wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 19, 2023 – 03:27 PM EST

PDB ID	:	1IZL
Title	:	Crystal Structure of Photosystem II
Authors	:	Kamiya, N.; Shen, J.-R.
Deposited on	:	2002-10-04
Resolution	:	3.70 Å(reported)

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

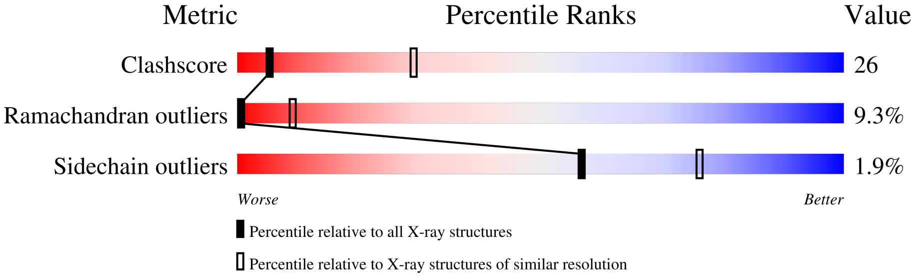
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.70 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)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1027 (3.86-3.54)
Ramachandran outliers	138981	1069 (3.88-3.52)
Sidechain outliers	138945	1065 (3.88-3.52)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	360	
1	J	360	
2	B	472	
2	L	472	
3	C	473	
3	M	473	
4	D	352	
4	N	352	

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Mol	Chain	Length	Quality of chain
5	E	83	35% 6% • 58%
5	P	83	19% • 80%
6	F	44	57% 11% 32%
6	Q	44	57% • 41%
7	G	220	99% •
7	R	220	98% •
8	H	33	97% •
8	S	33	94% • •
9	I	26	88% 12%
9	T	26	88% 8% •
10	K	37	62% 8% • 27%
10	W	37	62% 8% • 27%
11	O	205	93% 7%
11	Y	205	88% 5% 6%
12	U	97	97% •
12	Z	97	94% • 5%
13	0	137	75% 9% 16%
13	V	137	84% 10% 6%
14	1	25	88% 12%
14	X	25	92% 8%

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
16	CLA	A	365	X	-	-	-
16	CLA	A	366	X	-	-	-
16	CLA	A	368	X	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
16	CLA	A	369	X	-	-	-
16	CLA	B	1107	X	-	-	-
16	CLA	B	1108	X	-	-	-
16	CLA	B	1109	X	-	-	-
16	CLA	B	1110	X	-	-	-
16	CLA	B	1111	X	-	-	-
16	CLA	B	1112	X	-	-	-
16	CLA	B	1113	X	-	-	-
16	CLA	B	1114	X	-	-	-
16	CLA	B	1115	X	-	-	-
16	CLA	B	1116	X	-	-	-
16	CLA	B	1117	X	-	-	-
16	CLA	B	1118	X	-	-	-
16	CLA	B	1119	X	-	-	-
16	CLA	B	1120	X	-	-	-
16	CLA	B	1121	X	-	-	-
16	CLA	B	1122	X	-	-	-
16	CLA	C	1078	X	-	-	-
16	CLA	C	1079	X	-	-	-
16	CLA	C	1080	X	-	-	-
16	CLA	C	1081	X	-	-	-
16	CLA	C	1082	X	-	-	-
16	CLA	C	1083	X	-	-	-
16	CLA	C	1084	X	-	-	-
16	CLA	C	1085	X	-	-	-
16	CLA	C	1086	X	-	-	-
16	CLA	C	1087	X	-	-	-
16	CLA	C	1088	X	-	-	-
16	CLA	C	1089	X	-	X	-
16	CLA	D	354	X	-	-	-
16	CLA	D	355	X	-	-	-
16	CLA	D	357	X	-	-	-
16	CLA	G	221	X	-	-	-
16	CLA	J	365	X	-	-	-
16	CLA	J	367	X	-	X	-
16	CLA	J	368	X	-	-	-
16	CLA	L	1107	X	-	-	-
16	CLA	L	1108	X	-	-	-
16	CLA	L	1109	X	-	-	-
16	CLA	L	1110	X	-	-	-
16	CLA	L	1111	X	-	-	-
16	CLA	L	1112	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
16	CLA	L	1113	X	-	-	-
16	CLA	L	1114	X	-	-	-
16	CLA	L	1115	X	-	-	-
16	CLA	L	1116	X	-	-	-
16	CLA	L	1117	X	-	-	-
16	CLA	L	1118	X	-	-	-
16	CLA	L	1119	X	-	X	-
16	CLA	L	1120	X	-	X	-
16	CLA	L	1121	X	-	-	-
16	CLA	L	1122	X	-	-	-
16	CLA	M	1078	X	-	-	-
16	CLA	M	1079	X	-	-	-
16	CLA	M	1080	X	-	-	-
16	CLA	M	1081	X	-	-	-
16	CLA	M	1082	X	-	-	-
16	CLA	M	1083	X	-	-	-
16	CLA	M	1084	X	-	-	-
16	CLA	M	1085	X	-	-	-
16	CLA	M	1086	X	-	-	-
16	CLA	M	1087	X	-	-	-
16	CLA	M	1088	X	-	-	-
16	CLA	N	354	X	-	-	-
16	CLA	N	355	X	-	-	-
16	CLA	N	356	X	-	-	-
16	CLA	N	358	X	-	-	-
16	CLA	R	221	X	-	-	-
16	CLA	W	64	X	-	-	-
17	PHO	N	357	-	-	X	-
19	PLA	N	359	-	X	-	-

2 Entry composition ⓘ

There are 21 unique types of molecules in this entry. The entry contains 22804 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 II: Subunit PsbA.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
1	A	299	1595	975	310	310	0	0	0
1	J	299	1602	984	308	310	0	0	0

- Molecule 2 is a protein called Photosystem II: Subunit PsbB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	427	2004	1238	386	379	1	0	0	48
			Total	C	N	O				
2	L	424	2001	1242	383	376		0	0	48

- Molecule 3 is a protein called Photosystem II: Subunit PsbC.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	349	1792	1082	358	352	0	0	0
3	M	347	1759	1057	354	348	0	0	0

- Molecule 4 is a protein called Photosystem II: Subunit PsbD.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	D	277	1460	899	282	279	0	0	0
4	N	277	1451	888	284	279	0	0	0

- Molecule 5 is a protein called Photosystem II: Subunit PsbE.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
5	E	35	Total C N O 175 105 35 35	0	0	0
5	P	17	Total C N O 83 49 17 17	0	0	0

- Molecule 6 is a protein called Photosystem II: Subunit PsbF.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
6	F	30	Total C N O 166 105 31 30	0	0	0
6	Q	26	Total C N O 129 77 26 26	0	0	0

- Molecule 7 is a protein called Photosystem II: Subunit PsbG.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
7	G	220	Total C 220 220	0	0	220
7	R	220	Total C 220 220	0	0	220

- Molecule 8 is a protein called Photosystem II: Subunit PsbH.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
8	H	33	Total C N O 165 99 33 33	0	0	0
8	S	32	Total C N O 160 96 32 32	0	0	0

- Molecule 9 is a protein called Photosystem II: Subunit PsbI.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
9	I	26	Total C N O 130 78 26 26	0	0	0
9	T	25	Total C N O 125 75 25 25	0	0	0

- Molecule 10 is a protein called Photosystem II: Subunit PsbK.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
10	K	27	Total C N O 137 83 27 27	0	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
10	W	27	Total C N O 137 83 27 27	0	0	0

- Molecule 11 is a protein called Photosystem II: Subunit PsbO.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
11	O	205	Total C N O 1025 615 205 205	0	0	0
11	Y	192	Total C N O 960 576 192 192	0	0	0

- Molecule 12 is a protein called Photosystem II: Subunit PsbU.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
12	U	97	Total C N O 485 291 97 97	0	0	0
12	Z	92	Total C N O 460 276 92 92	0	0	0

- Molecule 13 is a protein called Photosystem II: Subunit PsbV.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
13	V	129	Total C N O 676 410 136 130	0	0	0
13	0	115	Total C N O 597 360 121 116	0	0	0

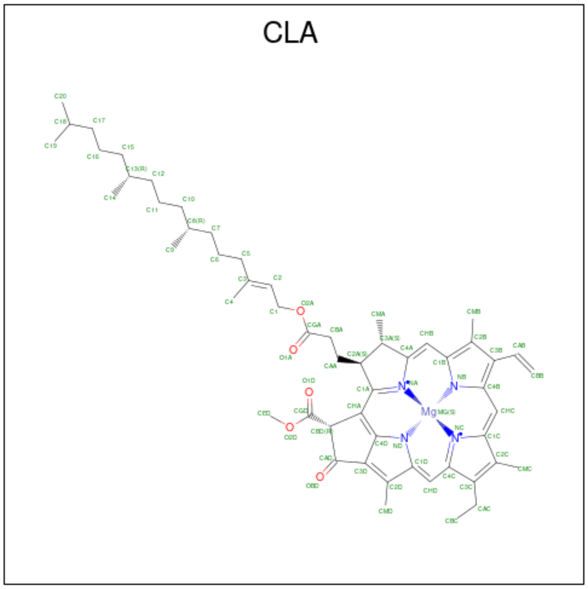
- Molecule 14 is a protein called Photosystem II: Subunit PsbX.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
14	X	25	Total C N O 125 75 25 25	0	0	0
14	1	25	Total C N O 125 75 25 25	0	0	0

- Molecule 15 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	A	4	Total Mn 4 4	0	0
15	J	4	Total Mn 4 4	0	0

- Molecule 16 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	A	1	Total C Mg N O 35 29 1 4 1	0	0
16	A	1	Total C Mg N O 35 29 1 4 1	0	0
16	A	1	Total C Mg N O 35 29 1 4 1	0	0
16	A	1	Total C Mg N O 35 29 1 4 1	0	0
16	B	1	Total C Mg N O 35 29 1 4 1	0	0
16	B	1	Total C Mg N O 35 29 1 4 1	0	0
16	B	1	Total C Mg N O 35 29 1 4 1	0	0
16	B	1	Total C Mg N O 35 29 1 4 1	0	0
16	B	1	Total C Mg N O 35 29 1 4 1	0	0
16	B	1	Total C Mg N O 35 29 1 4 1	0	0
16	B	1	Total C Mg N O 35 29 1 4 1	0	0
16	B	1	Total C Mg N O 35 29 1 4 1	0	0
16	B	1	Total C Mg N O 35 29 1 4 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	B	1	Total C Mg N O 35 29 1 4 1	0	0
16	B	1	Total C Mg N O 35 29 1 4 1	0	0
16	B	1	Total C Mg N O 35 29 1 4 1	0	0
16	B	1	Total C Mg N O 35 29 1 4 1	0	0
16	B	1	Total C Mg N O 35 29 1 4 1	0	0
16	B	1	Total C Mg N O 35 29 1 4 1	0	0
16	B	1	Total C Mg N O 35 29 1 4 1	0	0
16	C	1	Total C Mg N O 35 29 1 4 1	0	0
16	C	1	Total C Mg N O 35 29 1 4 1	0	0
16	C	1	Total C Mg N O 35 29 1 4 1	0	0
16	C	1	Total C Mg N O 35 29 1 4 1	0	0
16	C	1	Total C Mg N O 35 29 1 4 1	0	0
16	C	1	Total C Mg N O 35 29 1 4 1	0	0
16	C	1	Total C Mg N O 35 29 1 4 1	0	0
16	C	1	Total C Mg N O 35 29 1 4 1	0	0
16	C	1	Total C Mg N O 35 29 1 4 1	0	0
16	C	1	Total C Mg N O 35 29 1 4 1	0	0
16	C	1	Total C Mg N O 35 29 1 4 1	0	0
16	C	1	Total C Mg N O 35 29 1 4 1	0	0
16	D	1	Total C Mg N O 35 29 1 4 1	0	0
16	D	1	Total C Mg N O 35 29 1 4 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	D	1	Total C Mg N O 35 29 1 4 1	0	0
16	G	1	Total C Mg N O 35 29 1 4 1	0	0
16	J	1	Total C Mg N O 35 29 1 4 1	0	0
16	J	1	Total C Mg N O 35 29 1 4 1	0	0
16	J	1	Total C Mg N O 35 29 1 4 1	0	0
16	L	1	Total C Mg N O 35 29 1 4 1	0	0
16	L	1	Total C Mg N O 35 29 1 4 1	0	0
16	L	1	Total C Mg N O 35 29 1 4 1	0	0
16	L	1	Total C Mg N O 35 29 1 4 1	0	0
16	L	1	Total C Mg N O 35 29 1 4 1	0	0
16	L	1	Total C Mg N O 35 29 1 4 1	0	0
16	L	1	Total C Mg N O 35 29 1 4 1	0	0
16	L	1	Total C Mg N O 35 29 1 4 1	0	0
16	L	1	Total C Mg N O 35 29 1 4 1	0	0
16	L	1	Total C Mg N O 35 29 1 4 1	0	0
16	L	1	Total C Mg N O 35 29 1 4 1	0	0
16	L	1	Total C Mg N O 35 29 1 4 1	0	0
16	L	1	Total C Mg N O 35 29 1 4 1	0	0
16	L	1	Total C Mg N O 35 29 1 4 1	0	0
16	L	1	Total C Mg N O 35 29 1 4 1	0	0
16	L	1	Total C Mg N O 35 29 1 4 1	0	0

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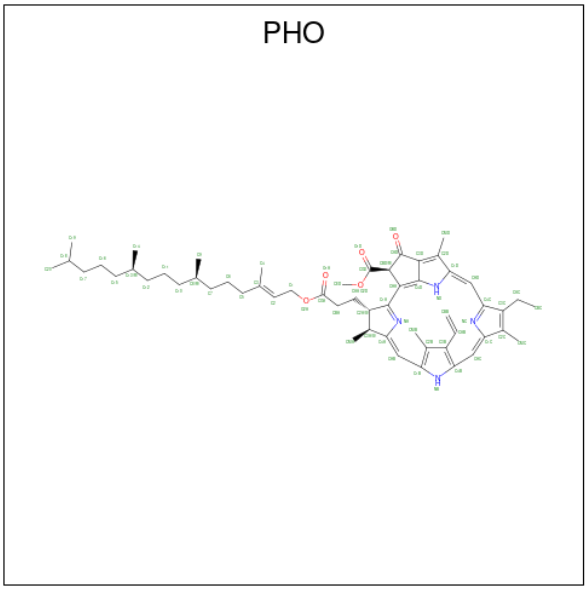
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	M	1	Total C Mg N O 35 29 1 4 1	0	0
16	M	1	Total C Mg N O 35 29 1 4 1	0	0
16	M	1	Total C Mg N O 35 29 1 4 1	0	0
16	M	1	Total C Mg N O 35 29 1 4 1	0	0
16	M	1	Total C Mg N O 35 29 1 4 1	0	0
16	M	1	Total C Mg N O 35 29 1 4 1	0	0
16	M	1	Total C Mg N O 35 29 1 4 1	0	0
16	M	1	Total C Mg N O 35 29 1 4 1	0	0
16	M	1	Total C Mg N O 35 29 1 4 1	0	0
16	M	1	Total C Mg N O 35 29 1 4 1	0	0
16	M	1	Total C Mg N O 35 29 1 4 1	0	0
16	N	1	Total C Mg N O 35 29 1 4 1	0	0
16	N	1	Total C Mg N O 35 29 1 4 1	0	0
16	N	1	Total C Mg N O 35 29 1 4 1	0	0
16	N	1	Total C Mg N O 35 29 1 4 1	0	0
16	R	1	Total C Mg N O 35 29 1 4 1	0	0
16	W	1	Total C Mg N O 35 29 1 4 1	0	0

- Molecule 17 is PHEOPHYTIN A (three-letter code: PHO) (formula: $C_{55}H_{74}N_4O_5$).

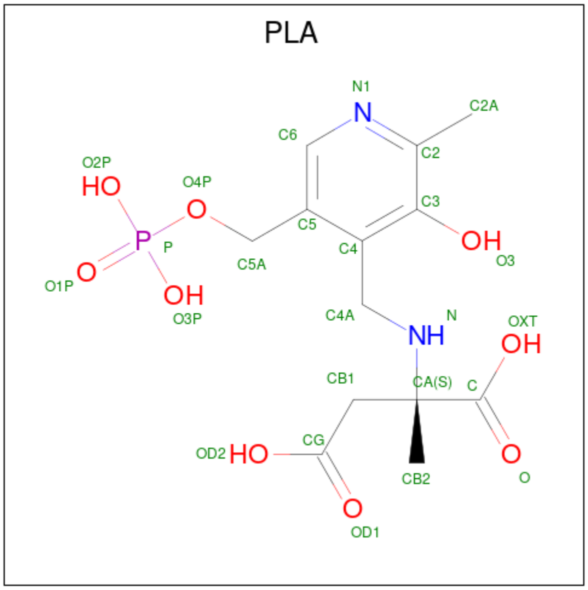


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	A	1	Total C N O 34 29 4 1	0	0
17	D	1	Total C N O 34 29 4 1	0	0
17	J	1	Total C N O 34 29 4 1	0	0
17	N	1	Total C N O 34 29 4 1	0	0

- Molecule 18 is FE (III) ION (three-letter code: FE) (formula: Fe).

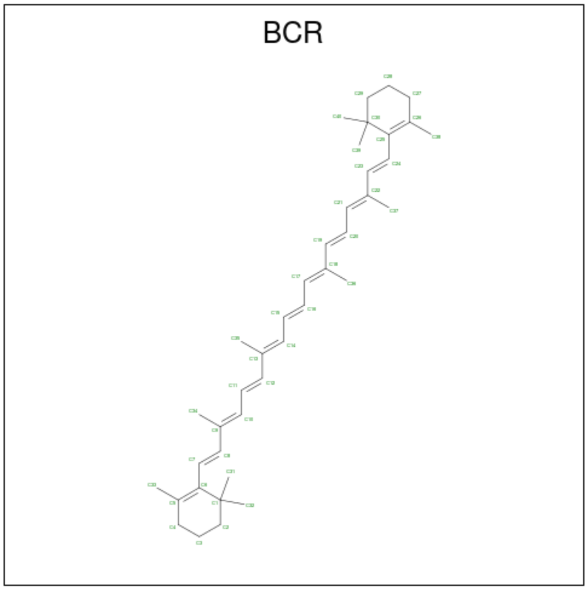
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	D	1	Total Fe 1 1	0	0
18	N	1	Total Fe 1 1	0	0

- Molecule 19 is 2-[(3-HYDROXY-2-METHYL-5-PHOSPHONOOXYMETHYL-PYRIDIN-4-YLMETHYL)-AMINO]-2-METHYL-SUCCINIC ACID (three-letter code: PLA) (formula: $C_{13}H_{19}N_2O_9P$).



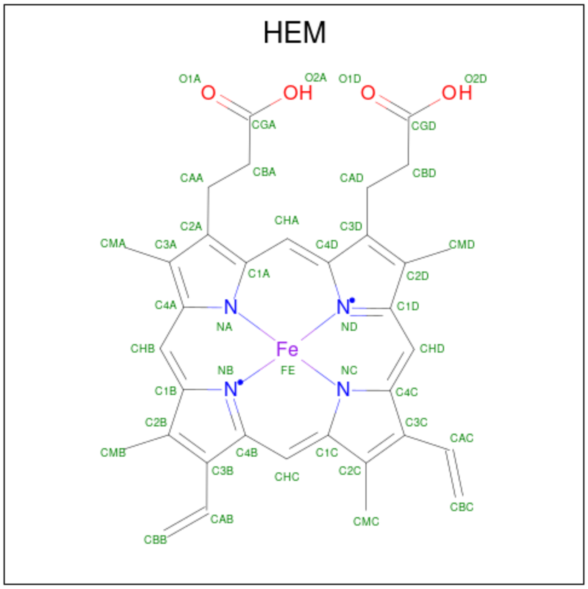
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	D	1	Total C N 6 5 1	0	0
19	N	1	Total C N 6 5 1	0	0

- Molecule 20 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	D	1	Total C 40 40	0	0
20	K	1	Total C 22 22	0	0

- Molecule 21 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



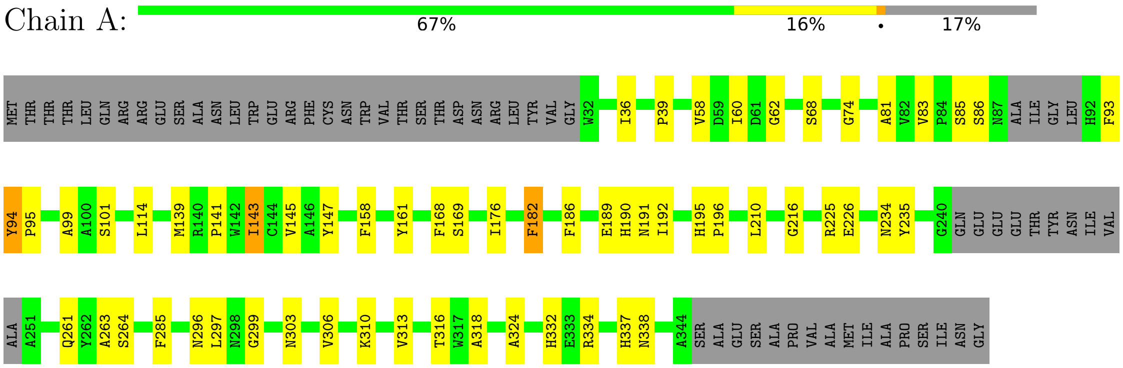
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	E	1	Total C Fe N 25 20 1 4	0	0
21	V	1	Total C Fe N 25 20 1 4	0	0
21	P	1	Total C Fe N 25 20 1 4	0	0
21	0	1	Total C Fe N 25 20 1 4	0	0

3 Residue-property plots ⓘ

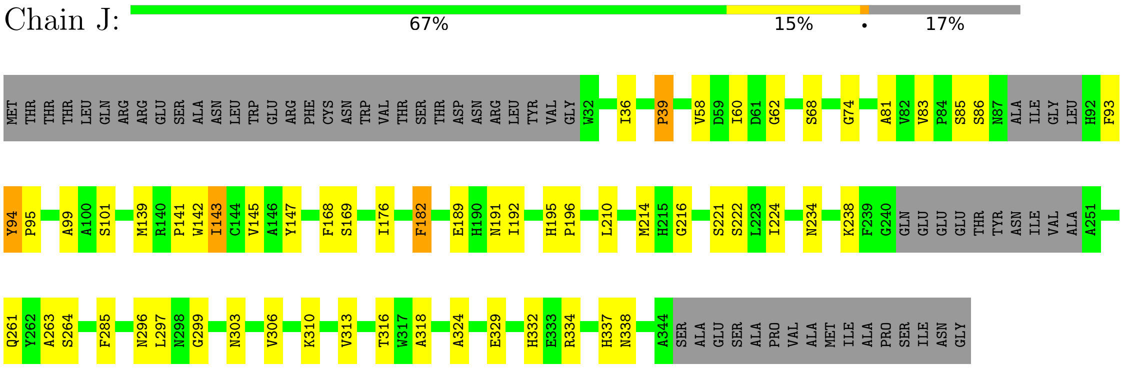
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS was not executed.

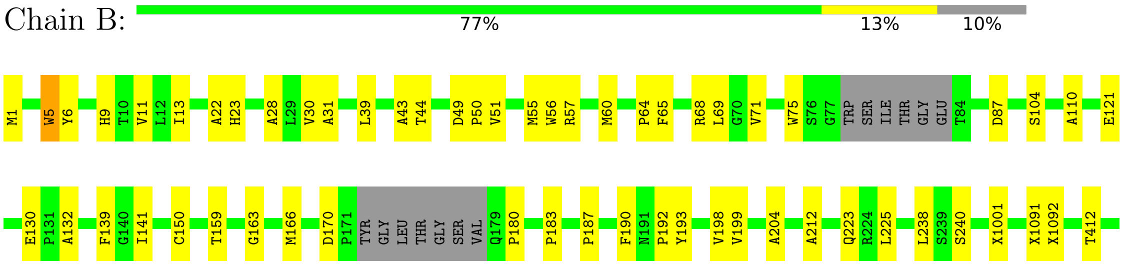
- Molecule 1: Photosystem II: Subunit PsbA

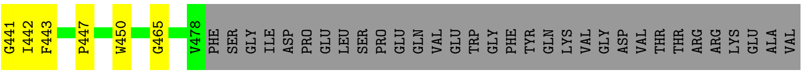


- Molecule 1: Photosystem II: Subunit PsbA

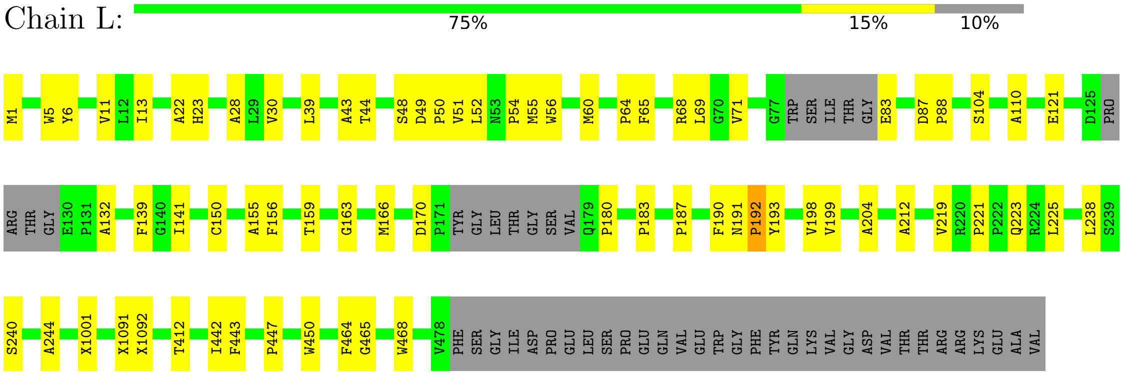


- Molecule 2: Photosystem II: Subunit PsbB

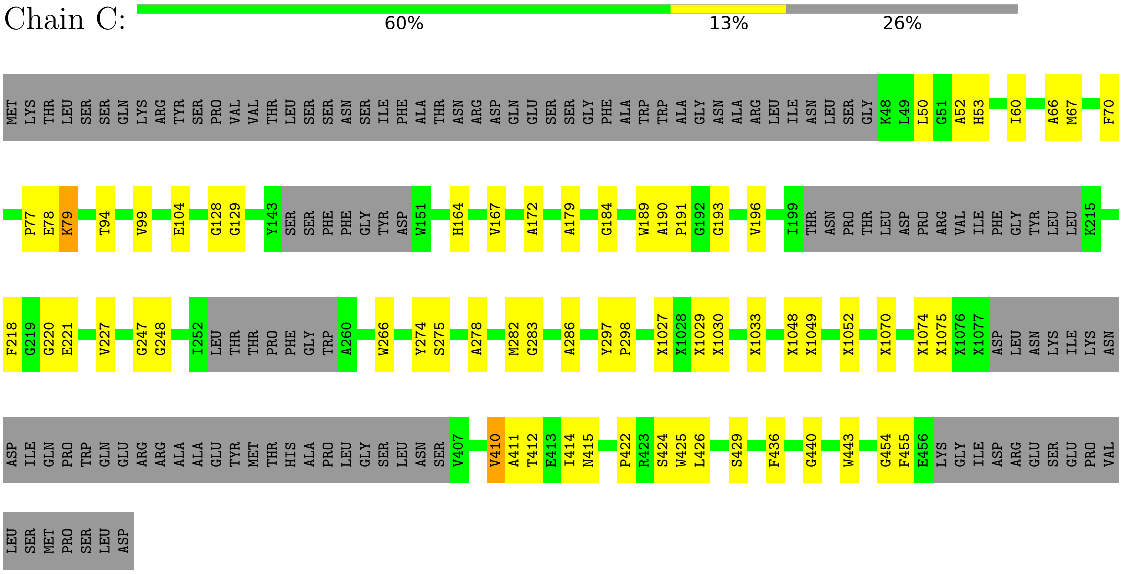




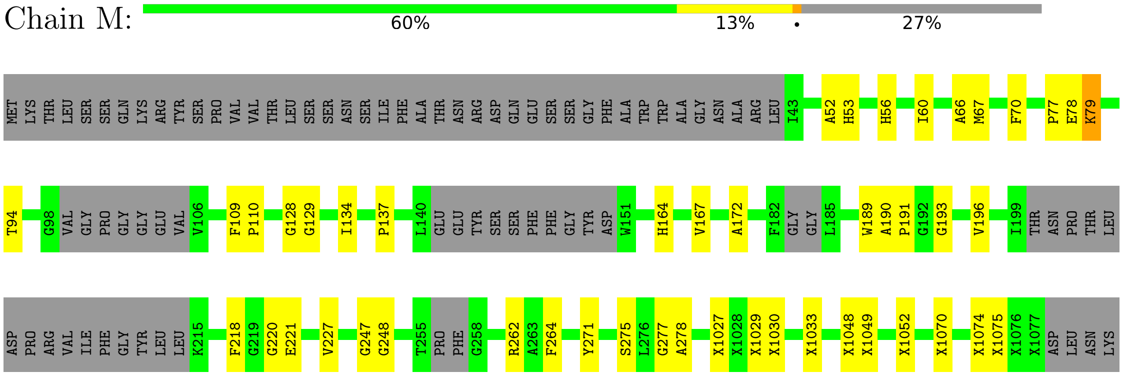
- Molecule 2: Photosystem II: Subunit PsbB

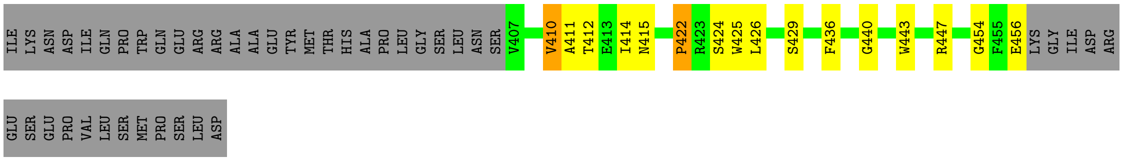


- Molecule 3: Photosystem II: Subunit PsbC



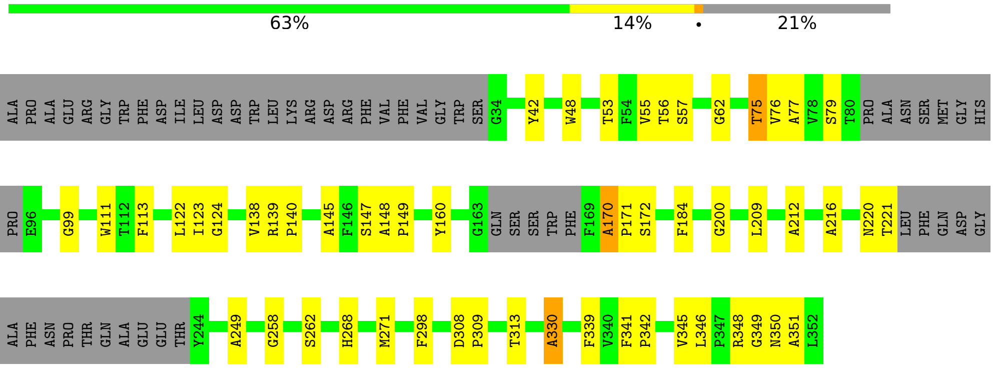
- Molecule 3: Photosystem II: Subunit PsbC





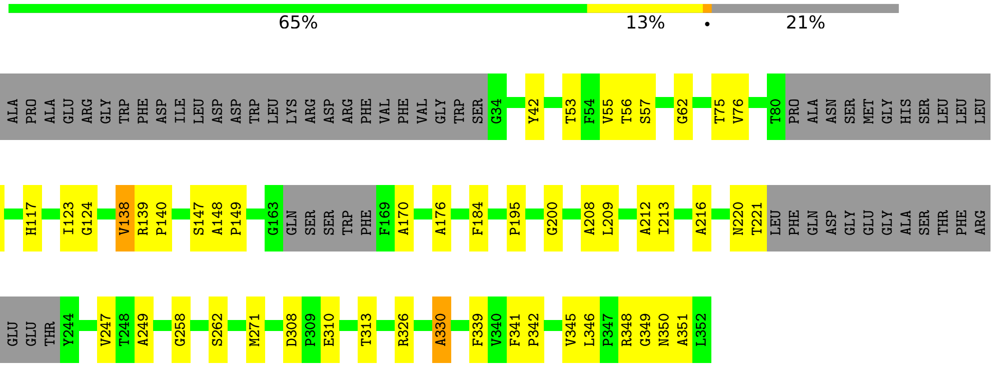
- Molecule 4: Photosystem II: Subunit PsbD

Chain D:



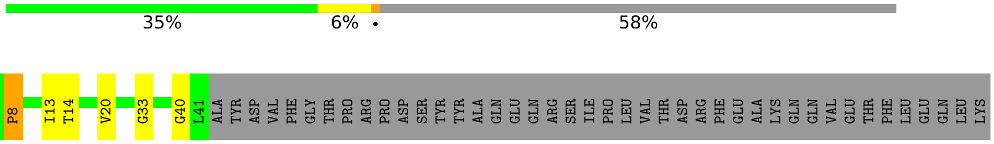
- Molecule 4: Photosystem II: Subunit PsbD

Chain N:



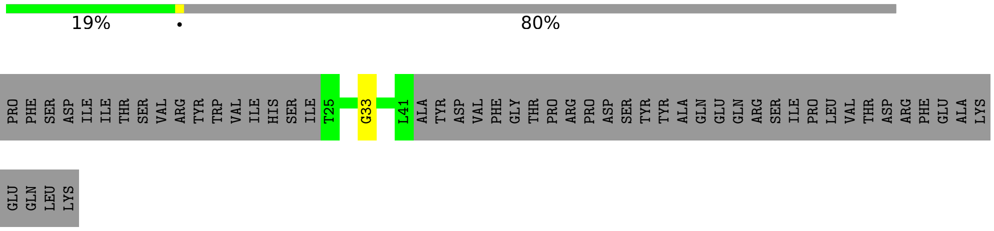
- Molecule 5: Photosystem II: Subunit PsbE

Chain E:



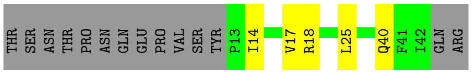
- Molecule 5: Photosystem II: Subunit PsbE

Chain P:



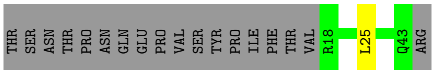
- Molecule 6: Photosystem II: Subunit PsbF

Chain F:



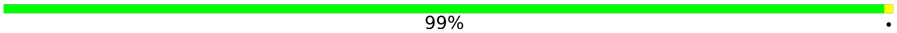
- Molecule 6: Photosystem II: Subunit PsbF

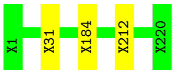
Chain Q:



- Molecule 7: Photosystem II: Subunit PsbG

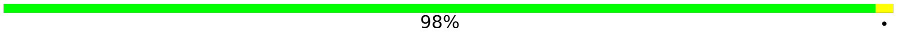
Chain G:

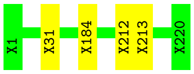




- Molecule 7: Photosystem II: Subunit PsbG

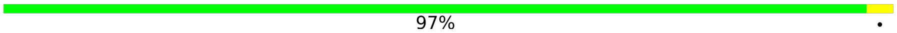
Chain R:

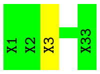




- Molecule 8: Photosystem II: Subunit PsbH

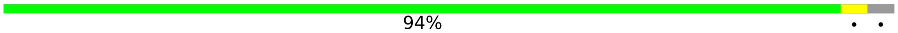
Chain H:

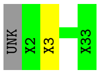




- Molecule 8: Photosystem II: Subunit PsbH

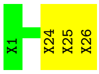
Chain S:





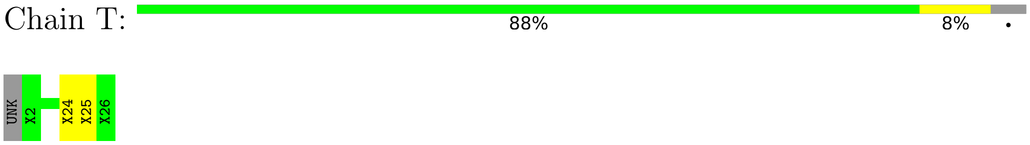
- Molecule 9: Photosystem II: Subunit PsbI

Chain I:



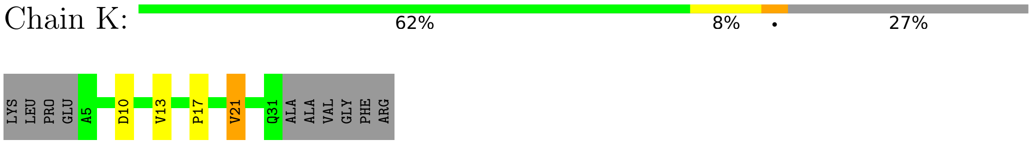
- Molecule 9: Photosystem II: Subunit PsbI

Chain T:



- Molecule 10: Photosystem II: Subunit PsbK

Chain K:

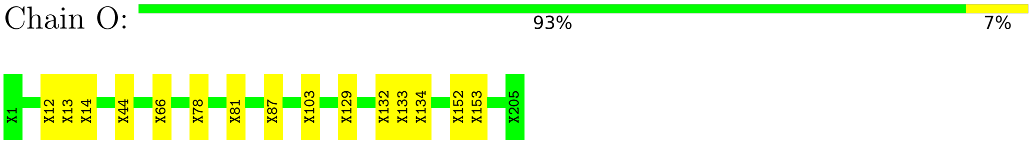


- Molecule 10: Photosystem II: Subunit PsbK

Chain W:

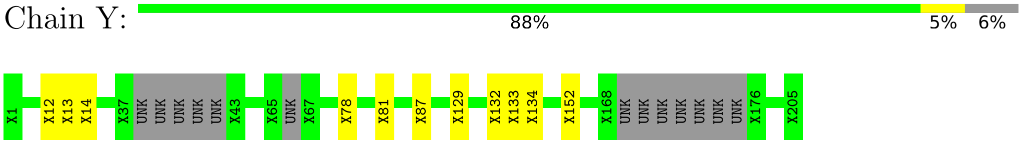
- Molecule 11: Photosystem II: Subunit PsbO

Chain O:



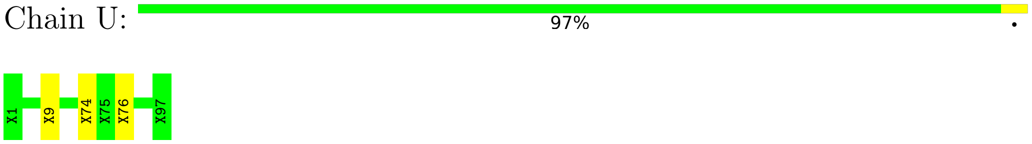
- Molecule 11: Photosystem II: Subunit PsbO

Chain Y:



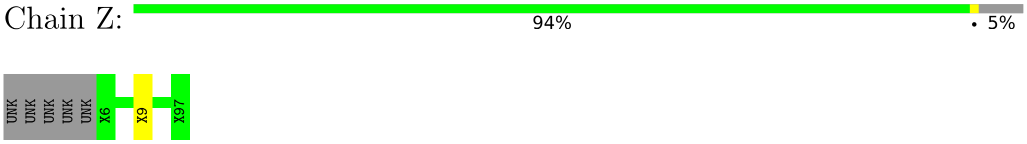
- Molecule 12: Photosystem II: Subunit PsbU

Chain U:



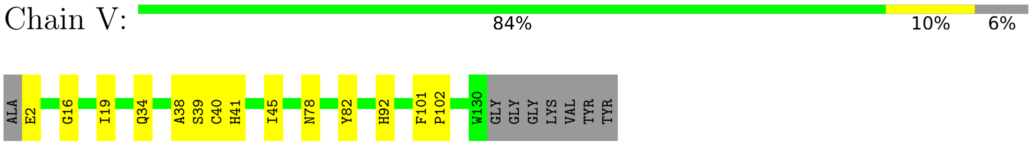
- Molecule 12: Photosystem II: Subunit PsbU

Chain Z:



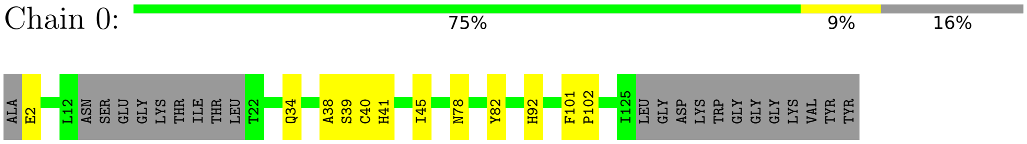
- Molecule 13: Photosystem II: Subunit PsbV

Chain V:



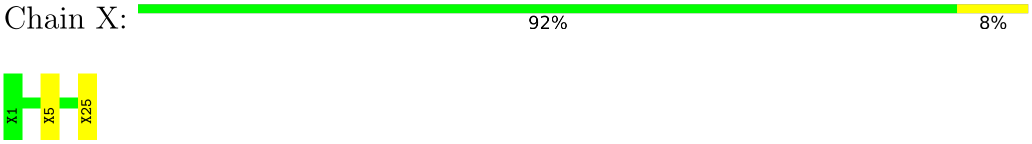
- Molecule 13: Photosystem II: Subunit PsbV

Chain 0:



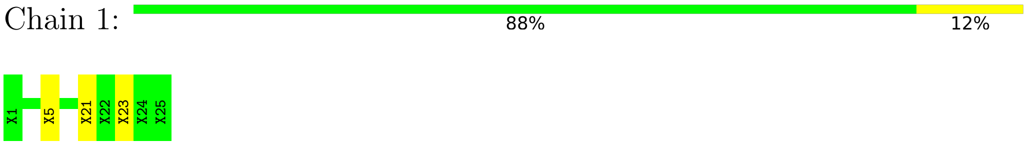
- Molecule 14: Photosystem II: Subunit PsbX

Chain X:



- Molecule 14: Photosystem II: Subunit PsbX

Chain 1:



4 Data and refinement statistics ⓘ

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	**Value**	**Source**
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	129.38Å 225.19Å 308.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 3.70	Depositor
% Data completeness (in resolution range)	100.0 (25.00-3.70)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program		Depositor
R, R_{free}	0.530 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	22804	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: BCR, HEM, CLA, MN, PLA, PHO, FE

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

Mol	**Chain**	**Bond lengths**		**Bond angles**	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.25	0/1613	0.40	0/2229
1	J	0.26	0/1621	0.40	0/2239
2	B	0.24	0/1685	0.41	0/2331
2	L	0.26	0/1682	0.40	0/2323
3	C	0.24	0/1421	0.40	0/1961
3	M	0.25	0/1379	0.40	0/1898
4	D	0.27	0/1475	0.40	0/2037
4	N	0.27	0/1464	0.39	0/2022
5	E	0.24	0/175	0.46	0/243
5	P	0.31	0/82	0.42	0/112
6	F	0.28	0/169	0.47	0/234
6	Q	0.26	0/128	0.40	0/177
10	K	0.25	0/137	0.45	0/191
10	W	0.25	0/137	0.45	0/191
13	0	0.24	0/600	0.37	0/831
13	V	0.23	0/683	0.38	0/949
All	All	0.25	0/14451	0.40	0/19968

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1595	0	834	95	0
1	J	1602	0	843	82	0
2	B	2004	0	968	147	0
2	L	2001	0	961	141	0
3	C	1792	0	842	126	0
3	M	1759	0	793	114	0
4	D	1460	0	761	71	0
4	N	1451	0	746	68	0
5	E	175	0	81	6	0
5	P	83	0	40	2	0
6	F	166	0	95	4	0
6	Q	129	0	66	4	0
7	G	220	0	0	8	0
7	R	220	0	0	10	0
8	H	165	0	36	1	0
8	S	160	0	35	2	0
9	I	130	0	30	2	0
9	T	125	0	29	1	0
10	K	137	0	68	11	0
10	W	137	0	68	11	0
11	O	1025	0	279	37	0
11	Y	960	0	265	34	0
12	U	485	0	112	5	0
12	Z	460	0	106	1	0
13	0	597	0	278	15	0
13	V	676	0	323	16	0
14	1	125	0	28	3	0
14	X	125	0	29	6	0
15	A	4	0	0	0	0
15	J	4	0	0	0	0
16	A	140	0	68	37	0
16	B	560	0	272	119	0
16	C	420	0	204	99	0
16	D	105	0	48	13	0
16	G	35	0	17	0	0
16	J	105	0	50	25	0
16	L	560	0	272	128	0
16	M	385	0	187	77	0
16	N	140	0	68	11	0
16	R	35	0	17	0	0
16	W	35	0	17	15	0
17	A	34	0	19	20	0
17	D	34	0	19	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	J	34	0	19	19	0
17	N	34	0	19	28	0
18	D	1	0	0	0	0
18	N	1	0	0	0	0
19	D	6	0	1	0	0
19	N	6	0	1	0	0
20	D	40	0	56	9	0
20	K	22	0	24	1	0
21	0	25	0	4	8	0
21	E	25	0	4	0	0
21	P	25	0	4	0	0
21	V	25	0	4	8	0
All	All	22804	0	10110	868	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 26.

The worst 5 of 868 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:450:TRP:HB3	16:B:1110:CLA:CMB	1.26	1.64
2:B:30:VAL:CB	16:B:1108:CLA:CAA	1.76	1.63
3:M:52:ALA:HB1	16:M:1081:CLA:CAB	1.27	1.62
2:B:465:GLY:CA	16:B:1119:CLA:HMA1	1.22	1.60
2:B:1:MET:HA	7:G:31:UNK:CA	1.20	1.60

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 X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	293/360 (81%)	195 (67%)	66 (22%)	32 (11%)	0	6
1	J	293/360 (81%)	199 (68%)	59 (20%)	35 (12%)	0	5
2	B	314/472 (66%)	219 (70%)	62 (20%)	33 (10%)	0	6
2	L	309/472 (66%)	215 (70%)	60 (19%)	34 (11%)	0	6
3	C	263/473 (56%)	198 (75%)	47 (18%)	18 (7%)	1	16
3	M	257/473 (54%)	189 (74%)	47 (18%)	21 (8%)	1	11
4	D	269/352 (76%)	187 (70%)	56 (21%)	26 (10%)	0	8
4	N	269/352 (76%)	184 (68%)	59 (22%)	26 (10%)	0	8
5	E	33/83 (40%)	23 (70%)	5 (15%)	5 (15%)	0	3
5	P	15/83 (18%)	11 (73%)	4 (27%)	0	100	100
6	F	28/44 (64%)	22 (79%)	3 (11%)	3 (11%)	0	6
6	Q	24/44 (54%)	22 (92%)	2 (8%)	0	100	100
10	K	25/37 (68%)	14 (56%)	9 (36%)	2 (8%)	1	12
10	W	25/37 (68%)	15 (60%)	8 (32%)	2 (8%)	1	12
13	0	111/137 (81%)	90 (81%)	17 (15%)	4 (4%)	3	29
13	V	127/137 (93%)	102 (80%)	19 (15%)	6 (5%)	2	23
All	All	2655/3916 (68%)	1885 (71%)	523 (20%)	247 (9%)	0	9

5 of 247 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	94	TYR
1	A	101	SER
1	A	168	PHE
1	A	191	ASN
1	A	192	ILE

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 X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	21/290 (7%)	20 (95%)	1 (5%)	25	56
1	J	22/290 (8%)	21 (96%)	1 (4%)	27	57
2	B	21/290 (7%)	21 (100%)	0	100	100
2	L	21/290 (7%)	21 (100%)	0	100	100
3	C	16/315 (5%)	16 (100%)	0	100	100
3	M	10/315 (3%)	9 (90%)	1 (10%)	7	32
4	D	16/283 (6%)	16 (100%)	0	100	100
4	N	14/283 (5%)	14 (100%)	0	100	100
5	E	1/72 (1%)	1 (100%)	0	100	100
6	F	3/38 (8%)	3 (100%)	0	100	100
10	K	1/30 (3%)	1 (100%)	0	100	100
10	W	1/30 (3%)	1 (100%)	0	100	100
13	0	5/117 (4%)	5 (100%)	0	100	100
13	V	7/117 (6%)	7 (100%)	0	100	100
All	All	159/2760 (6%)	156 (98%)	3 (2%)	57	76

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	182	PHE
1	J	182	PHE
3	M	422	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	J	332	HIS
3	M	164	HIS
4	N	117	HIS
2	B	9	HIS
1	A	332	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 ⓘ

Of 94 ligands modelled in this entry, 10 are monoatomic - leaving 84 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
21	HEM	E	84	-	22,32,50	2.71	7 (31%)	25,54,82	3.06	13 (52%)
17	PHO	A	367	-	22,39,69	1.38	4 (18%)	17,62,99	2.52	7 (41%)
16	CLA	L	1110	-	36,43,73	1.99	9 (25%)	45,76,113	2.24	9 (20%)
16	CLA	A	368	-	36,43,73	2.01	7 (19%)	45,76,113	2.19	8 (17%)
16	CLA	J	367	-	36,43,73	2.01	8 (22%)	45,76,113	2.19	8 (17%)
16	CLA	L	1108	-	36,43,73	1.99	8 (22%)	45,76,113	2.19	8 (17%)
16	CLA	M	1084	-	36,43,73	2.00	8 (22%)	45,76,113	2.21	7 (15%)
16	CLA	M	1083	-	36,43,73	1.99	8 (22%)	45,76,113	2.22	9 (20%)
16	CLA	R	221	-	36,43,73	1.93	11 (30%)	45,76,113	2.19	10 (22%)
16	CLA	L	1114	-	36,43,73	2.01	7 (19%)	45,76,113	2.24	10 (22%)
16	CLA	C	1082	-	36,43,73	2.00	8 (22%)	45,76,113	2.21	8 (17%)
16	CLA	D	354	4	36,43,73	1.85	9 (25%)	45,76,113	2.24	9 (20%)
17	PHO	J	366	-	22,39,69	1.37	3 (13%)	17,62,99	2.53	7 (41%)
16	CLA	J	368	-	36,43,73	1.99	8 (22%)	45,76,113	2.23	9 (20%)
16	CLA	M	1078	-	36,43,73	2.03	8 (22%)	45,76,113	2.20	7 (15%)
16	CLA	L	1111	-	36,43,73	2.01	8 (22%)	45,76,113	2.19	8 (17%)
16	CLA	N	355	-	36,43,73	1.90	11 (30%)	45,76,113	2.20	8 (17%)
16	CLA	B	1111	-	36,43,73	2.01	7 (19%)	45,76,113	2.21	8 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
16	CLA	L	1122	-	36,43,73	2.00	7 (19%)	45,76,113	2.21	8 (17%)
16	CLA	L	1118	-	36,43,73	2.00	8 (22%)	45,76,113	2.22	8 (17%)
16	CLA	L	1109	-	36,43,73	1.99	7 (19%)	45,76,113	2.19	9 (20%)
16	CLA	M	1079	-	36,43,73	2.00	7 (19%)	45,76,113	2.23	9 (20%)
16	CLA	L	1113	-	36,43,73	2.00	7 (19%)	45,76,113	2.22	8 (17%)
16	CLA	B	1113	-	36,43,73	1.99	7 (19%)	45,76,113	2.23	9 (20%)
16	CLA	C	1081	-	36,43,73	1.99	8 (22%)	45,76,113	2.22	8 (17%)
16	CLA	D	357	-	36,43,73	2.01	8 (22%)	45,76,113	2.25	9 (20%)
16	CLA	B	1110	-	36,43,73	1.99	9 (25%)	45,76,113	2.24	9 (20%)
16	CLA	L	1120	-	36,43,73	2.00	9 (25%)	45,76,113	2.20	9 (20%)
21	HEM	P	92	-	22,32,50	2.70	7 (31%)	25,54,82	3.07	13 (52%)
16	CLA	B	1109	-	36,43,73	1.98	7 (19%)	45,76,113	2.20	8 (17%)
16	CLA	B	1117	-	36,43,73	2.01	8 (22%)	45,76,113	2.20	10 (22%)
21	HEM	V	138	13	22,32,50	2.71	7 (31%)	25,54,82	3.05	13 (52%)
16	CLA	M	1082	-	36,43,73	1.99	7 (19%)	45,76,113	2.21	8 (17%)
17	PHO	D	356	-	22,39,69	1.34	3 (13%)	17,62,99	2.50	7 (41%)
16	CLA	M	1087	3	36,43,73	2.00	8 (22%)	45,76,113	2.21	8 (17%)
16	CLA	L	1121	-	36,43,73	1.98	7 (19%)	45,76,113	2.23	10 (22%)
16	CLA	G	221	-	36,43,73	1.93	11 (30%)	45,76,113	2.17	10 (22%)
16	CLA	J	365	-	36,43,73	1.86	8 (22%)	45,76,113	2.68	14 (31%)
16	CLA	B	1112	-	36,43,73	1.99	9 (25%)	45,76,113	2.22	10 (22%)
16	CLA	B	1107	-	36,43,73	1.99	7 (19%)	45,76,113	2.20	8 (17%)
21	HEM	0	138	13	22,32,50	2.71	7 (31%)	25,54,82	3.06	13 (52%)
16	CLA	M	1086	-	36,43,73	2.00	8 (22%)	45,76,113	2.20	8 (17%)
16	CLA	B	1116	-	36,43,73	1.98	9 (25%)	45,76,113	2.20	8 (17%)
16	CLA	B	1108	-	36,43,73	1.99	7 (19%)	45,76,113	2.19	8 (17%)
16	CLA	D	355	-	36,43,73	1.91	7 (19%)	45,76,113	2.15	10 (22%)
16	CLA	C	1086	-	36,43,73	2.00	7 (19%)	45,76,113	2.23	9 (20%)
16	CLA	B	1115	-	36,43,73	1.99	8 (22%)	45,76,113	2.23	8 (17%)
16	CLA	C	1084	-	36,43,73	1.98	8 (22%)	45,76,113	2.21	9 (20%)
19	PLA	N	359	-	6,6,25	2.92	6 (100%)	6,6,37	0.89	0
16	CLA	C	1079	-	36,43,73	2.01	7 (19%)	45,76,113	2.22	9 (20%)
16	CLA	B	1114	2	36,43,73	2.00	7 (19%)	45,76,113	2.22	10 (22%)
16	CLA	A	369	-	36,43,73	2.02	8 (22%)	45,76,113	2.24	10 (22%)
16	CLA	A	365	-	36,43,73	1.98	9 (25%)	45,76,113	2.49	13 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
16	CLA	B	1119	-	36,43,73	2.00	9 (25%)	45,76,113	2.21	9 (20%)
16	CLA	C	1089	3	36,43,73	2.01	8 (22%)	45,76,113	2.25	9 (20%)
20	BCR	D	359	-	41,41,41	1.27	4 (9%)	56,56,56	1.74	17 (30%)
20	BCR	K	47	-	21,21,41	1.02	1 (4%)	24,24,56	1.49	4 (16%)
16	CLA	C	1085	-	36,43,73	2.01	7 (19%)	45,76,113	2.19	8 (17%)
16	CLA	M	1085	-	36,43,73	2.00	7 (19%)	45,76,113	2.23	9 (20%)
16	CLA	C	1087	-	36,43,73	2.01	7 (19%)	45,76,113	2.21	8 (17%)
16	CLA	A	366	-	36,43,73	1.89	11 (30%)	45,76,113	2.18	8 (17%)
17	PHO	N	357	-	22,39,69	1.35	3 (13%)	17,62,99	2.51	7 (41%)
16	CLA	B	1120	-	36,43,73	2.00	7 (19%)	45,76,113	2.20	9 (20%)
16	CLA	M	1088	-	36,43,73	2.01	9 (25%)	45,76,113	2.22	9 (20%)
16	CLA	C	1078	-	36,43,73	2.03	8 (22%)	45,76,113	2.20	6 (13%)
19	PLA	D	358	-	6,6,25	2.92	5 (83%)	6,6,37	0.89	0
16	CLA	L	1112	-	36,43,73	1.99	8 (22%)	45,76,113	2.24	10 (22%)
16	CLA	L	1107	-	36,43,73	2.00	8 (22%)	45,76,113	2.21	8 (17%)
16	CLA	L	1116	-	36,43,73	2.00	8 (22%)	45,76,113	2.19	9 (20%)
16	CLA	B	1122	-	36,43,73	2.01	7 (19%)	45,76,113	2.20	8 (17%)
16	CLA	C	1088	-	36,43,73	2.00	9 (25%)	45,76,113	2.20	9 (20%)
16	CLA	L	1119	-	36,43,73	2.01	8 (22%)	45,76,113	2.22	9 (20%)
16	CLA	N	354	4	36,43,73	1.84	9 (25%)	45,76,113	2.24	9 (20%)
16	CLA	M	1081	-	36,43,73	2.00	7 (19%)	45,76,113	2.21	7 (15%)
16	CLA	N	356	-	36,43,73	1.91	7 (19%)	45,76,113	2.16	10 (22%)
16	CLA	W	64	-	36,43,73	2.01	9 (25%)	45,76,113	2.20	9 (20%)
16	CLA	L	1115	-	36,43,73	2.01	8 (22%)	45,76,113	2.21	9 (20%)
16	CLA	B	1118	-	36,43,73	2.01	9 (25%)	45,76,113	2.21	8 (17%)
16	CLA	C	1080	-	36,43,73	2.00	9 (25%)	45,76,113	2.22	10 (22%)
16	CLA	M	1080	-	36,43,73	1.99	7 (19%)	45,76,113	2.23	8 (17%)
16	CLA	N	358	-	36,43,73	2.00	8 (22%)	45,76,113	2.25	9 (20%)
16	CLA	B	1121	-	36,43,73	1.98	7 (19%)	45,76,113	2.21	9 (20%)
16	CLA	L	1117	-	36,43,73	2.01	8 (22%)	45,76,113	2.20	9 (20%)
16	CLA	C	1083	-	36,43,73	1.99	7 (19%)	45,76,113	2.21	8 (17%)

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
17	PHO	A	367	-	-	0/0/60/103	0/5/6/6
16	CLA	L	1110	-	1/1/8/20	-	-
16	CLA	A	368	-	1/1/8/20	-	-
16	CLA	J	367	-	1/1/8/20	-	-
16	CLA	L	1108	-	1/1/8/20	-	-
16	CLA	M	1084	-	1/1/8/20	-	-
16	CLA	M	1083	-	1/1/8/20	-	-
16	CLA	R	221	-	1/1/8/20	-	-
16	CLA	L	1114	-	1/1/8/20	-	-
16	CLA	C	1082	-	1/1/8/20	-	-
16	CLA	D	354	4	1/1/8/20	-	-
17	PHO	J	366	-	-	0/0/60/103	0/5/6/6
16	CLA	J	368	-	1/1/8/20	-	-
16	CLA	M	1078	-	1/1/8/20	-	-
16	CLA	L	1111	-	1/1/8/20	-	-
16	CLA	N	355	-	1/1/8/20	-	-
16	CLA	B	1111	-	1/1/8/20	-	-
16	CLA	L	1122	-	1/1/8/20	-	-
16	CLA	L	1118	-	1/1/8/20	-	-
16	CLA	L	1109	-	1/1/8/20	-	-
16	CLA	M	1079	-	1/1/8/20	-	-
16	CLA	L	1113	-	1/1/8/20	-	-
16	CLA	B	1113	-	1/1/8/20	-	-
16	CLA	C	1081	-	1/1/8/20	-	-
16	CLA	D	357	-	1/1/8/20	-	-
16	CLA	B	1110	-	1/1/8/20	-	-
16	CLA	L	1120	-	1/1/8/20	-	-
16	CLA	B	1109	-	1/1/8/20	-	-
16	CLA	B	1117	-	1/1/8/20	-	-
16	CLA	M	1082	-	1/1/8/20	-	-
17	PHO	D	356	-	-	0/0/60/103	0/5/6/6
16	CLA	M	1087	3	1/1/8/20	-	-
16	CLA	L	1121	-	1/1/8/20	-	-
16	CLA	G	221	-	1/1/8/20	-	-
16	CLA	J	365	-	1/1/8/20	-	-
16	CLA	B	1112	-	1/1/8/20	-	-
16	CLA	B	1107	-	1/1/8/20	-	-
16	CLA	M	1086	-	1/1/8/20	-	-
16	CLA	B	1116	-	1/1/8/20	-	-
16	CLA	B	1108	-	1/1/8/20	-	-
16	CLA	D	355	-	1/1/8/20	-	-
16	CLA	C	1086	-	1/1/8/20	-	-
16	CLA	B	1115	-	1/1/8/20	-	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	C	1084	-	1/1/8/20	-	-
19	PLA	N	359	-	-	-	0/1/1/1
16	CLA	C	1079	-	1/1/8/20	-	-
16	CLA	B	1114	2	1/1/8/20	-	-
16	CLA	A	369	-	1/1/8/20	-	-
16	CLA	A	365	-	1/1/8/20	-	-
16	CLA	B	1119	-	1/1/8/20	-	-
16	CLA	C	1089	3	2/2/8/20	-	-
20	BCR	D	359	-	-	3/29/63/63	0/2/2/2
20	BCR	K	47	-	-	1/23/23/63	-
16	CLA	C	1085	-	1/1/8/20	-	-
16	CLA	M	1085	-	1/1/8/20	-	-
16	CLA	C	1087	-	1/1/8/20	-	-
16	CLA	A	366	-	1/1/8/20	-	-
17	PHO	N	357	-	-	0/0/60/103	0/5/6/6
16	CLA	B	1120	-	1/1/8/20	-	-
16	CLA	M	1088	-	1/1/8/20	-	-
16	CLA	C	1078	-	1/1/8/20	-	-
16	CLA	L	1112	-	1/1/8/20	-	-
19	PLA	D	358	-	-	-	0/1/1/1
16	CLA	L	1107	-	1/1/8/20	-	-
16	CLA	L	1116	-	1/1/8/20	-	-
16	CLA	B	1122	-	1/1/8/20	-	-
16	CLA	C	1088	-	1/1/8/20	-	-
16	CLA	L	1119	-	1/1/8/20	-	-
16	CLA	N	354	4	1/1/8/20	-	-
16	CLA	M	1081	-	1/1/8/20	-	-
16	CLA	N	356	-	1/1/8/20	-	-
16	CLA	W	64	-	1/1/8/20	-	-
16	CLA	L	1115	-	1/1/8/20	-	-
16	CLA	B	1118	-	1/1/8/20	-	-
16	CLA	C	1080	-	1/1/8/20	-	-
16	CLA	M	1080	-	1/1/8/20	-	-
16	CLA	N	358	-	1/1/8/20	-	-
16	CLA	B	1121	-	1/1/8/20	-	-
16	CLA	L	1117	-	1/1/8/20	-	-
16	CLA	C	1083	-	1/1/8/20	-	-

The worst 5 of 632 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	E	84	HEM	C2A-C1A	7.38	1.52	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	0	138	HEM	C2A-C1A	7.34	1.52	1.39
21	V	138	HEM	C2A-C1A	7.31	1.52	1.39
21	P	92	HEM	C2A-C1A	7.29	1.52	1.39
21	V	138	HEM	C3A-C4A	6.78	1.51	1.39

The worst 5 of 734 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	N	354	CLA	C4A-NA-C1A	10.53	111.44	106.71
16	D	354	CLA	C4A-NA-C1A	10.52	111.44	106.71
16	C	1089	CLA	C4A-NA-C1A	10.43	111.39	106.71
16	D	357	CLA	C4A-NA-C1A	10.37	111.37	106.71
16	N	358	CLA	C4A-NA-C1A	10.30	111.34	106.71

5 of 73 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
16	A	365	CLA	ND
16	A	366	CLA	ND
16	A	368	CLA	ND
16	A	369	CLA	ND
16	B	1107	CLA	ND

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
20	D	359	BCR	C6-C7-C8-C9
20	D	359	BCR	C1-C6-C7-C8
20	D	359	BCR	C5-C6-C7-C8
20	K	47	BCR	C14-C15-C16-C17

There are no ring outliers.

70 monomers are involved in 601 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	A	367	PHO	20	0
16	L	1110	CLA	6	0
16	A	368	CLA	25	0
16	J	367	CLA	23	0
16	L	1108	CLA	13	0
16	M	1084	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	L	1114	CLA	12	0
16	C	1082	CLA	12	0
16	D	354	CLA	8	0
17	J	366	PHO	19	0
16	M	1078	CLA	3	0
16	L	1111	CLA	16	0
16	N	355	CLA	4	0
16	B	1111	CLA	19	0
16	L	1118	CLA	6	0
16	L	1109	CLA	14	0
16	M	1079	CLA	17	0
16	L	1113	CLA	4	0
16	B	1113	CLA	3	0
16	C	1081	CLA	5	0
16	D	357	CLA	5	0
16	B	1110	CLA	10	0
16	L	1120	CLA	22	0
16	B	1109	CLA	15	0
16	B	1117	CLA	13	0
21	V	138	HEM	8	0
16	M	1082	CLA	6	0
17	D	356	PHO	9	0
16	M	1087	CLA	12	0
16	L	1121	CLA	3	0
16	J	365	CLA	2	0
16	B	1112	CLA	3	0
16	B	1107	CLA	11	0
21	0	138	HEM	8	0
16	M	1086	CLA	3	0
16	B	1116	CLA	7	0
16	B	1108	CLA	9	0
16	C	1086	CLA	9	0
16	C	1079	CLA	16	0
16	B	1114	CLA	15	0
16	A	369	CLA	2	0
16	A	365	CLA	5	0
16	B	1119	CLA	15	0
16	C	1089	CLA	25	0
20	D	359	BCR	9	0
20	K	47	BCR	1	0
16	C	1085	CLA	3	0
16	M	1085	CLA	4	0

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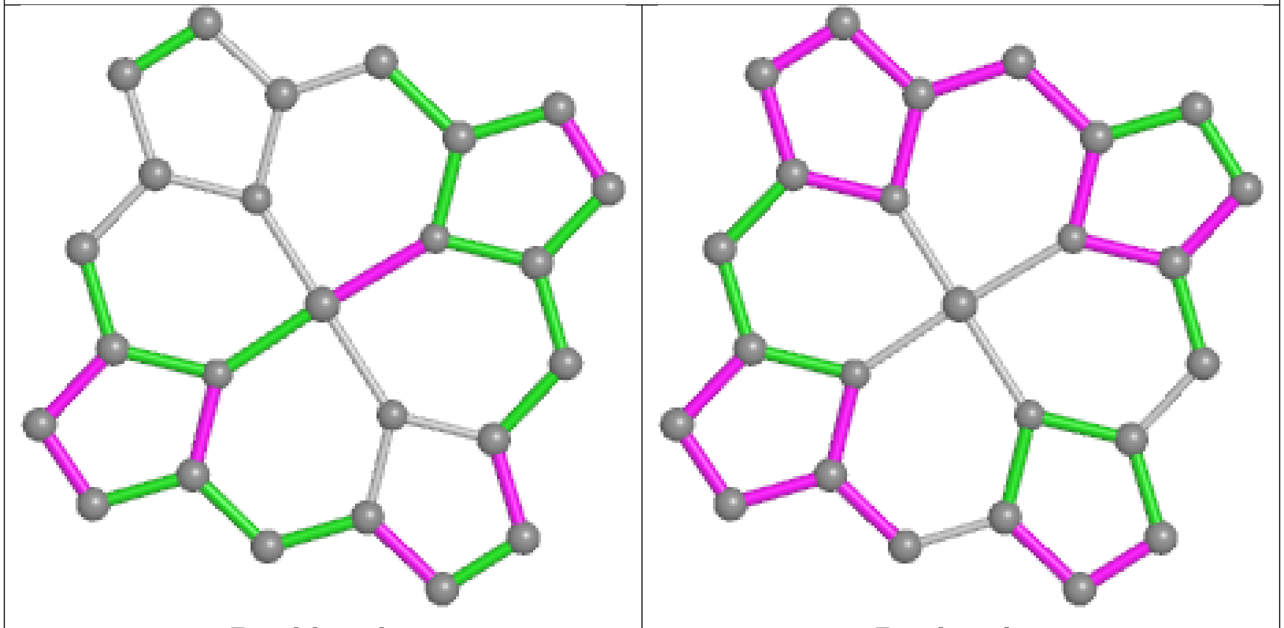
Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	C	1087	CLA	3	0
16	A	366	CLA	5	0
17	N	357	PHO	28	0
16	B	1120	CLA	5	0
16	M	1088	CLA	15	0
16	C	1078	CLA	11	0
16	L	1112	CLA	3	0
16	L	1107	CLA	9	0
16	C	1088	CLA	15	0
16	L	1119	CLA	23	0
16	N	354	CLA	5	0
16	M	1081	CLA	14	0
16	N	356	CLA	1	0
16	W	64	CLA	15	0
16	L	1115	CLA	2	0
16	B	1118	CLA	6	0
16	C	1080	CLA	11	0
16	M	1080	CLA	1	0
16	N	358	CLA	1	0
16	B	1121	CLA	3	0
16	L	1117	CLA	13	0
16	C	1083	CLA	6	0

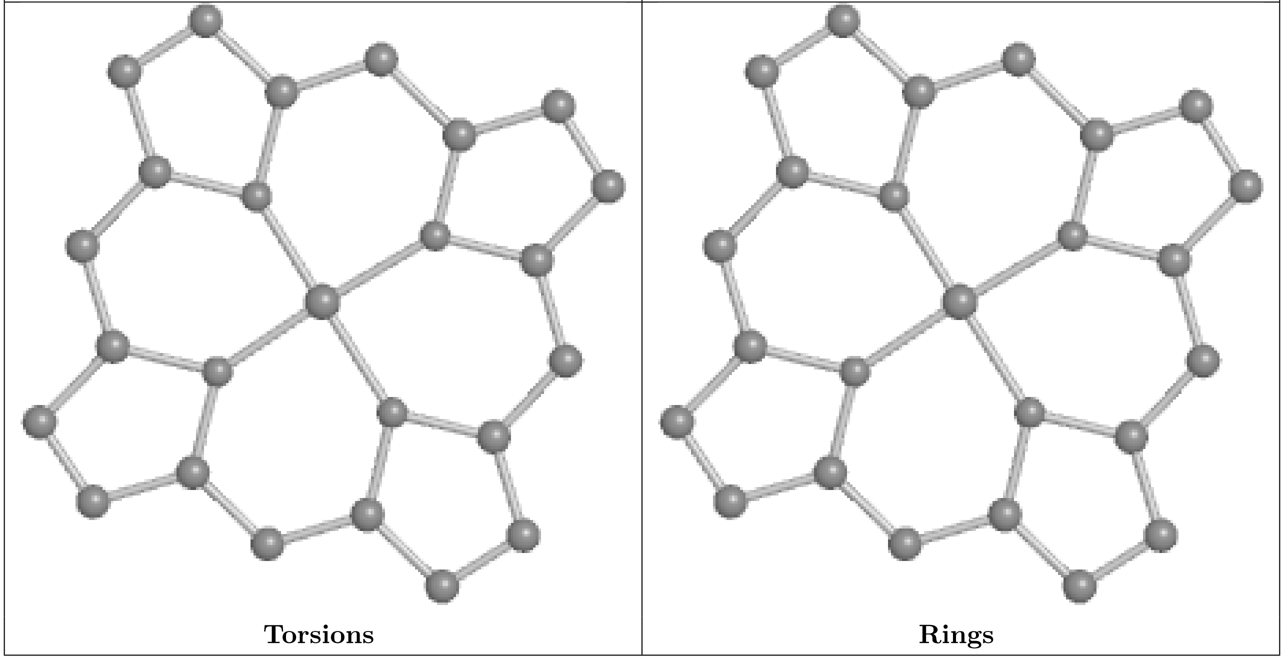
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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 HEM E 84



Bond lengths

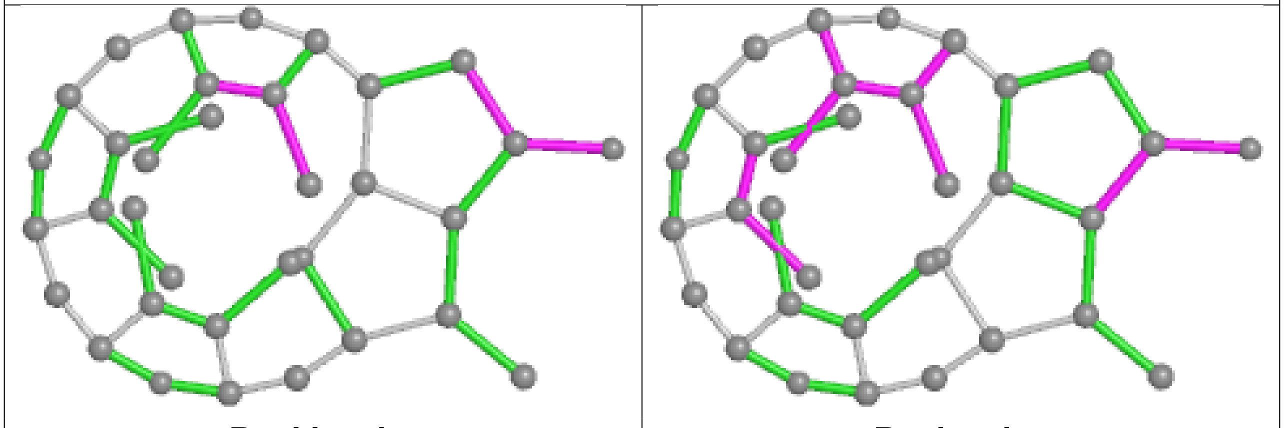
Bond angles



Torsions

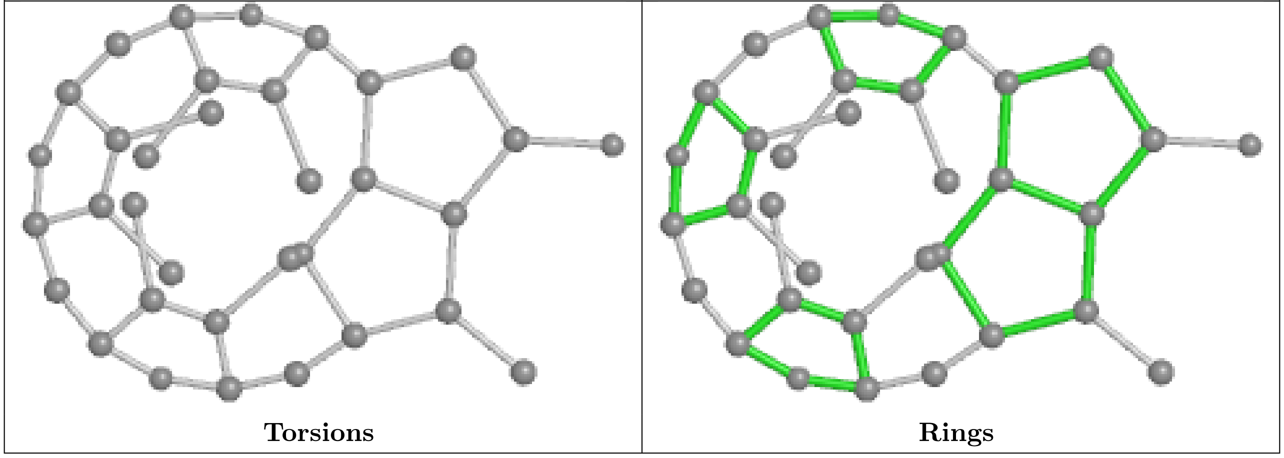
Rings

Ligand PHO A 367



Bond lengths

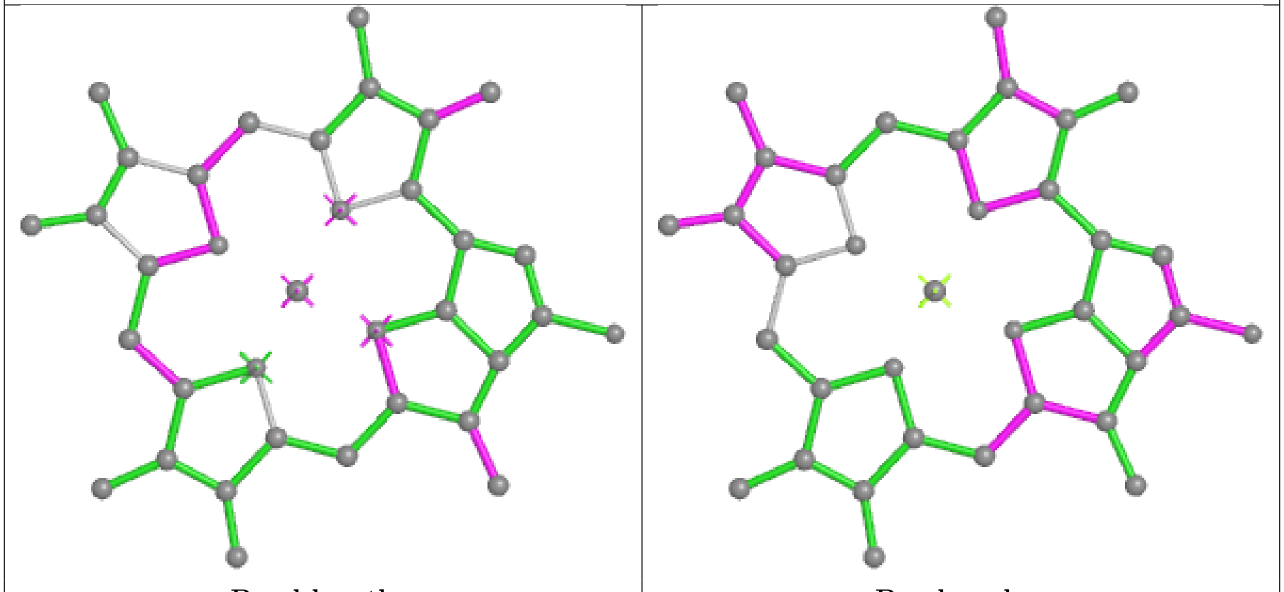
Bond angles



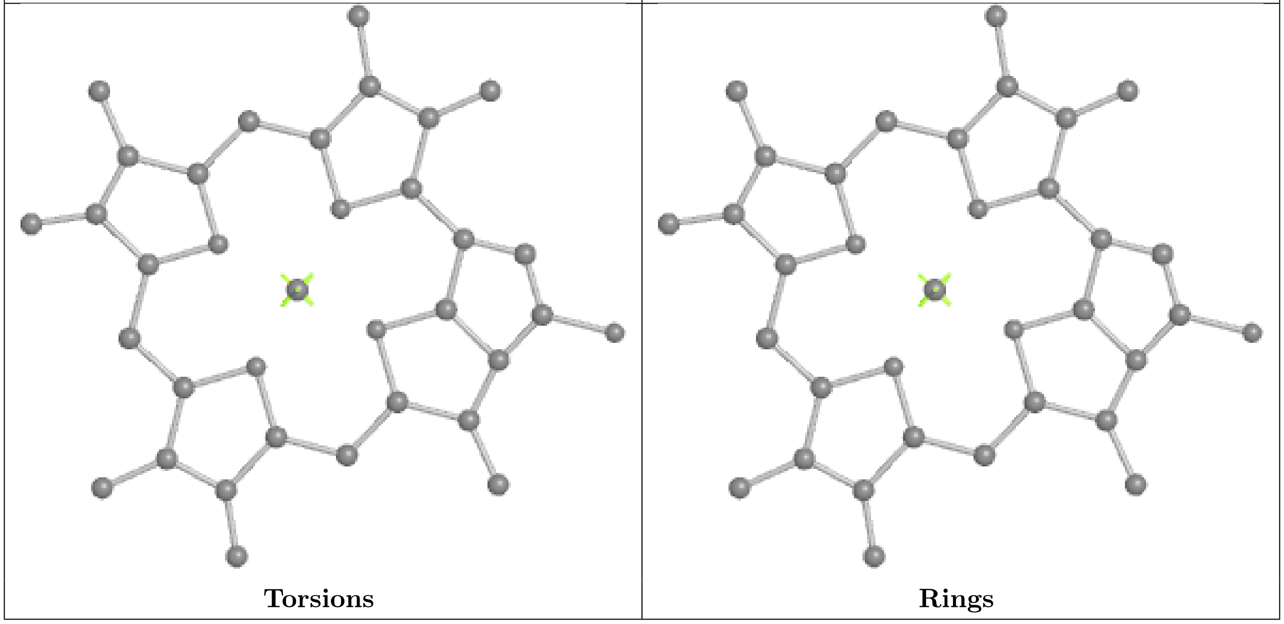
Torsions

Rings

Ligand CLA L 1110

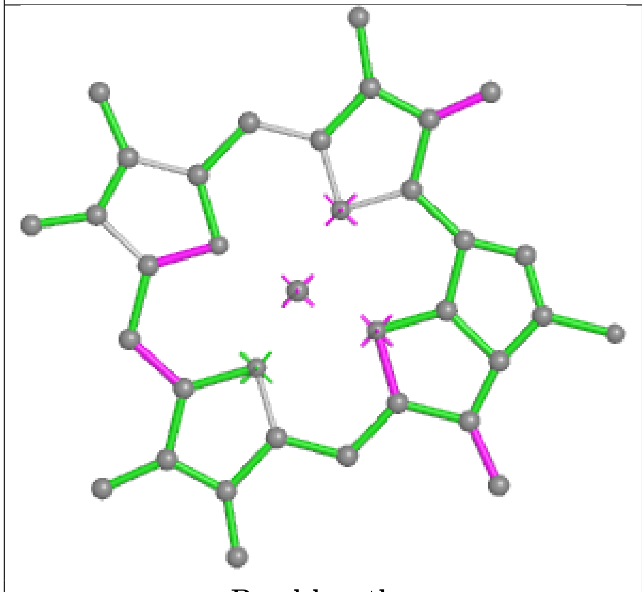


Bond lengths **Bond angles**

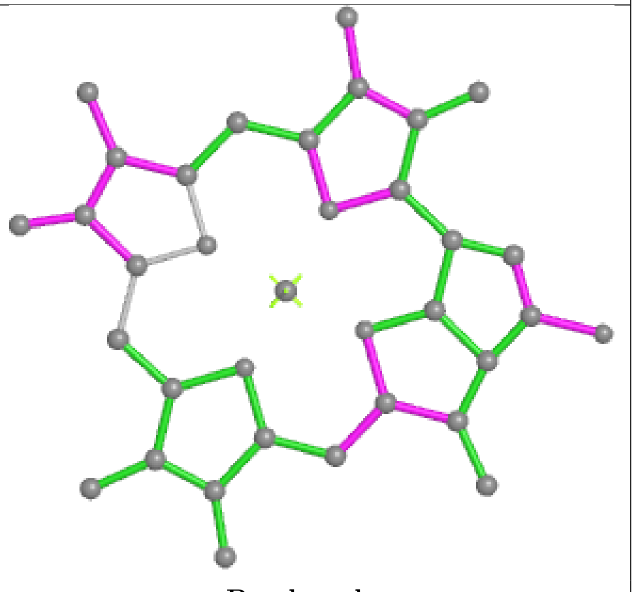


Torsions **Rings**

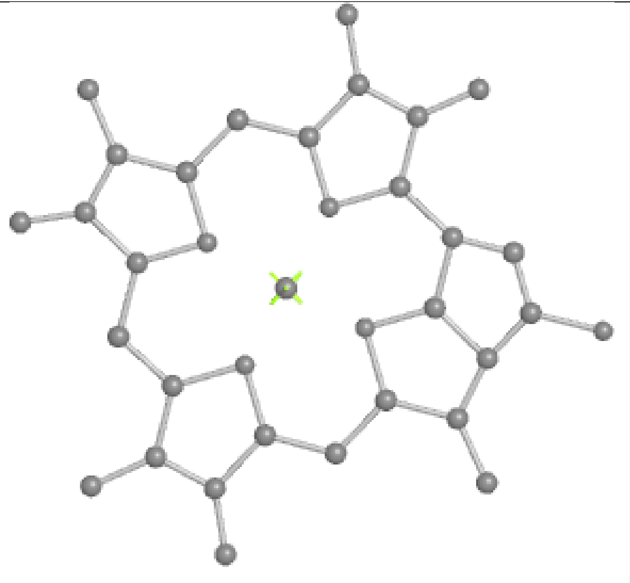
Ligand CLA A 368



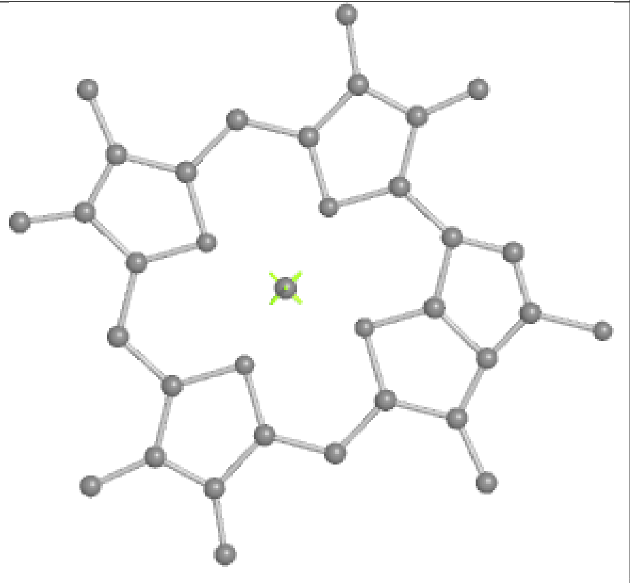
Bond lengths



Bond angles

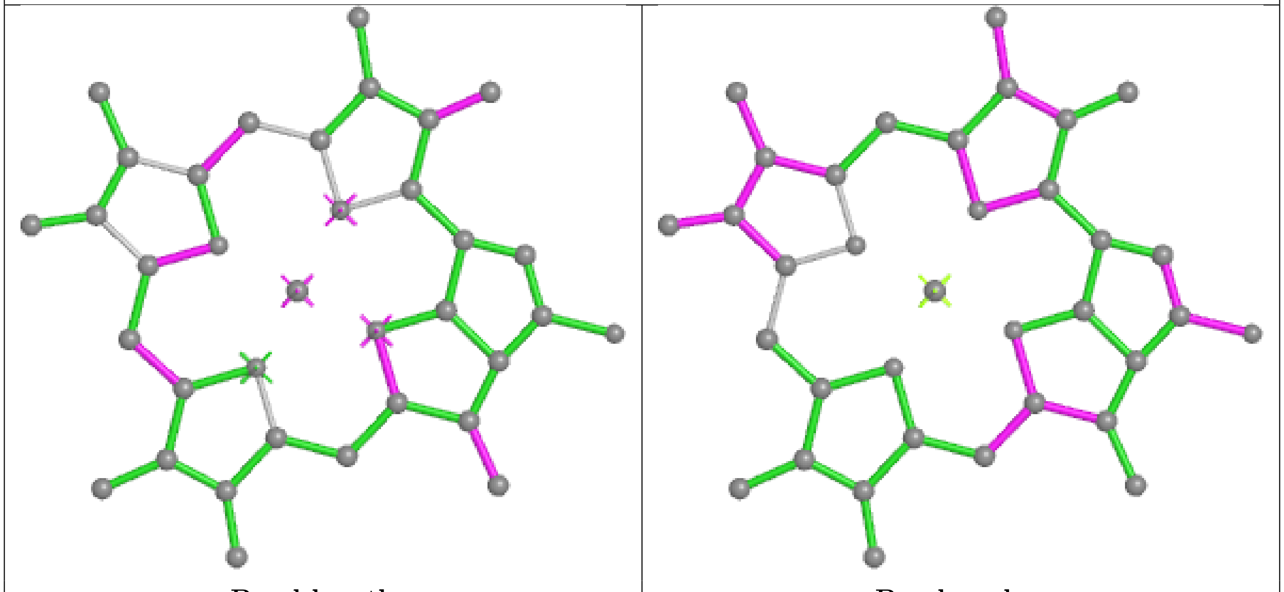


Torsions



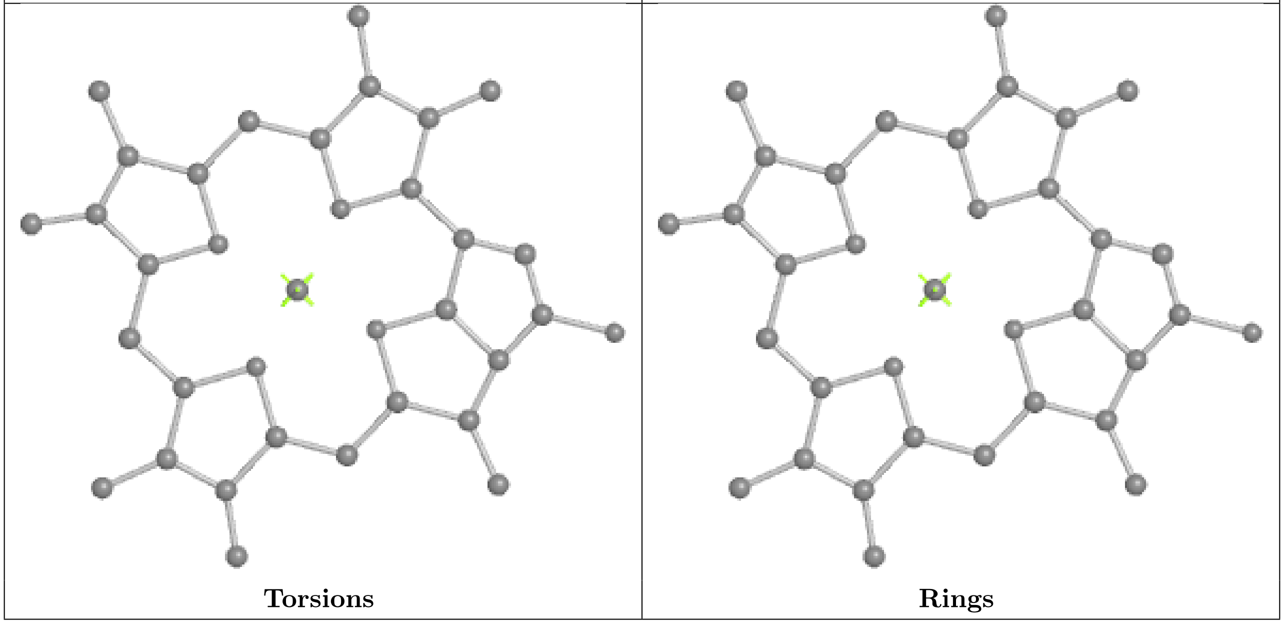
Rings

Ligand CLA J 367



Bond lengths

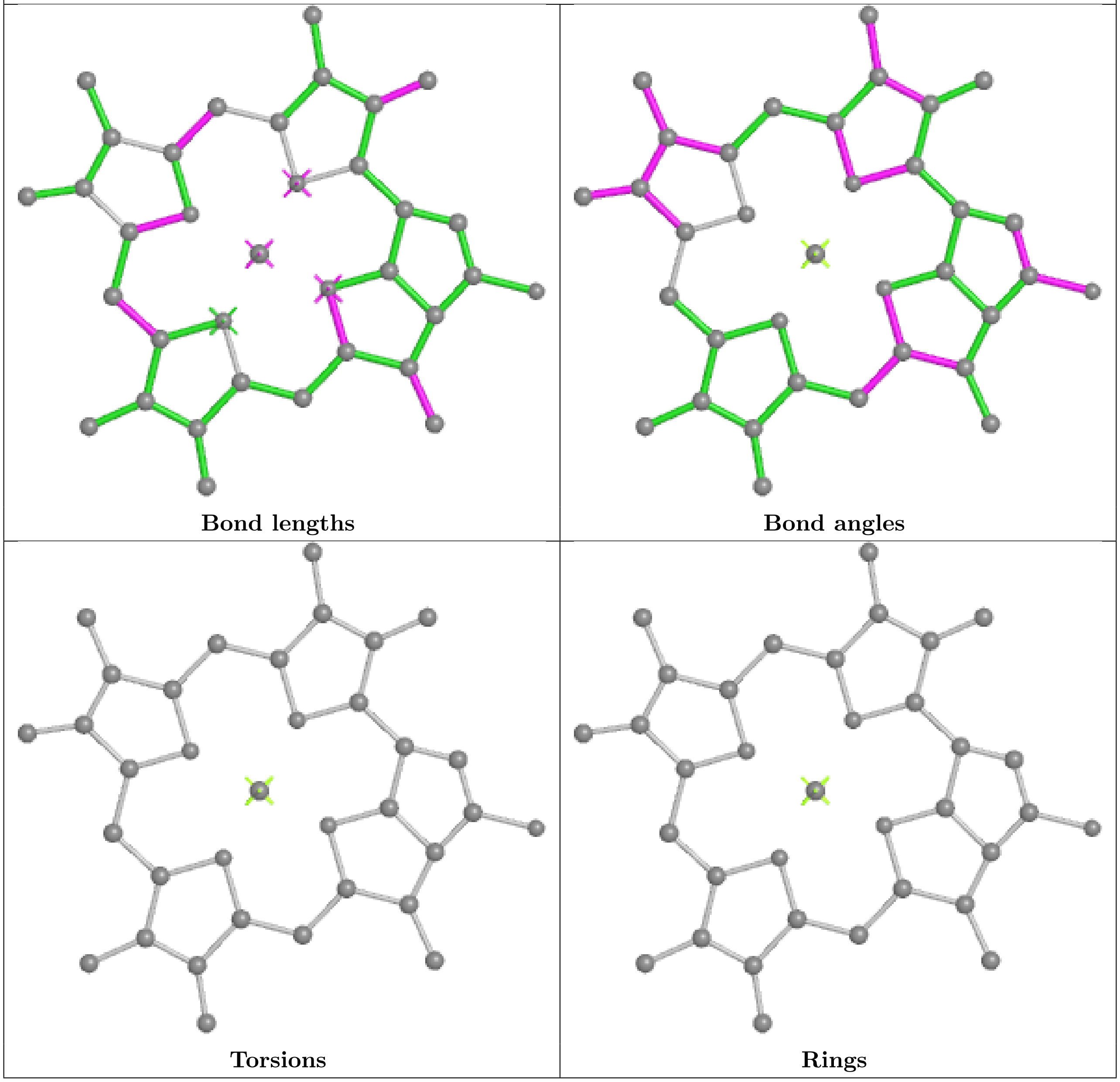
Bond angles



Torsions

Rings

Ligand CLA L 1108



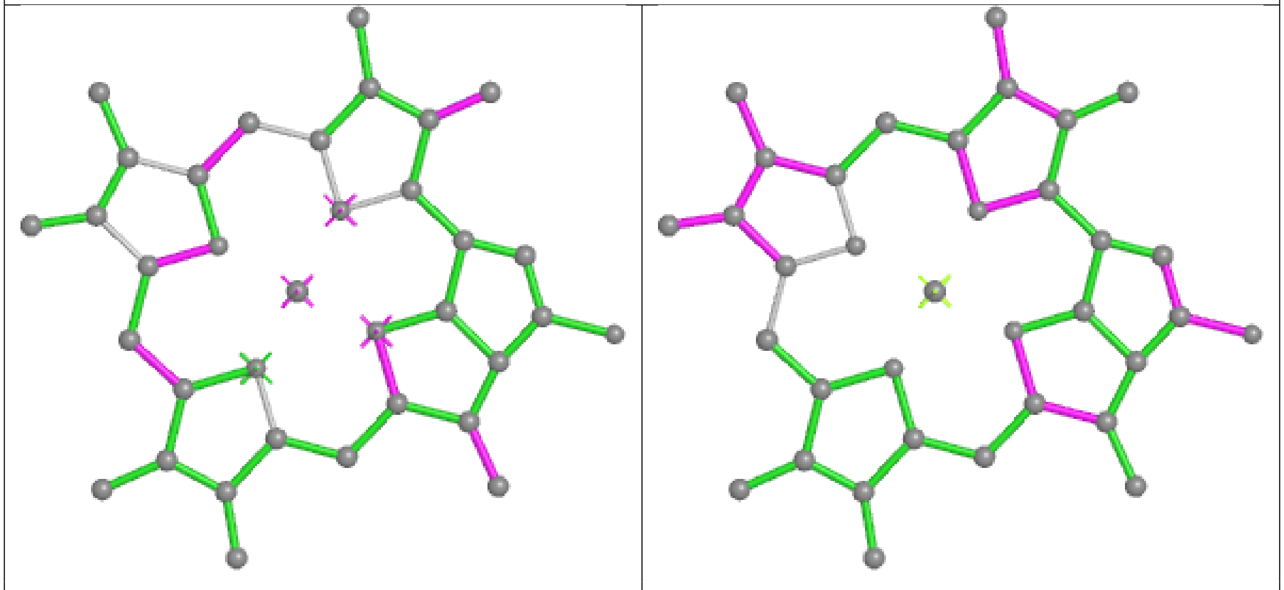
Bond lengths

Bond angles

Torsions

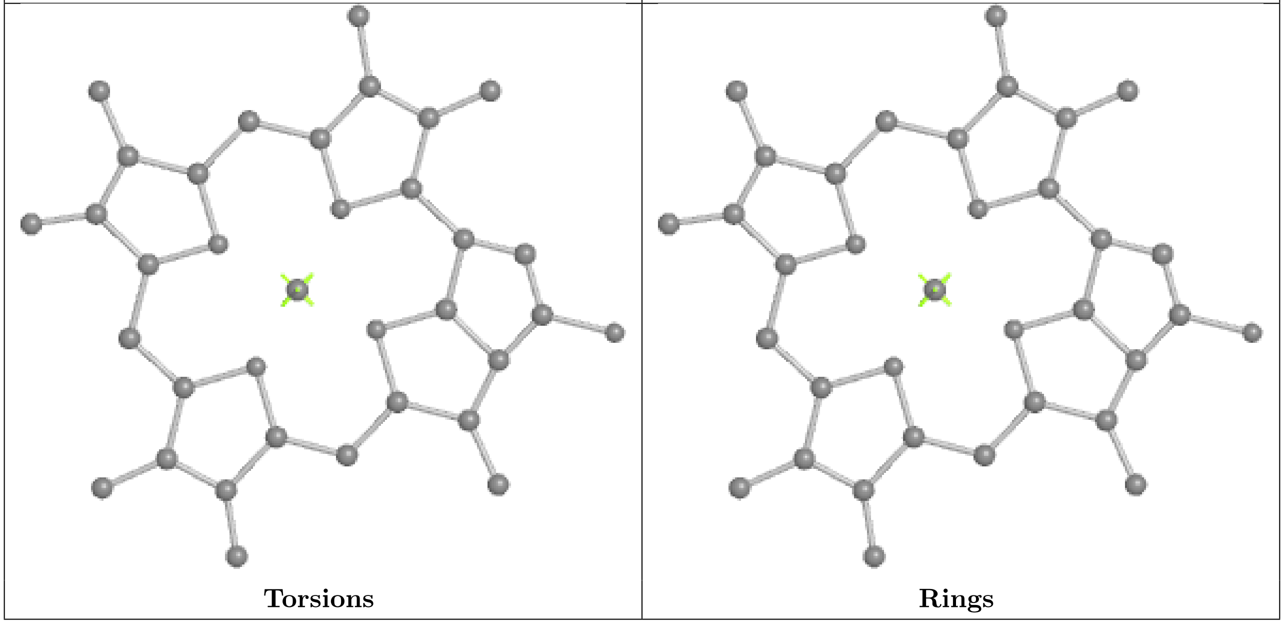
Rings

Ligand CLA M 1084



Bond lengths

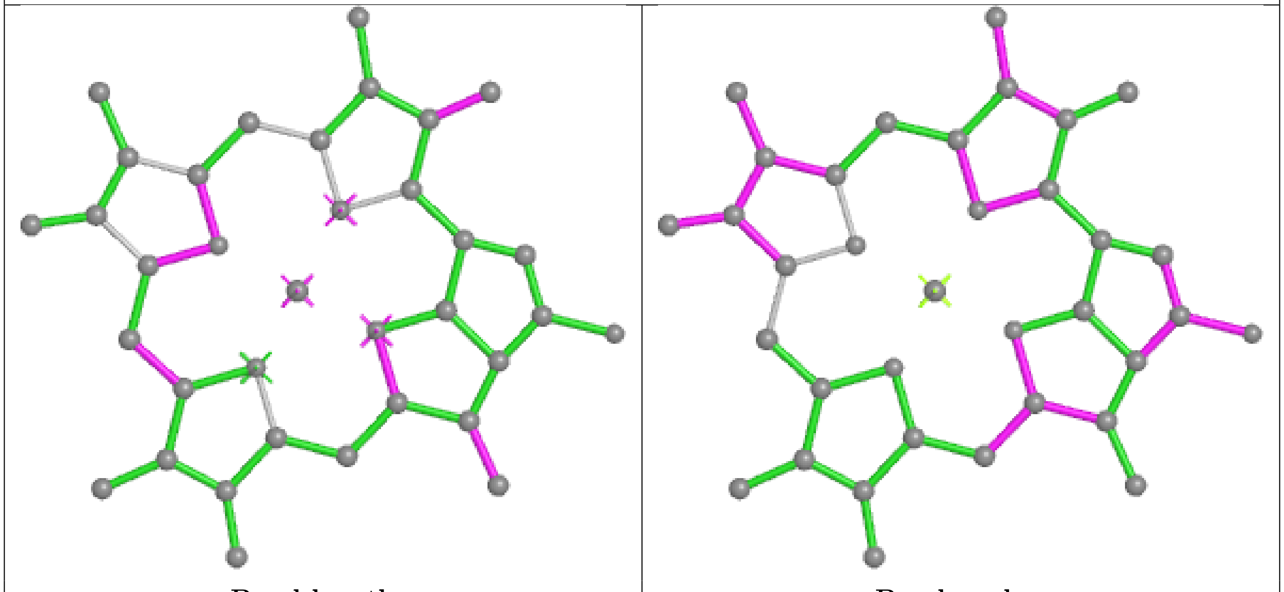
Bond angles



Torsions

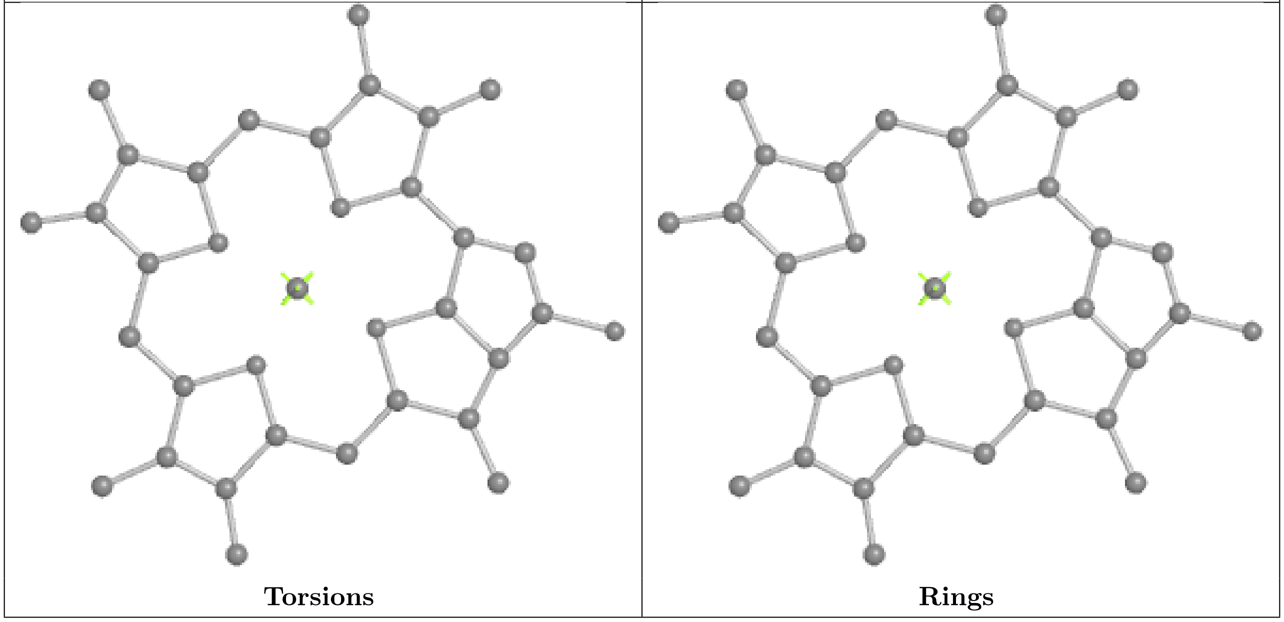
Rings

Ligand CLA M 1083



Bond lengths

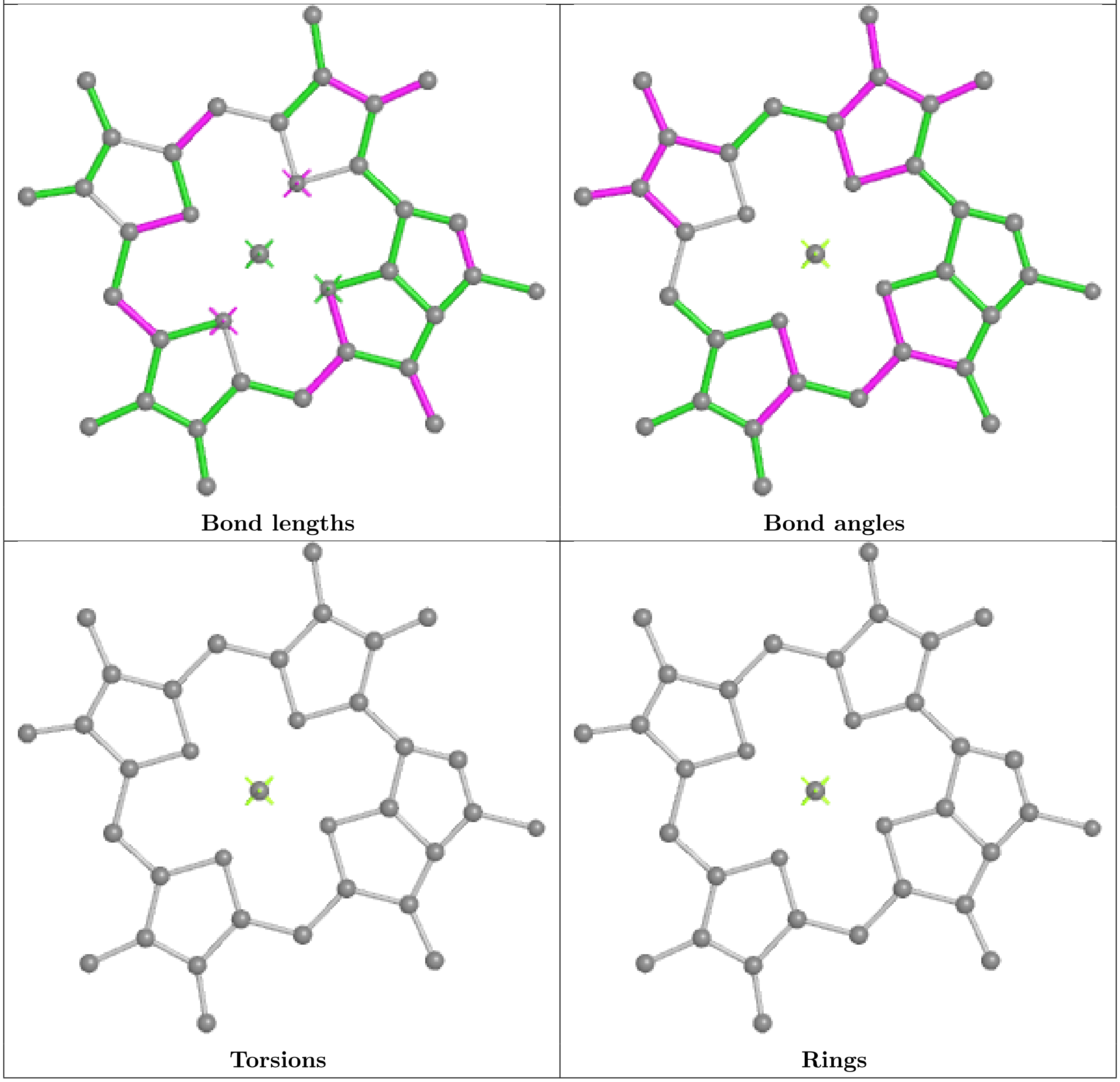
Bond angles



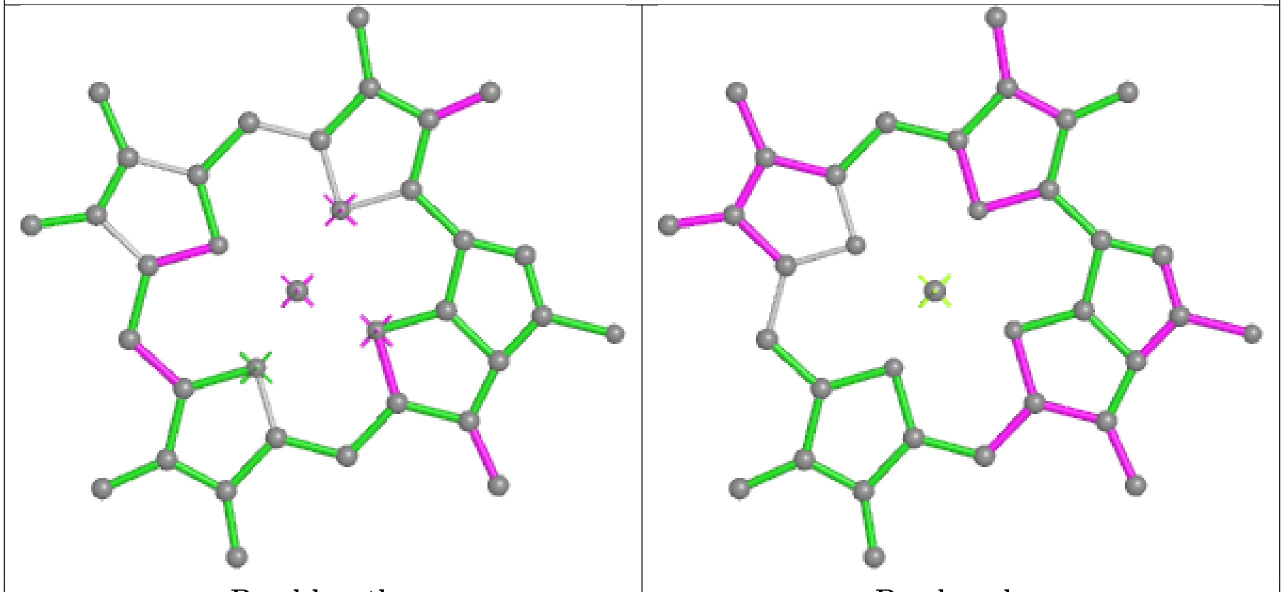
Torsions

Rings

Ligand CLA R 221

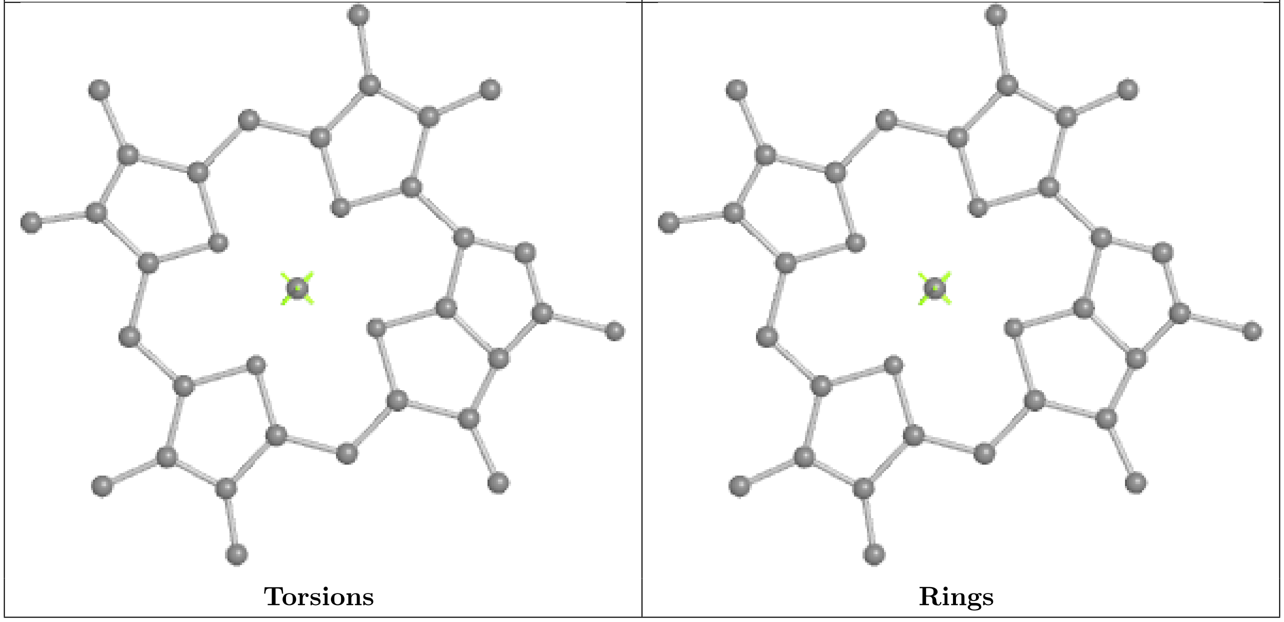


Ligand CLA L 1114



Bond lengths

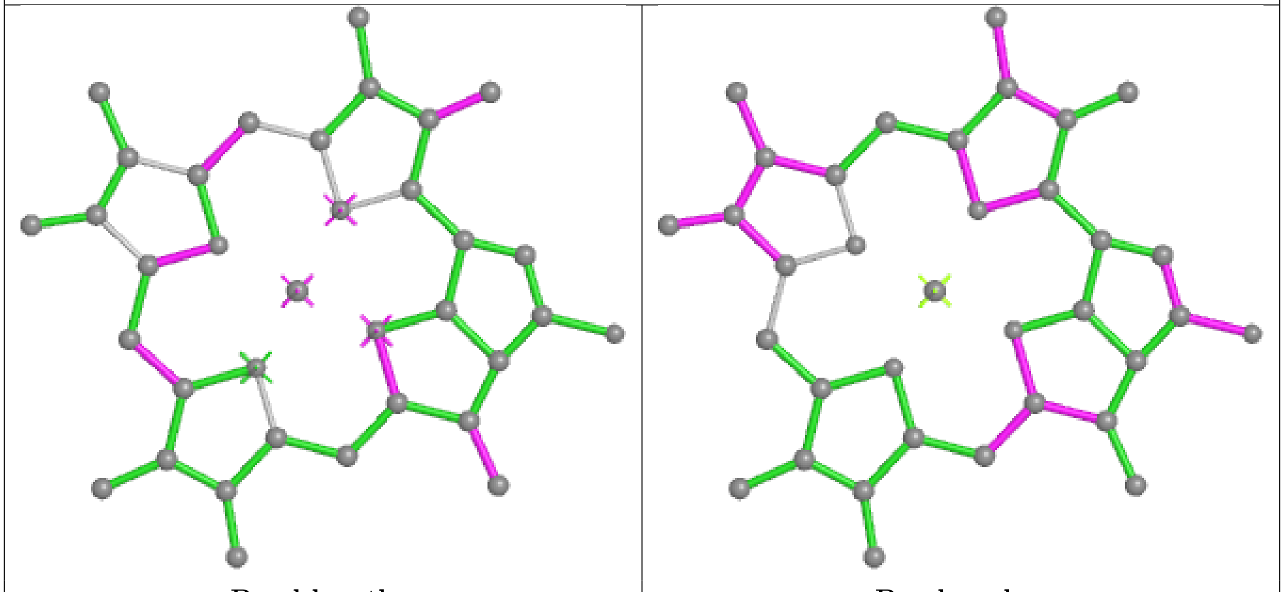
Bond angles



Torsions

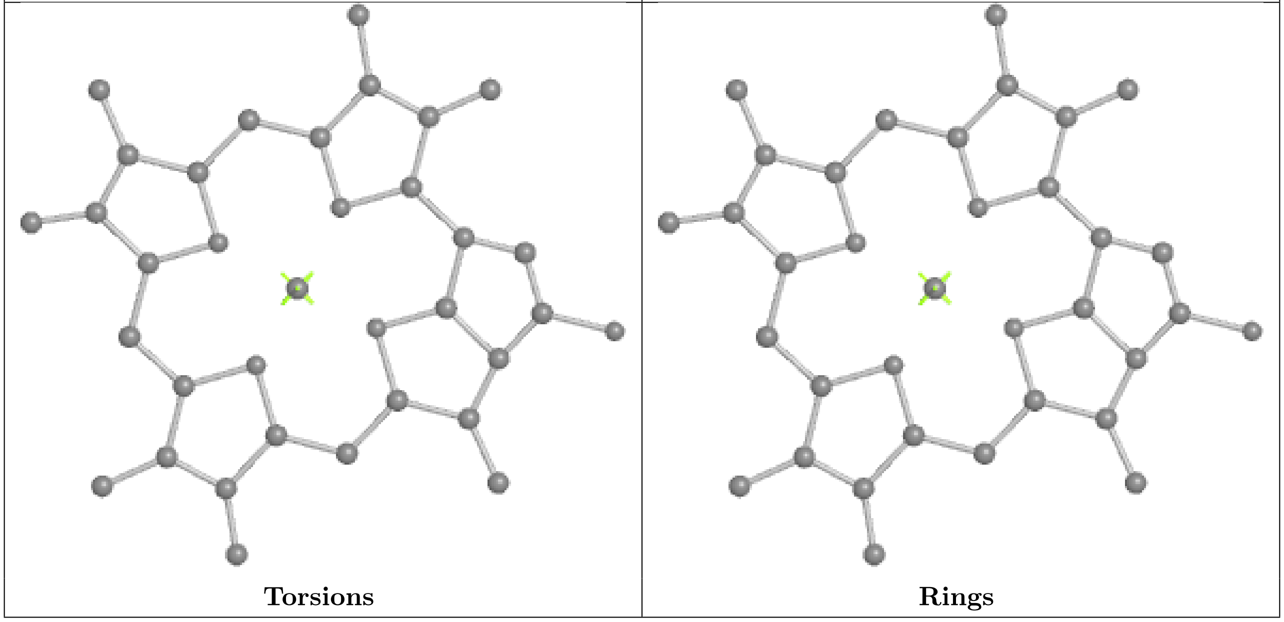
Rings

Ligand CLA C 1082



Bond lengths

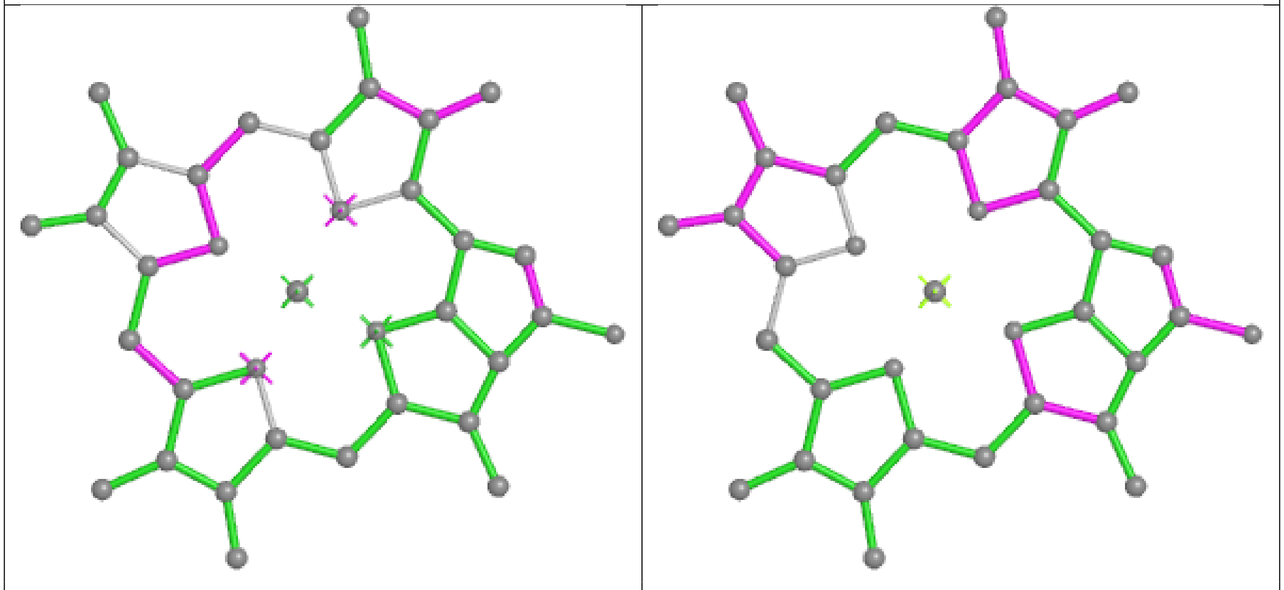
Bond angles



Torsions

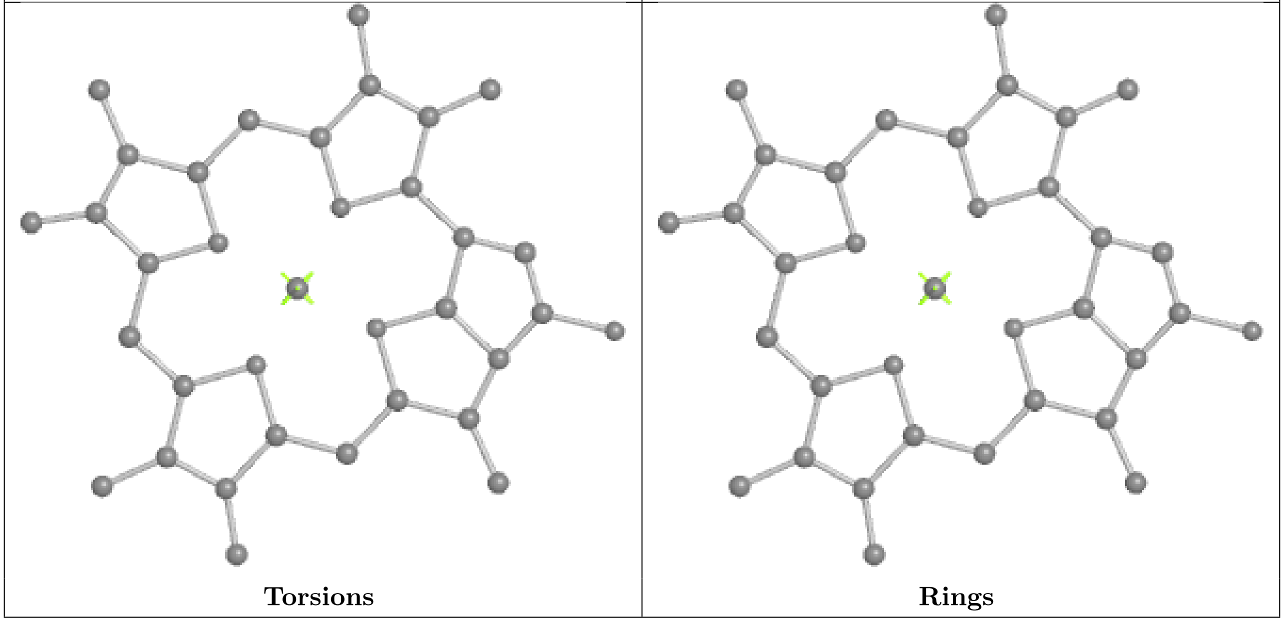
Rings

Ligand CLA D 354



Bond lengths

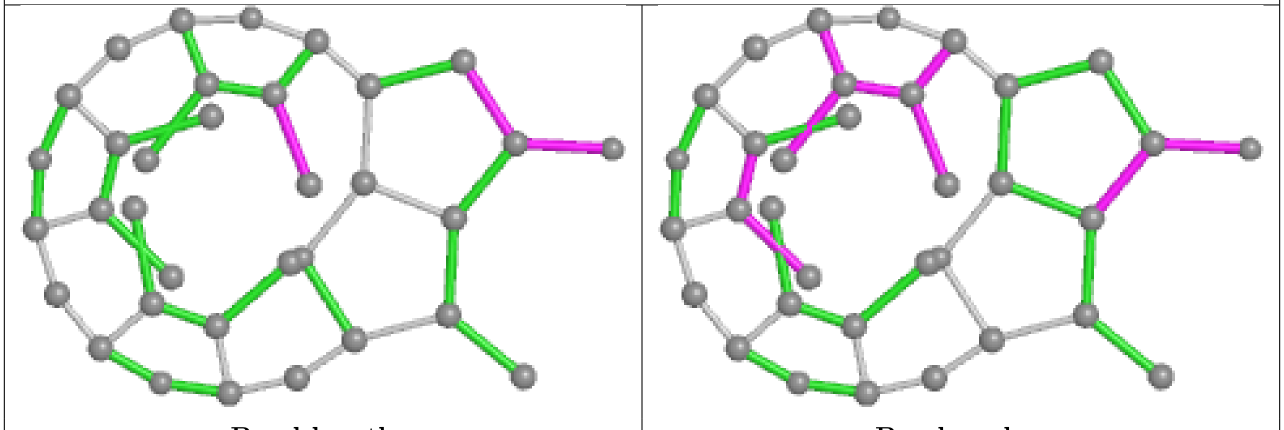
Bond angles



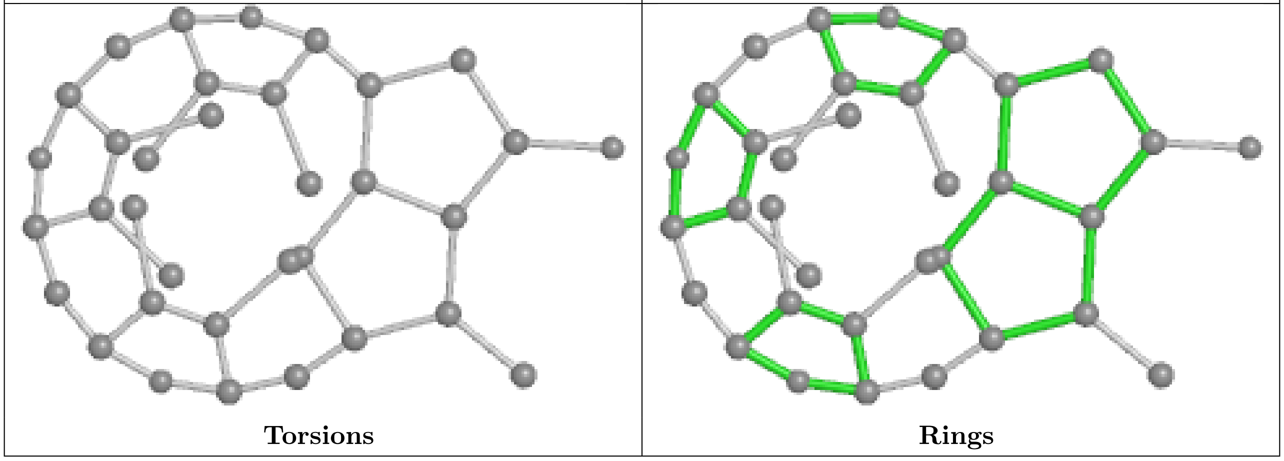
Torsions

Rings

Ligand PHO J 366

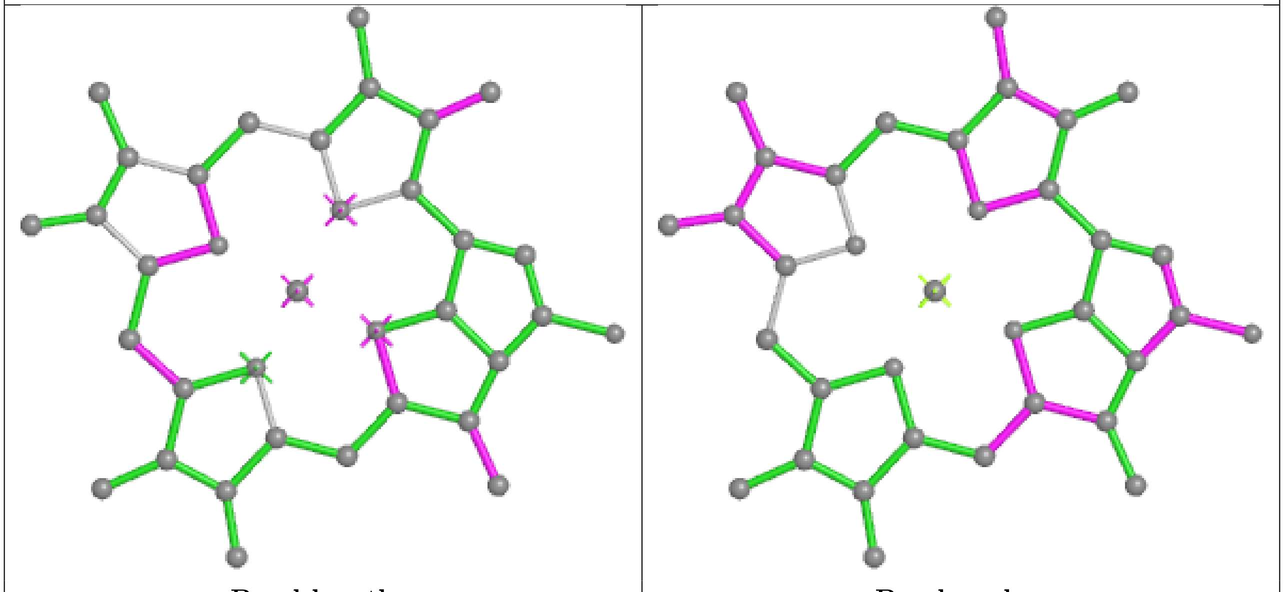


Bond lengths **Bond angles**

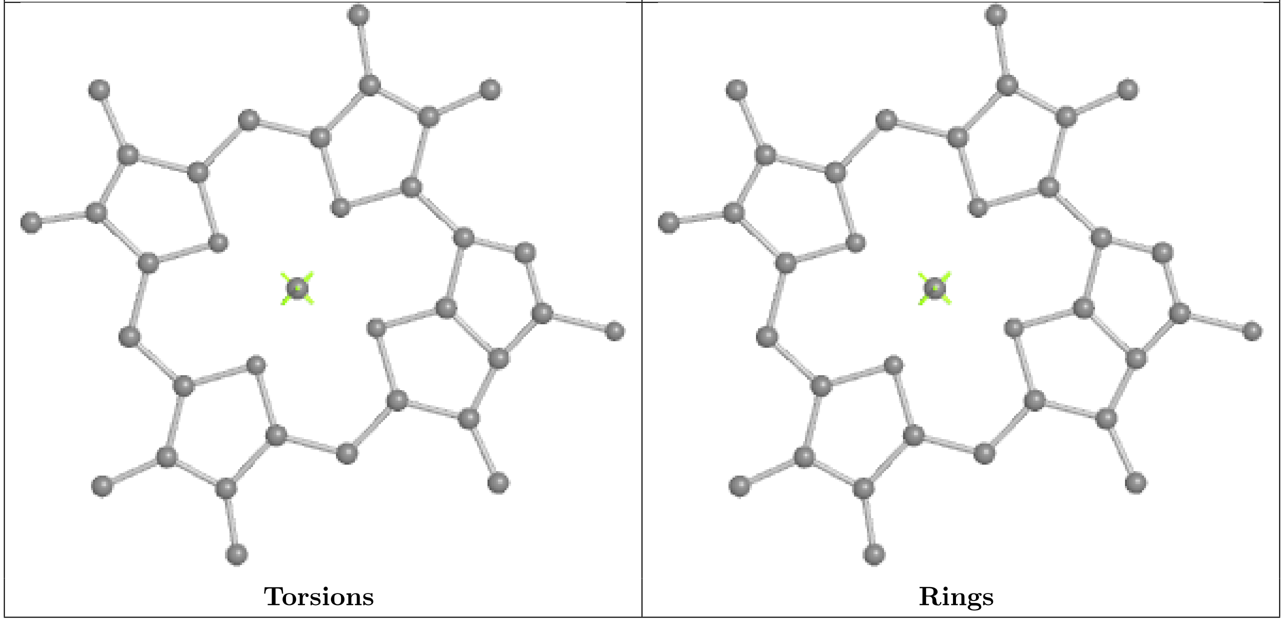


Torsions **Rings**

Ligand CLA J 368

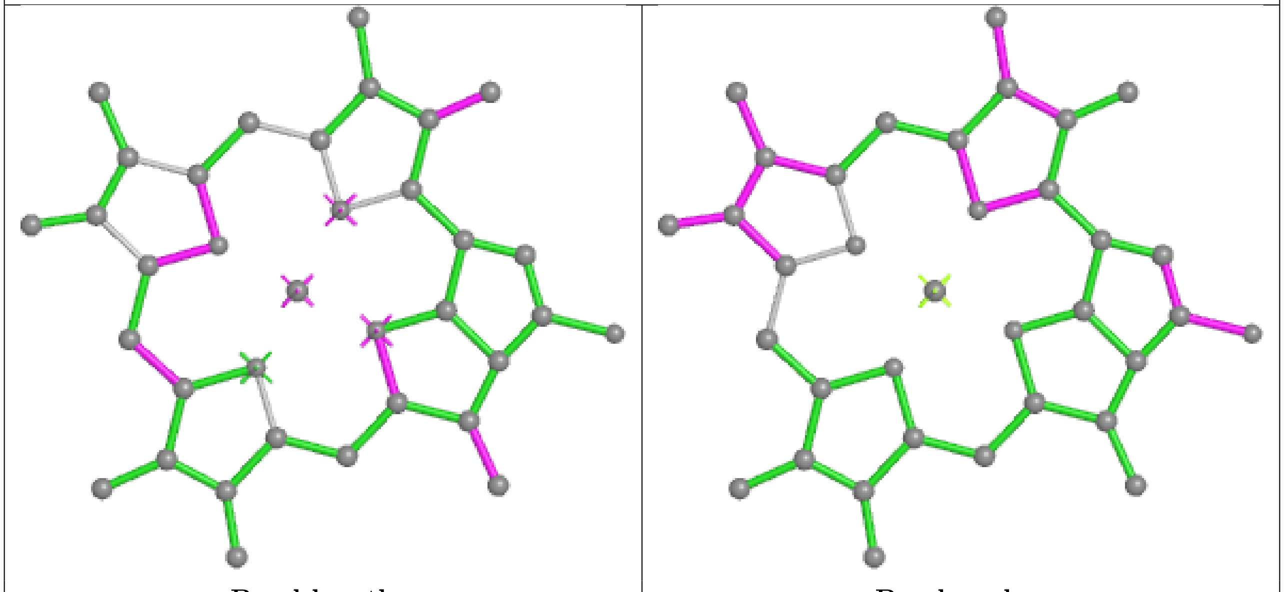


Bond lengths **Bond angles**

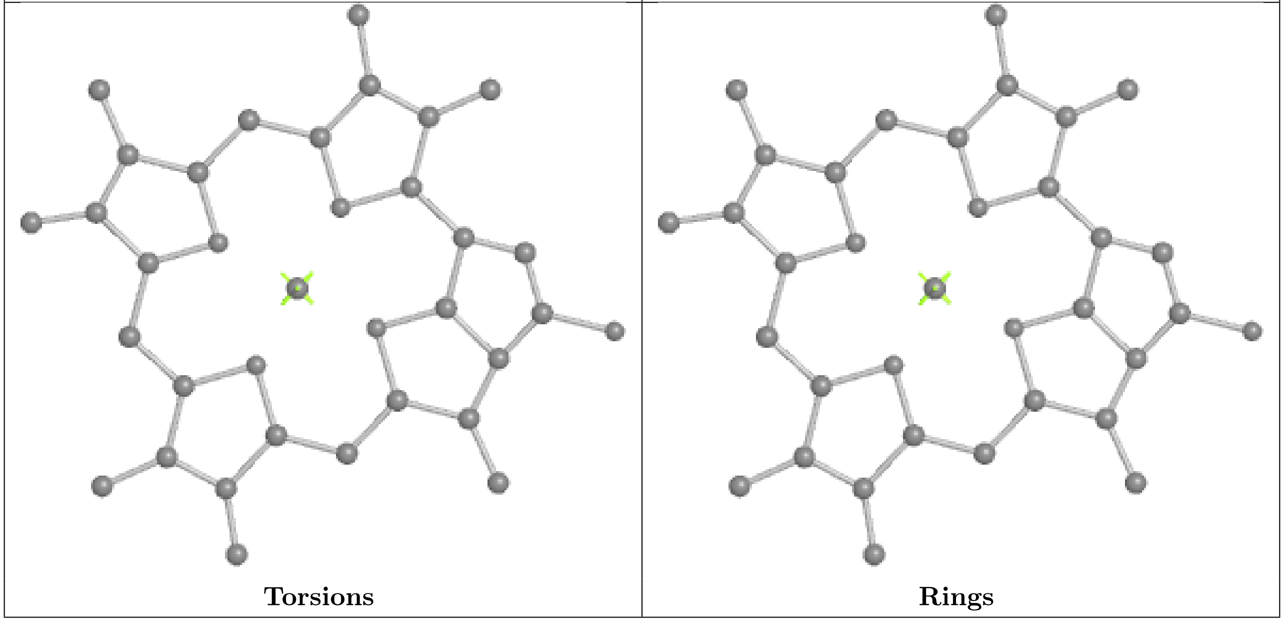


Torsions **Rings**

Ligand CLA M 1078

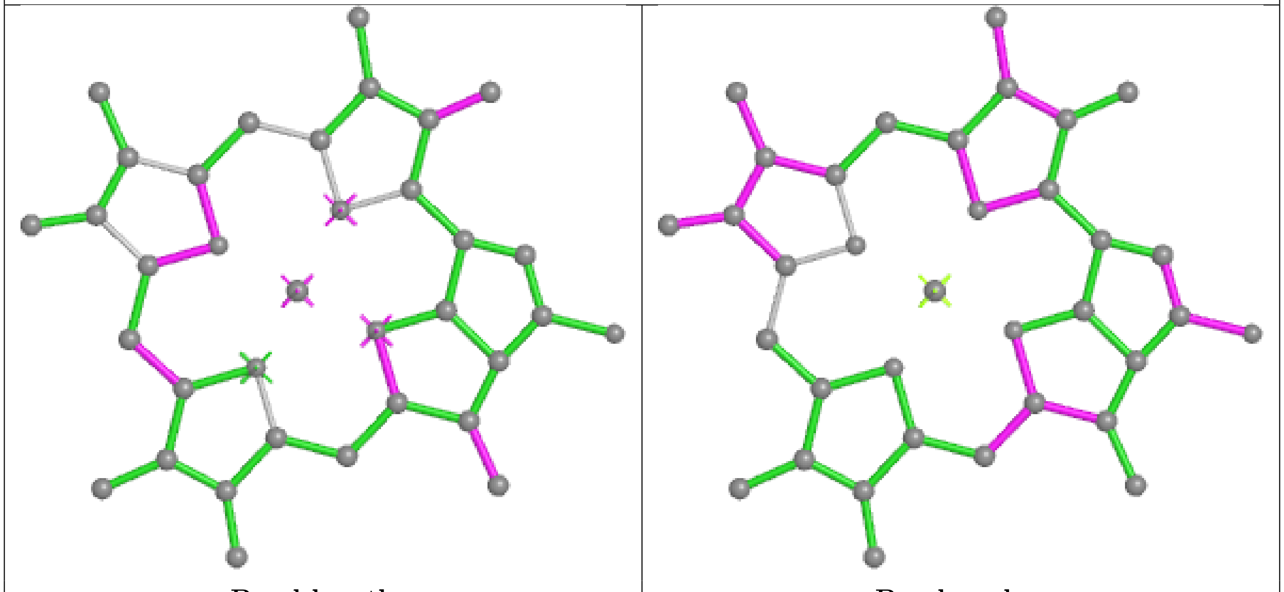


Bond lengths **Bond angles**

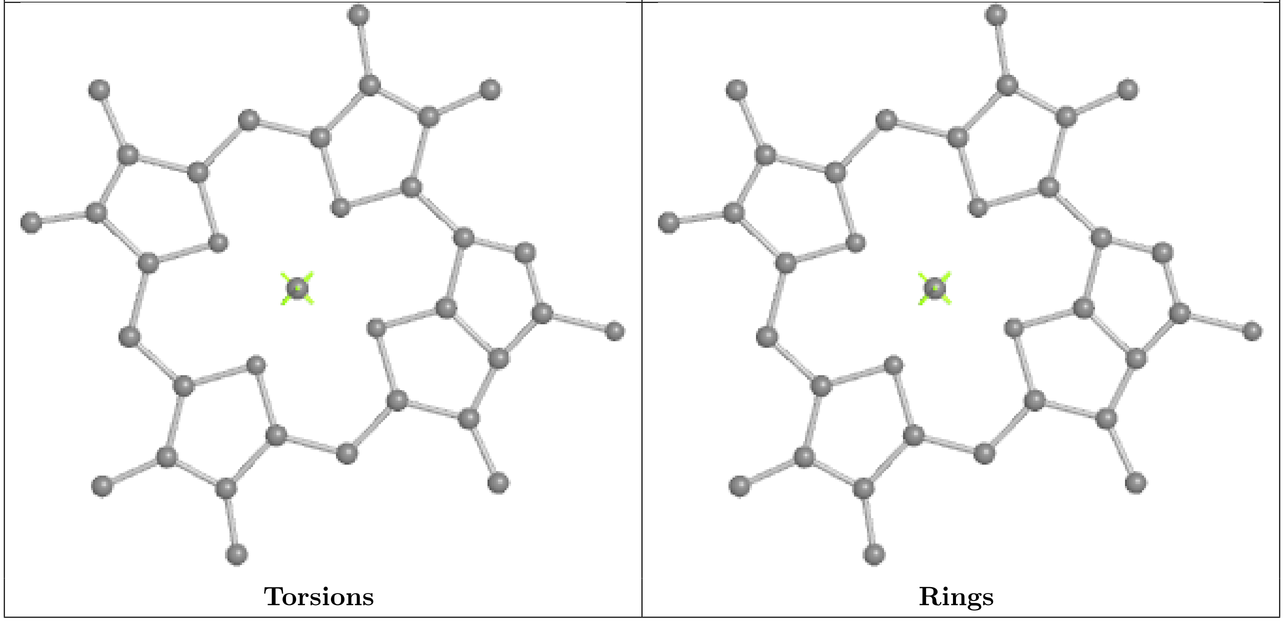


Torsions **Rings**

Ligand CLA L 1111

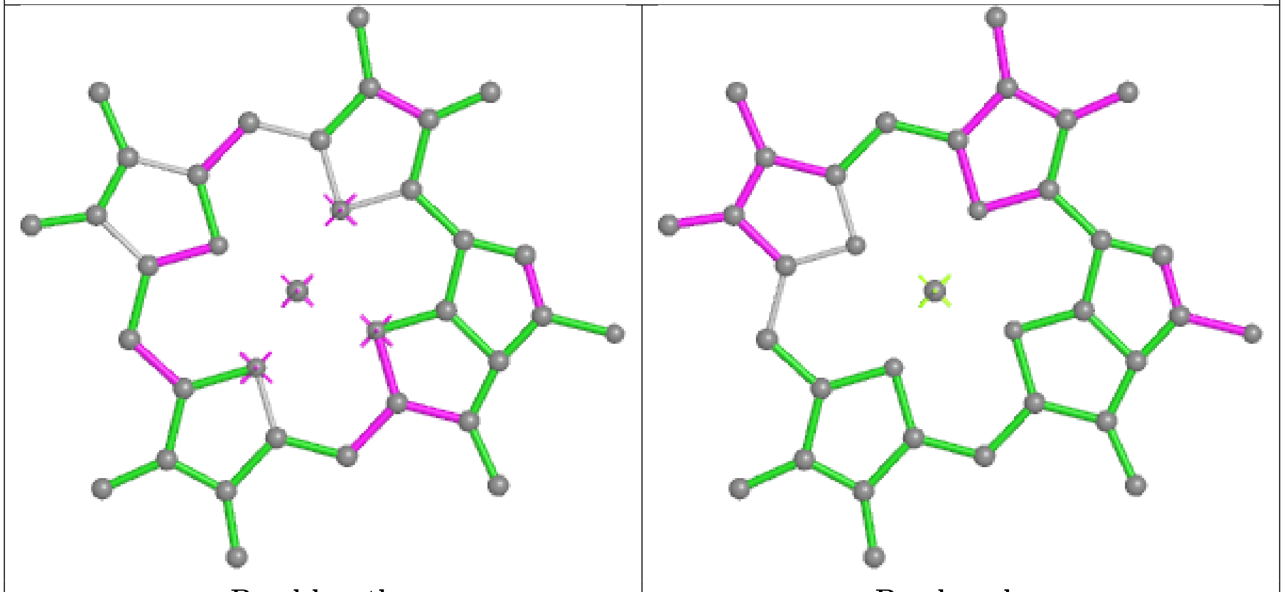


Bond lengths **Bond angles**



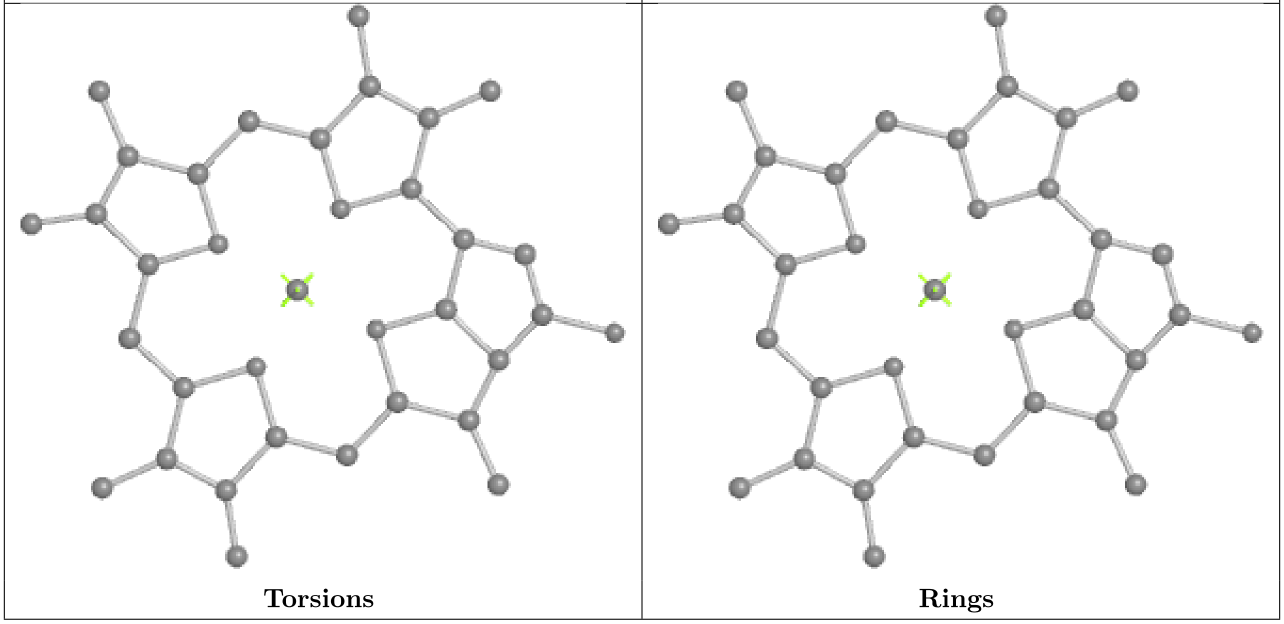
Torsions **Rings**

Ligand CLA N 355



Bond lengths

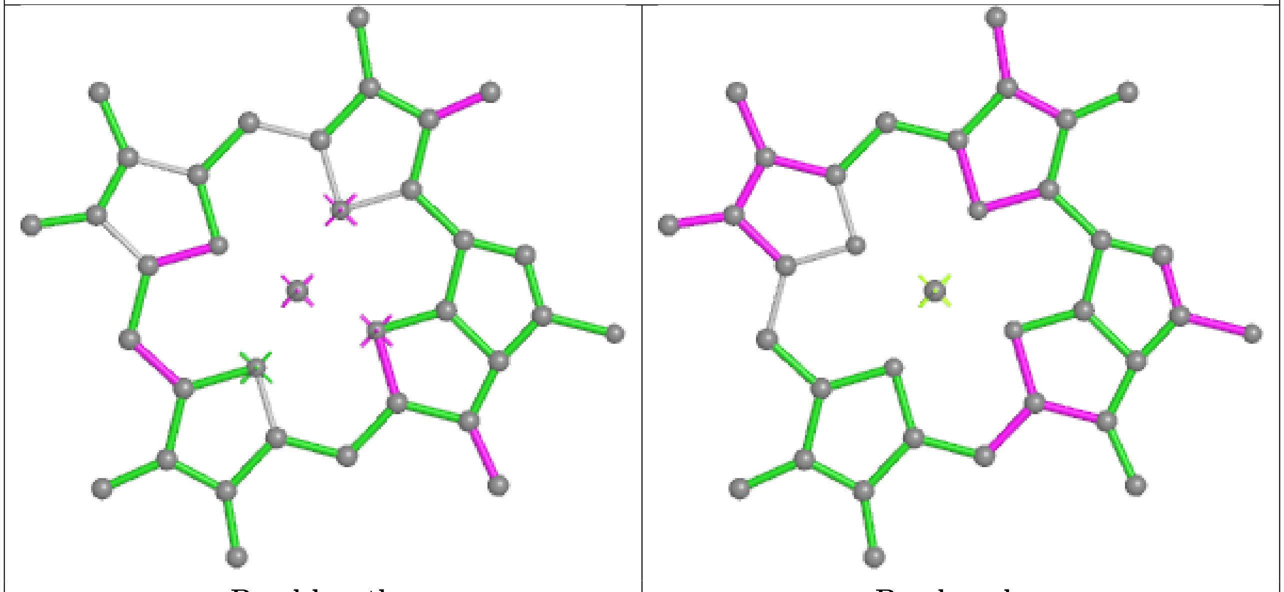
Bond angles



Torsions

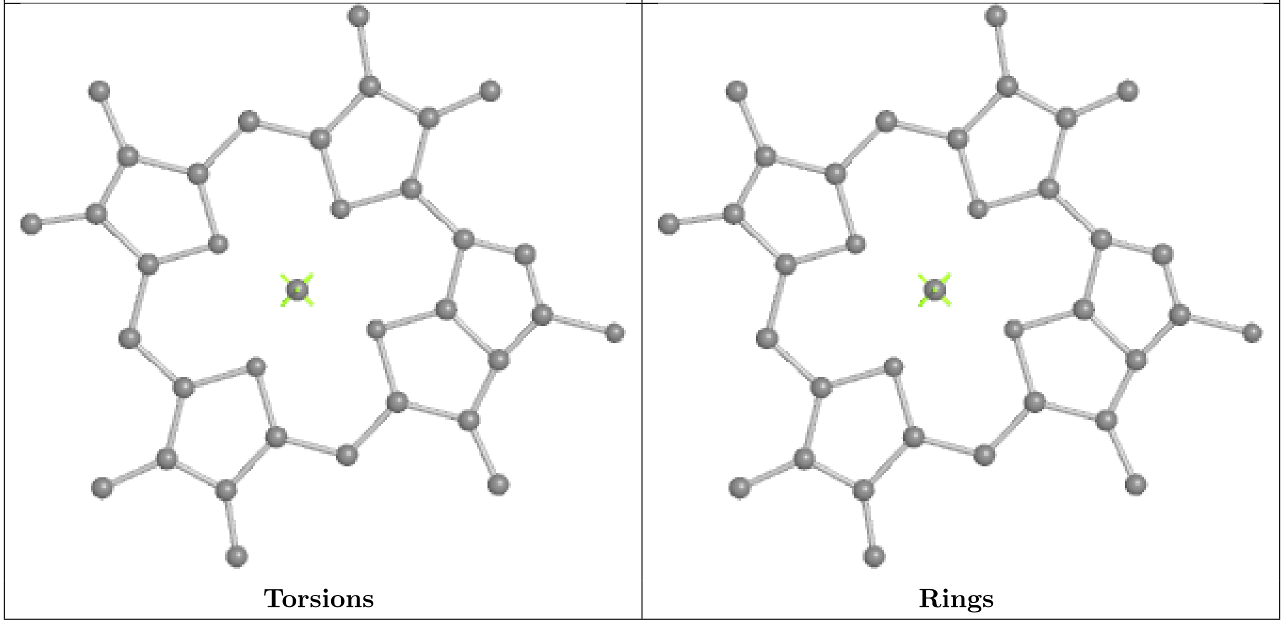
Rings

Ligand CLA B 1111



Bond lengths

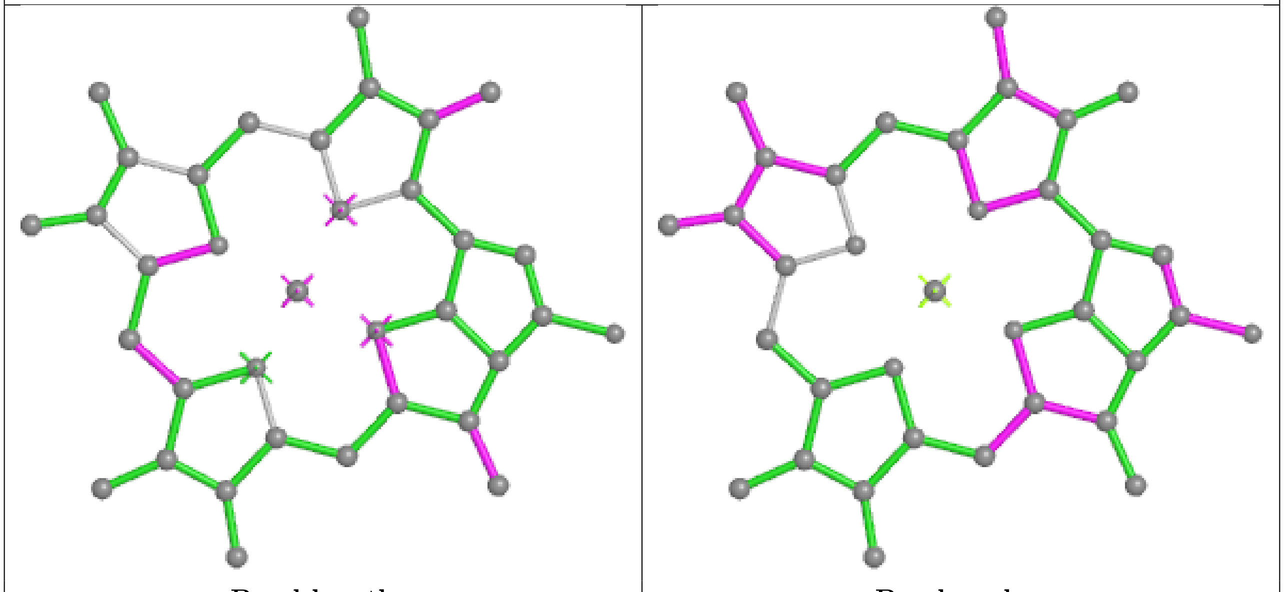
Bond angles



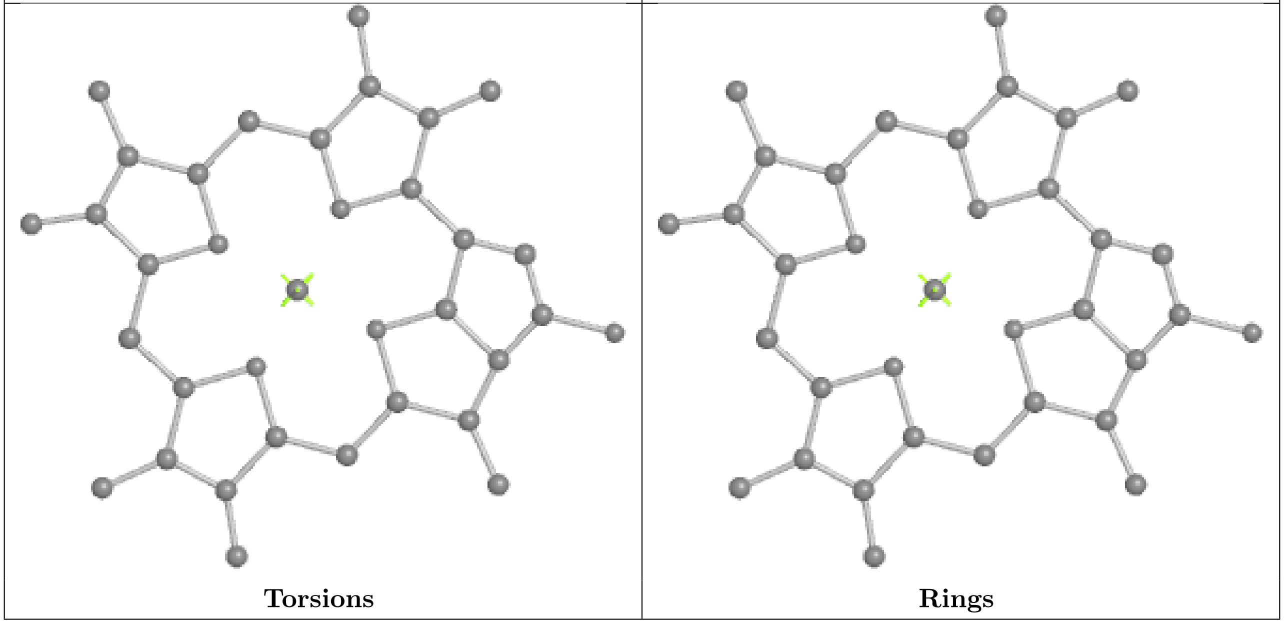
Torsions

Rings

Ligand CLA L 1122

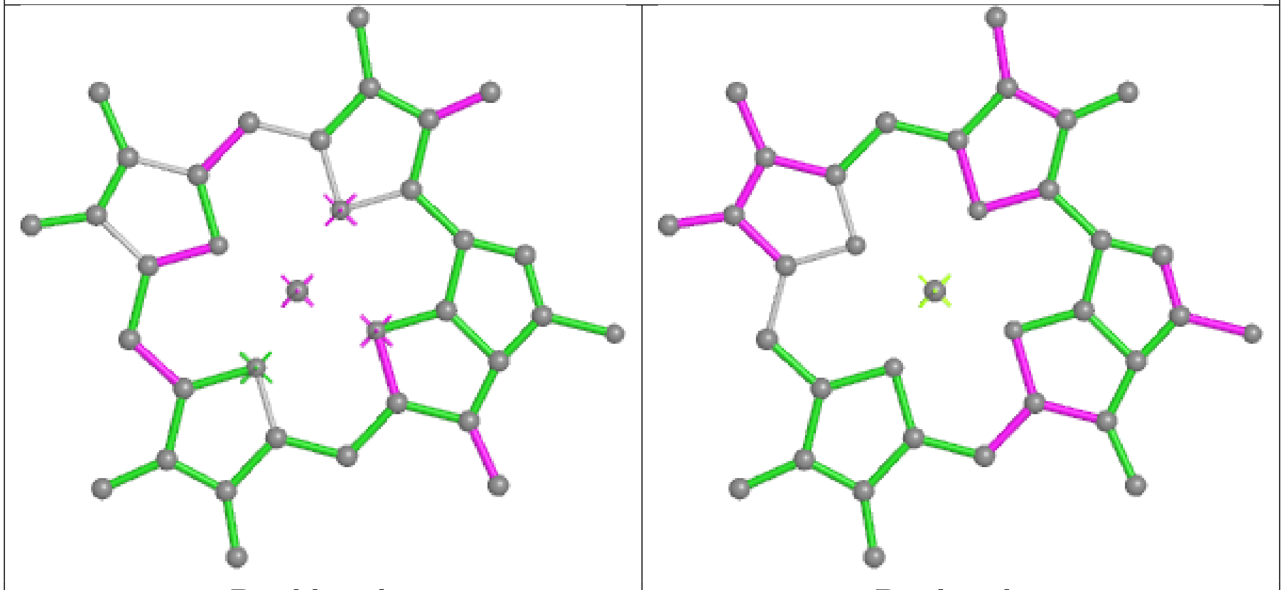


Bond lengths **Bond angles**



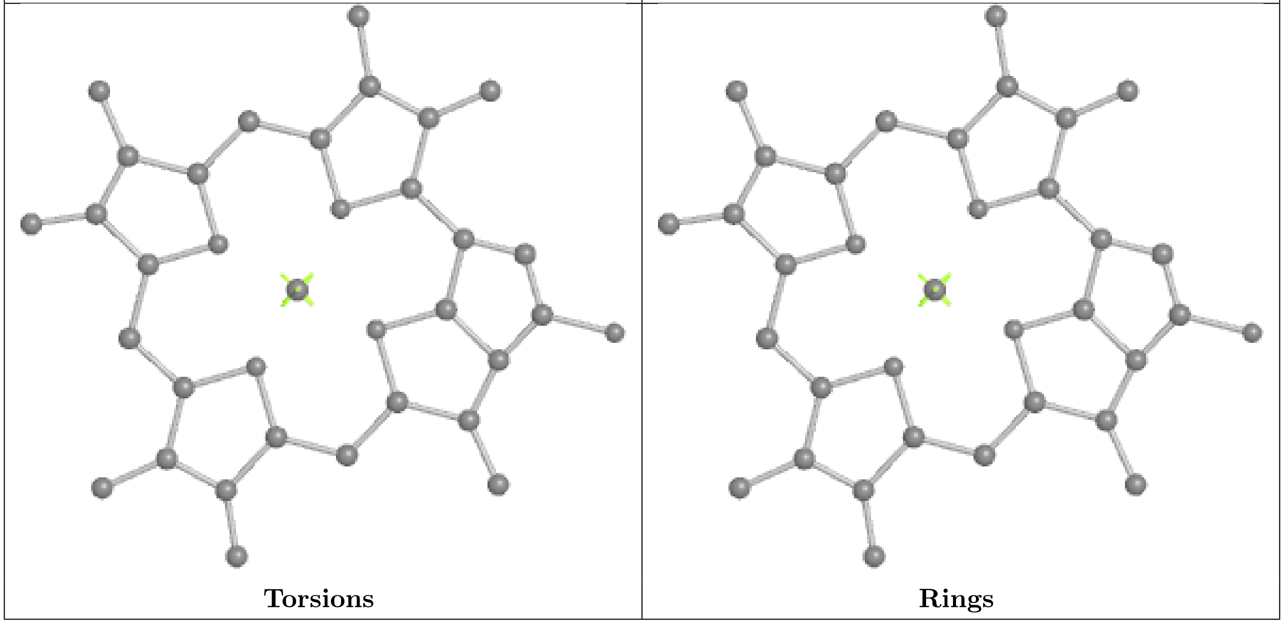
Torsions **Rings**

Ligand CLA L 1118



Bond lengths

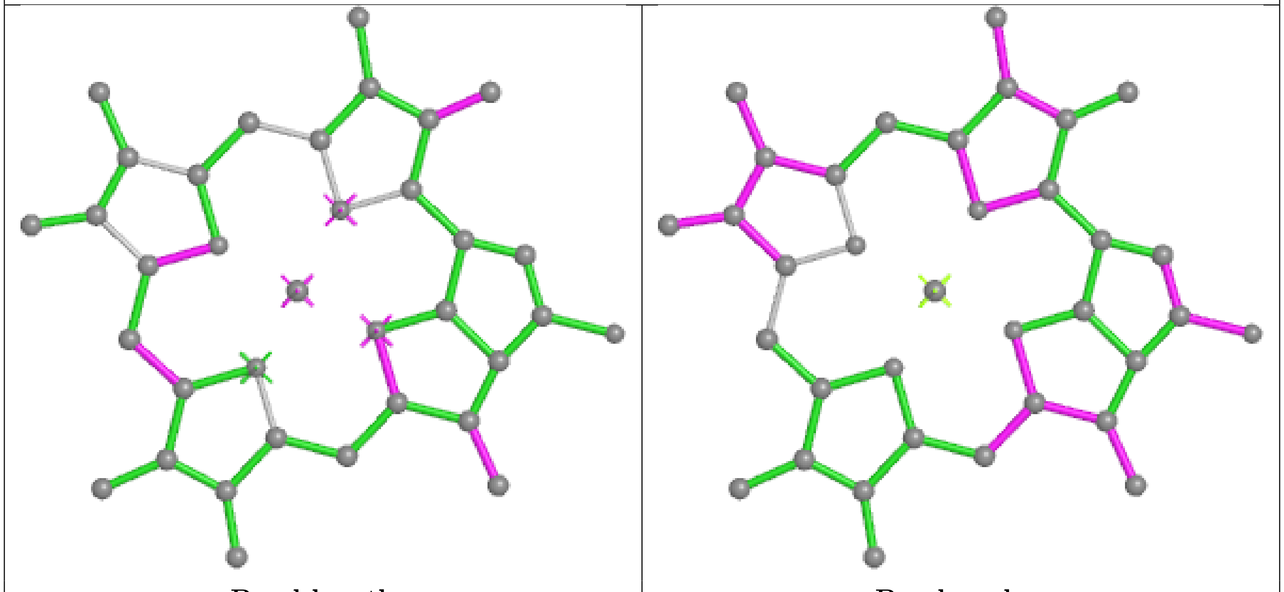
Bond angles



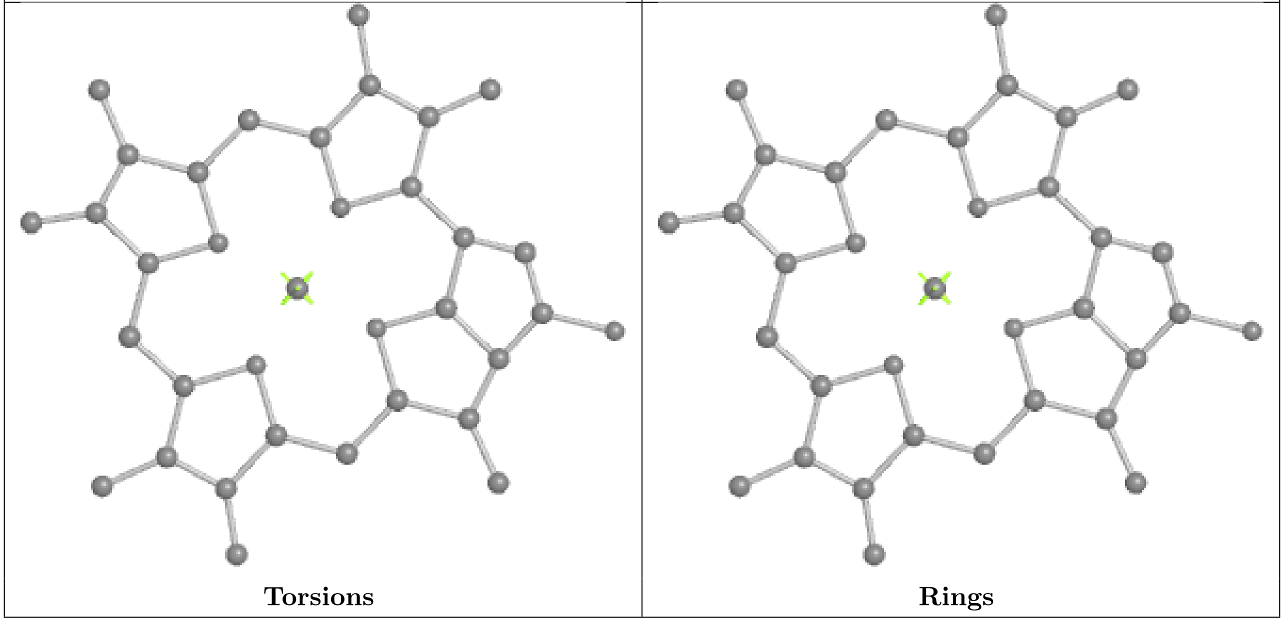
Torsions

Rings

Ligand CLA L 1109

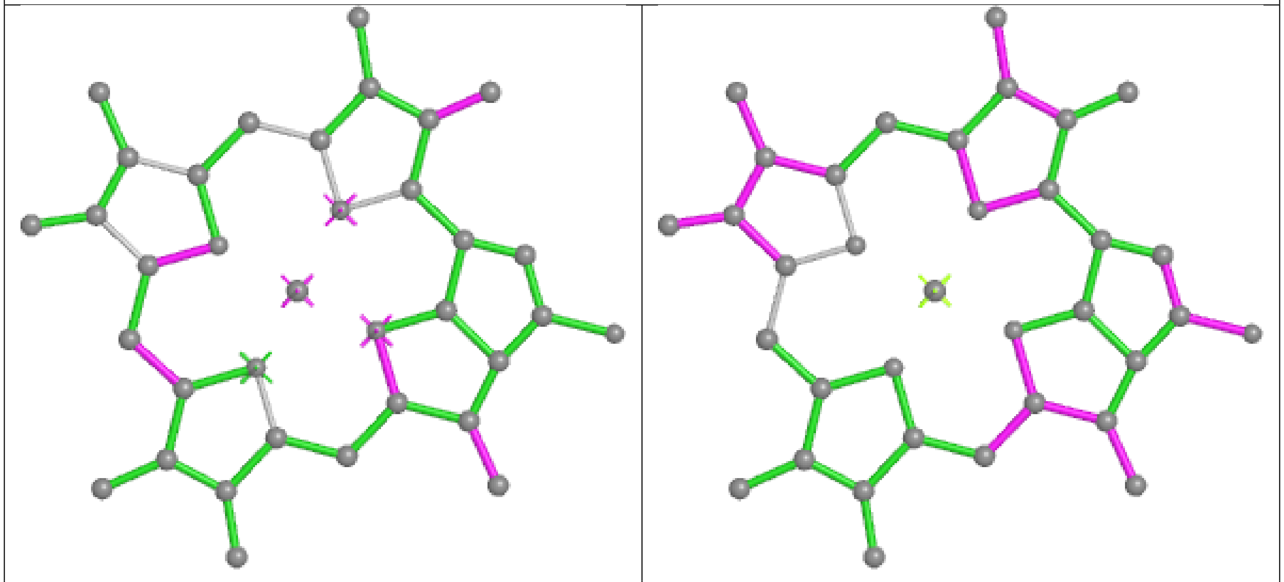


Bond lengths **Bond angles**



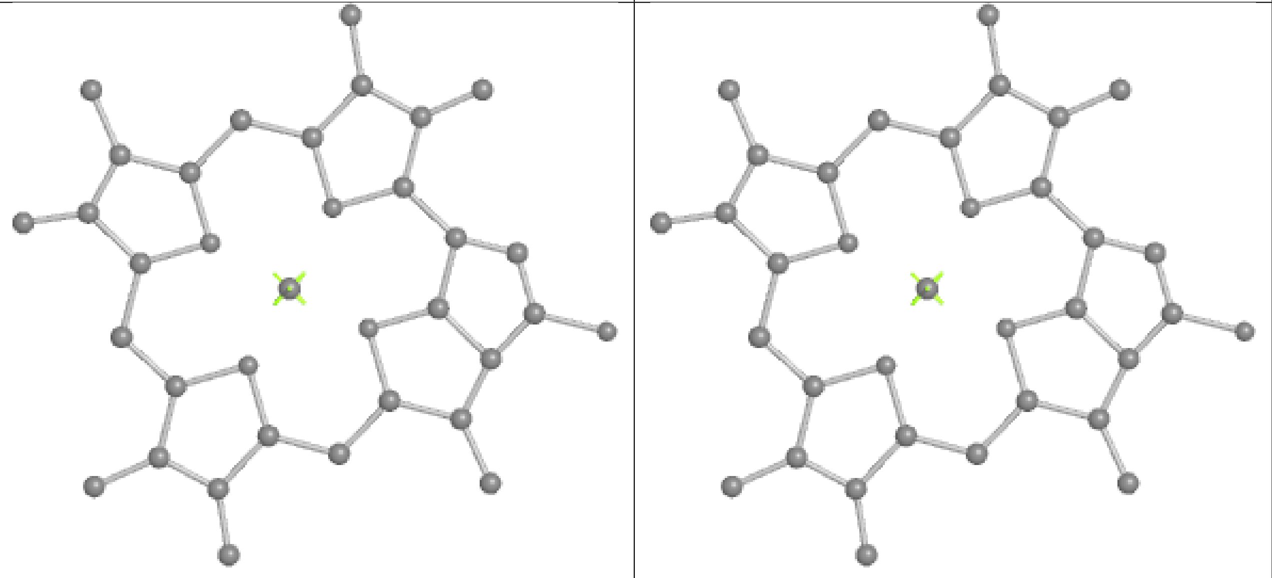
Torsions **Rings**

Ligand CLA M 1079



Bond lengths

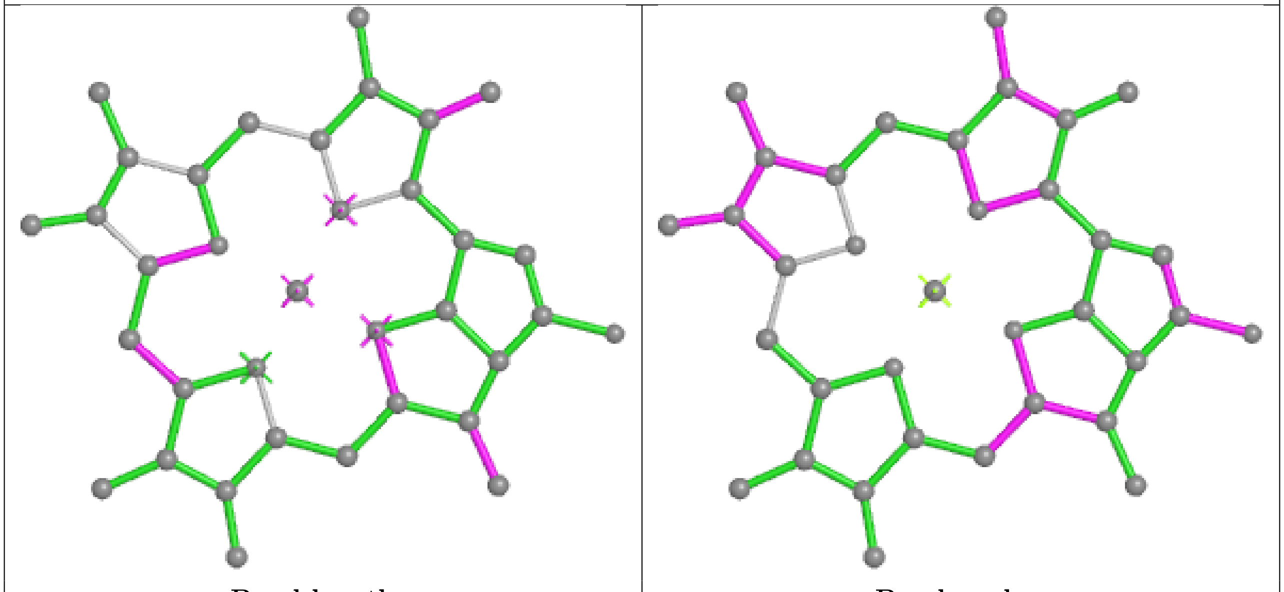
Bond angles



Torsions

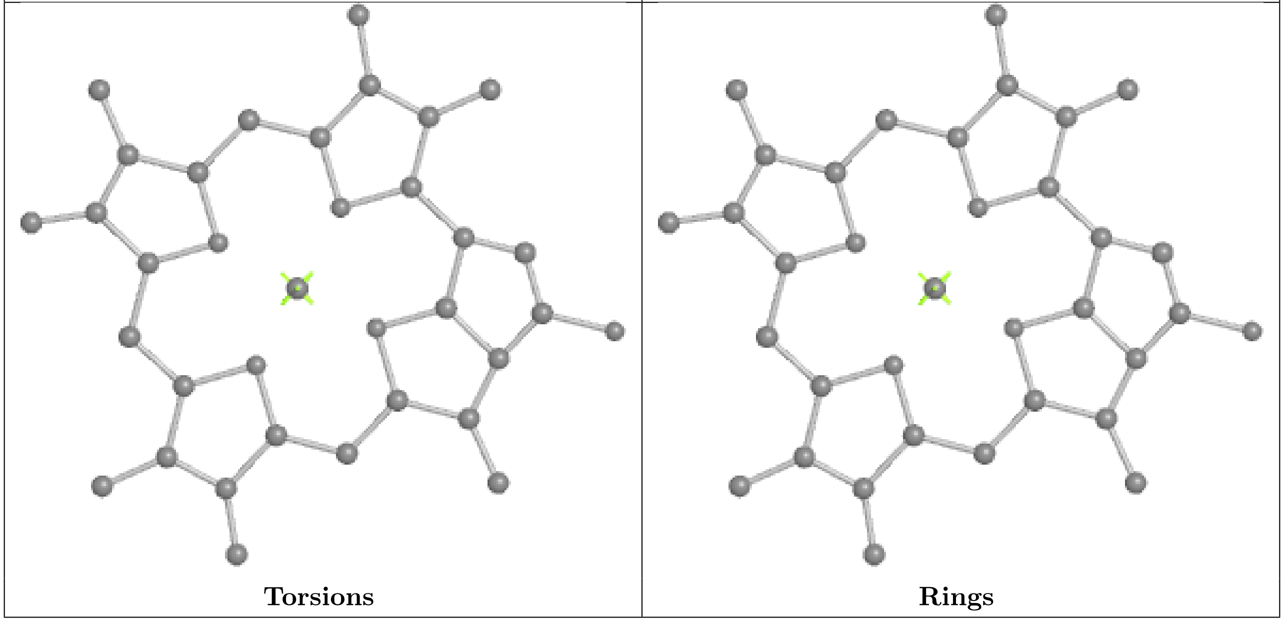
Rings

Ligand CLA L 1113



Bond lengths

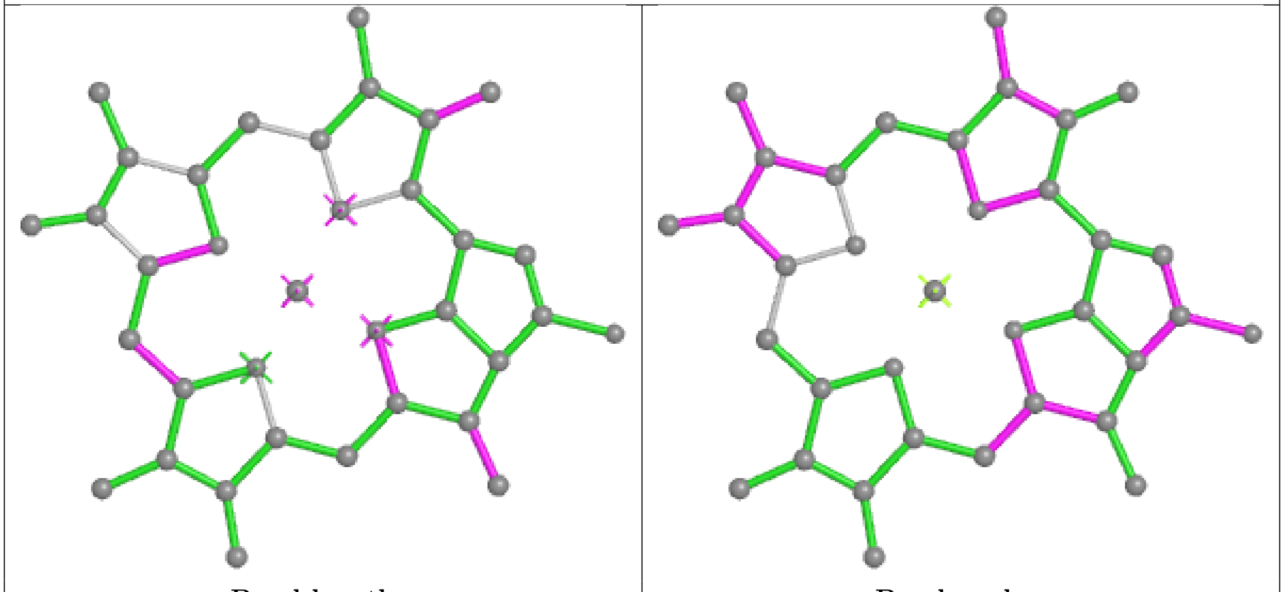
Bond angles



Torsions

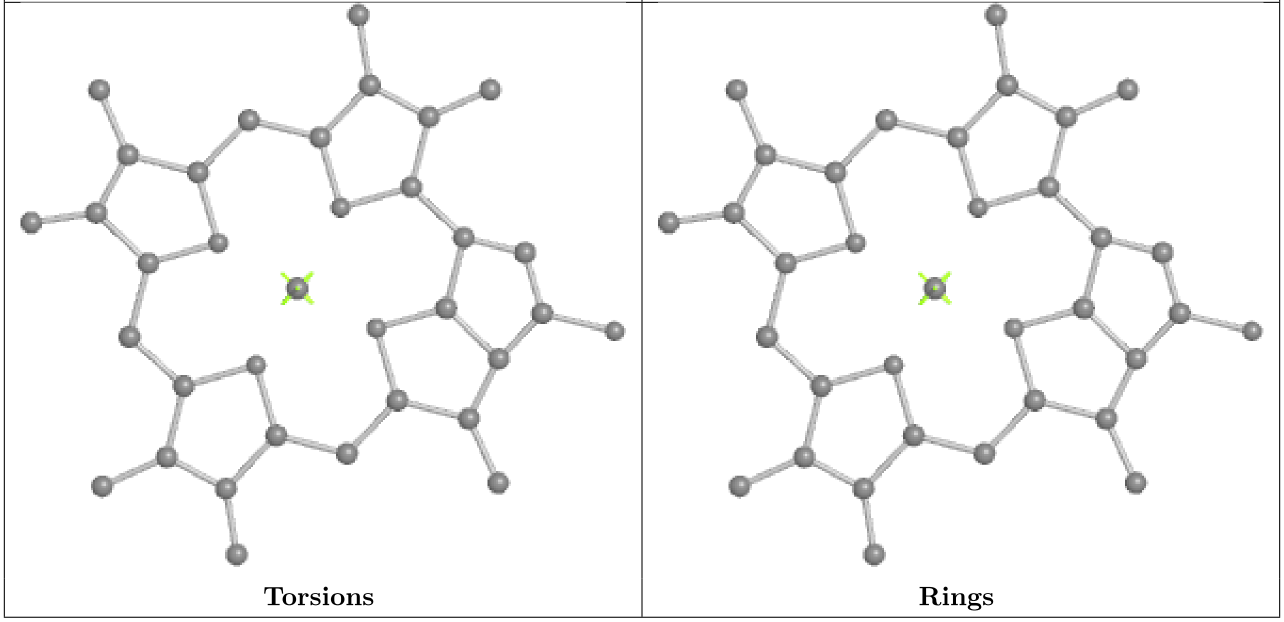
Rings

Ligand CLA B 1113



Bond lengths

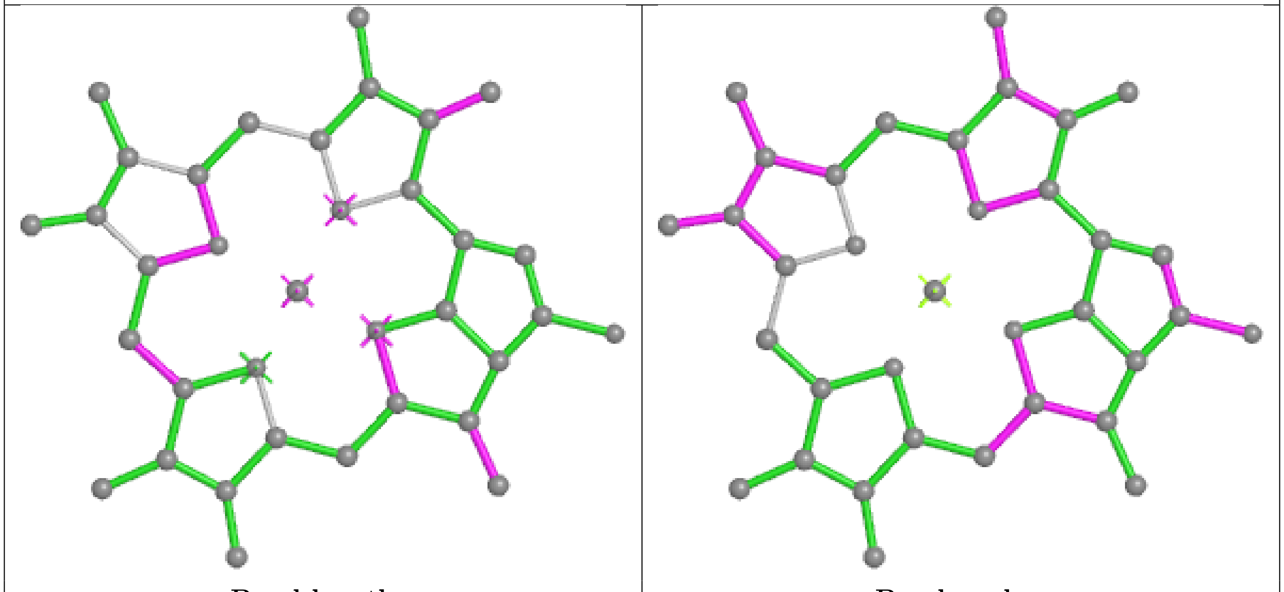
Bond angles



Torsions

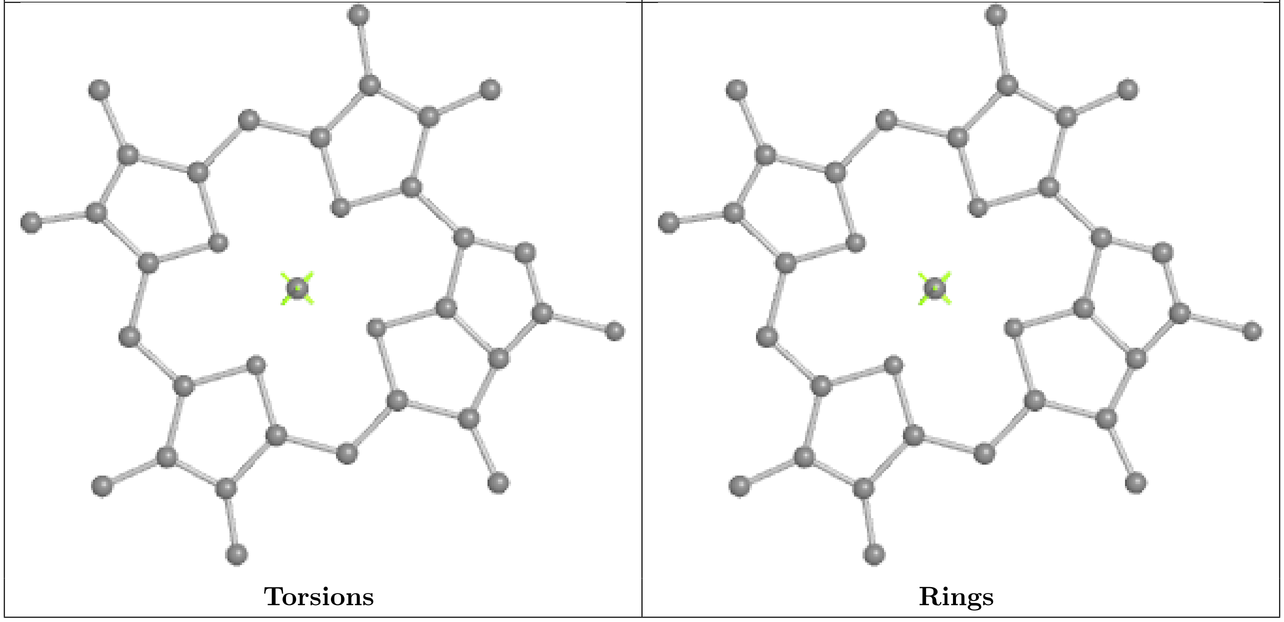
Rings

Ligand CLA C 1081



Bond lengths

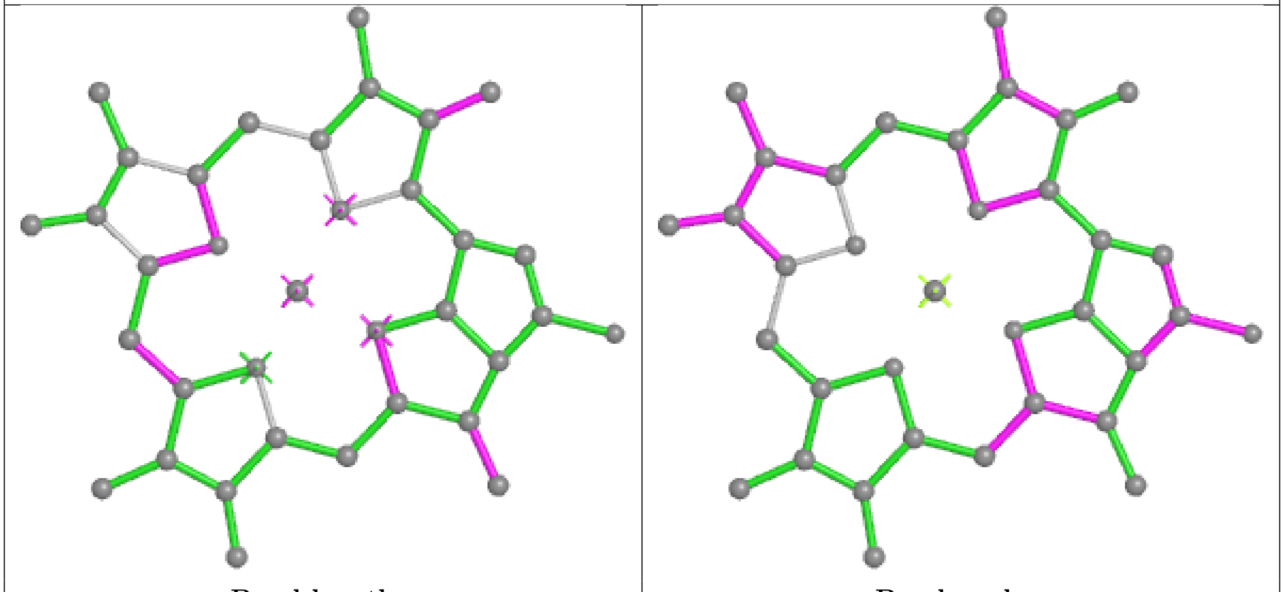
Bond angles



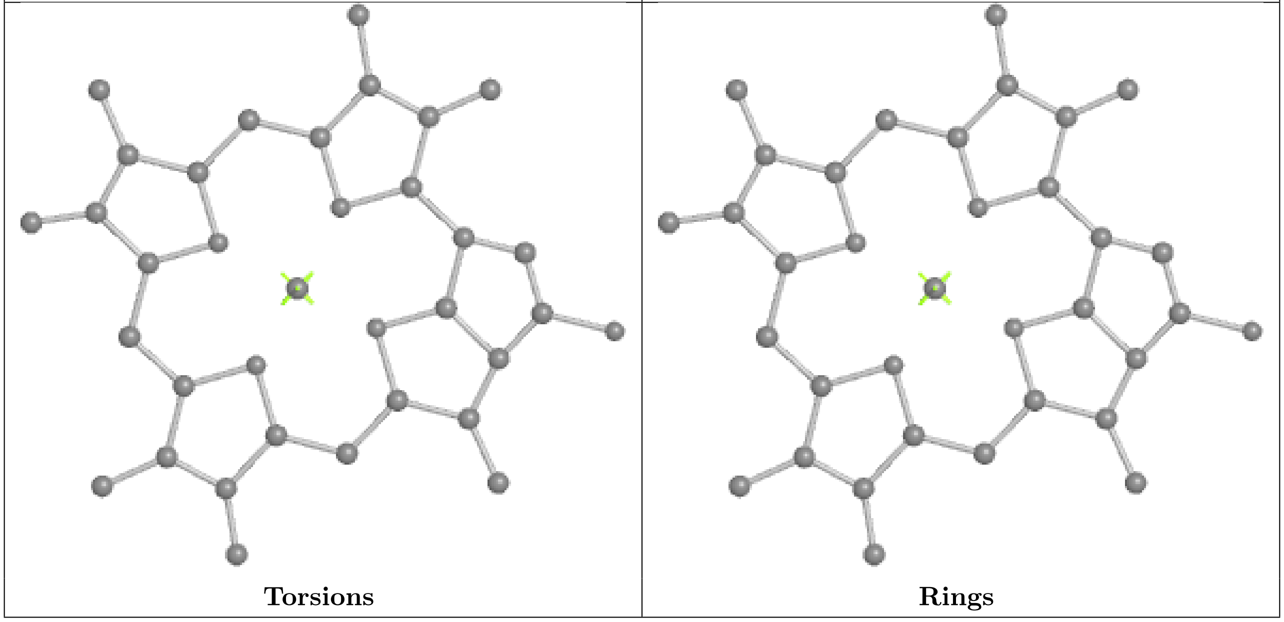
Torsions

Rings

Ligand CLA D 357

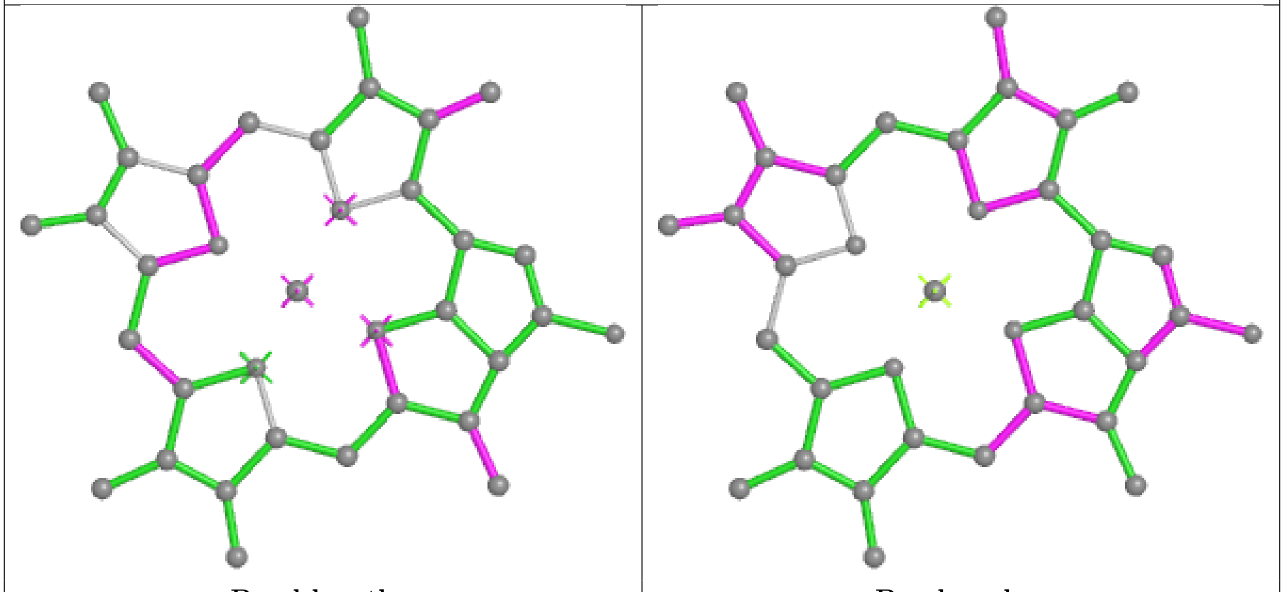


Bond lengths **Bond angles**

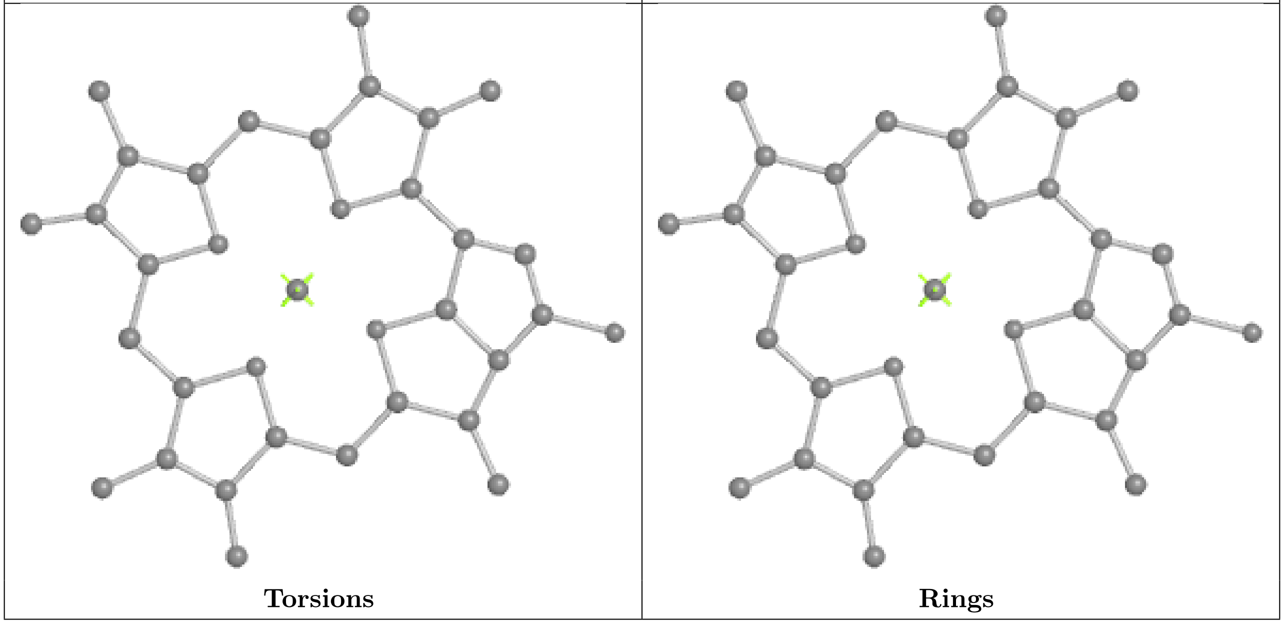


Torsions **Rings**

Ligand CLA B 1110

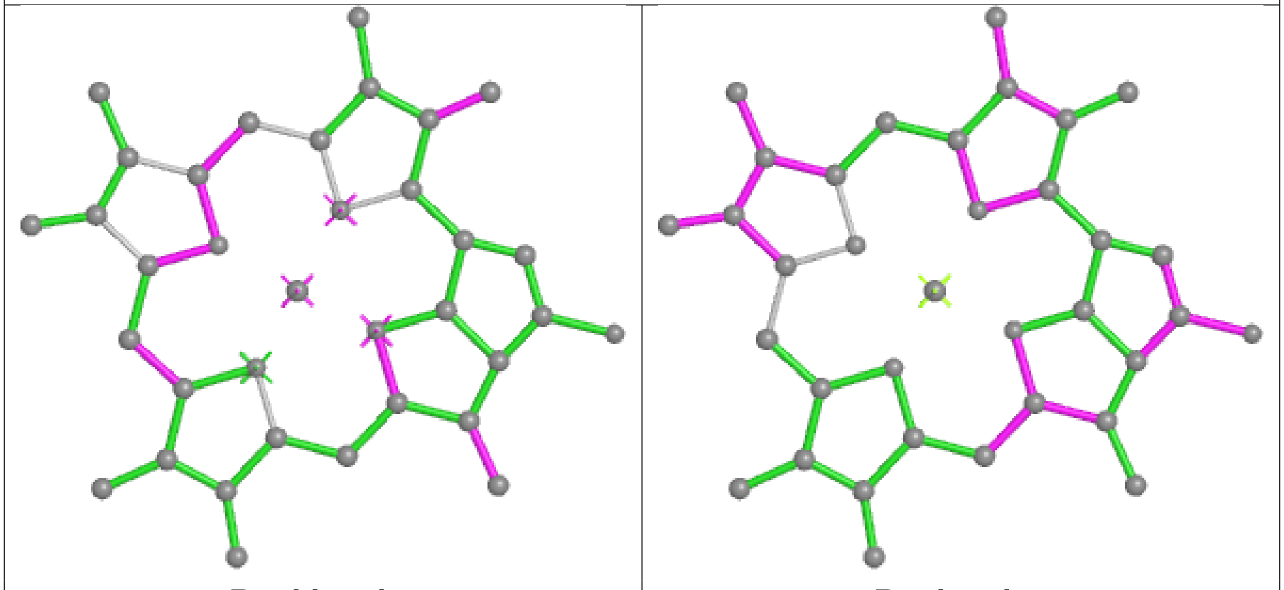


Bond lengths Bond angles

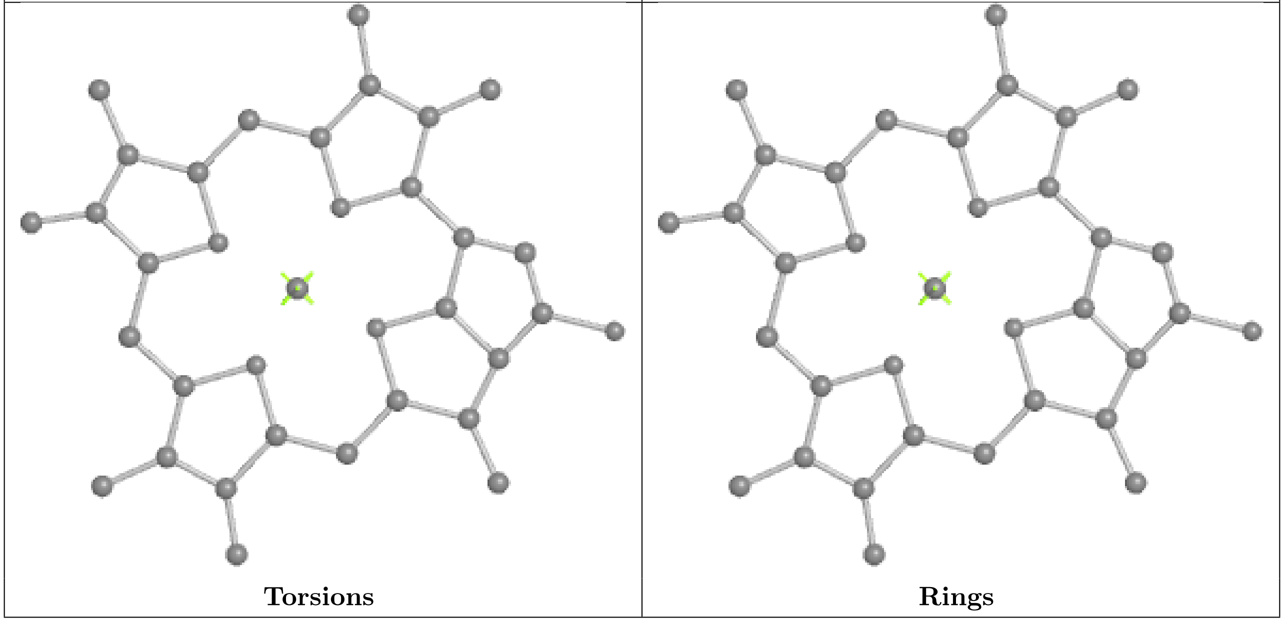


Torsions Rings

Ligand CLA L 1120

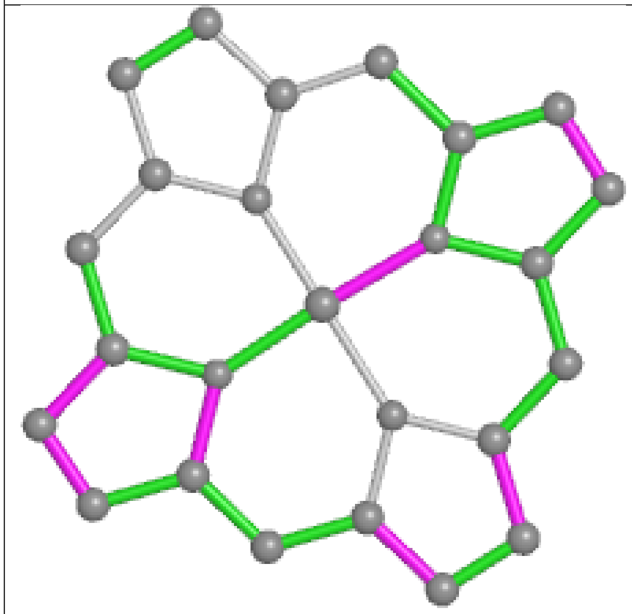


Bond lengths **Bond angles**

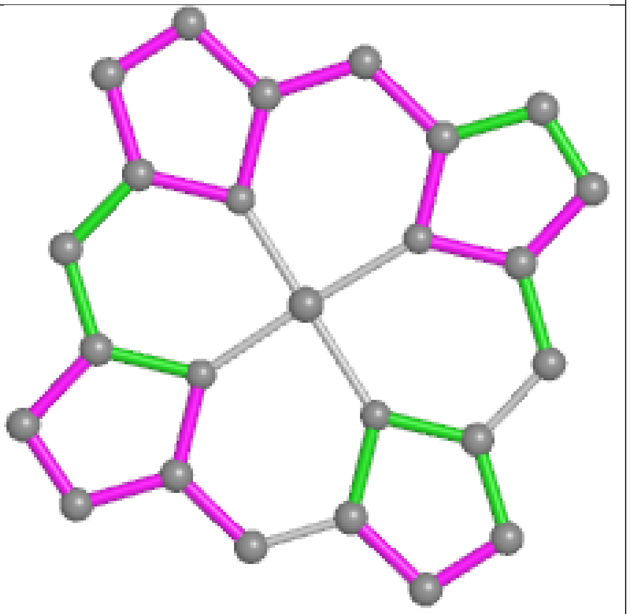


Torsions **Rings**

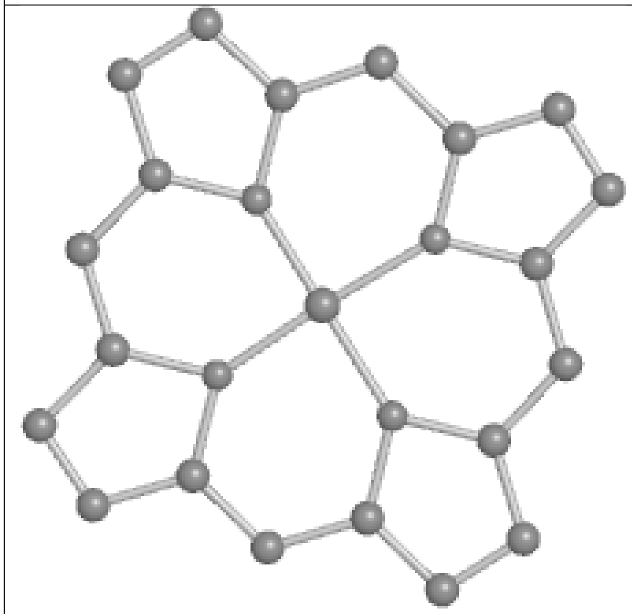
Ligand HEM P 92



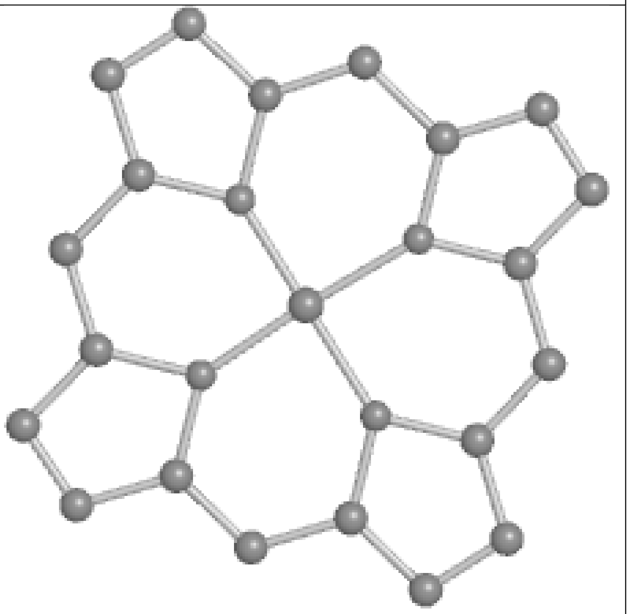
Bond lengths



Bond angles

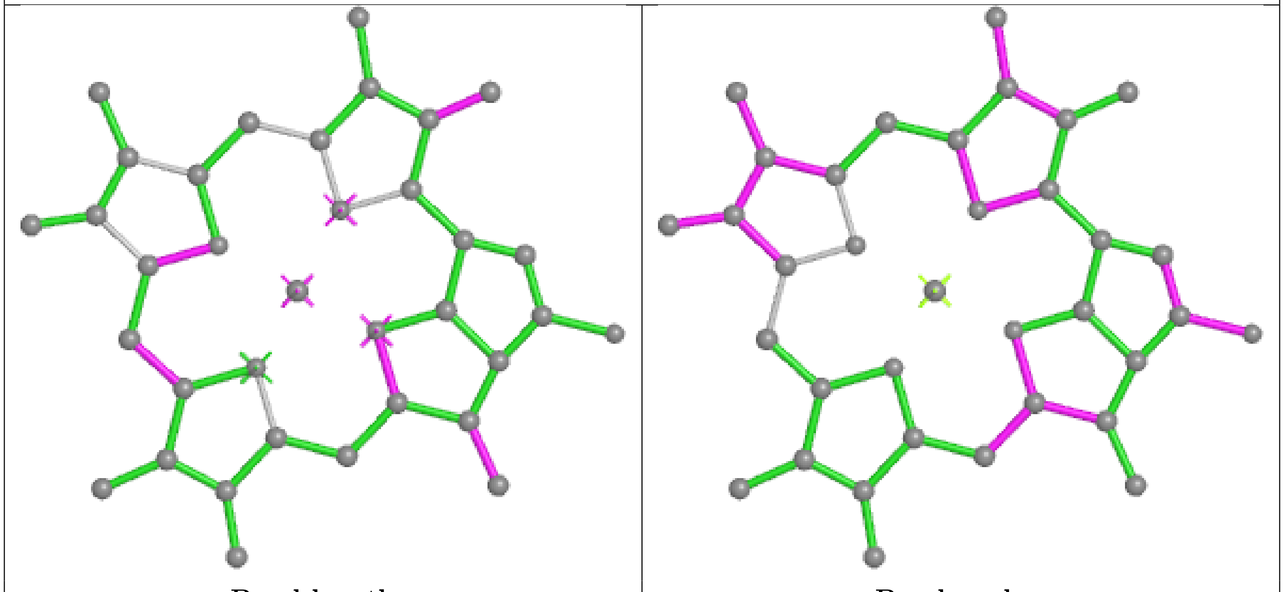


Torsions



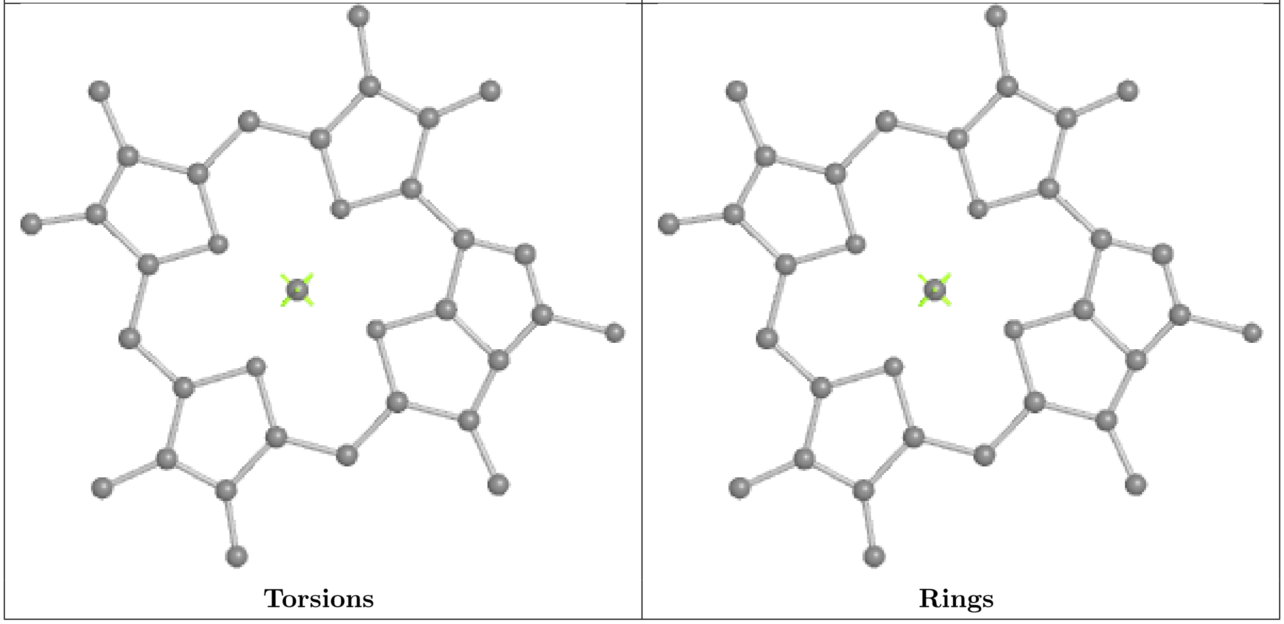
Rings

Ligand CLA B 1109



Bond lengths

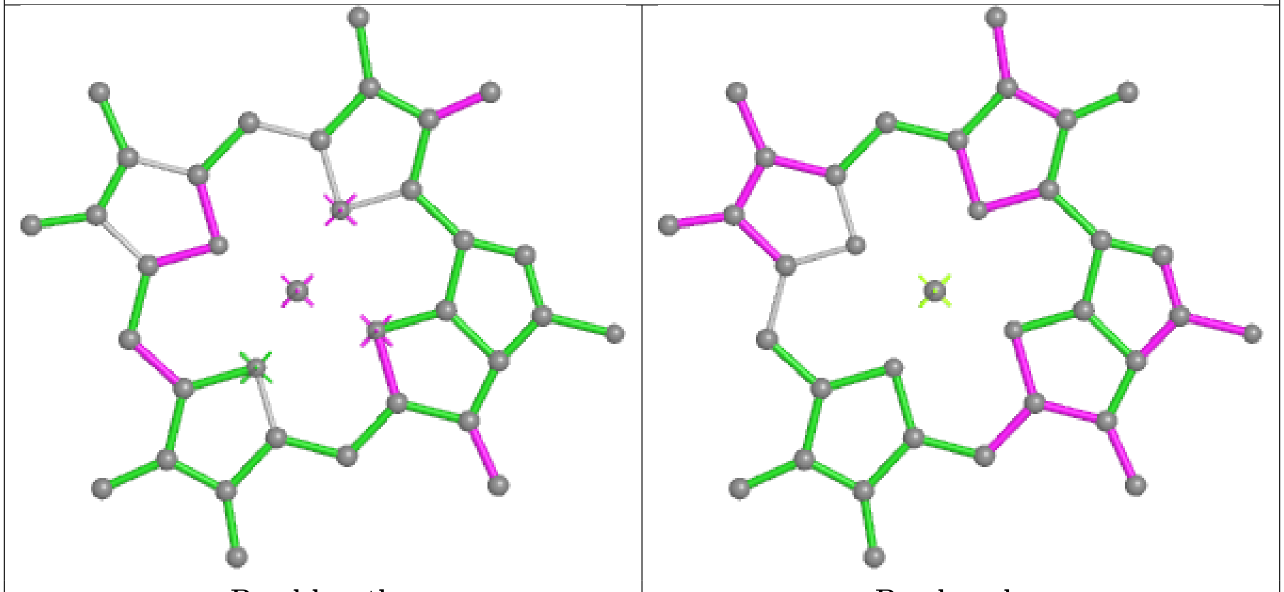
Bond angles



Torsions

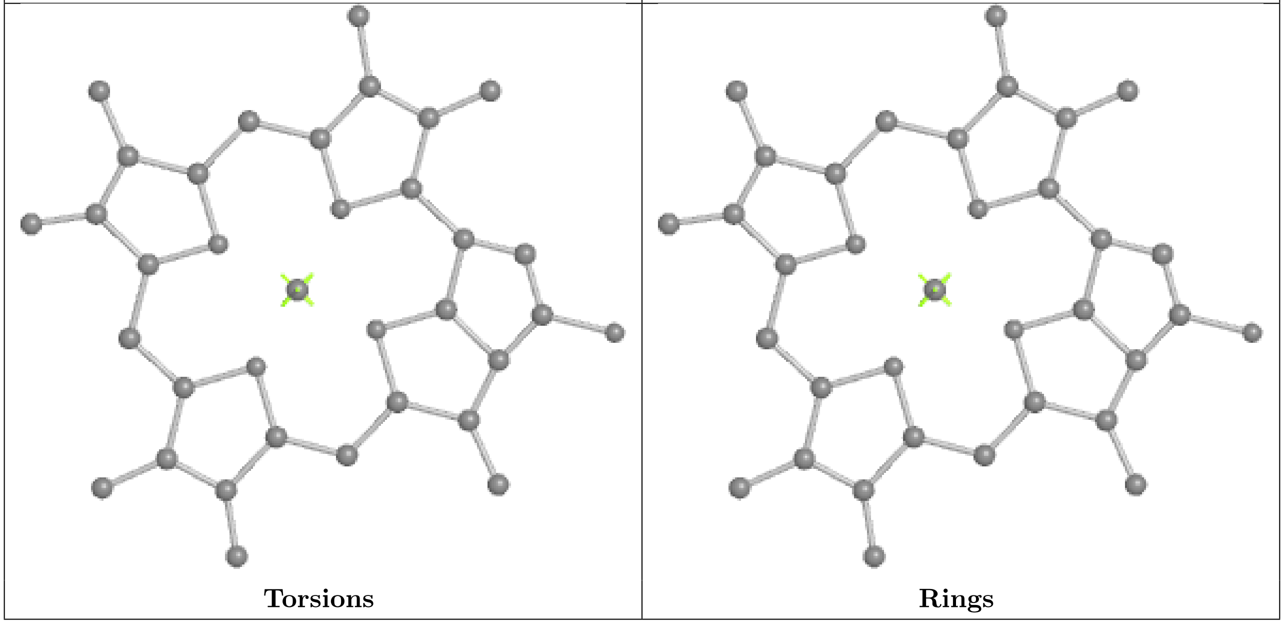
Rings

Ligand CLA B 1117



Bond lengths

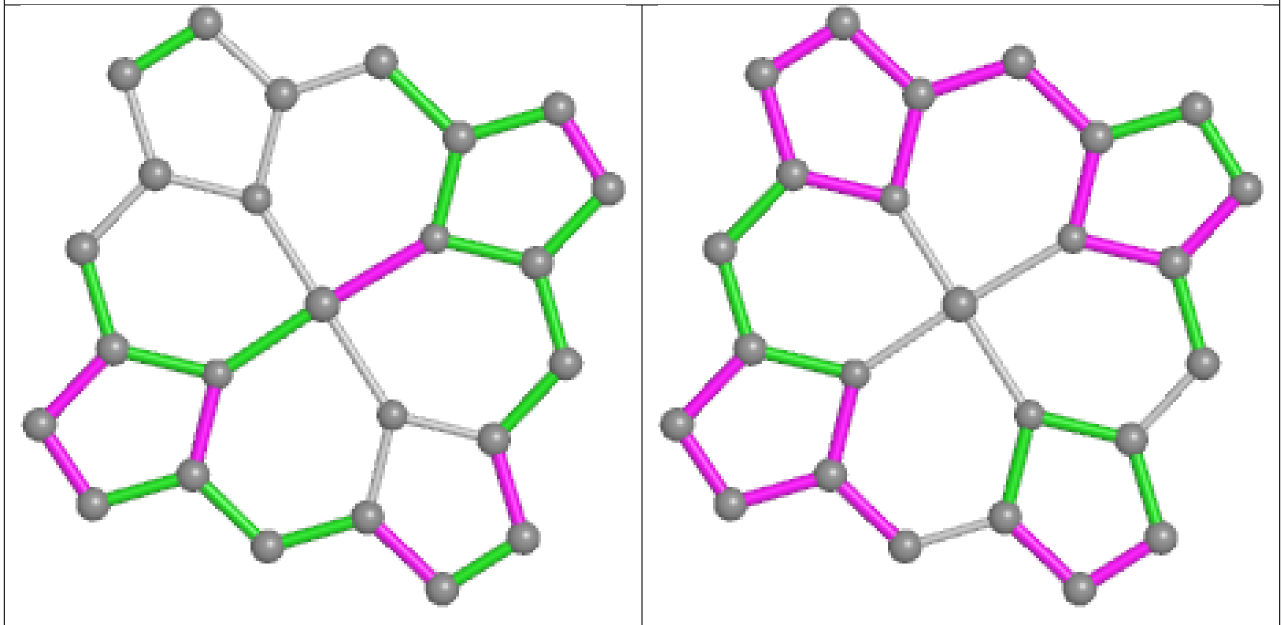
Bond angles



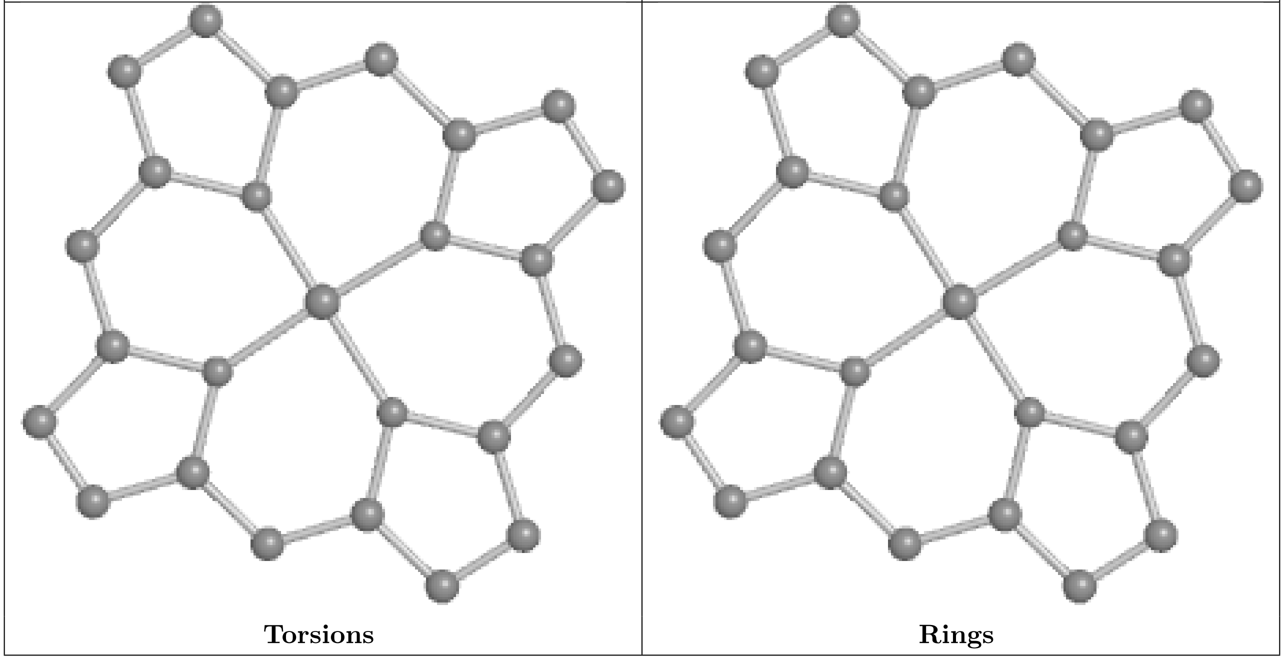
Torsions

Rings

Ligand HEM V 138

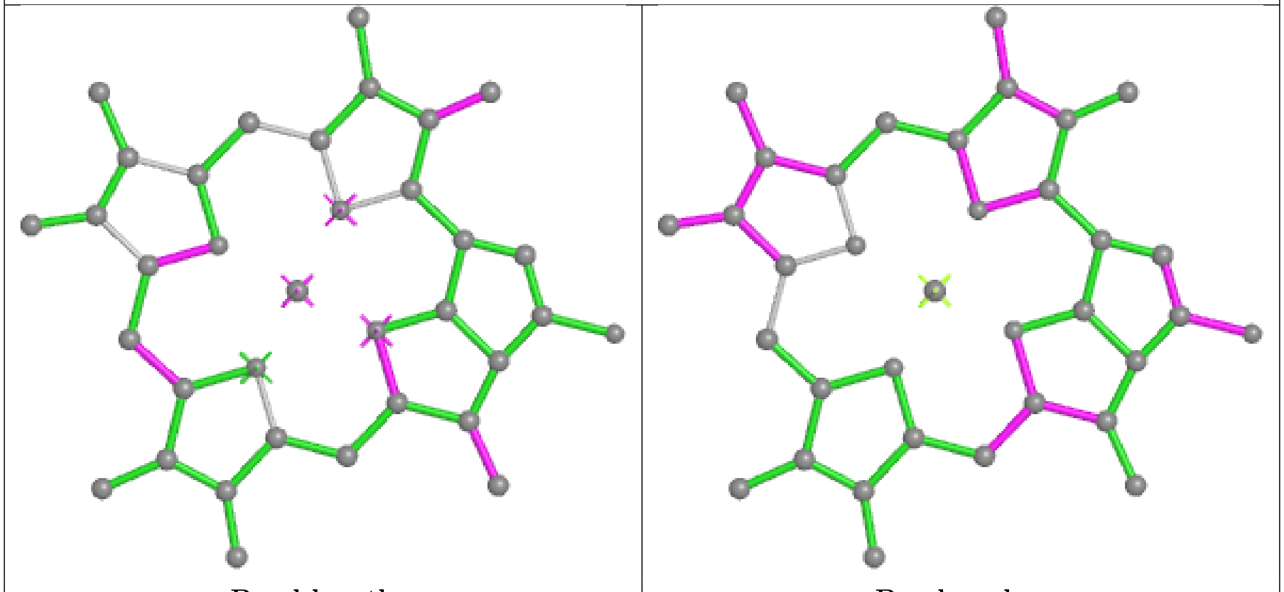


Bond lengths **Bond angles**



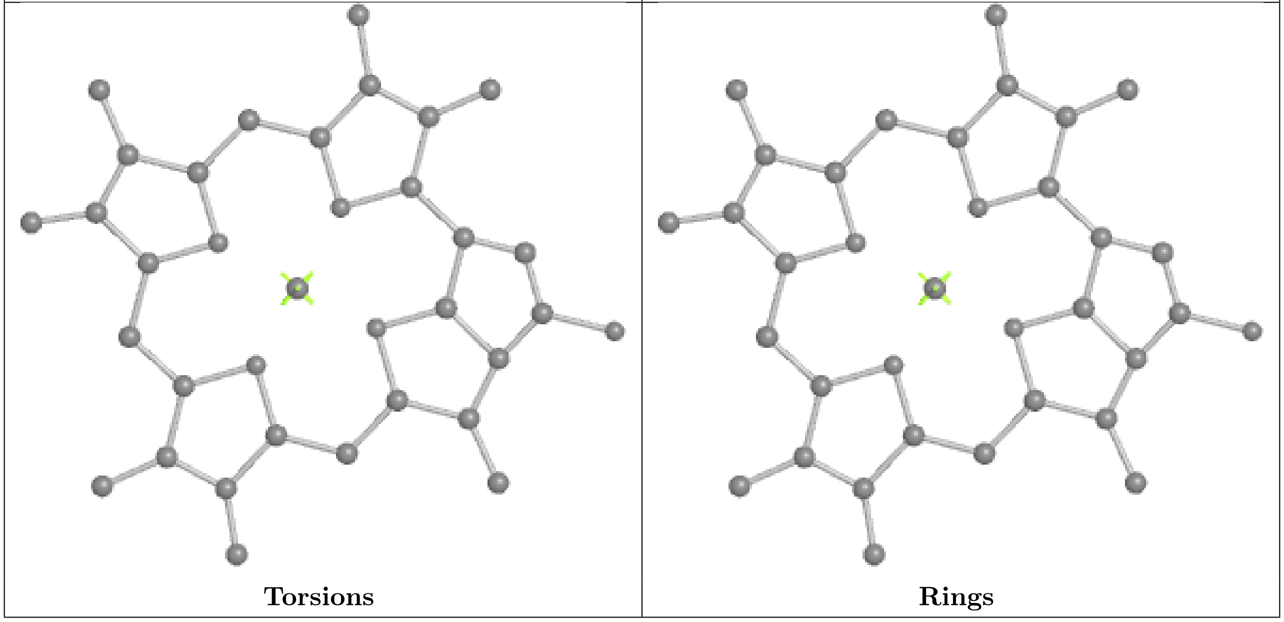
Torsions **Rings**

Ligand CLA M 1082



Bond lengths

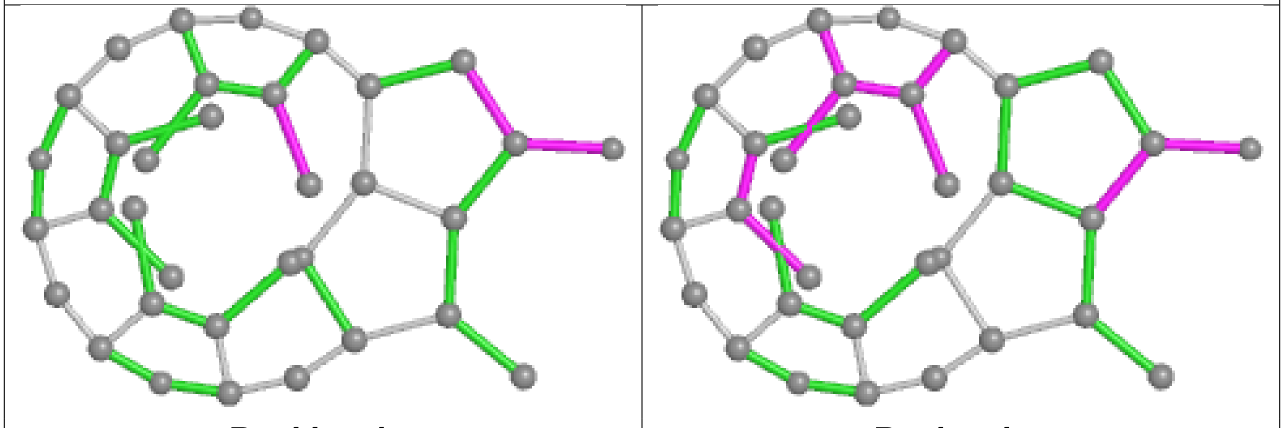
Bond angles



Torsions

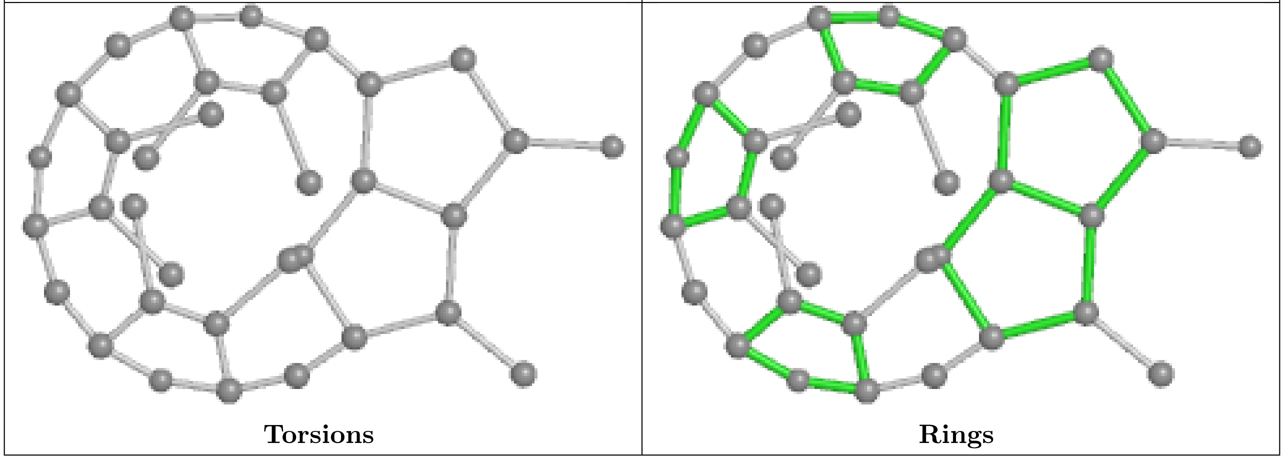
Rings

Ligand PHO D 356



Bond lengths

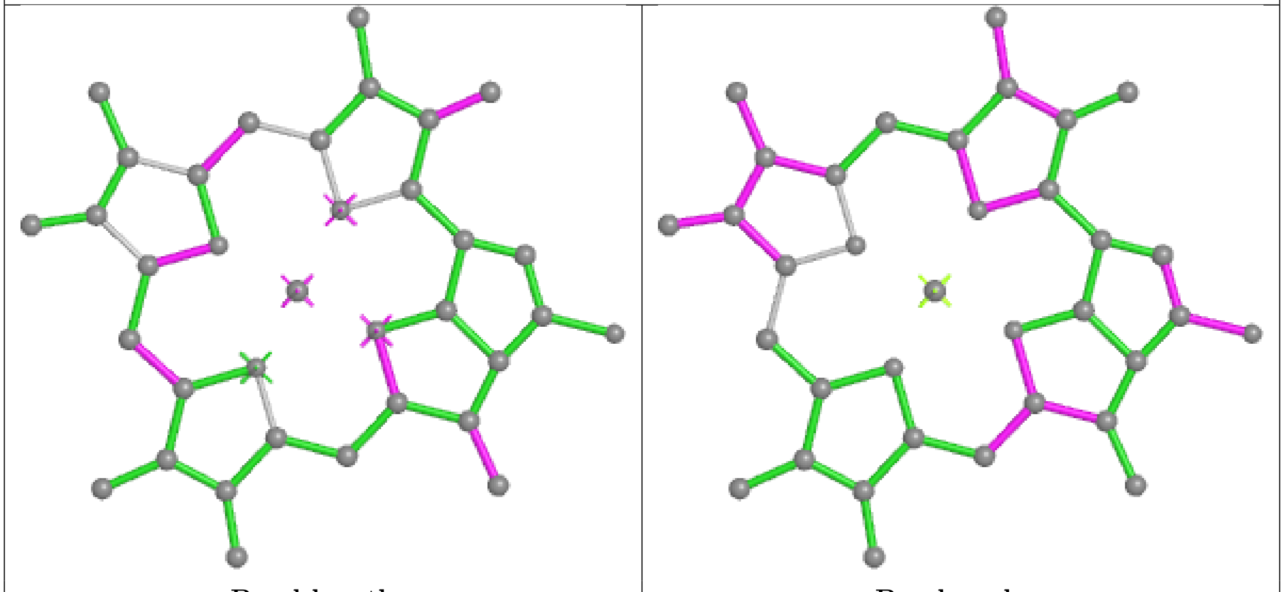
Bond angles



Torsions

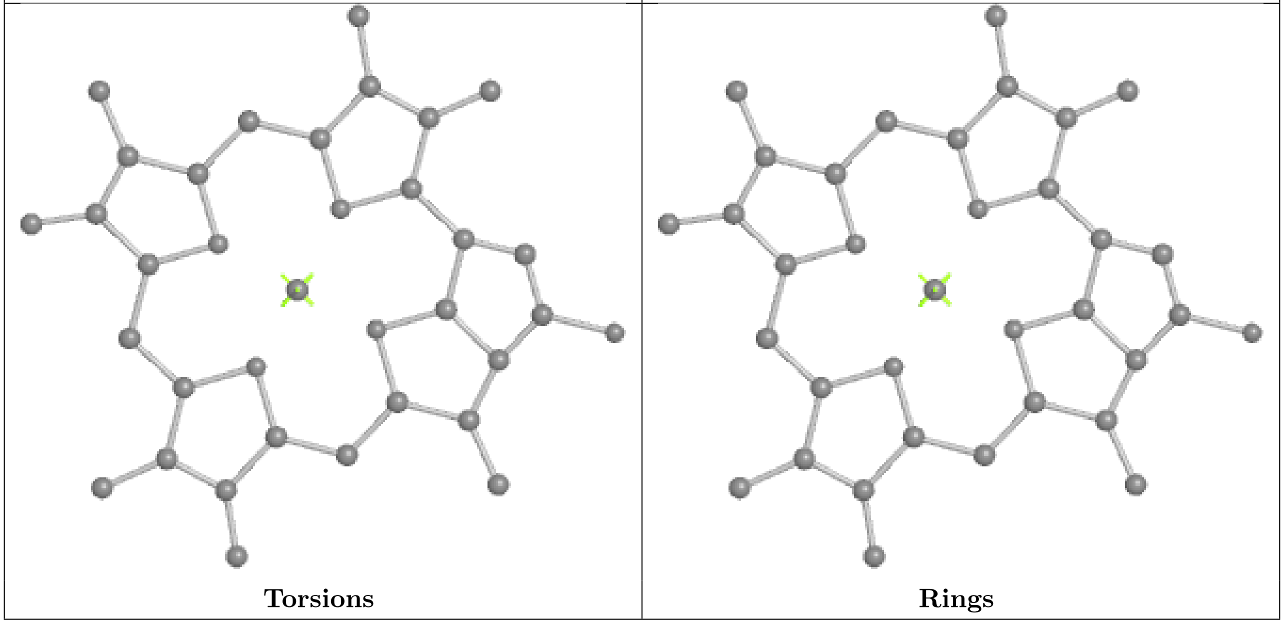
Rings

Ligand CLA M 1087



Bond lengths

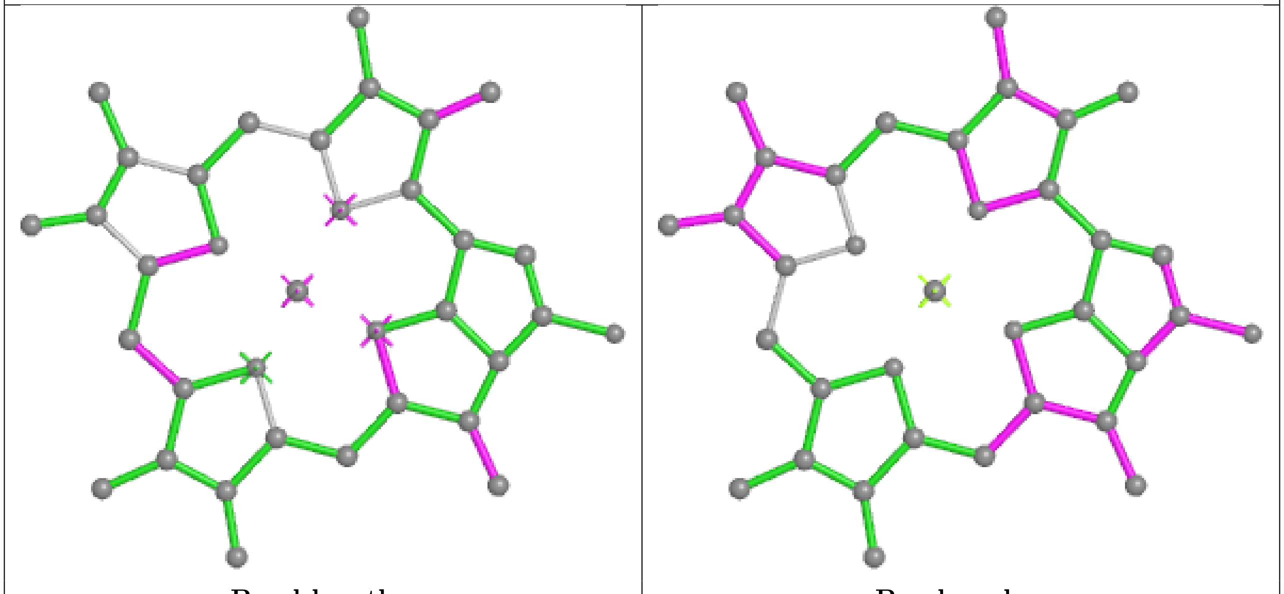
Bond angles



Torsions

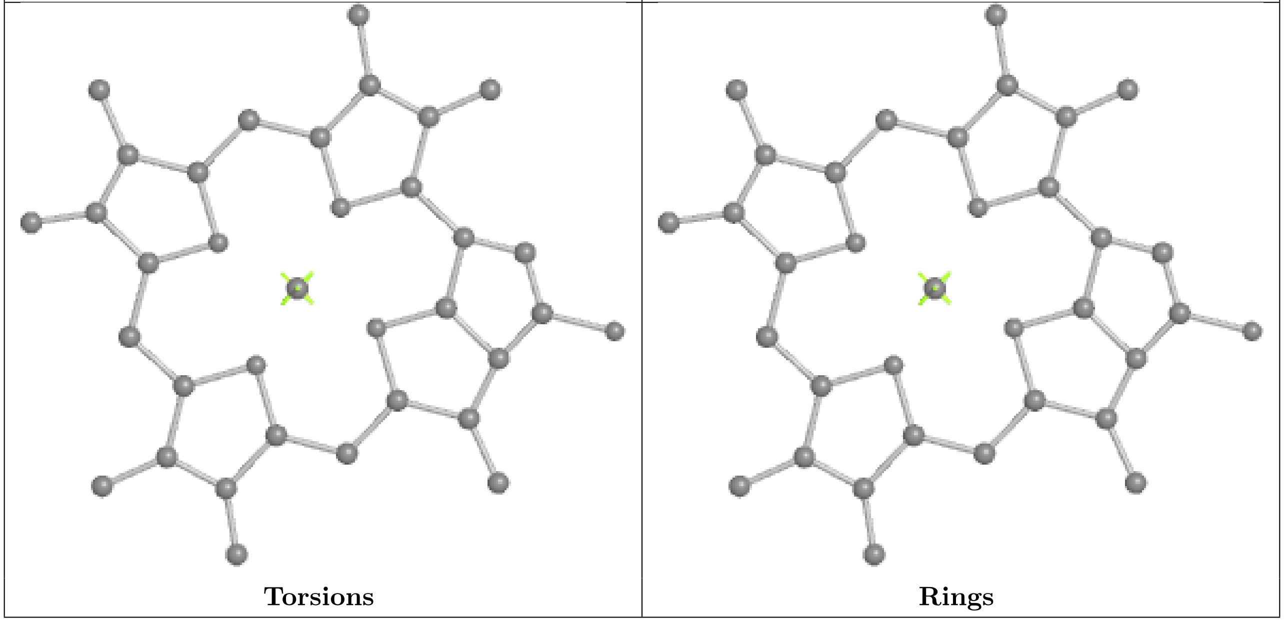
Rings

Ligand CLA L 1121



Bond lengths

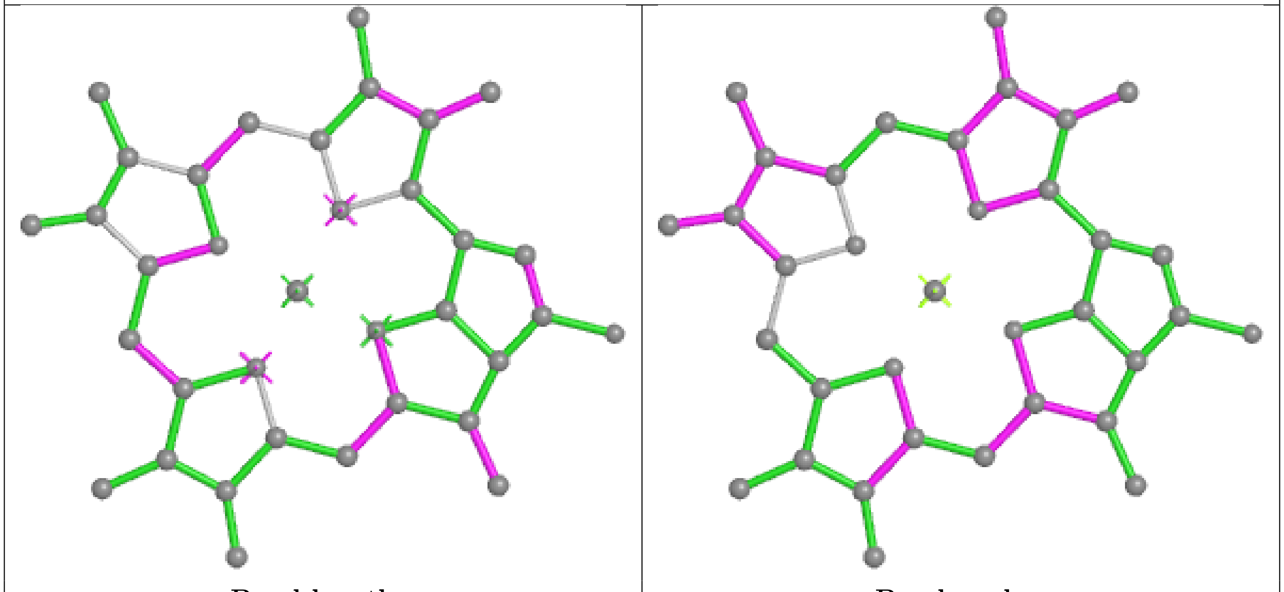
Bond angles



Torsions

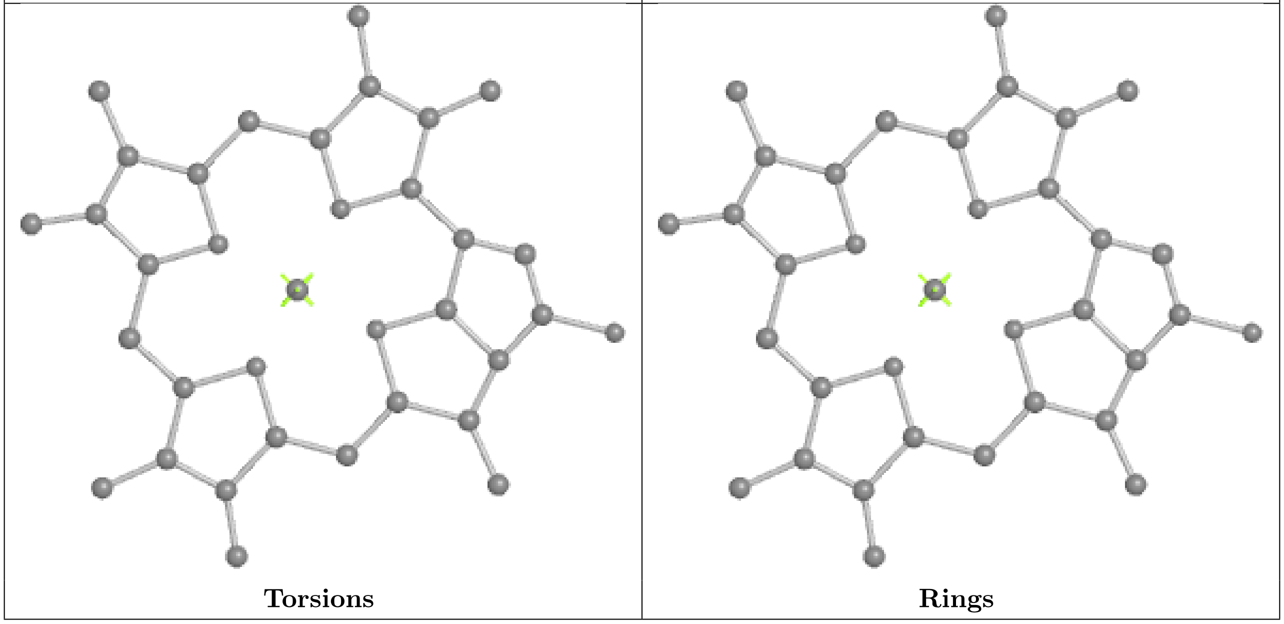
Rings

Ligand CLA G 221



Bond lengths

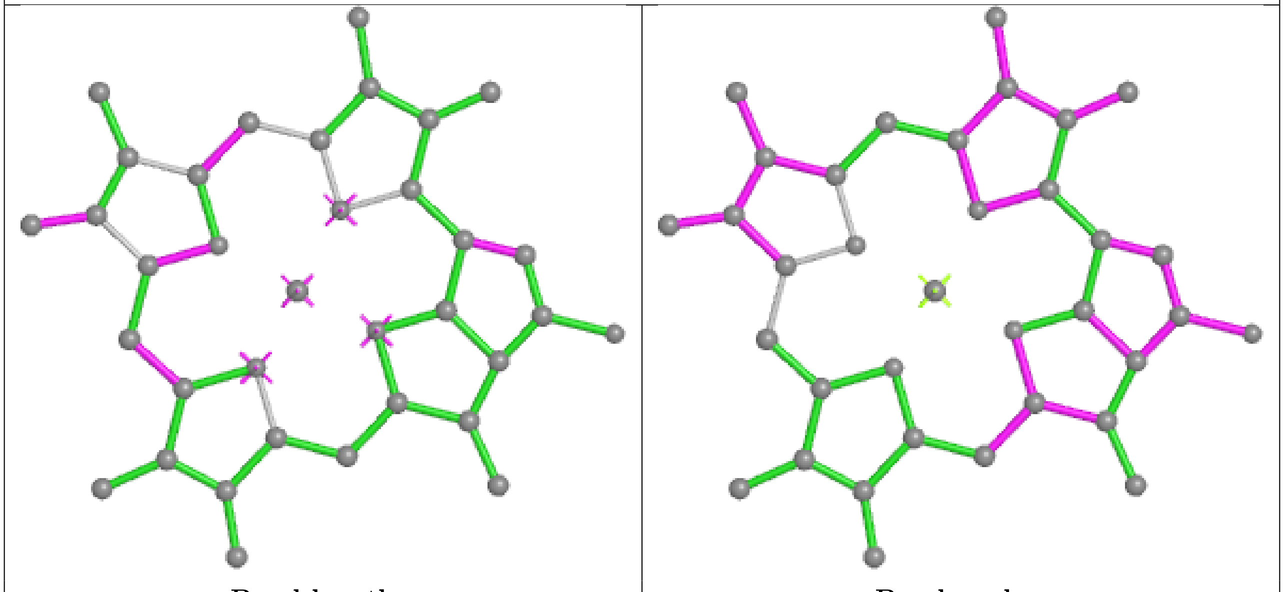
Bond angles



Torsions

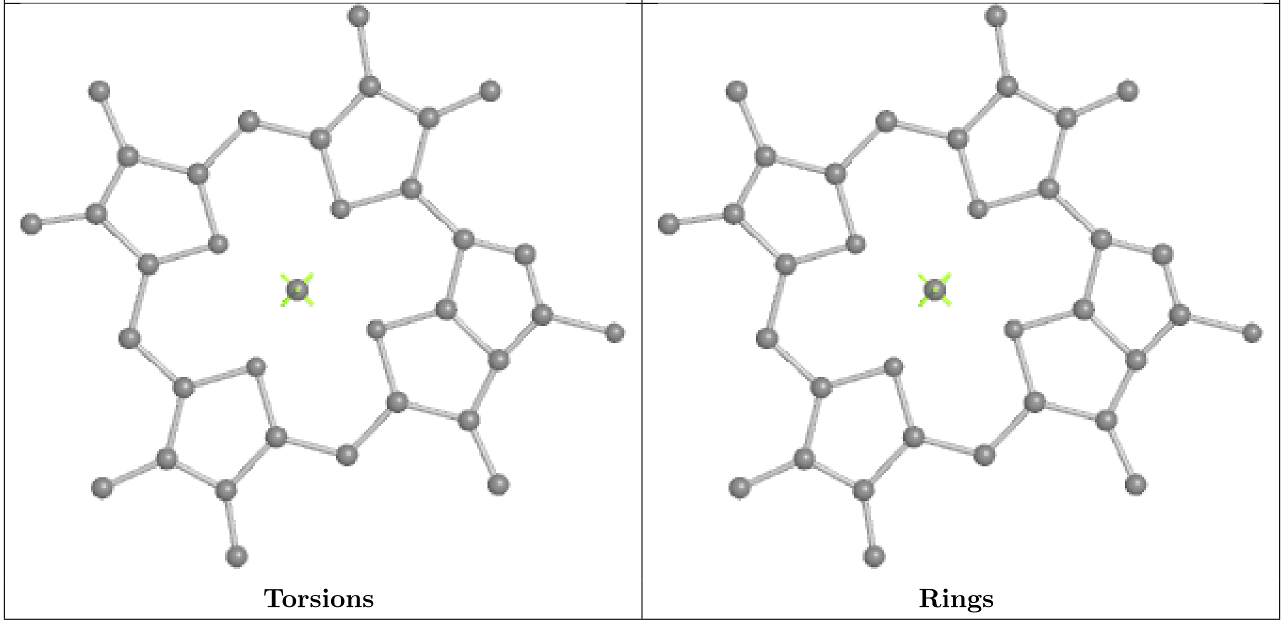
Rings

Ligand CLA J 365



Bond lengths

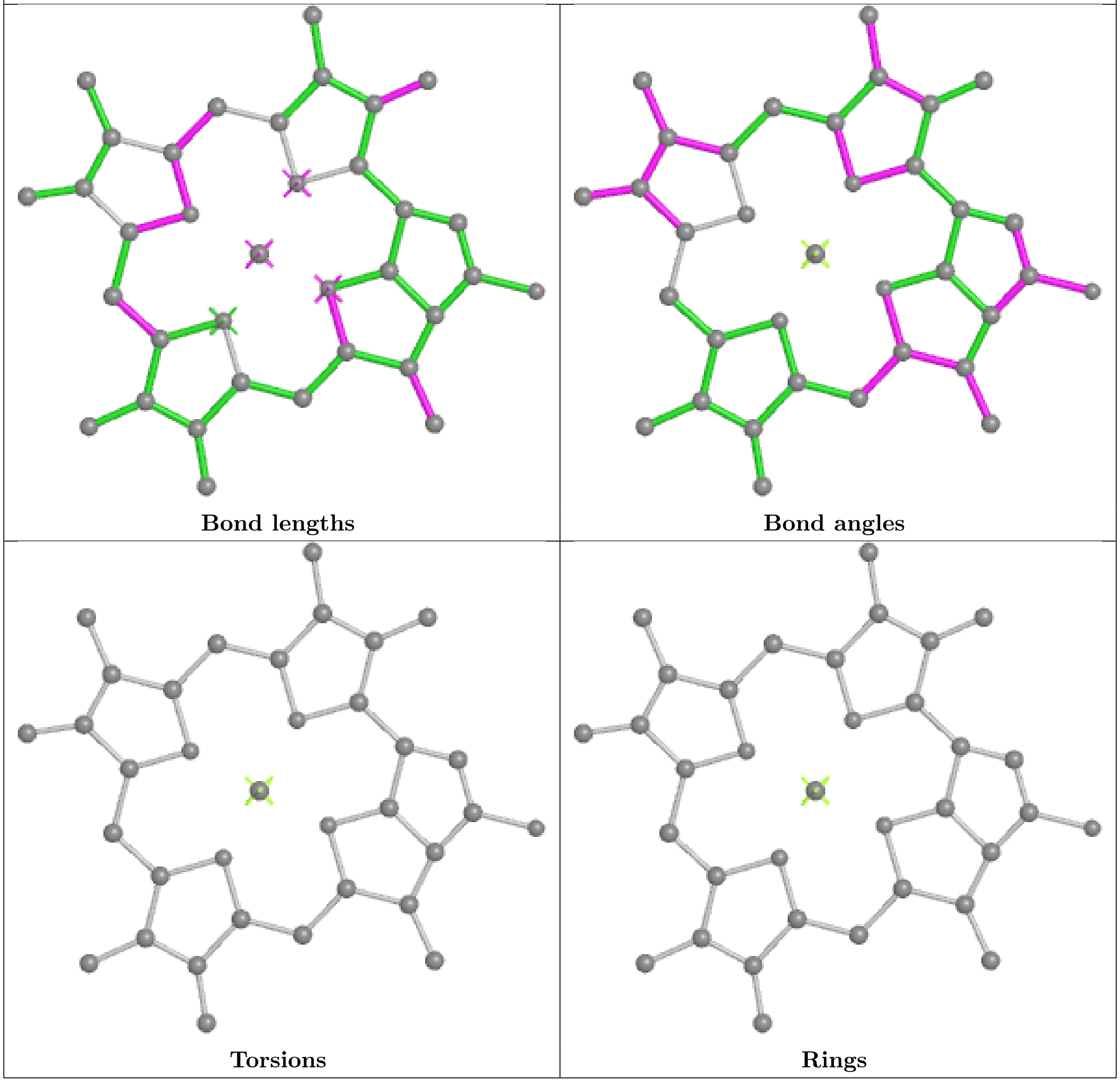
Bond angles



Torsions

Rings

Ligand CLA B 1112



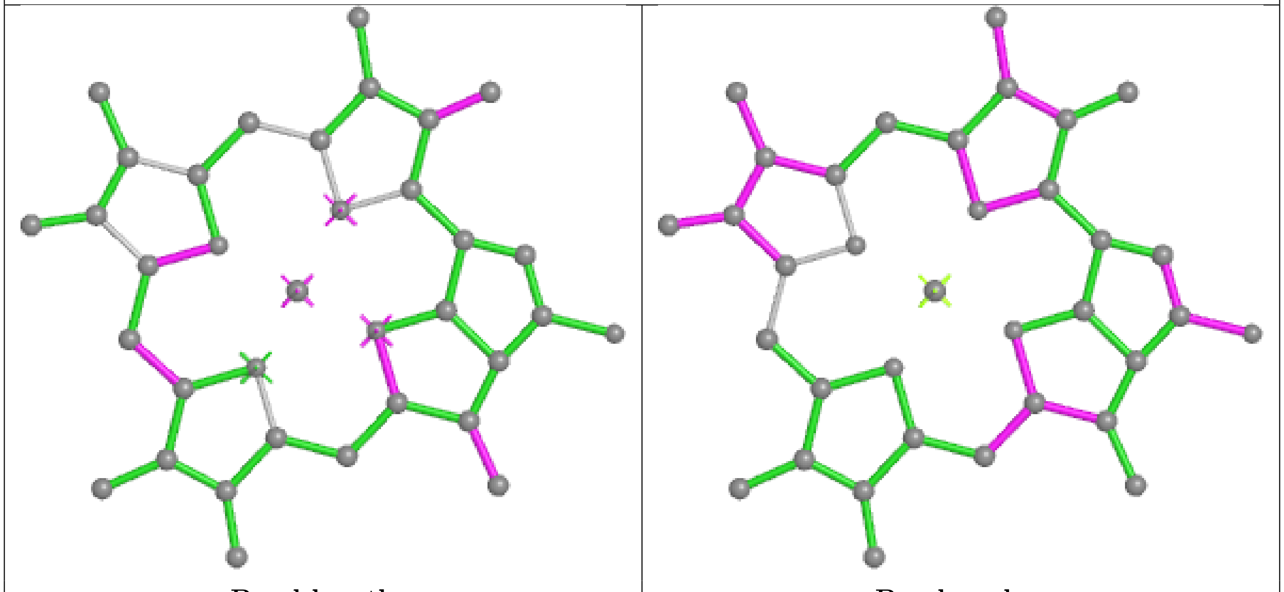
Bond lengths

Bond angles

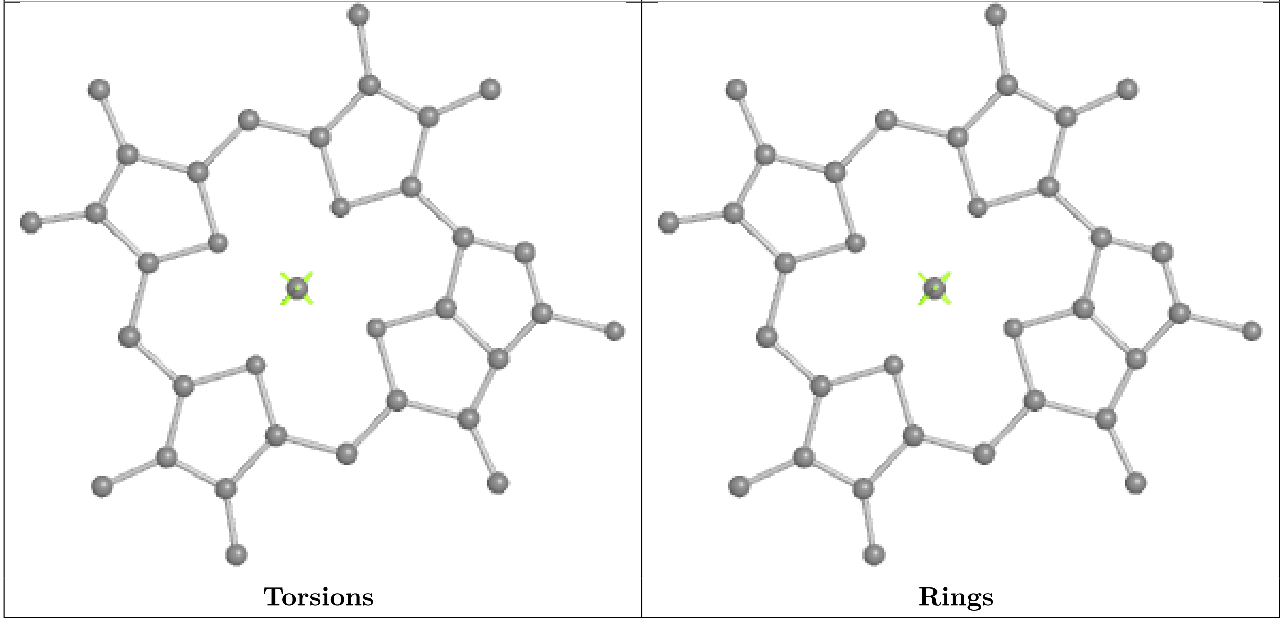
Torsions

Rings

Ligand CLA B 1107

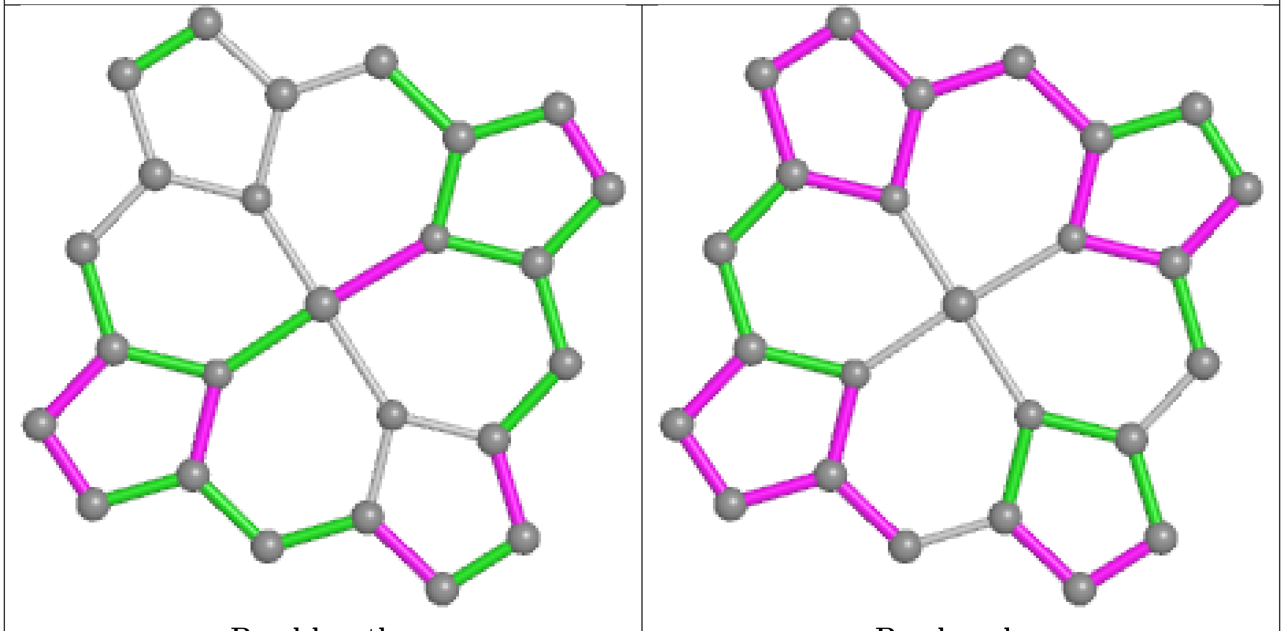


Bond lengths **Bond angles**

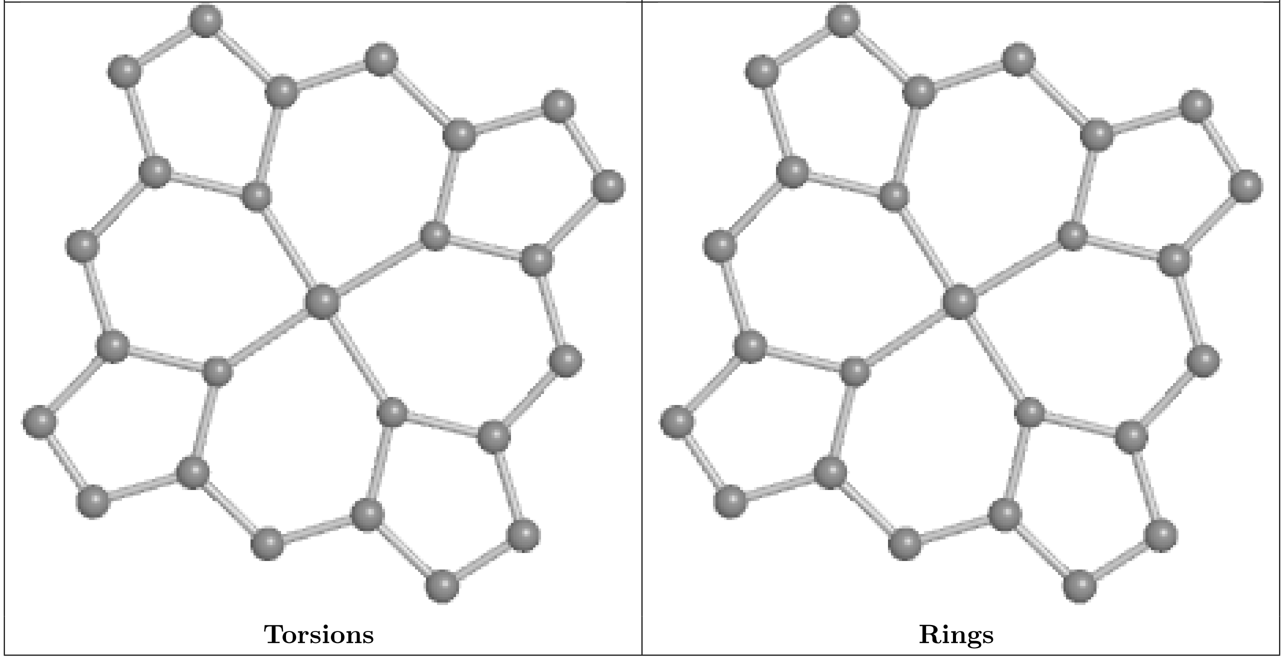


Torsions **Rings**

Ligand HEM 0 138

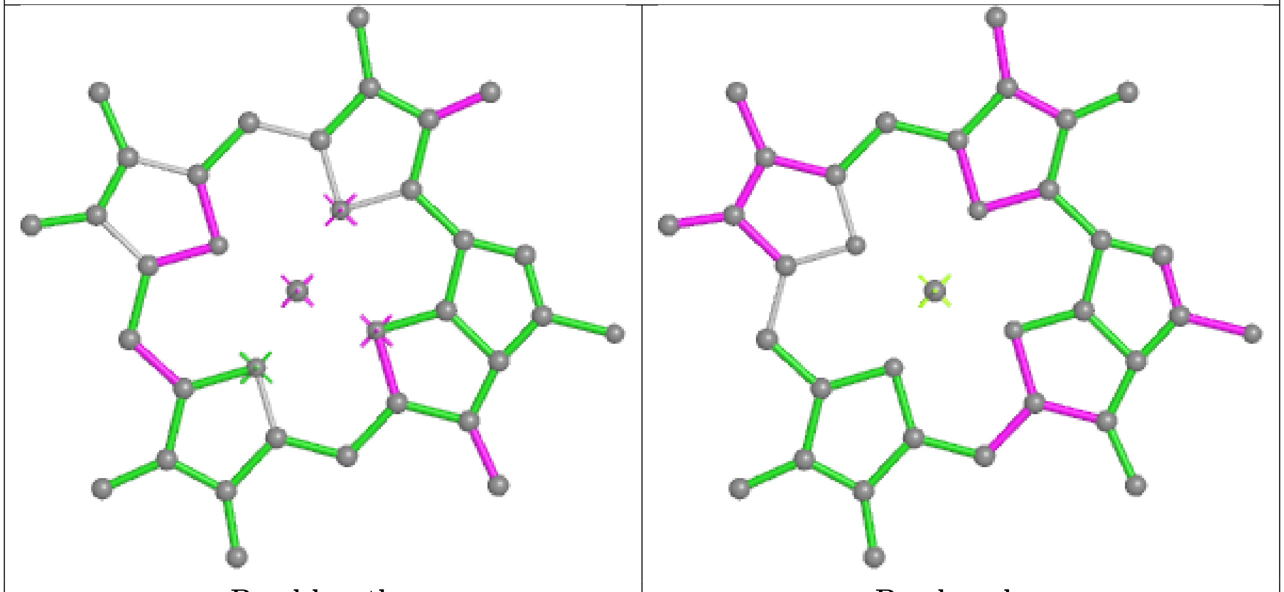


Bond lengths **Bond angles**



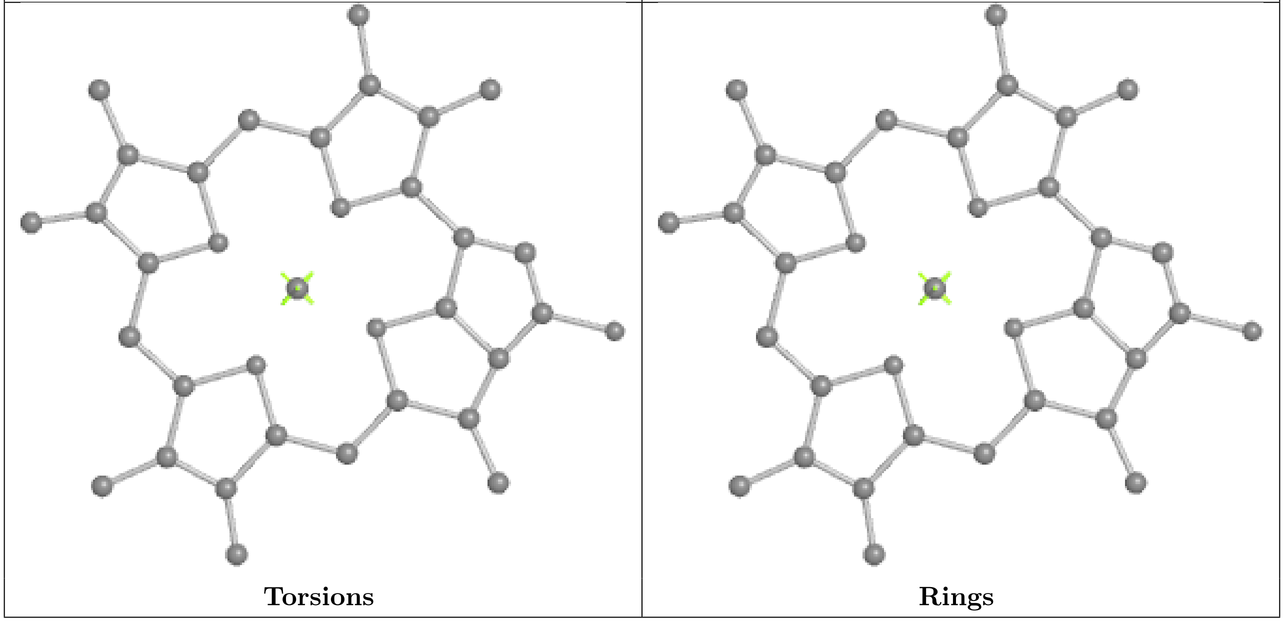
Torsions **Rings**

Ligand CLA M 1086



Bond lengths

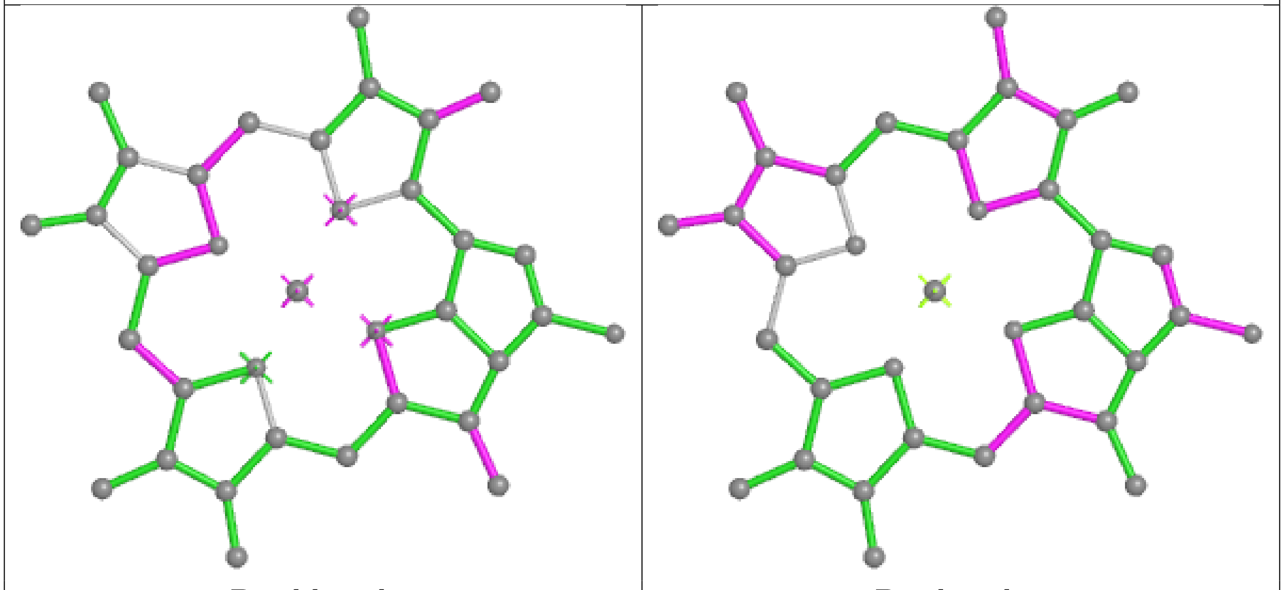
Bond angles



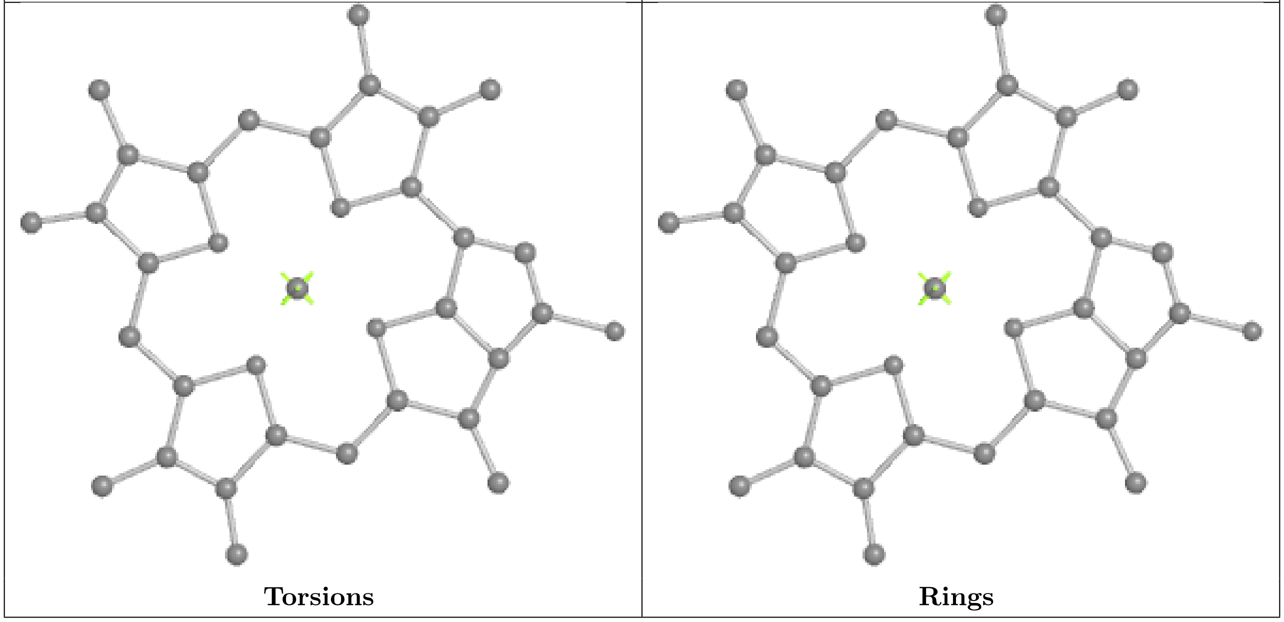
Torsions

Rings

Ligand CLA B 1116

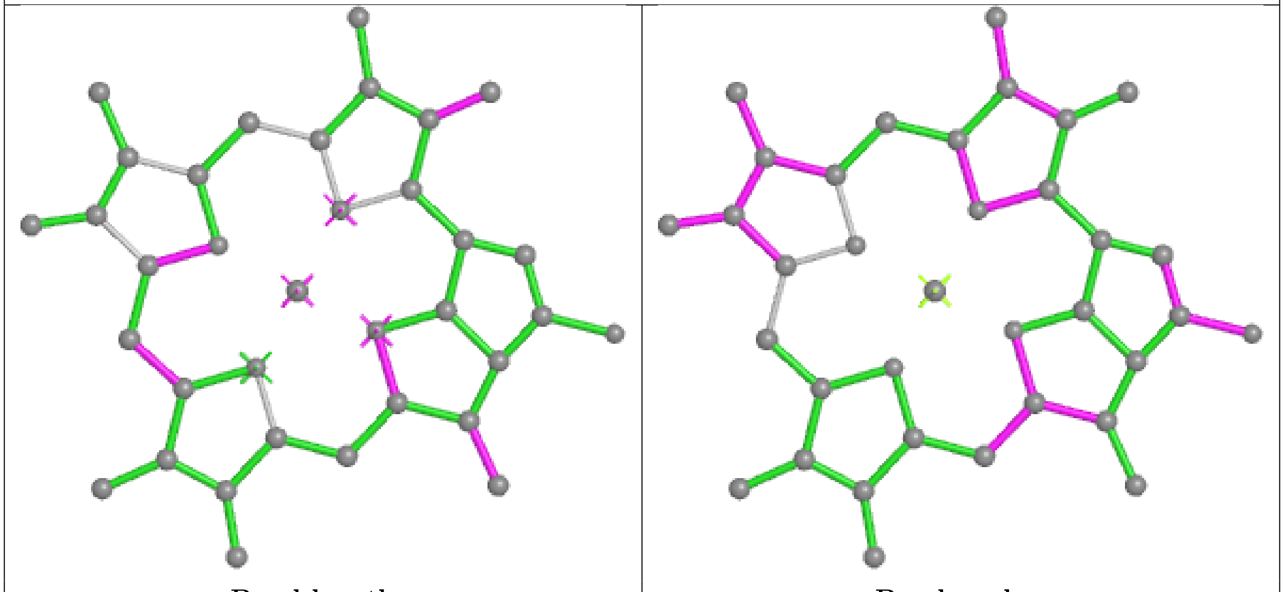


Bond lengths **Bond angles**

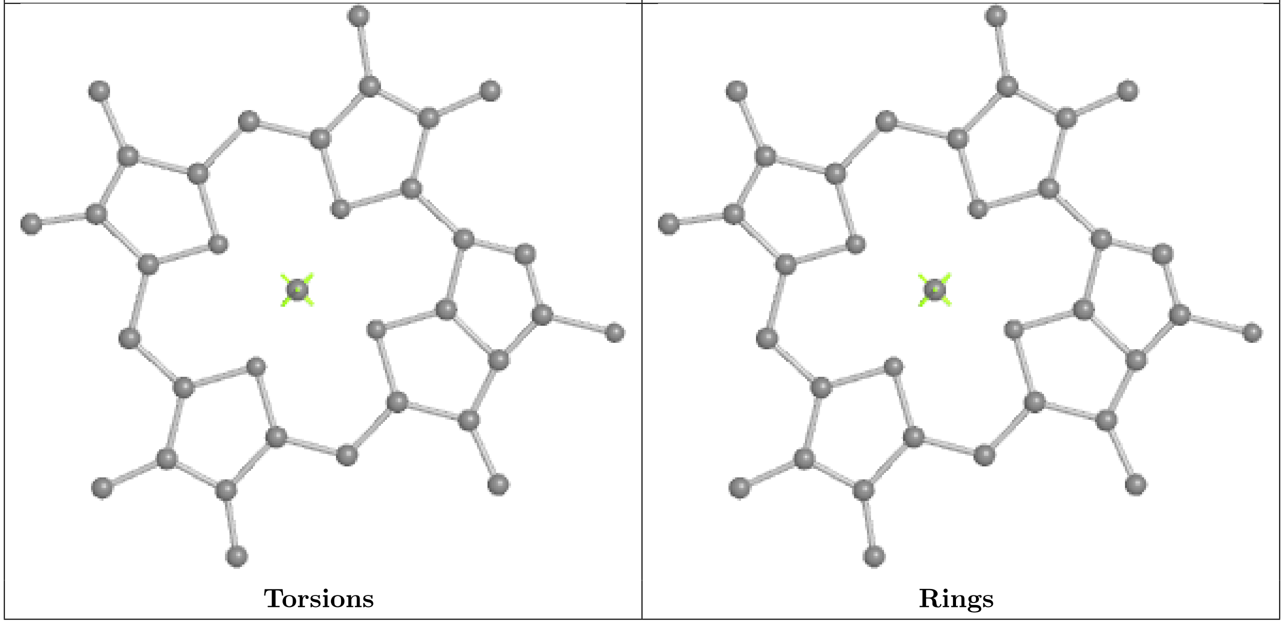


Torsions **Rings**

Ligand CLA B 1108

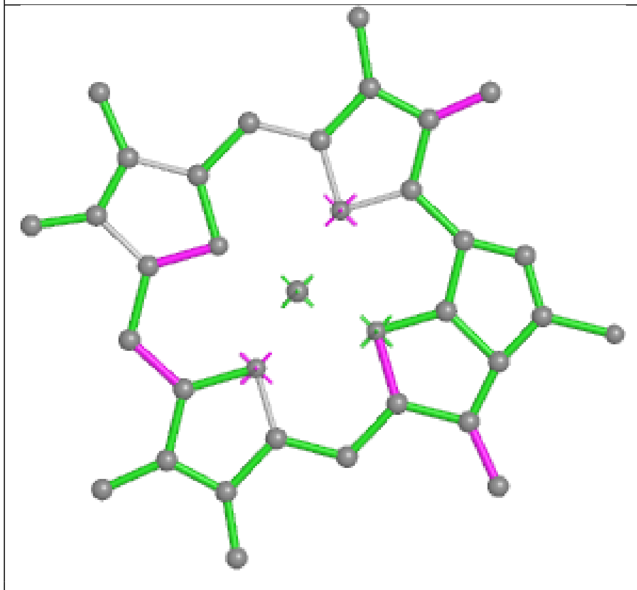


Bond lengths **Bond angles**

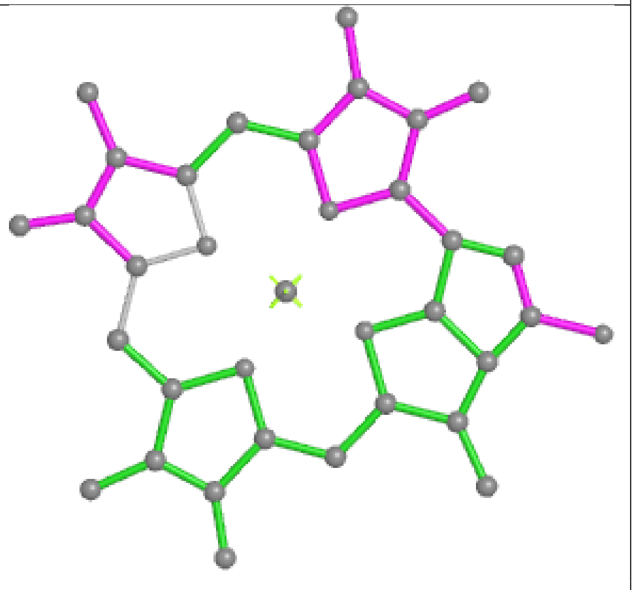


Torsions **Rings**

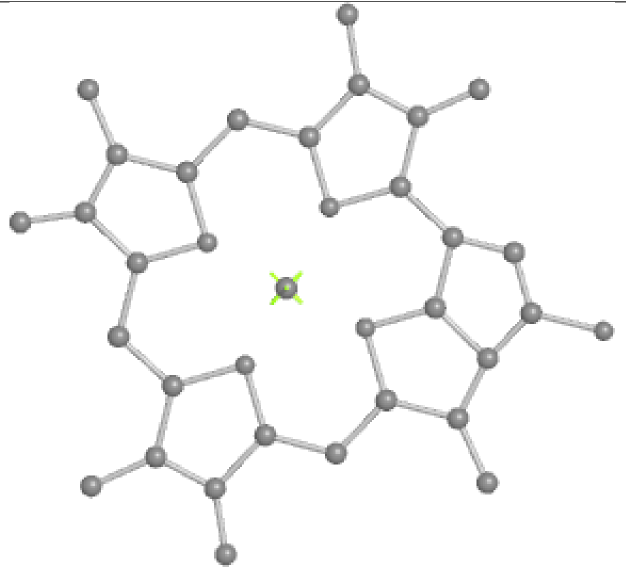
Ligand CLA D 355



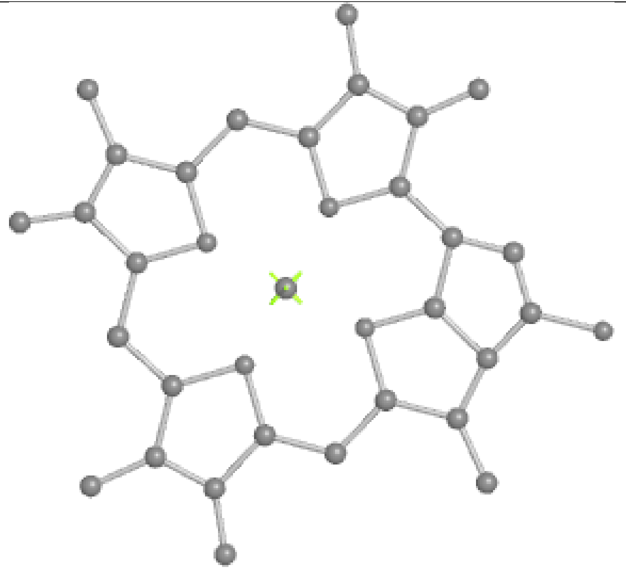
Bond lengths



Bond angles

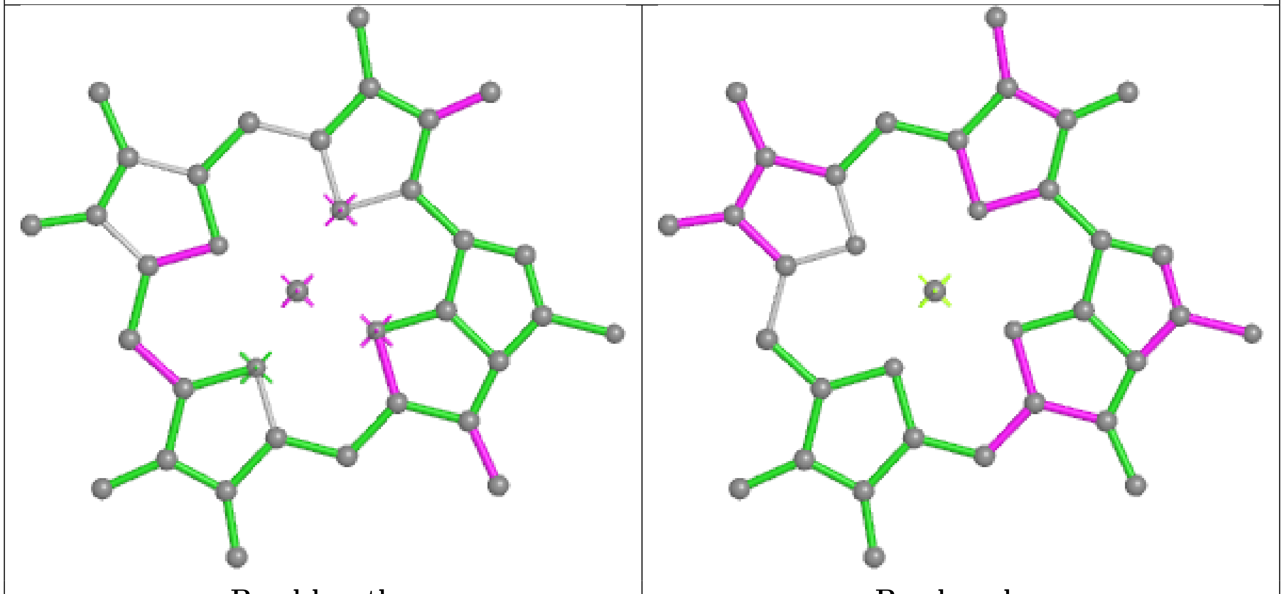


Torsions

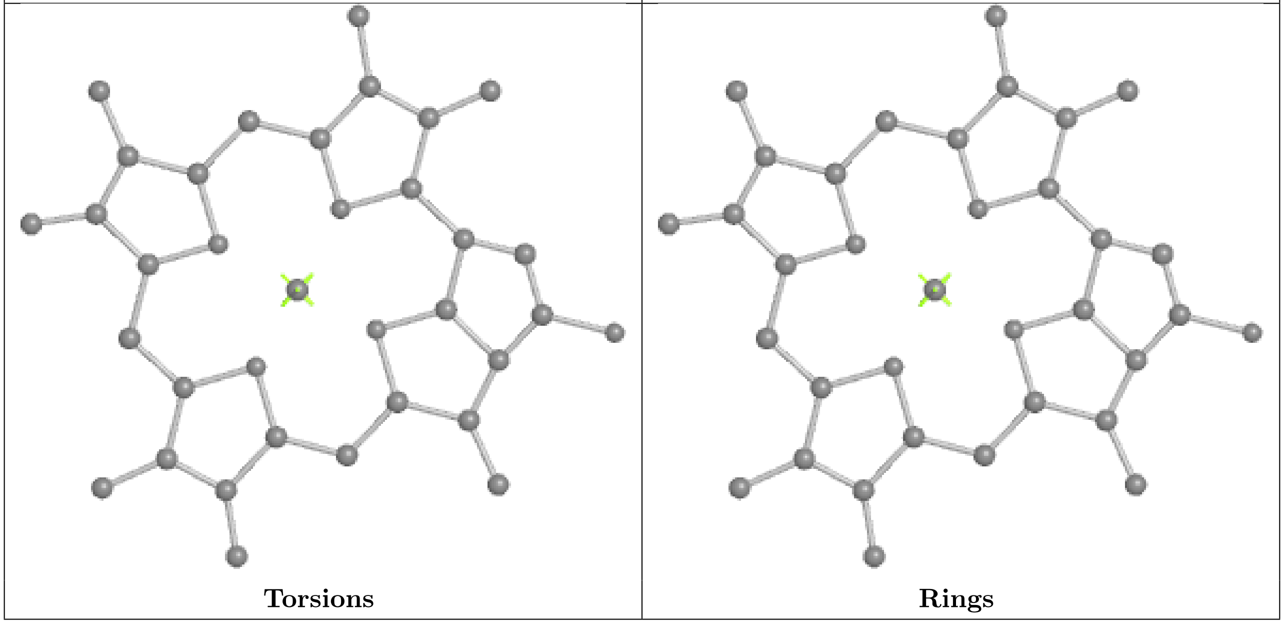


Rings

Ligand CLA C 1086

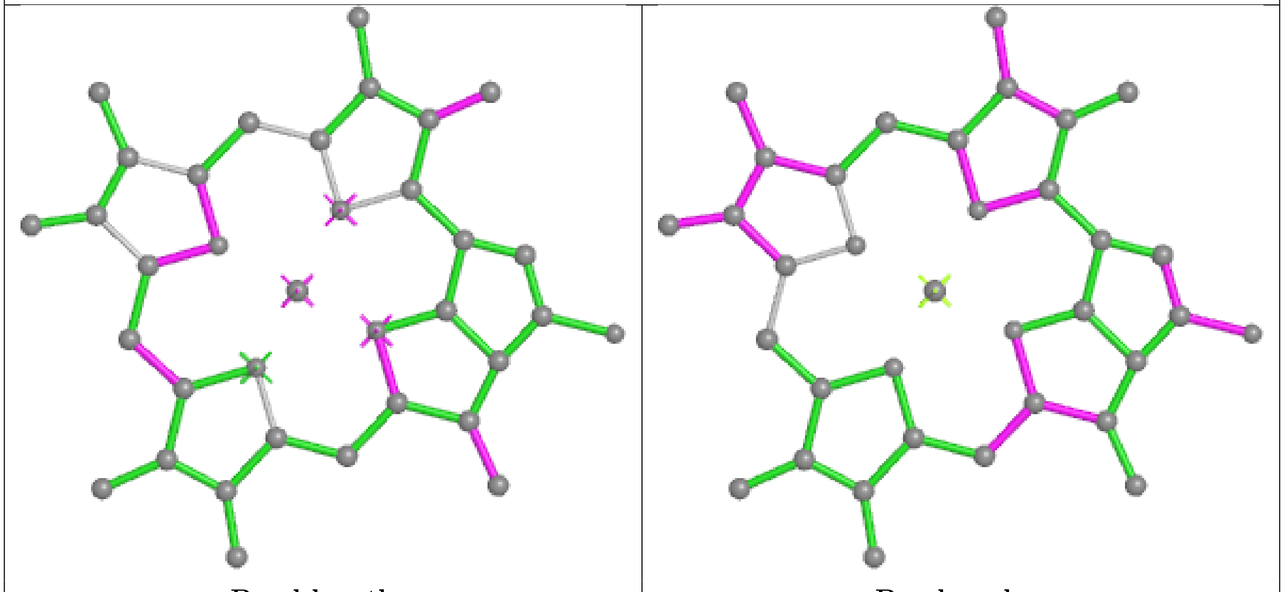


Bond lengths **Bond angles**

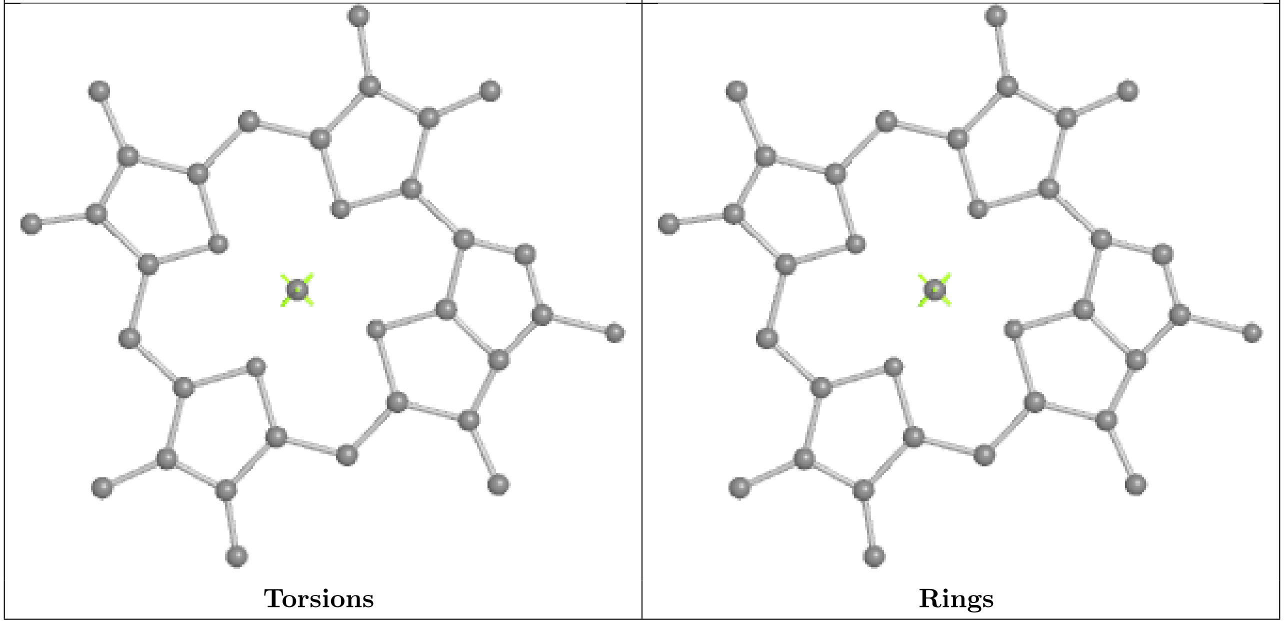


Torsions **Rings**

Ligand CLA B 1115

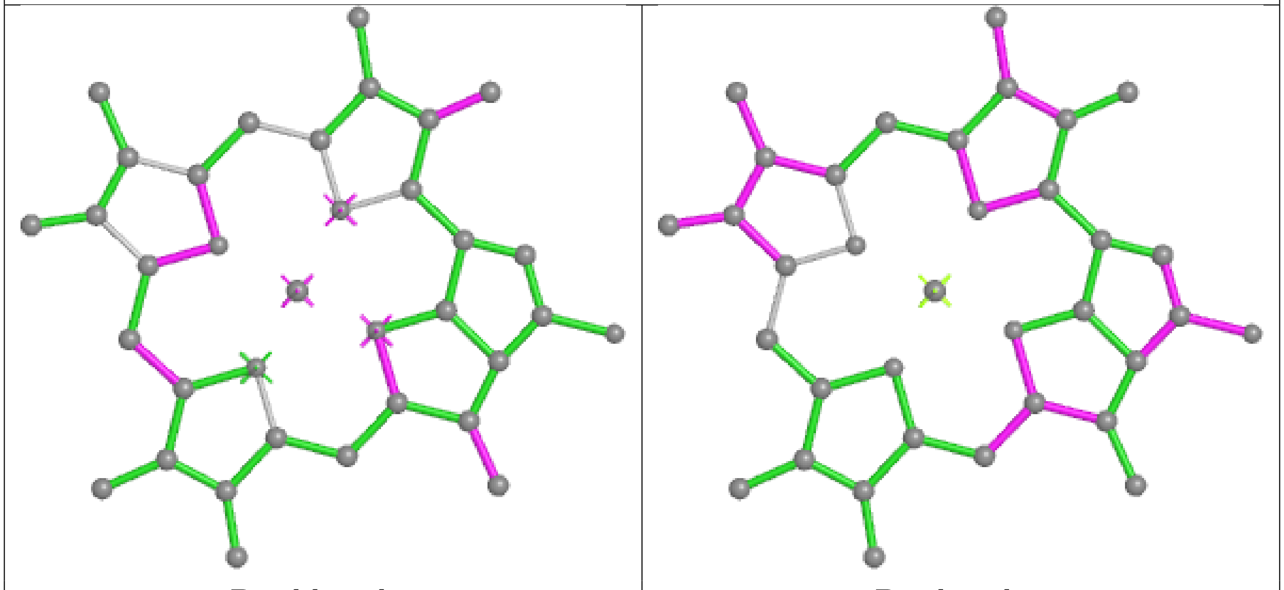


Bond lengths **Bond angles**



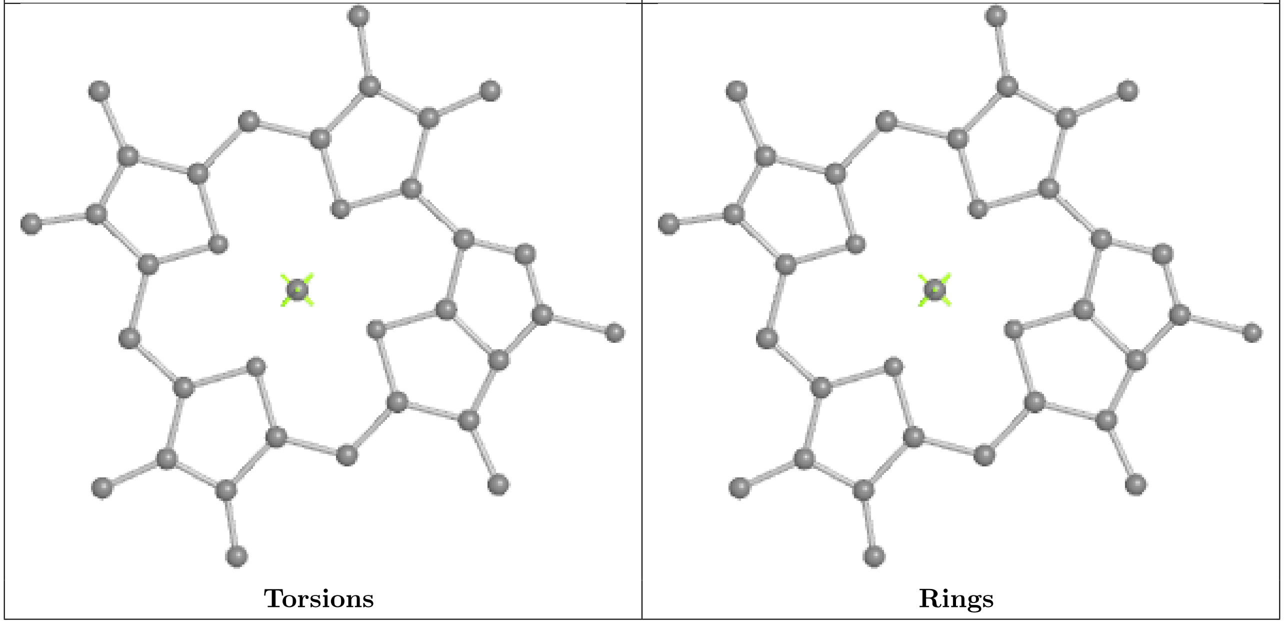
Torsions **Rings**

Ligand CLA C 1084



Bond lengths

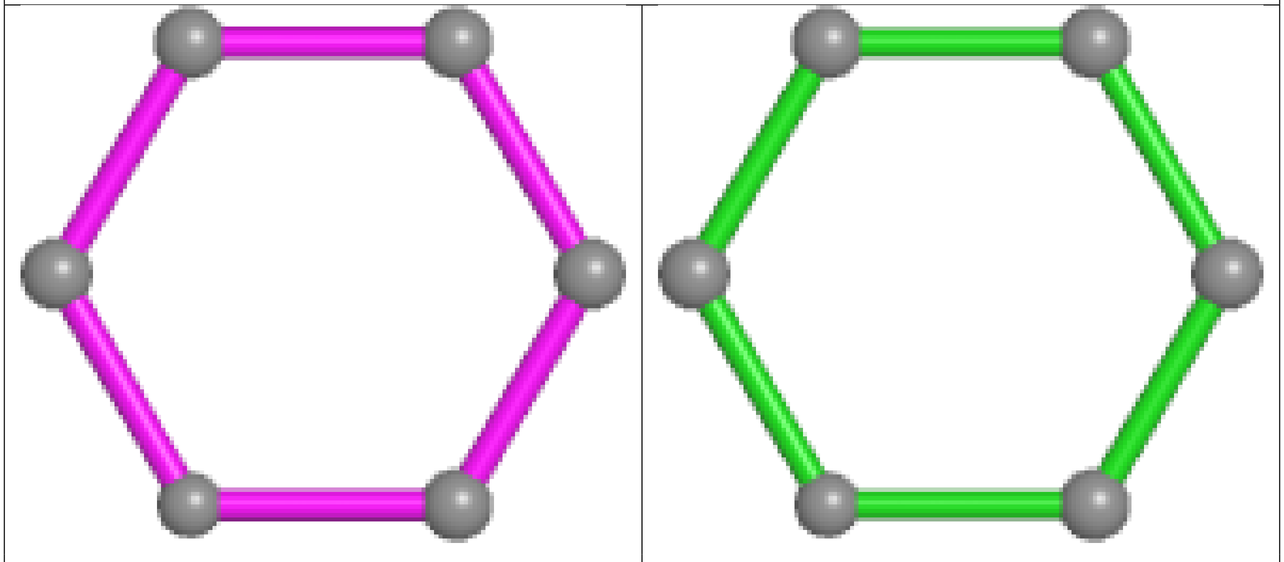
Bond angles



Torsions

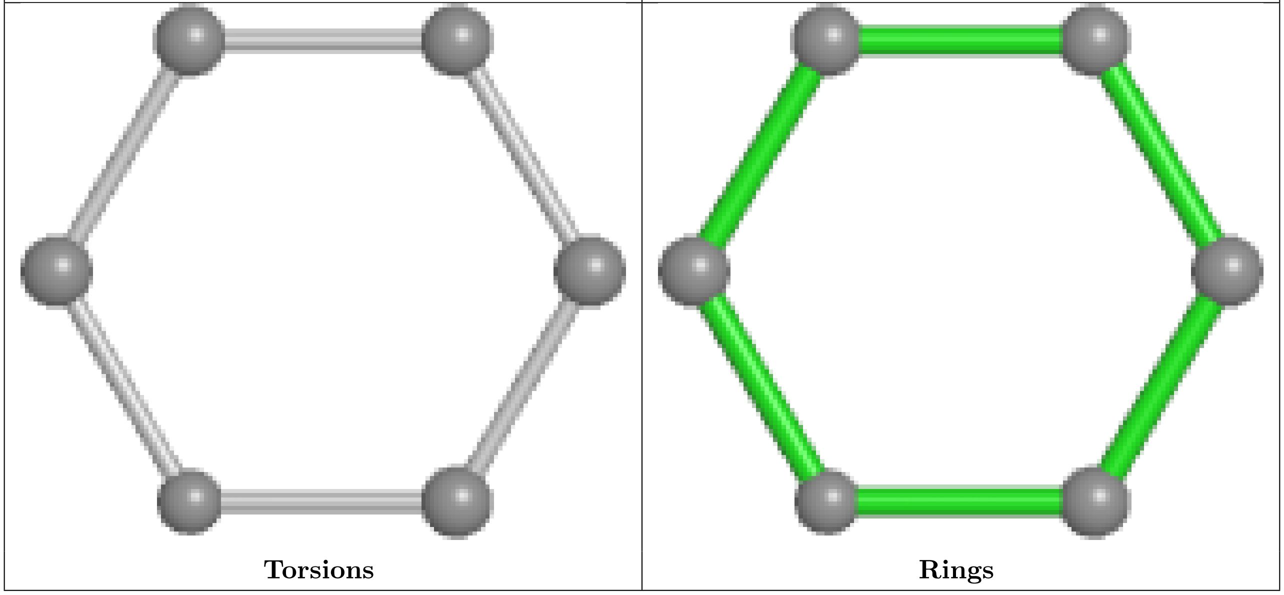
Rings

Ligand PLA N 359



Bond lengths

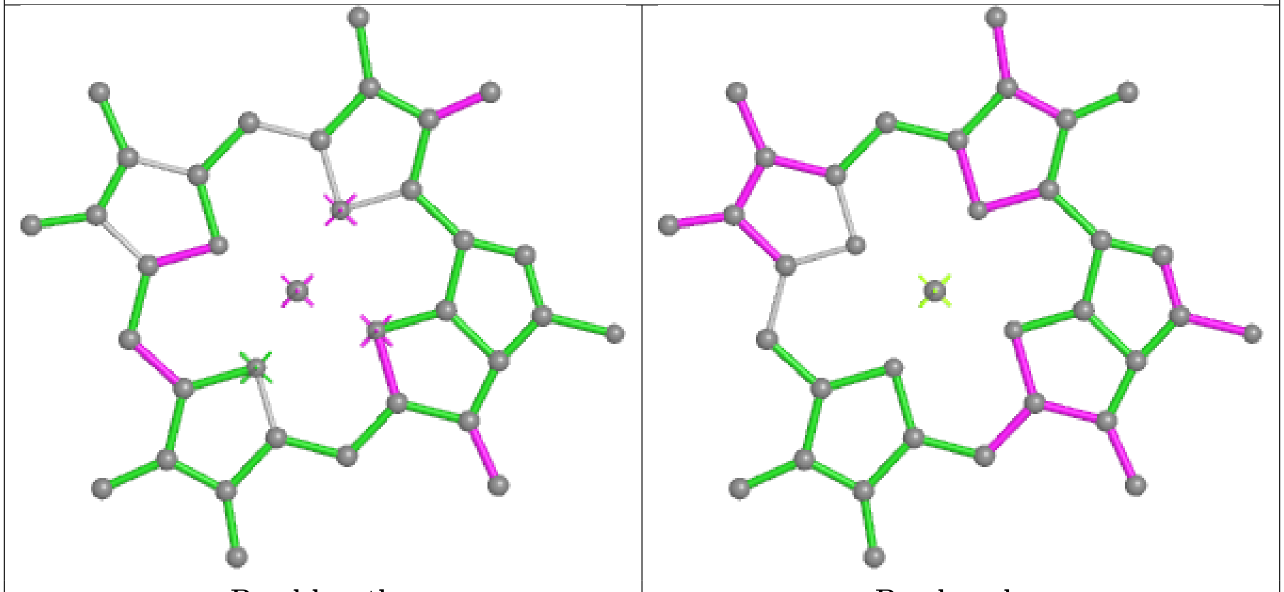
Bond angles



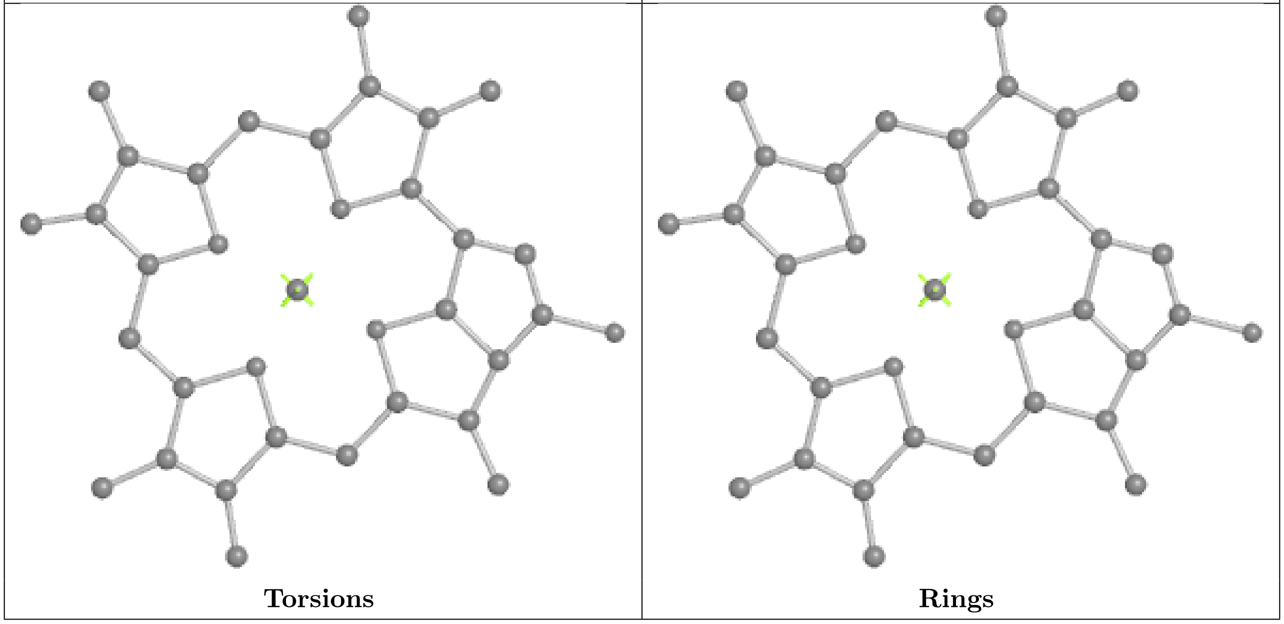
Torsions

Rings

Ligand CLA C 1079

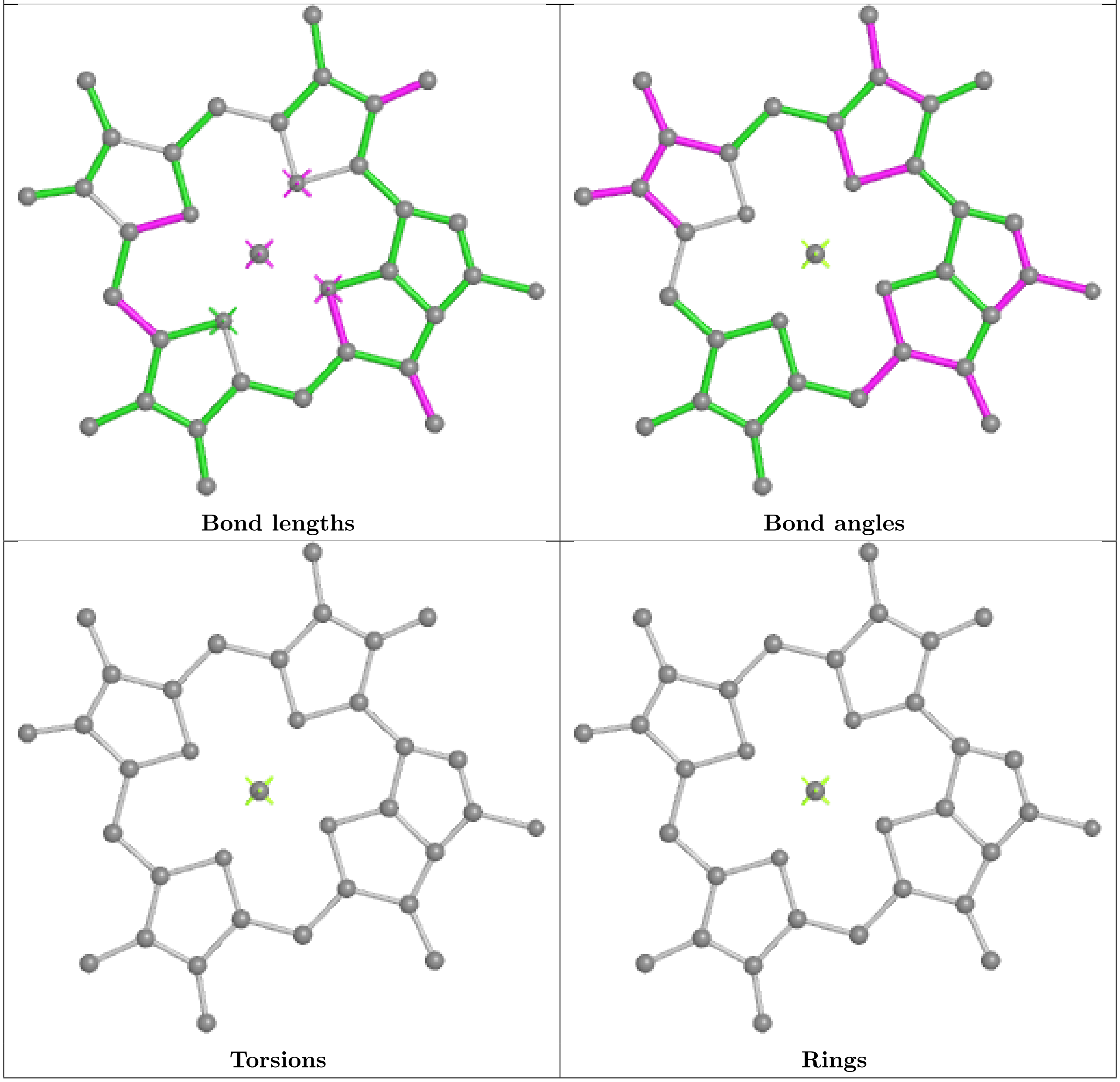


Bond lengths **Bond angles**



Torsions **Rings**

Ligand CLA B 1114



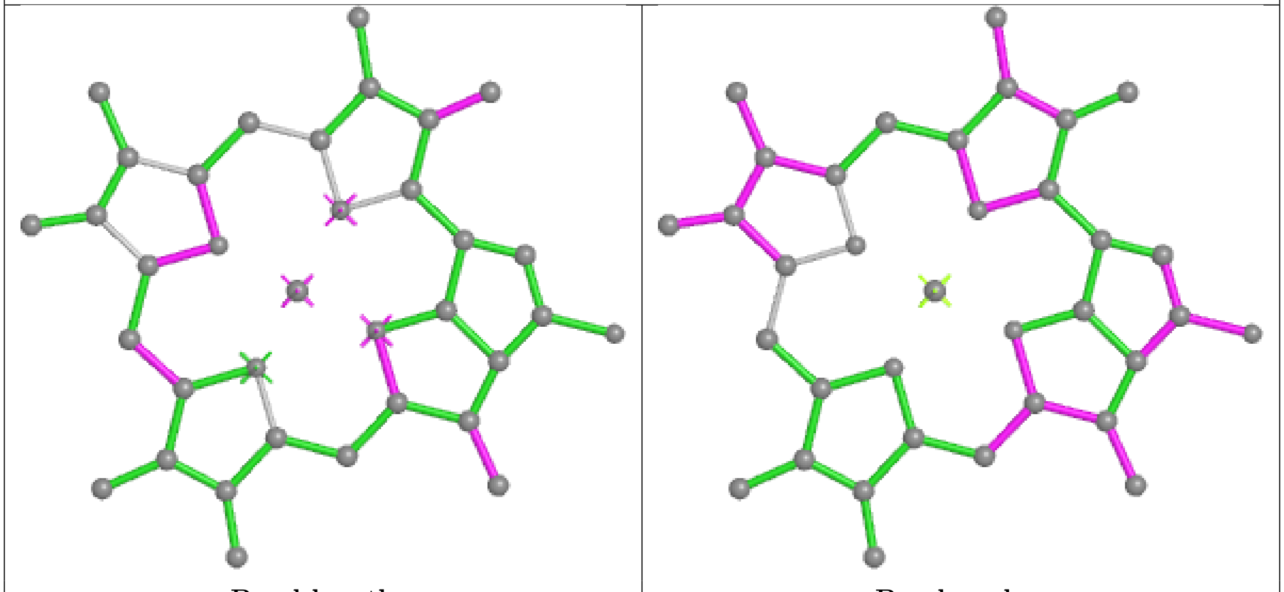
Bond lengths

Bond angles

Torsions

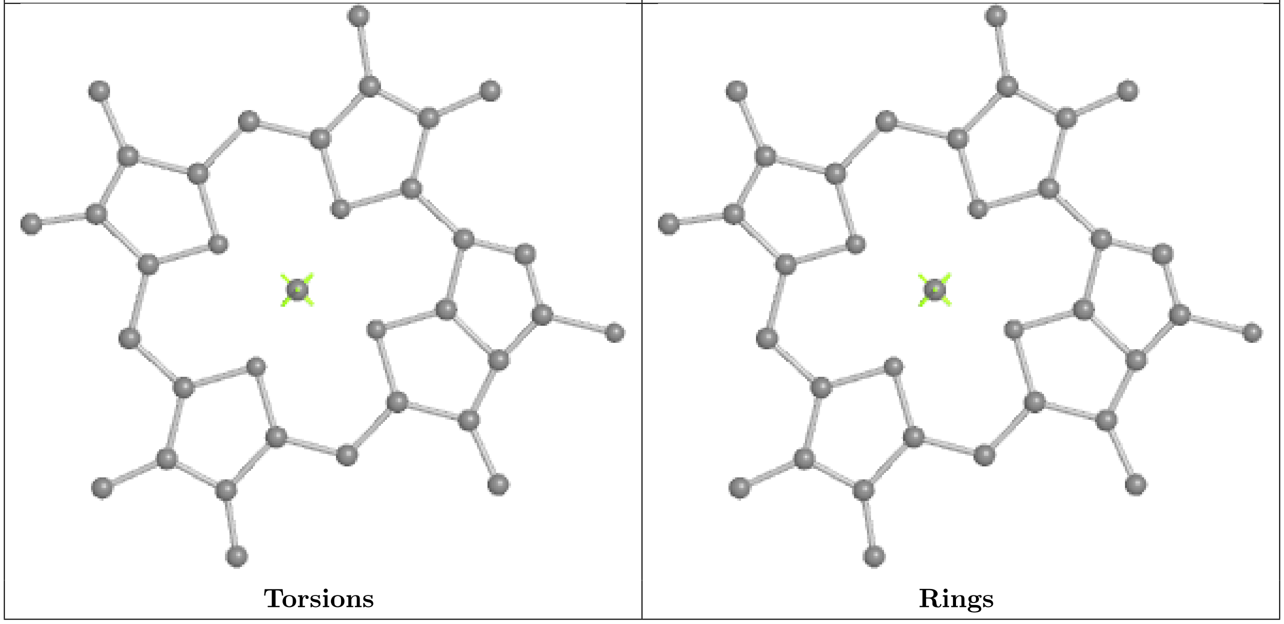
Rings

Ligand CLA A 369



Bond lengths

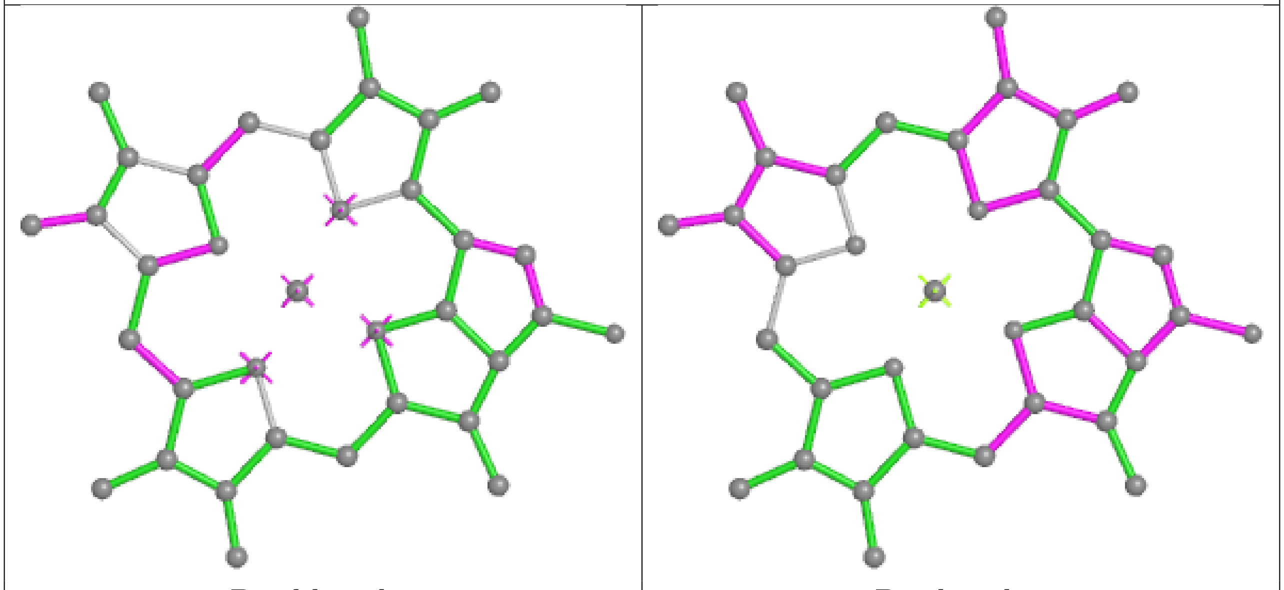
Bond angles



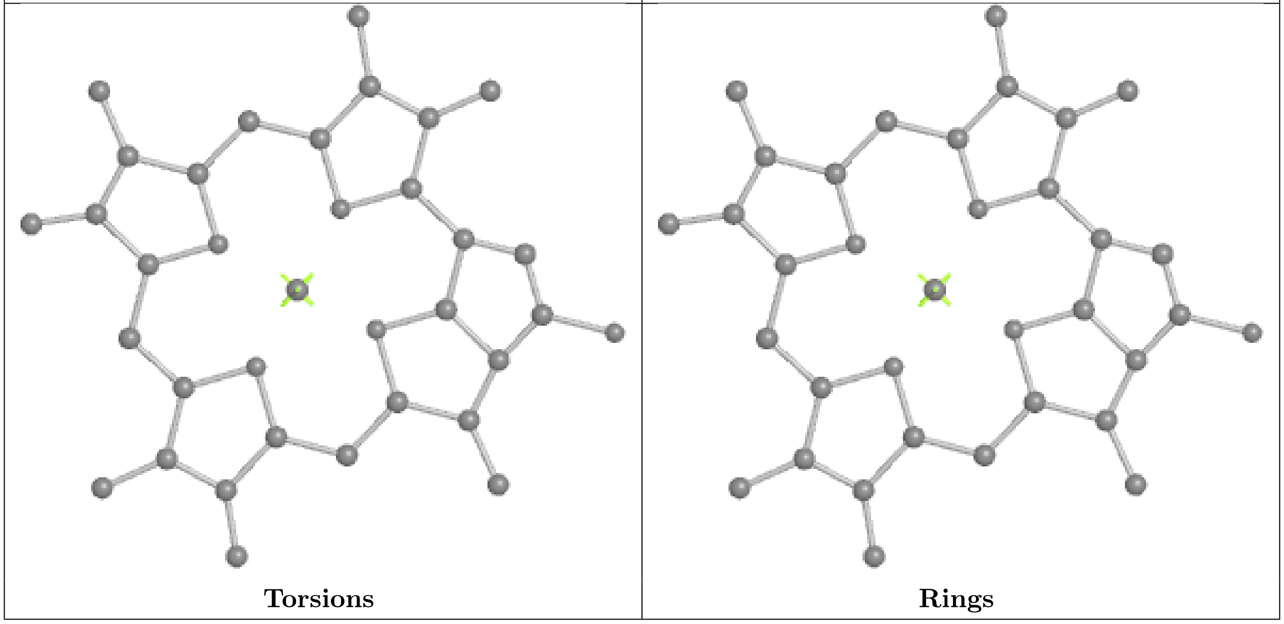
Torsions

Rings

Ligand CLA A 365

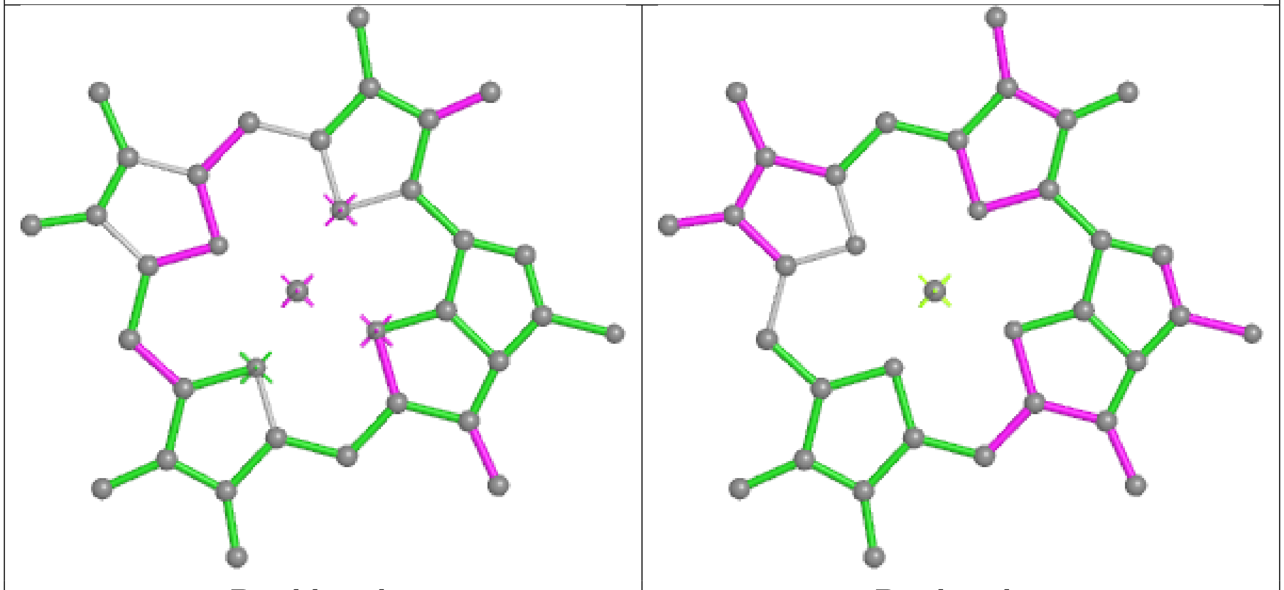


Bond lengths Bond angles

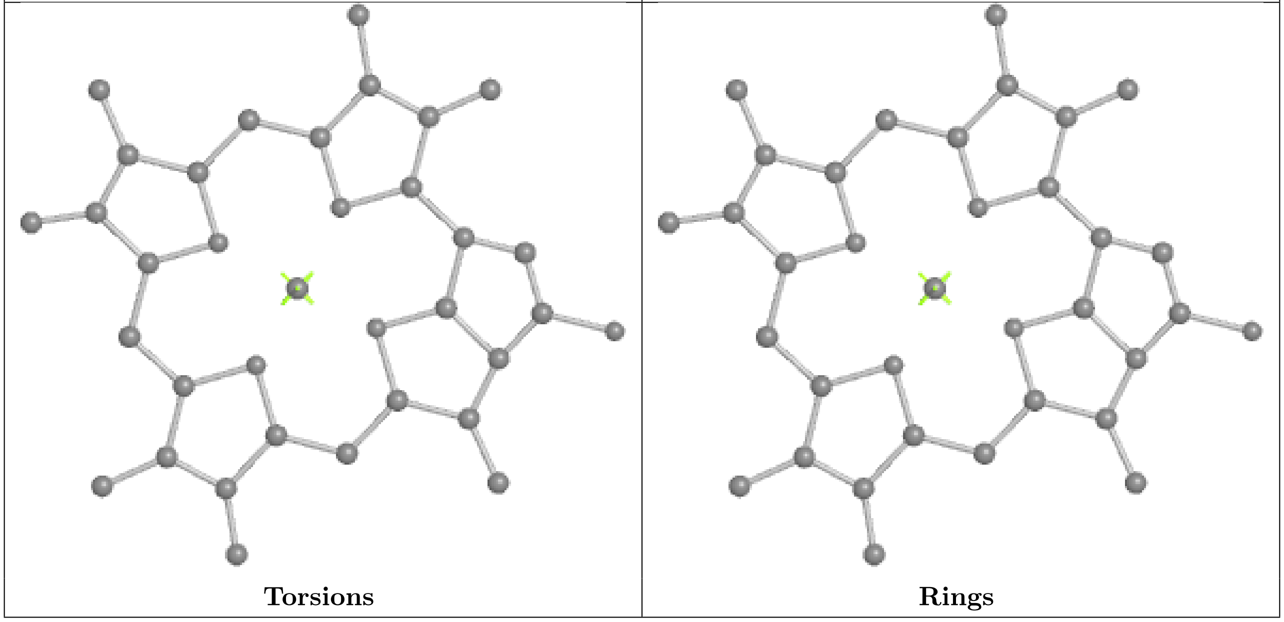


Torsions Rings

Ligand CLA B 1119

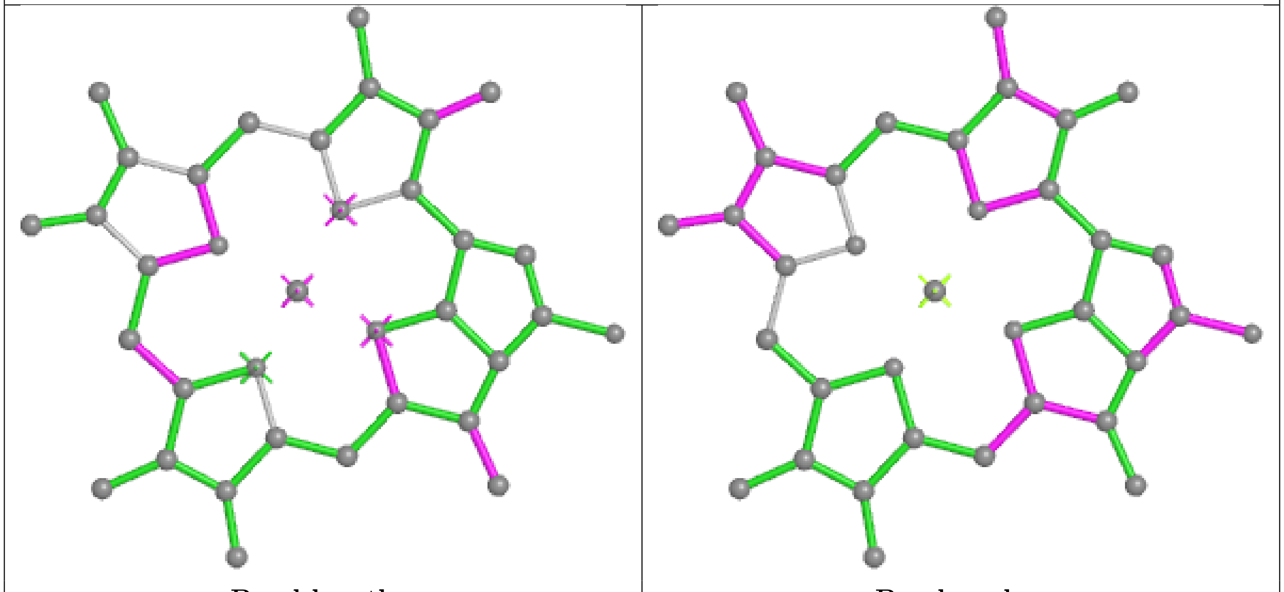


Bond lengths Bond angles



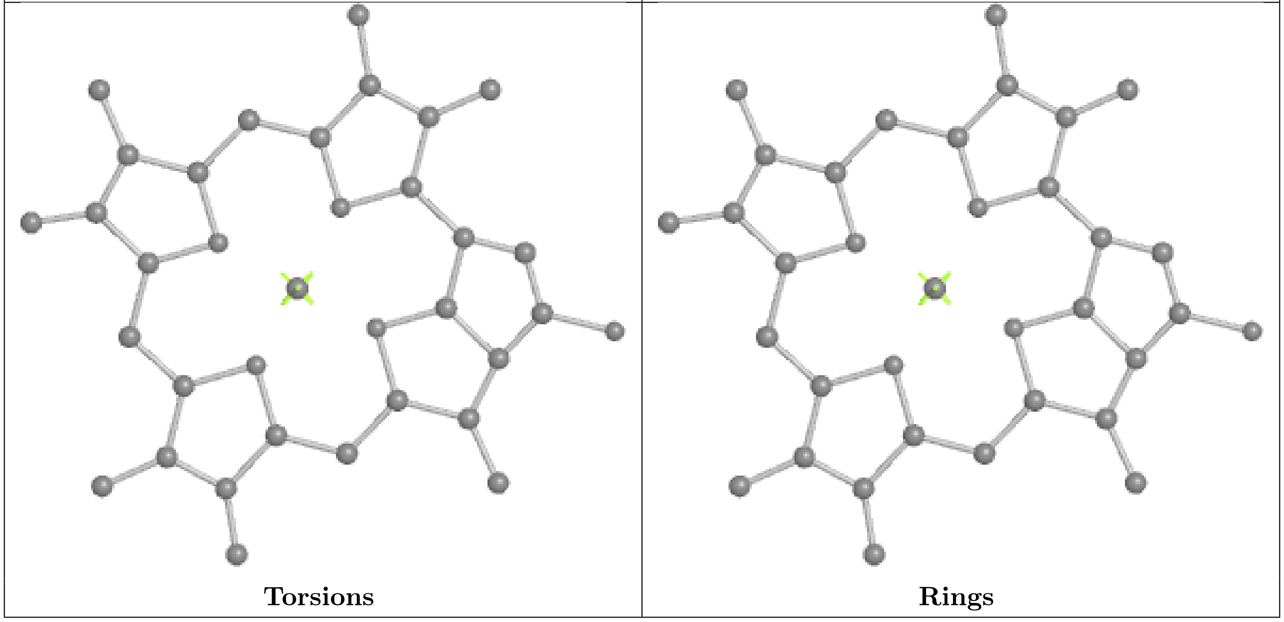
Torsions Rings

Ligand CLA C 1089



Bond lengths

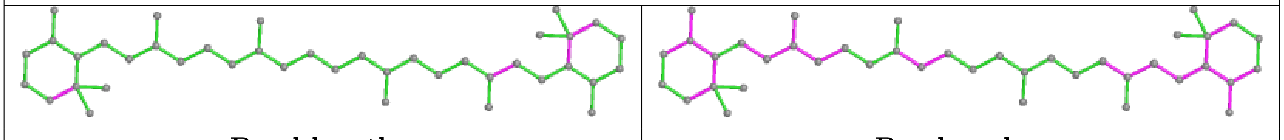
Bond angles



Torsions

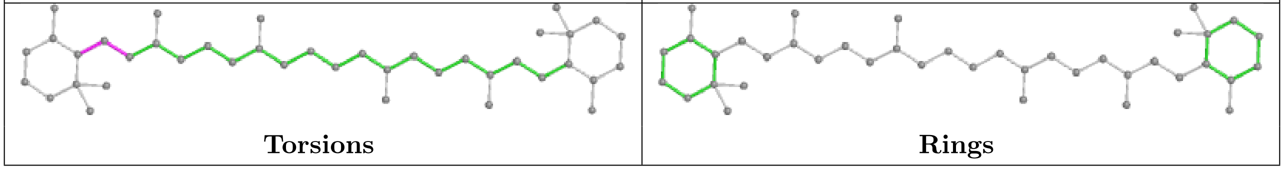
Rings

Ligand BCR D 359



Bond lengths

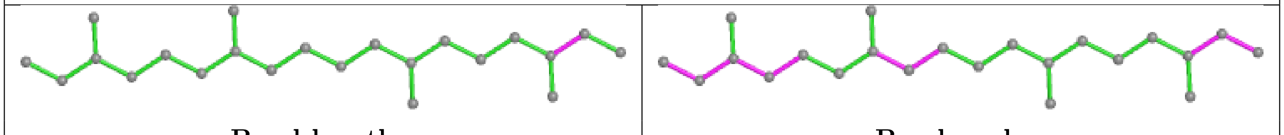
Bond angles



Torsions

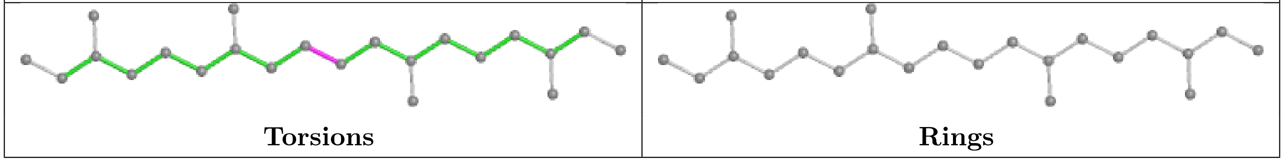
Rings

Ligand BCR K 47



Bond lengths

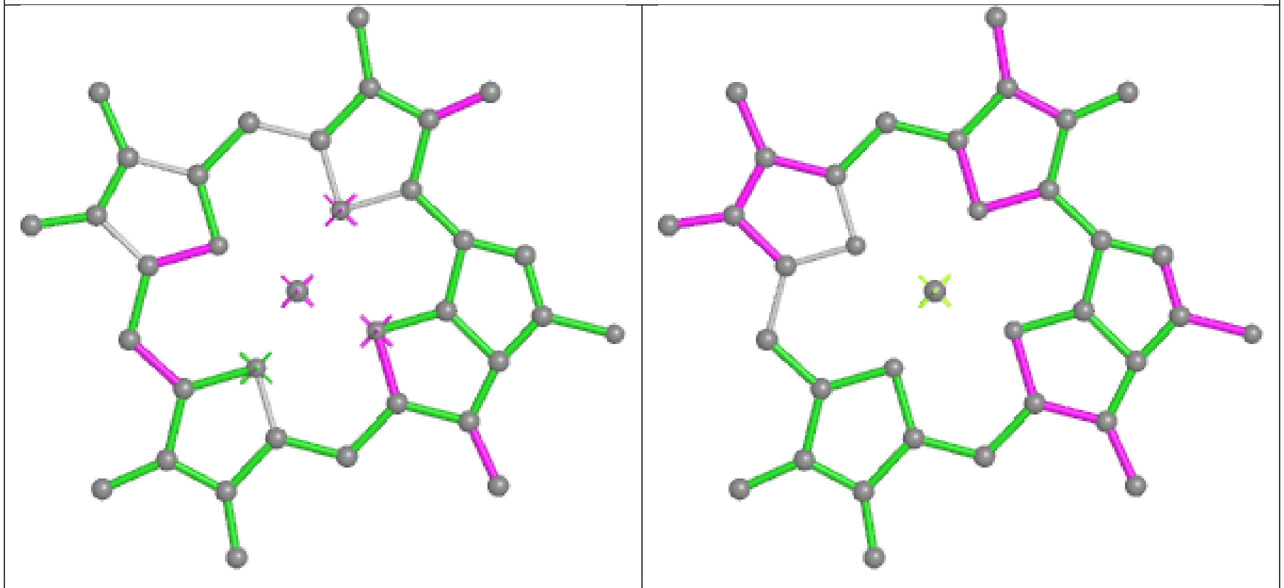
Bond angles



Torsions

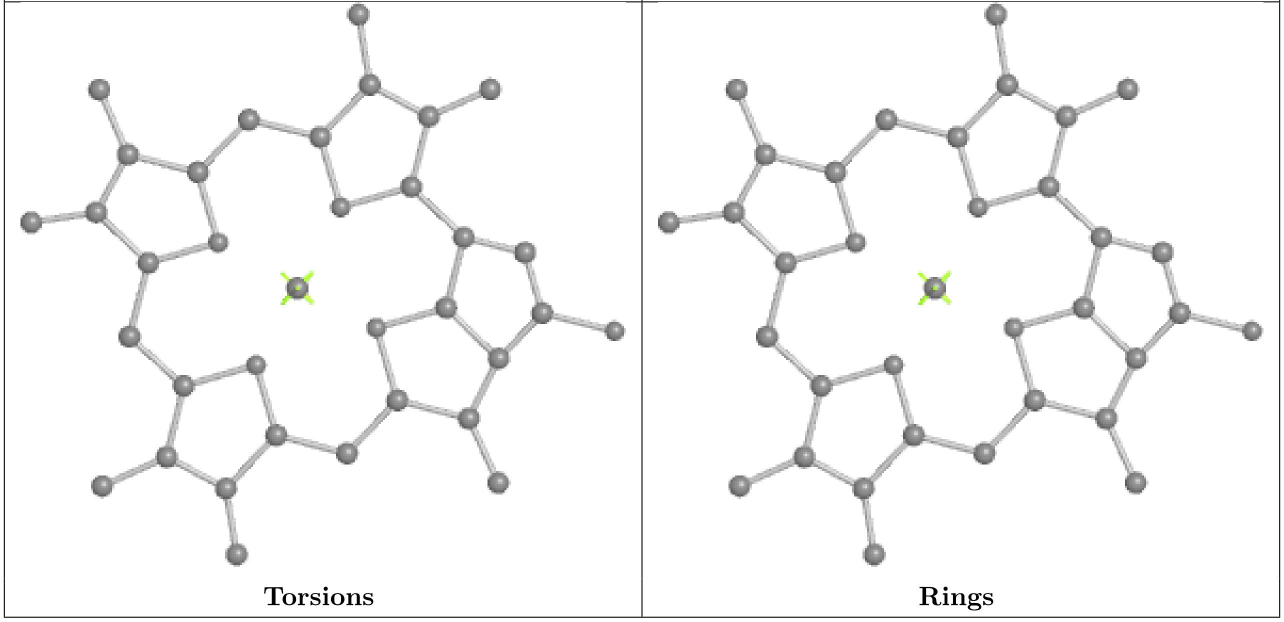
Rings

Ligand CLA C 1085



Bond lengths

Bond angles



Torsions

Rings

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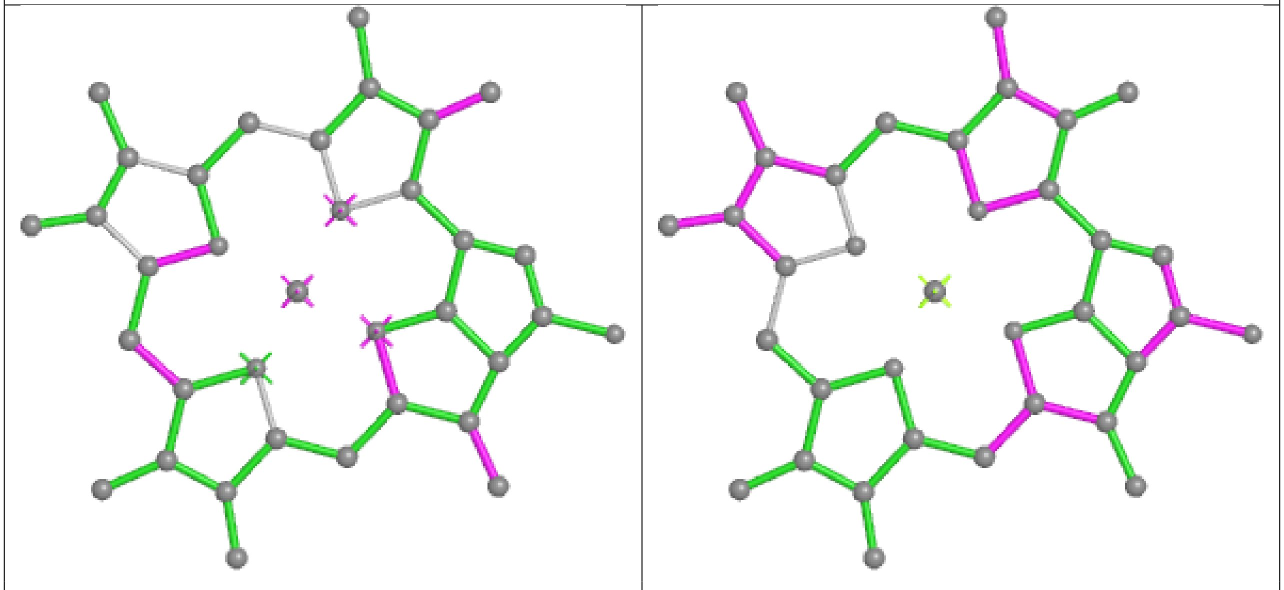
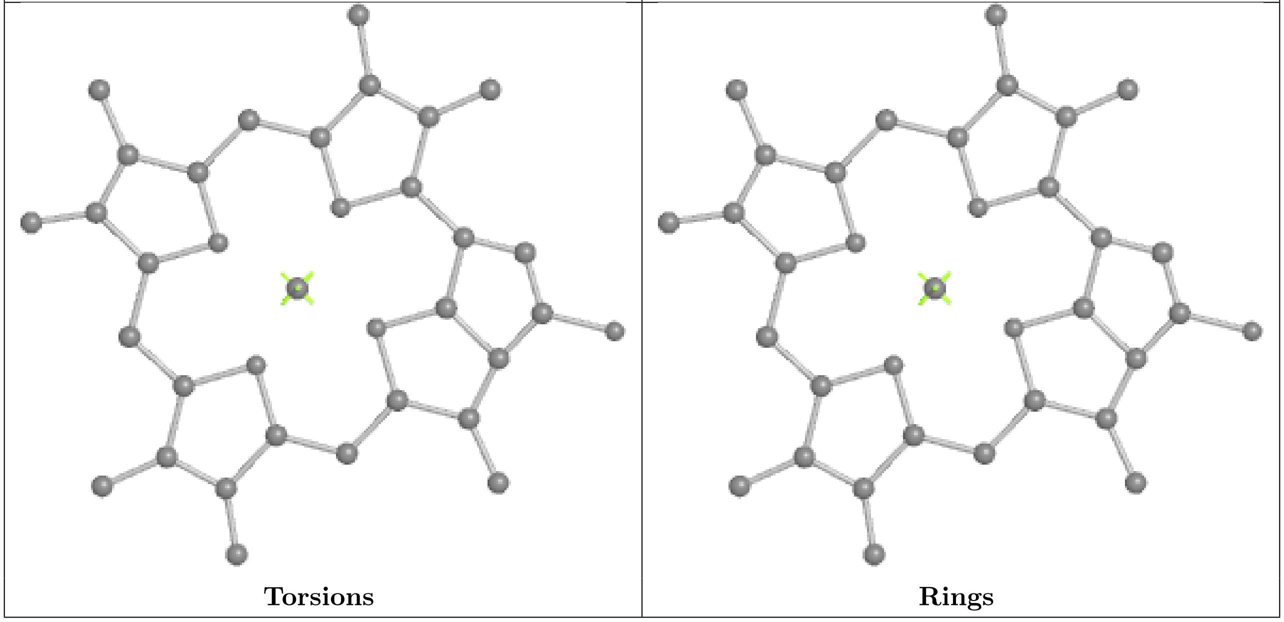


Bond lengths

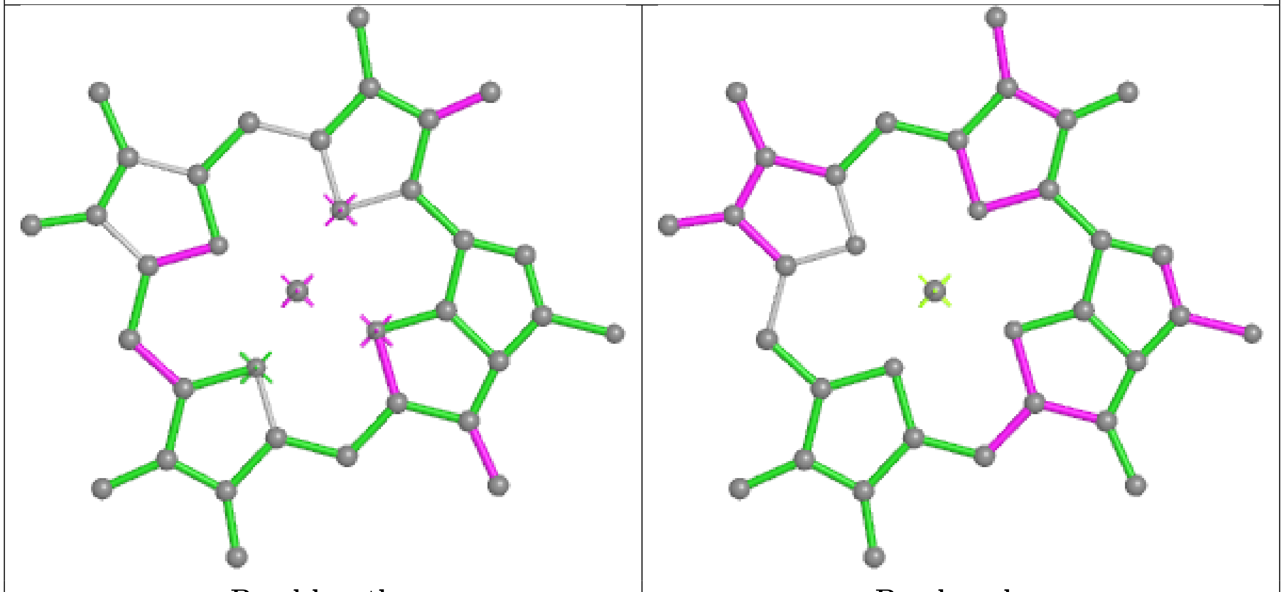
Bond angles



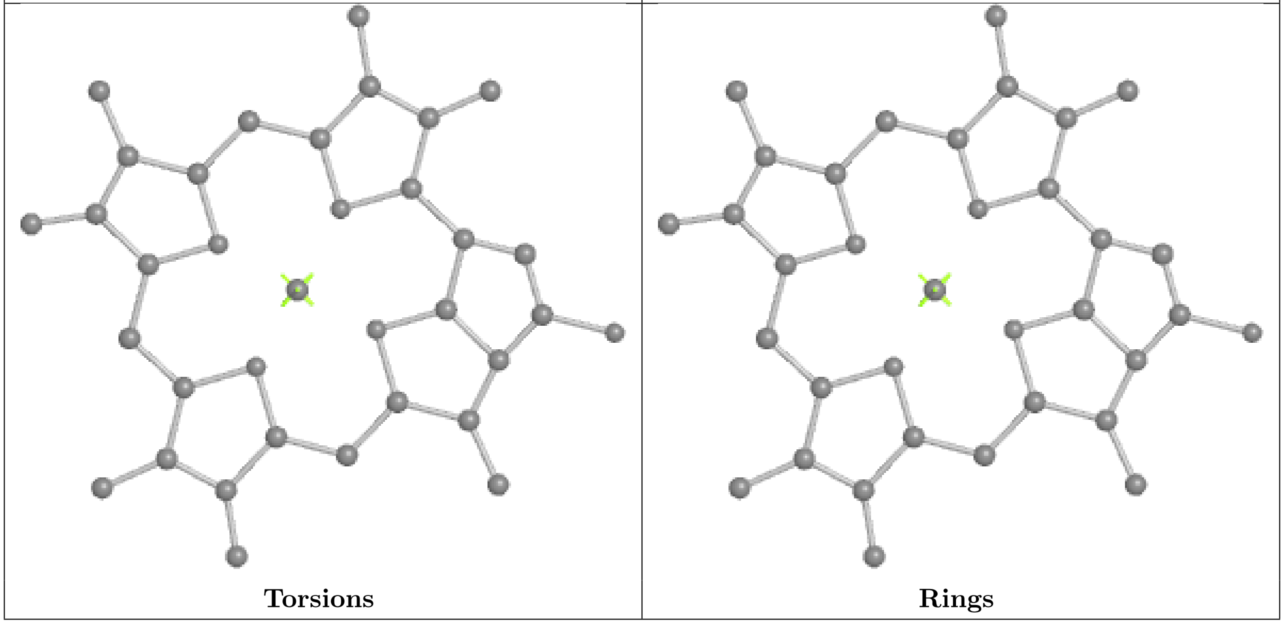
Torsions

Rings

Ligand CLA C 1087

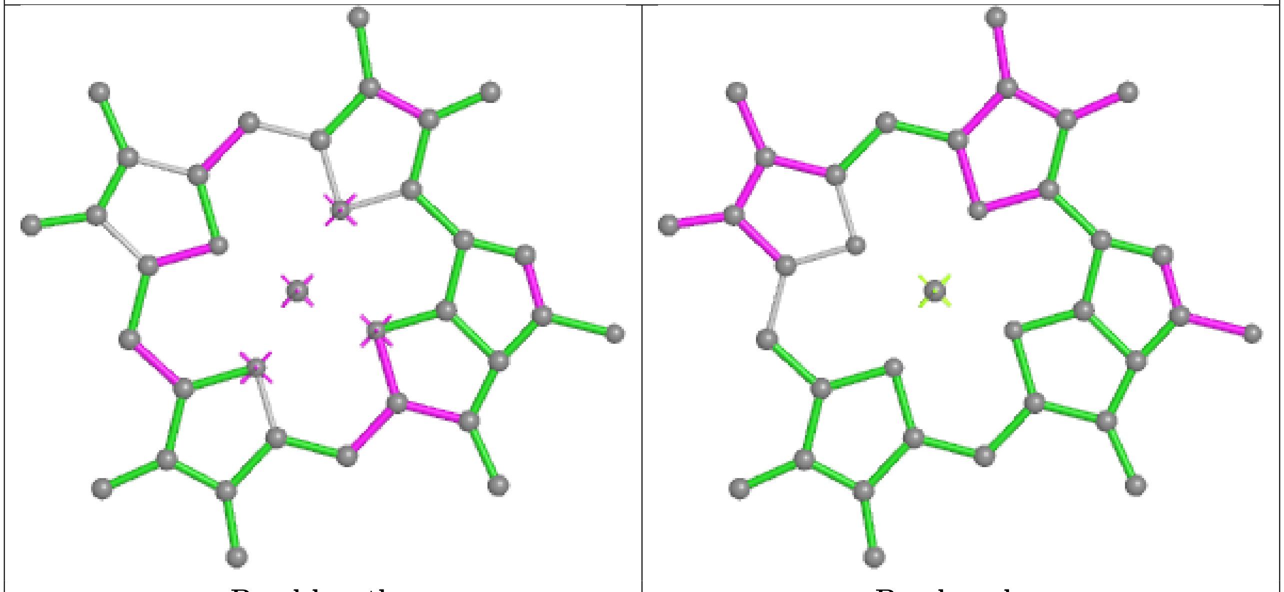


Bond lengths **Bond angles**

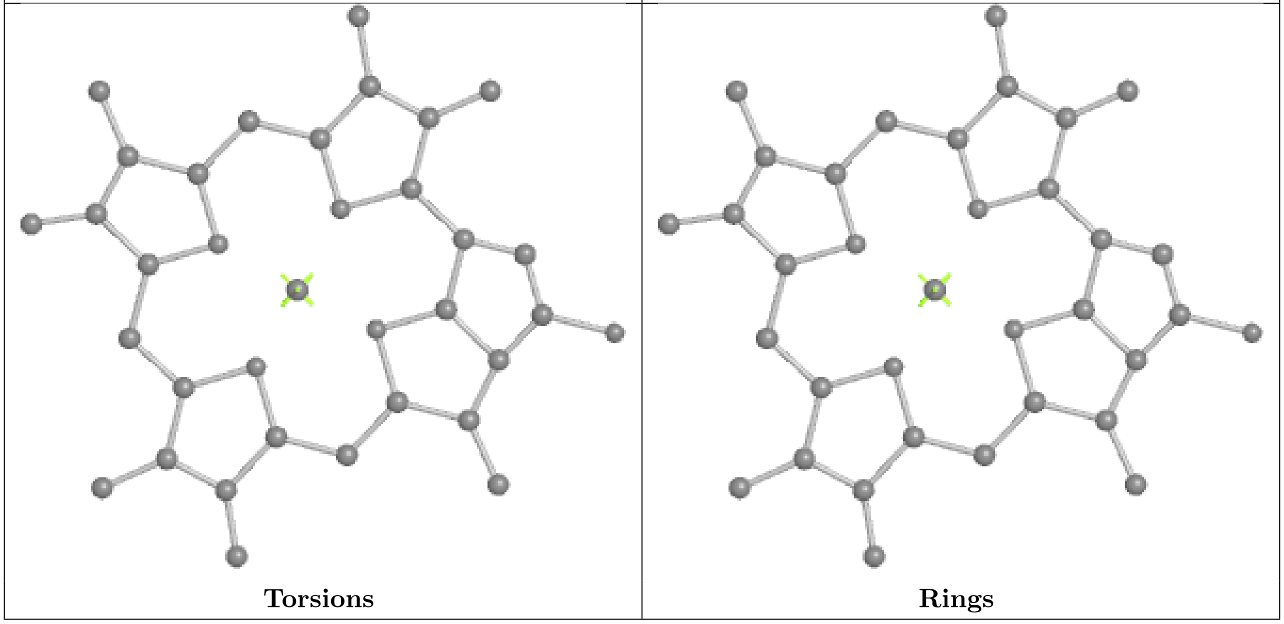


Torsions **Rings**

Ligand CLA A 366

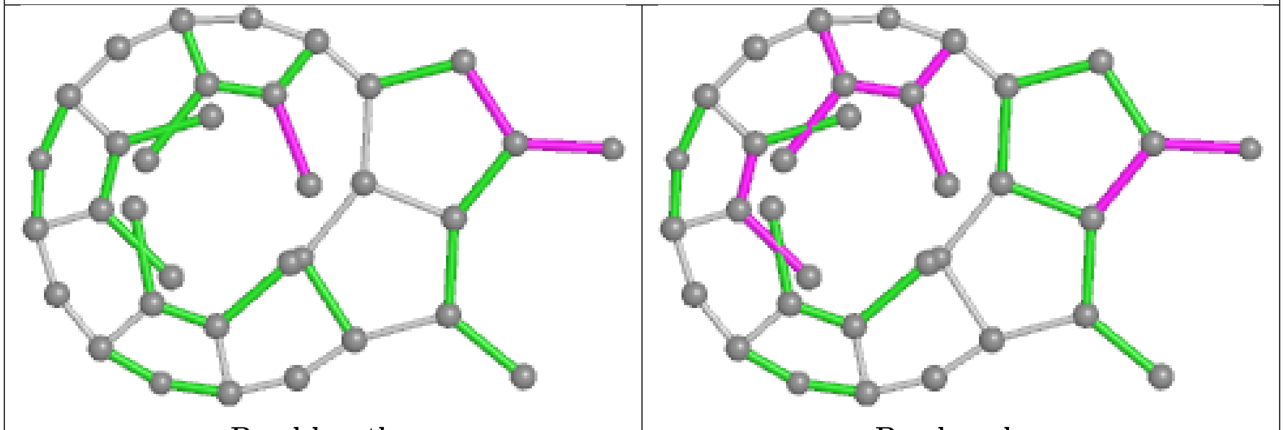


Bond lengths **Bond angles**



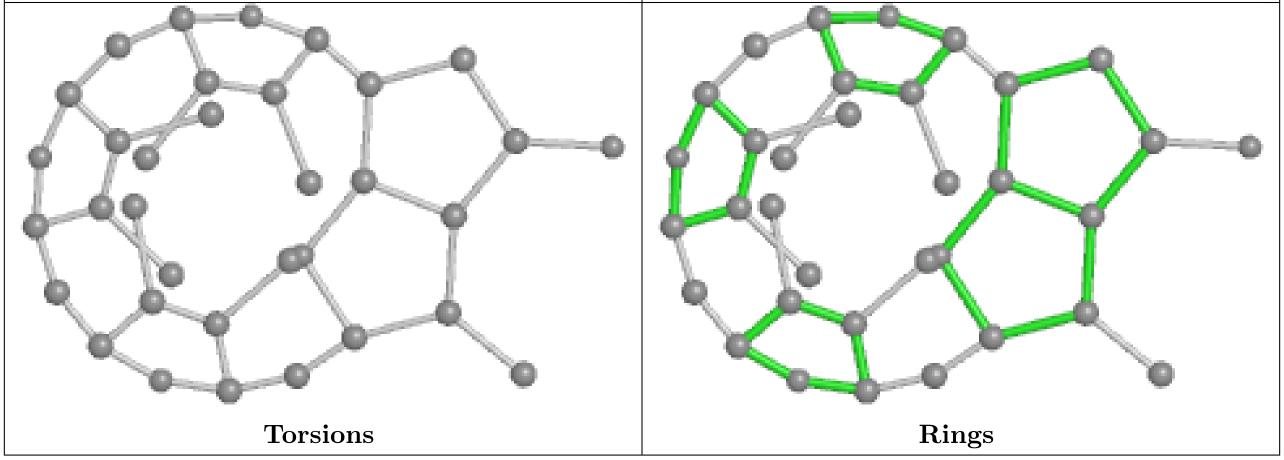
Torsions **Rings**

Ligand PHO N 357



Bond lengths

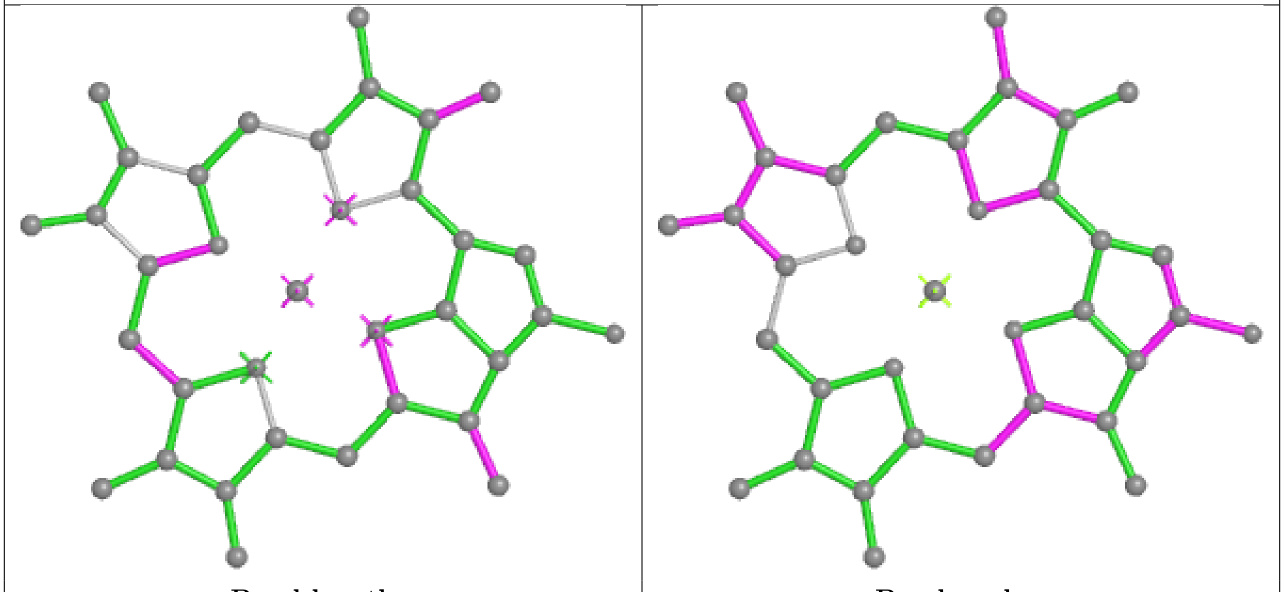
Bond angles



Torsions

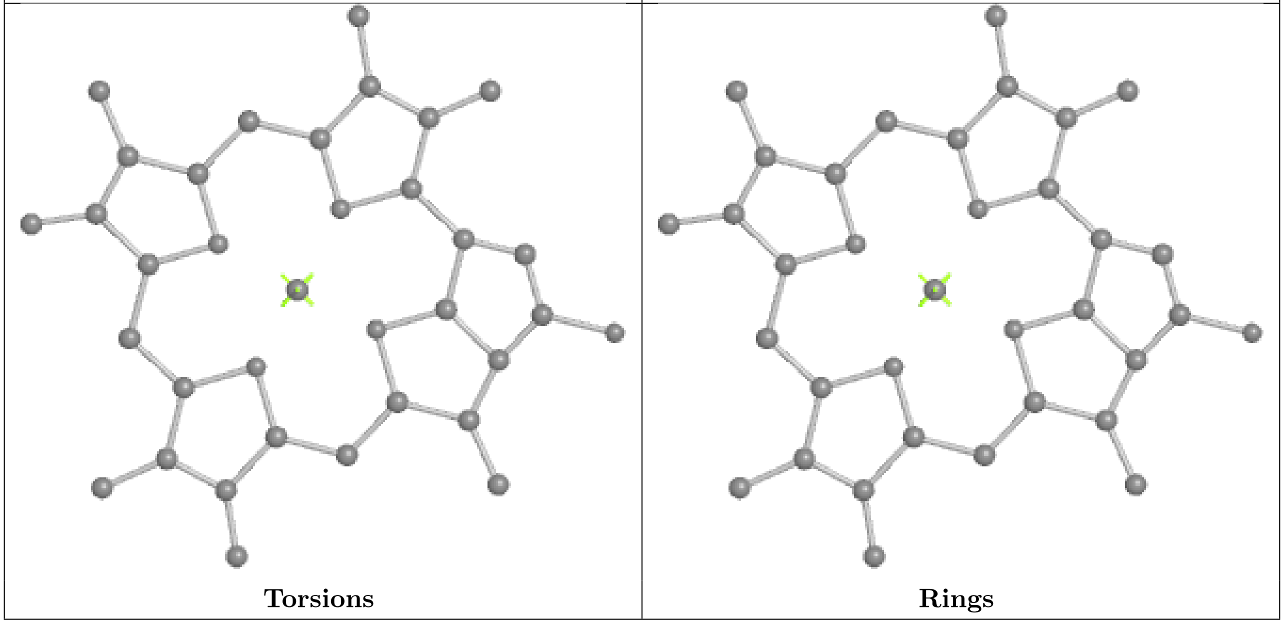
Rings

Ligand CLA B 1120



Bond lengths

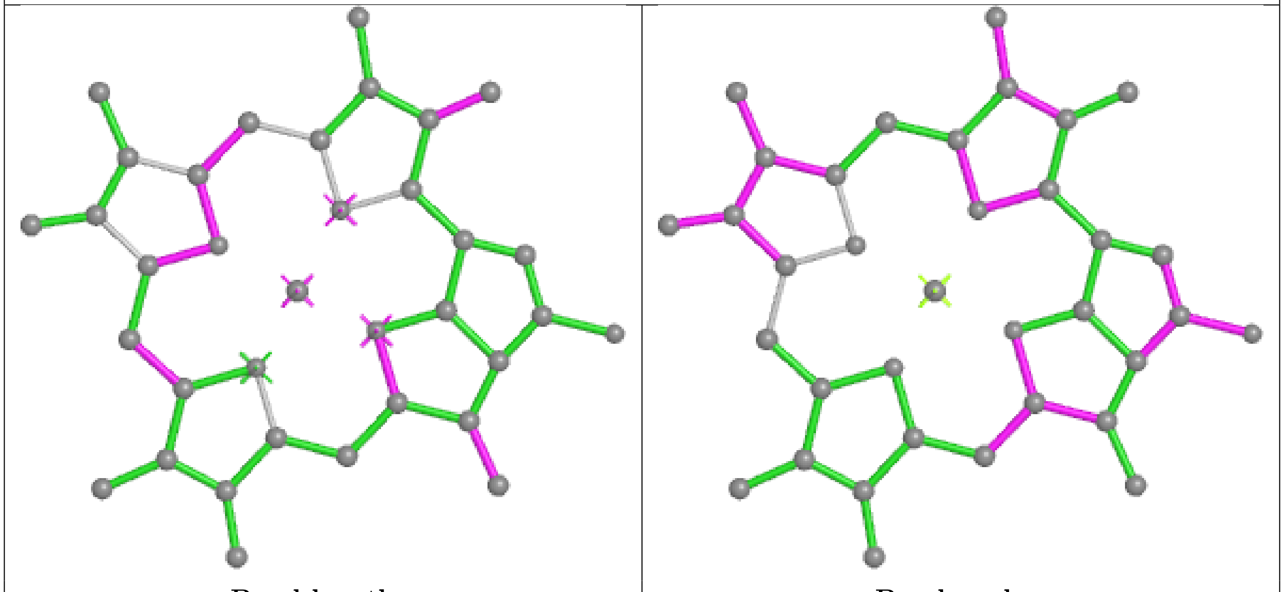
Bond angles



Torsions

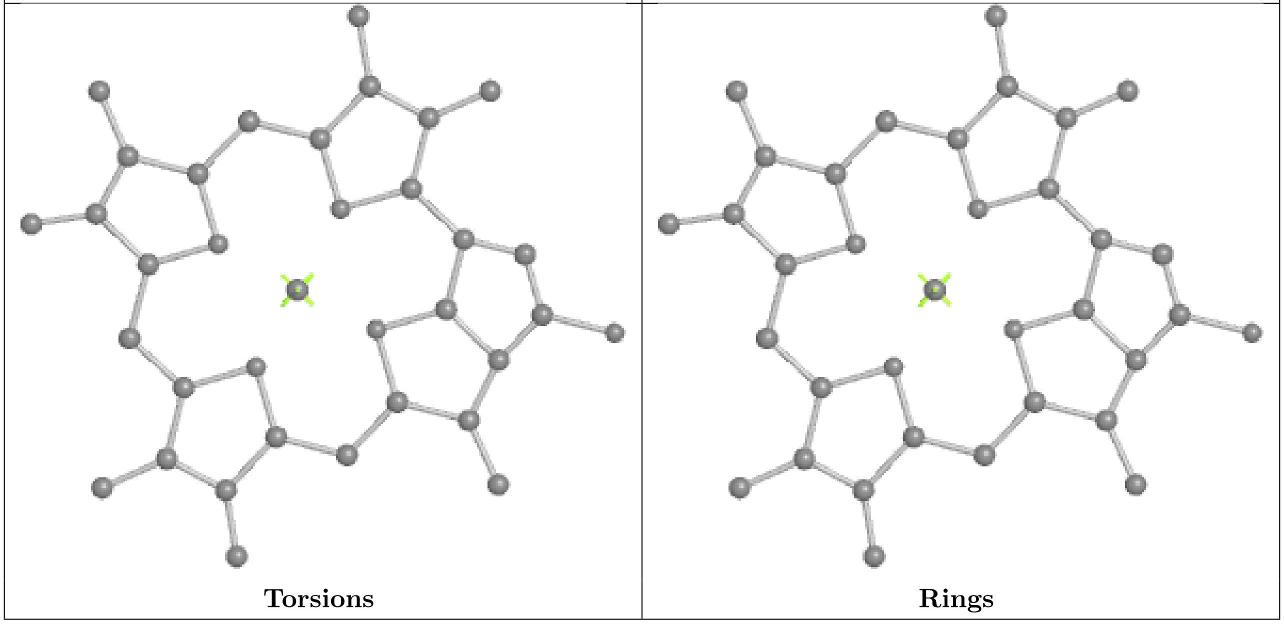
Rings

Ligand CLA M 1088



Bond lengths

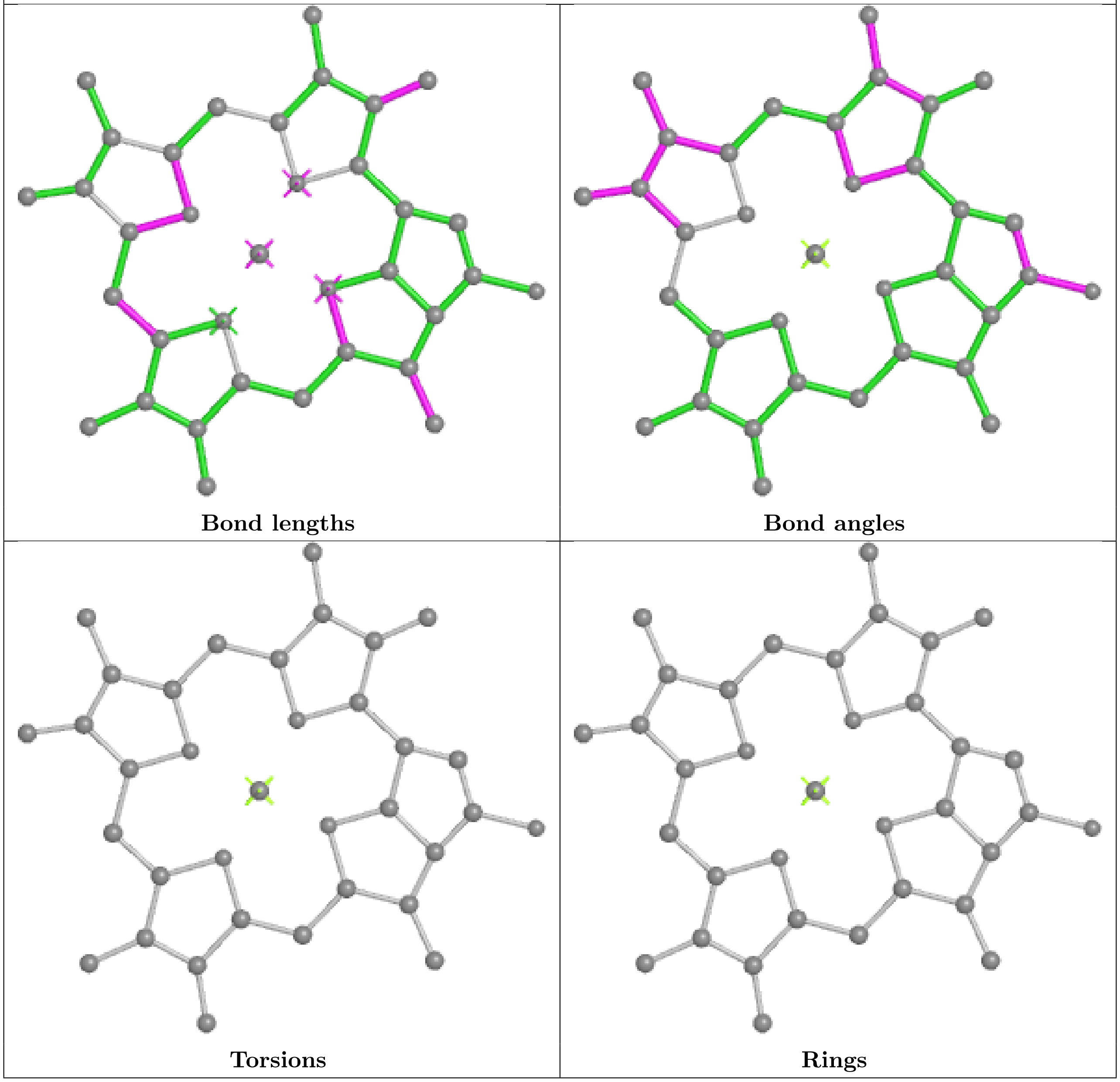
Bond angles



Torsions

Rings

Ligand CLA C 1078



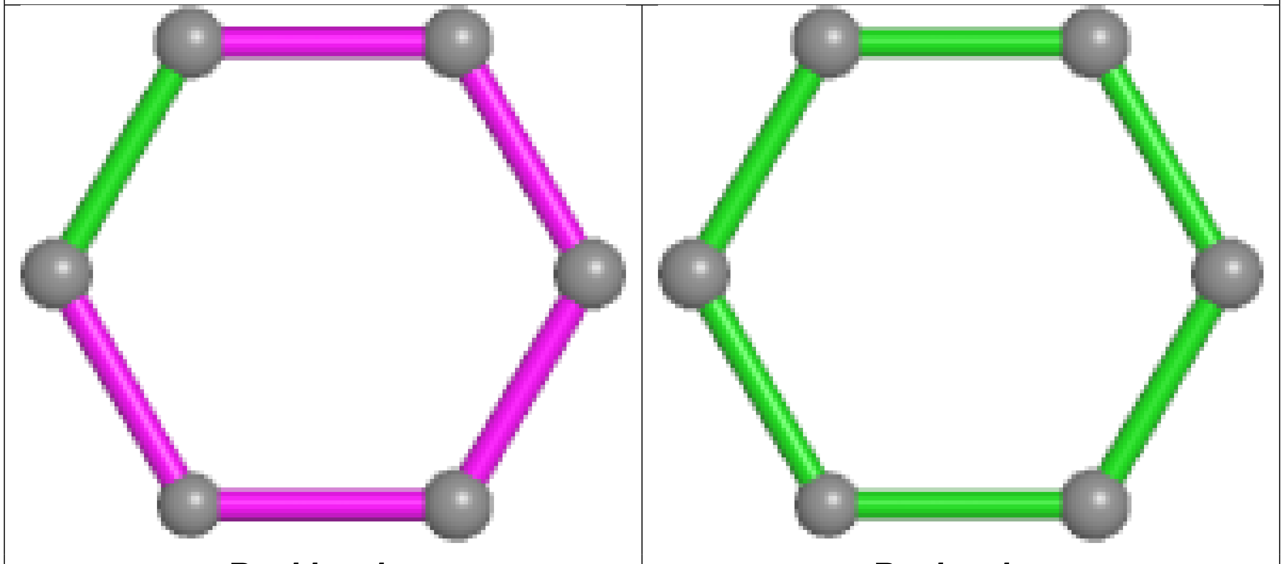
Bond lengths

Bond angles

Torsions

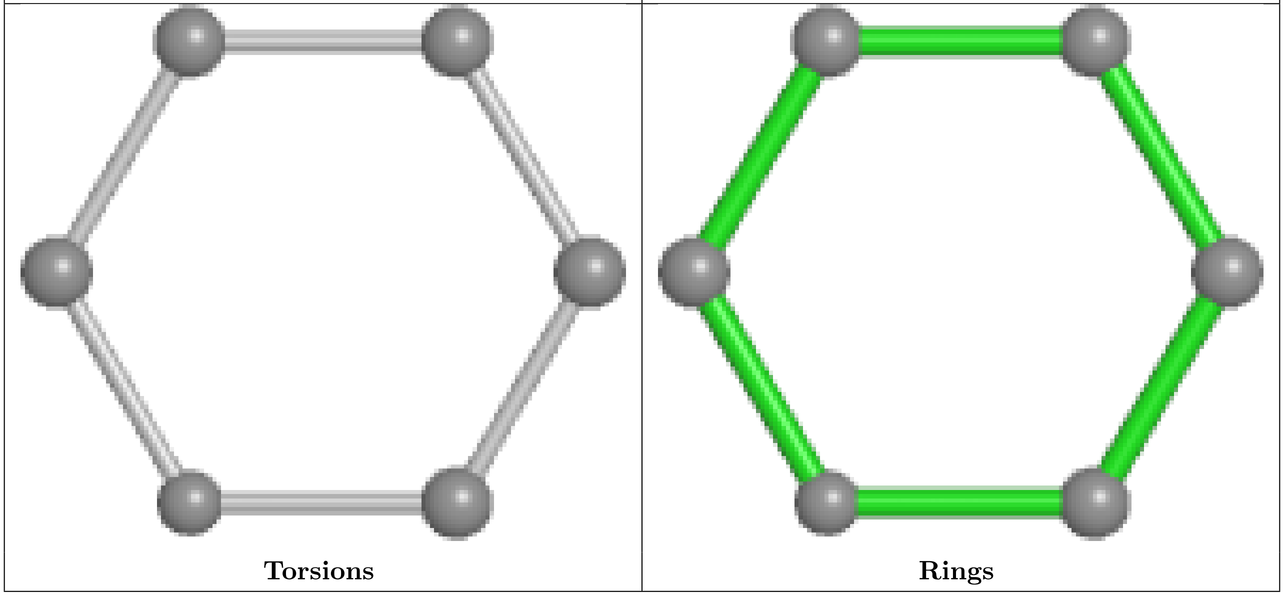
Rings

Ligand PLA D 358



Bond lengths

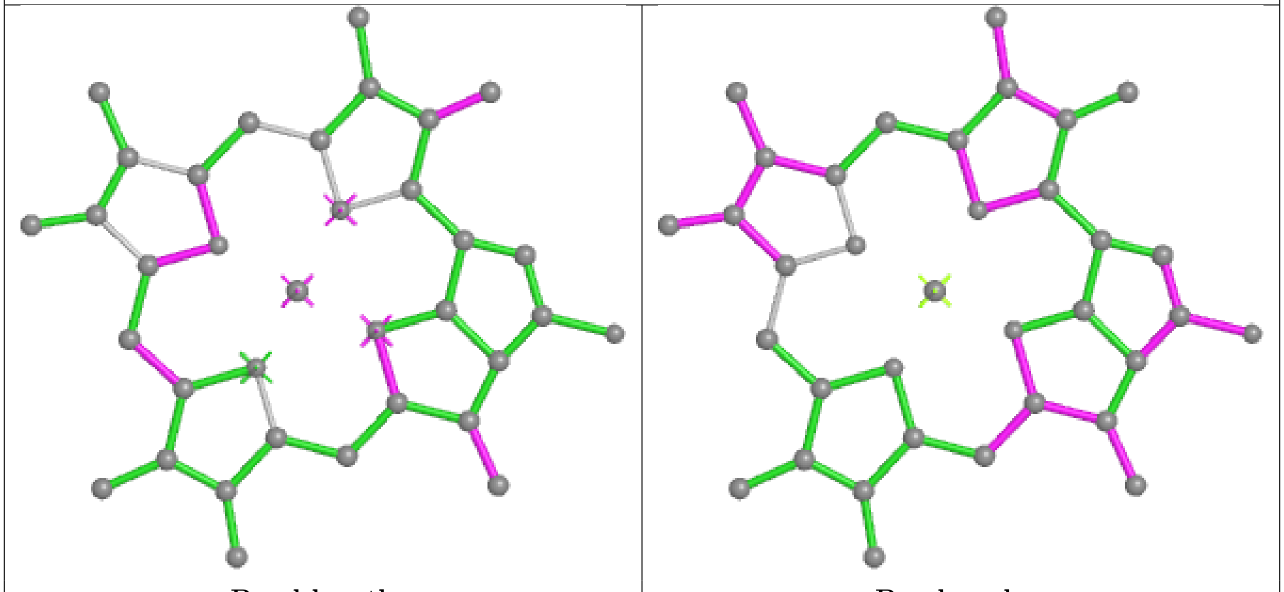
Bond angles



Torsions

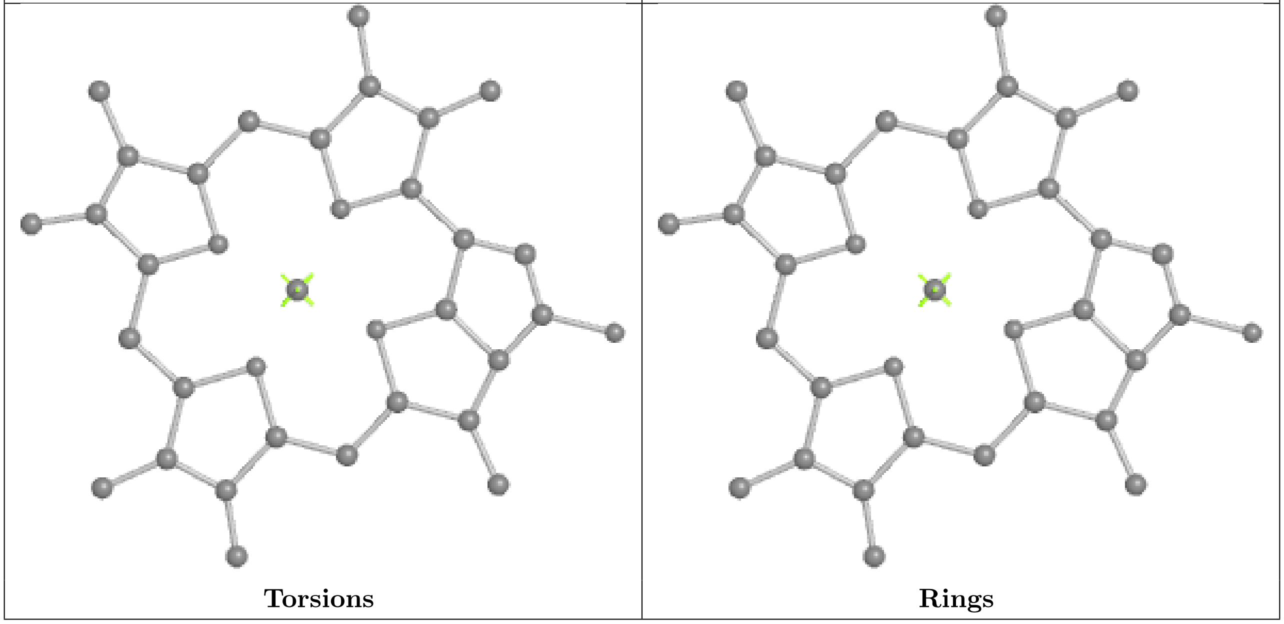
Rings

Ligand CLA L 1112



Bond lengths

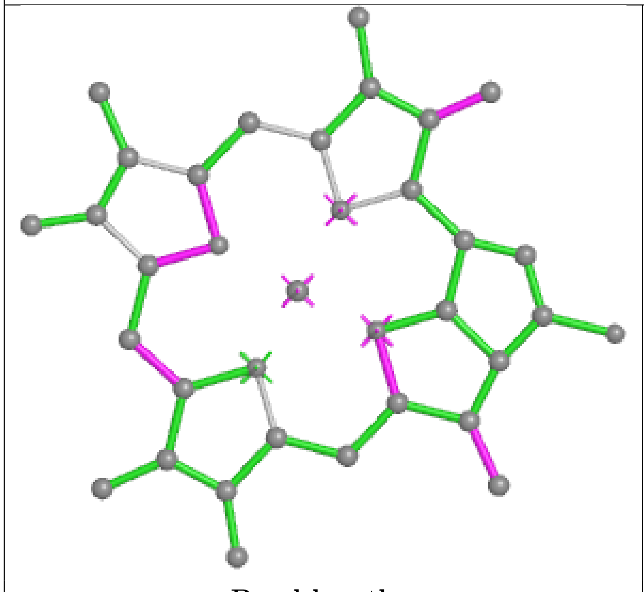
Bond angles



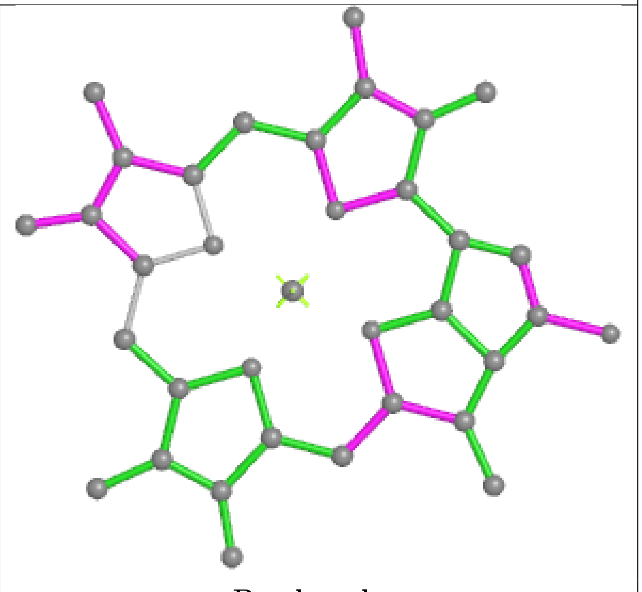
Torsions

Rings

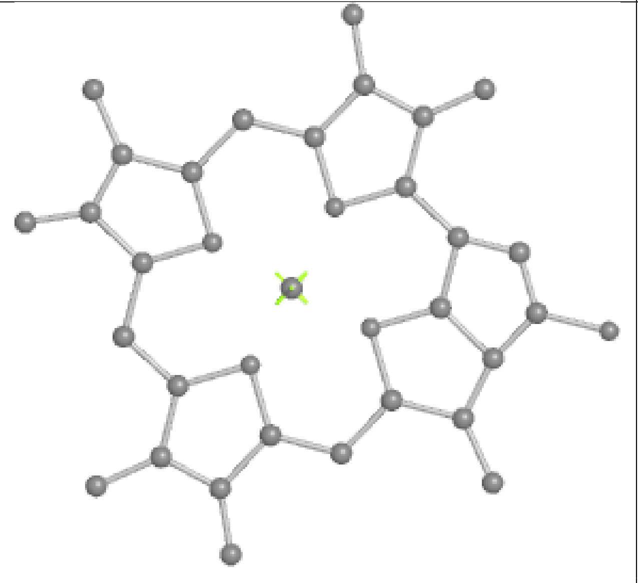
Ligand CLA L 1107



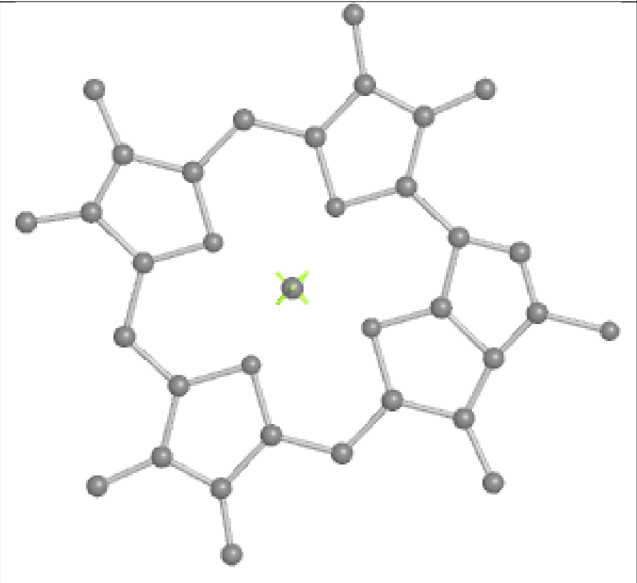
Bond lengths



Bond angles

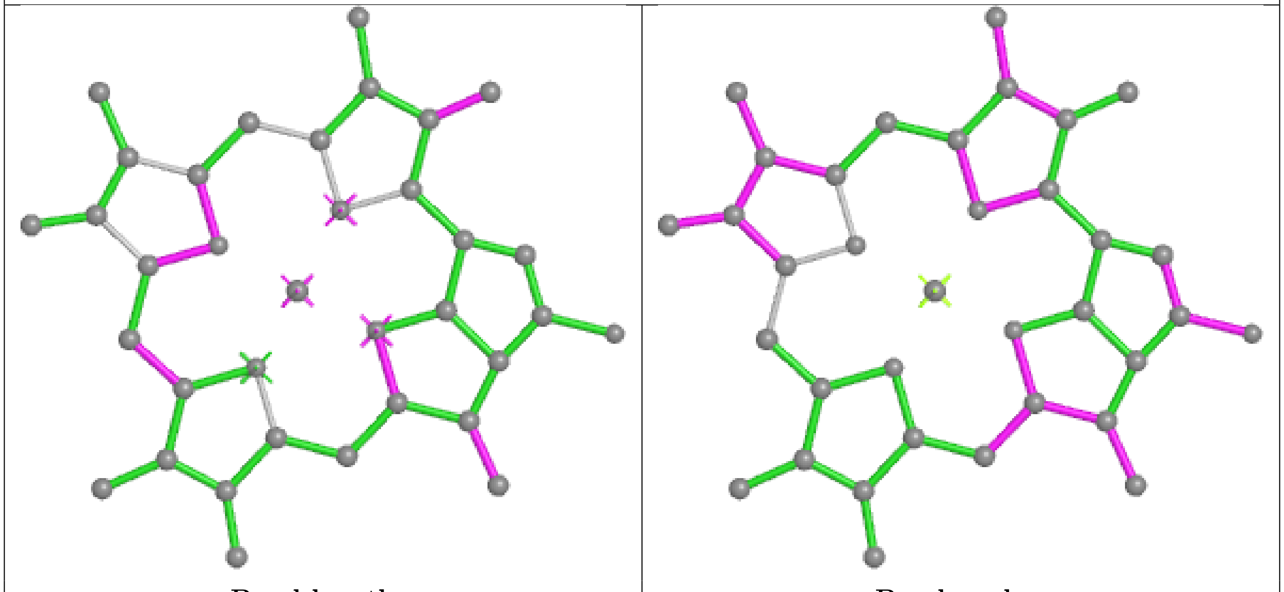


Torsions

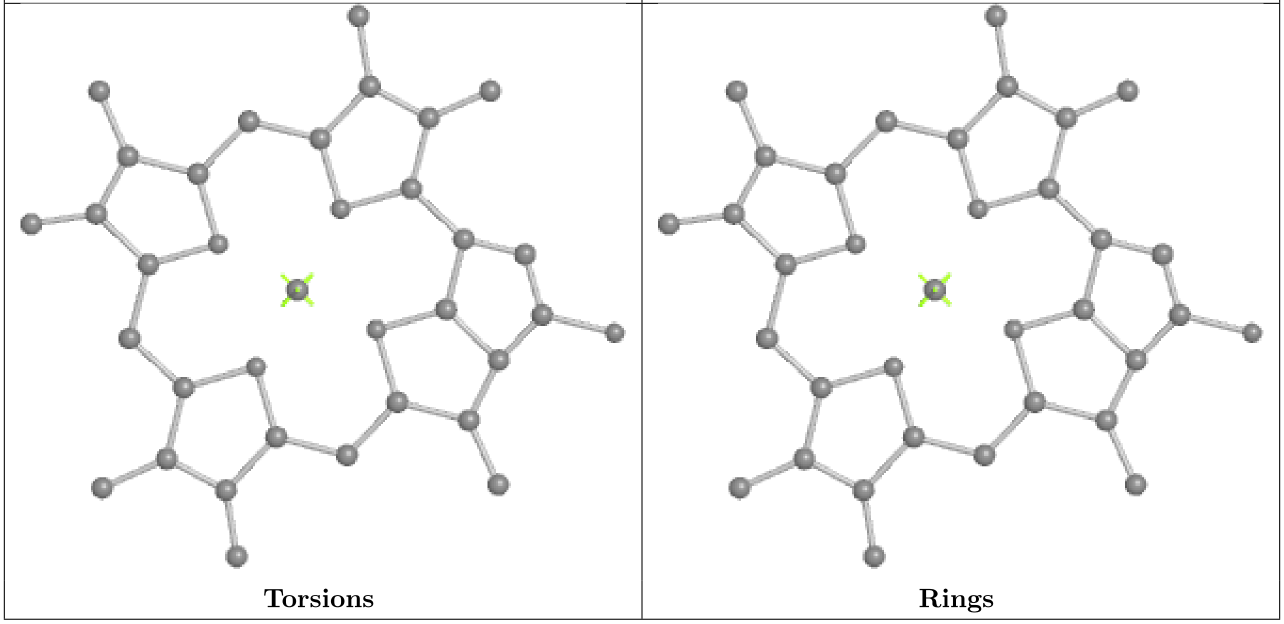


Rings

Ligand CLA L 1116

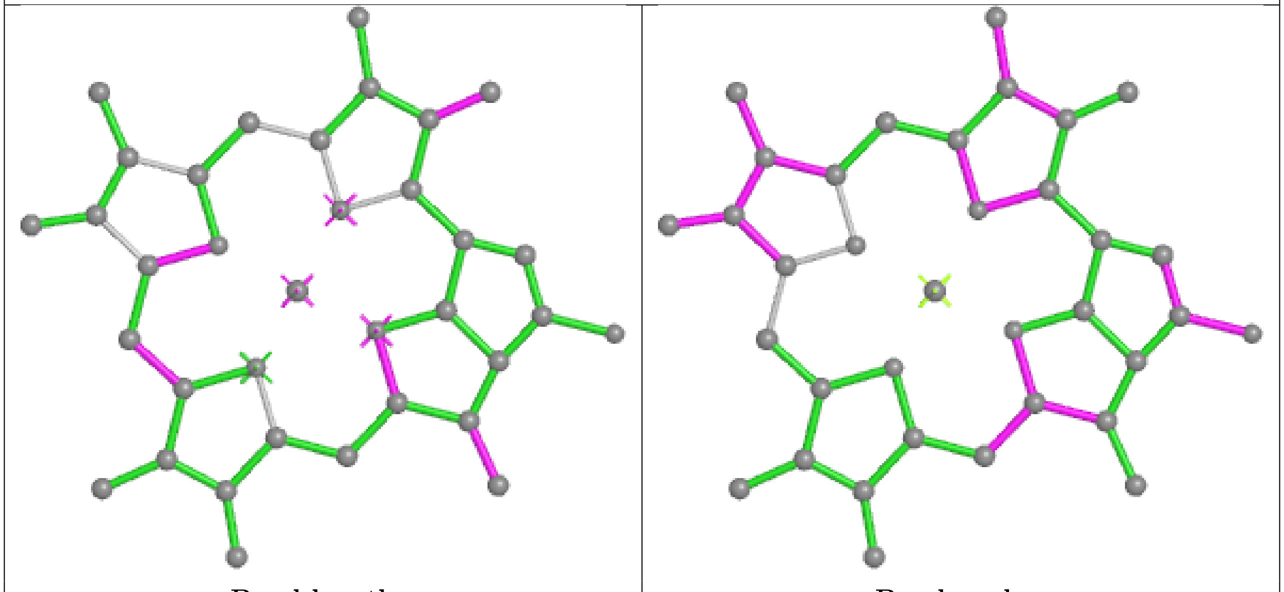


Bond lengths **Bond angles**



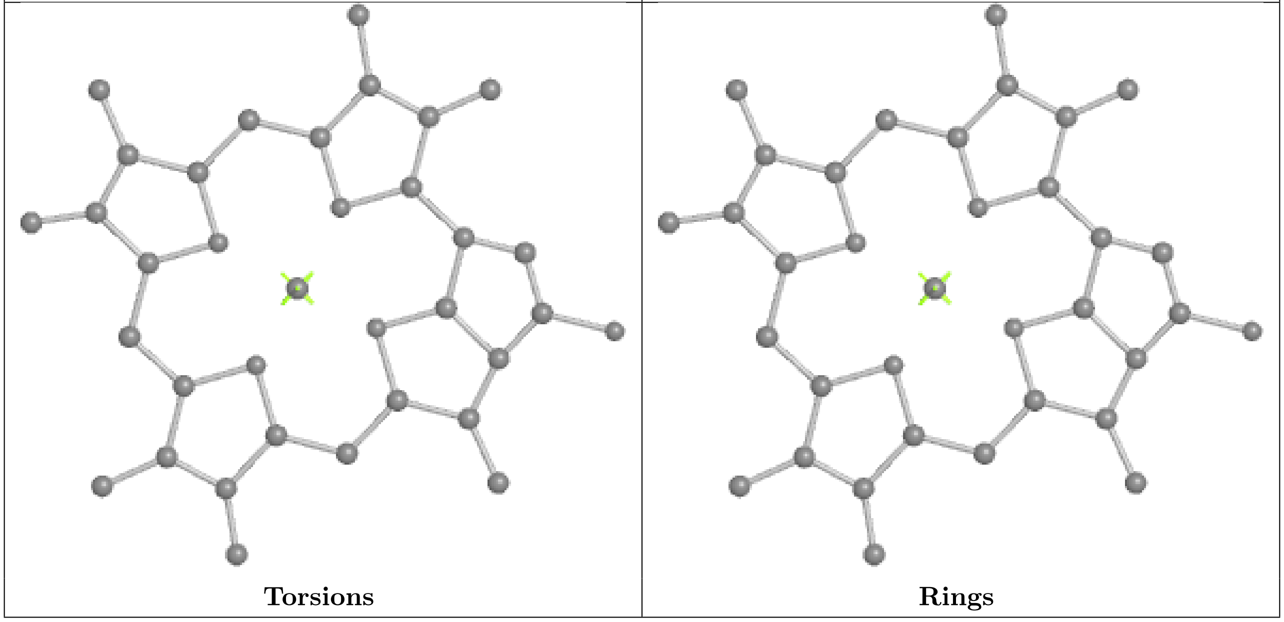
Torsions **Rings**

Ligand CLA B 1122



Bond lengths

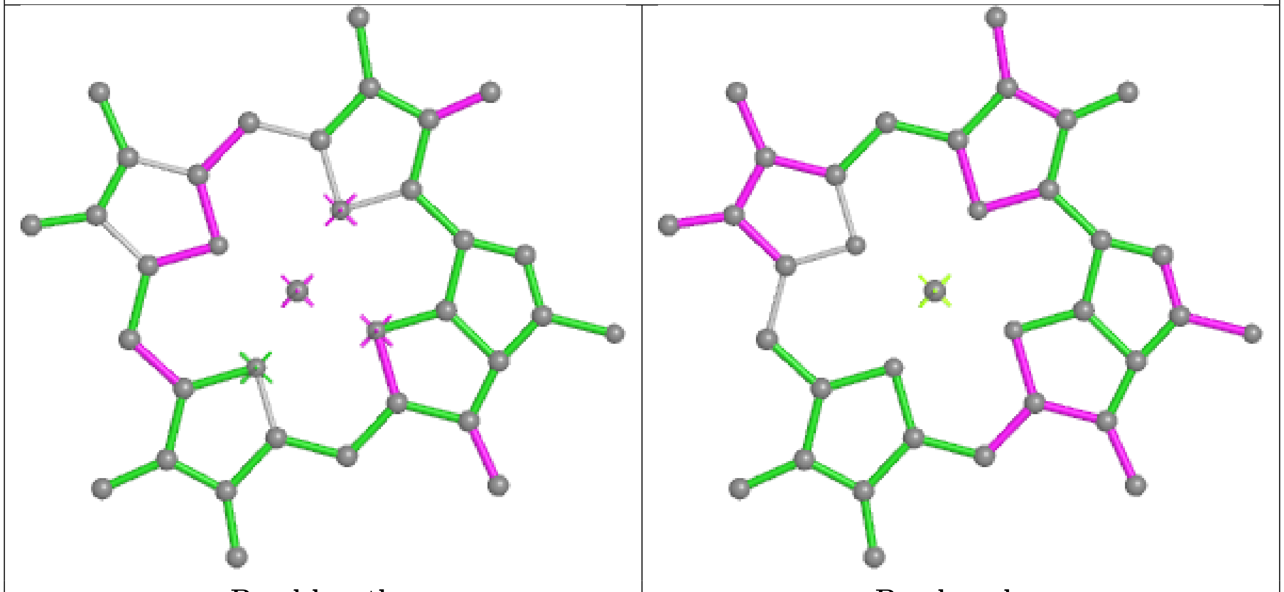
Bond angles



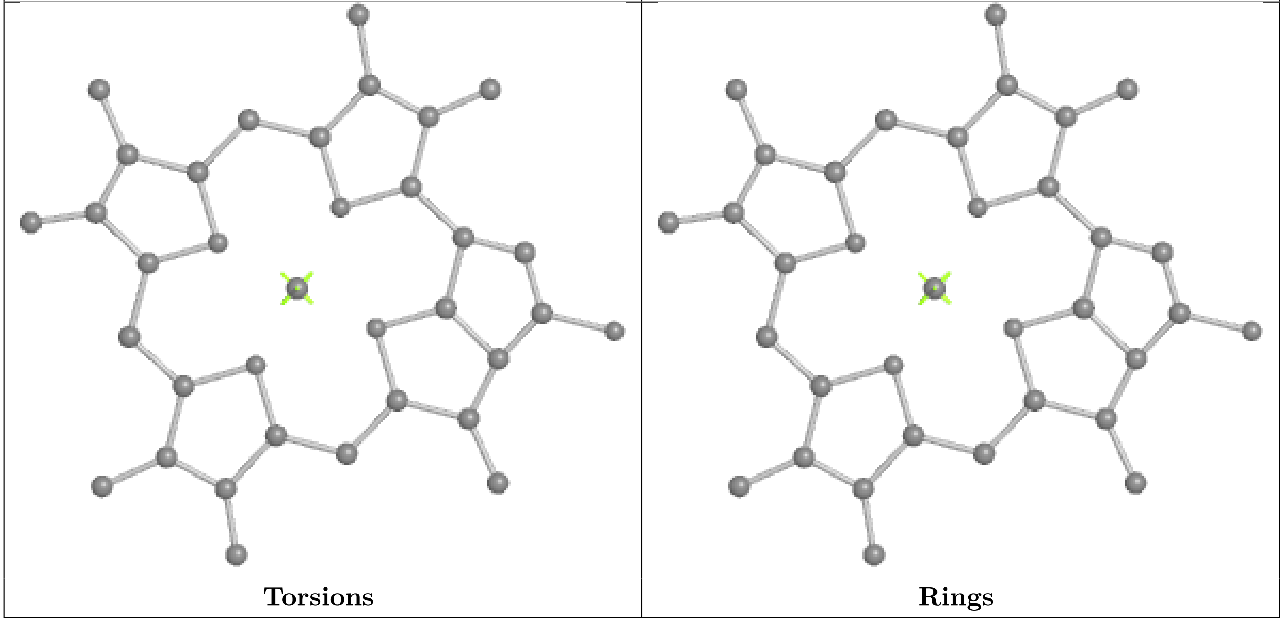
Torsions

Rings

Ligand CLA C 1088

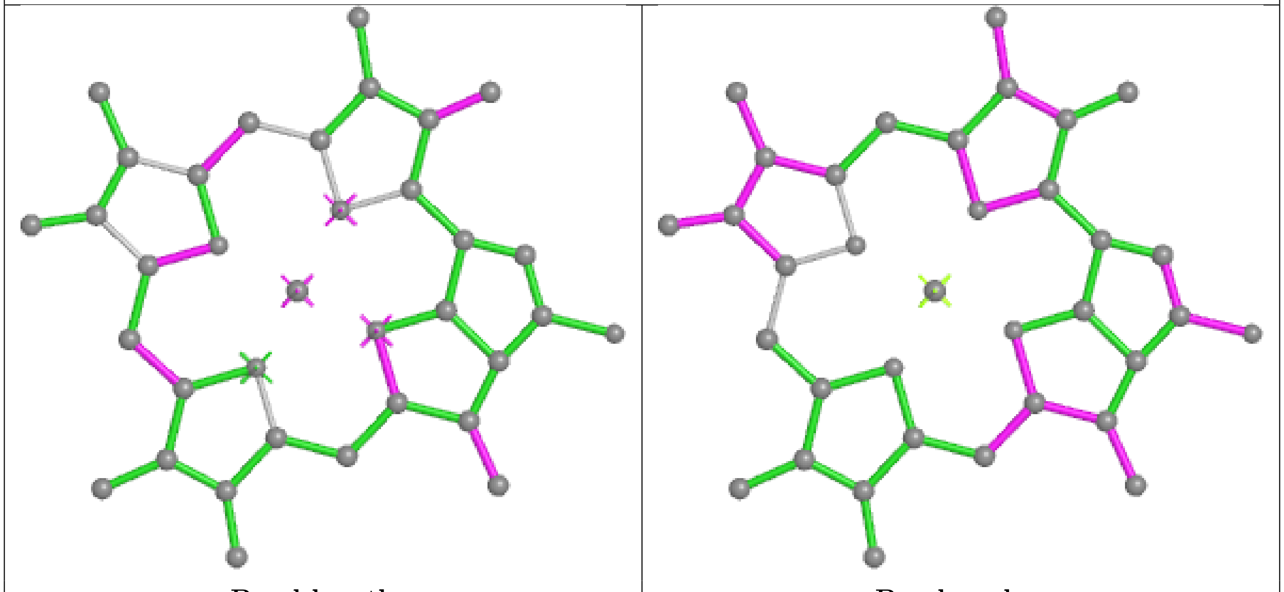


Bond lengths **Bond angles**



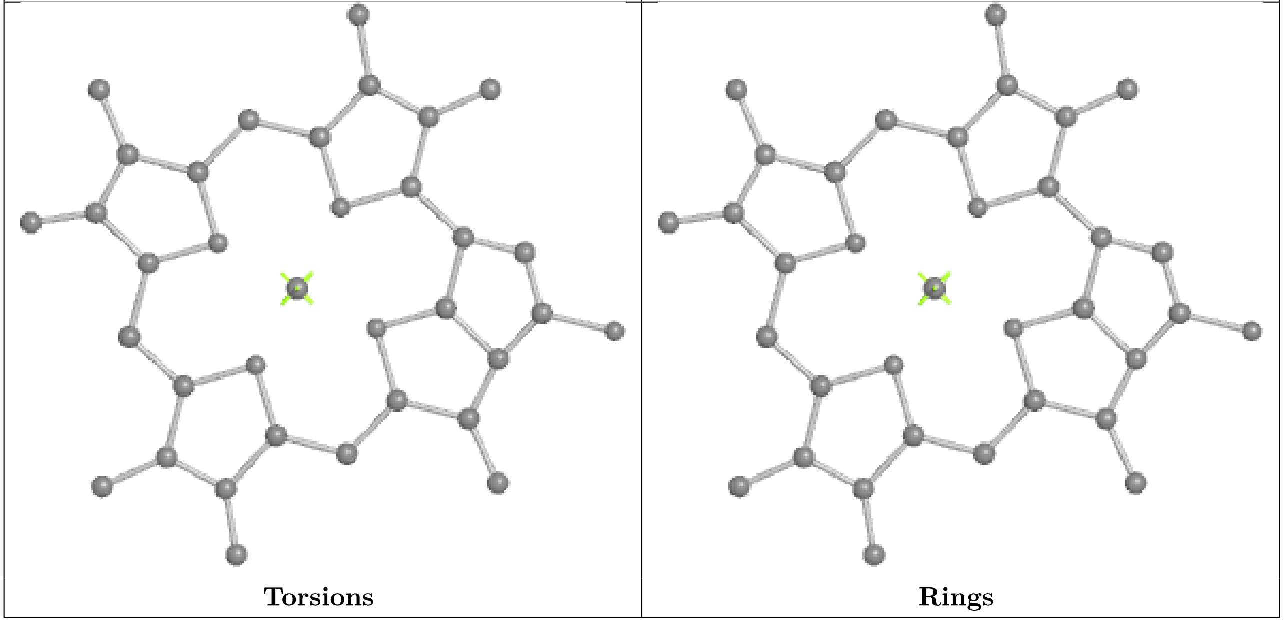
Torsions **Rings**

Ligand CLA L 1119



Bond lengths

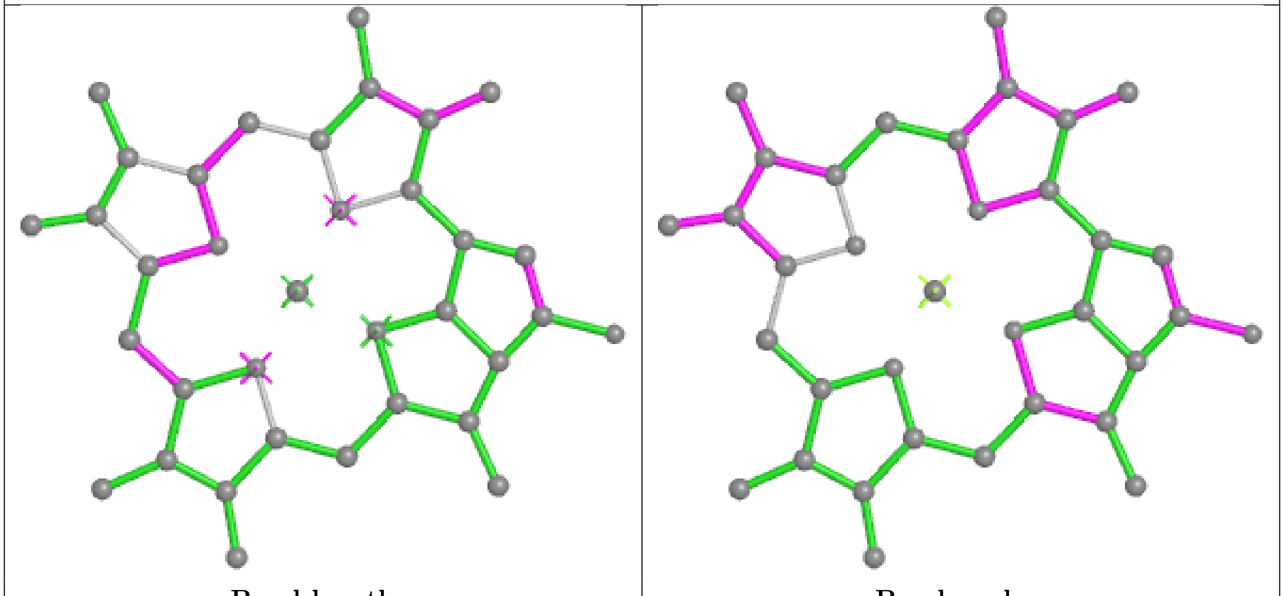
Bond angles



Torsions

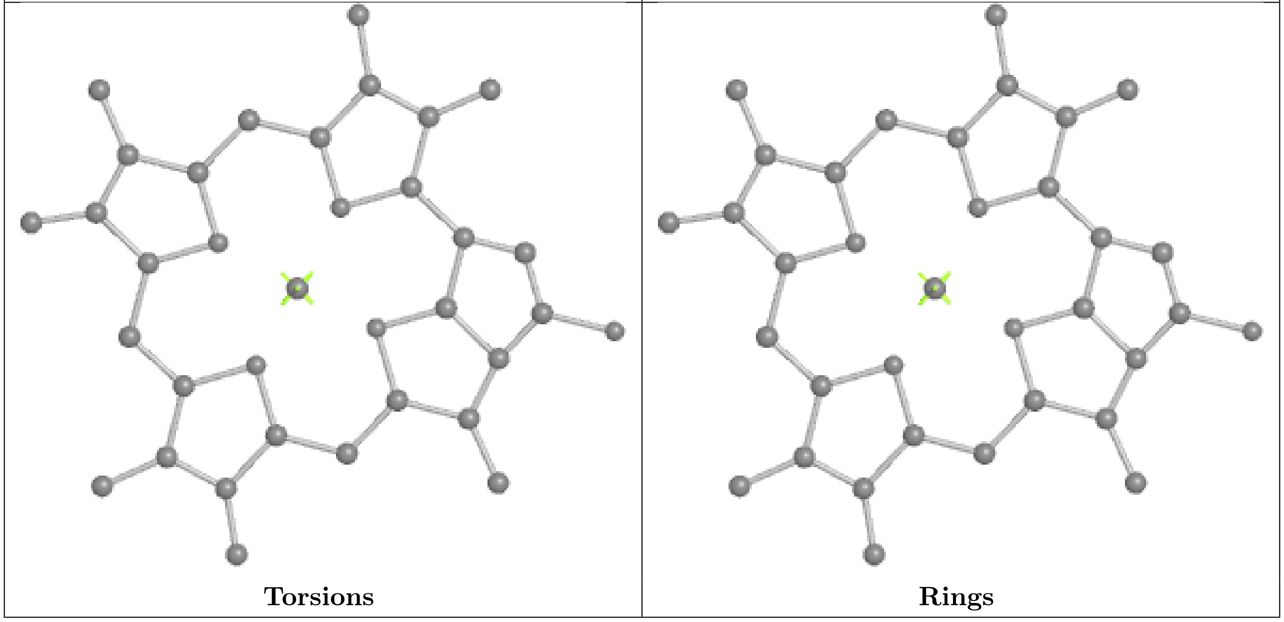
Rings

Ligand CLA N 354



Bond lengths

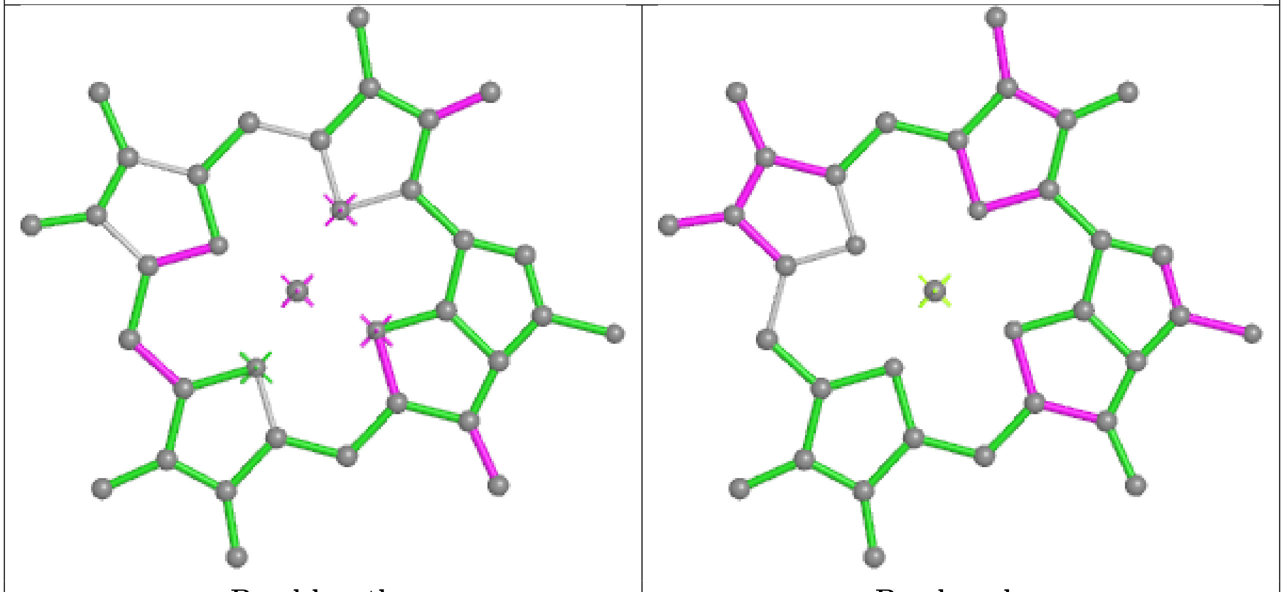
Bond angles



Torsions

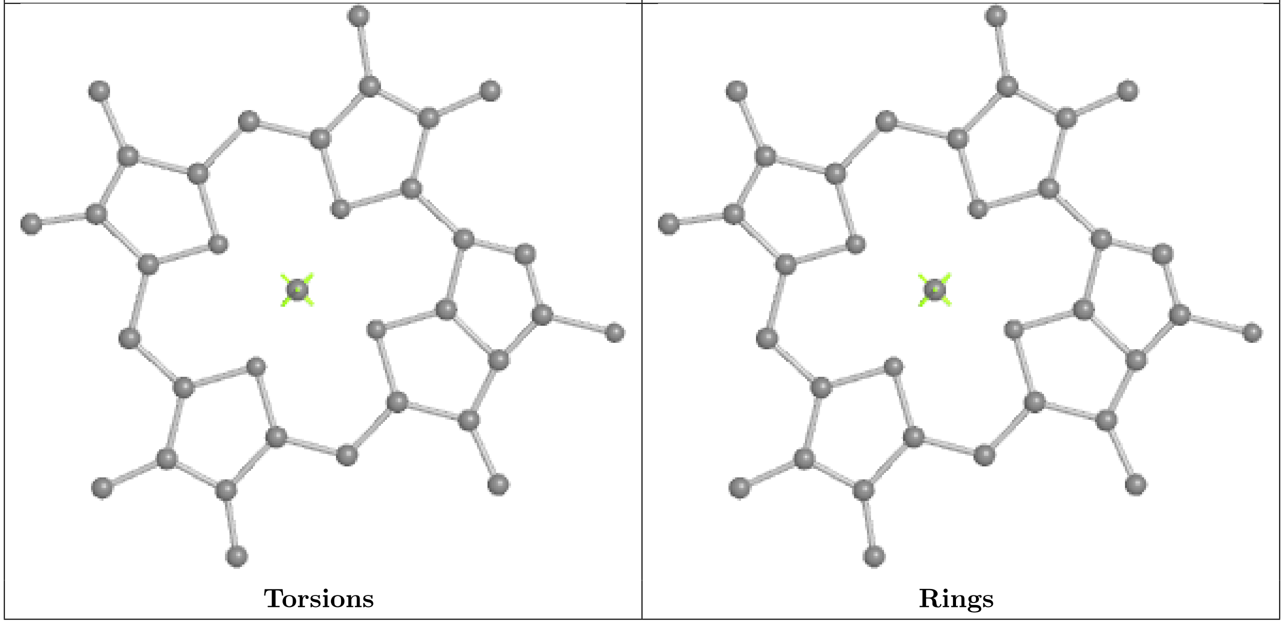
Rings

Ligand CLA M 1081



Bond lengths

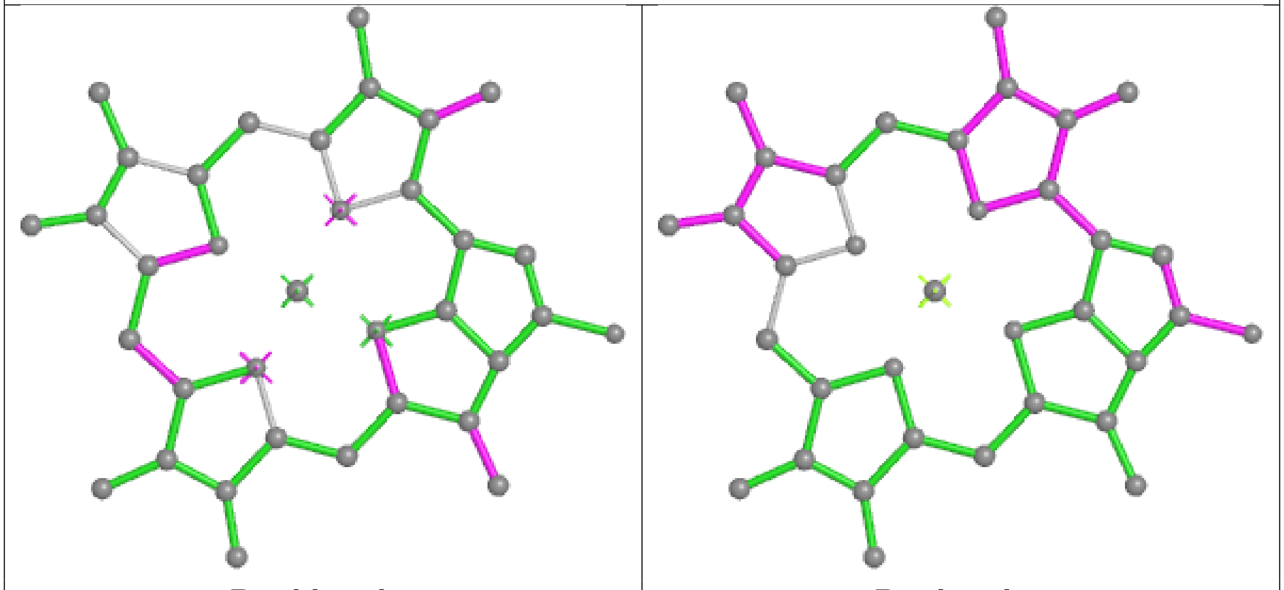
Bond angles



Torsions

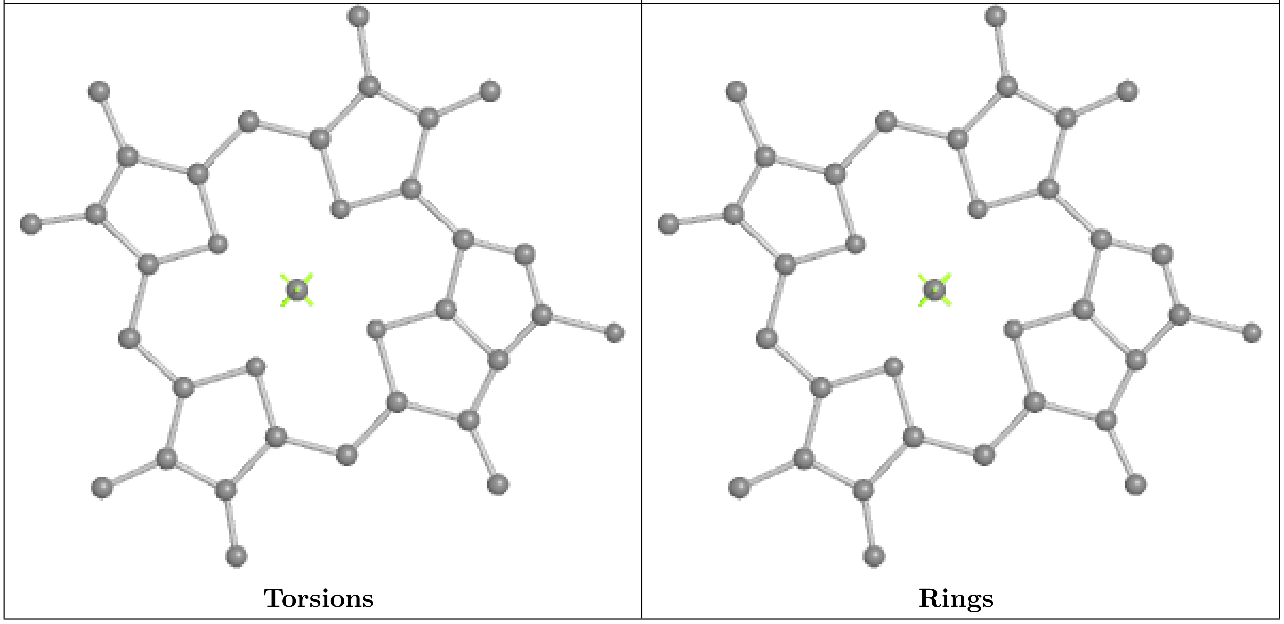
Rings

Ligand CLA N 356



Bond lengths

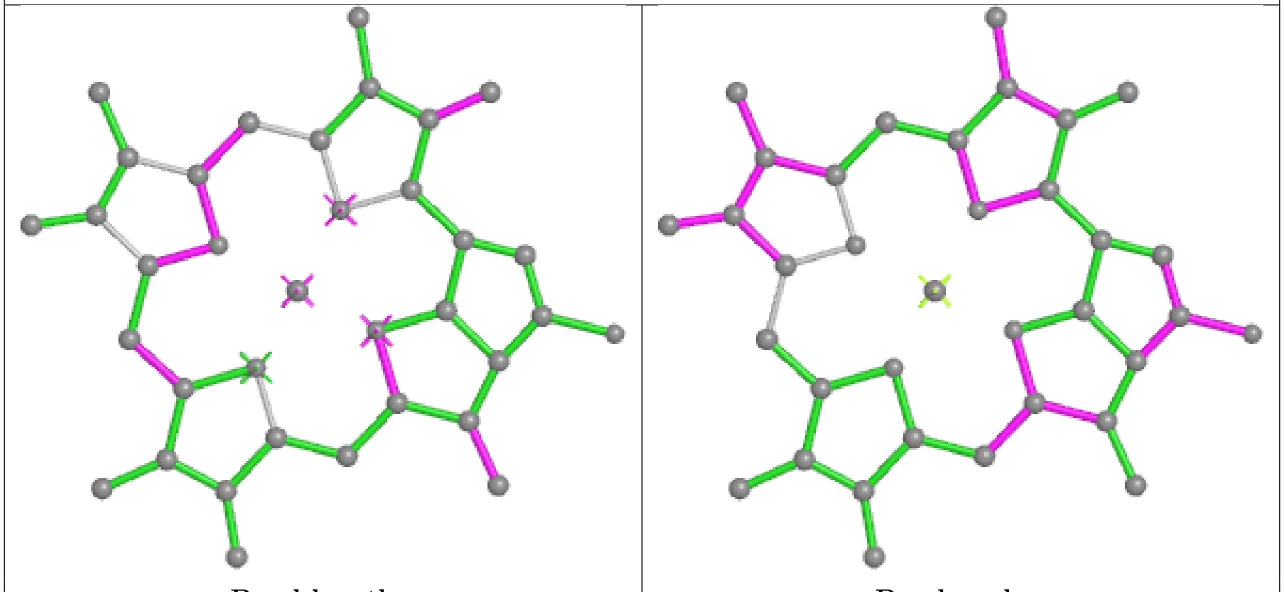
Bond angles



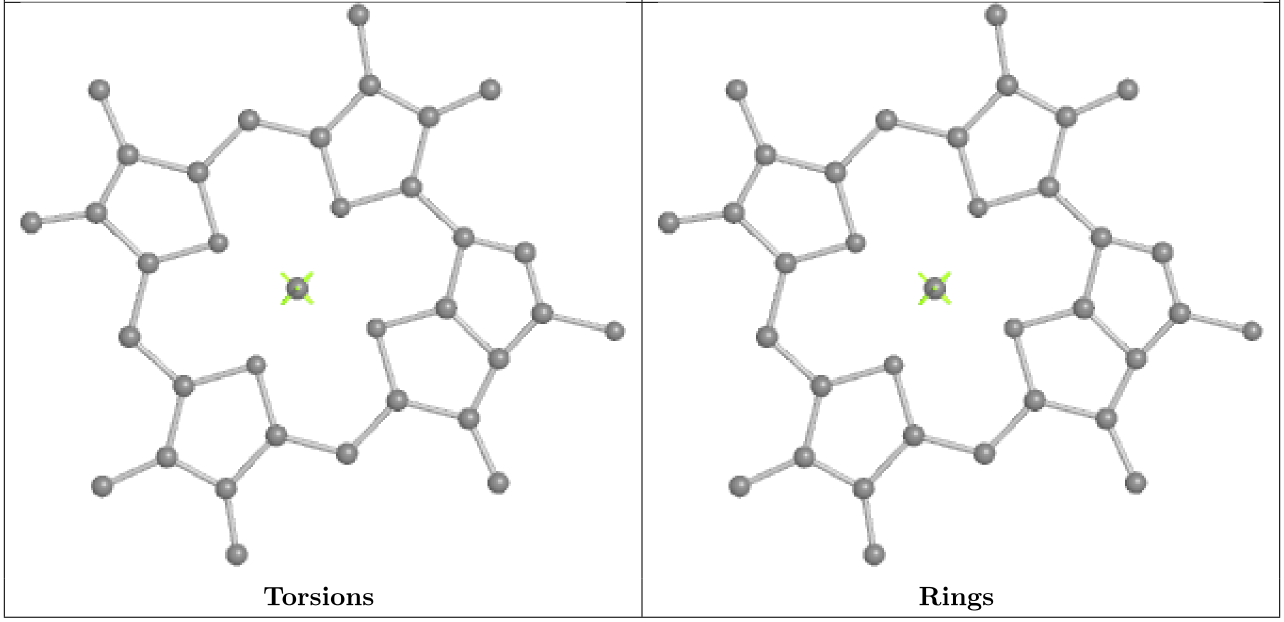
Torsions

Rings

Ligand CLA W 64

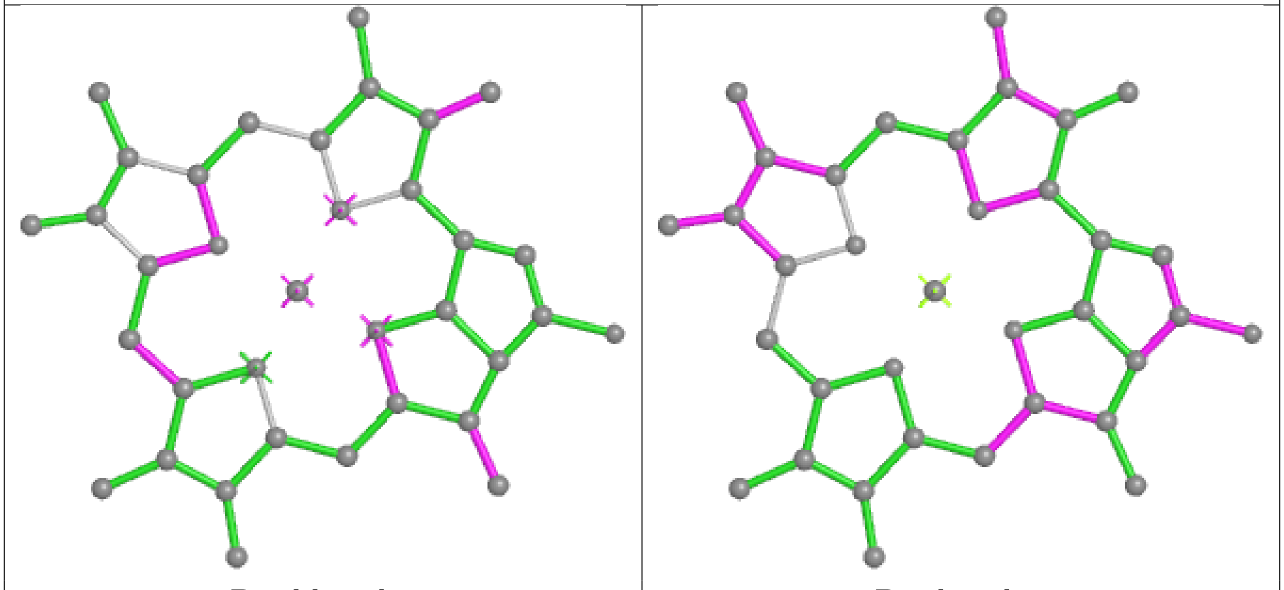


Bond lengths **Bond angles**

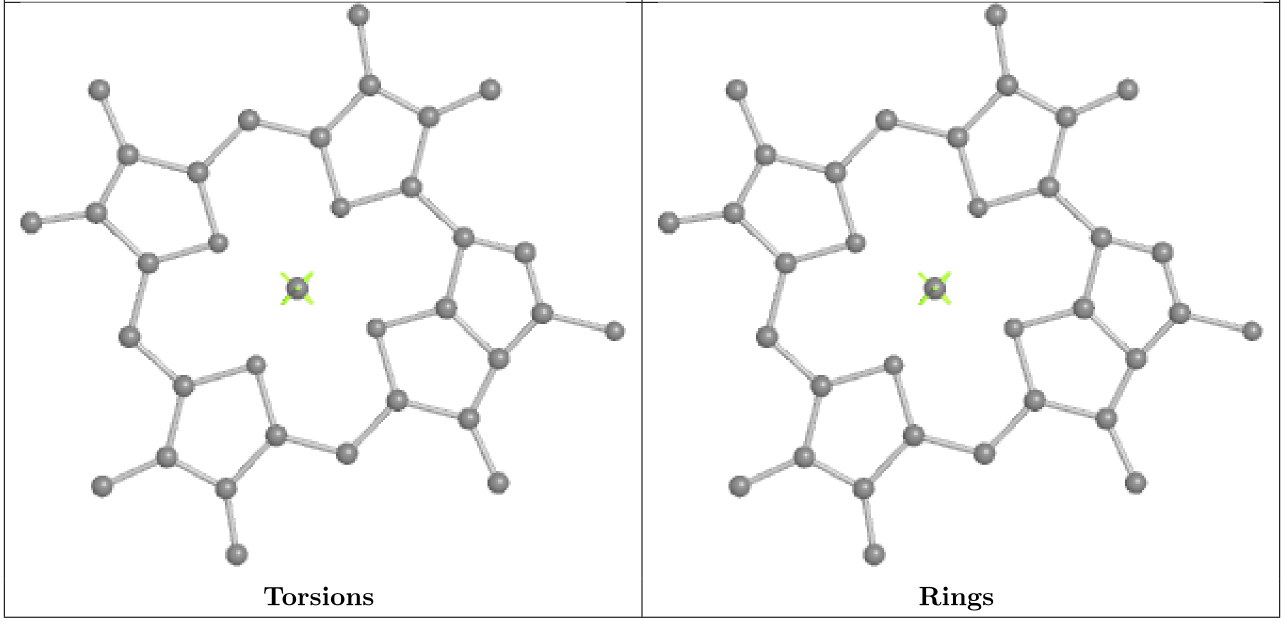


Torsions **Rings**

Ligand CLA L 1115

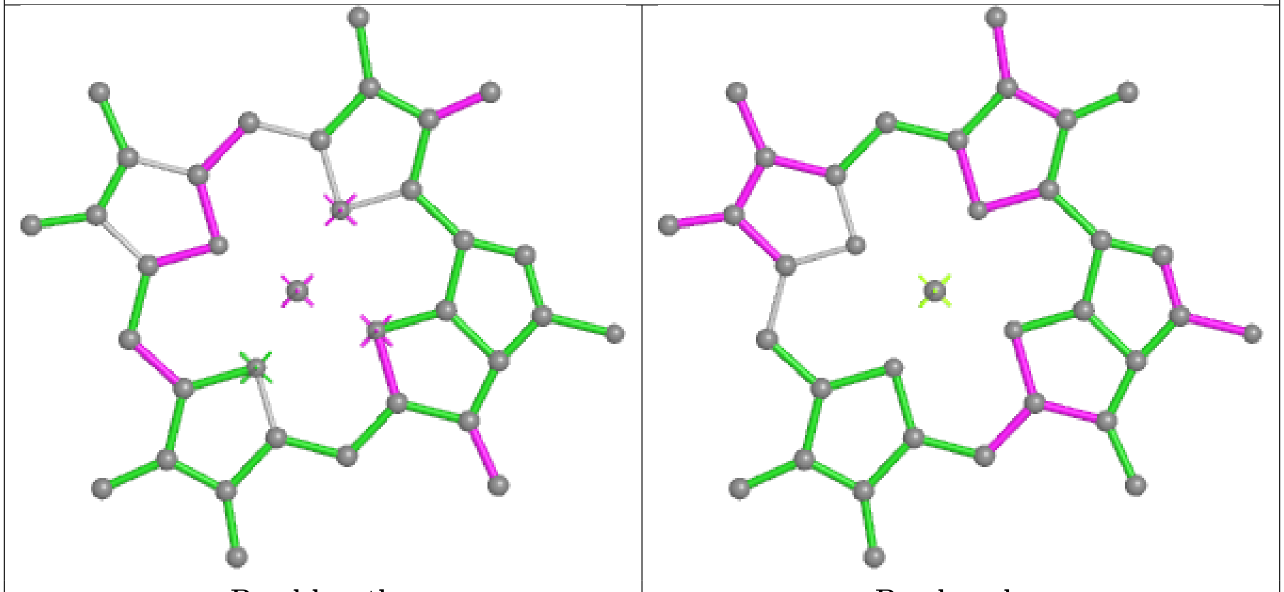


Bond lengths **Bond angles**

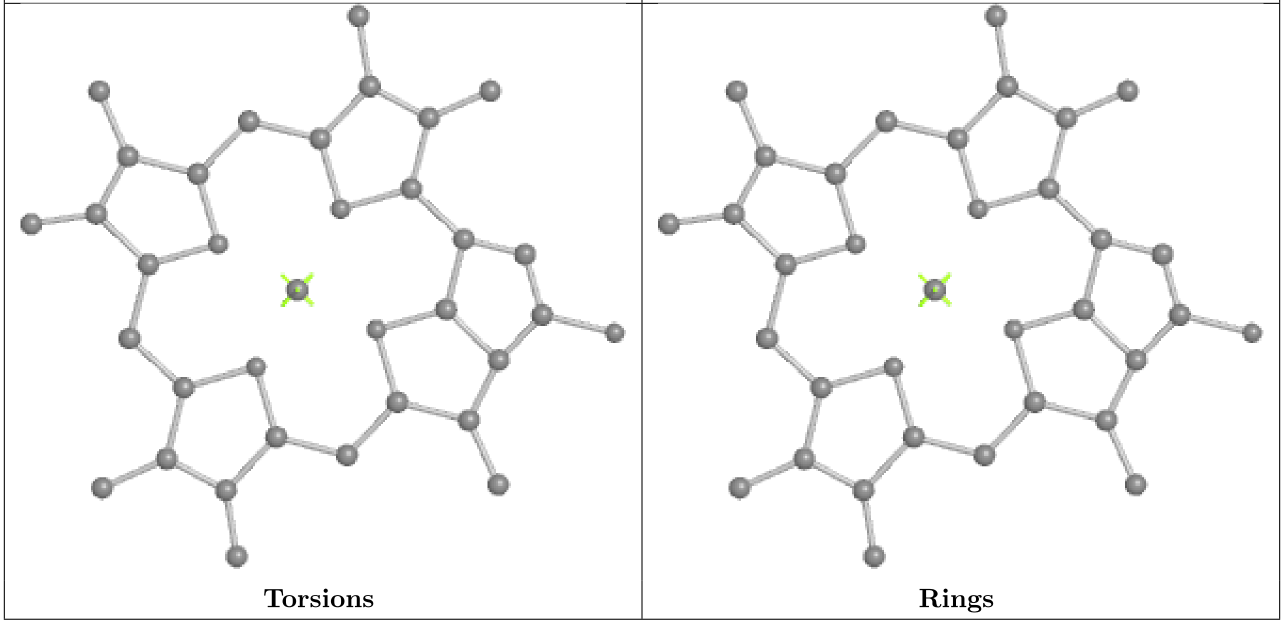


Torsions **Rings**

Ligand CLA B 1118

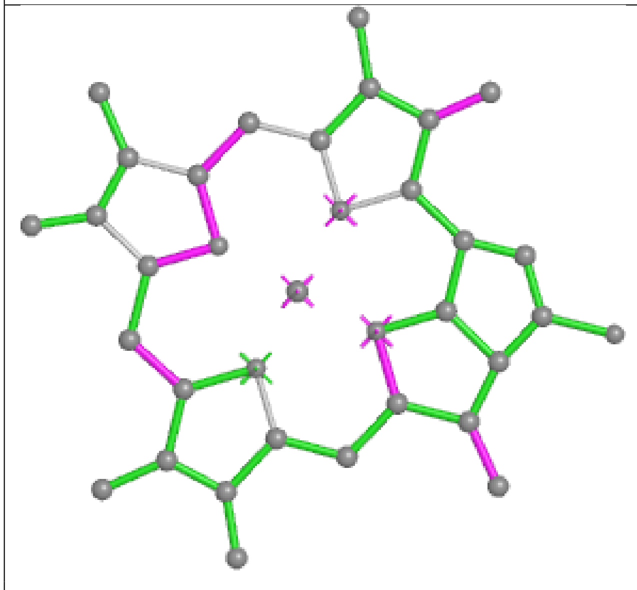


Bond lengths **Bond angles**

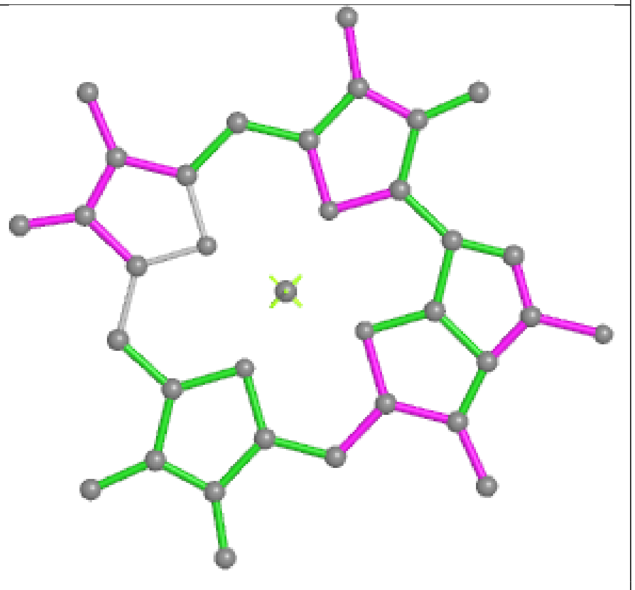


Torsions **Rings**

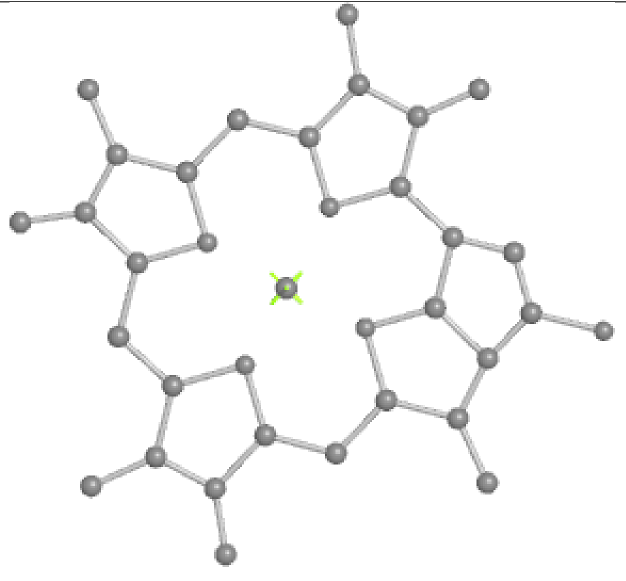
Ligand CLA C 1080



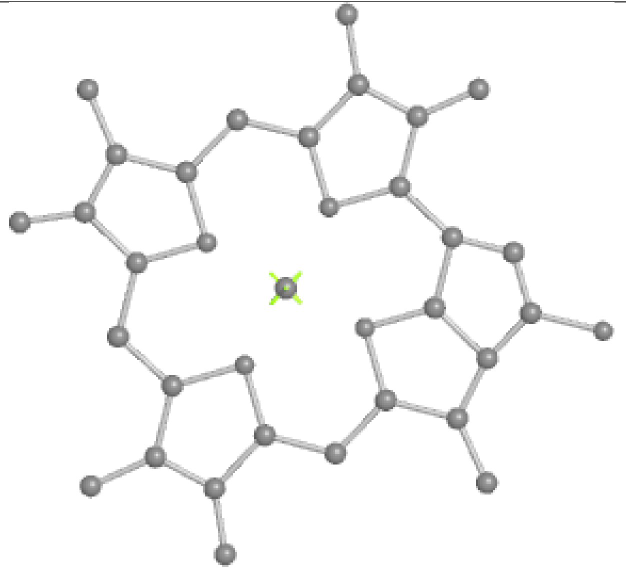
Bond lengths



Bond angles

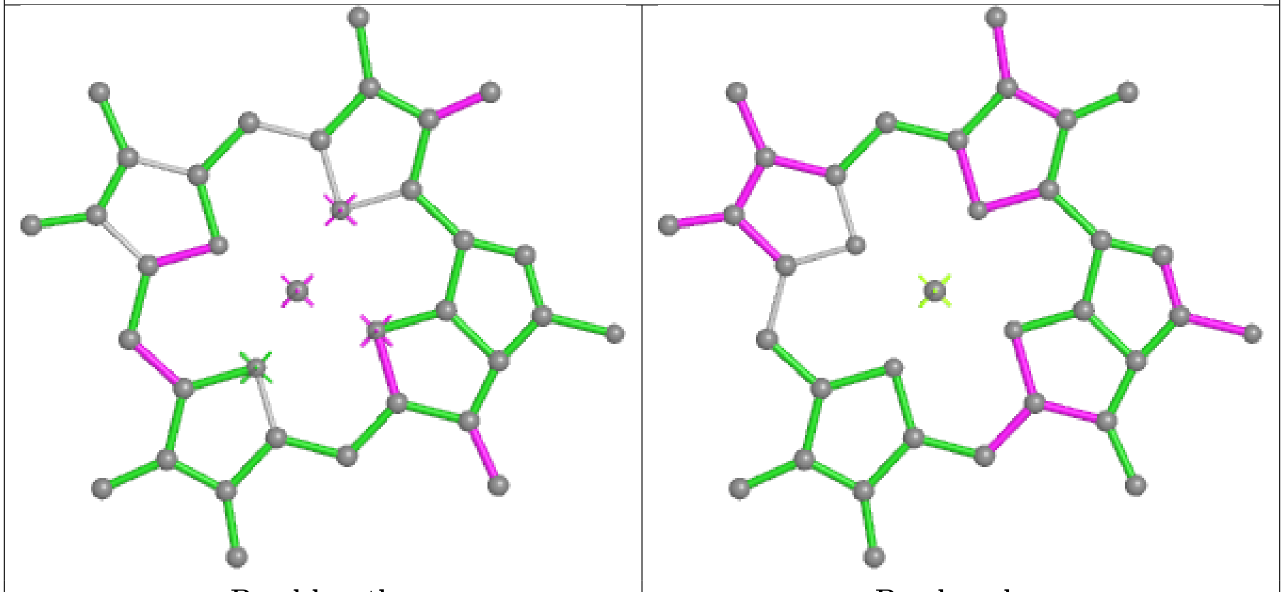


Torsions



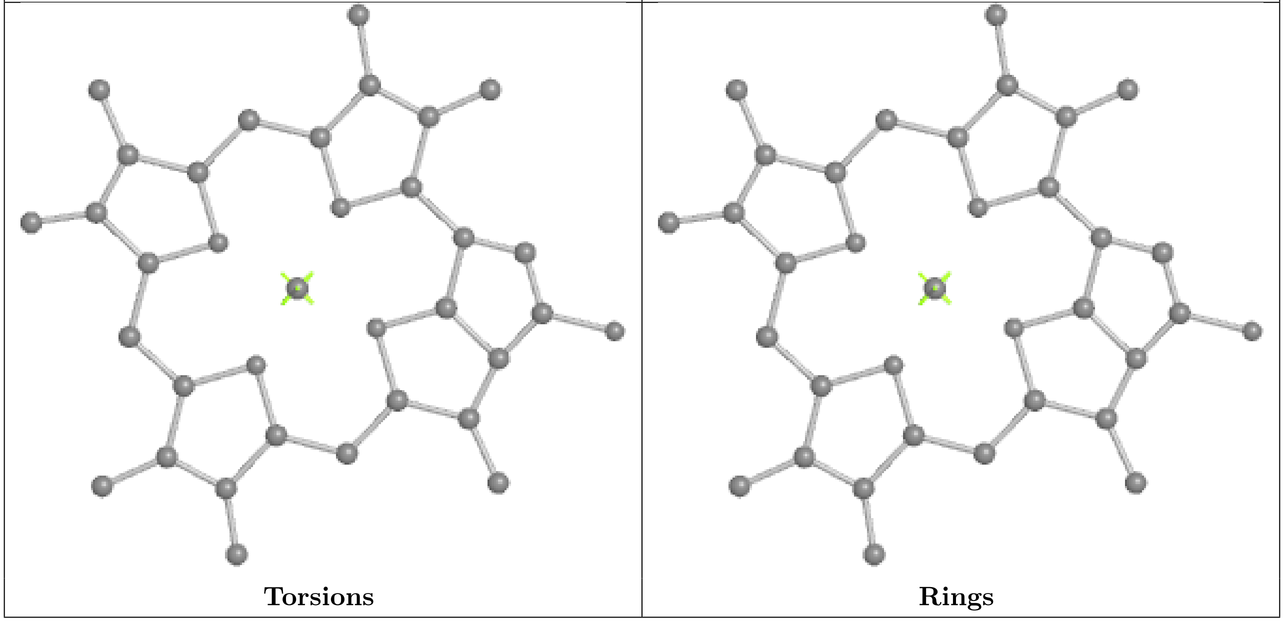
Rings

Ligand CLA M 1080



Bond lengths

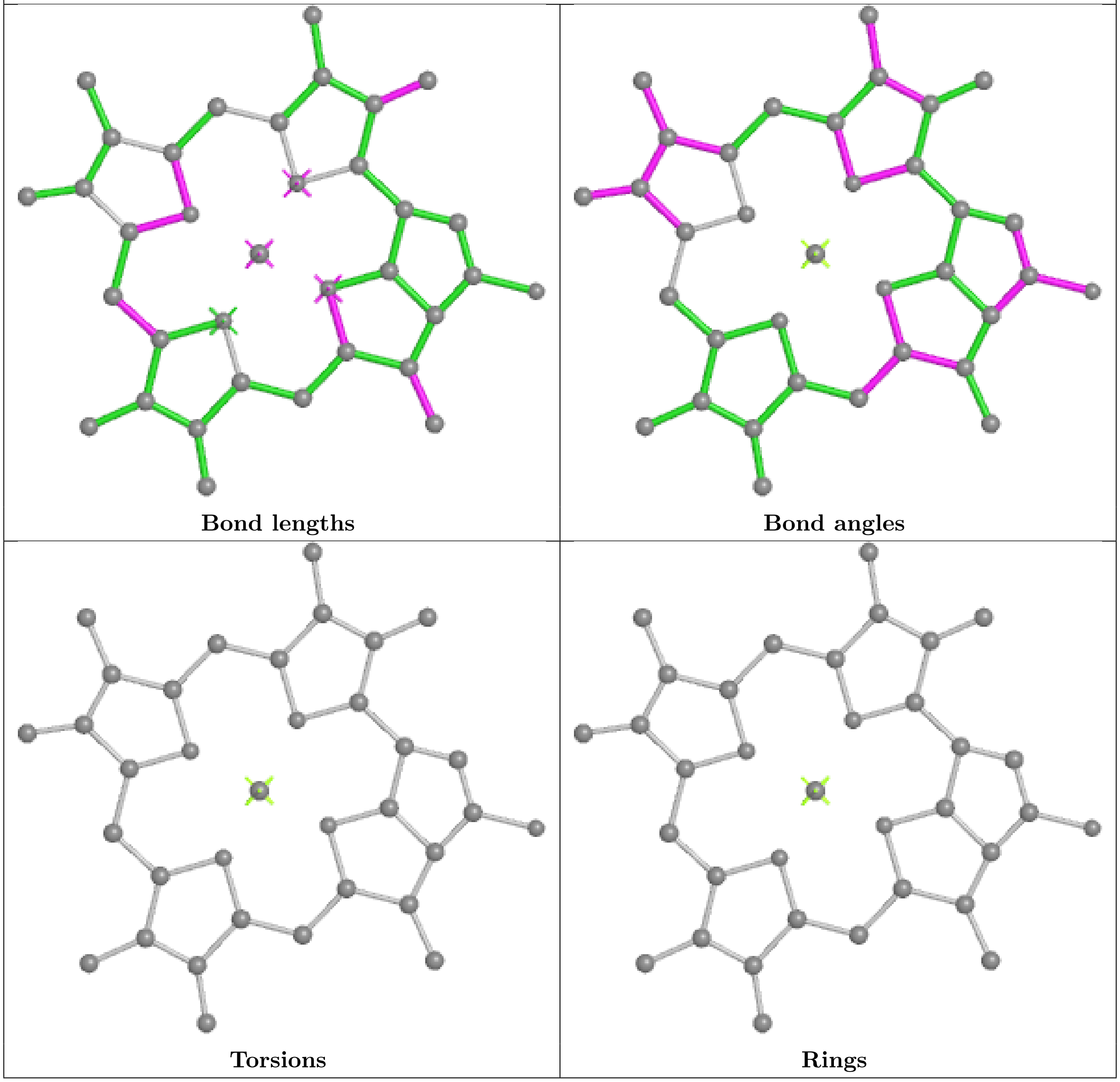
Bond angles



Torsions

Rings

Ligand CLA N 358



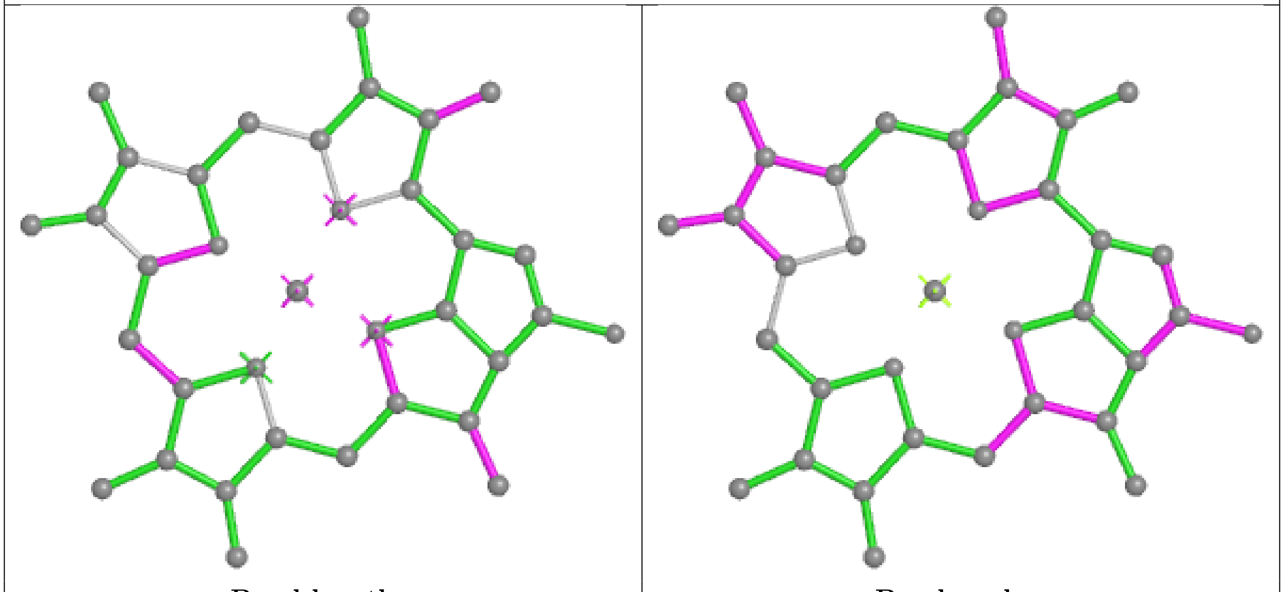
Bond lengths

Bond angles

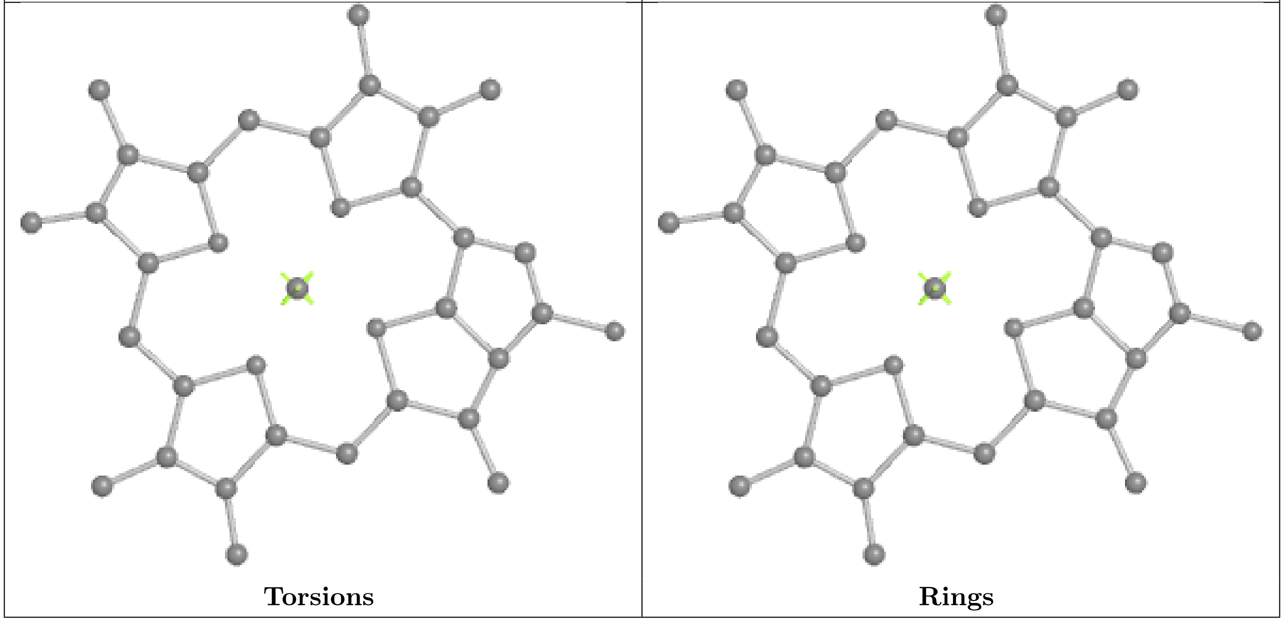
Torsions

Rings

Ligand CLA B 1121

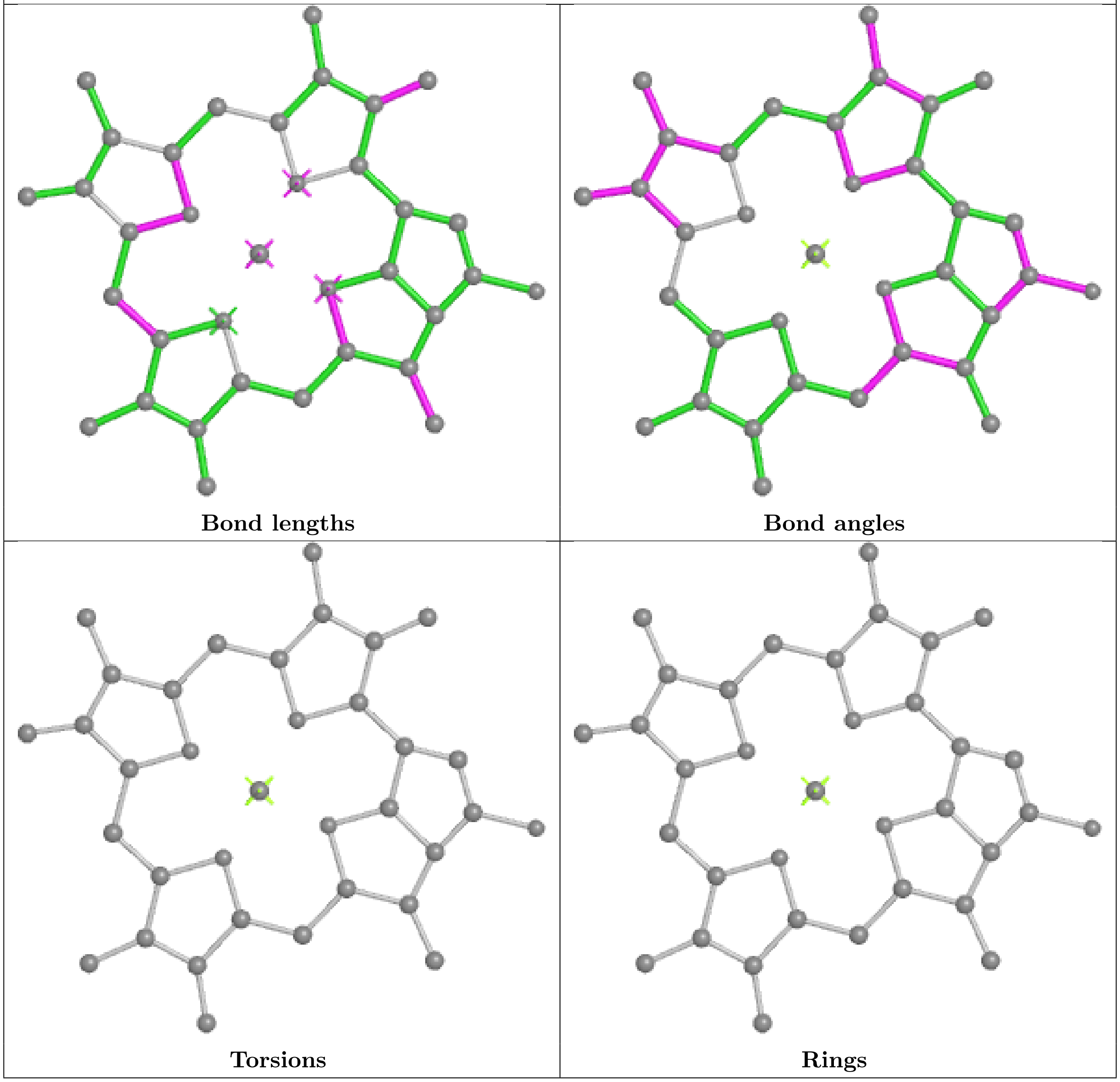


Bond lengths **Bond angles**



Torsions **Rings**

Ligand CLA L 1117



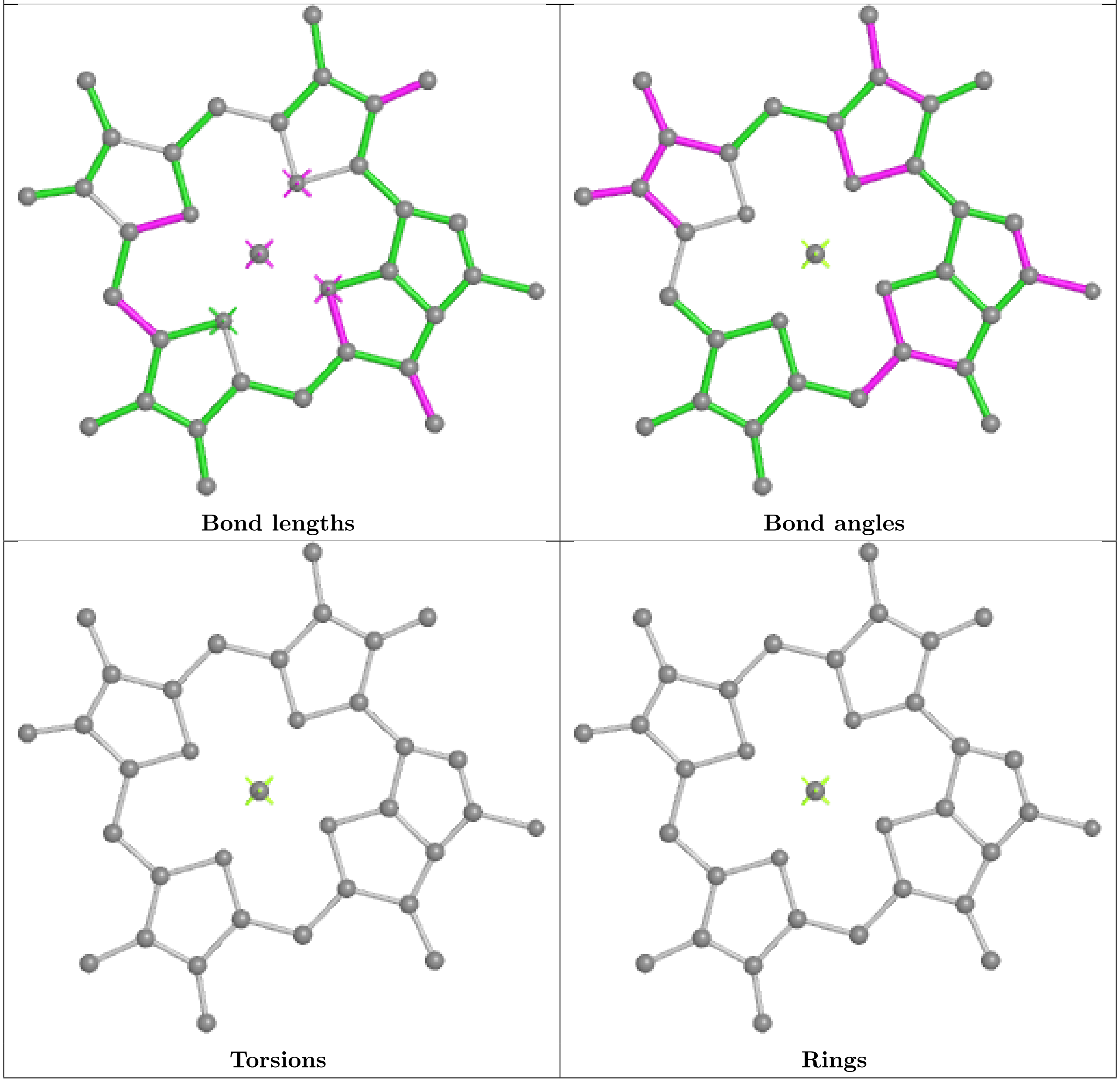
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA C 1083



Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
11	O	2

Continued on next page...

Continued from previous page...

Mol	Chain	Number of breaks
11	Y	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	O	175:UNK	C	176:UNK	N	9.74
1	O	9:UNK	C	10:UNK	N	6.01
1	Y	9:UNK	C	10:UNK	N	5.91

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.