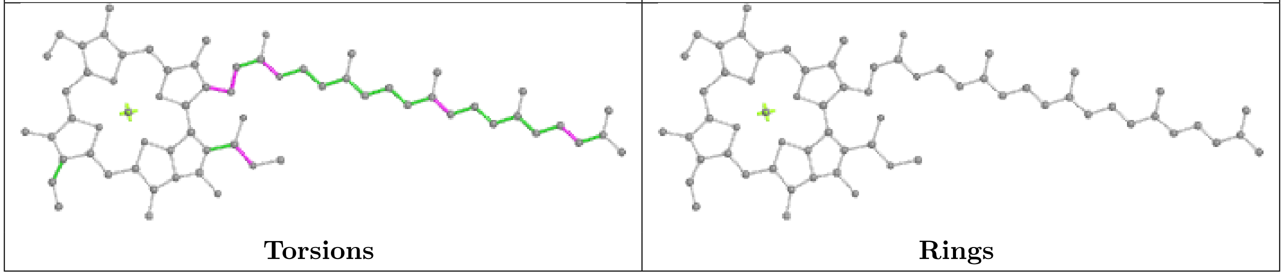


Torsions Rings

Ligand CLA cL 202

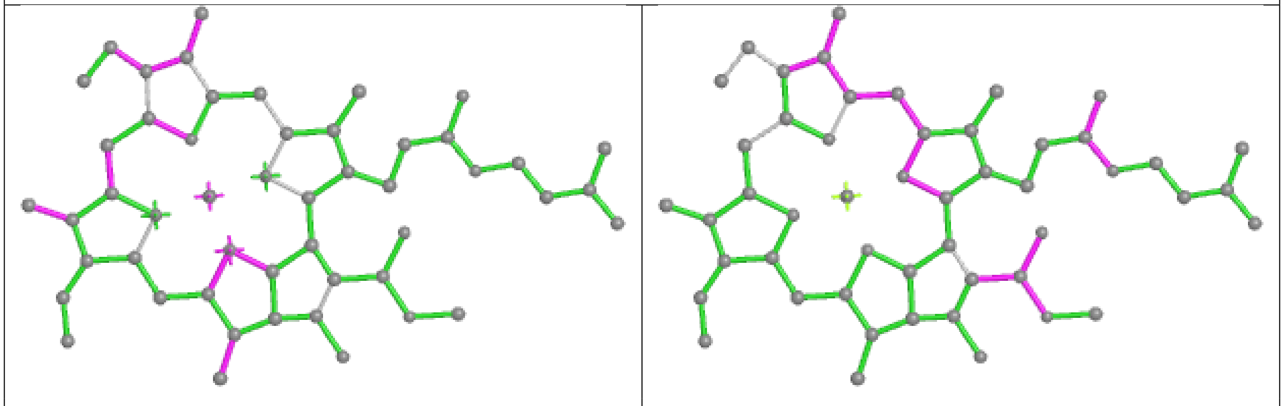


Bond lengths Bond angles



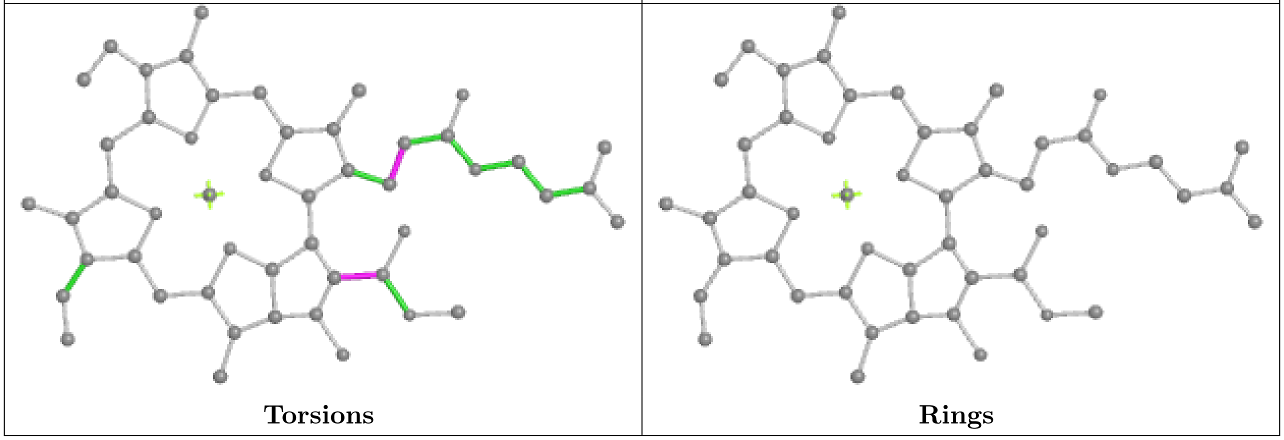
Torsions Rings

Ligand CLA dA 831



Bond lengths

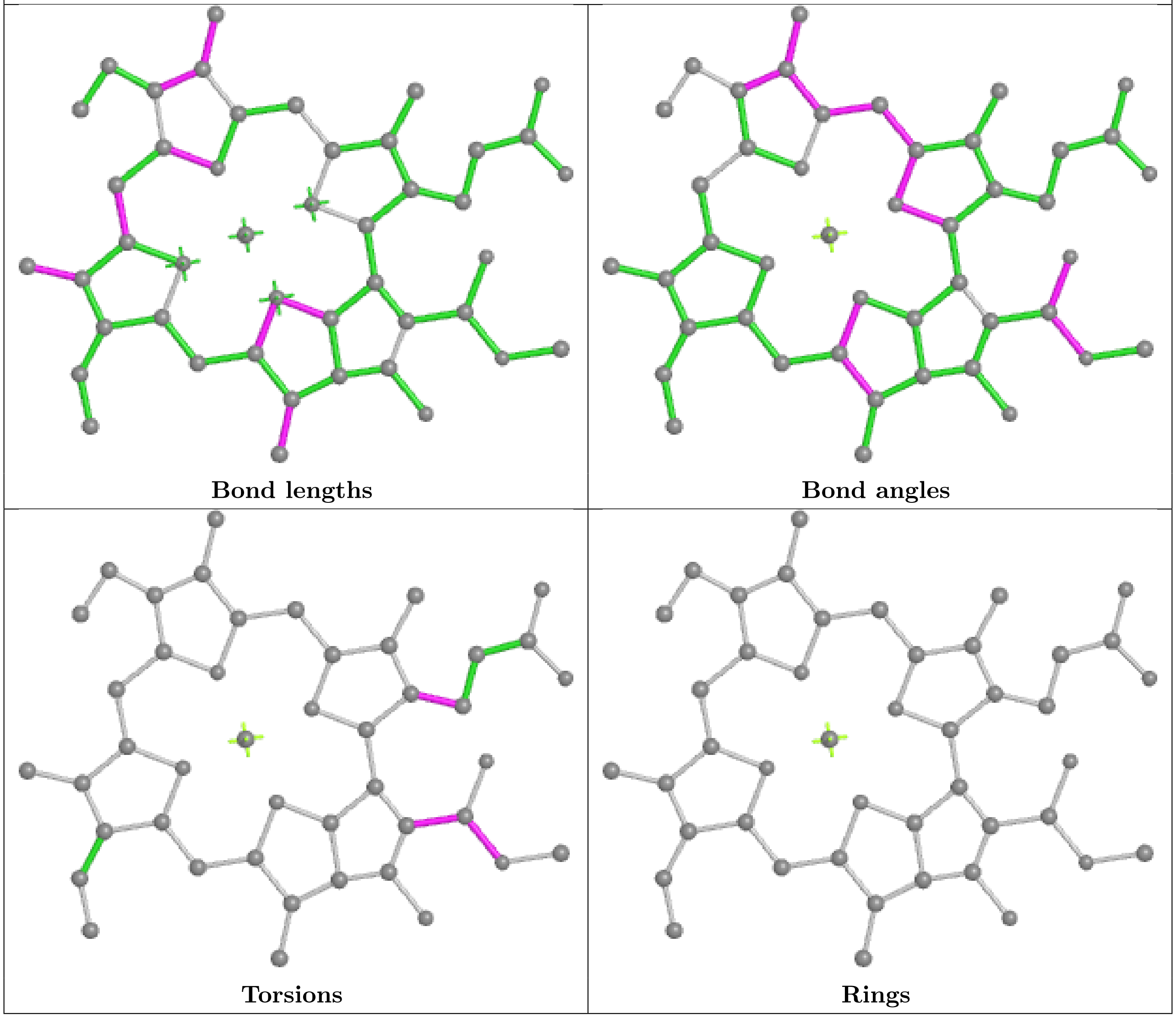
Bond angles



Torsions

Rings

Ligand CLA cB 811



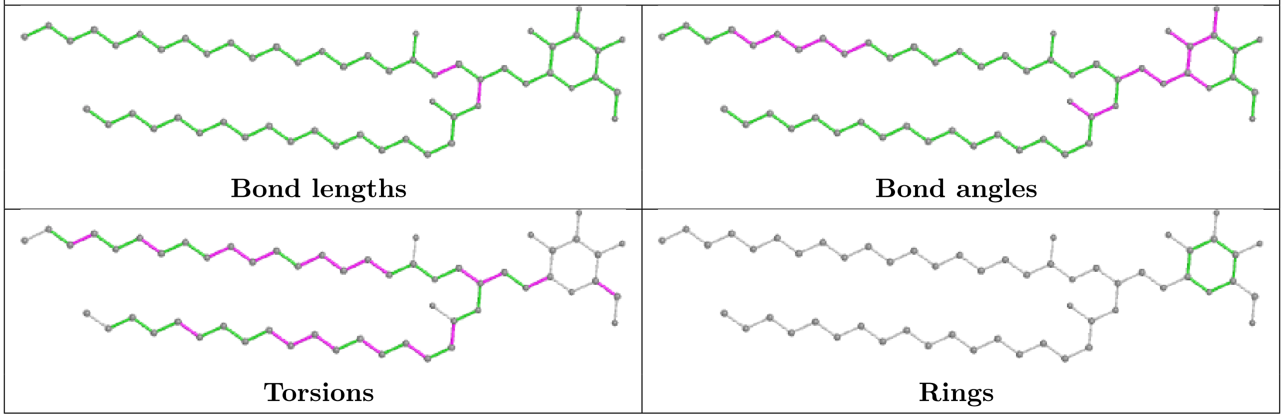
Bond lengths

Bond angles

Torsions

Rings

Ligand LMG aB 849



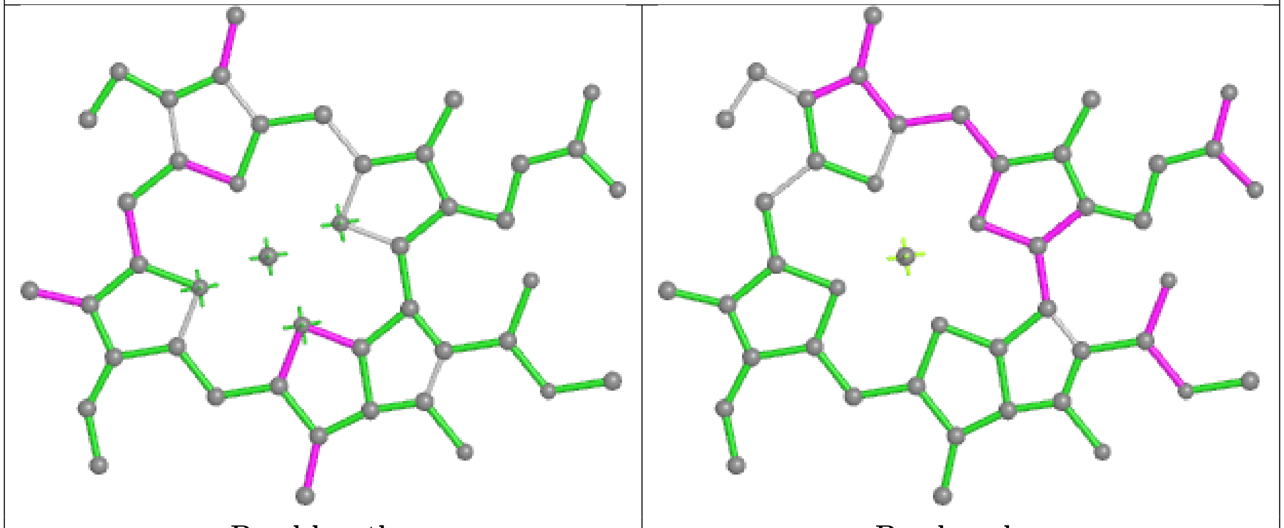
Bond lengths

Bond angles

Torsions

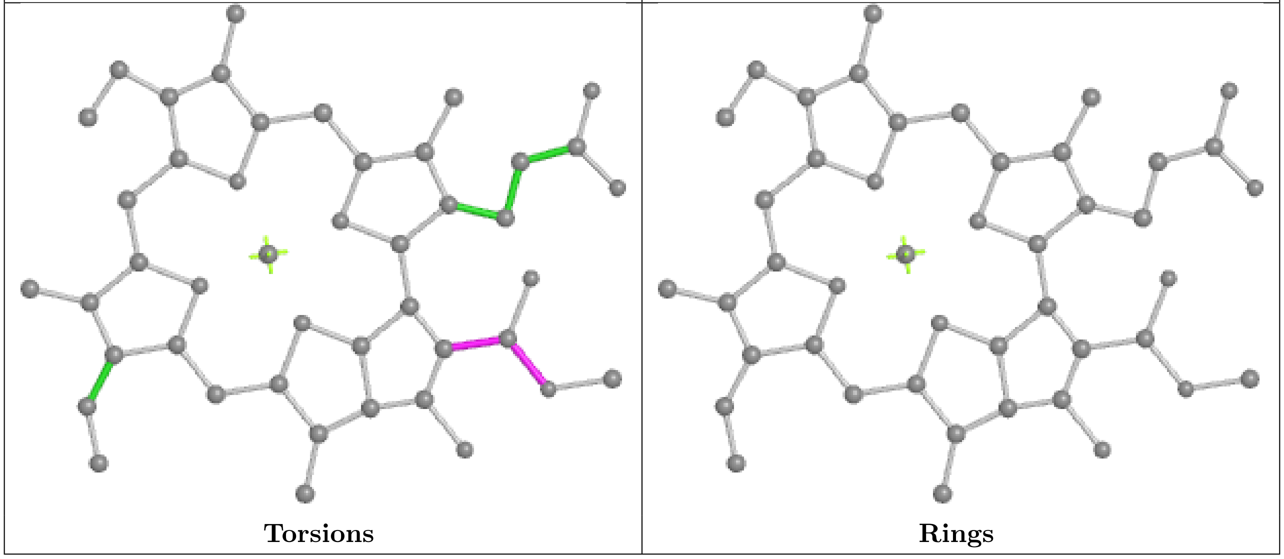
Rings

Ligand CLA aA 814



Bond lengths

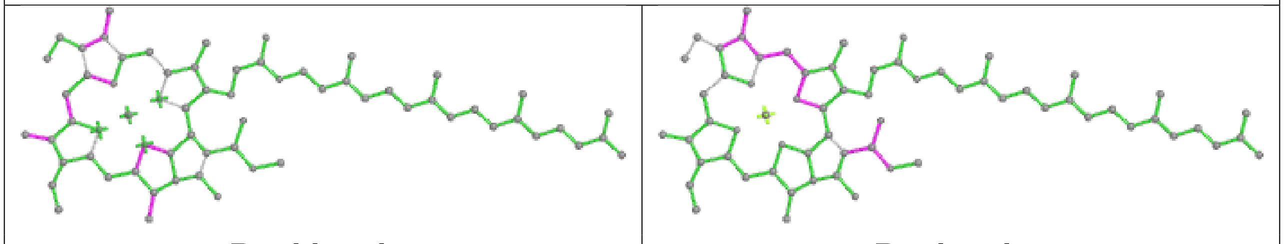
Bond angles



Torsions

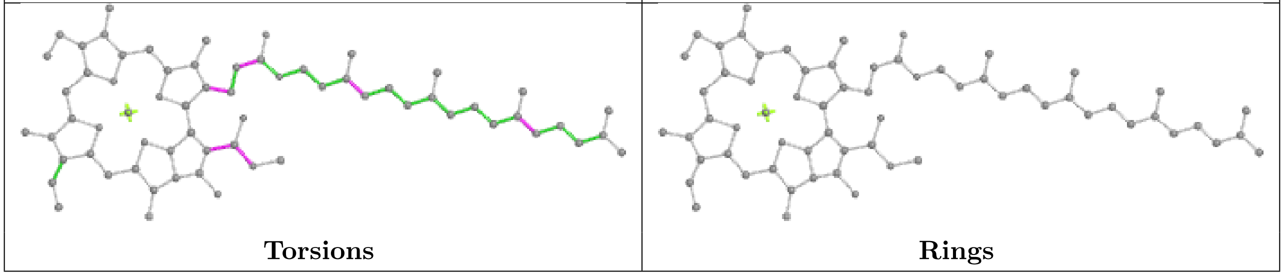
Rings

Ligand CLA aA 834



Bond lengths

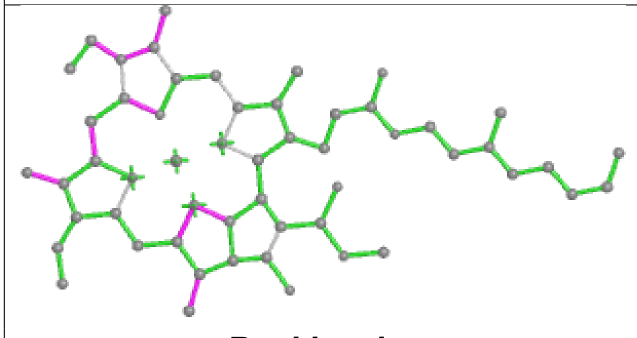
Bond angles

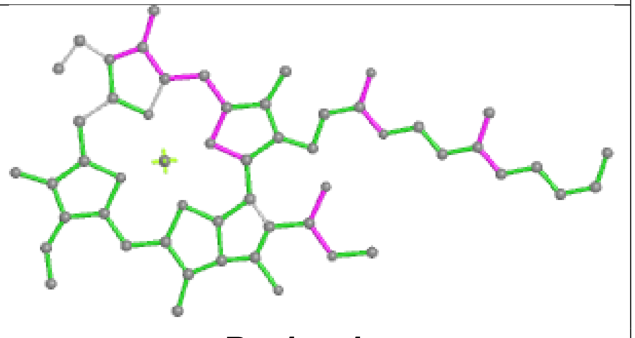


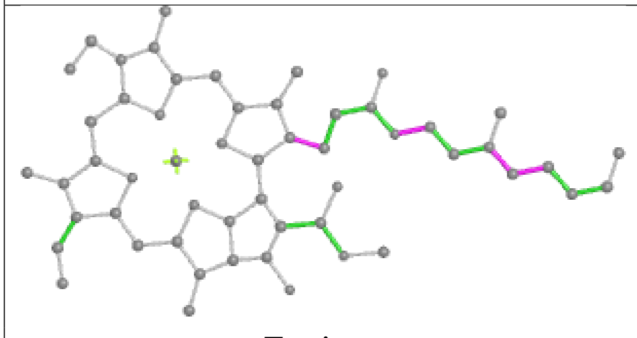
Torsions

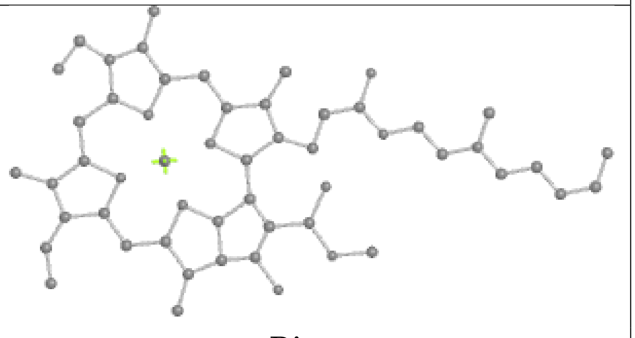
Rings

Ligand CLA cA 835

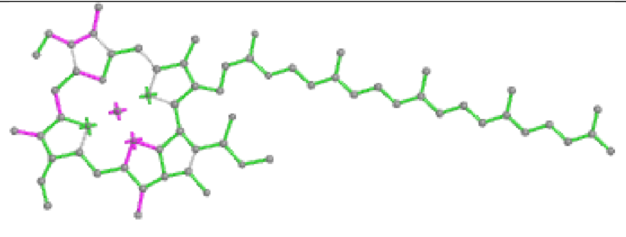

Bond lengths

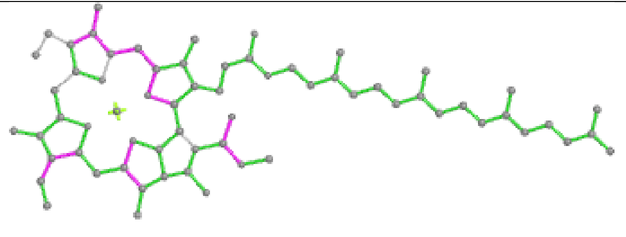

Bond angles

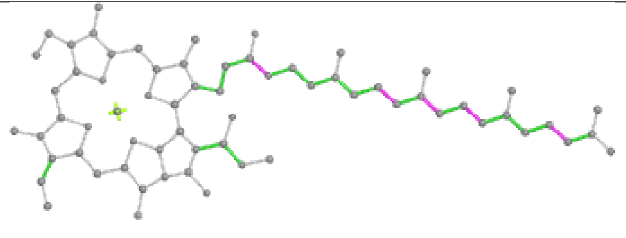

Torsions

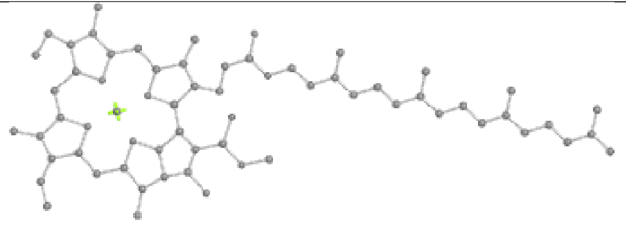

Rings

Ligand CLA dL 201

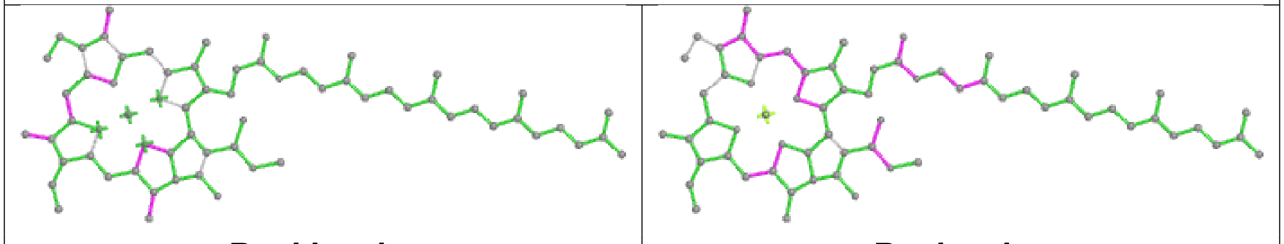

Bond lengths


Bond angles

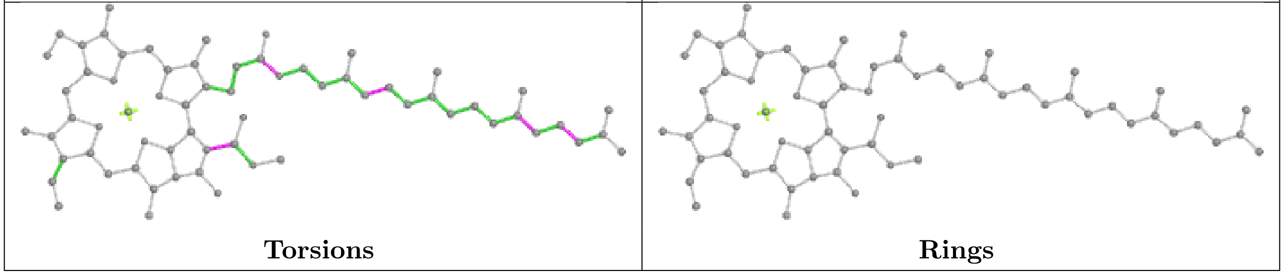

Torsions


Rings

Ligand CLA aB 838

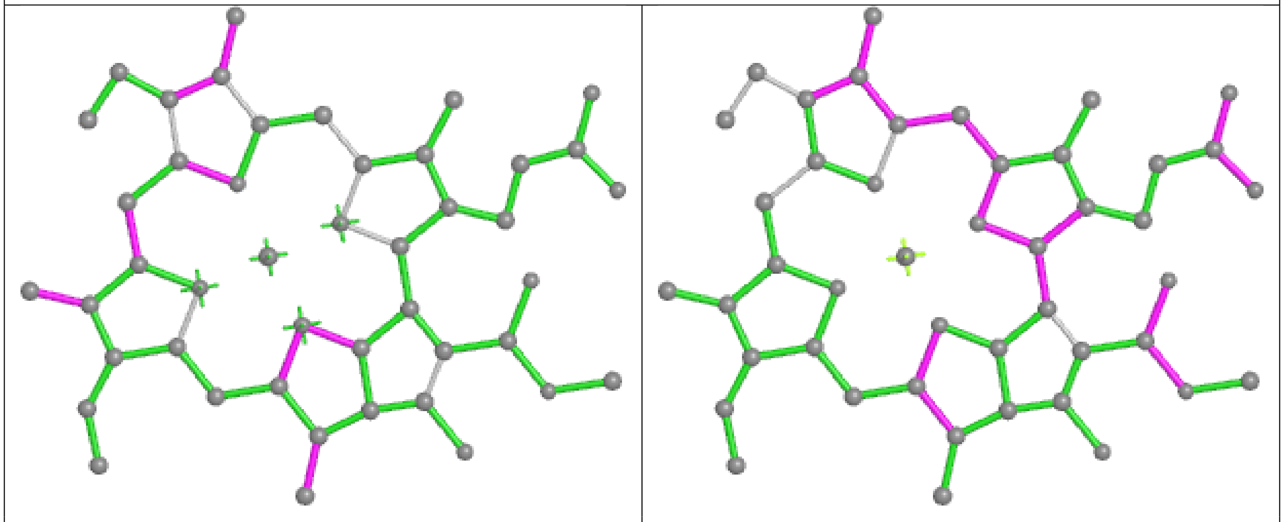


Bond lengths **Bond angles**

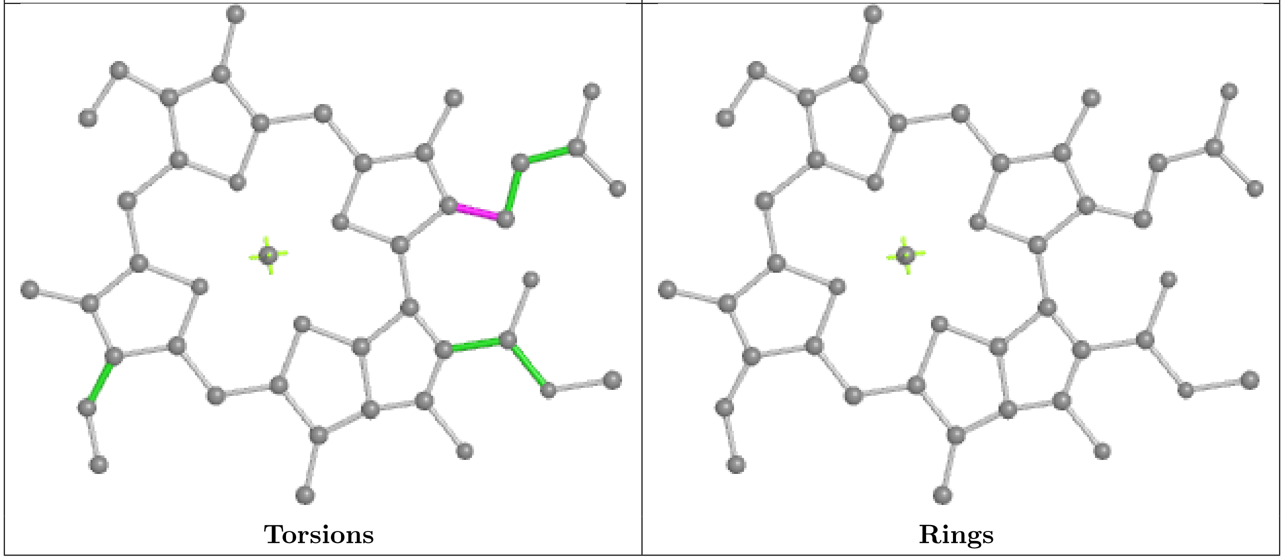


Torsions **Rings**

Ligand CLA bB 836

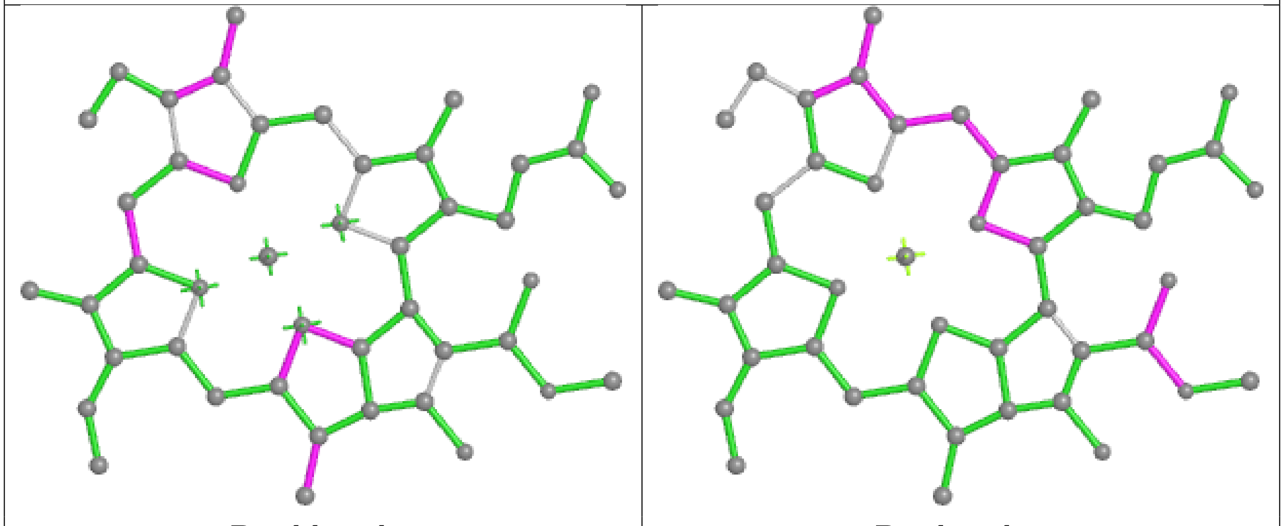


Bond lengths **Bond angles**



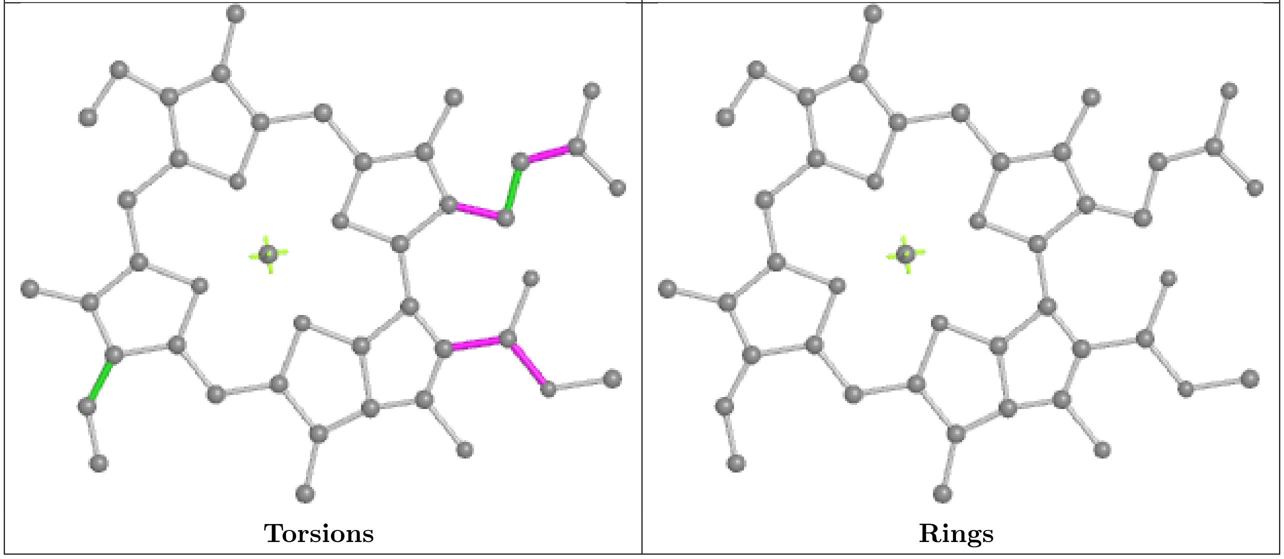
Torsions **Rings**

Ligand CLA aJ 101



Bond lengths

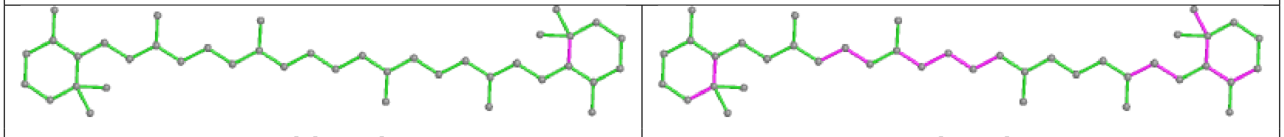
Bond angles



Torsions

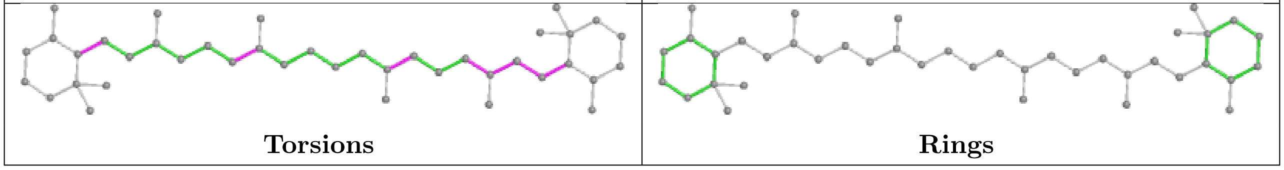
Rings

Ligand BCR aL 206



Bond lengths

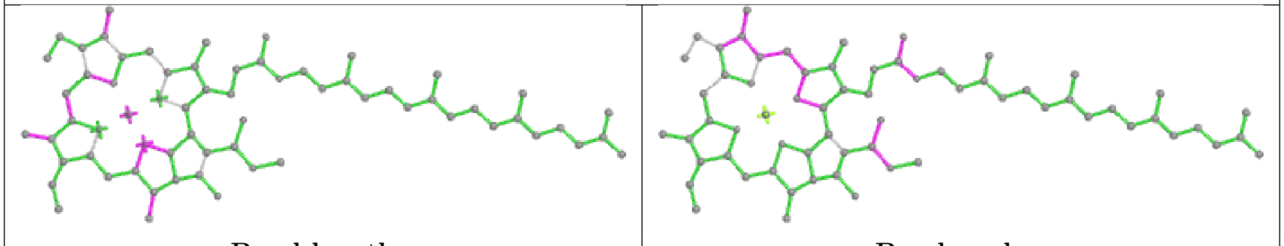
Bond angles



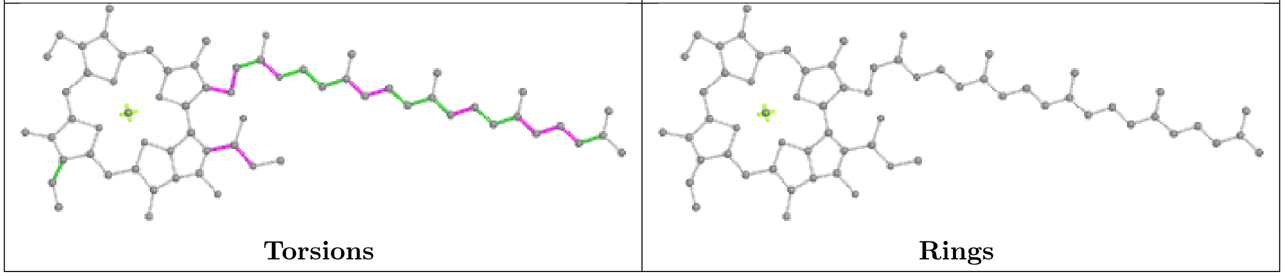
Torsions

Rings

Ligand CLA aB 803

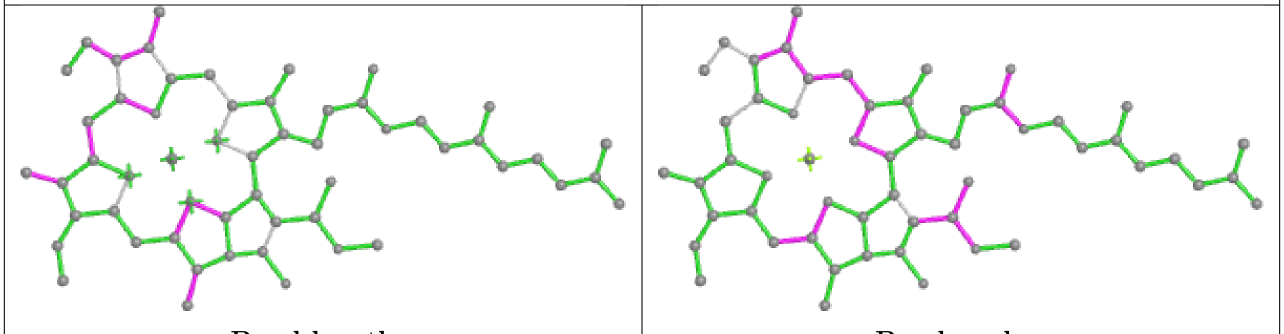


Bond lengths Bond angles

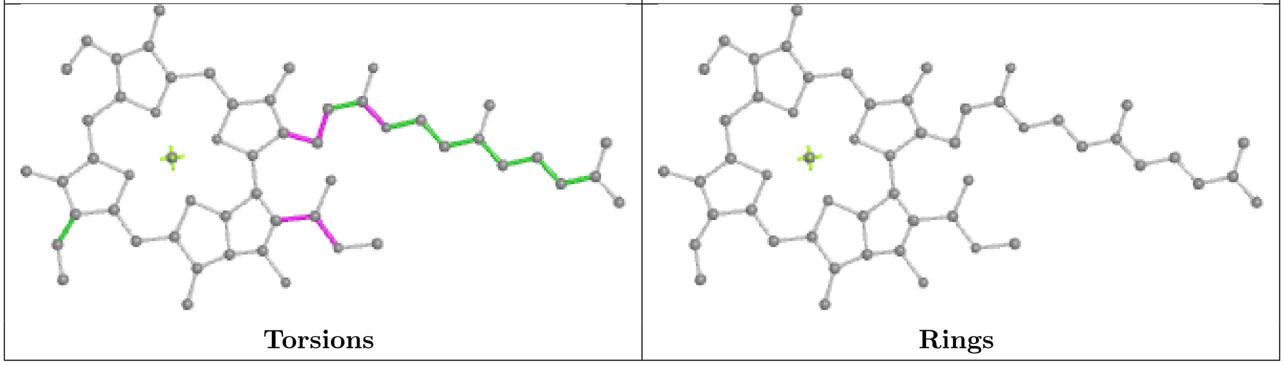


Torsions Rings

Ligand CLA cB 816

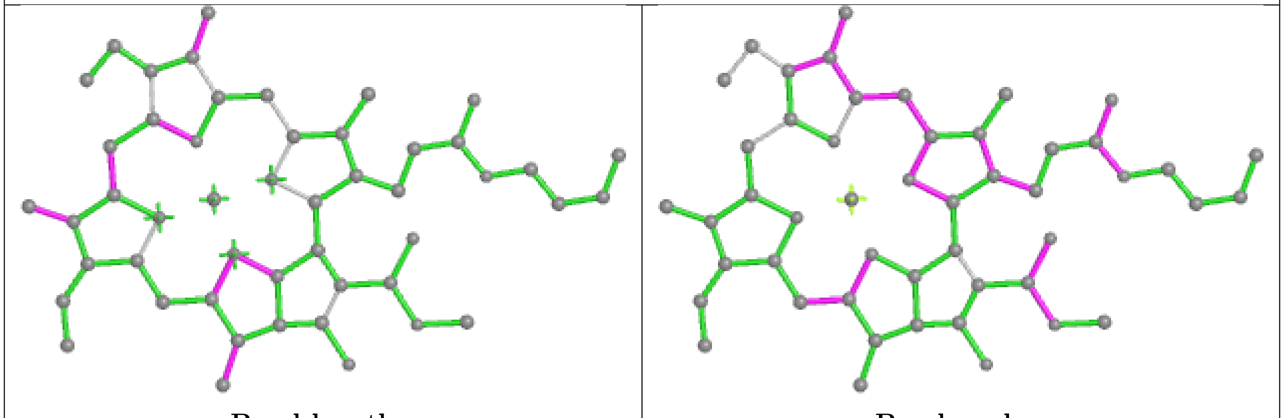


Bond lengths Bond angles



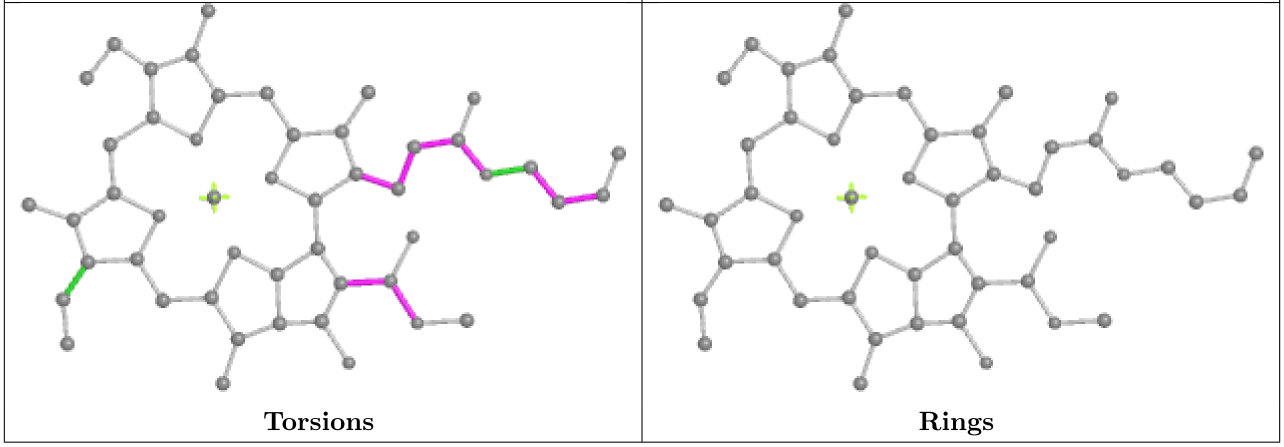
Torsions Rings

Ligand CLA dB 832



Bond lengths

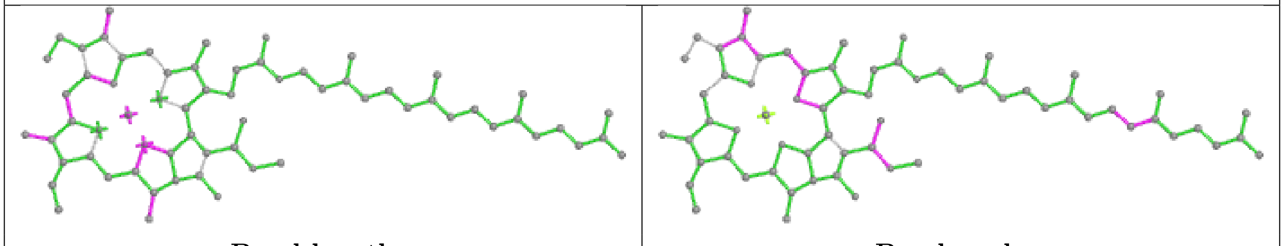
Bond angles



Torsions

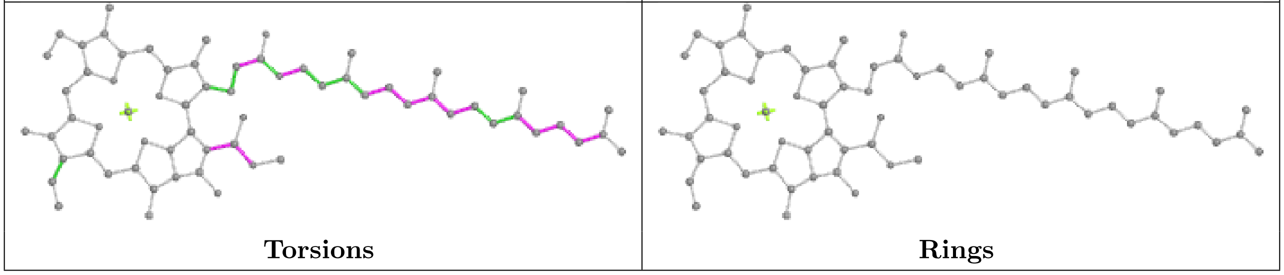
Rings

Ligand CLA cB 807



Bond lengths

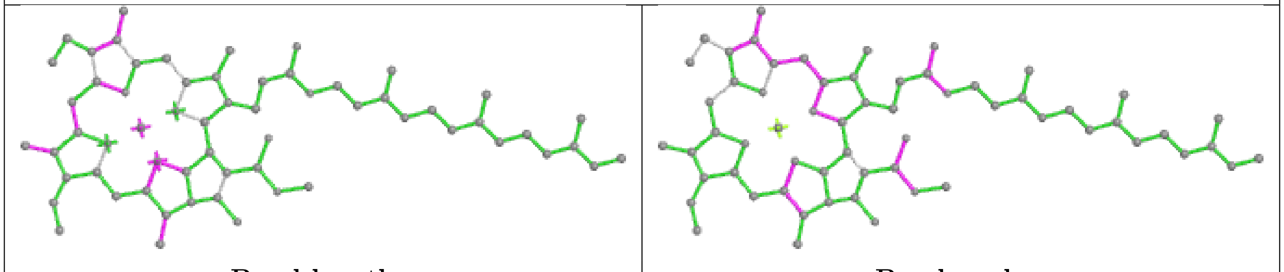
Bond angles



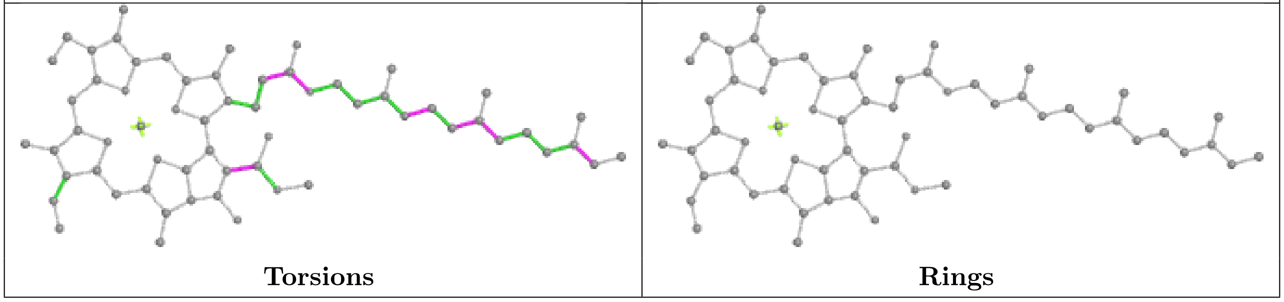
Torsions

Rings

Ligand CLA bA 820

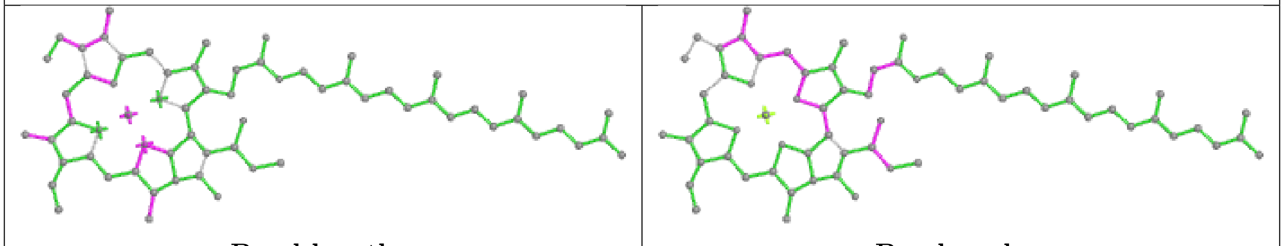


Bond lengths **Bond angles**

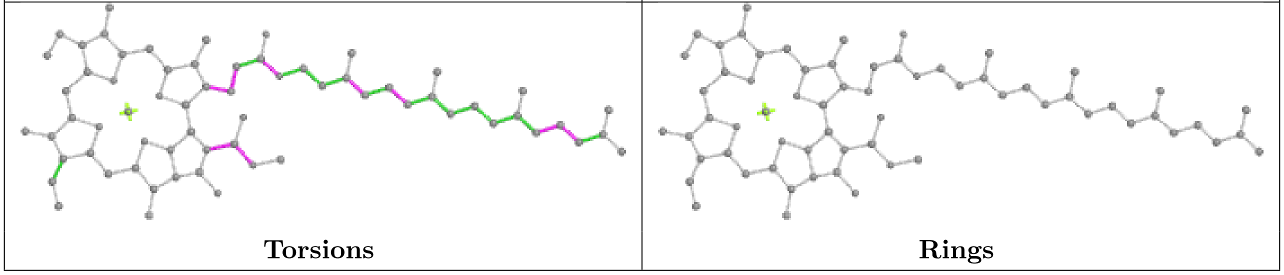


Torsions **Rings**

Ligand CLA cB 801

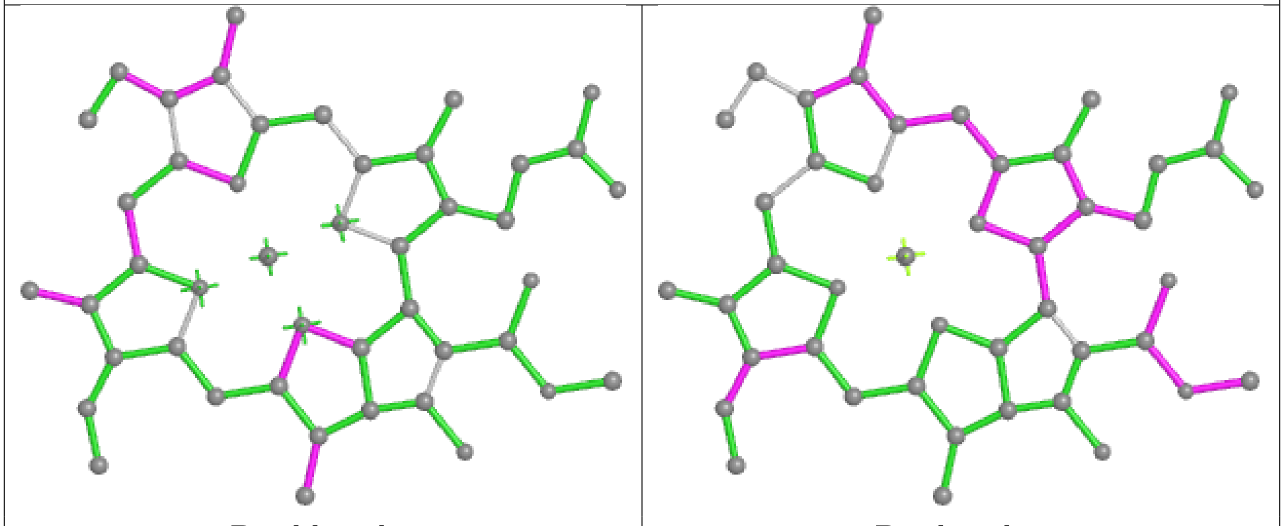


Bond lengths **Bond angles**



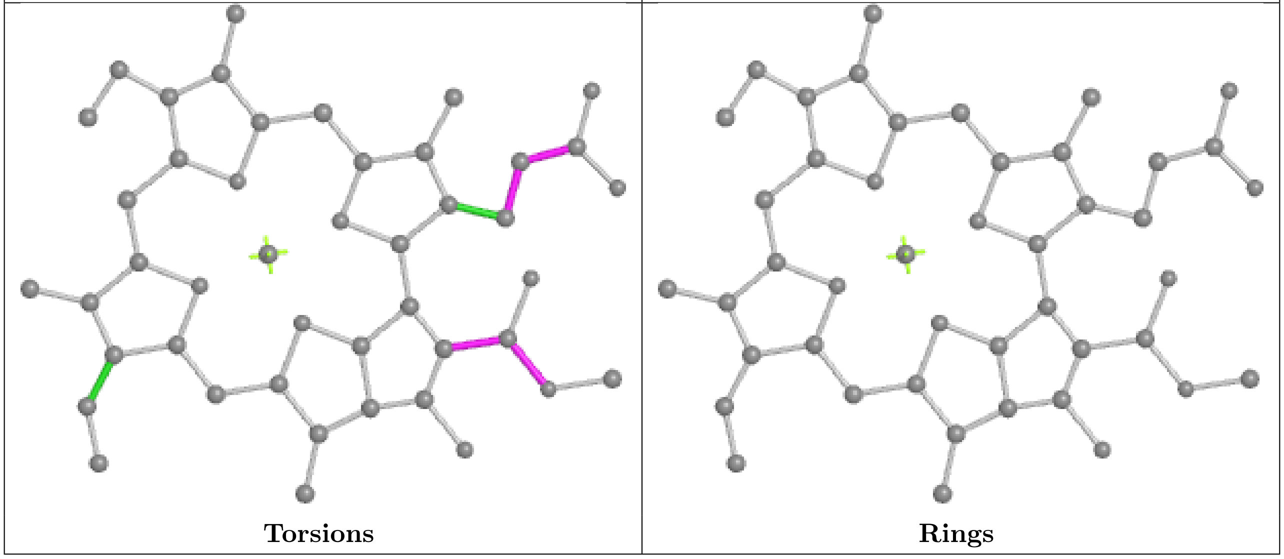
Torsions **Rings**

Ligand CLA bA 813



Bond lengths

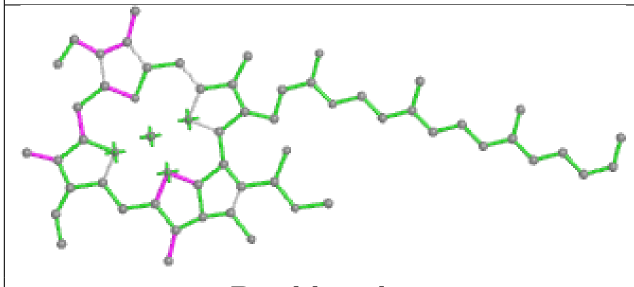
Bond angles



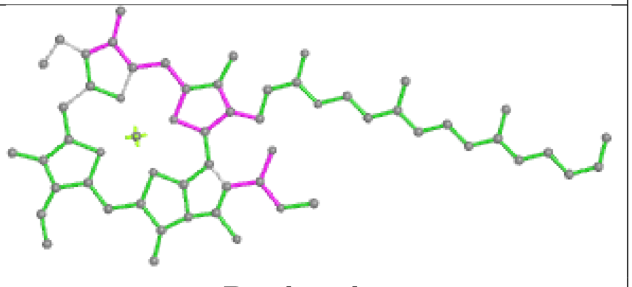
Torsions

Rings

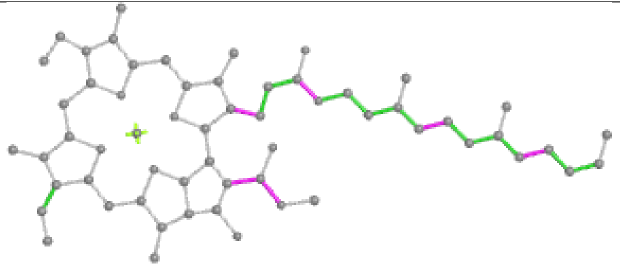
Ligand CLA dB 818



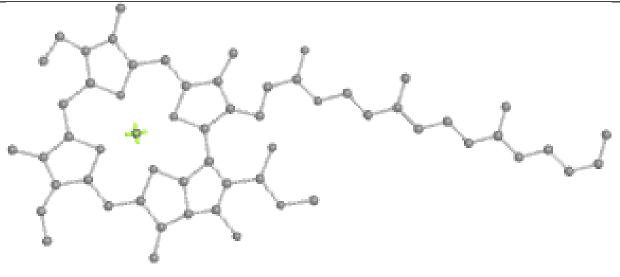
Bond lengths



Bond angles

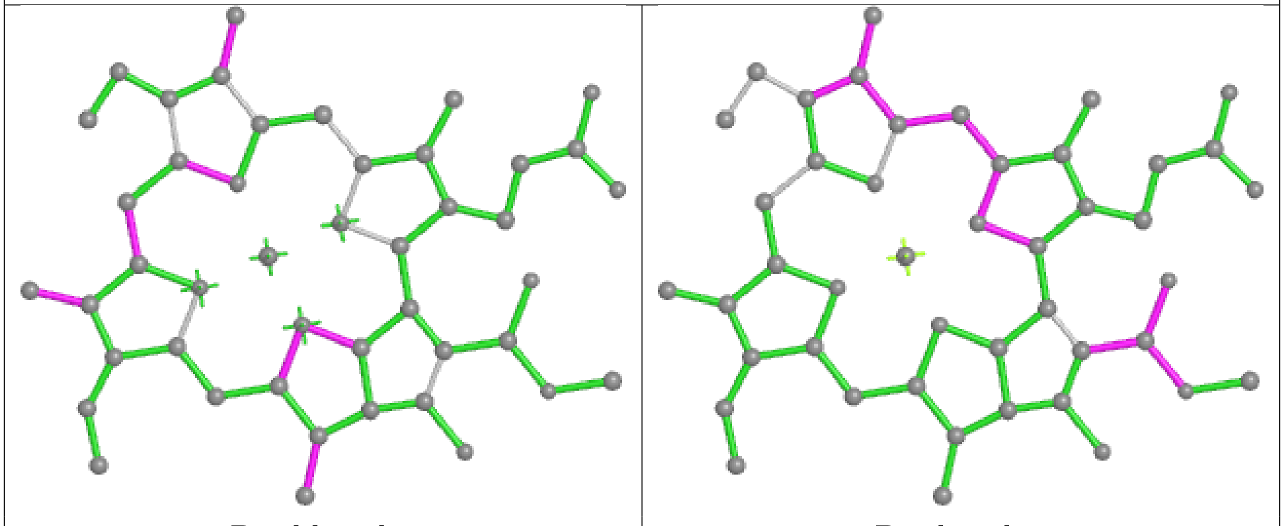


Torsions

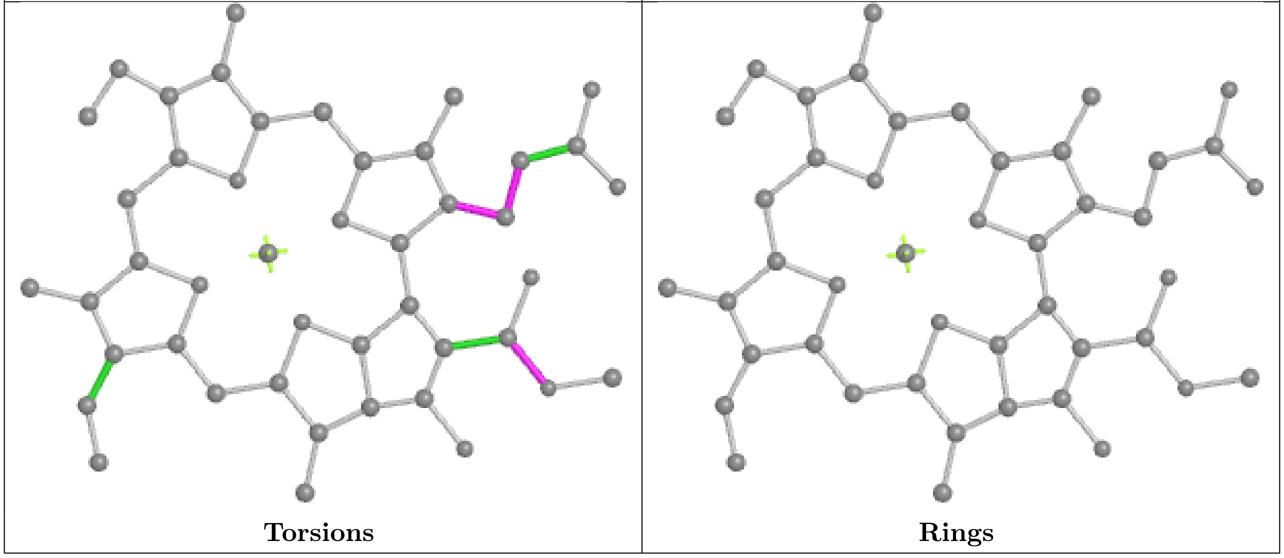


Rings

Ligand CLA bB 816

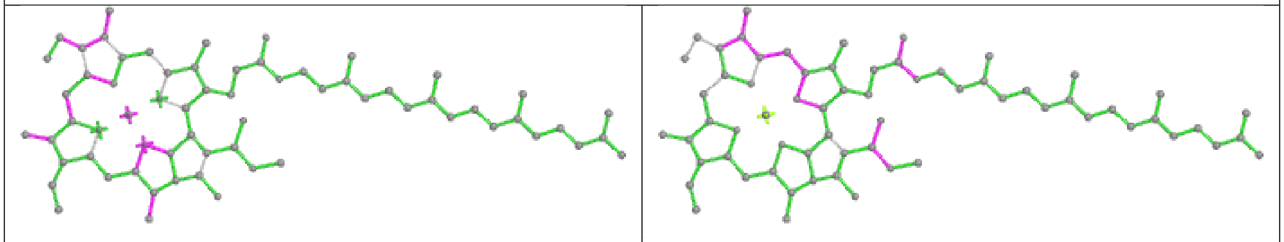


Bond lengths Bond angles

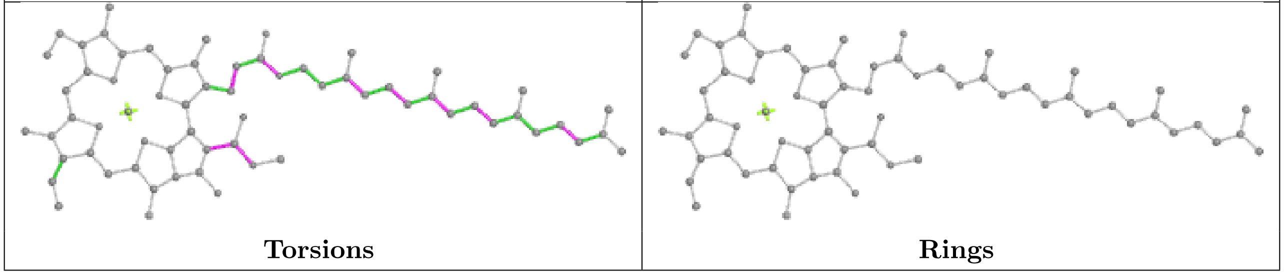


Torsions Rings

Ligand CLA aA 821

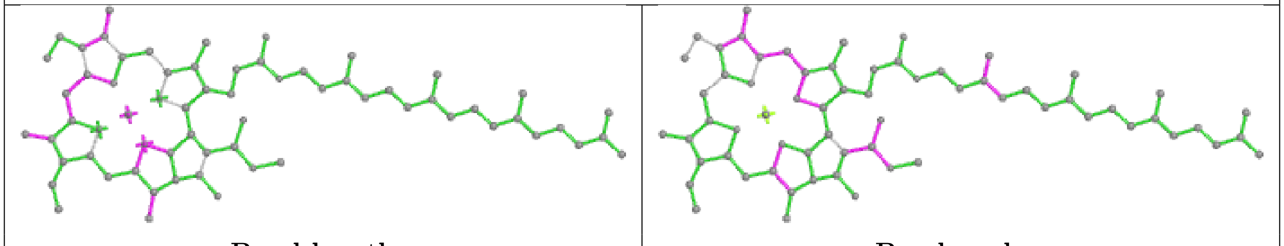


Bond lengths Bond angles

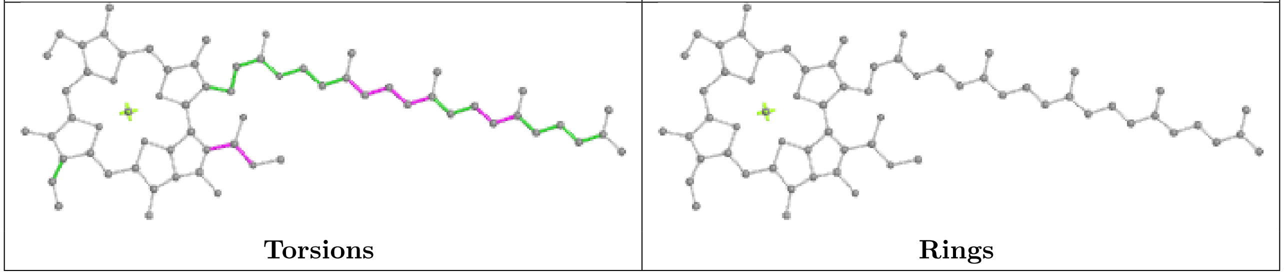


Torsions Rings

Ligand CLA bB 830

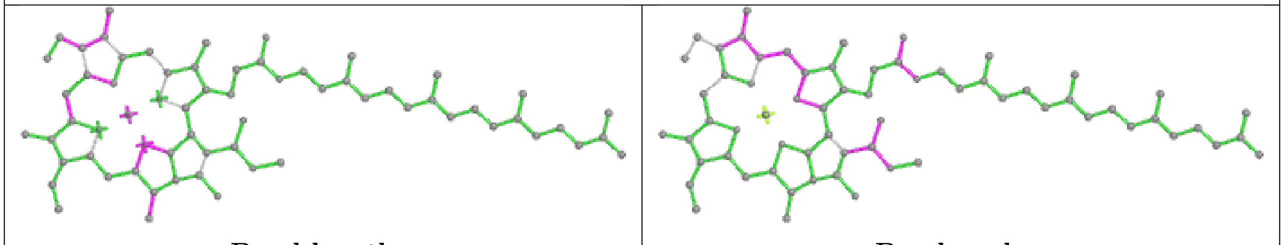


Bond lengths Bond angles

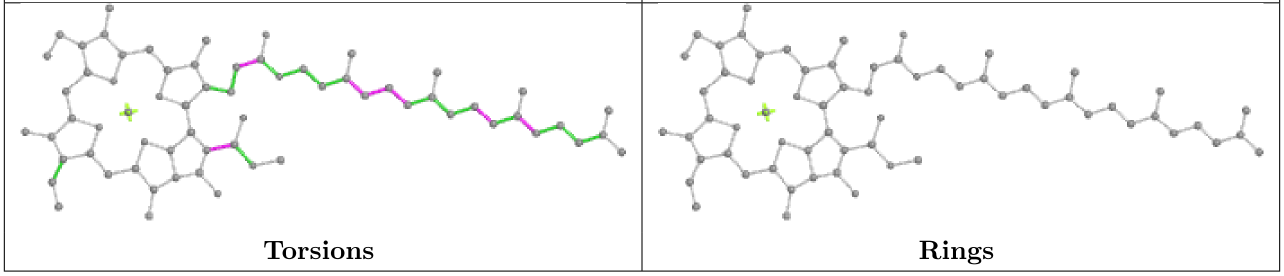


Torsions Rings

Ligand CLA aA 839

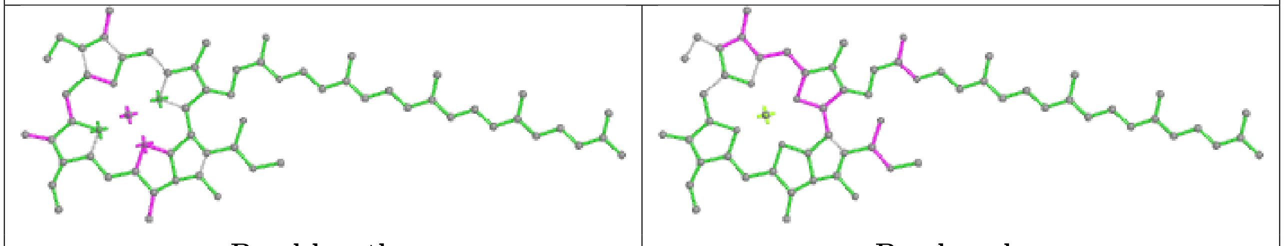


Bond lengths Bond angles

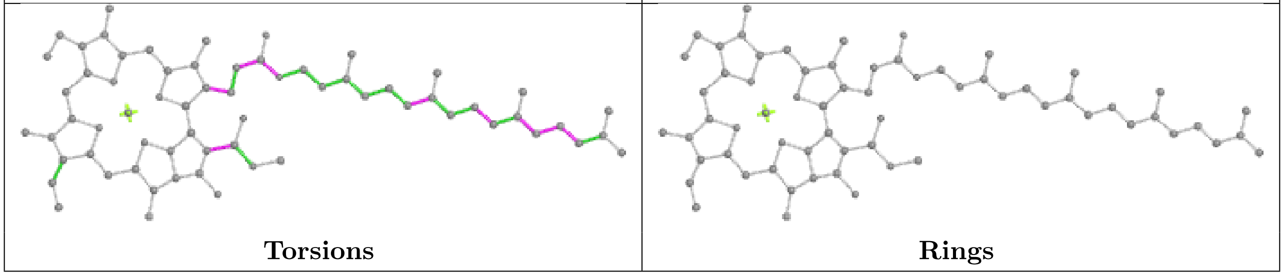


Torsions Rings

Ligand CLA cB 806

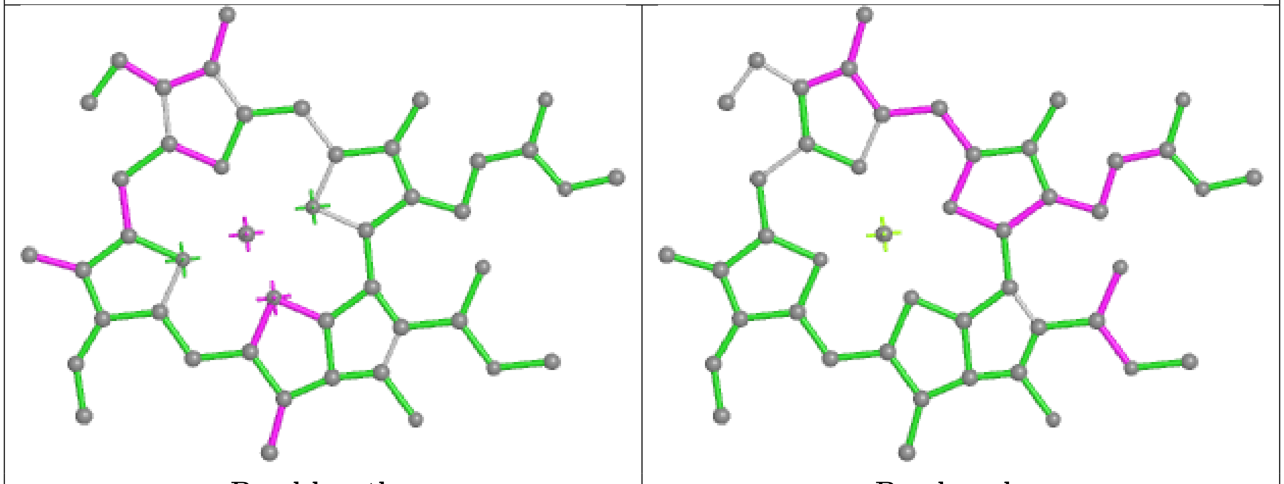


Bond lengths Bond angles

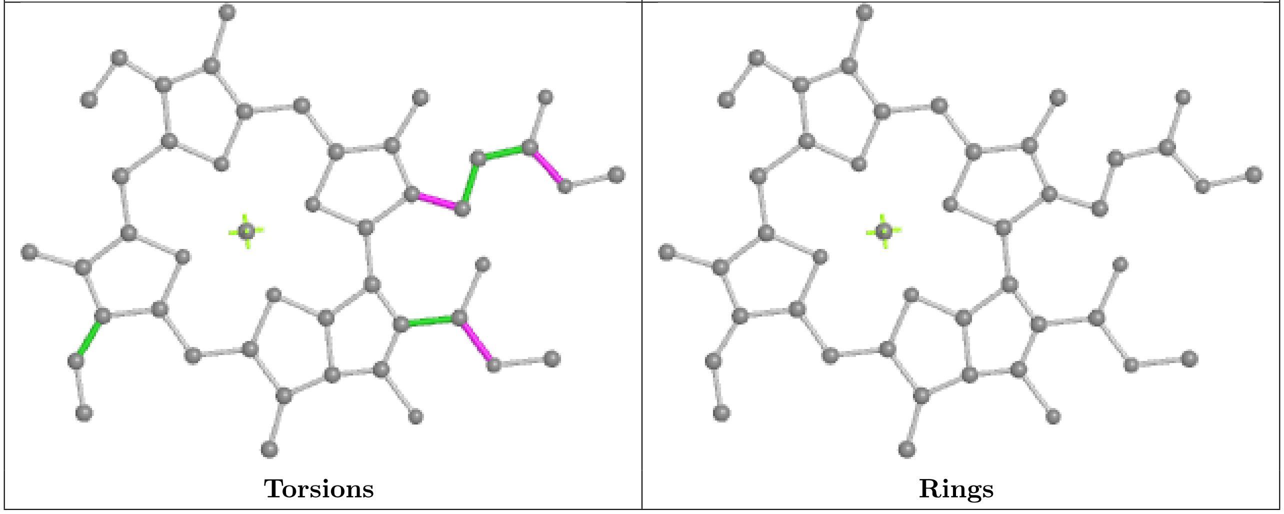


Torsions Rings

Ligand CLA dB 826

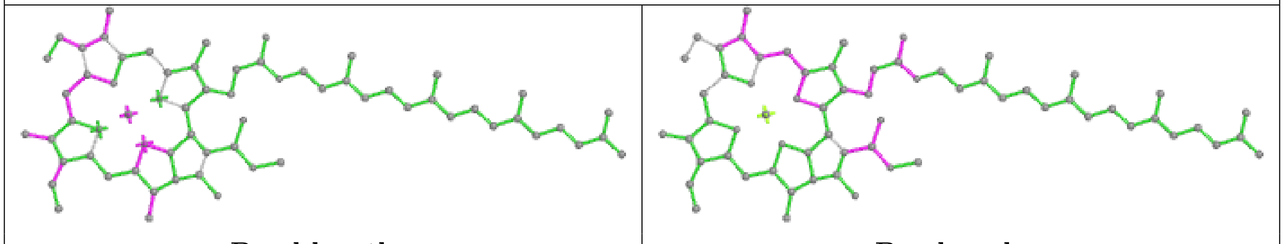

Bond lengths

Bond angles

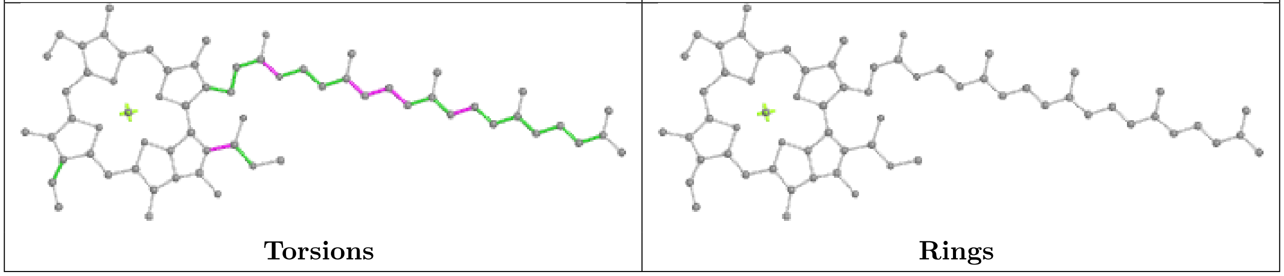

Torsions

Rings

Ligand CLA bB 809

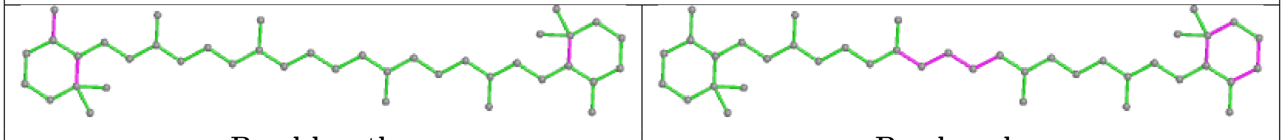

Bond lengths

Bond angles

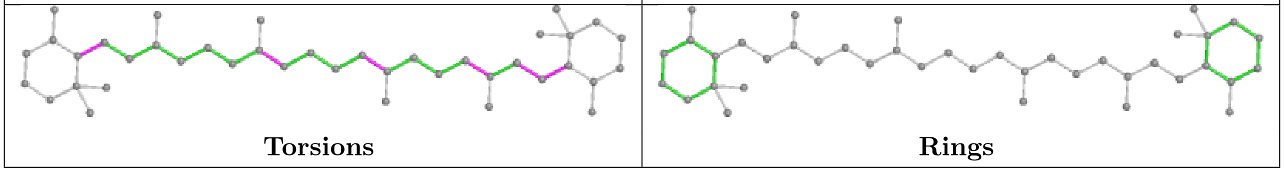

Torsions

Rings

Ligand BCR cJ 104

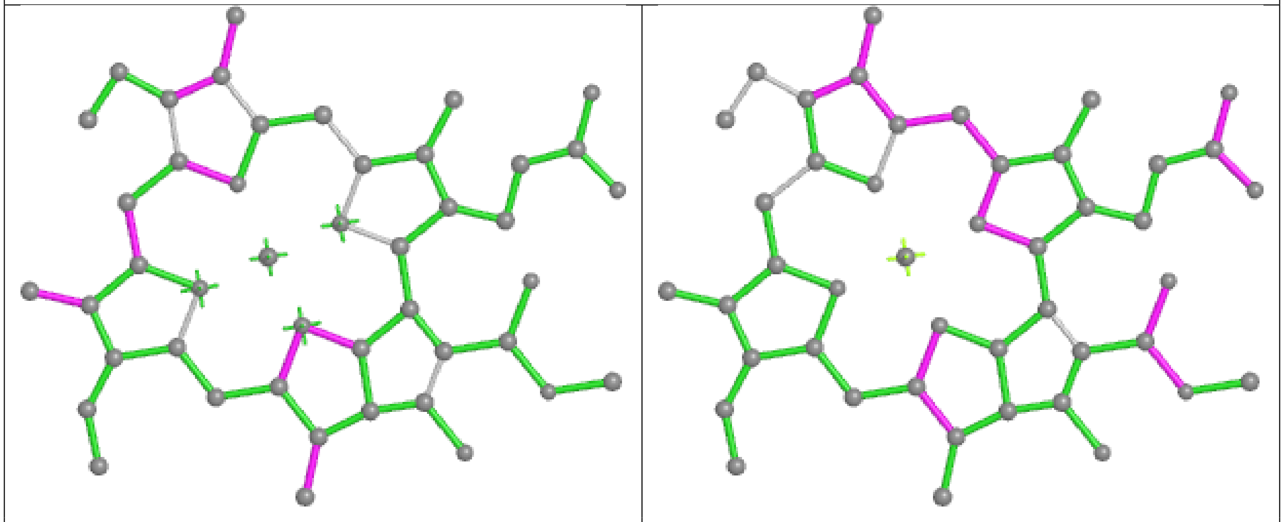


Bond lengths Bond angles

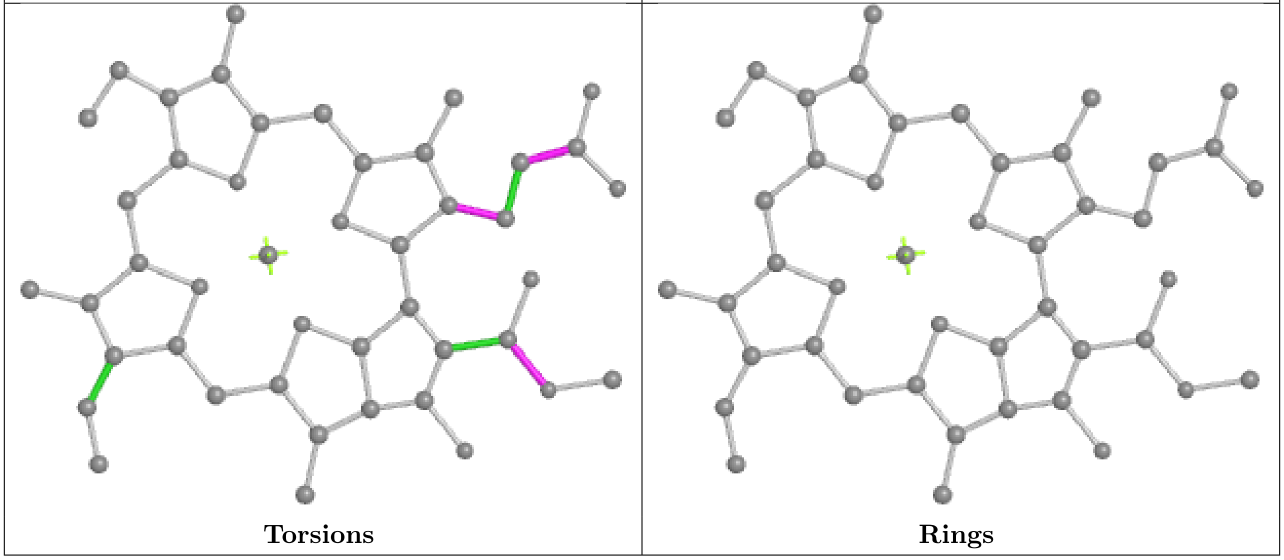


Torsions Rings

Ligand CLA dB 824

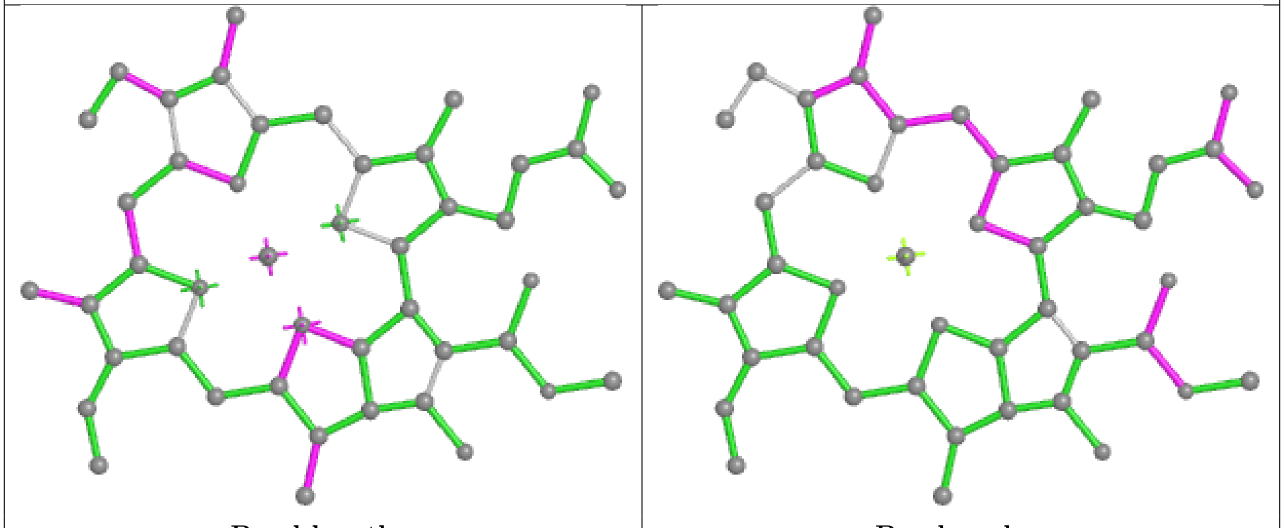


Bond lengths Bond angles



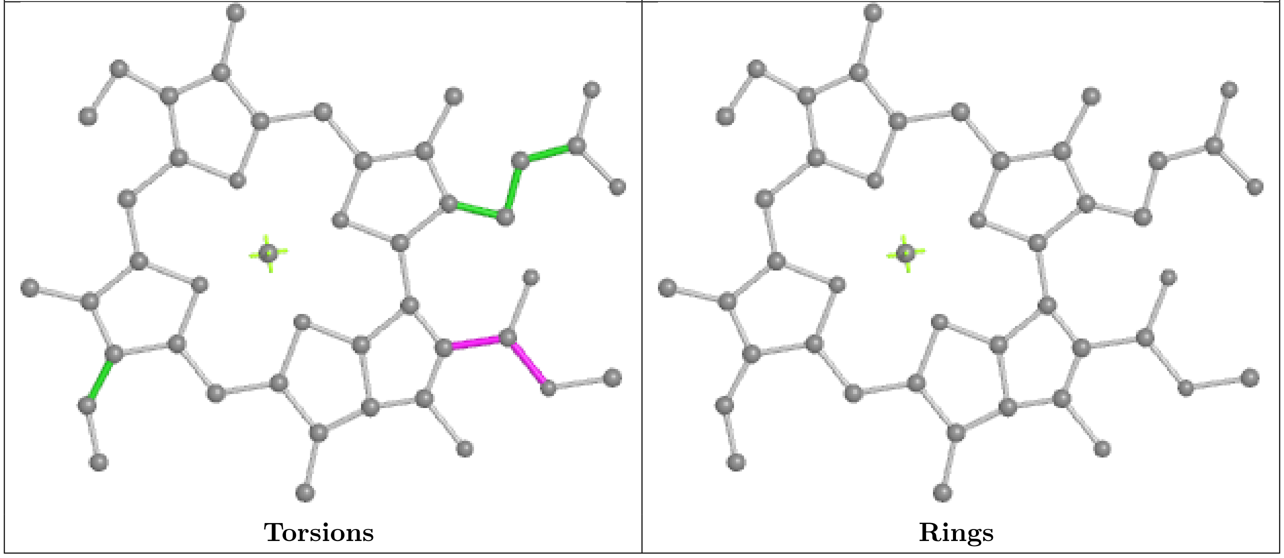
Torsions Rings

Ligand CLA dB 822



Bond lengths

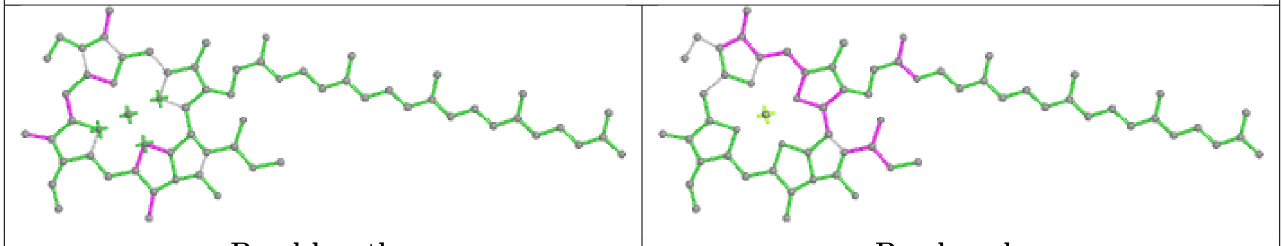
Bond angles



Torsions

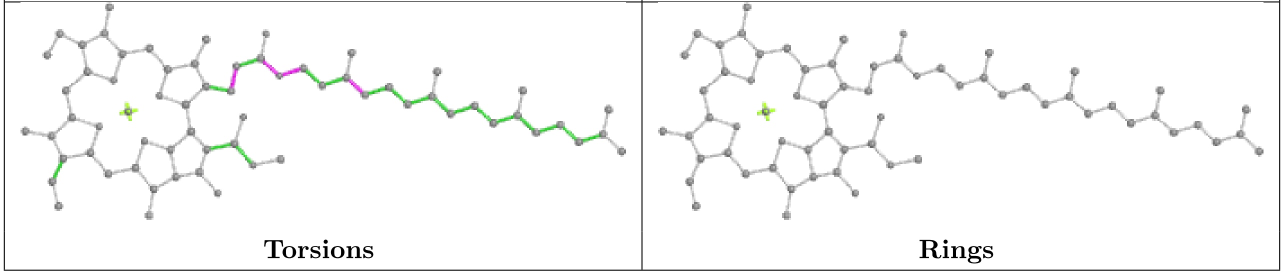
Rings

Ligand CLA aA 828



Bond lengths

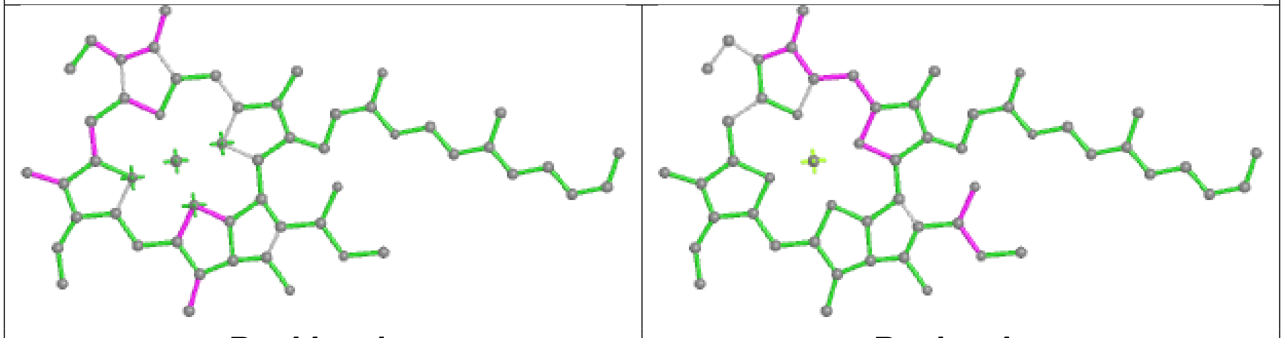
Bond angles



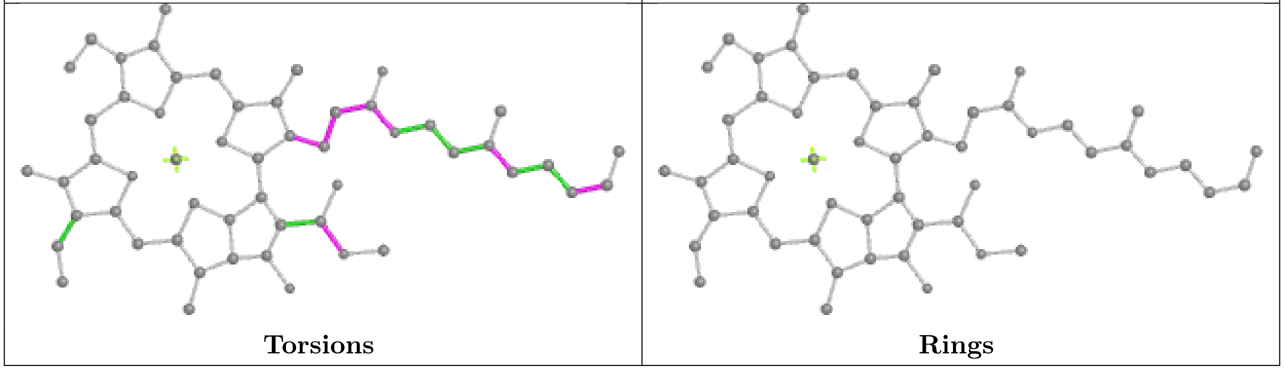
Torsions

Rings

Ligand CLA dA 812

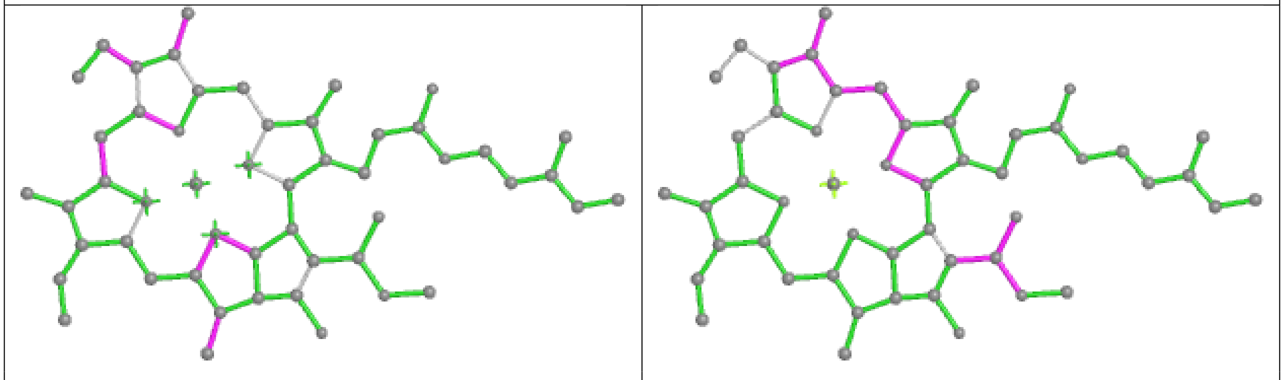


Bond lengths **Bond angles**

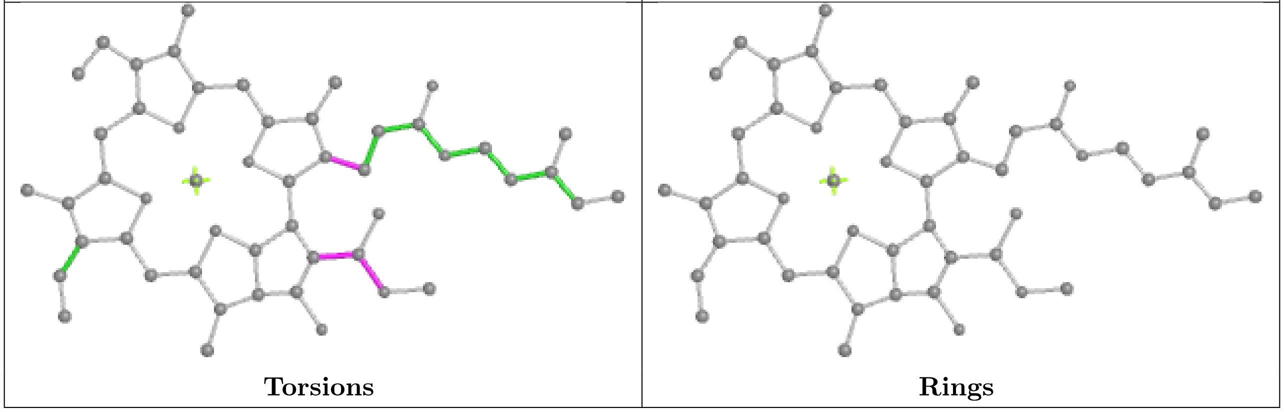


Torsions **Rings**

Ligand CLA dF 201

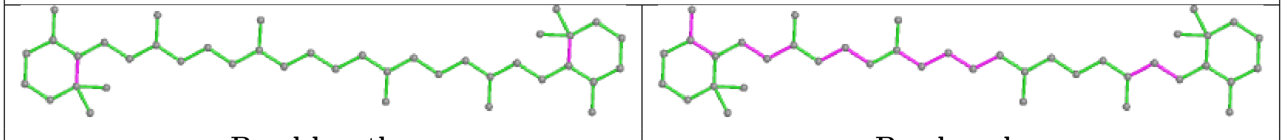


Bond lengths **Bond angles**

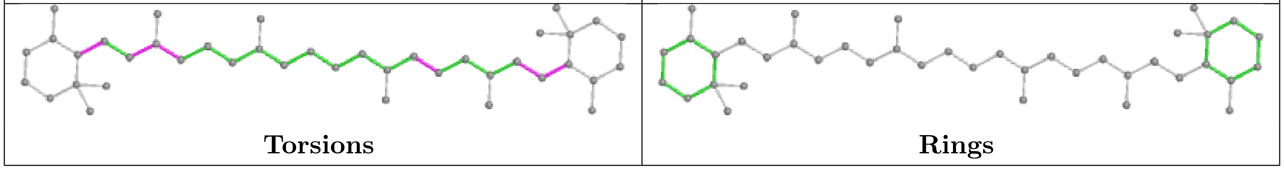


Torsions **Rings**

Ligand BCR aM 101

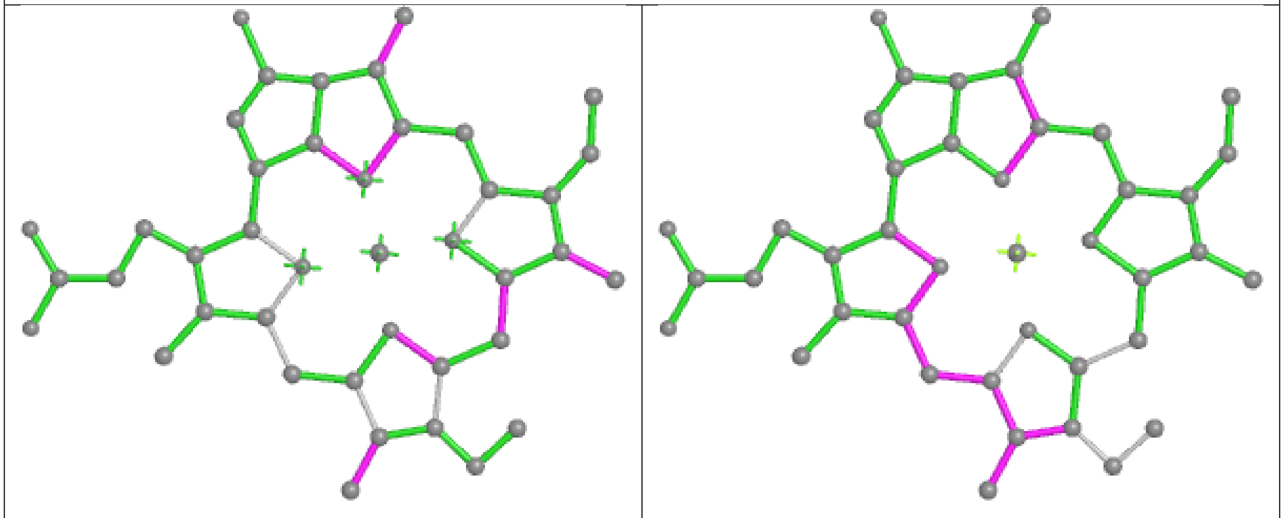


Bond lengths Bond angles

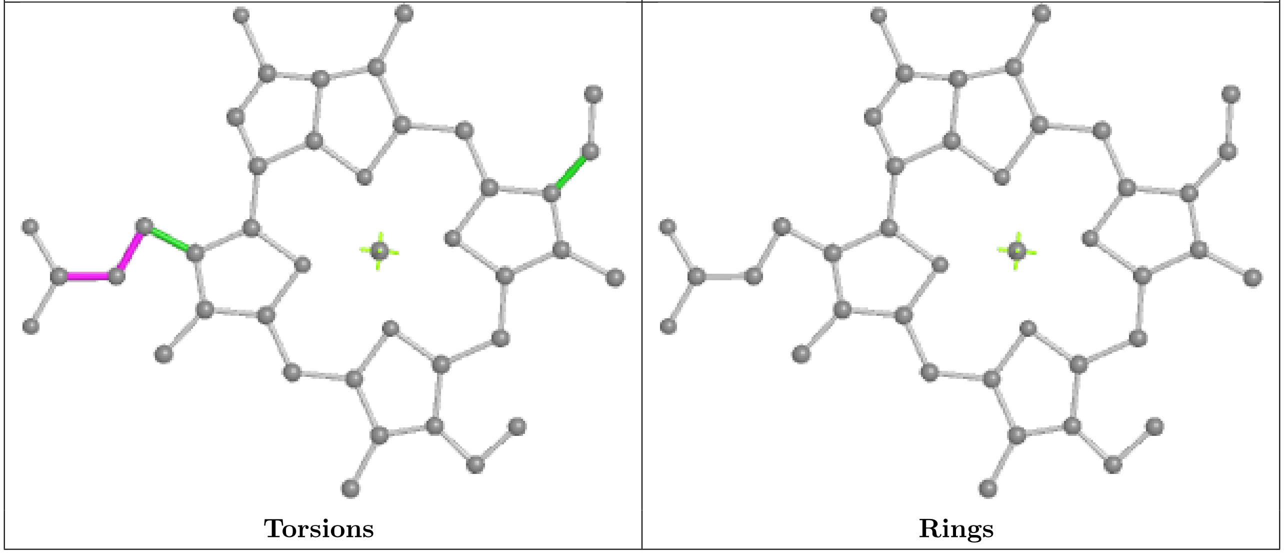


Torsions Rings

Ligand CLA dK 101

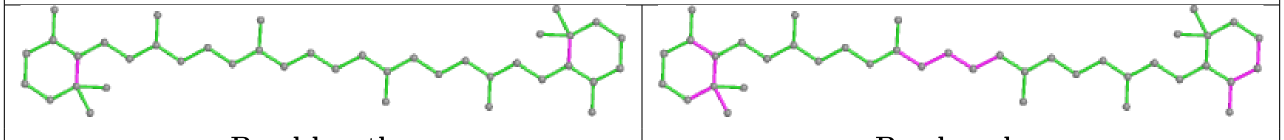


Bond lengths Bond angles



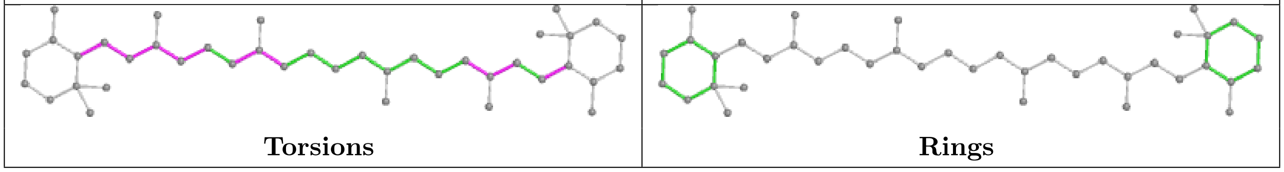
Torsions Rings

Ligand BCR dI 101



Bond lengths

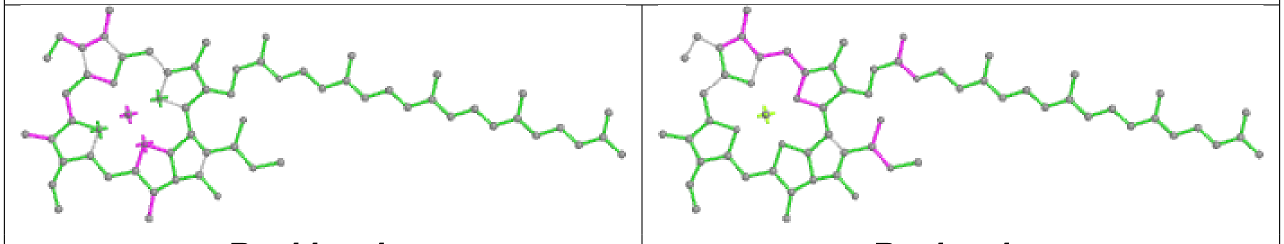
Bond angles



Torsions

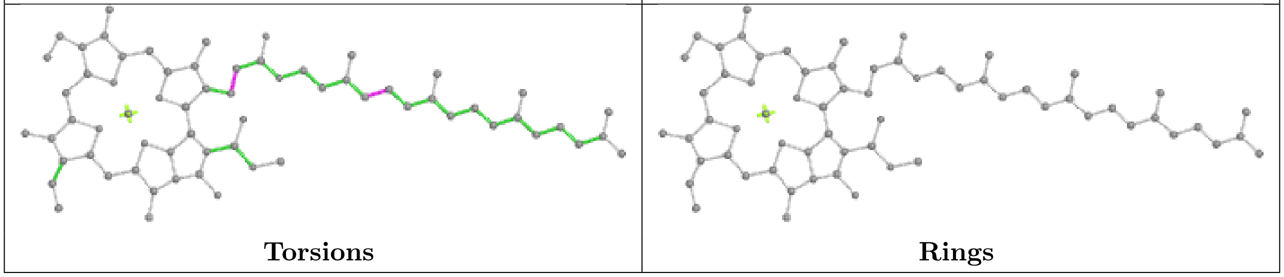
Rings

Ligand CLA aB 840



Bond lengths

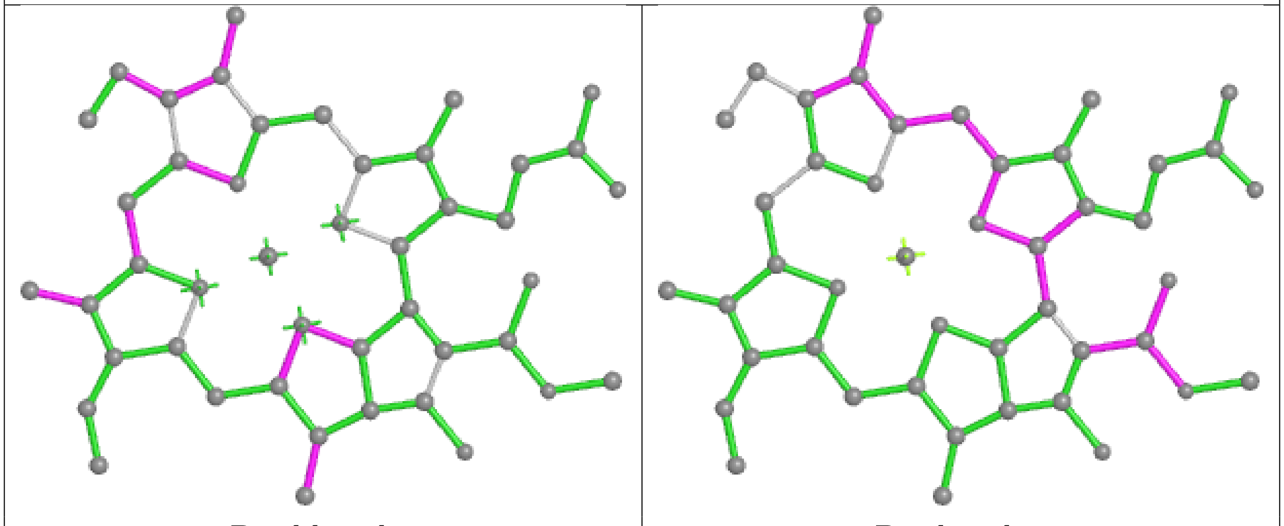
Bond angles

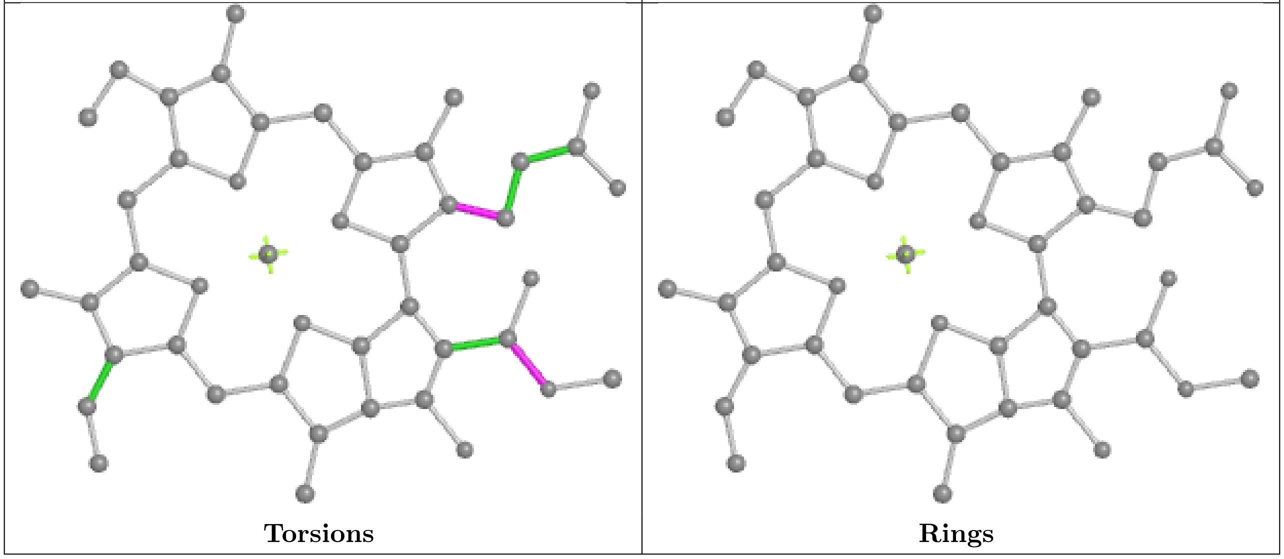


Torsions

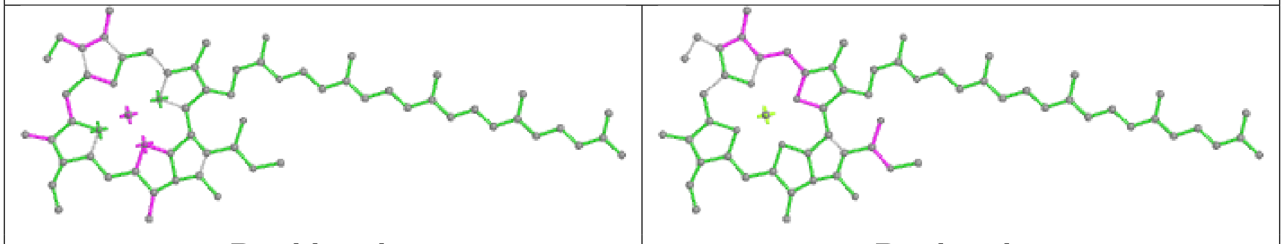
Rings

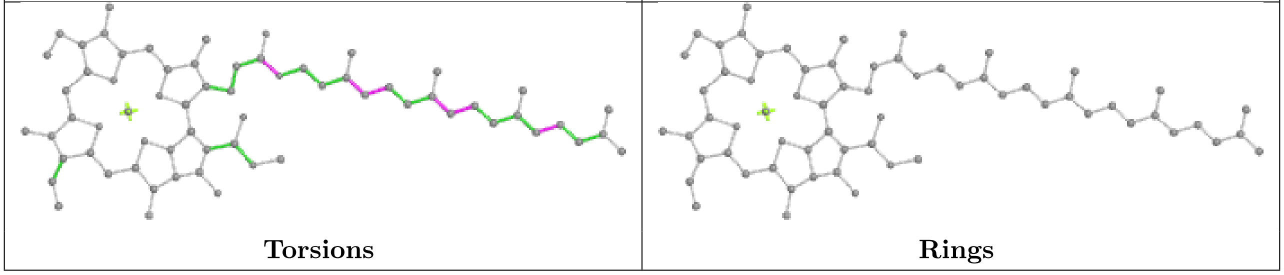
Ligand CLA bA 804


Bond lengths Bond angles

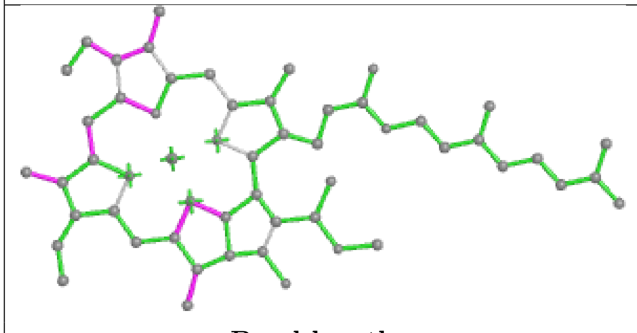

Torsions Rings

Ligand CLA dB 810

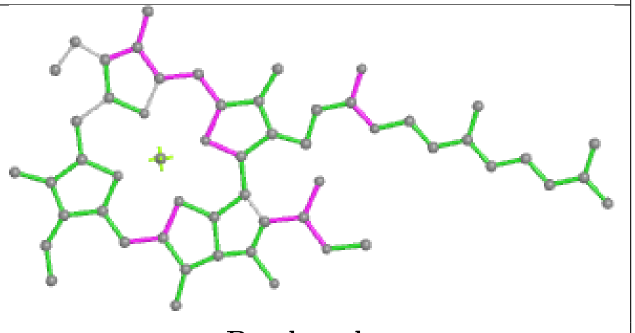

Bond lengths Bond angles


Torsions Rings

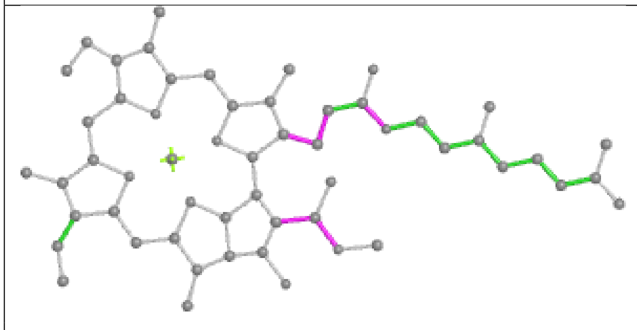
Ligand CLA aB 816



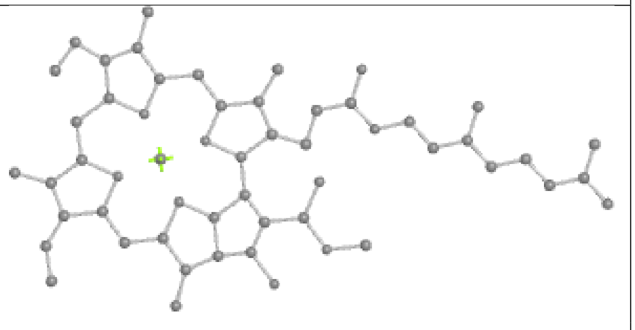
Bond lengths



Bond angles

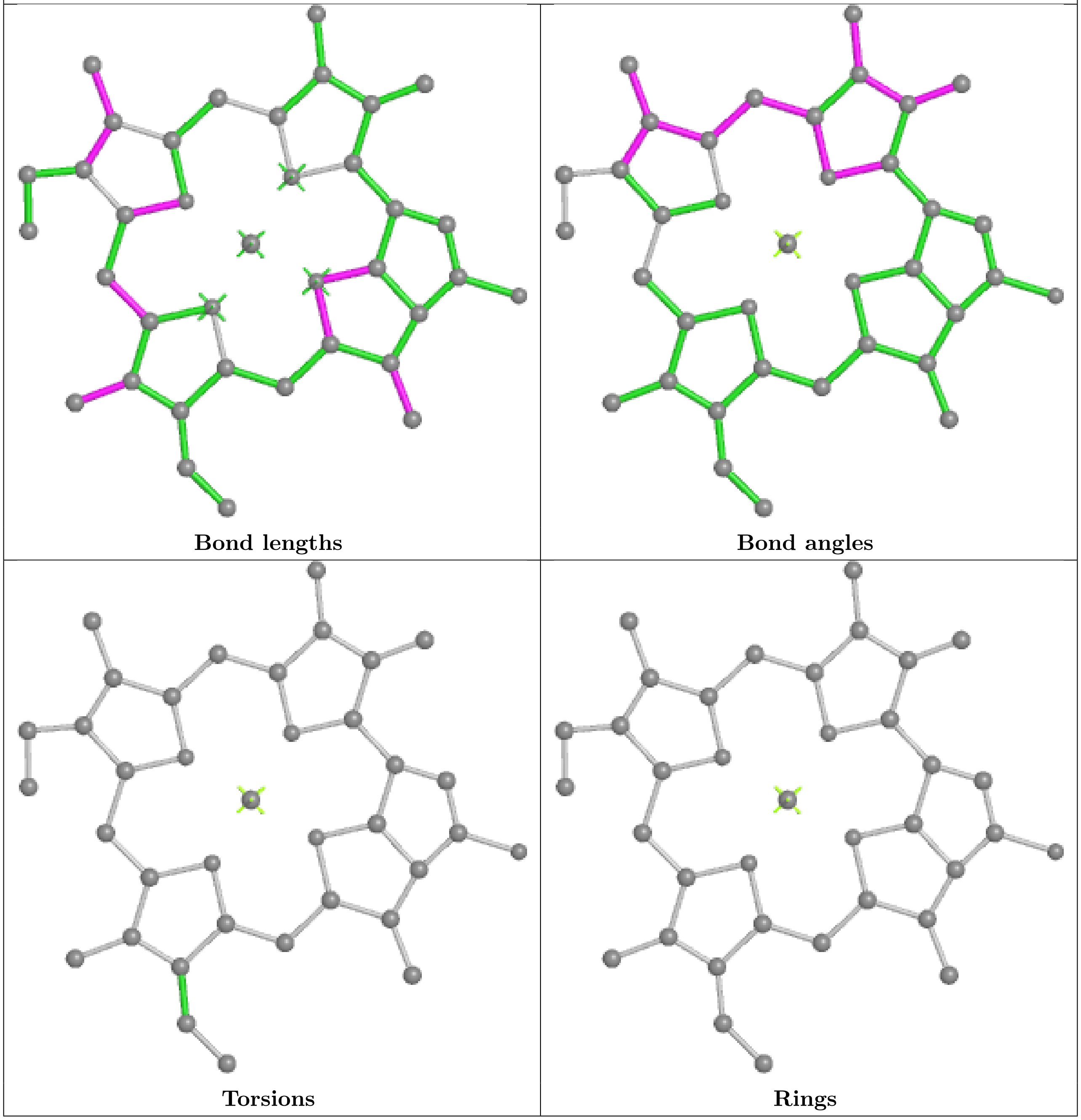


Torsions



Rings

Ligand CLA dJ 102



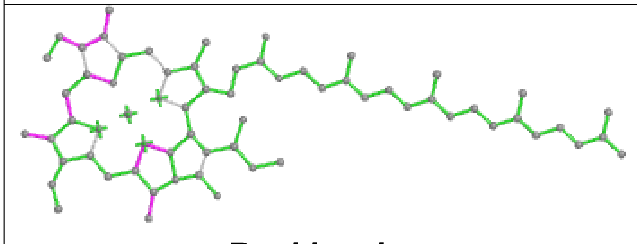
Bond lengths

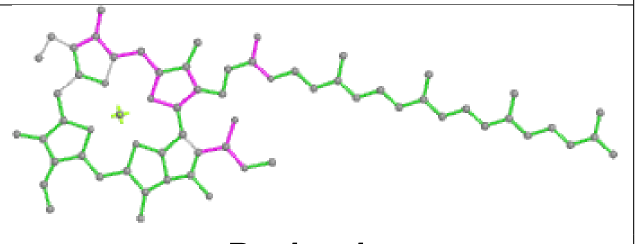
Bond angles

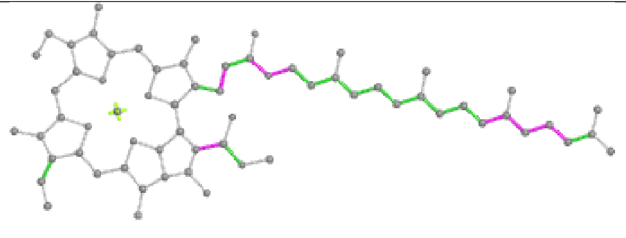
Torsions

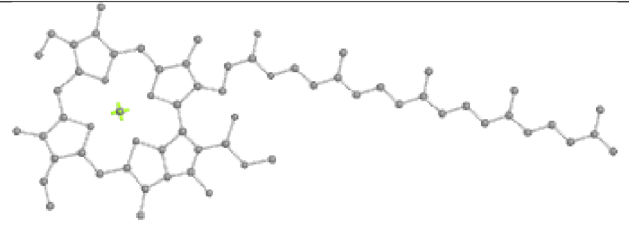
Rings

Ligand CLA aA 838

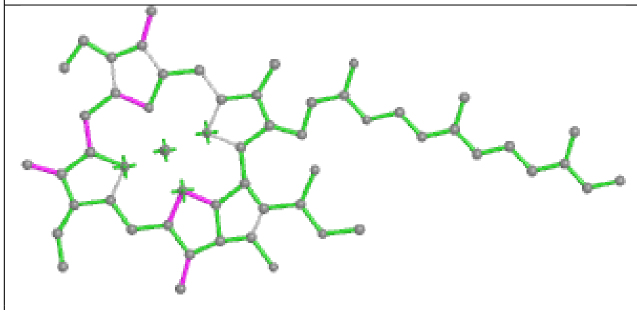

Bond lengths

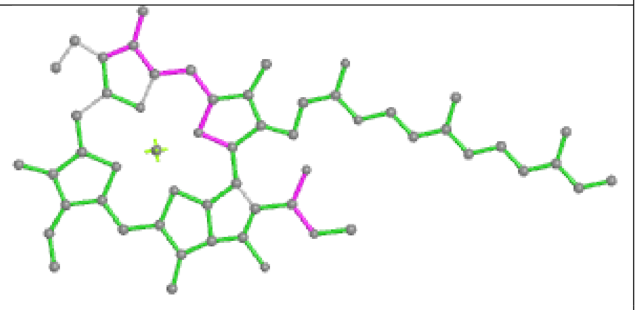

Bond angles

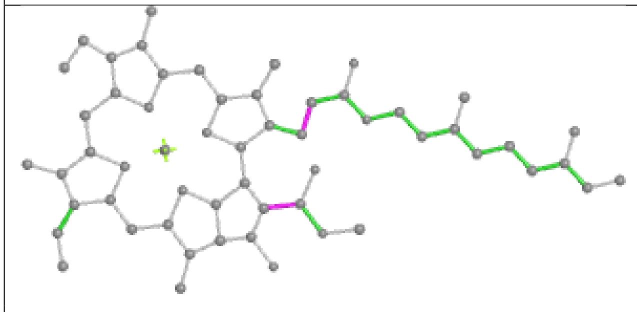

Torsions

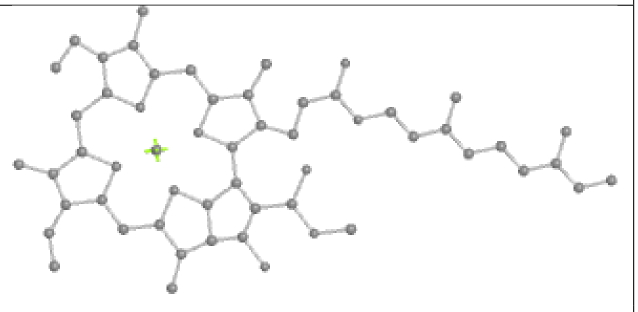

Rings

Ligand CLA bB 815

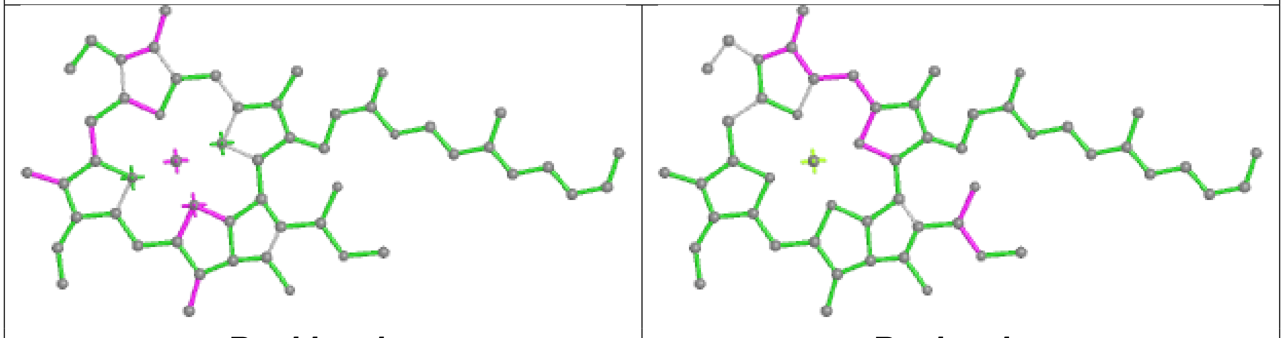

Bond lengths


Bond angles


Torsions

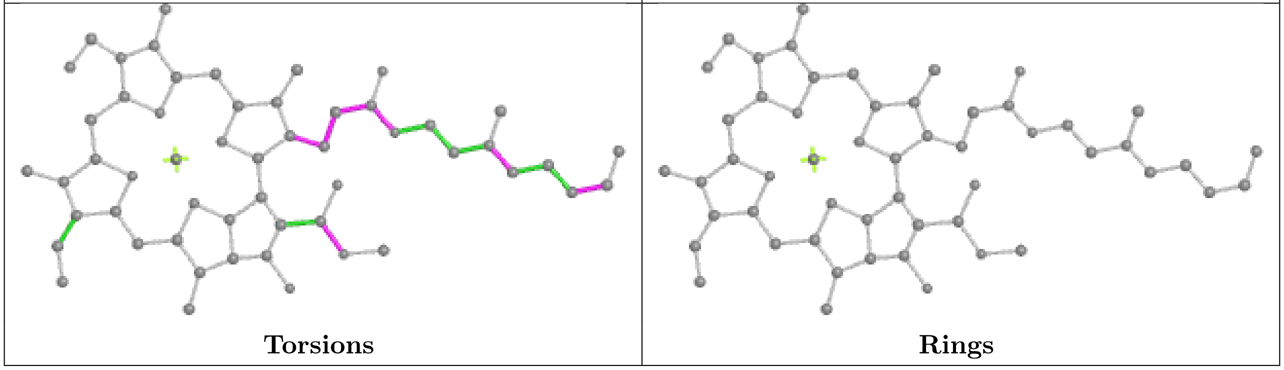

Rings

Ligand CLA cA 812



Bond lengths

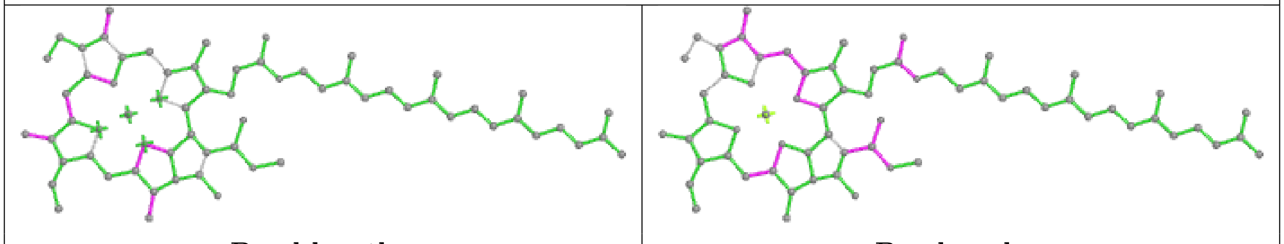
Bond angles



Torsions

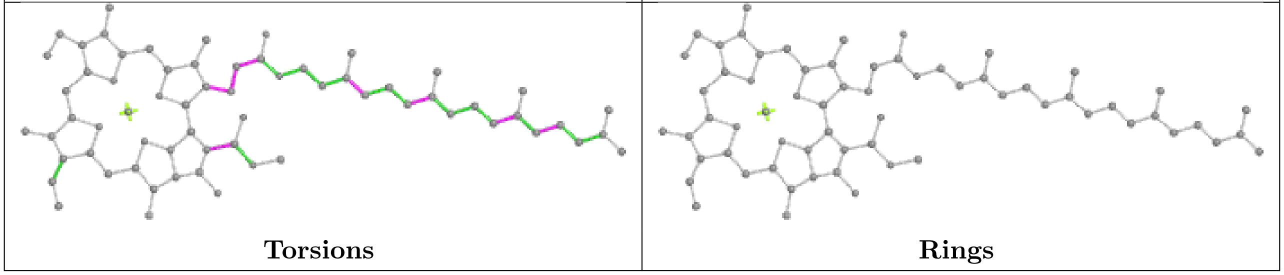
Rings

Ligand CLA aB 827



Bond lengths

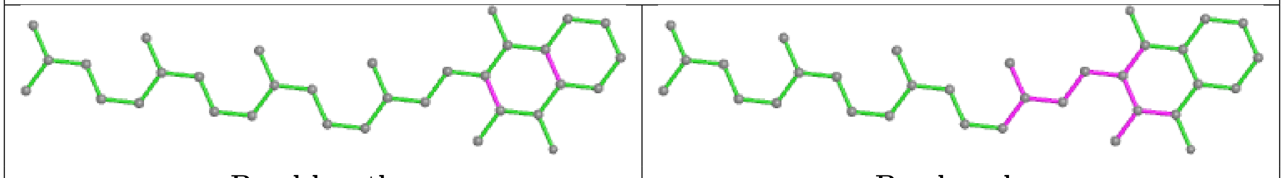
Bond angles



Torsions

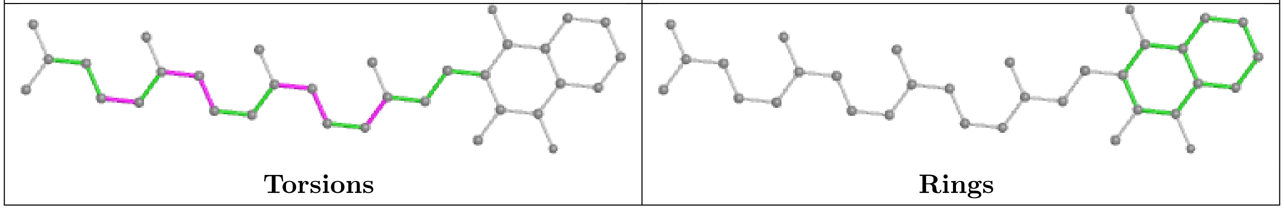
Rings

Ligand PQN cB 842



Bond lengths

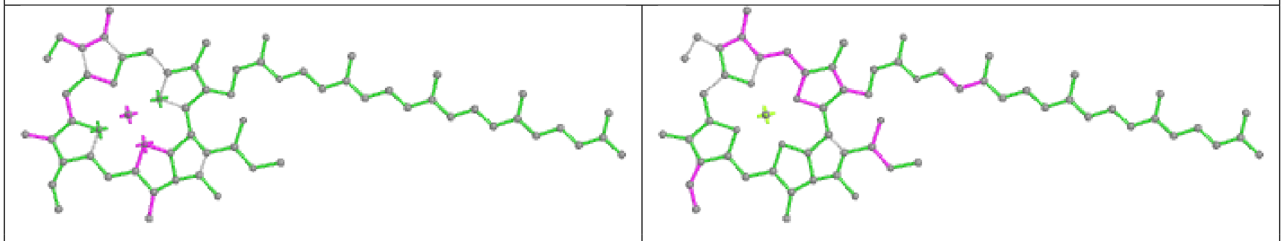
Bond angles



Torsions

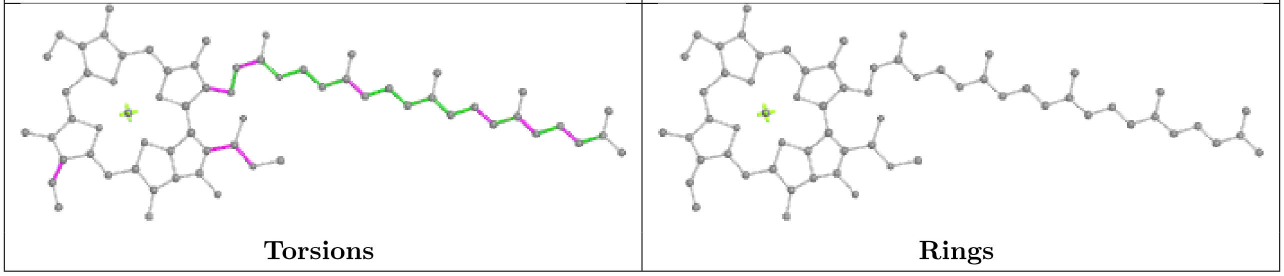
Rings

Ligand CLA cB 813



Bond lengths

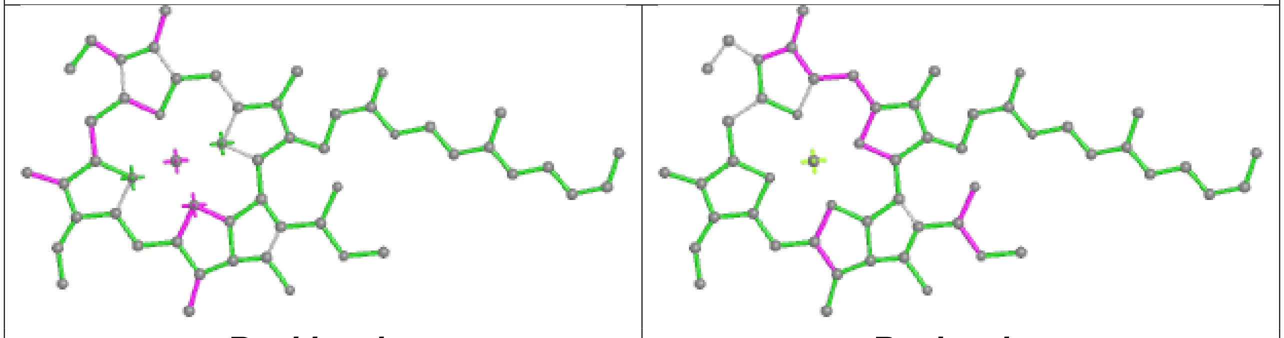
Bond angles



Torsions

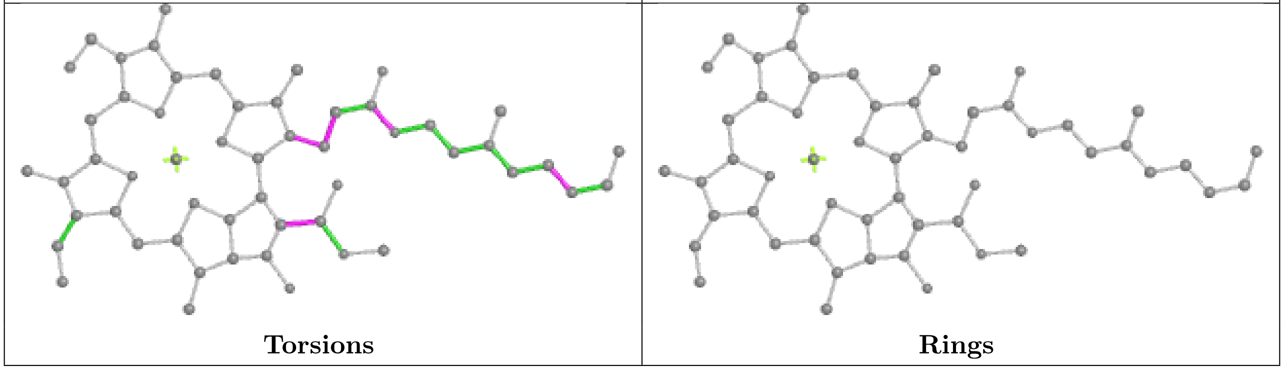
Rings

Ligand CLA cA 818



Bond lengths

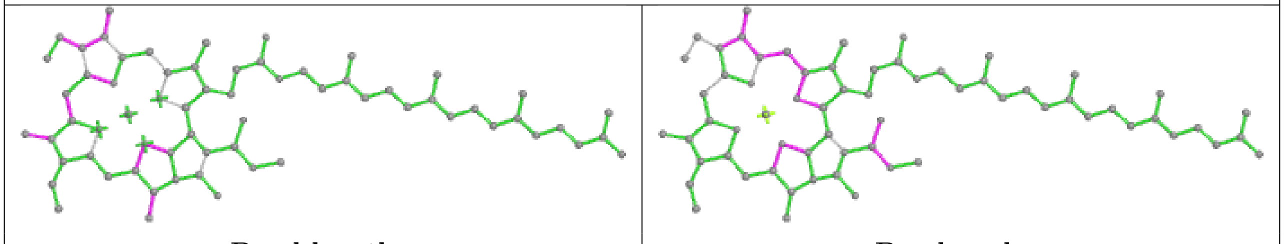
Bond angles



Torsions

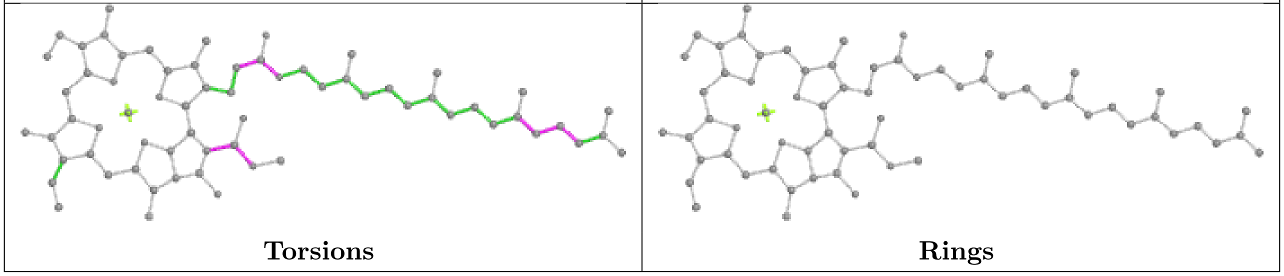
Rings

Ligand CLA bB 802



Bond lengths

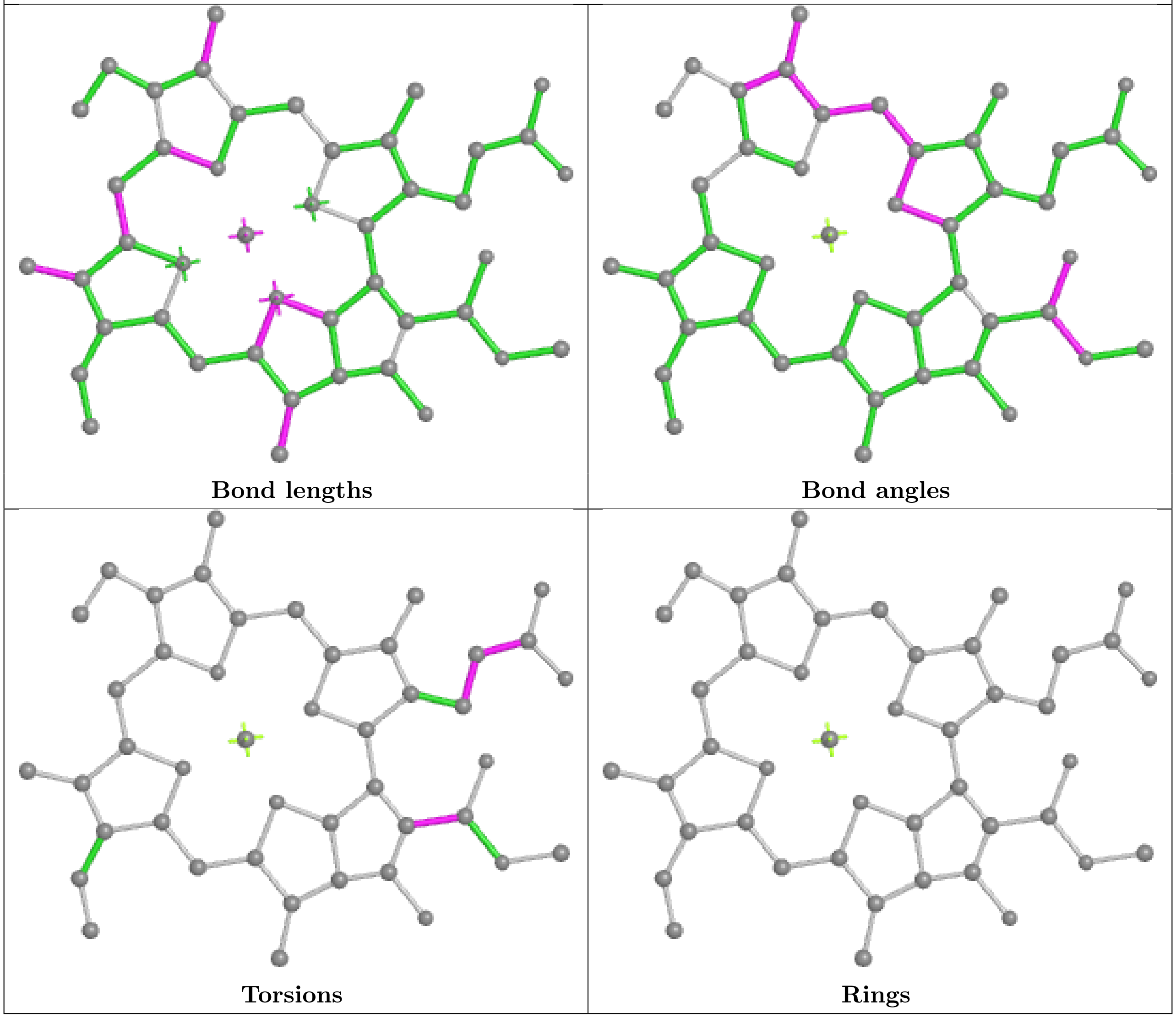
Bond angles



Torsions

Rings

Ligand CLA cF 203



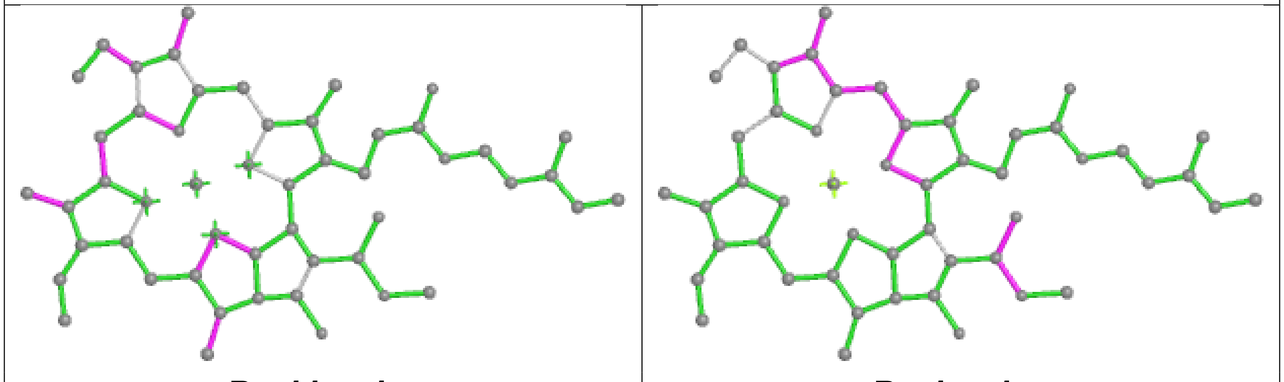
Bond lengths

Bond angles

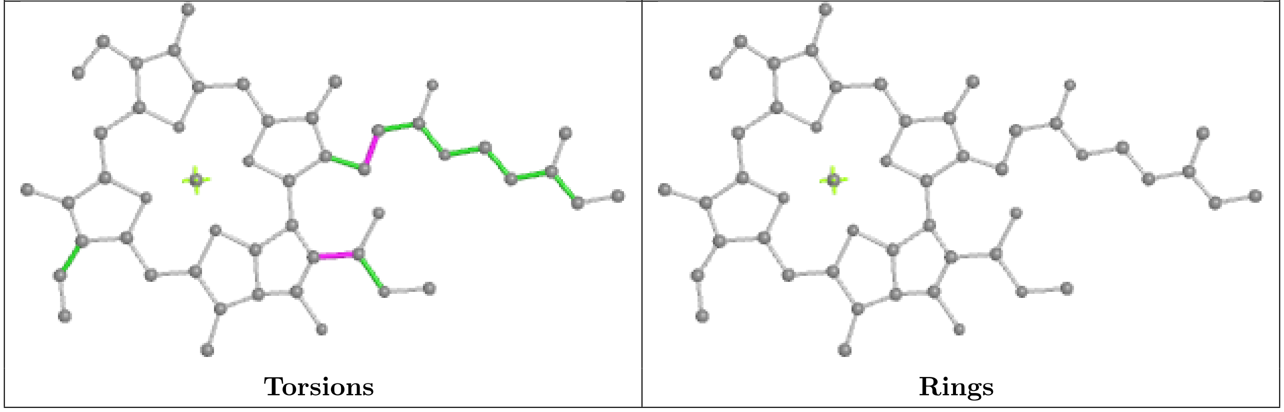
Torsions

Rings

Ligand CLA aA 807

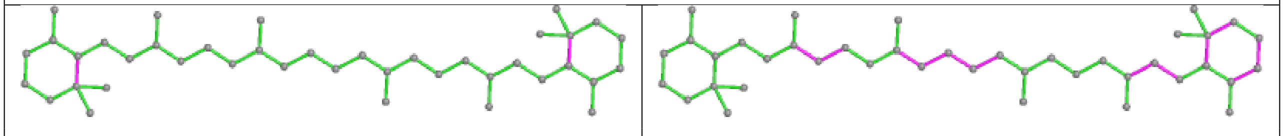


Bond lengths Bond angles

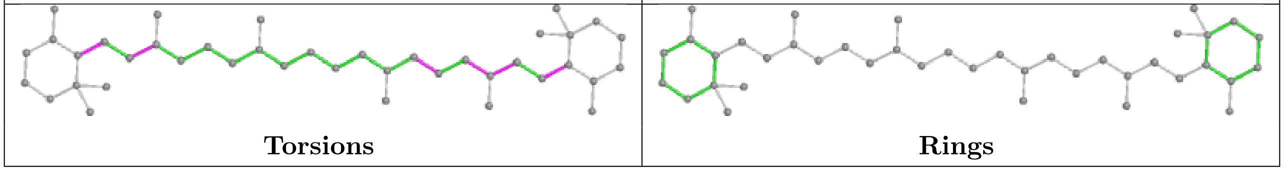


Torsions Rings

Ligand BCR bB 844

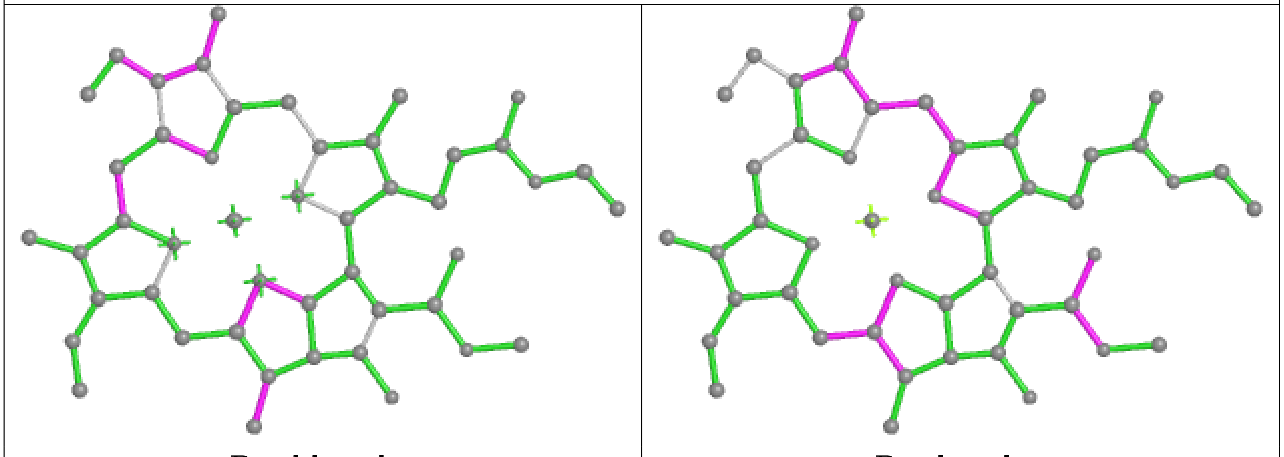


Bond lengths Bond angles



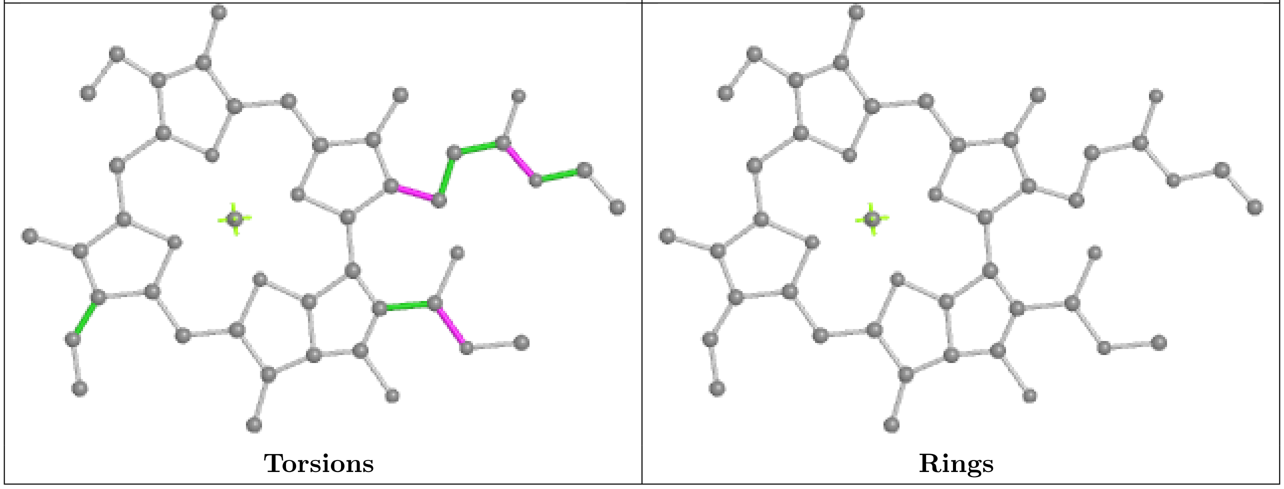
Torsions Rings

Ligand CLA dA 824



Bond lengths

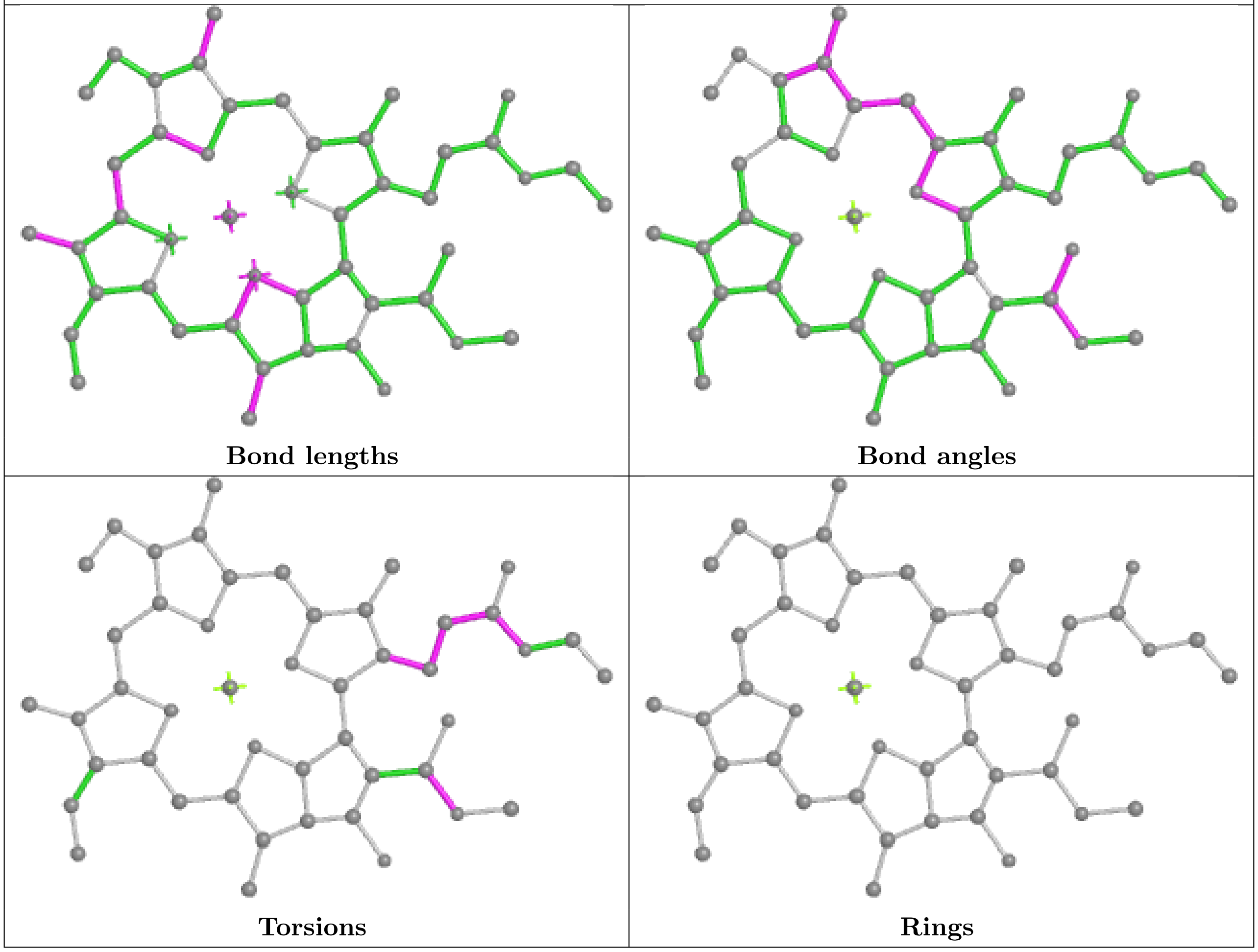
Bond angles



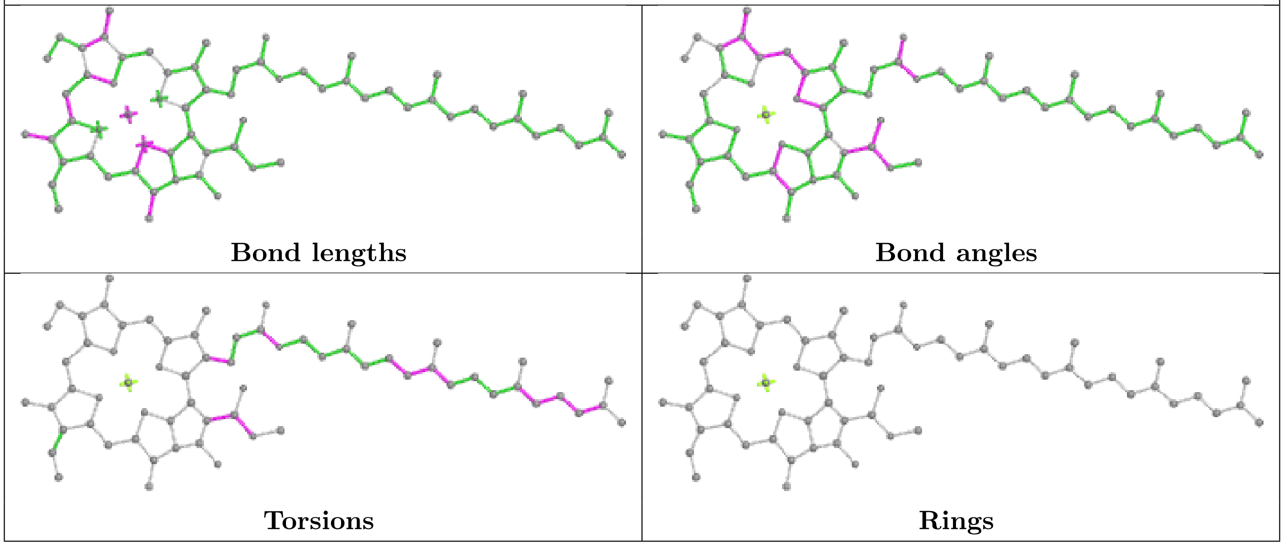
Torsions

Rings

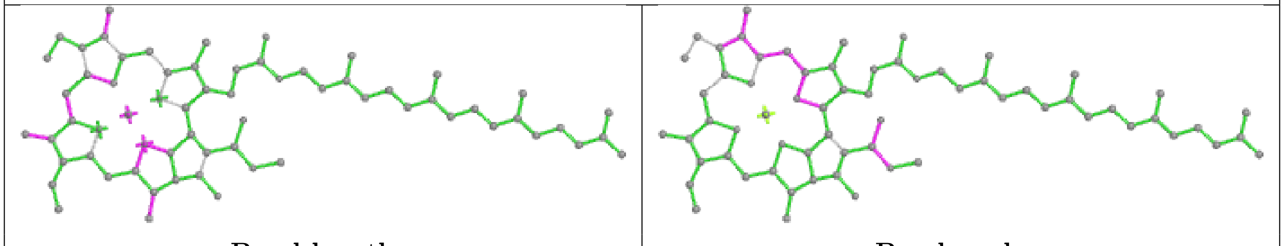
Ligand CLA dB 821


Bond lengths
Bond angles
Torsions
Rings

Ligand CLA cA 819

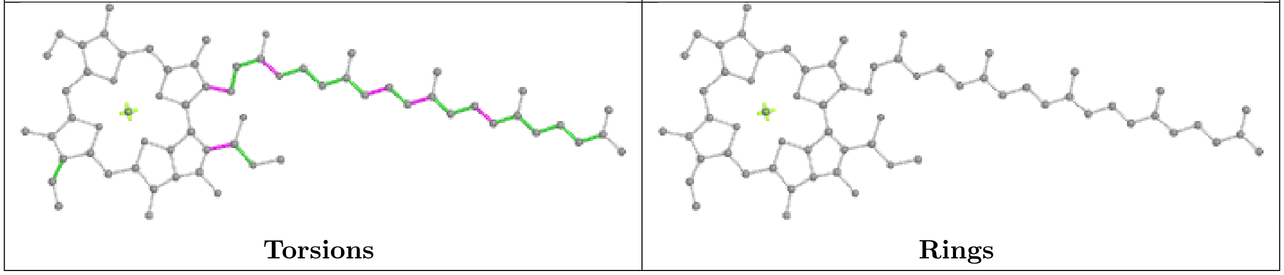

Bond lengths
Bond angles
Torsions
Rings

Ligand CLA cB 819



Bond lengths

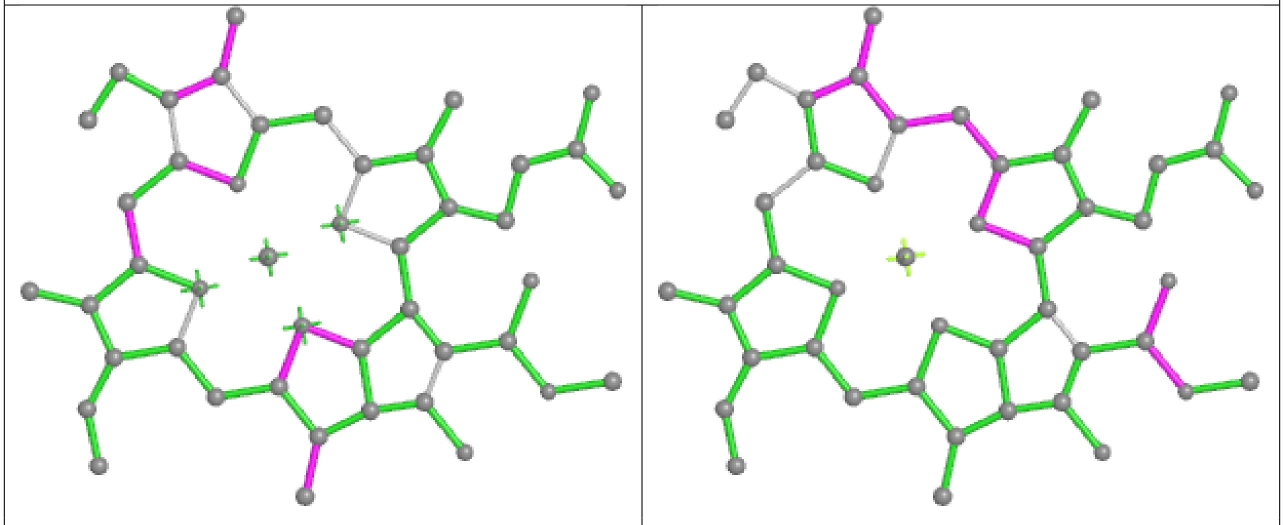
Bond angles



Torsions

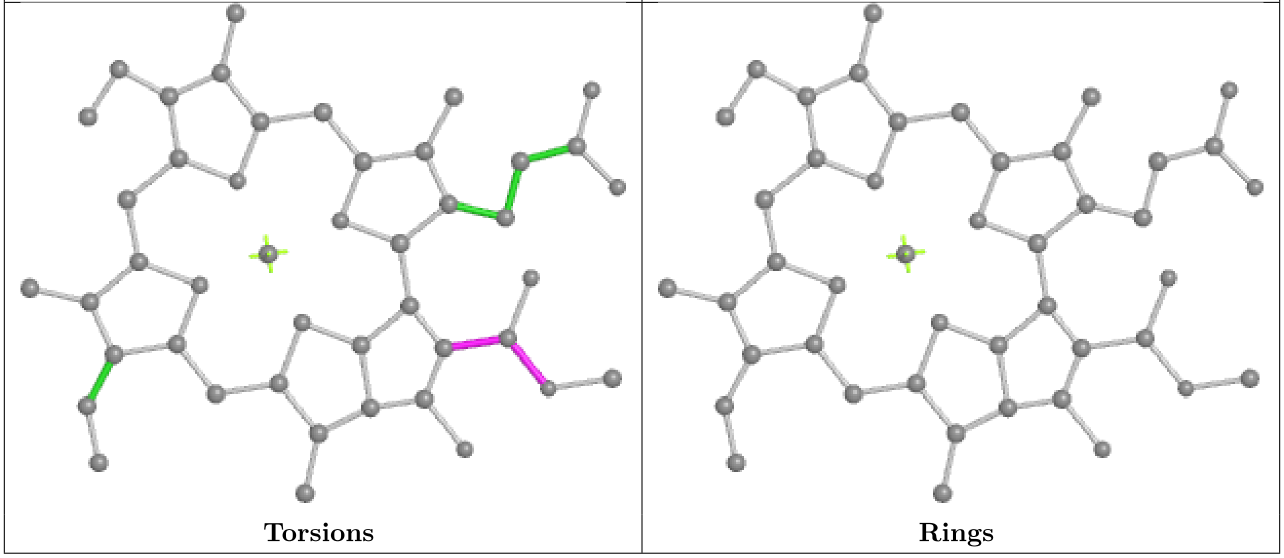
Rings

Ligand CLA dA 815



Bond lengths

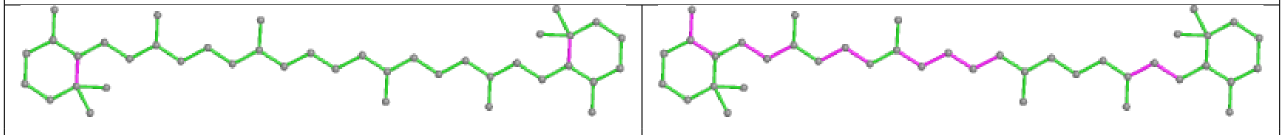
Bond angles



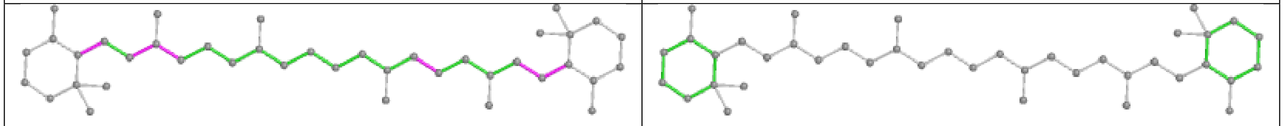
Torsions

Rings

Ligand BCR bM 101

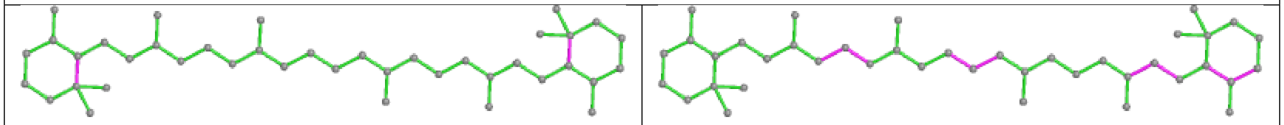


Bond lengths Bond angles

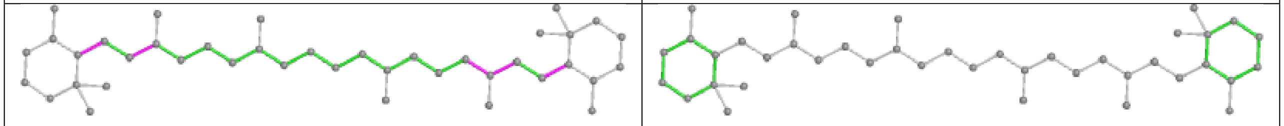


Torsions Rings

Ligand BCR aB 848

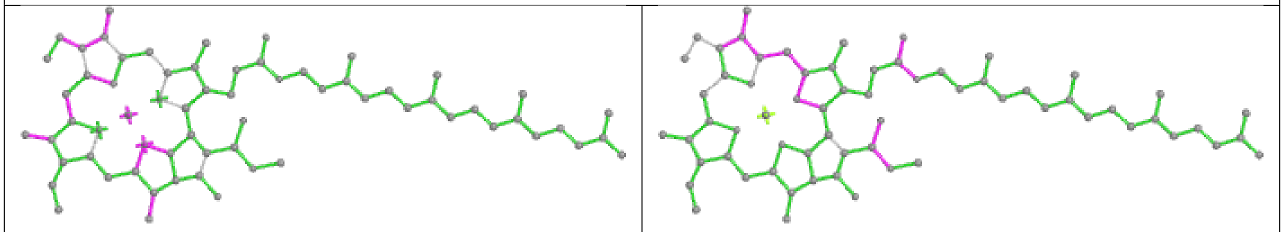


Bond lengths Bond angles

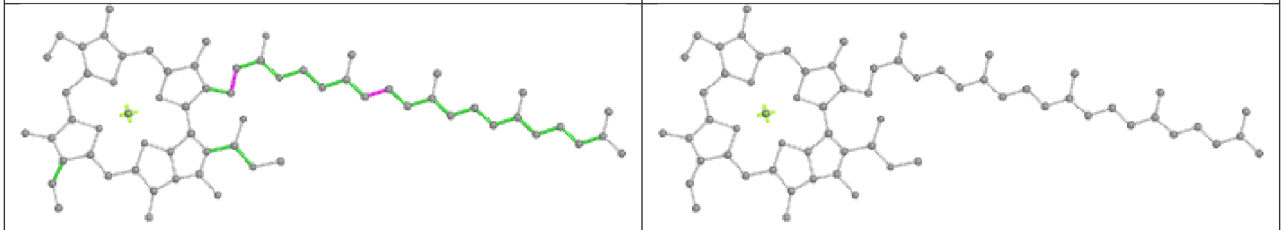


Torsions Rings

Ligand CLA dB 841

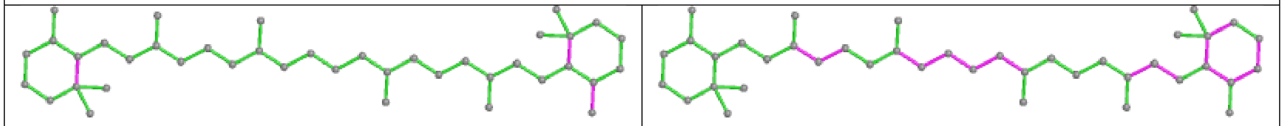


Bond lengths Bond angles

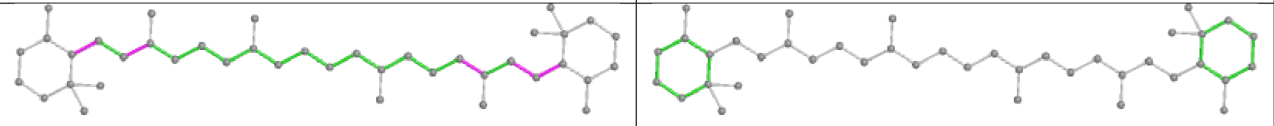


Torsions Rings

Ligand BCR bA 845

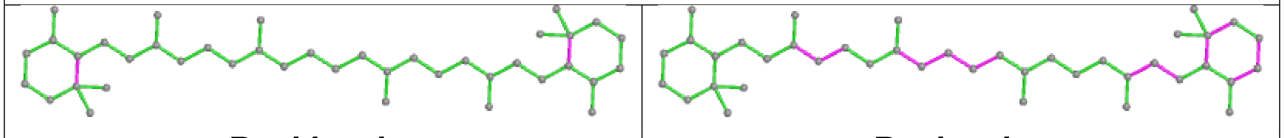


Bond lengths Bond angles



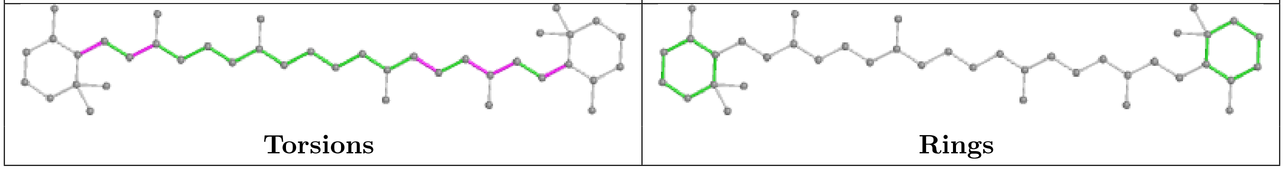
Torsions Rings

Ligand BCR cB 843



Bond lengths

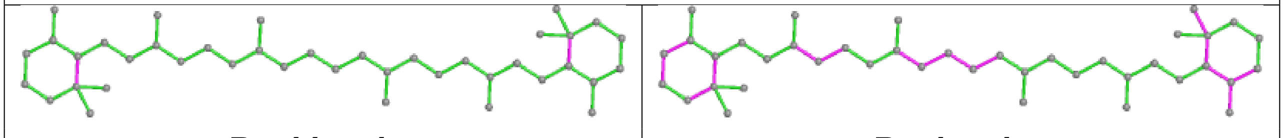
Bond angles



Torsions

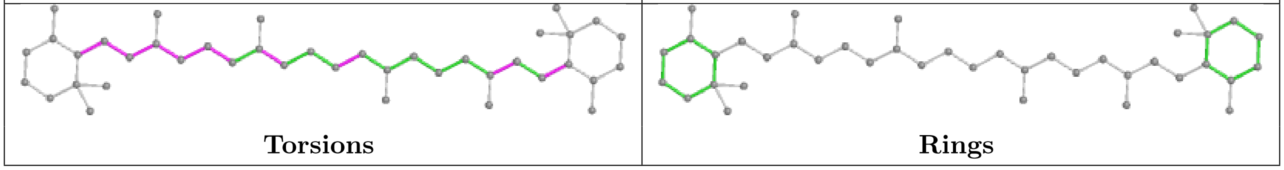
Rings

Ligand BCR dL 208



Bond lengths

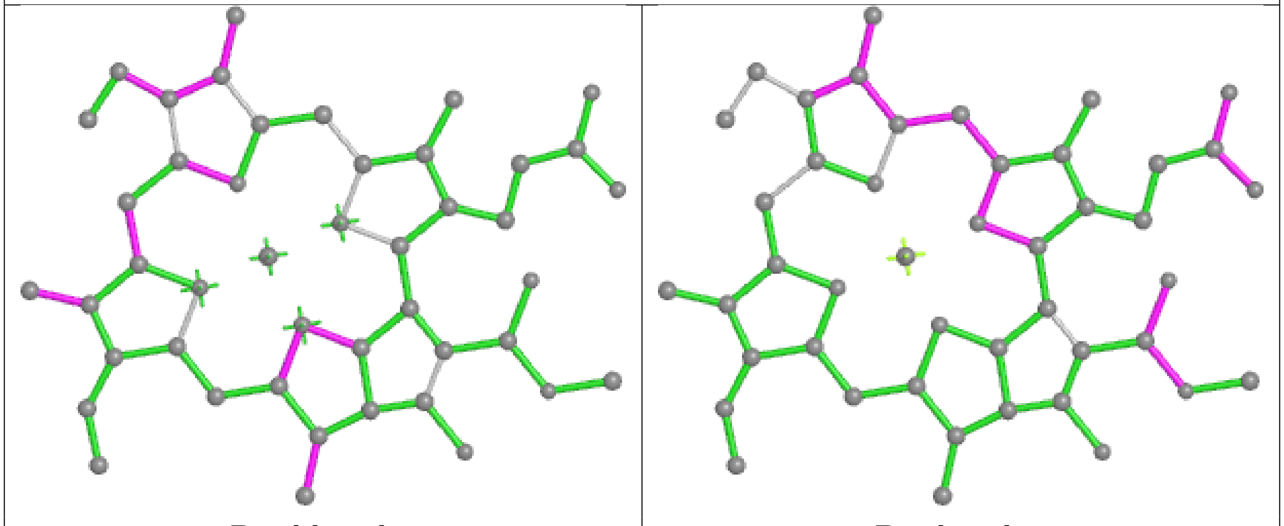
Bond angles



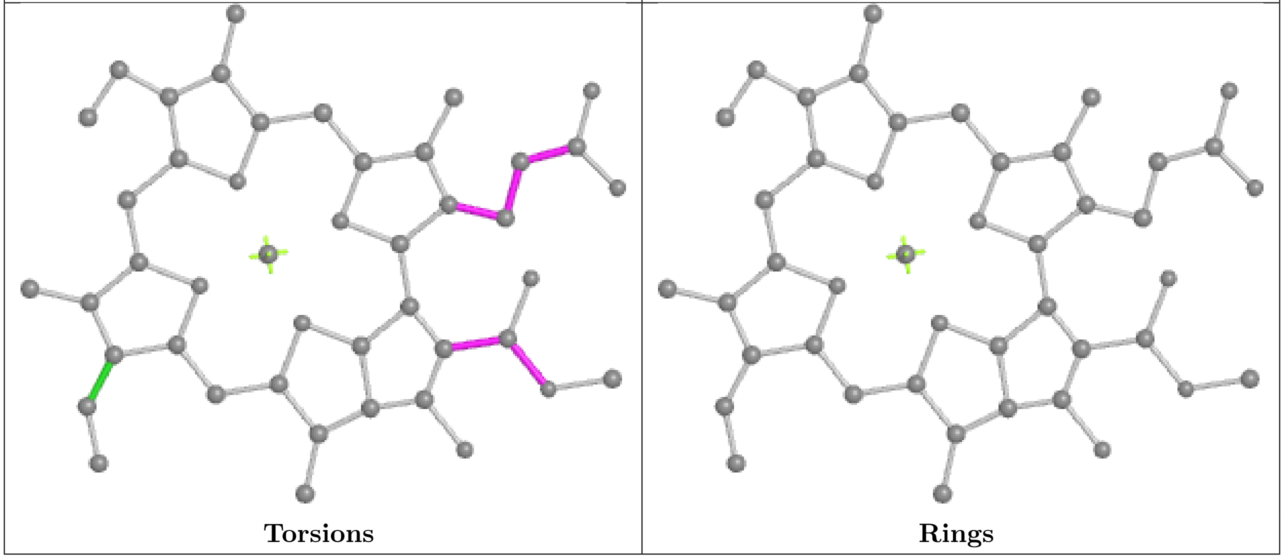
Torsions

Rings

Ligand CLA bB 813

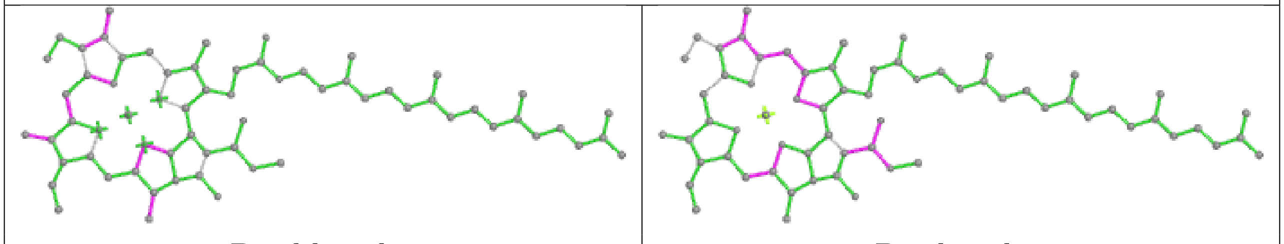


Bond lengths Bond angles

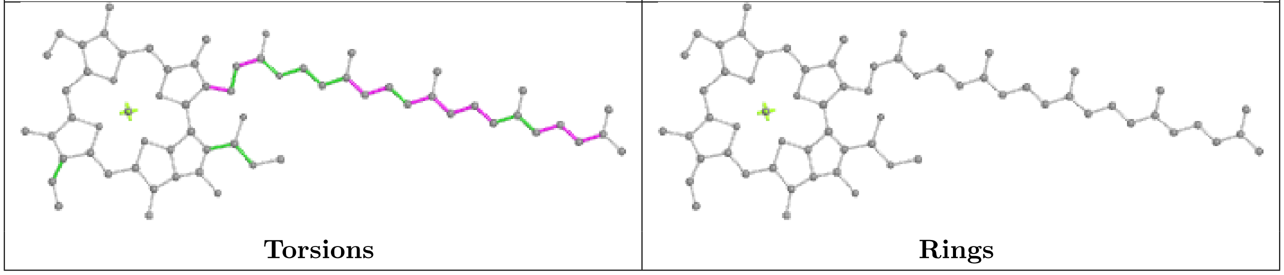


Torsions Rings

Ligand CLA bB 833

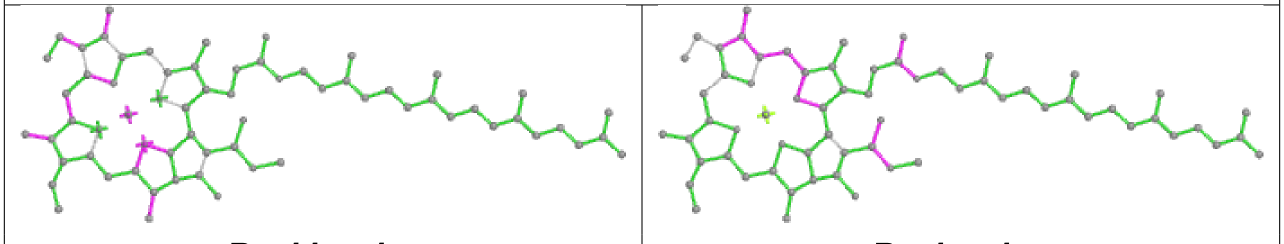


Bond lengths Bond angles



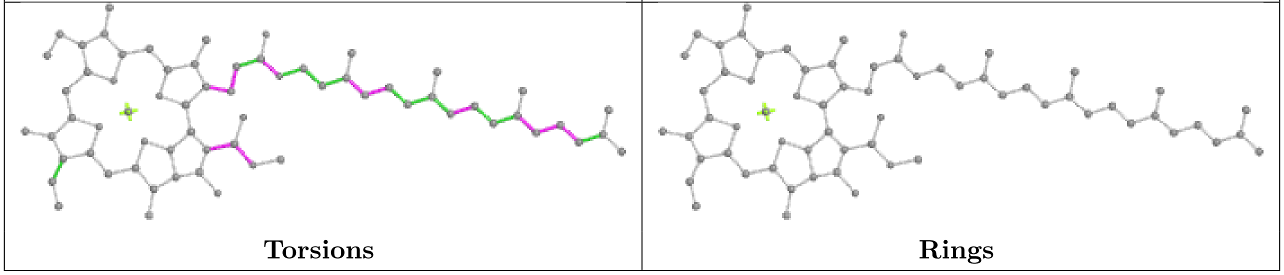
Torsions Rings

Ligand CLA bB 803



Bond lengths

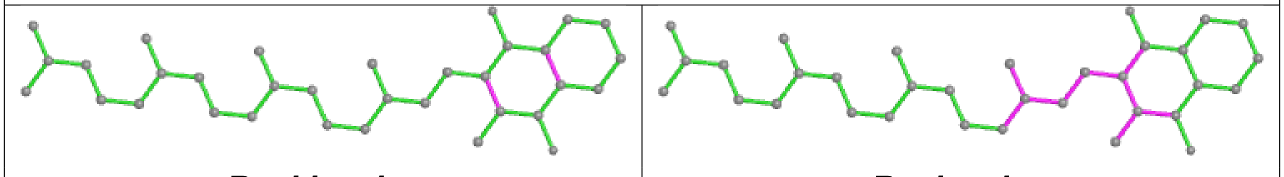
Bond angles



Torsions

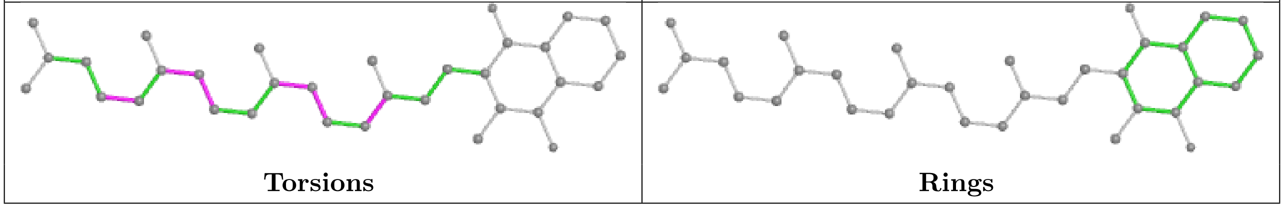
Rings

Ligand PQN aB 842



Bond lengths

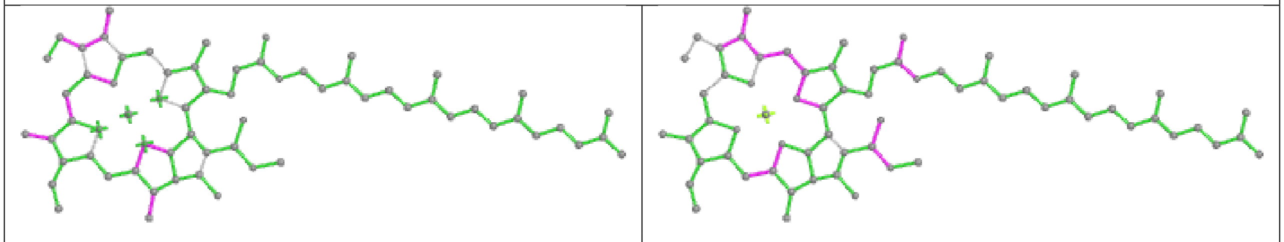
Bond angles



Torsions

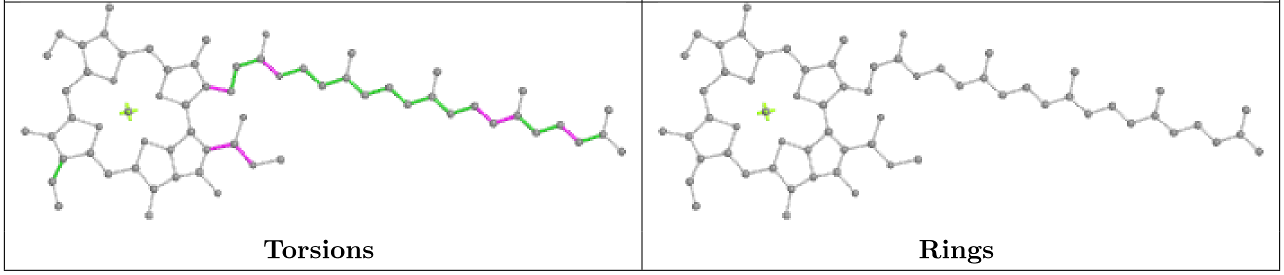
Rings

Ligand CLA aA 811



Bond lengths

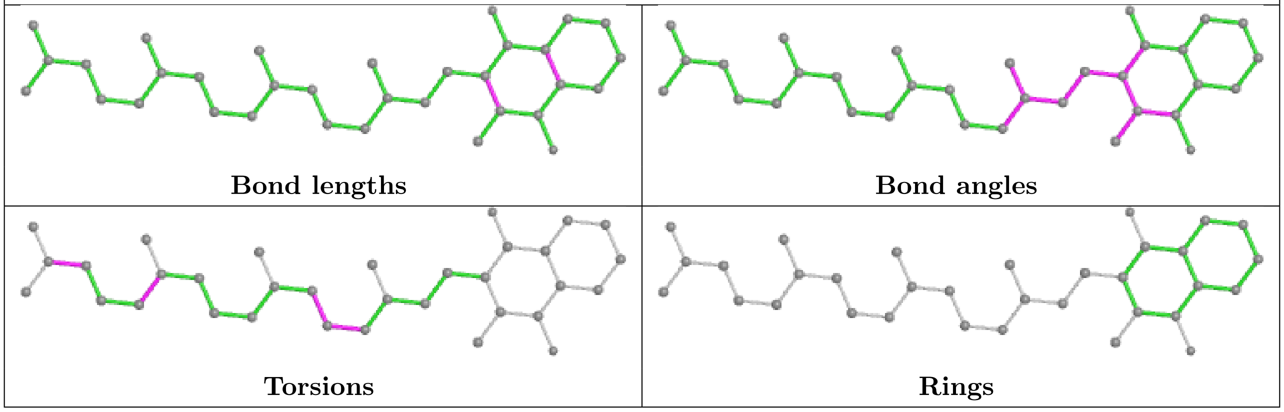
Bond angles



Torsions

Rings

Ligand PQN bA 843



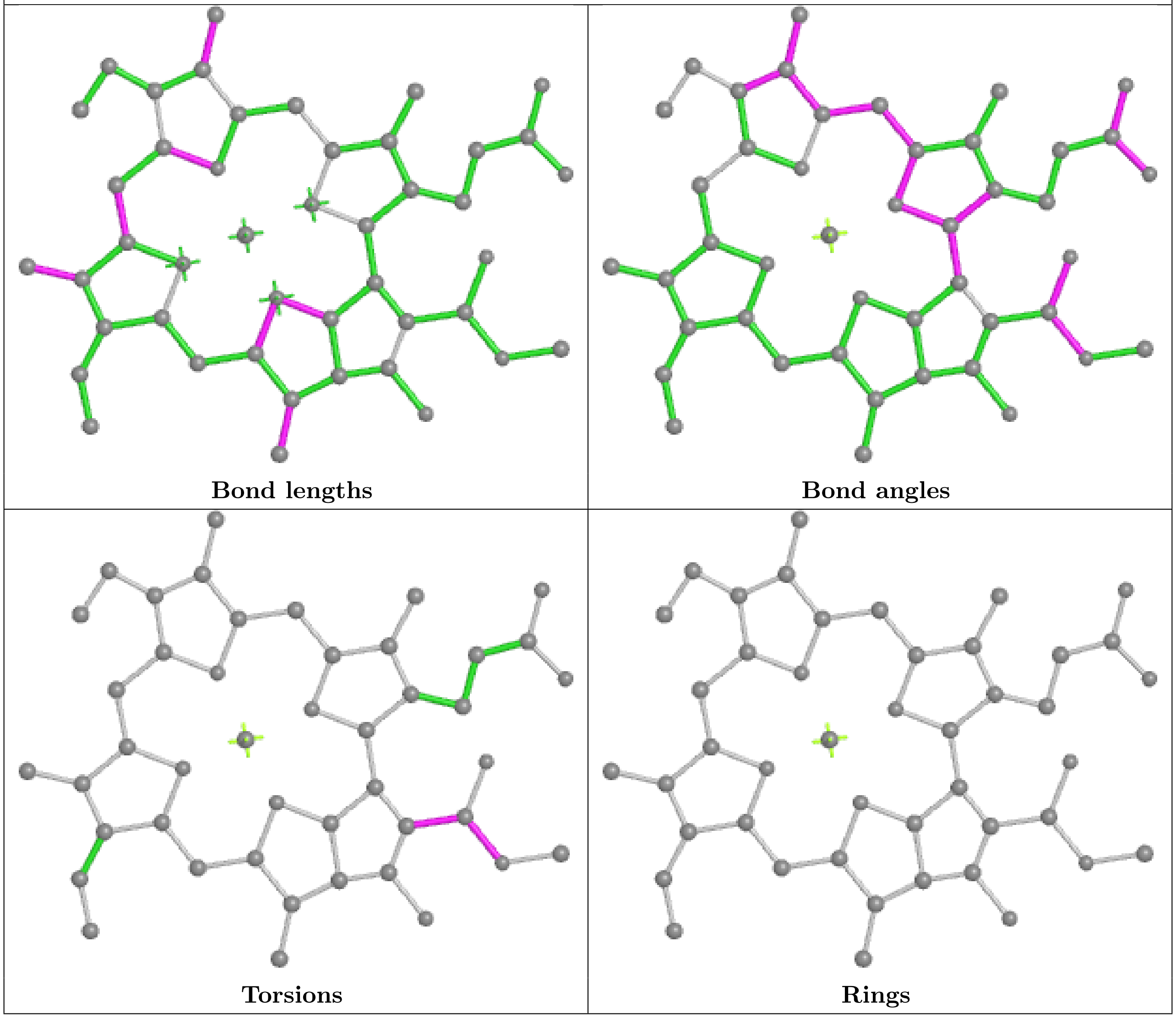
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA bA 814



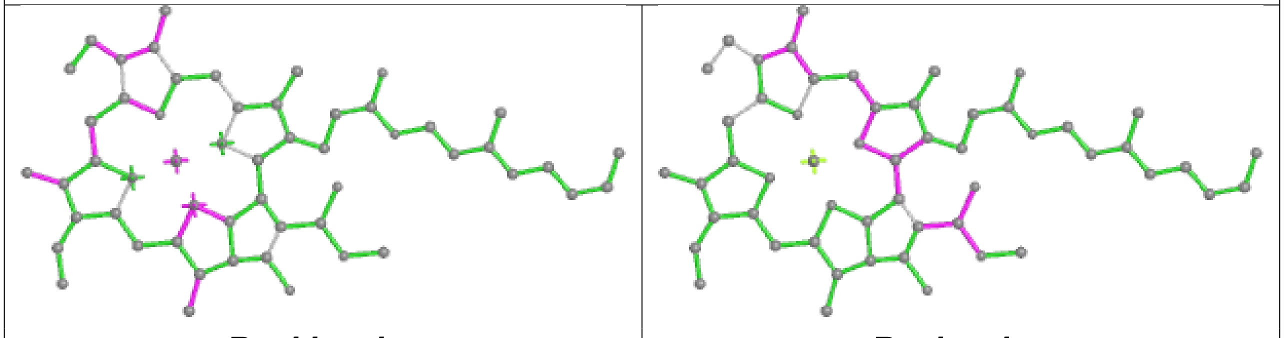
Bond lengths

Bond angles

Torsions

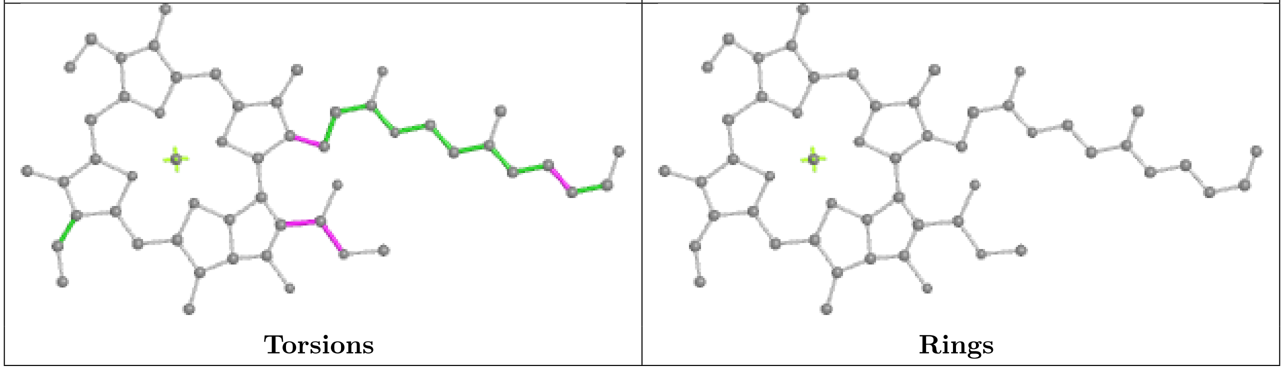
Rings

Ligand CLA bB 825



Bond lengths

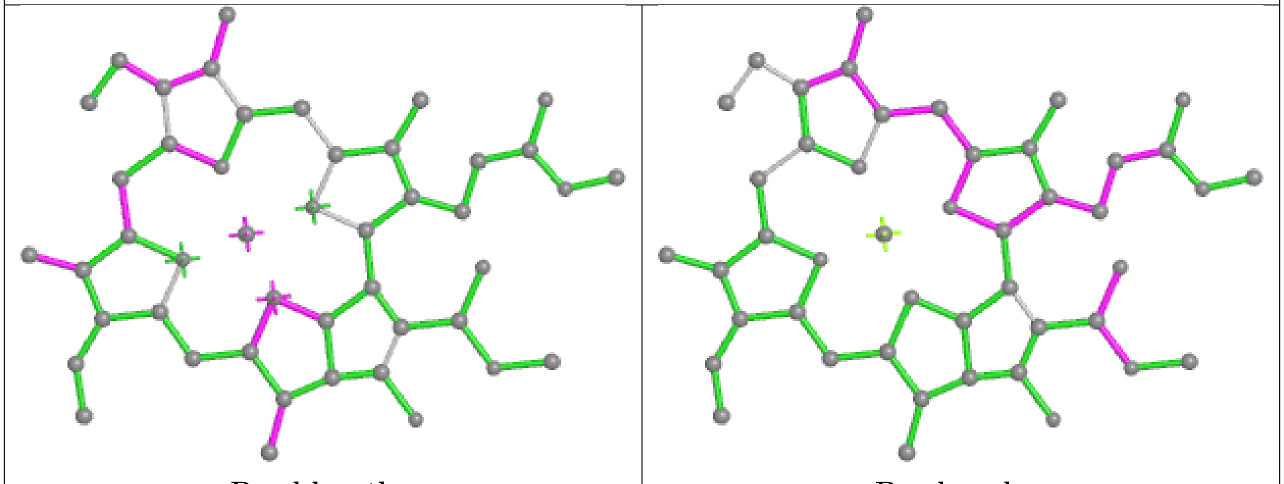
Bond angles



Torsions

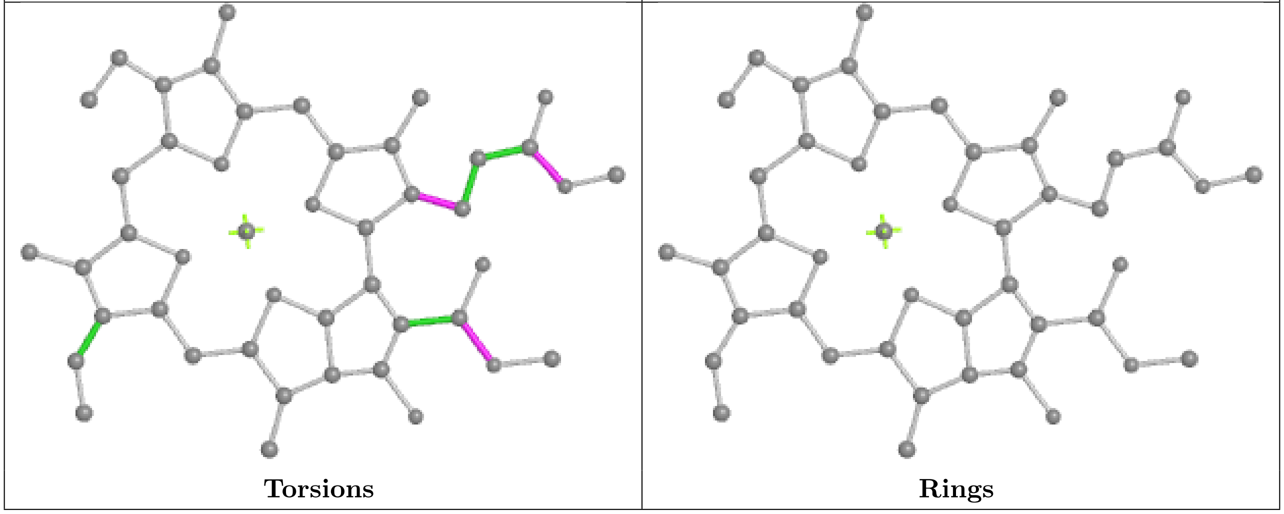
Rings

Ligand CLA aB 825



Bond lengths

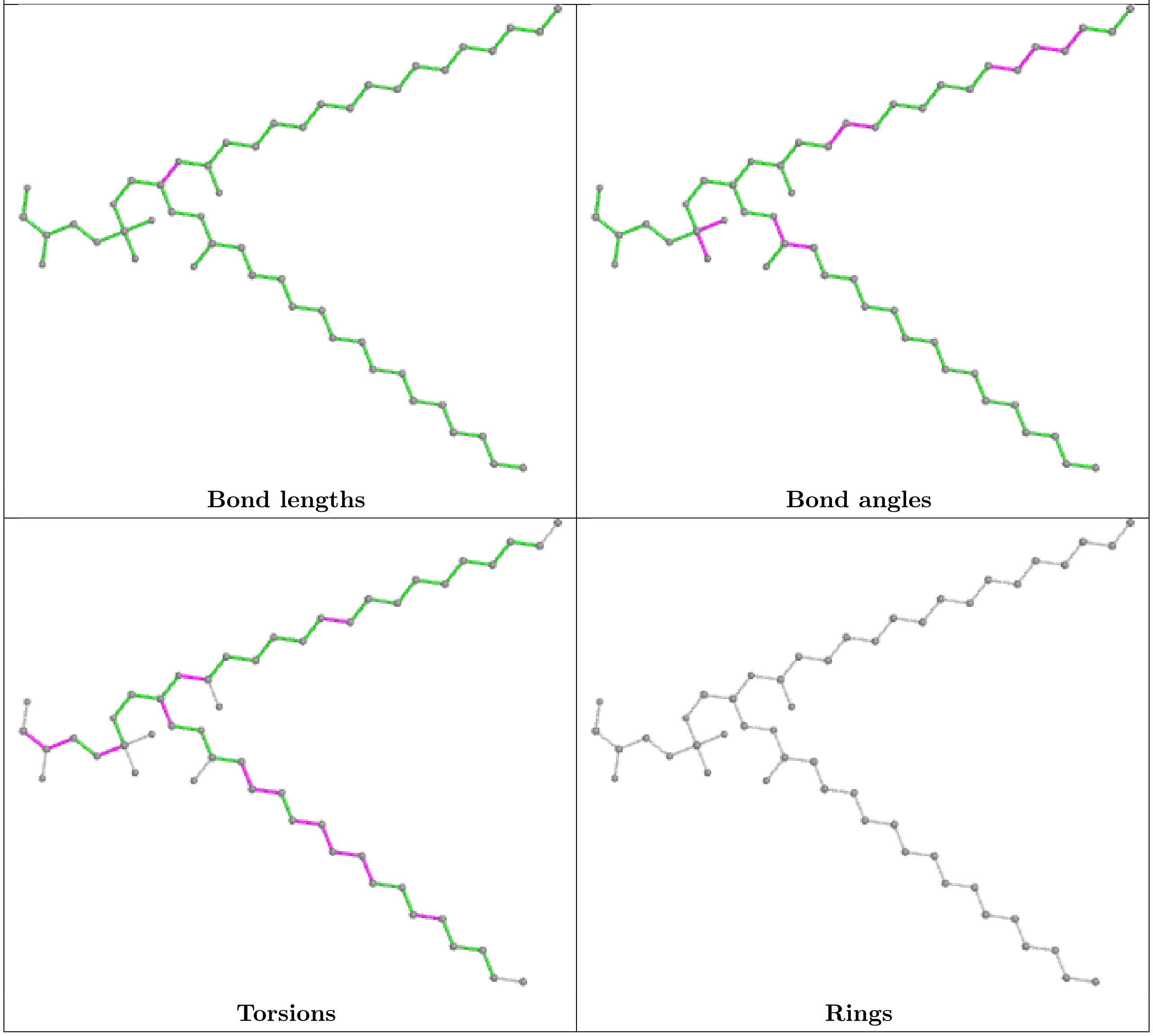
Bond angles



Torsions

Rings

Ligand LHG cA 852



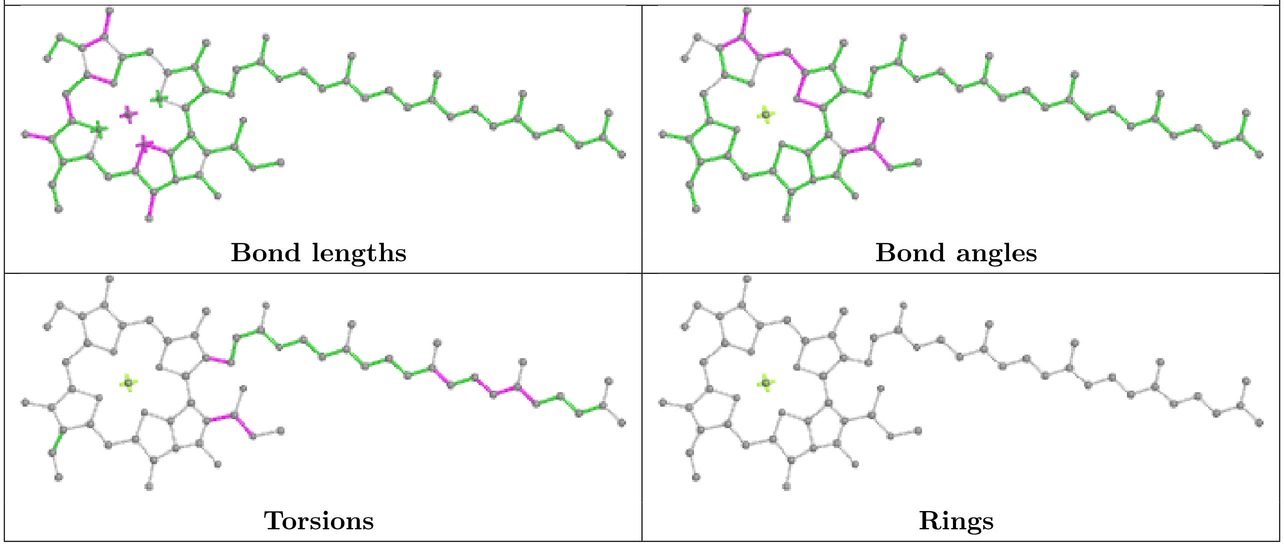
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA dA 830



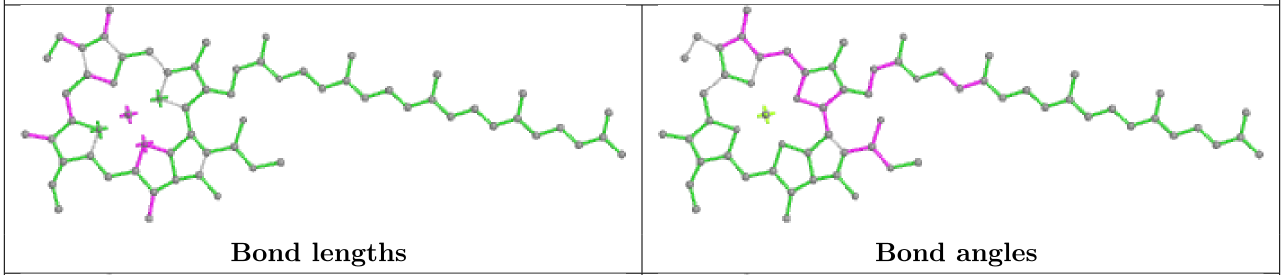
Bond lengths

Bond angles

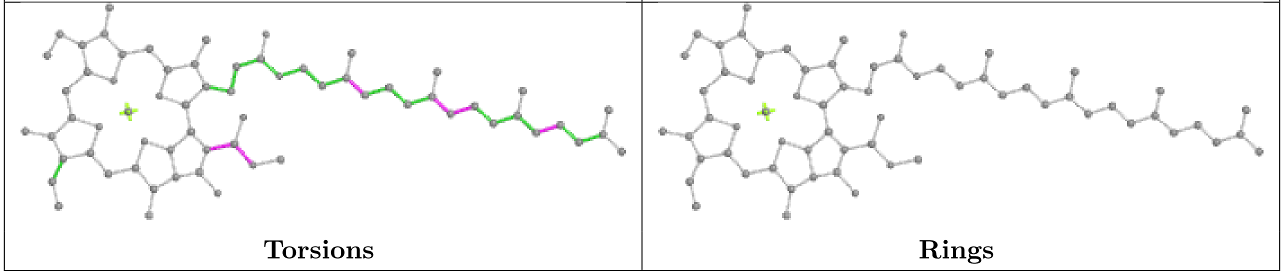
Torsions

Rings

Ligand CLA dA 833

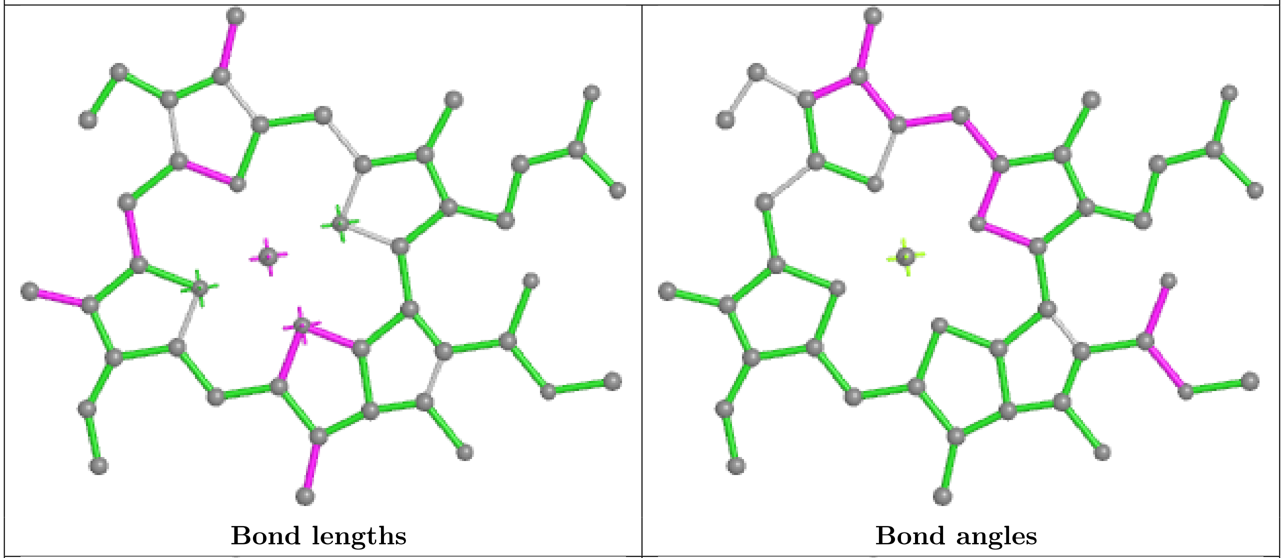


Bond lengths Bond angles

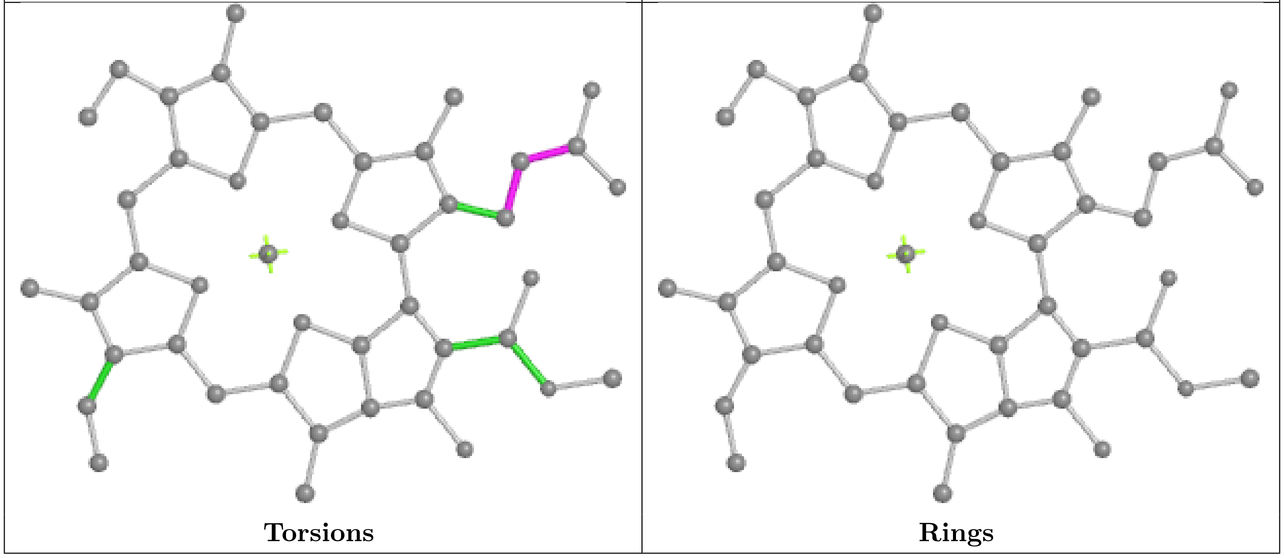


Torsions Rings

Ligand CLA bA 802

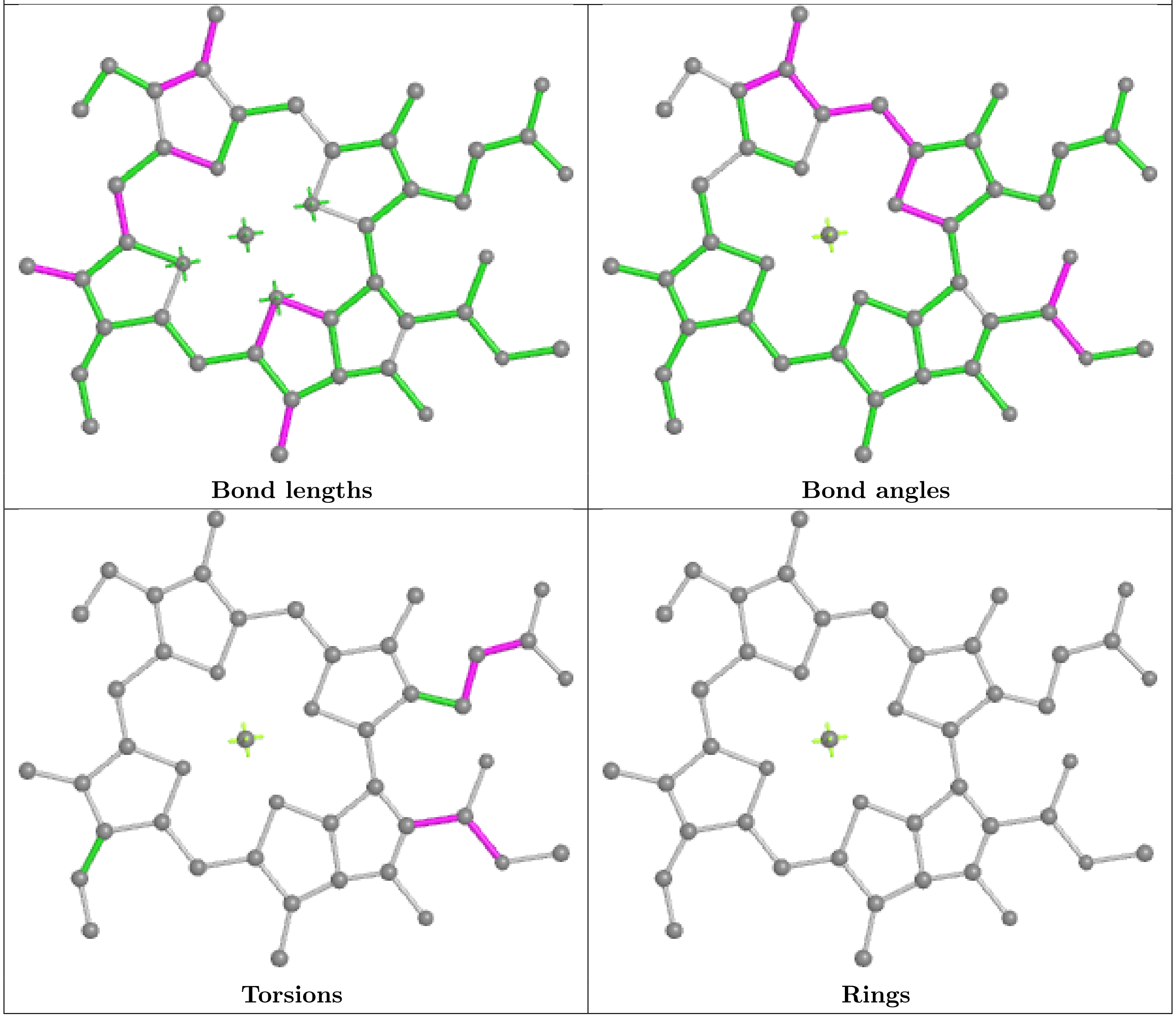


Bond lengths Bond angles

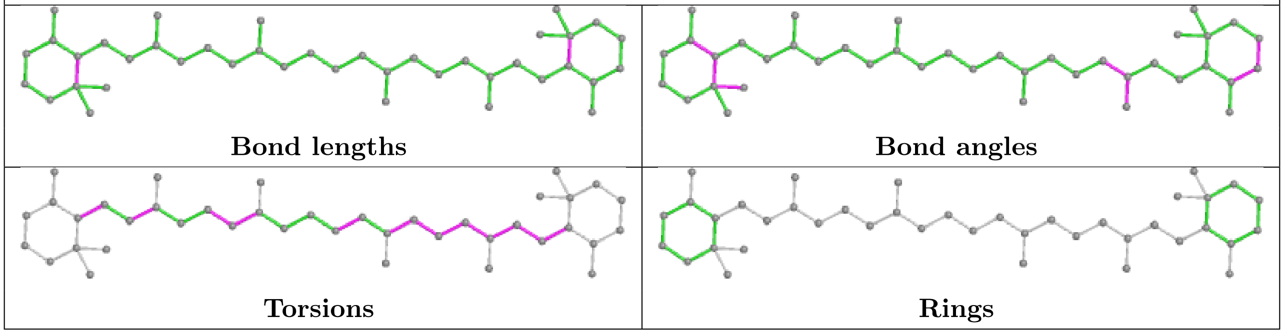


Torsions Rings

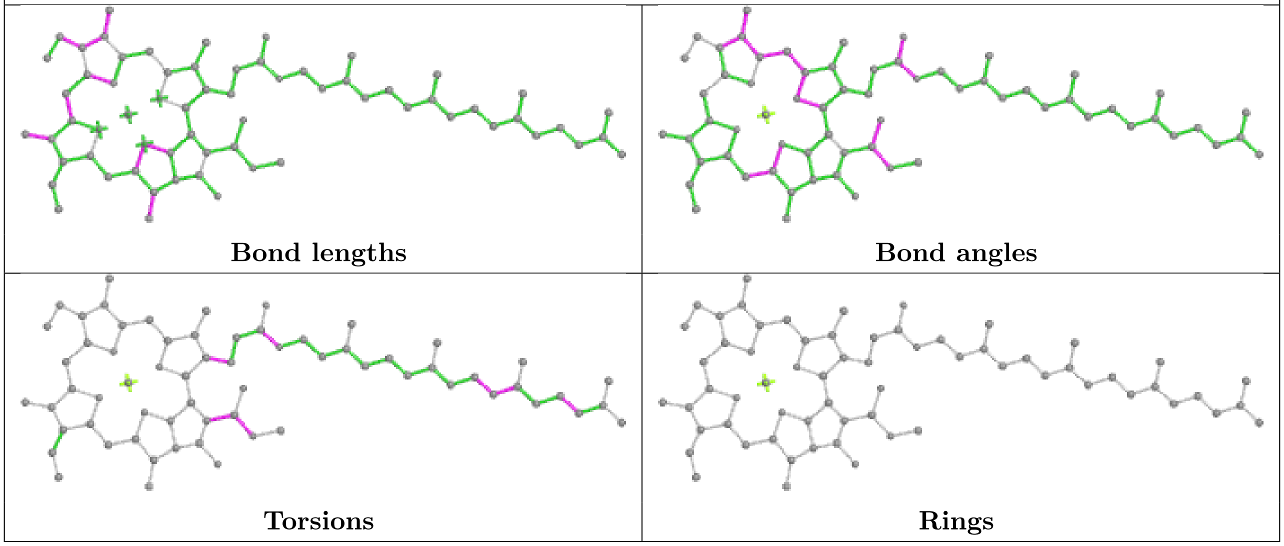
Ligand CLA cX 101



Ligand BCR cB 846



Ligand CLA cA 811



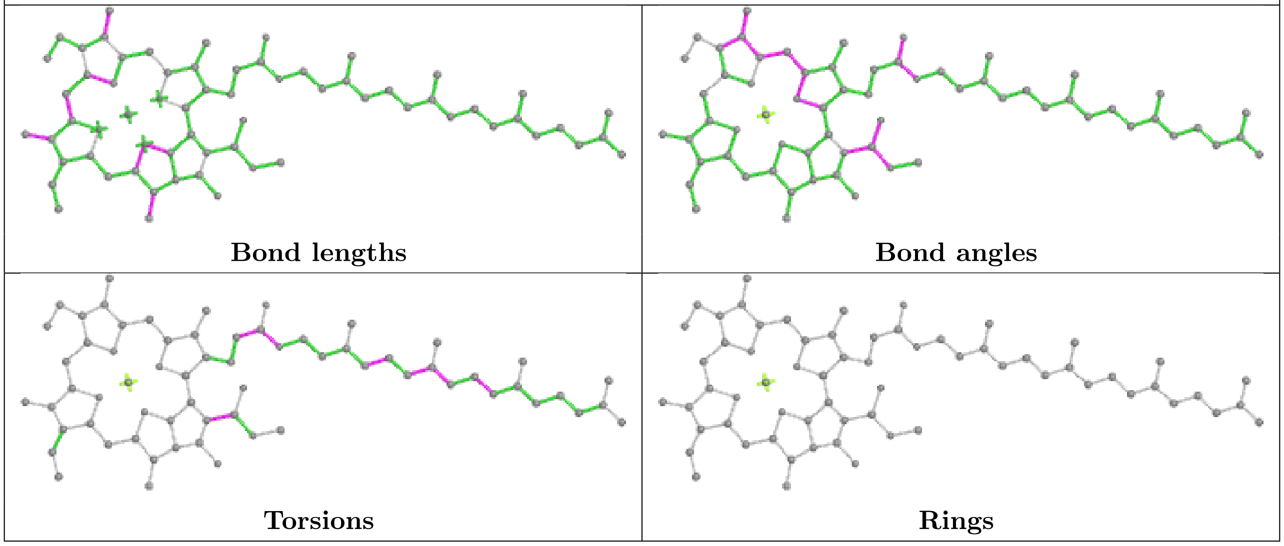
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA bA 827



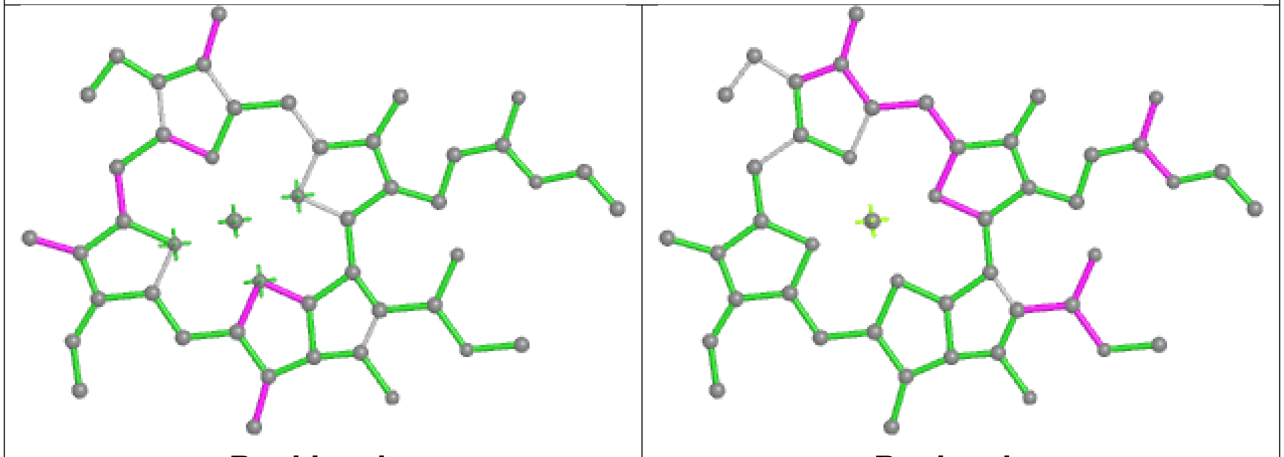
Bond lengths

Bond angles

Torsions

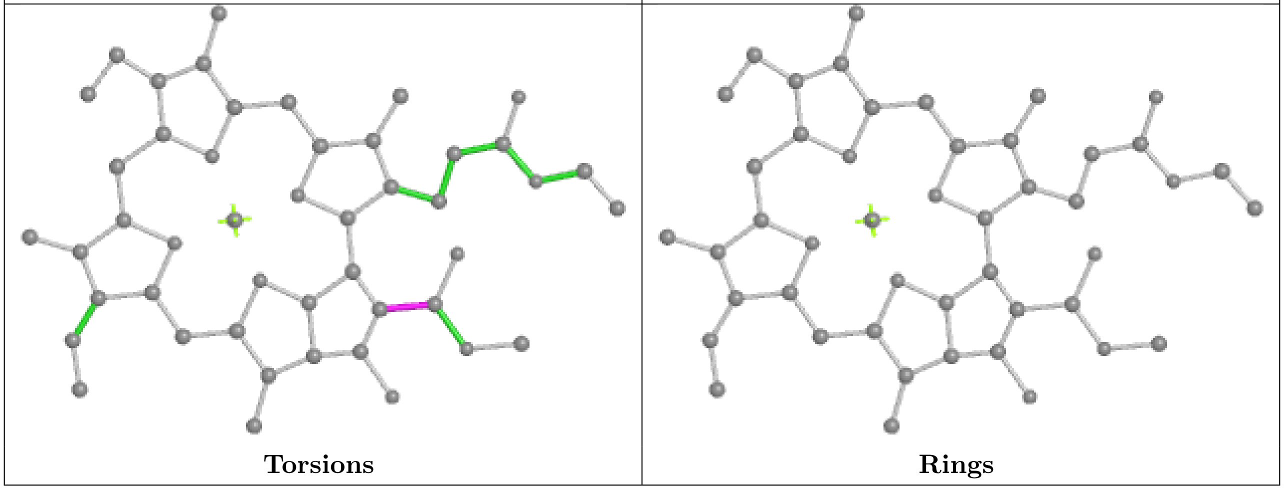
Rings

Ligand CLA bB 840



Bond lengths

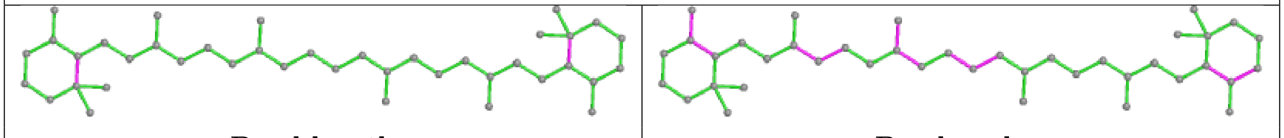
Bond angles



Torsions

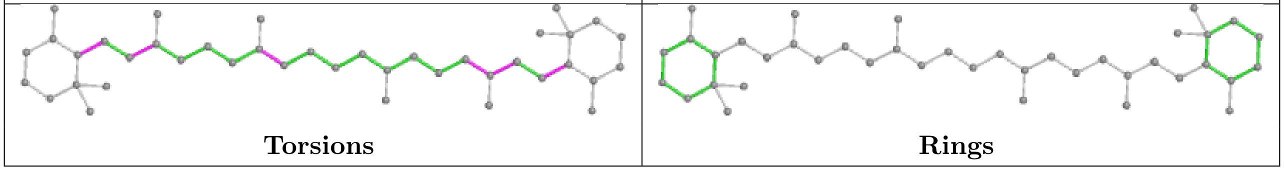
Rings

Ligand BCR cA 850



Bond lengths

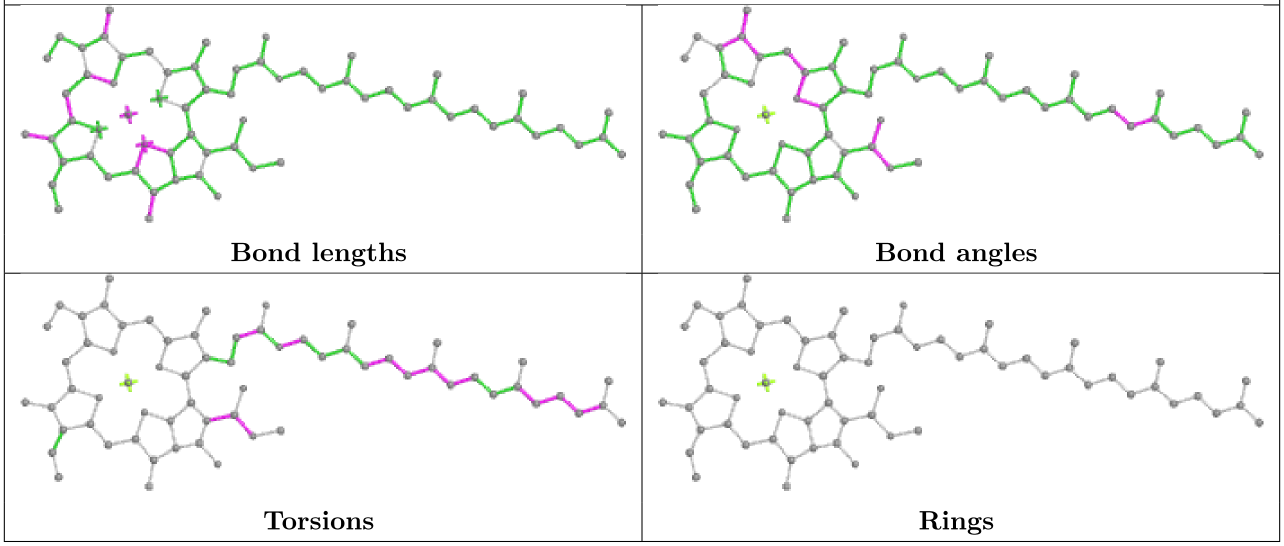
Bond angles



Torsions

Rings

Ligand CLA dB 807



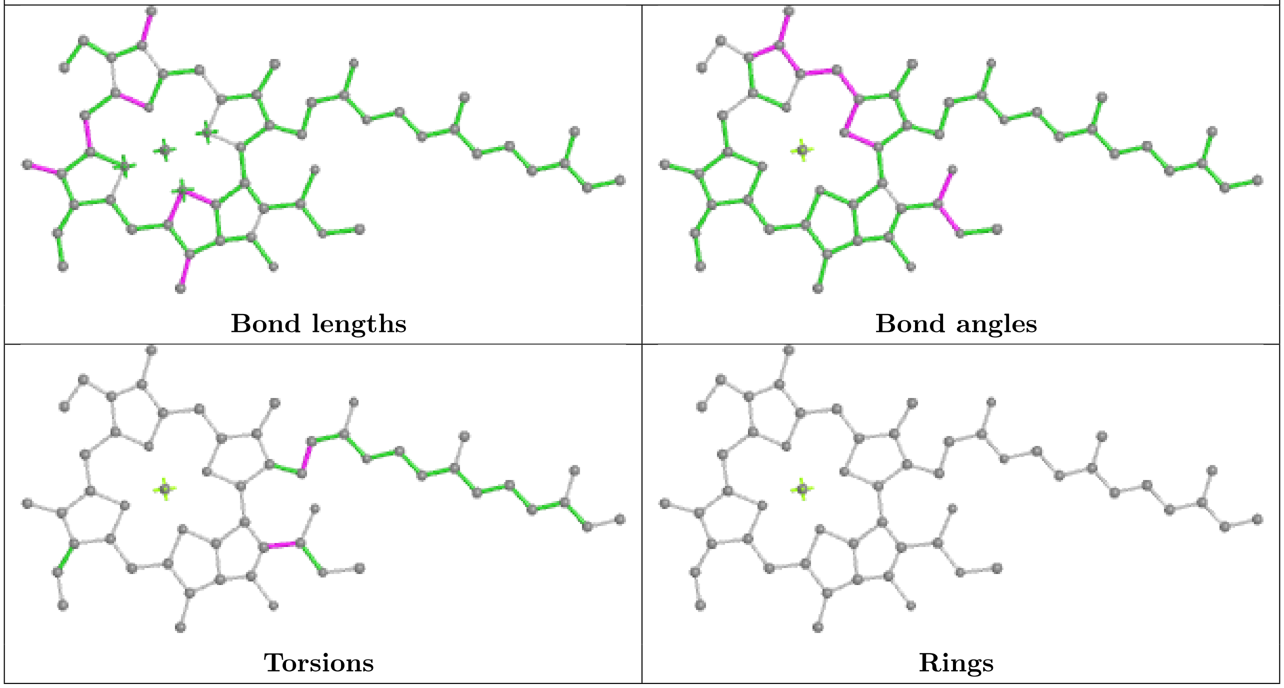
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA dB 815



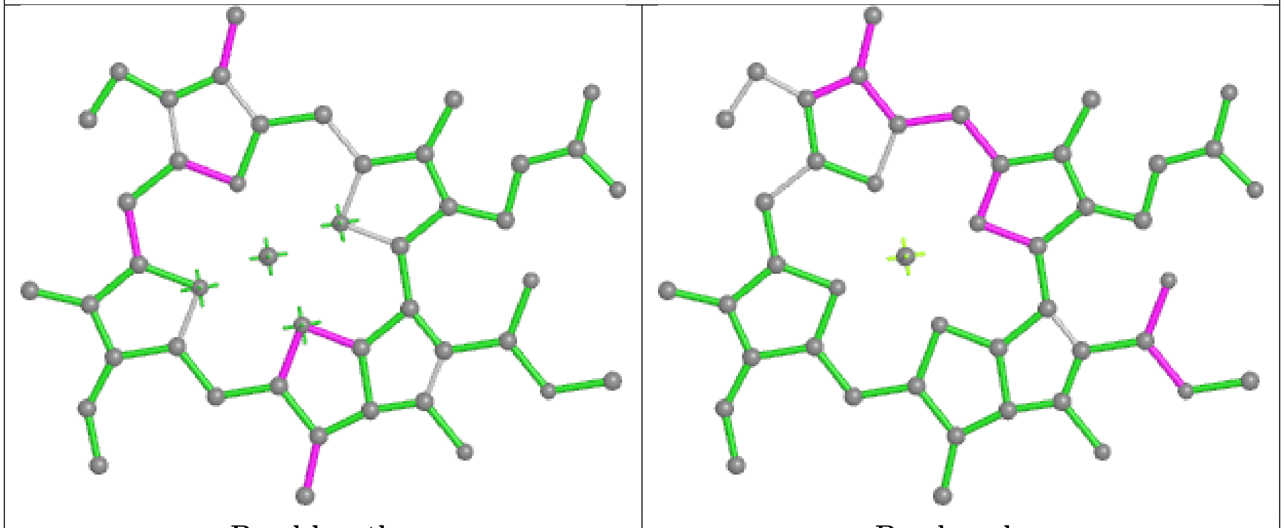
Bond lengths

Bond angles

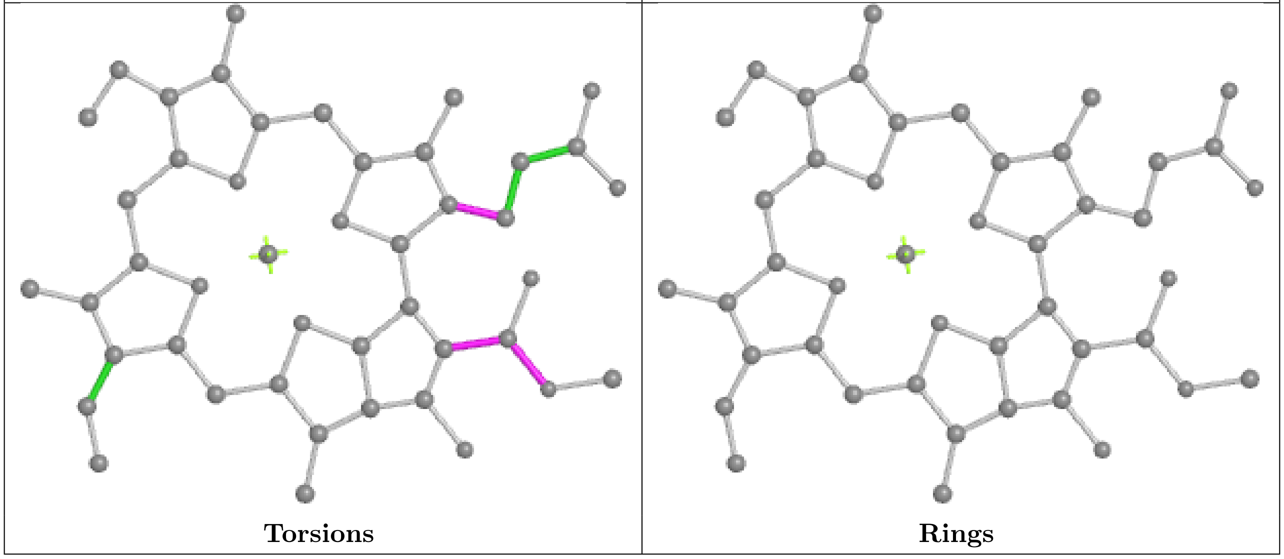
Torsions

Rings

Ligand CLA cA 810

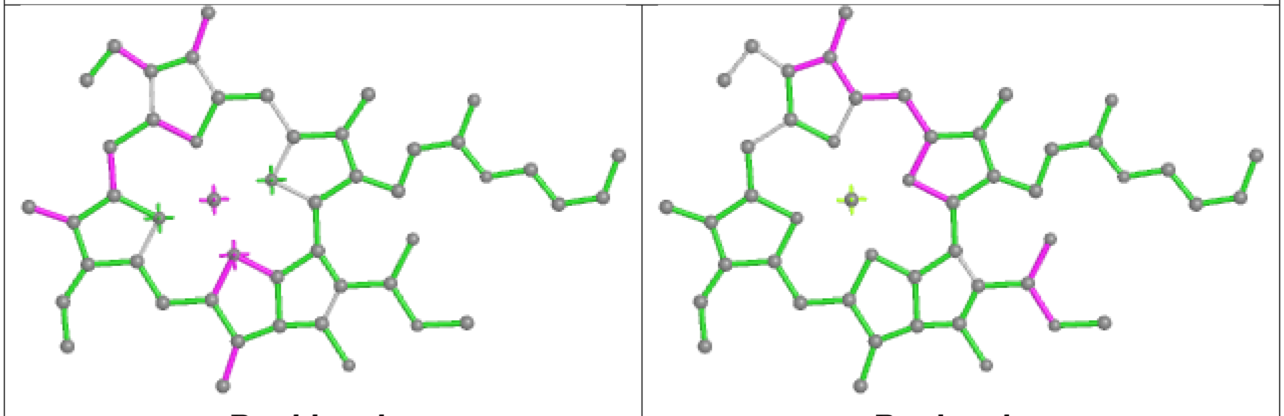


Bond lengths **Bond angles**



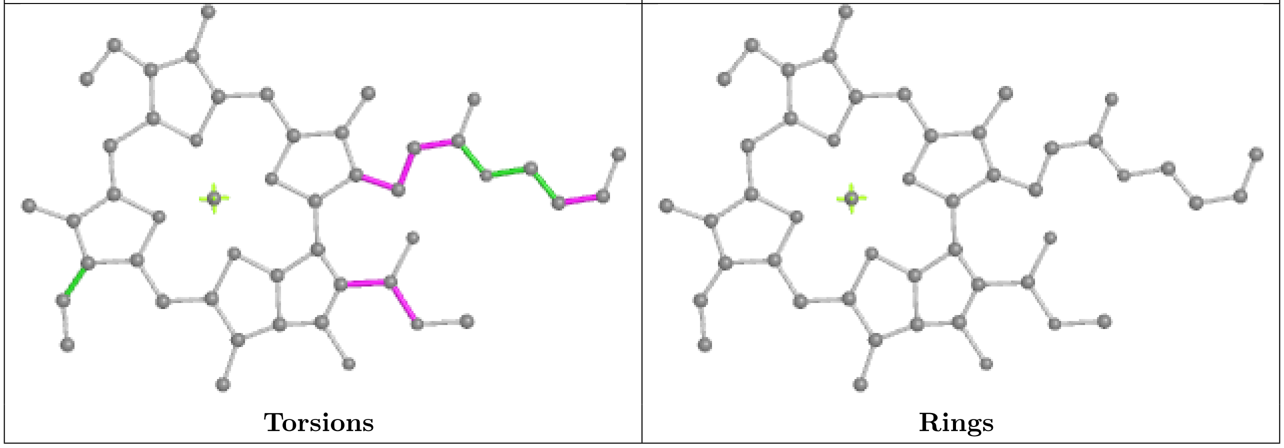
Torsions **Rings**

Ligand CLA aA 822



Bond lengths

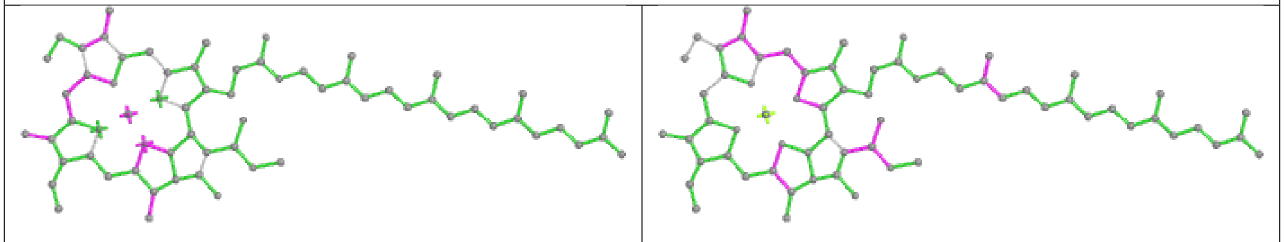
Bond angles



Torsions

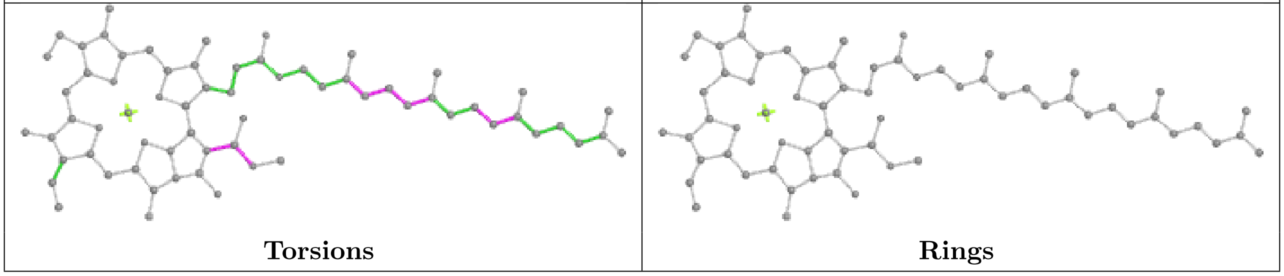
Rings

Ligand CLA cB 829



Bond lengths

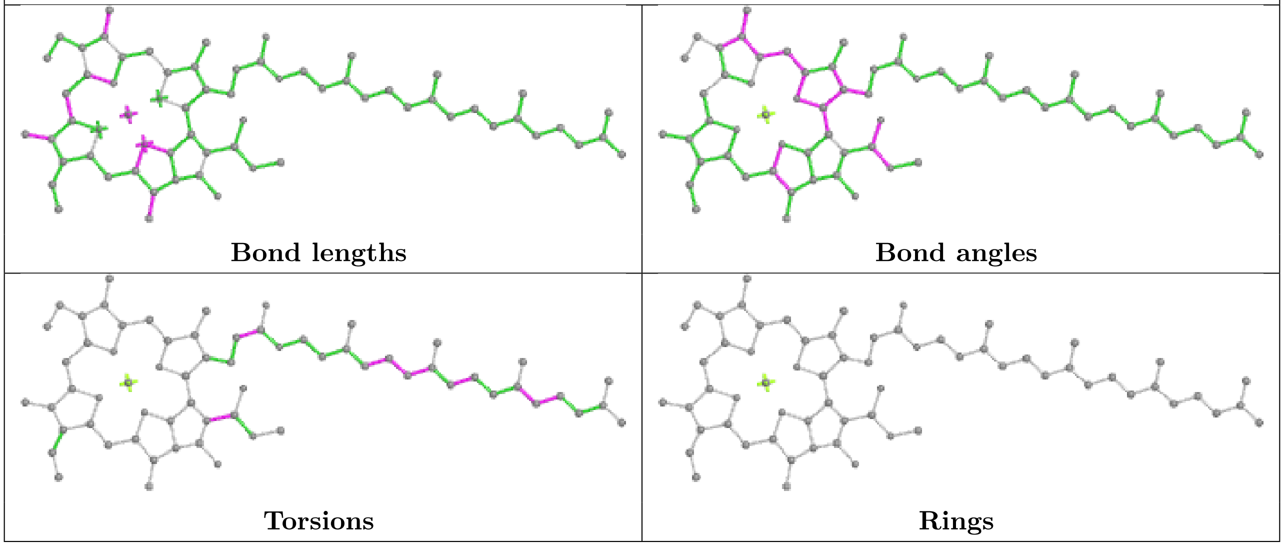
Bond angles



Torsions

Rings

Ligand CLA dA 825



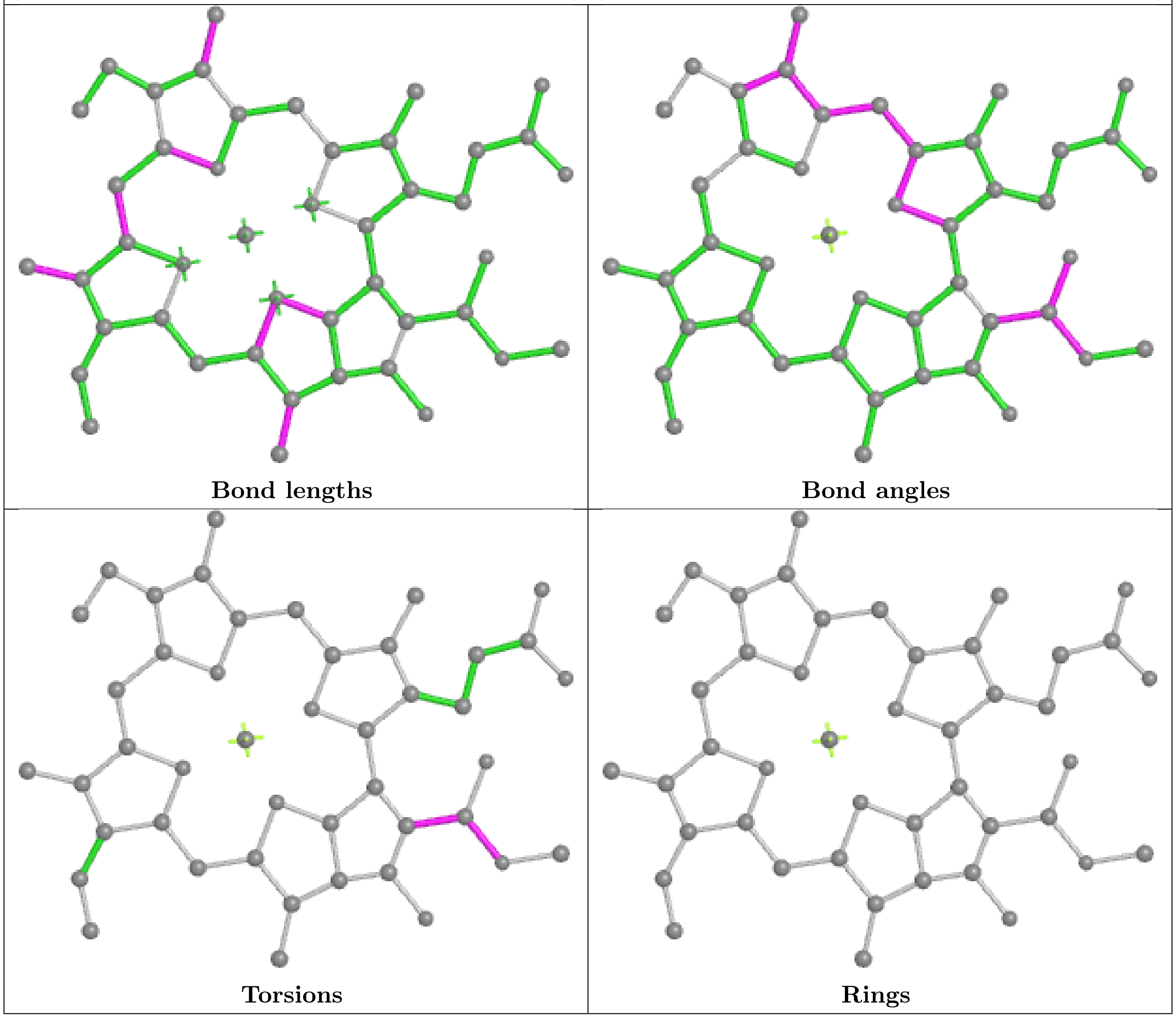
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA dB 835



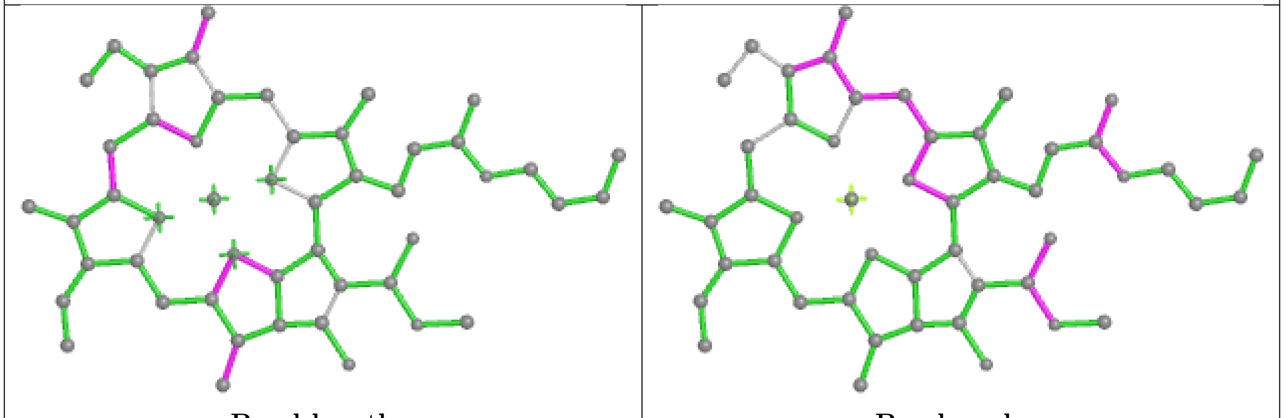
Bond lengths

Bond angles

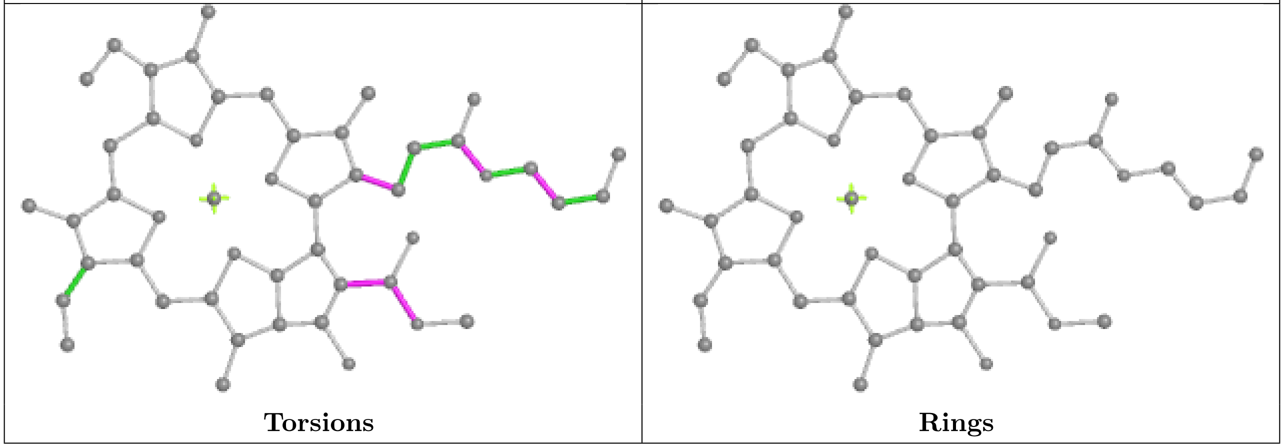
Torsions

Rings

Ligand CLA aA 816

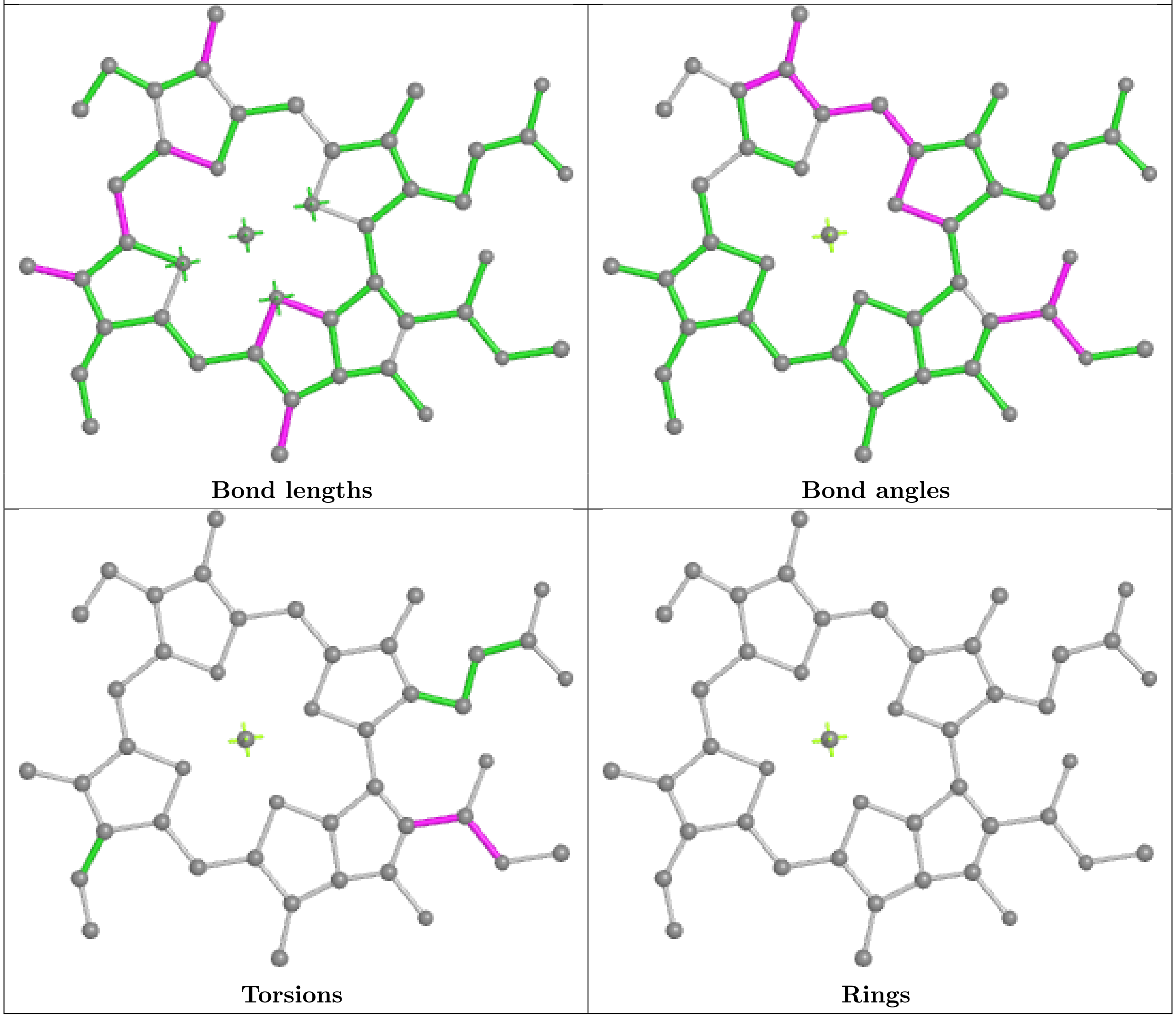


Bond lengths **Bond angles**



Torsions **Rings**

Ligand CLA cB 834



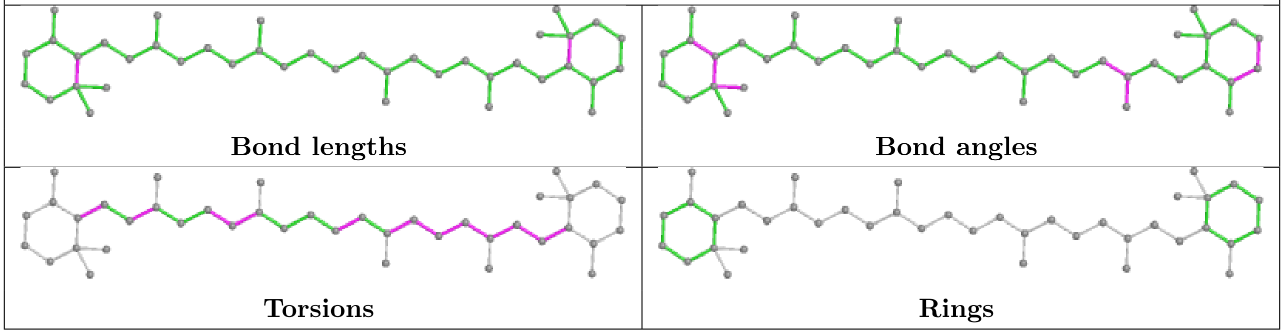
Bond lengths

Bond angles

Torsions

Rings

Ligand BCR aB 846



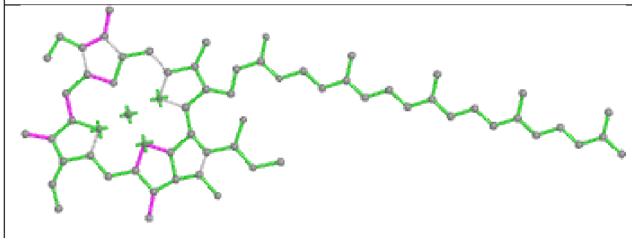
Bond lengths

Bond angles

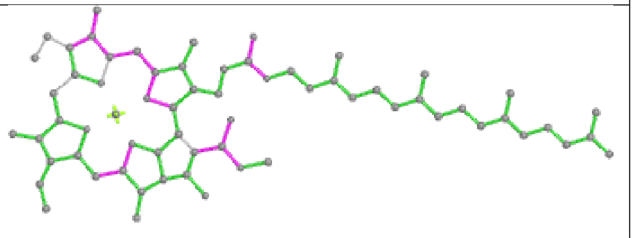
Torsions

Rings

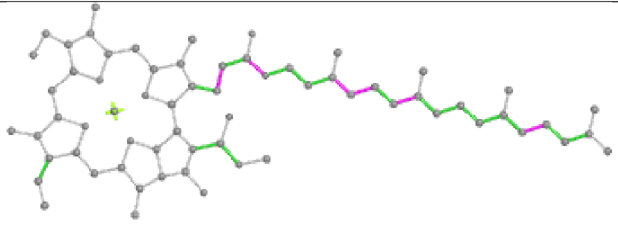
Ligand CLA dB 808



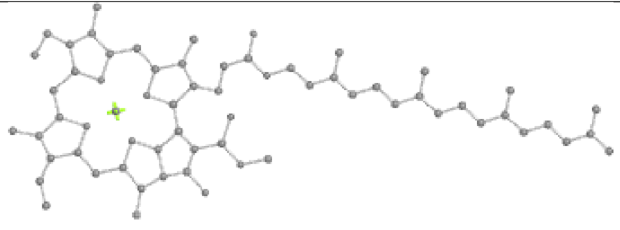
Bond lengths



Bond angles

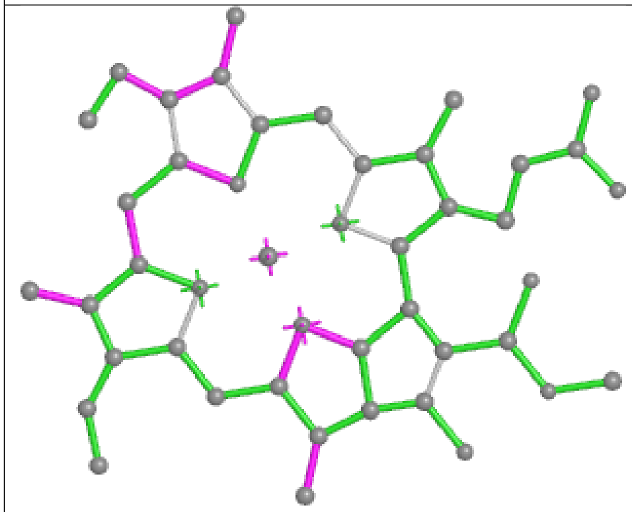


Torsions

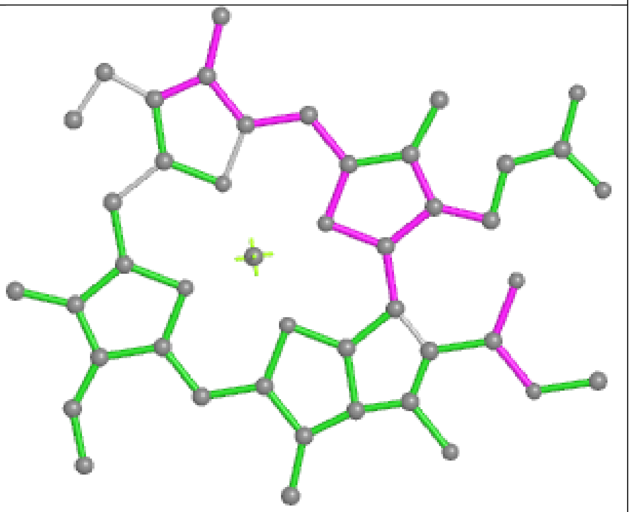


Rings

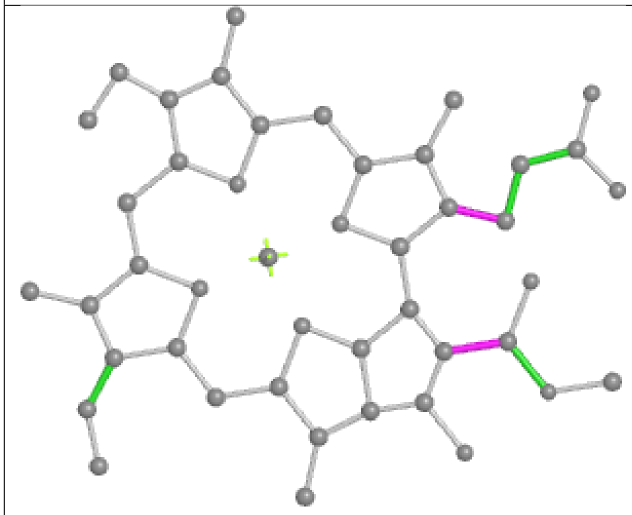
Ligand CLA bA 805



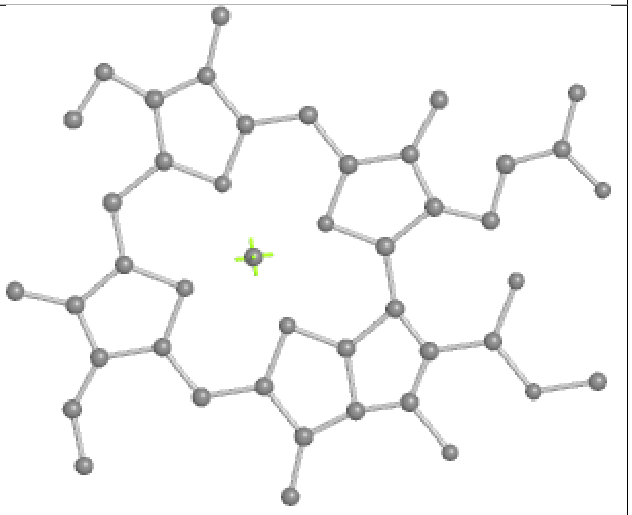
Bond lengths



Bond angles

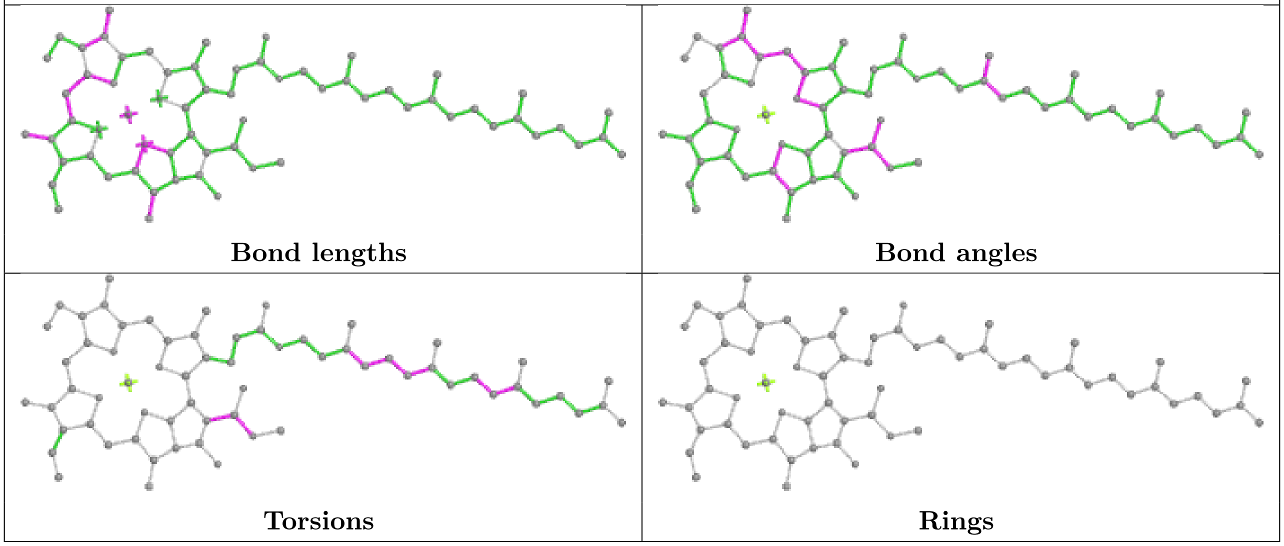


Torsions



Rings

Ligand CLA aB 829



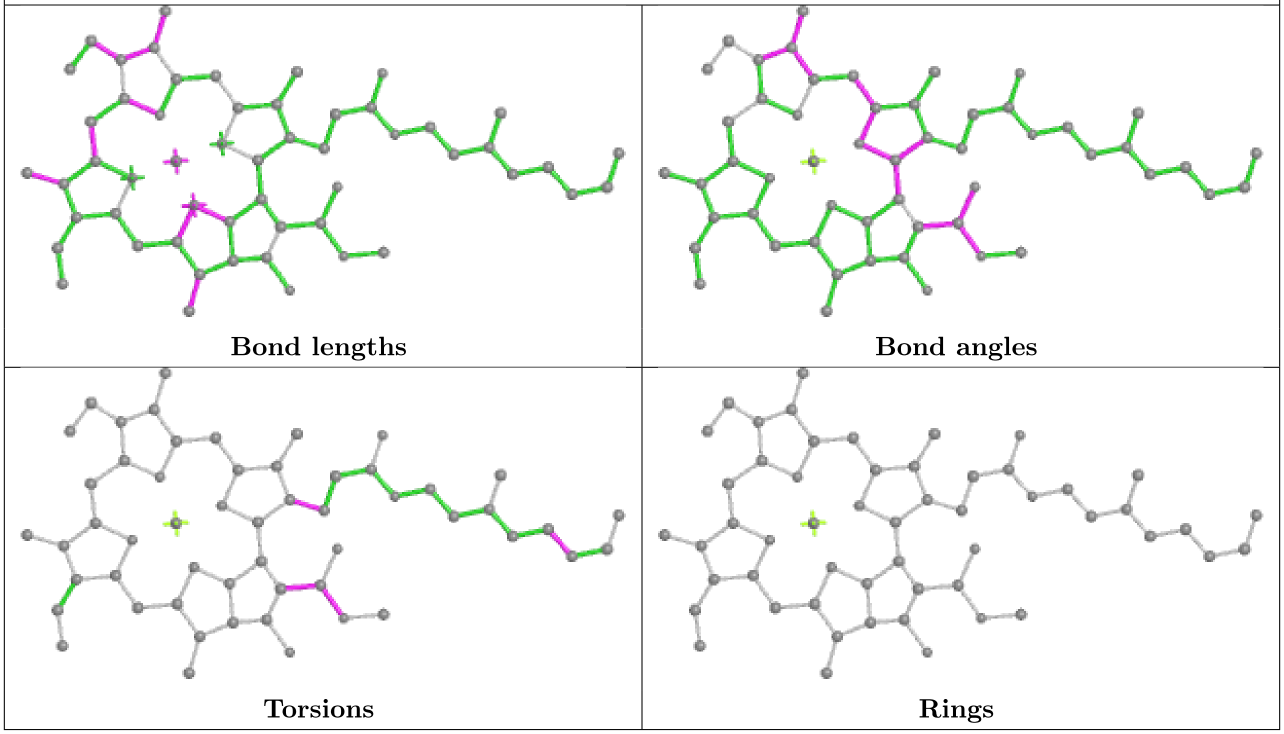
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA aB 824



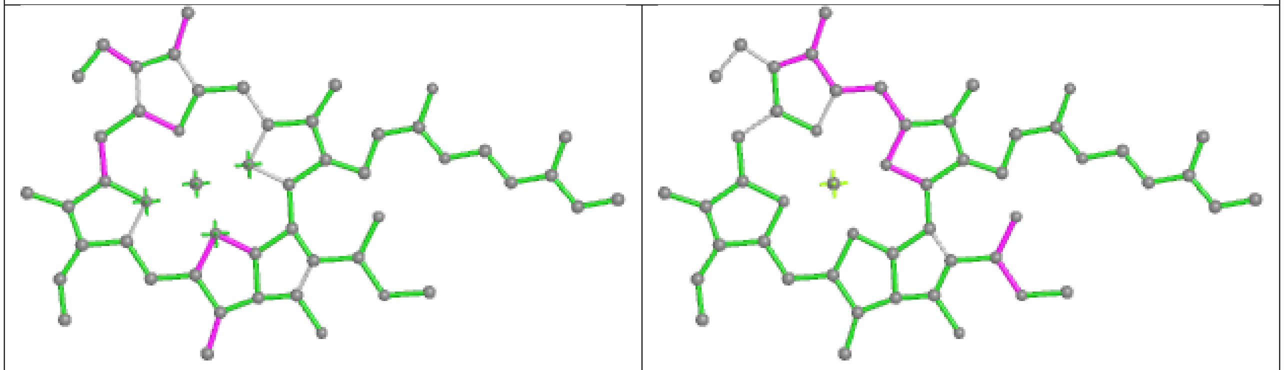
Bond lengths

Bond angles

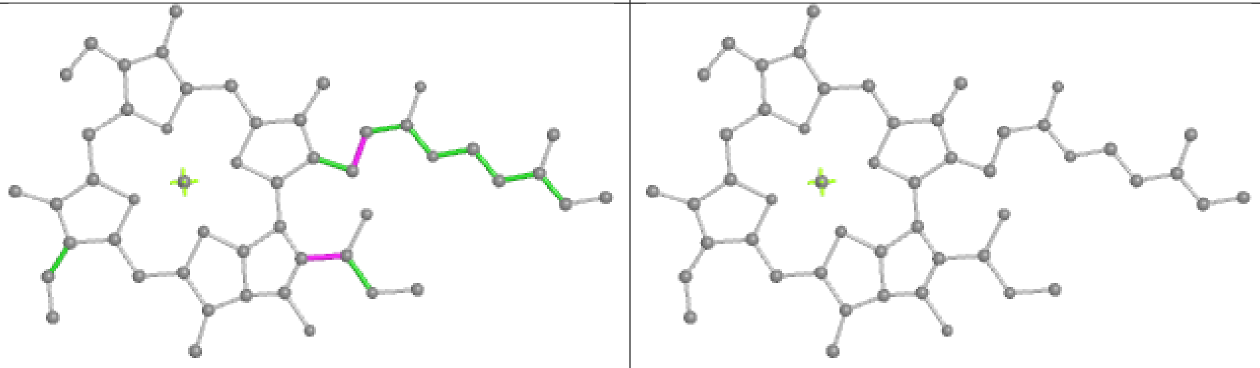
Torsions

Rings

Ligand CLA cA 807

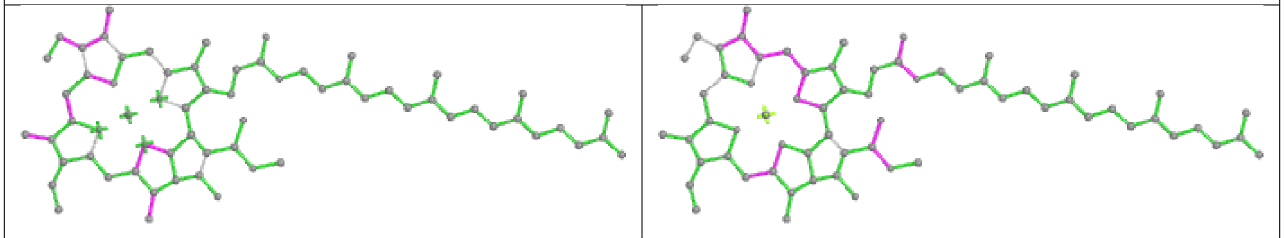


Bond lengths **Bond angles**

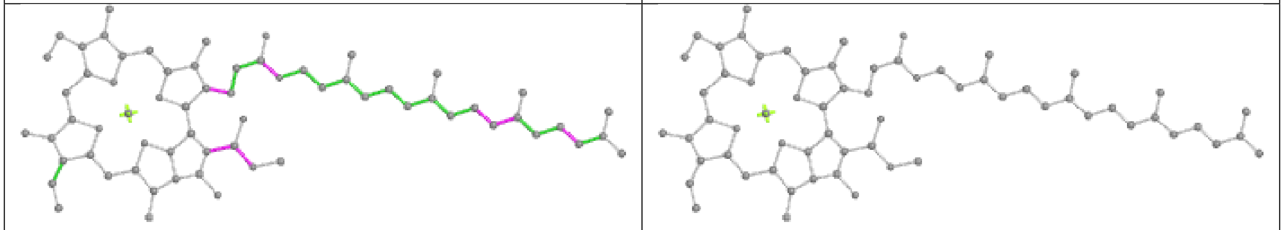


Torsions **Rings**

Ligand CLA bA 811

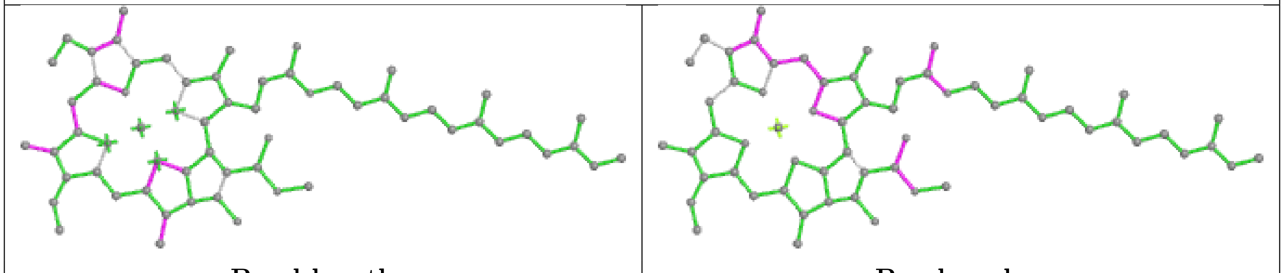


Bond lengths **Bond angles**



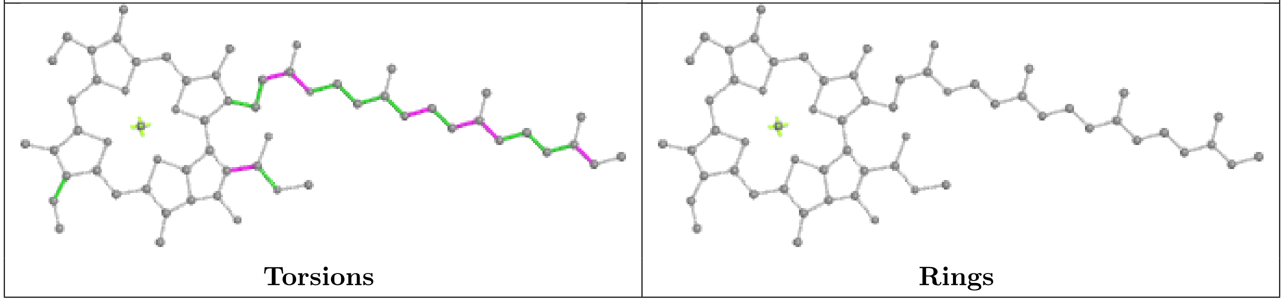
Torsions **Rings**

Ligand CLA cA 820



Bond lengths

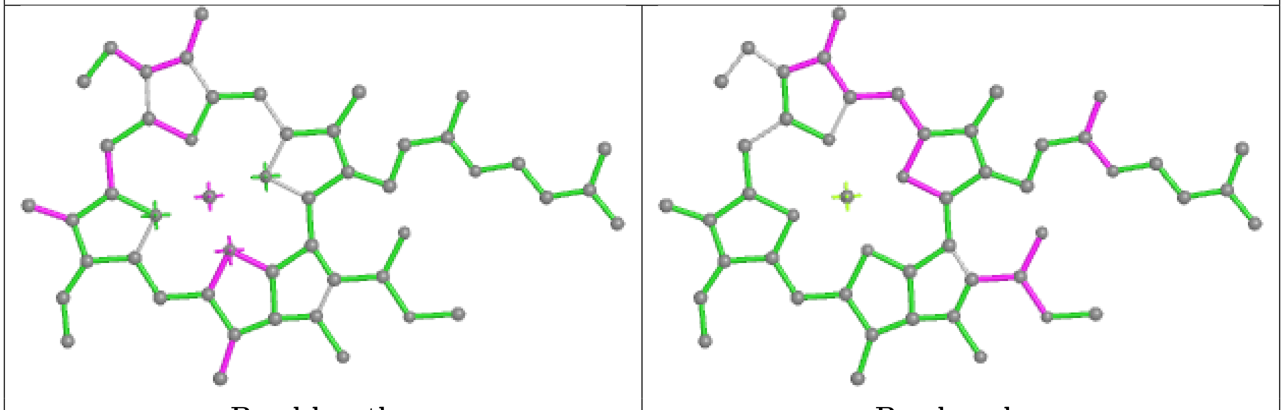
Bond angles



Torsions

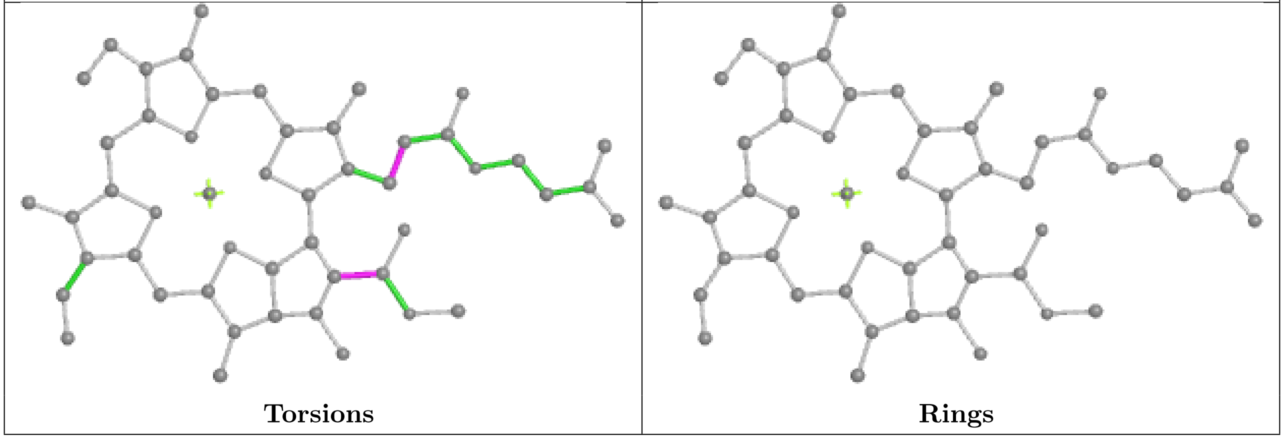
Rings

Ligand CLA aA 831



Bond lengths

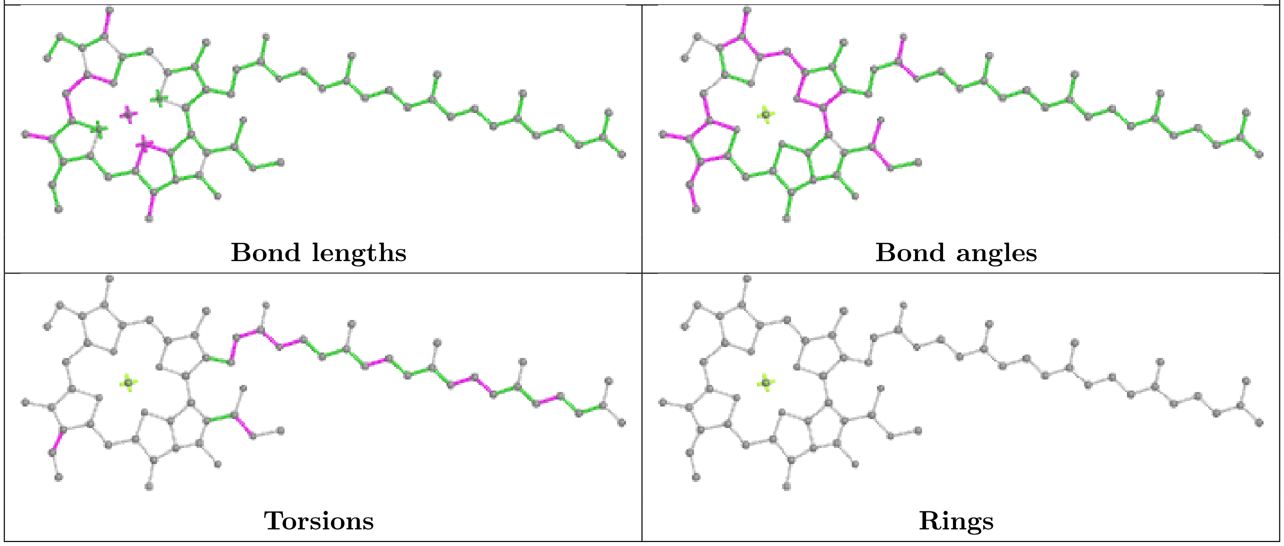
Bond angles



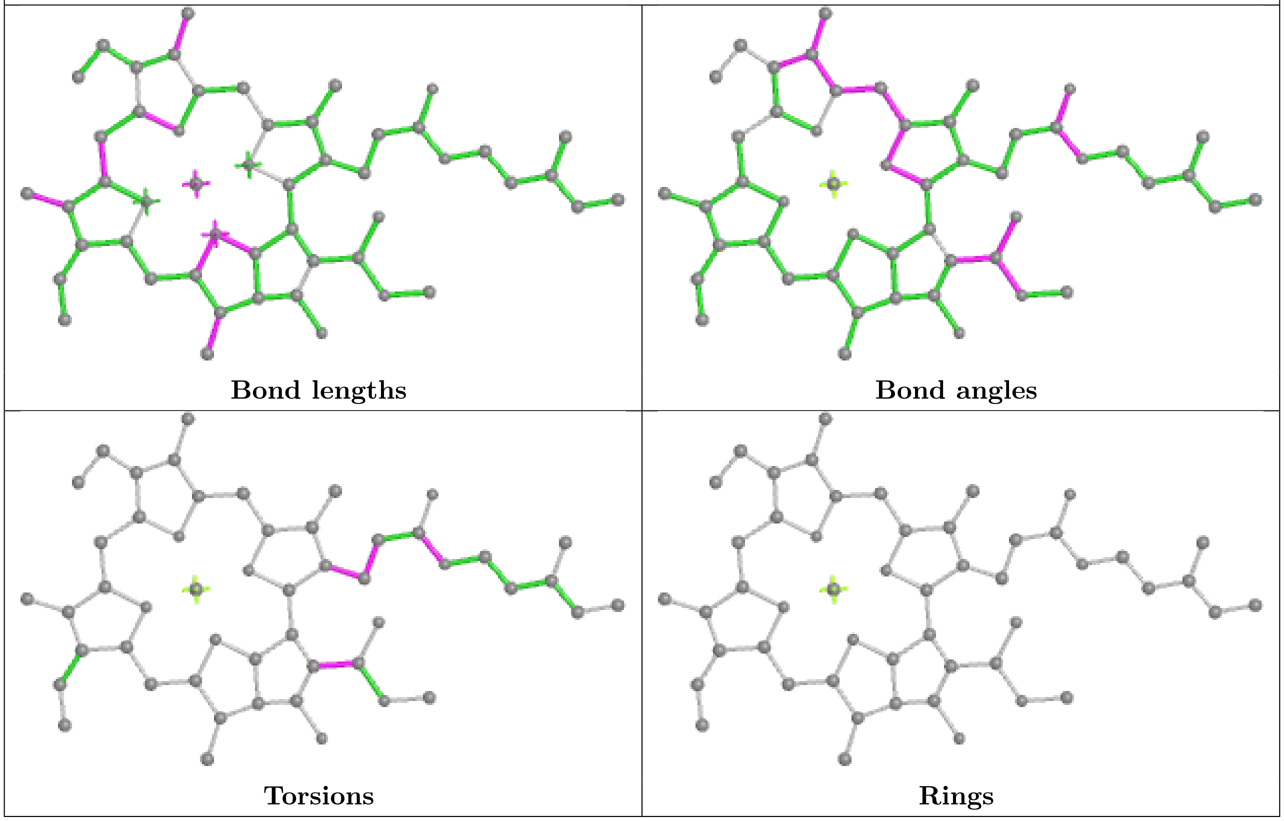
Torsions

Rings

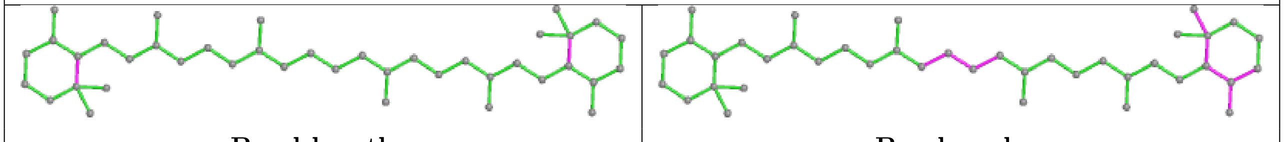
Ligand CLA bB 804



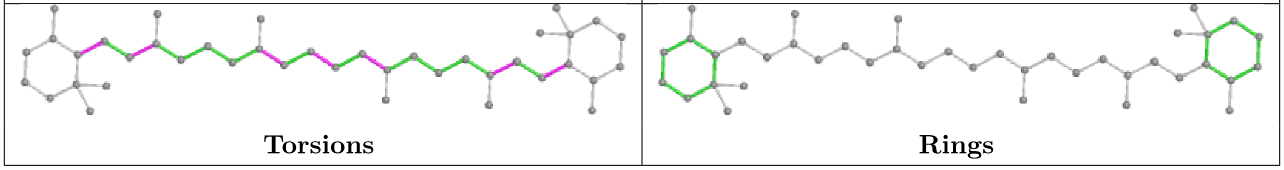
Ligand CLA bA 837



Ligand BCR cF 202

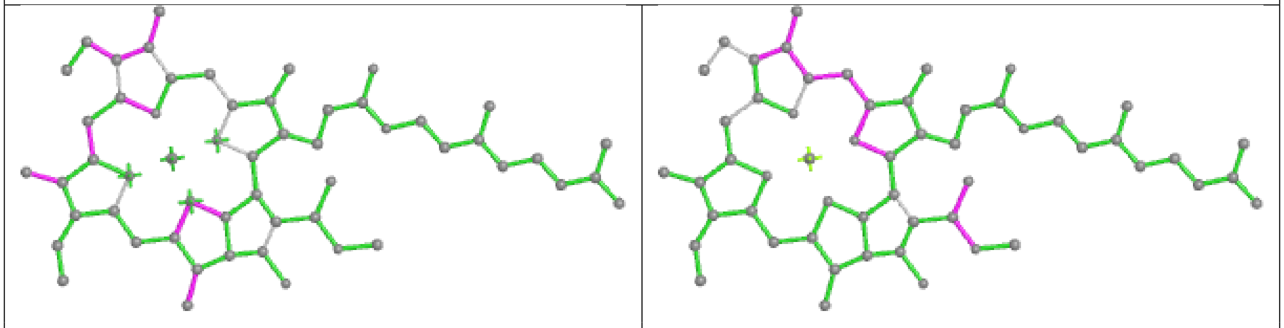


Bond lengths Bond angles

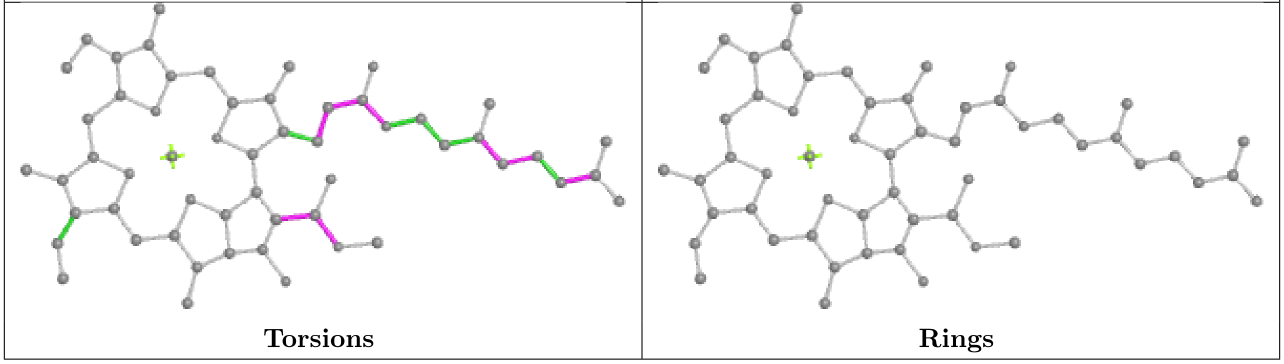


Torsions Rings

Ligand CLA dB 823

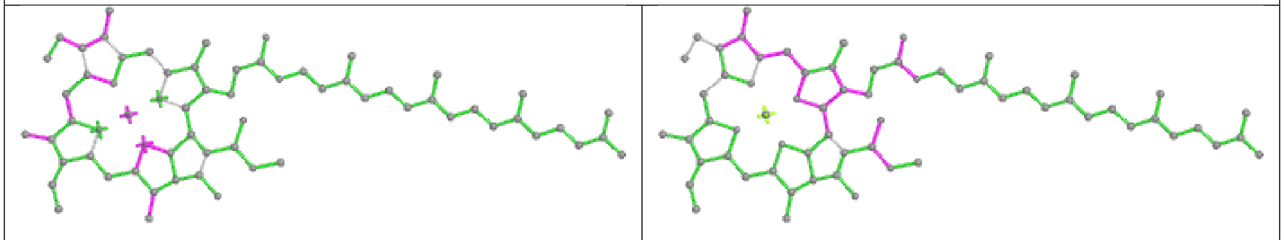


Bond lengths Bond angles

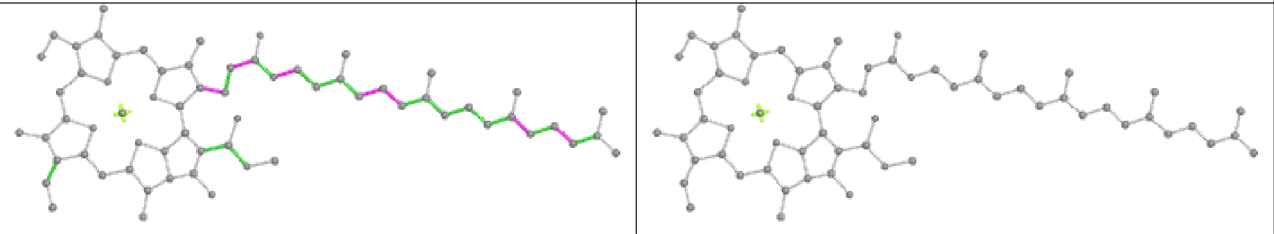


Torsions Rings

Ligand CLA cA 806

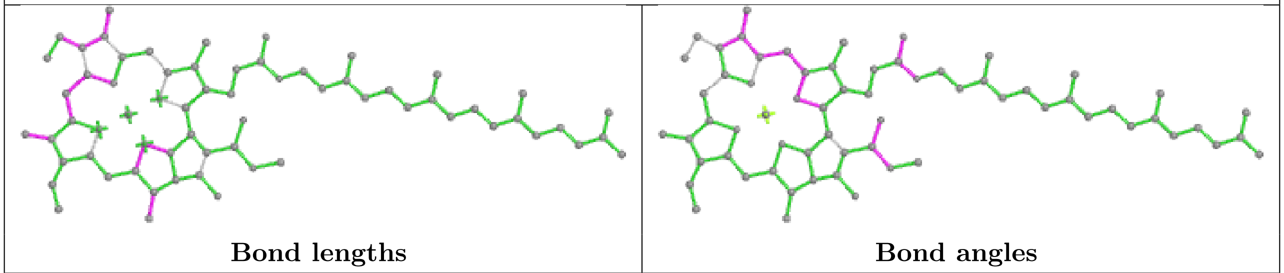


Bond lengths Bond angles



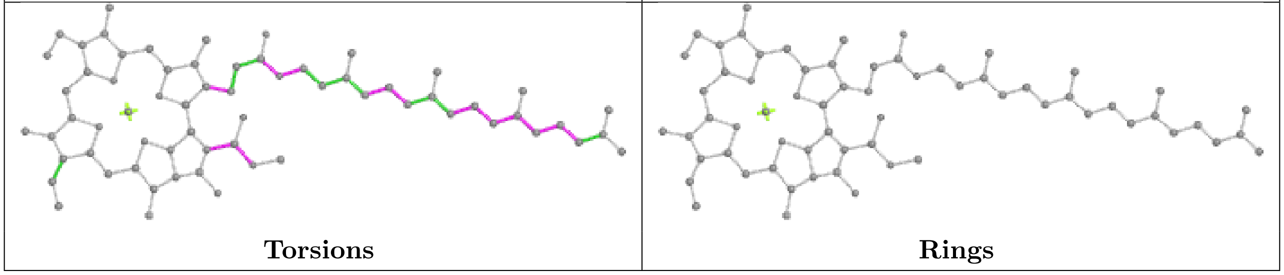
Torsions Rings

Ligand CLA aB 841



Bond lengths

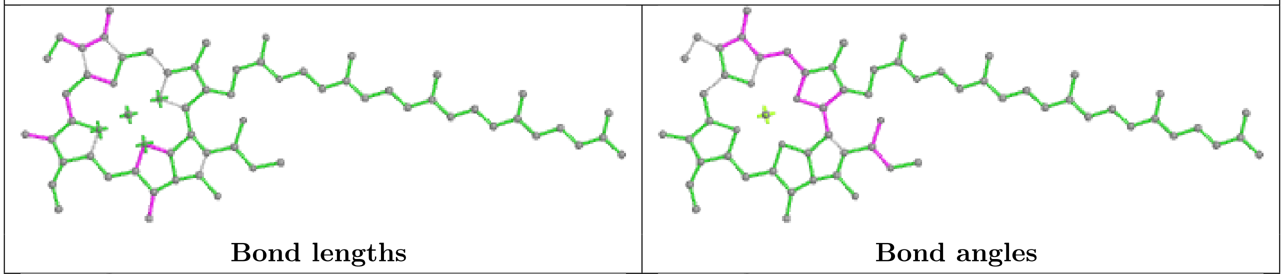
Bond angles



Torsions

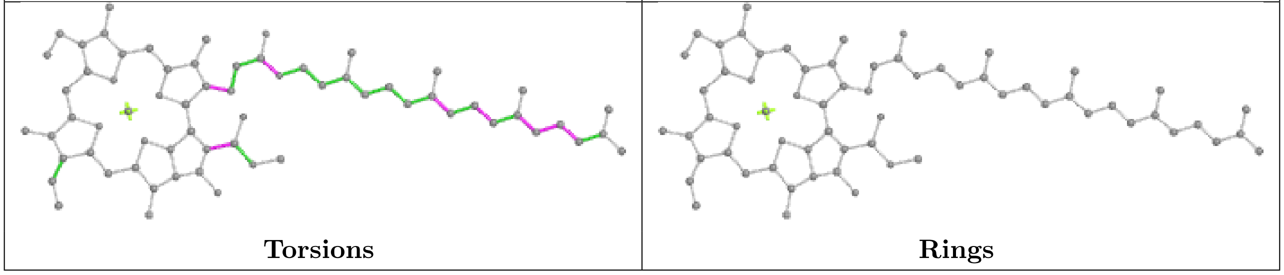
Rings

Ligand CLA cA 841



Bond lengths

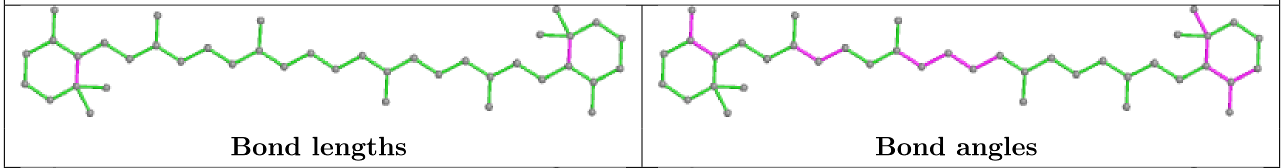
Bond angles



Torsions

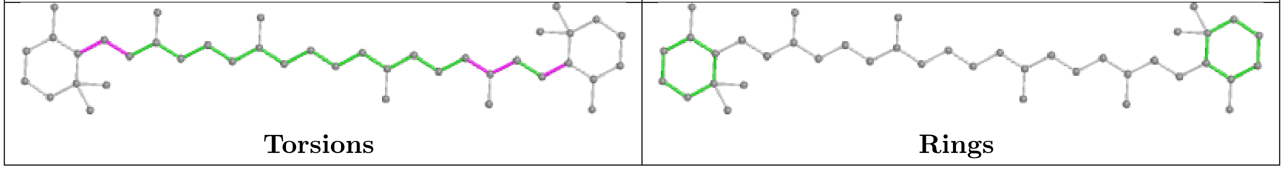
Rings

Ligand BCR aA 848



Bond lengths

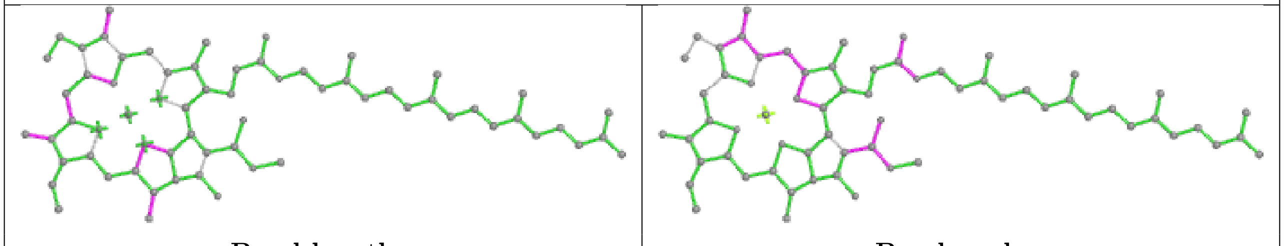
Bond angles



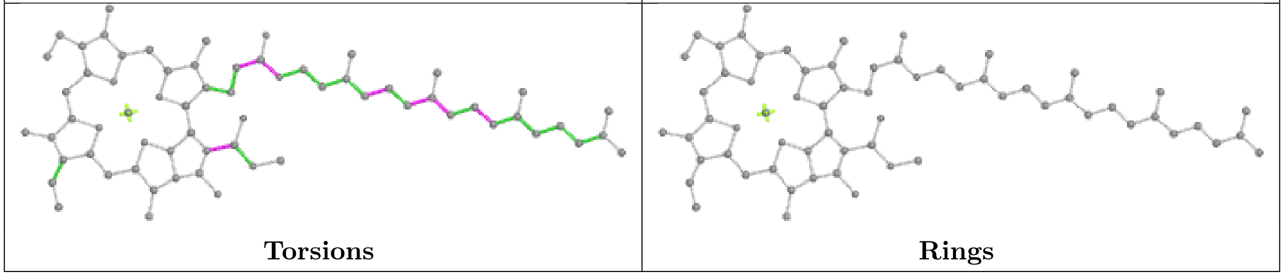
Torsions

Rings

Ligand CLA cA 827

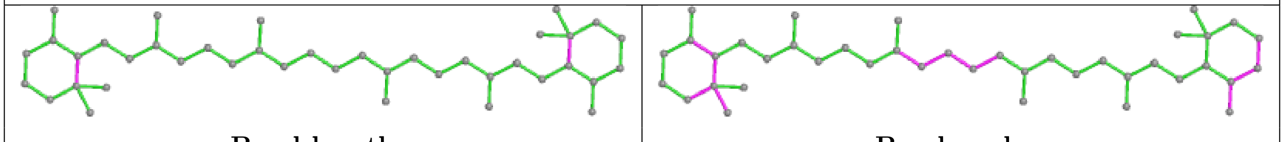


Bond lengths Bond angles

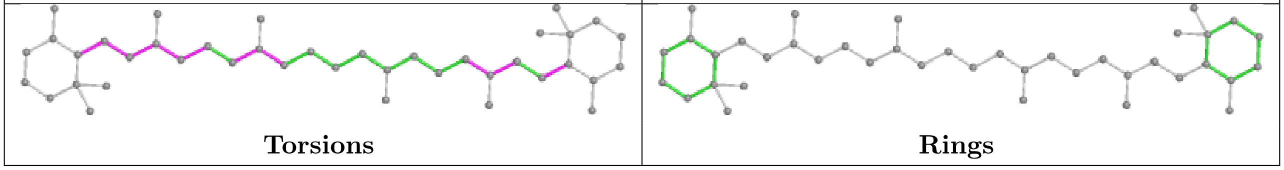


Torsions Rings

Ligand BCR aI 101

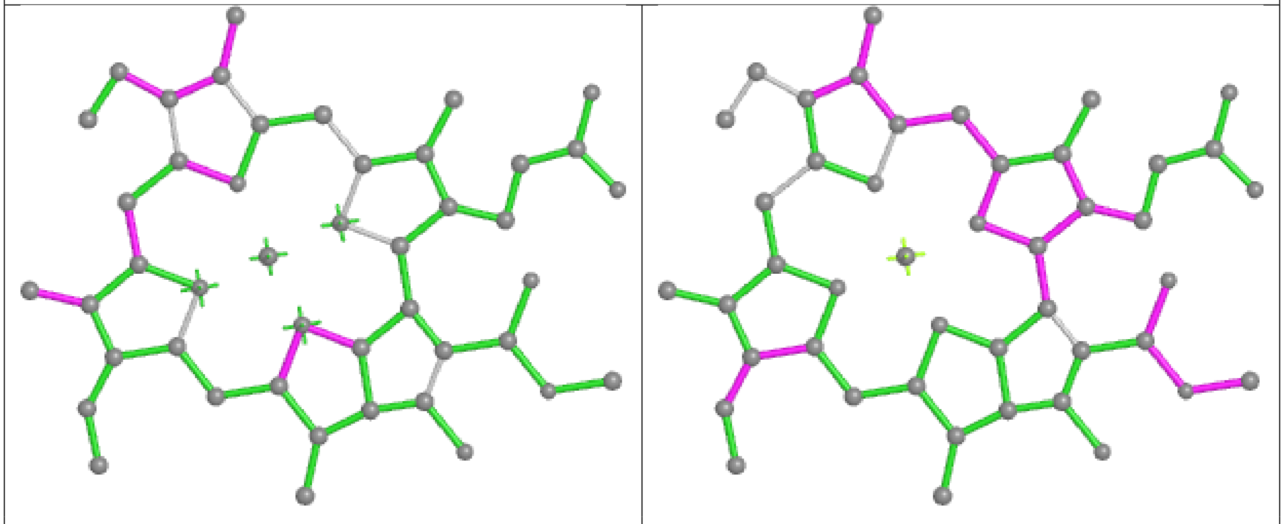


Bond lengths Bond angles

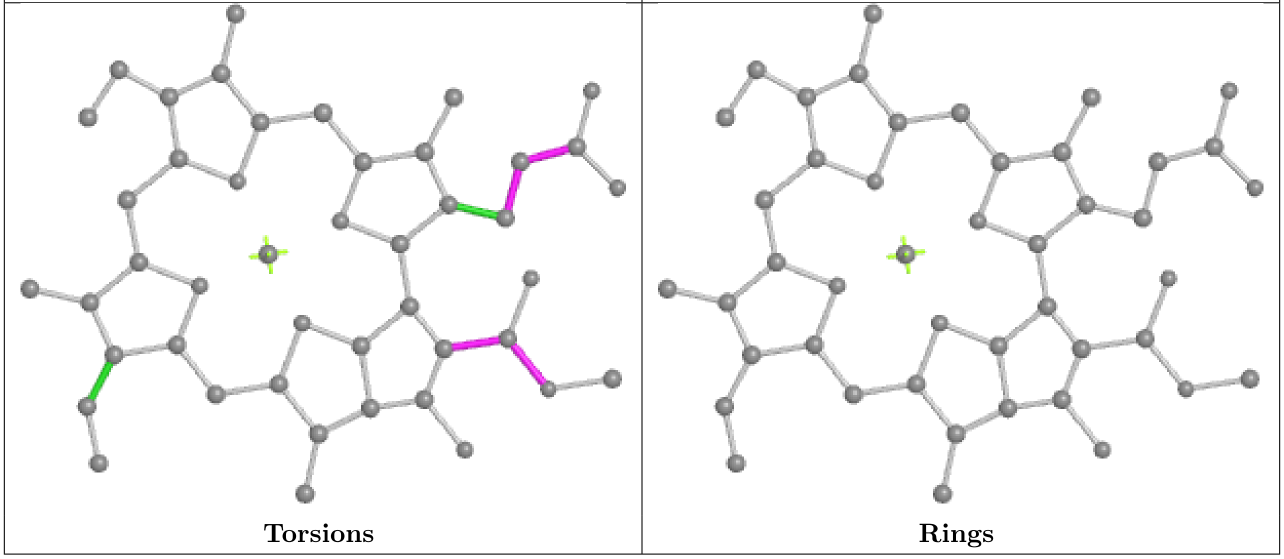


Torsions Rings

Ligand CLA dA 813

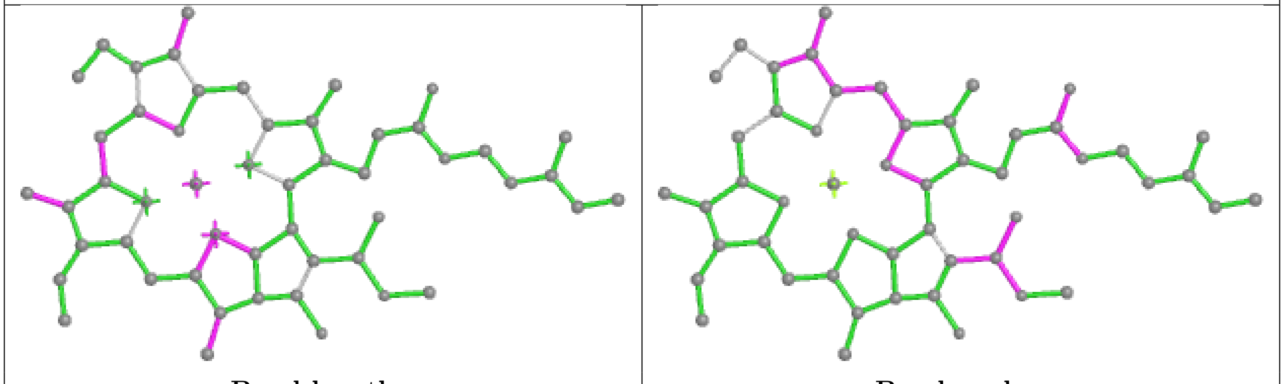


Bond lengths **Bond angles**



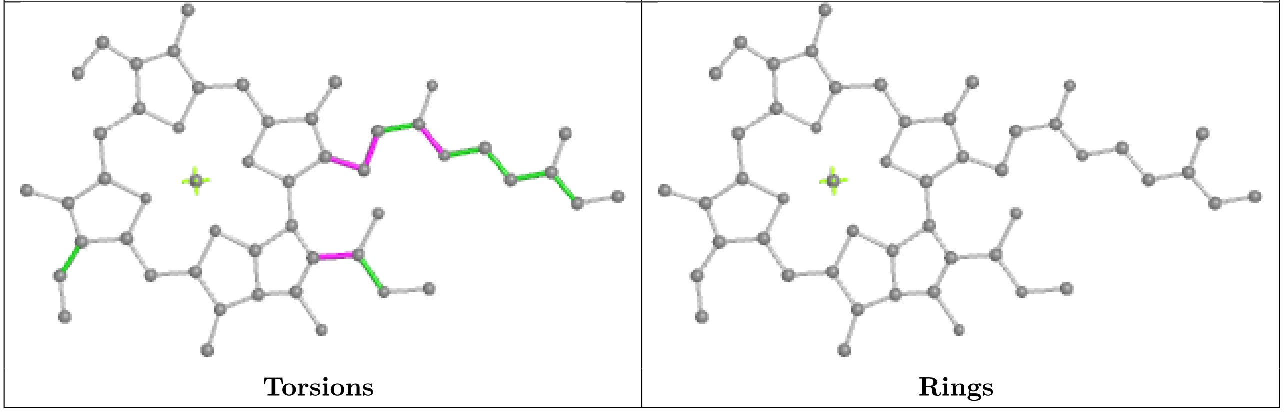
Torsions **Rings**

Ligand CLA cA 837



Bond lengths

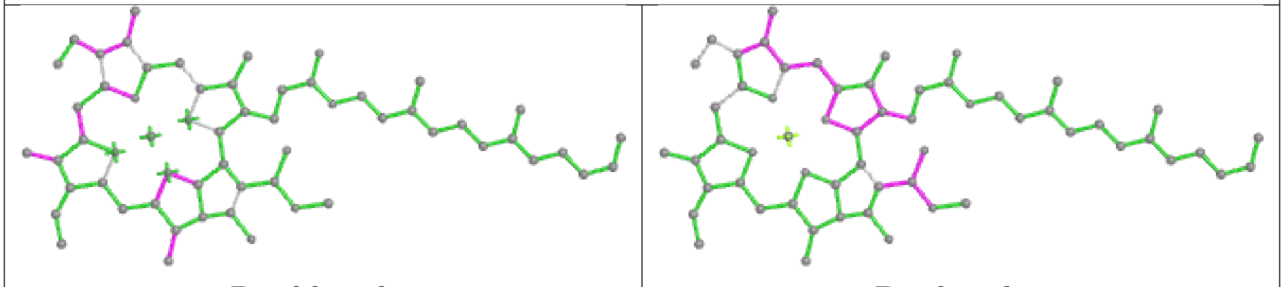
Bond angles



Torsions

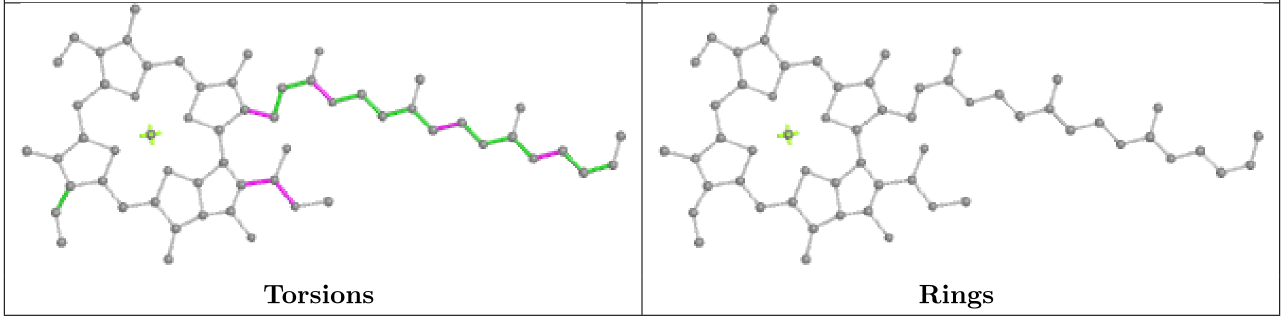
Rings

Ligand CLA bB 818



Bond lengths

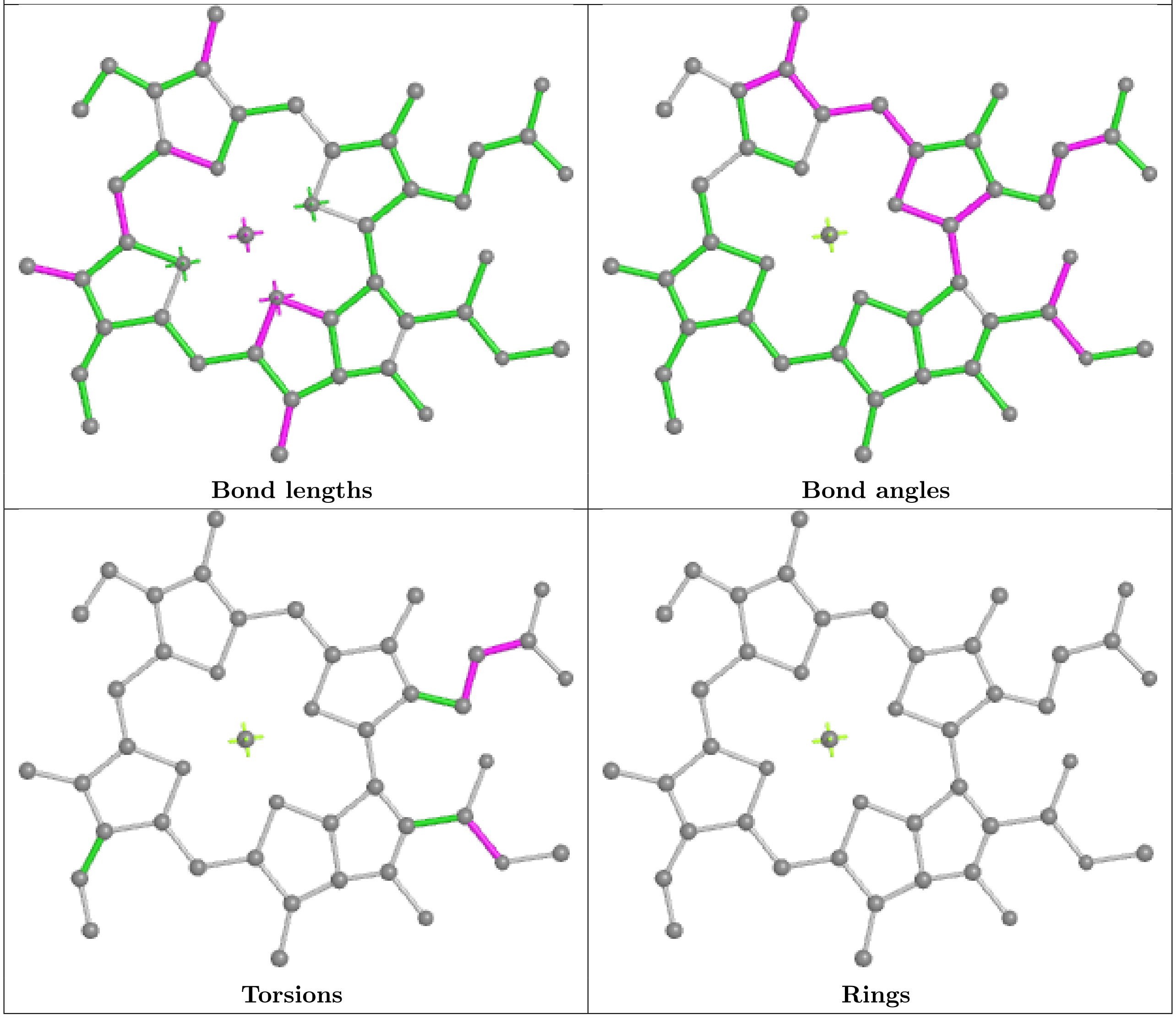
Bond angles



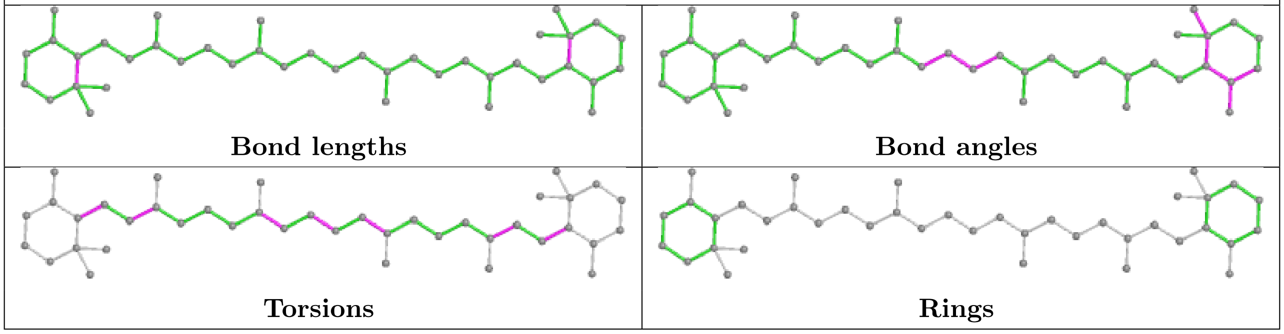
Torsions

Rings

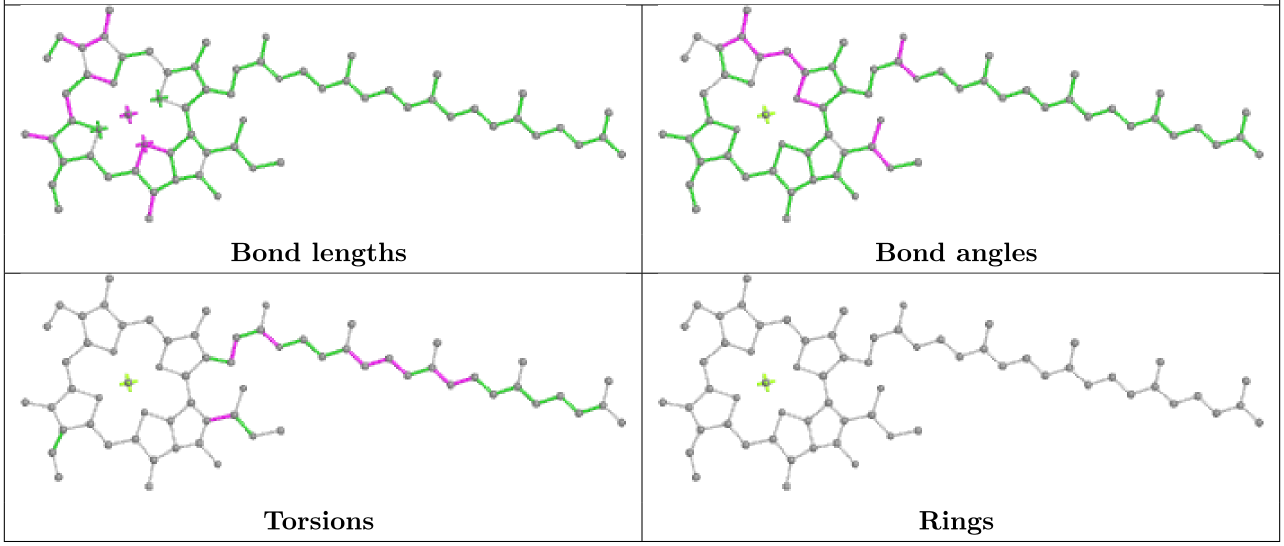
Ligand CLA dA 809



Ligand BCR dF 202



Ligand CLA bA 840



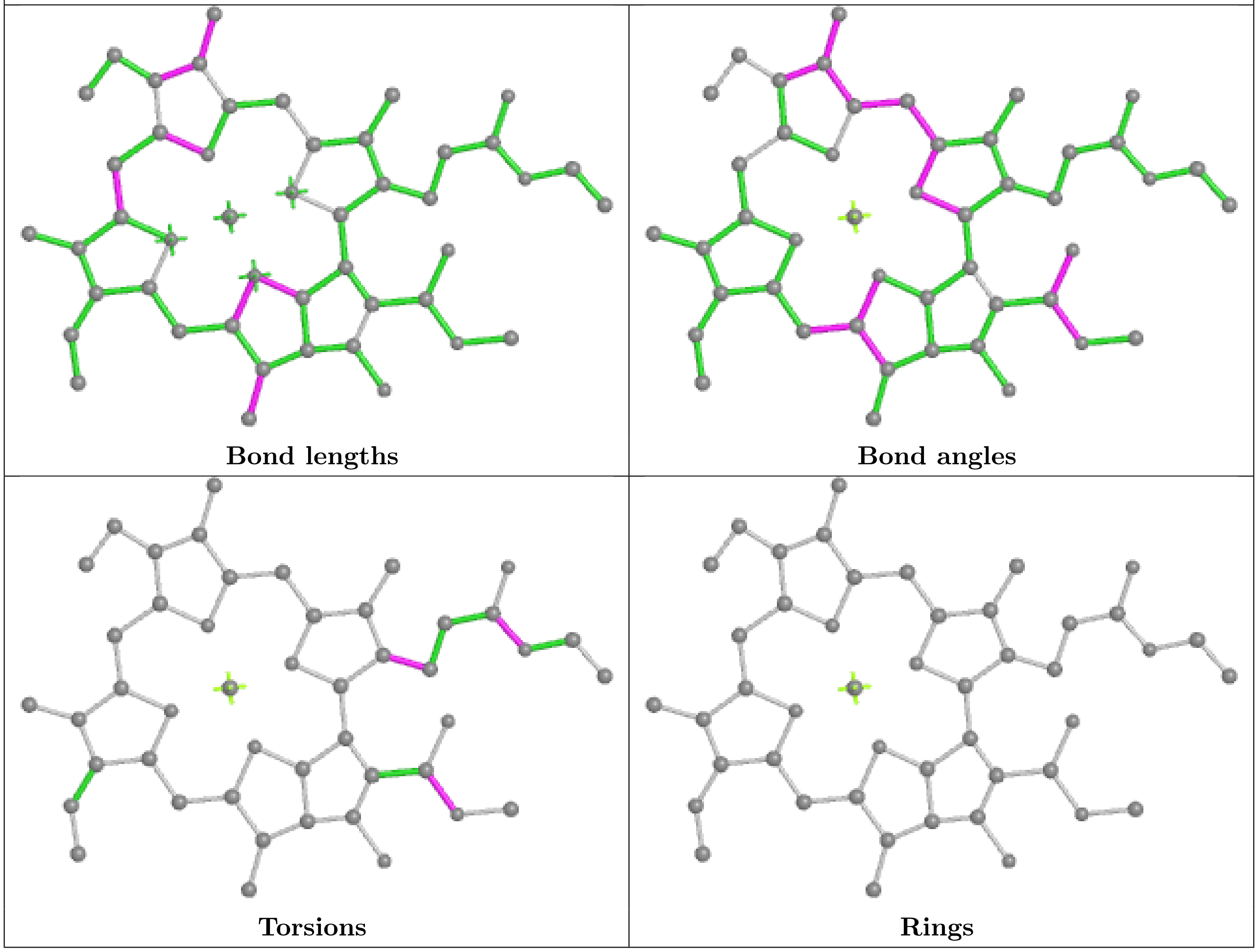
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA bA 824



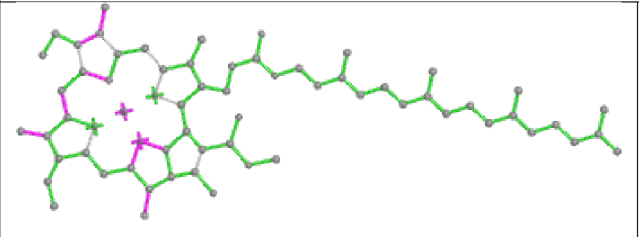
Bond lengths

Bond angles

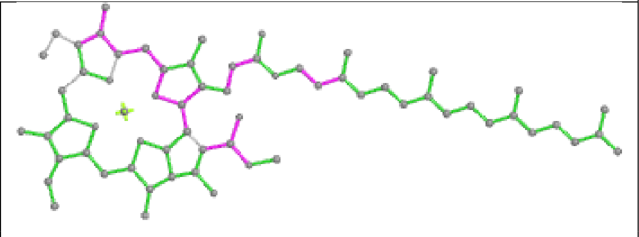
Torsions

Rings

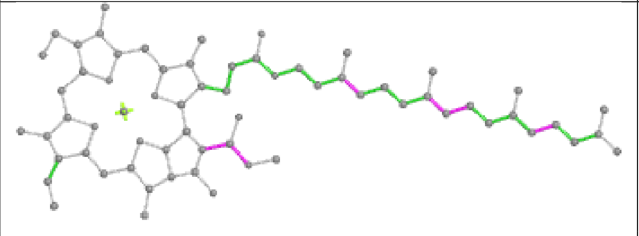
Ligand CLA bA 833



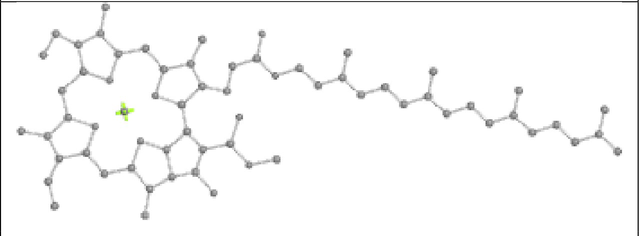
Bond lengths



Bond angles

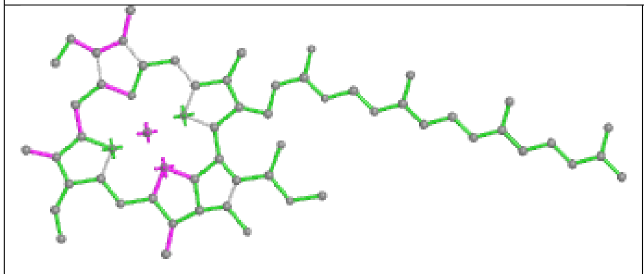


Torsions

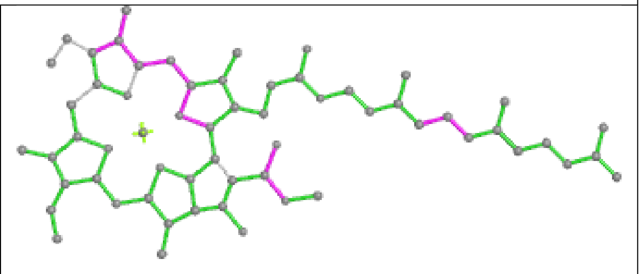


Rings

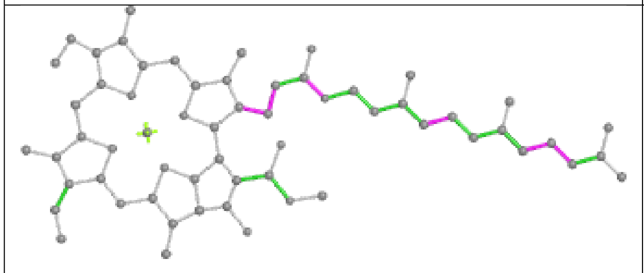
Ligand CLA aB 818



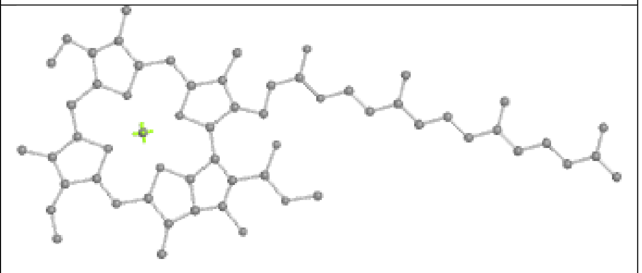
Bond lengths



Bond angles

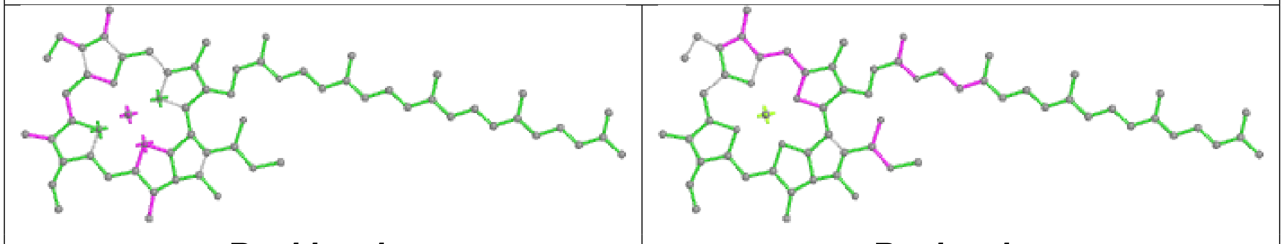


Torsions



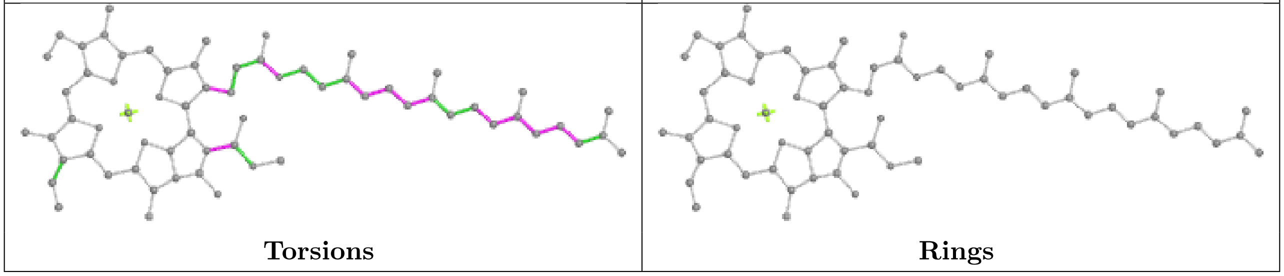
Rings

Ligand CLA cB 826



Bond lengths

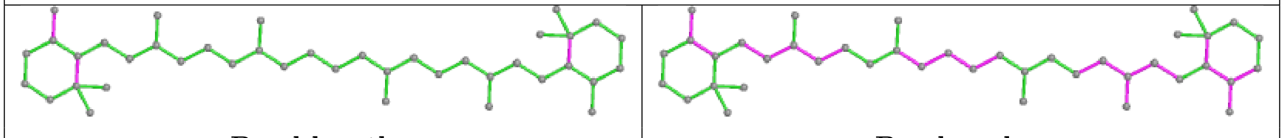
Bond angles



Torsions

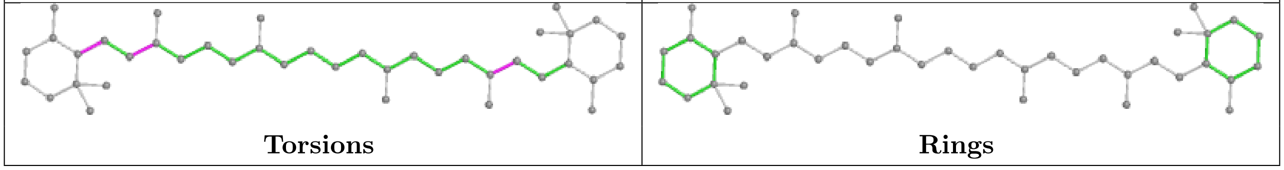
Rings

Ligand BCR aA 846



Bond lengths

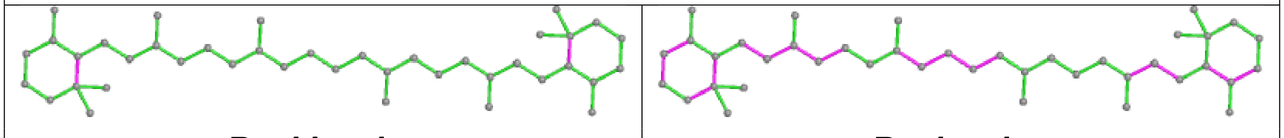
Bond angles



Torsions

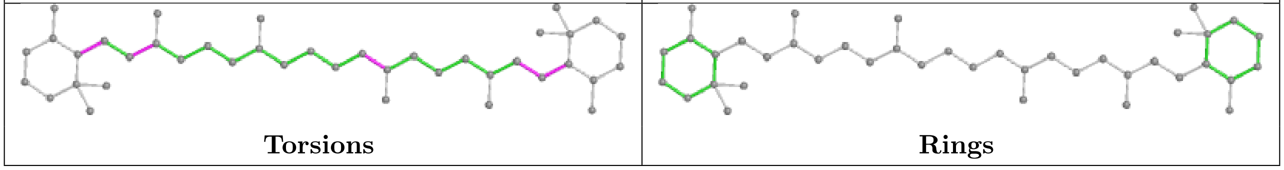
Rings

Ligand BCR cB 851



Bond lengths

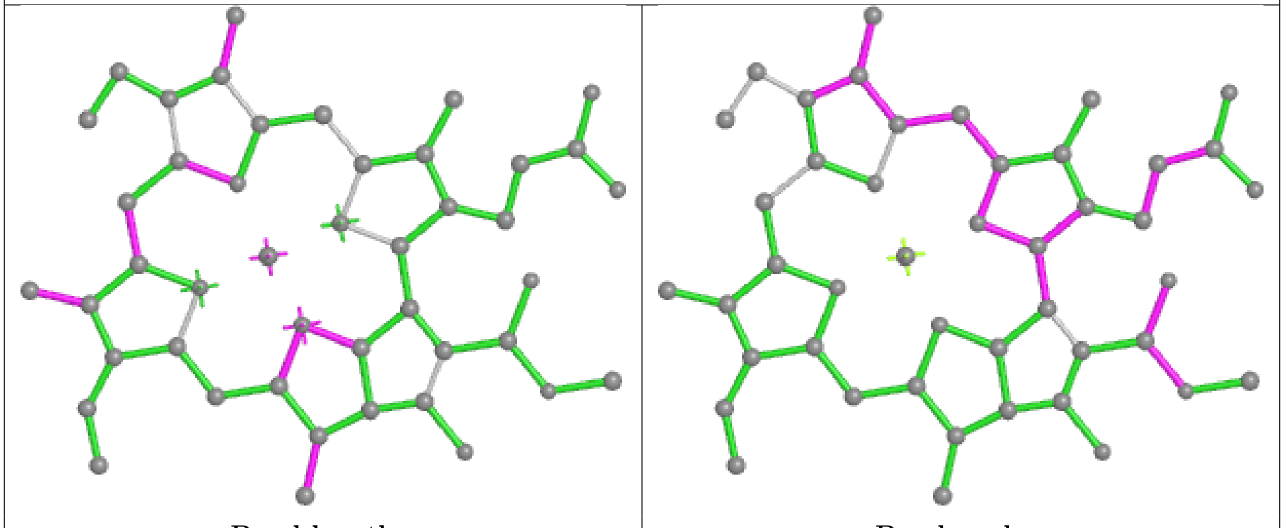
Bond angles



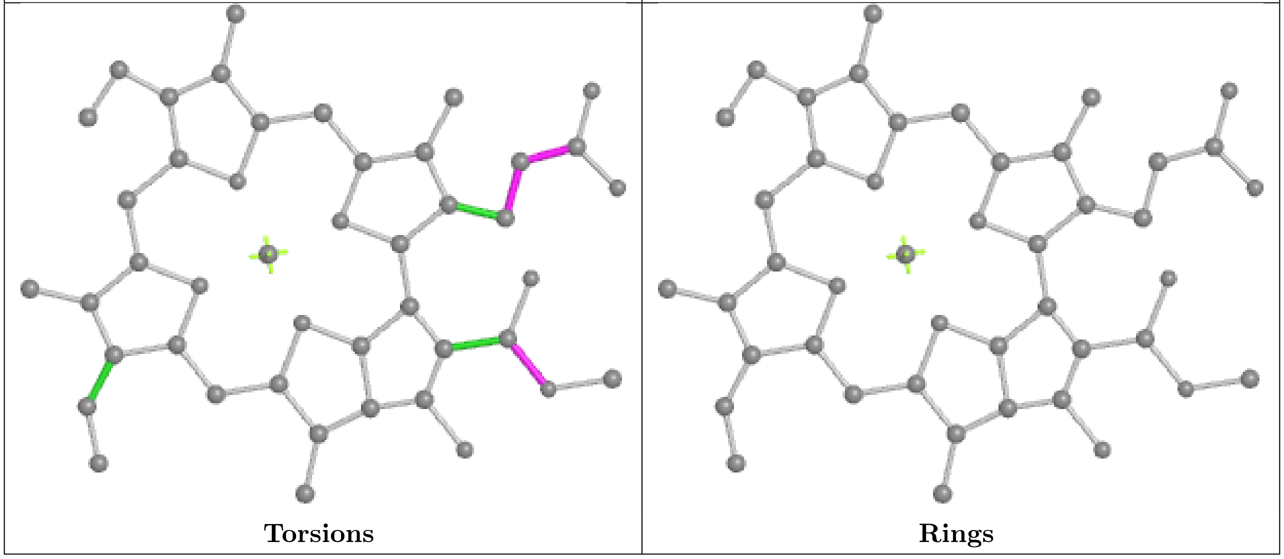
Torsions

Rings

Ligand CLA bA 809

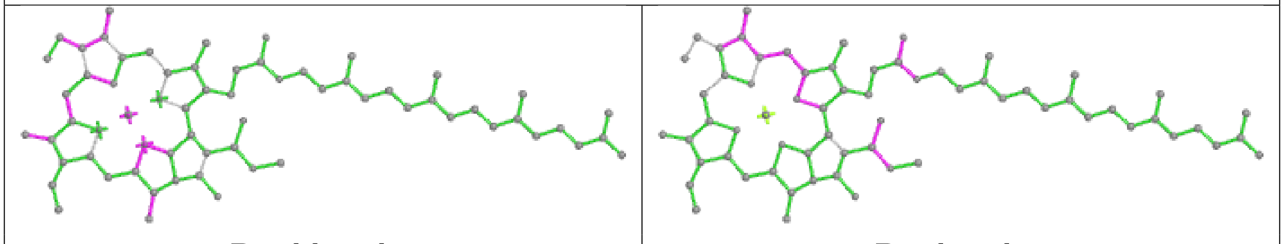


Bond lengths Bond angles

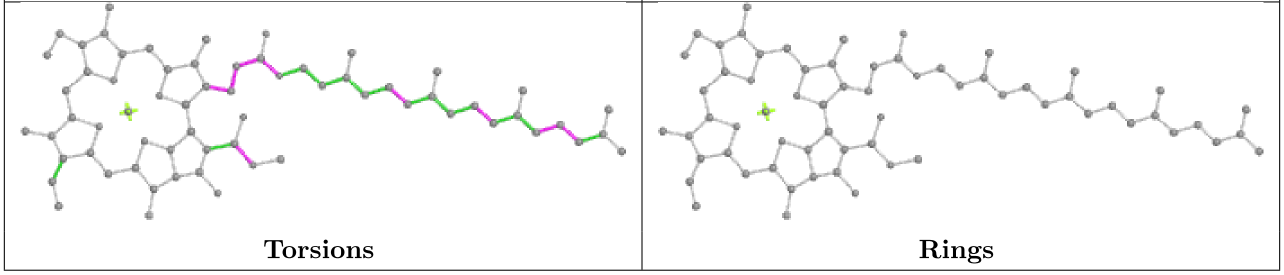


Torsions Rings

Ligand CLA bA 842

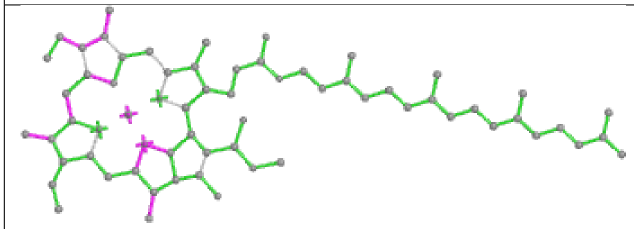
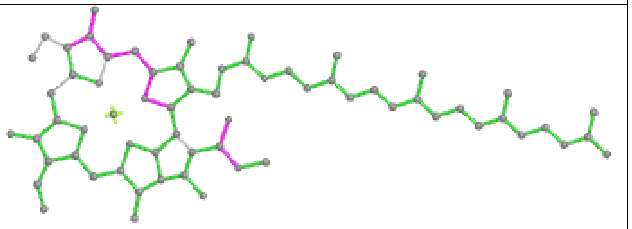
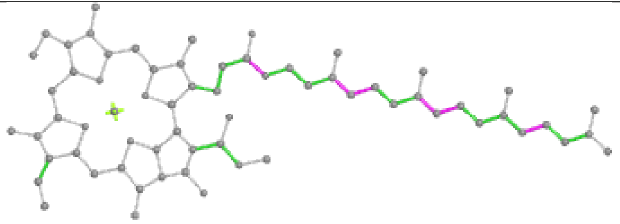
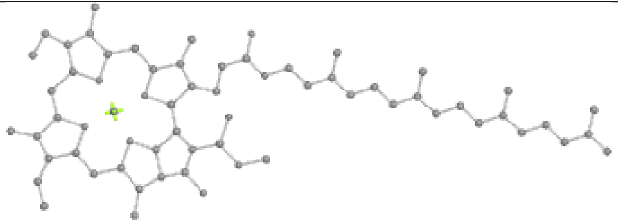


Bond lengths Bond angles

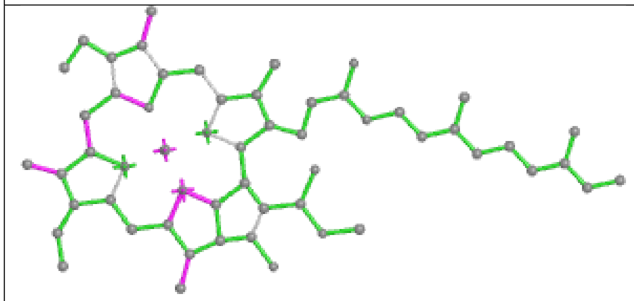
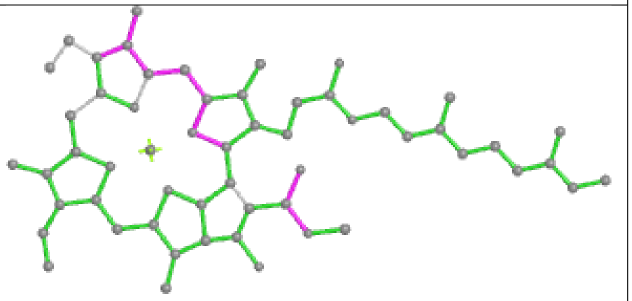
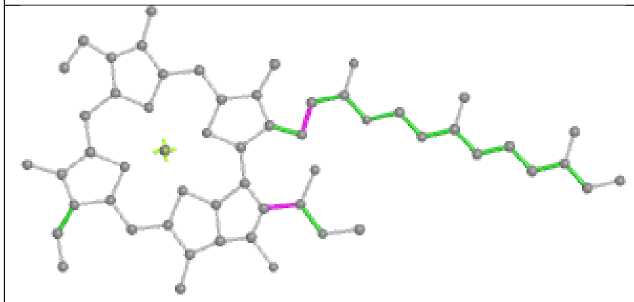
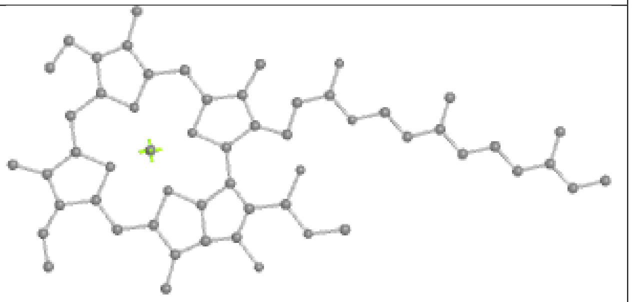


Torsions Rings

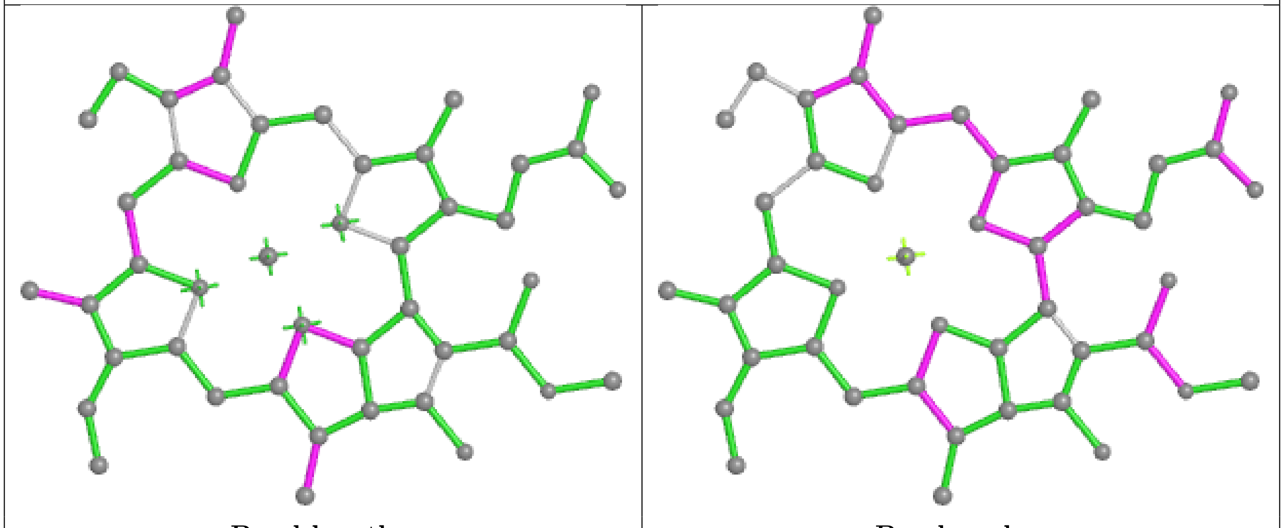
Ligand CLA cB 810

 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

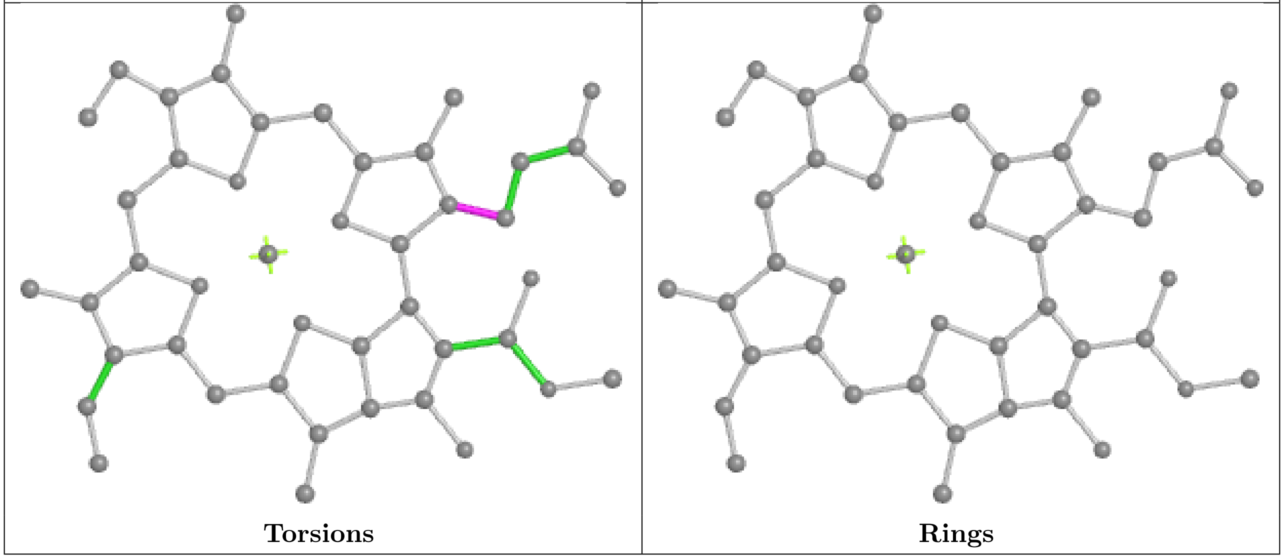
Ligand CLA cB 814

 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

Ligand CLA dB 836

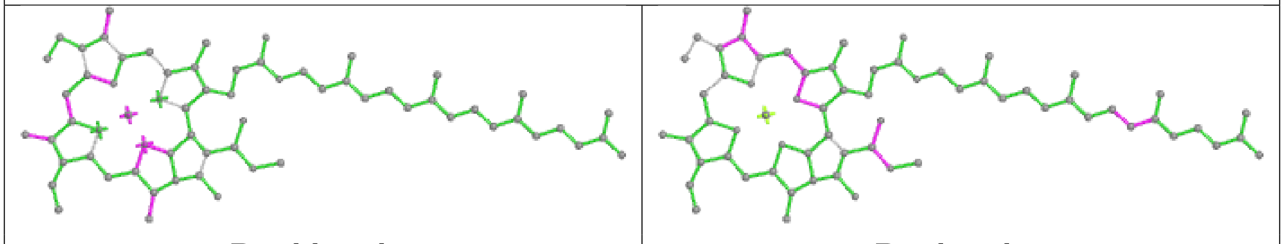


Bond lengths Bond angles

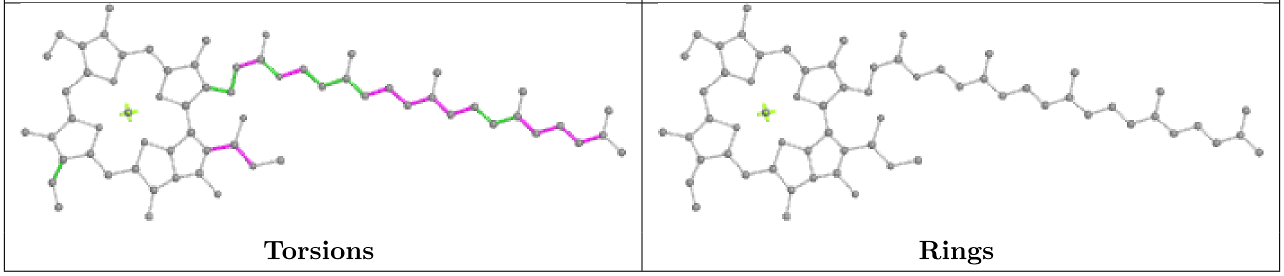


Torsions Rings

Ligand CLA aB 807

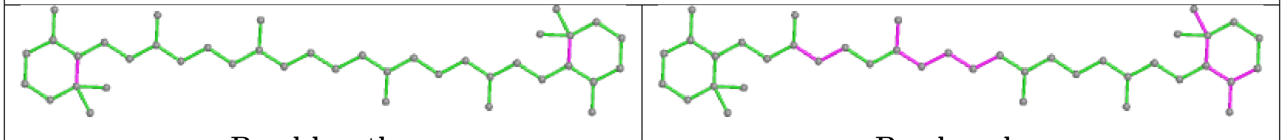


Bond lengths Bond angles



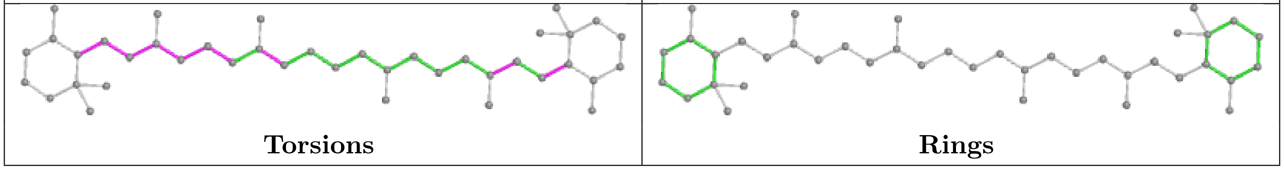
Torsions Rings

Ligand BCR aF 204



Bond lengths

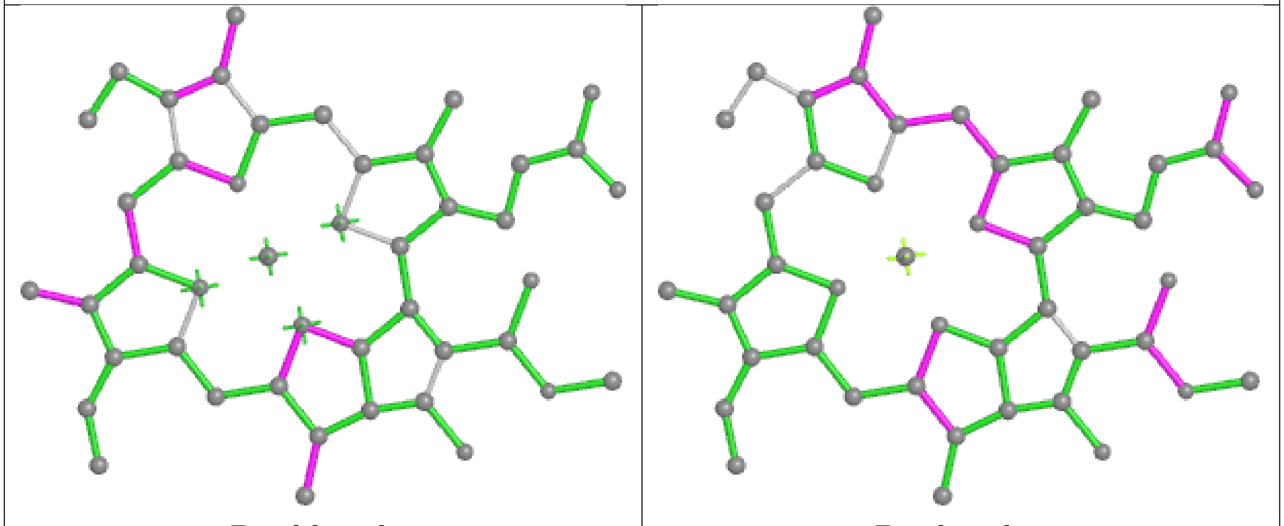
Bond angles



Torsions

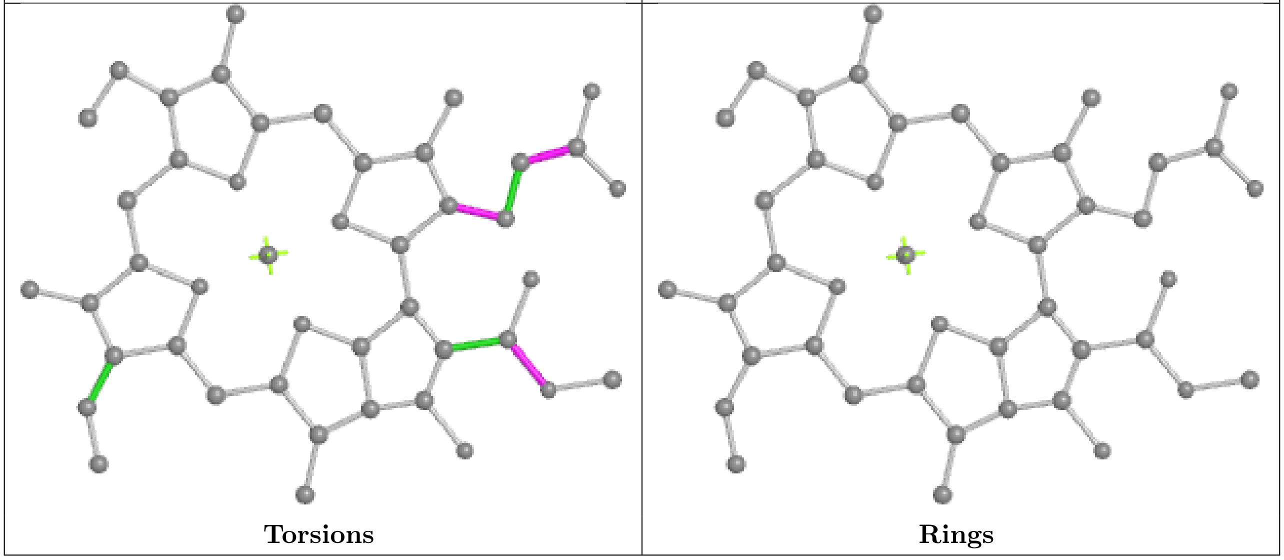
Rings

Ligand CLA aB 823



Bond lengths

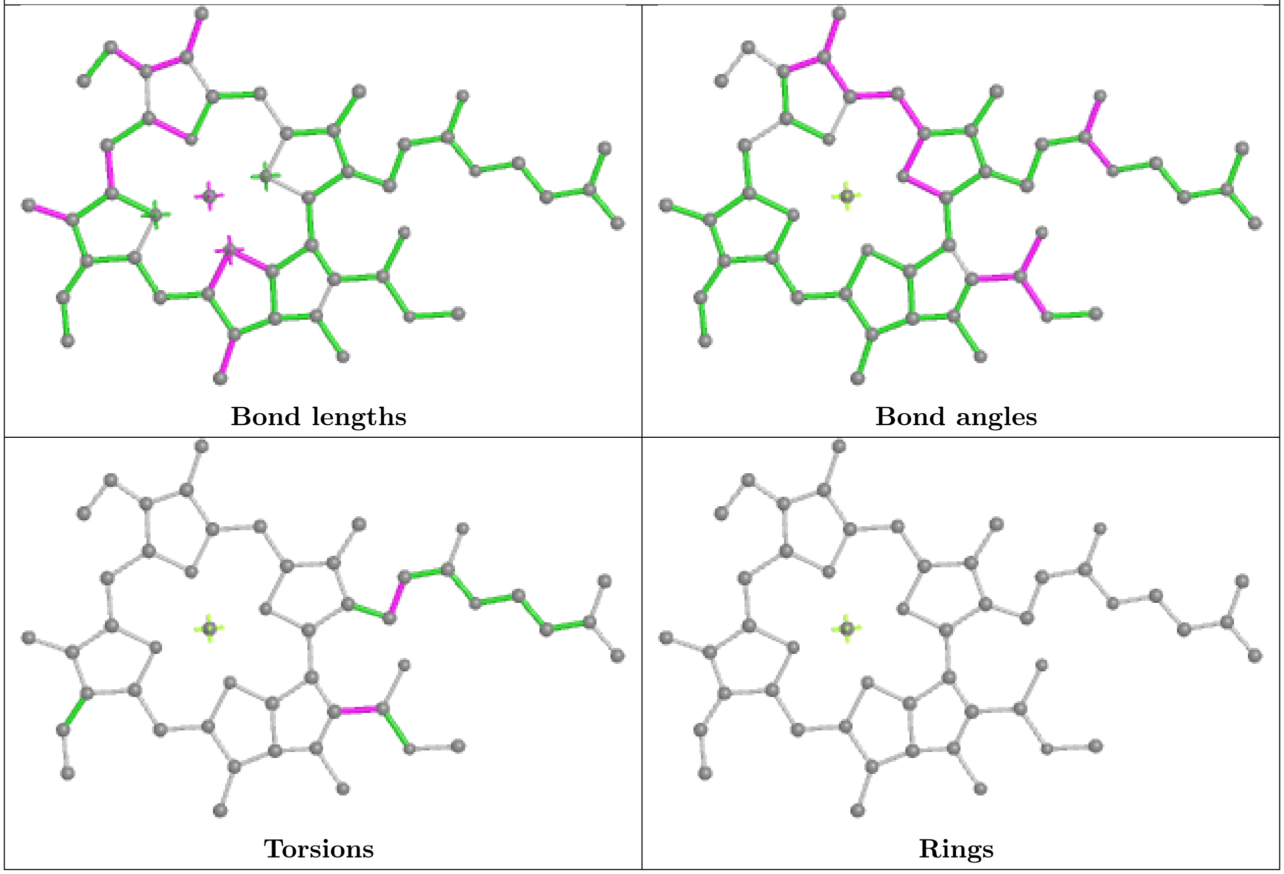
Bond angles



Torsions

Rings

Ligand CLA bA 831



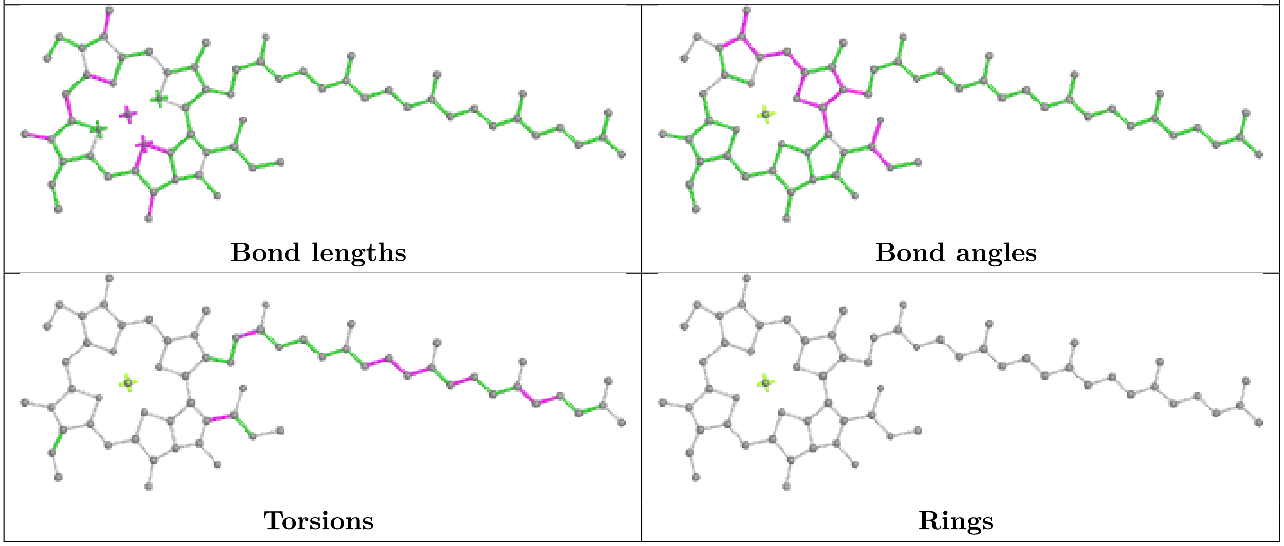
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA aA 825



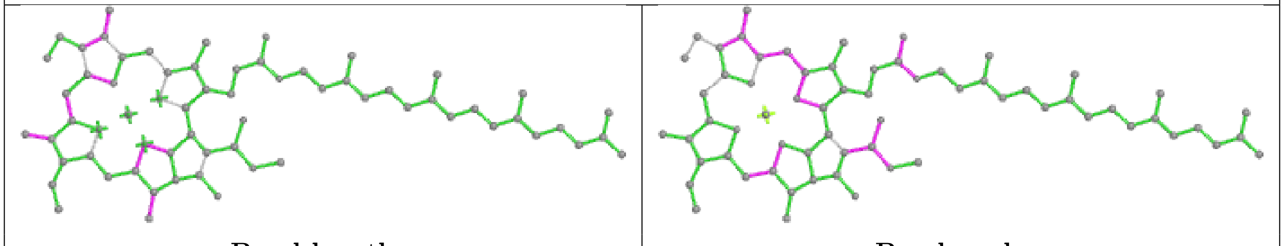
Bond lengths

Bond angles

Torsions

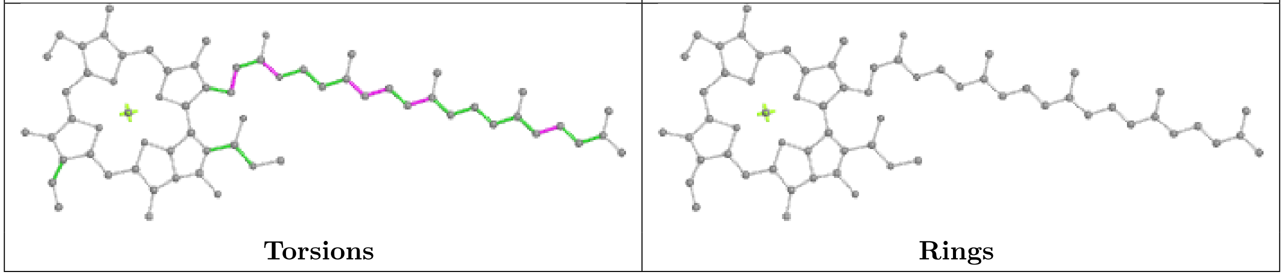
Rings

Ligand CLA aB 808



Bond lengths

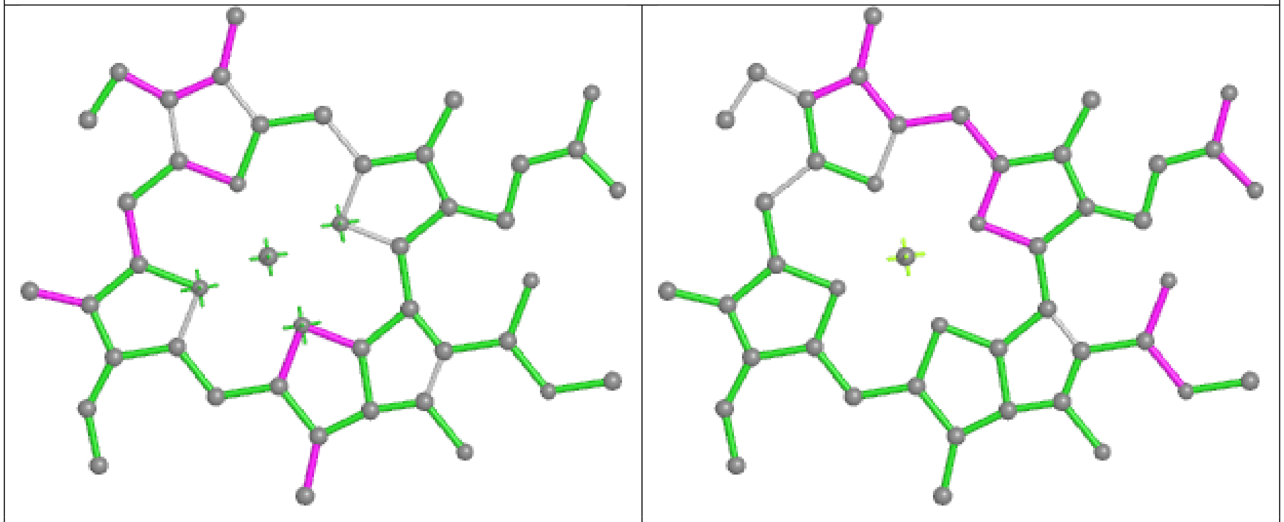
Bond angles



Torsions

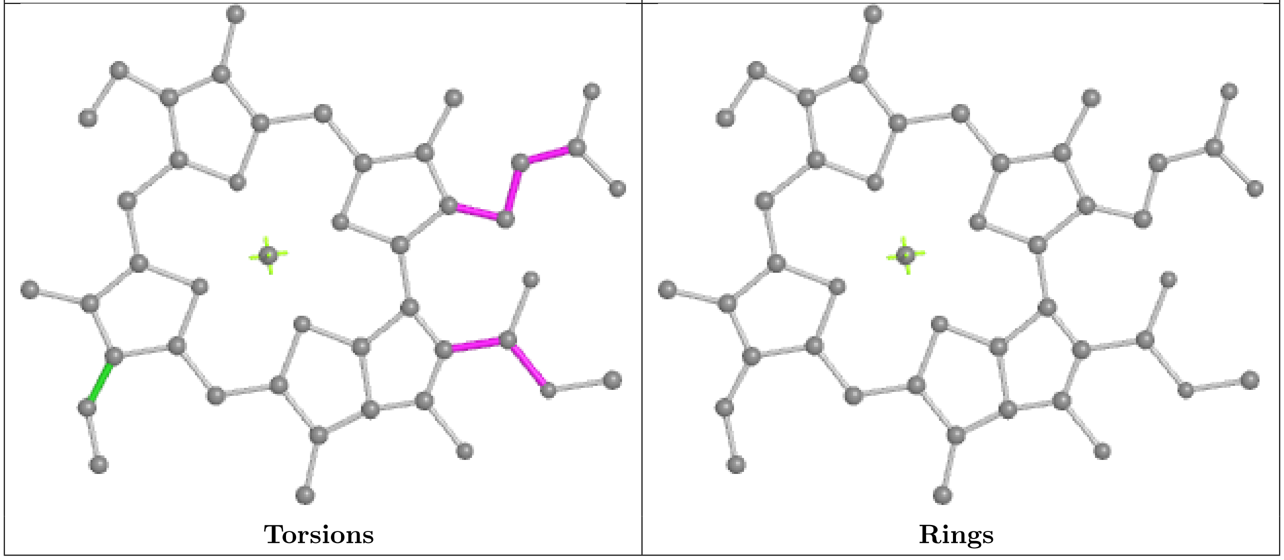
Rings

Ligand CLA aB 812



Bond lengths

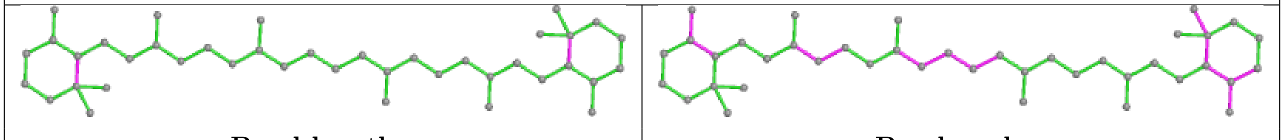
Bond angles



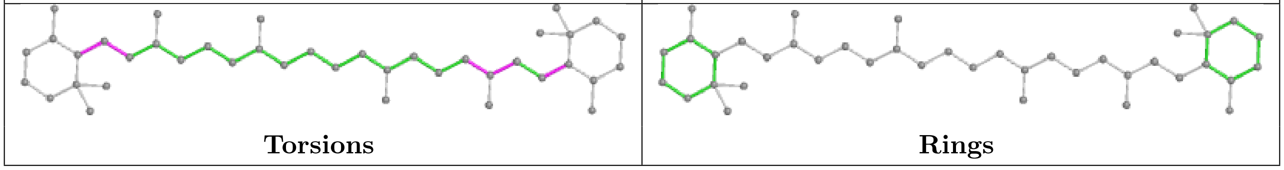
Torsions

Rings

Ligand BCR cA 848

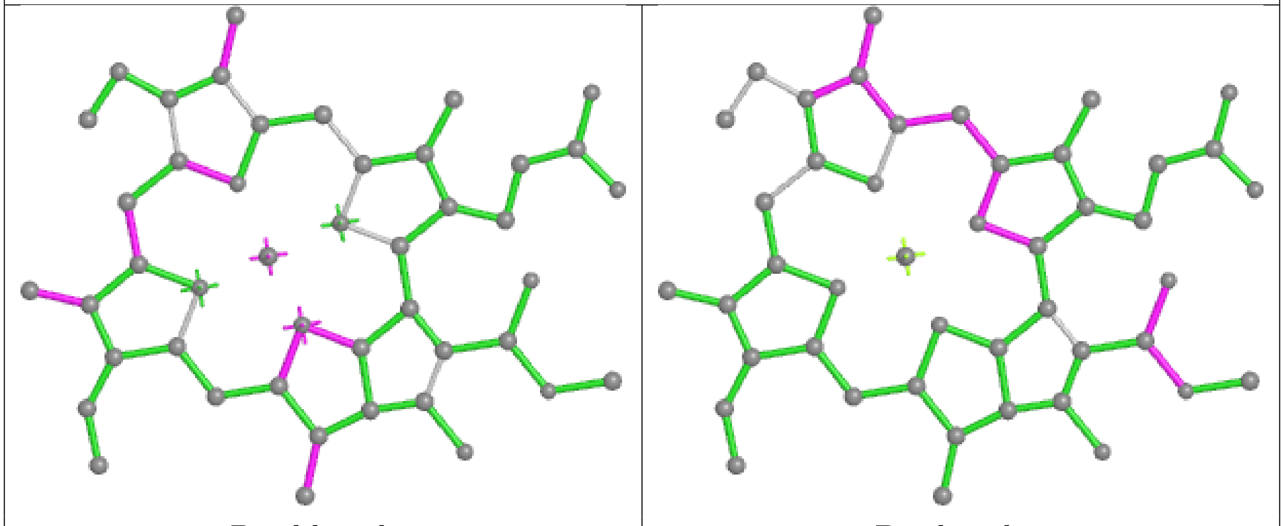


Bond lengths Bond angles

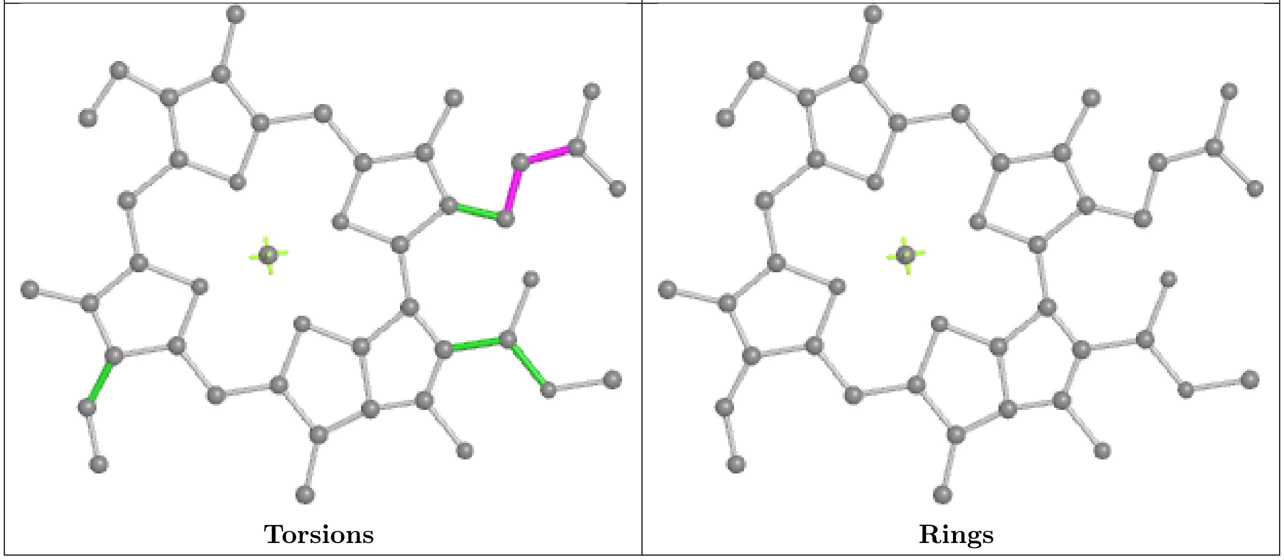


Torsions Rings

Ligand CLA cA 802

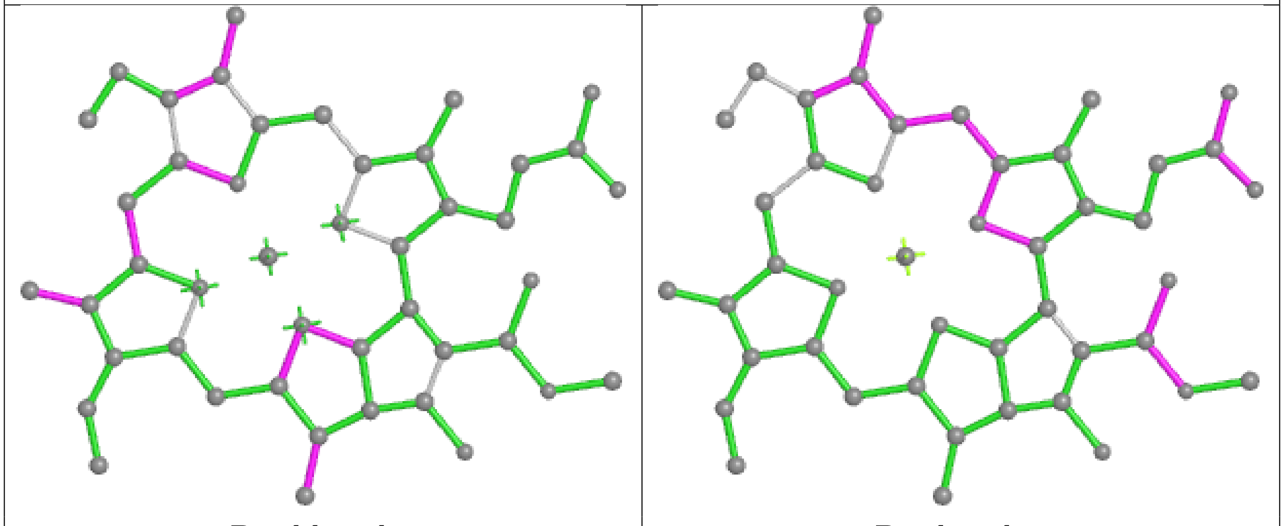


Bond lengths Bond angles



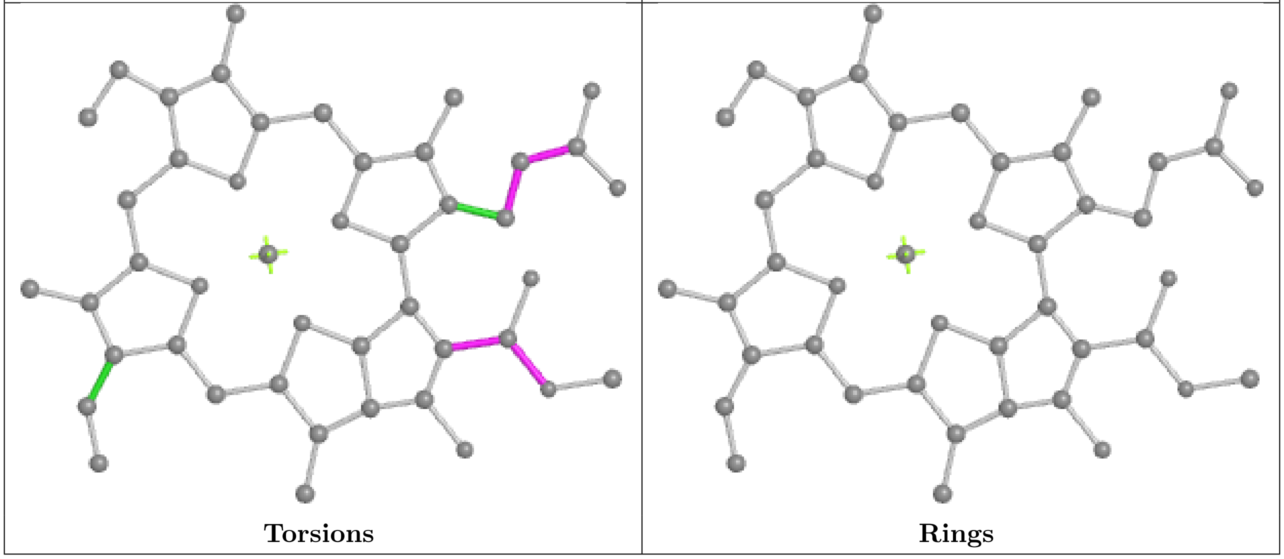
Torsions Rings

Ligand CLA bB 837



Bond lengths

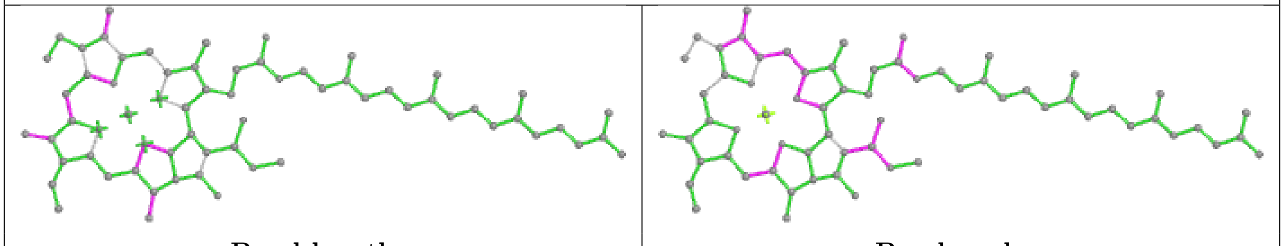
Bond angles



Torsions

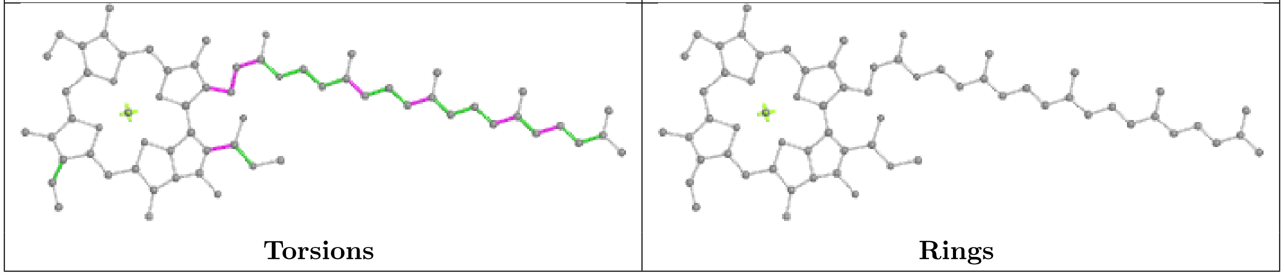
Rings

Ligand CLA bB 828



Bond lengths

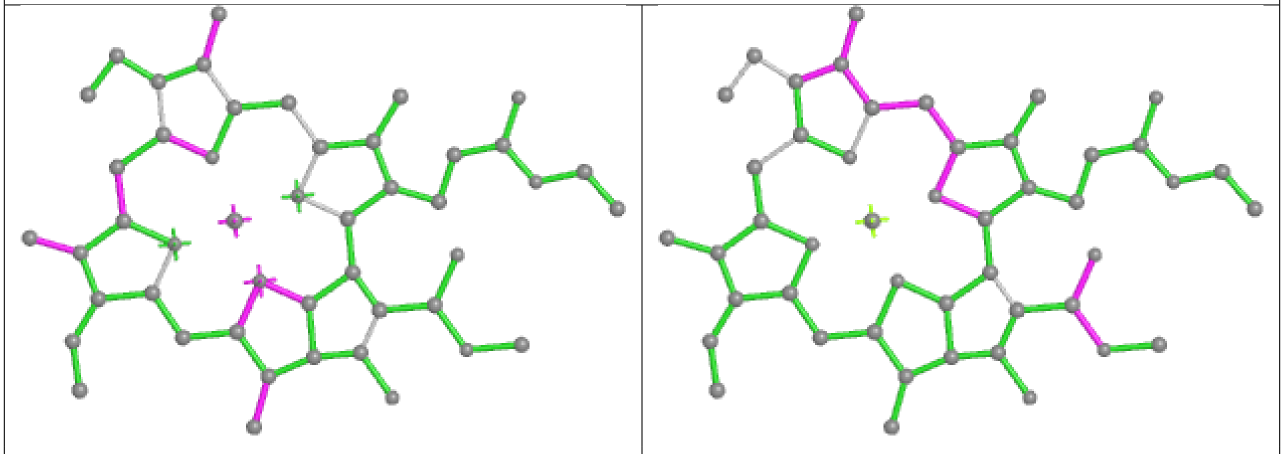
Bond angles



Torsions

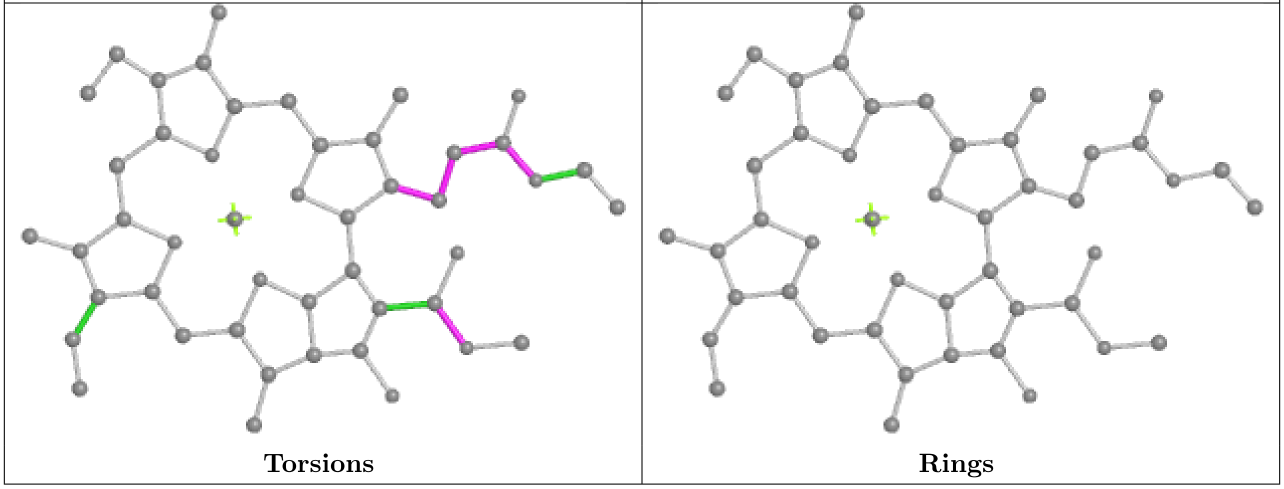
Rings

Ligand CLA cB 820



Bond lengths

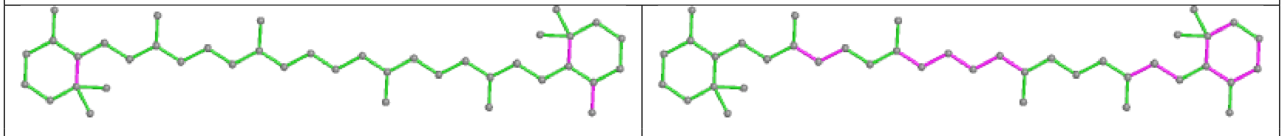
Bond angles



Torsions

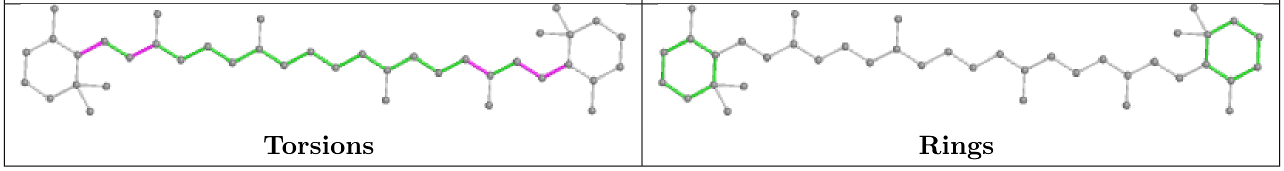
Rings

Ligand BCR aA 847



Bond lengths

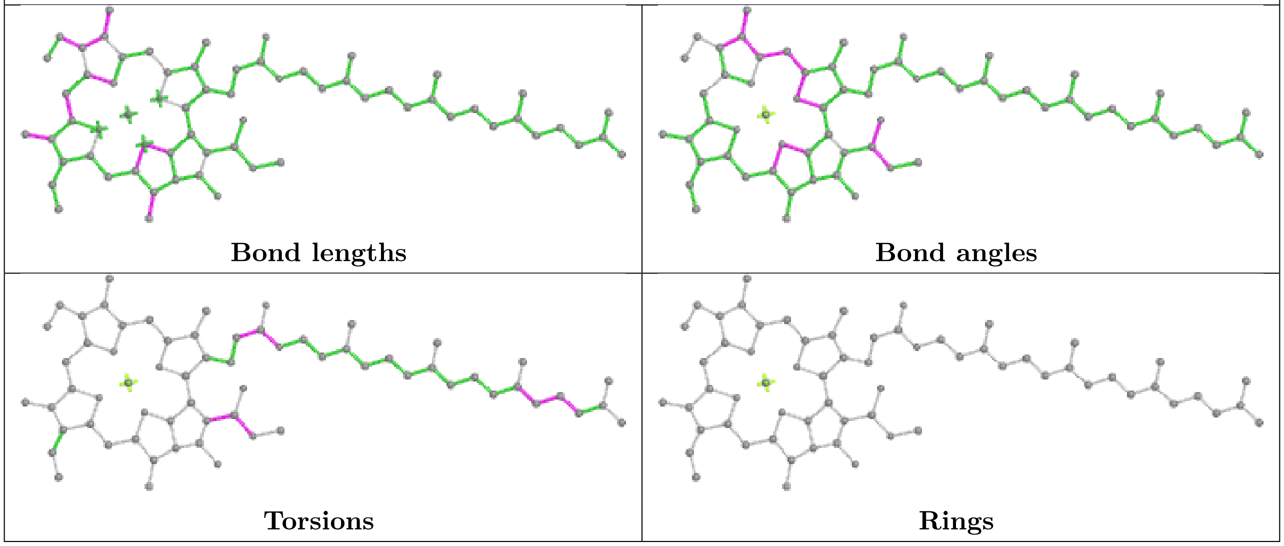
Bond angles



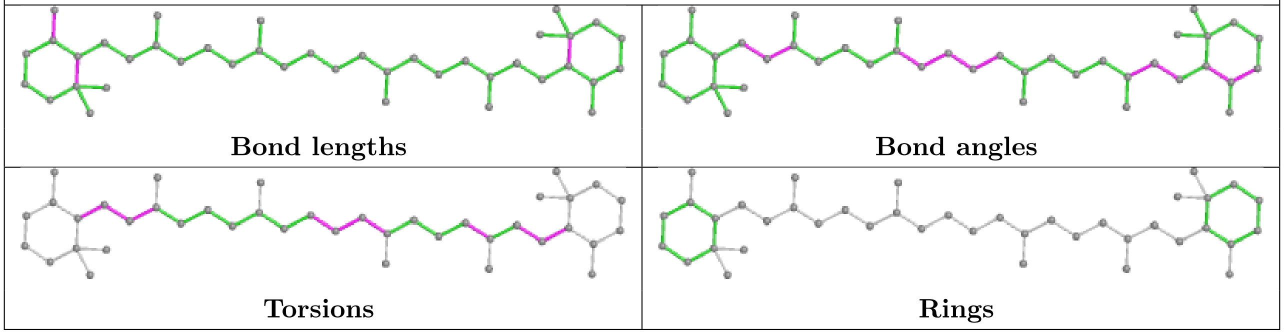
Torsions

Rings

Ligand CLA dB 802



Ligand BCR dL 203



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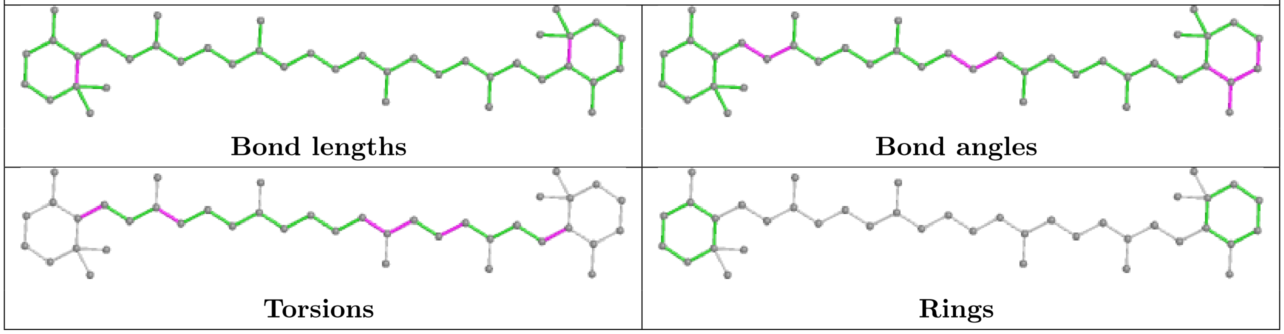
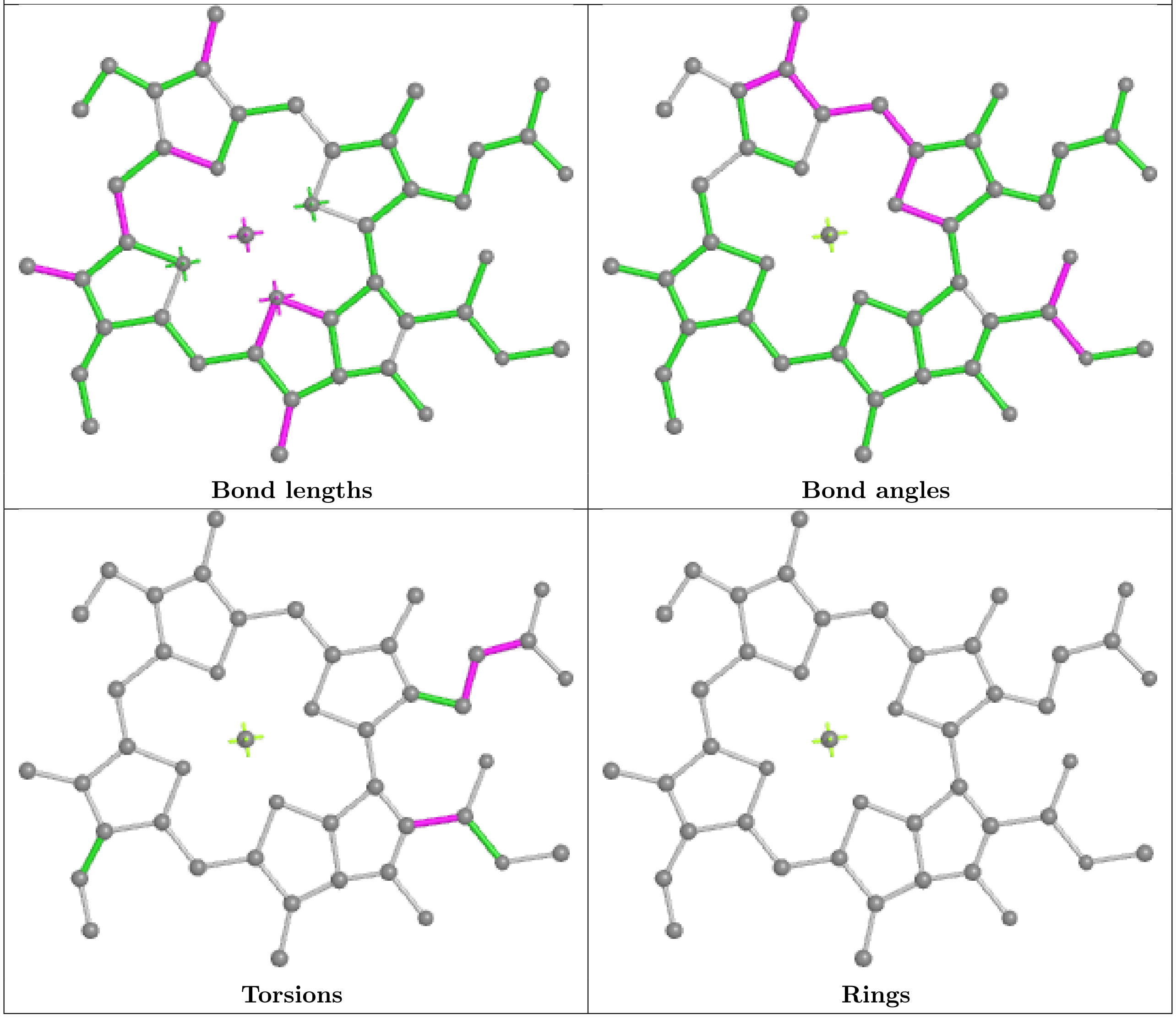


Ligand CLA aF 203



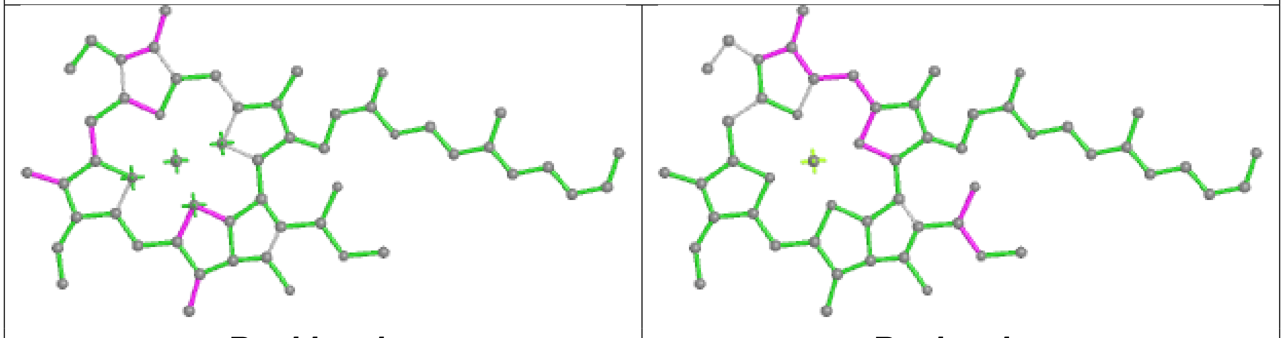
Bond lengths

Bond angles

Torsions

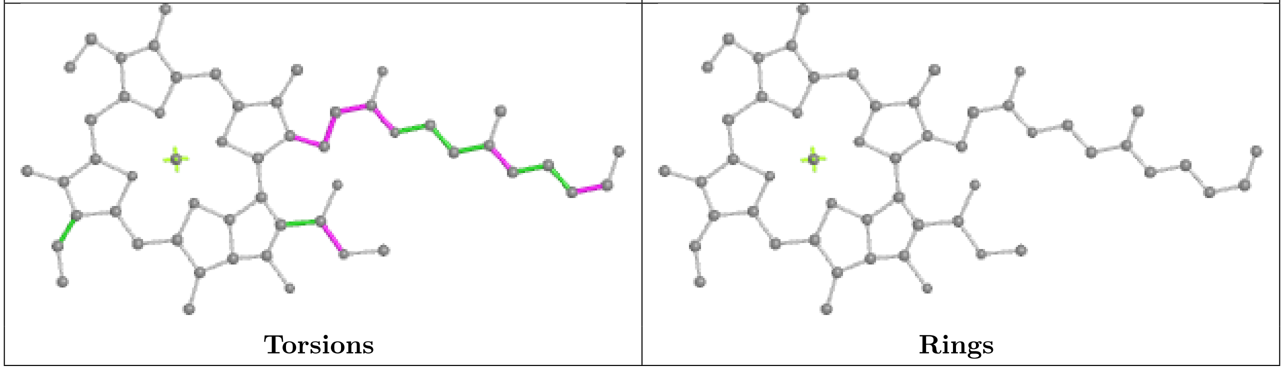
Rings

Ligand CLA aA 812



Bond lengths

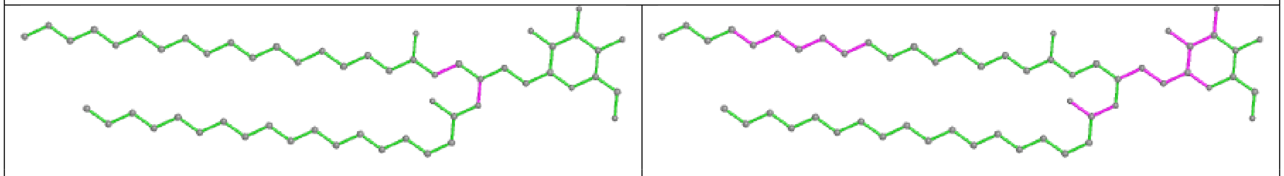
Bond angles



Torsions

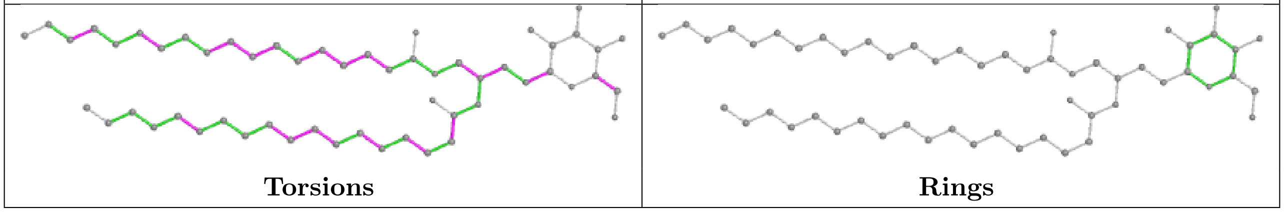
Rings

Ligand LMG cB 849



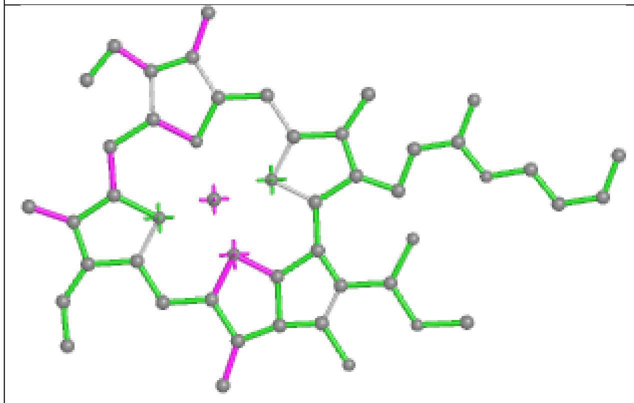
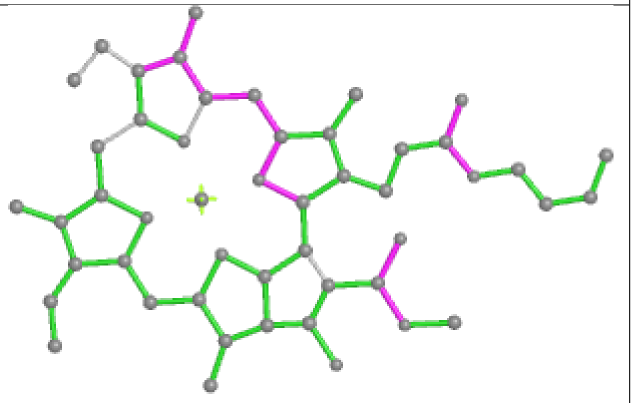
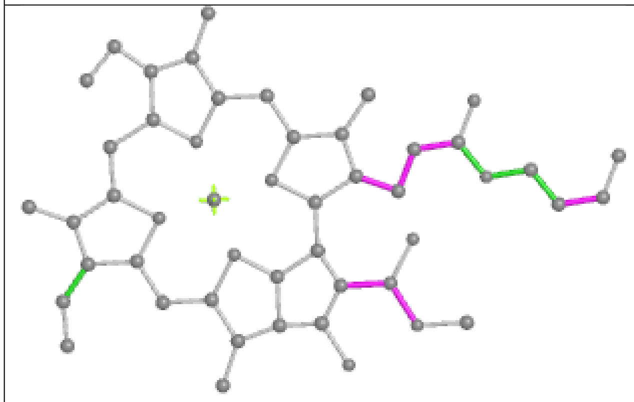
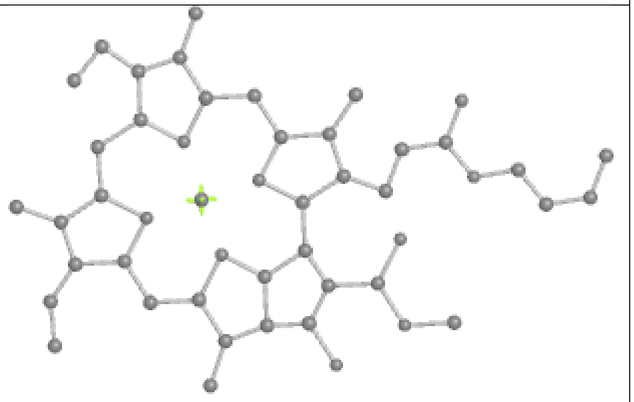
Bond lengths

Bond angles

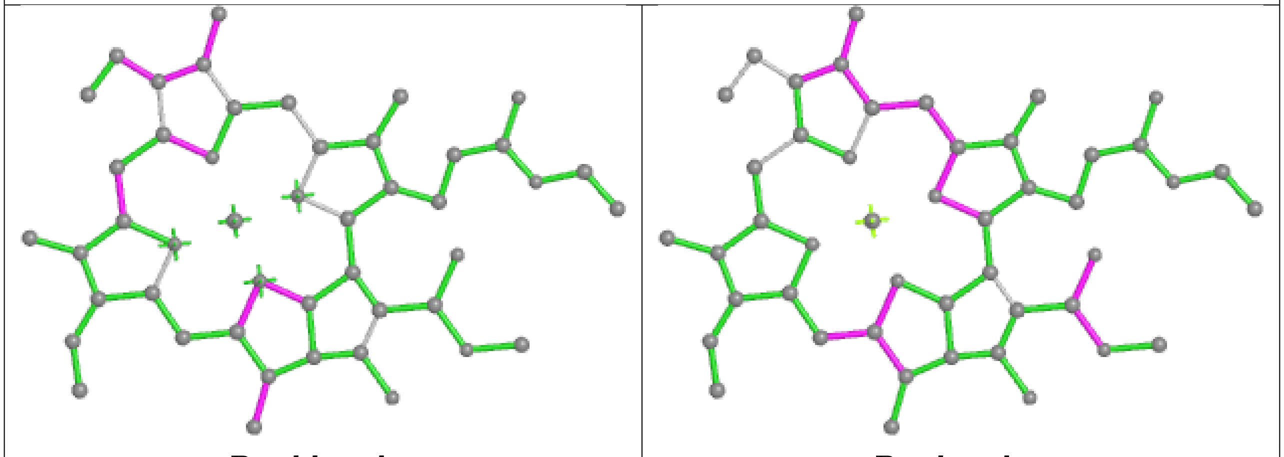


Torsions

Rings

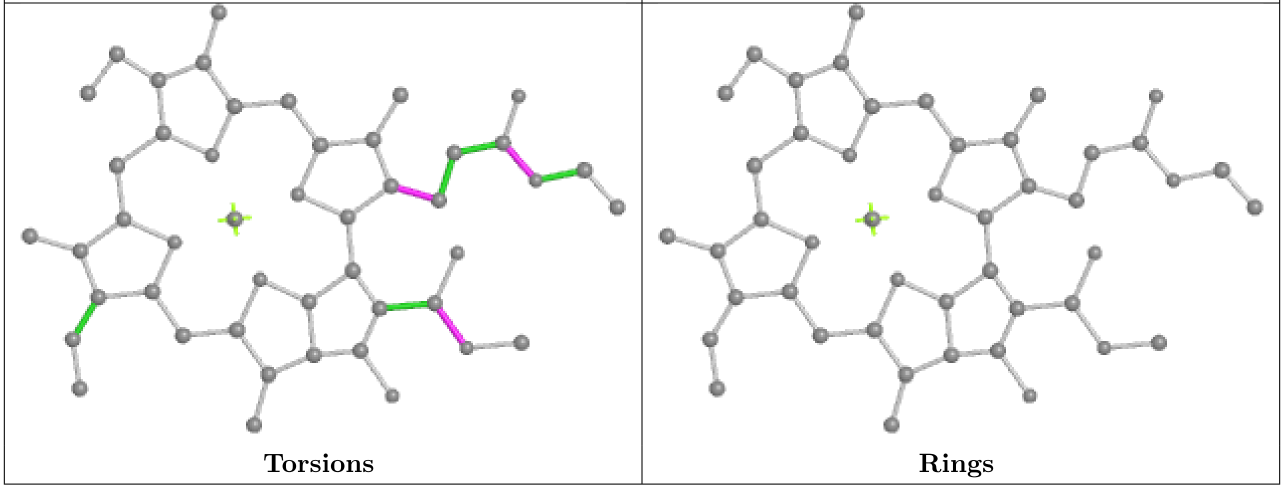
Ligand CLA cA 822	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

Ligand CLA aA 824



Bond lengths

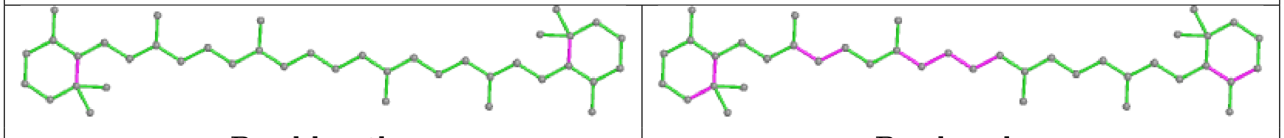
Bond angles



Torsions

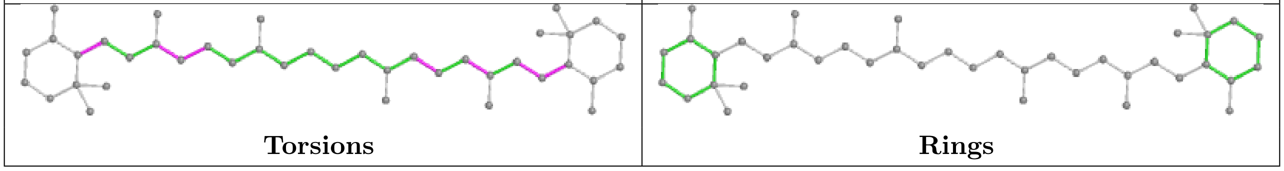
Rings

Ligand BCR aB 847



Bond lengths

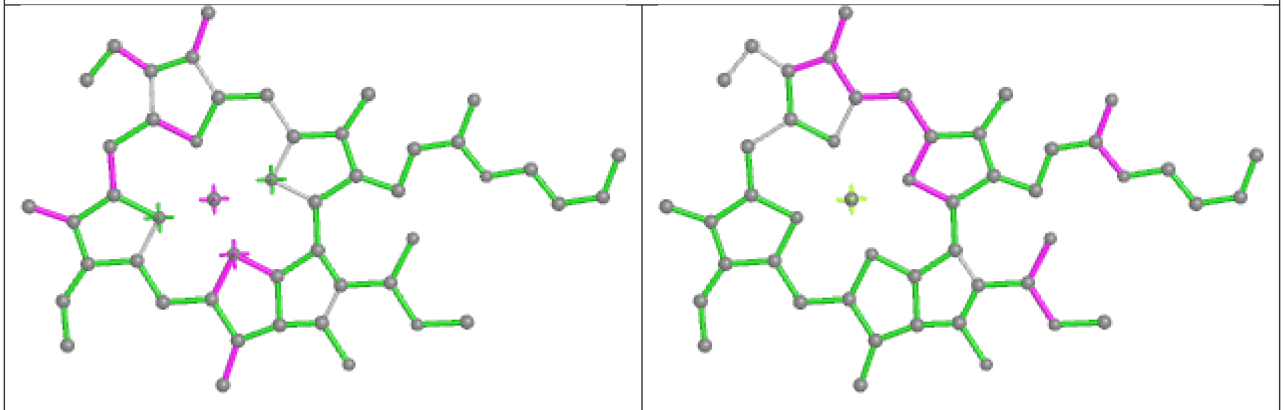
Bond angles



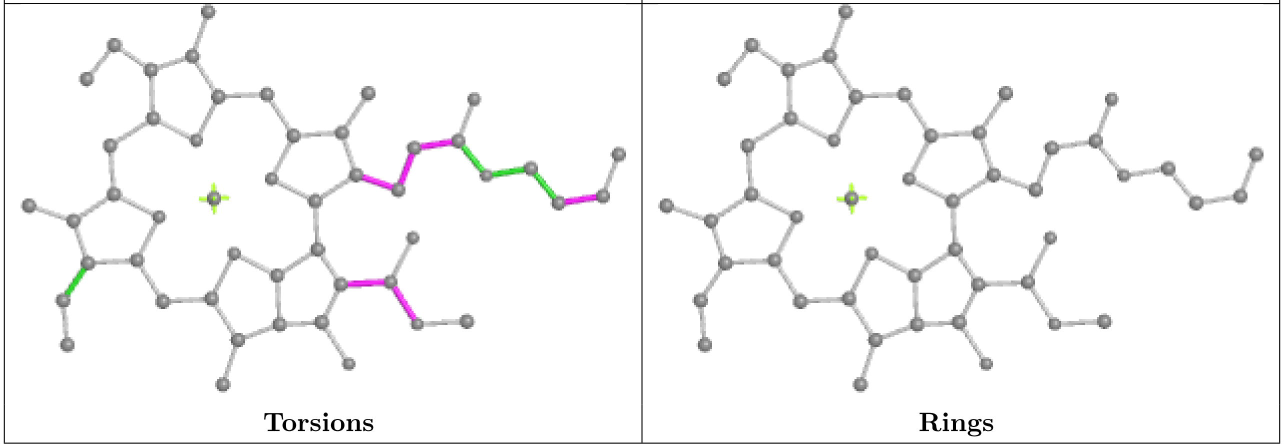
Torsions

Rings

Ligand CLA dA 822

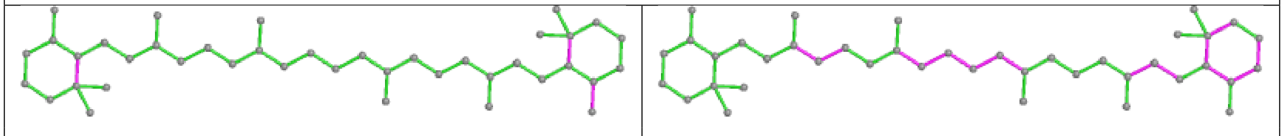


Bond lengths Bond angles

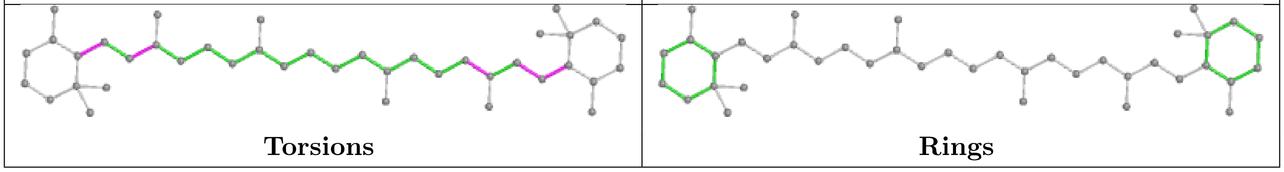


Torsions Rings

Ligand BCR cA 847

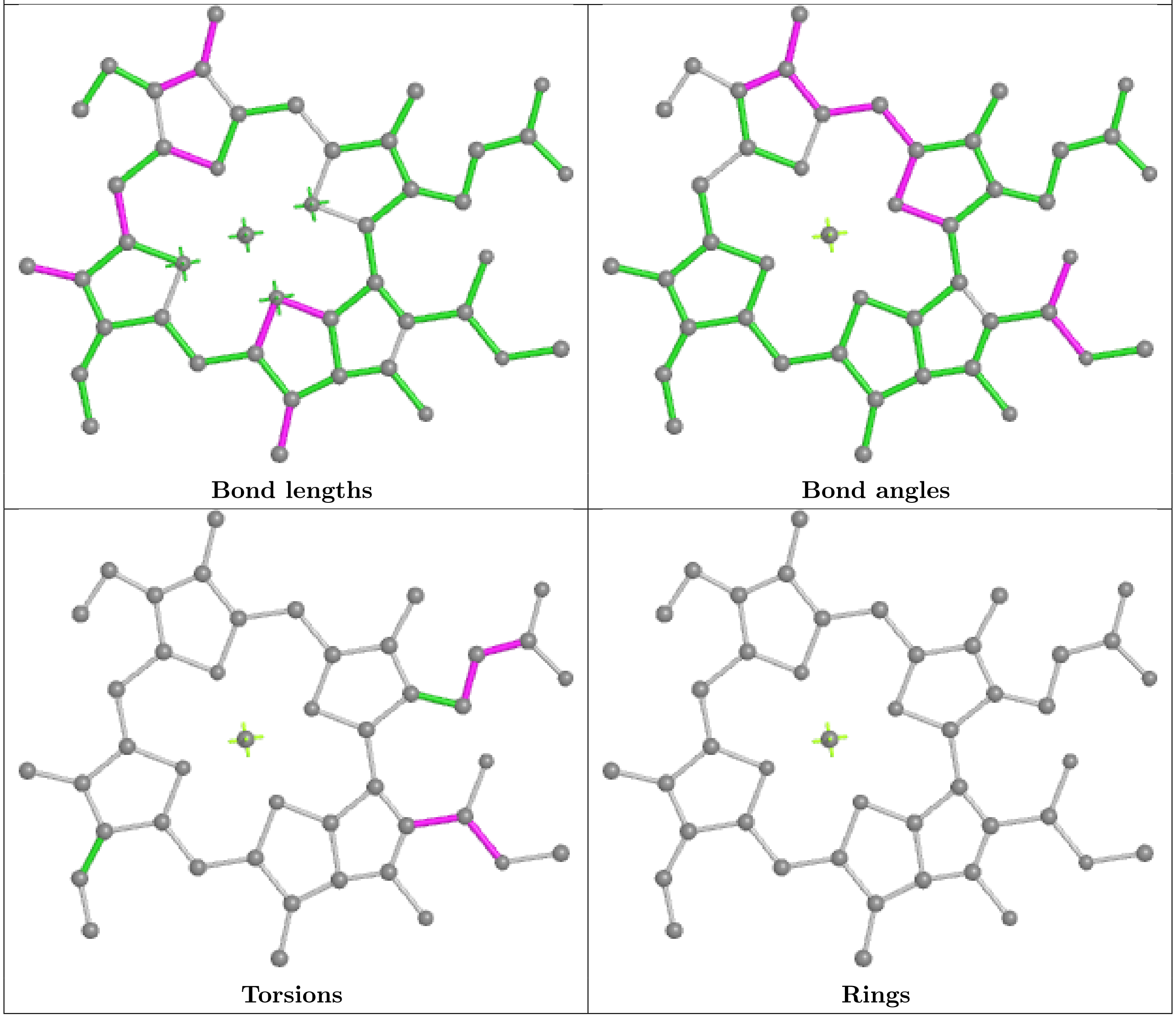


Bond lengths Bond angles



Torsions Rings

Ligand CLA aX 101



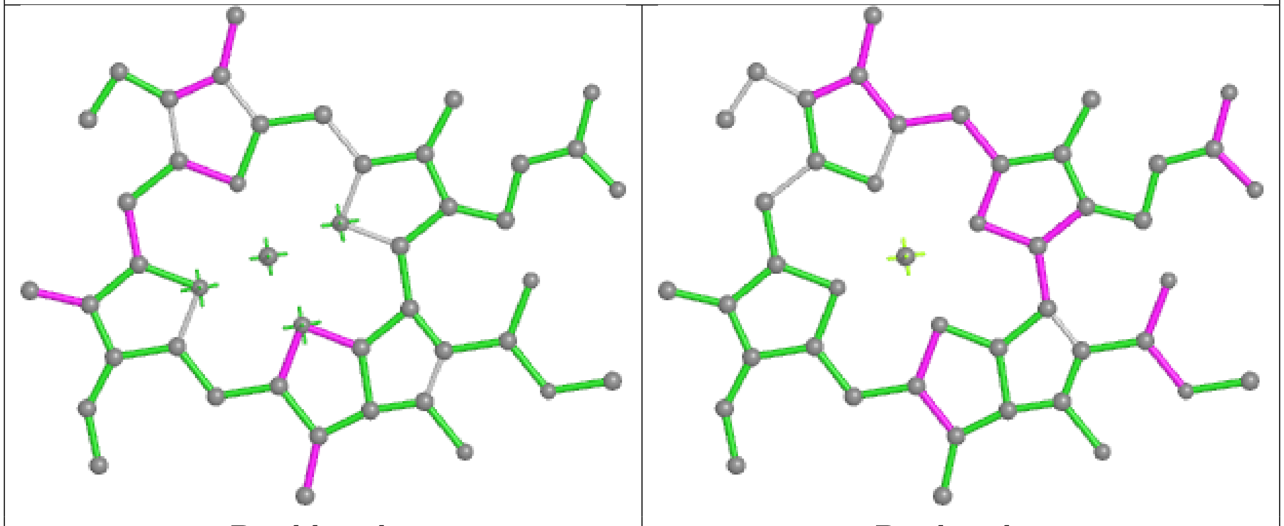
Bond lengths

Bond angles

Torsions

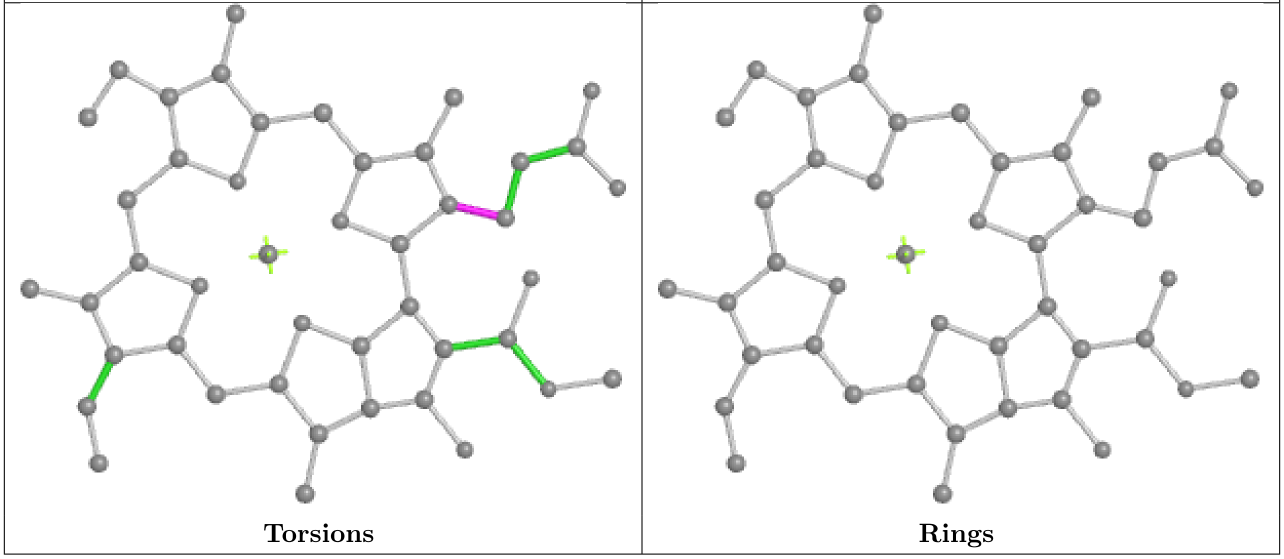
Rings

Ligand CLA aB 835



Bond lengths

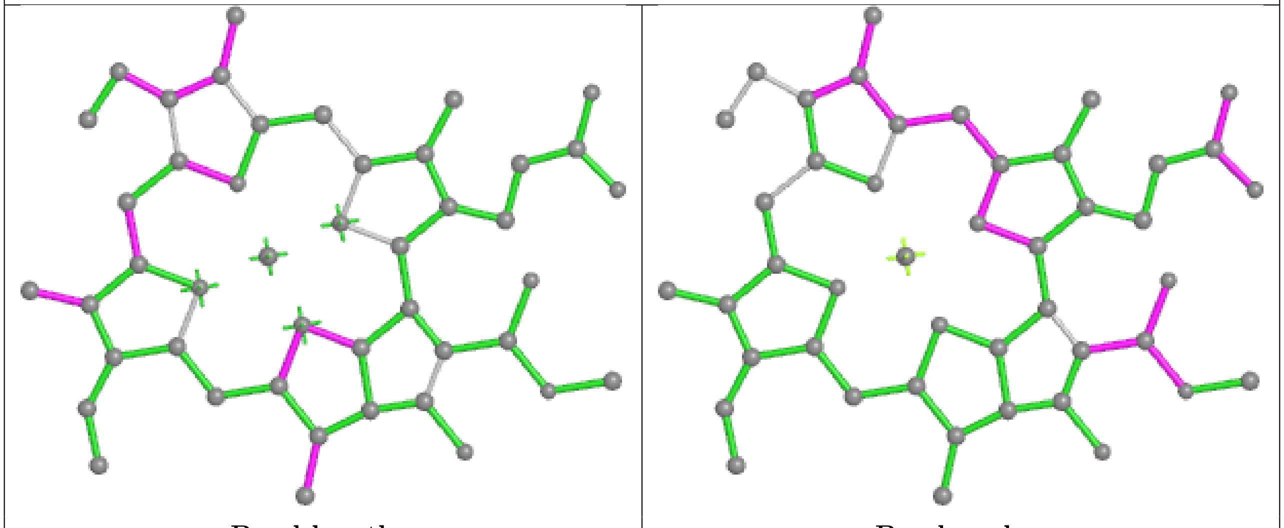
Bond angles



Torsions

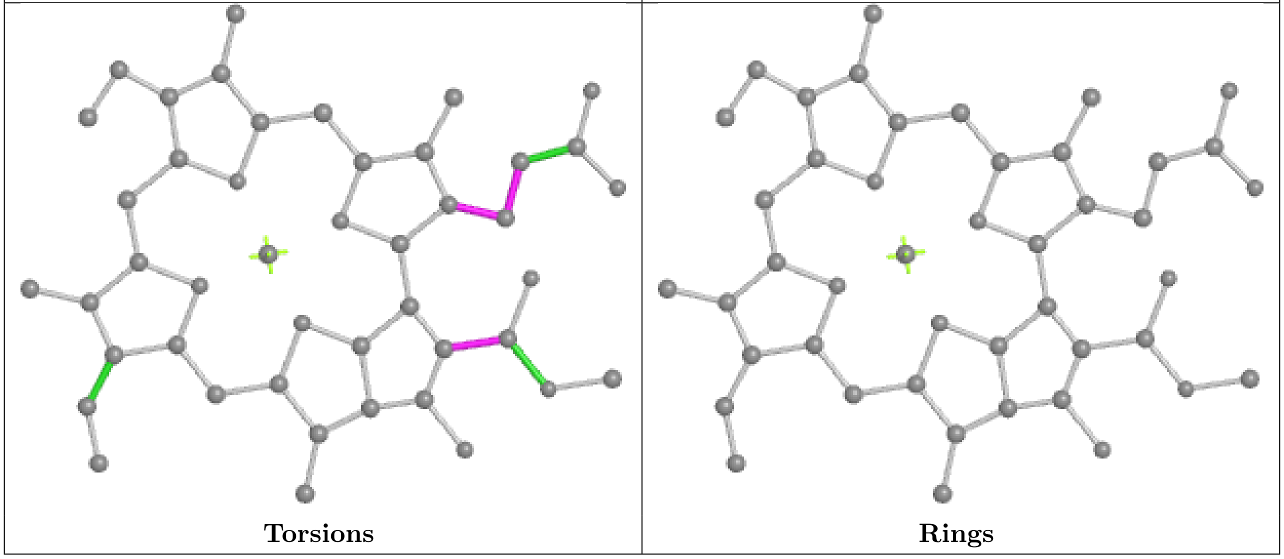
Rings

Ligand CLA aA 808



Bond lengths

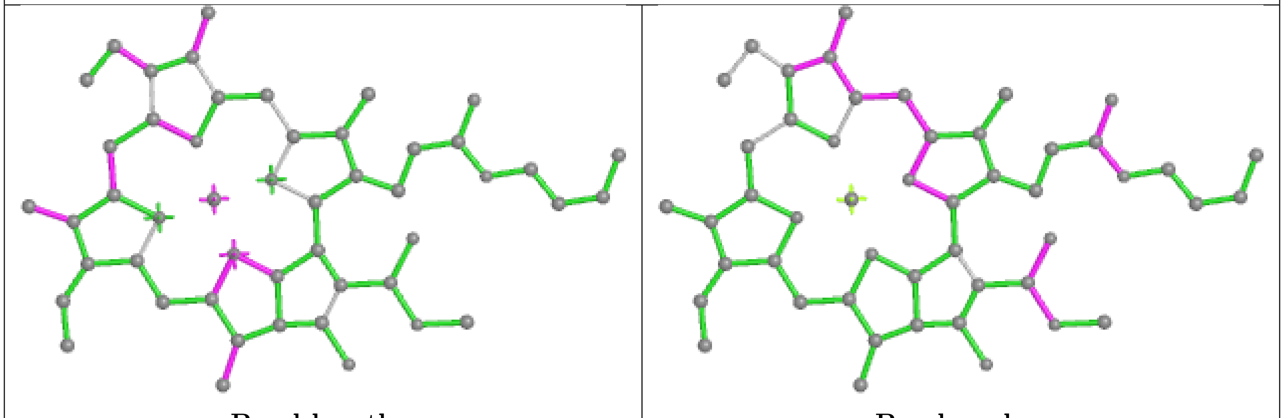
Bond angles



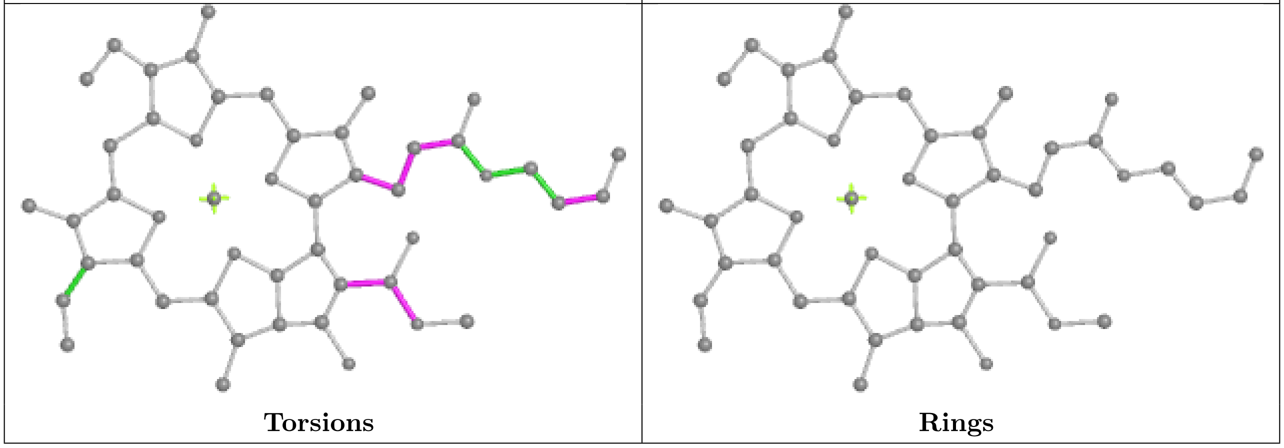
Torsions

Rings

Ligand CLA bA 822

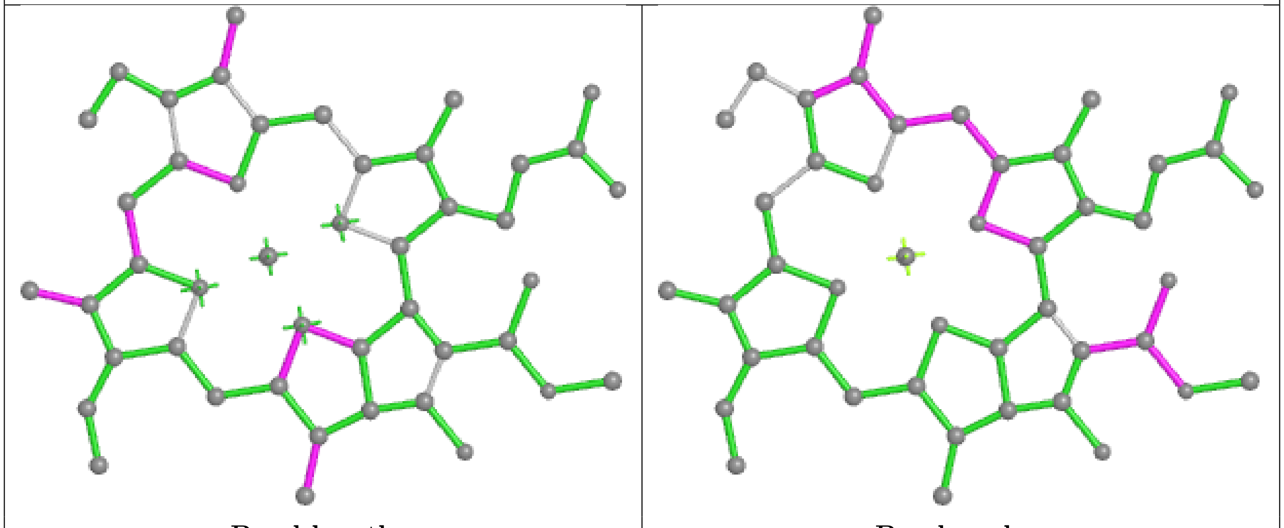


Bond lengths **Bond angles**

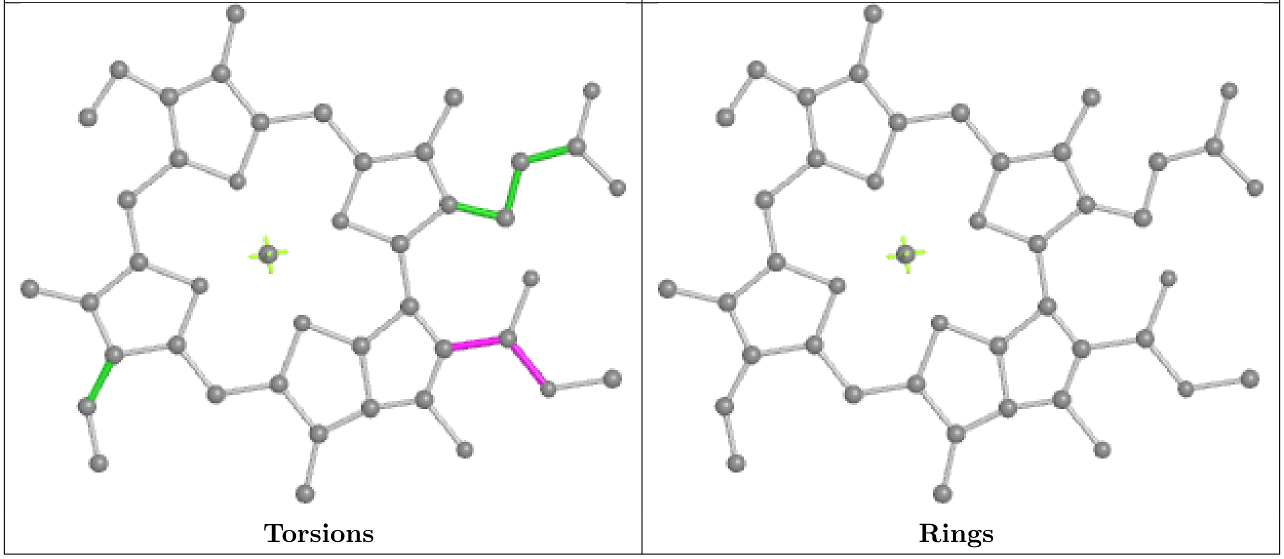


Torsions **Rings**

Ligand CLA bB 835

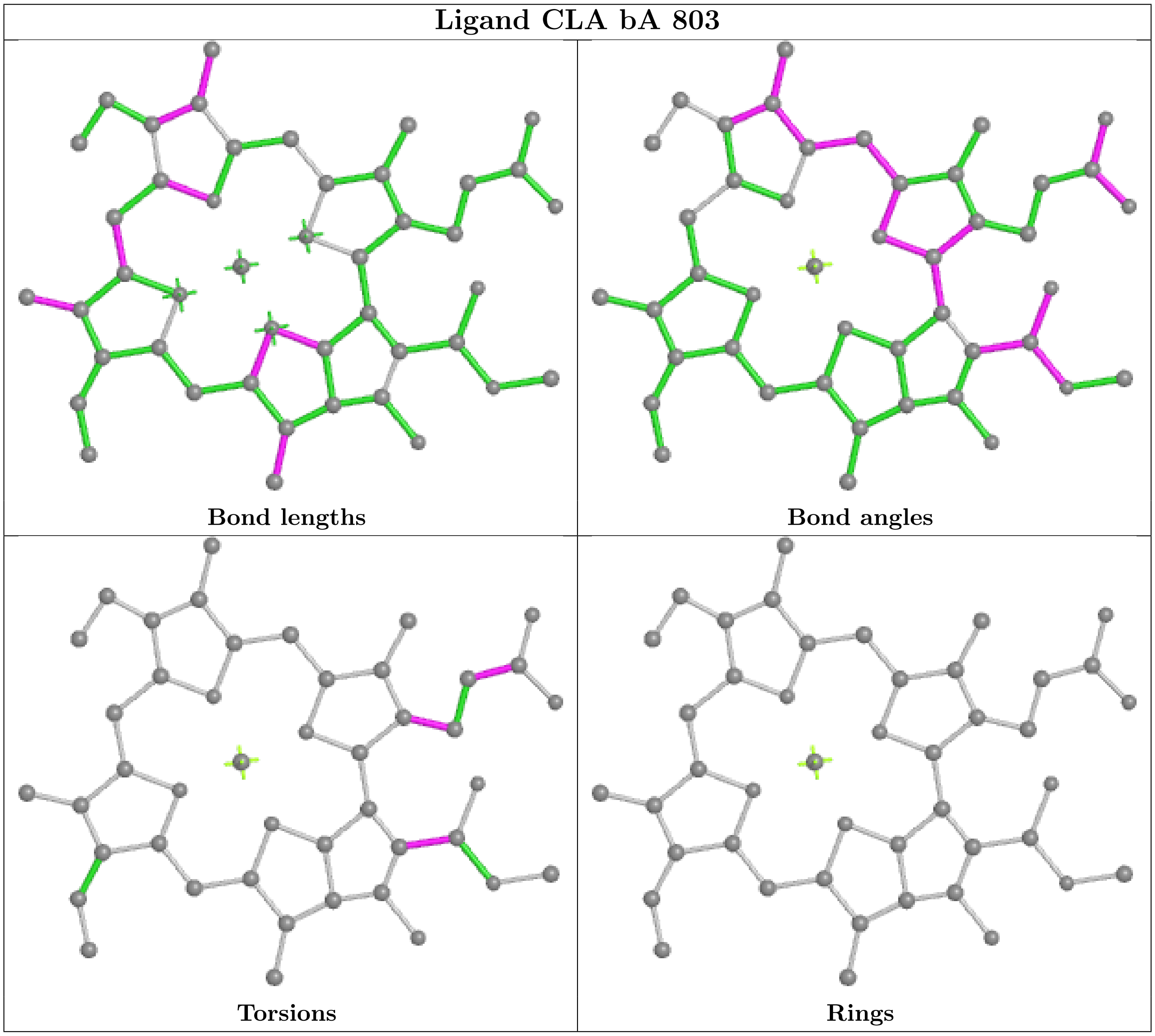


Bond lengths **Bond angles**



Torsions **Rings**

Ligand CLA bA 803



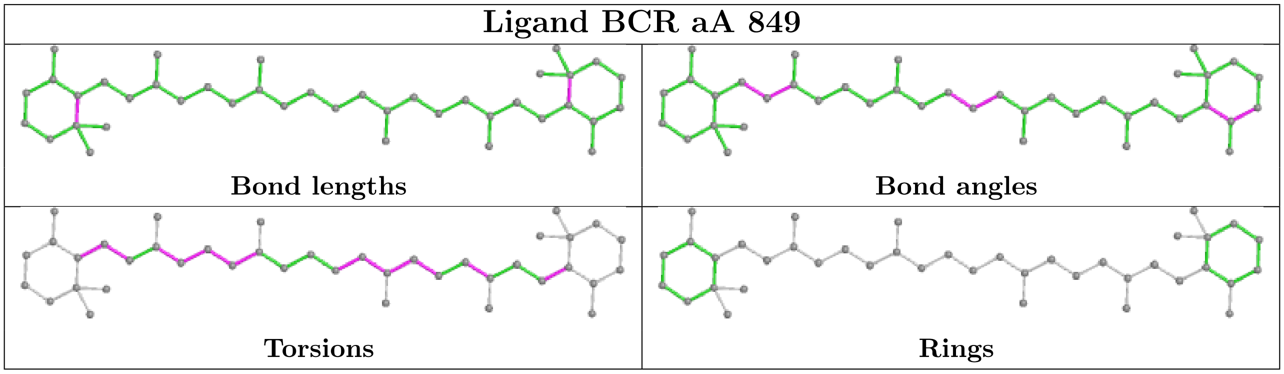
Bond lengths

Bond angles

Torsions

Rings

Ligand BCR aA 849



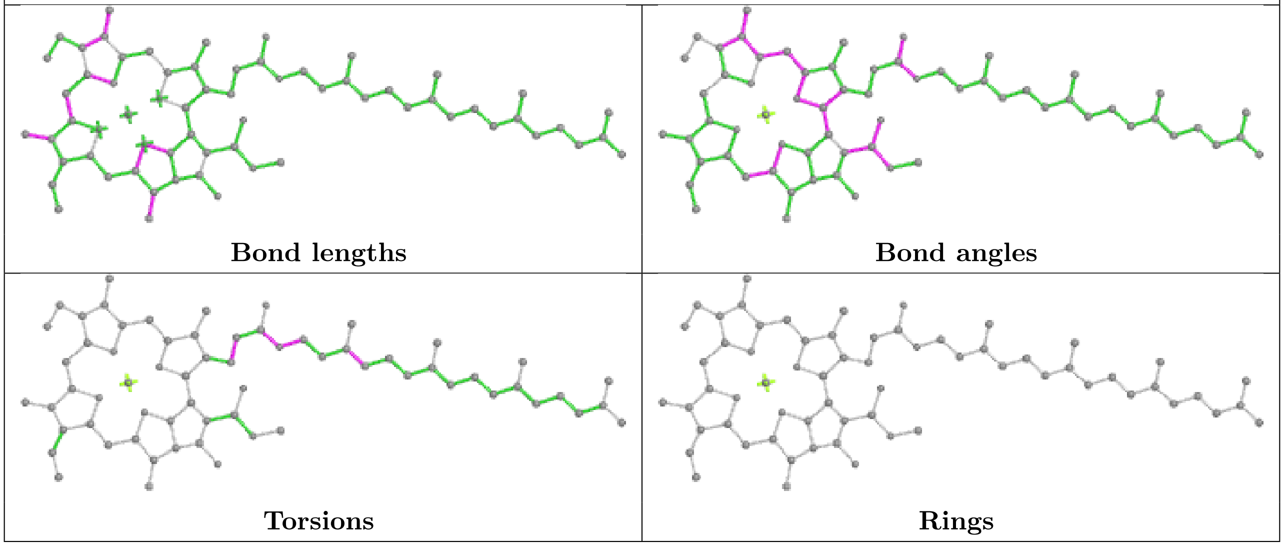
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA dA 828



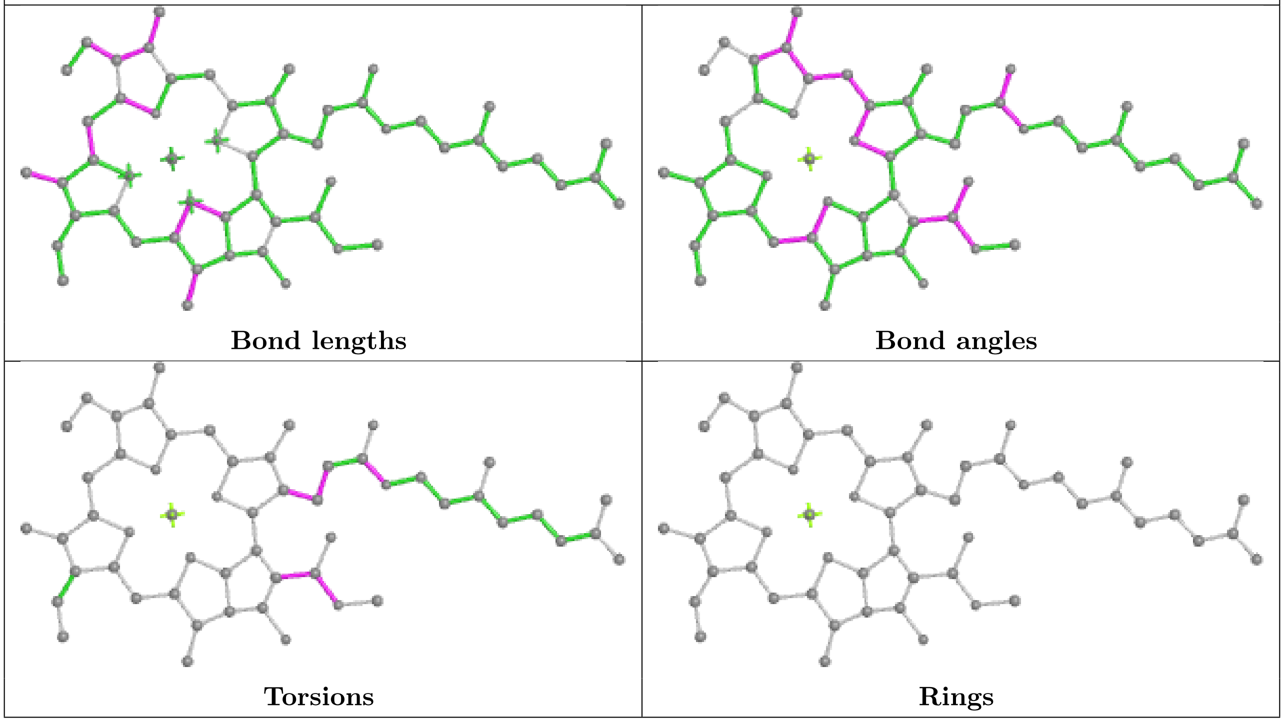
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA dB 817



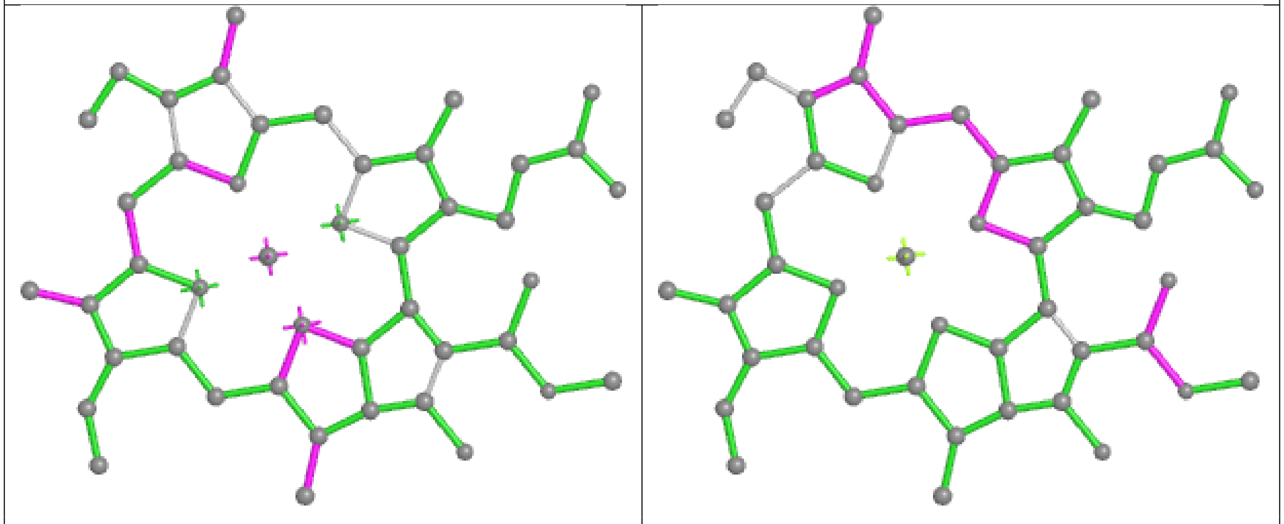
Bond lengths

Bond angles

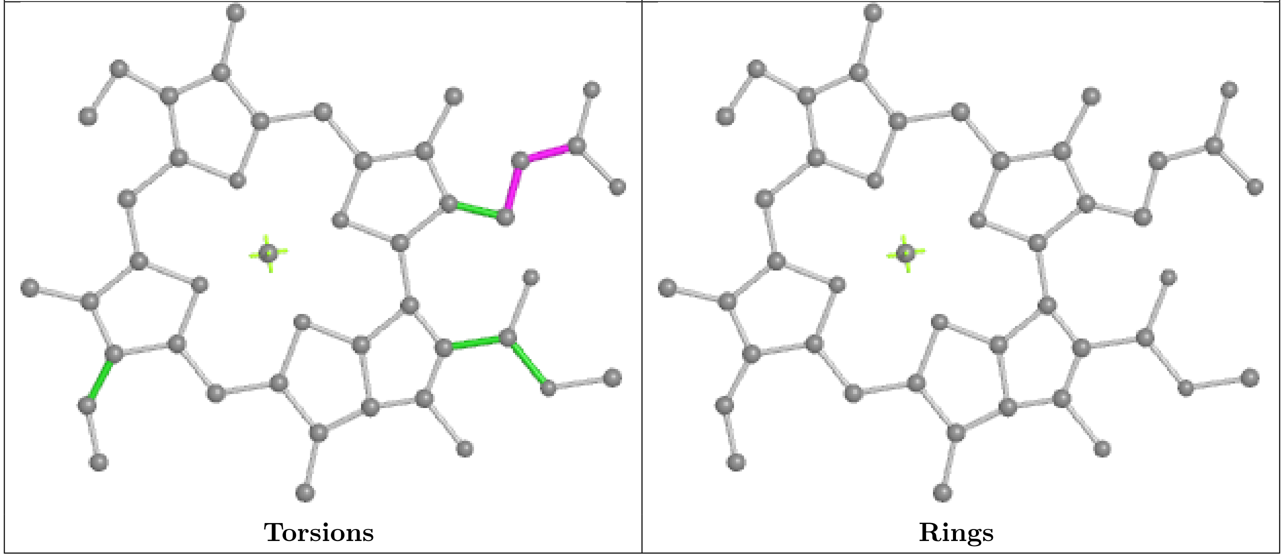
Torsions

Rings

Ligand CLA dA 802

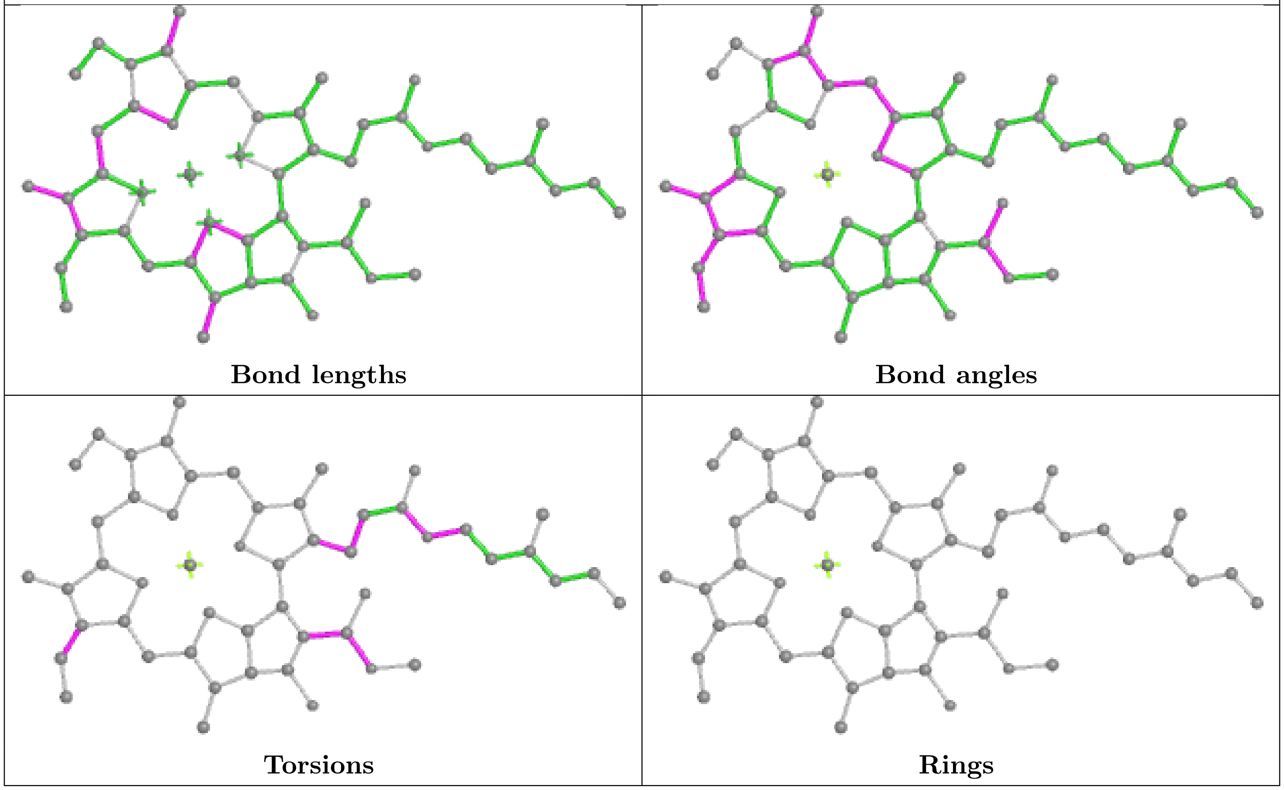


Bond lengths Bond angles

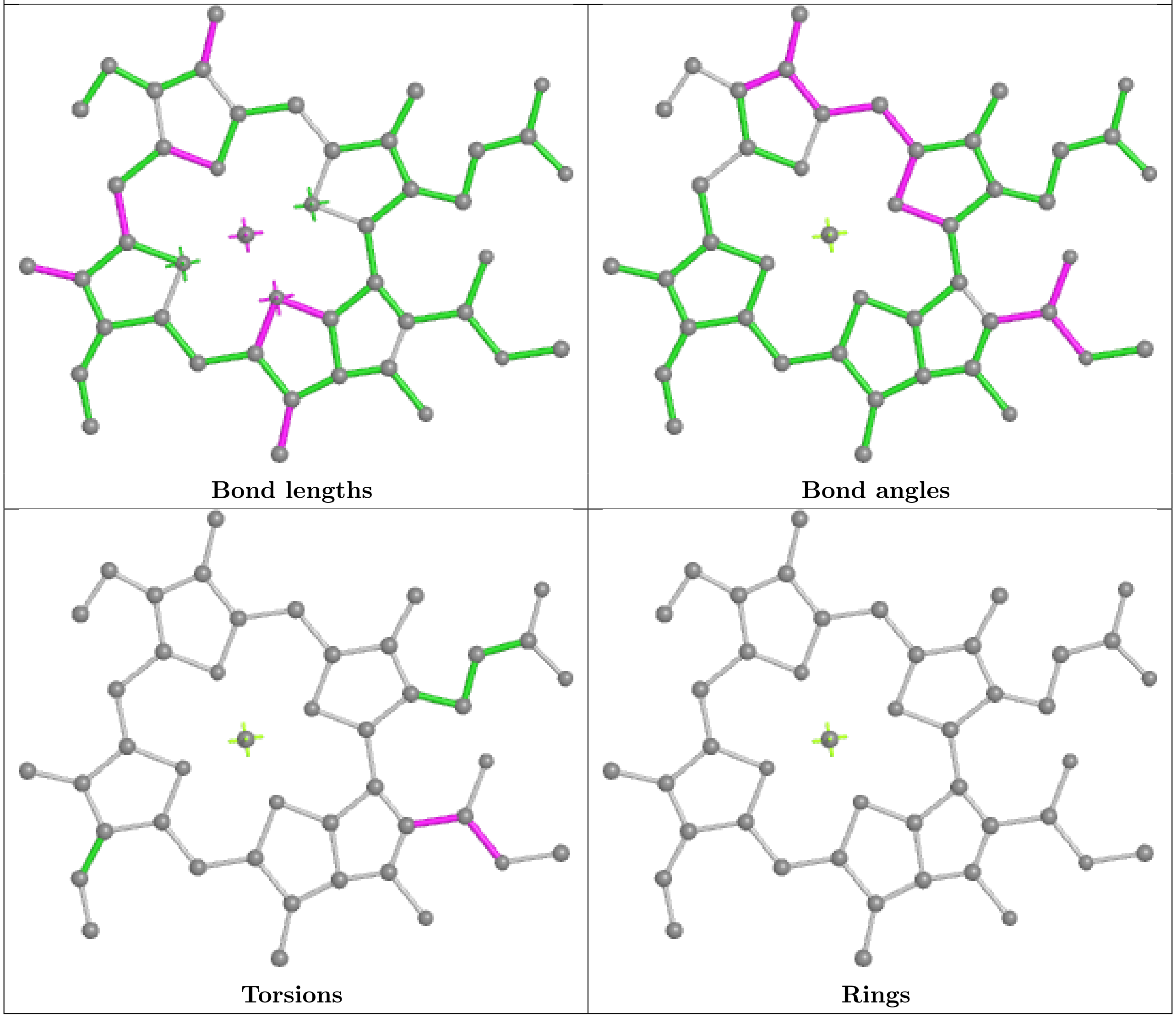


Torsions Rings

Ligand CLA dL 202



Ligand CLA bF 203



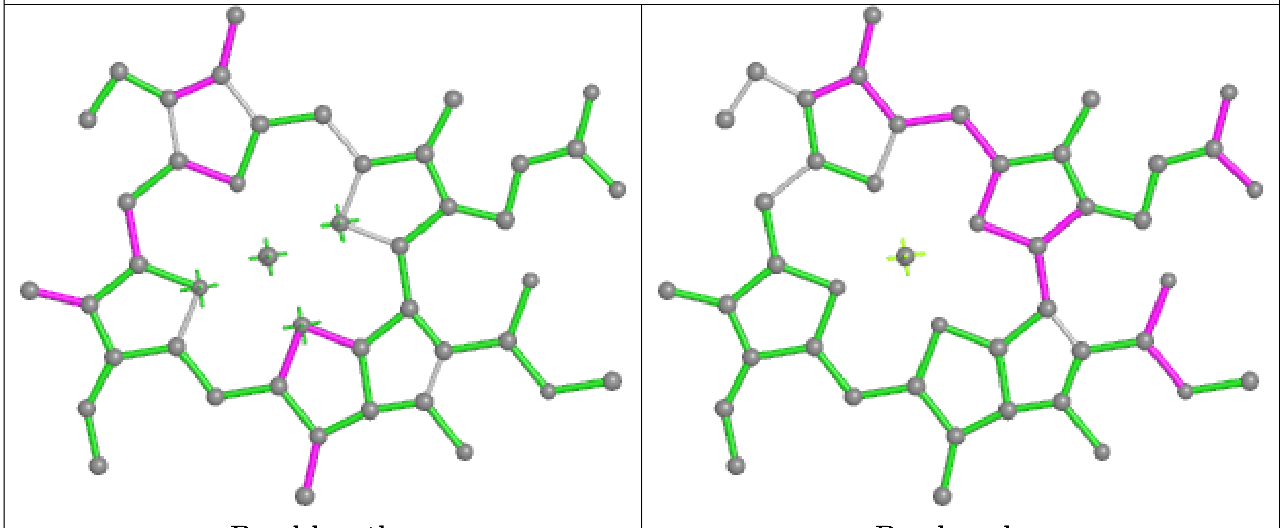
Bond lengths

Bond angles

Torsions

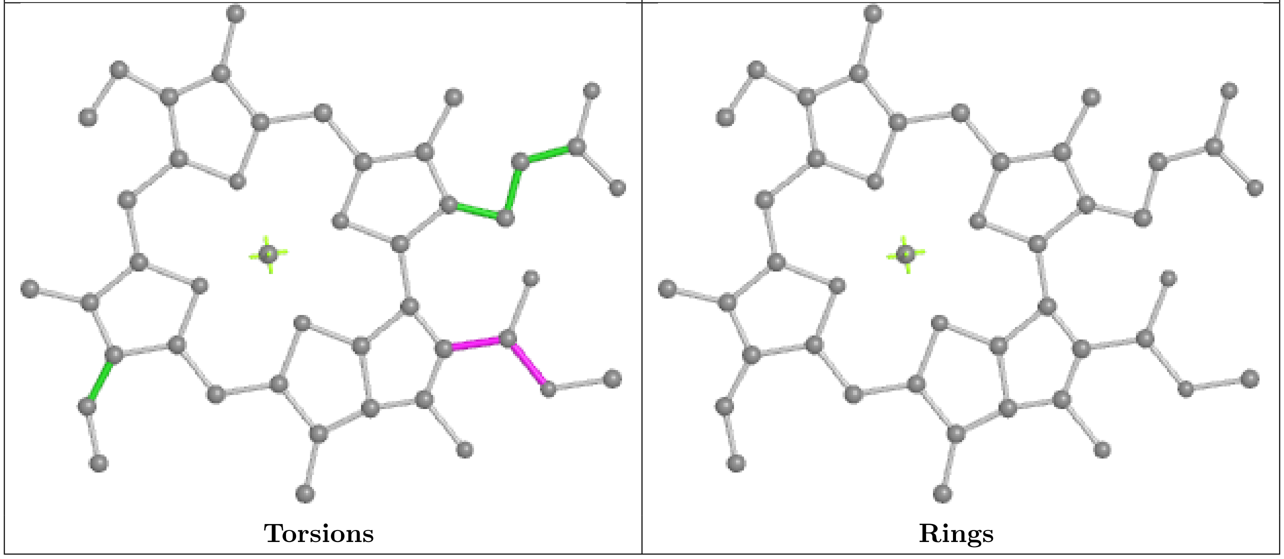
Rings

Ligand CLA cA 814



Bond lengths

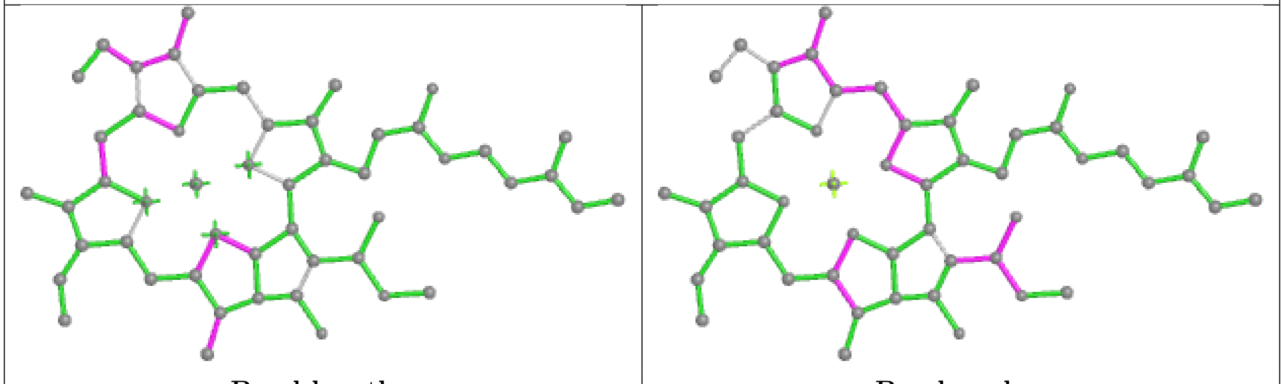
Bond angles



Torsions

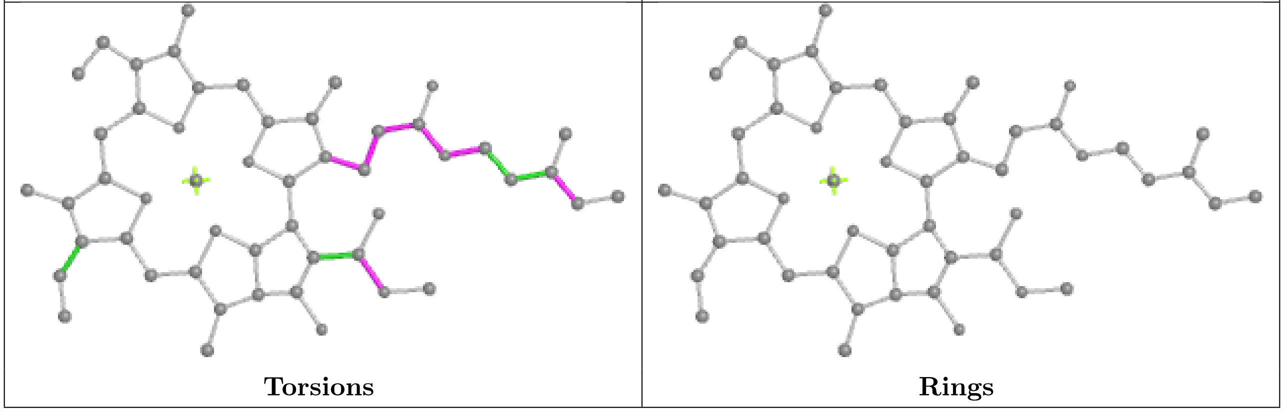
Rings

Ligand CLA bA 823



Bond lengths

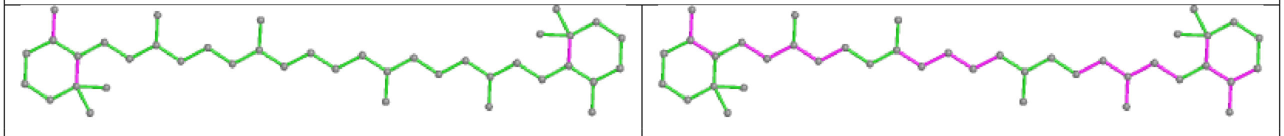
Bond angles



Torsions

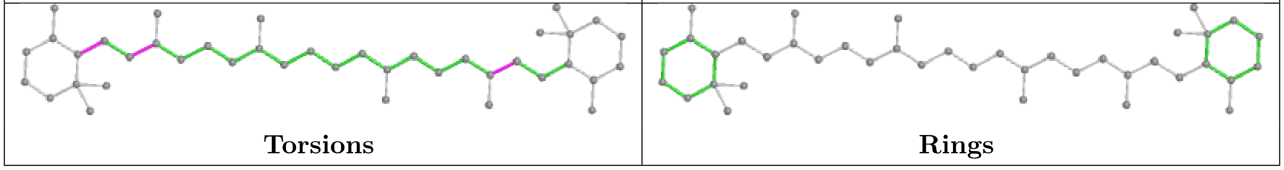
Rings

Ligand BCR cA 846



Bond lengths

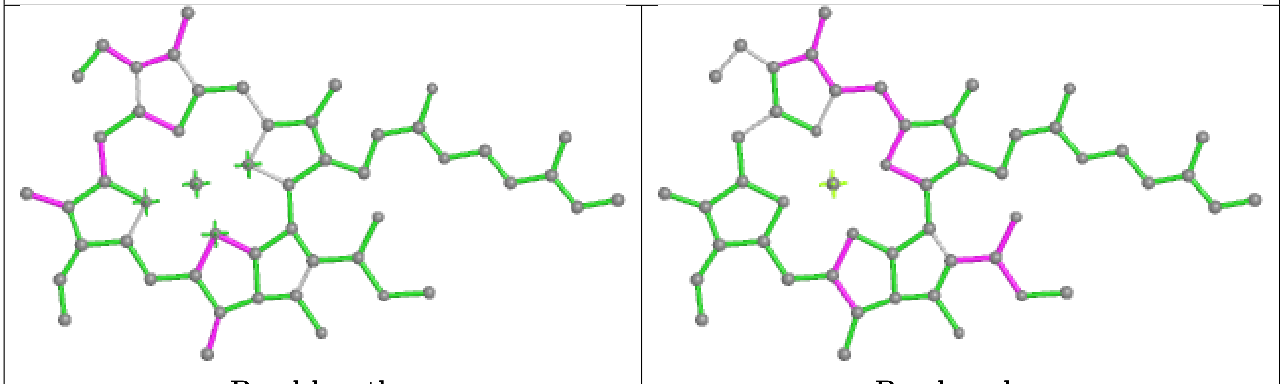
Bond angles



Torsions

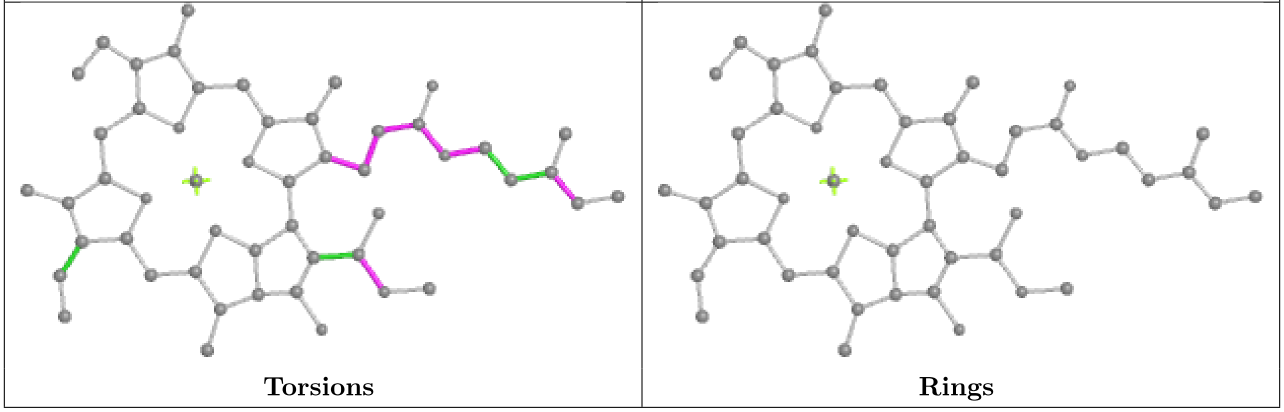
Rings

Ligand CLA dA 823



Bond lengths

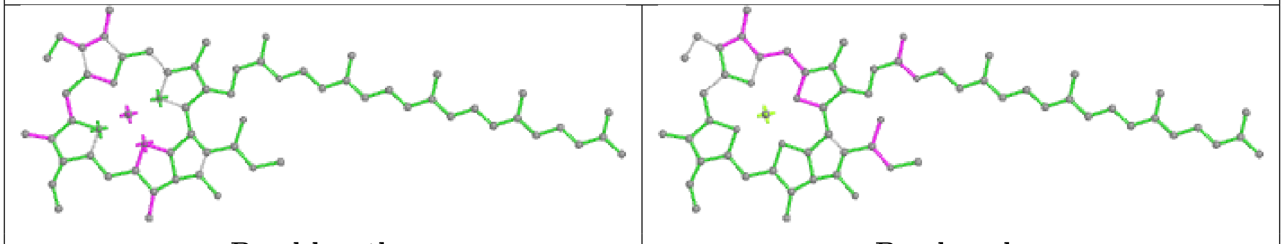
Bond angles



Torsions

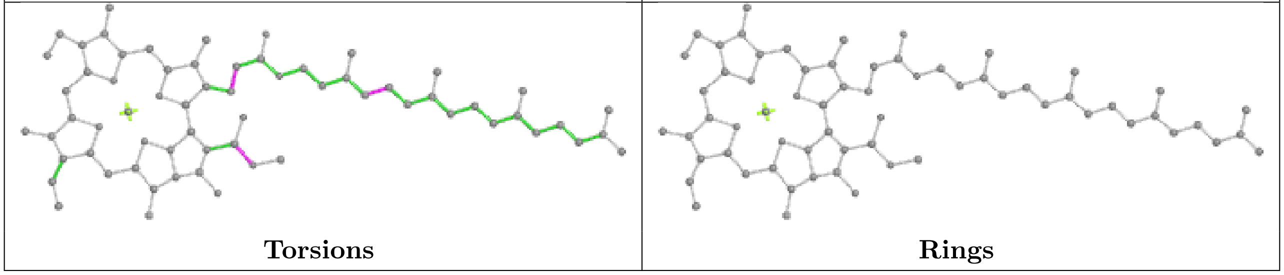
Rings

Ligand CLA cB 840



Bond lengths

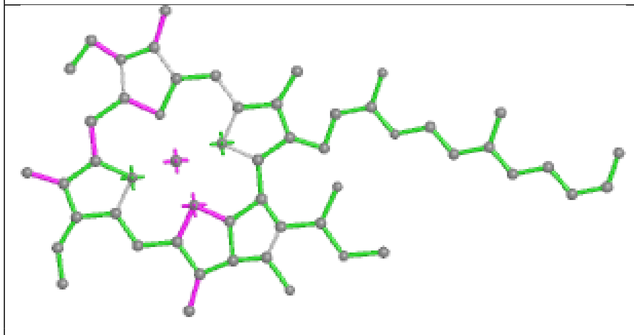
Bond angles



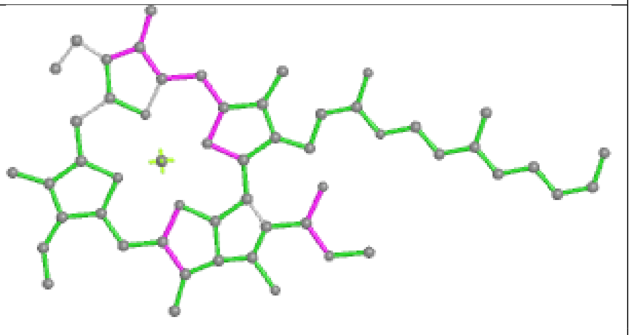
Torsions

Rings

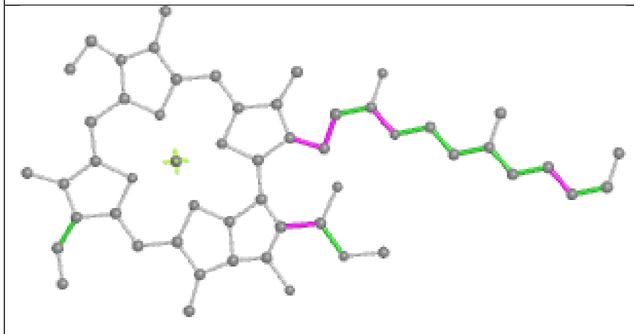
Ligand CLA aA 818



Bond lengths



Bond angles



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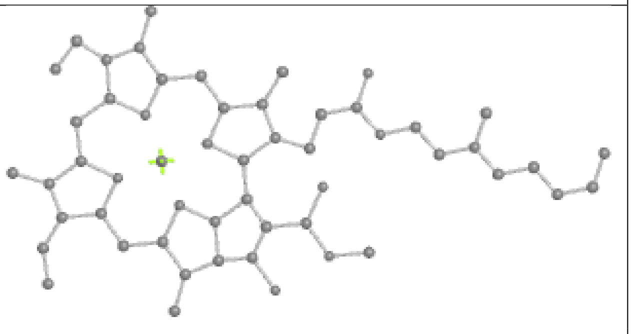
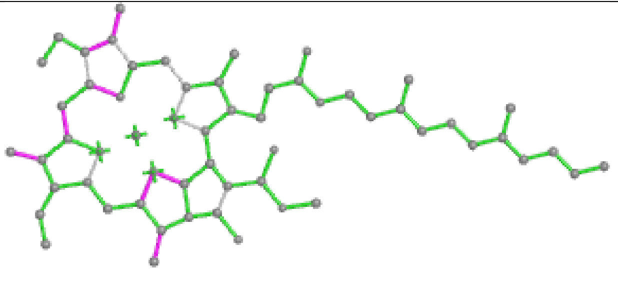


Rings

Ligand CLA cB 833



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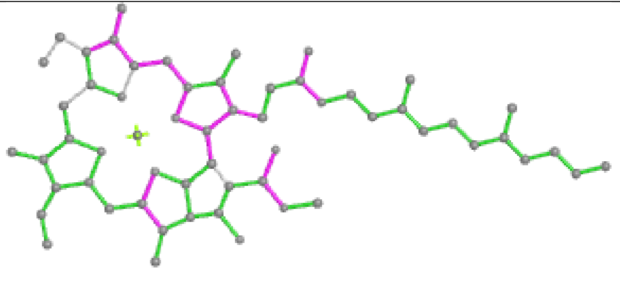
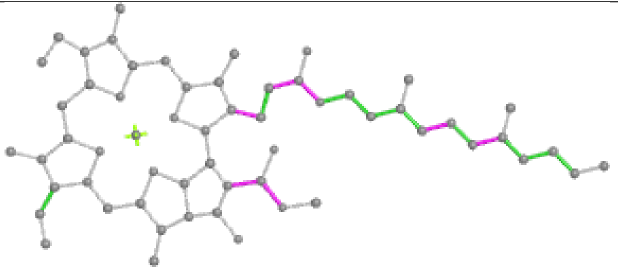
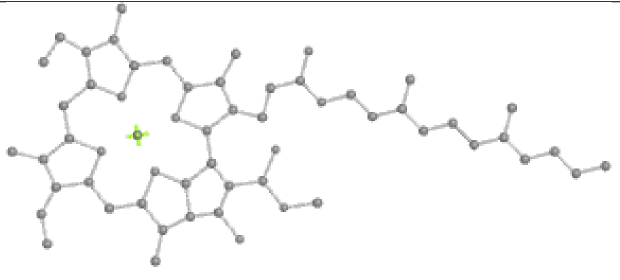


Bond angles

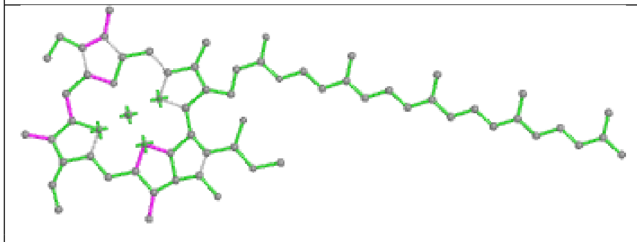


Torsions

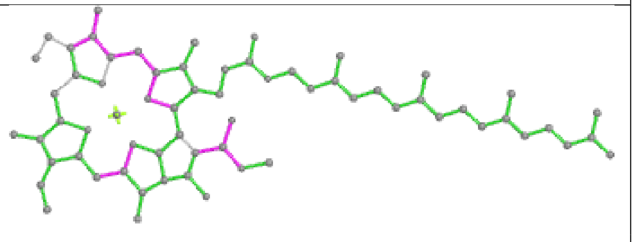


Rings

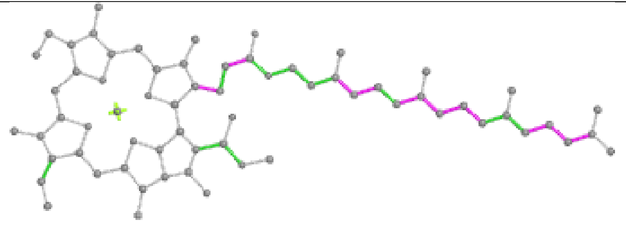
Ligand CLA aB 832



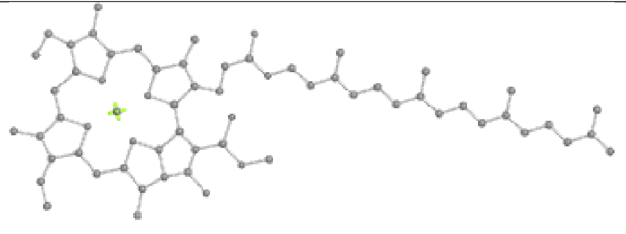
Bond lengths



Bond angles

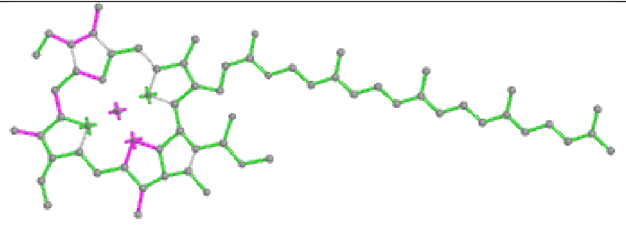


Torsions



Rings

Ligand CLA cA 829



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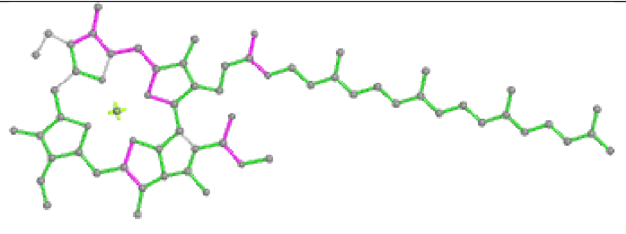
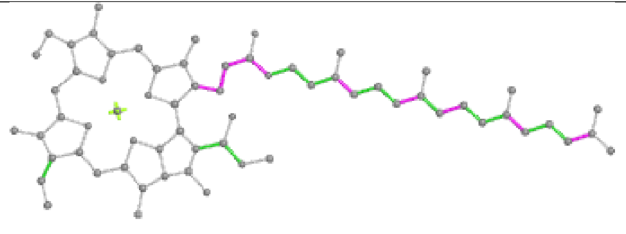


Bond angles



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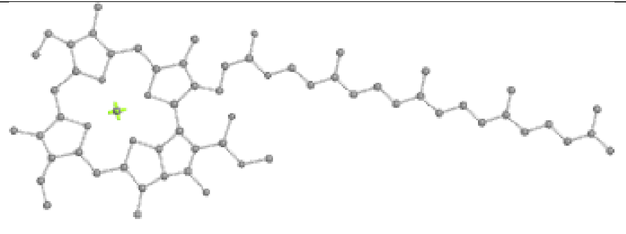
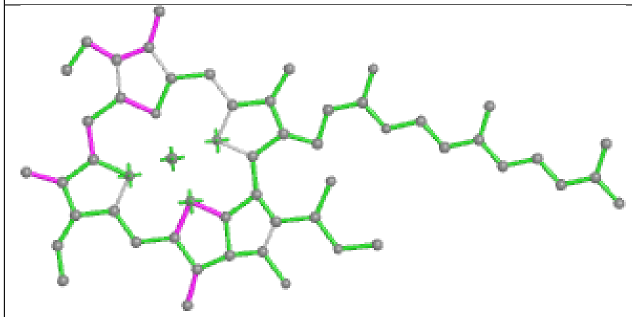


Rings

Ligand CLA bB 823



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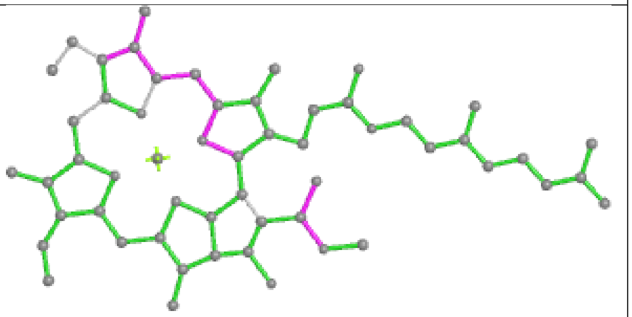
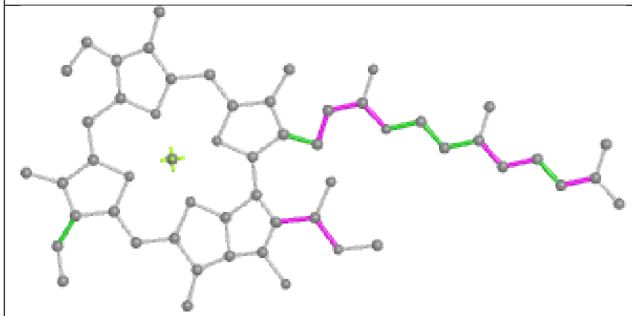


Bond angles



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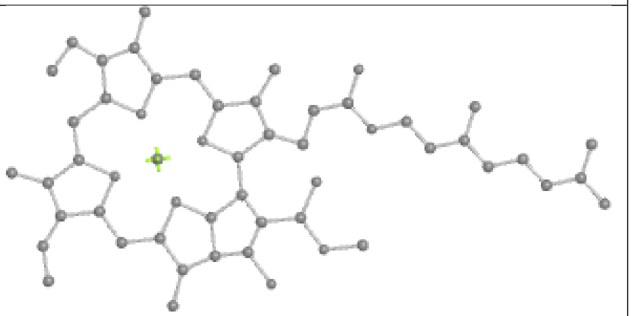
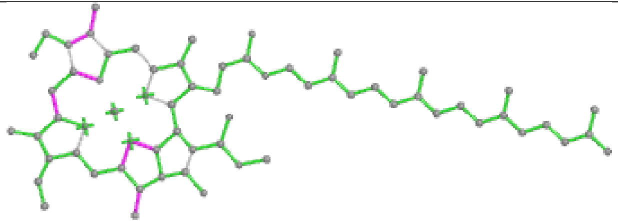
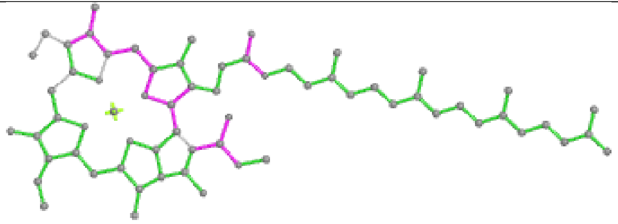


Rings

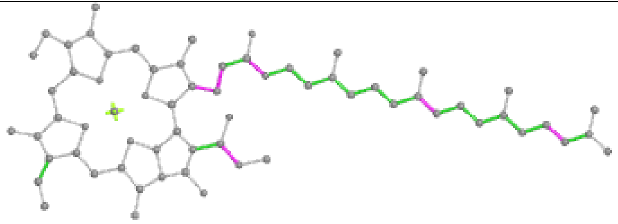
Ligand CLA aL 202



Bond lengths



Bond angles



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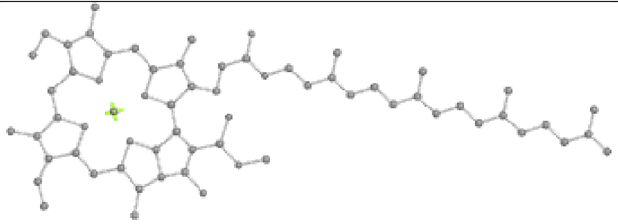
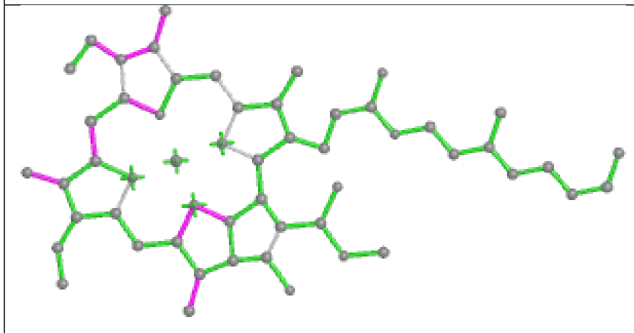


Rings

Ligand CLA dA 835



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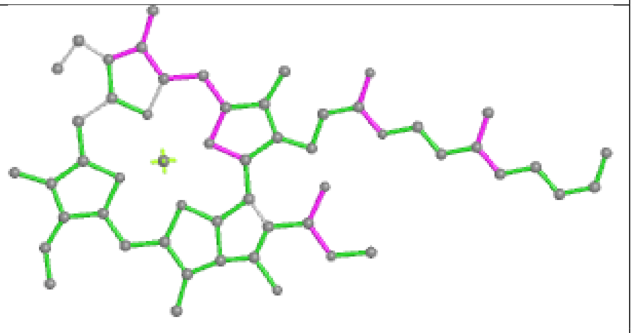
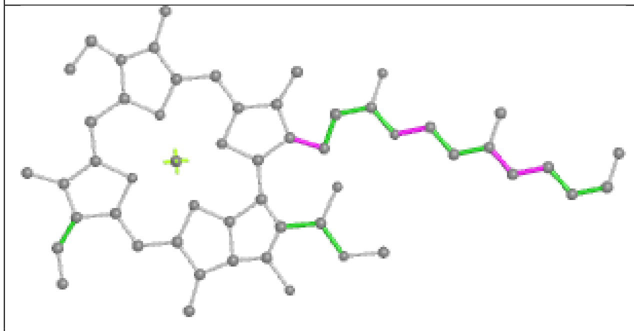


Bond angles



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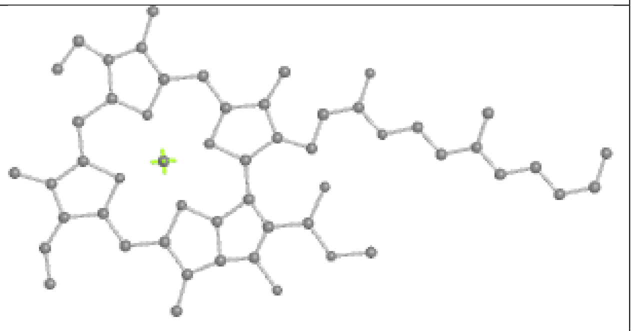
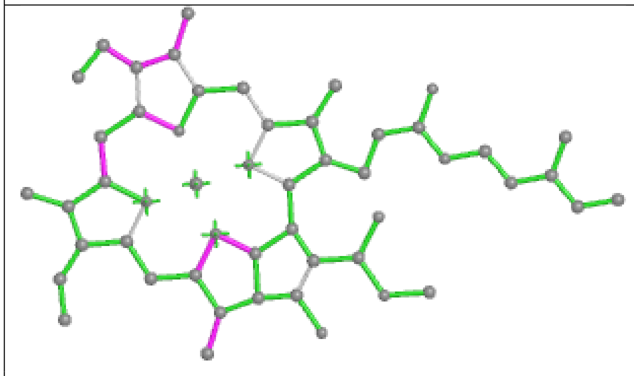


Rings

Ligand CLA aA 823



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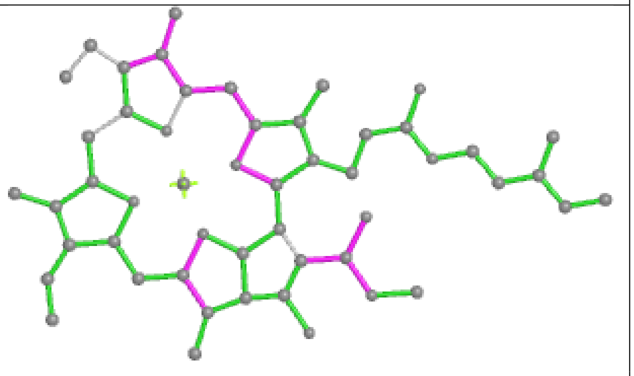
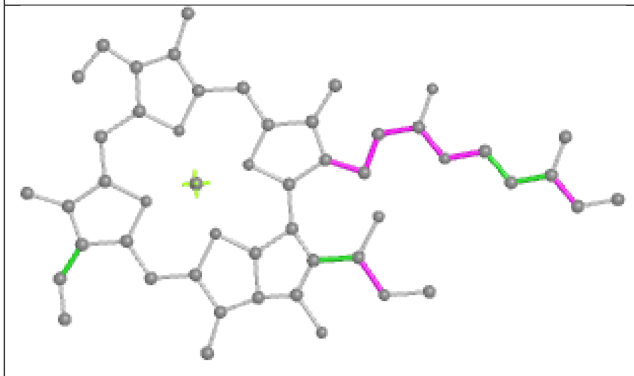
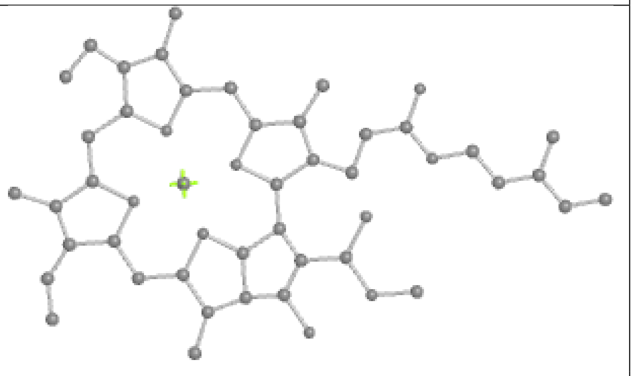


Bond angles

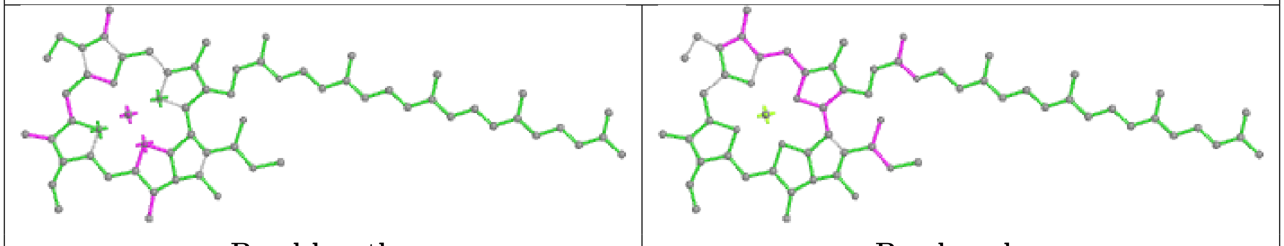


Torsions



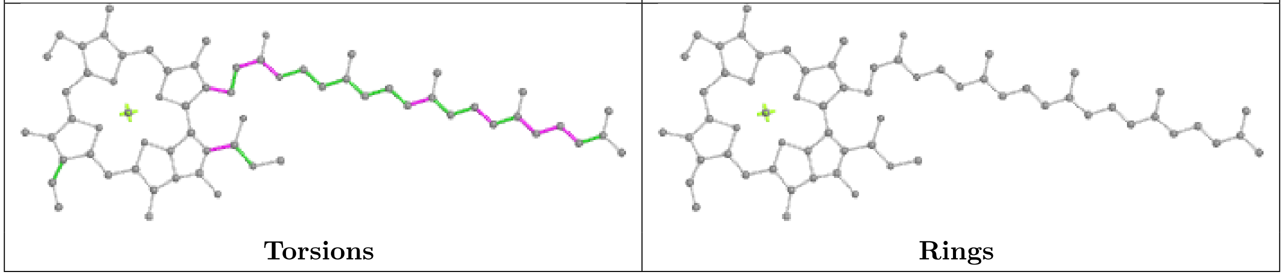
Rings

Ligand CLA aB 806



Bond lengths

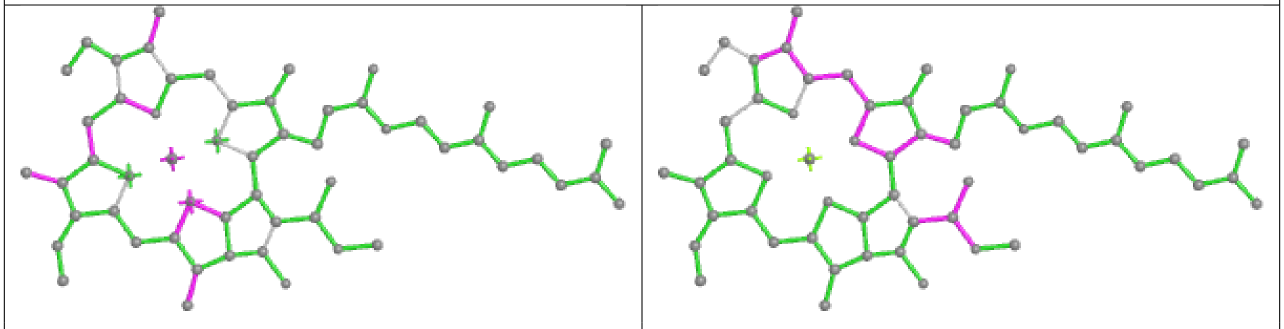
Bond angles



Torsions

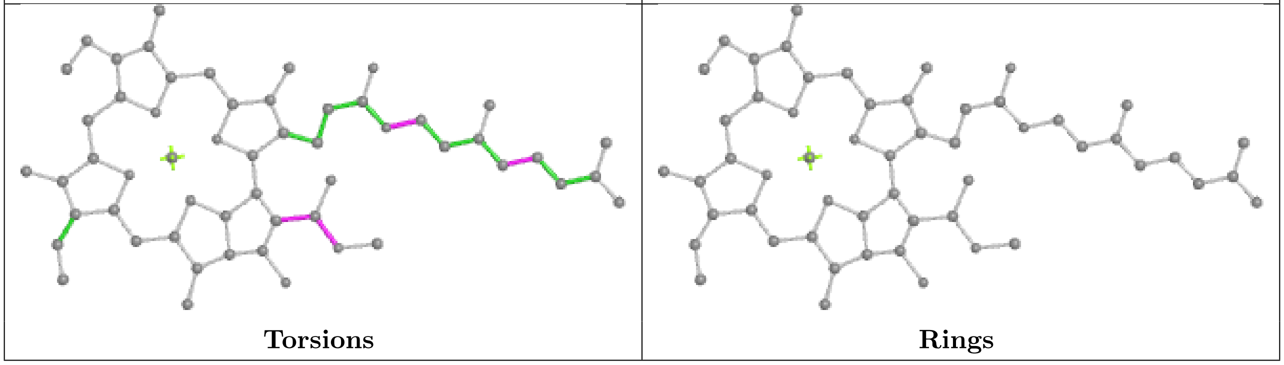
Rings

Ligand CLA aA 826



Bond lengths

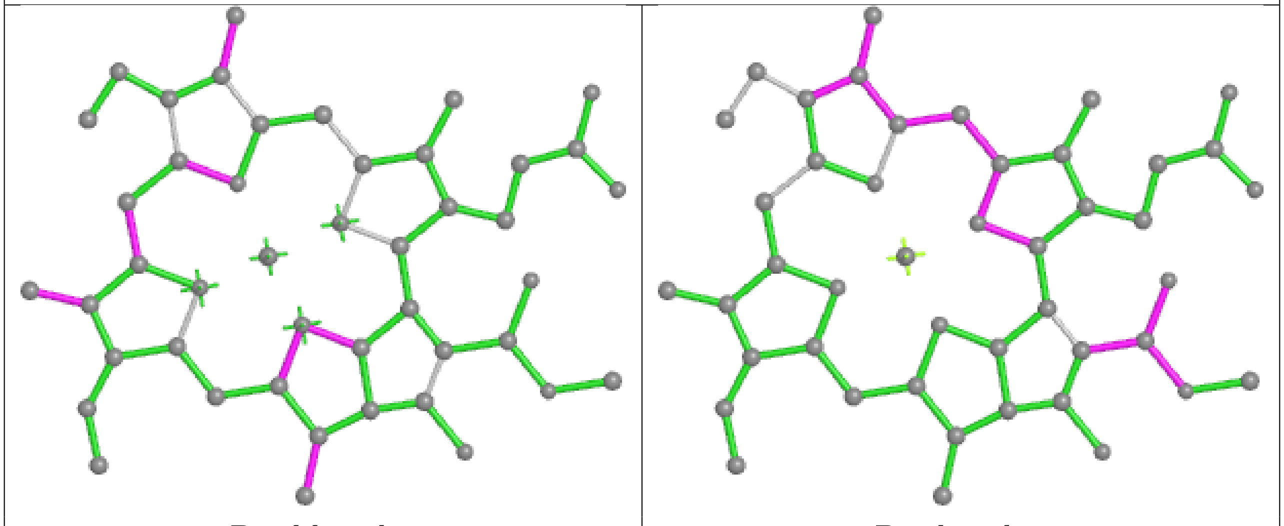
Bond angles



Torsions

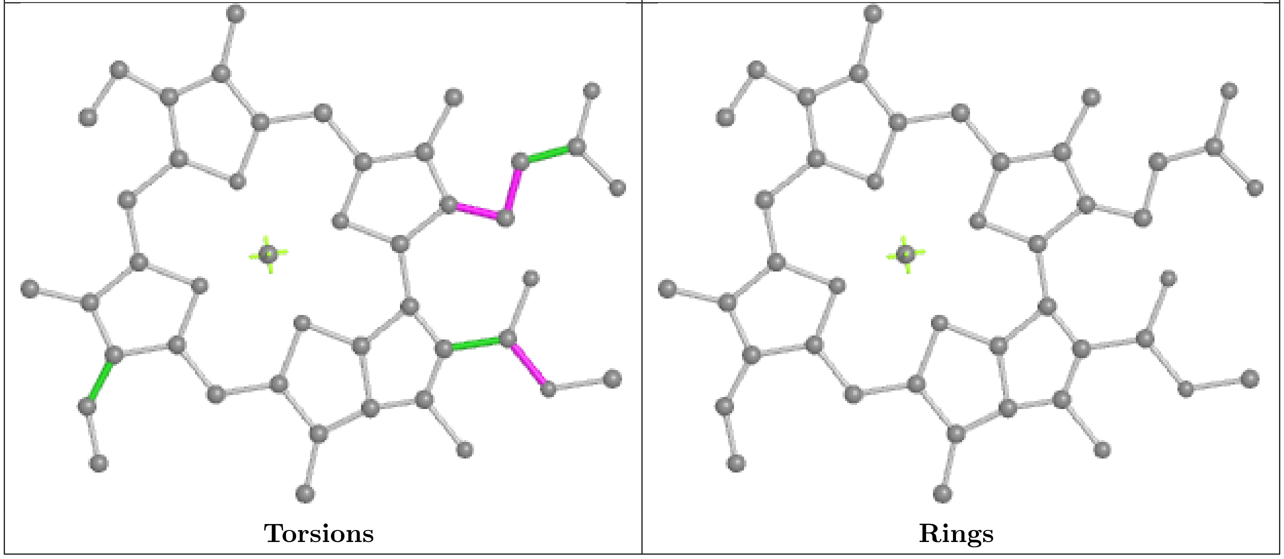
Rings

Ligand CLA cB 815



Bond lengths

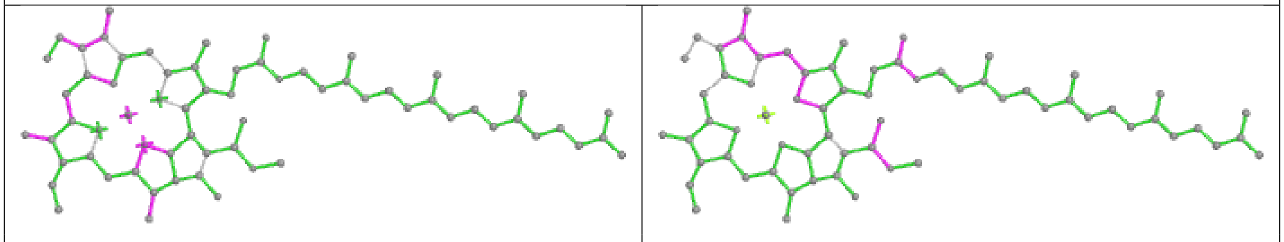
Bond angles



Torsions

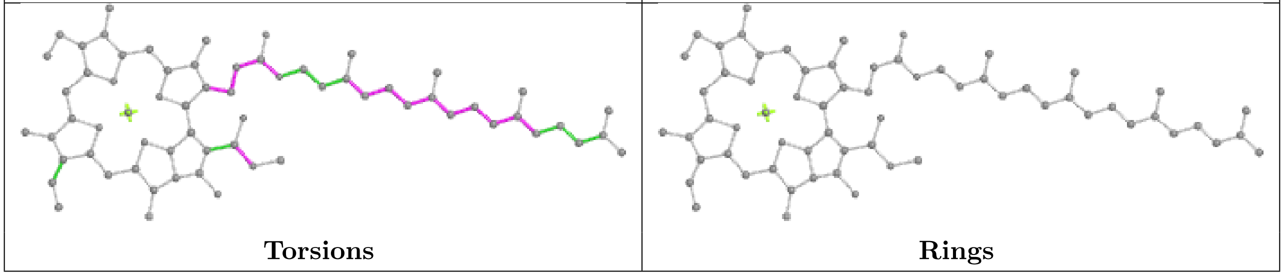
Rings

Ligand CLA bL 206



Bond lengths

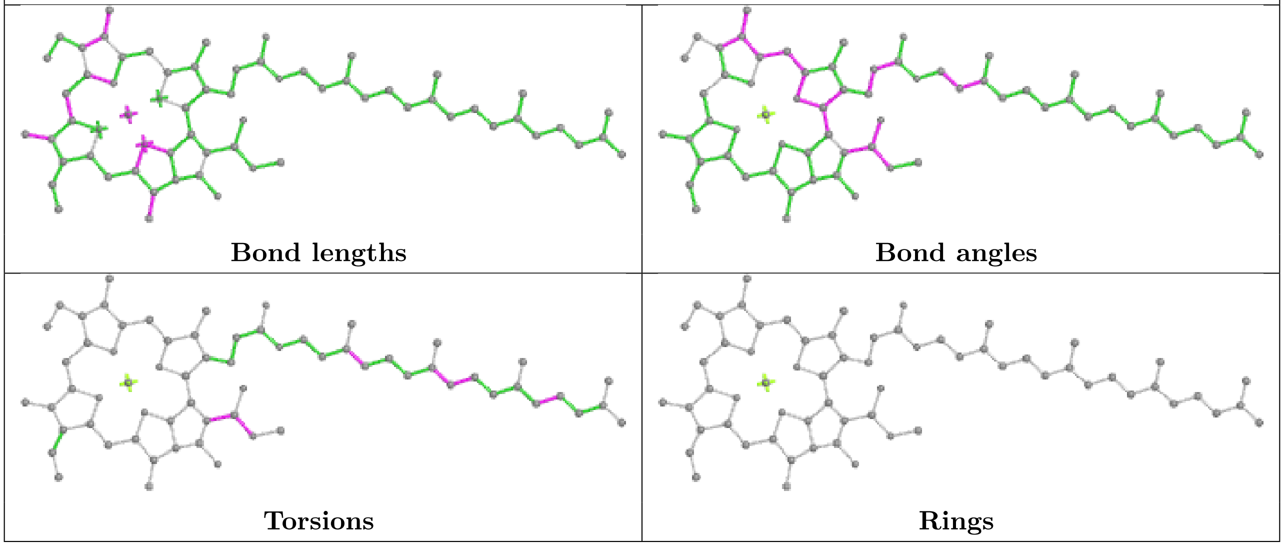
Bond angles



Torsions

Rings

Ligand CLA aA 833



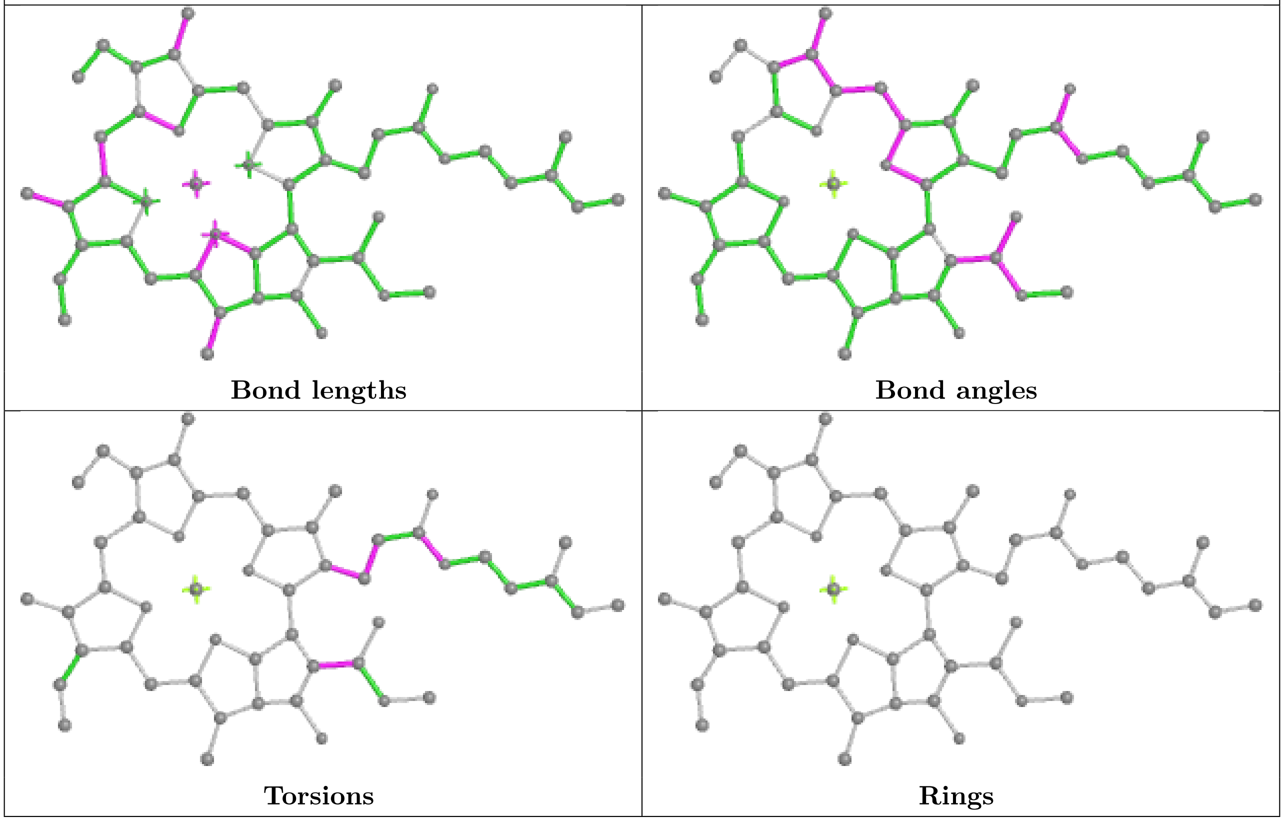
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA dA 837



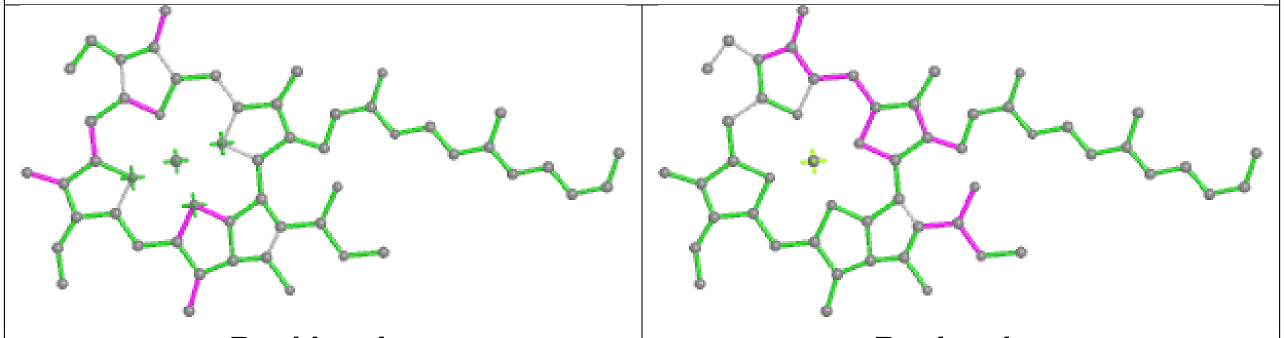
Bond lengths

Bond angles

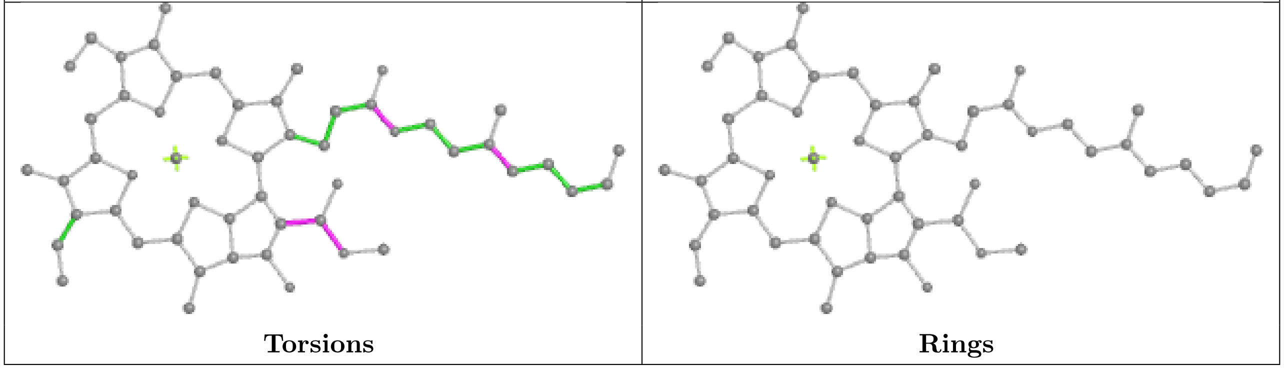
Torsions

Rings

Ligand CLA dB 805

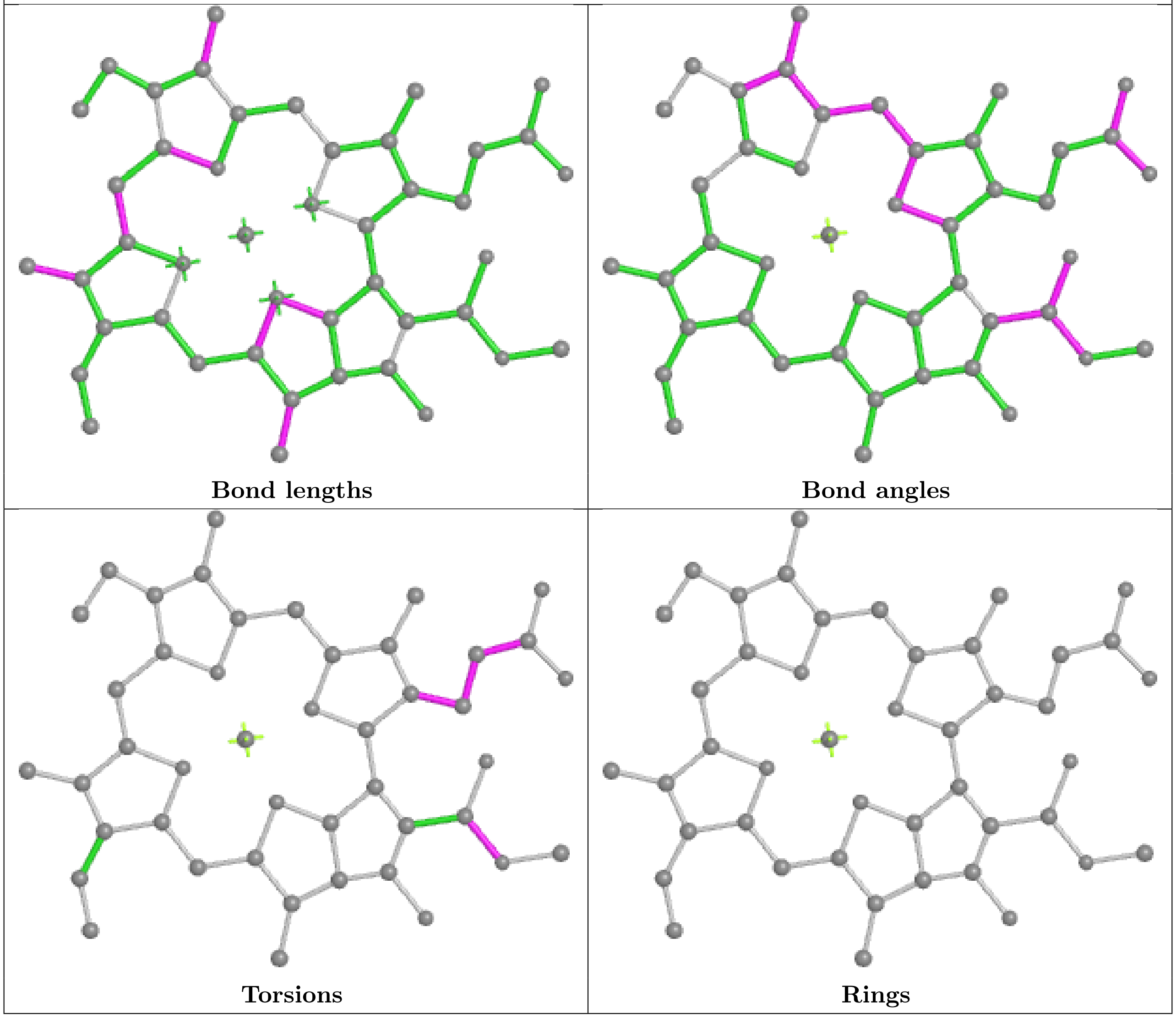


Bond lengths **Bond angles**



Torsions **Rings**

Ligand CLA bA 836



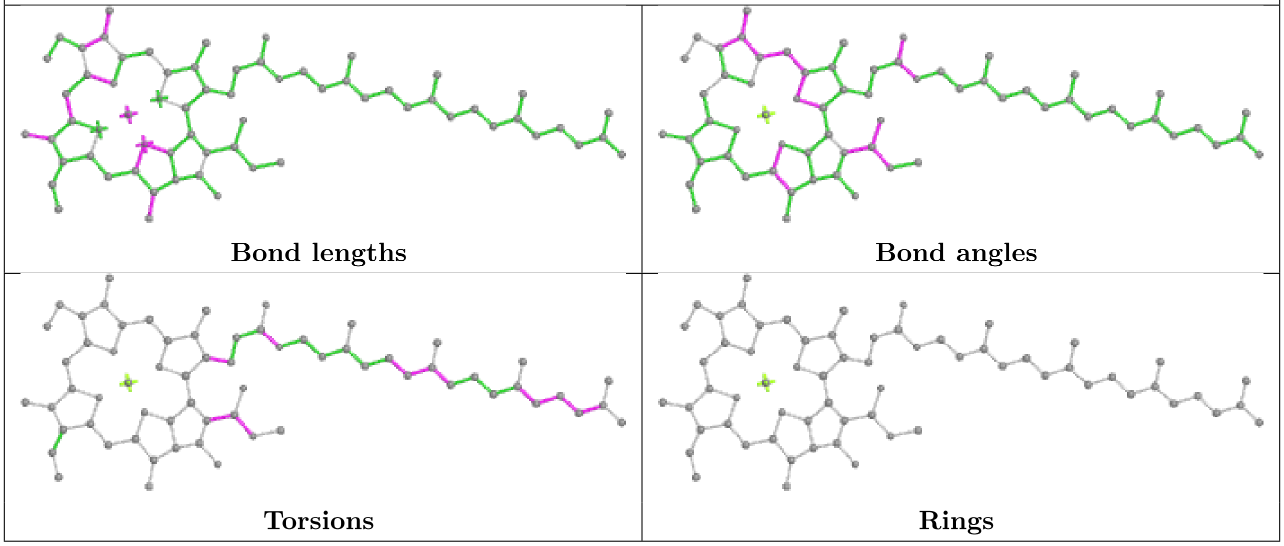
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA aA 819



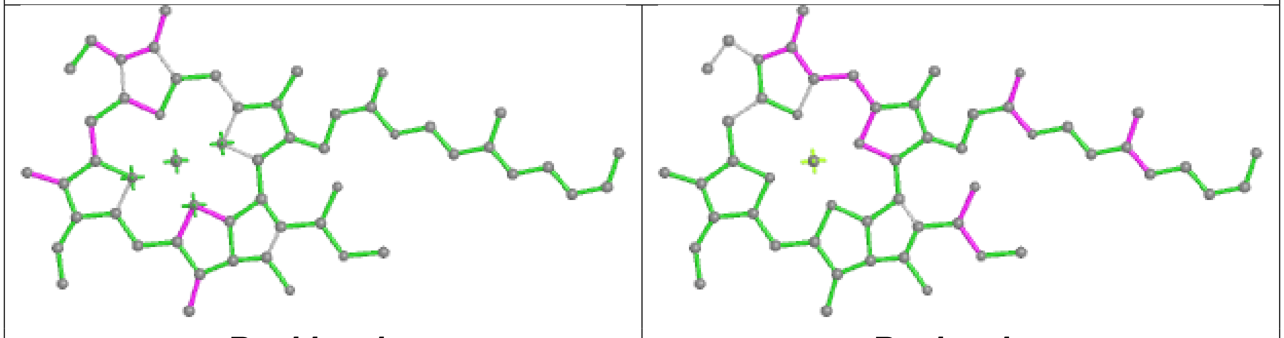
Bond lengths

Bond angles

Torsions

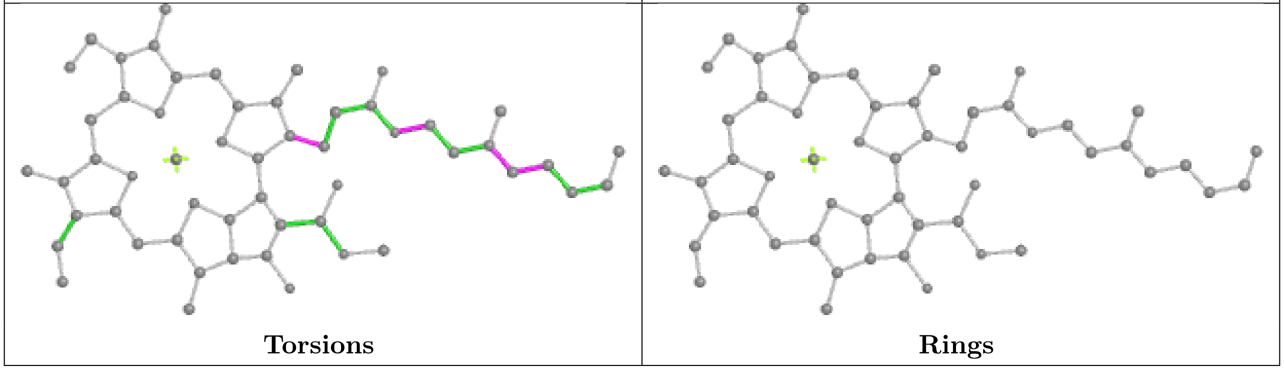
Rings

Ligand CLA aA 835



Bond lengths

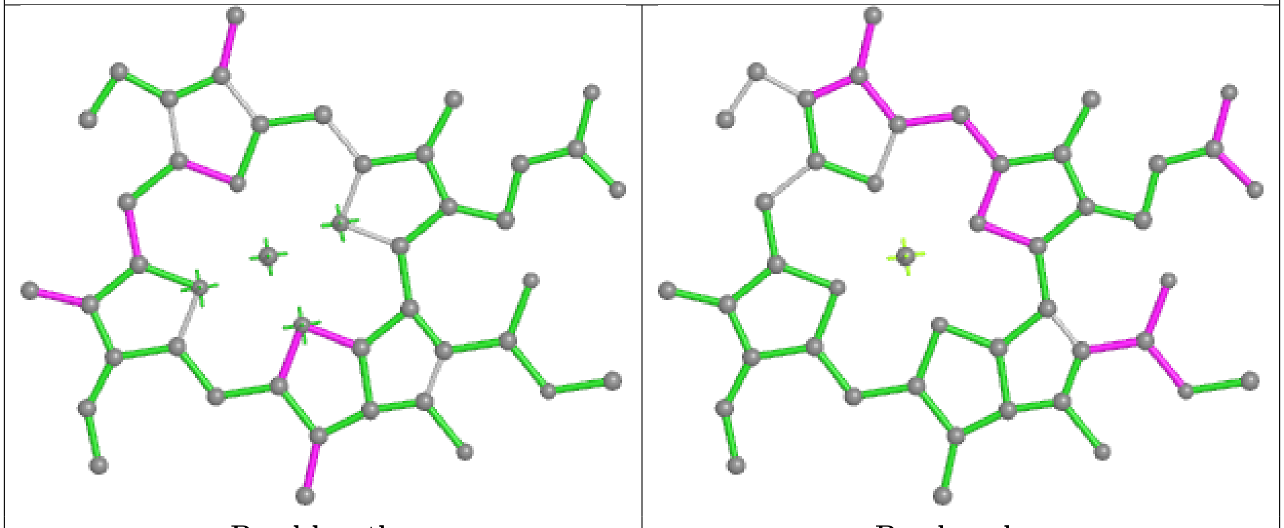
Bond angles



Torsions

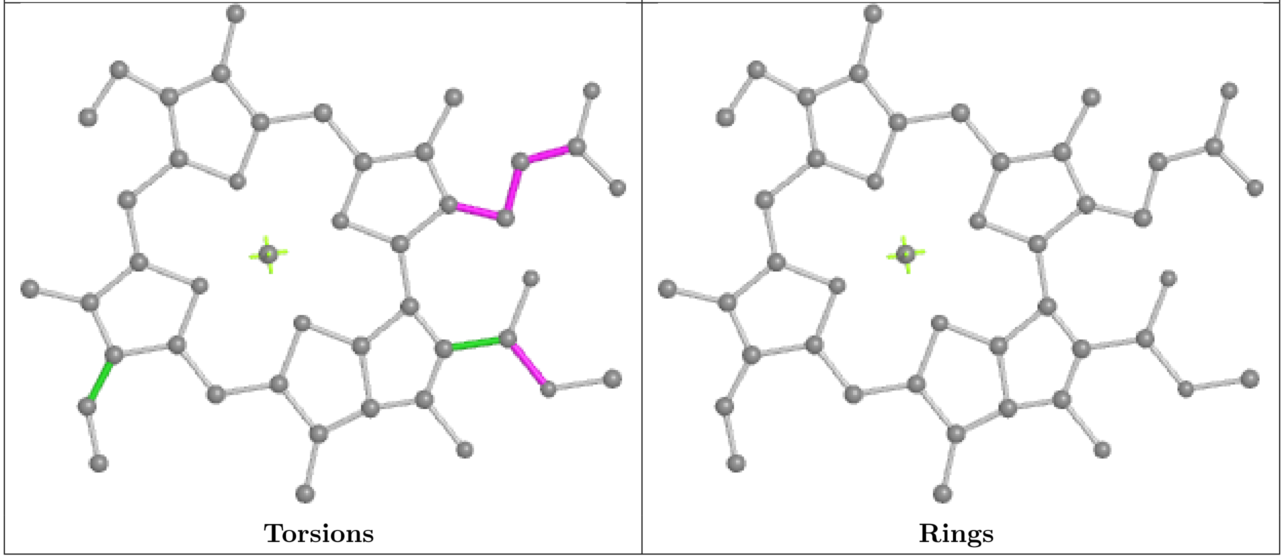
Rings

Ligand CLA cA 836



Bond lengths

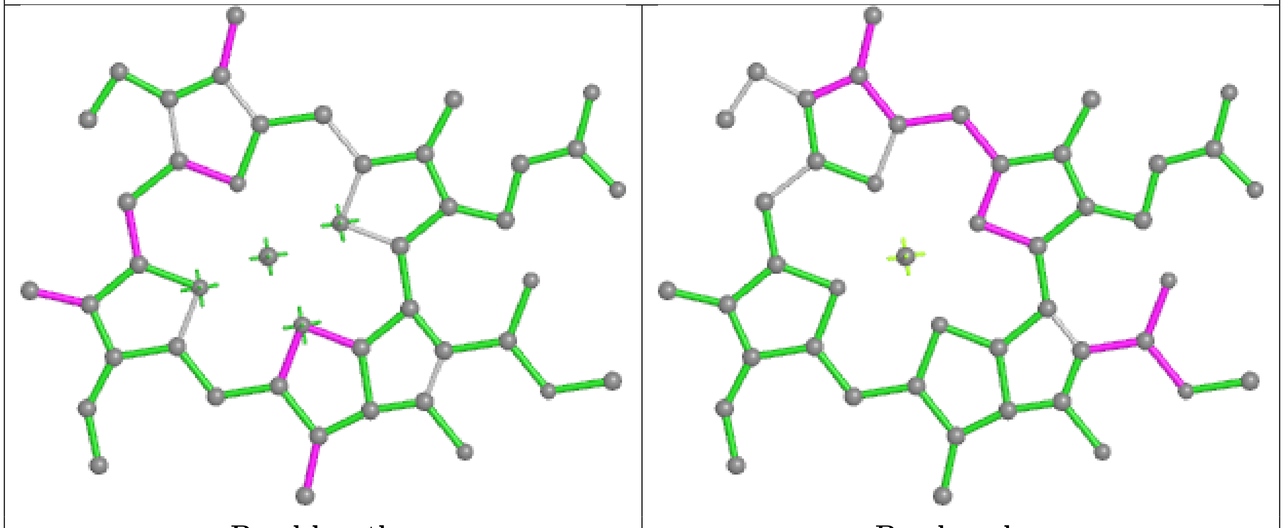
Bond angles



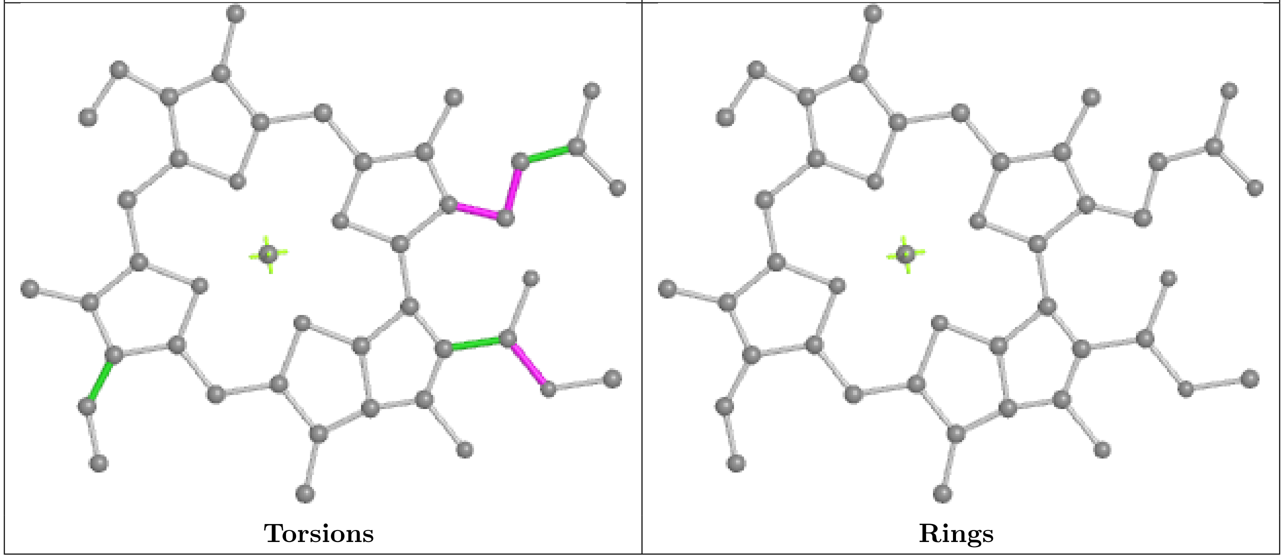
Torsions

Rings

Ligand CLA aB 815

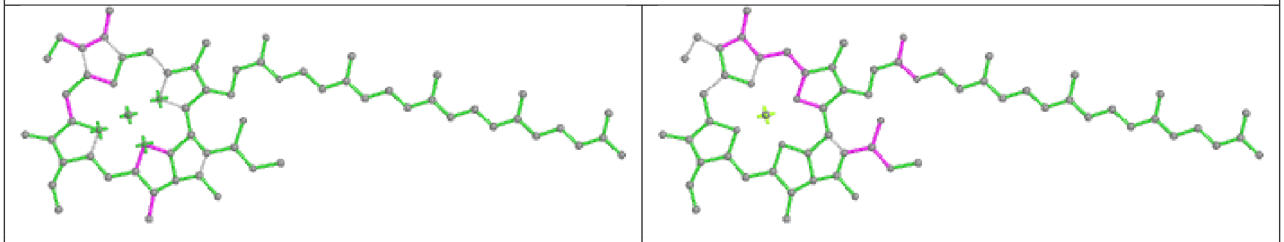


Bond lengths Bond angles

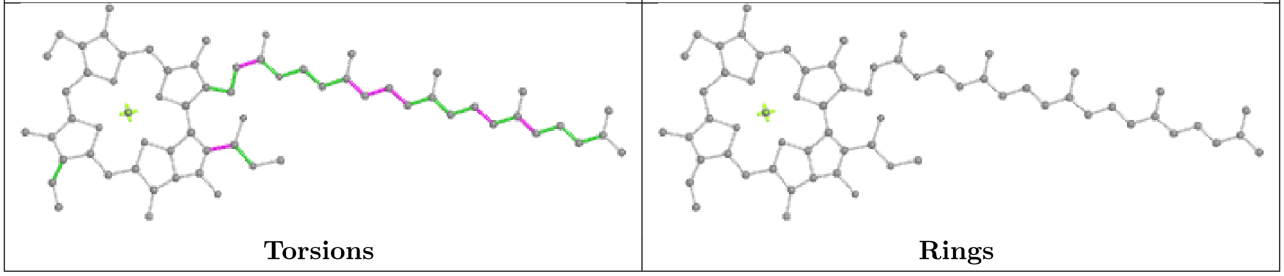


Torsions Rings

Ligand CLA cA 839

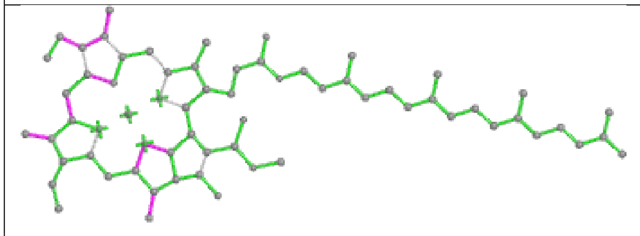


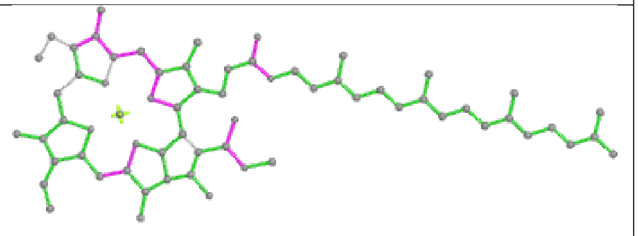
Bond lengths Bond angles

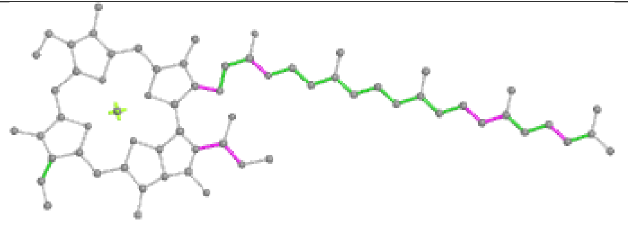


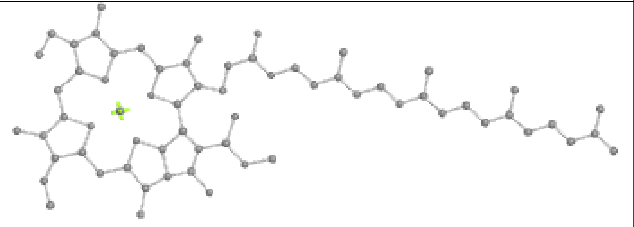
Torsions Rings

Ligand CLA dA 811

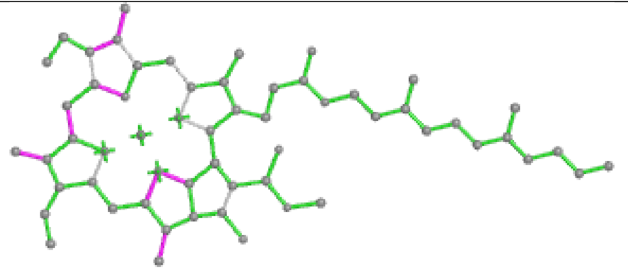

Bond lengths

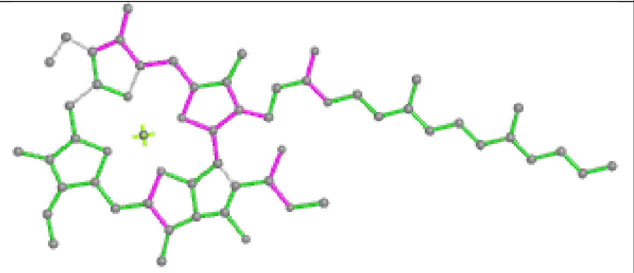

Bond angles

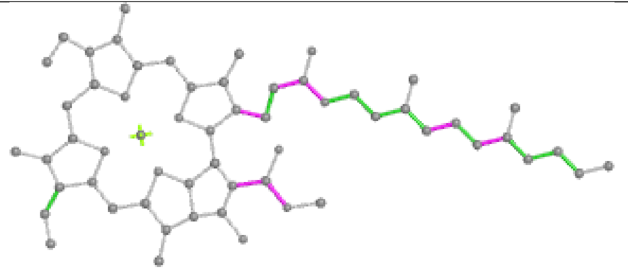

Torsions

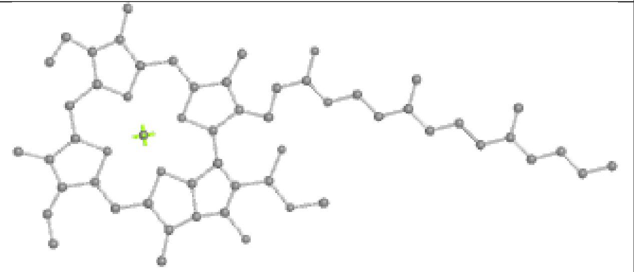

Rings

Ligand CLA aB 833

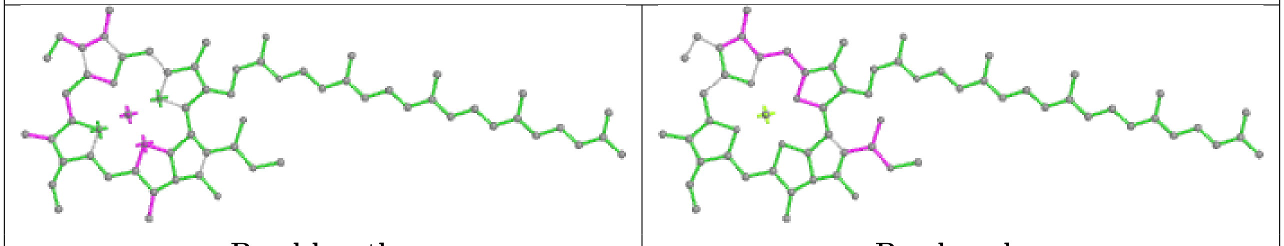

Bond lengths


Bond angles


Torsions

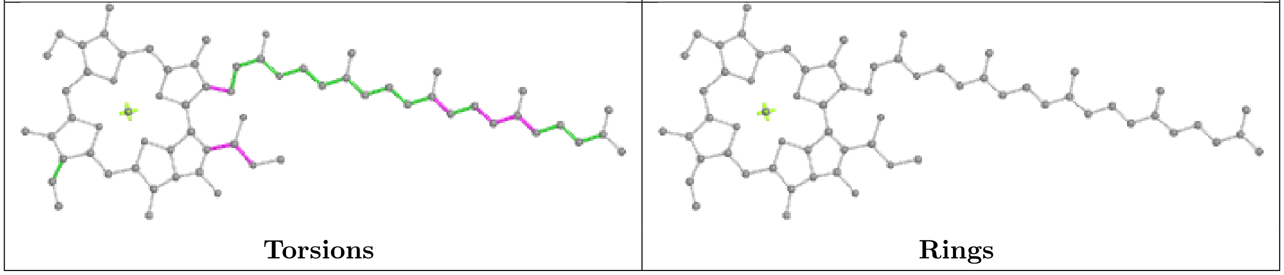

Rings

Ligand CLA cA 830



Bond lengths

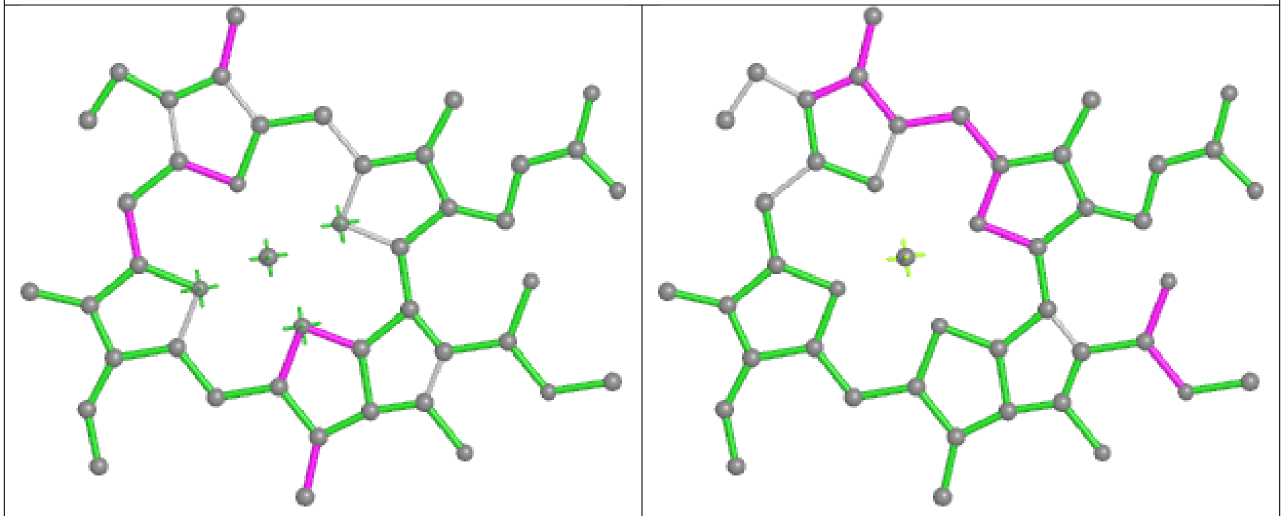
Bond angles



Torsions

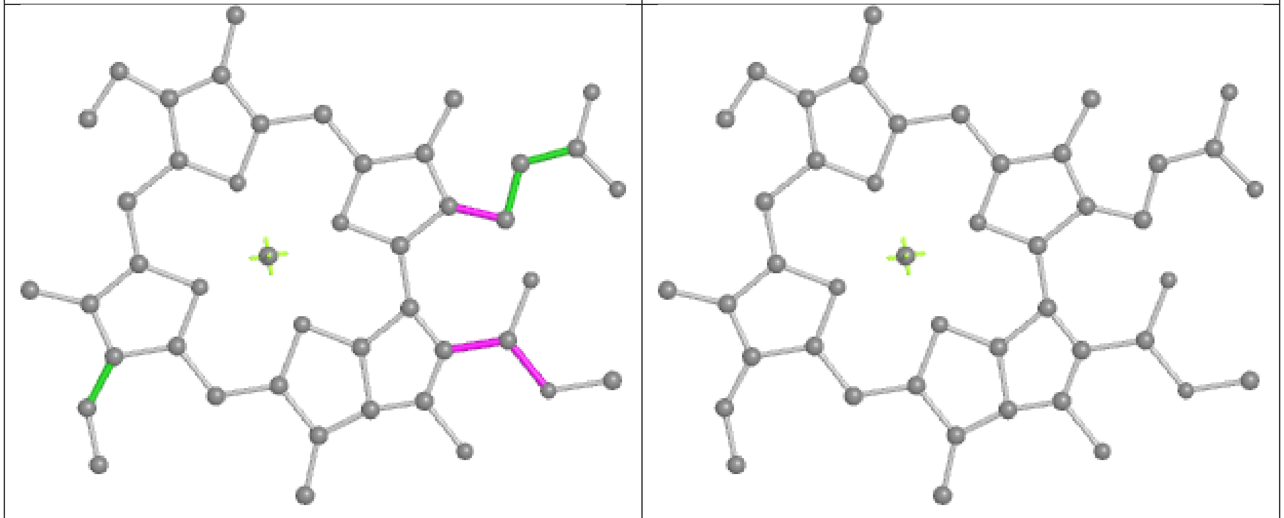
Rings

Ligand CLA dA 810



Bond lengths

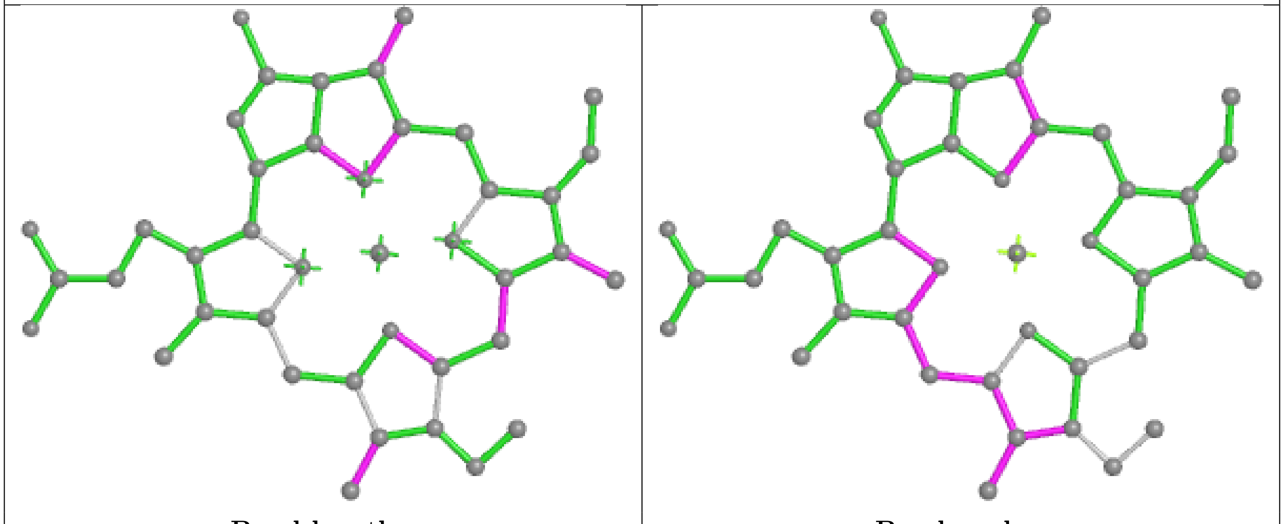
Bond angles



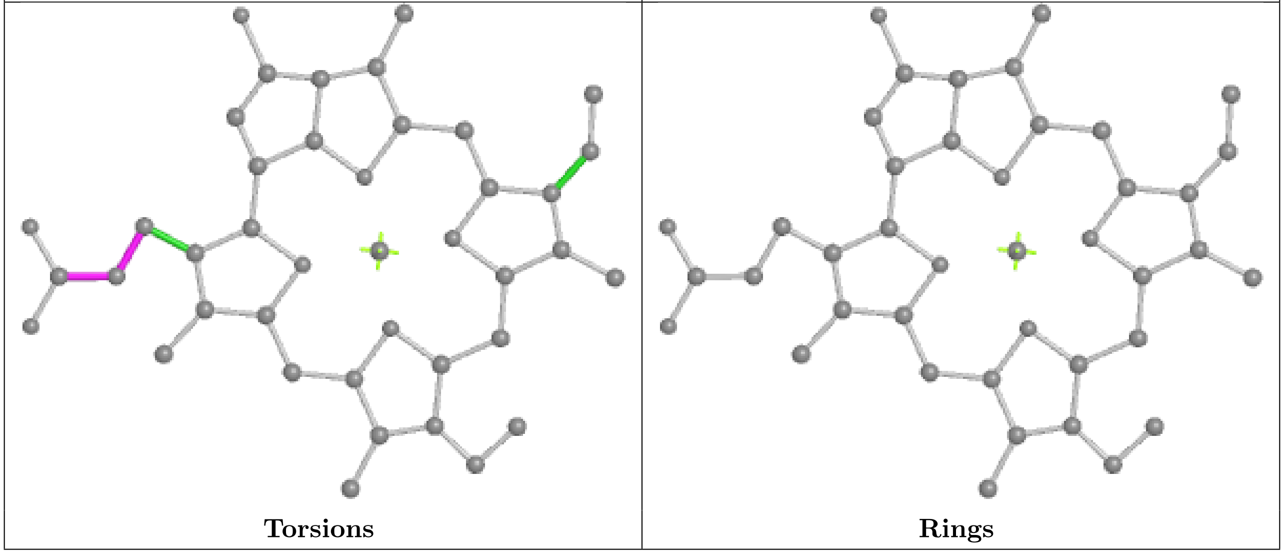
Torsions

Rings

Ligand CLA bK 101

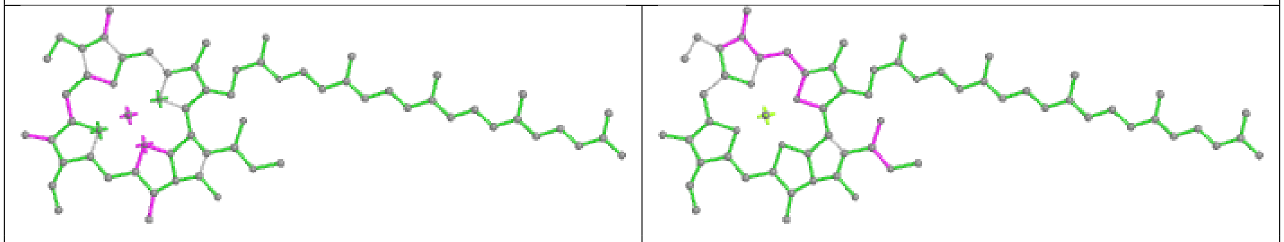


Bond lengths Bond angles

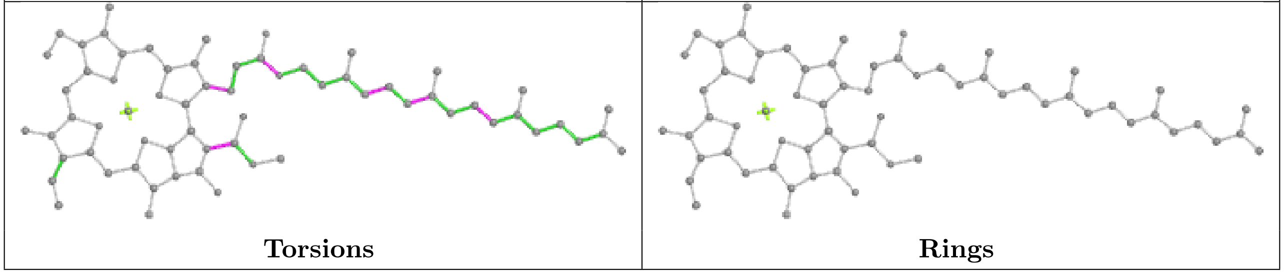


Torsions Rings

Ligand CLA dB 820

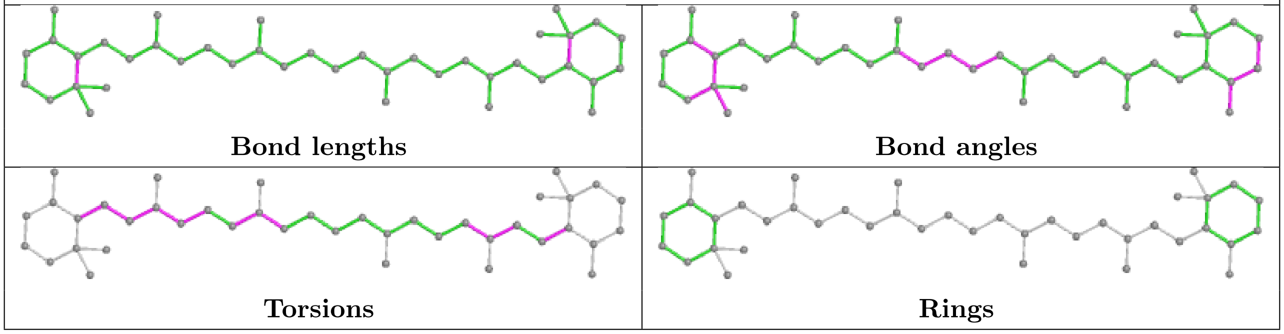


Bond lengths Bond angles

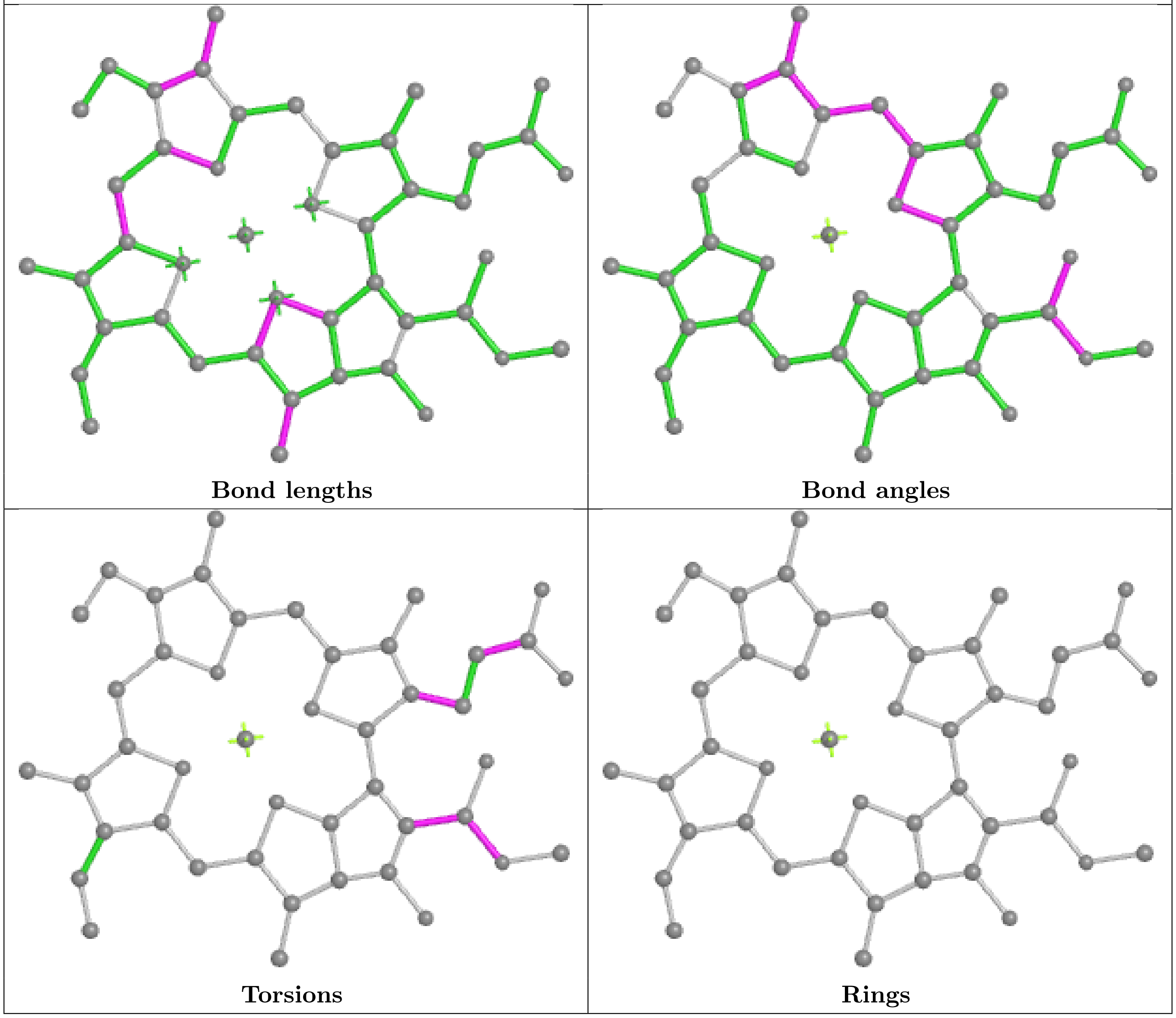


Torsions Rings

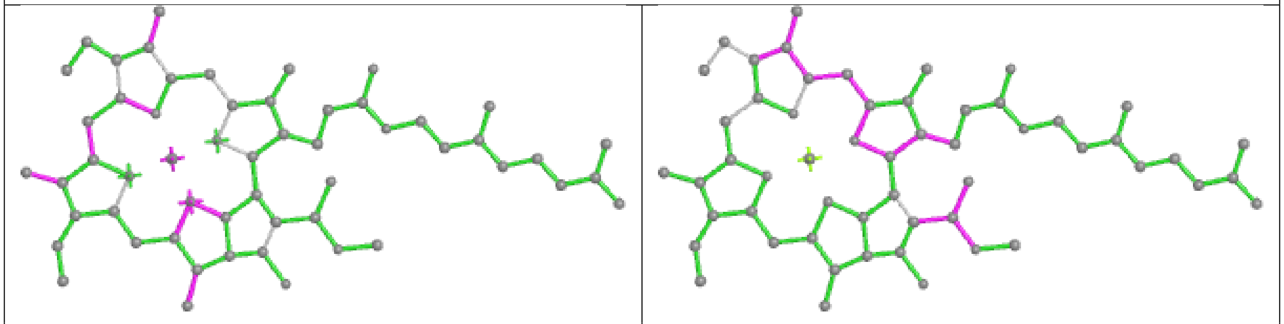
Ligand BCR bI 101



Ligand CLA cJ 101

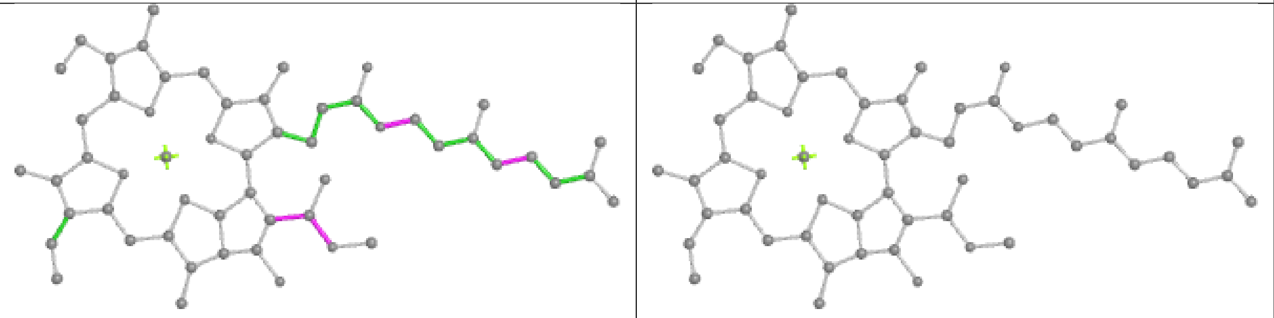


Ligand CLA cA 826



Bond lengths

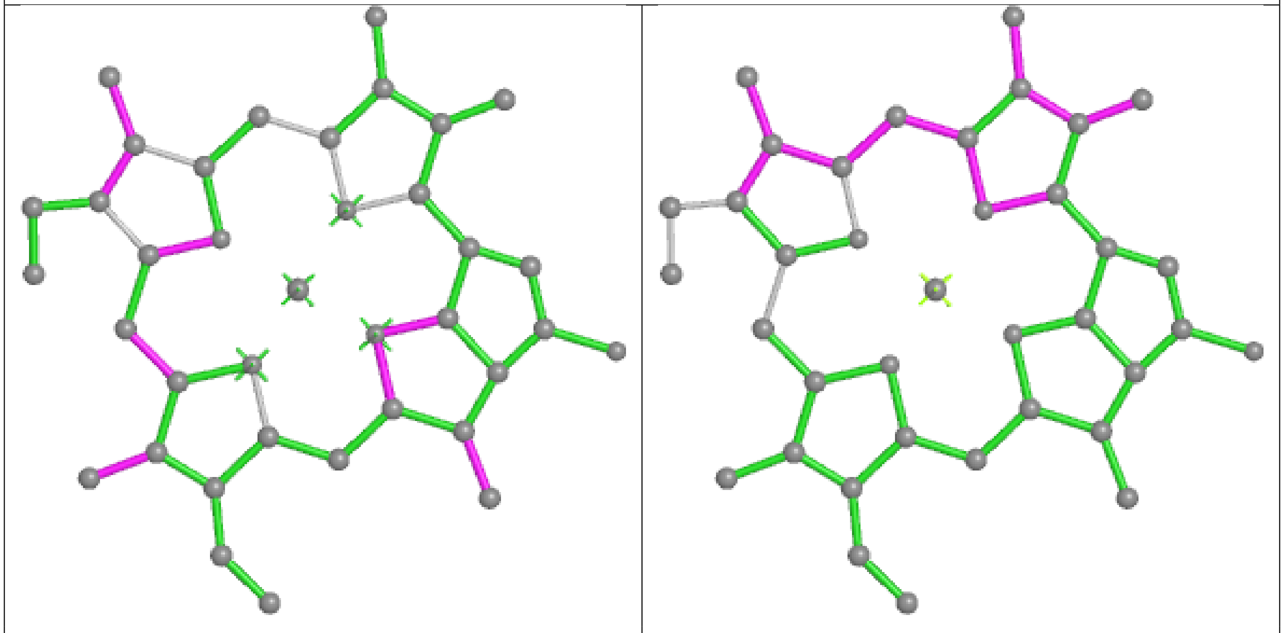
Bond angles



Torsions

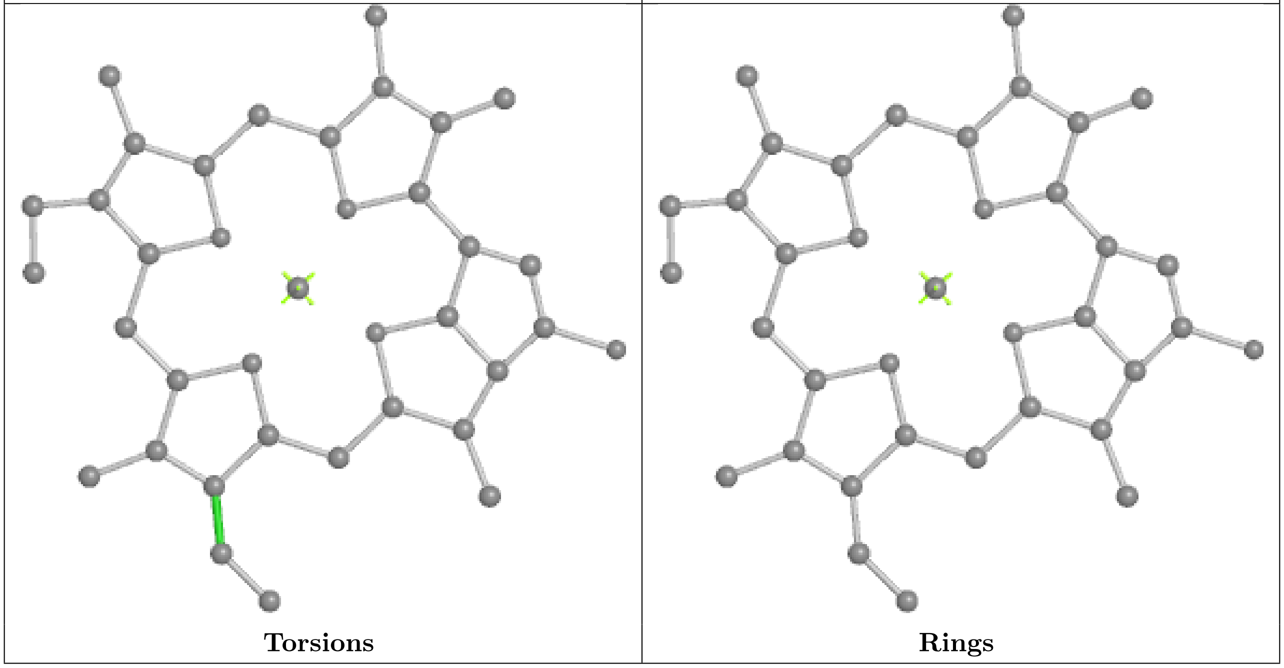
Rings

Ligand CLA cJ 102



Bond lengths

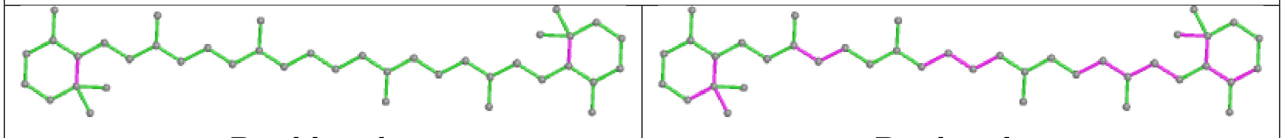
Bond angles



Torsions

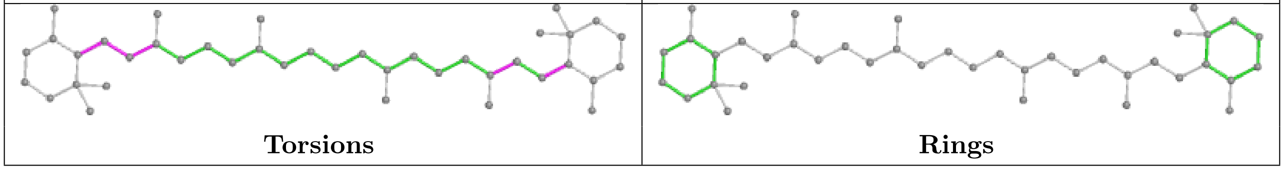
Rings

Ligand BCR cL 205



Bond lengths

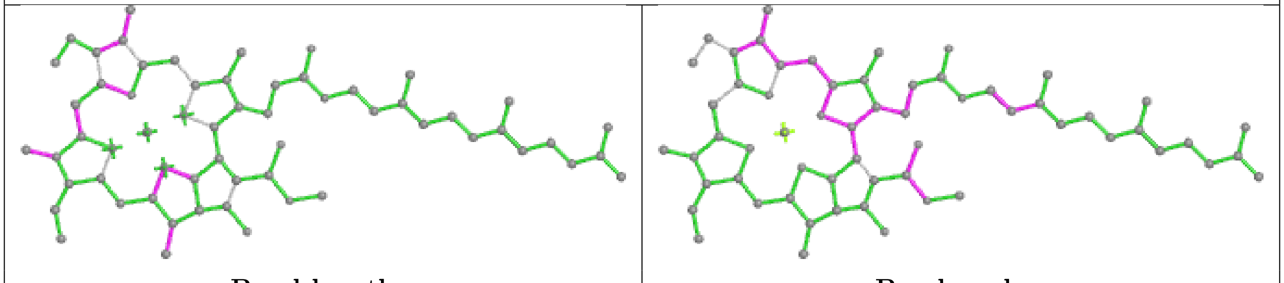
Bond angles



Torsions

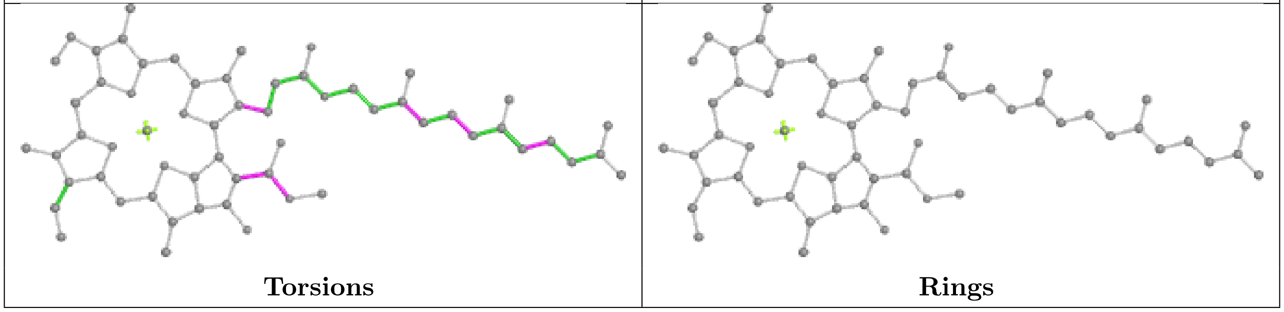
Rings

Ligand CLA bB 838



Bond lengths

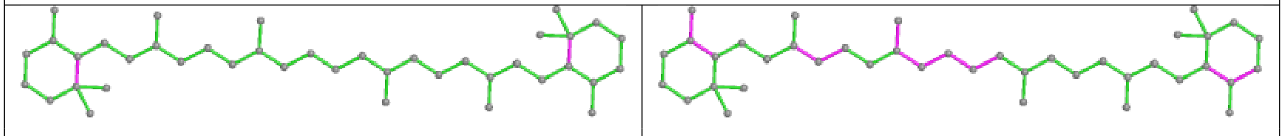
Bond angles



Torsions

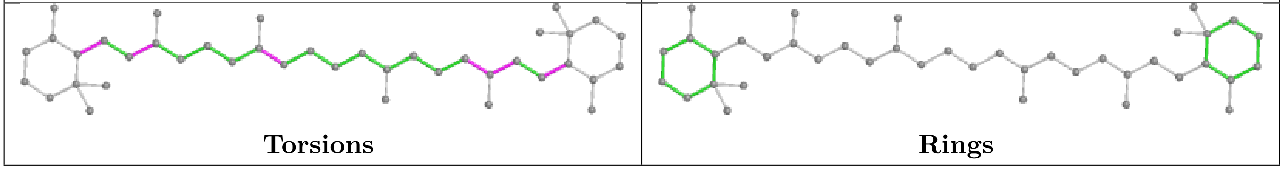
Rings

Ligand BCR dA 848



Bond lengths

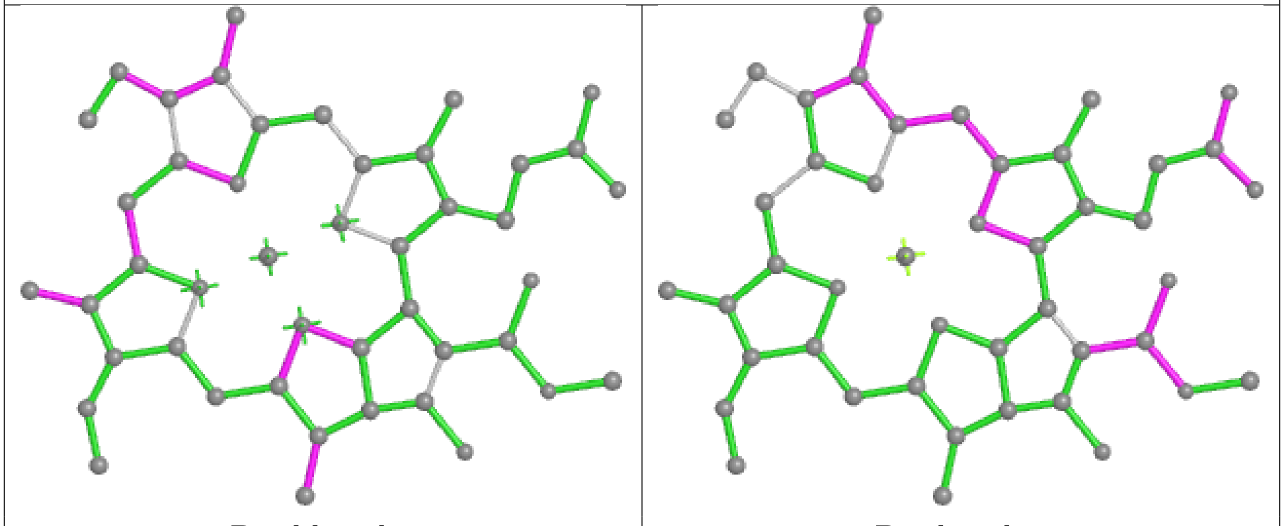
Bond angles



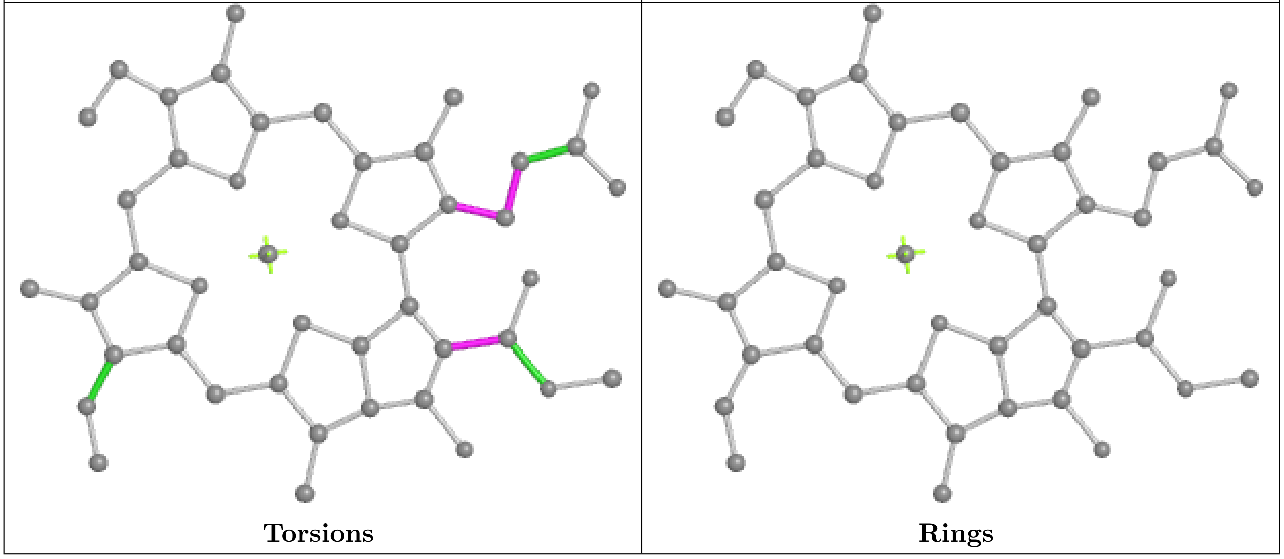
Torsions

Rings

Ligand CLA cA 808

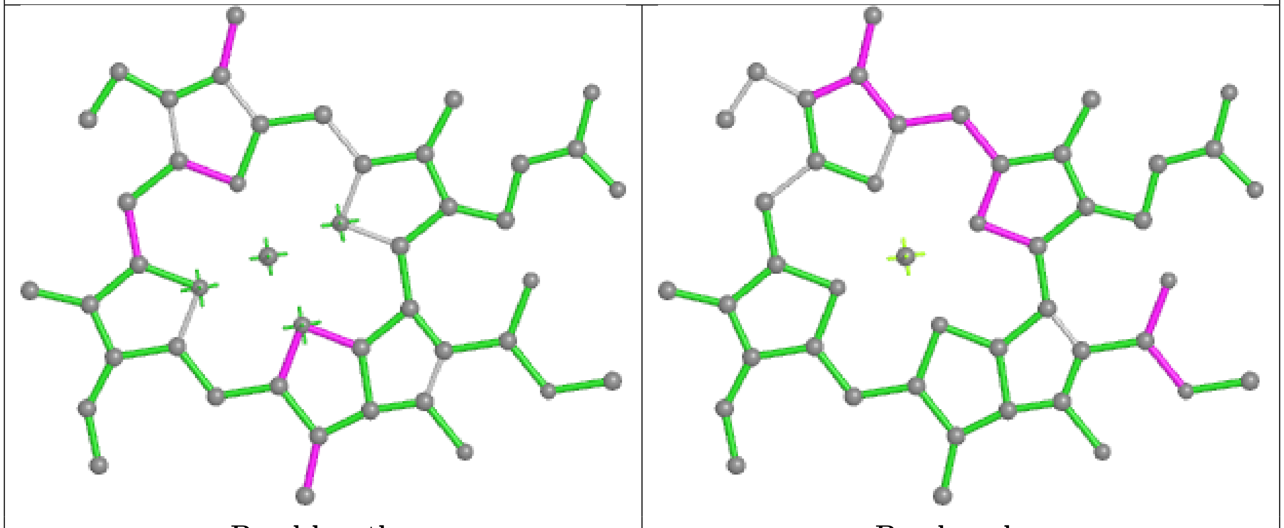


Bond lengths **Bond angles**

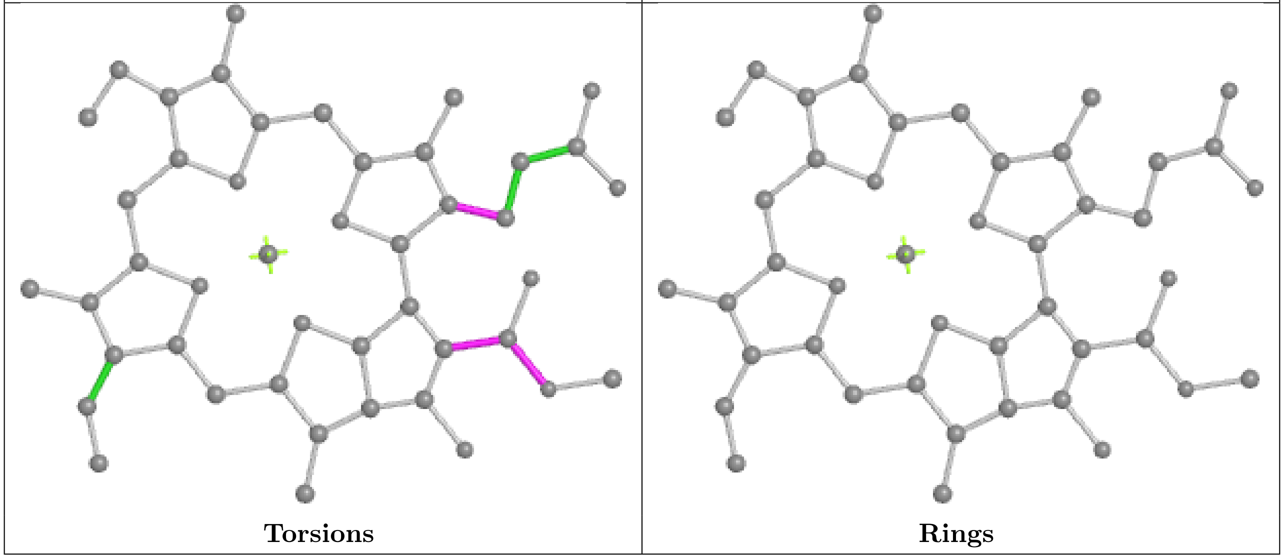


Torsions **Rings**

Ligand CLA bA 810

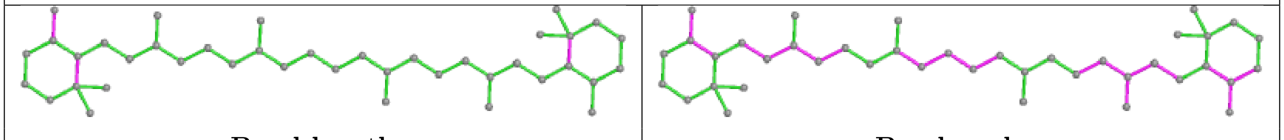


Bond lengths Bond angles

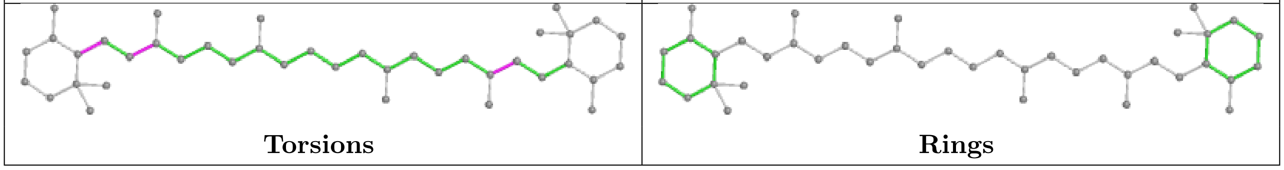


Torsions Rings

Ligand BCR dK 102

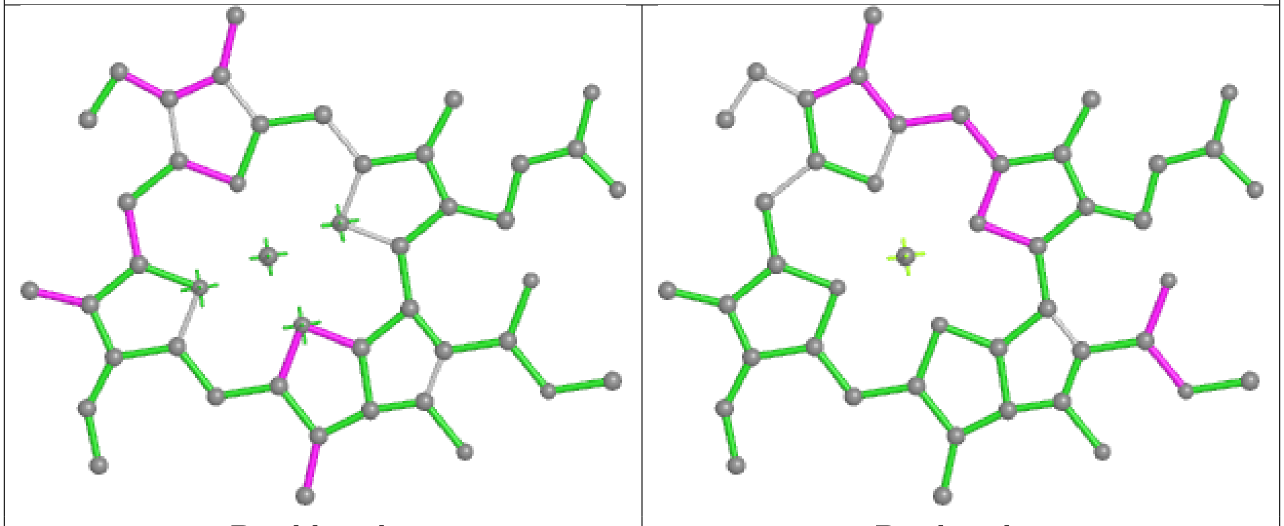


Bond lengths Bond angles

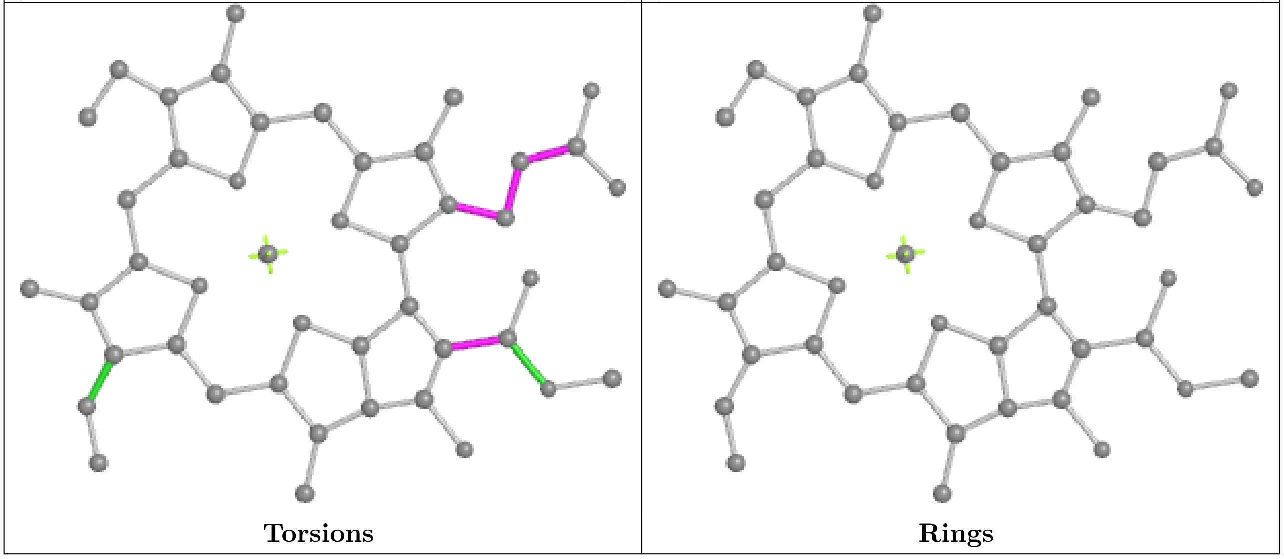


Torsions Rings

Ligand CLA bB 831

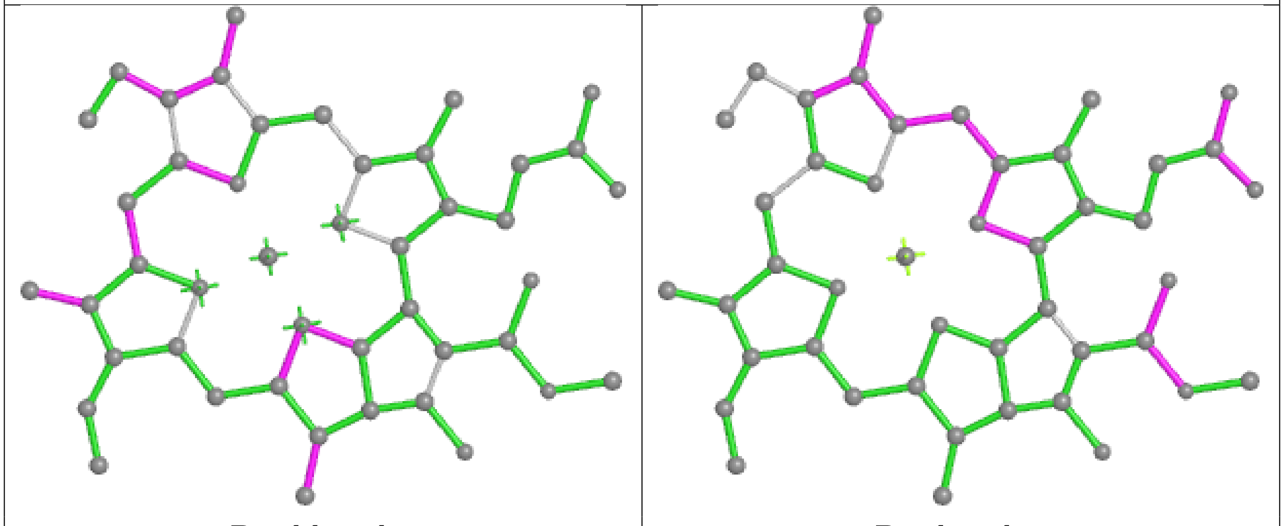


Bond lengths **Bond angles**



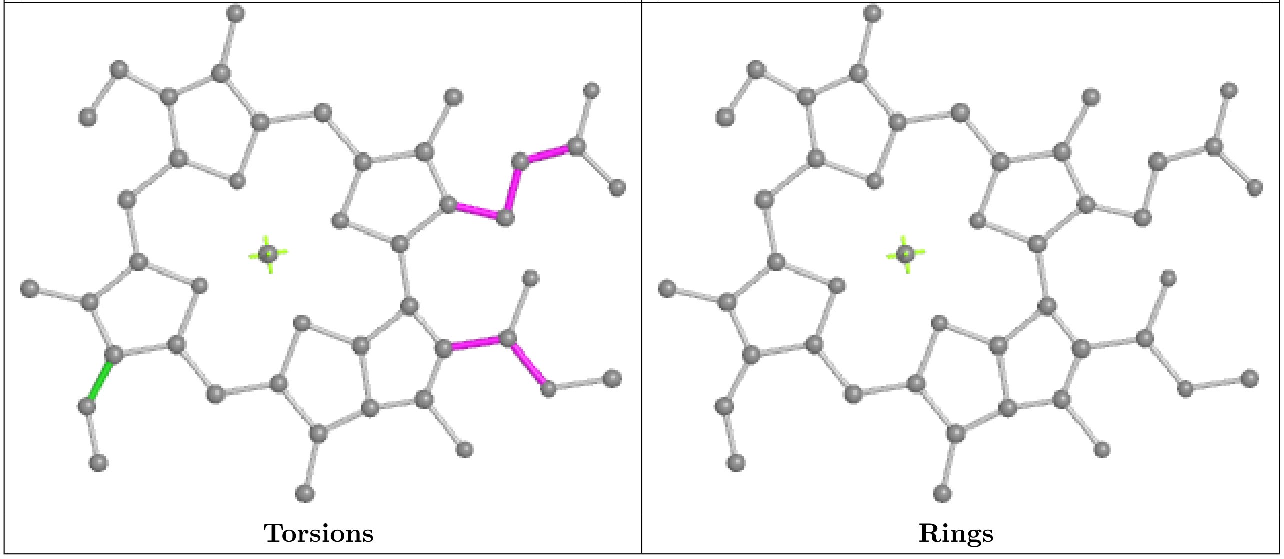
Torsions **Rings**

Ligand CLA dB 813



Bond lengths

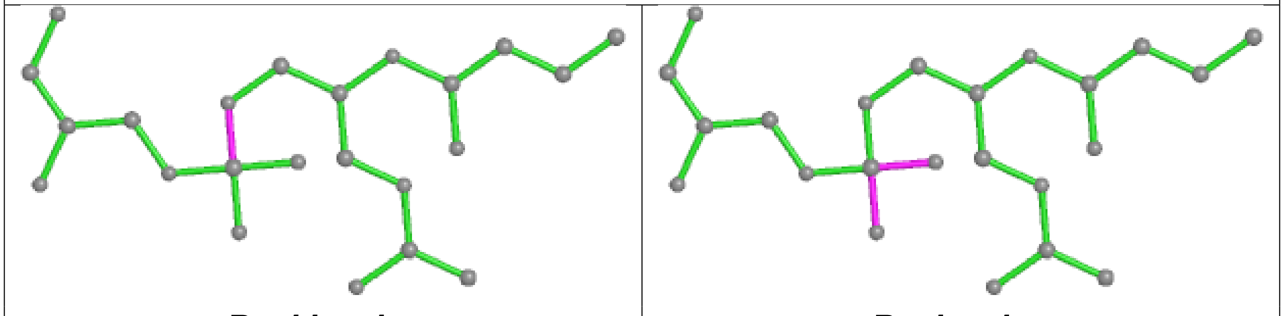
Bond angles



Torsions

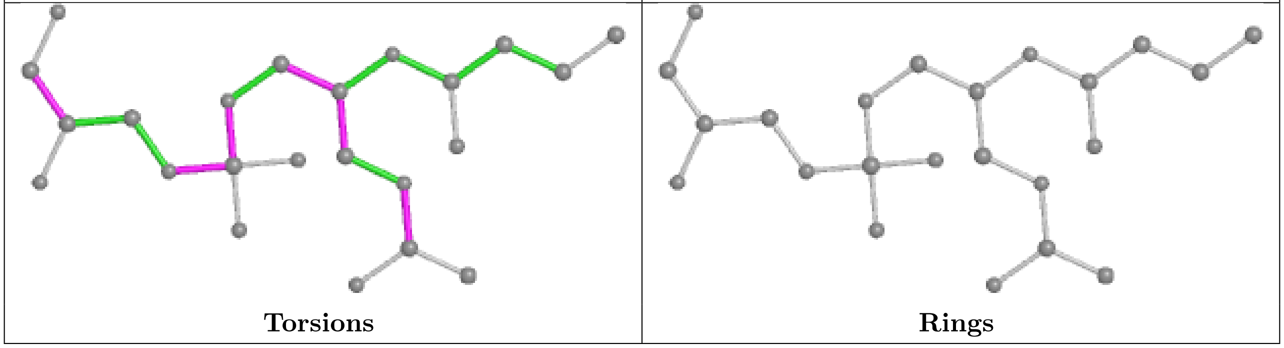
Rings

Ligand LHG aB 850



Bond lengths

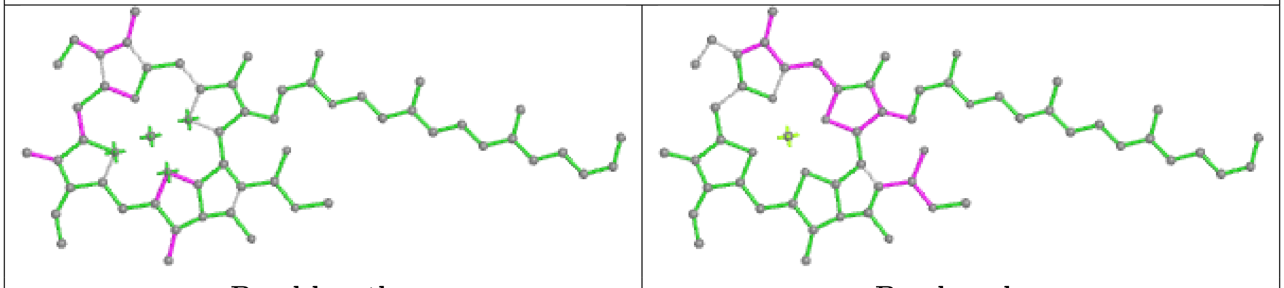
Bond angles



Torsions

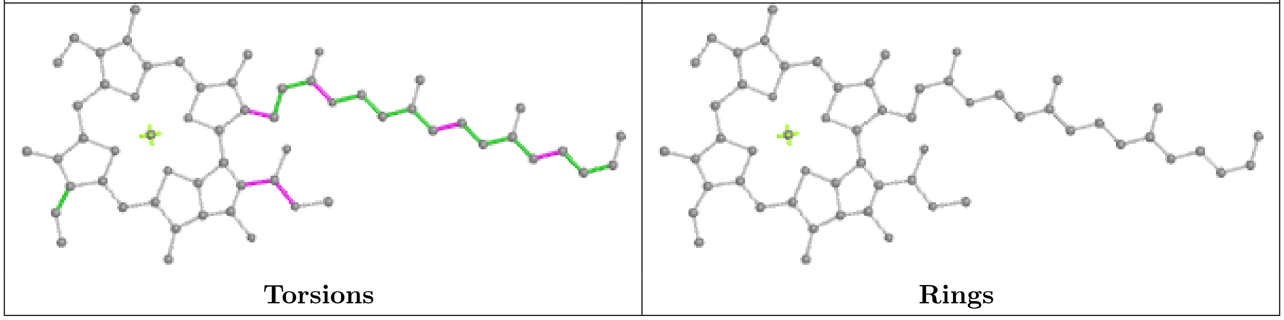
Rings

Ligand CLA cB 817



Bond lengths

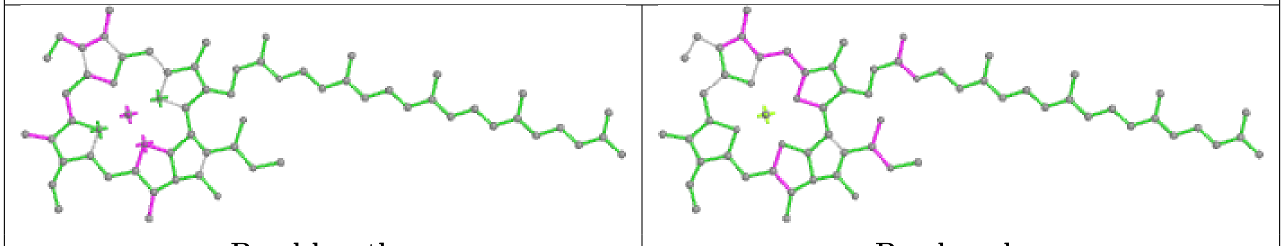
Bond angles



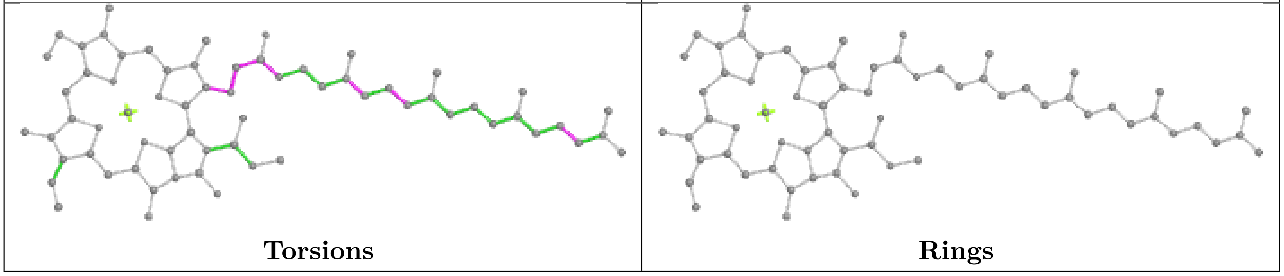
Torsions

Rings

Ligand CLA dB 829

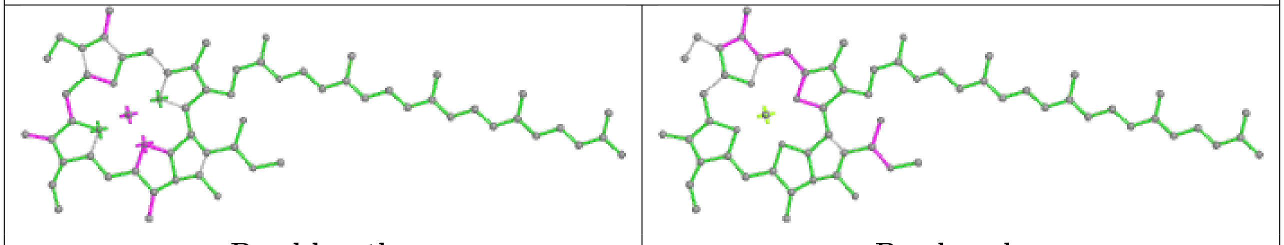


Bond lengths Bond angles

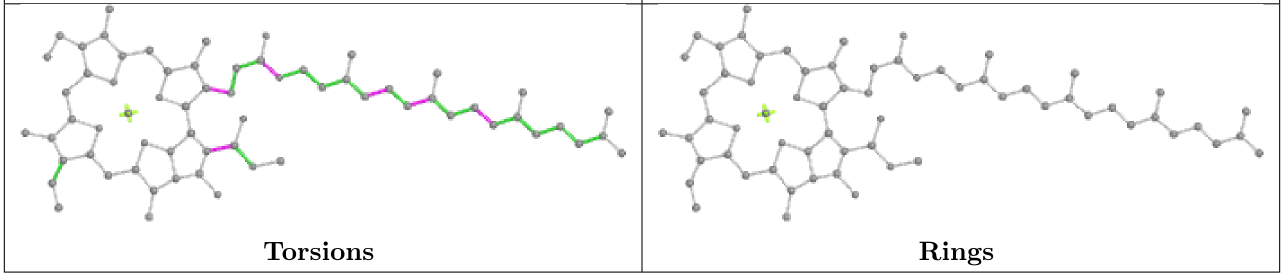


Torsions Rings

Ligand CLA bB 820

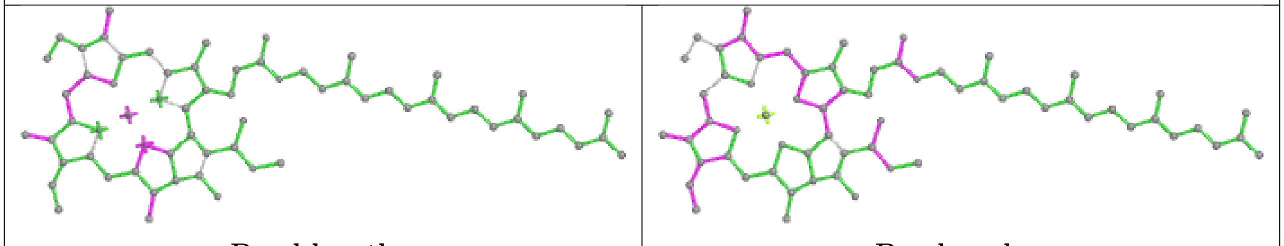


Bond lengths Bond angles

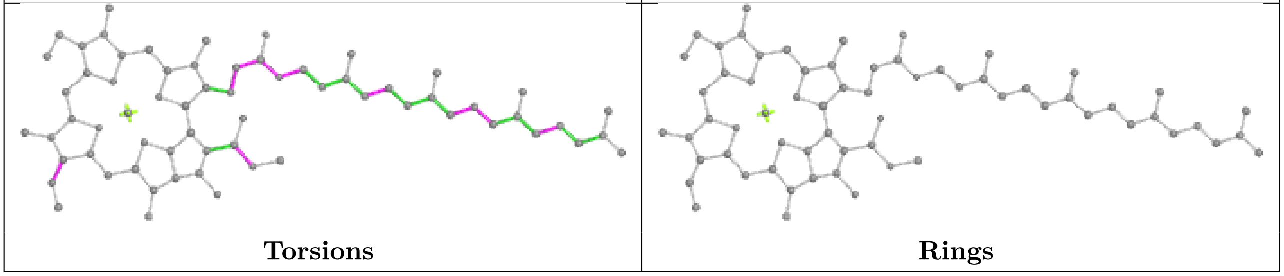


Torsions Rings

Ligand CLA dB 804

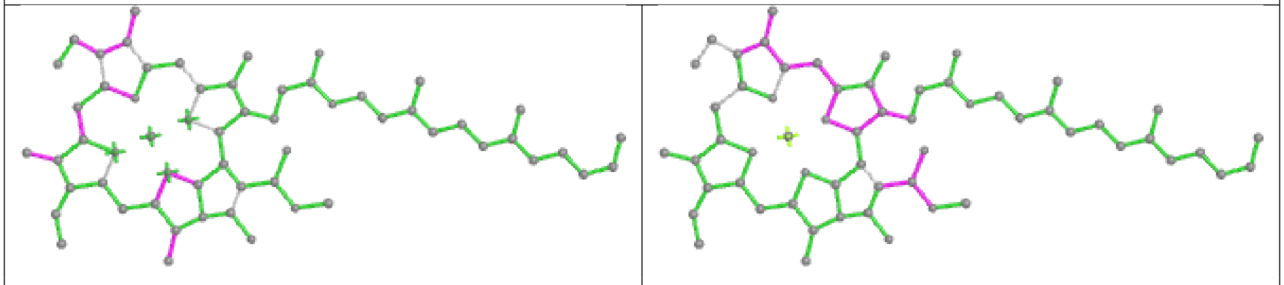


Bond lengths Bond angles



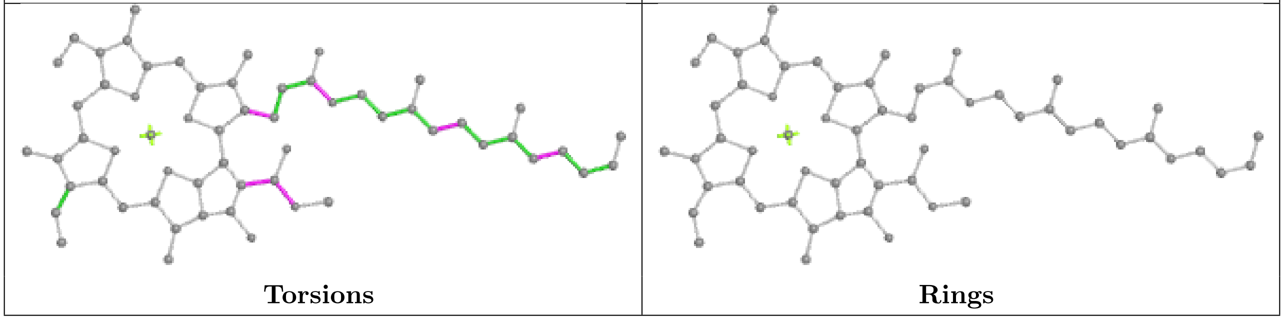
Torsions Rings

Ligand CLA aB 817



Bond lengths

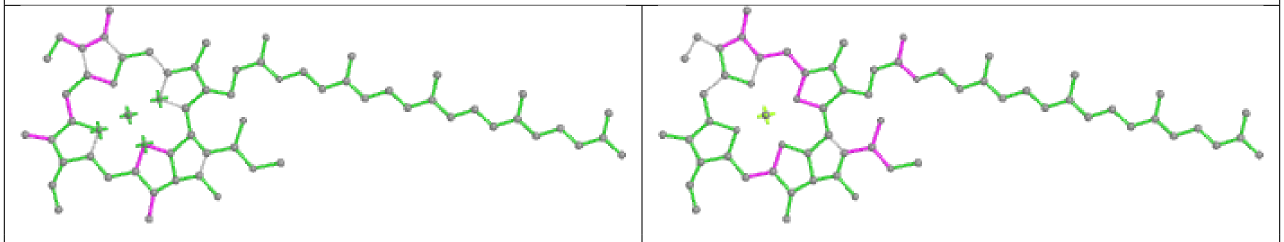
Bond angles



Torsions

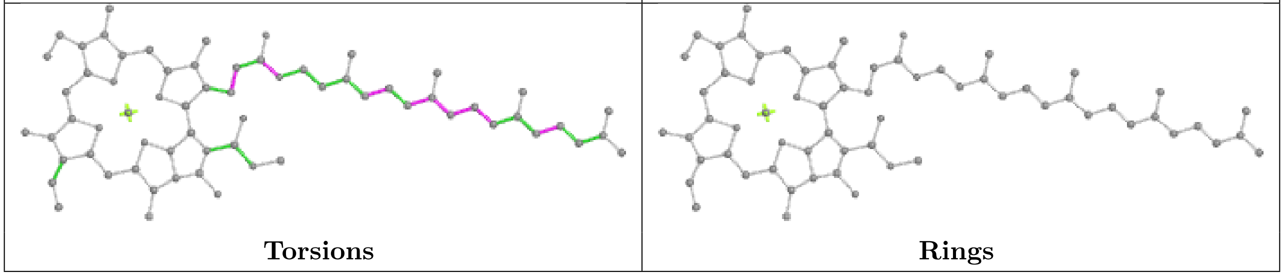
Rings

Ligand CLA dL 205



Bond lengths

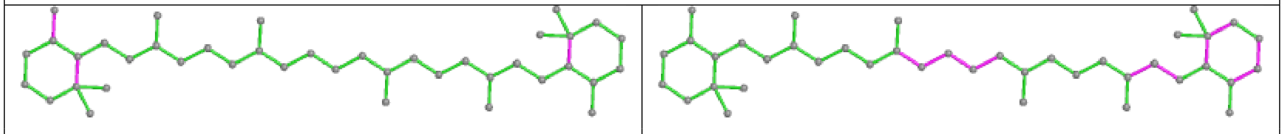
Bond angles



Torsions

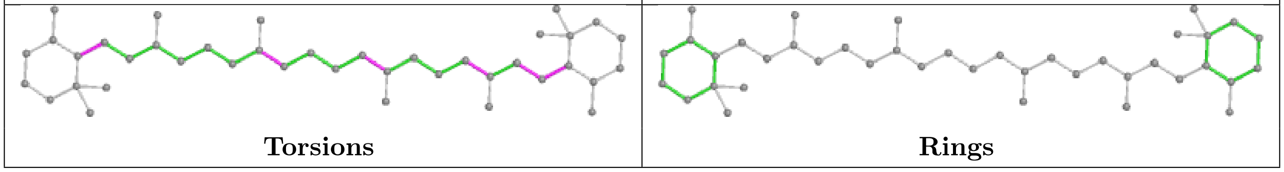
Rings

Ligand BCR bJ 104



Bond lengths

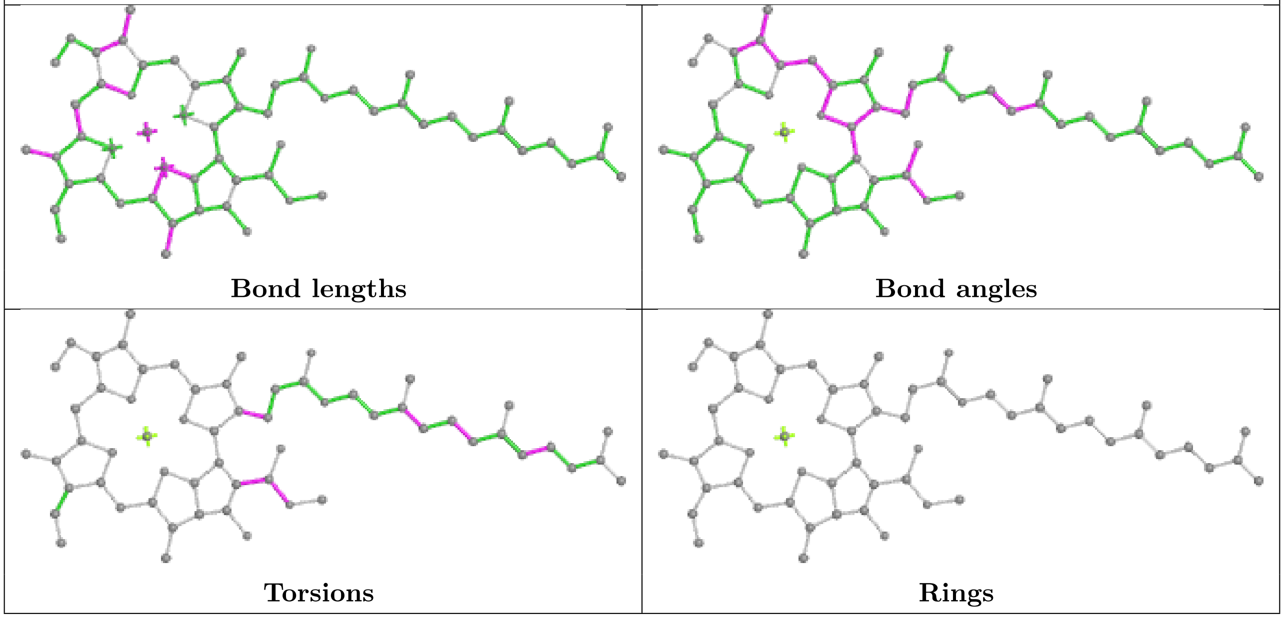
Bond angles



Torsions

Rings

Ligand CLA cB 837



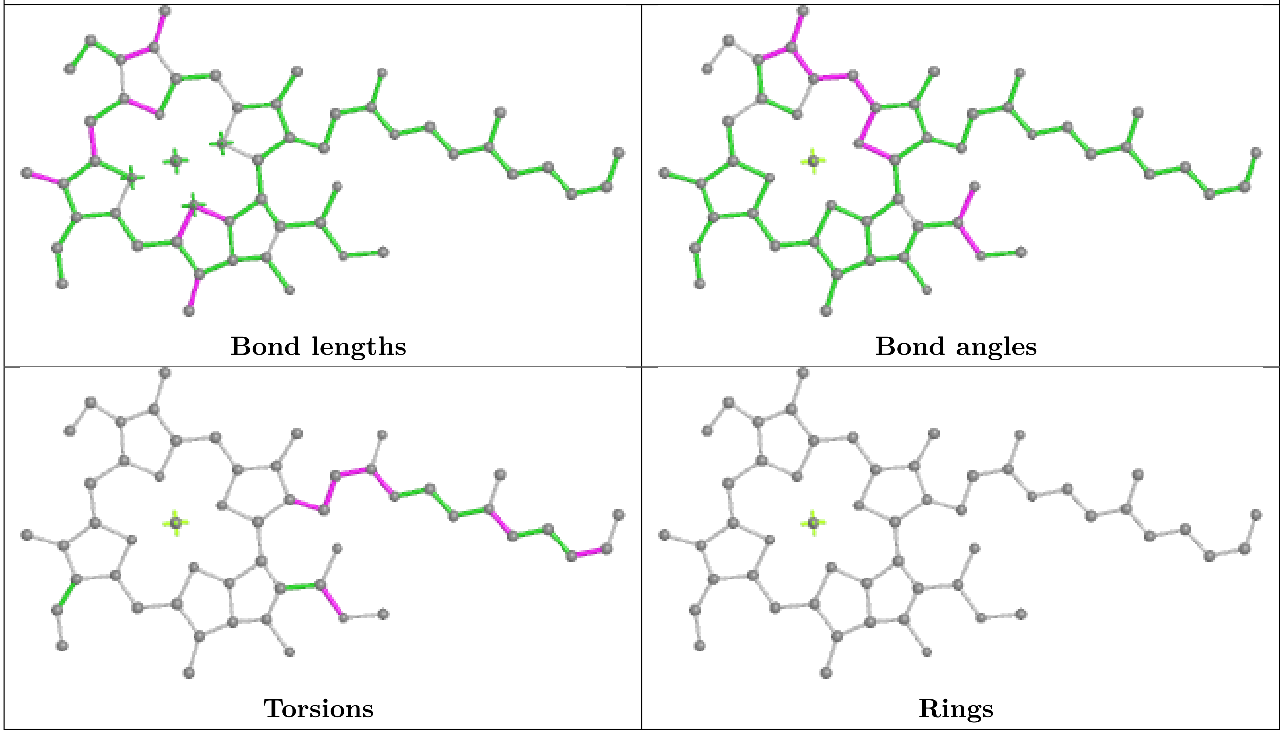
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA bA 812



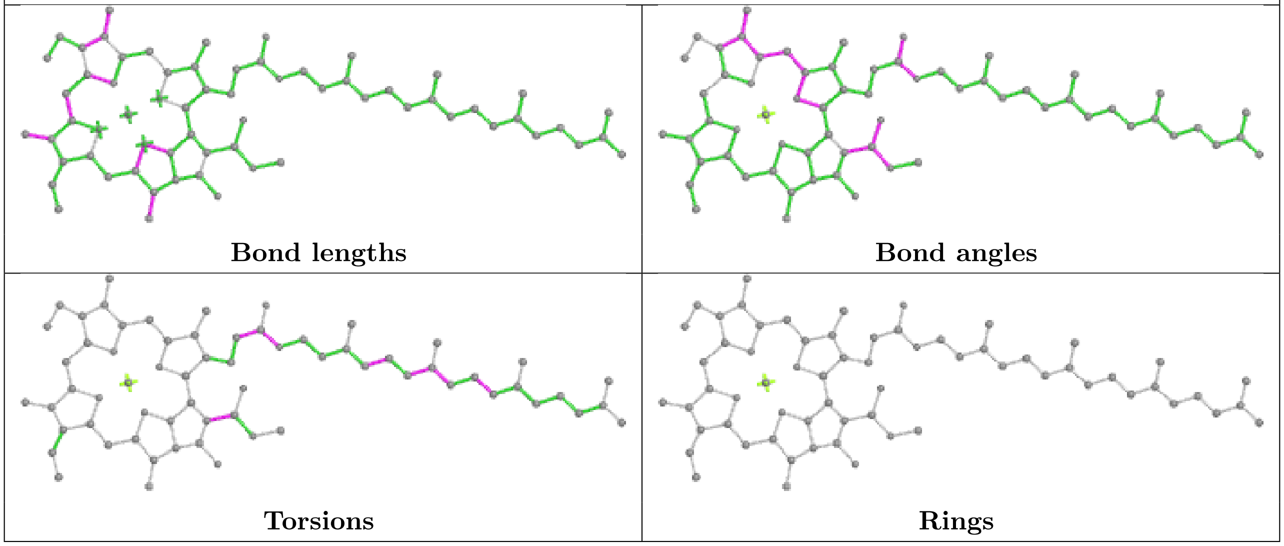
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA aA 827



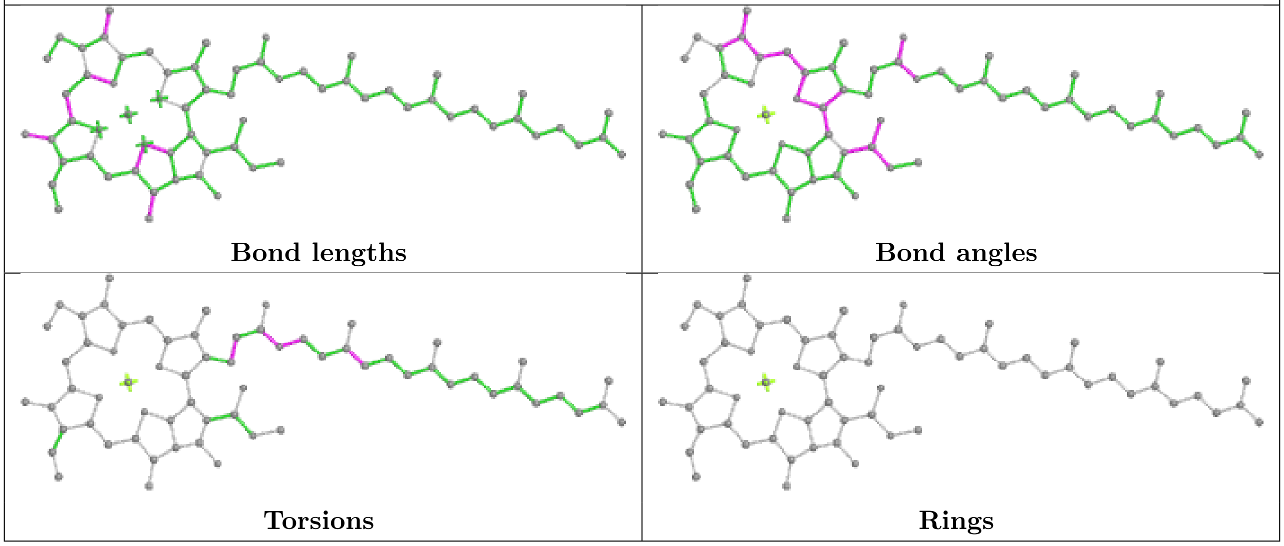
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA cA 828



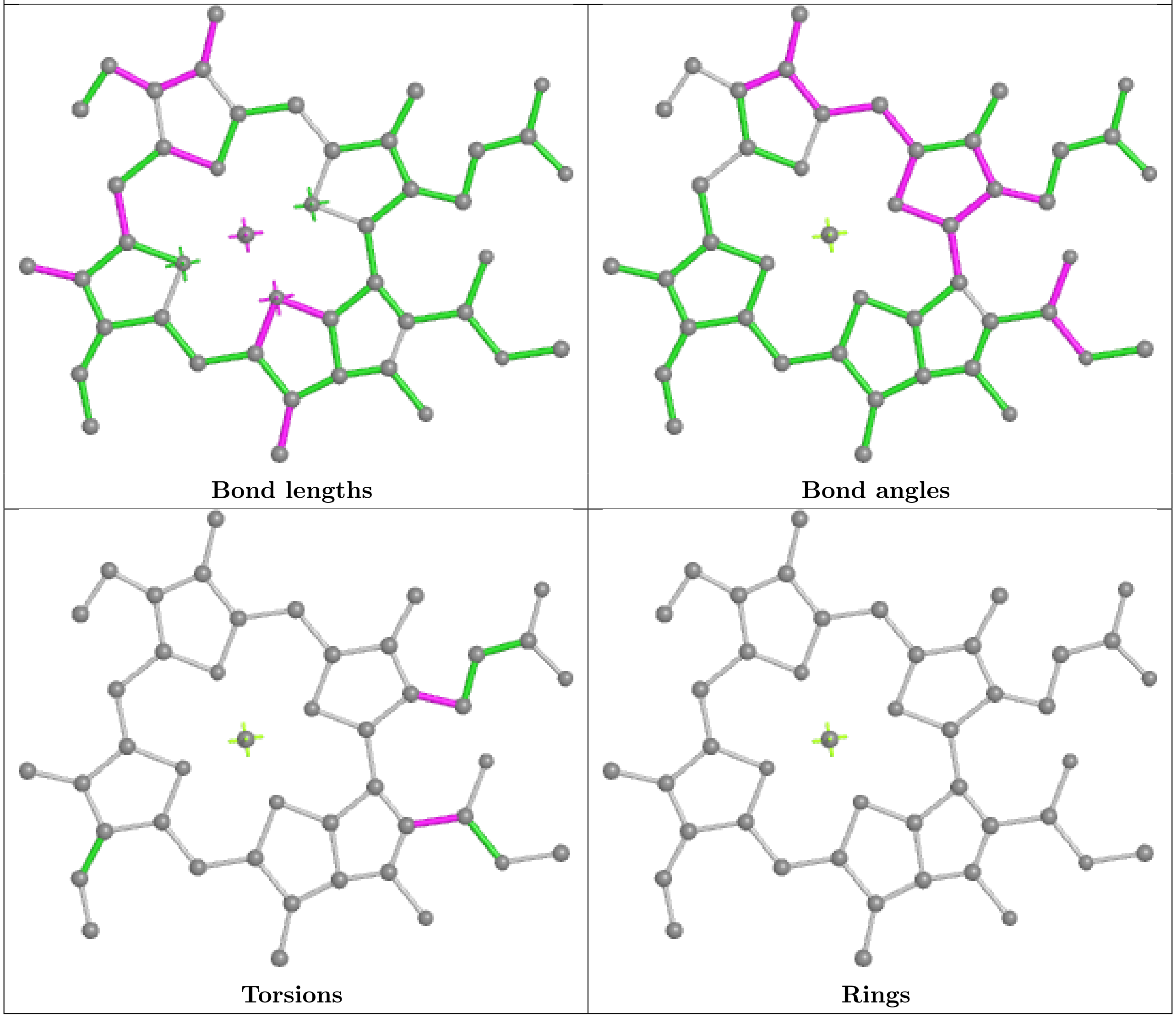
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA dA 805



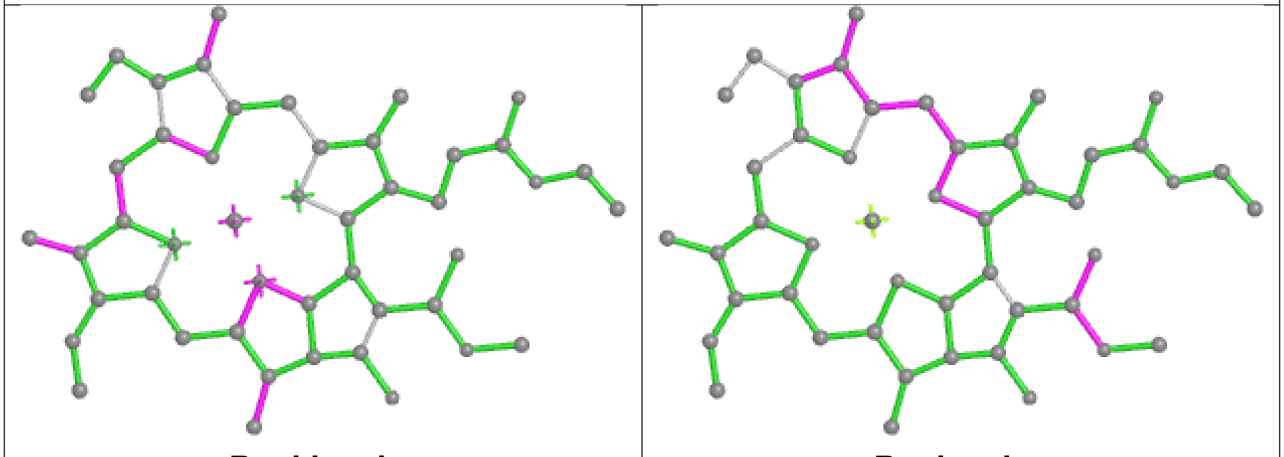
Bond lengths

Bond angles

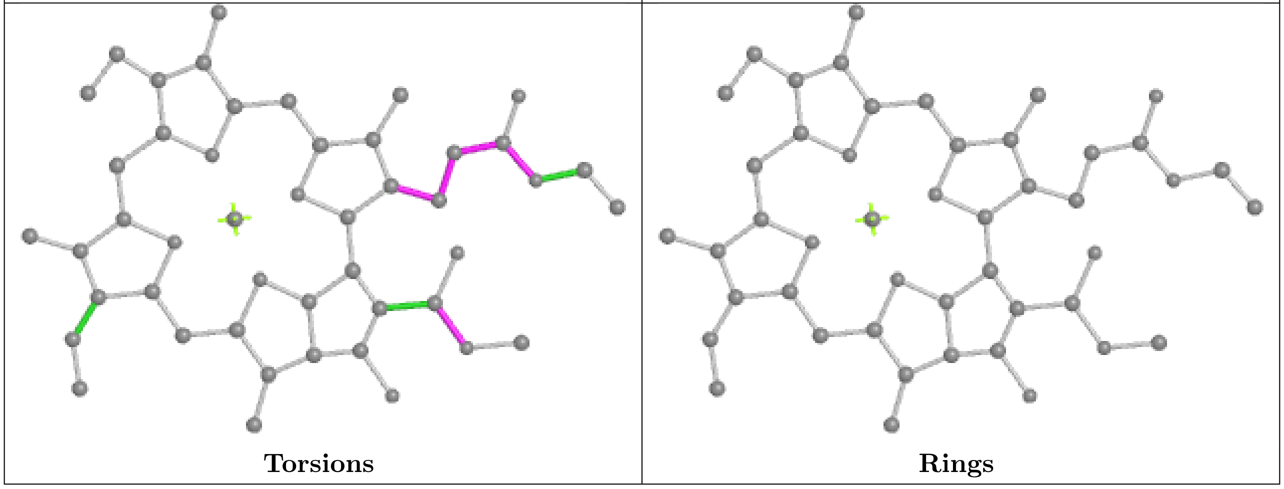
Torsions

Rings

Ligand CLA bB 821

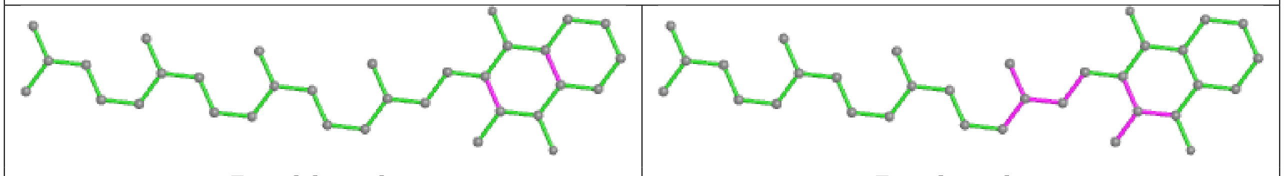


Bond lengths **Bond angles**

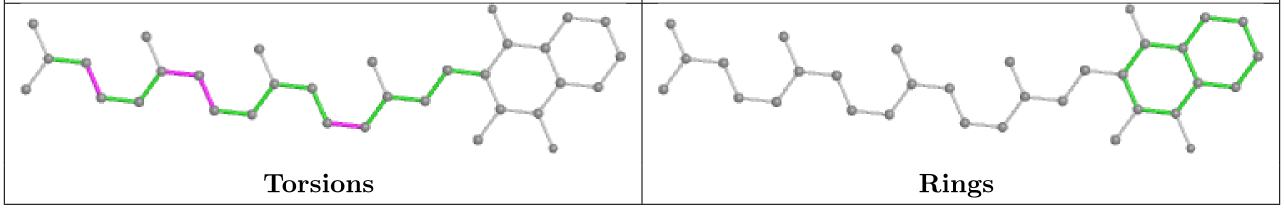


Torsions **Rings**

Ligand PQN dB 843

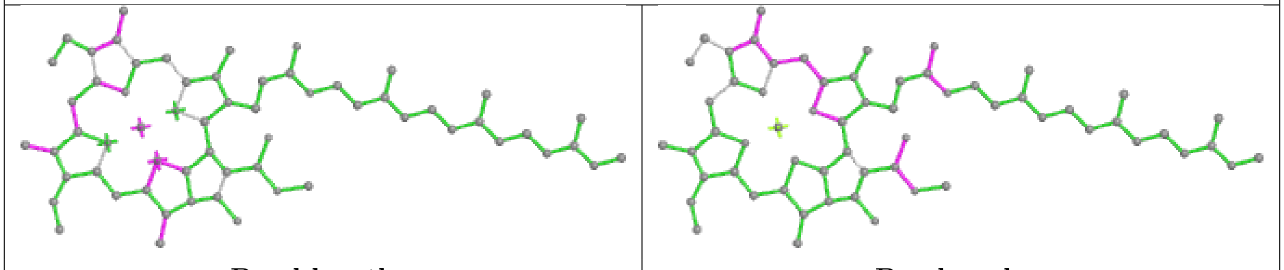


Bond lengths **Bond angles**



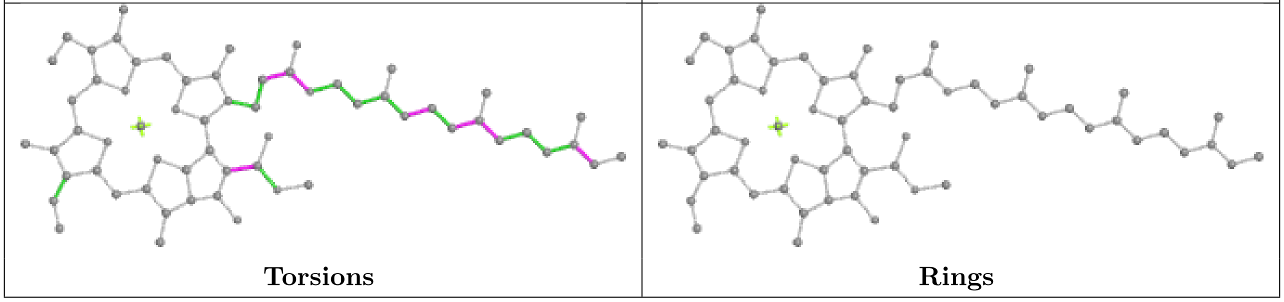
Torsions **Rings**

Ligand CLA dA 820



Bond lengths

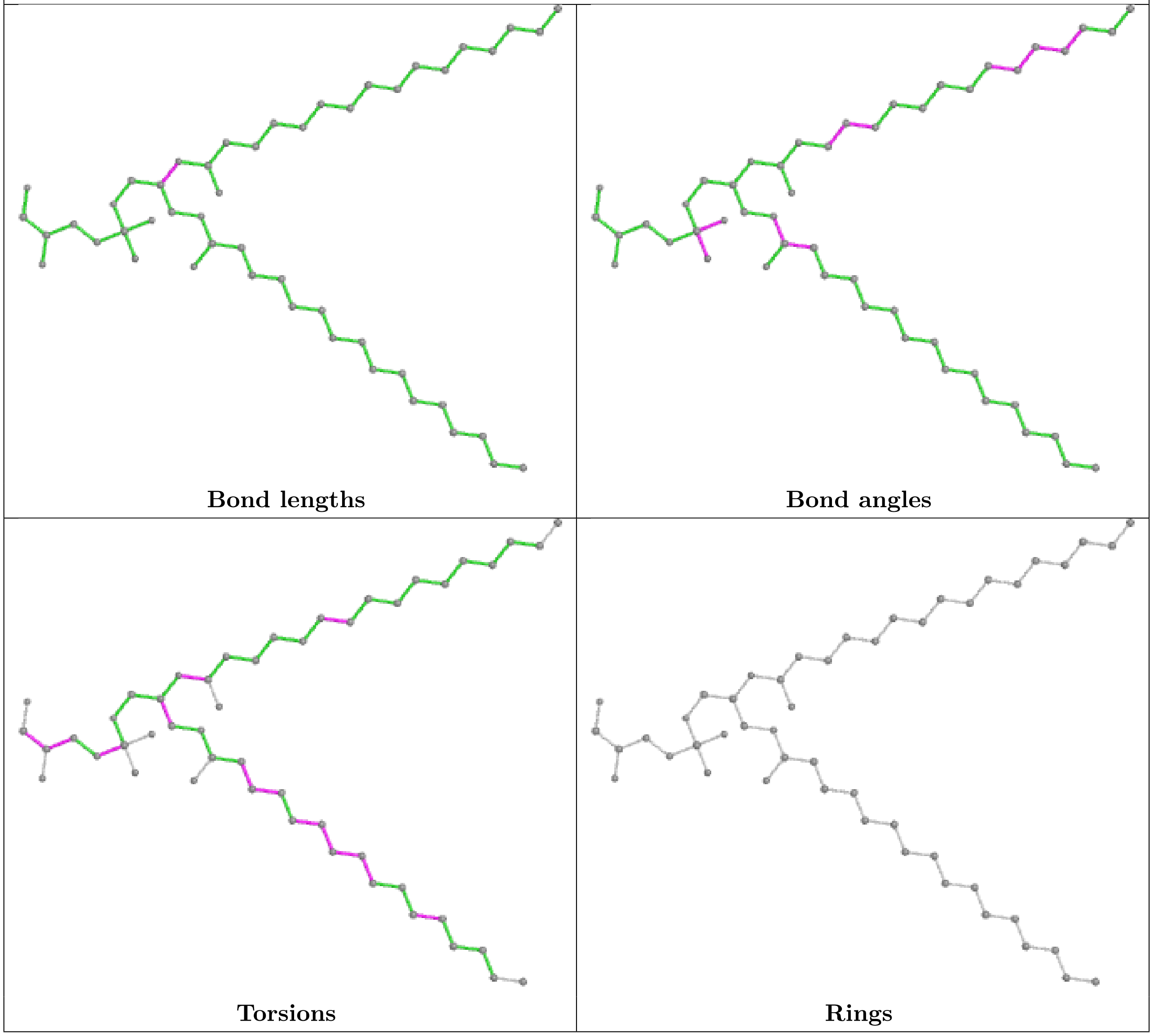
Bond angles



Torsions

Rings

Ligand LHG dA 850



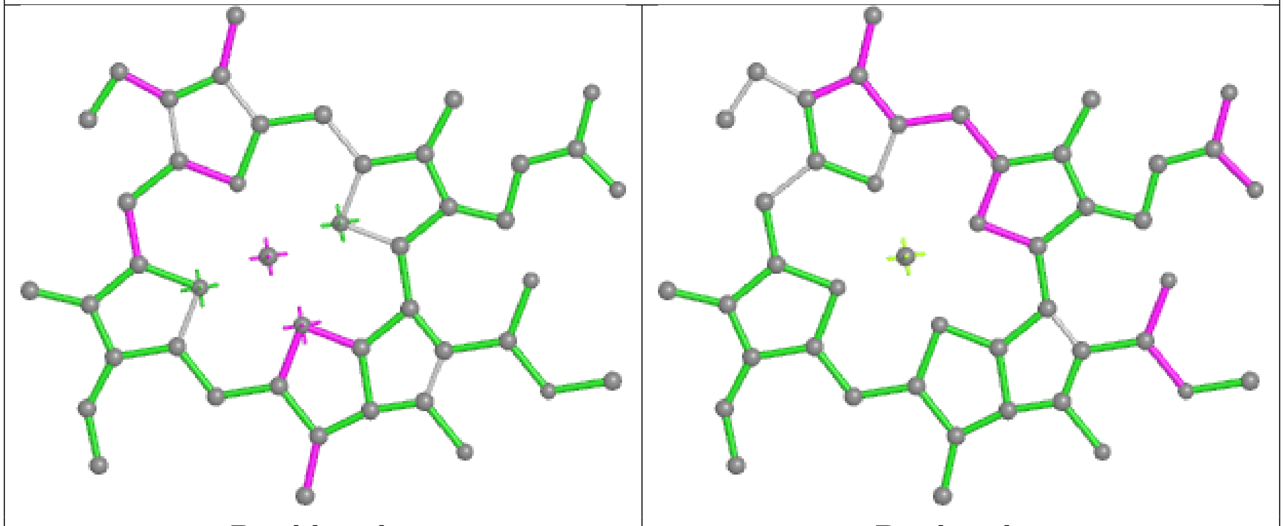
Bond lengths

Bond angles

Torsions

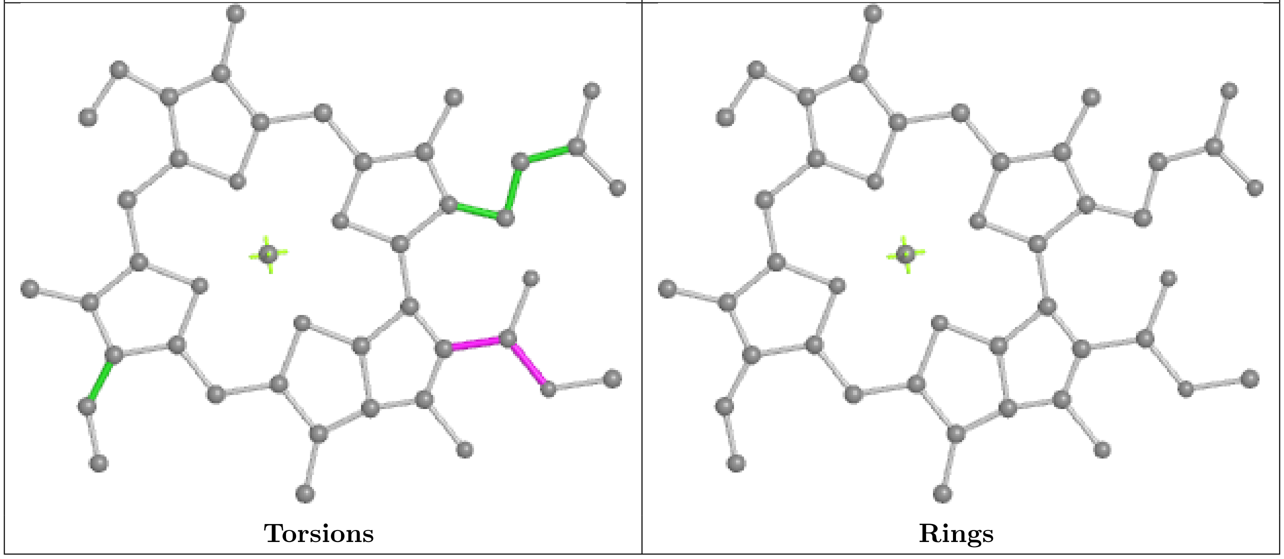
Rings

Ligand CLA bB 822



Bond lengths

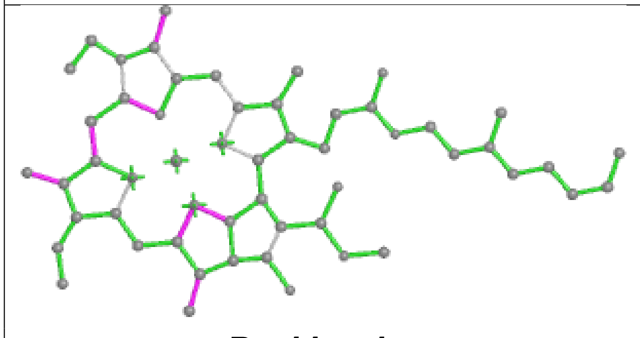
Bond angles



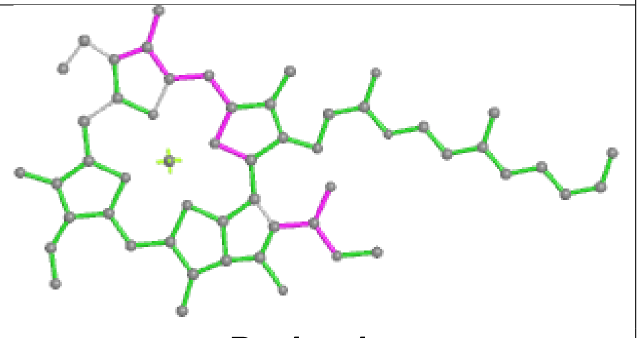
Torsions

Rings

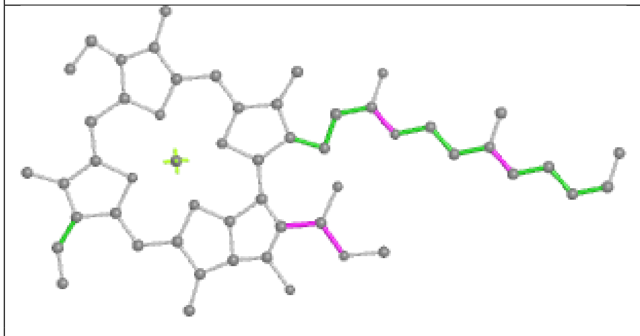
Ligand CLA bB 805



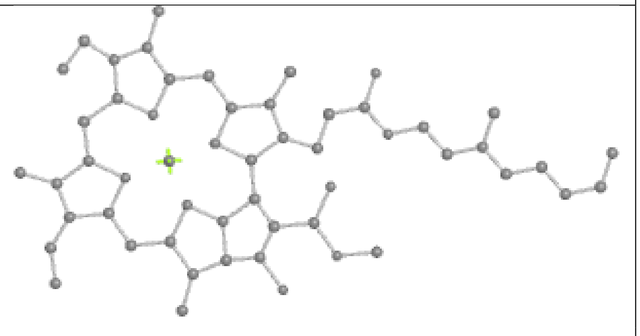
Bond lengths



Bond angles

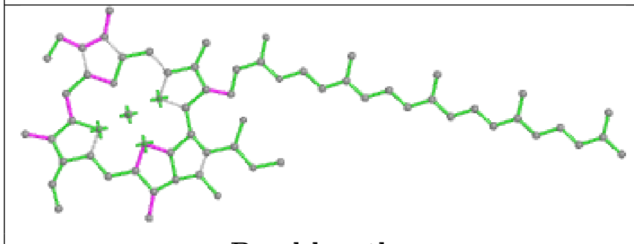


Torsions

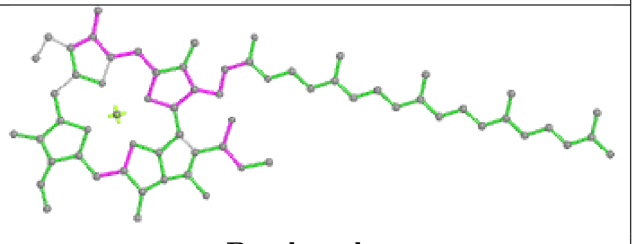


Rings

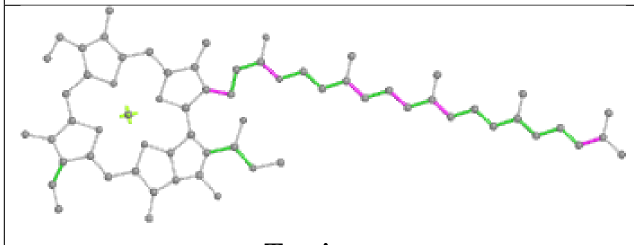
Ligand CLA aA 832



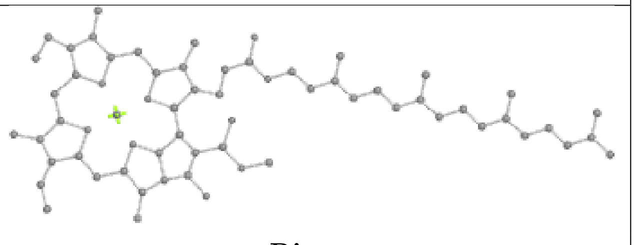
Bond lengths



Bond angles

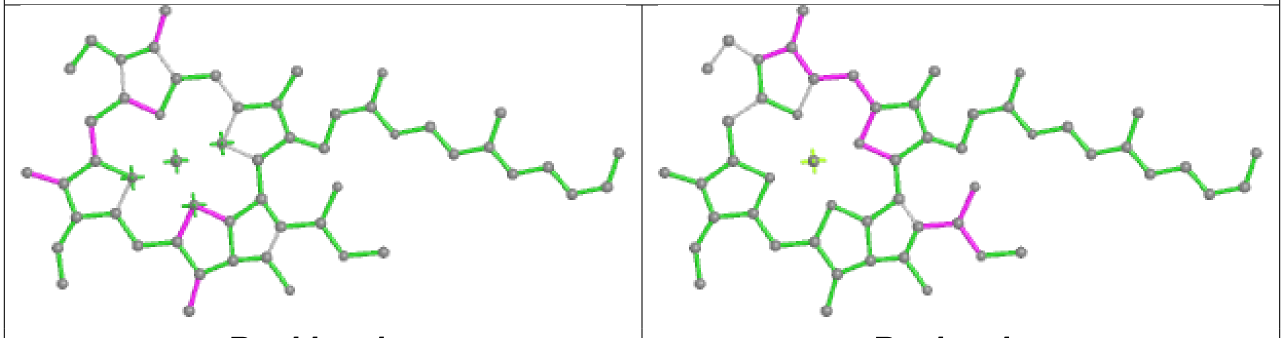


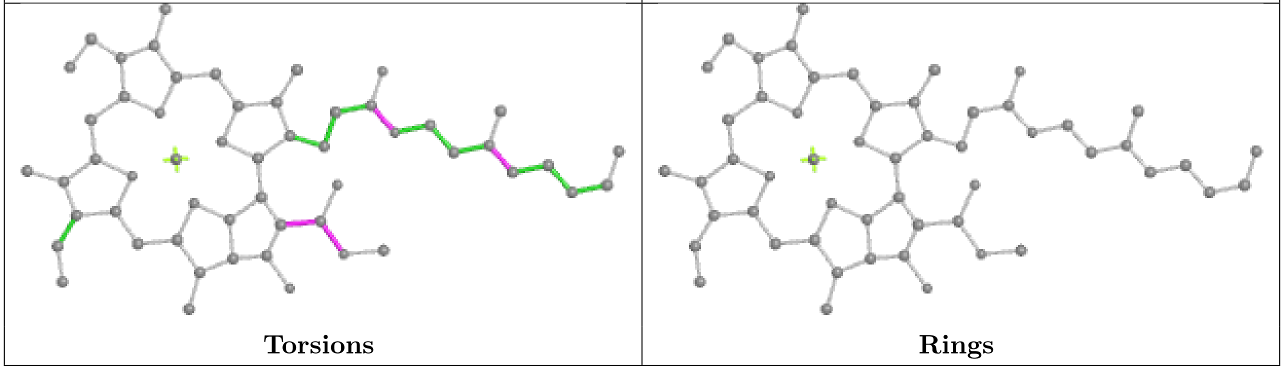
Torsions



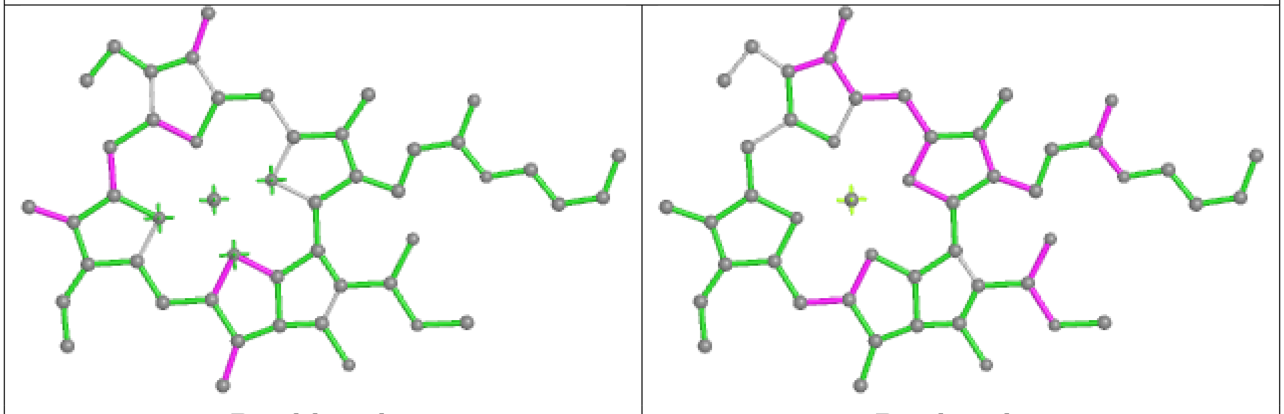
Rings

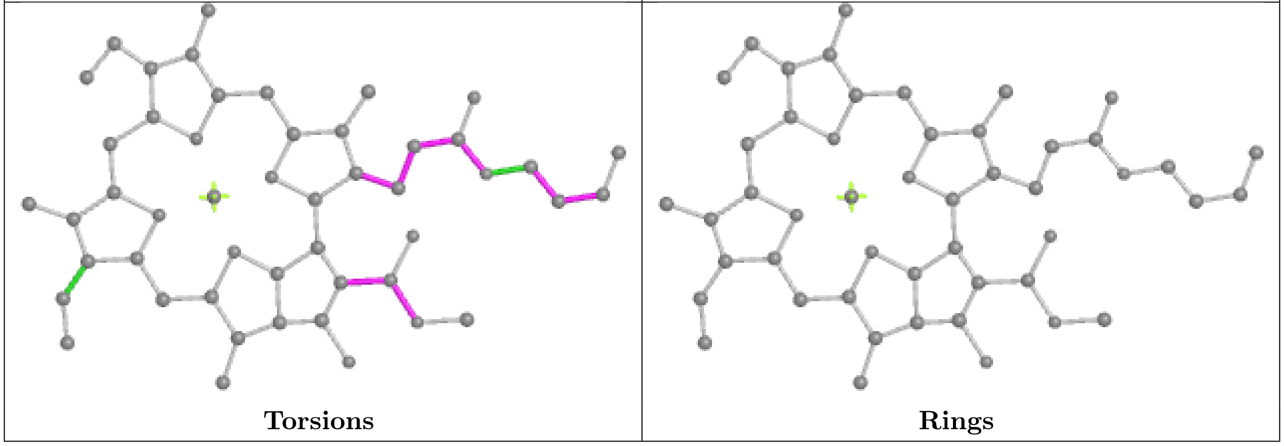
Ligand CLA aB 805


Bond lengths Bond angles

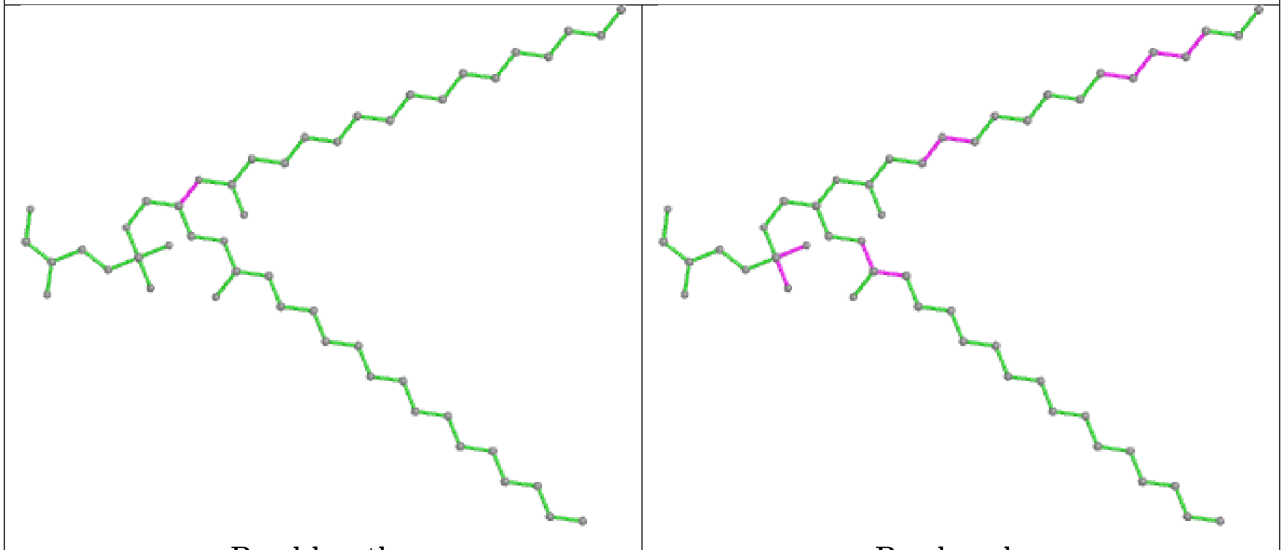

Torsions Rings

Ligand CLA aB 831


Bond lengths Bond angles

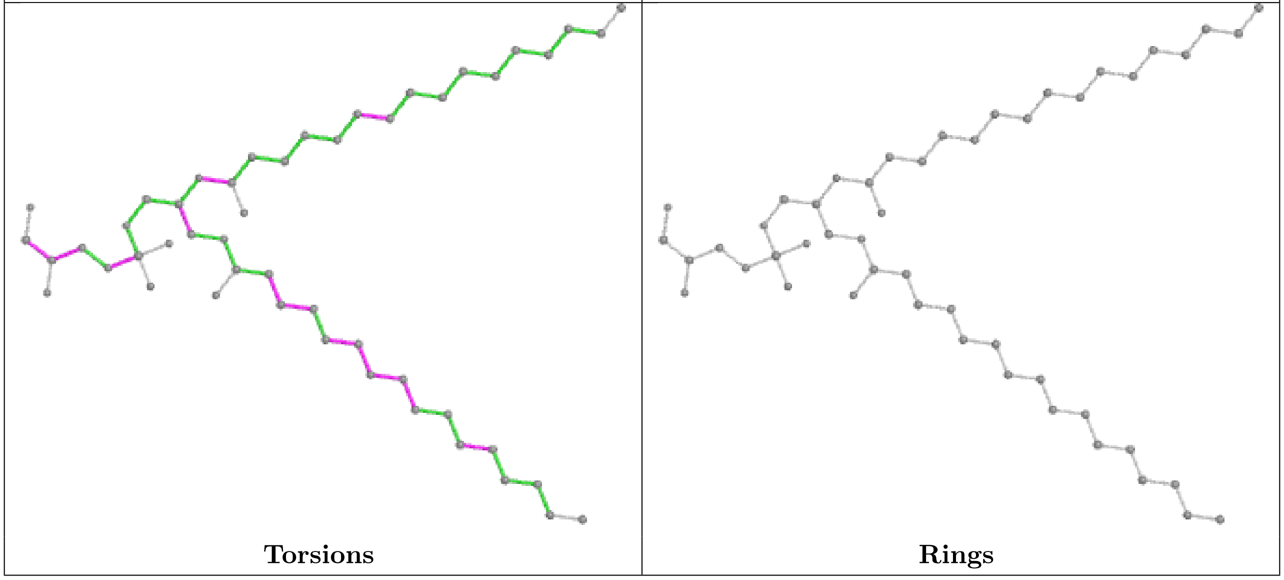

Torsions Rings

Ligand LHG bA 850



Bond lengths

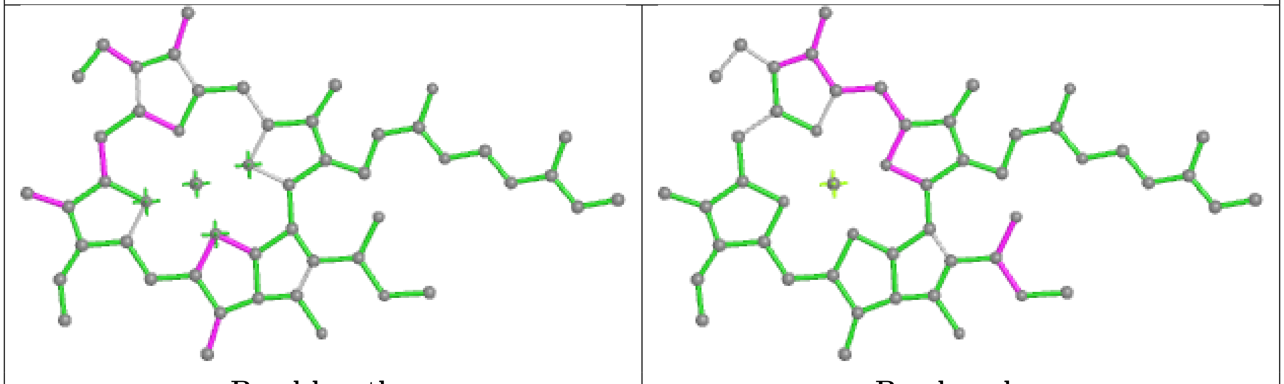
Bond angles



Torsions

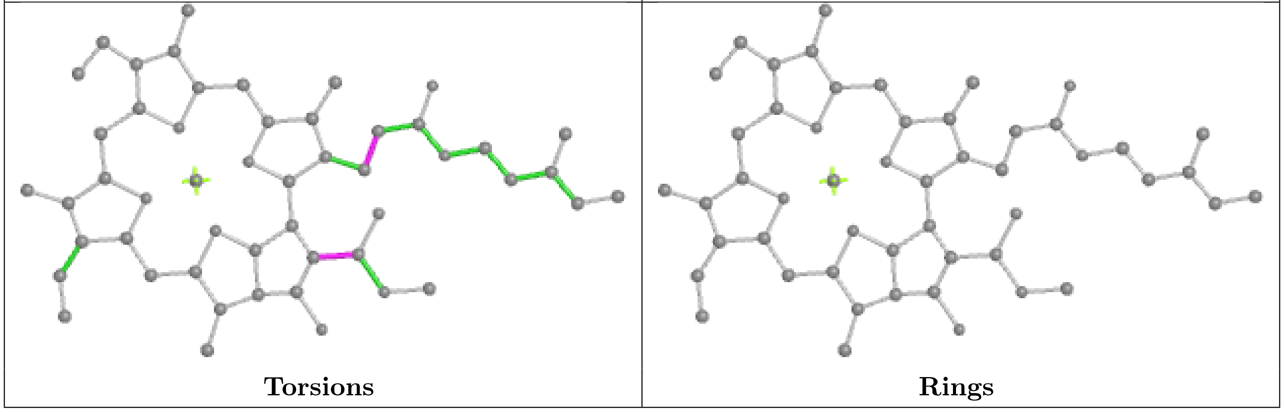
Rings

Ligand CLA dA 807



Bond lengths

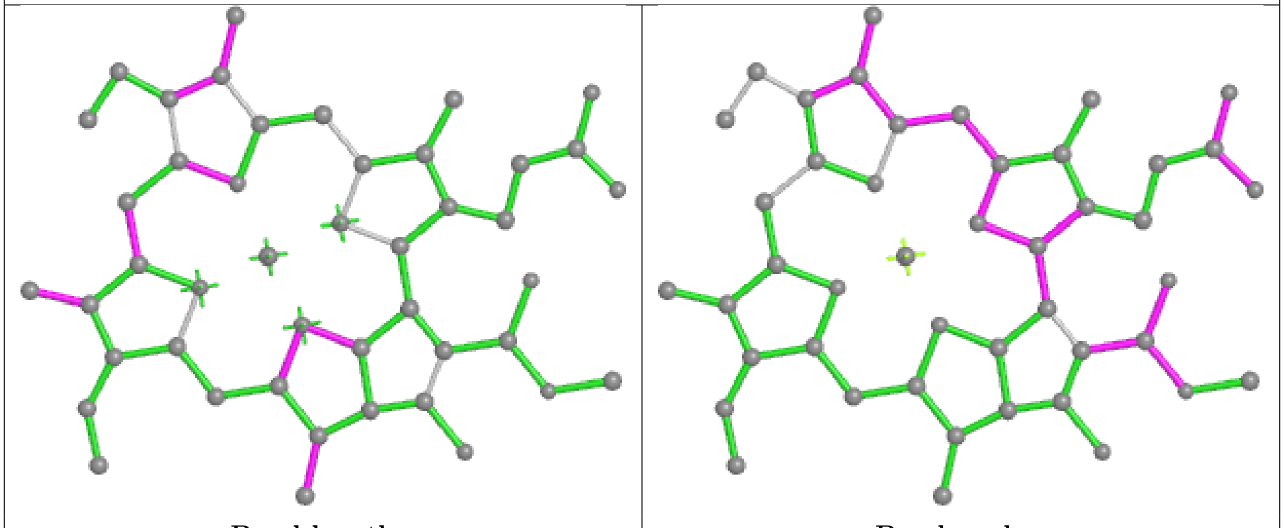
Bond angles



Torsions

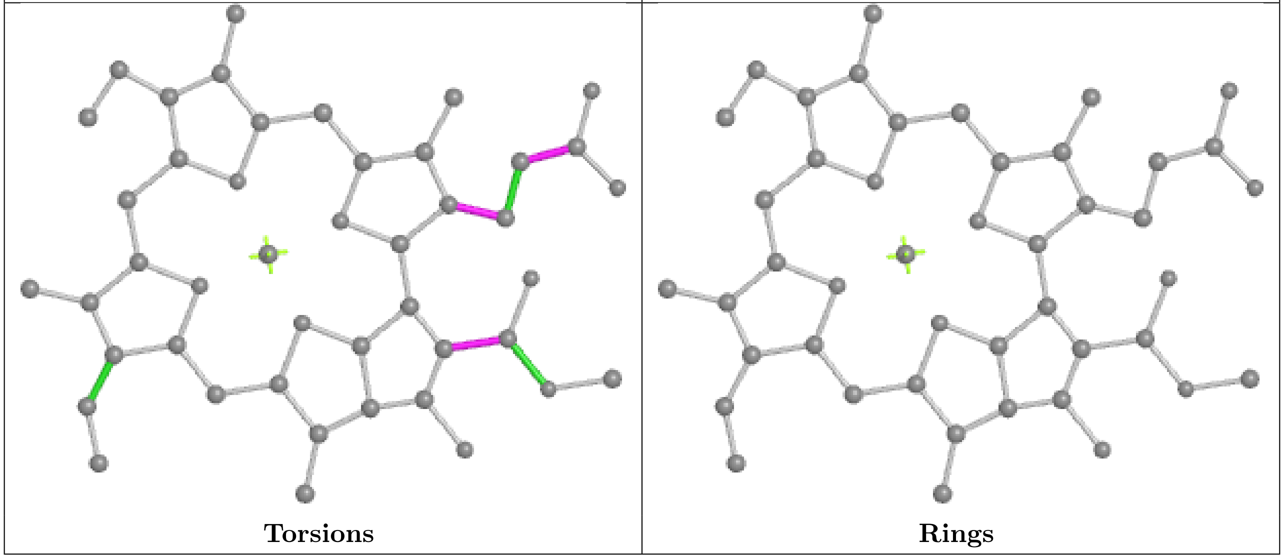
Rings

Ligand CLA cA 803



Bond lengths

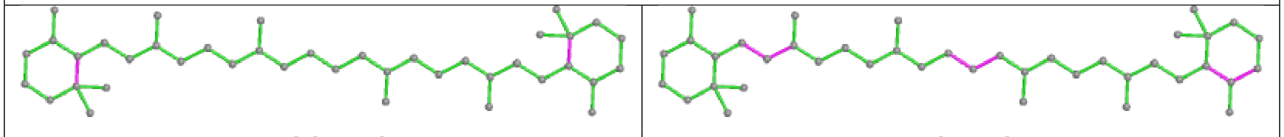
Bond angles



Torsions

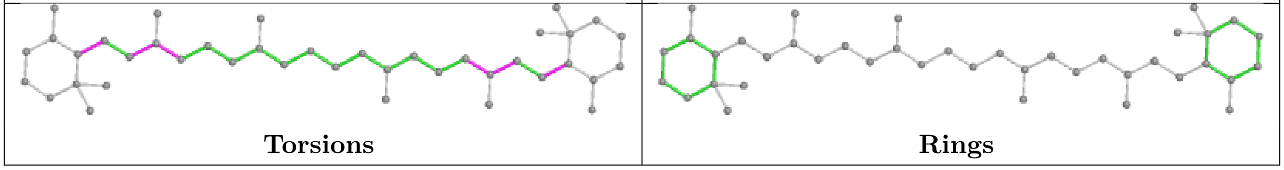
Rings

Ligand BCR dB 846



Bond lengths

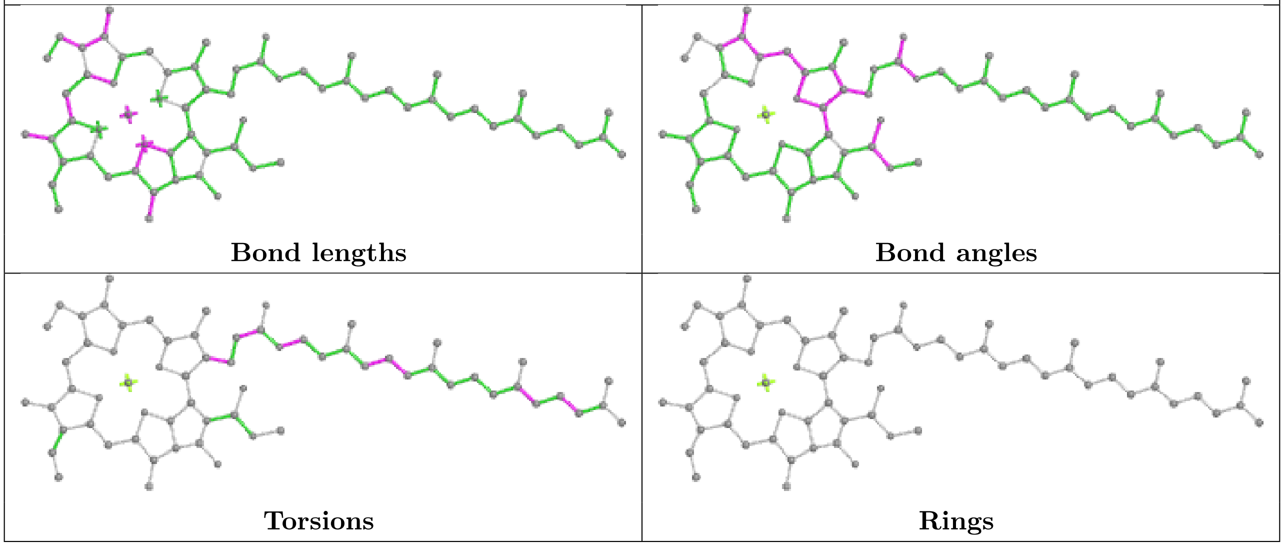
Bond angles



Torsions

Rings

Ligand CLA aA 806



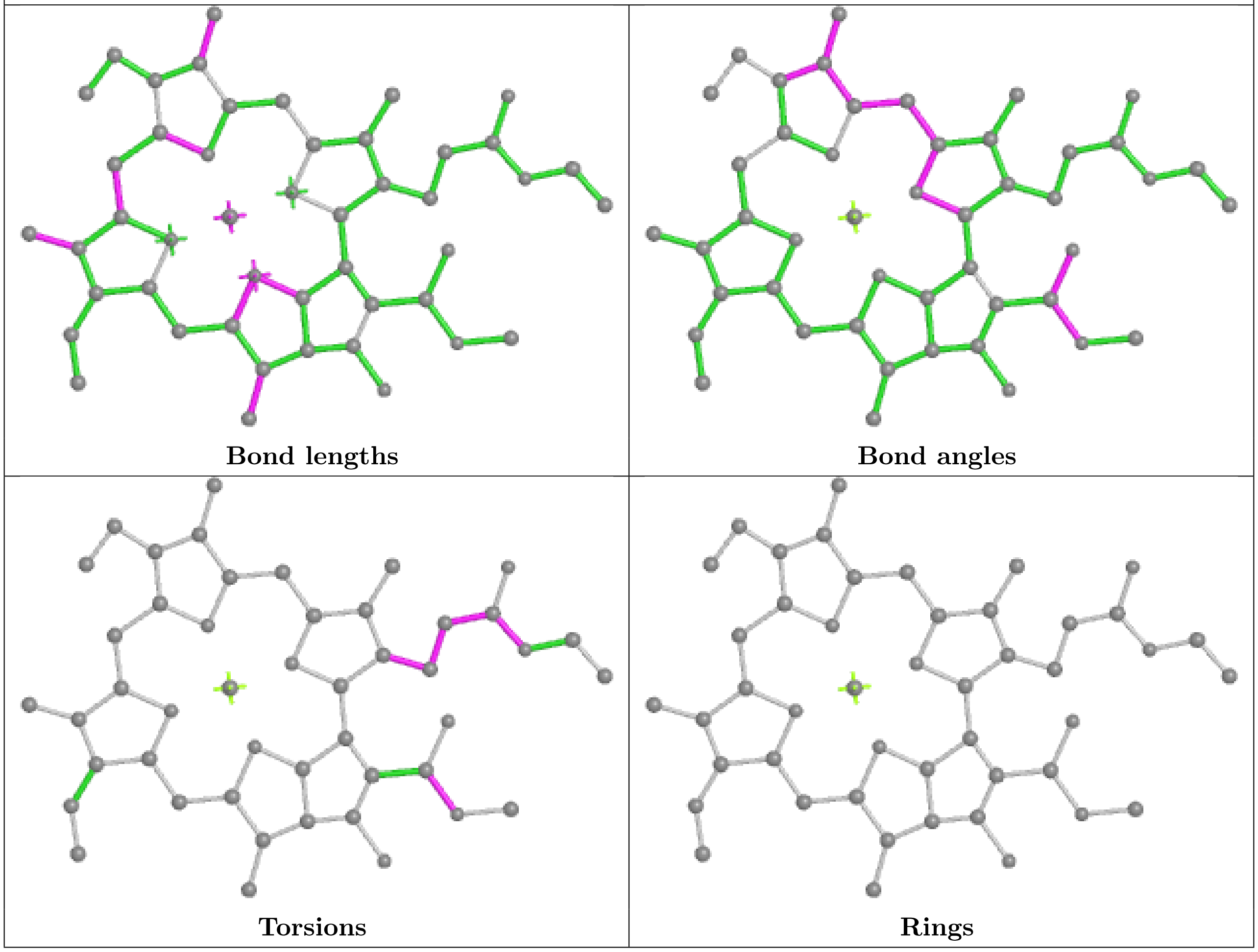
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA aB 820



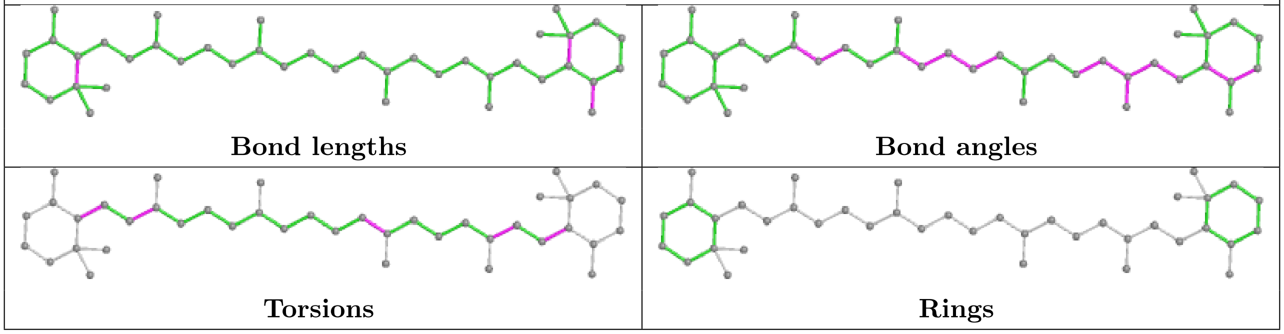
Bond lengths

Bond angles

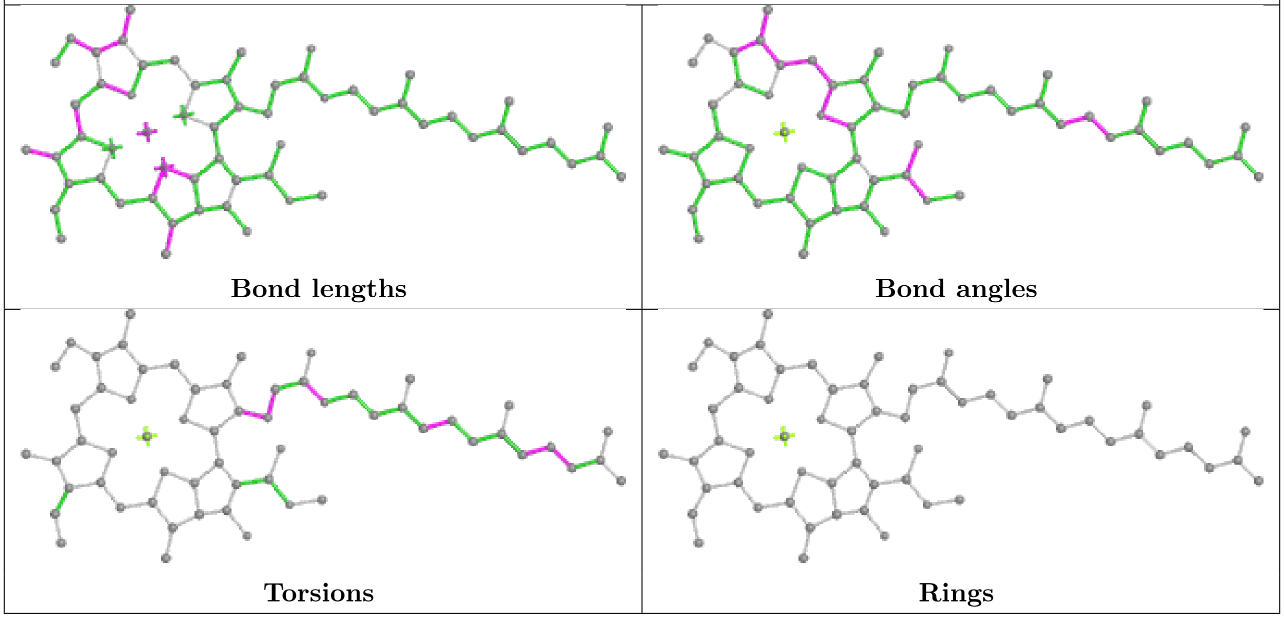
Torsions

Rings

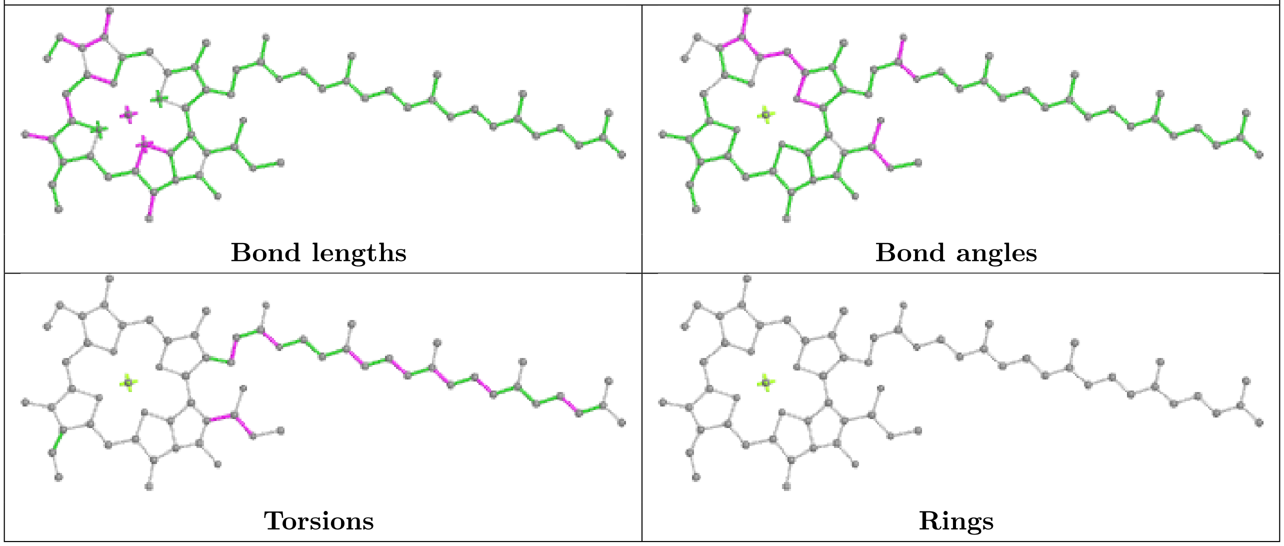
Ligand BCR bL 207



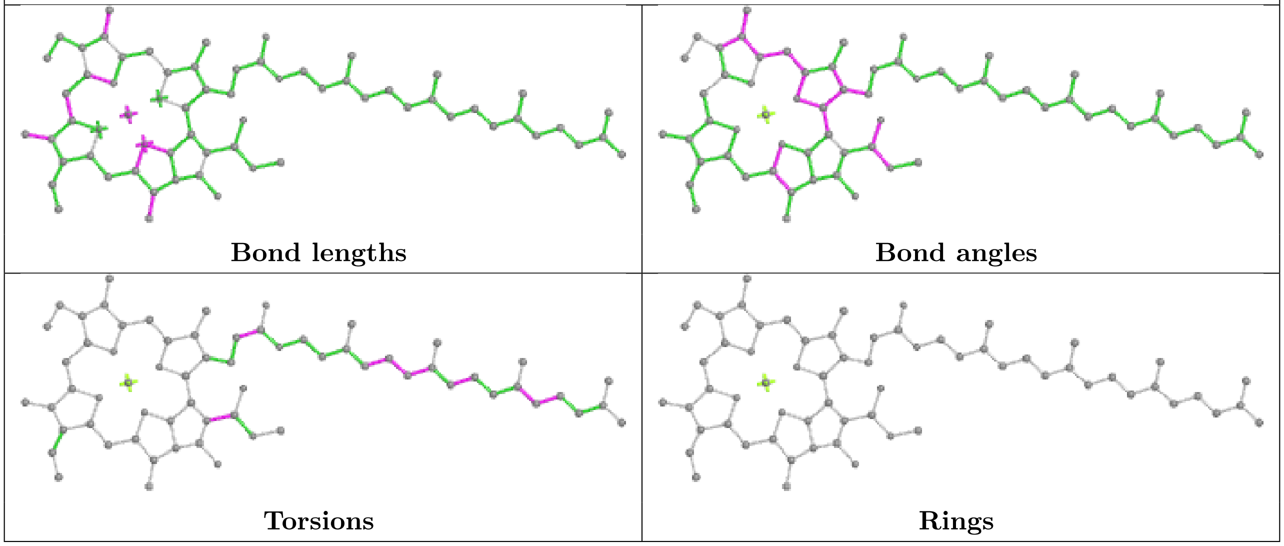
Ligand CLA cB 818



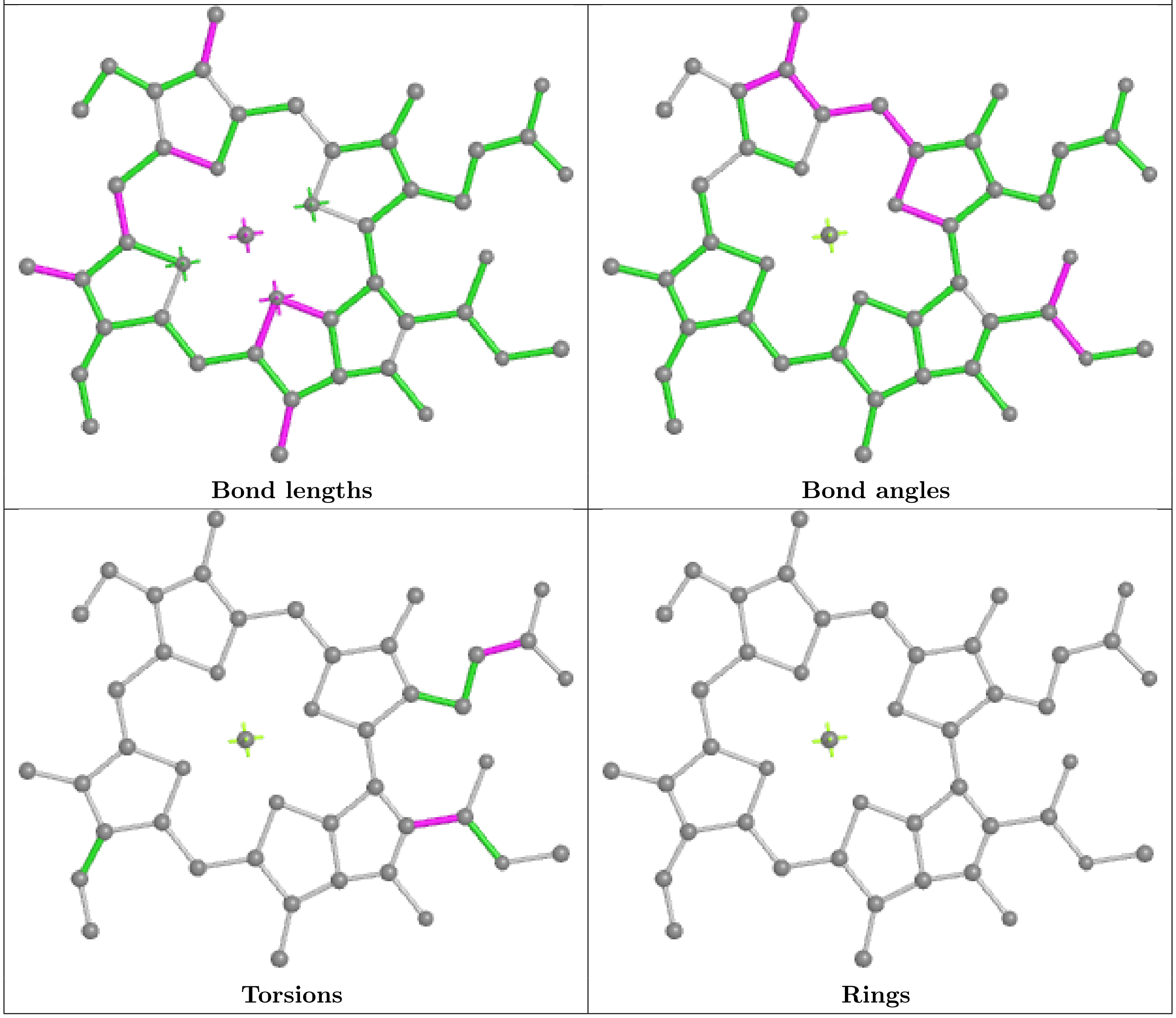
Ligand CLA dA 821



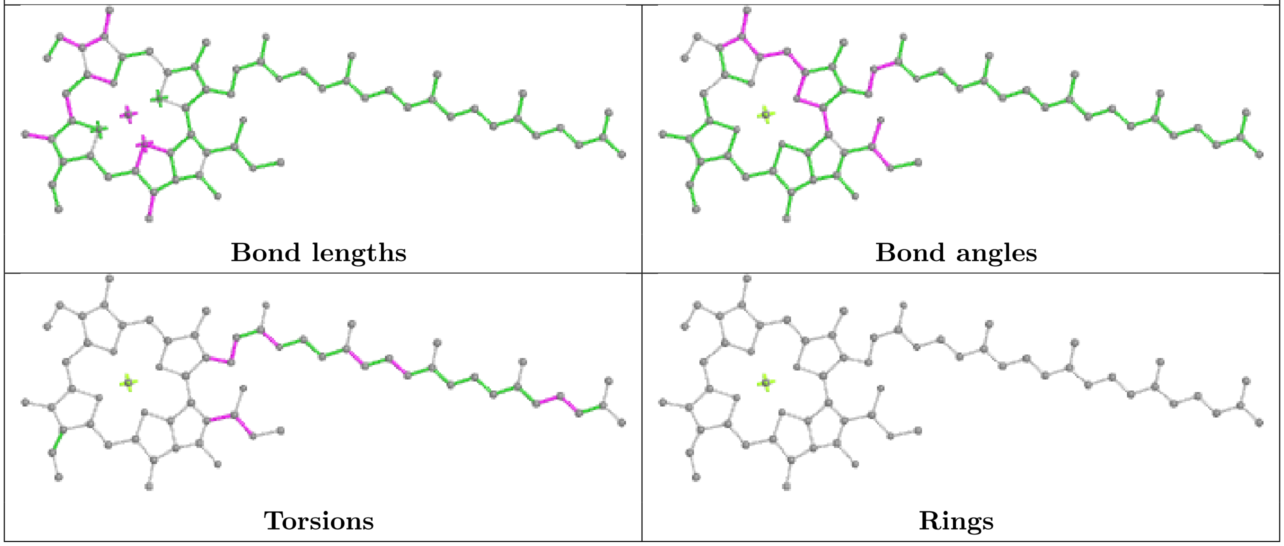
Ligand CLA cA 825



Ligand CLA bK 103



Ligand CLA dB 801



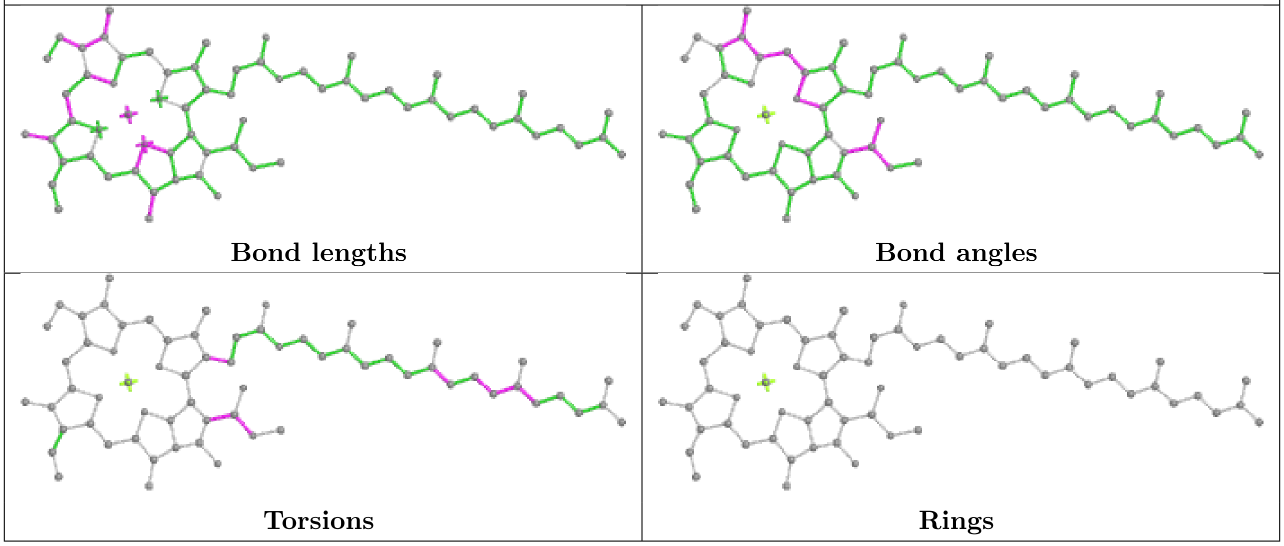
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA aA 830



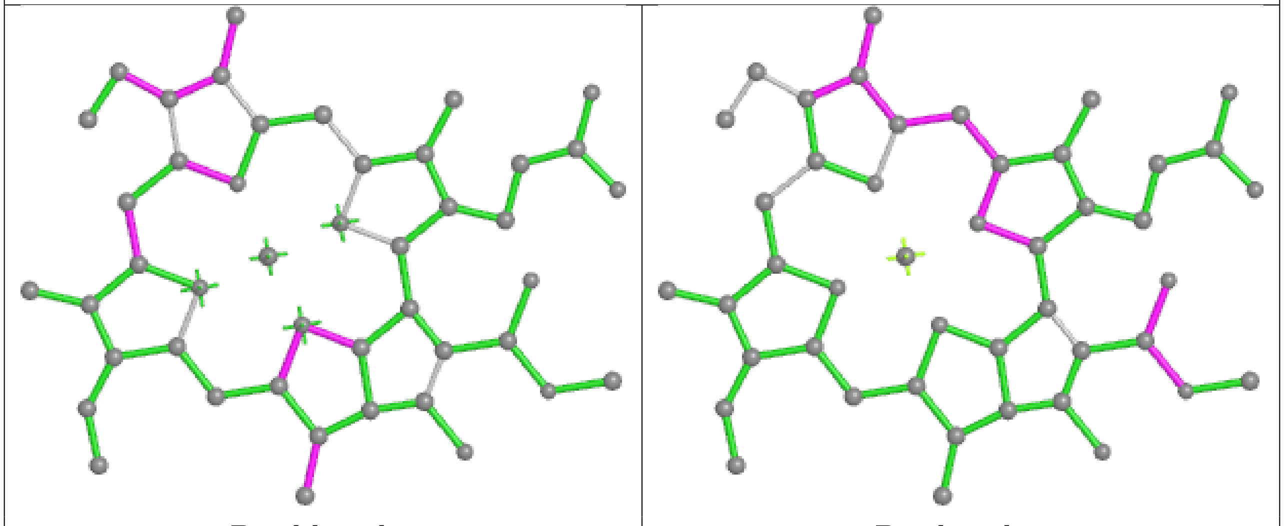
Bond lengths

Bond angles

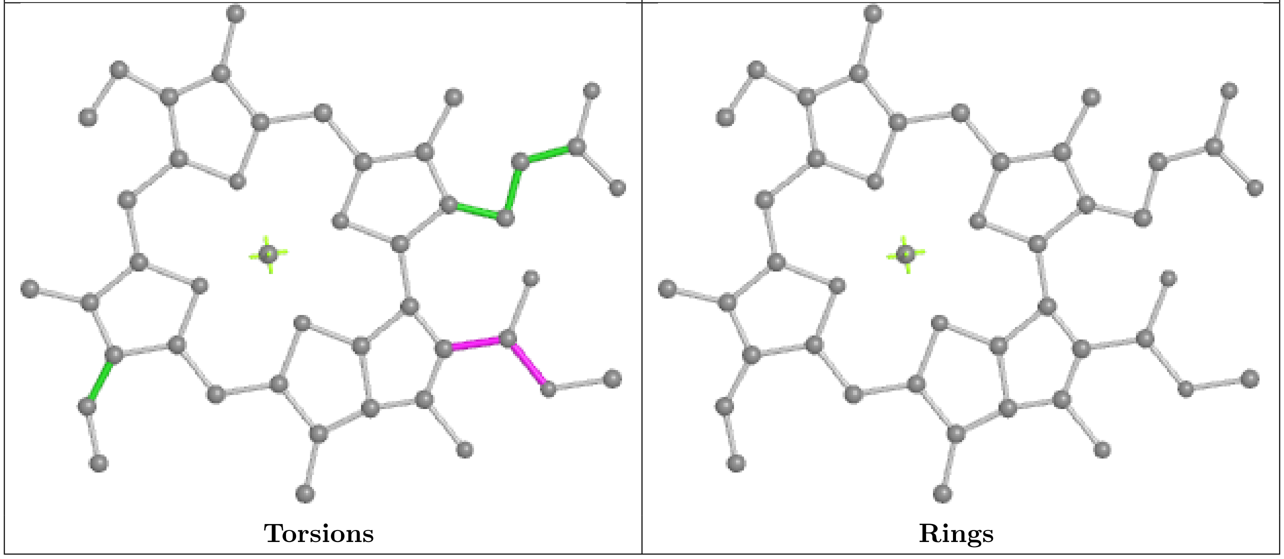
Torsions

Rings

Ligand CLA aA 815

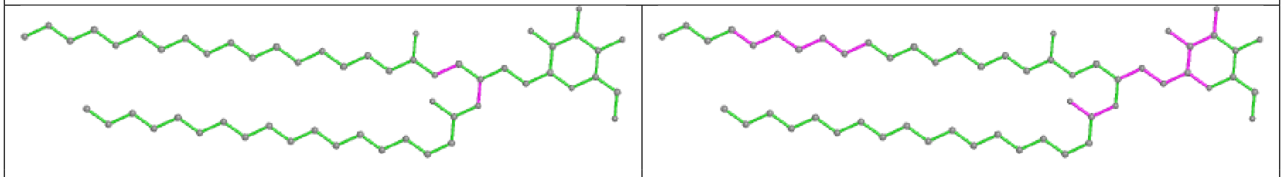


Bond lengths Bond angles

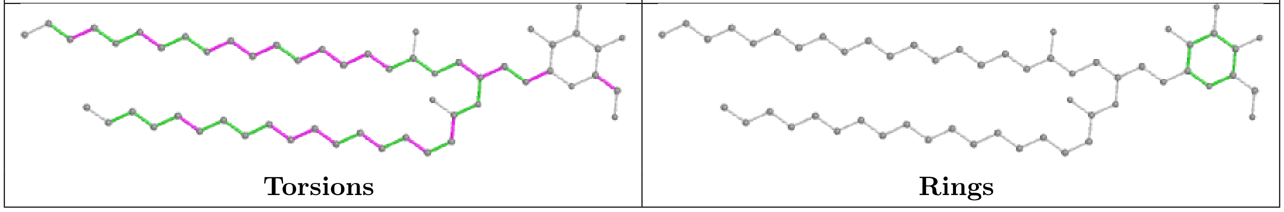


Torsions Rings

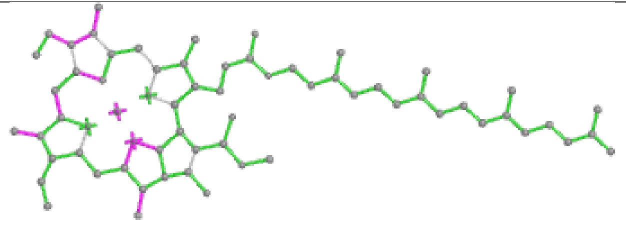
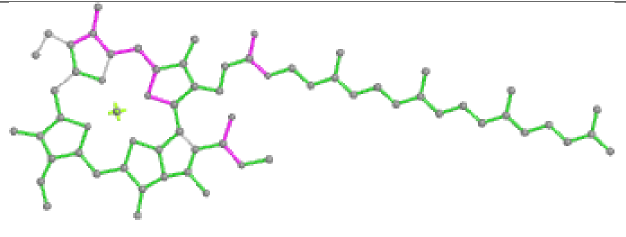
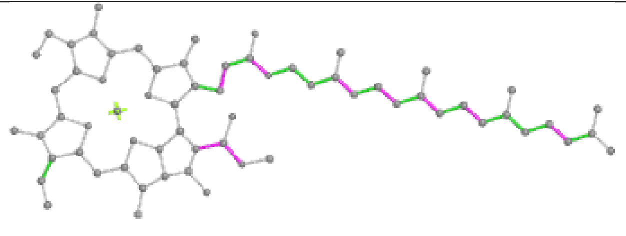
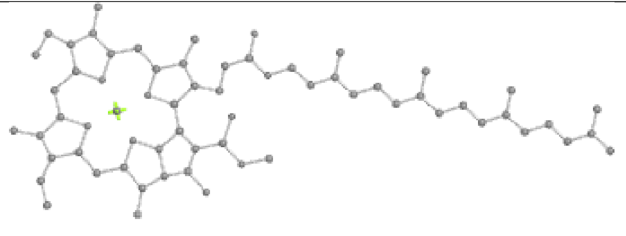
Ligand LMG dB 850

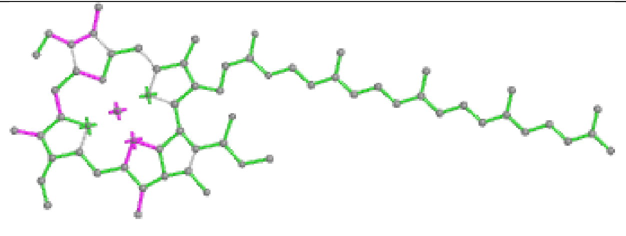
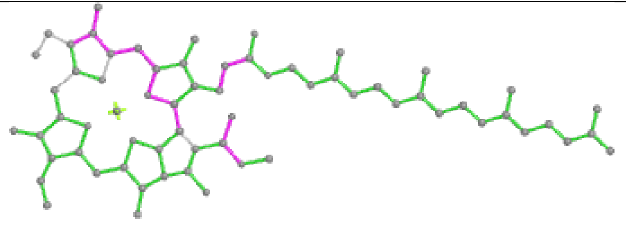
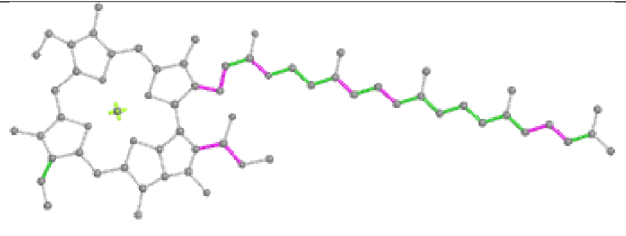
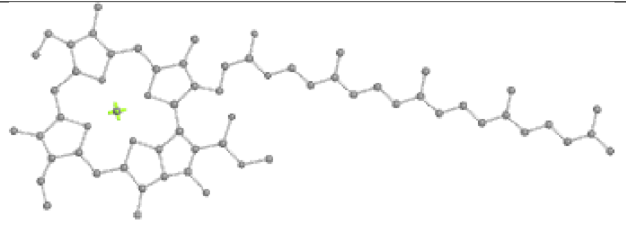


Bond lengths Bond angles



Torsions Rings

Ligand CLA bA 821	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA aB 801	
 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.

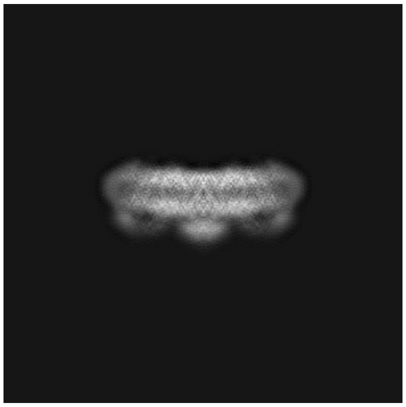
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-9807. These allow visual inspection of the internal detail of the map and identification of artifacts.

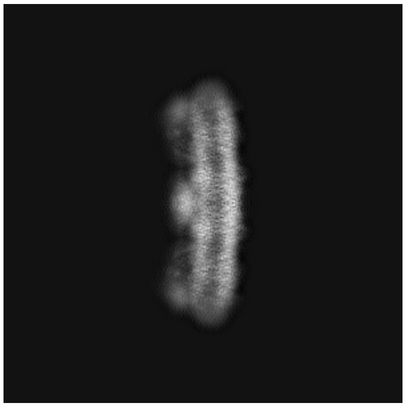
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

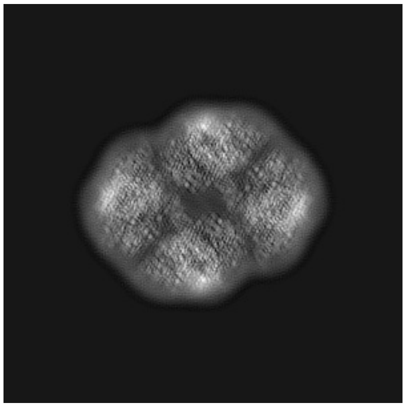
6.1.1 Primary map



X



Y

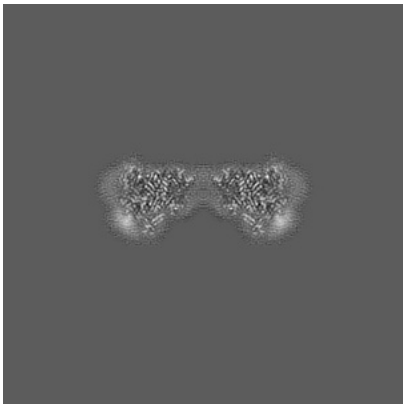


Z

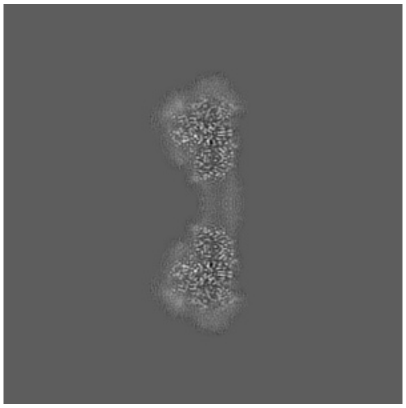
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

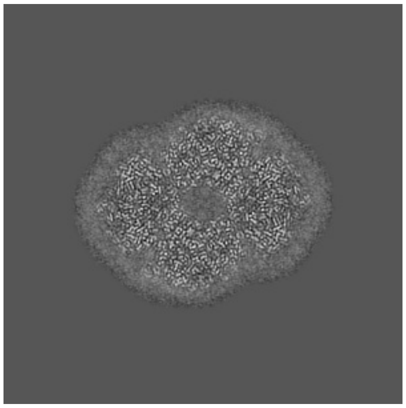
6.2.1 Primary map



X Index: 220



Y Index: 220

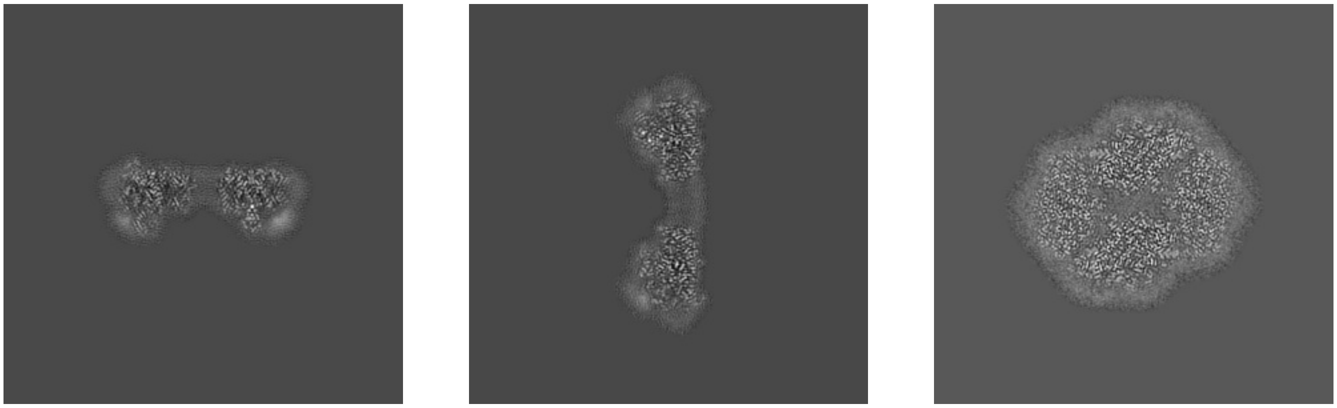


Z Index: 220

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

6.3 Largest variance slices

6.3.1 Primary map

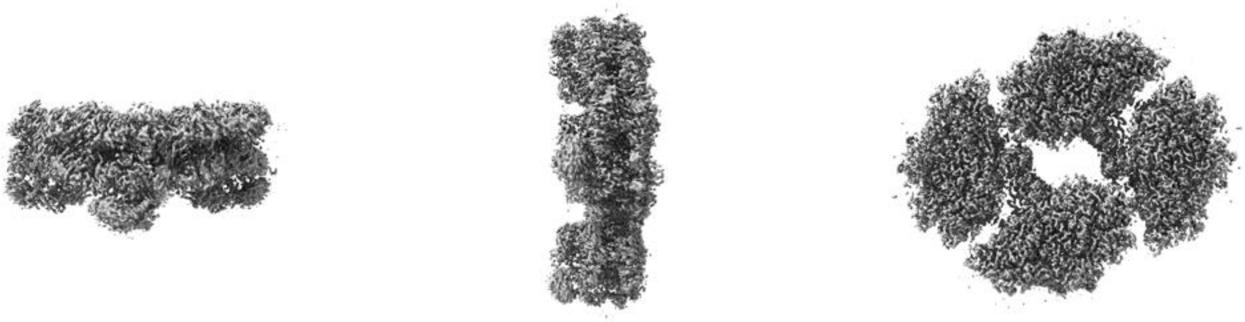


X Index: 226 Y Index: 222 Z Index: 245

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

6.4 Orthogonal surface views

6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.06. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

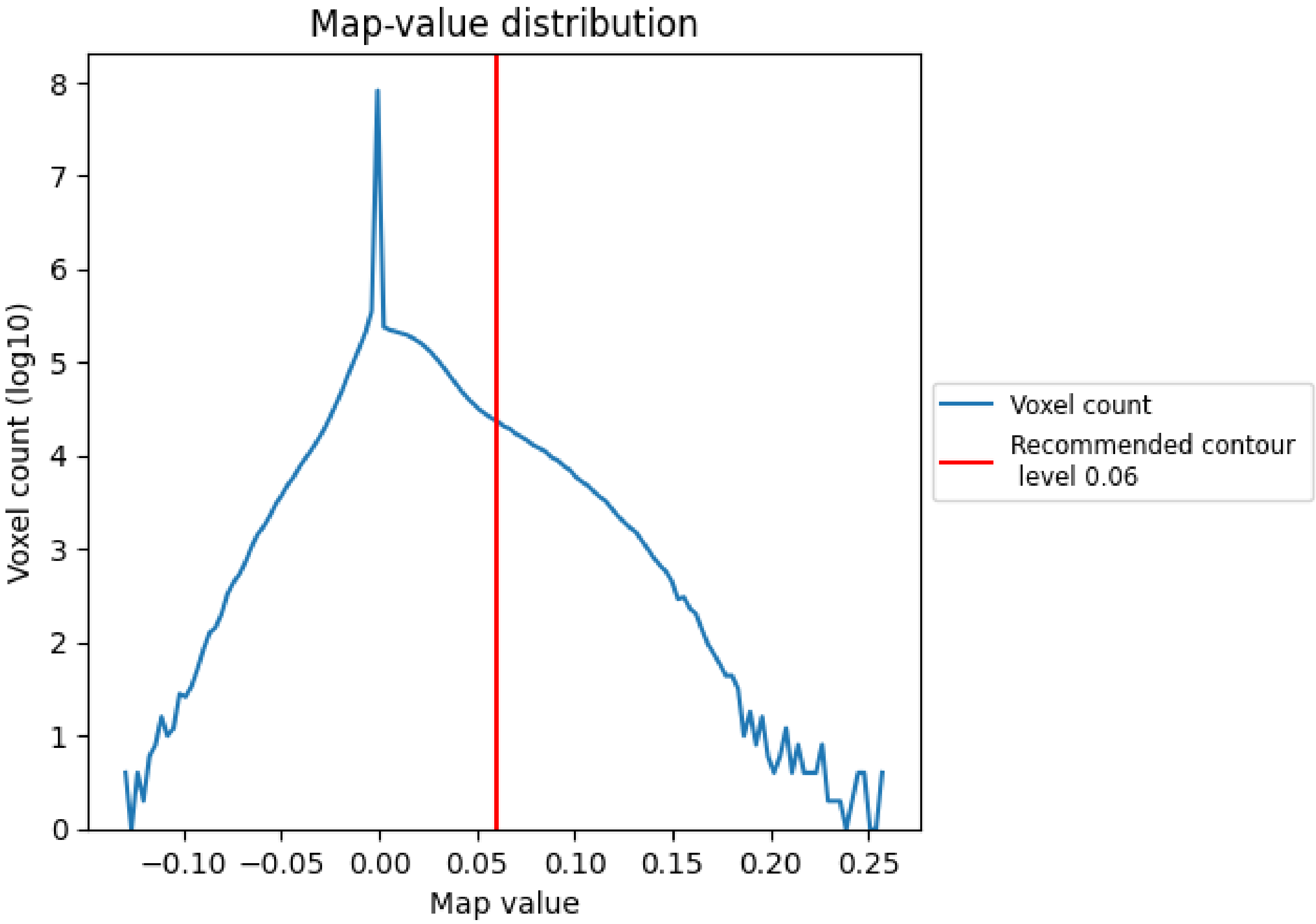
6.5 Mask visualisation ⓘ

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

7 Map analysis ⓘ

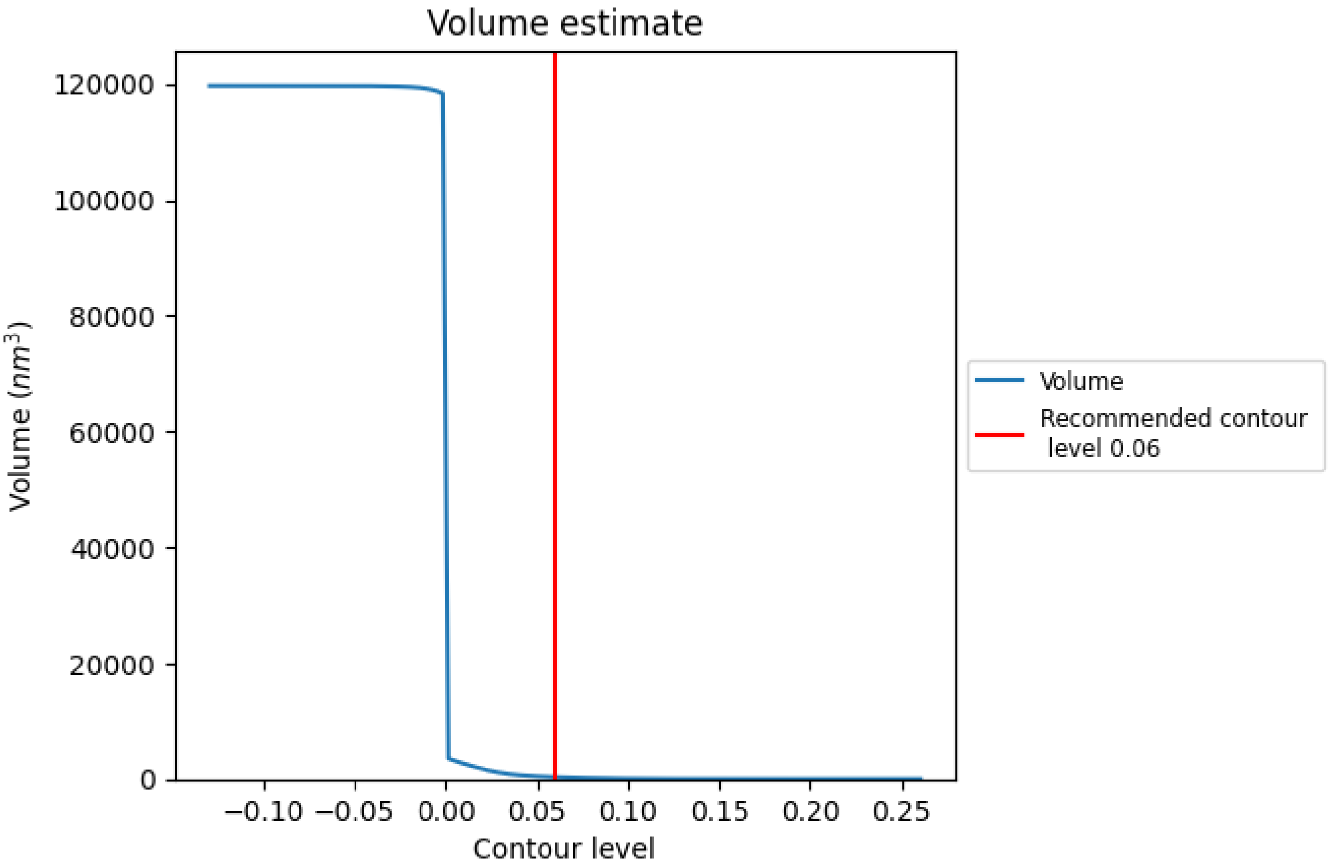
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ



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.

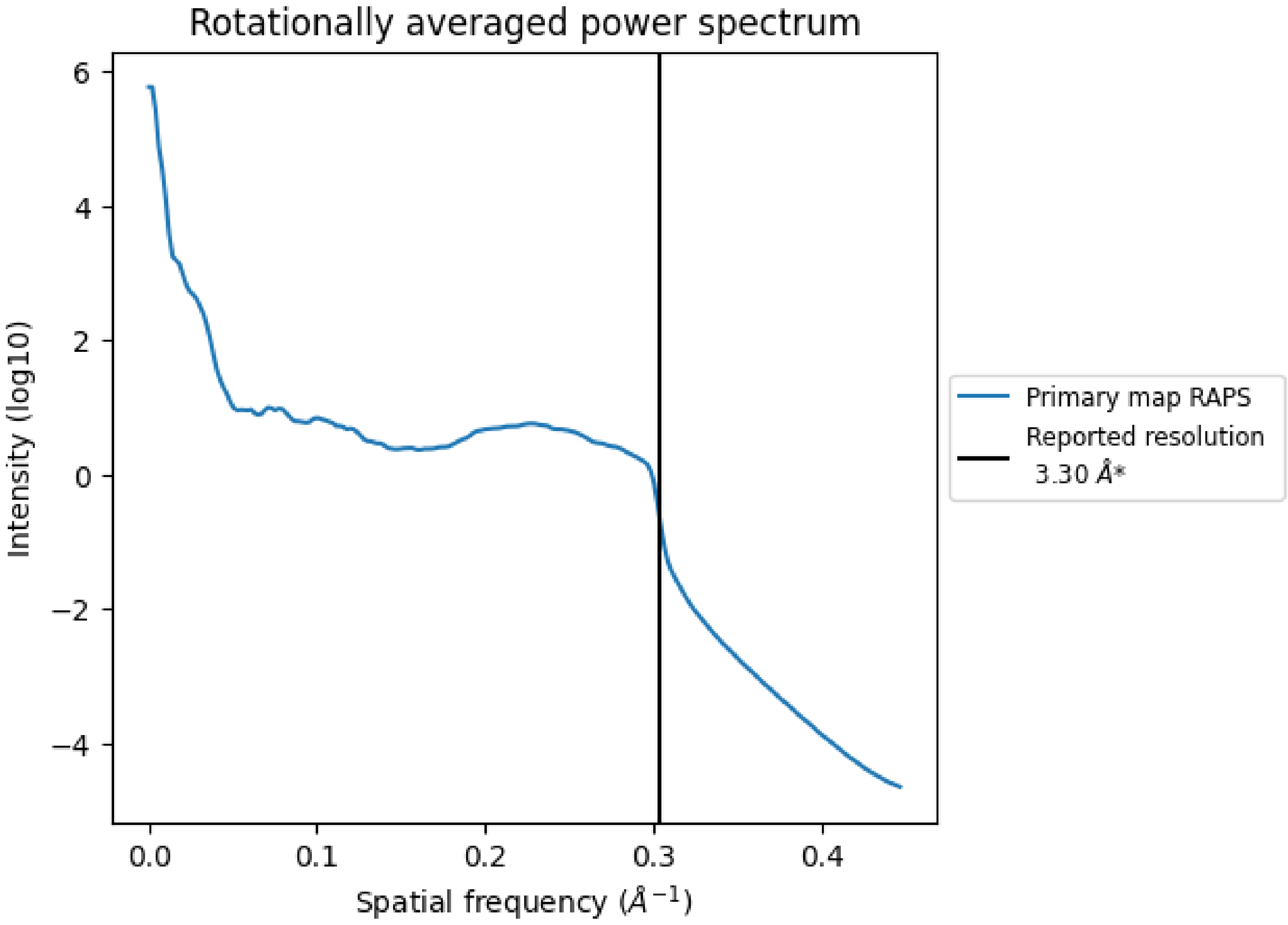
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 322 nm^3; this corresponds to an approximate mass of 291 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 ⓘ

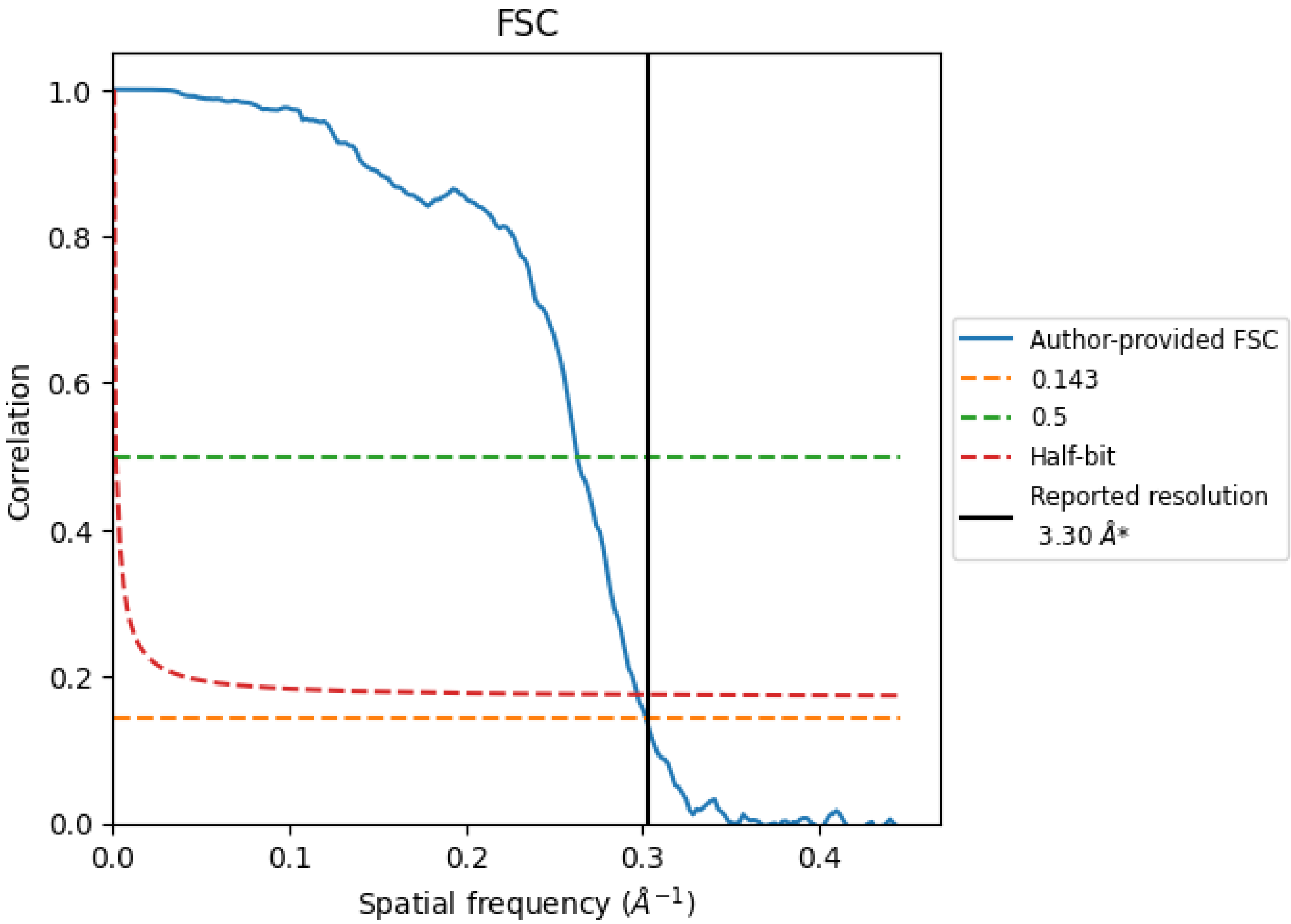


*Reported resolution corresponds to spatial frequency of 0.303 $Å^{-1}$

8 Fourier-Shell correlation ⓘ

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

8.1 FSC ⓘ



*Reported resolution corresponds to spatial frequency of 0.303 $Å^{-1}$

8.2 Resolution estimates (i)

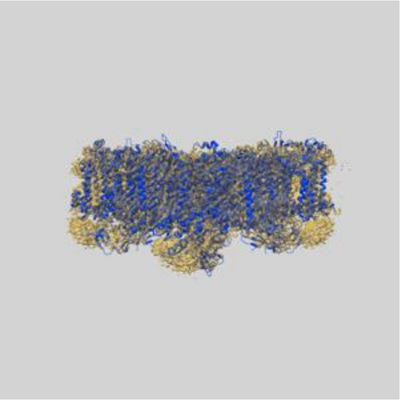
Resolution estimate (Å)	**Estimation criterion (FSC cut-off)**		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.31	3.80	3.37
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

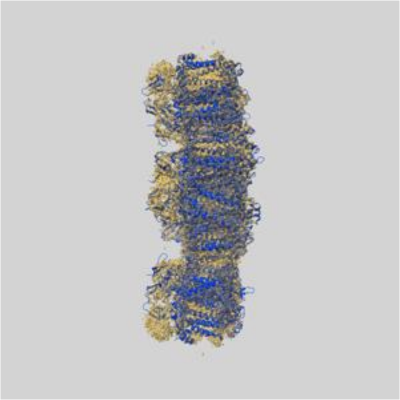
9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-9807 and PDB model 6JEO. Per-residue inclusion information can be found in section 3 on page 46.

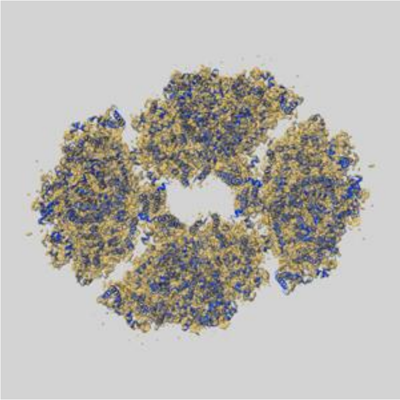
9.1 Map-model overlay ⓘ



X



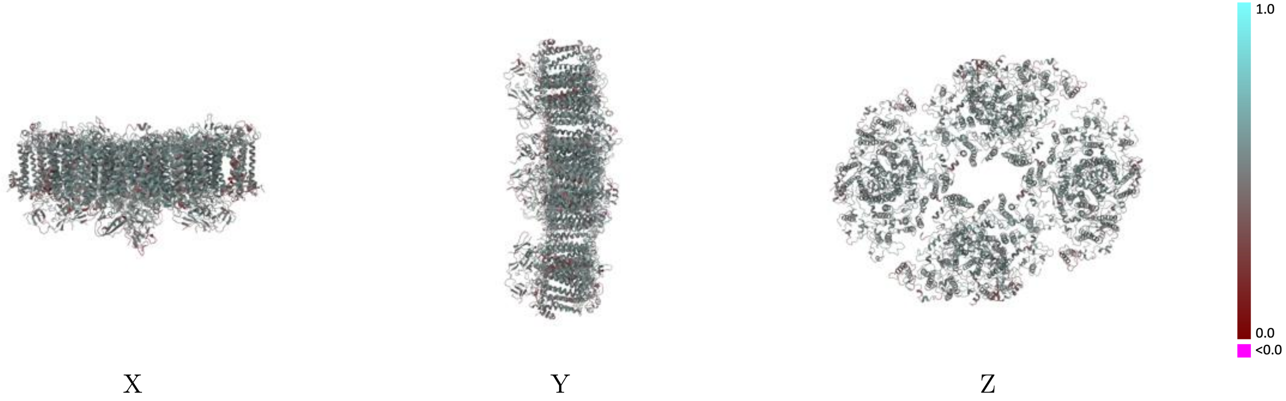
Y



Z

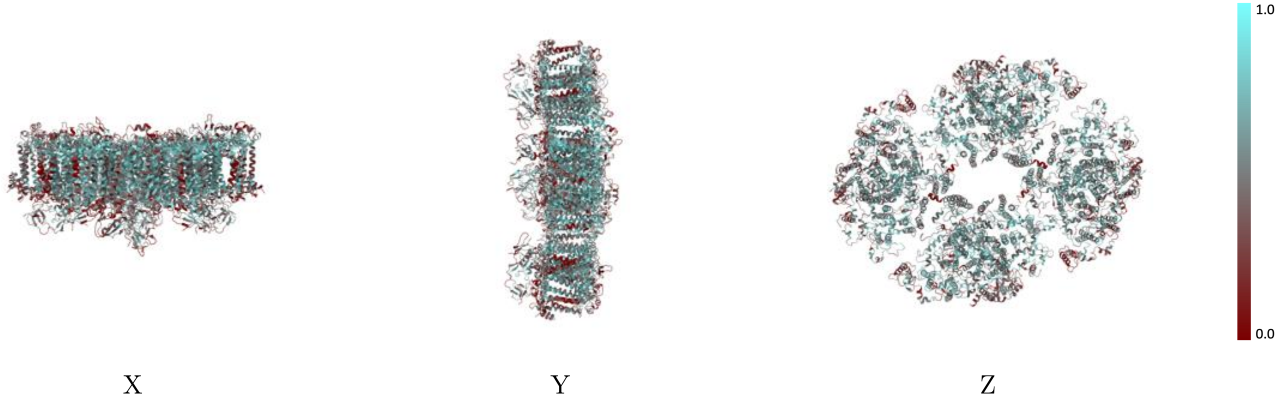
The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model ⓘ



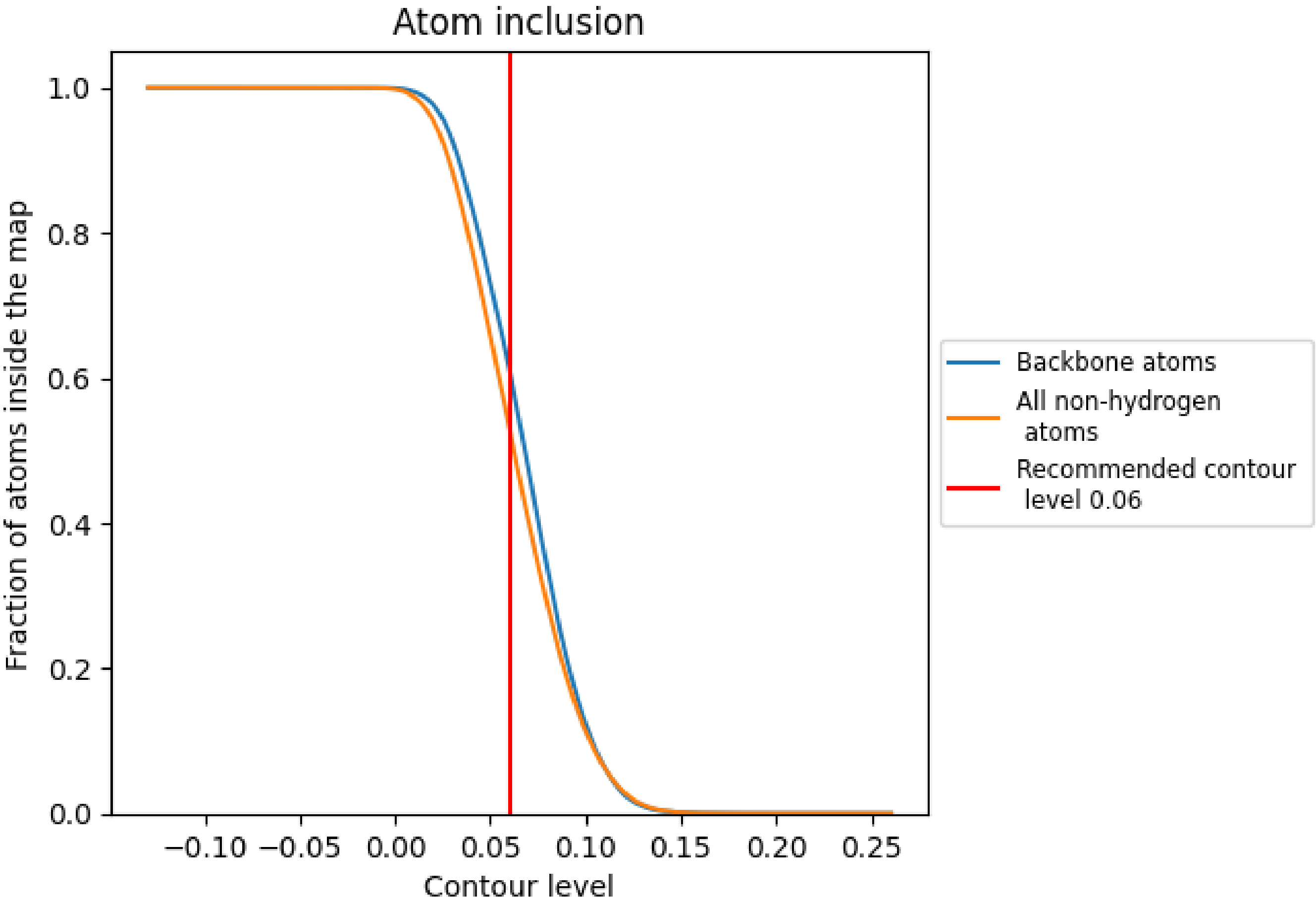
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.06).

9.4 Atom inclusion ⓘ



At the recommended contour level, 61% of all backbone atoms, 53% 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 (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5323	0.5160
aA	0.5500	0.5240
aB	0.5835	0.5350
aC	0.5341	0.5000
aD	0.3480	0.4530
aE	0.3640	0.4150
aF	0.3388	0.4610
aI	0.4844	0.5240
aJ	0.3320	0.4990
aK	0.1715	0.3790
aL	0.5004	0.5250
aM	0.4481	0.5030
aX	0.2626	0.4440
bA	0.5938	0.5280
bB	0.5997	0.5390
bC	0.5724	0.5060
bD	0.3777	0.4650
bE	0.3975	0.4320
bF	0.3782	0.4630
bI	0.3979	0.5150
bJ	0.3903	0.4860
bK	0.3064	0.4020
bL	0.4761	0.5040
bM	0.4444	0.4930
bX	0.4065	0.4720
cA	0.5505	0.5250
cB	0.5811	0.5360
cC	0.5424	0.5000
cD	0.3409	0.4580
cE	0.3577	0.4210
cF	0.3396	0.4590
cI	0.4740	0.5250
cJ	0.3300	0.5000
cK	0.1679	0.3800
cL	0.5004	0.5250

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Chain	Atom inclusion	Q-score
cM	0.4296	0.4980
cX	0.2590	0.4400
dA	0.5921	0.5270
dB	0.5968	0.5390
dC	0.5740	0.5010
dD	0.3723	0.4640
dE	0.3891	0.4270
dF	0.3782	0.4600
dI	0.3806	0.5140
dJ	0.4044	0.4890
dK	0.3047	0.3920
dL	0.4754	0.5020
dM	0.4333	0.4980
dX	0.3921	0.4780