wwPDB EM Validation Summary Report (i)

Oct 23, 2023 – 10:32 pm BST

PDB ID	:	8BCW
EMDB ID	:	EMD-15970
Title	:	Photosystem I assembly intermediate of Avena sativa
Authors	:	Naschberger, A.; Amunts, A.; Nelson, N.
Deposited on	:	2022-10-17
Resolution	:	2.11 Å(reported)

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

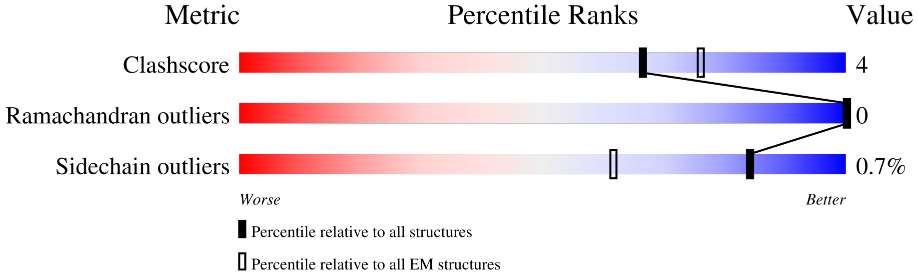
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance ⓘ

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

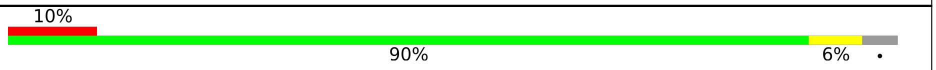
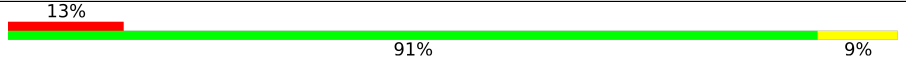
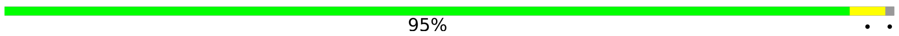
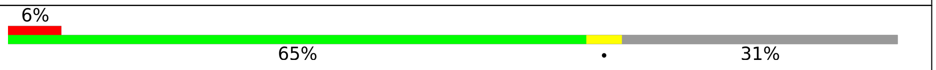
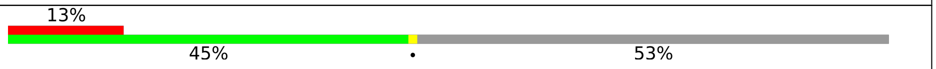
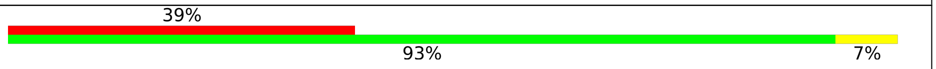
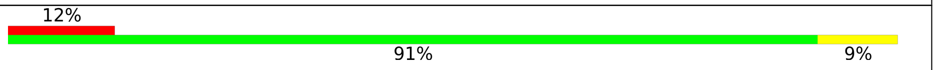
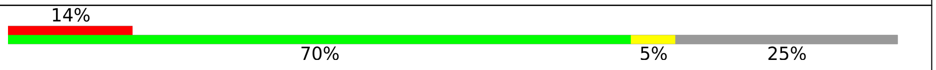
The reported resolution of this entry is 2.11 Å.

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	A	750	
2	B	734	
3	C	81	
4	D	206	
5	E	143	
6	H	94	
7	I	33	
8	L	213	

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
10	CLA	A	802	X	-	-	-
10	CLA	A	803	X	-	-	-
10	CLA	A	804	X	-	-	-
10	CLA	A	805	X	-	-	-
10	CLA	A	806	X	-	-	-
10	CLA	A	807	X	-	-	-
10	CLA	A	808	X	-	-	-
10	CLA	A	809	X	-	-	-
10	CLA	A	810	X	-	-	-
10	CLA	A	811	X	-	-	-
10	CLA	A	812	X	-	-	-
10	CLA	A	813	X	-	-	-
10	CLA	A	814	X	-	-	-
10	CLA	A	815	X	-	-	-
10	CLA	A	816	X	-	-	-
10	CLA	A	817	X	-	-	-
10	CLA	A	818	X	-	-	-
10	CLA	A	819	X	-	-	-
10	CLA	A	820	X	-	-	-
10	CLA	A	821	X	-	-	-
10	CLA	A	822	X	-	-	-
10	CLA	A	823	X	-	-	-
10	CLA	A	824	X	-	-	-
10	CLA	A	825	X	-	-	-
10	CLA	A	826	X	-	-	-
10	CLA	A	827	X	-	-	-
10	CLA	A	828	X	-	-	-
10	CLA	A	829	X	-	-	-
10	CLA	A	830	X	-	-	-
10	CLA	A	831	X	-	-	-
10	CLA	A	832	X	-	-	-
10	CLA	A	833	X	-	-	-
10	CLA	A	834	X	-	-	-
10	CLA	A	835	X	-	-	-
10	CLA	A	836	X	-	-	-
10	CLA	A	837	X	-	-	-
10	CLA	A	838	X	-	-	-
10	CLA	A	839	X	-	-	-
10	CLA	A	840	X	-	-	-
10	CLA	A	841	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	CLA	A	842	X	-	-	-
10	CLA	A	843	X	-	-	-
10	CLA	A	845	X	-	-	-
10	CLA	A	854	X	-	-	-
10	CLA	A	856	X	-	-	-
10	CLA	B	801	X	-	-	-
10	CLA	B	802	X	-	-	-
10	CLA	B	803	X	-	-	-
10	CLA	B	804	X	-	-	-
10	CLA	B	805	X	-	-	-
10	CLA	B	806	X	-	-	-
10	CLA	B	807	X	-	-	-
10	CLA	B	808	X	-	-	-
10	CLA	B	809	X	-	-	-
10	CLA	B	810	X	-	-	-
10	CLA	B	811	X	-	-	-
10	CLA	B	812	X	-	-	-
10	CLA	B	813	X	-	-	-
10	CLA	B	814	X	-	-	-
10	CLA	B	815	X	-	-	-
10	CLA	B	816	X	-	-	-
10	CLA	B	817	X	-	-	-
10	CLA	B	818	X	-	-	-
10	CLA	B	819	X	-	-	-
10	CLA	B	820	X	-	-	-
10	CLA	B	821	X	-	-	-
10	CLA	B	822	X	-	-	-
10	CLA	B	823	X	-	-	-
10	CLA	B	824	X	-	-	-
10	CLA	B	825	X	-	-	-
10	CLA	B	826	X	-	-	-
10	CLA	B	827	X	-	-	-
10	CLA	B	828	X	-	-	-
10	CLA	B	829	X	-	-	-
10	CLA	B	830	X	-	-	-
10	CLA	B	831	X	-	-	-
10	CLA	B	832	X	-	-	-
10	CLA	B	833	X	-	-	-
10	CLA	B	834	X	-	-	-
10	CLA	B	835	X	-	-	-
10	CLA	B	836	X	-	-	-
10	CLA	B	837	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	CLA	B	838	X	-	-	-
10	CLA	L	302	X	-	-	-
10	CLA	L	303	X	-	-	-
10	CLA	L	304	X	-	-	-
9	CL0	A	801	X	-	-	-
9	CL0	H	201	X	-	-	-

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 22313 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	720	5660	3711	961	969	19	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	733	5864	3848	996	1007	13	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	80	605	372	104	118	11	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	143	1124	722	196	203	3	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	E	67	533	340	94	99	0	0

- Molecule 6 is a protein called Photosystem I reaction center subunit VI, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	H	94	715	469	114	132	0	0

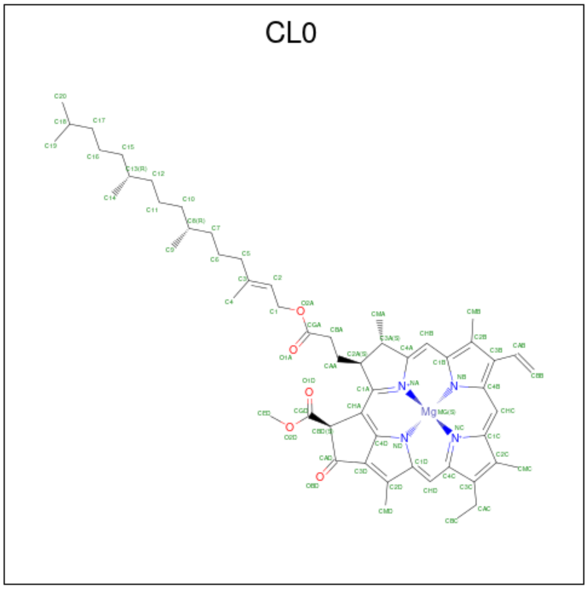
- Molecule 7 is a protein called Photosystem I reaction center subunit VIII.

Mol	Chain	Residues	Atoms	AltConf	Trace
7	I	33	Total C N O S 258 178 38 41 1	0	0

- Molecule 8 is a protein called PSI subunit V.

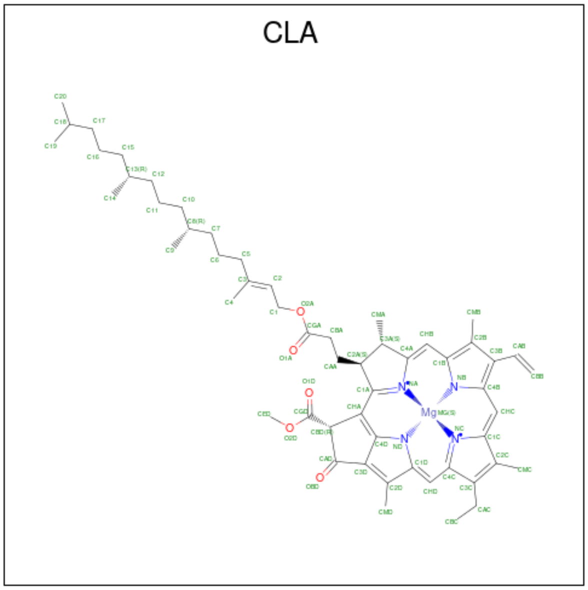
Mol	Chain	Residues	Atoms	AltConf	Trace
8	L	159	Total C N O S 1192 788 189 214 1	0	0

- Molecule 9 is CHLOROPHYLL A ISOMER (three-letter code: CL0) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
9	A	1	Total C Mg N O 65 55 1 4 5	0
9	H	1	Total C Mg N O 55 45 1 4 5	0

- Molecule 10 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
10	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
10	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
10	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
10	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
10	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
10	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
10	A	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
10	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
10	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
10	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
10	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
10	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
10	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
10	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	

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Mol	Chain	Residues	Atoms	AltConf
10	A	1	Total C Mg N O 60 50 1 4 5	0
10	A	1	Total C Mg N O 45 35 1 4 5	0
10	A	1	Total C Mg N O 45 35 1 4 5	0
10	A	1	Total C Mg N O 56 46 1 4 5	0
10	A	1	Total C Mg N O 65 55 1 4 5	0
10	A	1	Total C Mg N O 45 35 1 4 5	0
10	A	1	Total C Mg N O 65 55 1 4 5	0
10	A	1	Total C Mg N O 52 42 1 4 5	0
10	A	1	Total C Mg N O 45 35 1 4 5	0
10	A	1	Total C Mg N O 60 50 1 4 5	0
10	A	1	Total C Mg N O 65 55 1 4 5	0
10	A	1	Total C Mg N O 55 45 1 4 5	0
10	A	1	Total C Mg N O 65 55 1 4 5	0
10	A	1	Total C Mg N O 60 50 1 4 5	0
10	A	1	Total C Mg N O 65 55 1 4 5	0
10	A	1	Total C Mg N O 65 55 1 4 5	0
10	A	1	Total C Mg N O 45 35 1 4 5	0
10	A	1	Total C Mg N O 55 45 1 4 5	0
10	A	1	Total C Mg N O 65 55 1 4 5	0
10	A	1	Total C Mg N O 65 55 1 4 5	0
10	A	1	Total C Mg N O 65 55 1 4 5	0

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Mol	Chain	Residues	Atoms	AltConf
10	A	1	Total C Mg N O 45 35 1 4 5	0
10	A	1	Total C Mg N O 51 41 1 4 5	0
10	A	1	Total C Mg N O 65 55 1 4 5	0
10	A	1	Total C Mg N O 55 45 1 4 5	0
10	A	1	Total C Mg N O 55 45 1 4 5	0
10	A	1	Total C Mg N O 45 35 1 4 5	0
10	A	1	Total C Mg N O 65 55 1 4 5	0
10	A	1	Total C Mg N O 45 35 1 4 5	0
10	A	1	Total C Mg N O 55 45 1 4 5	0
10	A	1	Total C Mg N O 50 40 1 4 5	0
10	B	1	Total C Mg N O 65 55 1 4 5	0
10	B	1	Total C Mg N O 65 55 1 4 5	0
10	B	1	Total C Mg N O 45 35 1 4 5	0
10	B	1	Total C Mg N O 65 55 1 4 5	0
10	B	1	Total C Mg N O 65 55 1 4 5	0
10	B	1	Total C Mg N O 60 50 1 4 5	0
10	B	1	Total C Mg N O 65 55 1 4 5	0
10	B	1	Total C Mg N O 65 55 1 4 5	0
10	B	1	Total C Mg N O 65 55 1 4 5	0
10	B	1	Total C Mg N O 56 46 1 4 5	0
10	B	1	Total C Mg N O 45 35 1 4 5	0

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Mol	Chain	Residues	Atoms					AltConf
10	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
10	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
10	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
10	B	1	Total 57	C 47	Mg 1	N 4	O 5	0
10	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
10	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
10	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
10	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
10	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
10	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
10	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
10	B	1	Total 56	C 46	Mg 1	N 4	O 5	0
10	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
10	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
10	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
10	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
10	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
10	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
10	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
10	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
10	B	1	Total 45	C 35	Mg 1	N 4	O 5	0

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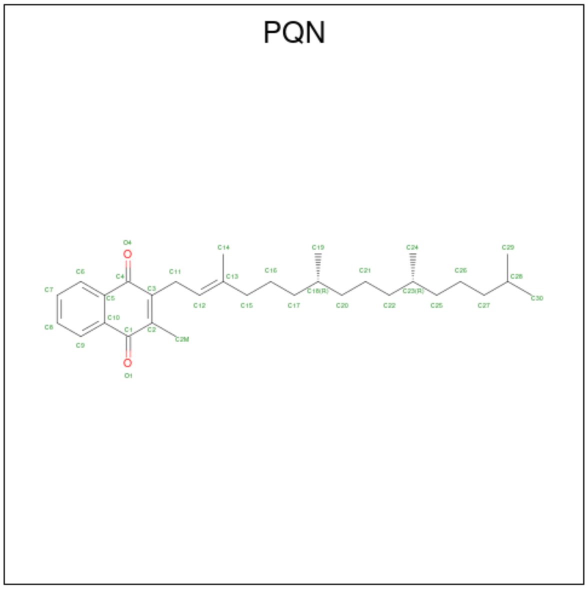
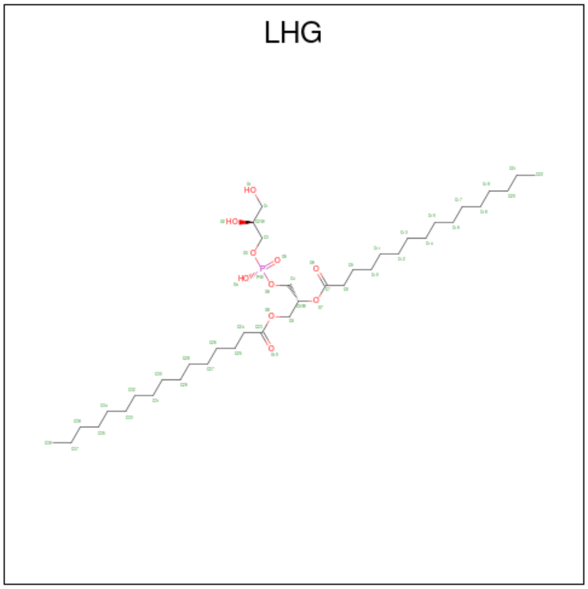
Mol	Chain	Residues	Atoms					AltConf
10	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
10	B	1	Total 51	C 41	Mg 1	N 4	O 5	0
10	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
10	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
10	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
10	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
10	L	1	Total 45	C 35	Mg 1	N 4	O 5	0
10	L	1	Total 60	C 50	Mg 1	N 4	O 5	0
10	L	1	Total 45	C 35	Mg 1	N 4	O 5	0

- Molecule 11 is PHYLLOQUINONE (three-letter code: PQN) (formula: $C_{31}H_{46}O_2$) (labeled as "Ligand of Interest" by depositor).



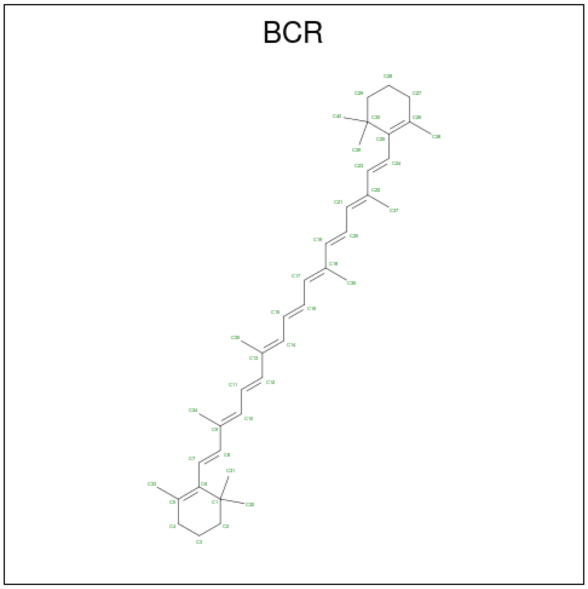
Mol	Chain	Residues	Atoms			AltConf
11	A	1	Total 33	C 31	O 2	0
11	B	1	Total 33	C 31	O 2	0

- Molecule 12 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$) (labeled as "Ligand of Interest" by depositor).



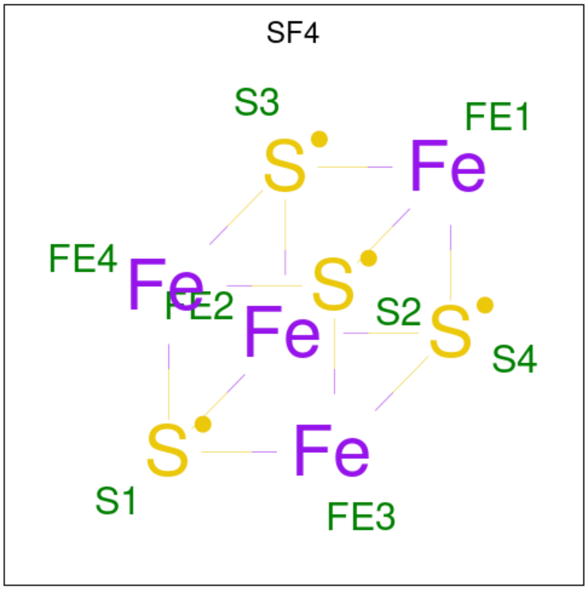
Mol	Chain	Residues	Atoms				AltConf
12	A	1	Total 41	C 30	O 10	P 1	0
12	A	1	Total 31	C 20	O 10	P 1	0
12	B	1	Total 49	C 38	O 10	P 1	0

- Molecule 13 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$) (labeled as "Ligand of Interest" by depositor).



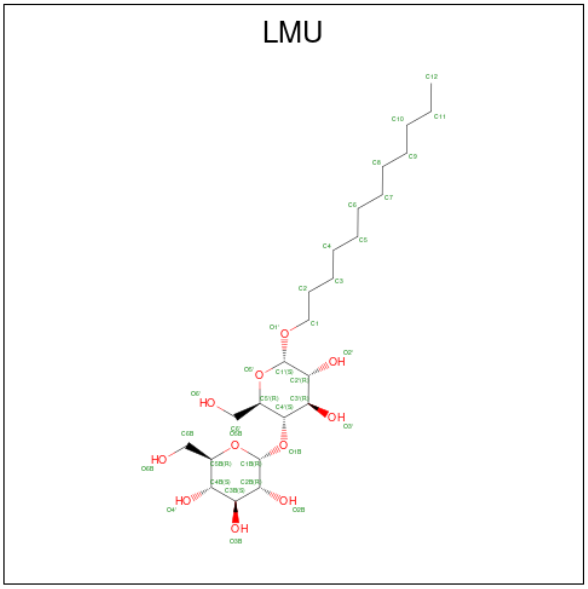
Mol	Chain	Residues	Atoms	AltConf
13	A	1	Total C 40 40	0
13	A	1	Total C 40 40	0
13	A	1	Total C 40 40	0
13	A	1	Total C 40 40	0
13	A	1	Total C 40 40	0
13	B	1	Total C 40 40	0
13	B	1	Total C 40 40	0
13	B	1	Total C 40 40	0
13	B	1	Total C 40 40	0
13	I	1	Total C 40 40	0
13	L	1	Total C 40 40	0
13	L	1	Total C 40 40	0
13	L	1	Total C 40 40	0

- Molecule 14 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



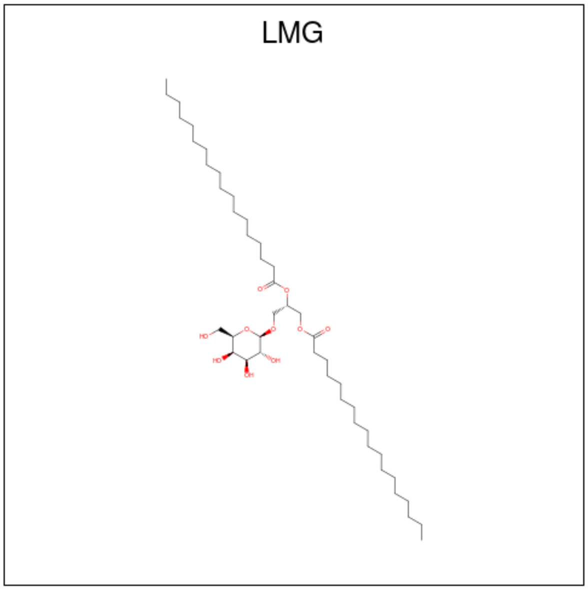
Mol	Chain	Residues	Atoms	AltConf
14	A	1	Total Fe S 8 4 4	0
14	C	1	Total Fe S 8 4 4	0
14	C	1	Total Fe S 8 4 4	0

- Molecule 15 is DODECYL-ALPHA-D-MALTOSIDE (three-letter code: LMU) (formula: $C_{24}H_{46}O_{11}$).



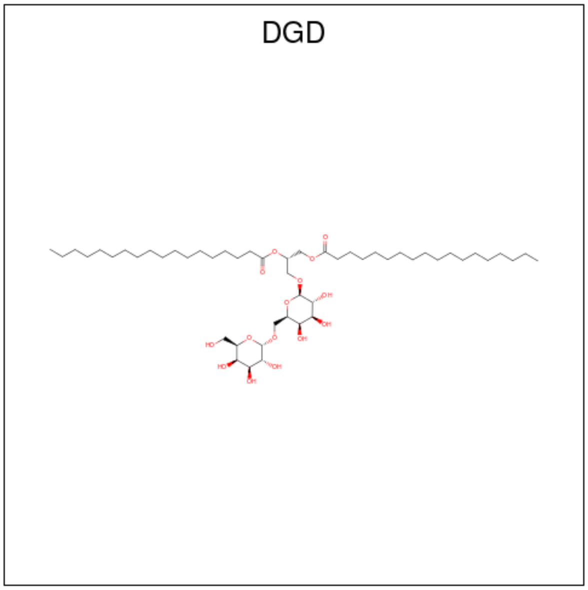
Mol	Chain	Residues	Atoms	AltConf
15	A	1	Total C O 35 24 11	0
15	A	1	Total C O 24 18 6	0
15	A	1	Total C O 21 15 6	0

- Molecule 16 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
16	A	1	Total C O 43 33 10	0

- Molecule 17 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
17	B	1	Total C O 61 46 15	0

- Molecule 18 is water.

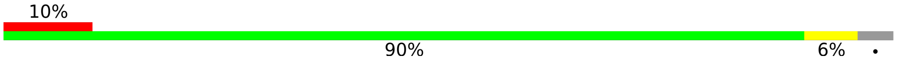
Mol	Chain	Residues	Atoms	AltConf
18	A	155	Total O 155 155	0
18	B	203	Total O 203 203	0
18	C	62	Total O 62 62	0
18	D	47	Total O 47 47	0
18	E	13	Total O 13 13	0
18	H	9	Total O 9 9	0
18	I	4	Total O 4 4	0
18	L	24	Total O 24 24	0

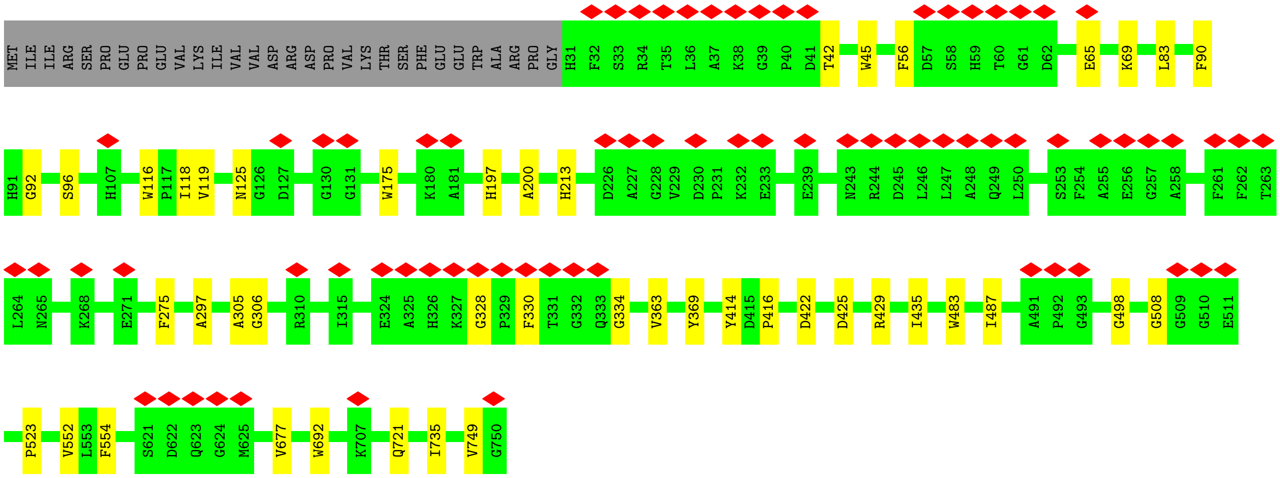
3 Residue-property plots ⓘ

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

- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

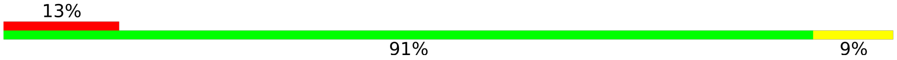
Chain A:

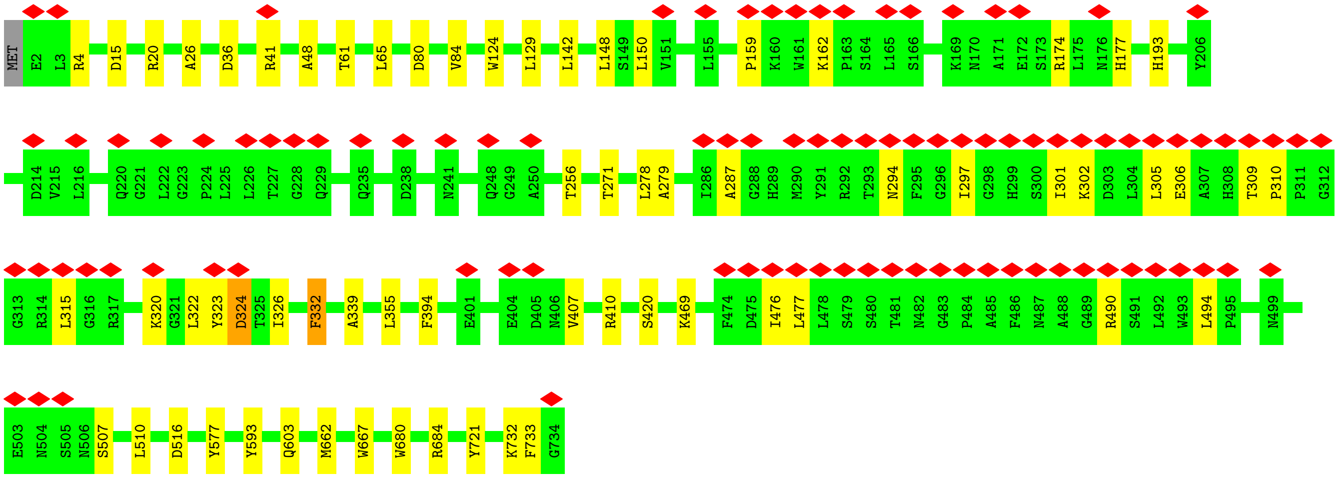




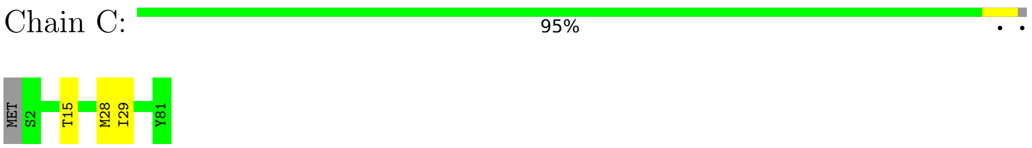
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain B:

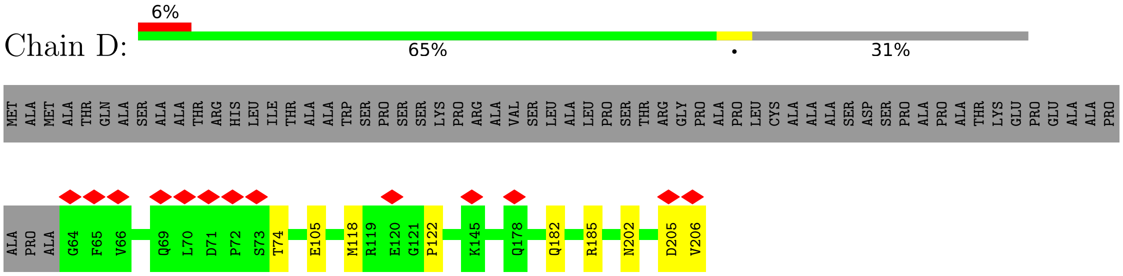




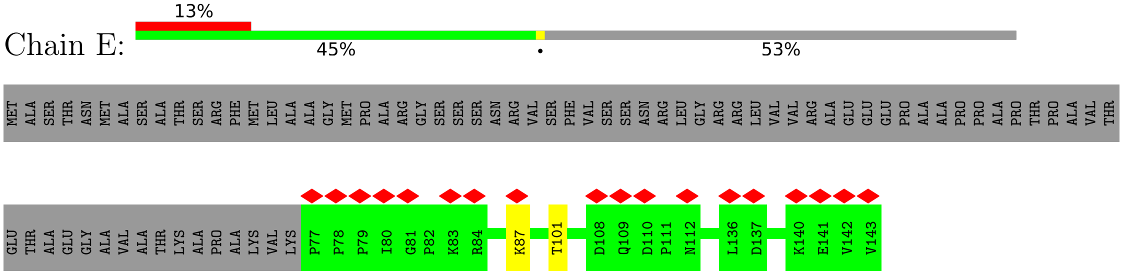
- Molecule 3: Photosystem I iron-sulfur center



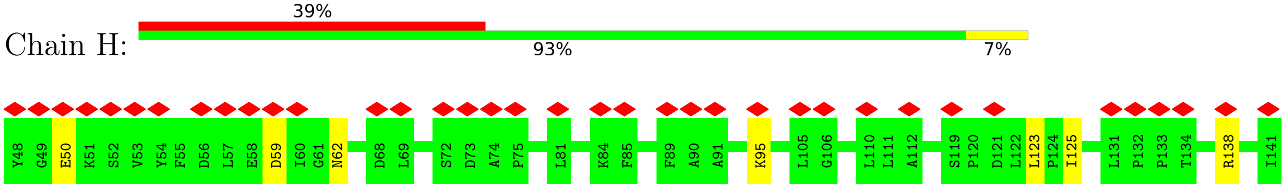
- Molecule 4: Photosystem I reaction center subunit II, chloroplastic



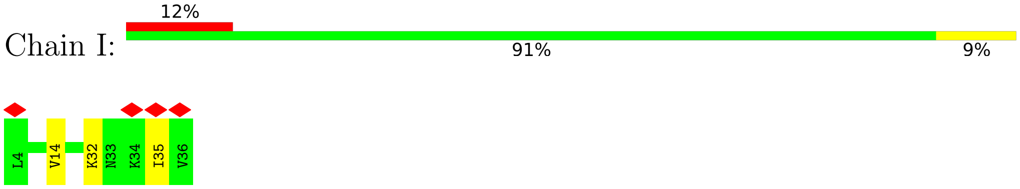
- Molecule 5: Photosystem I reaction center subunit IV A, chloroplastic



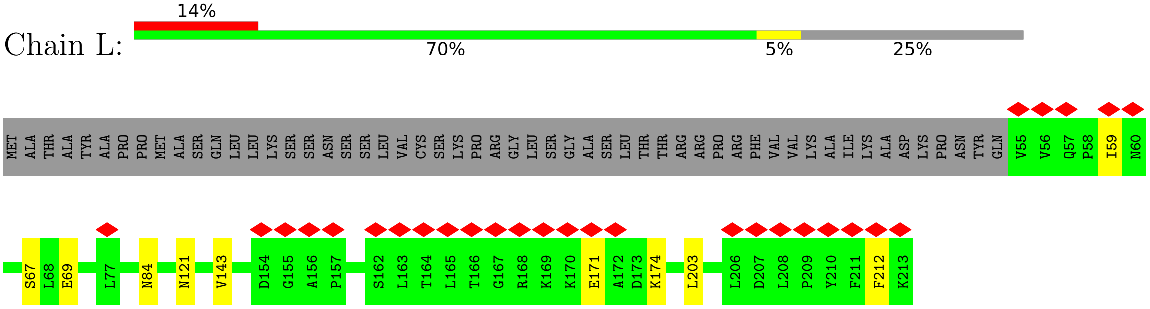
- Molecule 6: Photosystem I reaction center subunit VI, chloroplastic



- Molecule 7: Photosystem I reaction center subunit VIII



- Molecule 8: PSI subunit V



4 Experimental information ⓘ

Property	**Value**	**Source**
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	169213	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 $(e^-/\text{Å}^2)$	51.346	Depositor
Minimum defocus (nm)	300	Depositor
Maximum defocus (nm)	2100	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.470	Depositor
Minimum map value	-0.159	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.053	Depositor
Map size (Å)	336.0, 336.0, 336.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.84, 0.84, 0.84	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PQN, LMG, BCR, DGD, LMU, SF4, CLA, CL0, 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	A	0.26	0/5853	0.45	0/7985
2	B	0.26	0/6075	0.45	0/8297
3	C	0.23	0/616	0.54	0/834
4	D	0.26	0/1153	0.52	0/1557
5	E	0.25	0/546	0.50	0/743
6	H	0.25	0/737	0.43	0/1002
7	I	0.26	0/264	0.41	0/359
8	L	0.26	0/1228	0.44	0/1681
All	All	0.26	0/16472	0.46	0/22458

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	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	667	TRP	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	A	5660	0	5513	33	0
2	B	5864	0	5642	46	0
3	C	605	0	587	2	0
4	D	1124	0	1128	5	0
5	E	533	0	538	1	0
6	H	715	0	715	4	0
7	I	258	0	285	2	0
8	L	1192	0	1197	7	0
9	A	65	0	72	0	0
9	H	55	0	49	1	0
10	A	2520	0	2393	50	0
10	B	2140	0	2054	45	0
10	L	150	0	125	3	0
11	A	33	0	46	2	0
11	B	33	0	46	1	0
12	A	72	0	87	3	0
12	B	49	0	74	6	0
13	A	200	0	280	15	0
13	B	160	0	224	8	0
13	I	40	0	56	2	0
13	L	120	0	168	3	0
14	A	8	0	0	0	0
14	C	16	0	0	0	0
15	A	80	0	107	3	0
16	A	43	0	56	1	0
17	B	61	0	83	1	0
18	A	155	0	0	1	0
18	B	203	0	0	1	0
18	C	62	0	0	0	0
18	D	47	0	0	0	0
18	E	13	0	0	0	0
18	H	9	0	0	0	0
18	I	4	0	0	0	0
18	L	24	0	0	1	0
All	All	22313	0	21525	174	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 4.

The worst 5 of 174 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:ASN:ND2	15:A:855:LMU:O6’	2.24	0.70
2:B:490:ARG:HA	2:B:494:LEU:HD12	1.76	0.68
10:B:802:CLA:H143	13:B:843:BCR:H362	1.76	0.66
2:B:150:LEU:HD11	12:B:845:LHG:H382	1.80	0.63
8:L:59:ILE:HA	8:L:69:GLU:HG3	1.79	0.63

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	718/750 (96%)	703 (98%)	15 (2%)	0	100	100
2	B	731/734 (100%)	716 (98%)	15 (2%)	0	100	100
3	C	78/81 (96%)	76 (97%)	2 (3%)	0	100	100
4	D	141/206 (68%)	138 (98%)	3 (2%)	0	100	100
5	E	65/143 (46%)	65 (100%)	0	0	100	100
6	H	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
7	I	31/33 (94%)	31 (100%)	0	0	100	100
8	L	157/213 (74%)	154 (98%)	3 (2%)	0	100	100
All	All	2013/2254 (89%)	1974 (98%)	39 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	580/608 (95%)	577 (100%)	3 (0%)	88	92
2	B	598/599 (100%)	592 (99%)	6 (1%)	76	81
3	C	70/71 (99%)	70 (100%)	0	100	100
4	D	120/163 (74%)	120 (100%)	0	100	100
5	E	59/115 (51%)	59 (100%)	0	100	100
6	H	76/76 (100%)	75 (99%)	1 (1%)	69	74
7	I	30/30 (100%)	30 (100%)	0	100	100
8	L	123/168 (73%)	122 (99%)	1 (1%)	81	86
All	All	1656/1830 (90%)	1645 (99%)	11 (1%)	84	88

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	394	PHE
2	B	577	TYR
8	L	143	VAL
6	H	50	GLU
2	B	297	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	125	ASN
2	B	603	GLN
6	H	66	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

114 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	$\#\|Z\| > 2$
10	CLA	A	830	-	65,73,73	1.03	3 (4%)	76,113,113	0.82	2 (2%)
9	CL0	H	201	6	55,63,73	2.23	7 (12%)	64,101,113	1.27	6 (9%)
10	CLA	A	835	-	65,73,73	1.03	3 (4%)	76,113,113	0.84	2 (2%)
10	CLA	A	813	-	45,53,73	1.25	3 (6%)	52,89,113	1.04	2 (3%)
13	BCR	B	842	-	41,41,41	0.13	0	56,56,56	0.41	0
10	CLA	B	803	-	45,53,73	1.24	3 (6%)	52,89,113	1.01	2 (3%)
10	CLA	B	819	-	45,53,73	1.26	3 (6%)	52,89,113	1.04	2 (3%)
13	BCR	L	305	-	41,41,41	0.27	0	56,56,56	0.46	1 (1%)
14	SF4	C	102	3	0,12,12	-	-	-		
9	CL0	A	801	-	65,73,73	2.00	8 (12%)	76,113,113	1.12	6 (7%)
10	CLA	B	816	-	60,68,73	1.08	3 (5%)	70,107,113	0.88	2 (2%)
13	BCR	B	841	-	41,41,41	0.14	0	56,56,56	0.30	0
10	CLA	B	806	-	60,68,73	1.04	3 (5%)	70,107,113	0.88	2 (2%)
10	CLA	A	822	18	65,73,73	1.02	3 (4%)	76,113,113	0.88	2 (2%)
10	CLA	A	820	-	65,73,73	1.02	3 (4%)	76,113,113	0.89	2 (2%)
10	CLA	A	812	10	65,73,73	1.01	3 (4%)	76,113,113	0.84	2 (2%)
10	CLA	B	827	-	65,73,73	1.01	3 (4%)	76,113,113	0.89	3 (3%)
10	CLA	B	808	2	65,73,73	1.01	3 (4%)	76,113,113	0.83	2 (2%)
10	CLA	A	811	-	45,53,73	1.23	3 (6%)	52,89,113	1.04	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
10	CLA	B	834	-	51,59,73	1.18	3 (5%)	59,96,113	0.97	2 (3%)
15	LMU	A	855	-	36,36,36	0.12	0	47,47,47	0.25	0
10	CLA	B	811	-	45,53,73	1.25	3 (6%)	52,89,113	1.04	2 (3%)
10	CLA	A	805	10	50,58,73	1.17	3 (6%)	58,95,113	0.93	2 (3%)
10	CLA	A	832	-	45,53,73	1.24	3 (6%)	52,89,113	1.02	2 (3%)
13	BCR	A	851	-	41,41,41	0.18	0	56,56,56	0.34	0
10	CLA	A	819	-	56,64,73	1.12	3 (5%)	65,102,113	0.91	2 (3%)
10	CLA	A	821	-	45,53,73	1.24	3 (6%)	52,89,113	1.01	2 (3%)
10	CLA	B	802	-	65,73,73	0.98	3 (4%)	76,113,113	0.82	3 (3%)
10	CLA	A	804	-	45,53,73	1.25	3 (6%)	52,89,113	1.05	2 (3%)
10	CLA	A	839	-	65,73,73	1.03	3 (4%)	76,113,113	0.85	2 (2%)
10	CLA	A	827	18	55,63,73	1.09	3 (5%)	64,101,113	0.90	2 (3%)
10	CLA	B	838	-	65,73,73	1.03	3 (4%)	76,113,113	0.86	2 (2%)
10	CLA	A	843	18	65,73,73	1.01	3 (4%)	76,113,113	0.88	2 (2%)
10	CLA	A	818	-	45,53,73	1.25	3 (6%)	52,89,113	1.02	2 (3%)
10	CLA	A	842	-	45,53,73	1.25	3 (6%)	52,89,113	1.03	2 (3%)
10	CLA	B	835	-	55,63,73	1.09	3 (5%)	64,101,113	0.94	2 (3%)
10	CLA	B	814	-	55,63,73	1.10	3 (5%)	64,101,113	0.91	2 (3%)
13	BCR	I	101	-	41,41,41	0.16	0	56,56,56	0.44	0
10	CLA	B	810	-	56,64,73	1.12	3 (5%)	65,102,113	0.90	2 (3%)
10	CLA	B	818	18	55,63,73	1.14	3 (5%)	64,101,113	0.95	2 (3%)
14	SF4	C	101	3	0,12,12	-	-	-		
10	CLA	A	823	-	52,60,73	1.16	3 (5%)	60,97,113	0.97	2 (3%)
10	CLA	A	814	-	65,73,73	1.04	3 (4%)	76,113,113	0.85	2 (2%)
10	CLA	A	807	1	65,73,73	1.02	3 (4%)	76,113,113	0.85	2 (2%)
10	CLA	B	828	-	65,73,73	0.95	4 (6%)	76,113,113	0.85	2 (2%)
10	CLA	B	821	-	45,53,73	1.25	3 (6%)	52,89,113	1.03	2 (3%)
10	CLA	A	845	12	45,53,73	1.25	3 (6%)	52,89,113	1.04	2 (3%)
10	CLA	B	809	-	65,73,73	1.04	3 (4%)	76,113,113	0.83	2 (2%)
13	BCR	A	850	-	41,41,41	0.15	0	56,56,56	0.34	0
12	LHG	A	847	10	30,30,48	0.29	0	33,36,54	0.31	0
10	CLA	B	805	2	65,73,73	1.03	3 (4%)	76,113,113	0.81	2 (2%)
10	CLA	B	830	-	45,53,73	1.24	3 (6%)	52,89,113	1.02	2 (3%)
13	BCR	L	306	-	41,41,41	0.12	0	56,56,56	0.24	0
10	CLA	B	837	18	65,73,73	0.99	3 (4%)	76,113,113	0.85	2 (2%)
10	CLA	A	841	-	55,63,73	1.10	3 (5%)	64,101,113	0.91	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
10	CLA	B	829	-	45,53,73	1.25	3 (6%)	52,89,113	1.05	2 (3%)
10	CLA	B	801	-	65,73,73	1.00	3 (4%)	76,113,113	0.80	2 (2%)
10	CLA	A	828	-	65,73,73	1.03	3 (4%)	76,113,113	0.86	2 (2%)
16	LMG	A	858	-	43,43,55	0.18	0	51,51,63	0.17	0
13	BCR	L	301	-	41,41,41	0.14	0	56,56,56	0.32	0
10	CLA	B	813	-	65,73,73	1.03	3 (4%)	76,113,113	0.84	2 (2%)
10	CLA	B	832	-	45,53,73	1.21	3 (6%)	52,89,113	1.04	2 (3%)
10	CLA	A	816	-	60,68,73	1.04	3 (5%)	70,107,113	0.89	2 (2%)
10	CLA	A	837	1	45,53,73	1.24	3 (6%)	52,89,113	1.04	2 (3%)
10	CLA	L	303	-	60,68,73	1.04	3 (5%)	70,107,113	0.90	2 (2%)
11	PQN	A	844	-	34,34,34	0.32	0	42,45,45	0.35	0
10	CLA	A	833	-	55,63,73	1.08	3 (5%)	64,101,113	0.92	2 (3%)
10	CLA	A	854	18	55,63,73	1.07	3 (5%)	64,101,113	1.00	3 (4%)
10	CLA	A	829	-	60,68,73	1.07	3 (5%)	70,107,113	0.87	2 (2%)
10	CLA	A	834	-	65,73,73	1.00	3 (4%)	76,113,113	0.88	2 (2%)
13	BCR	B	843	-	41,41,41	0.14	0	56,56,56	0.42	0
10	CLA	A	824	-	45,53,73	1.25	3 (6%)	52,89,113	1.04	2 (3%)
14	SF4	A	853	1,2	0,12,12	-	-	-		
10	CLA	B	817	-	65,73,73	1.02	3 (4%)	76,113,113	0.88	2 (2%)
13	BCR	B	840	-	41,41,41	0.19	0	56,56,56	0.44	0
10	CLA	A	825	-	60,68,73	1.07	3 (5%)	70,107,113	0.88	2 (2%)
10	CLA	B	812	-	65,73,73	1.05	3 (4%)	76,113,113	0.85	2 (2%)
15	LMU	A	857	-	24,24,36	0.13	0	29,29,47	0.29	0
10	CLA	A	806	-	65,73,73	1.03	3 (4%)	76,113,113	0.85	2 (2%)
12	LHG	A	846	-	40,40,48	0.26	0	43,46,54	0.28	0
10	CLA	A	836	-	65,73,73	1.01	3 (4%)	76,113,113	0.84	2 (2%)
10	CLA	B	807	-	65,73,73	1.03	3 (4%)	76,113,113	0.84	2 (2%)
13	BCR	A	849	-	41,41,41	0.13	0	56,56,56	0.28	0
10	CLA	B	825	-	65,73,73	1.02	3 (4%)	76,113,113	0.83	2 (2%)
10	CLA	A	838	-	51,59,73	1.18	3 (5%)	59,96,113	0.97	2 (3%)
10	CLA	B	823	18	56,64,73	1.14	3 (5%)	65,102,113	0.90	2 (3%)
10	CLA	A	856	18	50,58,73	1.17	3 (6%)	58,95,113	0.97	2 (3%)
10	CLA	L	302	8	45,53,73	1.24	3 (6%)	52,89,113	1.02	2 (3%)
10	CLA	A	802	-	65,73,73	0.97	3 (4%)	76,113,113	0.86	2 (2%)
17	DGD	B	844	-	62,62,67	0.18	0	76,76,81	0.30	0
10	CLA	A	826	18	65,73,73	1.06	3 (4%)	76,113,113	0.85	2 (2%)
10	CLA	B	815	-	57,65,73	1.10	3 (5%)	66,103,113	0.91	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
13	BCR	A	852	-	41,41,41	0.27	0	56,56,56	0.83	1 (1%)
13	BCR	A	848	-	41,41,41	0.12	0	56,56,56	0.26	0
10	CLA	B	831	-	45,53,73	1.22	3 (6%)	52,89,113	1.08	3 (5%)
10	CLA	B	804	-	65,73,73	1.01	3 (4%)	76,113,113	0.87	2 (2%)
10	CLA	L	304	18	45,53,73	1.24	3 (6%)	52,89,113	1.02	2 (3%)
10	CLA	B	833	-	45,53,73	1.22	3 (6%)	52,89,113	1.05	2 (3%)
10	CLA	B	820	-	45,53,73	1.25	3 (6%)	52,89,113	1.05	2 (3%)
10	CLA	B	824	18	50,58,73	1.13	3 (6%)	58,95,113	0.95	2 (3%)
10	CLA	A	817	18	45,53,73	1.28	3 (6%)	52,89,113	1.04	2 (3%)
10	CLA	A	803	18	65,73,73	1.06	3 (4%)	76,113,113	0.88	3 (3%)
10	CLA	A	815	-	54,62,73	1.15	3 (5%)	62,99,113	0.93	2 (3%)
12	LHG	B	845	-	48,48,48	0.23	0	51,54,54	0.24	0
11	PQN	B	839	-	34,34,34	0.32	0	42,45,45	0.32	0
10	CLA	A	831	-	65,73,73	1.01	3 (4%)	76,113,113	0.81	2 (2%)
10	CLA	B	826	-	65,73,73	1.01	3 (4%)	76,113,113	0.89	3 (3%)
10	CLA	A	808	-	47,55,73	1.20	3 (6%)	54,91,113	1.00	2 (3%)
10	CLA	A	809	1	55,63,73	1.09	3 (5%)	64,101,113	0.91	2 (3%)
10	CLA	A	810	1	50,58,73	1.17	3 (6%)	58,95,113	0.97	2 (3%)
10	CLA	B	836	-	50,58,73	1.17	3 (6%)	58,95,113	0.94	2 (3%)
10	CLA	A	840	-	55,63,73	1.07	3 (5%)	64,101,113	0.93	2 (3%)
15	LMU	A	859	-	21,21,36	0.13	0	26,26,47	0.28	0
10	CLA	B	822	-	45,53,73	1.24	3 (6%)	52,89,113	1.03	2 (3%)

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
10	CLA	A	830	-	1/1/15/20	2/37/115/115	-
9	CL0	H	201	6	3/3/18/25	4/25/123/135	-
10	CLA	A	835	-	1/1/15/20	2/37/115/115	-
10	CLA	A	813	-	1/1/11/20	3/13/91/115	-
13	BCR	B	842	-	-	2/29/63/63	0/2/2/2
10	CLA	B	803	-	1/1/11/20	4/13/91/115	-
10	CLA	B	819	-	1/1/11/20	2/13/91/115	-
13	BCR	L	305	-	-	2/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	SF4	C	102	3	-	-	0/6/5/5
9	CL0	A	801	-	3/3/20/25	2/37/135/135	-
10	CLA	B	816	-	1/1/14/20	4/31/109/115	-
13	BCR	B	841	-	-	6/29/63/63	0/2/2/2
10	CLA	B	806	-	1/1/14/20	4/31/109/115	-
10	CLA	A	822	18	1/1/15/20	0/37/115/115	-
10	CLA	A	820	-	1/1/15/20	6/37/115/115	-
10	CLA	A	812	10	1/1/15/20	7/37/115/115	-
10	CLA	B	827	-	1/1/15/20	8/37/115/115	-
10	CLA	B	808	2	1/1/15/20	6/37/115/115	-
10	CLA	A	811	-	1/1/11/20	1/13/91/115	-
10	CLA	B	834	-	1/1/12/20	4/21/99/115	-
15	LMU	A	855	-	-	4/21/61/61	0/2/2/2
10	CLA	B	811	-	1/1/11/20	3/13/91/115	-
10	CLA	A	805	10	1/1/12/20	3/19/97/115	-
10	CLA	A	832	-	1/1/11/20	3/13/91/115	-
13	BCR	A	851	-	-	2/29/63/63	0/2/2/2
10	CLA	A	819	-	1/1/13/20	5/27/105/115	-
10	CLA	A	821	-	1/1/11/20	3/13/91/115	-
10	CLA	B	802	-	1/1/15/20	1/37/115/115	-
10	CLA	A	804	-	1/1/11/20	4/13/91/115	-
10	CLA	A	839	-	1/1/15/20	4/37/115/115	-
10	CLA	A	827	18	1/1/13/20	1/25/103/115	-
10	CLA	B	838	-	1/1/15/20	2/37/115/115	-
10	CLA	A	843	18	1/1/15/20	5/37/115/115	-
10	CLA	A	818	-	1/1/11/20	4/13/91/115	-
10	CLA	A	842	-	1/1/11/20	2/13/91/115	-
10	CLA	B	835	-	1/1/13/20	2/25/103/115	-
10	CLA	B	814	-	1/1/13/20	5/25/103/115	-
13	BCR	I	101	-	-	0/29/63/63	0/2/2/2
10	CLA	B	810	-	1/1/13/20	4/27/105/115	-
10	CLA	B	818	18	1/1/13/20	2/25/103/115	-
14	SF4	C	101	3	-	-	0/6/5/5
10	CLA	A	823	-	1/1/12/20	5/22/100/115	-
10	CLA	A	814	-	1/1/15/20	6/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	CLA	A	807	1	1/1/15/20	6/37/115/115	-
10	CLA	B	828	-	1/1/15/20	8/37/115/115	-
10	CLA	B	821	-	1/1/11/20	5/13/91/115	-
10	CLA	A	845	12	1/1/11/20	5/13/91/115	-
10	CLA	B	809	-	1/1/15/20	2/37/115/115	-
13	BCR	A	850	-	-	2/29/63/63	0/2/2/2
12	LHG	A	847	10	-	10/35/35/53	-
10	CLA	B	805	2	1/1/15/20	2/37/115/115	-
10	CLA	B	830	-	1/1/11/20	2/13/91/115	-
13	BCR	L	306	-	-	1/29/63/63	0/2/2/2
10	CLA	B	837	18	1/1/15/20	3/37/115/115	-
10	CLA	A	841	-	1/1/13/20	2/25/103/115	-
10	CLA	B	829	-	1/1/11/20	4/13/91/115	-
10	CLA	B	801	-	1/1/15/20	4/37/115/115	-
10	CLA	A	828	-	1/1/15/20	2/37/115/115	-
16	LMG	A	858	-	-	2/38/58/70	0/1/1/1
13	BCR	L	301	-	-	4/29/63/63	0/2/2/2
10	CLA	B	813	-	1/1/15/20	4/37/115/115	-
10	CLA	B	832	-	1/1/11/20	3/13/91/115	-
10	CLA	A	816	-	1/1/14/20	4/31/109/115	-
10	CLA	A	837	1	1/1/11/20	1/13/91/115	-
10	CLA	L	303	-	1/1/14/20	3/31/109/115	-
11	PQN	A	844	-	-	0/23/43/43	0/2/2/2
10	CLA	A	833	-	1/1/13/20	0/25/103/115	-
10	CLA	A	854	18	1/1/13/20	3/25/103/115	-
10	CLA	A	829	-	1/1/14/20	2/31/109/115	-
10	CLA	A	834	-	1/1/15/20	3/37/115/115	-
13	BCR	B	843	-	-	1/29/63/63	0/2/2/2
10	CLA	A	824	-	1/1/11/20	3/13/91/115	-
14	SF4	A	853	1,2	-	-	0/6/5/5
10	CLA	B	817	-	1/1/15/20	4/37/115/115	-
13	BCR	B	840	-	-	1/29/63/63	0/2/2/2
10	CLA	A	825	-	1/1/14/20	2/31/109/115	-
10	CLA	B	812	-	1/1/15/20	7/37/115/115	-
15	LMU	A	857	-	-	3/15/35/61	0/1/1/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	CLA	A	806	-	1/1/15/20	3/37/115/115	-
12	LHG	A	846	-	-	7/45/45/53	-
10	CLA	A	836	-	1/1/15/20	5/37/115/115	-
10	CLA	B	807	-	1/1/15/20	5/37/115/115	-
13	BCR	A	849	-	-	2/29/63/63	0/2/2/2
10	CLA	B	825	-	1/1/15/20	3/37/115/115	-
10	CLA	A	838	-	1/1/12/20	1/21/99/115	-
10	CLA	B	823	18	1/1/13/20	5/27/105/115	-
10	CLA	A	856	18	1/1/12/20	0/19/97/115	-
10	CLA	L	302	8	1/1/11/20	2/13/91/115	-
10	CLA	A	802	-	1/1/15/20	0/37/115/115	-
17	DGD	B	844	-	-	11/50/90/95	0/2/2/2
10	CLA	A	826	18	1/1/15/20	7/37/115/115	-
10	CLA	B	815	-	1/1/13/20	4/28/106/115	-
13	BCR	A	852	-	-	4/29/63/63	0/2/2/2
13	BCR	A	848	-	-	4/29/63/63	0/2/2/2
10	CLA	B	831	-	1/1/11/20	2/13/91/115	-
10	CLA	B	804	-	1/1/15/20	5/37/115/115	-
10	CLA	L	304	18	1/1/11/20	0/13/91/115	-
10	CLA	B	833	-	1/1/11/20	2/13/91/115	-
10	CLA	B	820	-	1/1/11/20	4/13/91/115	-
10	CLA	B	824	18	1/1/12/20	2/19/97/115	-
10	CLA	A	817	18	1/1/11/20	1/13/91/115	-
10	CLA	A	803	18	1/1/15/20	1/37/115/115	-
10	CLA	A	815	-	1/1/12/20	3/24/102/115	-
12	LHG	B	845	-	-	18/53/53/53	-
11	PQN	B	839	-	-	3/23/43/43	0/2/2/2
10	CLA	A	831	-	1/1/15/20	2/37/115/115	-
10	CLA	B	826	-	1/1/15/20	6/37/115/115	-
10	CLA	A	808	-	1/1/11/20	2/16/94/115	-
10	CLA	A	809	1	1/1/13/20	7/25/103/115	-
10	CLA	A	810	1	1/1/12/20	2/19/97/115	-
10	CLA	B	836	-	1/1/12/20	0/19/97/115	-
10	CLA	A	840	-	1/1/13/20	2/25/103/115	-
15	LMU	A	859	-	-	4/12/32/61	0/1/1/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	CLA	B	822	-	1/1/11/20	3/13/91/115	-

The worst 5 of 274 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	801	CL0	C4B-NB	10.89	1.44	1.35
9	H	201	CL0	C4B-NB	10.55	1.44	1.35
9	H	201	CL0	C1B-NB	7.30	1.41	1.35
9	A	801	CL0	C1B-NB	6.71	1.41	1.35
10	B	823	CLA	C1D-ND	5.91	1.45	1.37

The worst 5 of 192 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	831	CLA	C1D-ND-C4D	-4.27	103.30	106.33
10	A	820	CLA	C1D-ND-C4D	-4.25	103.31	106.33
10	A	828	CLA	C1D-ND-C4D	-4.21	103.34	106.33
10	A	804	CLA	C1D-ND-C4D	-4.21	103.34	106.33
10	B	807	CLA	C1D-ND-C4D	-4.20	103.35	106.33

5 of 92 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
9	A	801	CL0	NA
9	A	801	CL0	NC
9	A	801	CL0	ND
9	H	201	CL0	NA
9	H	201	CL0	NC

5 of 379 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	A	812	CLA	CHA-CBD-CGD-O2D
10	A	818	CLA	CHA-CBD-CGD-O2D
10	A	819	CLA	C1A-C2A-CAA-CBA
10	A	819	CLA	C3A-C2A-CAA-CBA
10	A	823	CLA	C2-C3-C5-C6

There are no ring outliers.

81 monomers are involved in 123 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	A	830	CLA	2	0
9	H	201	CL0	1	0
13	B	842	BCR	5	0
10	B	803	CLA	1	0
13	L	305	BCR	1	0
10	B	816	CLA	2	0
13	B	841	BCR	1	0
10	B	806	CLA	3	0
10	A	822	CLA	5	0
10	A	820	CLA	1	0
10	A	812	CLA	3	0
10	B	827	CLA	2	0
10	B	808	CLA	1	0
10	B	834	CLA	1	0
15	A	855	LMU	2	0
10	A	805	CLA	1	0
10	A	832	CLA	1	0
13	A	851	BCR	2	0
10	A	819	CLA	2	0
10	B	802	CLA	2	0
10	A	804	CLA	1	0
10	A	843	CLA	4	0
10	A	818	CLA	1	0
10	A	842	CLA	2	0
10	B	814	CLA	1	0
13	I	101	BCR	2	0
10	B	818	CLA	4	0
10	A	814	CLA	3	0
10	A	807	CLA	1	0
10	B	828	CLA	1	0
10	B	821	CLA	1	0
13	A	850	BCR	3	0
12	A	847	LHG	3	0
13	L	306	BCR	1	0
10	B	837	CLA	1	0
10	A	841	CLA	2	0
10	B	829	CLA	2	0
10	B	801	CLA	1	0
10	A	828	CLA	2	0
16	A	858	LMG	1	0
13	L	301	BCR	1	0
10	B	813	CLA	4	0
10	A	837	CLA	1	0

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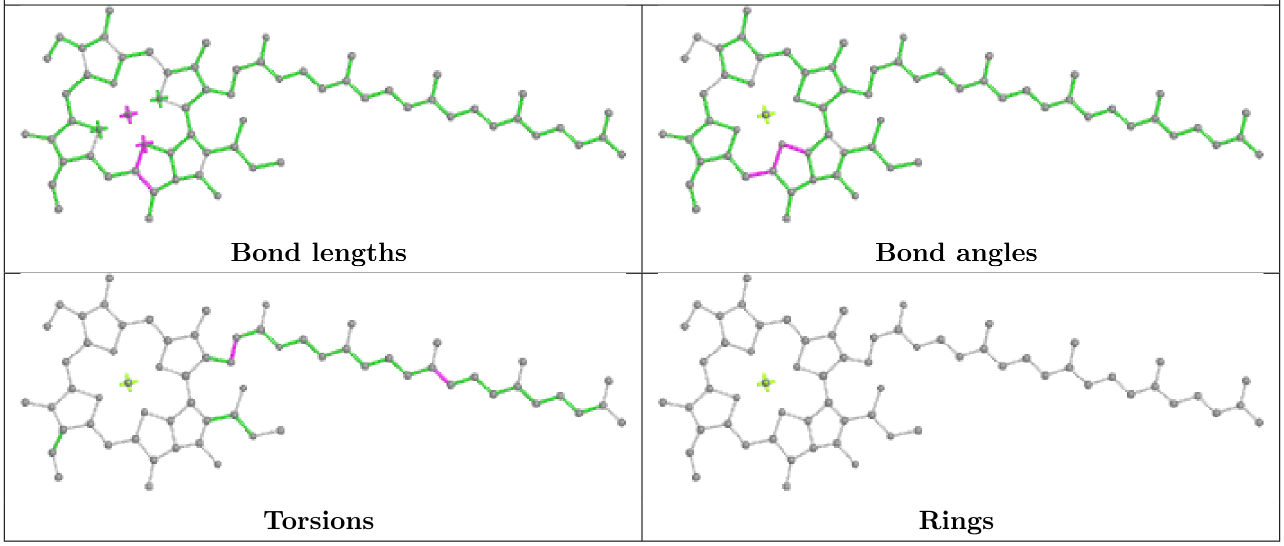
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	A	844	PQN	2	0
10	A	833	CLA	2	0
10	A	854	CLA	3	0
10	A	829	CLA	2	0
13	B	843	BCR	1	0
13	B	840	BCR	1	0
10	A	825	CLA	1	0
10	B	812	CLA	2	0
10	A	806	CLA	1	0
10	A	836	CLA	2	0
10	B	807	CLA	2	0
13	A	849	BCR	2	0
10	B	825	CLA	3	0
10	B	823	CLA	3	0
10	L	302	CLA	1	0
10	A	802	CLA	3	0
17	B	844	DGD	1	0
10	A	826	CLA	4	0
10	B	815	CLA	1	0
13	A	852	BCR	7	0
13	A	848	BCR	2	0
10	B	831	CLA	2	0
10	B	804	CLA	1	0
10	L	304	CLA	2	0
10	B	833	CLA	3	0
10	B	824	CLA	2	0
10	A	817	CLA	1	0
10	A	803	CLA	1	0
10	A	815	CLA	3	0
12	B	845	LHG	6	0
11	B	839	PQN	1	0
10	B	826	CLA	2	0
10	A	808	CLA	1	0
10	A	809	CLA	3	0
10	A	810	CLA	1	0
10	A	840	CLA	1	0
15	A	859	LMU	1	0
10	B	822	CLA	2	0

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

Ligand CLA A 830



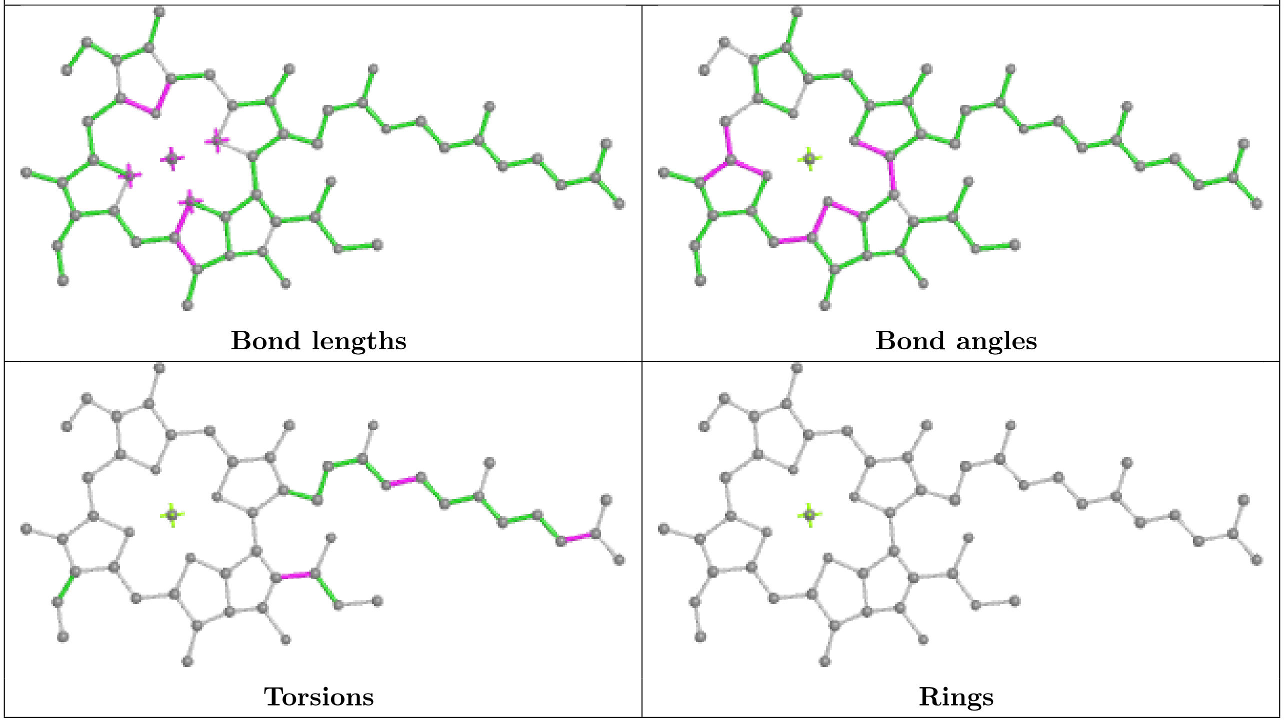
Bond lengths

Bond angles

Torsions

Rings

Ligand CL0 H 201



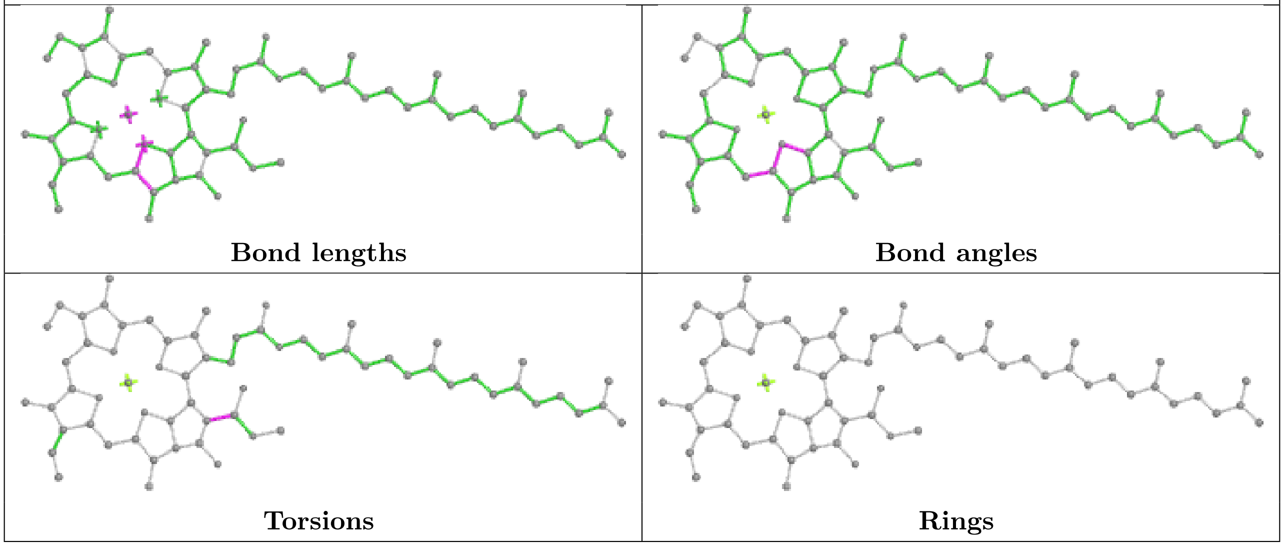
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA A 835



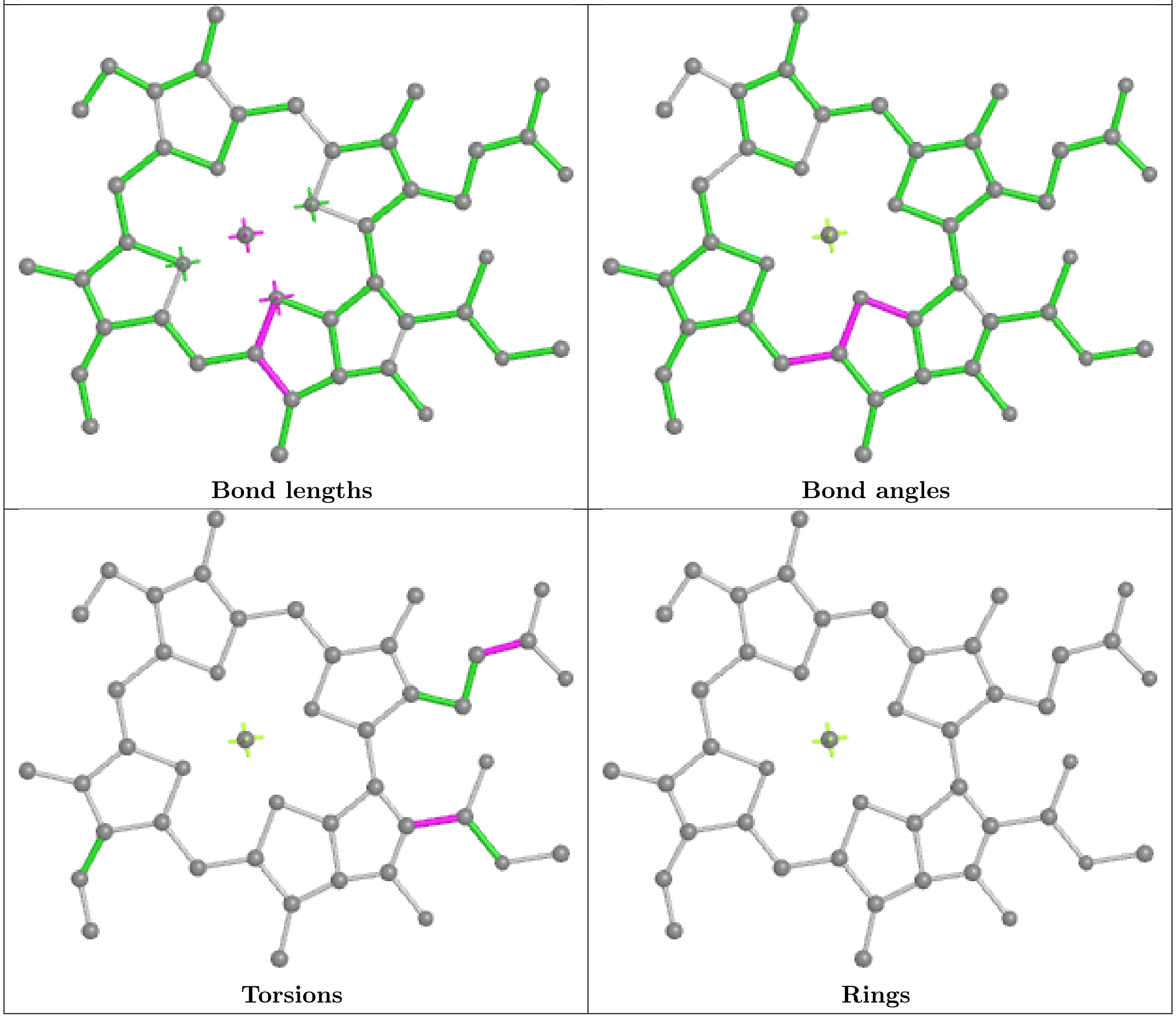
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA A 813



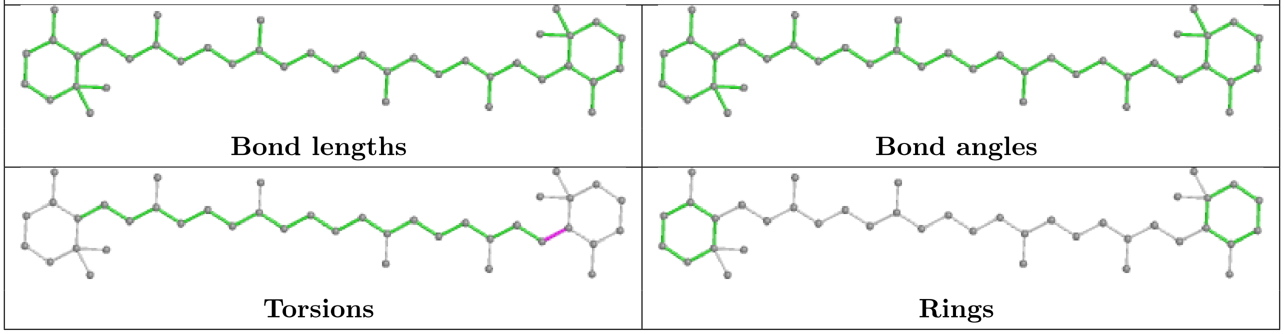
Bond lengths

Bond angles

Torsions

Rings

Ligand BCR B 842



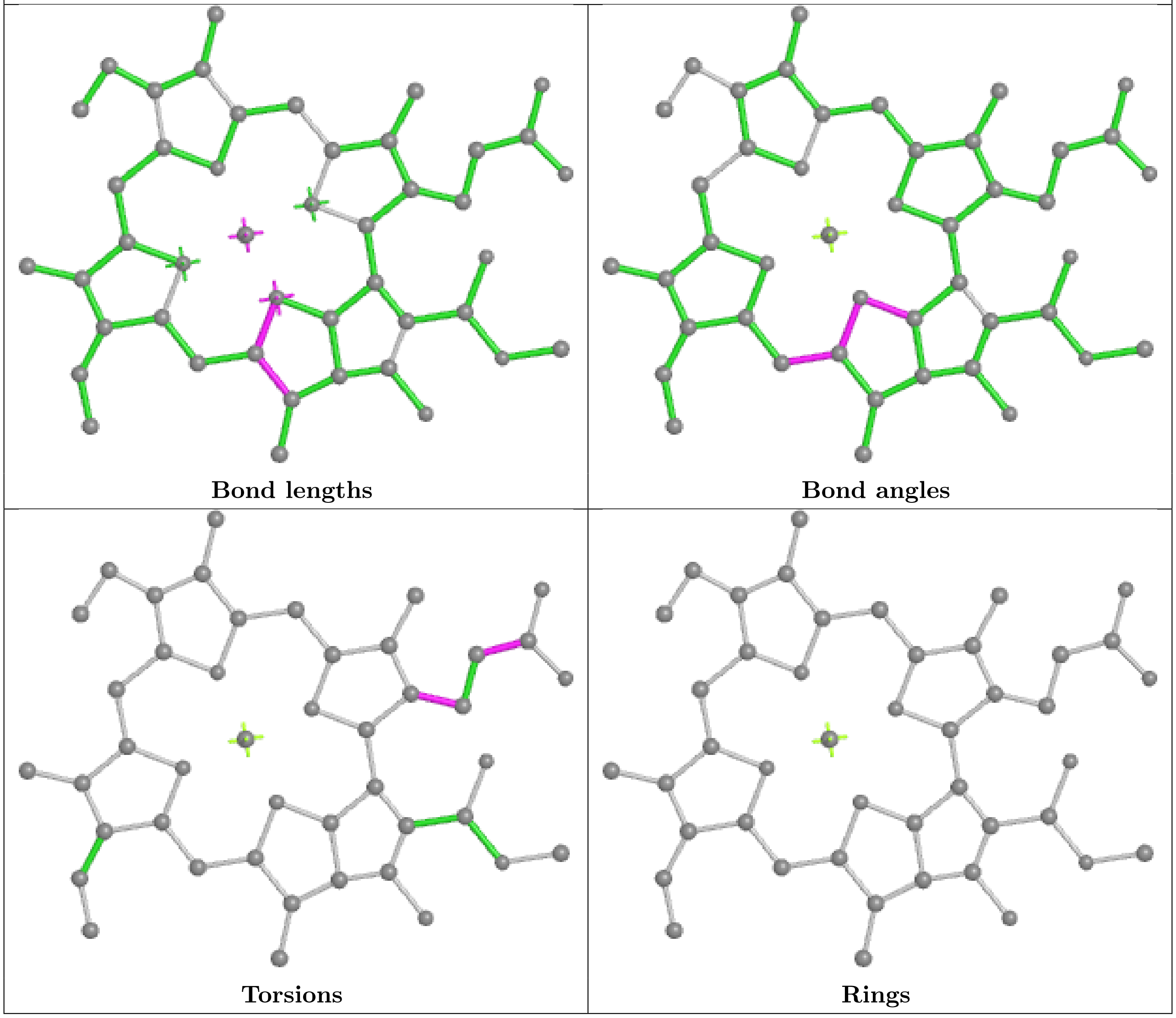
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA B 803



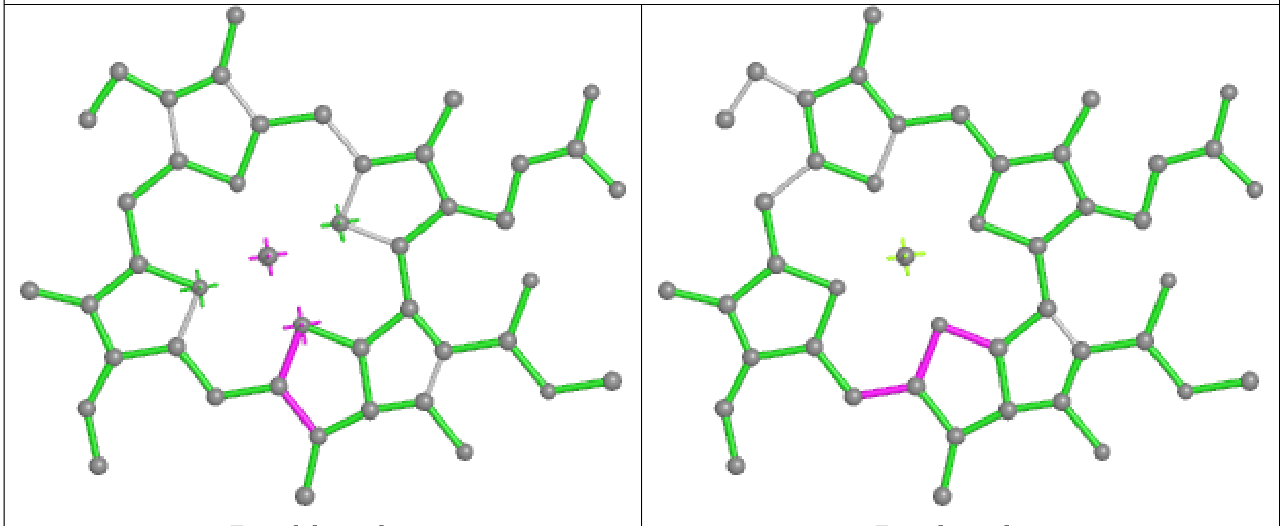
Bond lengths

Bond angles

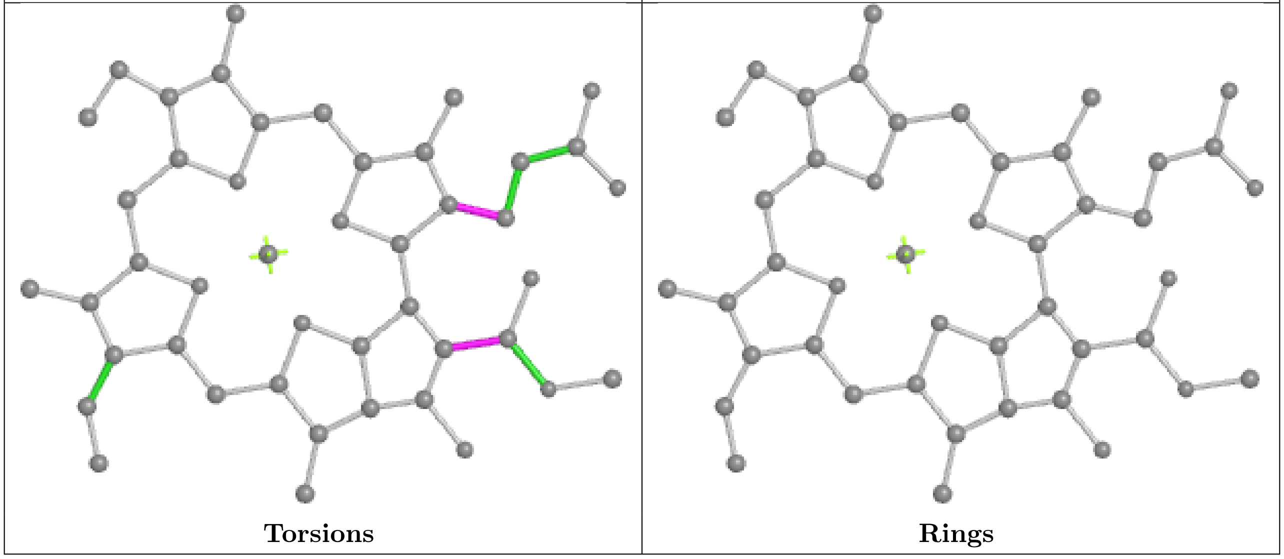
Torsions

Rings

Ligand CLA B 819

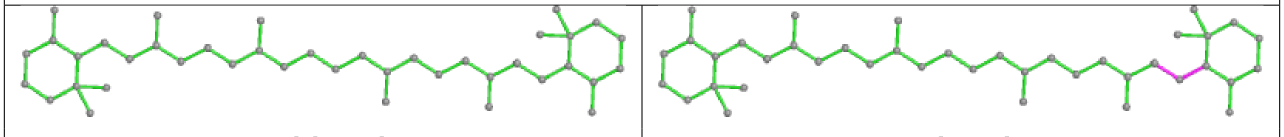


Bond lengths Bond angles

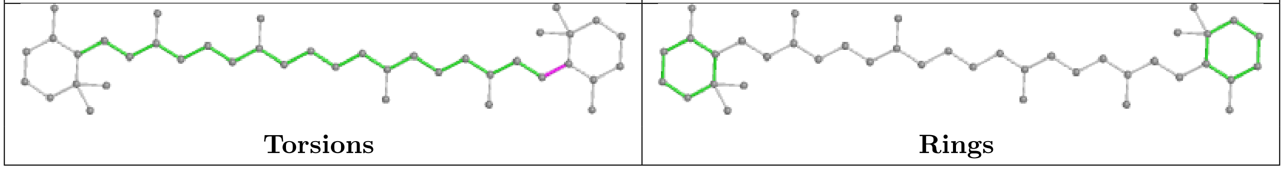


Torsions Rings

Ligand BCR L 305

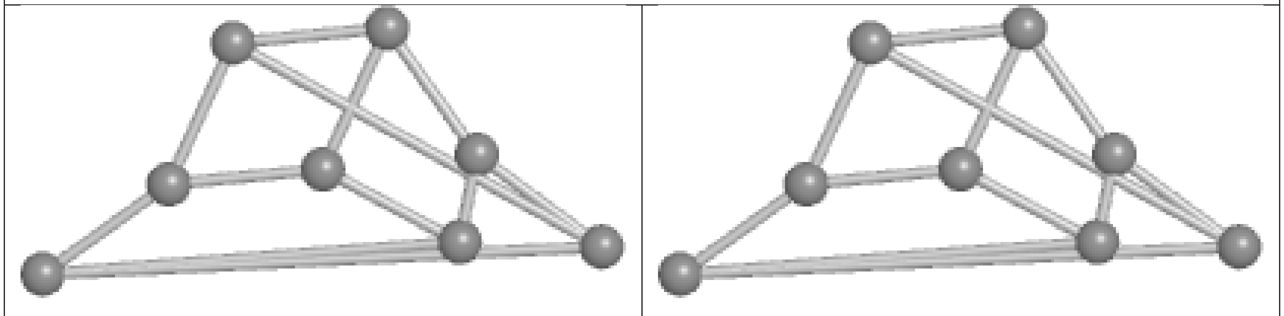


Bond lengths Bond angles



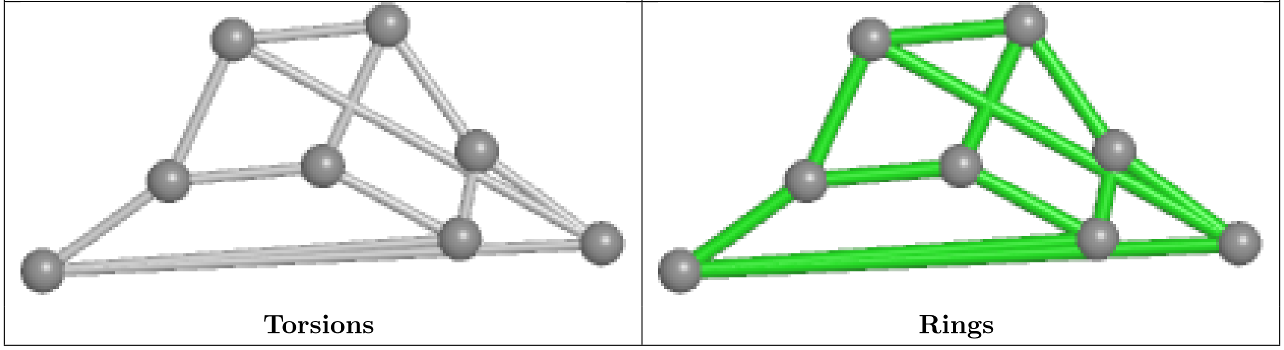
Torsions Rings

Ligand SF4 C 102



Bond lengths

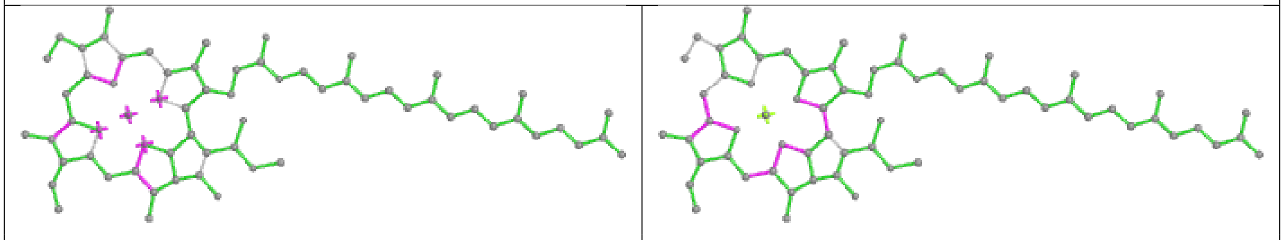
Bond angles



Torsions

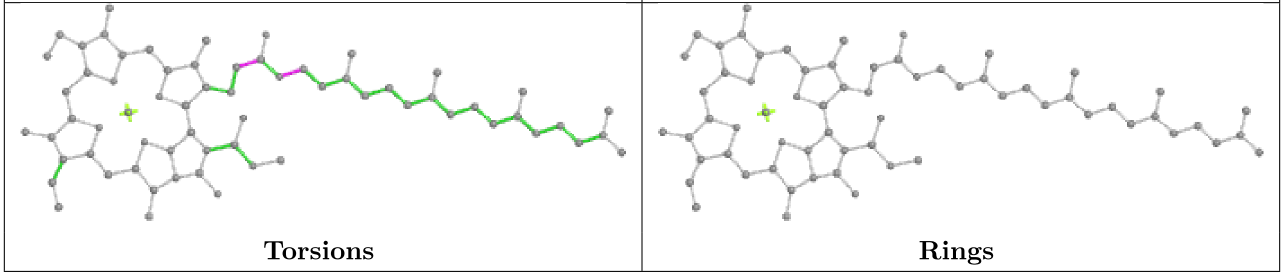
Rings

Ligand CL0 A 801



Bond lengths

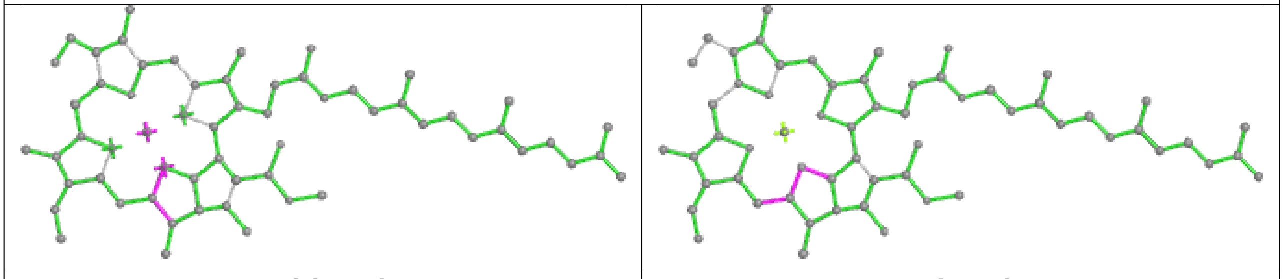
Bond angles



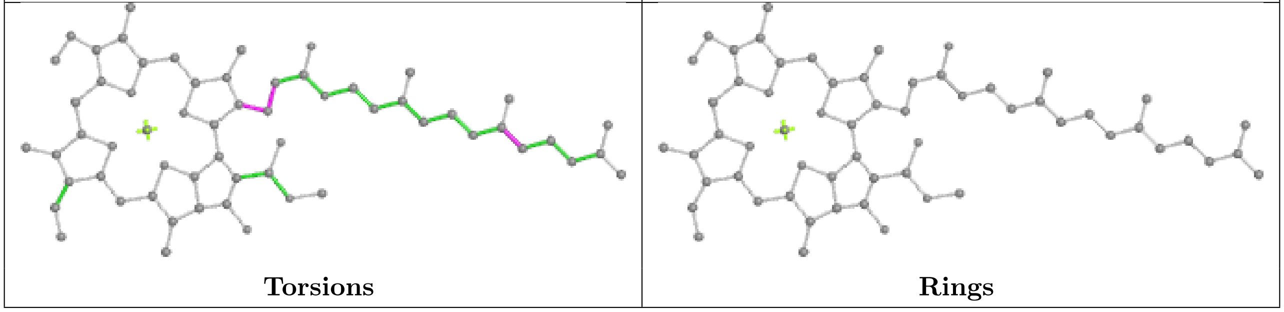
Torsions

Rings

Ligand CLA B 816

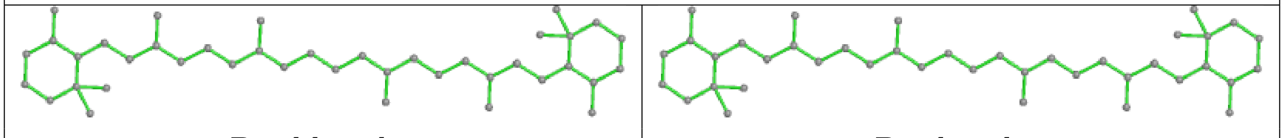


Bond lengths **Bond angles**

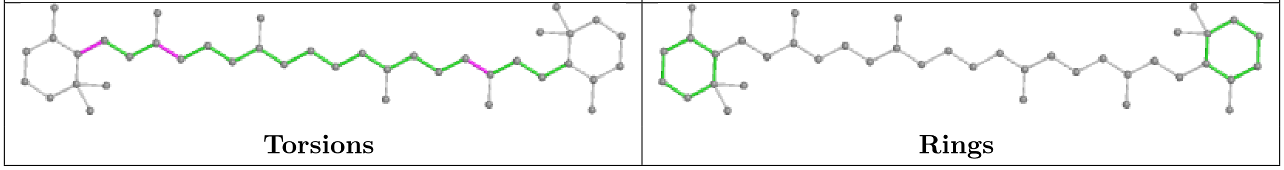


Torsions **Rings**

Ligand BCR B 841

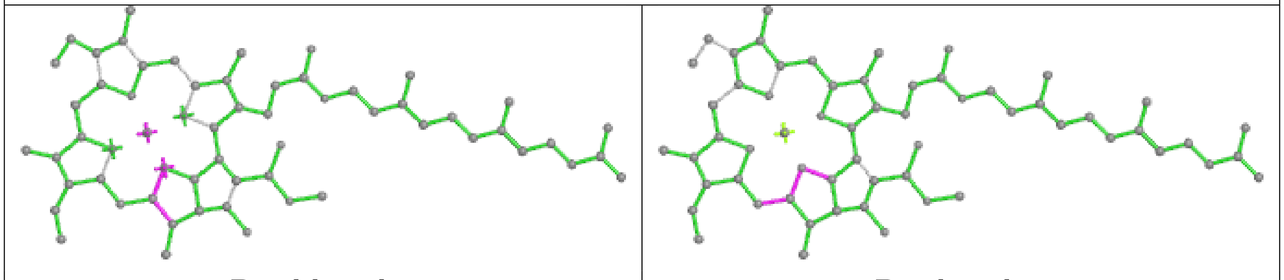


Bond lengths **Bond angles**

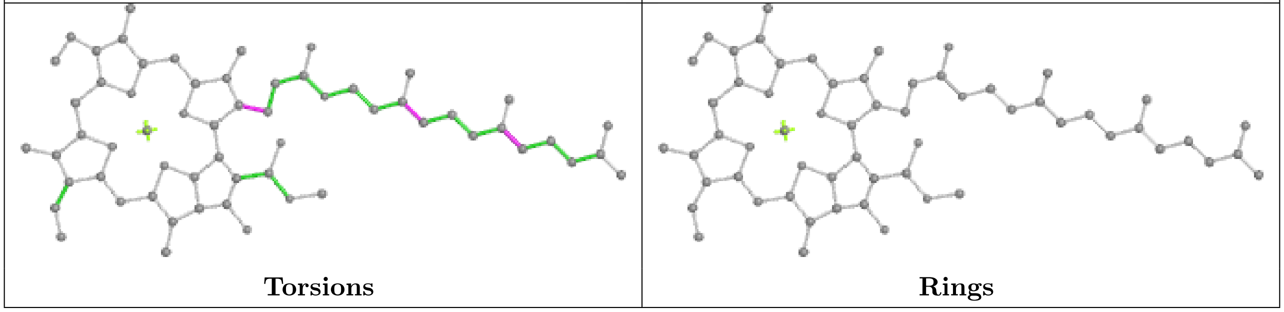


Torsions **Rings**

Ligand CLA B 806

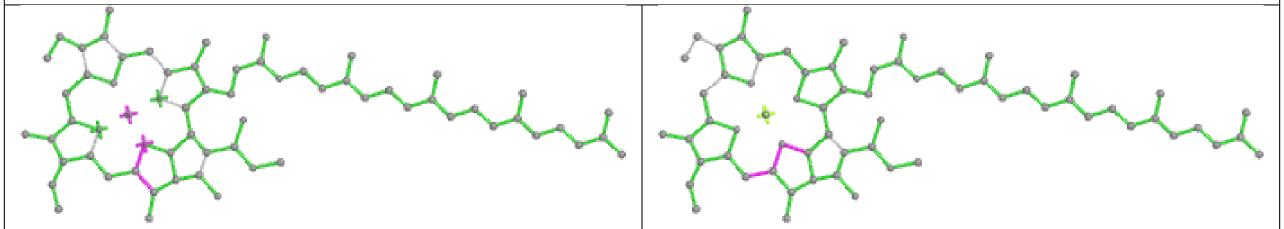


Bond lengths **Bond angles**

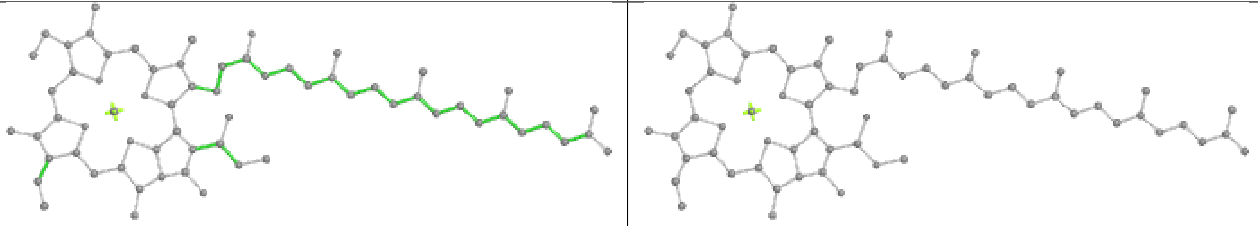


Torsions **Rings**

Ligand CLA A 822

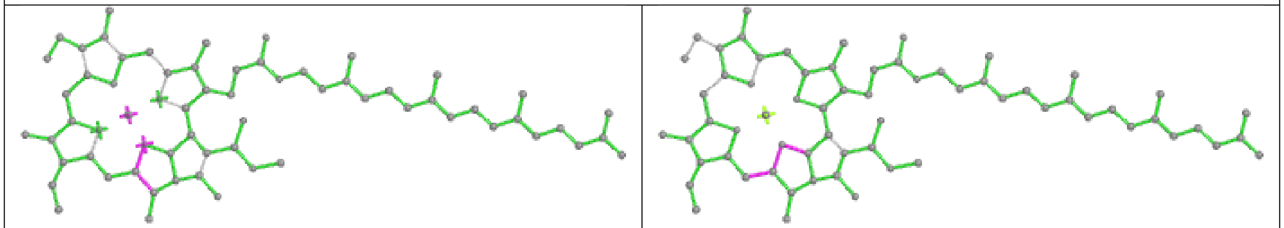


Bond lengths Bond angles

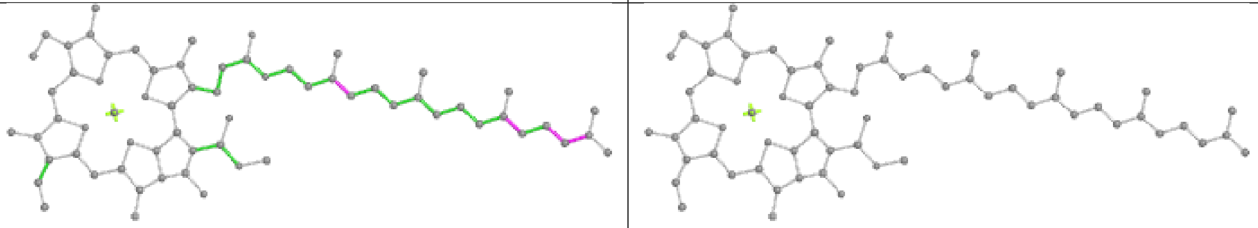


Torsions Rings

Ligand CLA A 820

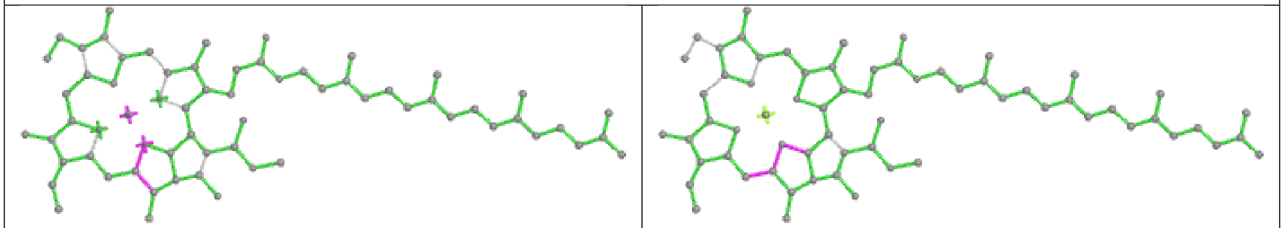


Bond lengths Bond angles

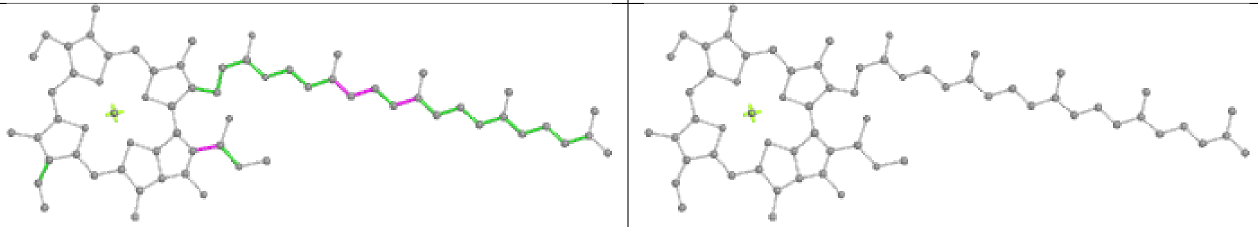


Torsions Rings

Ligand CLA A 812

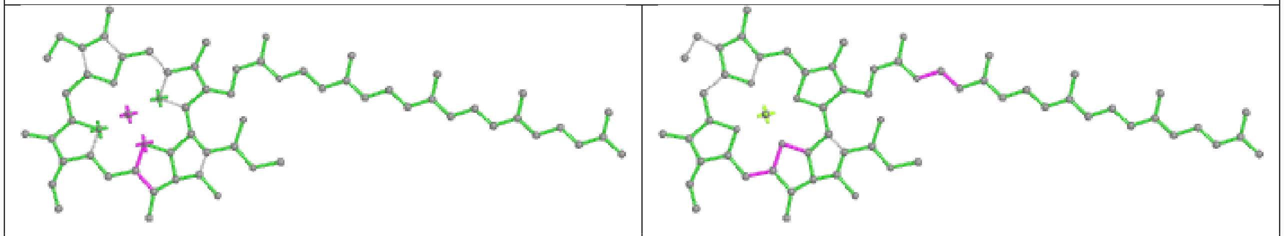


Bond lengths Bond angles



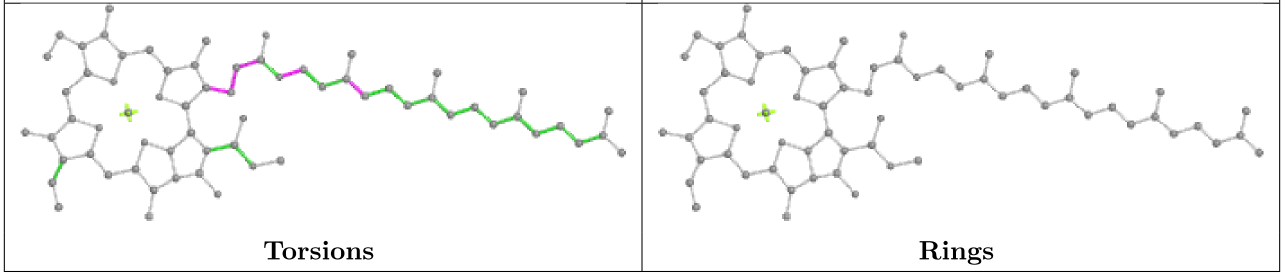
Torsions Rings

Ligand CLA B 827



Bond lengths

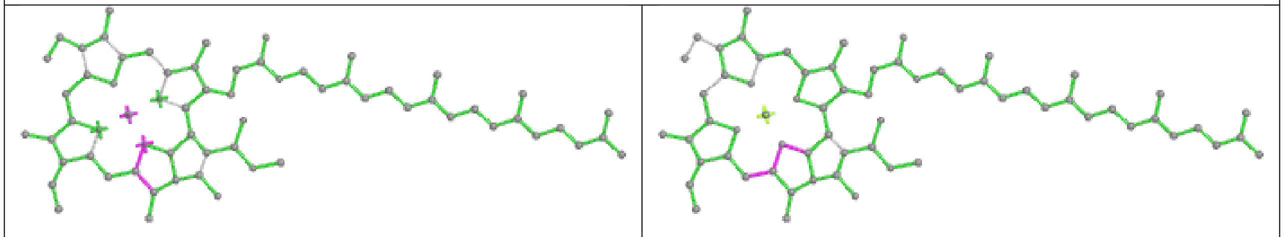
Bond angles



Torsions

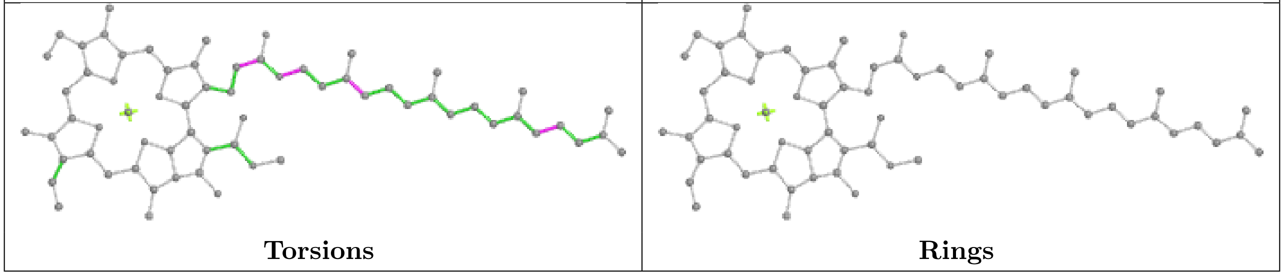
Rings

Ligand CLA B 808



Bond lengths

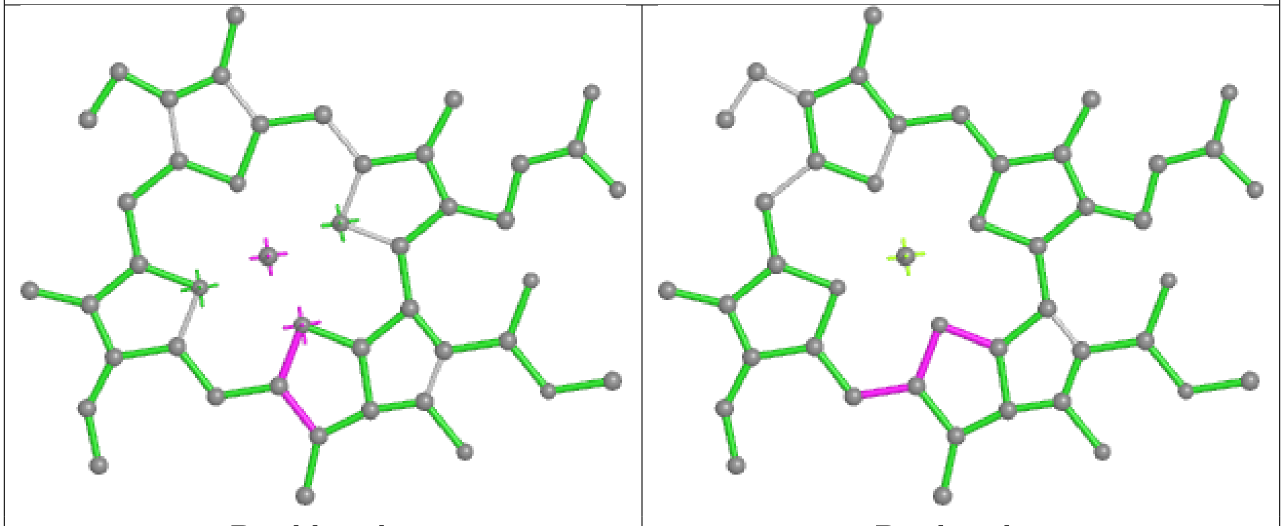
Bond angles



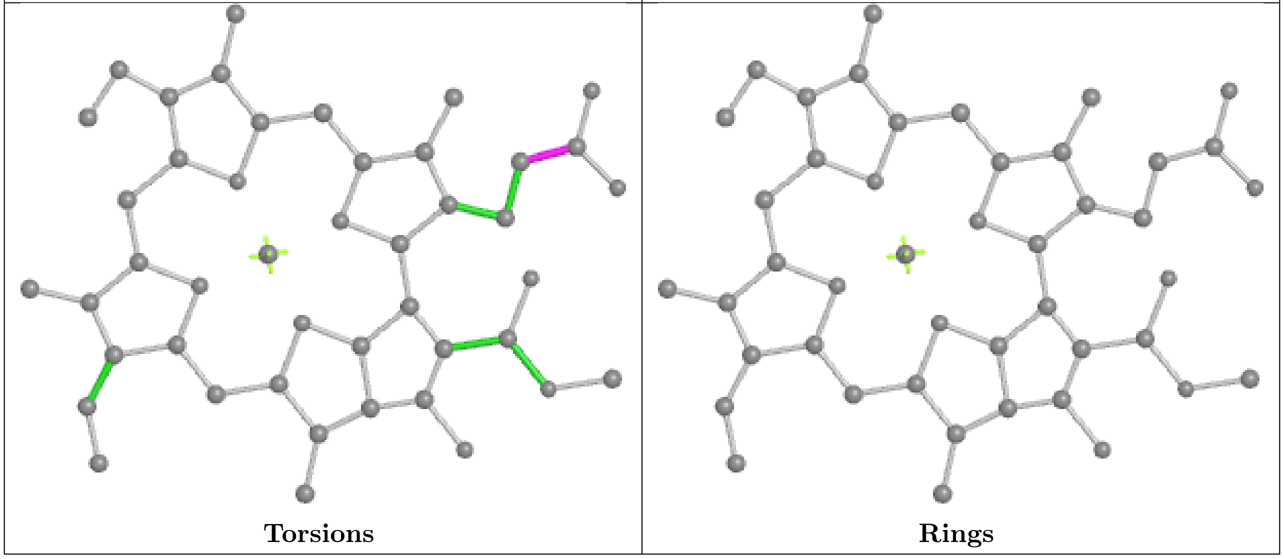
Torsions

Rings

Ligand CLA A 811

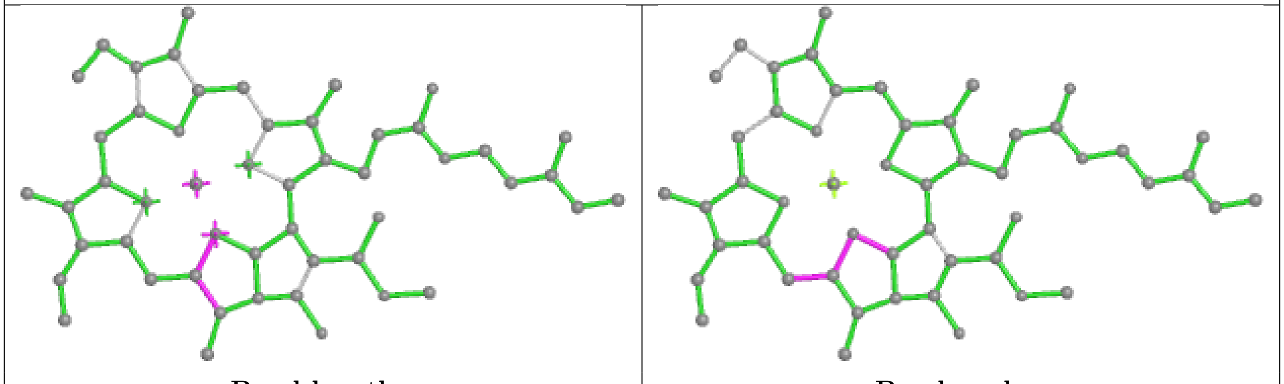


Bond lengths **Bond angles**

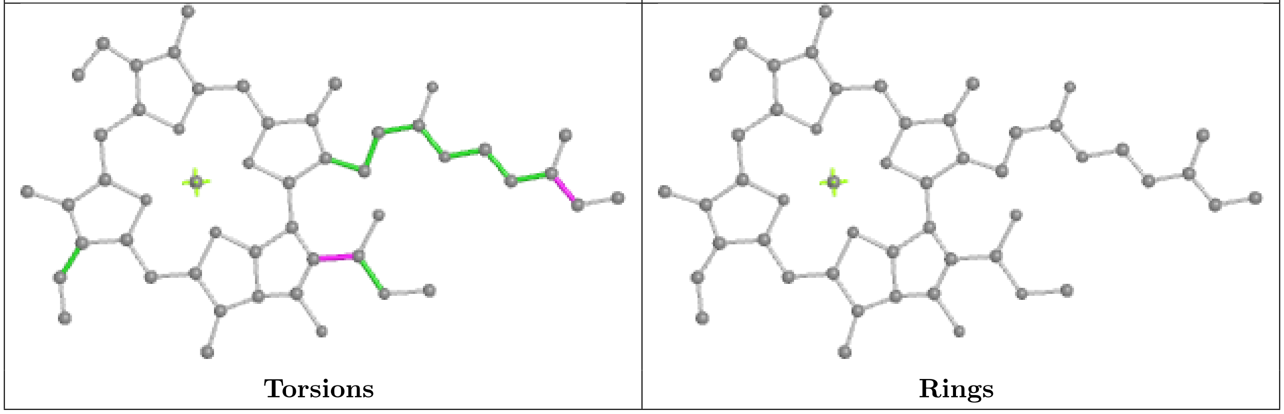


Torsions **Rings**

Ligand CLA B 834

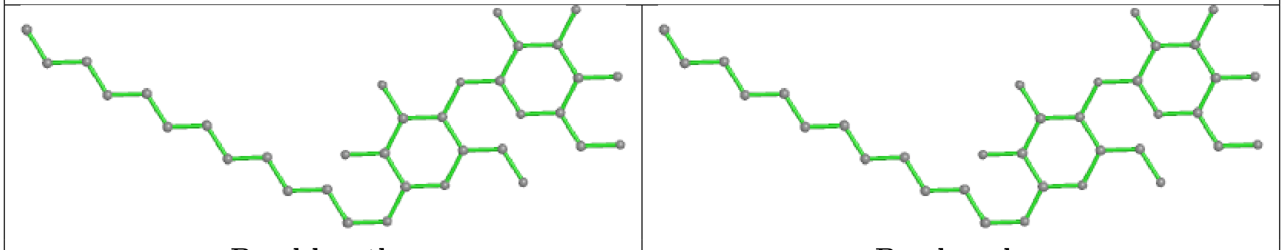


Bond lengths Bond angles

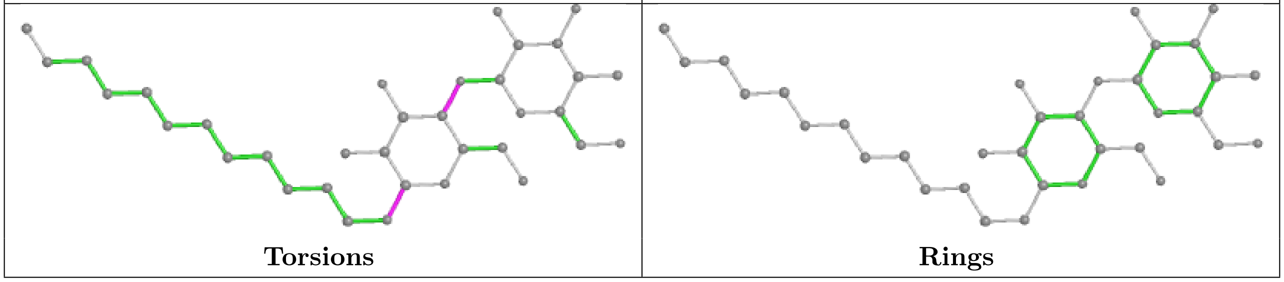


Torsions Rings

Ligand LMU A 855

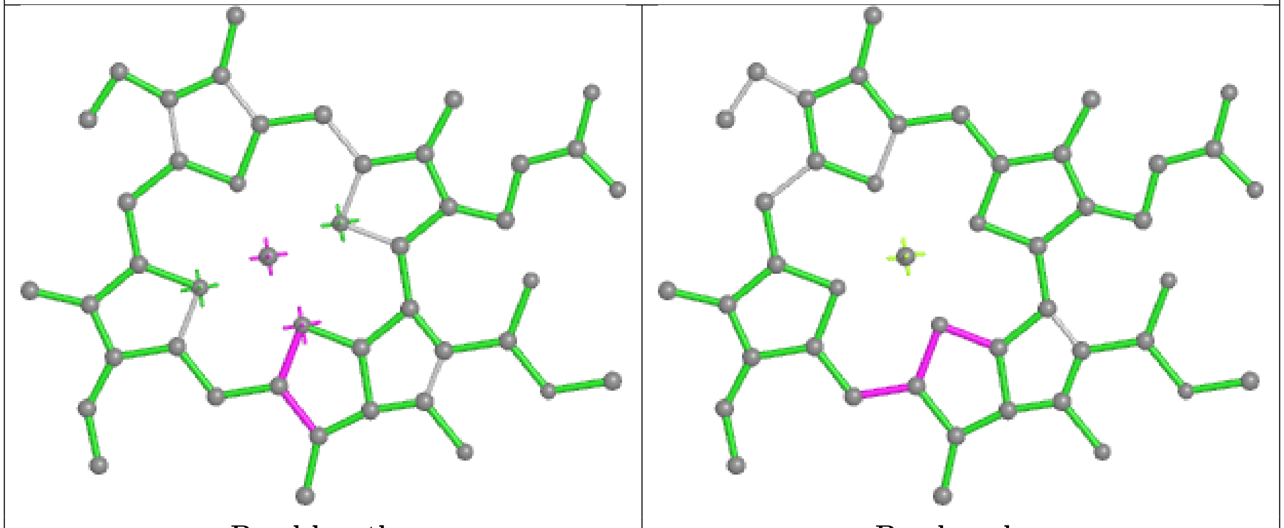


Bond lengths Bond angles



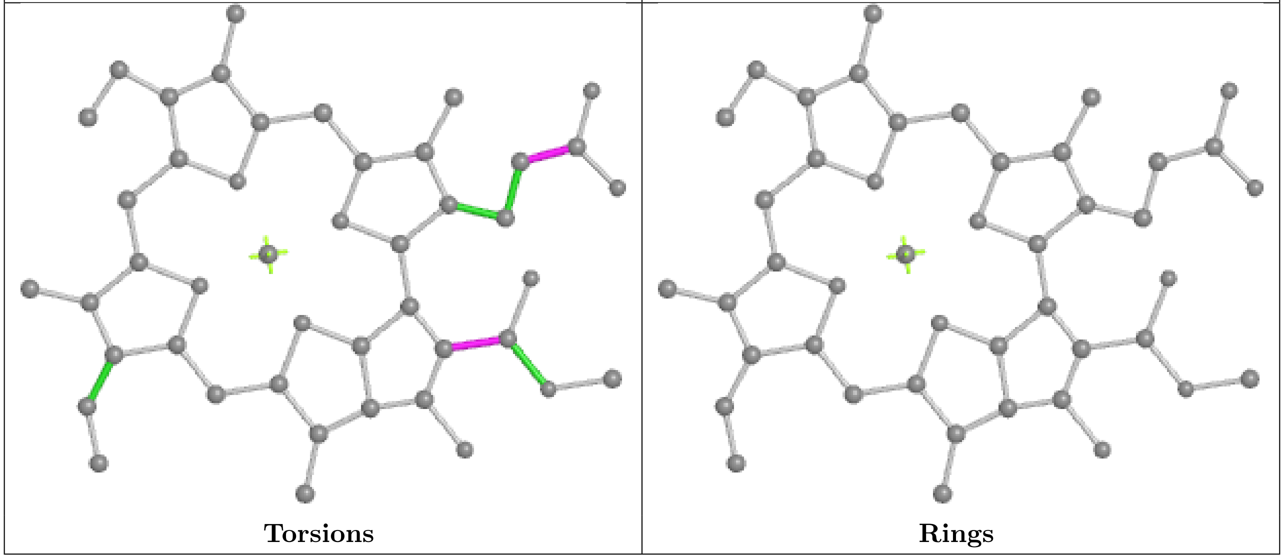
Torsions Rings

Ligand CLA B 811



Bond lengths

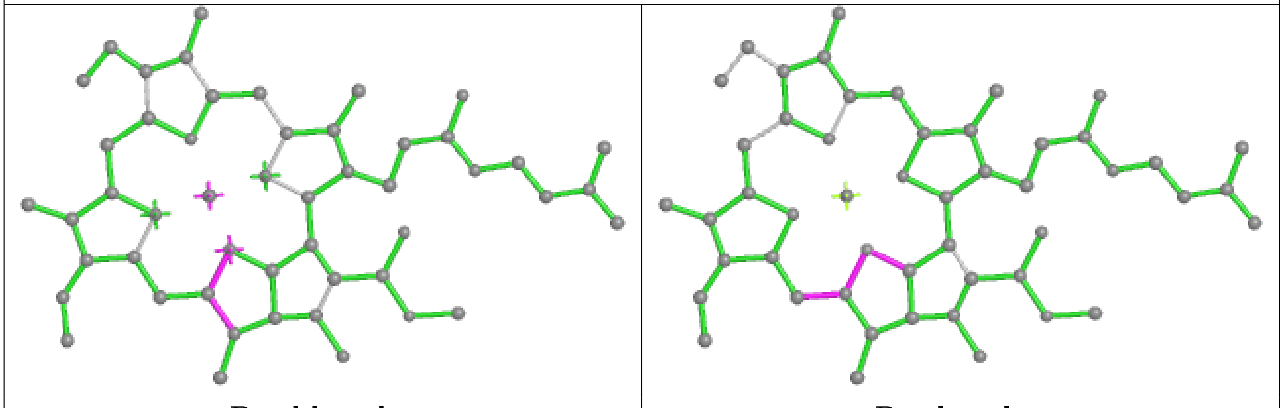
Bond angles



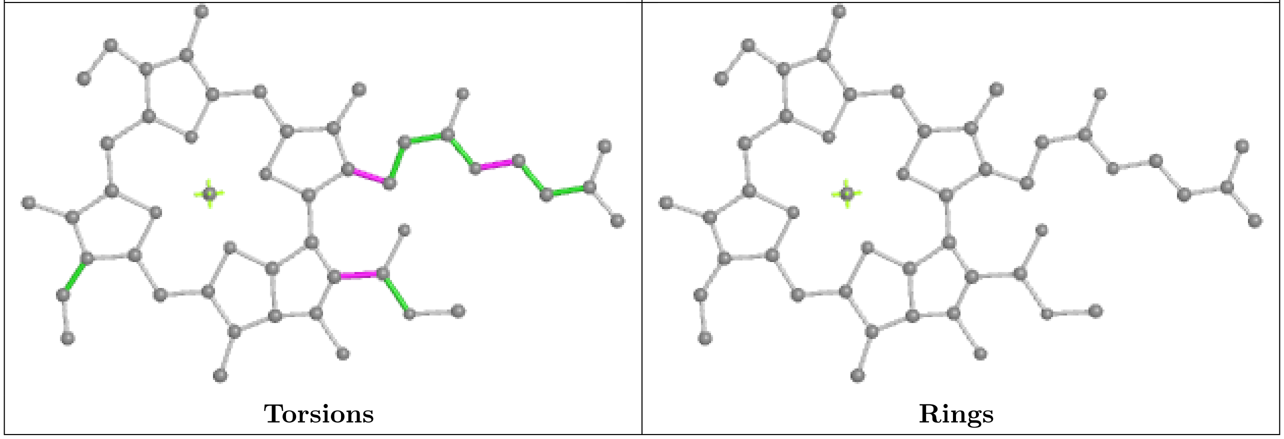
Torsions

Rings

Ligand CLA A 805

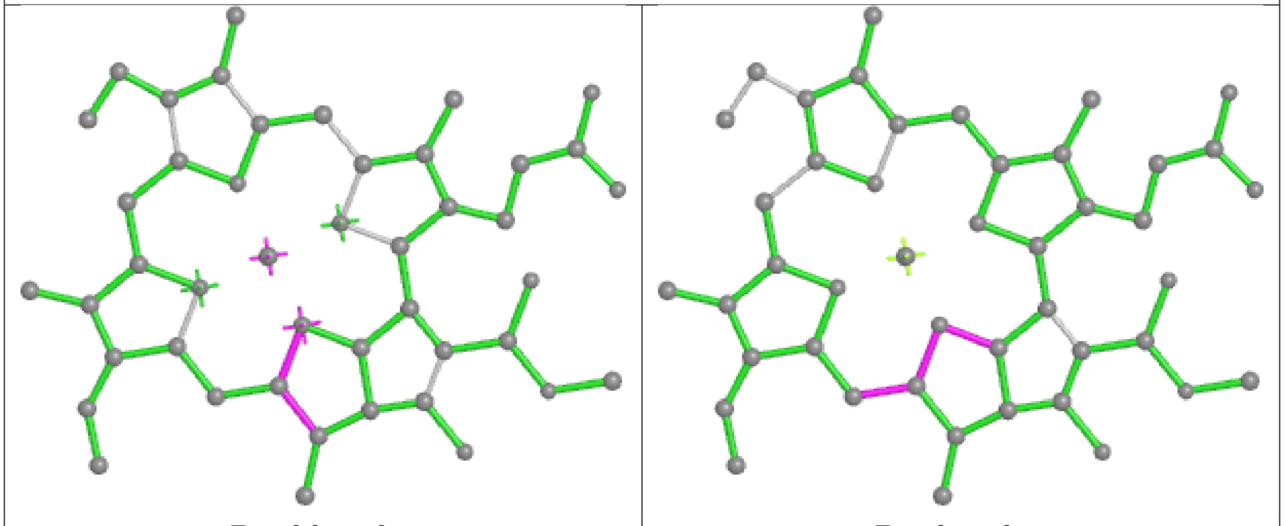


Bond lengths **Bond angles**



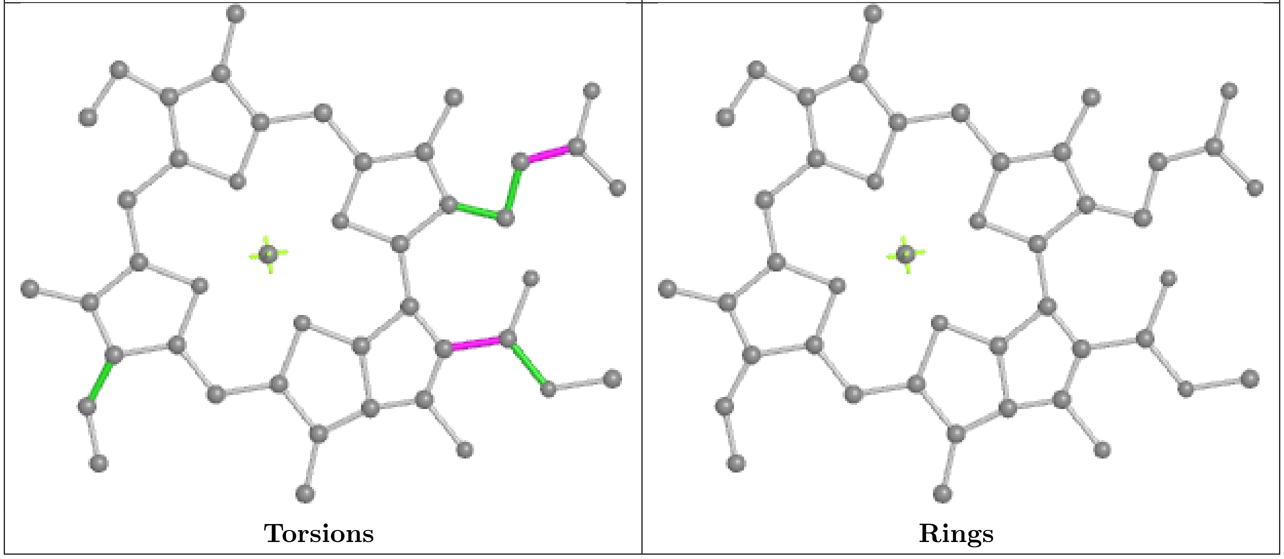
Torsions **Rings**

Ligand CLA A 832



Bond lengths

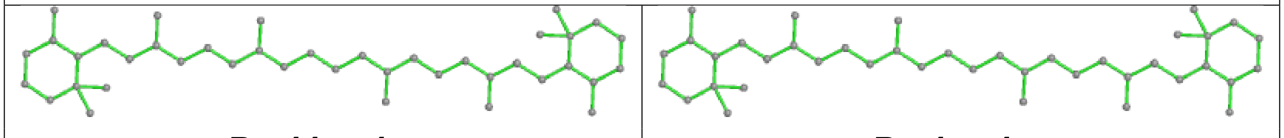
Bond angles



Torsions

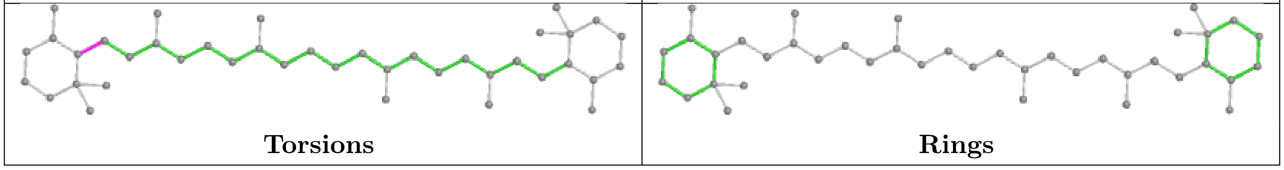
Rings

Ligand BCR A 851



Bond lengths

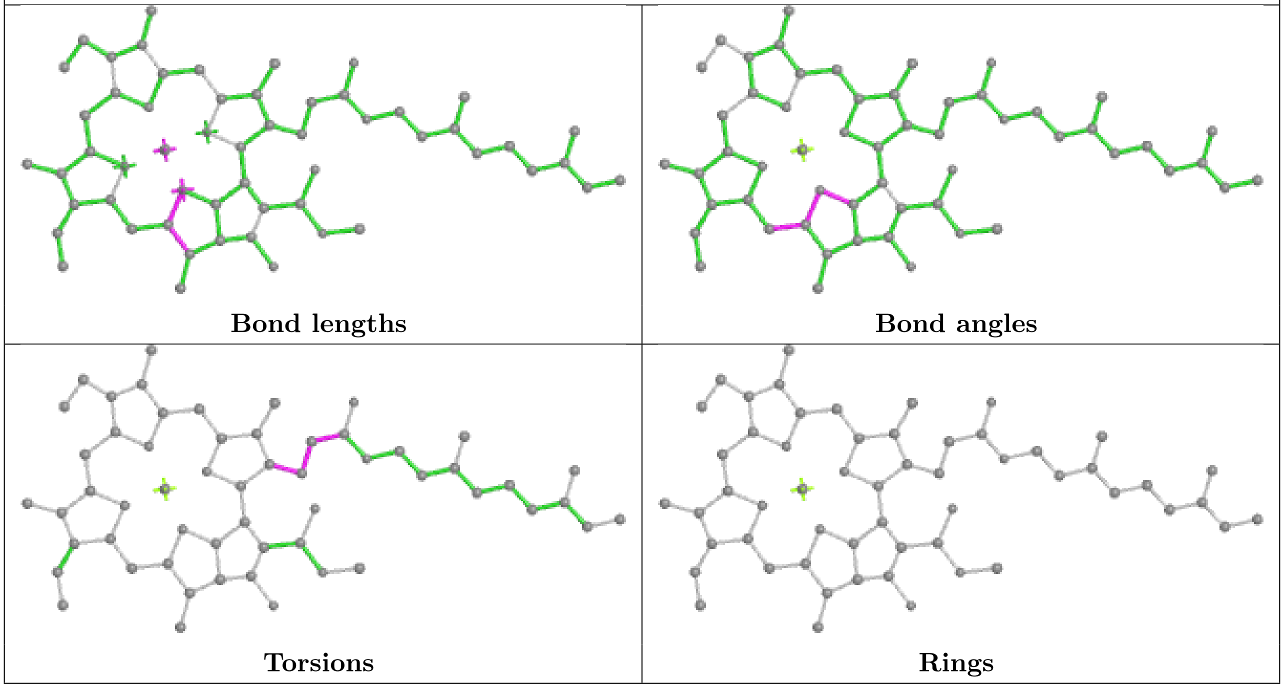
Bond angles



Torsions

Rings

Ligand CLA A 819



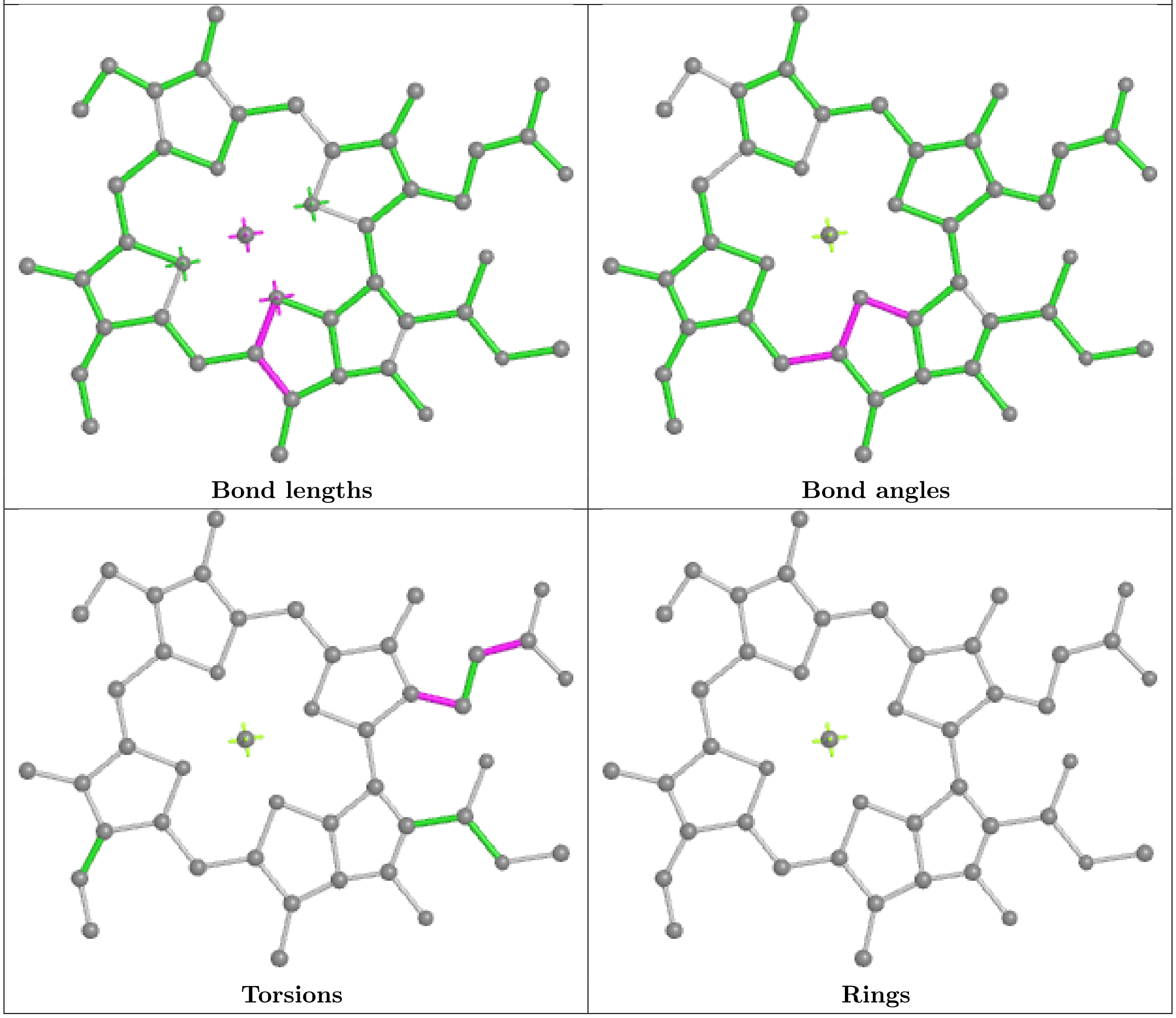
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA A 821



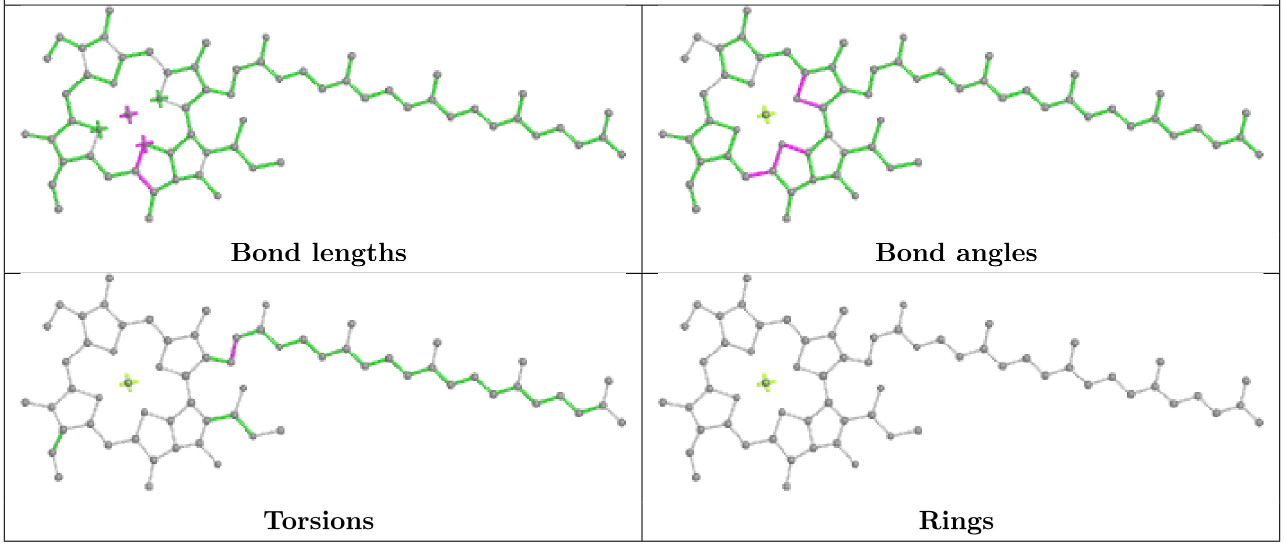
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA B 802



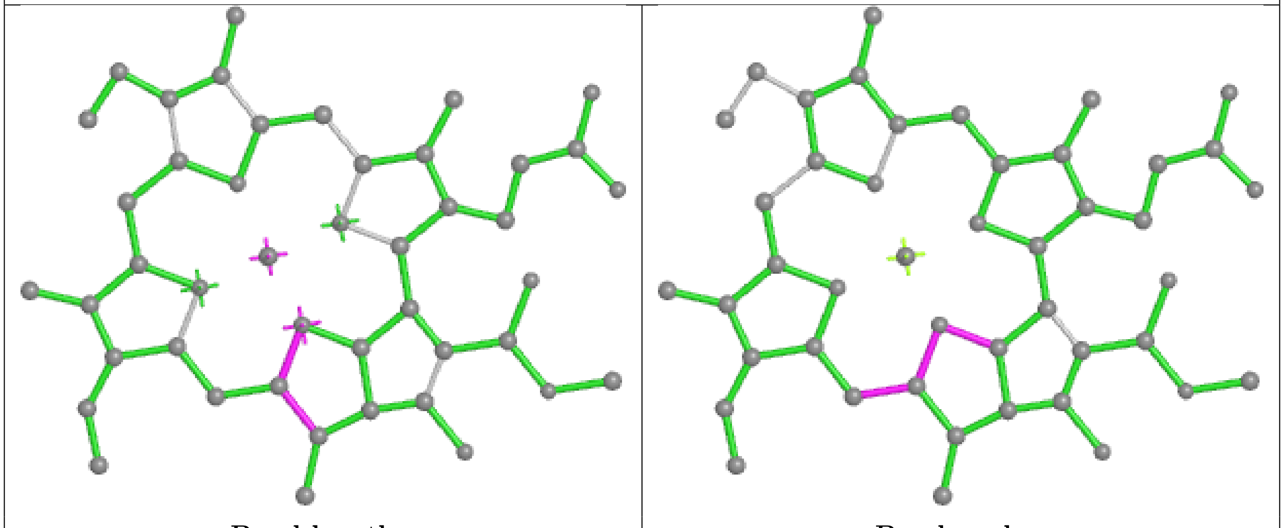
Bond lengths

Bond angles

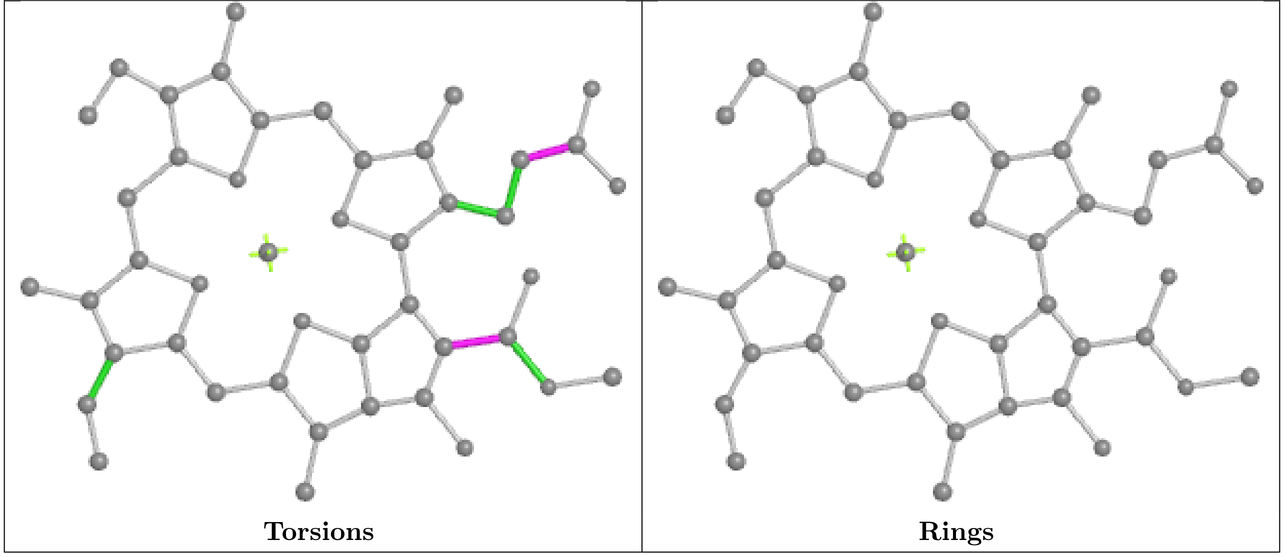
Torsions

Rings

Ligand CLA A 804

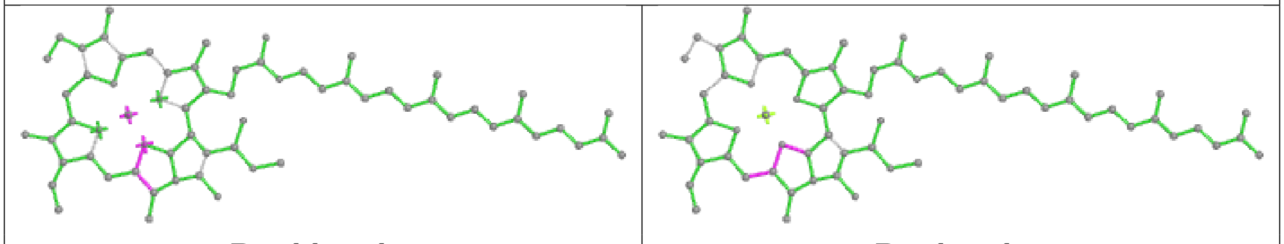


Bond lengths Bond angles

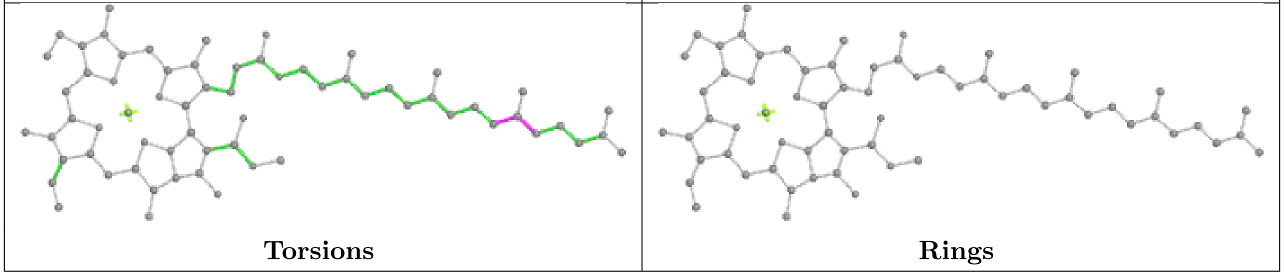


Torsions Rings

Ligand CLA A 839

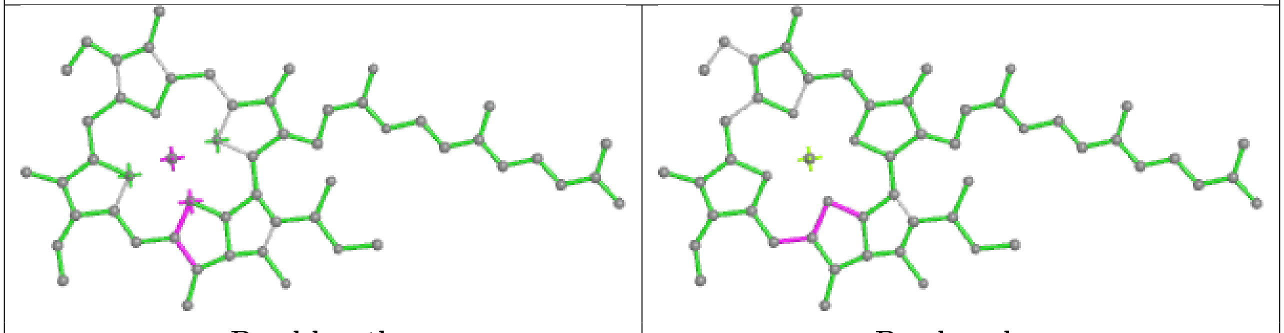


Bond lengths Bond angles



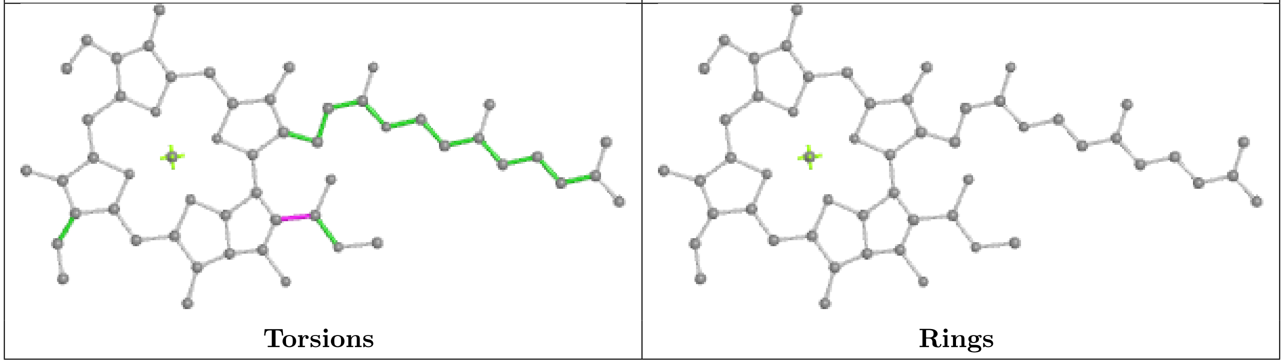
Torsions Rings

Ligand CLA A 827



Bond lengths

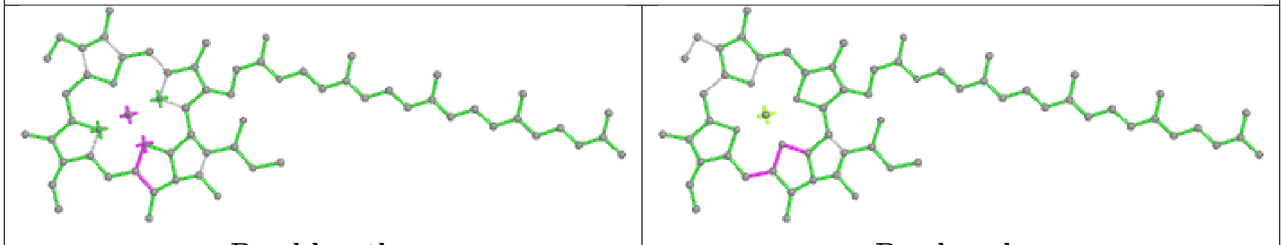
Bond angles



Torsions

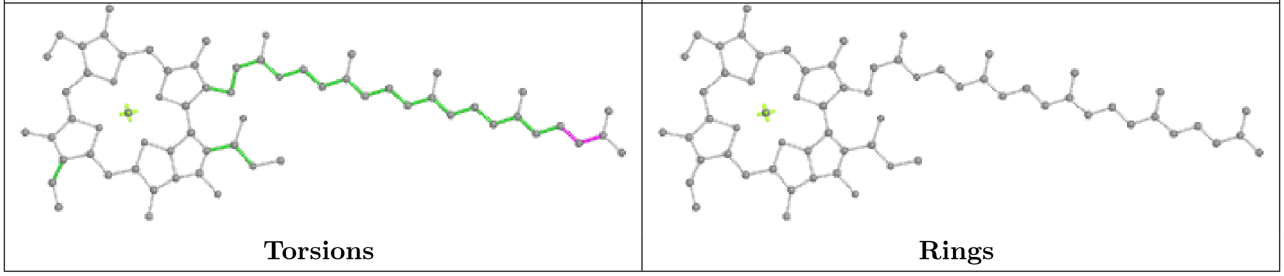
Rings

Ligand CLA B 838



Bond lengths

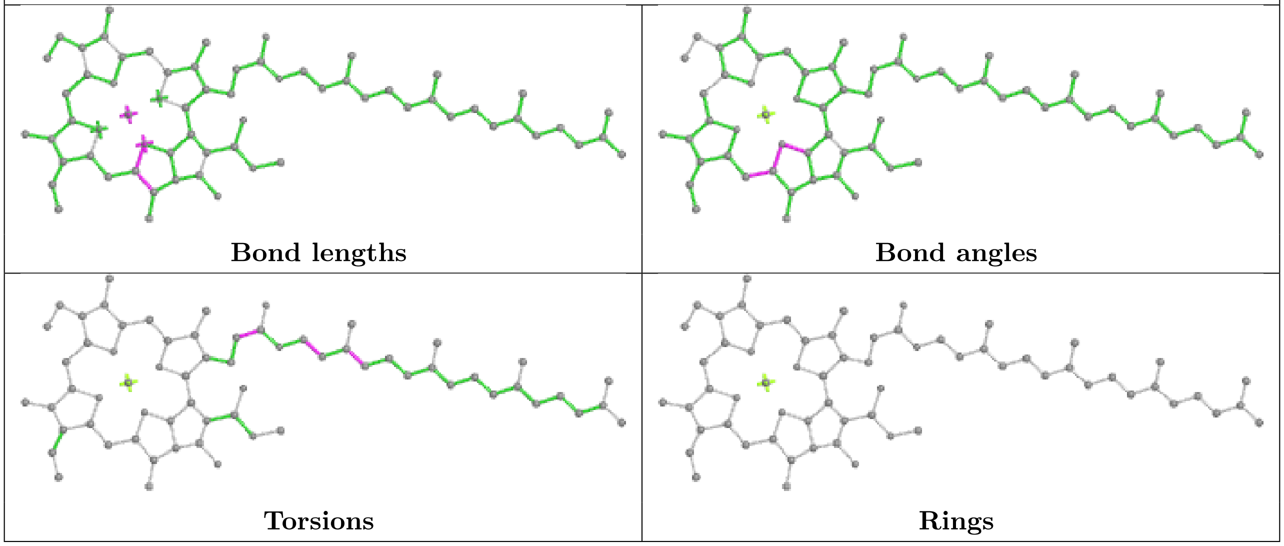
Bond angles



Torsions

Rings

Ligand CLA A 843



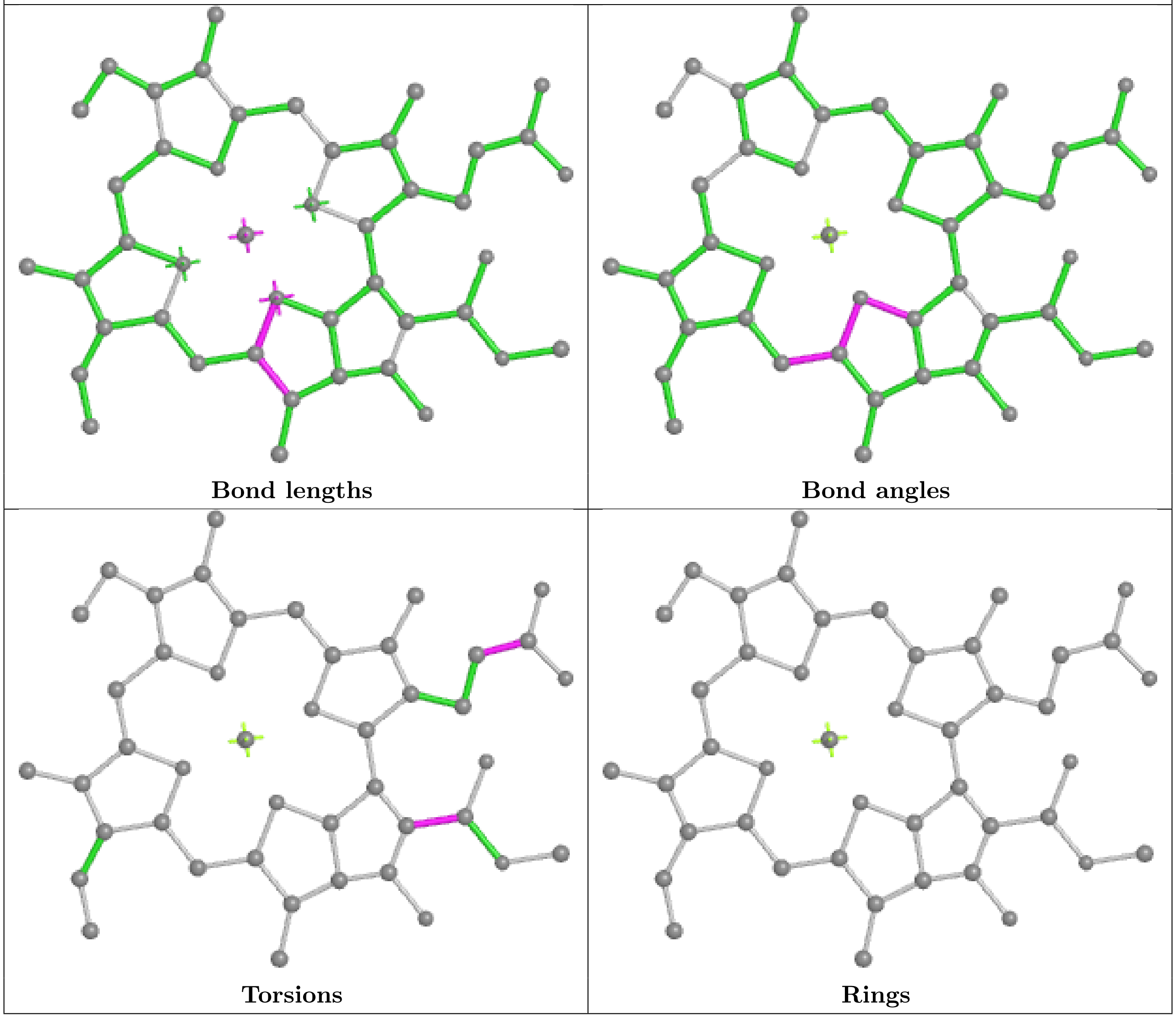
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA A 818



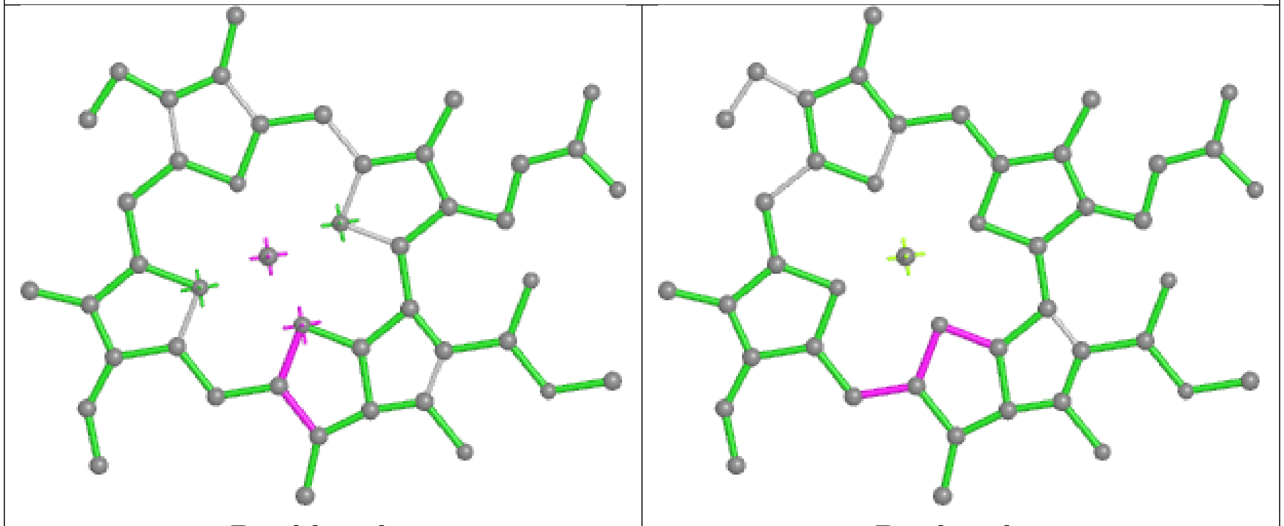
Bond lengths

Bond angles

Torsions

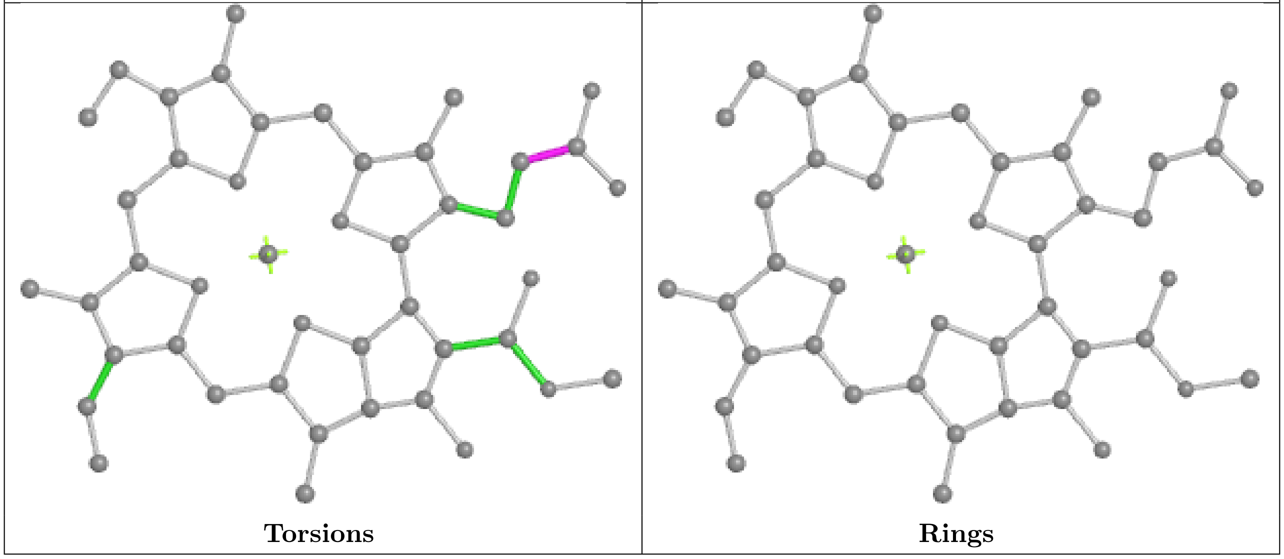
Rings

Ligand CLA A 842



Bond lengths

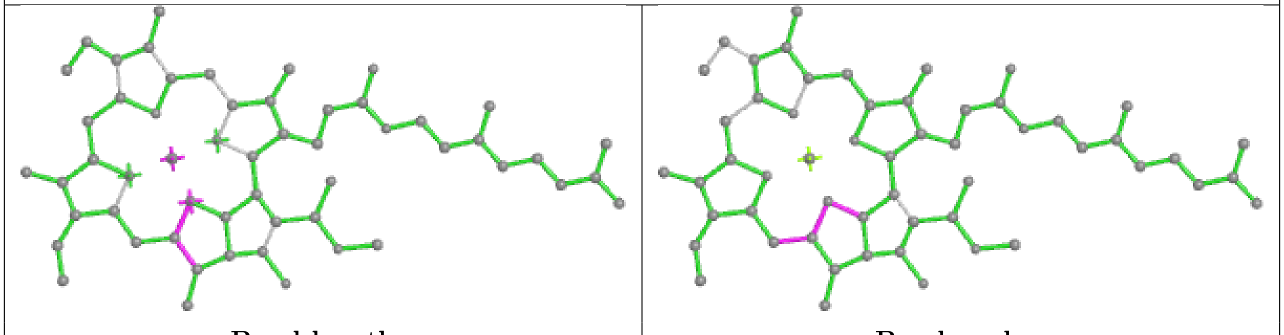
Bond angles



Torsions

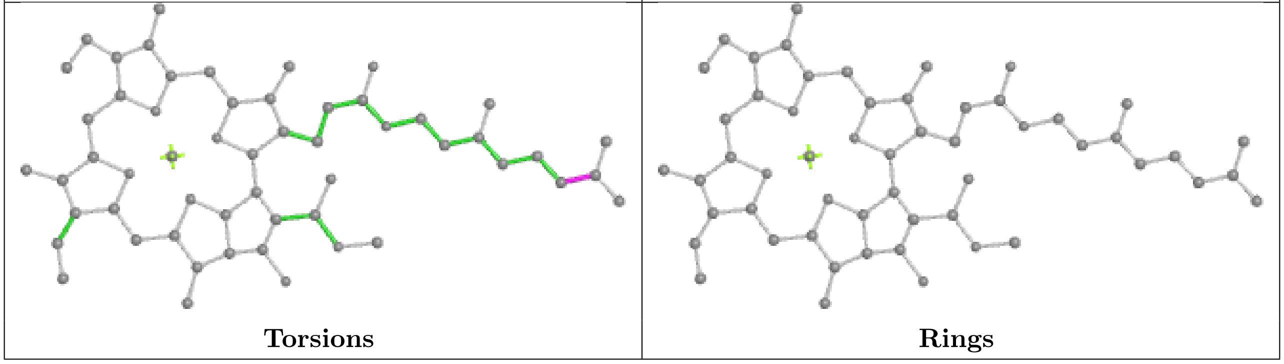
Rings

Ligand CLA B 835



Bond lengths

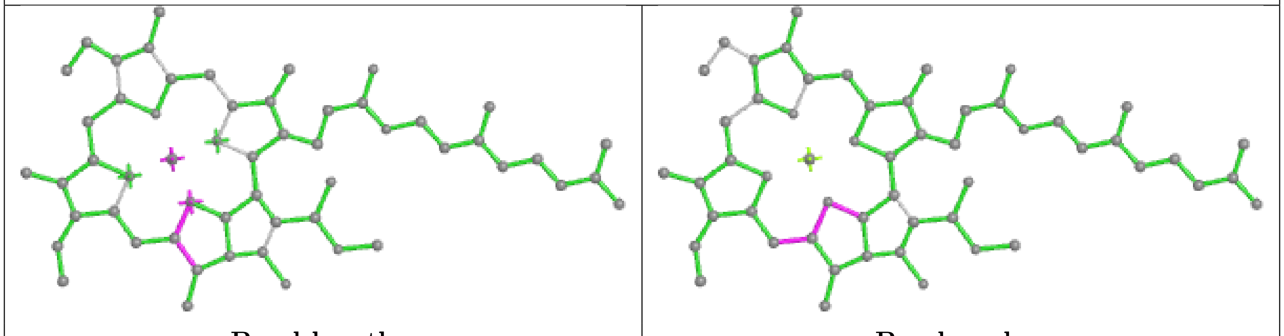
Bond angles



Torsions

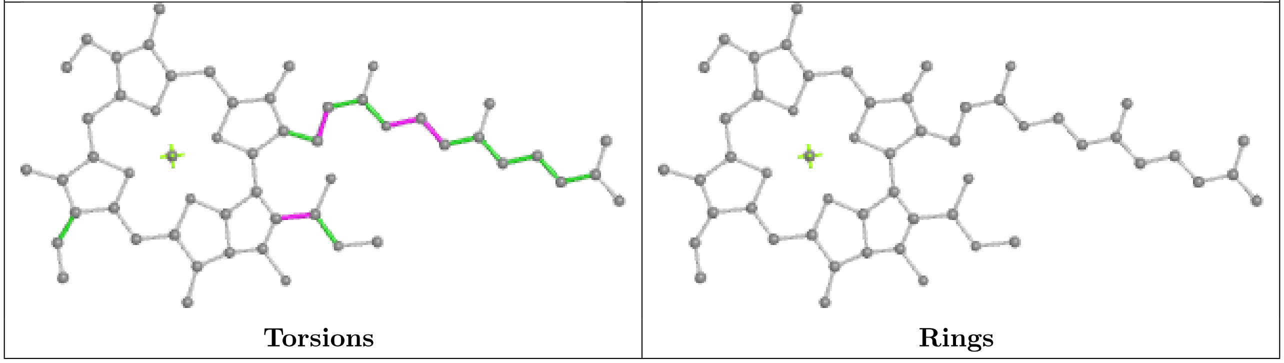
Rings

Ligand CLA B 814



Bond lengths

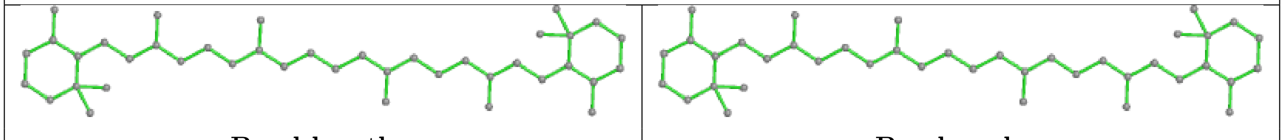
Bond angles



Torsions

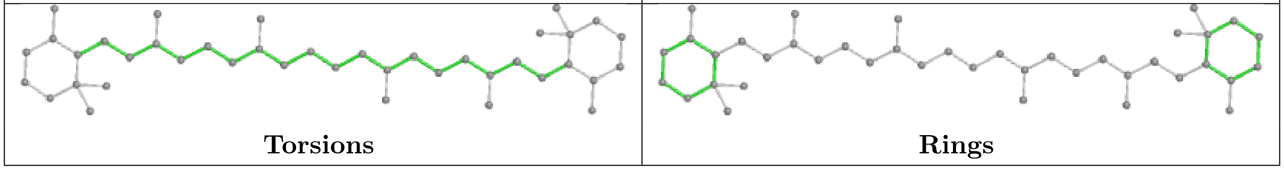
Rings

Ligand BCR I 101



Bond lengths

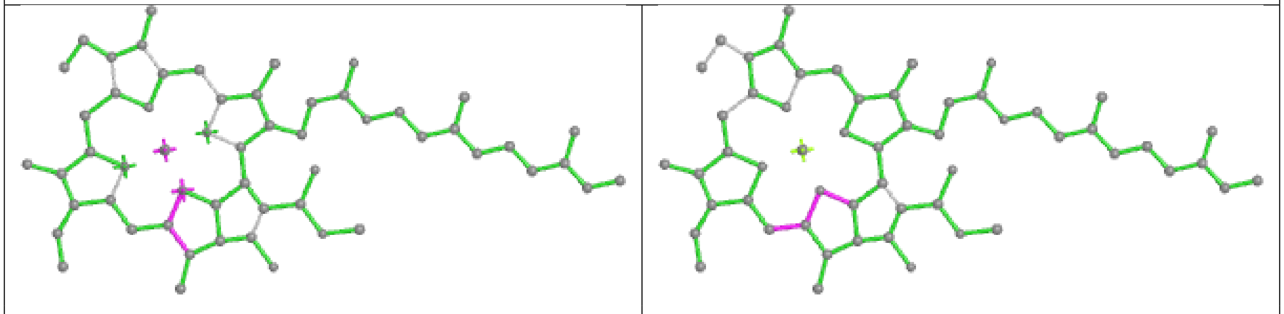
Bond angles



Torsions

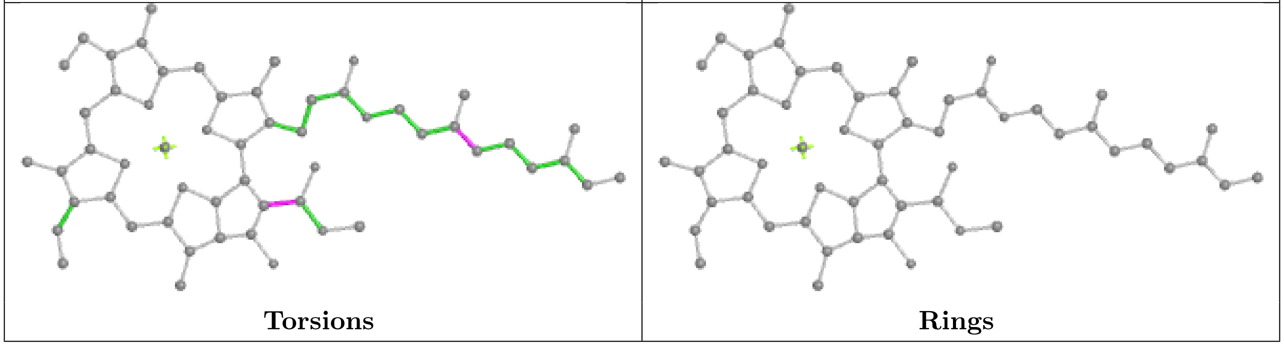
Rings

Ligand CLA B 810



Bond lengths

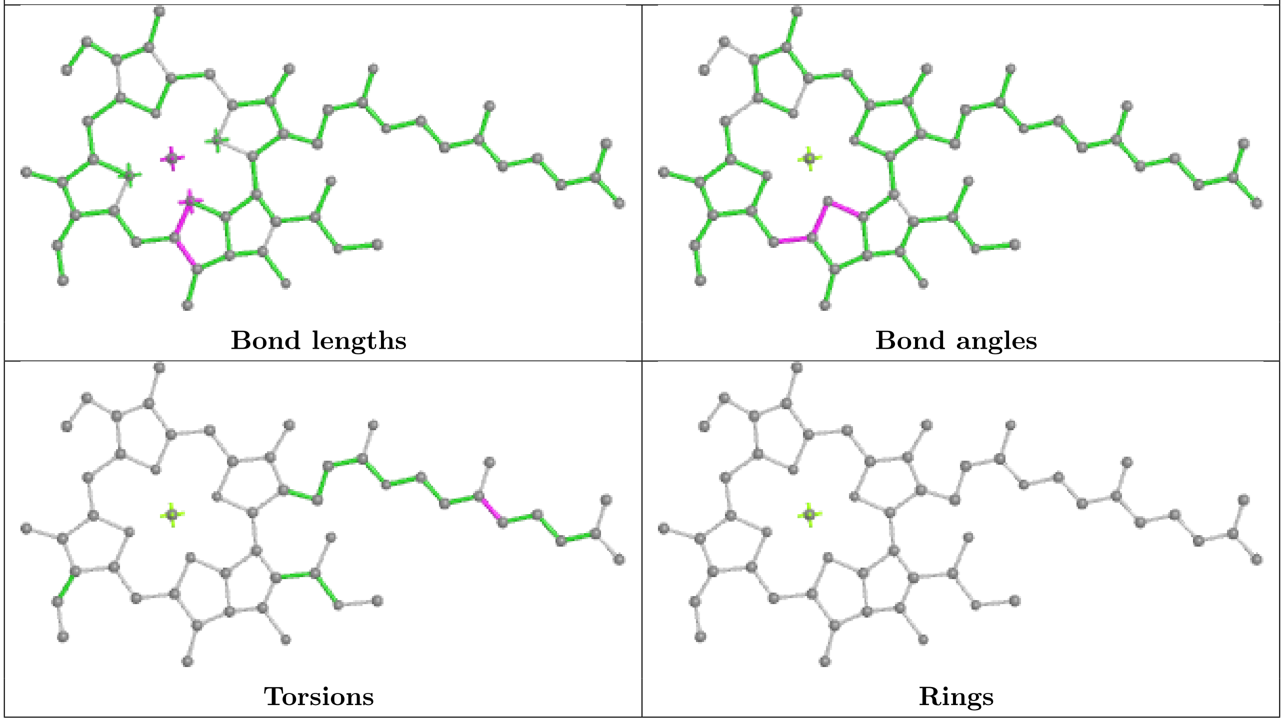
Bond angles



Torsions

Rings

Ligand CLA B 818



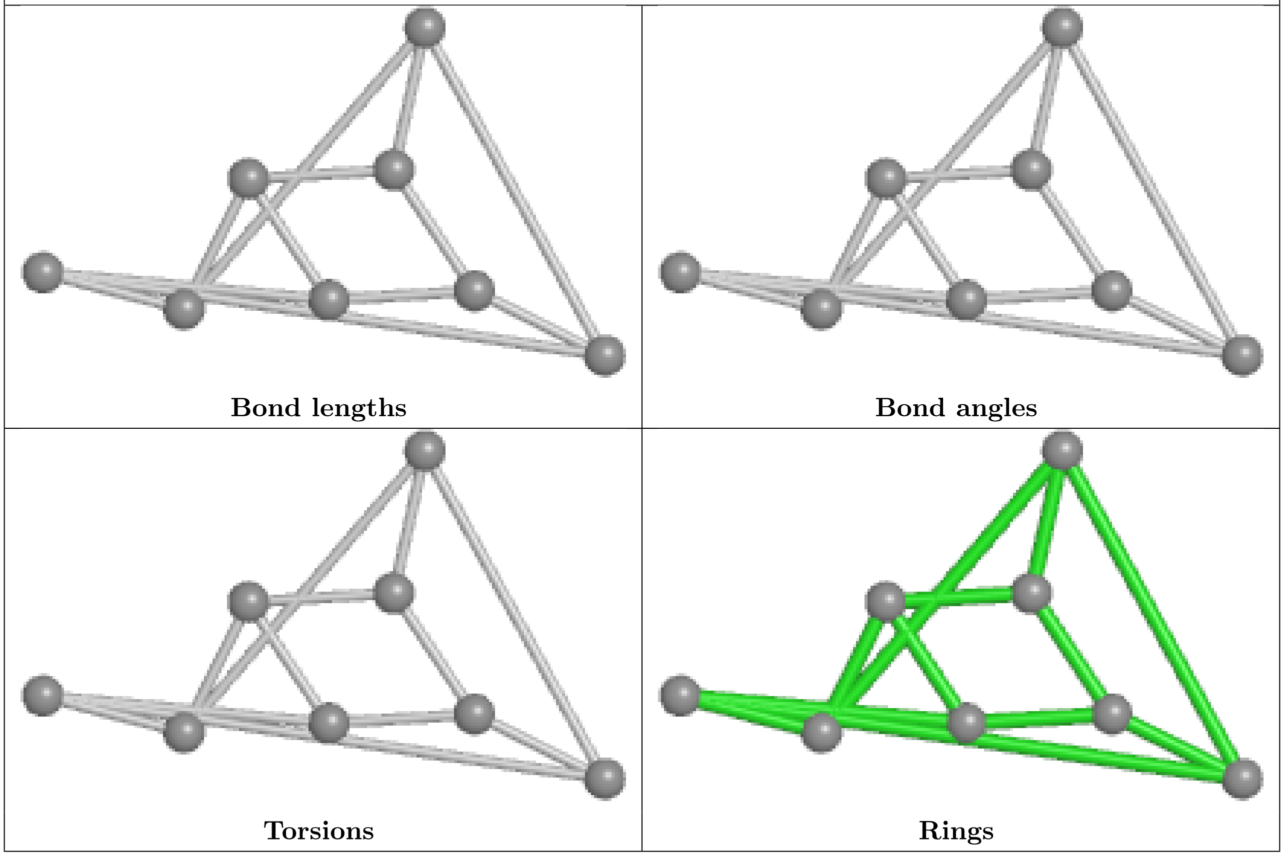
Bond lengths

Bond angles

Torsions

Rings

Ligand SF4 C 101



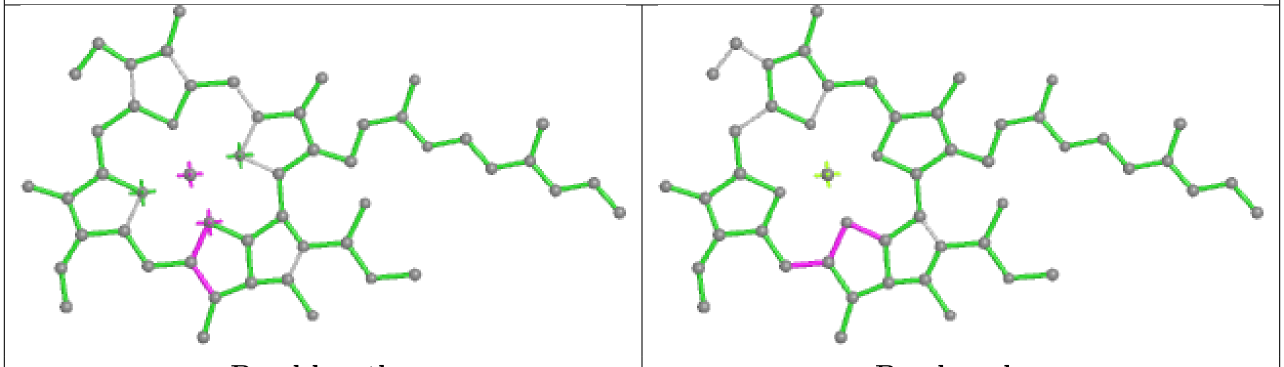
Bond lengths

Bond angles

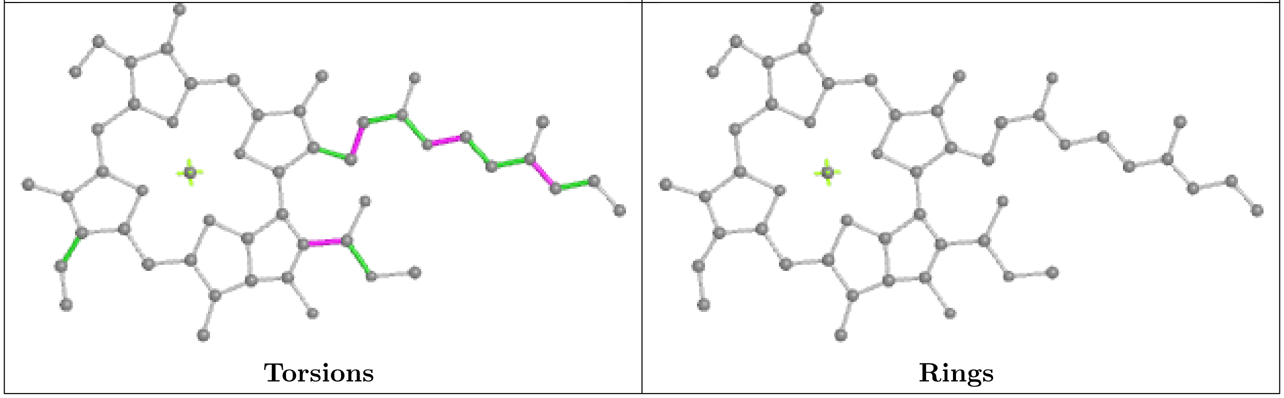
Torsions

Rings

Ligand CLA A 823

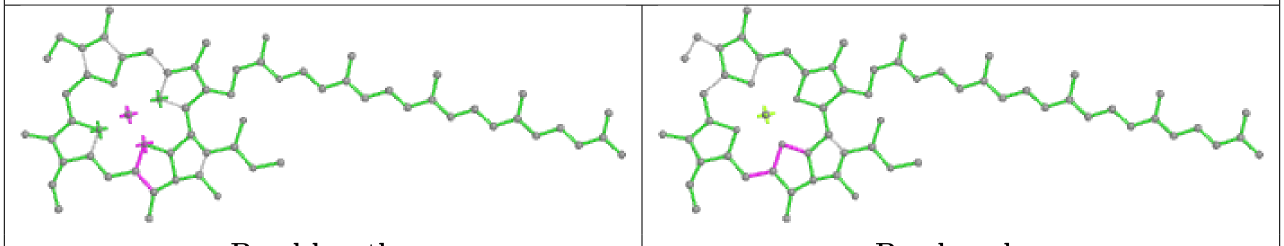


Bond lengths **Bond angles**

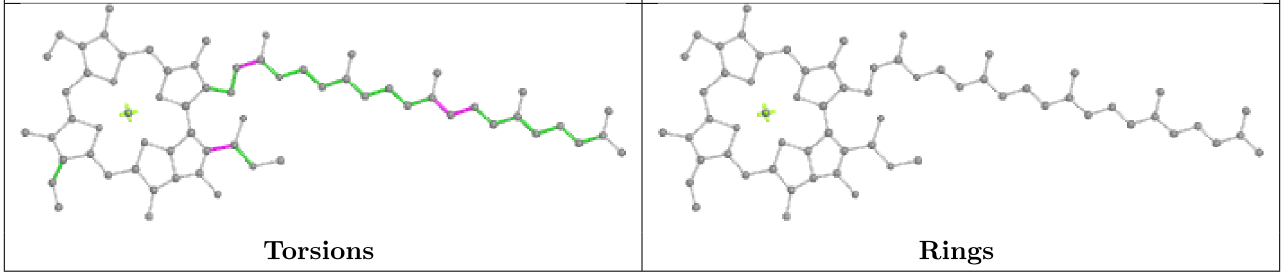


Torsions **Rings**

Ligand CLA A 814

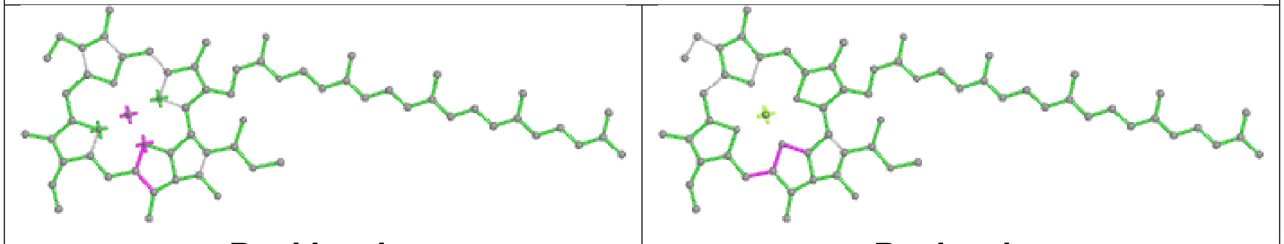


Bond lengths **Bond angles**



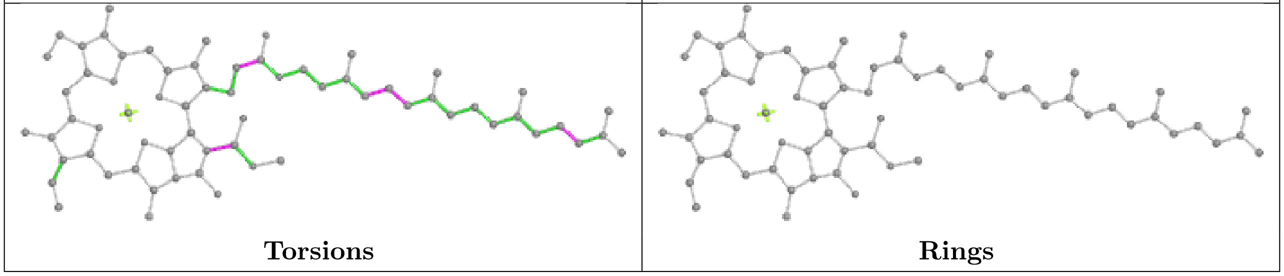
Torsions **Rings**

Ligand CLA A 807



Bond lengths

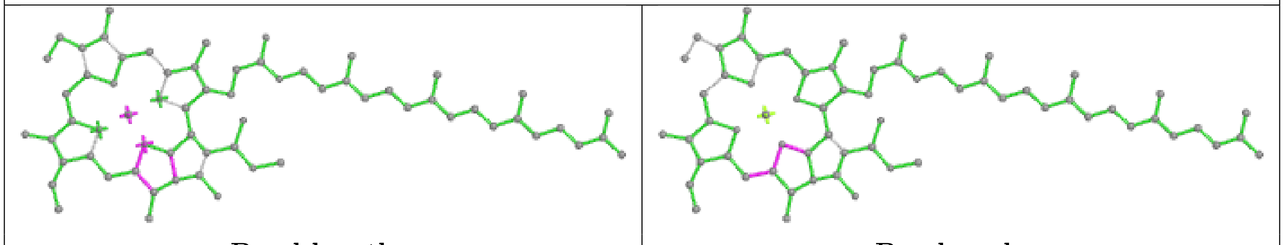
Bond angles



Torsions

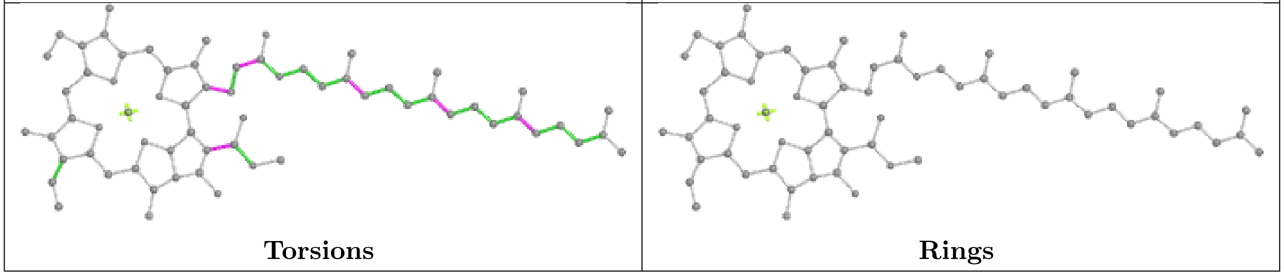
Rings

Ligand CLA B 828



Bond lengths

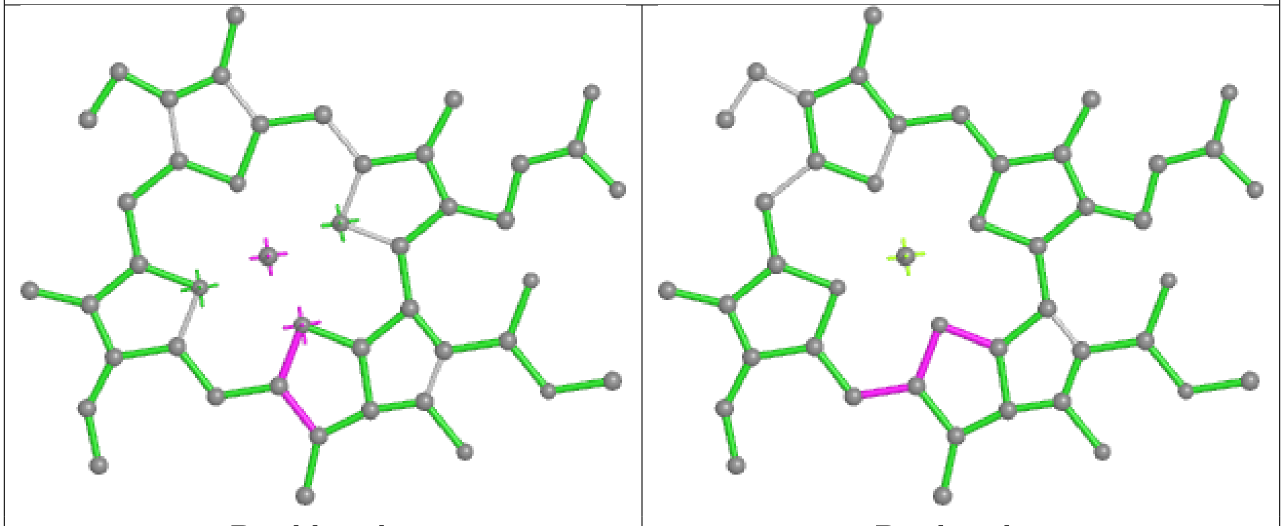
Bond angles



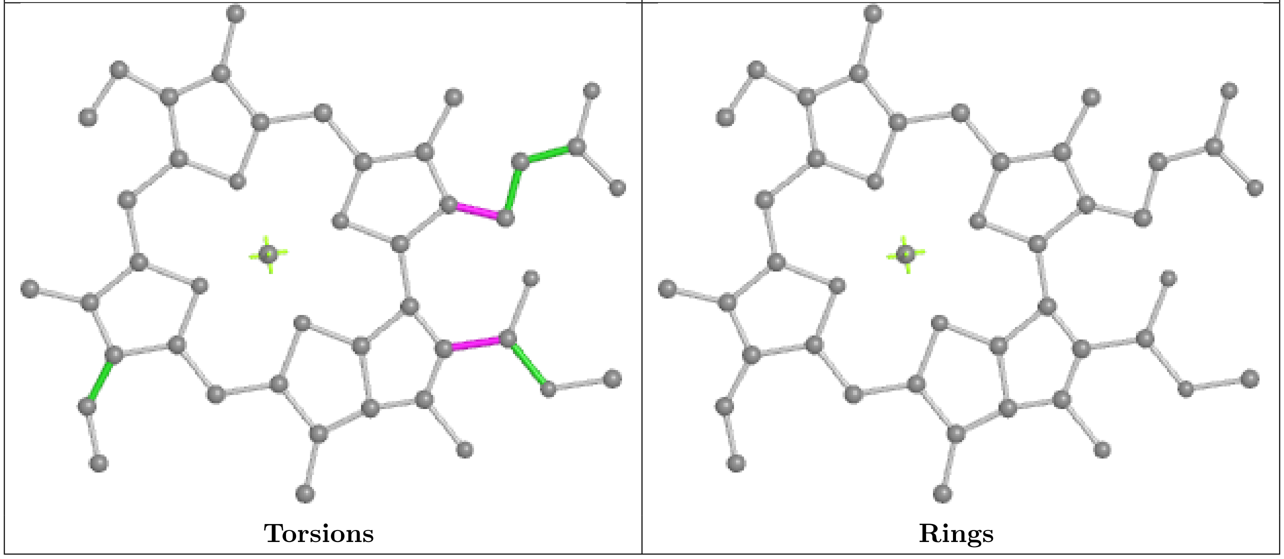
Torsions

Rings

Ligand CLA B 821

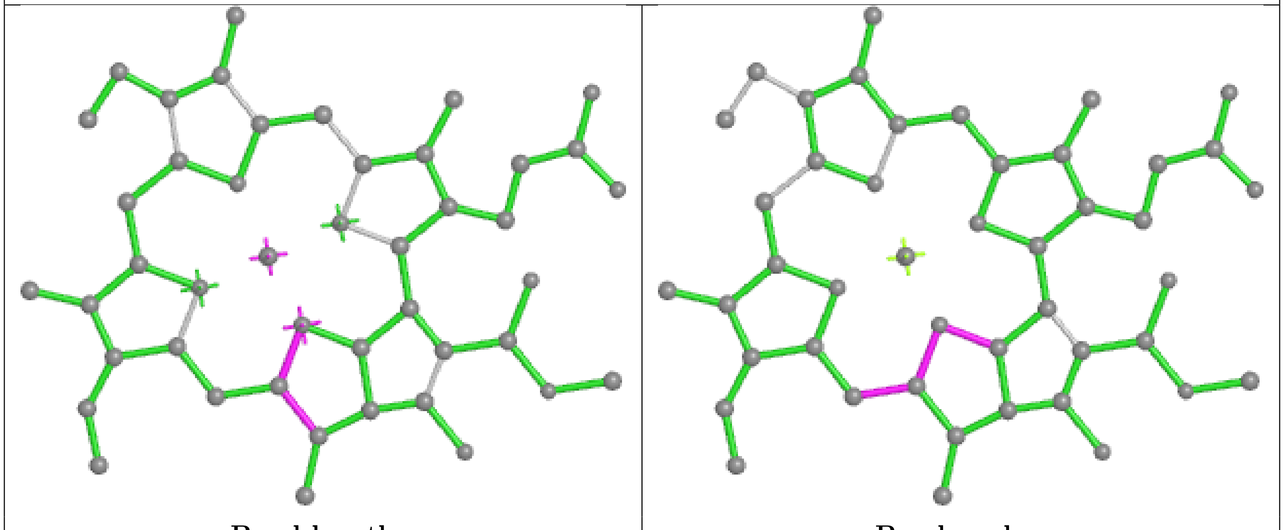


Bond lengths **Bond angles**

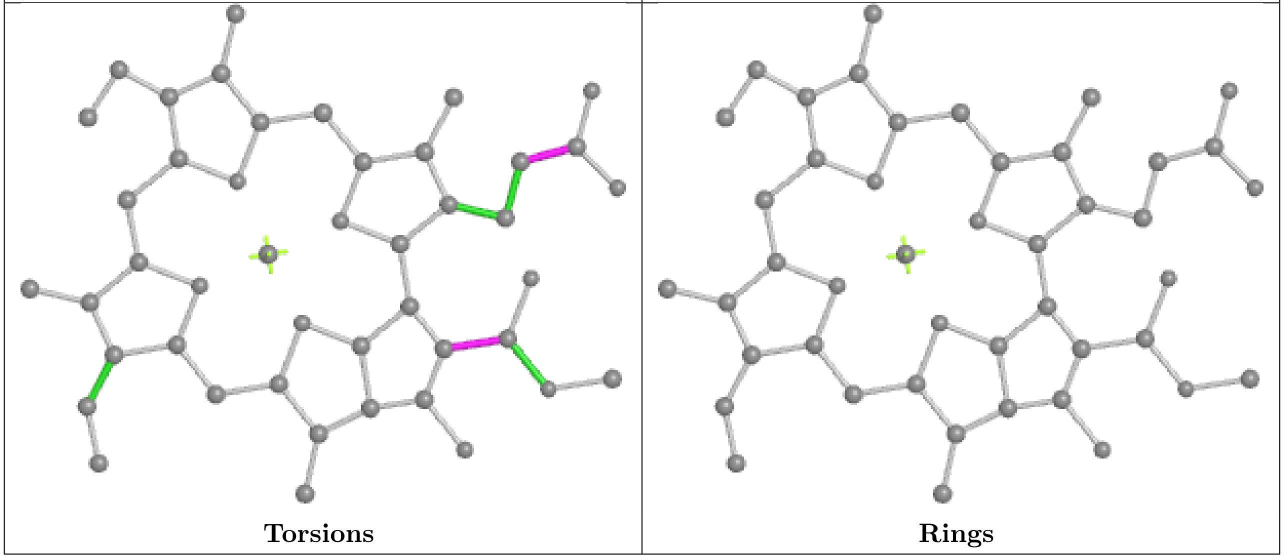


Torsions **Rings**

Ligand CLA A 845

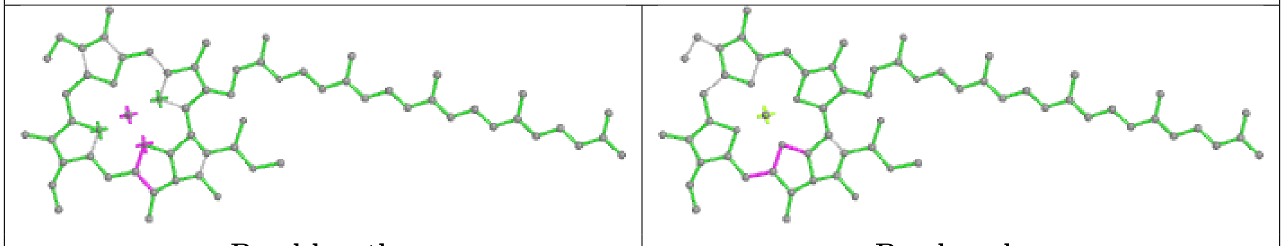


Bond lengths Bond angles

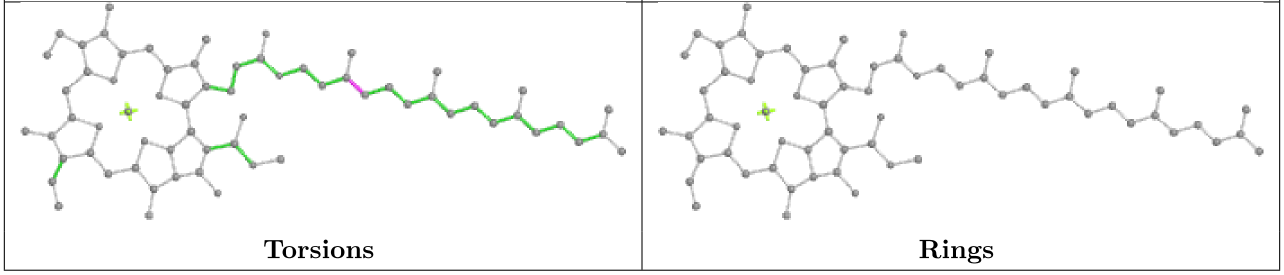


Torsions Rings

Ligand CLA B 809

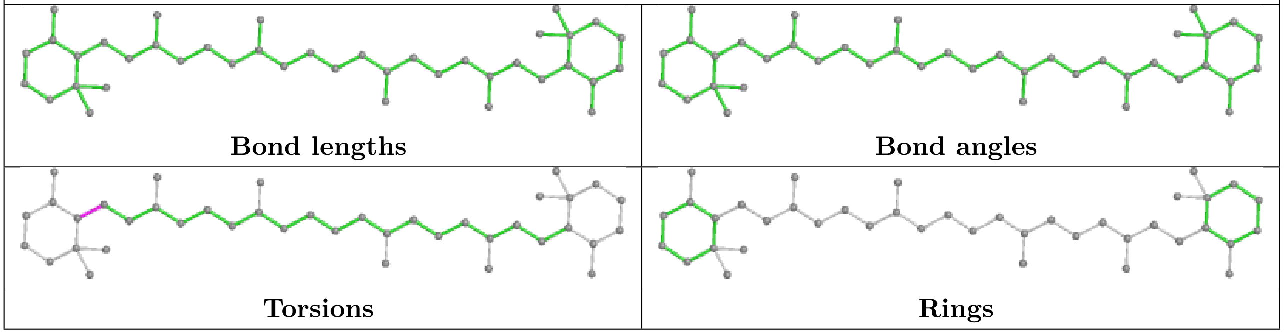


Bond lengths Bond angles



Torsions Rings

Ligand BCR A 850



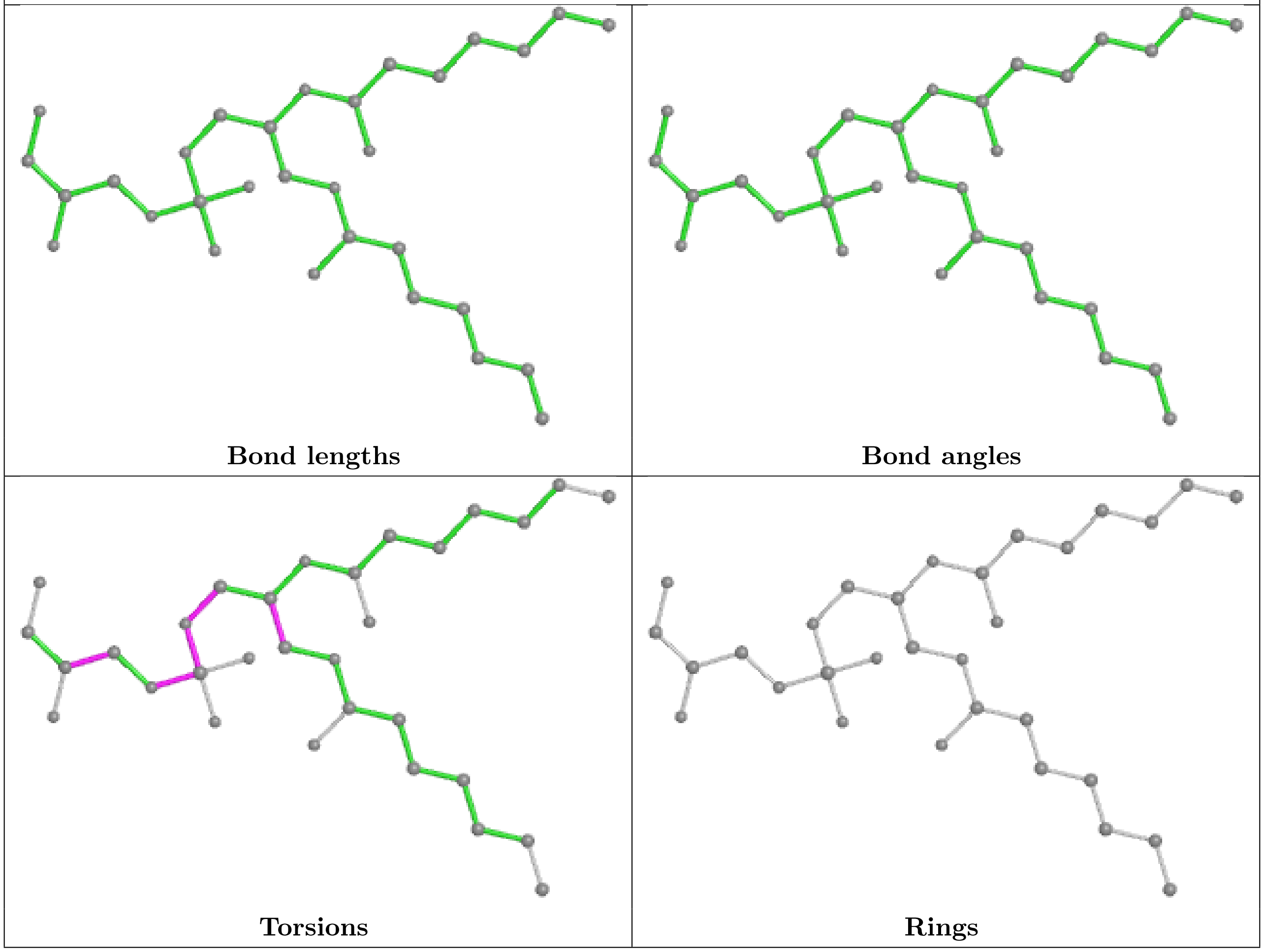
Bond lengths

Bond angles

Torsions

Rings

Ligand LHG A 847



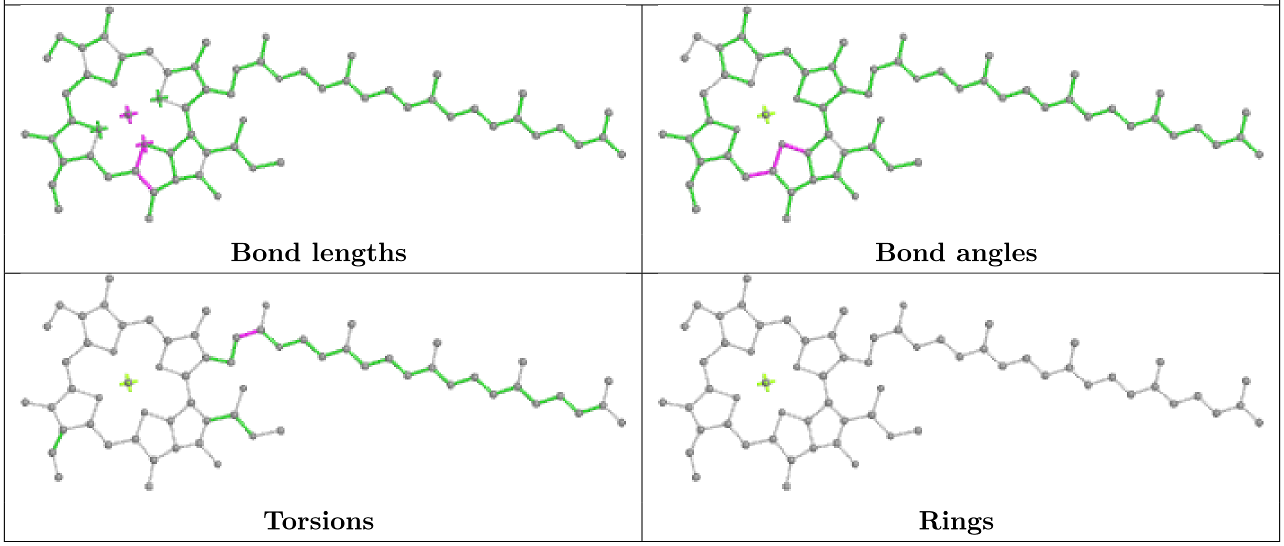
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA B 805



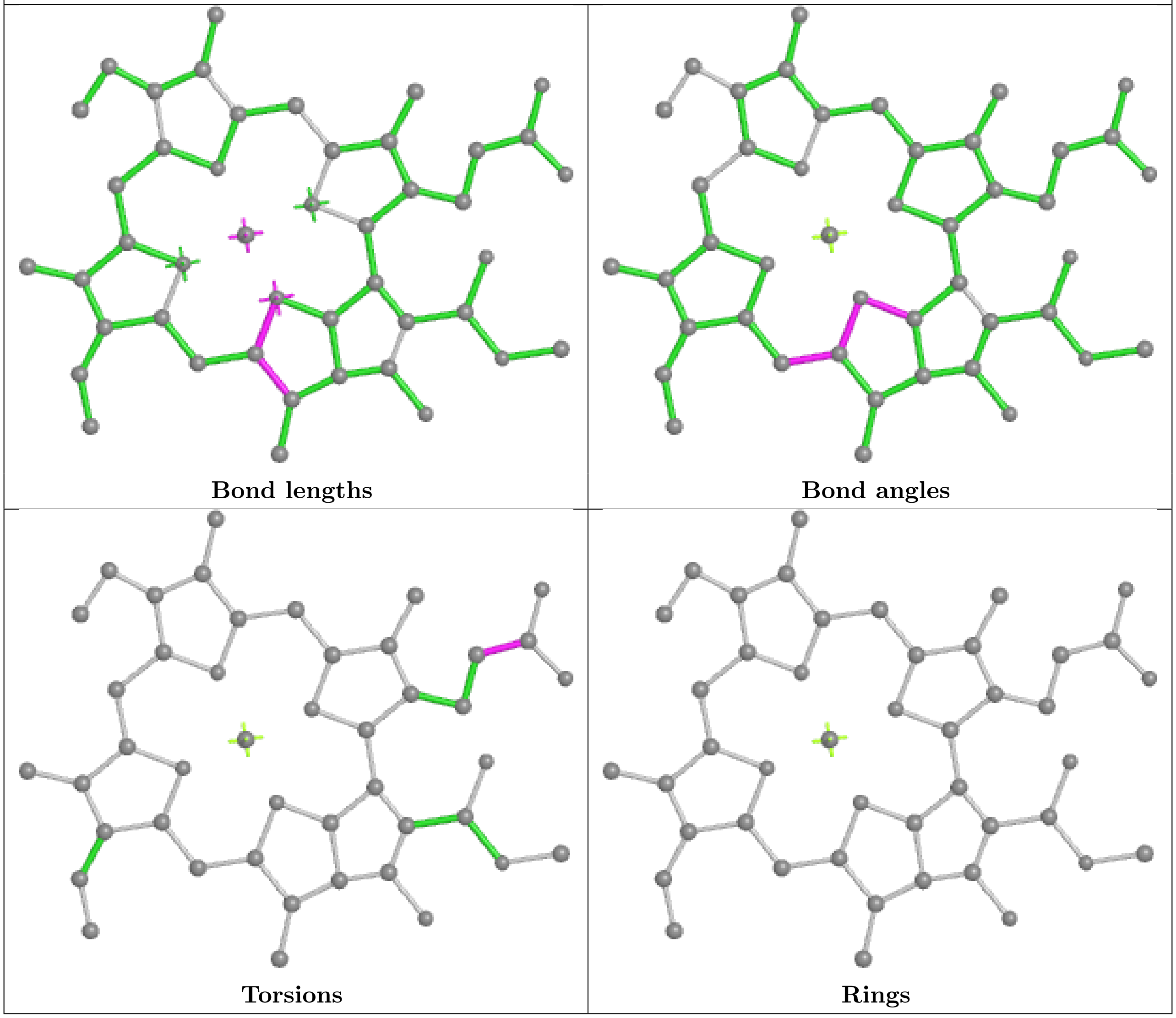
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA B 830



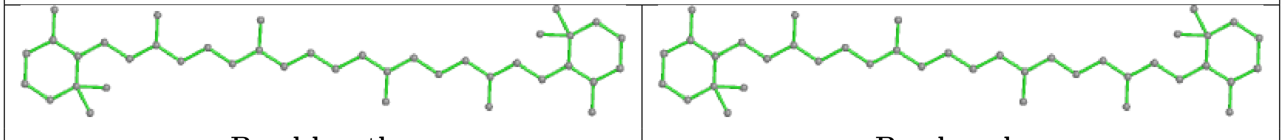
Bond lengths

Bond angles

Torsions

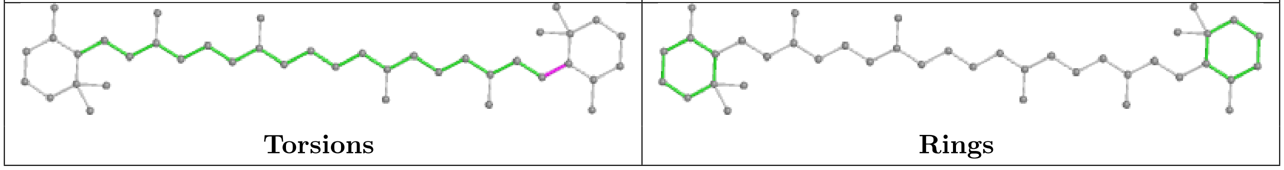
Rings

Ligand BCR L 306



Bond lengths

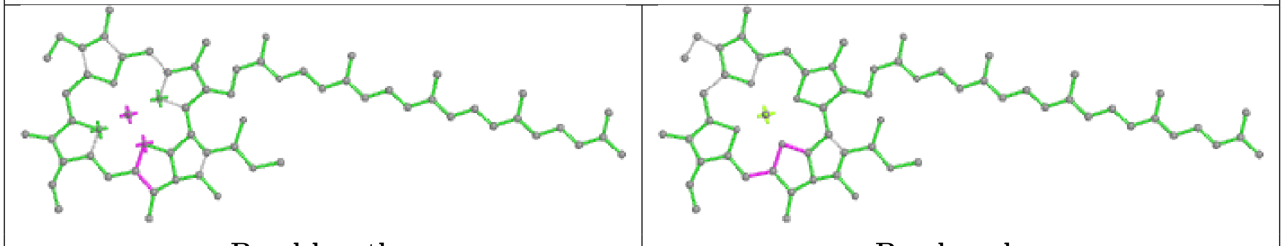
Bond angles



Torsions

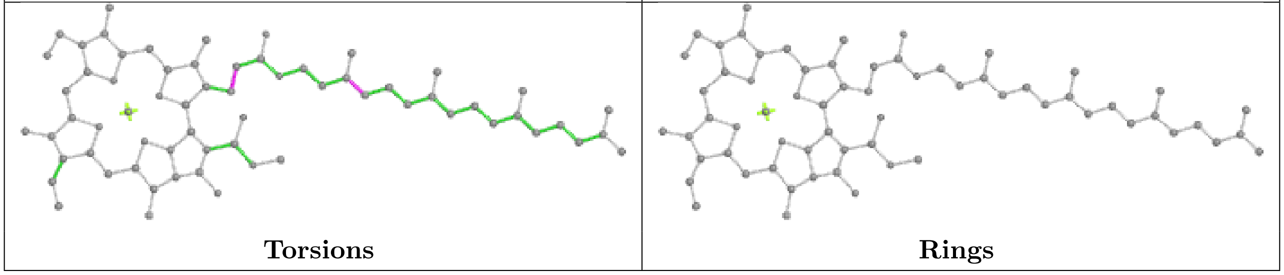
Rings

Ligand CLA B 837



Bond lengths

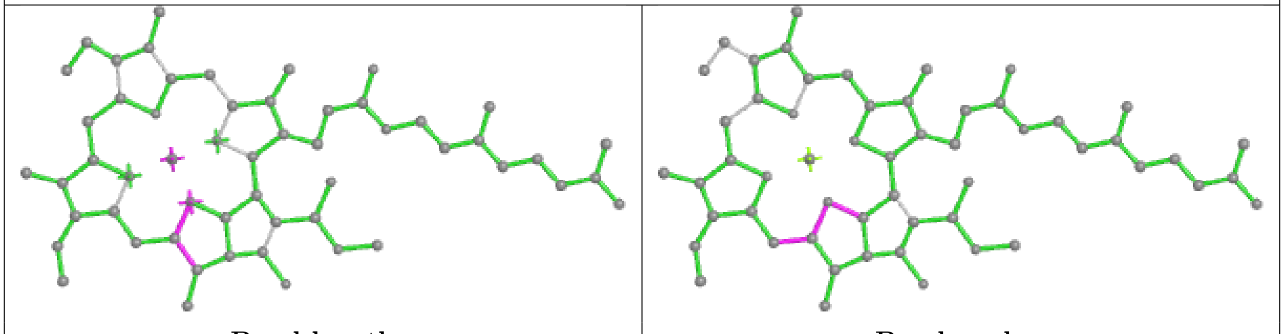
Bond angles



Torsions

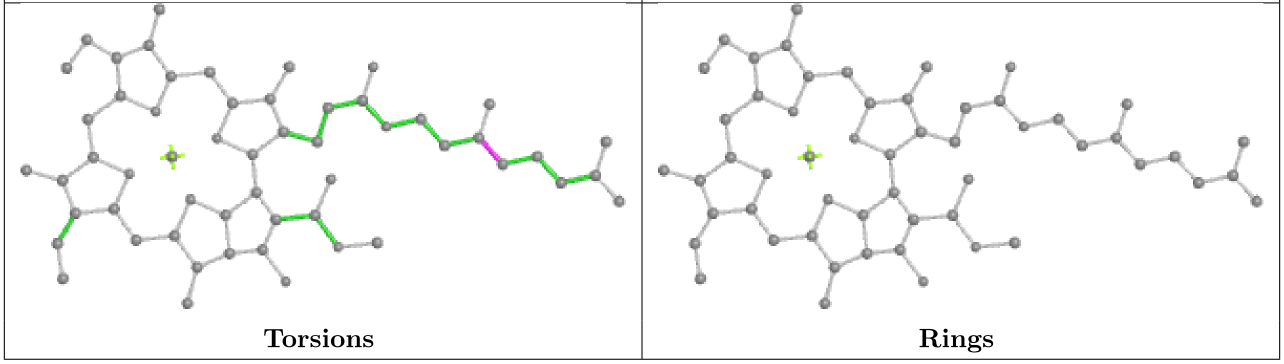
Rings

Ligand CLA A 841



Bond lengths

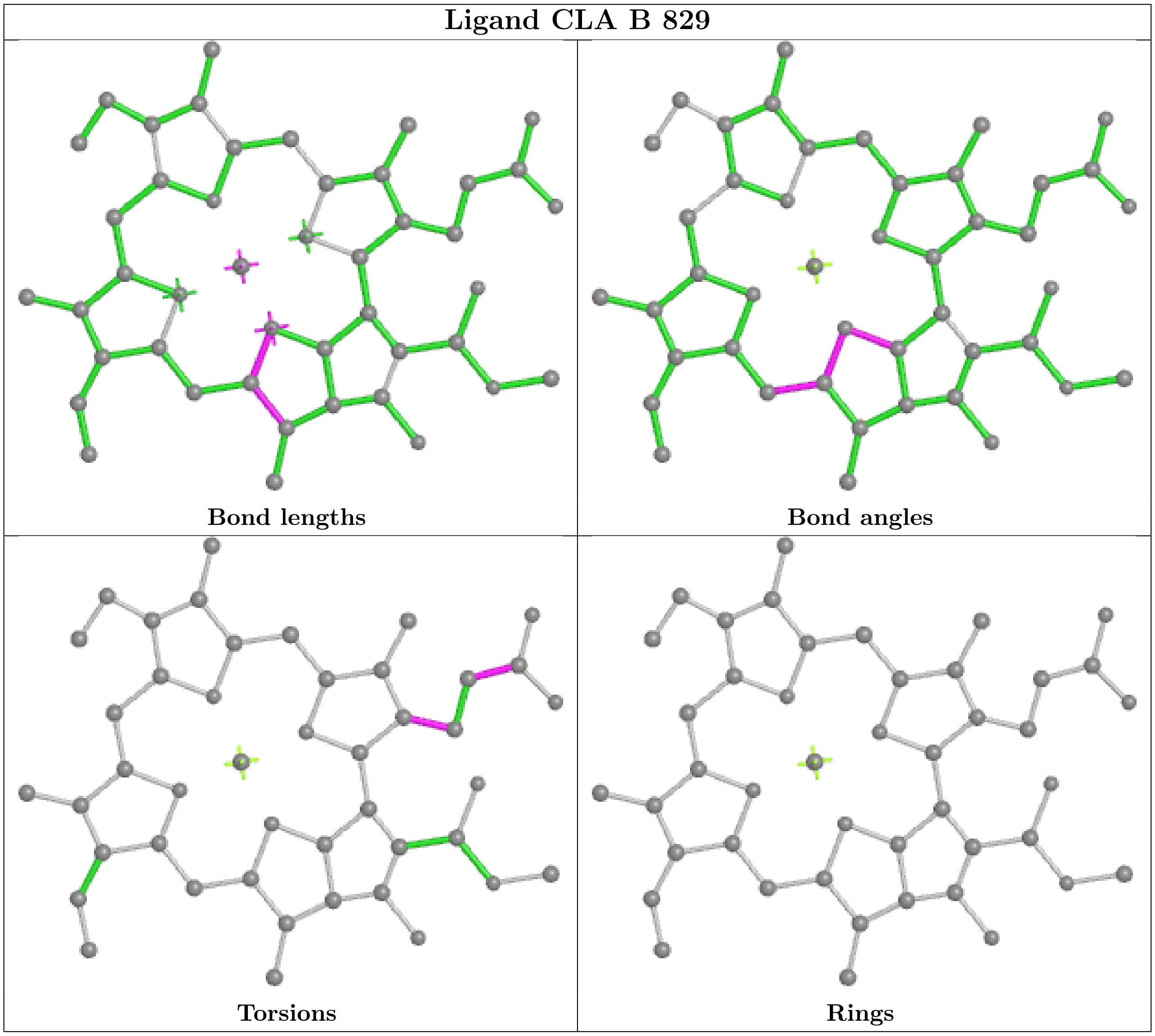
Bond angles



Torsions

Rings

Ligand CLA B 829

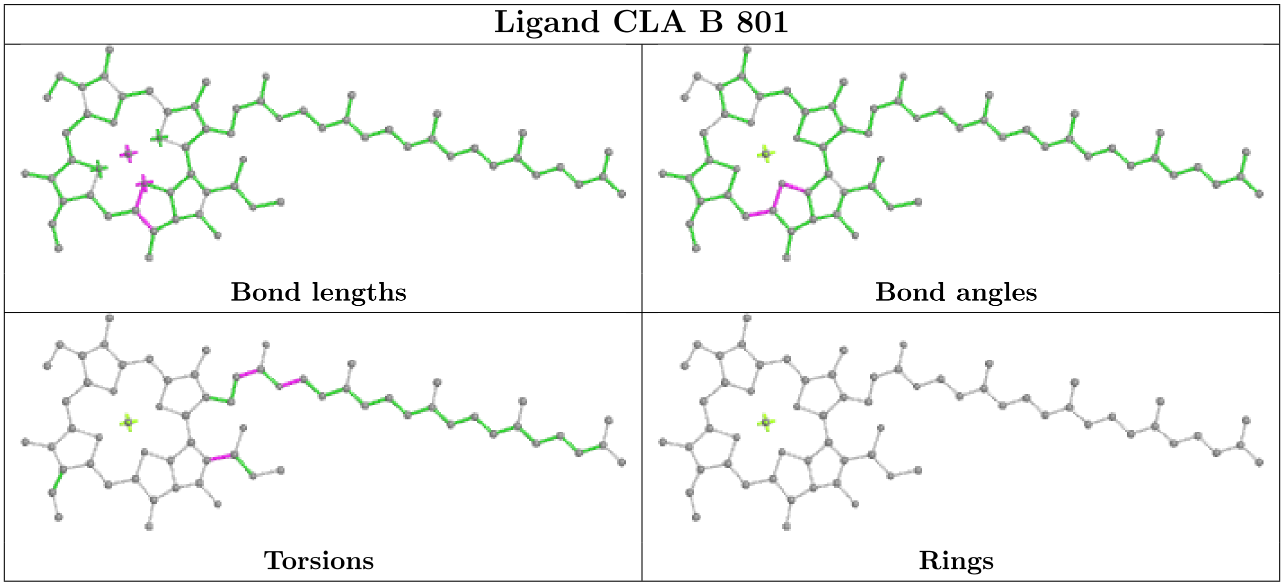

Bond lengths

Bond angles

Torsions

Rings

Ligand CLA B 801

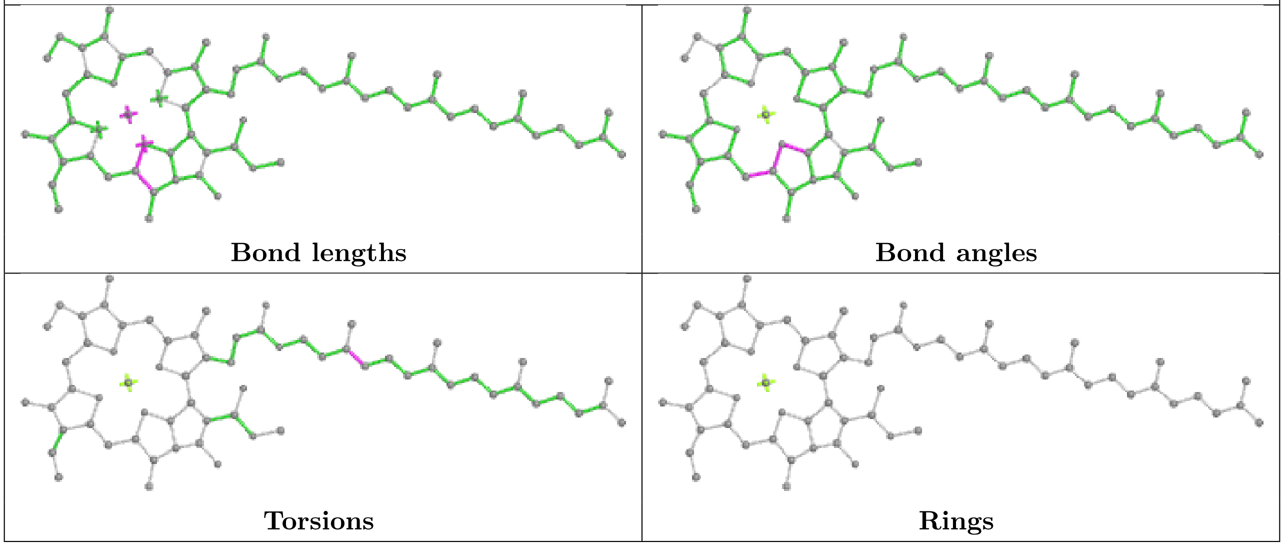

Bond lengths

Bond angles

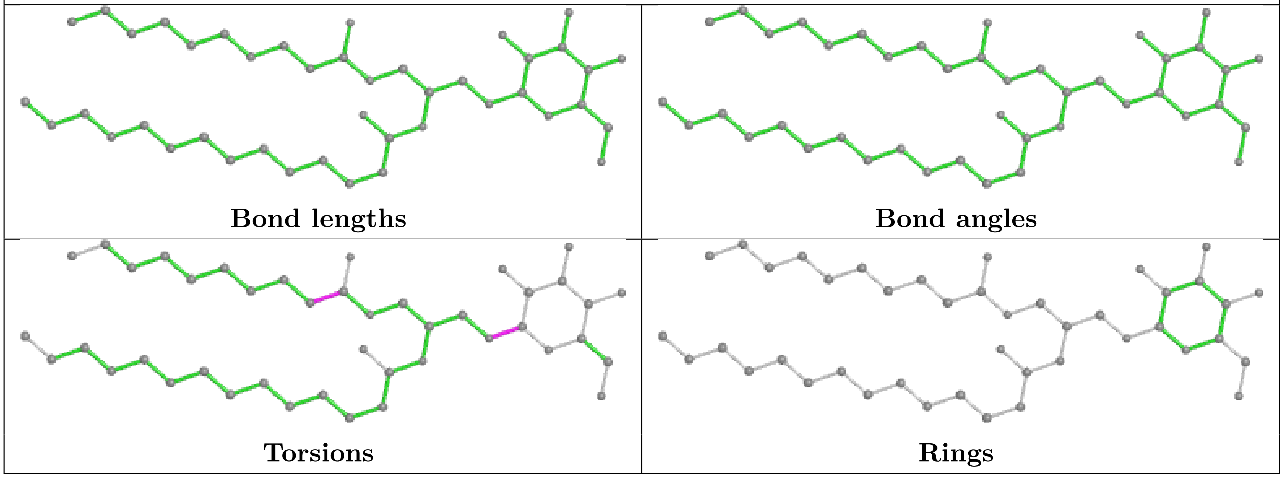
Torsions

Rings

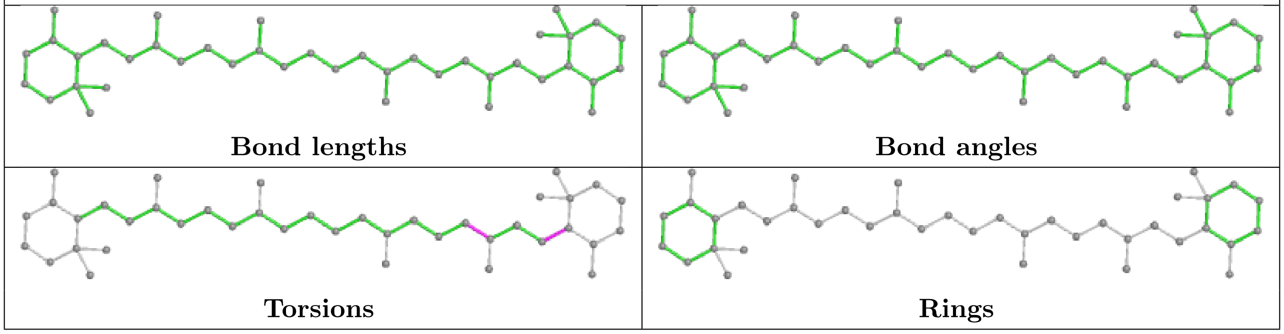
Ligand CLA A 828



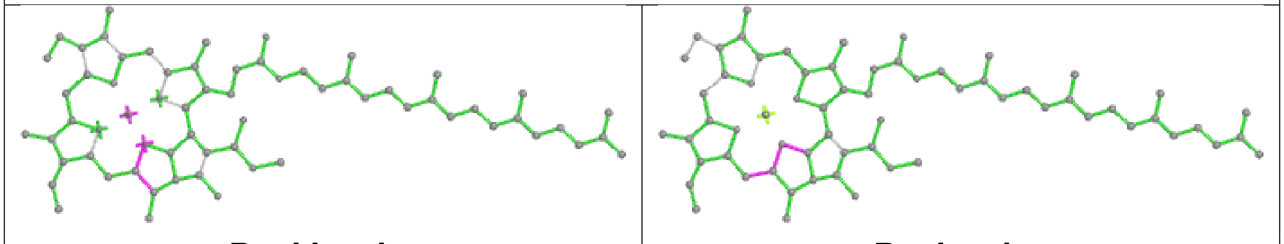
Ligand LMG A 858



Ligand BCR L 301

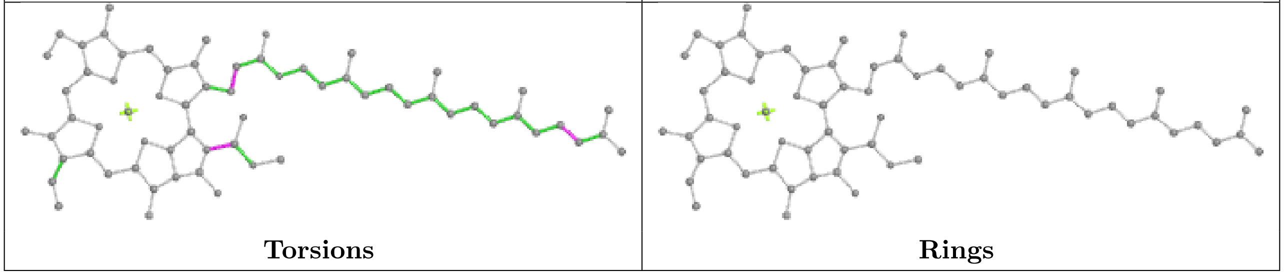


Ligand CLA B 813



Bond lengths

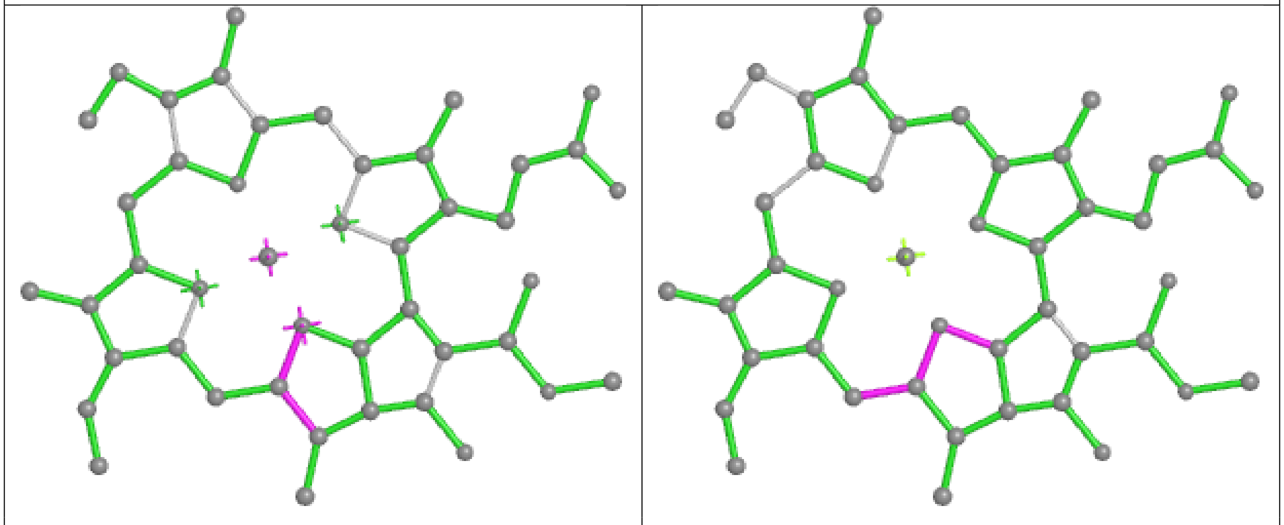
Bond angles



Torsions

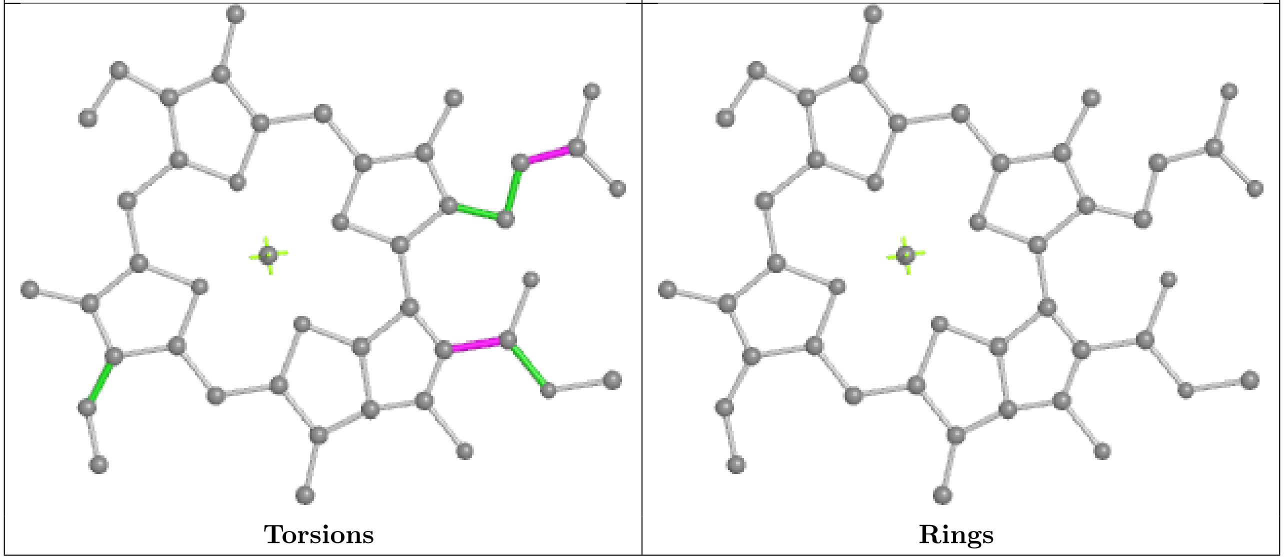
Rings

Ligand CLA B 832



Bond lengths

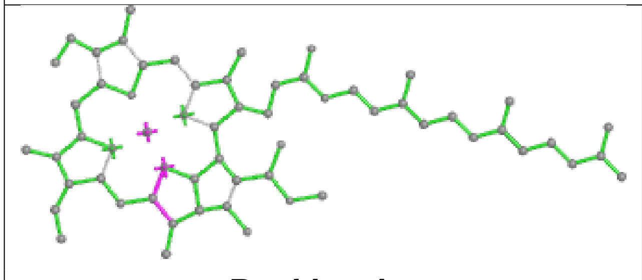
Bond angles



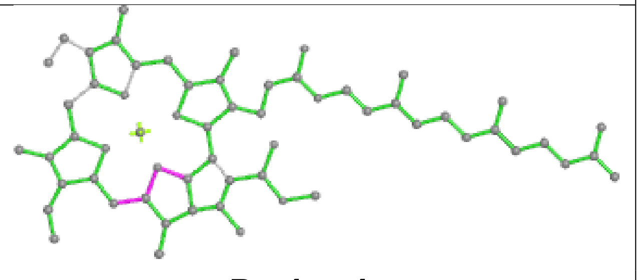
Torsions

Rings

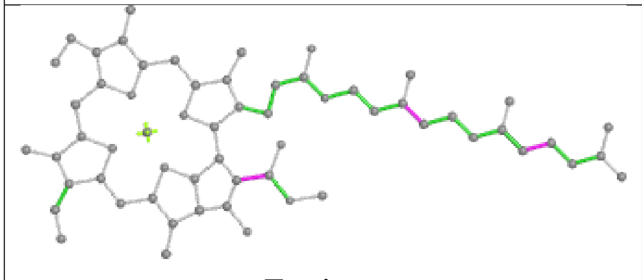
Ligand CLA A 816



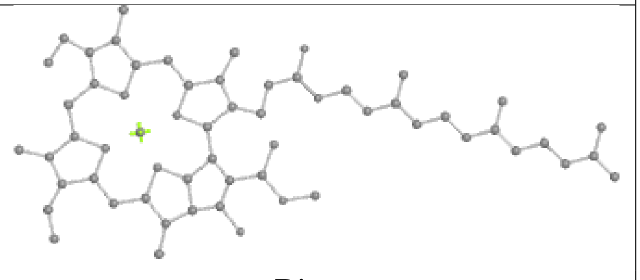
Bond lengths



Bond angles

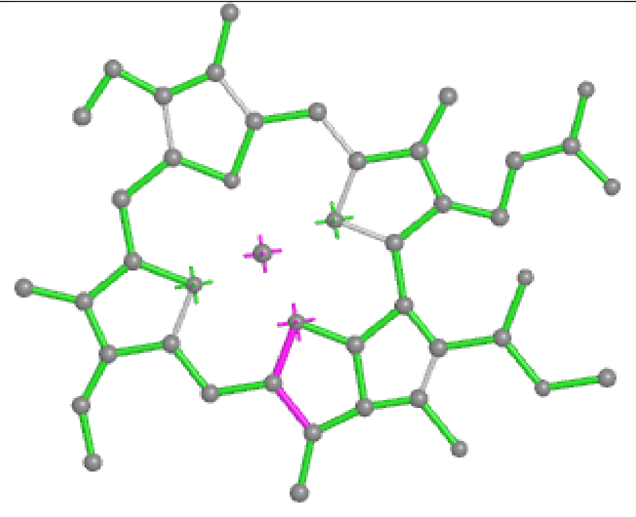


Torsions

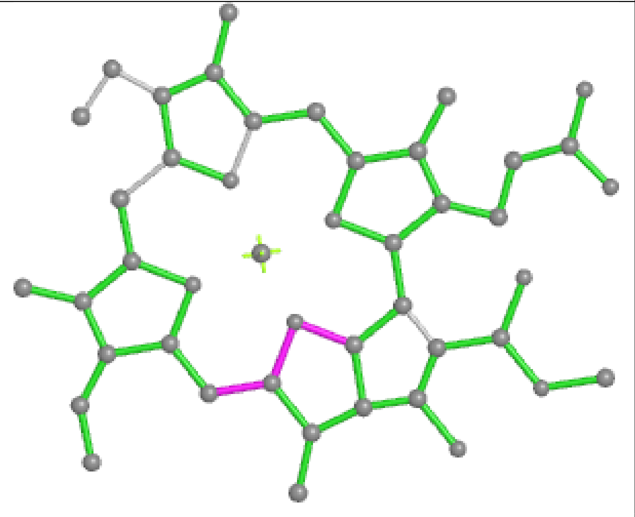


Rings

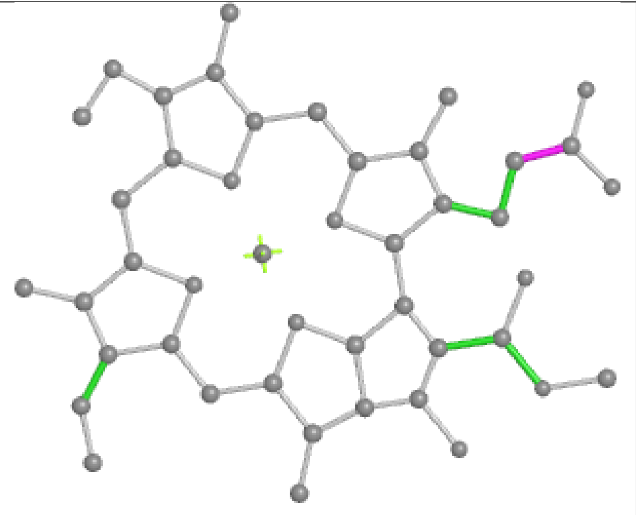
Ligand CLA A 837



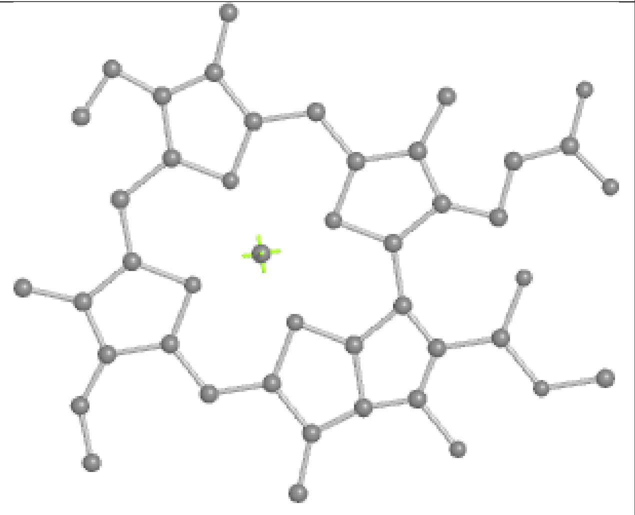
Bond lengths



Bond angles

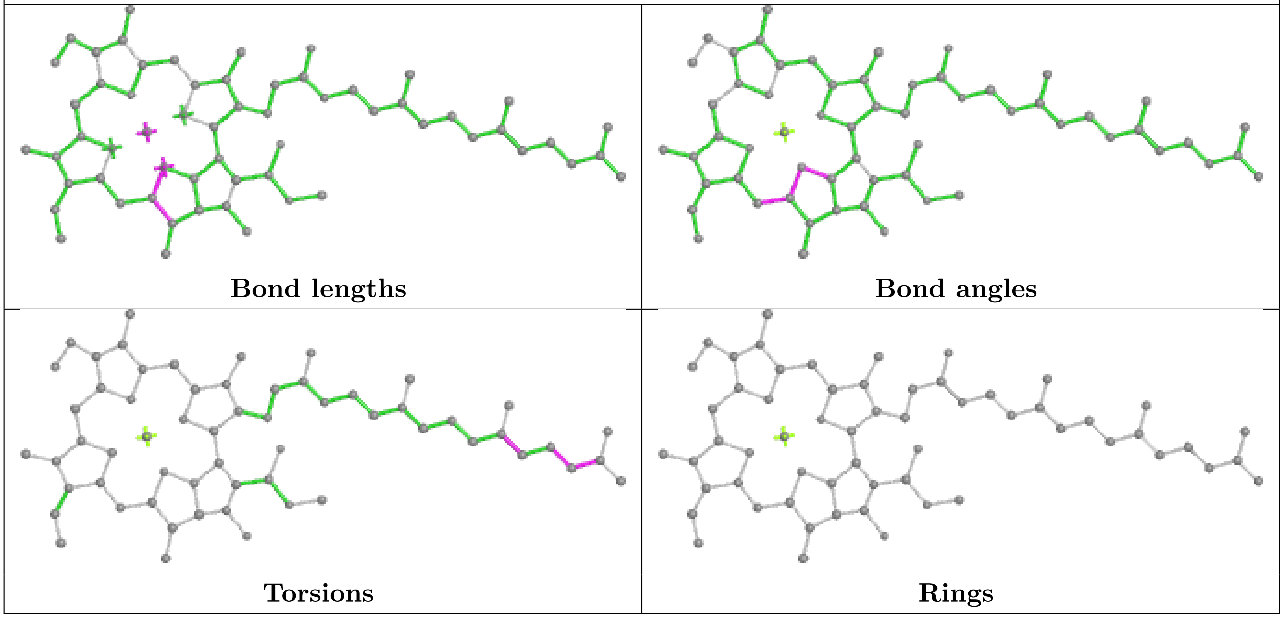


Torsions



Rings

Ligand CLA L 303



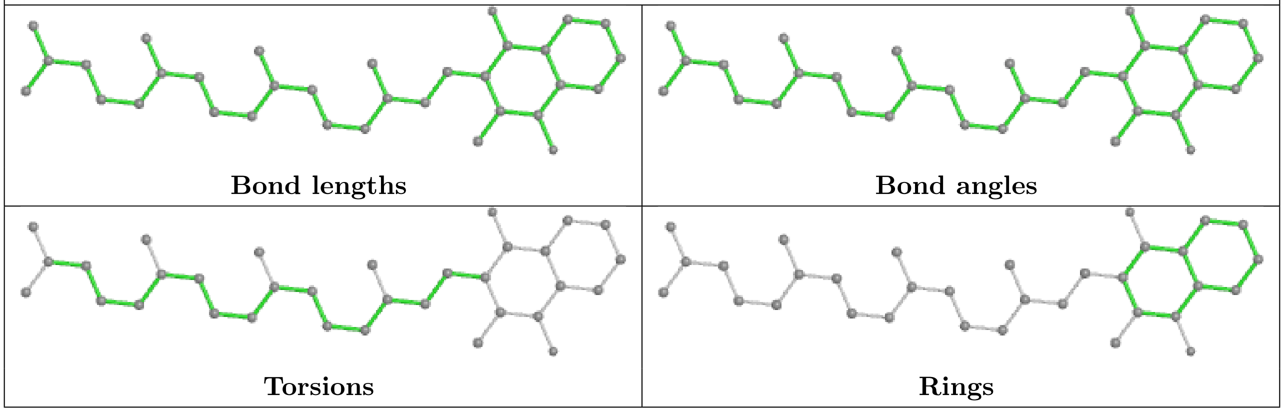
Bond lengths

Bond angles

Torsions

Rings

Ligand PQN A 844



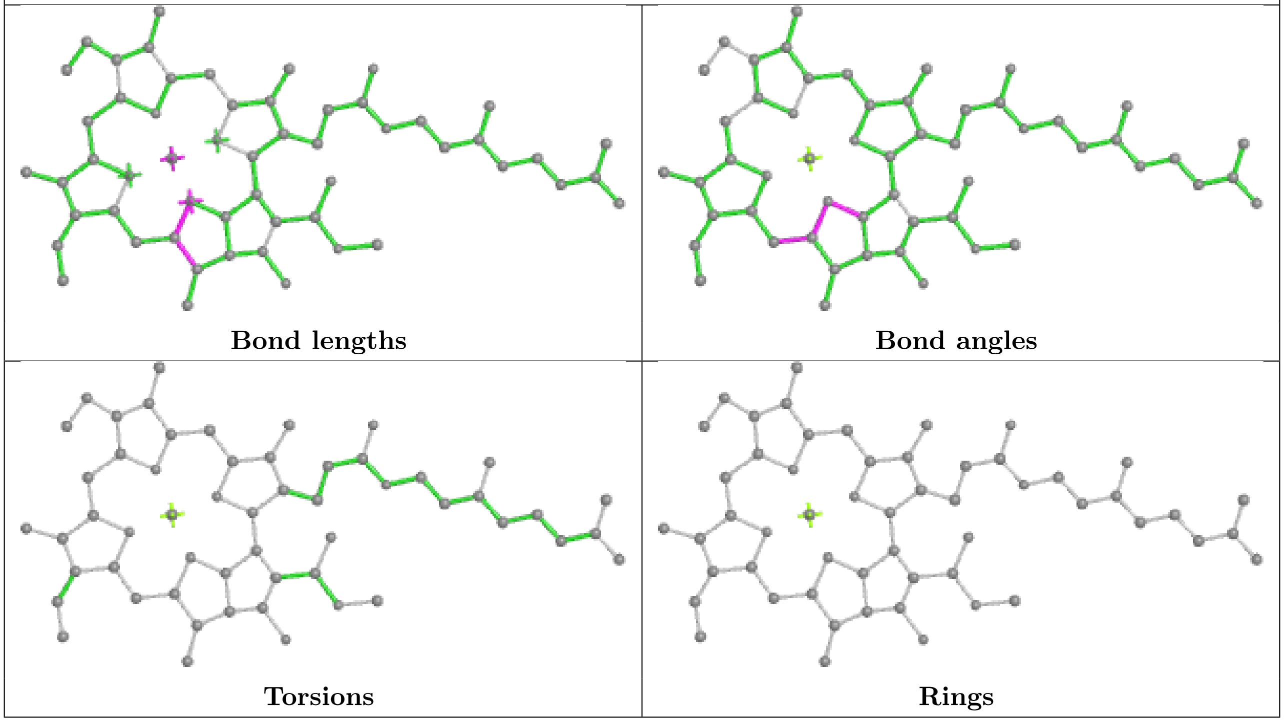
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA A 833



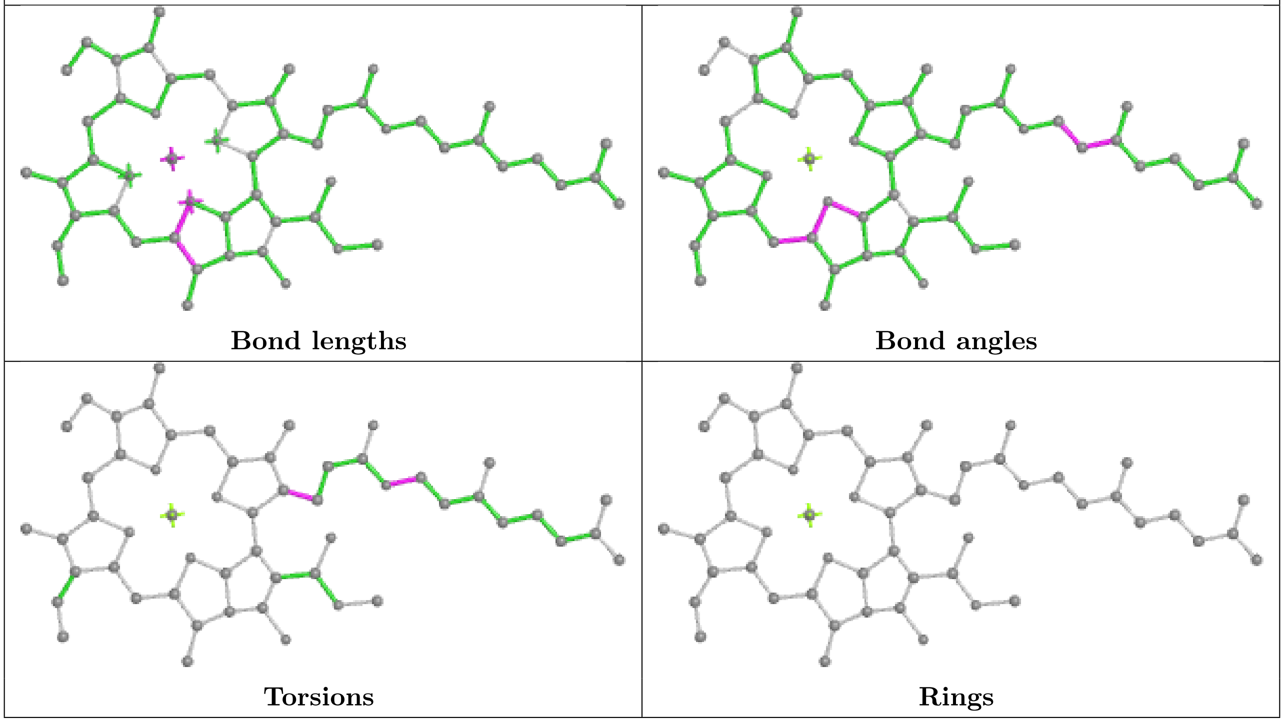
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA A 854



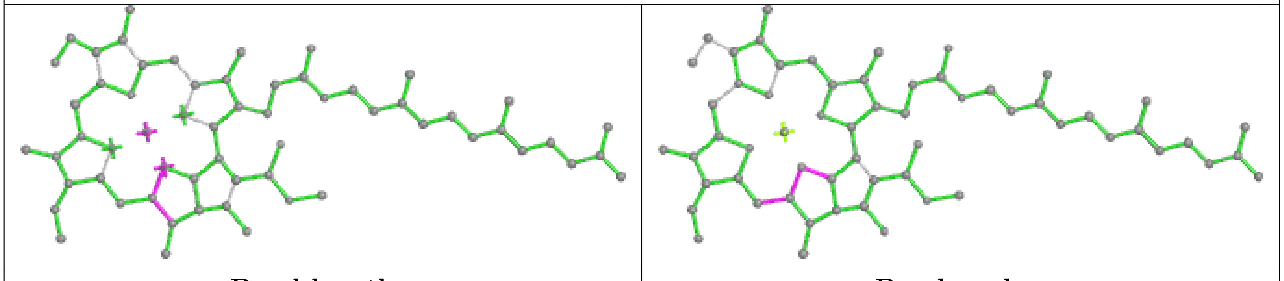
Bond lengths

Bond angles

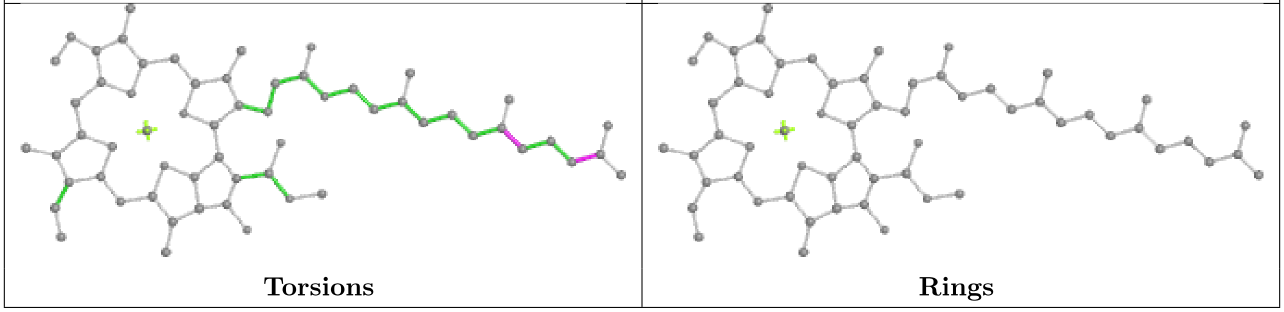
Torsions

Rings

Ligand CLA A 829

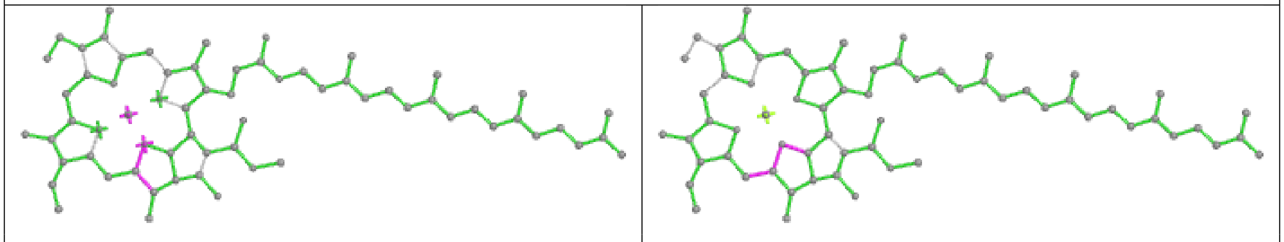


Bond lengths Bond angles

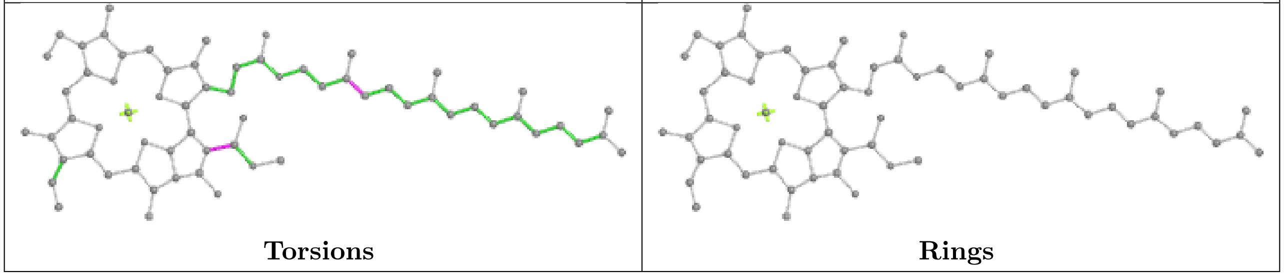


Torsions Rings

Ligand CLA A 834

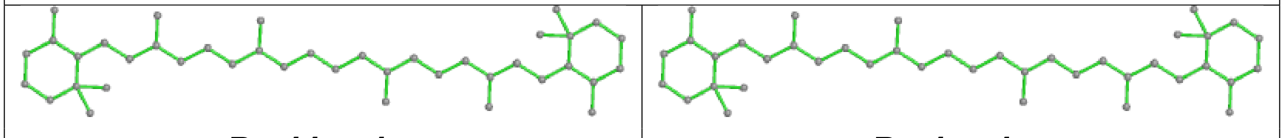


Bond lengths Bond angles

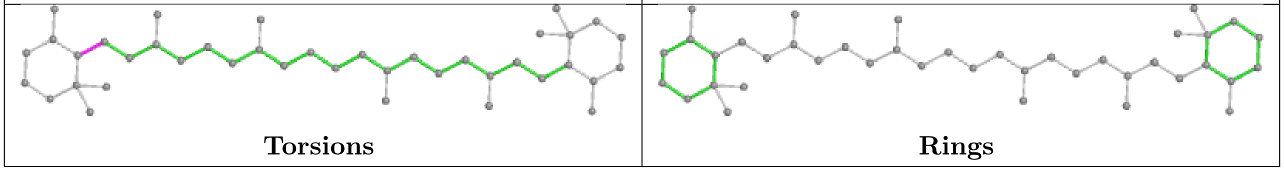


Torsions Rings

Ligand BCR B 843

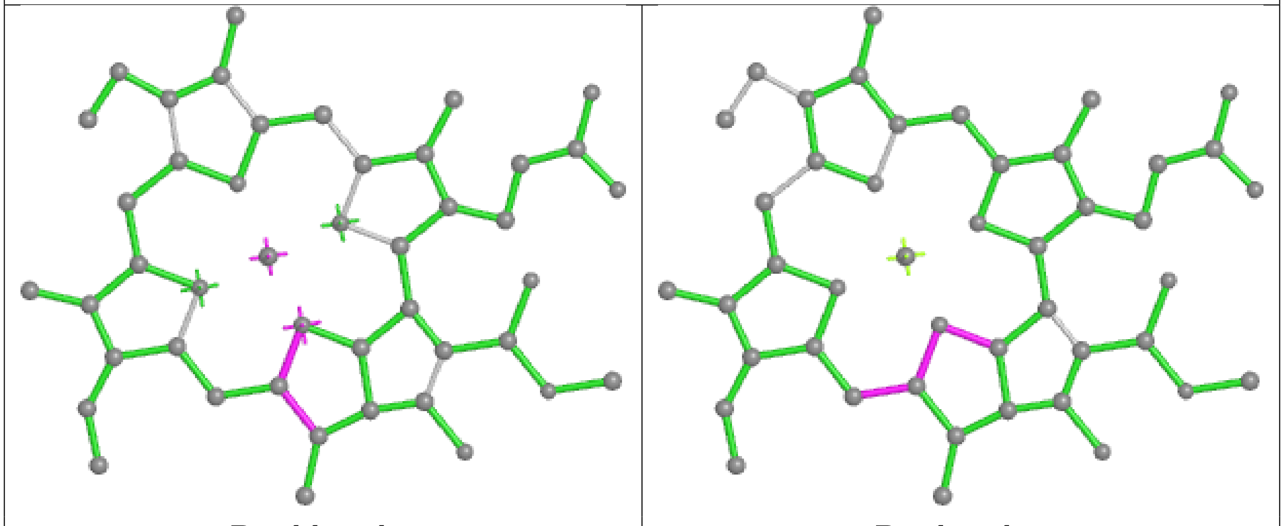


Bond lengths Bond angles

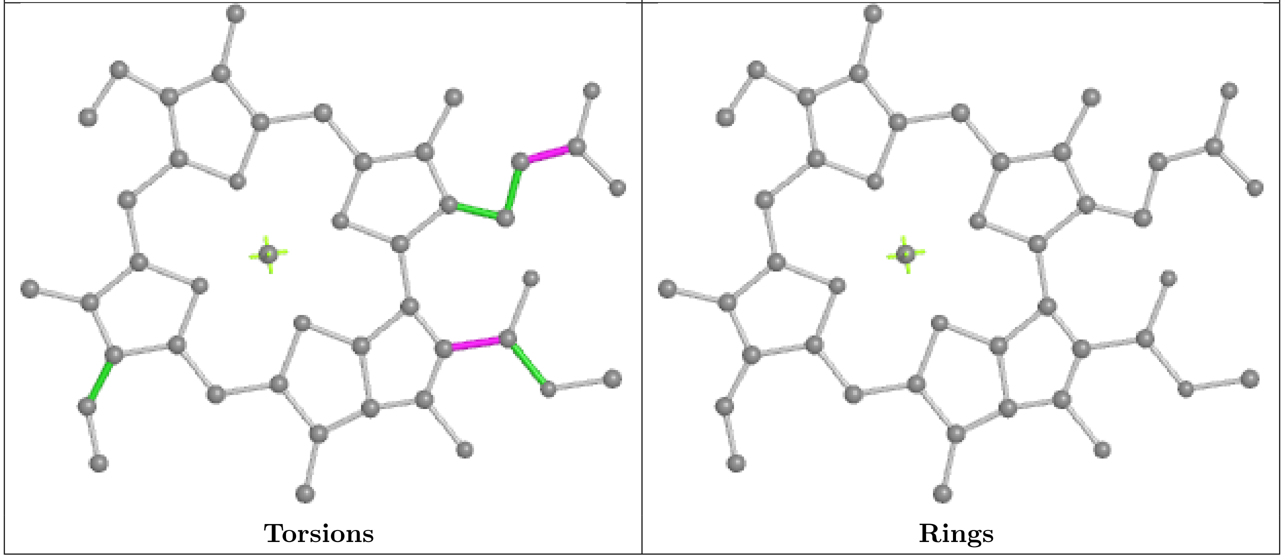


Torsions Rings

Ligand CLA A 824

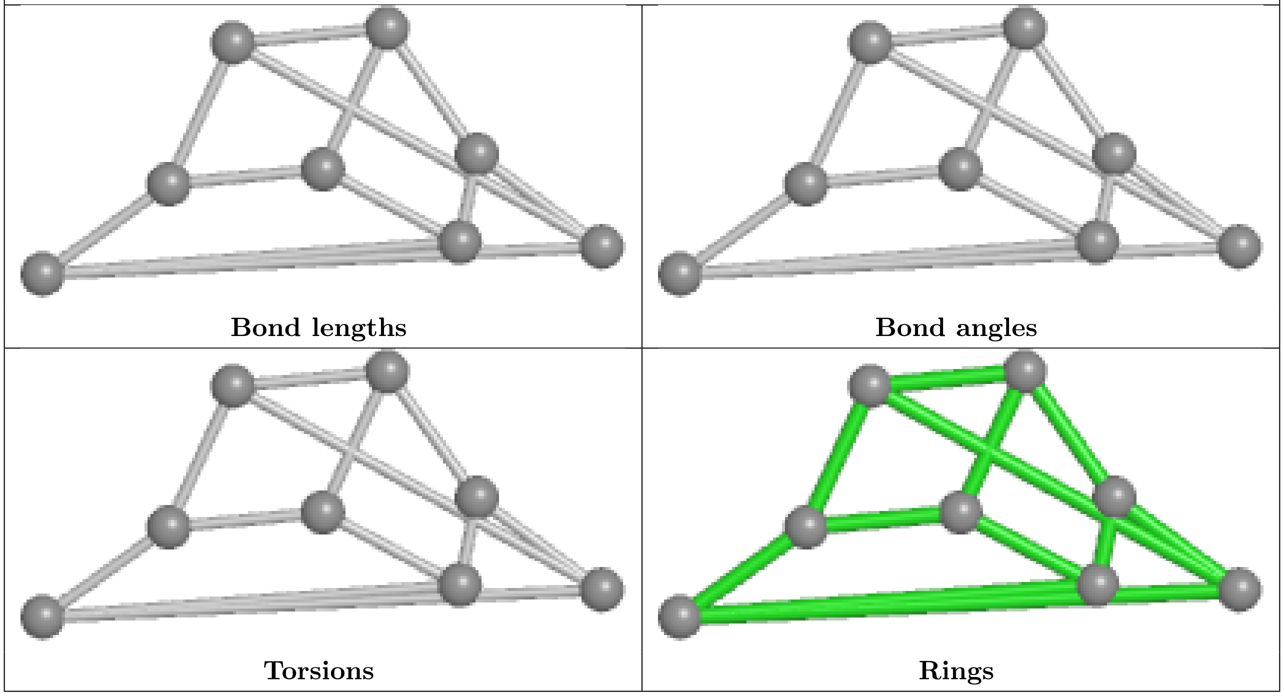


Bond lengths Bond angles



Torsions Rings

Ligand SF4 A 853



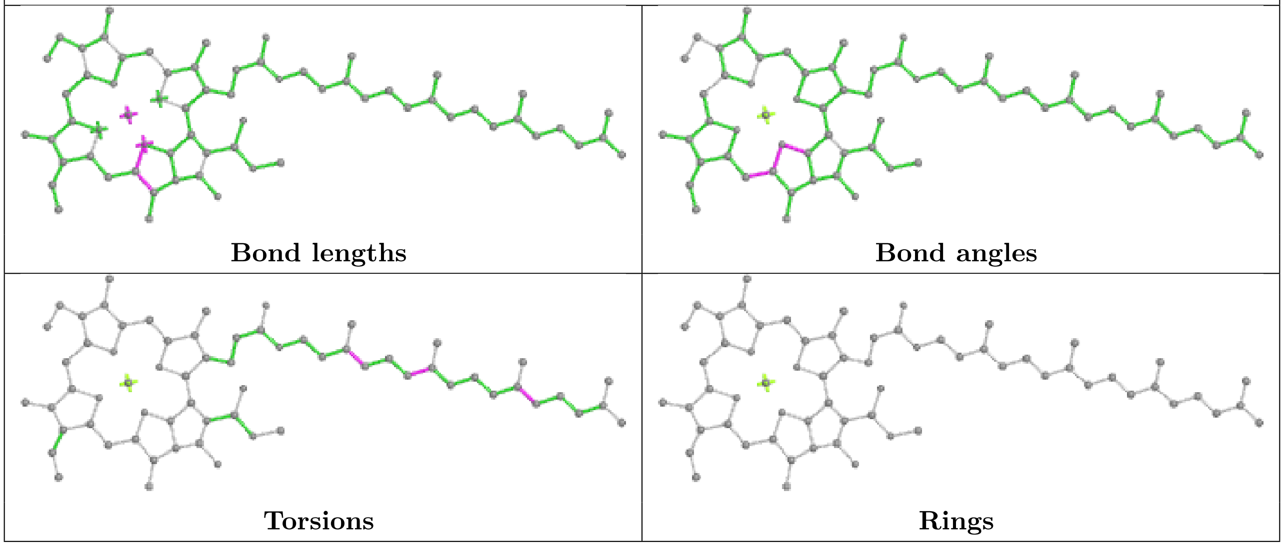
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA B 817



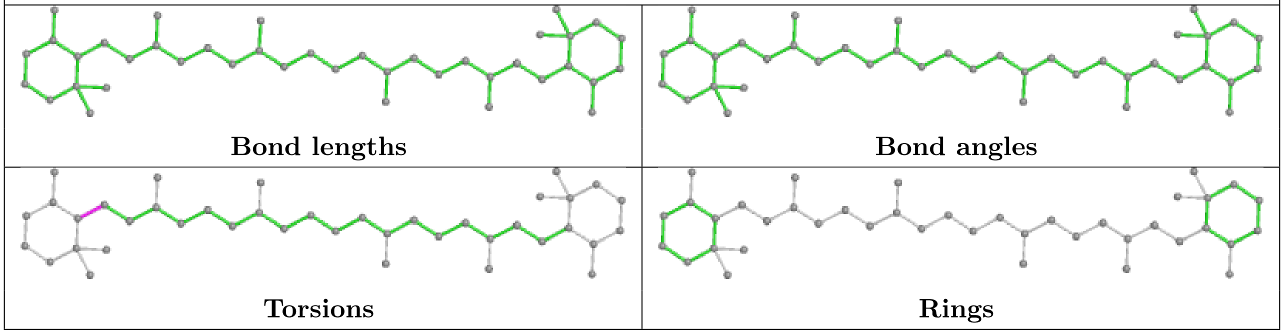
Bond lengths

Bond angles

Torsions

Rings

Ligand BCR B 840



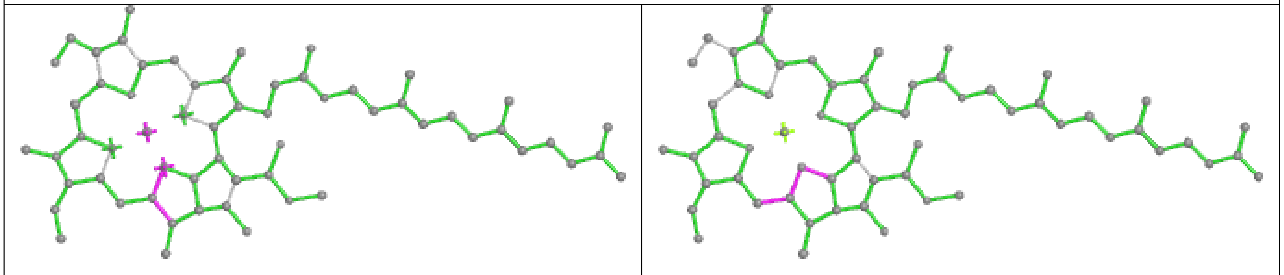
Bond lengths

Bond angles

Torsions

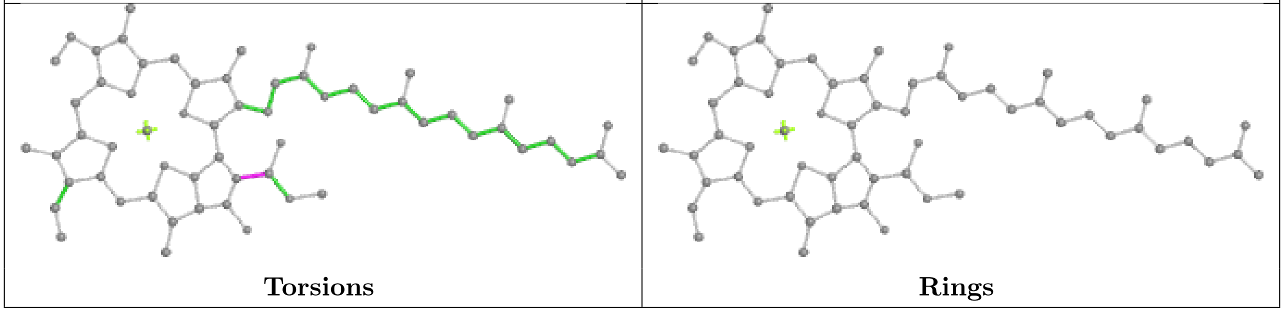
Rings

Ligand CLA A 825



Bond lengths

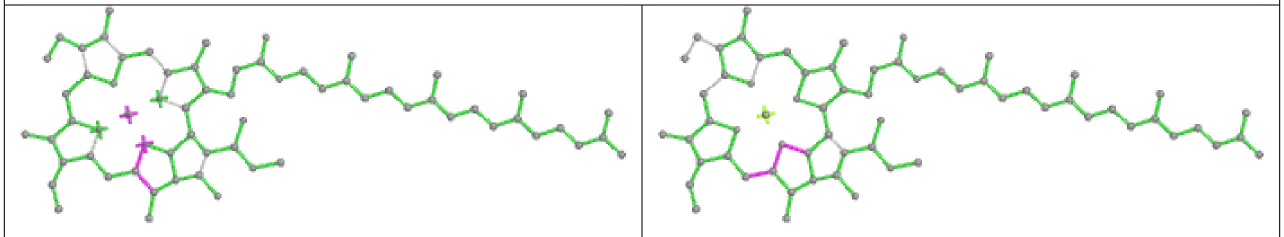
Bond angles



Torsions

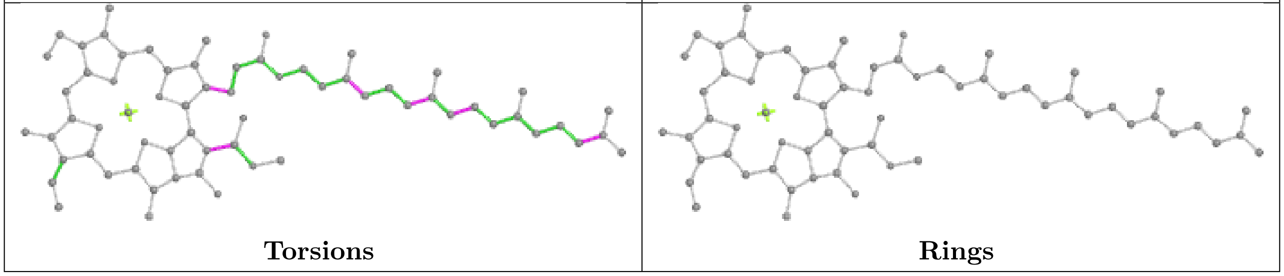
Rings

Ligand CLA B 812



Bond lengths

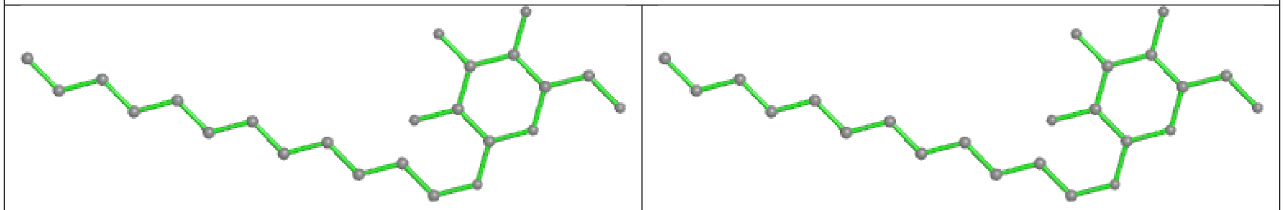
Bond angles



Torsions

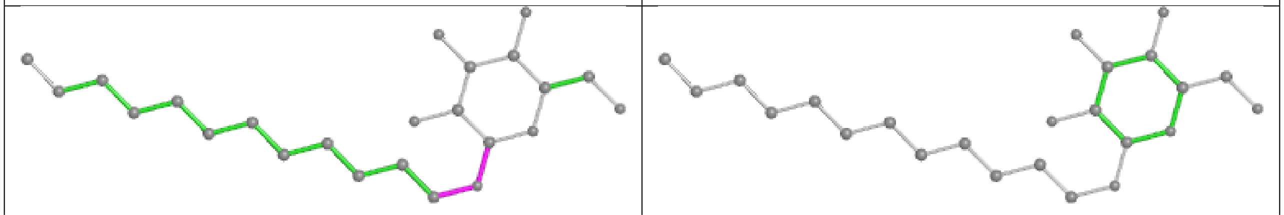
Rings

Ligand LMU A 857



Bond lengths

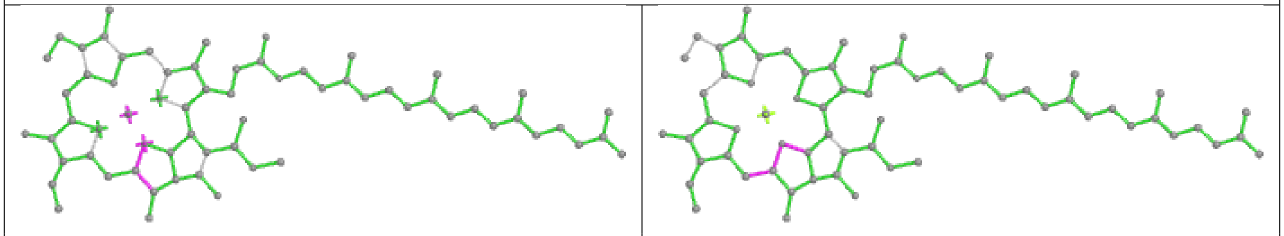
Bond angles



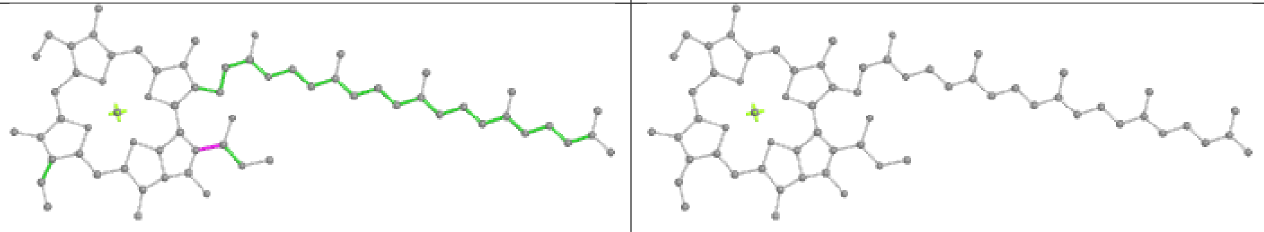
Torsions

Rings

Ligand CLA A 806

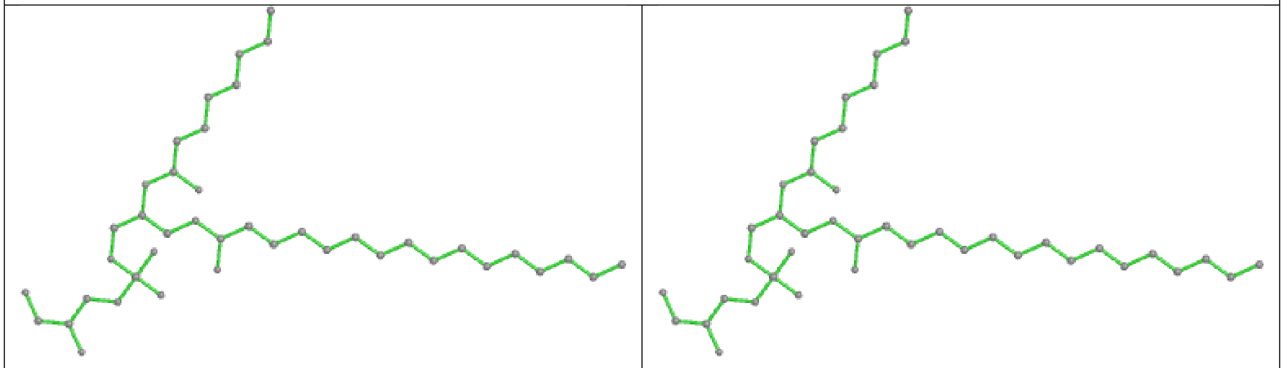


Bond lengths Bond angles

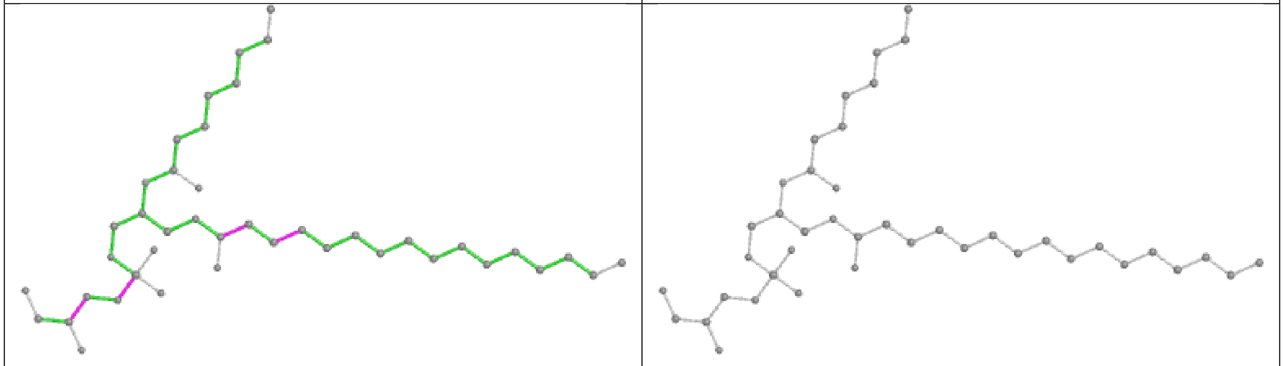


Torsions Rings

Ligand LHG A 846

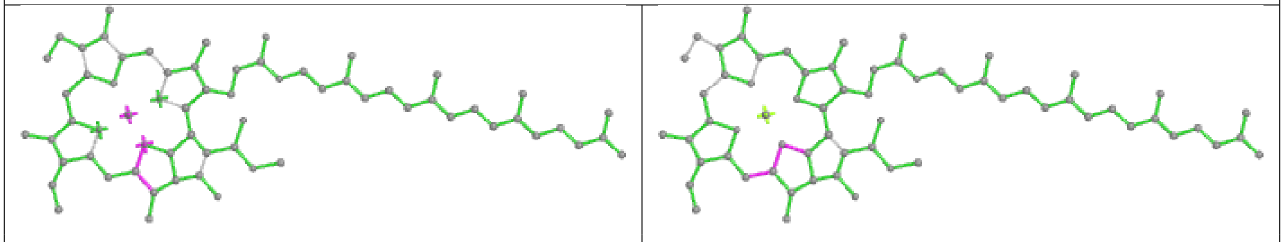


Bond lengths Bond angles

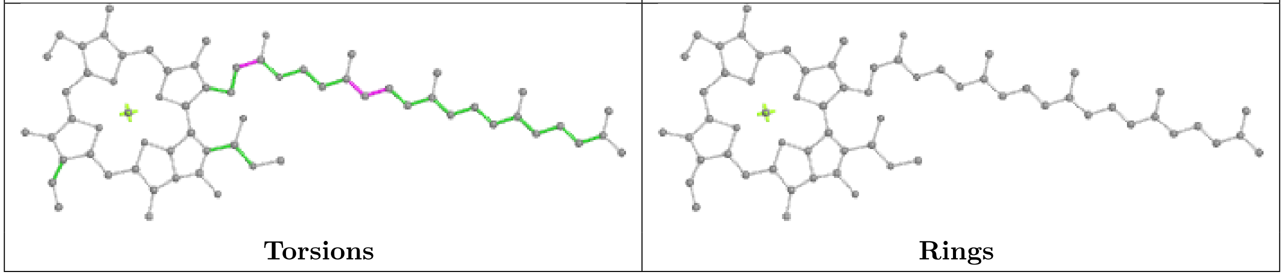


Torsions Rings

Ligand CLA A 836

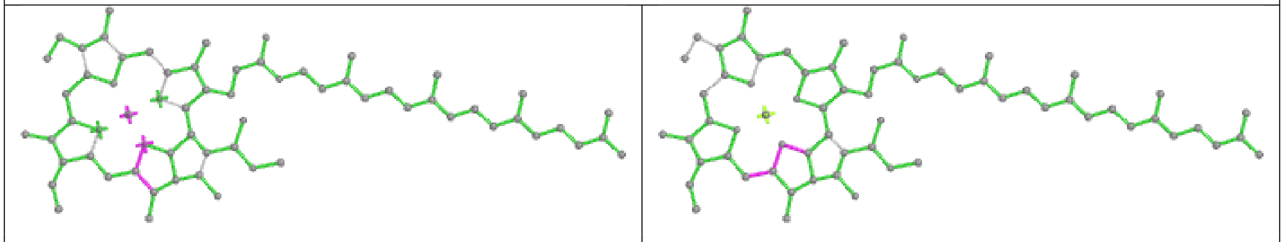


Bond lengths Bond angles

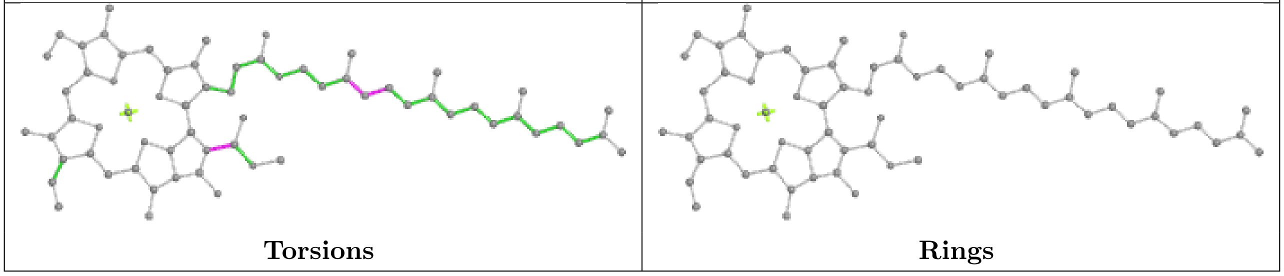


Torsions Rings

Ligand CLA B 807

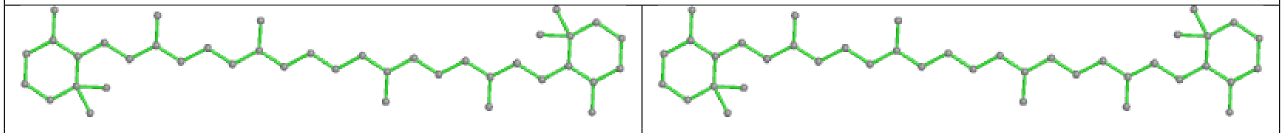


Bond lengths Bond angles

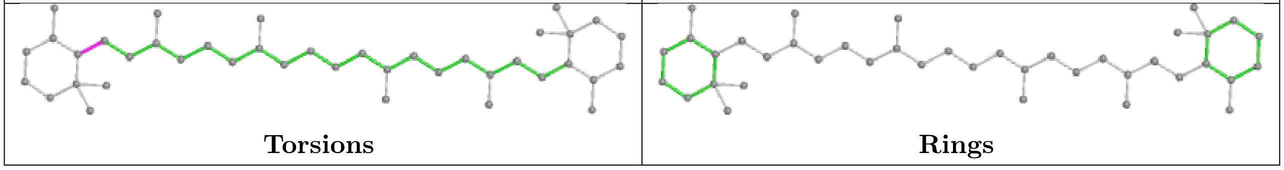


Torsions Rings

Ligand BCR A 849

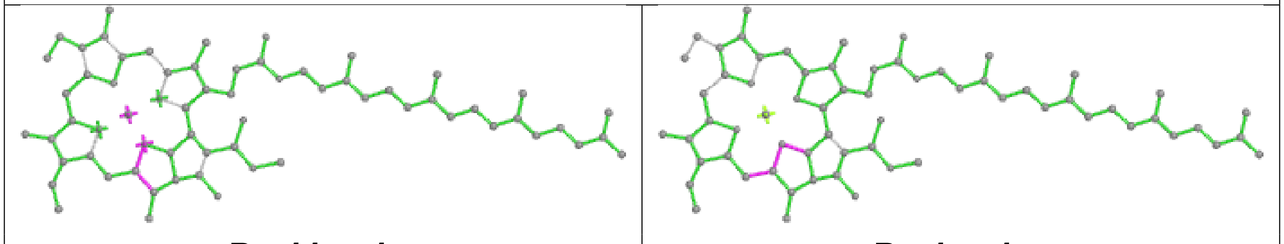


Bond lengths Bond angles



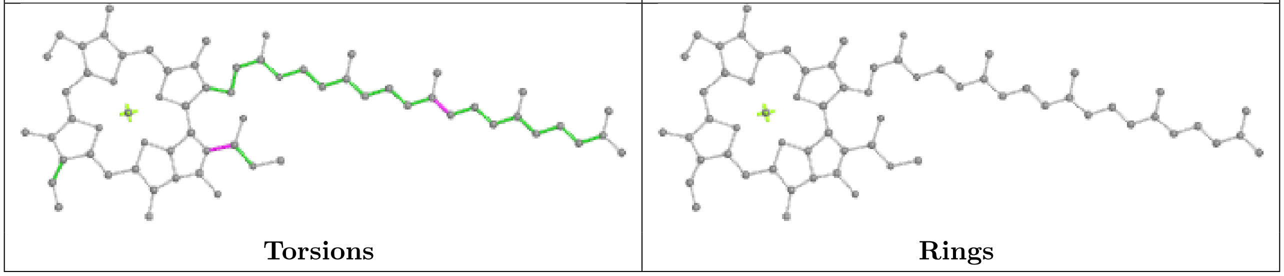
Torsions Rings

Ligand CLA B 825



Bond lengths

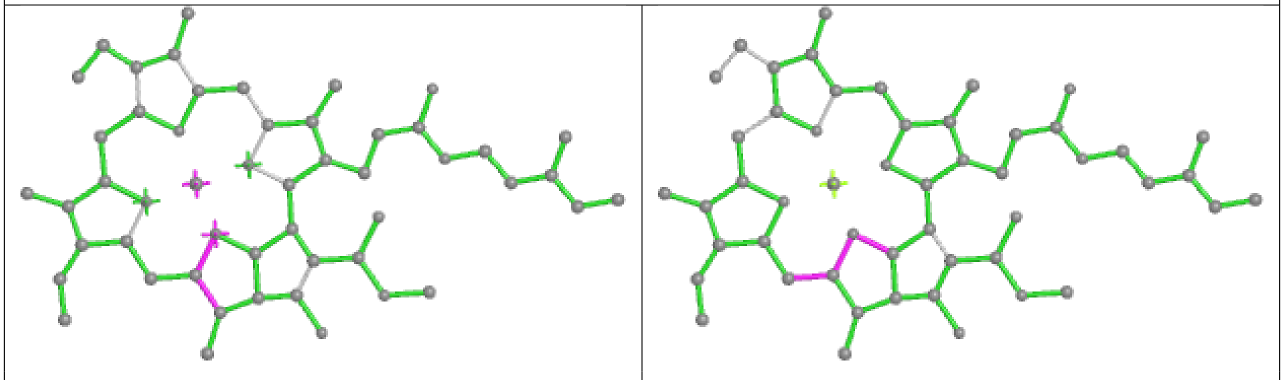
Bond angles



Torsions

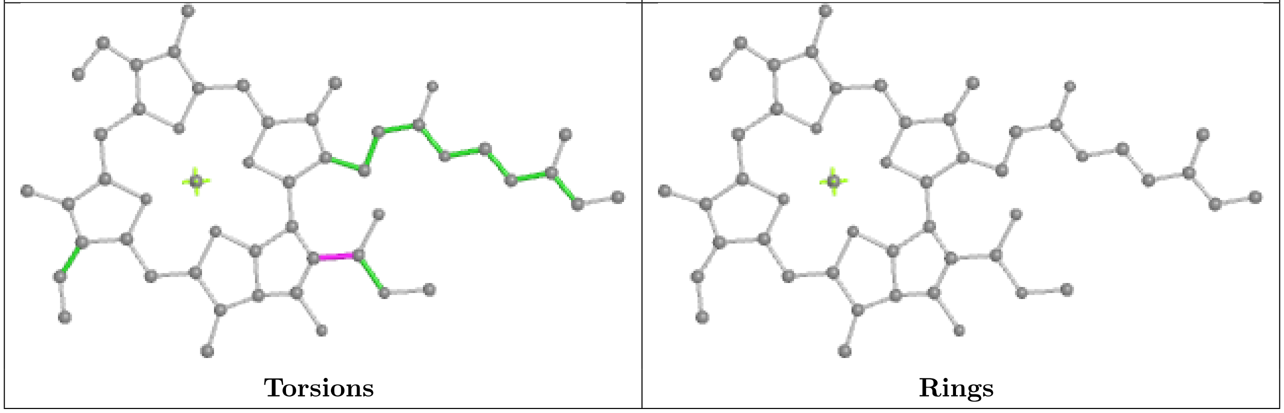
Rings

Ligand CLA A 838



Bond lengths

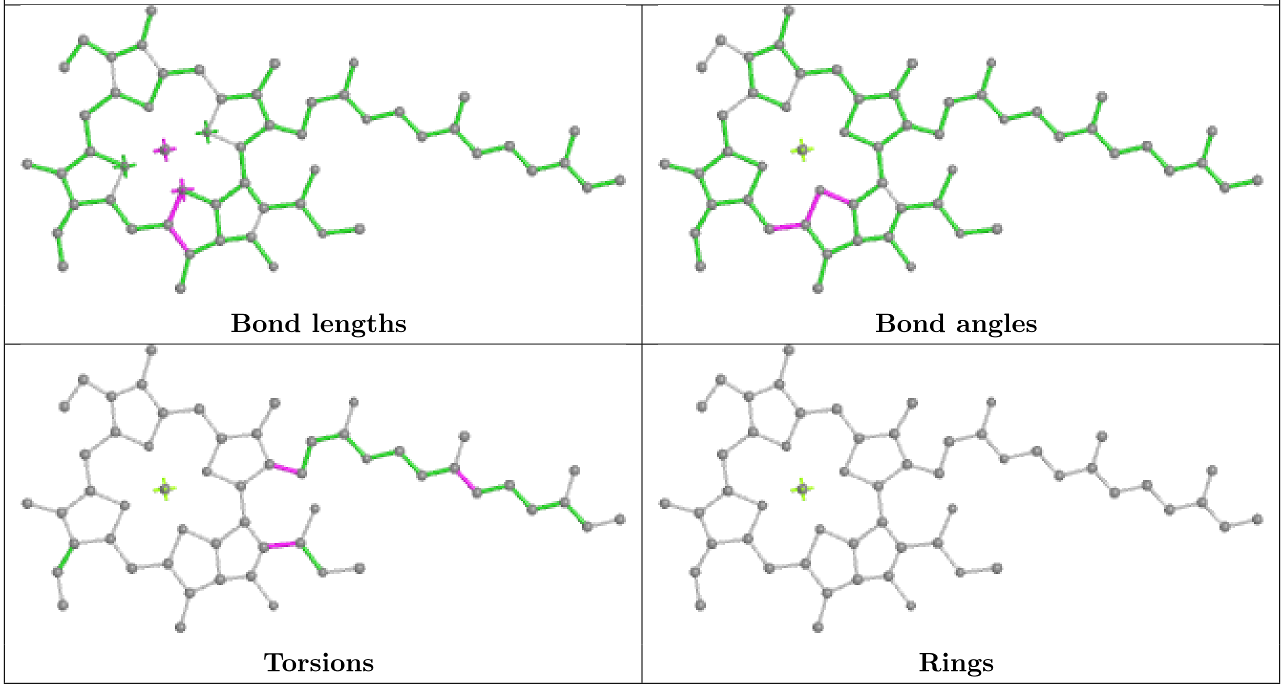
Bond angles



Torsions

Rings

Ligand CLA B 823



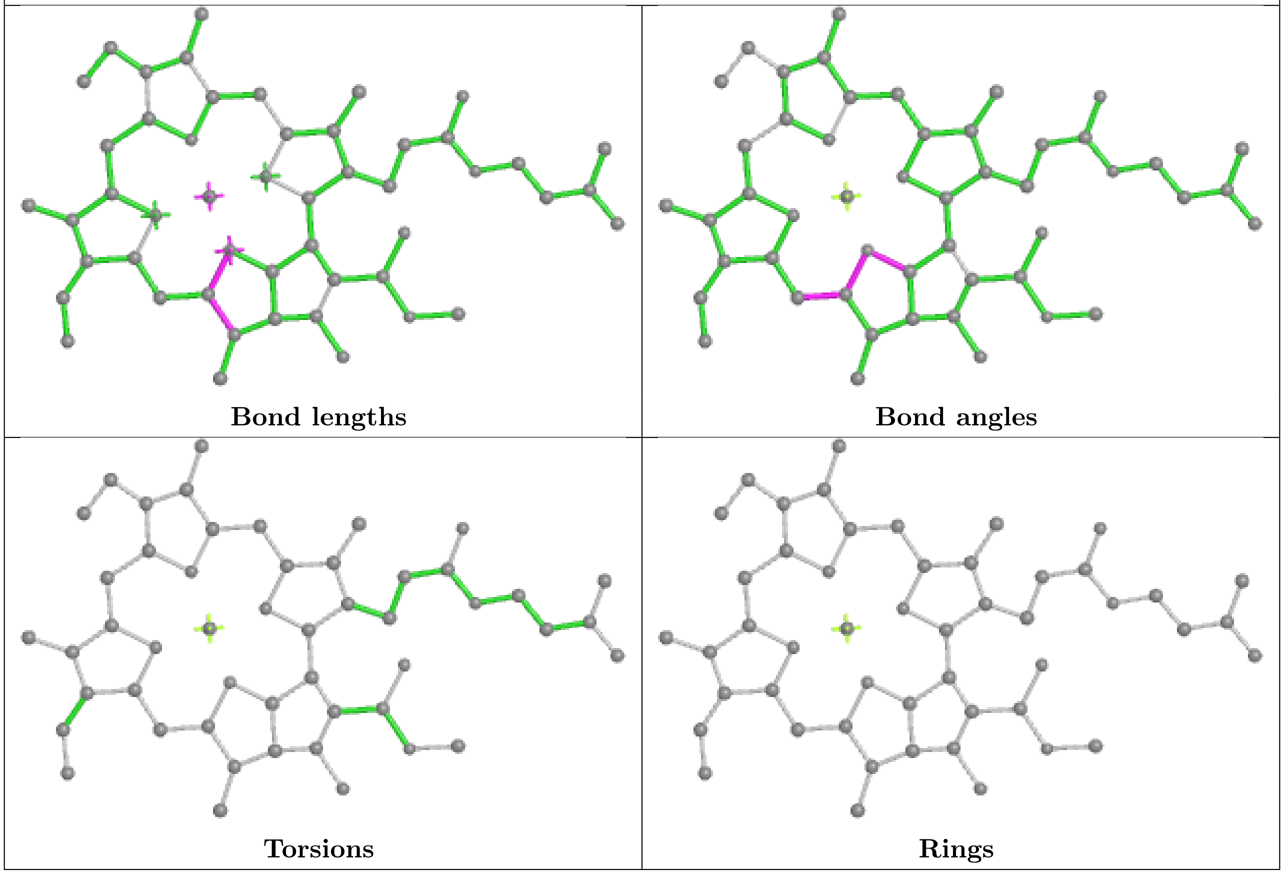
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA A 856



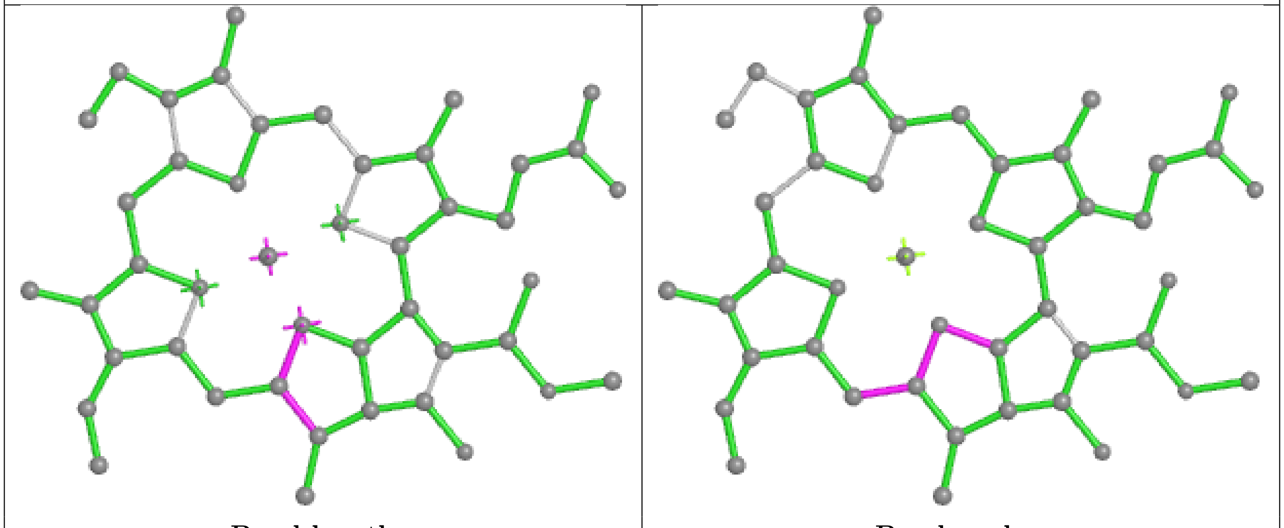
Bond lengths

Bond angles

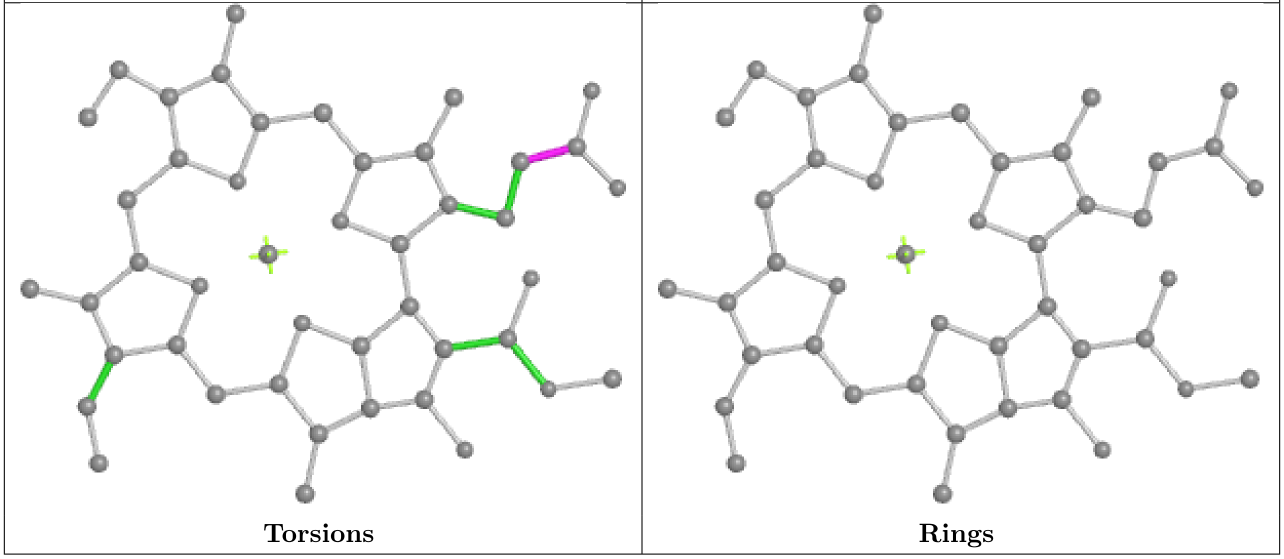
Torsions

Rings

Ligand CLA L 302

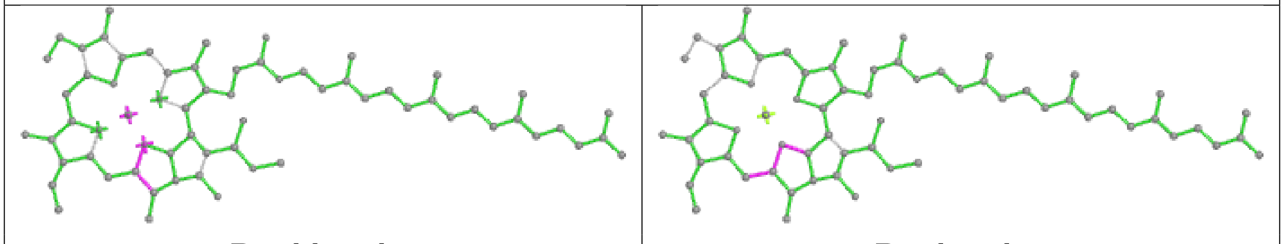


Bond lengths Bond angles

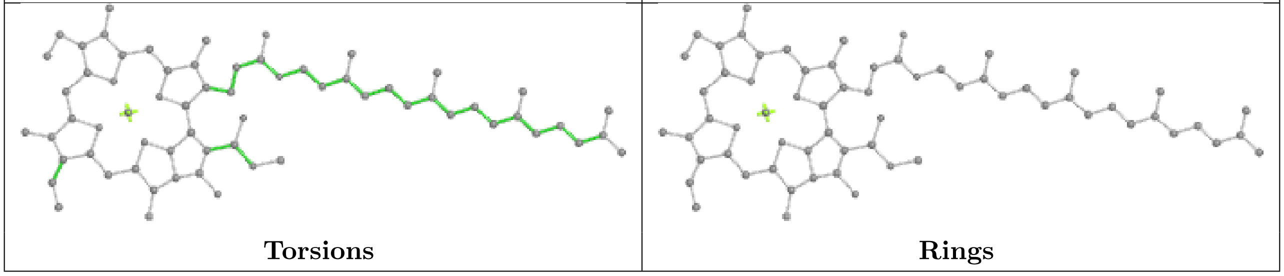


Torsions Rings

Ligand CLA A 802

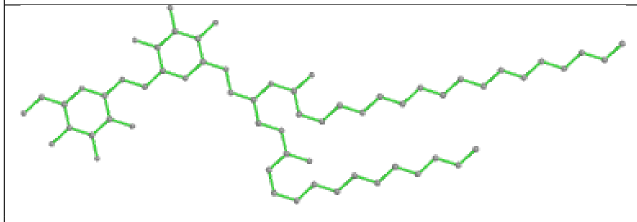


Bond lengths Bond angles

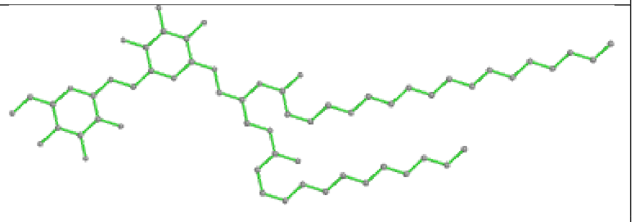


Torsions Rings

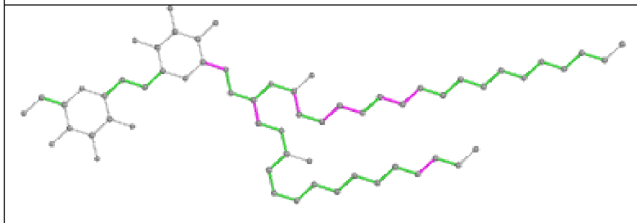
Ligand DGD B 844



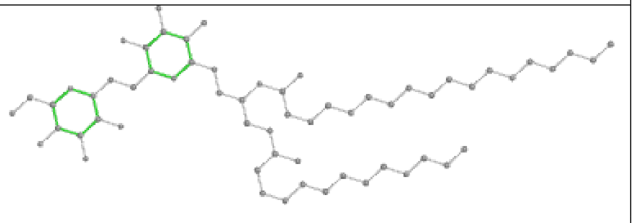
Bond lengths



Bond angles

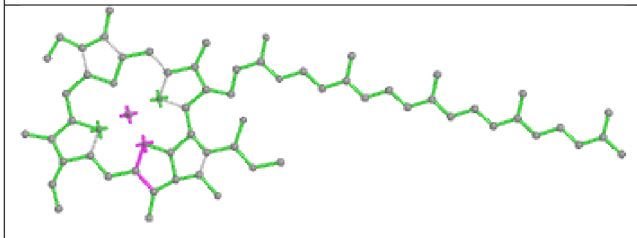


Torsions

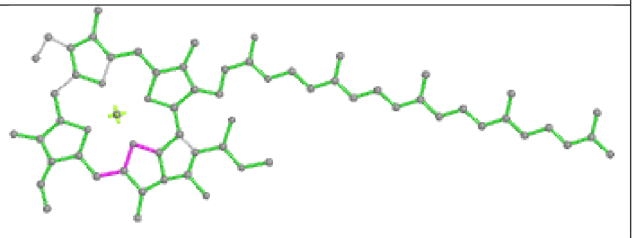


Rings

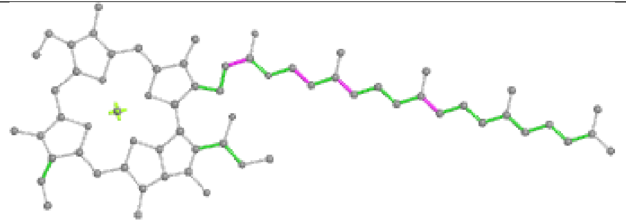
Ligand CLA A 826



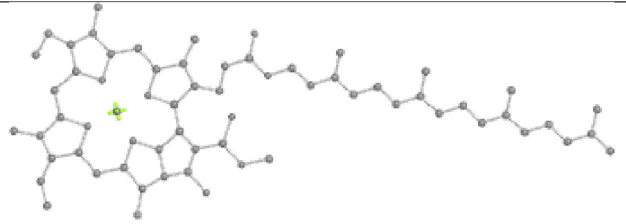
Bond lengths



Bond angles

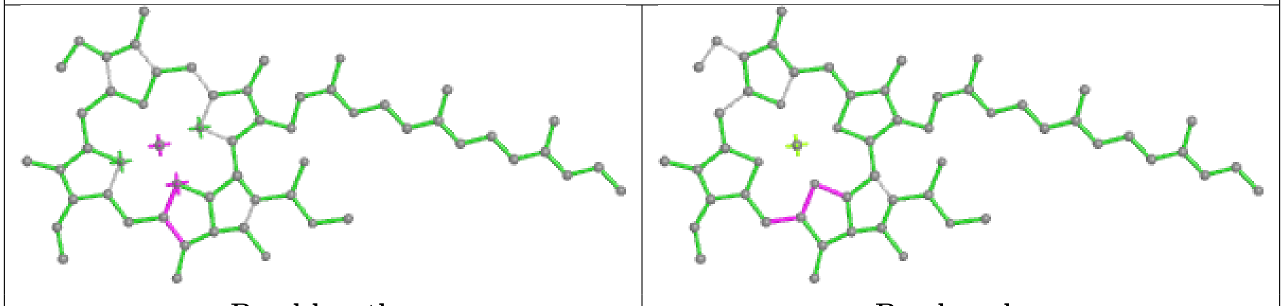


Torsions



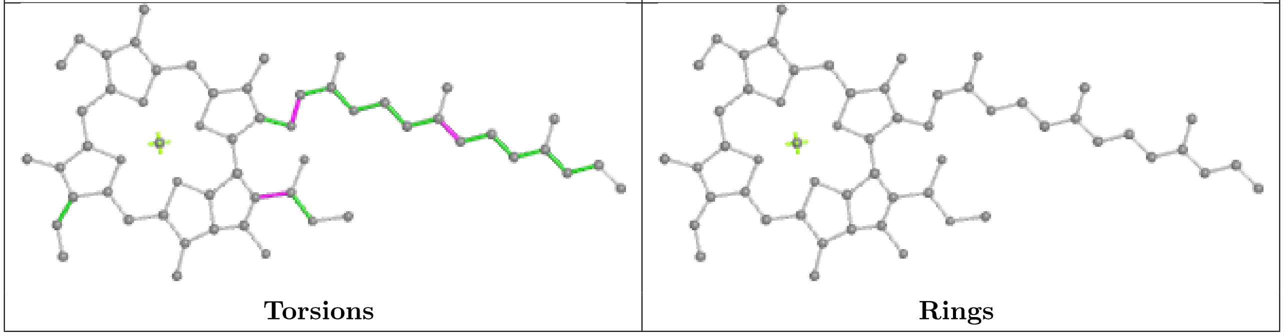
Rings

Ligand CLA B 815



Bond lengths

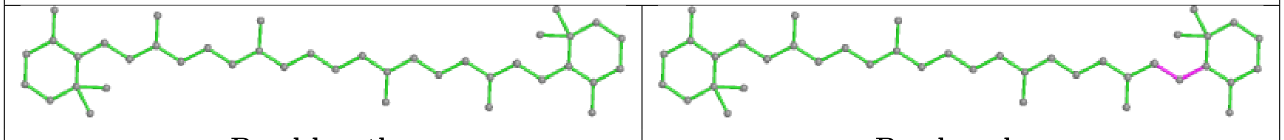
Bond angles



Torsions

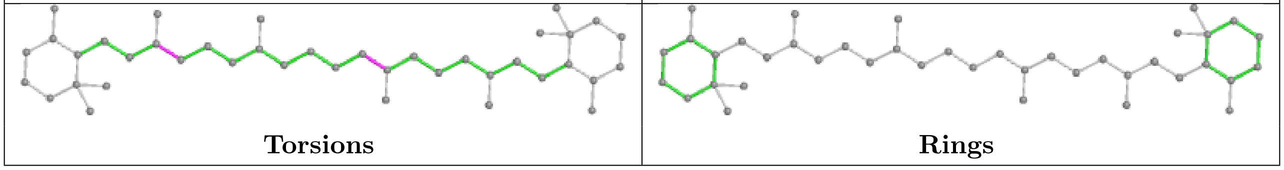
Rings

Ligand BCR A 852



Bond lengths

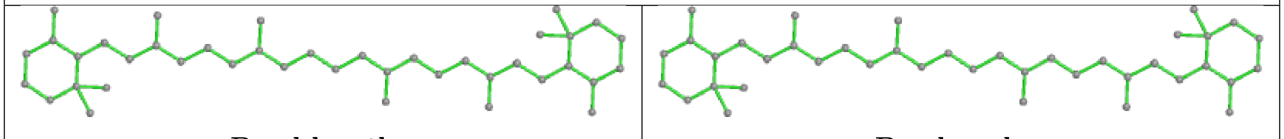
Bond angles



Torsions

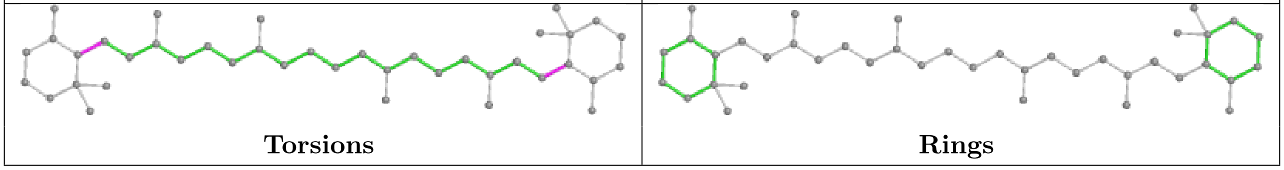
Rings

Ligand BCR A 848



Bond lengths

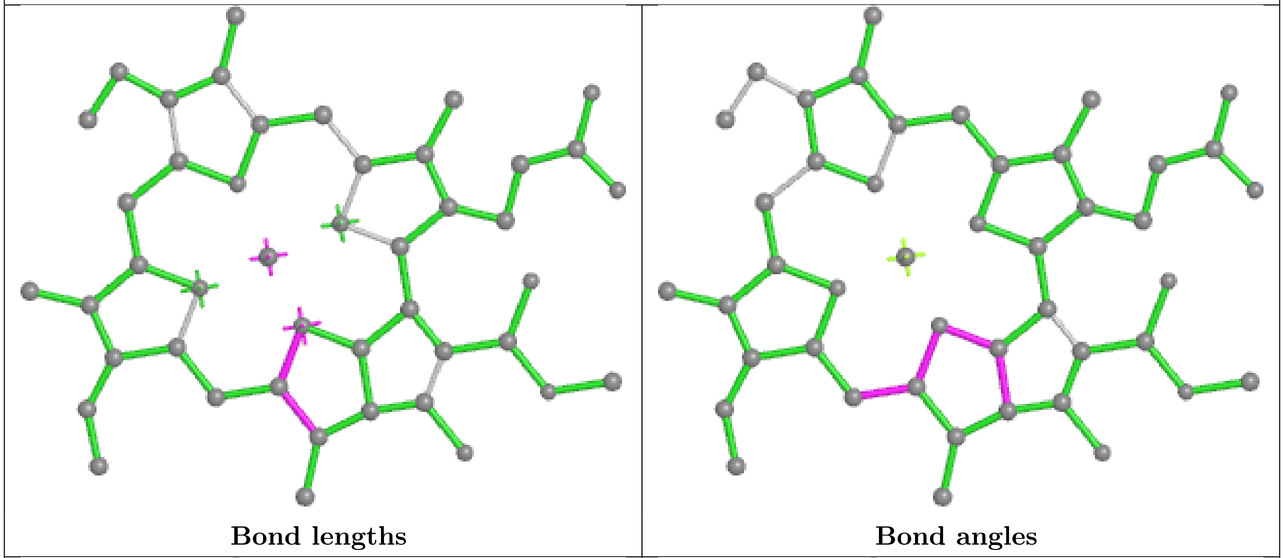
Bond angles



Torsions

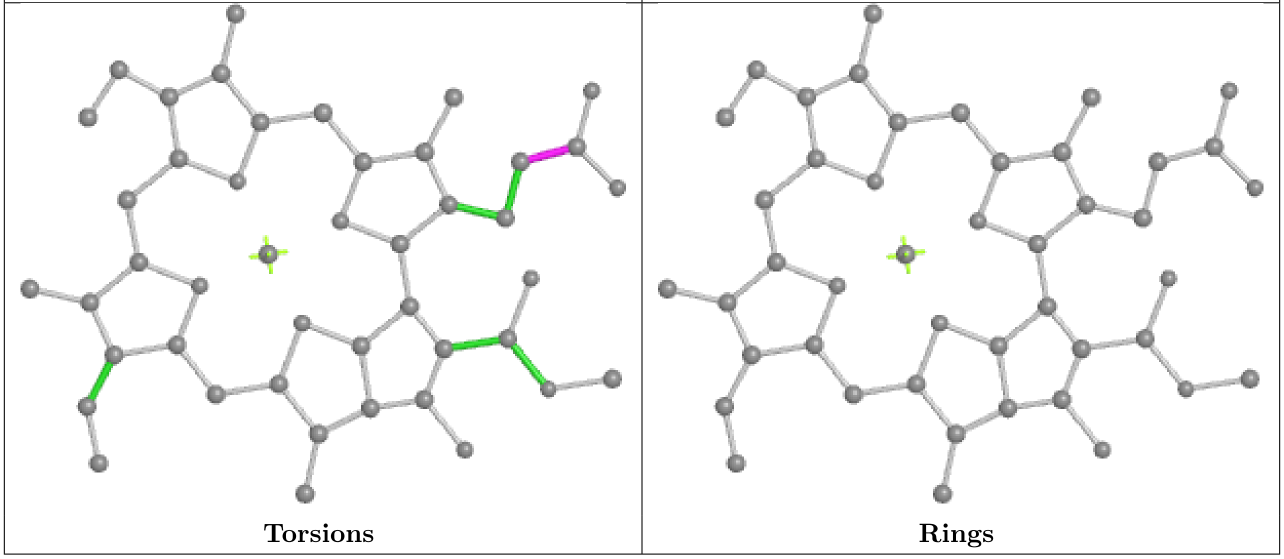
Rings

Ligand CLA B 831



Bond lengths

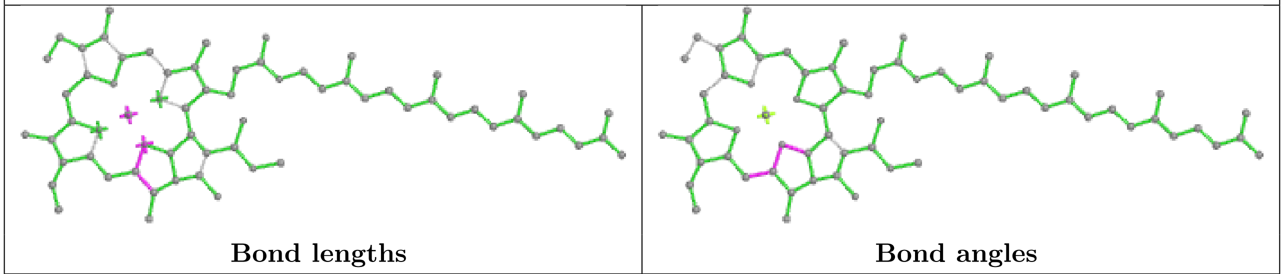
Bond angles



Torsions

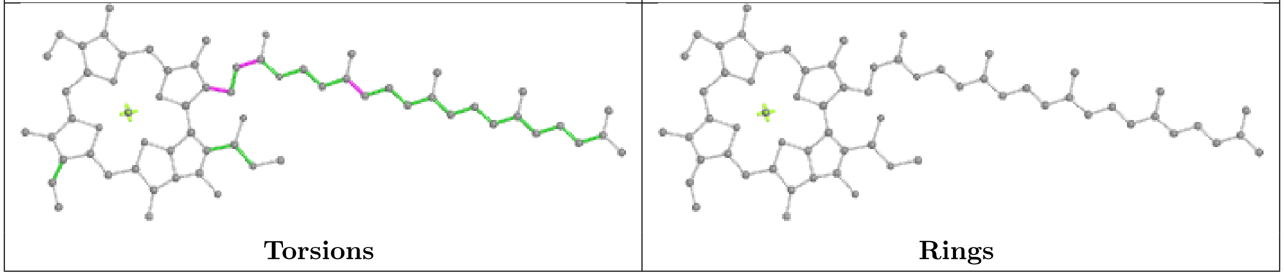
Rings

Ligand CLA B 804



Bond lengths

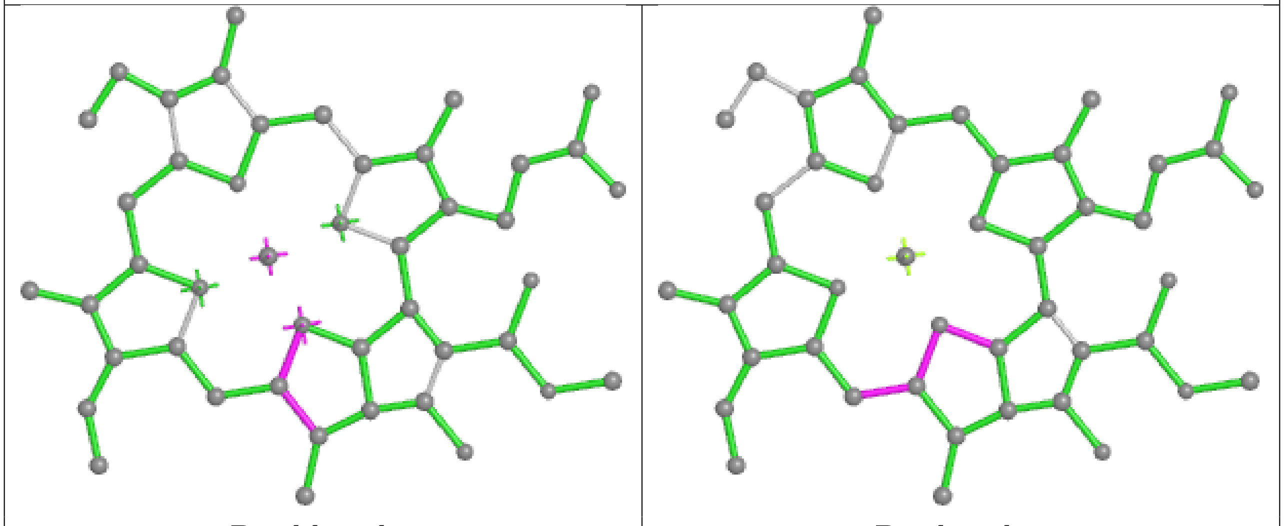
Bond angles



Torsions

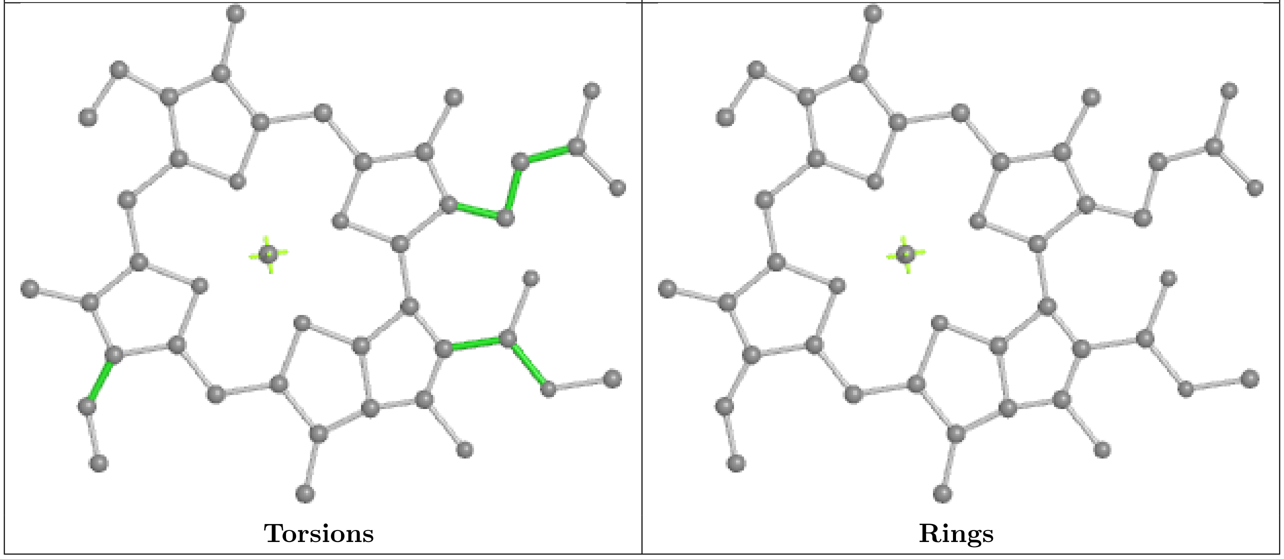
Rings

Ligand CLA L 304



Bond lengths

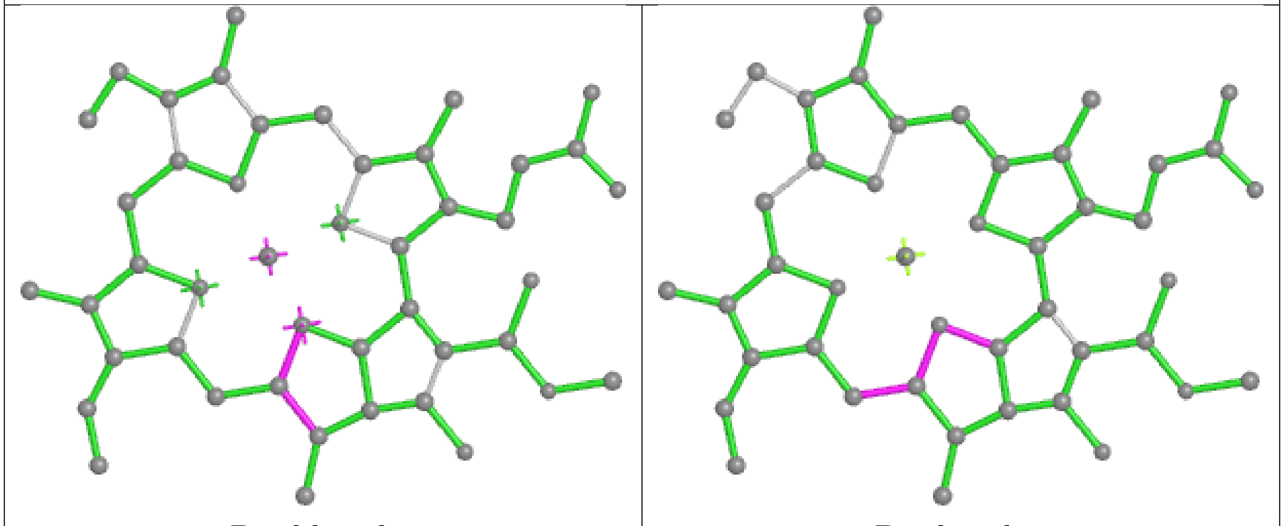
Bond angles



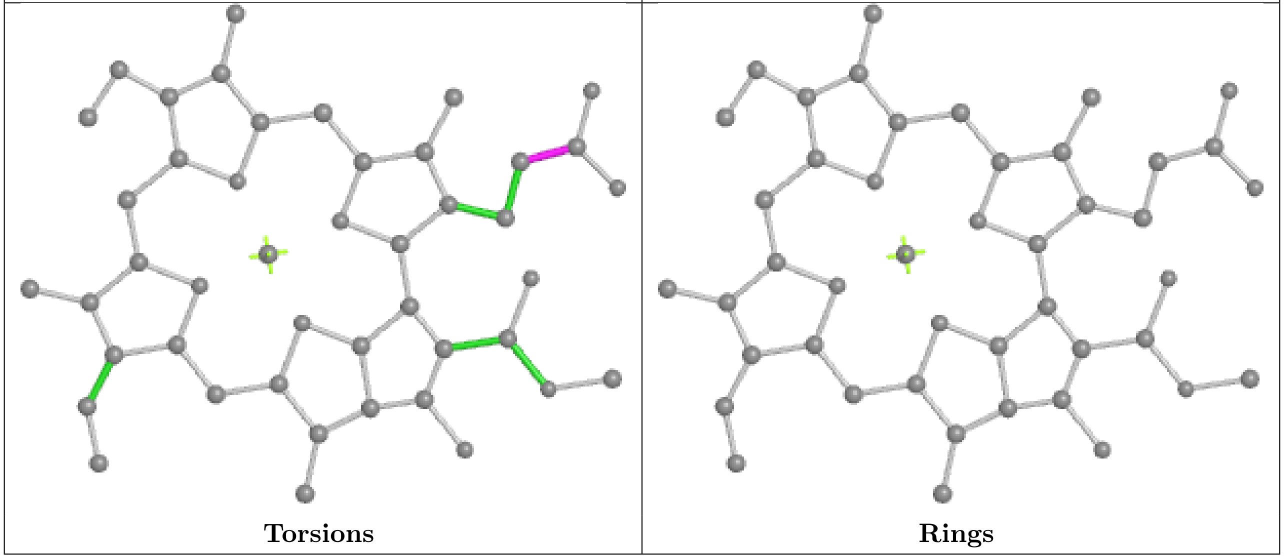
Torsions

Rings

Ligand CLA B 833

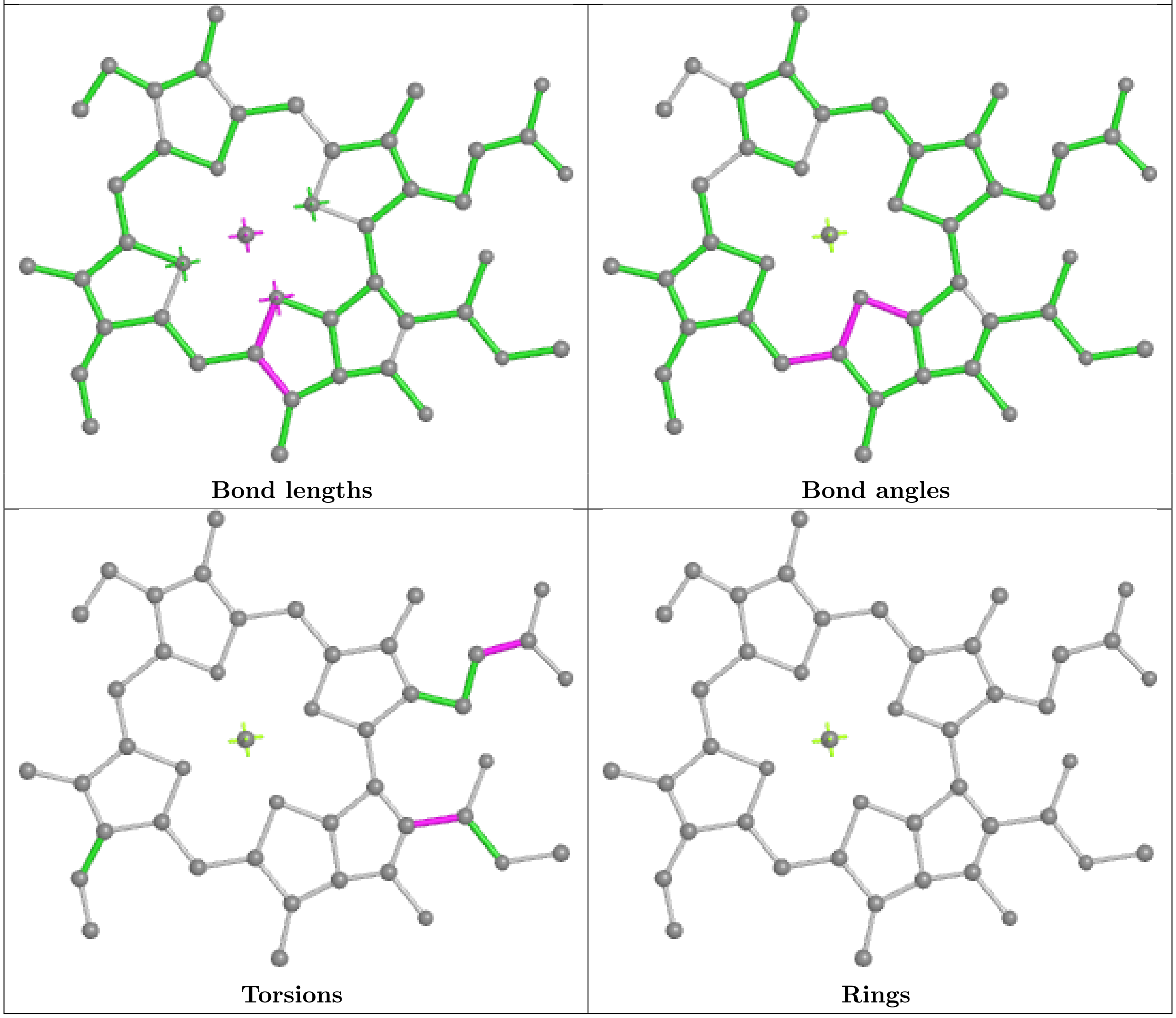


Bond lengths Bond angles

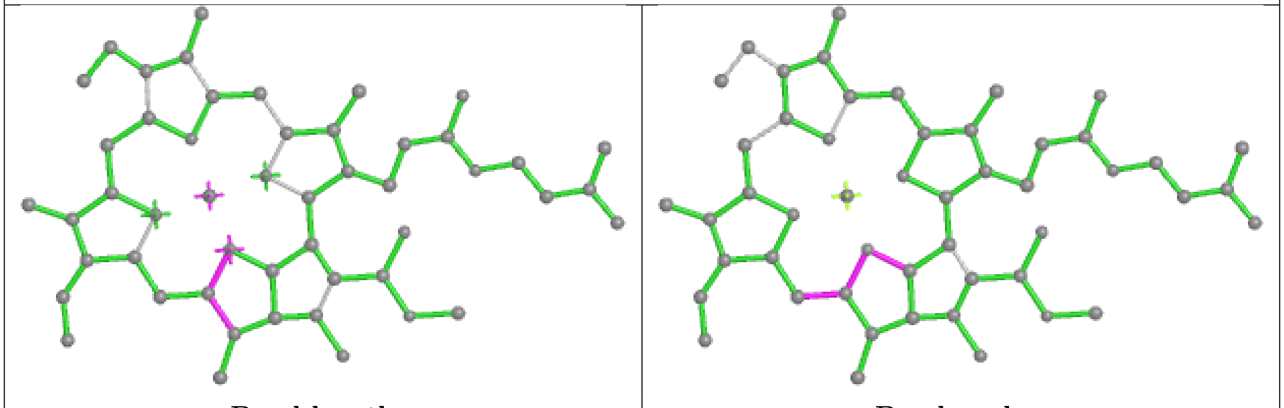


Torsions Rings

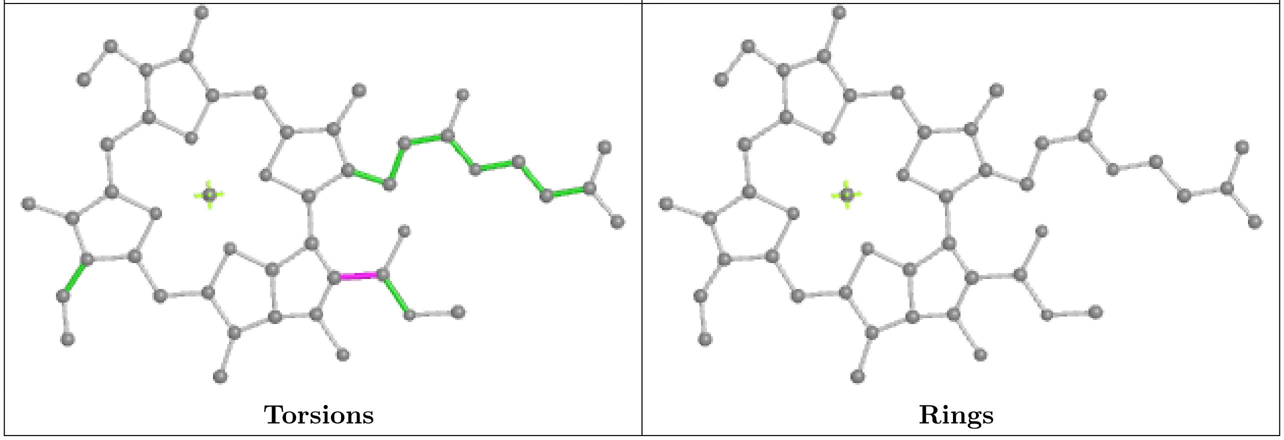
Ligand CLA B 820



Ligand CLA B 824

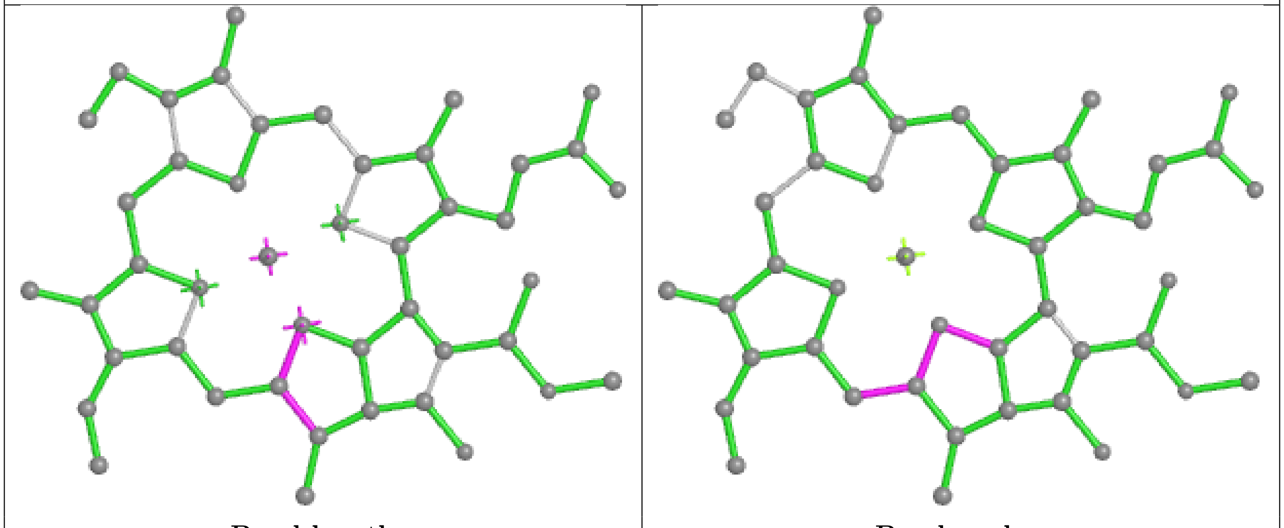


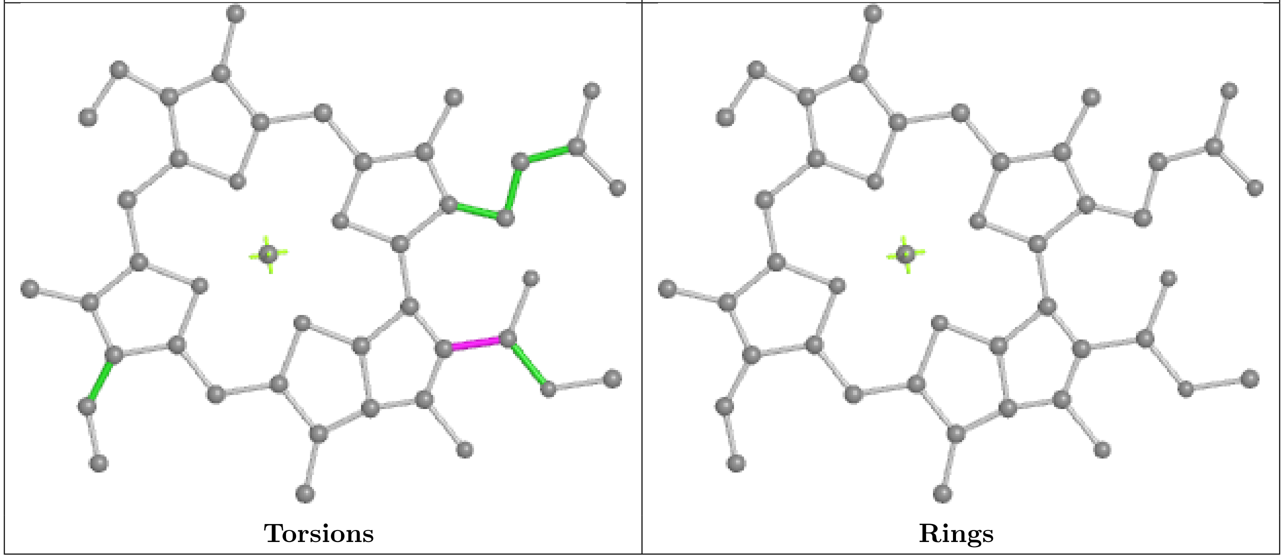
Bond lengths **Bond angles**



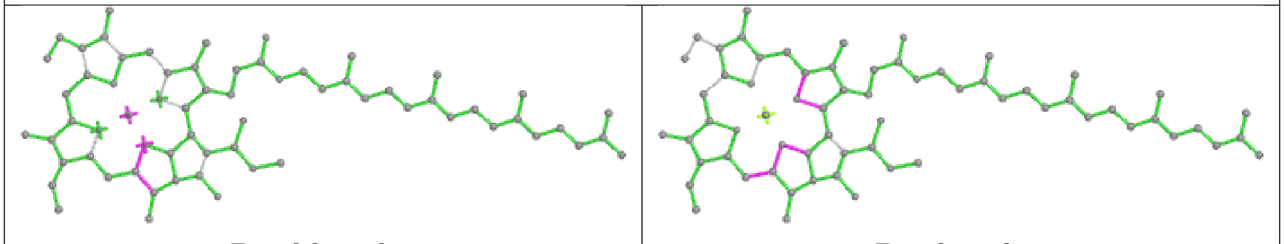
Torsions **Rings**

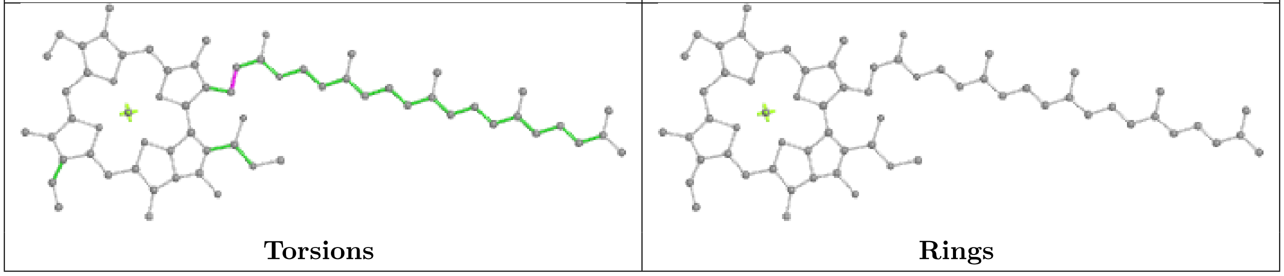
Ligand CLA A 817


Bond lengths Bond angles

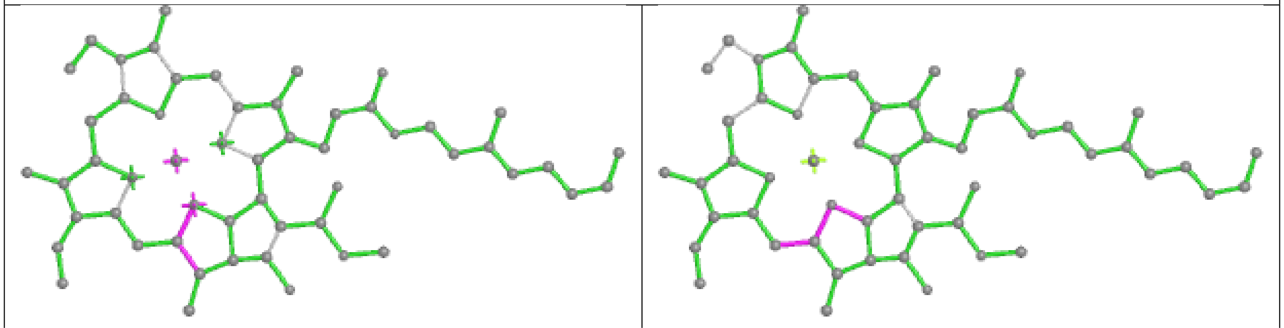

Torsions Rings

Ligand CLA A 803


Bond lengths Bond angles

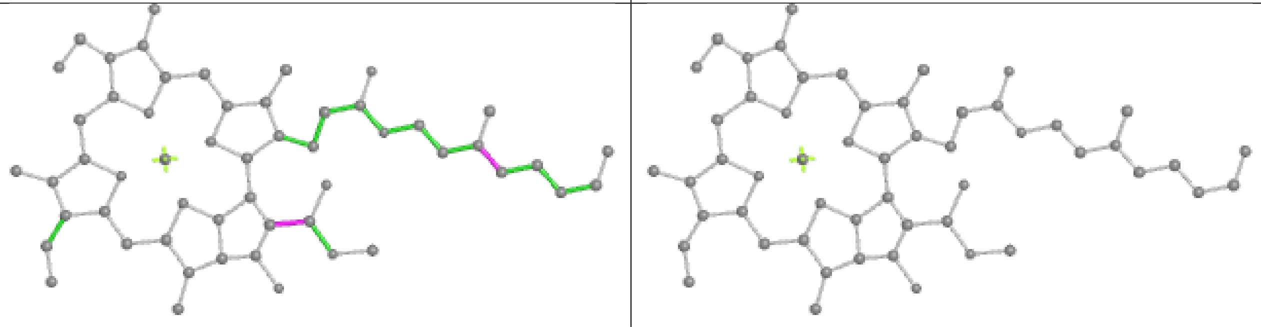

Torsions Rings

Ligand CLA A 815



Bond lengths

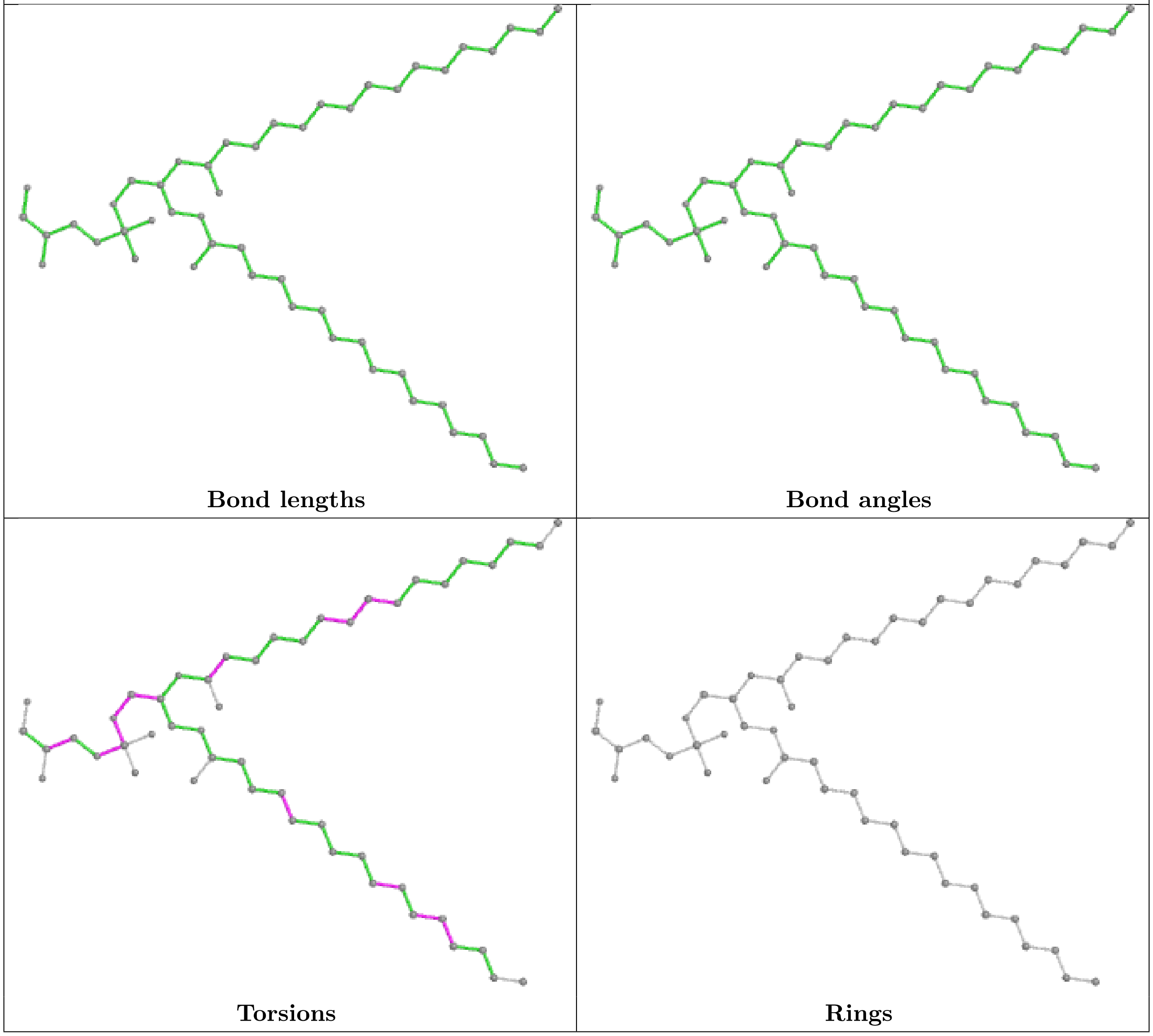
Bond angles



Torsions

Rings

Ligand LHG B 845



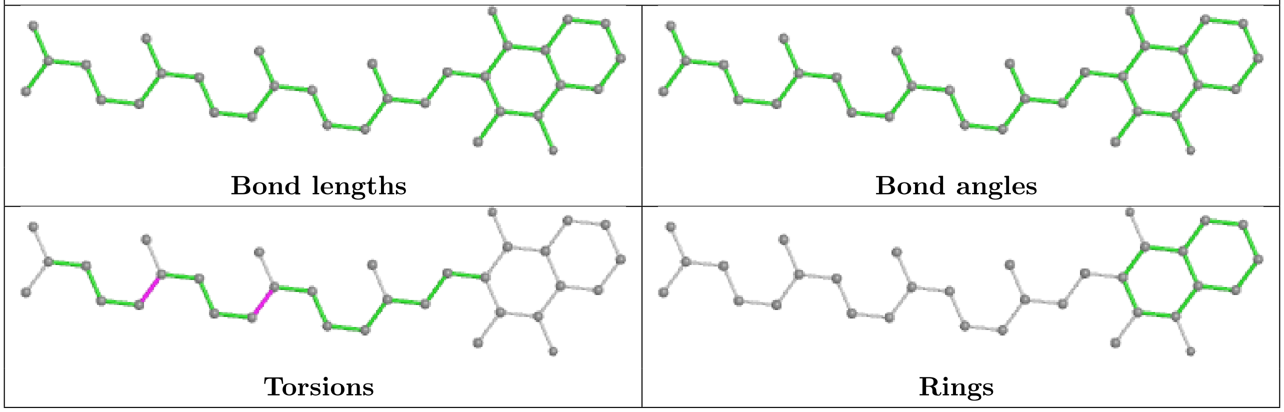
Bond lengths

Bond angles

Torsions

Rings

Ligand PQN B 839



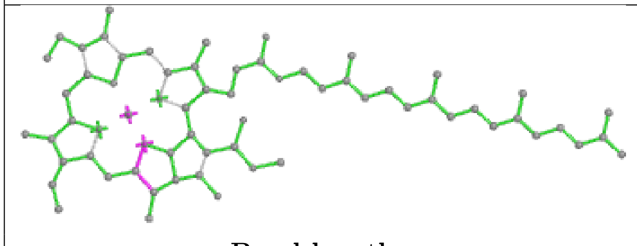
Bond lengths

Bond angles

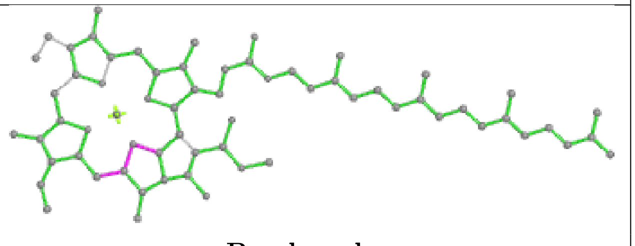
Torsions

Rings

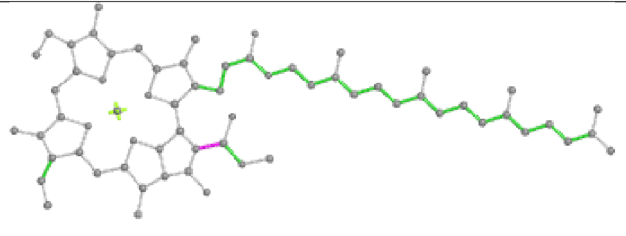
Ligand CLA A 831



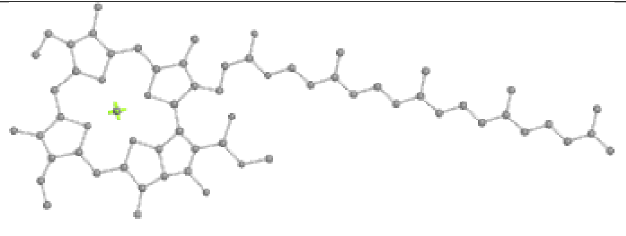
Bond lengths



Bond angles



Torsions



Rings

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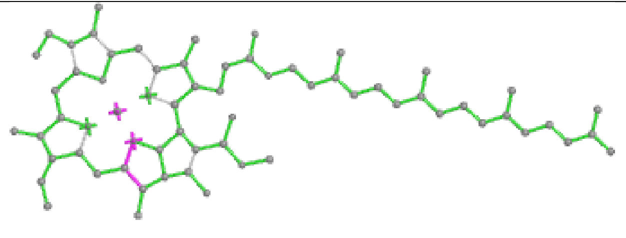
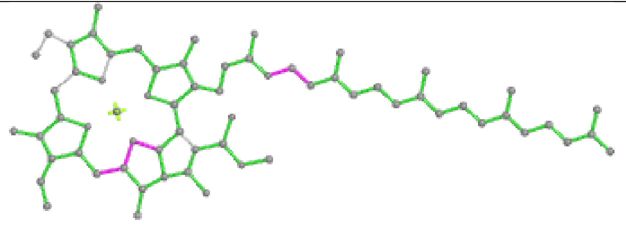
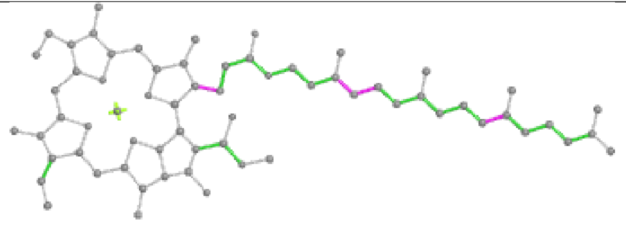


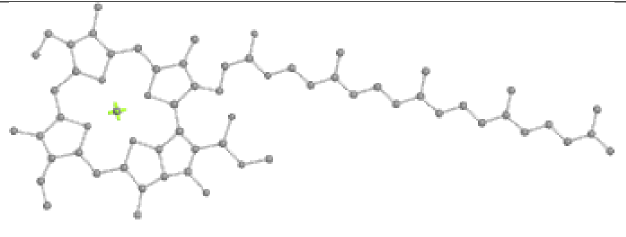
Bond lengths



Bond angles

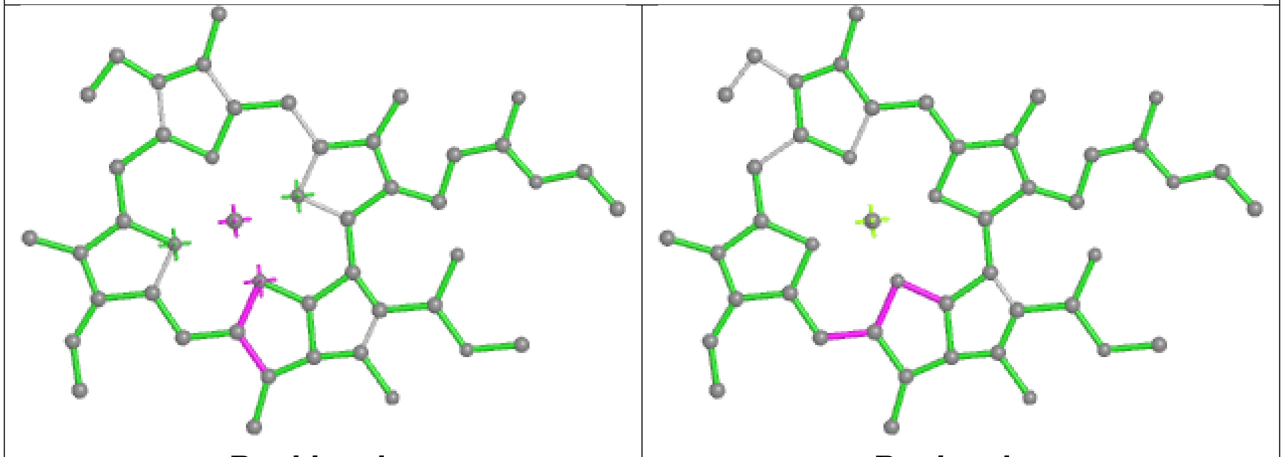


Torsions

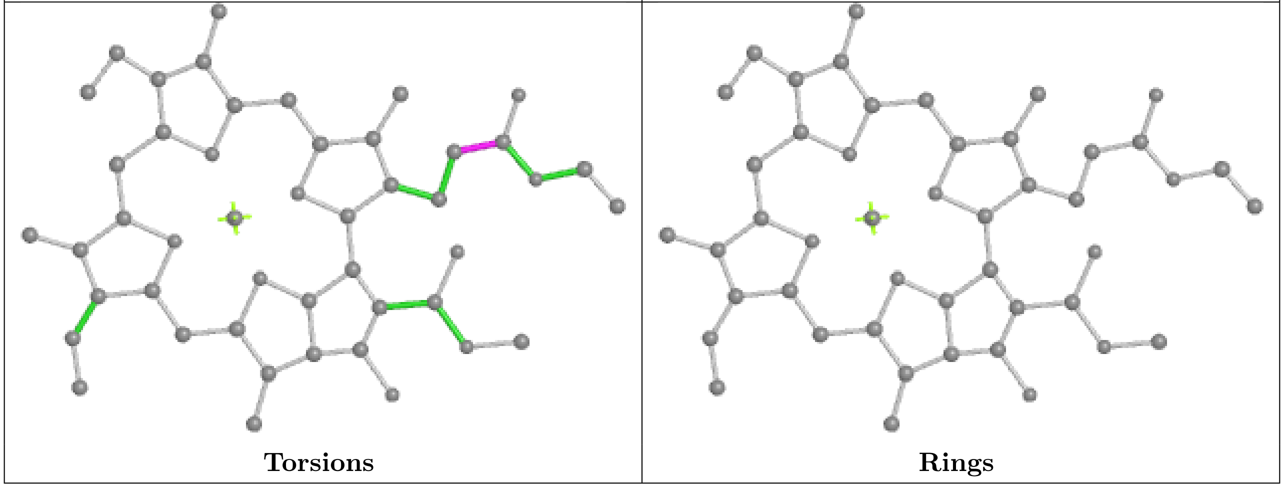


Rings

Ligand CLA A 808

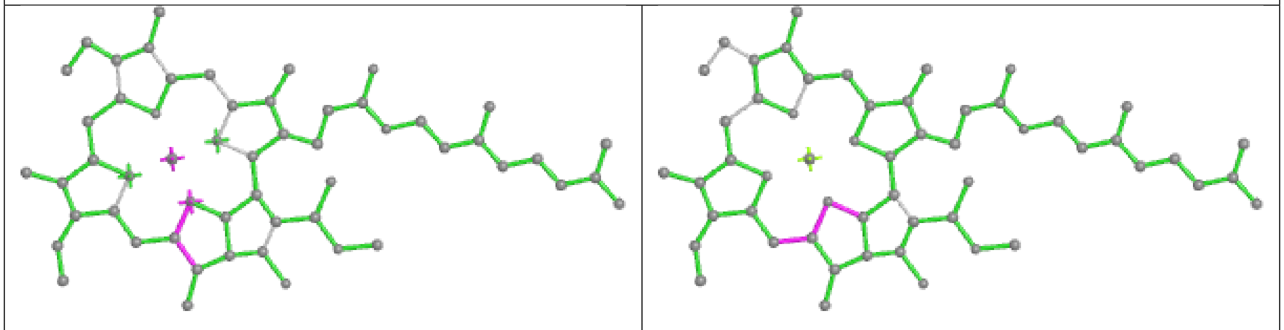


Bond lengths Bond angles

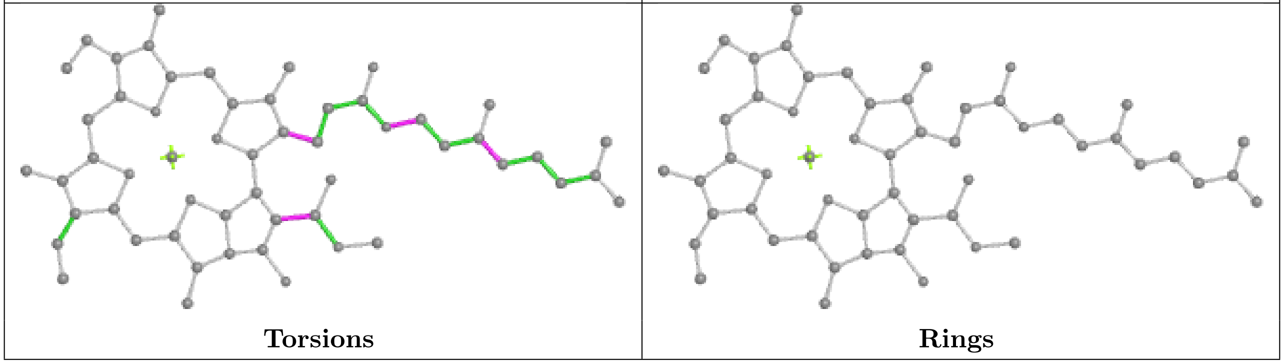


Torsions Rings

Ligand CLA A 809

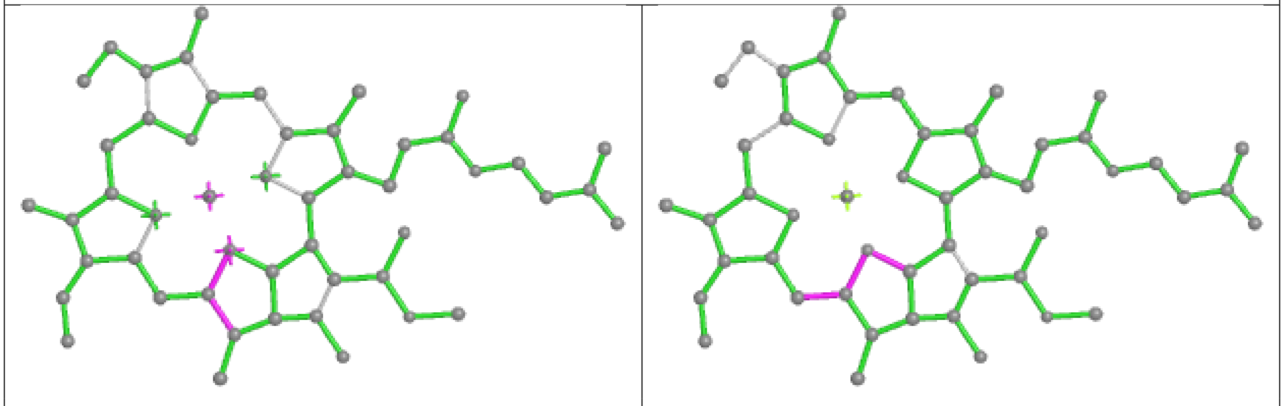


Bond lengths Bond angles

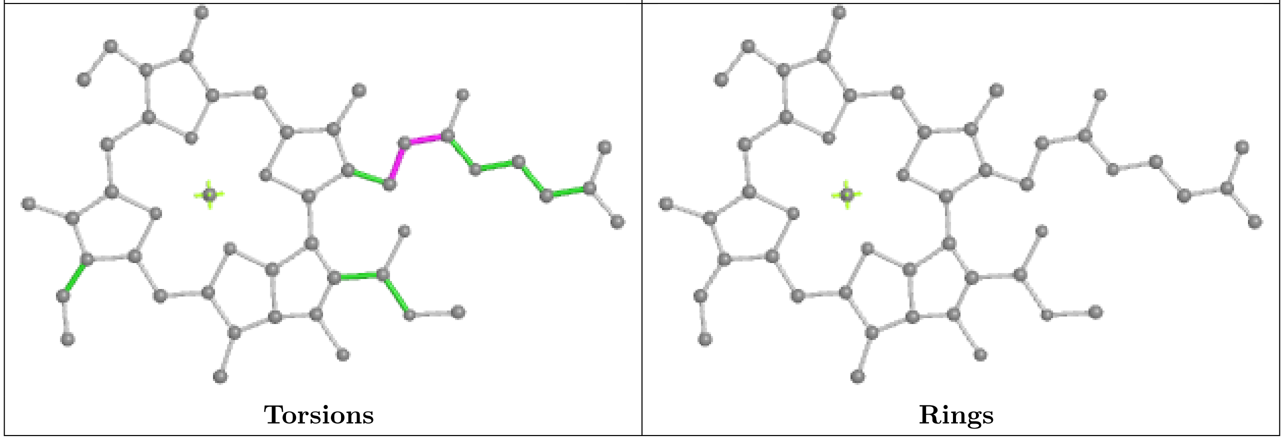


Torsions Rings

Ligand CLA A 810

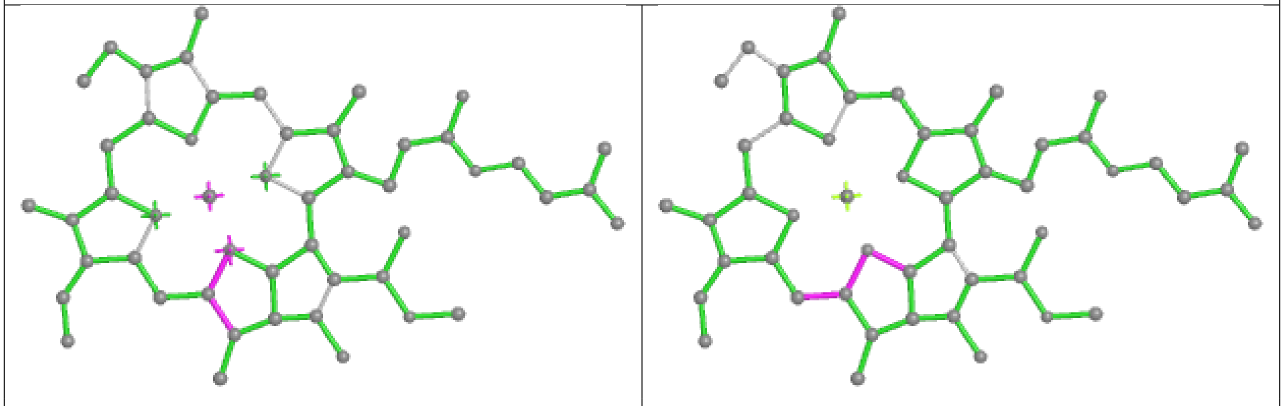


Bond lengths Bond angles

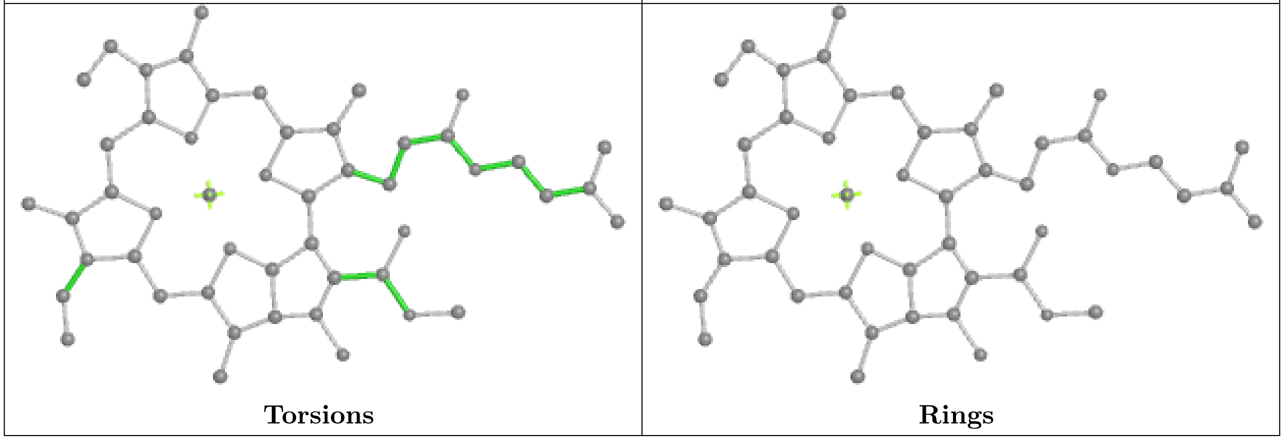


Torsions Rings

Ligand CLA B 836

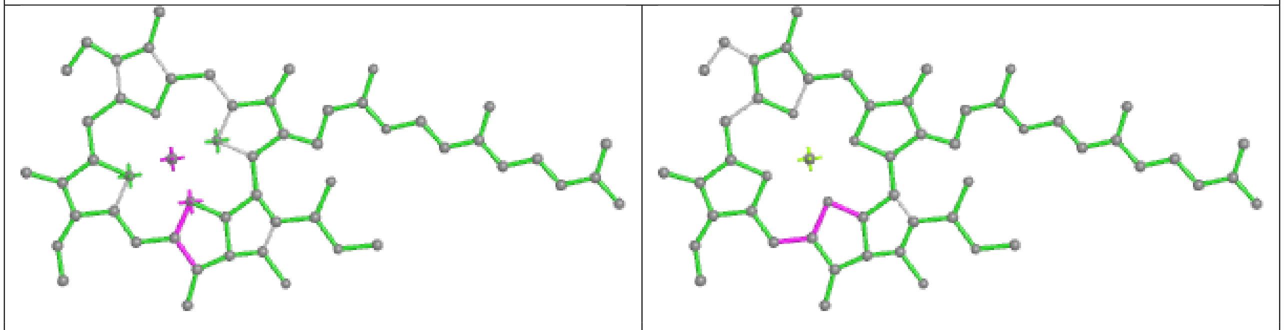


Bond lengths Bond angles

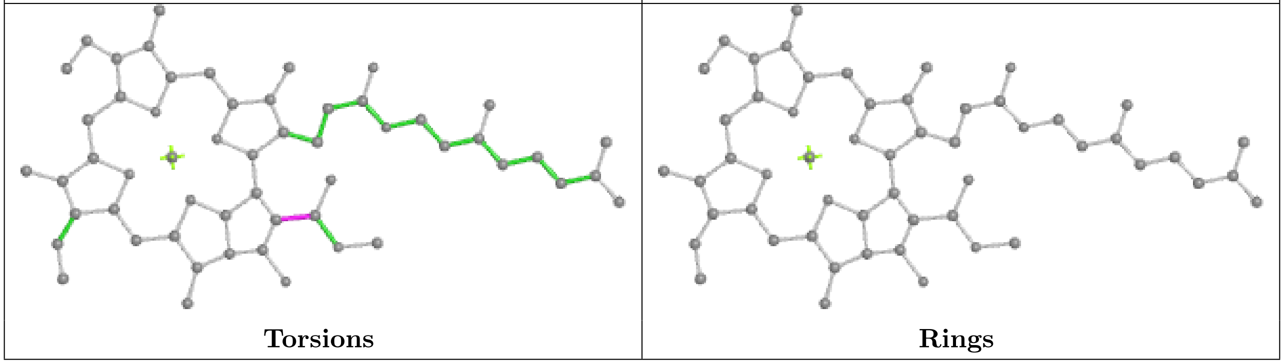


Torsions Rings

Ligand CLA A 840

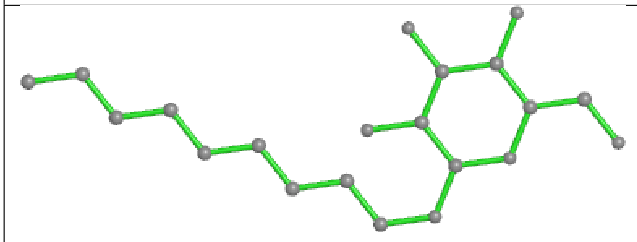


Bond lengths Bond angles

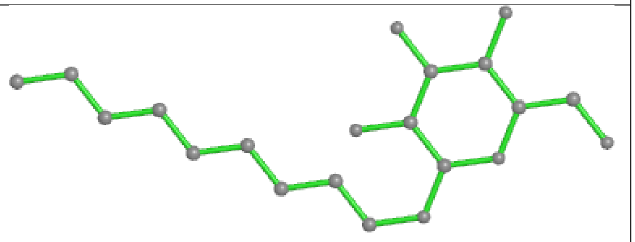


Torsions Rings

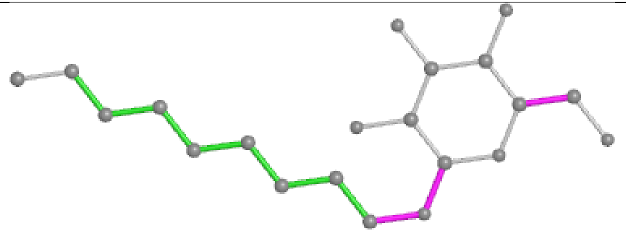
Ligand LMU A 859



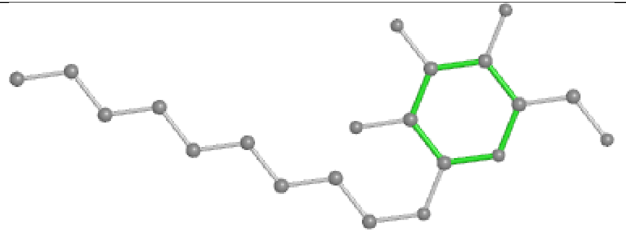
Bond lengths



Bond angles

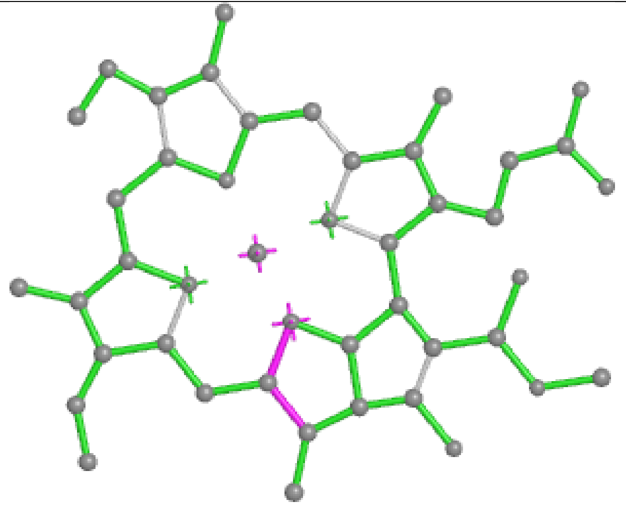


Torsions

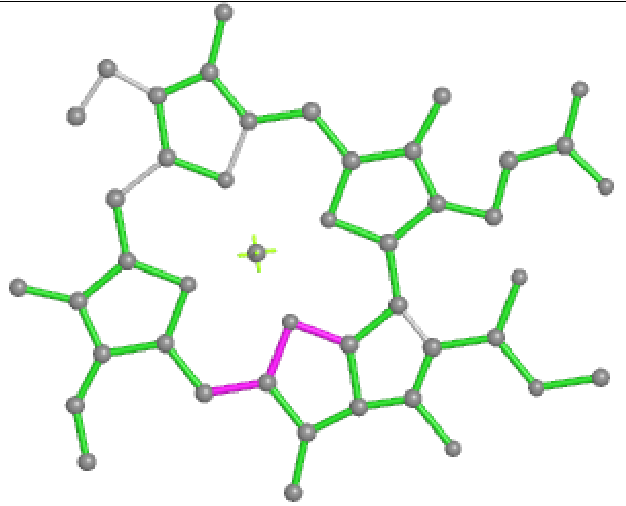


Rings

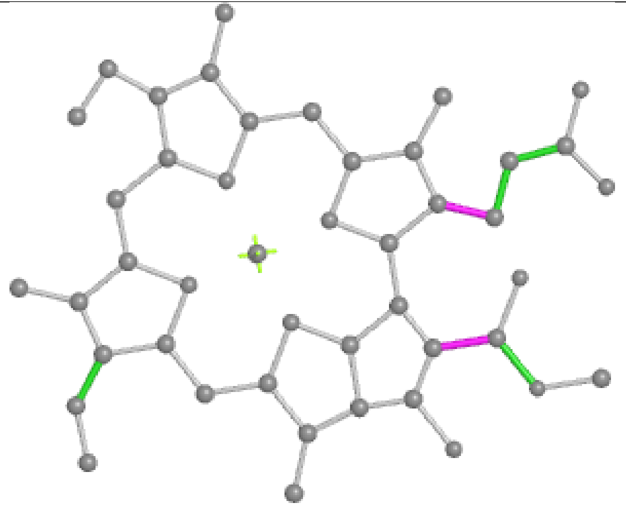
Ligand CLA B 822



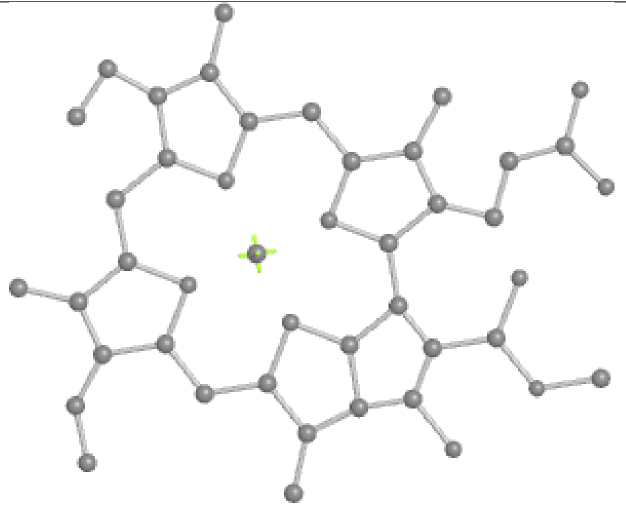
Bond lengths



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.

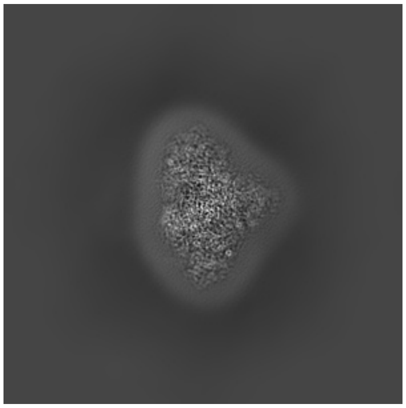
6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-15970. These allow visual inspection of the internal detail of the map and identification of artifacts.

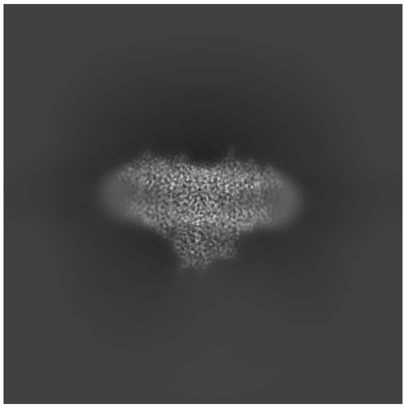
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections ⓘ

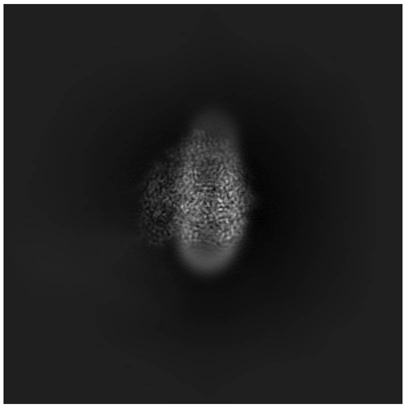
6.1.1 Primary map



X

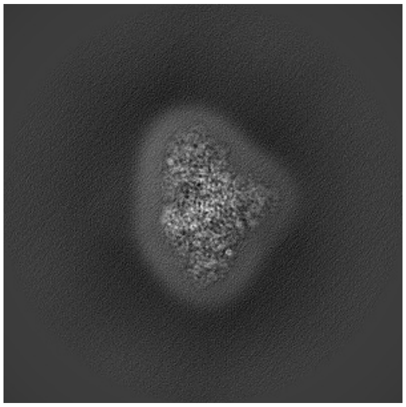


Y

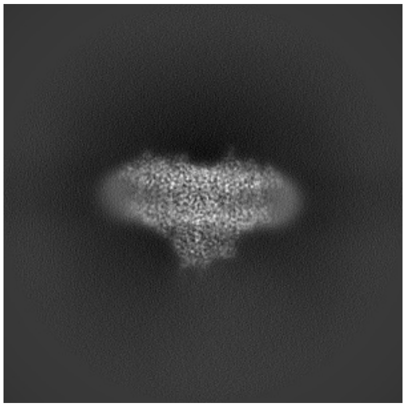


Z

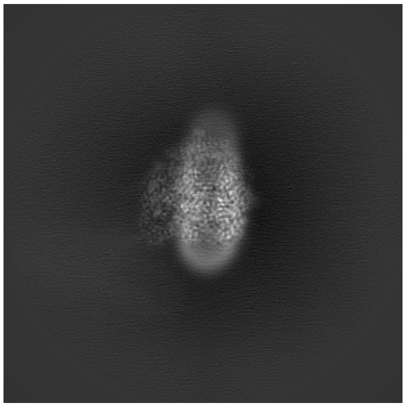
6.1.2 Raw map



X



Y

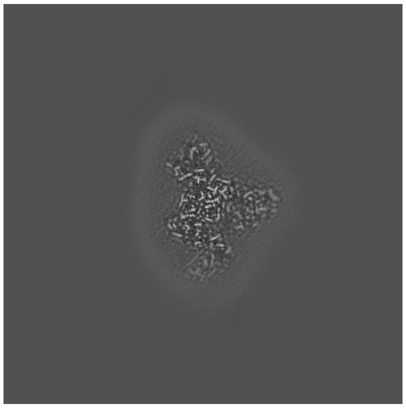


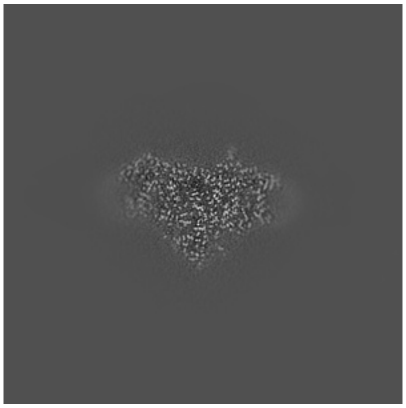
Z

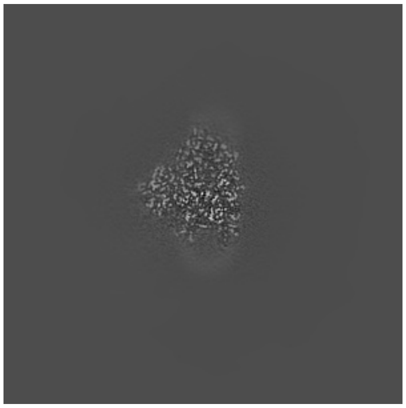
The images above show the map projected in three orthogonal directions.

6.2 Central slices

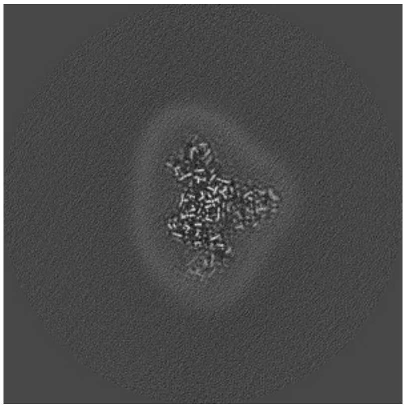
6.2.1 Primary map

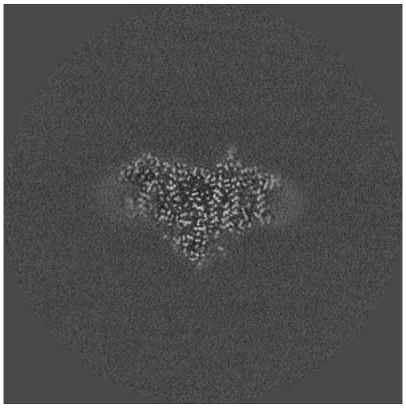

X Index: 200

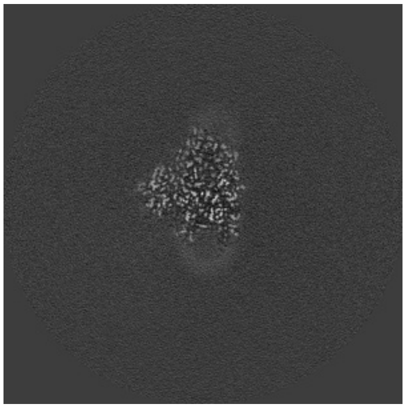

Y Index: 200


Z Index: 200

6.2.2 Raw map


X Index: 200

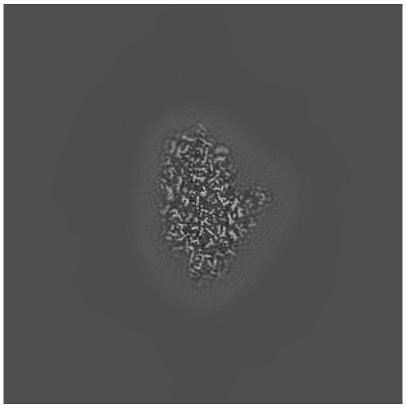

Y Index: 200


Z Index: 200

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

6.3 Largest variance slices ⓘ

6.3.1 Primary map

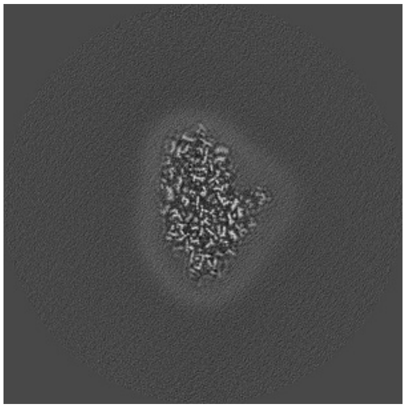


X Index: 219

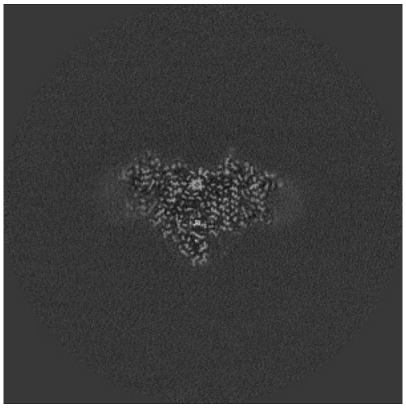
Y Index: 198

Z Index: 193

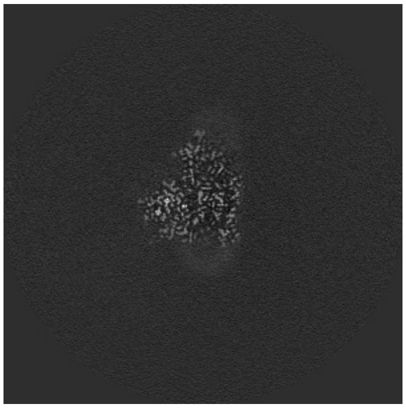
6.3.2 Raw map



X Index: 219



Y Index: 198

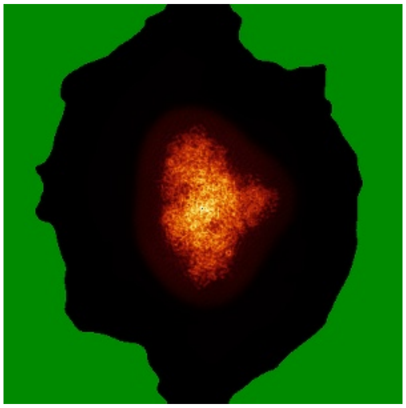


Z Index: 193

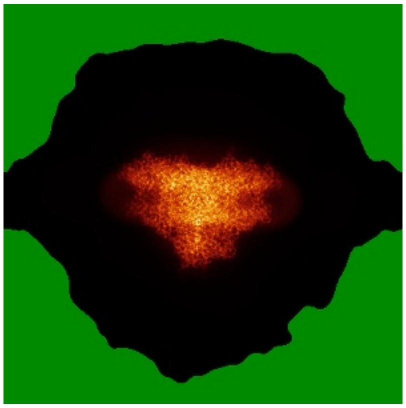
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color)

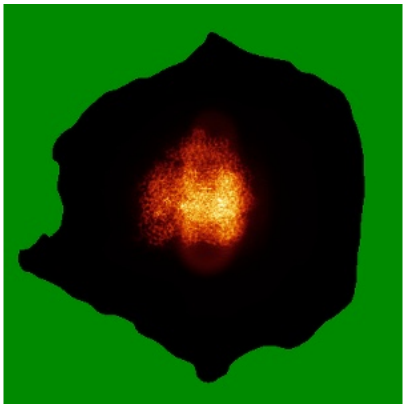
6.4.1 Primary map



X

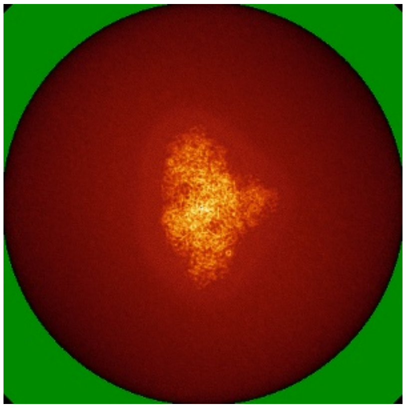


Y

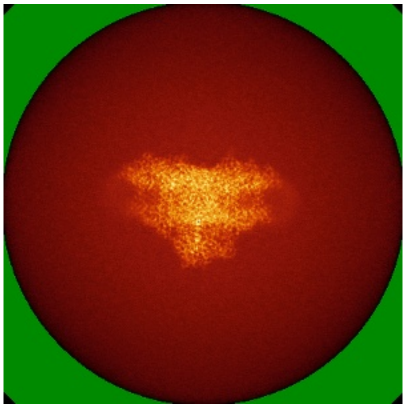


Z

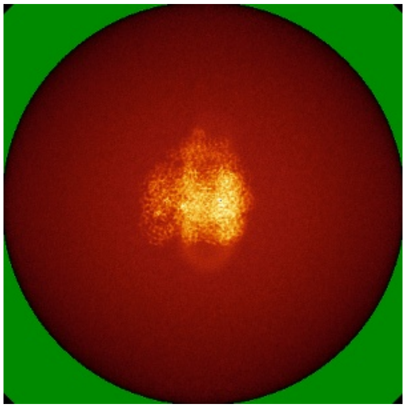
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views ⓘ

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.053. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

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

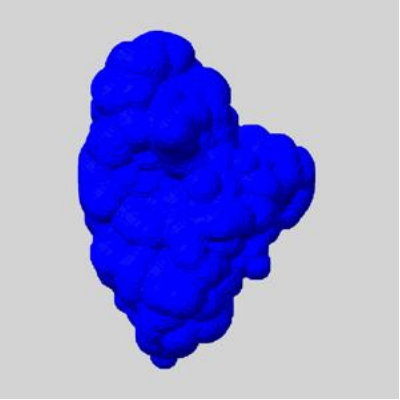
6.6 Mask visualisation ⓘ

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

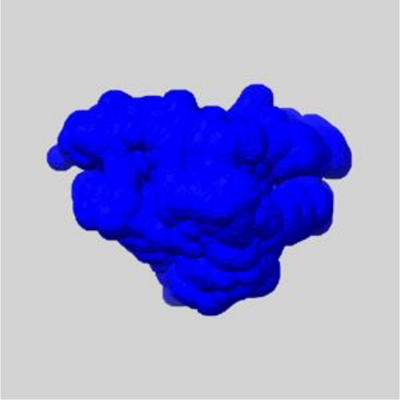
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

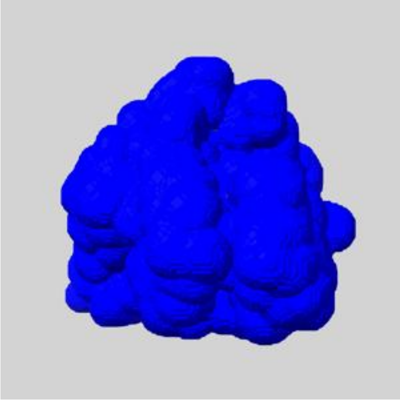
6.6.1 emd_15970_msk_1.map ⓘ



X



Y

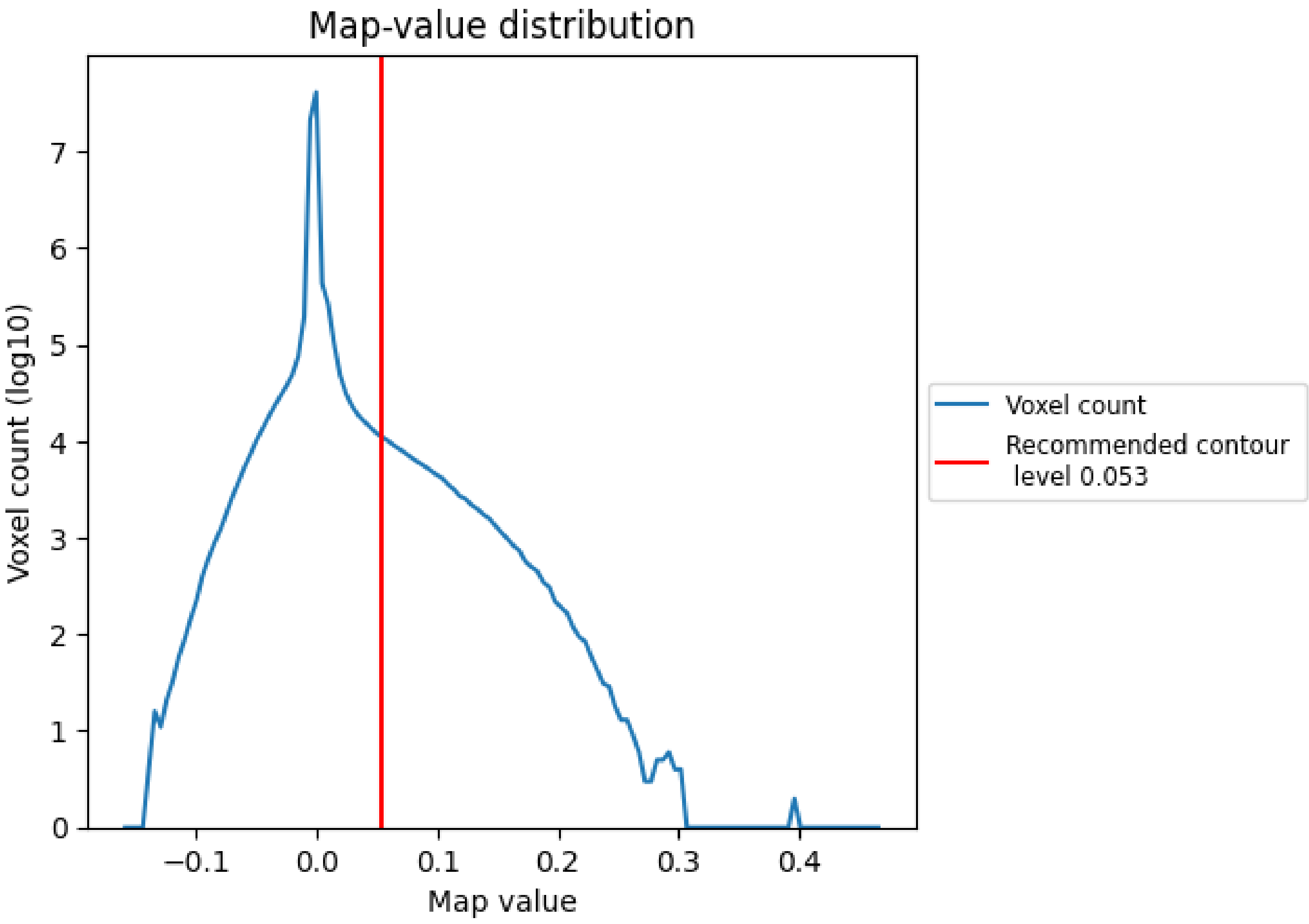


Z

7 Map analysis ⓘ

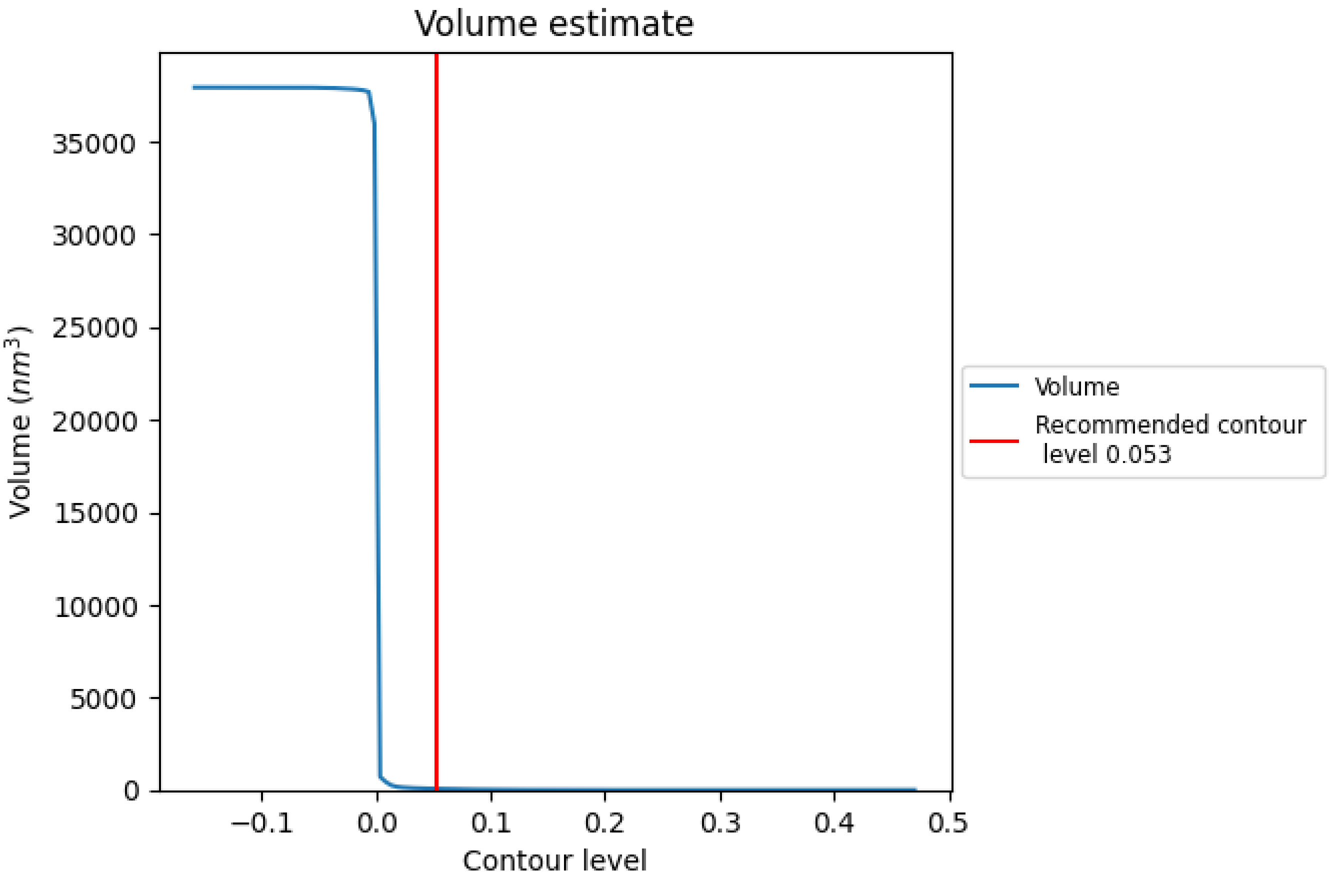
This section contains the results of statistical analysis of the map.

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.

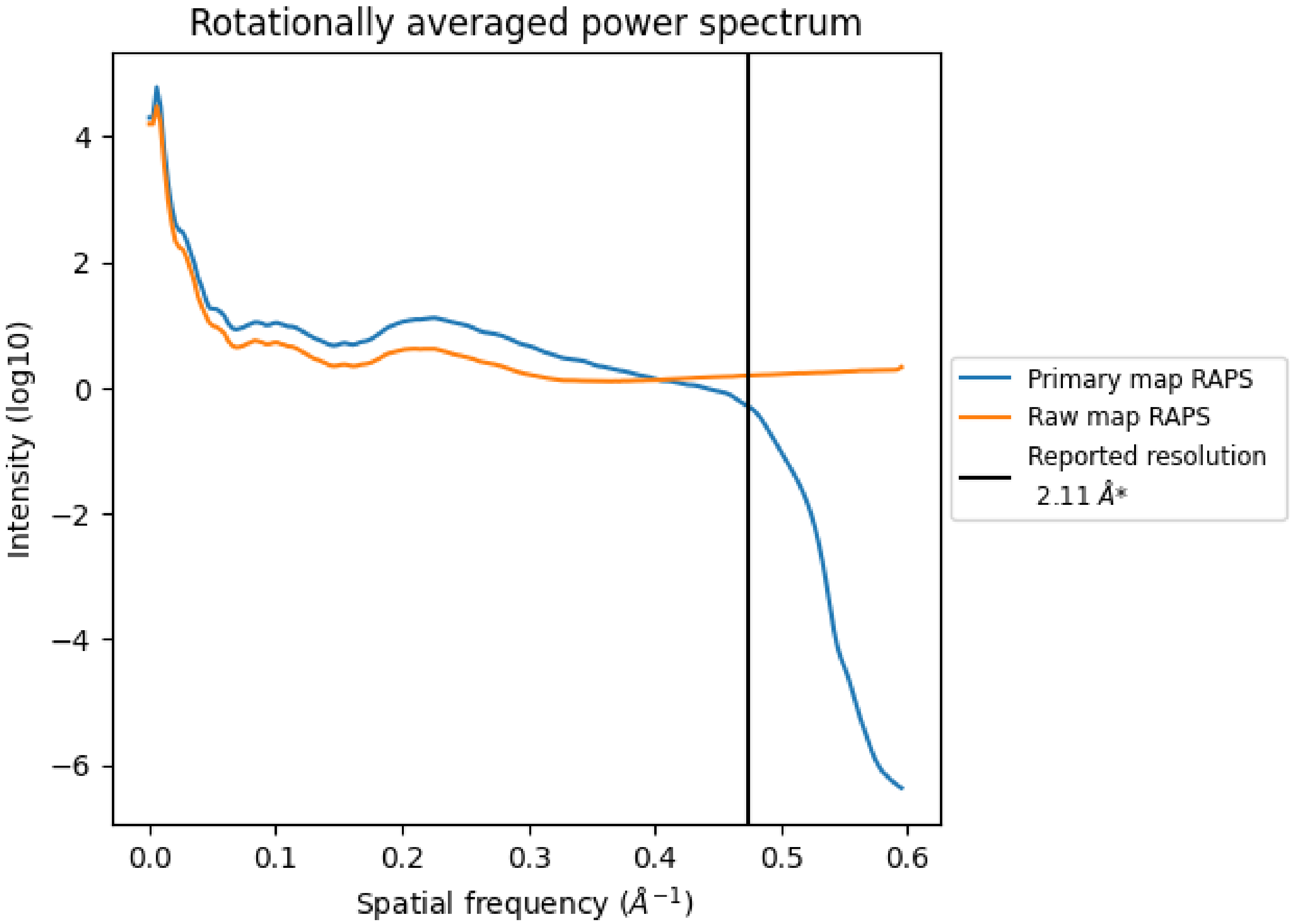
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 64 nm^3; this corresponds to an approximate mass of 58 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 (i)

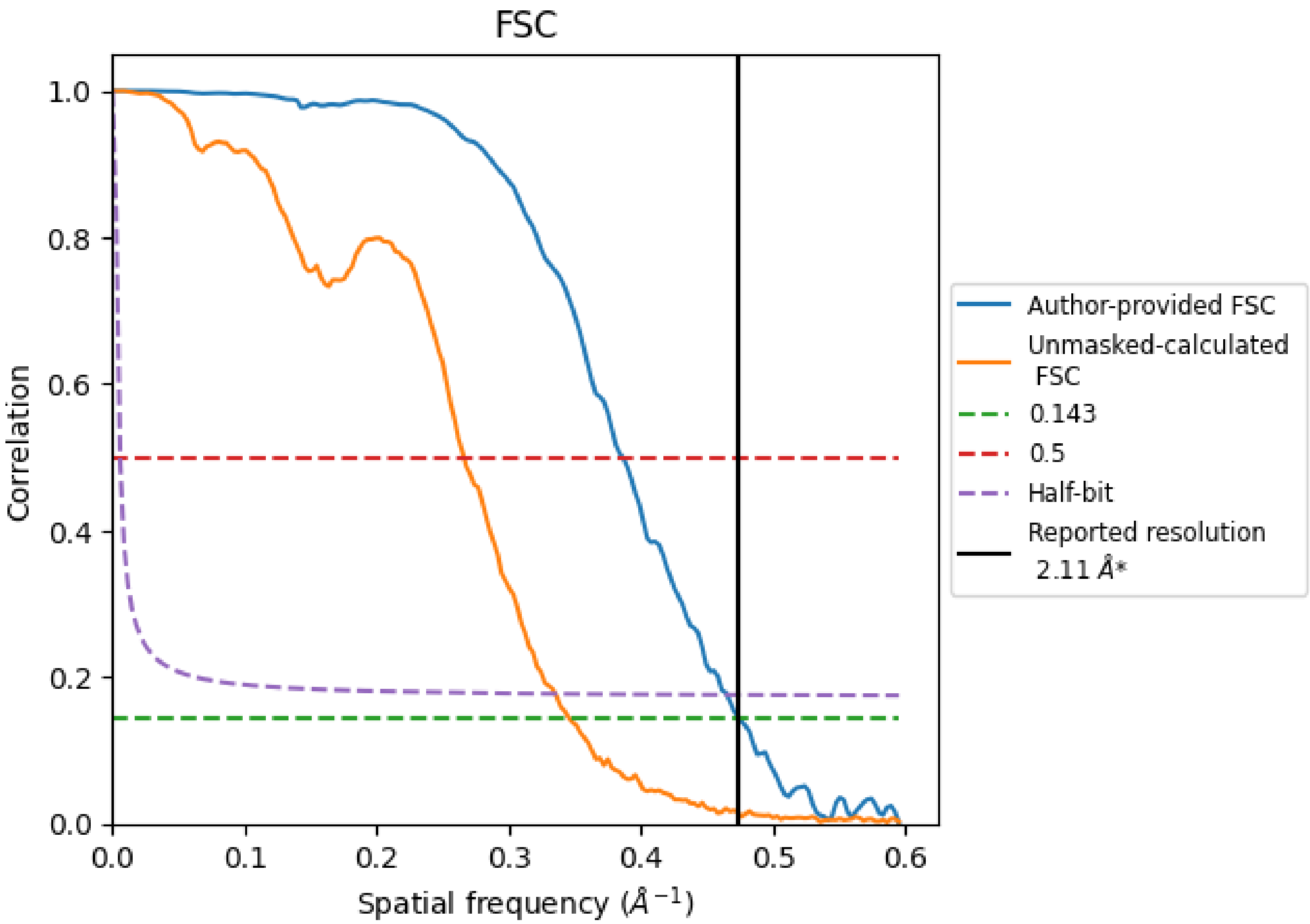


*Reported resolution corresponds to spatial frequency of 0.474 Å^{-1}

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 0.474 Å^{-1}

8.2 Resolution estimates ⓘ

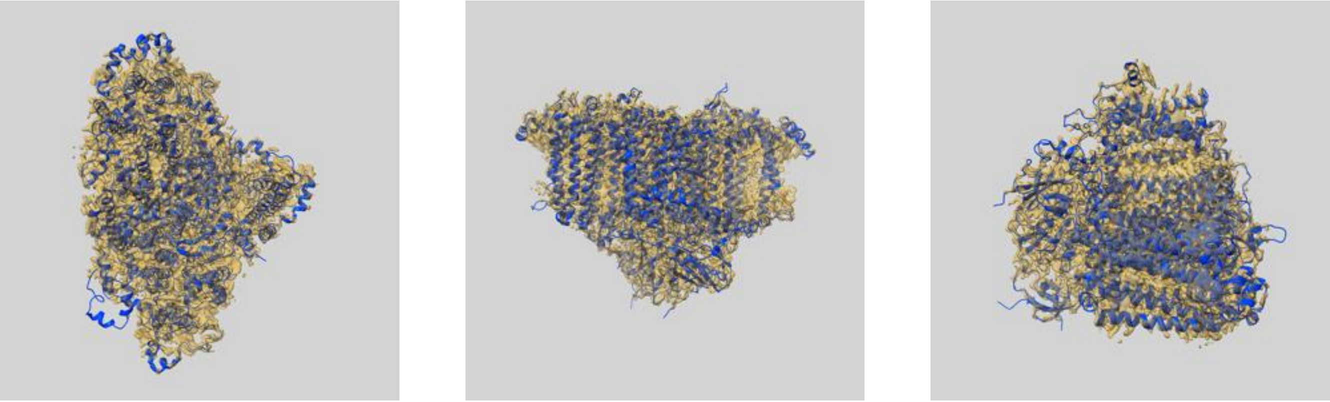
Resolution estimate (Å)	**Estimation criterion (FSC cut-off)**		
	0.143	0.5	Half-bit
Reported by author	2.11	-	-
Author-provided FSC curve	2.11	2.59	2.15
Unmasked-calculated*	2.89	3.76	2.98

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.89 differs from the reported value 2.11 by more than 10 %

9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-15970 and PDB model 8BCW. Per-residue inclusion information can be found in section 3 on page 18.

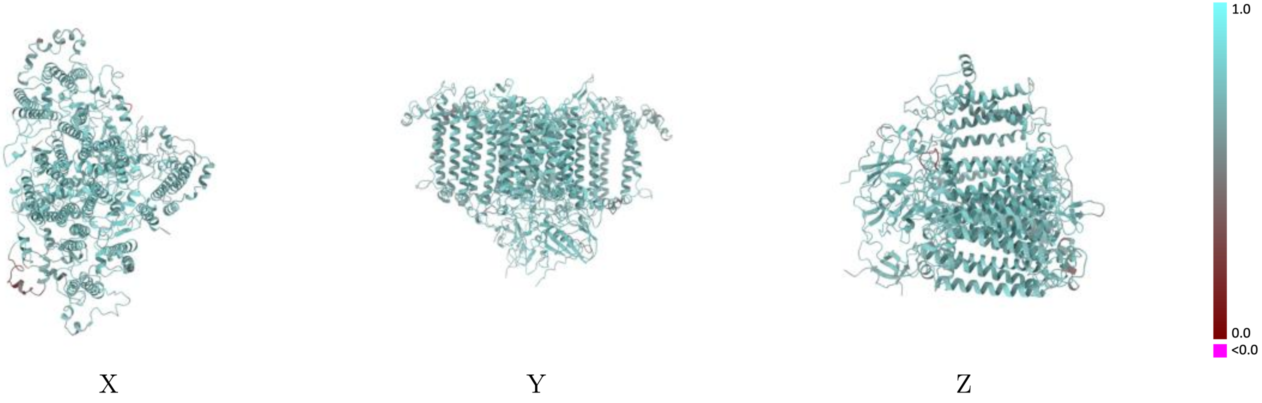
9.1 Map-model overlay ⓘ



X Y Z

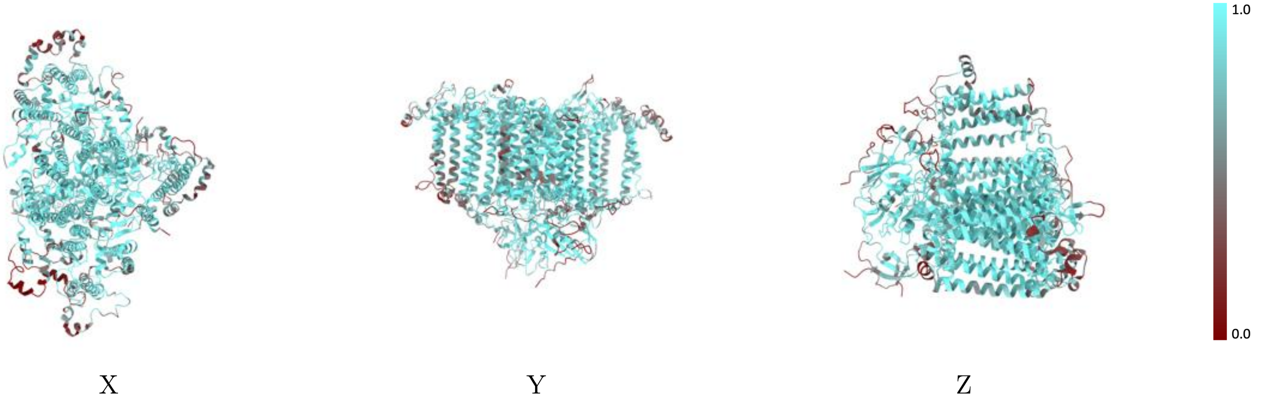
The images above show the 3D surface view of the map at the recommended contour level 0.053 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model



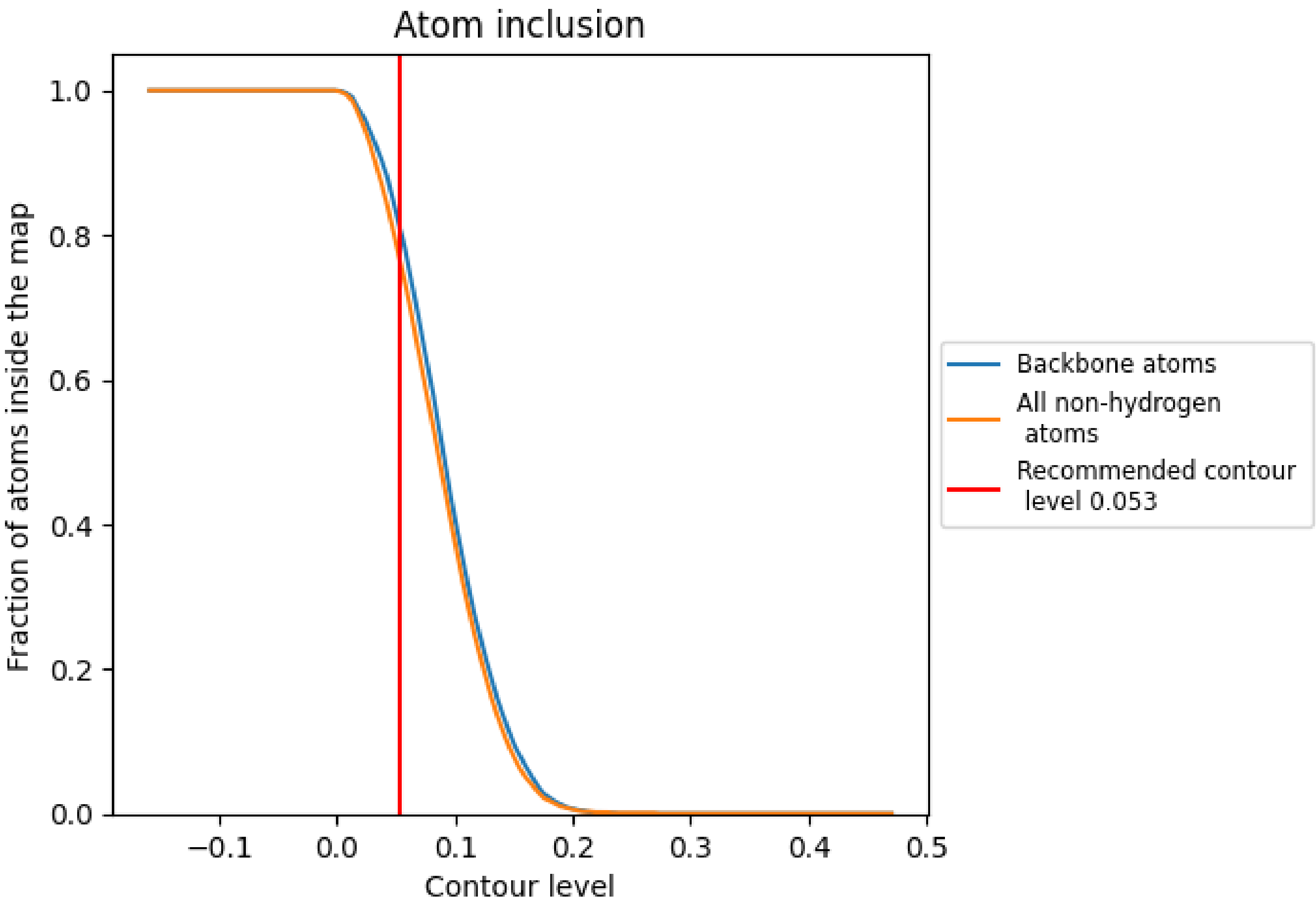
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.053).

9.4 Atom inclusion ⓘ



At the recommended contour level, 81% of all backbone atoms, 77% 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 (0.053) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	▬ 0.7680	▬ 0.7070
A	▬ 0.8030	▬ 0.7130
B	▬ 0.7530	▬ 0.7060
C	▬ 0.9490	▬ 0.7580
D	▬ 0.8140	▬ 0.7130
E	▬ 0.6400	▬ 0.6690
H	▬ 0.4850	▬ 0.6610
I	▬ 0.7610	▬ 0.7030
L	▬ 0.7210	▬ 0.6940