wwPDB EM Validation Summary Report ⓘ

Aug 8, 2023 – 03:35 pm BST

PDB ID	:	8AM5
EMDB ID	:	EMD-15522
Title	:	RCII/PSI complex, class 3
Authors	:	Zhao, Z.; Vercellino, I.; Knoppova, J.; Sobotka, R.; Murray, J.W.; Nixon, P.J.; Sazanov, L.A.; Komenda, J.
Deposited on	:	2022-08-02
Resolution	:	3.10 Å(reported)
Based on initial models	:	6WJ6, 2XBG, 5OY0

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

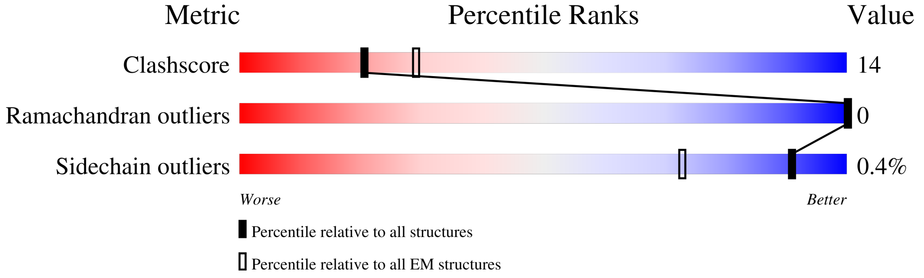
EMDB validation analysis	:	0.0.1.dev50
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

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

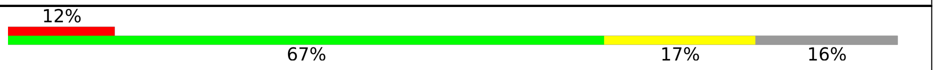
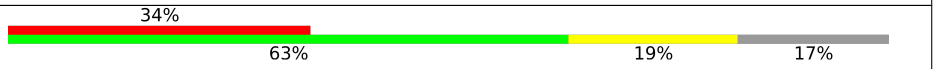
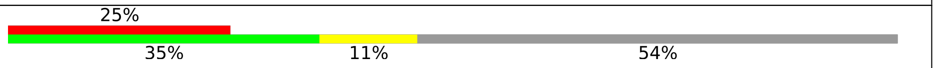
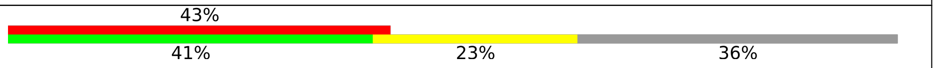
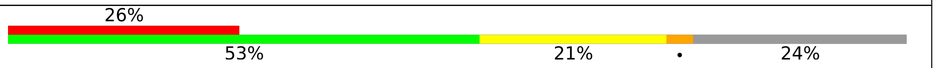
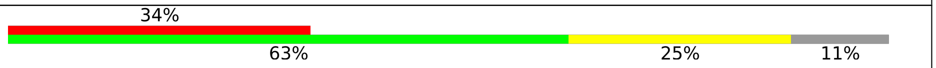
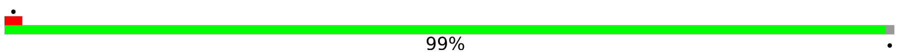
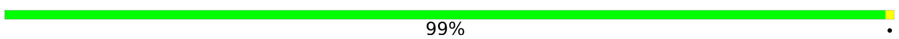
The reported resolution of this entry is 3.10 Å.

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.



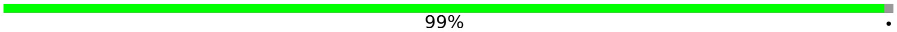
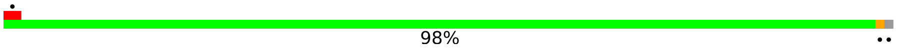
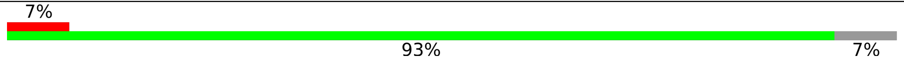
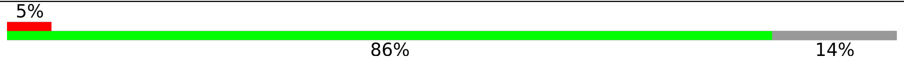
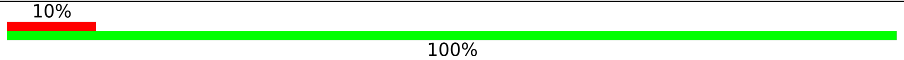
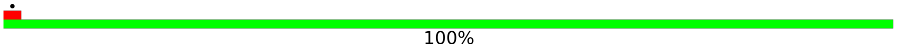
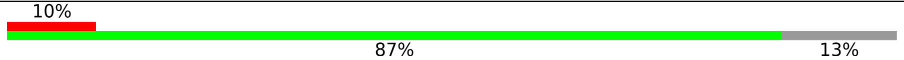
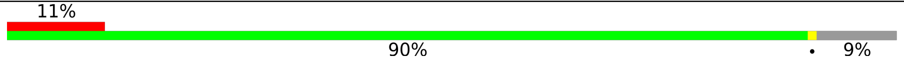
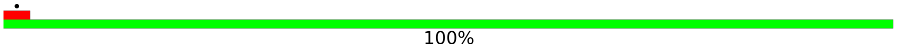
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	344	
2	D	336	
3	E	81	
4	F	44	
5	I	38	
6	S	342	
7	a	751	
8	b	731	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	c	81	
10	d	141	
11	e	74	
12	f	165	
13	i	40	
14	j	40	
15	k	86	
16	l	157	
17	m	31	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	A	402	X	-	-	-
19	CLA	A	403	X	-	-	-
19	CLA	A	405	X	-	-	-
19	CLA	A	407	X	-	-	-
19	CLA	D	402	X	-	-	-
19	CLA	D	403	X	-	-	-
19	CLA	a	802	X	-	-	-
19	CLA	a	803	X	-	-	-
19	CLA	a	804	X	-	-	-
19	CLA	a	805	X	-	-	-
19	CLA	a	806	X	-	-	-
19	CLA	a	807	X	-	-	-
19	CLA	a	808	X	-	-	-
19	CLA	a	809	X	-	-	-
19	CLA	a	810	X	-	-	-
19	CLA	a	811	X	-	-	-
19	CLA	a	812	X	-	-	-
19	CLA	a	813	X	-	-	-
19	CLA	a	815	X	-	-	-
19	CLA	a	816	X	-	-	-
19	CLA	a	817	X	-	-	-
19	CLA	a	818	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	a	819	X	-	-	-
19	CLA	a	820	X	-	-	-
19	CLA	a	821	X	-	-	-
19	CLA	a	822	X	-	-	-
19	CLA	a	823	X	-	-	-
19	CLA	a	824	X	-	-	-
19	CLA	a	825	X	-	-	-
19	CLA	a	826	X	-	-	-
19	CLA	a	827	X	-	-	-
19	CLA	a	828	X	-	-	-
19	CLA	a	829	X	-	-	-
19	CLA	a	830	X	-	-	-
19	CLA	a	831	X	-	-	-
19	CLA	a	832	X	-	-	-
19	CLA	a	833	X	-	-	-
19	CLA	a	834	X	-	-	-
19	CLA	a	835	X	-	-	-
19	CLA	a	836	X	-	-	-
19	CLA	a	837	X	-	-	-
19	CLA	a	838	X	-	-	-
19	CLA	a	839	X	-	-	-
19	CLA	a	840	X	-	-	-
19	CLA	a	841	X	-	-	-
19	CLA	a	842	X	-	-	-
19	CLA	a	843	X	-	-	-
19	CLA	a	856	X	-	-	-
19	CLA	a	857	X	-	-	-
19	CLA	a	860	X	-	-	-
19	CLA	b	801	X	-	-	-
19	CLA	b	802	X	-	-	-
19	CLA	b	803	X	-	-	-
19	CLA	b	804	X	-	-	-
19	CLA	b	805	X	-	-	-
19	CLA	b	806	X	-	-	-
19	CLA	b	807	X	-	-	-
19	CLA	b	808	X	-	-	-
19	CLA	b	809	X	-	-	-
19	CLA	b	810	X	-	-	-
19	CLA	b	811	X	-	-	-
19	CLA	b	812	X	-	-	-
19	CLA	b	813	X	-	-	-
19	CLA	b	814	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	b	815	X	-	-	-
19	CLA	b	816	X	-	-	-
19	CLA	b	817	X	-	-	-
19	CLA	b	818	X	-	-	-
19	CLA	b	819	X	-	-	-
19	CLA	b	820	X	-	-	-
19	CLA	b	821	X	-	-	-
19	CLA	b	822	X	-	-	-
19	CLA	b	823	X	-	-	-
19	CLA	b	824	X	-	-	-
19	CLA	b	825	X	-	-	-
19	CLA	b	826	X	-	-	-
19	CLA	b	827	X	-	-	-
19	CLA	b	828	X	-	-	-
19	CLA	b	829	X	-	-	-
19	CLA	b	830	X	-	-	-
19	CLA	b	831	X	-	-	-
19	CLA	b	832	X	-	-	-
19	CLA	b	833	X	-	-	-
19	CLA	b	834	X	-	-	-
19	CLA	b	835	X	-	-	-
19	CLA	b	836	X	-	-	-
19	CLA	b	837	X	-	-	-
19	CLA	b	838	X	-	-	-
19	CLA	b	839	X	-	-	-
19	CLA	b	840	X	-	-	-
19	CLA	f	201	X	-	-	-
19	CLA	f	203	X	-	-	-
19	CLA	f	204	X	-	-	-
19	CLA	j	103	X	-	-	-
19	CLA	j	104	X	-	-	-
19	CLA	k	101	X	-	-	-
19	CLA	k	102	X	-	-	-
19	CLA	l	202	X	-	-	-
19	CLA	l	203	X	-	-	-
19	CLA	l	204	X	-	-	-
23	CL0	a	801	X	-	-	-

2 Entry composition (i)

There are 32 unique types of molecules in this entry. The entry contains 32746 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 II protein D1 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	290	2256	1484	367	390	15	0	0

- Molecule 2 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	D	278	2188	1465	351	360	12	0	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-5	MET	-	initiating methionine	UNP P09192
D	-4	HIS	-	expression tag	UNP P09192
D	-3	HIS	-	expression tag	UNP P09192
D	-2	HIS	-	expression tag	UNP P09192
D	-1	HIS	-	expression tag	UNP P09192
D	0	HIS	-	expression tag	UNP P09192
D	1	HIS	-	expression tag	UNP P09192

- Molecule 3 is a protein called Cytochrome b559 subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	E	37	301	206	44	50	1	0	0

- Molecule 4 is a protein called Cytochrome b559 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	F	28	222	149	39	33	1	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
5	I	29	Total	C	N	O	0	0
			229	159	33	37		

- Molecule 6 is a protein called Photosystem II assembly lipoprotein Ycf48.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	S	303	Total	C	N	O	S	0	0
			2328	1481	393	451	3		

- Molecule 7 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	a	741	Total	C	N	O	S	0	0
			5795	3797	984	987	27		

- Molecule 8 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	b	729	Total	C	N	O	S	0	0
			5770	3798	967	990	15		

- Molecule 9 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	c	80	Total	C	N	O	S	0	0
			600	369	103	117	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	d	139	Total	C	N	O	S	0	0
			1087	688	188	208	3		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
11	e	69	Total	C	N	O	0	0
			538	337	95	106		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	f	142	1108	715	184	204	5	0	0

- Molecule 13 is a protein called Photosystem I reaction center subunit VIII.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	i	40	311	209	44	55	3	0	0

- Molecule 14 is a protein called Photosystem I reaction center subunit IX.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	j	40	319	215	47	54	3	0	0

- Molecule 15 is a protein called Photosystem I reaction center subunit PsaK 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	k	75	524	343	87	90	4	0	0

- Molecule 16 is a protein called Photosystem I reaction center subunit XI.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	l	143	1069	697	173	197	2	0	0

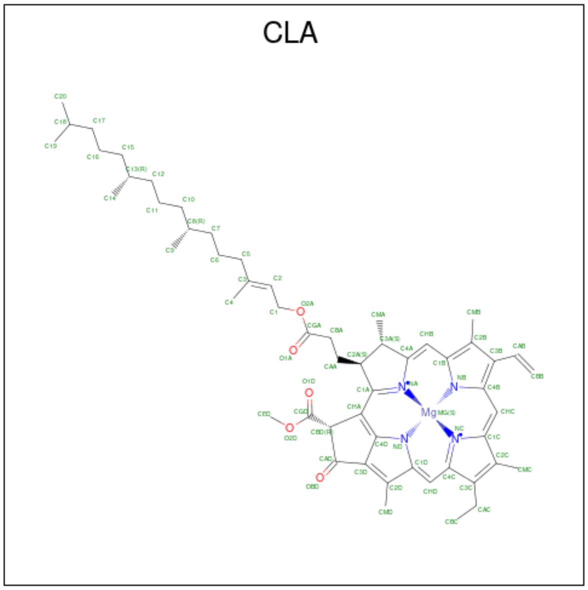
- Molecule 17 is a protein called Photosystem I reaction center subunit XII.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	m	31	238	159	36	42	1	0	0

- Molecule 18 is FE (II) ION (three-letter code: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		AltConf
			Total	Fe	
18	A	1	1	1	0

- Molecule 19 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
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 46	C 36	Mg 1	N 4	O 5	0
19	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	D	1	Total 55	C 45	Mg 1	N 4	O 5	0
19	D	1	Total 46	C 36	Mg 1	N 4	O 5	0
19	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	a	1	Total 65	C 55	Mg 1	N 4	O 5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
19	a	1	Total C Mg N O 51 41 1 4 5	0
19	a	1	Total C Mg N O 50 40 1 4 5	0
19	a	1	Total C Mg N O 65 55 1 4 5	0
19	a	1	Total C Mg N O 60 50 1 4 5	0
19	a	1	Total C Mg N O 65 55 1 4 5	0
19	a	1	Total C Mg N O 65 55 1 4 5	0
19	a	1	Total C Mg N O 46 36 1 4 5	0
19	a	1	Total C Mg N O 46 36 1 4 5	0
19	a	1	Total C Mg N O 65 55 1 4 5	0
19	a	1	Total C Mg N O 65 55 1 4 5	0
19	a	1	Total C Mg N O 65 55 1 4 5	0
19	a	1	Total C Mg N O 65 55 1 4 5	0
19	a	1	Total C Mg N O 65 55 1 4 5	0
19	a	1	Total C Mg N O 65 55 1 4 5	0
19	a	1	Total C Mg N O 65 55 1 4 5	0
19	a	1	Total C Mg N O 60 50 1 4 5	0
19	a	1	Total C Mg N O 65 55 1 4 5	0
19	a	1	Total C Mg N O 65 55 1 4 5	0
19	a	1	Total C Mg N O 65 55 1 4 5	0
19	a	1	Total C Mg N O 65 55 1 4 5	0
19	a	1	Total C Mg N O 65 55 1 4 5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
19	a	1	65	55	1	4	5	0
19	a	1	56	46	1	4	5	0
19	a	1	60	50	1	4	5	0
19	a	1	65	55	1	4	5	0
19	a	1	65	55	1	4	5	0
19	a	1	65	55	1	4	5	0
19	a	1	65	55	1	4	5	0
19	a	1	51	41	1	4	5	0
19	a	1	65	55	1	4	5	0
19	a	1	65	55	1	4	5	0
19	a	1	65	55	1	4	5	0
19	a	1	65	55	1	4	5	0
19	a	1	56	46	1	4	5	0
19	a	1	65	55	1	4	5	0
19	a	1	65	55	1	4	5	0
19	a	1	65	55	1	4	5	0
19	b	1	65	55	1	4	5	0
19	b	1	65	55	1	4	5	0
19	b	1	65	55	1	4	5	0
19	b	1	65	55	1	4	5	0
19	b	1	65	55	1	4	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
19	b	1	Total C Mg N O 65 55 1 4 5	0
19	b	1	Total C Mg N O 65 55 1 4 5	0
19	b	1	Total C Mg N O 65 55 1 4 5	0
19	b	1	Total C Mg N O 56 46 1 4 5	0
19	b	1	Total C Mg N O 56 46 1 4 5	0
19	b	1	Total C Mg N O 50 40 1 4 5	0
19	b	1	Total C Mg N O 65 55 1 4 5	0
19	b	1	Total C Mg N O 65 55 1 4 5	0
19	b	1	Total C Mg N O 55 45 1 4 5	0
19	b	1	Total C Mg N O 56 46 1 4 5	0
19	b	1	Total C Mg N O 65 55 1 4 5	0
19	b	1	Total C Mg N O 65 55 1 4 5	0
19	b	1	Total C Mg N O 60 50 1 4 5	0
19	b	1	Total C Mg N O 65 55 1 4 5	0
19	b	1	Total C Mg N O 60 50 1 4 5	0
19	b	1	Total C Mg N O 46 36 1 4 5	0
19	b	1	Total C Mg N O 57 47 1 4 5	0
19	b	1	Total C Mg N O 65 55 1 4 5	0
19	b	1	Total C Mg N O 55 45 1 4 5	0
19	b	1	Total C Mg N O 65 55 1 4 5	0
19	b	1	Total C Mg N O 65 55 1 4 5	0

Continued on next page...

Continued from previous page...

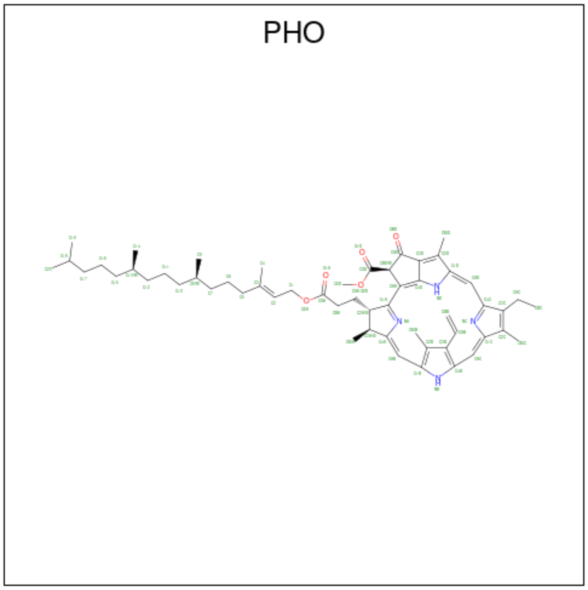
Mol	Chain	Residues	Atoms	AltConf
19	b	1	Total C Mg N O 65 55 1 4 5	0
19	b	1	Total C Mg N O 65 55 1 4 5	0
19	b	1	Total C Mg N O 51 41 1 4 5	0
19	b	1	Total C Mg N O 50 40 1 4 5	0
19	b	1	Total C Mg N O 65 55 1 4 5	0
19	b	1	Total C Mg N O 65 55 1 4 5	0
19	b	1	Total C Mg N O 65 55 1 4 5	0
19	b	1	Total C Mg N O 50 40 1 4 5	0
19	b	1	Total C Mg N O 52 42 1 4 5	0
19	b	1	Total C Mg N O 65 55 1 4 5	0
19	b	1	Total C Mg N O 50 40 1 4 5	0
19	b	1	Total C Mg N O 65 55 1 4 5	0
19	b	1	Total C Mg N O 65 55 1 4 5	0
19	b	1	Total C Mg N O 46 36 1 4 5	0
19	f	1	Total C Mg N O 65 55 1 4 5	0
19	f	1	Total C Mg N O 50 40 1 4 5	0
19	f	1	Total C Mg N O 50 40 1 4 5	0
19	j	1	Total C Mg N O 55 45 1 4 5	0
19	j	1	Total C Mg N O 46 36 1 4 5	0
19	k	1	Total C Mg N O 46 36 1 4 5	0
19	k	1	Total C Mg N O 45 35 1 4 5	0

Continued on next page...

Continued from previous page...

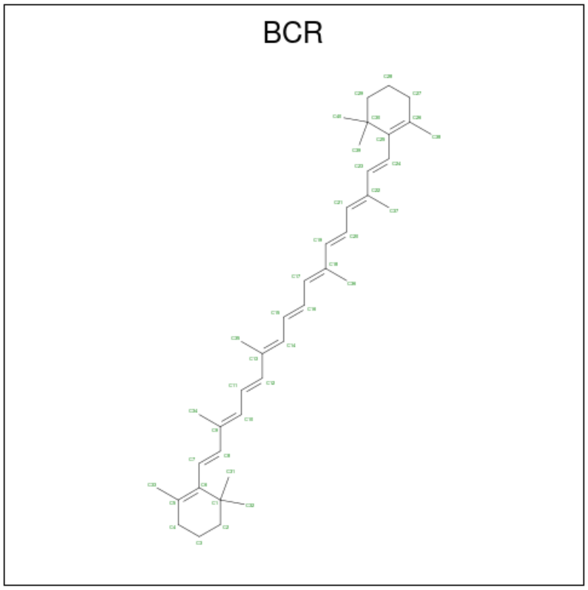
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
19	l	1	50	40	1	4	5	0
19	l	1	65	55	1	4	5	0
19	l	1	52	42	1	4	5	0

- Molecule 20 is PHEOPHYTIN A (three-letter code: PHO) (formula: $C_{55}H_{74}N_4O_5$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
20	A	1	64	55	4	5	0
20	D	1	64	55	4	5	0

- Molecule 21 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



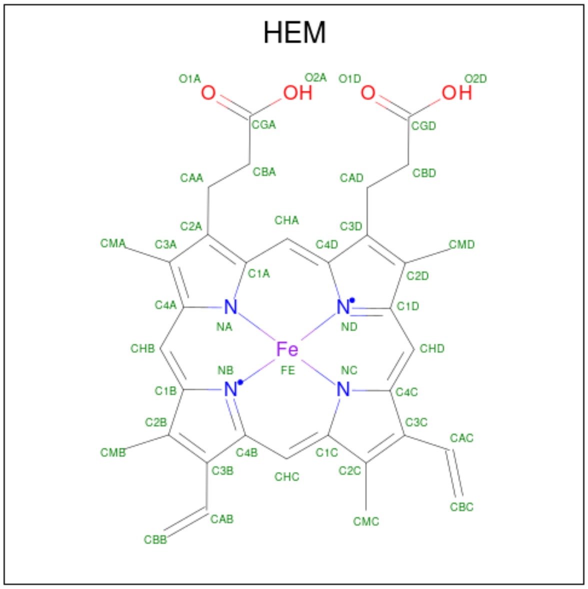
Mol	Chain	Residues	Atoms	AltConf
21	A	1	Total C 40 40	0
21	a	1	Total C 40 40	0
21	a	1	Total C 40 40	0
21	a	1	Total C 40 40	0
21	a	1	Total C 40 40	0
21	a	1	Total C 40 40	0
21	a	1	Total C 25 25	0
21	a	1	Total C 40 40	0
21	b	1	Total C 40 40	0
21	b	1	Total C 40 40	0
21	b	1	Total C 40 40	0
21	b	1	Total C 40 40	0
21	b	1	Total C 40 40	0
21	f	1	Total C 40 40	0

Continued on next page...

Continued from previous page...

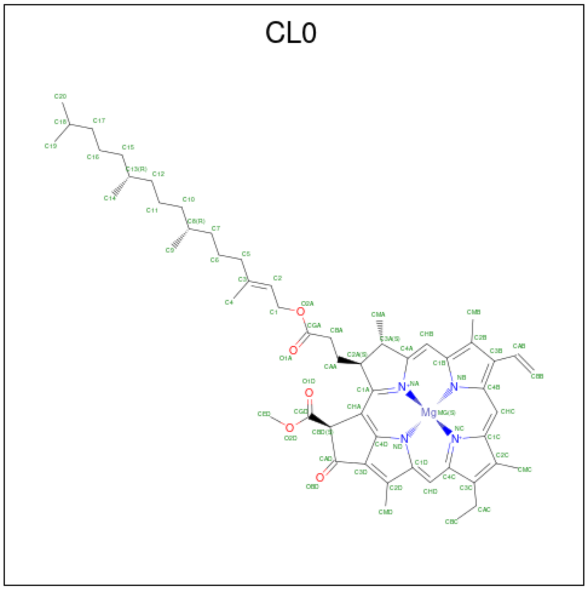
Mol	Chain	Residues	Atoms	AltConf
21	i	1	Total C 40 40	0
21	i	1	Total C 40 40	0
21	j	1	Total C 40 40	0
21	k	1	Total C 40 40	0
21	l	1	Total C 40 40	0

- Molecule 22 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



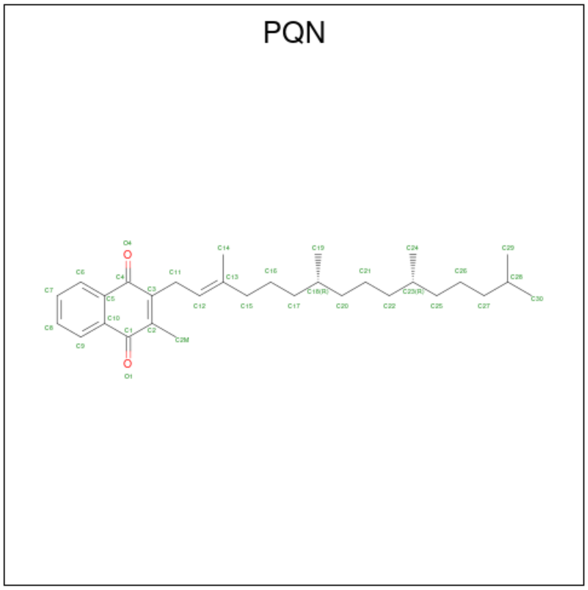
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Fe	N	O	
22	E	1	43	34	1	4	4	0

- Molecule 23 is CHLOROPHYLL A ISOMER (three-letter code: CL0) (formula: $C_{55}H_{72}MgN_4O_5$).



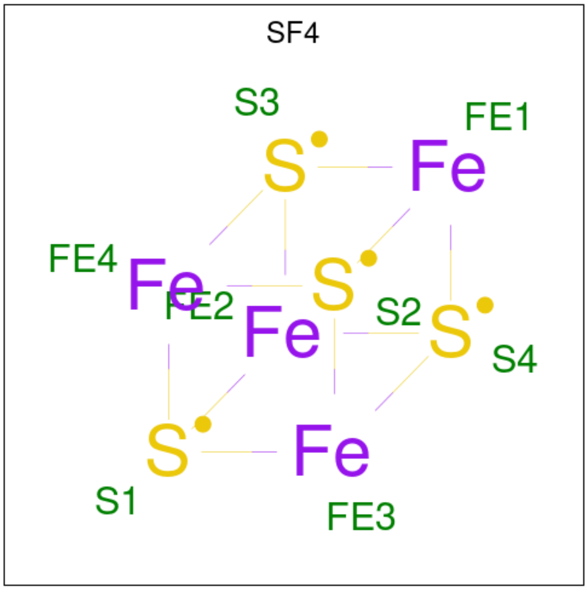
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
23	a	1	65	55	1	4	5	0

- Molecule 24 is PHYLLOQUINONE (three-letter code: PQN) (formula: $C_{31}H_{46}O_2$).



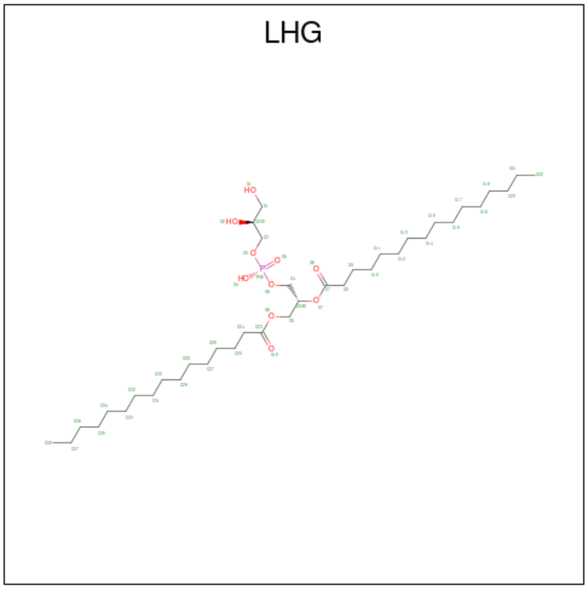
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
24	a	1	33	31	2	0
24	b	1	33	31	2	0

- Molecule 25 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



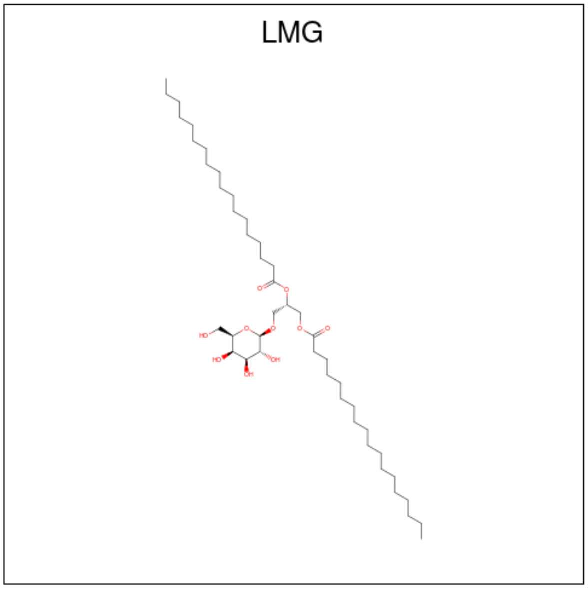
Mol	Chain	Residues	Atoms	AltConf
25	a	1	Total Fe S 8 4 4	0
25	c	1	Total Fe S 8 4 4	0
25	c	1	Total Fe S 8 4 4	0

- Molecule 26 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



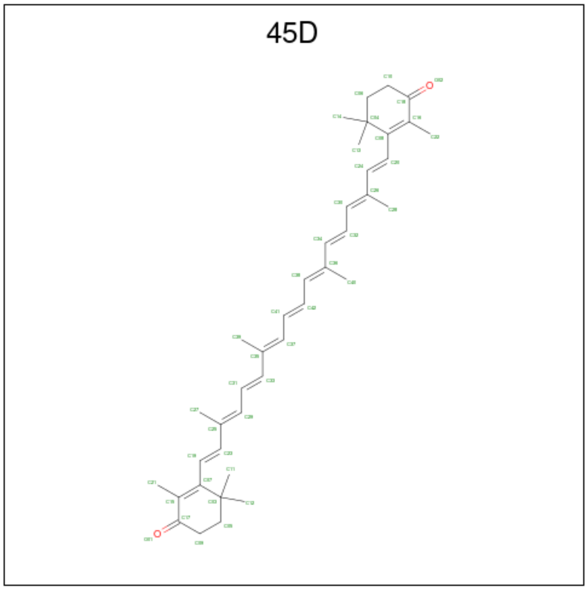
Mol	Chain	Residues	Atoms				AltConf
26	a	1	Total 49	C 38	O 10	P 1	0
26	a	1	Total 49	C 38	O 10	P 1	0
26	a	1	Total 49	C 38	O 10	P 1	0
26	b	1	Total 38	C 27	O 10	P 1	0
26	f	1	Total 49	C 38	O 10	P 1	0

- Molecule 27 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



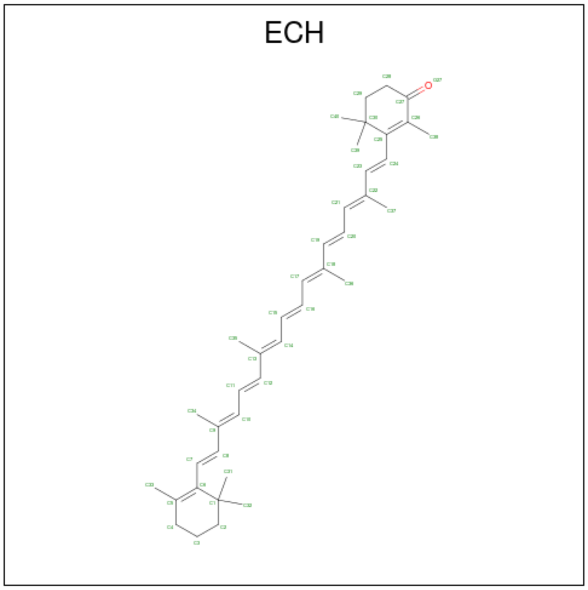
Mol	Chain	Residues	Atoms			AltConf
27	a	1	Total 40	C 30	O 10	0
27	b	1	Total 55	C 45	O 10	0
27	b	1	Total 55	C 45	O 10	0
27	l	1	Total 50	C 40	O 10	0

- Molecule 28 is beta,beta-carotene-4,4'-dione (three-letter code: 45D) (formula: $C_{40}H_{52}O_2$).



Mol	Chain	Residues	Atoms	AltConf
28	a	1	Total C O 42 40 2	0

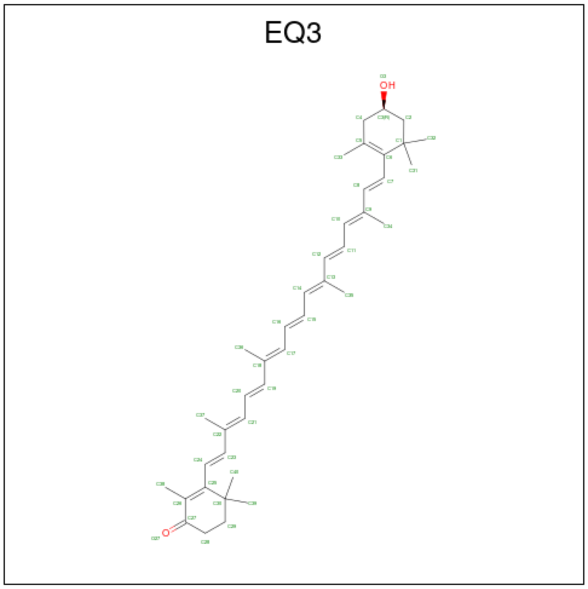
- Molecule 29 is beta,beta-caroten-4-one (three-letter code: ECH) (formula: $C_{40}H_{54}O$).



Mol	Chain	Residues	Atoms	AltConf
29	b	1	Total C O 41 40 1	0
29	m	1	Total C O 41 40 1	0

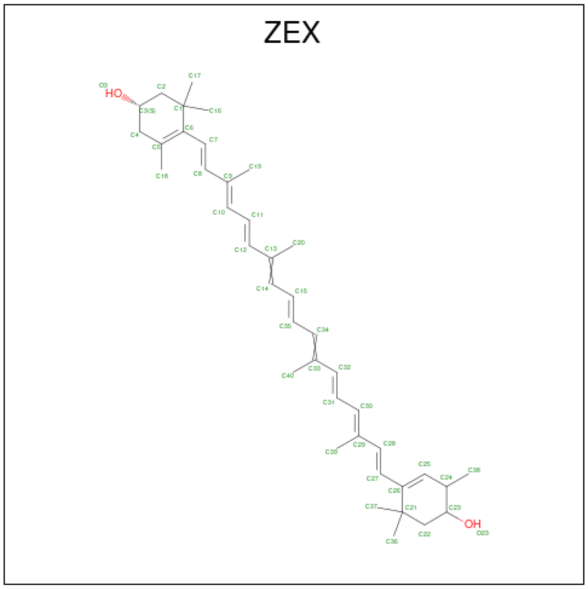
- Molecule 30 is (3'R)-3'-hydroxy-beta,beta-caroten-4-one (three-letter code: EQ3) (formula:

$C_{40}H_{54}O_2$).



Mol	Chain	Residues	Atoms	AltConf
30	b	1	Total C O 42 40 2	0

- Molecule 31 is (1R,2S)-4-{(1E,3E,5E,7E,9E,11E,13E,15E,17E)-18-[(4S)-4-hydroxy-2,6,6-trimethylcyclohex-1-en-1-yl]-3,7,12,16-tetramethyloctadeca-1,3,5,7,9,11,13,15,17-nonaen-1-yl}-2,5,5-trimethylcyclohex-3-en-1-ol (three-letter code: ZEX) (formula: $C_{40}H_{56}O_2$).



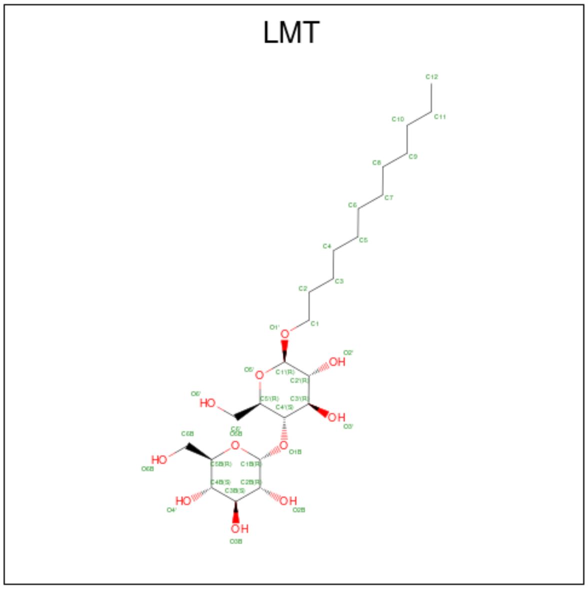
Mol	Chain	Residues	Atoms	AltConf
31	b	1	Total C O 42 40 2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
31	f	1	42	40	2	0

- Molecule 32 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



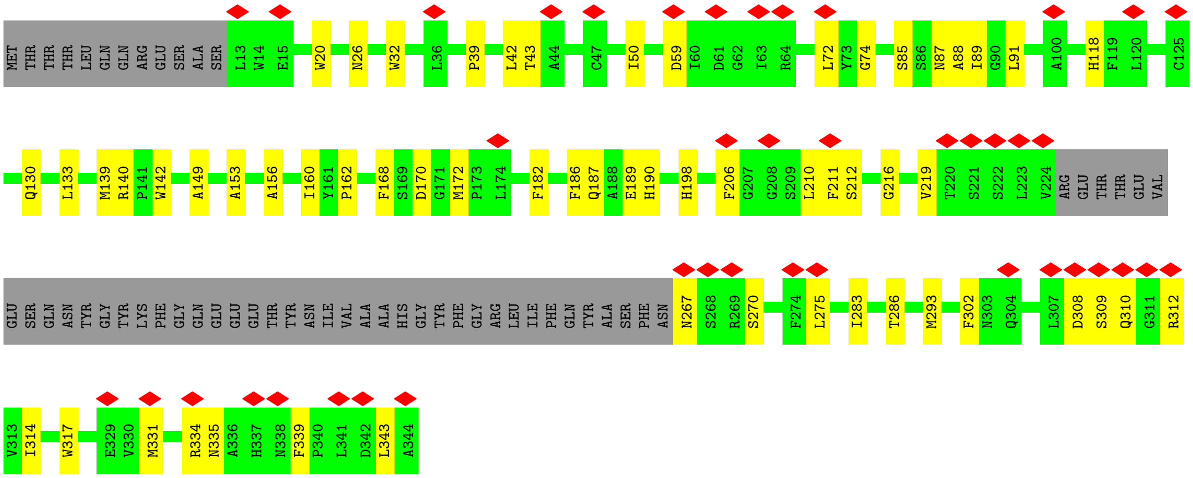
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
32	j	1	35	24	11	0

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.

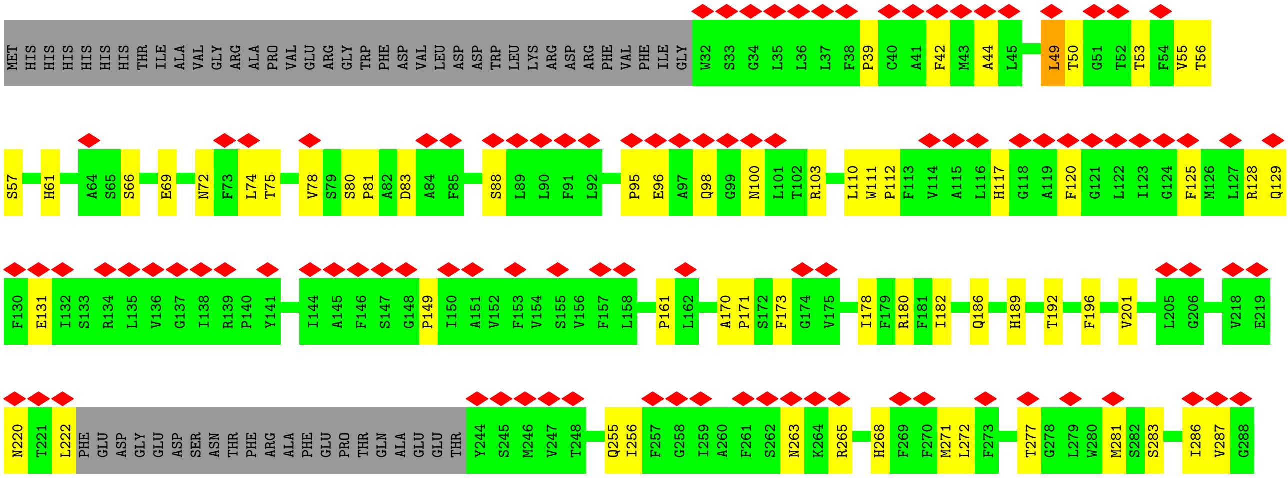
- Molecule 1: Photosystem II protein D1 2

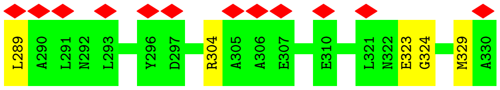
Chain A:



- Molecule 2: Photosystem II D2 protein

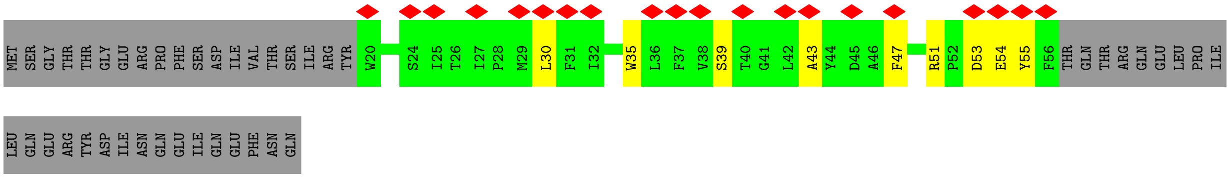
Chain D:





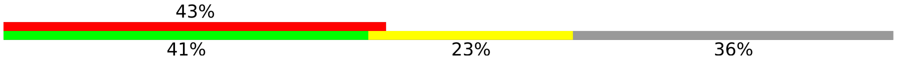
- Molecule 3: Cytochrome b559 subunit alpha

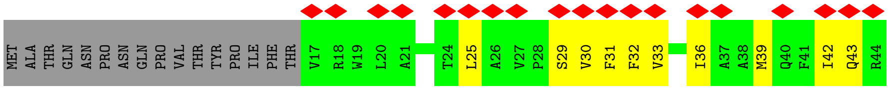
Chain E:



- Molecule 4: Cytochrome b559 subunit beta

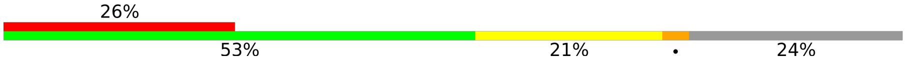
Chain F:

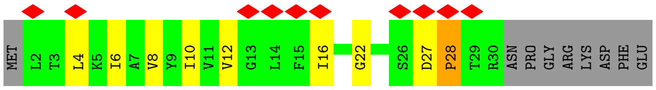




- Molecule 5: Photosystem II reaction center protein I

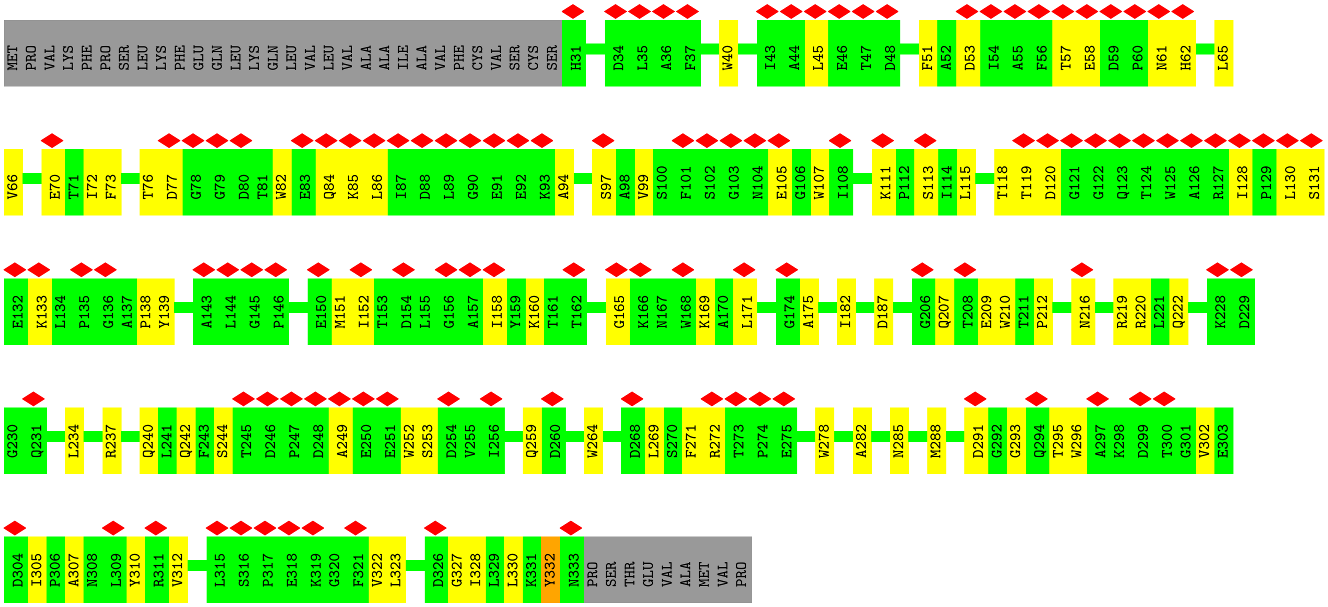
Chain I:





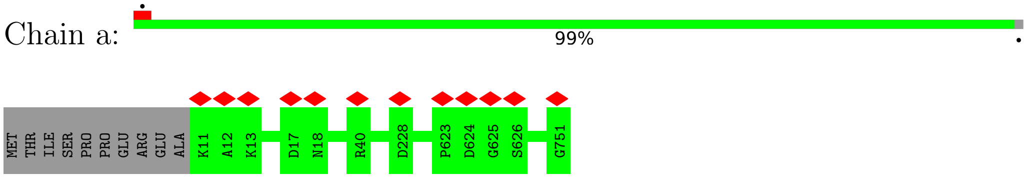
- Molecule 6: Photosystem II assembly lipoprotein Ycf48

Chain S:



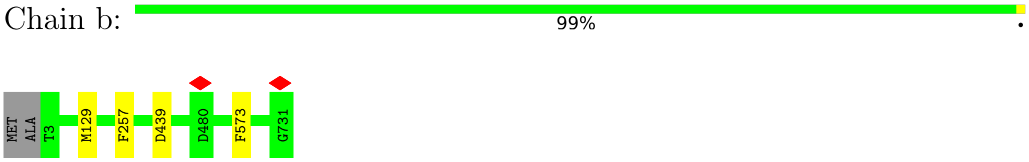
- Molecule 7: Photosystem I P700 chlorophyll a apoprotein A1

Chain a:



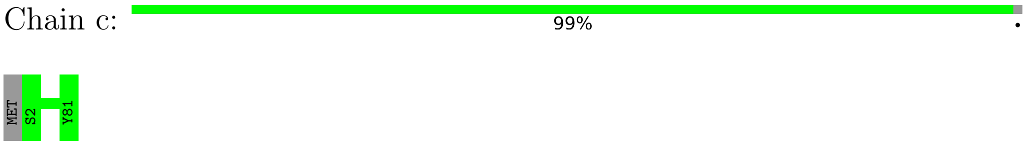
- Molecule 8: Photosystem I P700 chlorophyll a apoprotein A2

Chain b:



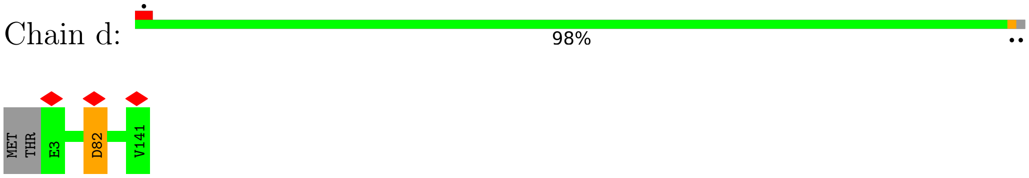
- Molecule 9: Photosystem I iron-sulfur center

Chain c:



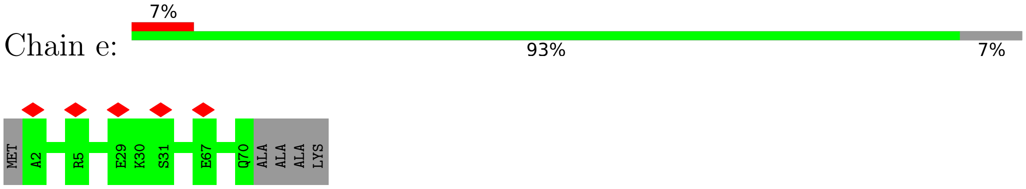
- Molecule 10: Photosystem I reaction center subunit II

Chain d:



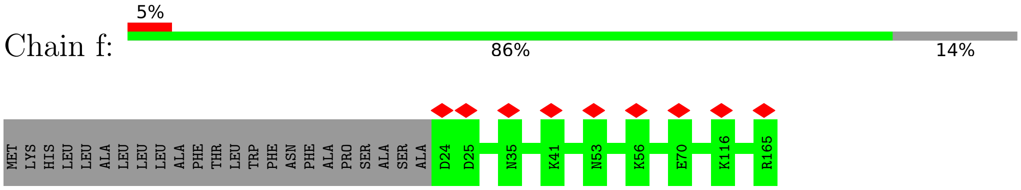
- Molecule 11: Photosystem I reaction center subunit IV

Chain e:



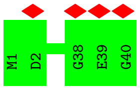
- Molecule 12: Photosystem I reaction center subunit III

Chain f:



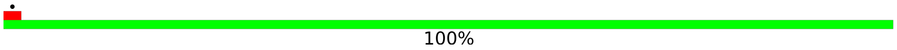
- Molecule 13: Photosystem I reaction center subunit VIII

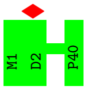
Chain i:



- Molecule 14: Photosystem I reaction center subunit IX

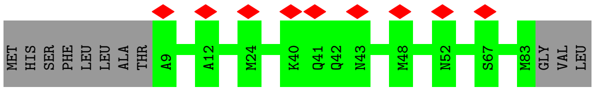
Chain j:





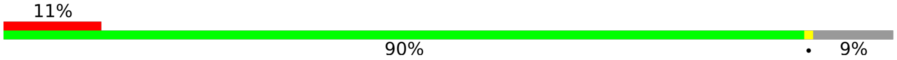
- Molecule 15: Photosystem I reaction center subunit PsaK 1

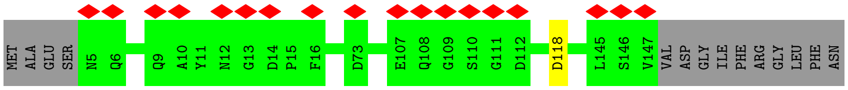
Chain k:



- Molecule 16: Photosystem I reaction center subunit XI

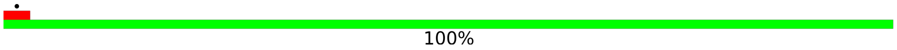
Chain l:

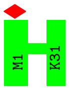




- Molecule 17: Photosystem I reaction center subunit XII

Chain m:





4 Experimental information ⓘ

Property	**Value**	**Source**
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	178513	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\AA^2$)	90.9	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	120000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.510	Depositor
Minimum map value	-0.104	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.0845	Depositor
Map size (Å)	488.0, 488.0, 488.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.22, 1.22, 1.22	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CLA, EQ3, ECH, CL0, PHO, BCR, HEM, FE2, 45D, PQN, LMG, SF4, LMT, ZEX, 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	0/2330	0.43	0/3180
2	D	0.26	0/2266	0.46	0/3086
3	E	0.26	0/314	0.40	0/431
4	F	0.27	0/228	0.53	0/309
5	I	0.31	0/234	0.65	1/317 (0.3%)
6	S	0.25	0/2390	0.49	0/3258
7	a	0.27	0/5993	0.43	0/8169
8	b	0.27	0/5981	0.43	0/8178
9	c	0.28	0/610	0.51	0/826
10	d	0.28	0/1111	0.51	1/1497 (0.1%)
11	e	0.28	0/547	0.52	0/741
12	f	0.26	0/1138	0.47	0/1546
13	i	0.28	0/322	0.44	0/438
14	j	0.27	0/328	0.48	0/443
15	k	0.26	0/535	0.47	0/726
16	l	0.27	0/1097	0.44	0/1493
17	m	0.26	0/241	0.42	0/326
All	All	0.27	0/25665	0.45	2/34964 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	I	28	PRO	CA-N-CD	-6.63	102.22	111.50
10	d	82	ASP	CB-CG-OD2	5.22	123.00	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	2256	0	2181	57	0
2	D	2188	0	2129	51	0
3	E	301	0	287	7	0
4	F	222	0	230	7	0
5	I	229	0	247	7	0
6	S	2328	0	2227	62	0
7	a	5795	0	5653	0	0
8	b	5770	0	5547	0	0
9	c	600	0	581	0	0
10	d	1087	0	1082	0	0
11	e	538	0	514	0	0
12	f	1108	0	1100	0	0
13	i	311	0	304	0	0
14	j	319	0	328	0	0
15	k	524	0	547	0	0
16	l	1069	0	1044	0	0
17	m	238	0	260	0	0
18	A	1	0	0	0	0
19	A	226	0	216	20	0
19	D	101	0	82	12	0
19	a	2811	0	2986	0	0
19	b	2410	0	2456	0	0
19	f	165	0	150	0	0
19	j	101	0	82	0	0
19	k	91	0	66	0	0
19	l	167	0	154	0	0
20	A	64	0	74	5	0
20	D	64	0	74	3	0
21	A	40	0	56	6	0
21	a	265	0	369	0	0
21	b	200	0	280	0	0
21	f	40	0	56	0	0
21	i	80	0	112	0	0
21	j	40	0	56	0	0
21	k	40	0	56	0	0
21	l	40	0	56	0	0
22	E	43	0	30	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	a	65	0	72	0	0
24	a	33	0	46	0	0
24	b	33	0	46	0	0
25	a	8	0	0	0	0
25	c	16	0	0	0	0
26	a	147	0	222	0	0
26	b	38	0	49	0	0
26	f	49	0	74	0	0
27	a	40	0	50	0	0
27	b	110	0	172	0	0
27	l	50	0	73	0	0
28	a	42	0	52	0	0
29	b	41	0	54	0	0
29	m	41	0	54	0	0
30	b	42	0	0	0	0
31	b	42	0	56	0	0
31	f	42	0	56	0	0
32	j	35	0	45	0	0
All	All	32746	0	32793	184	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 14.

The worst 5 of 184 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:186:GLN:HB2	19:D:402:CLA:HBC1	1.59	0.83
6:S:322:VAL:HB	6:S:330:LEU:HB2	1.67	0.76
1:A:211:PHE:HB3	1:A:275:LEU:HD13	1.72	0.71
6:S:113:SER:HB3	6:S:130:LEU:HD12	1.75	0.68
20:D:401:PHO:HAB	19:D:402:CLA:H11	1.76	0.68

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	286/344 (83%)	278 (97%)	8 (3%)	0	100	100
2	D	274/336 (82%)	264 (96%)	10 (4%)	0	100	100
3	E	35/81 (43%)	33 (94%)	2 (6%)	0	100	100
4	F	26/44 (59%)	26 (100%)	0	0	100	100
5	I	27/38 (71%)	26 (96%)	1 (4%)	0	100	100
6	S	301/342 (88%)	292 (97%)	9 (3%)	0	100	100
7	a	739/751 (98%)	715 (97%)	24 (3%)	0	100	100
8	b	727/731 (100%)	707 (97%)	20 (3%)	0	100	100
9	c	78/81 (96%)	74 (95%)	4 (5%)	0	100	100
10	d	137/141 (97%)	134 (98%)	3 (2%)	0	100	100
11	e	67/74 (90%)	63 (94%)	4 (6%)	0	100	100
12	f	140/165 (85%)	135 (96%)	5 (4%)	0	100	100
13	i	38/40 (95%)	37 (97%)	1 (3%)	0	100	100
14	j	38/40 (95%)	38 (100%)	0	0	100	100
15	k	73/86 (85%)	72 (99%)	1 (1%)	0	100	100
16	l	141/157 (90%)	137 (97%)	4 (3%)	0	100	100
17	m	29/31 (94%)	29 (100%)	0	0	100	100
All	All	3156/3482 (91%)	3060 (97%)	96 (3%)	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	236/283 (83%)	235 (100%)	1 (0%)	91	96
2	D	220/271 (81%)	218 (99%)	2 (1%)	78	91

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	E	31/73 (42%)	31 (100%)	0	100	100
4	F	22/37 (60%)	22 (100%)	0	100	100
5	I	26/34 (76%)	26 (100%)	0	100	100
6	S	239/279 (86%)	238 (100%)	1 (0%)	91	96
7	a	593/603 (98%)	593 (100%)	0	100	100
8	b	582/583 (100%)	578 (99%)	4 (1%)	84	93
9	c	68/69 (99%)	68 (100%)	0	100	100
10	d	114/116 (98%)	113 (99%)	1 (1%)	78	91
11	e	57/60 (95%)	57 (100%)	0	100	100
12	f	119/137 (87%)	119 (100%)	0	100	100
13	i	32/32 (100%)	32 (100%)	0	100	100
14	j	35/35 (100%)	35 (100%)	0	100	100
15	k	53/62 (86%)	53 (100%)	0	100	100
16	l	107/118 (91%)	106 (99%)	1 (1%)	78	91
17	m	25/25 (100%)	25 (100%)	0	100	100
All	All	2559/2817 (91%)	2549 (100%)	10 (0%)	91	96

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	b	573	PHE
10	d	82	ASP
16	l	118	ASP
6	S	332	TYR
8	b	129	MET

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

Mol	Chain	Res	Type
7	a	109	HIS
8	b	41	ASN
16	l	6	GLN
2	D	129	GLN
1	A	87	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 146 ligands modelled in this entry, 1 is monoatomic - leaving 145 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
19	CLA	b	814	-	55,63,73	1.59	8 (14%)	64,101,113	1.46	7 (10%)
19	CLA	a	807	-	65,73,73	1.45	6 (9%)	76,113,113	1.41	7 (9%)
21	BCR	a	846	-	41,41,41	1.16	2 (4%)	56,56,56	1.23	7 (12%)
19	CLA	a	820	-	65,73,73	1.46	6 (9%)	76,113,113	1.40	9 (11%)
19	CLA	a	816	-	46,54,73	1.73	7 (15%)	53,90,113	1.59	6 (11%)
30	EQ3	b	851	-	43,43,43	1.66	9 (20%)	56,60,60	1.55	11 (19%)
19	CLA	b	835	-	52,60,73	1.61	7 (13%)	60,97,113	1.56	9 (15%)
19	CLA	a	825	-	60,68,73	1.52	6 (10%)	70,107,113	1.43	7 (10%)
26	LHG	a	853	19	48,48,48	0.60	1 (2%)	51,54,54	1.26	6 (11%)
19	CLA	a	831	-	65,73,73	1.46	7 (10%)	76,113,113	1.51	9 (11%)
19	CLA	b	810	-	56,64,73	1.58	6 (10%)	65,102,113	1.47	6 (9%)
19	CLA	a	802	-	65,73,73	1.48	5 (7%)	76,113,113	1.40	8 (10%)
21	BCR	b	847	-	41,41,41	1.10	2 (4%)	56,56,56	1.14	6 (10%)
21	BCR	j	101	-	41,41,41	1.15	2 (4%)	56,56,56	1.22	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
19	CLA	D	403	-	46,54,73	1.75	5 (10%)	53,90,113	1.57	6 (11%)
19	CLA	b	808	8	65,73,73	1.48	6 (9%)	76,113,113	1.38	7 (9%)
31	ZEX	b	852	-	42,43,43	1.65	8 (19%)	55,60,60	1.58	11 (20%)
19	CLA	b	821	-	46,54,73	1.76	7 (15%)	53,90,113	1.56	6 (11%)
21	BCR	a	851	-	25,25,41	1.16	1 (4%)	33,33,56	1.30	3 (9%)
29	ECH	b	844	-	42,42,42	1.73	8 (19%)	55,58,58	2.37	16 (29%)
21	BCR	b	846	-	41,41,41	1.15	2 (4%)	56,56,56	1.15	4 (7%)
26	LHG	f	206	-	48,48,48	0.58	0	51,54,54	1.25	6 (11%)
19	CLA	k	101	-	46,54,73	1.75	6 (13%)	53,90,113	1.46	6 (11%)
25	SF4	c	102	9	0,12,12	-	-	-		
26	LHG	a	855	-	48,48,48	0.60	1 (2%)	51,54,54	1.27	6 (11%)
19	CLA	b	824	-	55,63,73	1.57	6 (10%)	64,101,113	1.53	7 (10%)
19	CLA	A	407	-	65,73,73	1.47	6 (9%)	76,113,113	1.39	6 (7%)
19	CLA	b	836	-	65,73,73	1.45	6 (9%)	76,113,113	1.40	8 (10%)
23	CL0	a	801	-	65,73,73	1.48	6 (9%)	76,113,113	1.36	8 (10%)
19	CLA	b	839	-	65,73,73	1.51	7 (10%)	76,113,113	1.36	7 (9%)
19	CLA	b	802	-	65,73,73	1.46	7 (10%)	76,113,113	1.41	7 (9%)
19	CLA	b	809	-	56,64,73	1.63	6 (10%)	65,102,113	1.41	7 (10%)
27	LMG	b	848	-	55,55,55	0.70	1 (1%)	63,63,63	1.40	8 (12%)
19	CLA	A	403	-	46,54,73	1.75	6 (13%)	53,90,113	1.54	7 (13%)
19	CLA	b	803	-	65,73,73	1.46	6 (9%)	76,113,113	1.37	8 (10%)
19	CLA	b	833	-	65,73,73	1.46	6 (9%)	76,113,113	1.39	8 (10%)
27	LMG	a	854	-	40,40,55	0.82	0	48,48,63	1.29	5 (10%)
19	CLA	A	405	-	50,58,73	1.69	6 (12%)	58,95,113	1.54	9 (15%)
19	CLA	a	812	-	65,73,73	1.47	6 (9%)	76,113,113	1.38	7 (9%)
19	CLA	a	842	-	65,73,73	1.47	6 (9%)	76,113,113	1.36	6 (7%)
19	CLA	b	805	-	65,73,73	1.45	7 (10%)	76,113,113	1.43	8 (10%)
19	CLA	a	808	-	65,73,73	1.46	6 (9%)	76,113,113	1.38	8 (10%)
21	BCR	a	859	-	41,41,41	1.17	3 (7%)	56,56,56	1.20	6 (10%)
19	CLA	b	827	-	65,73,73	1.45	7 (10%)	76,113,113	1.37	7 (9%)
19	CLA	D	402	-	55,63,73	1.61	7 (12%)	64,101,113	1.48	8 (12%)
19	CLA	a	806	-	65,73,73	1.45	7 (10%)	76,113,113	1.47	7 (9%)
19	CLA	b	813	-	65,73,73	1.46	6 (9%)	76,113,113	1.42	9 (11%)
21	BCR	b	842	-	41,41,41	1.19	2 (4%)	56,56,56	1.25	7 (12%)
21	BCR	a	849	-	41,41,41	1.18	2 (4%)	56,56,56	1.24	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
21	BCR	b	843	-	41,41,41	1.16	2 (4%)	56,56,56	1.20	6 (10%)
24	PQN	b	841	-	34,34,34	0.38	0	42,45,45	0.39	0
19	CLA	b	840	26	46,54,73	1.73	5 (10%)	53,90,113	1.56	6 (11%)
19	CLA	b	825	-	65,73,73	1.46	7 (10%)	76,113,113	1.36	7 (9%)
19	CLA	b	838	-	65,73,73	1.47	6 (9%)	76,113,113	1.39	9 (11%)
32	LMT	j	102	-	36,36,36	1.18	6 (16%)	47,47,47	0.95	2 (4%)
19	CLA	a	809	7	65,73,73	1.44	6 (9%)	76,113,113	1.43	9 (11%)
19	CLA	b	828	-	65,73,73	1.47	6 (9%)	76,113,113	1.43	6 (7%)
21	BCR	i	102	-	41,41,41	1.10	2 (4%)	56,56,56	1.24	7 (12%)
19	CLA	a	810	7	51,59,73	1.64	6 (11%)	59,96,113	1.59	8 (13%)
21	BCR	A	406	-	41,41,41	1.15	2 (4%)	56,56,56	1.23	6 (10%)
21	BCR	a	850	-	41,41,41	1.20	2 (4%)	56,56,56	1.26	6 (10%)
19	CLA	a	803	-	65,73,73	1.48	7 (10%)	76,113,113	1.41	8 (10%)
19	CLA	b	817	-	65,73,73	1.45	6 (9%)	76,113,113	1.37	6 (7%)
19	CLA	b	816	-	65,73,73	1.46	6 (9%)	76,113,113	1.42	9 (11%)
19	CLA	f	201	-	65,73,73	1.48	6 (9%)	76,113,113	1.37	6 (7%)
19	CLA	a	833	-	60,68,73	1.53	6 (10%)	70,107,113	1.41	9 (12%)
19	CLA	a	836	-	65,73,73	1.47	6 (9%)	76,113,113	1.37	8 (10%)
21	BCR	f	202	-	41,41,41	1.17	2 (4%)	56,56,56	1.20	5 (8%)
19	CLA	a	827	-	65,73,73	1.48	6 (9%)	76,113,113	1.38	8 (10%)
19	CLA	a	857	-	65,73,73	1.48	6 (9%)	76,113,113	1.36	6 (7%)
19	CLA	a	821	-	65,73,73	1.50	7 (10%)	76,113,113	1.37	7 (9%)
19	CLA	a	813	-	60,68,73	1.55	8 (13%)	70,107,113	1.39	8 (11%)
19	CLA	b	818	-	60,68,73	1.51	6 (10%)	70,107,113	1.39	6 (8%)
19	CLA	a	840	-	65,73,73	1.50	7 (10%)	76,113,113	1.38	6 (7%)
19	CLA	b	834	-	50,58,73	1.66	6 (12%)	58,95,113	1.57	7 (12%)
21	BCR	a	848	-	41,41,41	1.16	2 (4%)	56,56,56	1.20	6 (10%)
25	SF4	a	845	7,8	0,12,12	-	-	-		
19	CLA	a	843	26	56,64,73	1.57	7 (12%)	65,102,113	1.50	8 (12%)
19	CLA	b	801	-	65,73,73	1.49	7 (10%)	76,113,113	1.32	7 (9%)
19	CLA	b	812	-	65,73,73	1.45	7 (10%)	76,113,113	1.40	8 (10%)
19	CLA	a	856	-	65,73,73	1.46	7 (10%)	76,113,113	1.35	7 (9%)
21	BCR	b	845	-	41,41,41	1.15	2 (4%)	56,56,56	1.29	5 (8%)
19	CLA	a	860	-	65,73,73	1.46	5 (7%)	76,113,113	1.37	8 (10%)
19	CLA	l	202	-	50,58,73	1.70	5 (10%)	58,95,113	1.53	9 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
19	CLA	a	834	-	65,73,73	1.46	6 (9%)	76,113,113	1.37	7 (9%)
19	CLA	k	102	15	45,53,73	1.79	6 (13%)	52,89,113	1.56	6 (11%)
19	CLA	b	820	-	60,68,73	1.52	6 (10%)	70,107,113	1.42	7 (10%)
19	CLA	b	822	-	57,65,73	1.57	6 (10%)	66,103,113	1.48	8 (12%)
19	CLA	A	402	-	65,73,73	1.47	7 (10%)	76,113,113	1.37	6 (7%)
19	CLA	b	832	-	65,73,73	1.45	7 (10%)	76,113,113	1.44	8 (10%)
19	CLA	f	203	-	50,58,73	1.69	6 (12%)	58,95,113	1.53	8 (13%)
19	CLA	b	807	-	65,73,73	1.47	7 (10%)	76,113,113	1.35	8 (10%)
27	LMG	b	850	-	55,55,55	0.78	1 (1%)	63,63,63	1.34	9 (14%)
21	BCR	i	101	-	41,41,41	1.15	2 (4%)	56,56,56	1.21	5 (8%)
19	CLA	a	832	-	56,64,73	1.59	6 (10%)	65,102,113	1.44	8 (12%)
26	LHG	b	849	19	37,37,48	0.71	1 (2%)	40,43,54	1.21	3 (7%)
19	CLA	a	804	-	65,73,73	1.48	7 (10%)	76,113,113	1.37	7 (9%)
27	LMG	l	201	-	50,50,55	0.73	0	58,58,63	1.34	7 (12%)
19	CLA	b	829	-	51,59,73	1.68	6 (11%)	59,96,113	1.51	8 (13%)
25	SF4	c	101	9	0,12,12	-	-	-		
19	CLA	b	831	-	65,73,73	1.50	7 (10%)	76,113,113	1.34	7 (9%)
31	ZEX	f	205	-	42,43,43	1.66	8 (19%)	55,60,60	1.56	11 (20%)
19	CLA	a	818	-	65,73,73	1.45	7 (10%)	76,113,113	1.40	7 (9%)
19	CLA	j	104	-	46,54,73	1.77	6 (13%)	53,90,113	1.53	7 (13%)
19	CLA	a	828	-	65,73,73	1.45	7 (10%)	76,113,113	1.38	7 (9%)
21	BCR	a	847	-	41,41,41	1.18	2 (4%)	56,56,56	1.22	5 (8%)
28	45D	a	858	-	43,43,43	1.70	9 (20%)	54,60,60	1.63	11 (20%)
19	CLA	l	203	-	65,73,73	1.46	7 (10%)	76,113,113	1.38	7 (9%)
19	CLA	a	814	-	65,73,73	1.45	7 (10%)	76,113,113	1.46	8 (10%)
19	CLA	a	829	-	65,73,73	1.46	6 (9%)	76,113,113	1.41	7 (9%)
19	CLA	a	824	-	65,73,73	1.49	6 (9%)	76,113,113	1.43	9 (11%)
19	CLA	a	830	-	65,73,73	1.46	6 (9%)	76,113,113	1.34	6 (7%)
19	CLA	a	838	-	51,59,73	1.64	6 (11%)	59,96,113	1.52	7 (11%)
19	CLA	b	811	-	50,58,73	1.68	6 (12%)	58,95,113	1.52	7 (12%)
19	CLA	b	830	-	50,58,73	1.65	6 (12%)	58,95,113	1.57	8 (13%)
19	CLA	b	819	-	65,73,73	1.47	6 (9%)	76,113,113	1.34	7 (9%)
19	CLA	a	819	-	65,73,73	1.48	8 (12%)	76,113,113	1.39	6 (7%)
19	CLA	a	839	-	65,73,73	1.47	6 (9%)	76,113,113	1.33	8 (10%)
19	CLA	b	826	-	65,73,73	1.46	6 (9%)	76,113,113	1.41	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
19	CLA	a	837	7	65,73,73	1.47	6 (9%)	76,113,113	1.41	7 (9%)
19	CLA	b	815	-	56,64,73	1.55	6 (10%)	65,102,113	1.51	8 (12%)
19	CLA	a	815	-	65,73,73	1.46	6 (9%)	76,113,113	1.43	9 (11%)
19	CLA	a	835	-	65,73,73	1.46	6 (9%)	76,113,113	1.45	8 (10%)
19	CLA	a	811	-	50,58,73	1.65	6 (12%)	58,95,113	1.55	8 (13%)
19	CLA	a	822	-	65,73,73	1.48	6 (9%)	76,113,113	1.37	6 (7%)
19	CLA	b	823	-	65,73,73	1.47	7 (10%)	76,113,113	1.41	7 (9%)
20	PHO	D	401	-	51,69,69	1.03	6 (11%)	47,99,99	1.14	5 (10%)
22	HEM	E	101	4,3	41,50,50	1.54	5 (12%)	45,82,82	1.28	5 (11%)
19	CLA	l	204	-	52,60,73	1.63	6 (11%)	60,97,113	1.51	7 (11%)
24	PQN	a	844	-	34,34,34	0.37	0	42,45,45	0.40	0
19	CLA	b	804	-	65,73,73	1.44	6 (9%)	76,113,113	1.45	8 (10%)
19	CLA	a	805	-	65,73,73	1.47	7 (10%)	76,113,113	1.36	6 (7%)
19	CLA	j	103	14	55,63,73	1.63	5 (9%)	64,101,113	1.45	7 (10%)
19	CLA	f	204	12	50,58,73	1.70	5 (10%)	58,95,113	1.52	8 (13%)
19	CLA	a	823	-	65,73,73	1.46	5 (7%)	76,113,113	1.42	7 (9%)
19	CLA	b	837	-	50,58,73	1.71	7 (14%)	58,95,113	1.54	7 (12%)
20	PHO	A	404	-	51,69,69	1.01	4 (7%)	47,99,99	1.09	5 (10%)
19	CLA	a	817	-	46,54,73	1.72	6 (13%)	53,90,113	1.58	6 (11%)
19	CLA	b	806	-	65,73,73	1.45	6 (9%)	76,113,113	1.38	7 (9%)
26	LHG	a	852	-	48,48,48	0.62	1 (2%)	51,54,54	1.29	6 (11%)
29	ECH	m	101	-	42,42,42	1.78	9 (21%)	55,58,58	1.85	13 (23%)
21	BCR	k	103	-	41,41,41	1.15	2 (4%)	56,56,56	1.26	6 (10%)
19	CLA	a	841	-	65,73,73	1.47	7 (10%)	76,113,113	1.40	8 (10%)
19	CLA	a	826	-	65,73,73	1.45	7 (10%)	76,113,113	1.42	8 (10%)
21	BCR	l	205	-	41,41,41	1.12	2 (4%)	56,56,56	1.21	4 (7%)

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
19	CLA	b	814	-	1/1/13/20	12/25/103/115	-
19	CLA	a	807	-	1/1/15/20	10/37/115/115	-
21	BCR	a	846	-	-	8/29/63/63	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	a	820	-	1/1/15/20	14/37/115/115	-
19	CLA	a	816	-	1/1/11/20	7/15/93/115	-
30	EQ3	b	851	-	-	3/29/68/68	0/2/2/2
19	CLA	b	835	-	1/1/12/20	6/22/100/115	-
19	CLA	a	825	-	1/1/14/20	11/31/109/115	-
26	LHG	a	853	19	-	23/53/53/53	-
19	CLA	a	831	-	1/1/15/20	16/37/115/115	-
19	CLA	b	810	-	1/1/13/20	8/27/105/115	-
19	CLA	a	802	-	1/1/15/20	13/37/115/115	-
21	BCR	b	847	-	-	15/29/63/63	0/2/2/2
21	BCR	j	101	-	-	7/29/63/63	0/2/2/2
19	CLA	D	403	-	1/1/11/20	6/15/93/115	-
19	CLA	b	808	8	1/1/15/20	9/37/115/115	-
31	ZEX	b	852	-	-	3/29/67/67	0/2/2/2
19	CLA	b	821	-	1/1/11/20	5/15/93/115	-
21	BCR	a	851	-	-	7/18/35/63	0/1/1/2
29	ECH	b	844	-	-	10/29/66/66	0/2/2/2
21	BCR	b	846	-	-	7/29/63/63	0/2/2/2
26	LHG	f	206	-	-	30/53/53/53	-
19	CLA	k	101	-	1/1/11/20	11/15/93/115	-
25	SF4	c	102	9	-	-	0/6/5/5
26	LHG	a	855	-	-	20/53/53/53	-
19	CLA	b	824	-	1/1/13/20	6/25/103/115	-
19	CLA	A	407	-	1/1/15/20	15/37/115/115	-
19	CLA	b	836	-	1/1/15/20	17/37/115/115	-
23	CL0	a	801	-	3/3/20/25	10/37/135/135	-
19	CLA	b	839	-	1/1/15/20	10/37/115/115	-
19	CLA	b	802	-	1/1/15/20	15/37/115/115	-
19	CLA	b	809	-	1/1/13/20	8/27/105/115	-
27	LMG	b	848	-	-	22/50/70/70	0/1/1/1
19	CLA	A	403	-	1/1/11/20	10/15/93/115	-
19	CLA	b	803	-	1/1/15/20	13/37/115/115	-
19	CLA	b	833	-	1/1/15/20	19/37/115/115	-
27	LMG	a	854	-	-	18/35/55/70	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	A	405	-	1/1/12/20	7/19/97/115	-
19	CLA	a	812	-	1/1/15/20	13/37/115/115	-
19	CLA	a	842	-	1/1/15/20	12/37/115/115	-
19	CLA	b	805	-	1/1/15/20	16/37/115/115	-
19	CLA	a	808	-	1/1/15/20	14/37/115/115	-
21	BCR	a	859	-	-	6/29/63/63	0/2/2/2
19	CLA	b	827	-	1/1/15/20	10/37/115/115	-
19	CLA	D	402	-	1/1/13/20	13/25/103/115	-
19	CLA	a	806	-	1/1/15/20	11/37/115/115	-
19	CLA	b	813	-	1/1/15/20	12/37/115/115	-
21	BCR	b	842	-	-	11/29/63/63	0/2/2/2
21	BCR	a	849	-	-	6/29/63/63	0/2/2/2
21	BCR	b	843	-	-	6/29/63/63	0/2/2/2
24	PQN	b	841	-	-	0/23/43/43	0/2/2/2
19	CLA	b	840	26	1/1/11/20	9/15/93/115	-
19	CLA	b	825	-	1/1/15/20	5/37/115/115	-
19	CLA	b	838	-	1/1/15/20	12/37/115/115	-
32	LMT	j	102	-	-	5/21/61/61	0/2/2/2
19	CLA	a	809	7	1/1/15/20	14/37/115/115	-
19	CLA	b	828	-	1/1/15/20	16/37/115/115	-
21	BCR	i	102	-	-	12/29/63/63	0/2/2/2
19	CLA	a	810	7	1/1/12/20	3/21/99/115	-
21	BCR	A	406	-	-	9/29/63/63	0/2/2/2
21	BCR	a	850	-	-	10/29/63/63	0/2/2/2
19	CLA	a	803	-	1/1/15/20	10/37/115/115	-
19	CLA	b	817	-	1/1/15/20	13/37/115/115	-
19	CLA	b	816	-	1/1/15/20	9/37/115/115	-
19	CLA	f	201	-	1/1/15/20	15/37/115/115	-
19	CLA	a	833	-	1/1/14/20	13/31/109/115	-
19	CLA	a	836	-	1/1/15/20	11/37/115/115	-
21	BCR	f	202	-	-	10/29/63/63	0/2/2/2
19	CLA	a	827	-	1/1/15/20	7/37/115/115	-
19	CLA	a	857	-	1/1/15/20	19/37/115/115	-
19	CLA	a	821	-	1/1/15/20	22/37/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	a	813	-	1/1/14/20	14/31/109/115	-
19	CLA	b	818	-	1/1/14/20	6/31/109/115	-
19	CLA	a	840	-	1/1/15/20	18/37/115/115	-
19	CLA	b	834	-	1/1/12/20	8/19/97/115	-
21	BCR	a	848	-	-	6/29/63/63	0/2/2/2
25	SF4	a	845	7,8	-	-	0/6/5/5
19	CLA	a	843	26	1/1/13/20	10/27/105/115	-
19	CLA	b	801	-	1/1/15/20	16/37/115/115	-
19	CLA	b	812	-	1/1/15/20	15/37/115/115	-
19	CLA	a	856	-	1/1/15/20	5/37/115/115	-
21	BCR	b	845	-	-	5/29/63/63	0/2/2/2
19	CLA	a	860	-	1/1/15/20	14/37/115/115	-
19	CLA	l	202	-	1/1/12/20	10/19/97/115	-
19	CLA	a	834	-	1/1/15/20	12/37/115/115	-
19	CLA	k	102	15	1/1/11/20	4/13/91/115	-
19	CLA	b	820	-	1/1/14/20	11/31/109/115	-
19	CLA	b	822	-	1/1/13/20	15/28/106/115	-
19	CLA	A	402	-	1/1/15/20	10/37/115/115	-
19	CLA	b	832	-	1/1/15/20	18/37/115/115	-
19	CLA	f	203	-	1/1/12/20	3/19/97/115	-
19	CLA	b	807	-	1/1/15/20	8/37/115/115	-
27	LMG	b	850	-	-	24/50/70/70	0/1/1/1
21	BCR	i	101	-	-	7/29/63/63	0/2/2/2
19	CLA	a	832	-	1/1/13/20	10/27/105/115	-
26	LHG	b	849	19	-	20/42/42/53	-
19	CLA	a	804	-	1/1/15/20	10/37/115/115	-
27	LMG	l	201	-	-	25/45/65/70	0/1/1/1
19	CLA	b	829	-	1/1/12/20	6/21/99/115	-
25	SF4	c	101	9	-	-	0/6/5/5
19	CLA	b	831	-	1/1/15/20	13/37/115/115	-
31	ZEX	f	205	-	-	4/29/67/67	0/2/2/2
19	CLA	a	818	-	1/1/15/20	14/37/115/115	-
19	CLA	j	104	-	1/1/11/20	7/15/93/115	-
19	CLA	a	828	-	1/1/15/20	16/37/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	BCR	a	847	-	-	6/29/63/63	0/2/2/2
28	45D	a	858	-	-	4/29/69/69	0/2/2/2
19	CLA	l	203	-	1/1/15/20	13/37/115/115	-
19	CLA	a	814	-	-	11/37/115/115	-
19	CLA	a	829	-	1/1/15/20	10/37/115/115	-
19	CLA	a	824	-	1/1/15/20	16/37/115/115	-
19	CLA	a	830	-	1/1/15/20	19/37/115/115	-
19	CLA	a	838	-	1/1/12/20	5/21/99/115	-
19	CLA	b	811	-	1/1/12/20	6/19/97/115	-
19	CLA	b	830	-	1/1/12/20	5/19/97/115	-
19	CLA	b	819	-	1/1/15/20	10/37/115/115	-
19	CLA	a	819	-	1/1/15/20	18/37/115/115	-
19	CLA	a	839	-	1/1/15/20	12/37/115/115	-
19	CLA	b	826	-	1/1/15/20	15/37/115/115	-
19	CLA	a	837	7	1/1/15/20	13/37/115/115	-
19	CLA	b	815	-	1/1/13/20	8/27/105/115	-
19	CLA	a	815	-	1/1/15/20	17/37/115/115	-
19	CLA	a	835	-	1/1/15/20	15/37/115/115	-
19	CLA	a	811	-	1/1/12/20	6/19/97/115	-
19	CLA	a	822	-	1/1/15/20	10/37/115/115	-
19	CLA	b	823	-	1/1/15/20	13/37/115/115	-
20	PHO	D	401	-	-	10/37/103/103	0/5/6/6
22	HEM	E	101	4,3	-	1/12/54/54	-
19	CLA	l	204	-	1/1/12/20	8/22/100/115	-
24	PQN	a	844	-	-	1/23/43/43	0/2/2/2
19	CLA	b	804	-	1/1/15/20	15/37/115/115	-
19	CLA	a	805	-	1/1/15/20	11/37/115/115	-
19	CLA	j	103	14	1/1/13/20	11/25/103/115	-
19	CLA	f	204	12	1/1/12/20	5/19/97/115	-
19	CLA	a	823	-	1/1/15/20	15/37/115/115	-
19	CLA	b	837	-	1/1/12/20	4/19/97/115	-
20	PHO	A	404	-	-	11/37/103/103	0/5/6/6
19	CLA	a	817	-	1/1/11/20	5/15/93/115	-
19	CLA	b	806	-	1/1/15/20	15/37/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	LHG	a	852	-	-	25/53/53/53	-
29	ECH	m	101	-	-	6/29/66/66	0/2/2/2
21	BCR	k	103	-	-	8/29/63/63	0/2/2/2
19	CLA	a	841	-	1/1/15/20	13/37/115/115	-
19	CLA	a	826	-	1/1/15/20	13/37/115/115	-
21	BCR	l	205	-	-	10/29/63/63	0/2/2/2

The worst 5 of 758 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	b	809	CLA	C4B-NB	7.74	1.42	1.35
19	b	821	CLA	C4B-NB	7.74	1.42	1.35
19	j	103	CLA	C4B-NB	7.70	1.42	1.35
19	b	839	CLA	C4B-NB	7.62	1.42	1.35
19	b	837	CLA	C4B-NB	7.58	1.42	1.35

The worst 5 of 1003 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	b	844	ECH	C15-C16-C17	8.39	140.66	123.47
19	a	806	CLA	C4A-NA-C1A	7.20	109.94	106.71
19	a	842	CLA	C4A-NA-C1A	7.09	109.89	106.71
19	a	841	CLA	C4A-NA-C1A	7.05	109.88	106.71
19	a	818	CLA	C4A-NA-C1A	7.04	109.87	106.71

5 of 103 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
19	A	402	CLA	ND
19	A	403	CLA	ND
19	A	405	CLA	ND
19	A	407	CLA	ND
19	D	402	CLA	ND

5 of 1568 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	A	403	CLA	C1A-C2A-CAA-CBA
19	A	403	CLA	C3A-C2A-CAA-CBA
19	A	403	CLA	CHA-CBD-CGD-O1D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
19	A	403	CLA	CHA-CBD-CGD-O2D
19	A	405	CLA	C1A-C2A-CAA-CBA

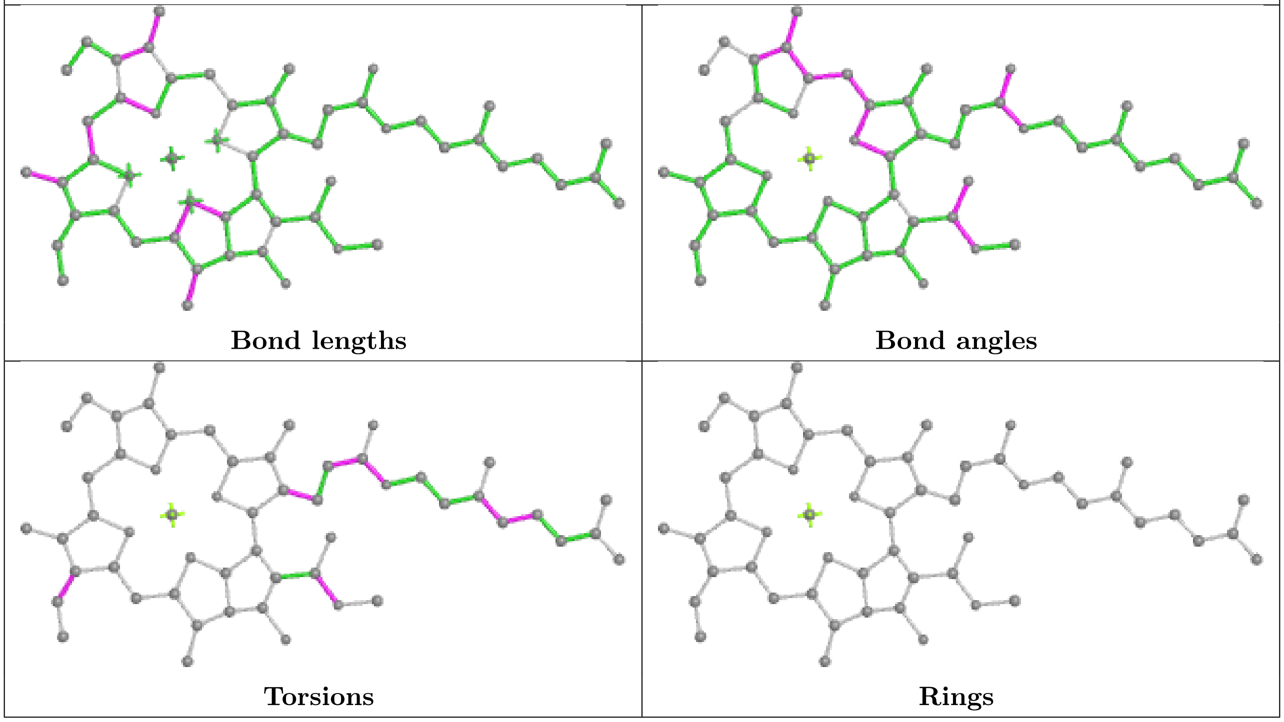
There are no ring outliers.

10 monomers are involved in 40 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	D	403	CLA	1	0
19	A	407	CLA	6	0
19	A	403	CLA	4	0
19	A	405	CLA	5	0
19	D	402	CLA	11	0
21	A	406	BCR	6	0
19	A	402	CLA	5	0
20	D	401	PHO	3	0
22	E	101	HEM	3	0
20	A	404	PHO	5	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 b 814



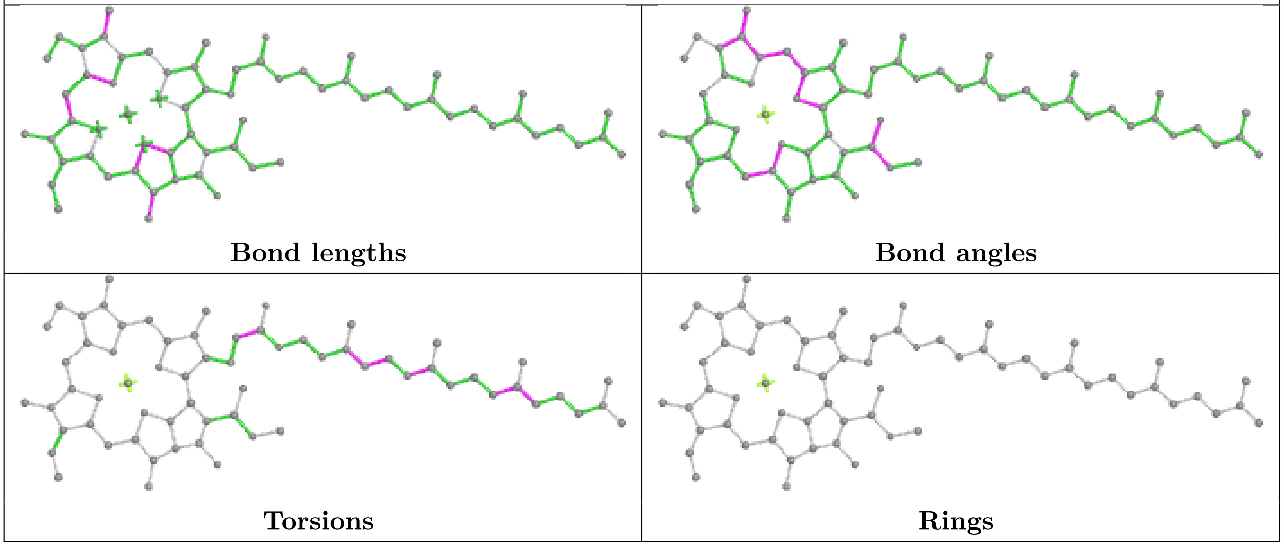
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA a 807



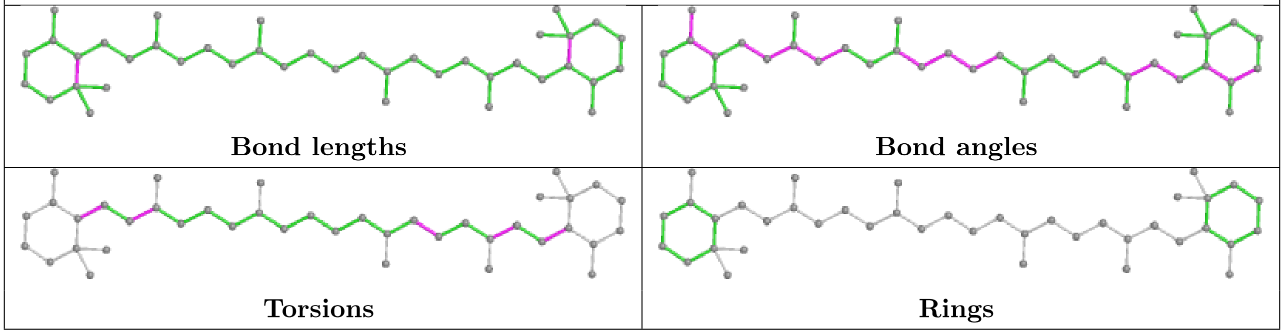
Bond lengths

Bond angles

Torsions

Rings

Ligand BCR a 846



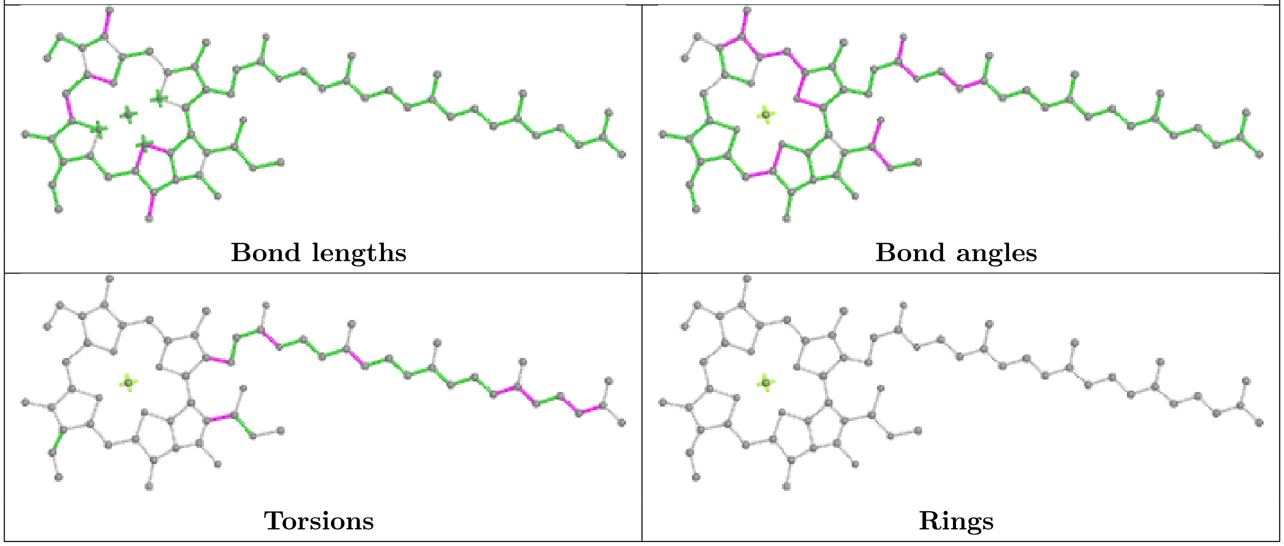
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA a 820



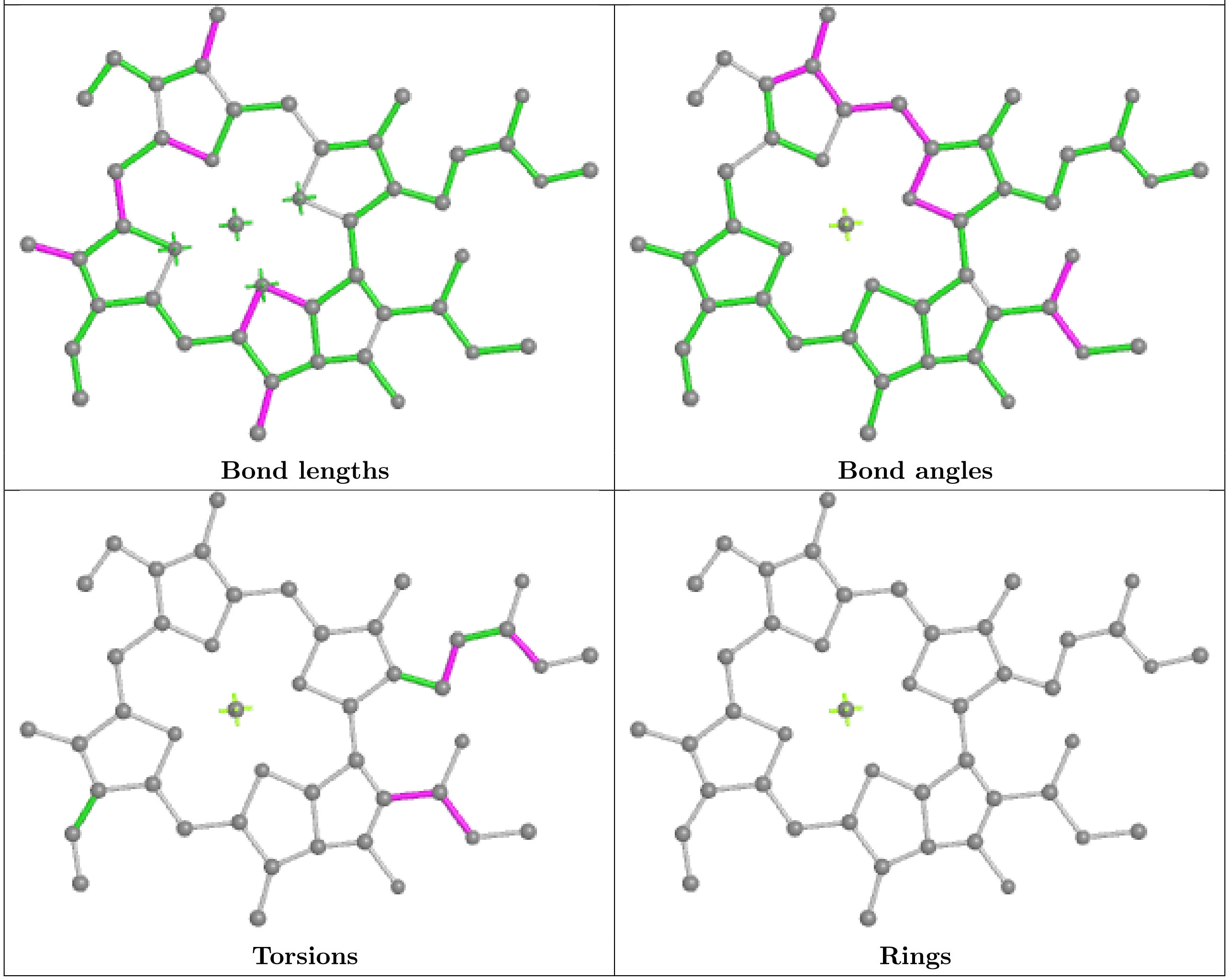
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA a 816



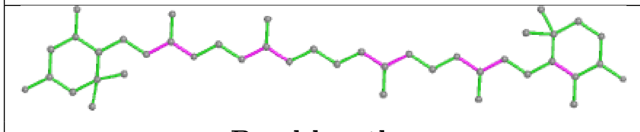
Bond lengths

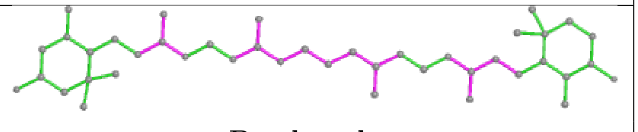
Bond angles

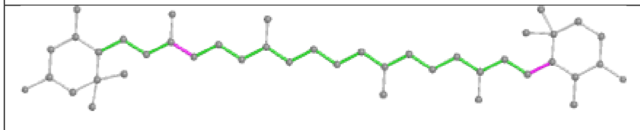
Torsions

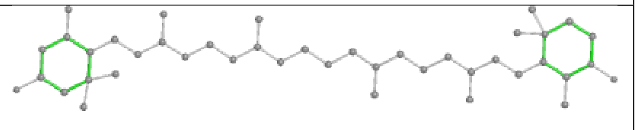
Rings

Ligand EQ3 b 851

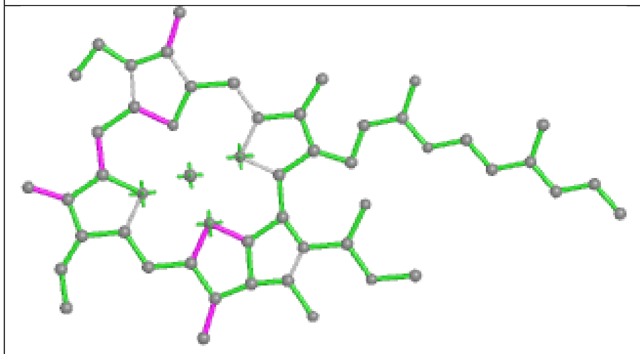

Bond lengths

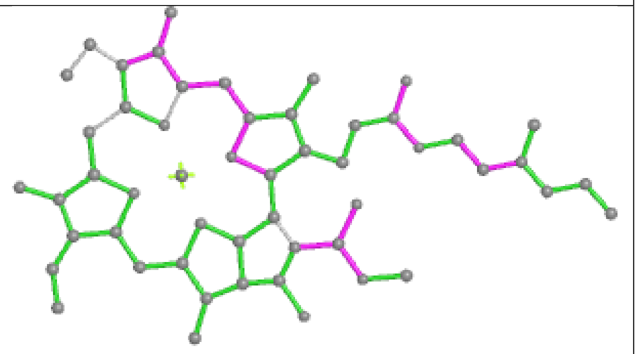

Bond angles

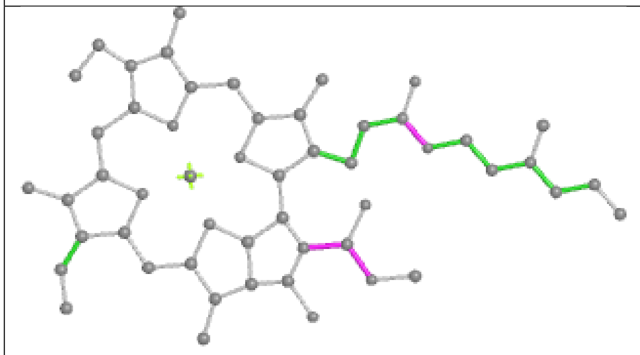

Torsions

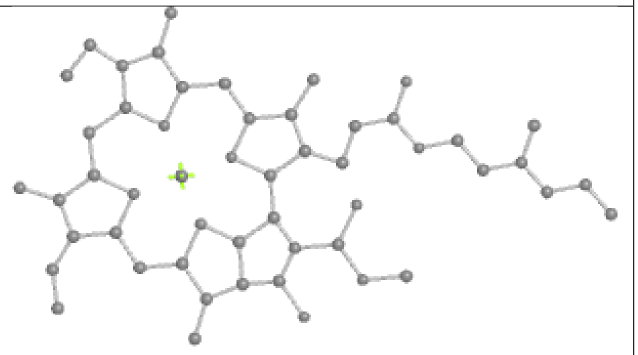

Rings

Ligand CLA b 835

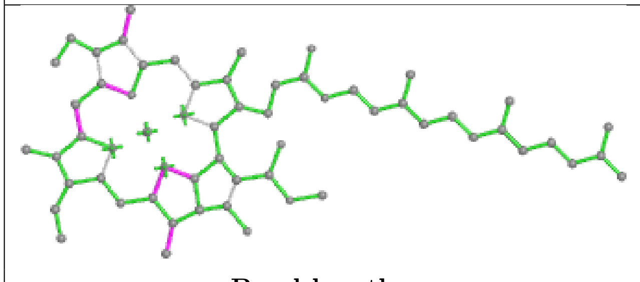

Bond lengths


Bond angles

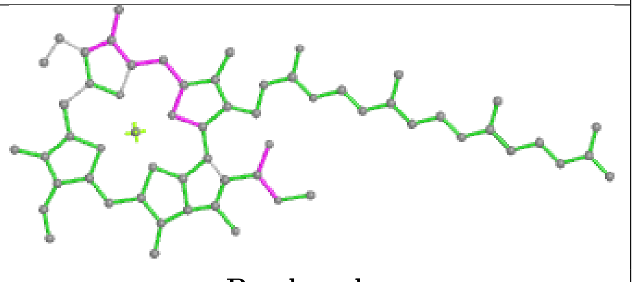

Torsions


Rings

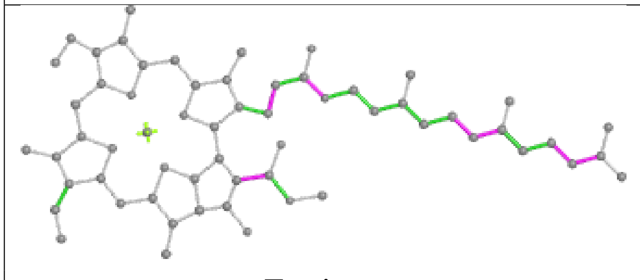
Ligand CLA a 825



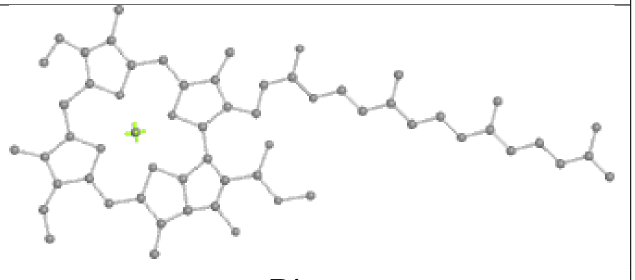
Bond lengths



Bond angles

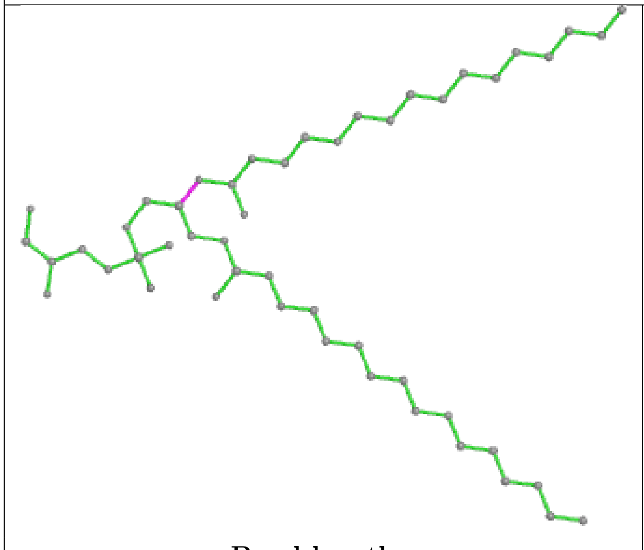


Torsions

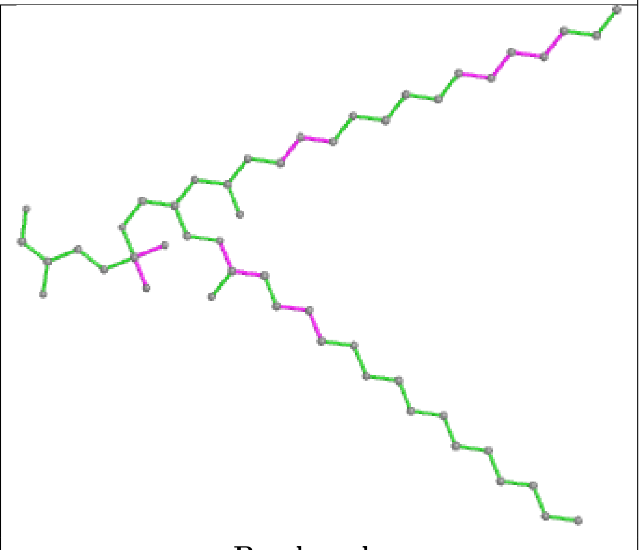


Rings

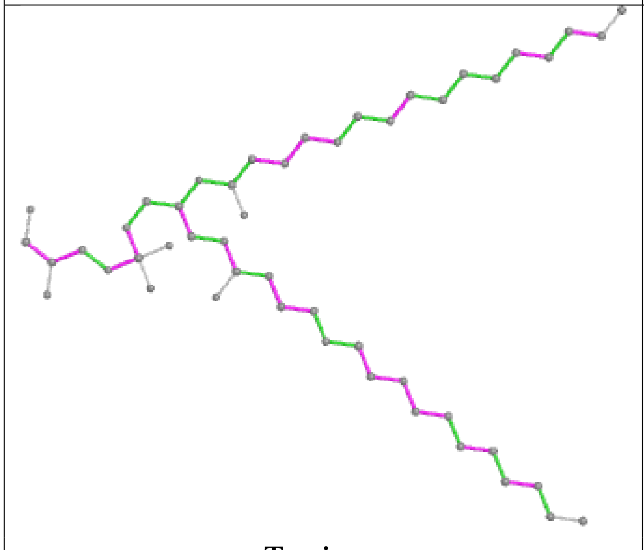
Ligand LHG a 853



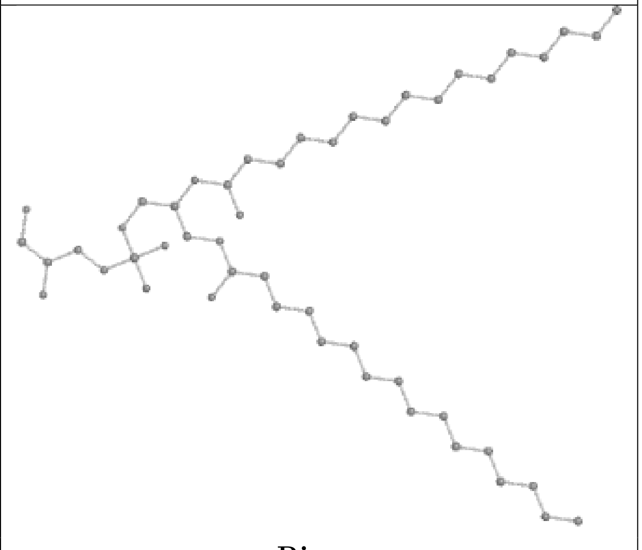
Bond lengths



Bond angles

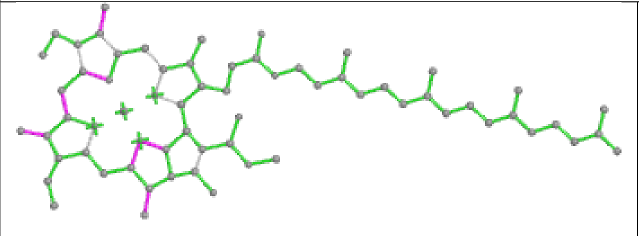


Torsions

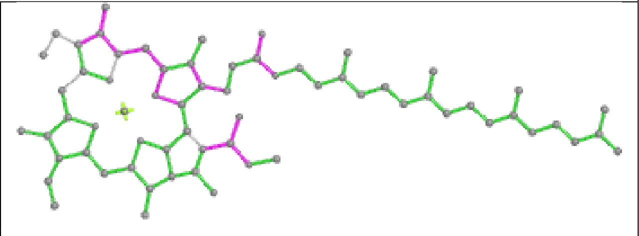


Rings

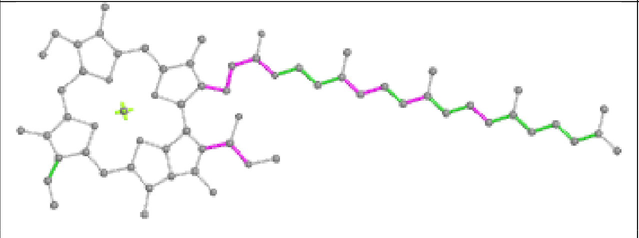
Ligand CLA a 831



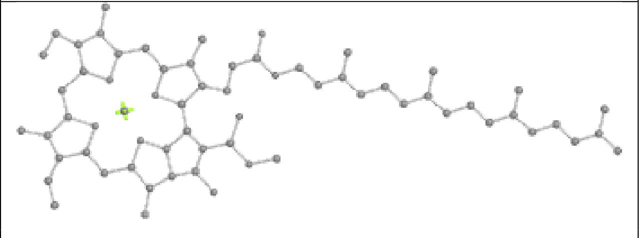
Bond lengths



Bond angles

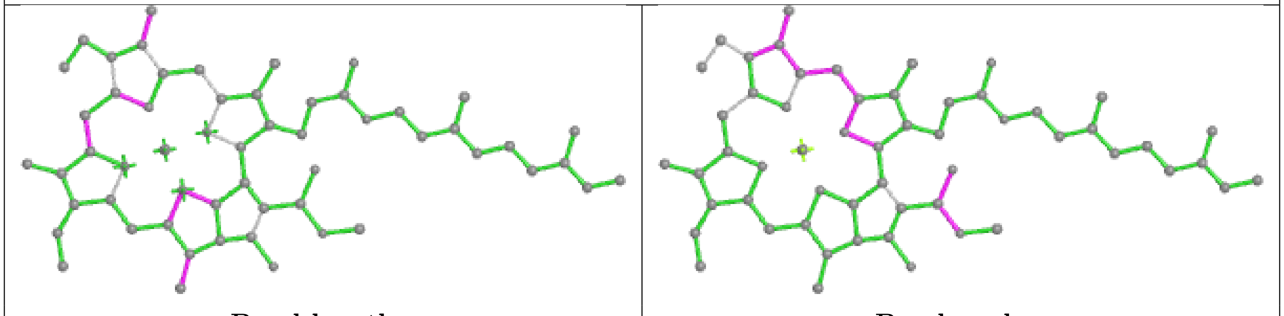


Torsions

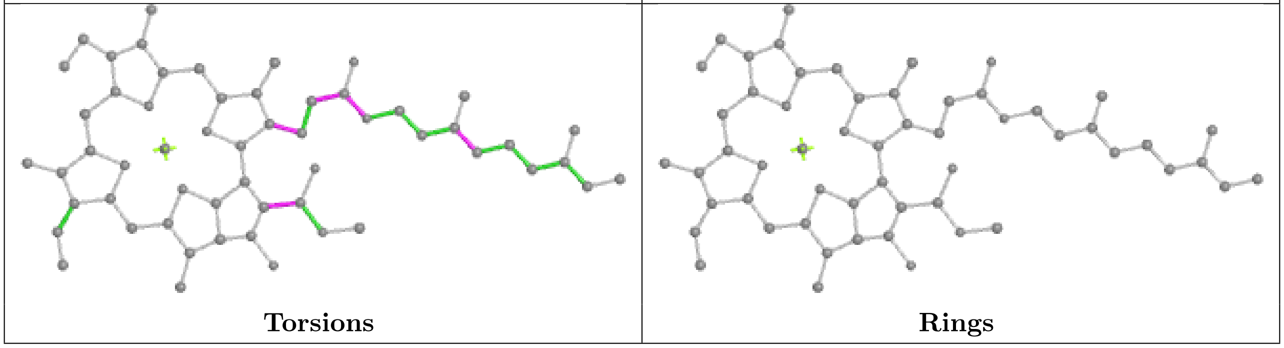


Rings

Ligand CLA b 810

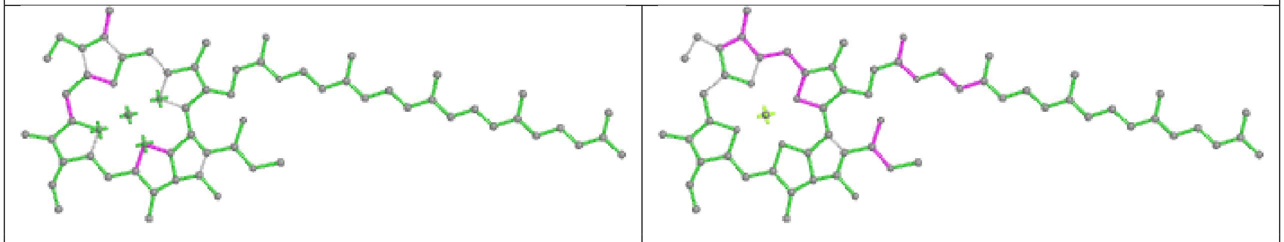


Bond lengths Bond angles

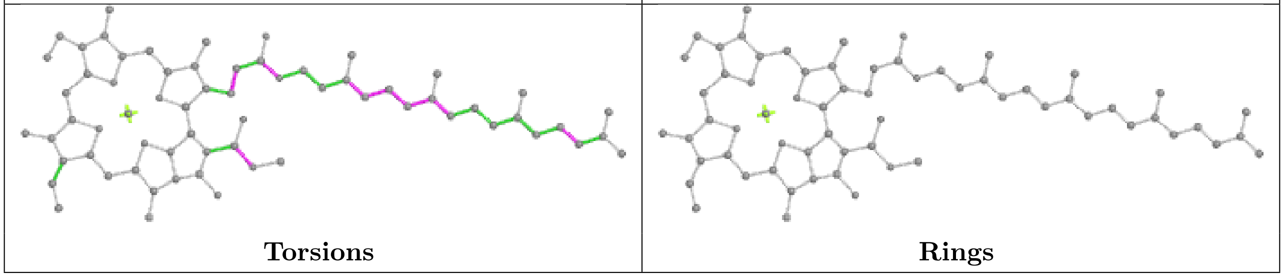


Torsions Rings

Ligand CLA a 802

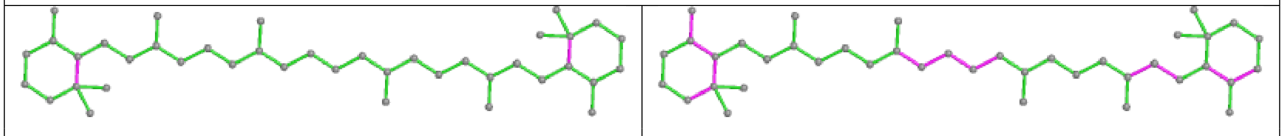


Bond lengths Bond angles

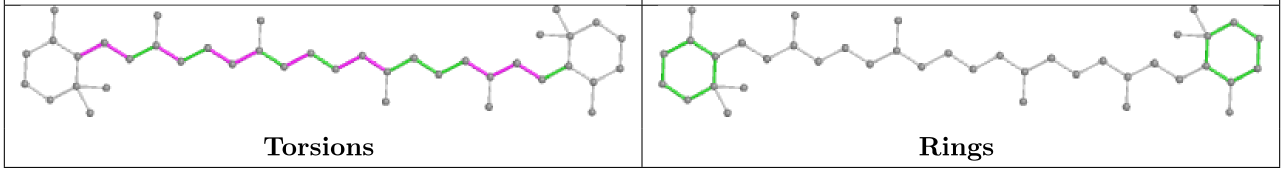


Torsions Rings

Ligand BCR b 847

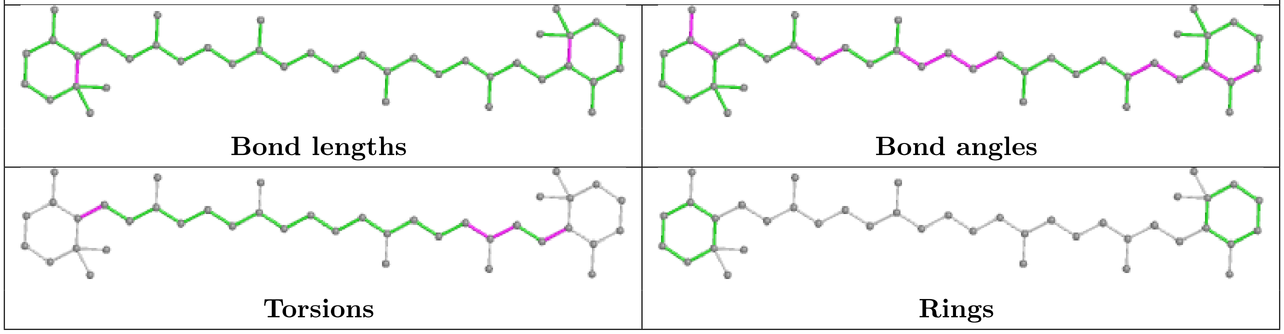


Bond lengths Bond angles



Torsions Rings

Ligand BCR j 101



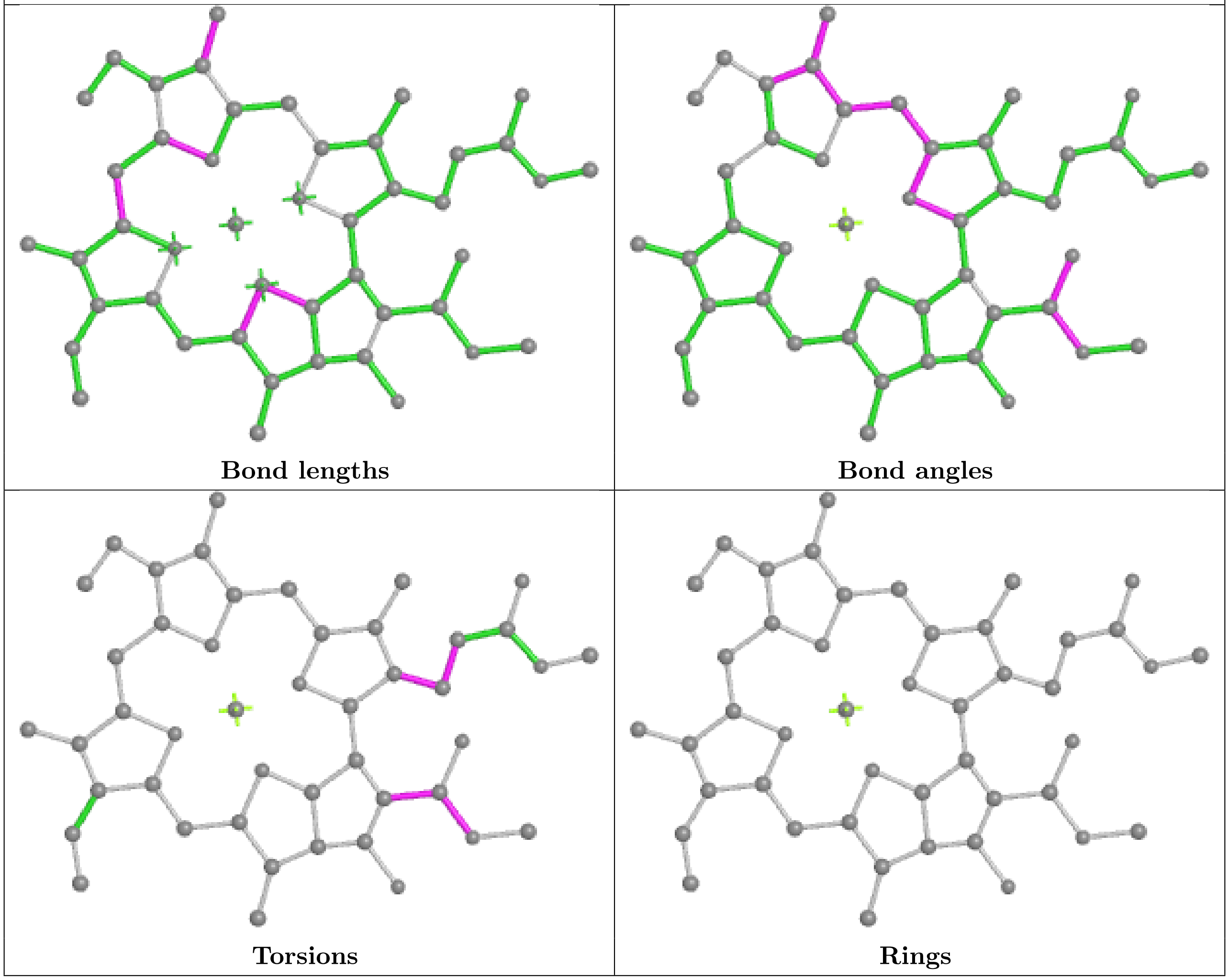
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA D 403



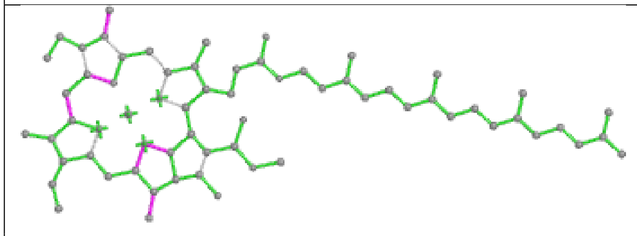
Bond lengths

Bond angles

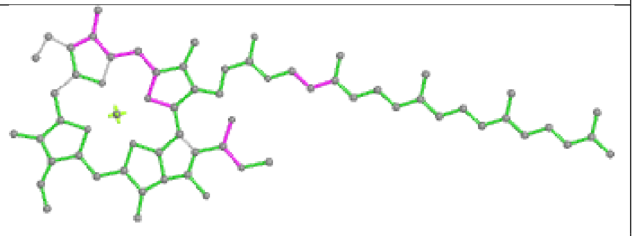
Torsions

Rings

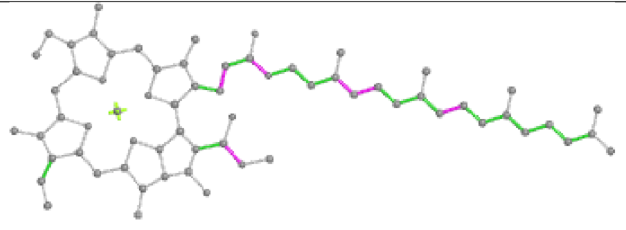
Ligand CLA b 808



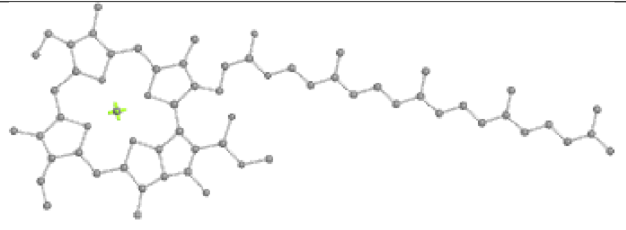
Bond lengths



Bond angles

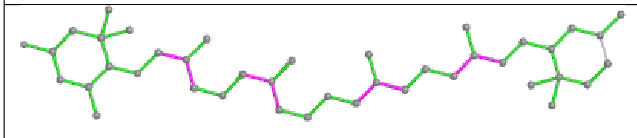


Torsions



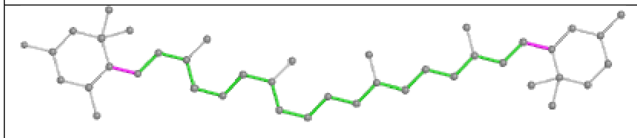
Rings

Ligand ZEX b 852

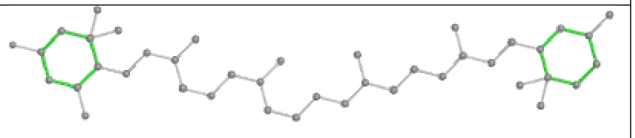


Bond lengths

Bond angles

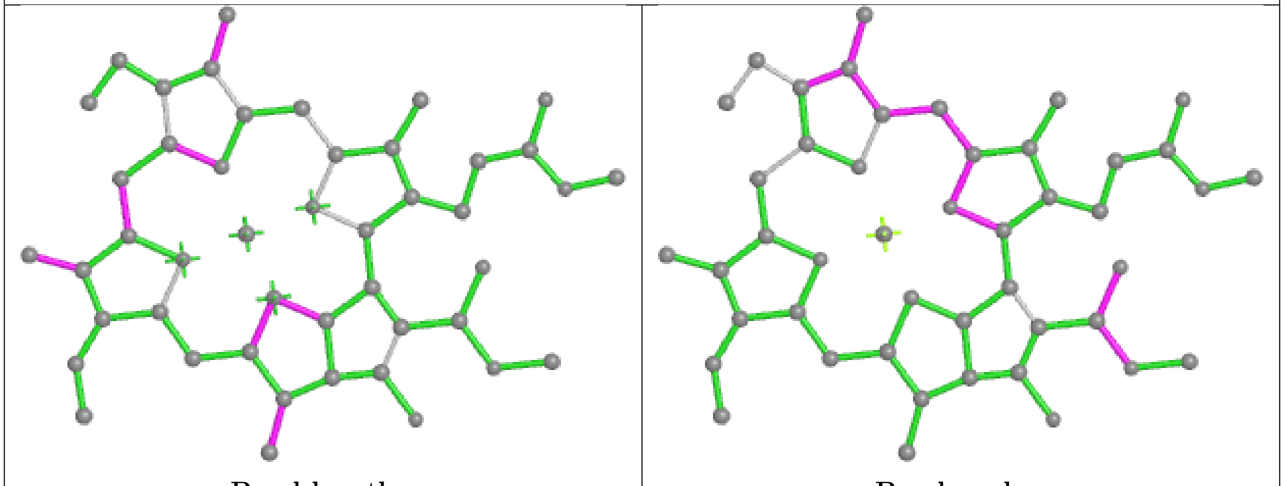


Torsions

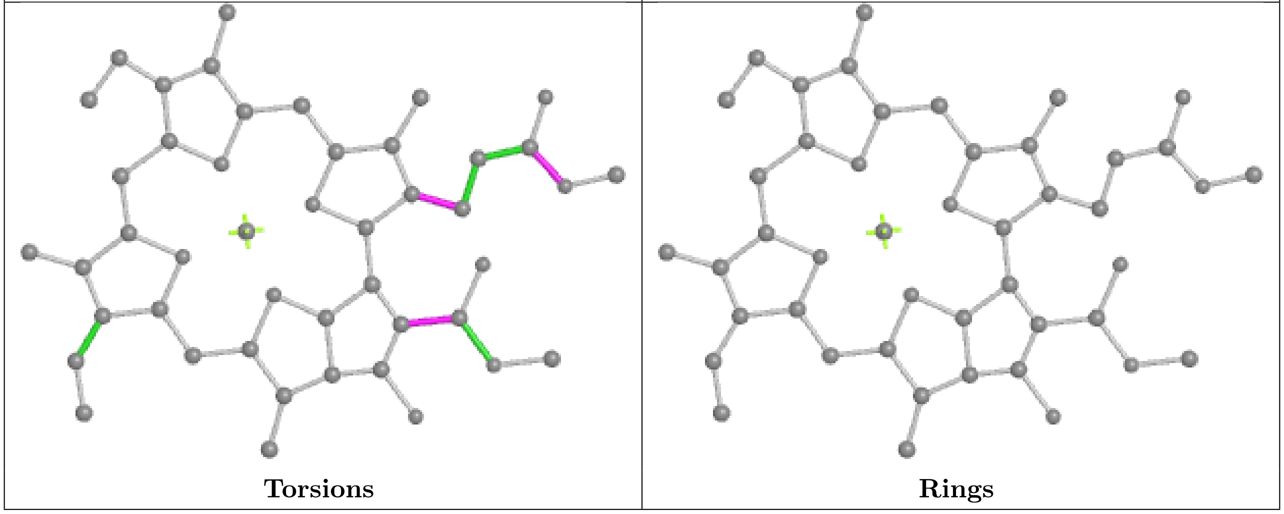


Rings

Ligand CLA b 821

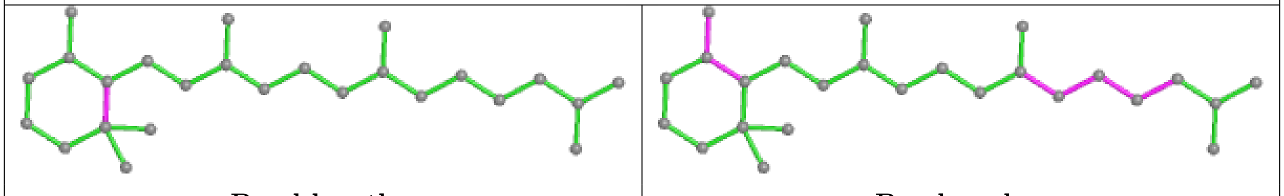


Bond lengths **Bond angles**

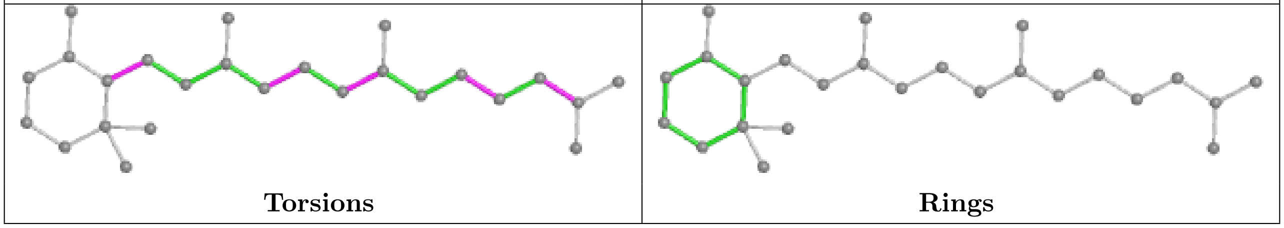


Torsions **Rings**

Ligand BCR a 851

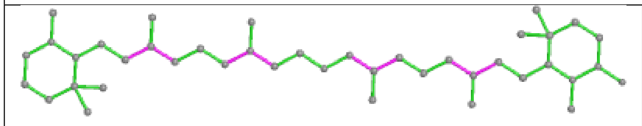
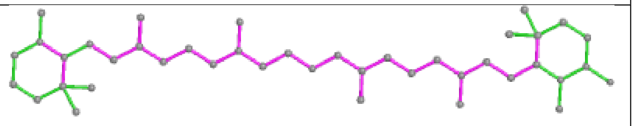
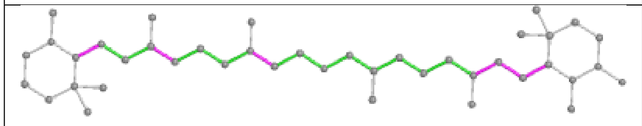
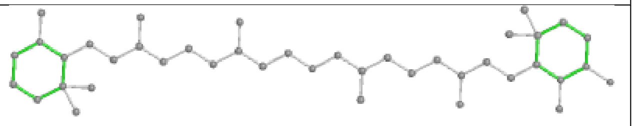


Bond lengths **Bond angles**

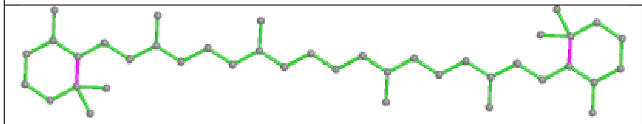
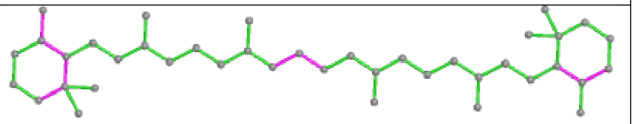
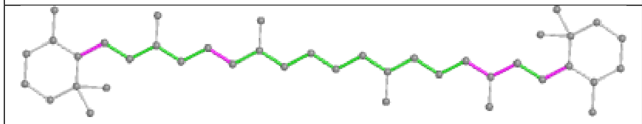
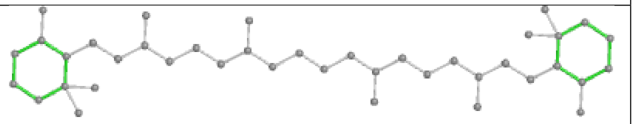


Torsions **Rings**

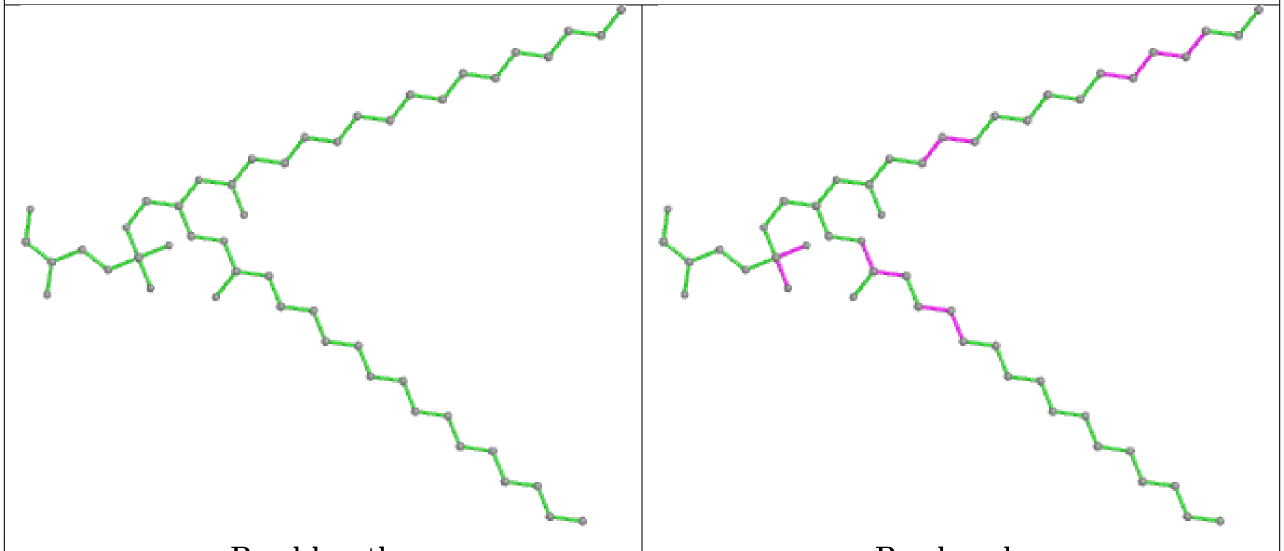
Ligand ECH b 844

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

Ligand BCR b 846

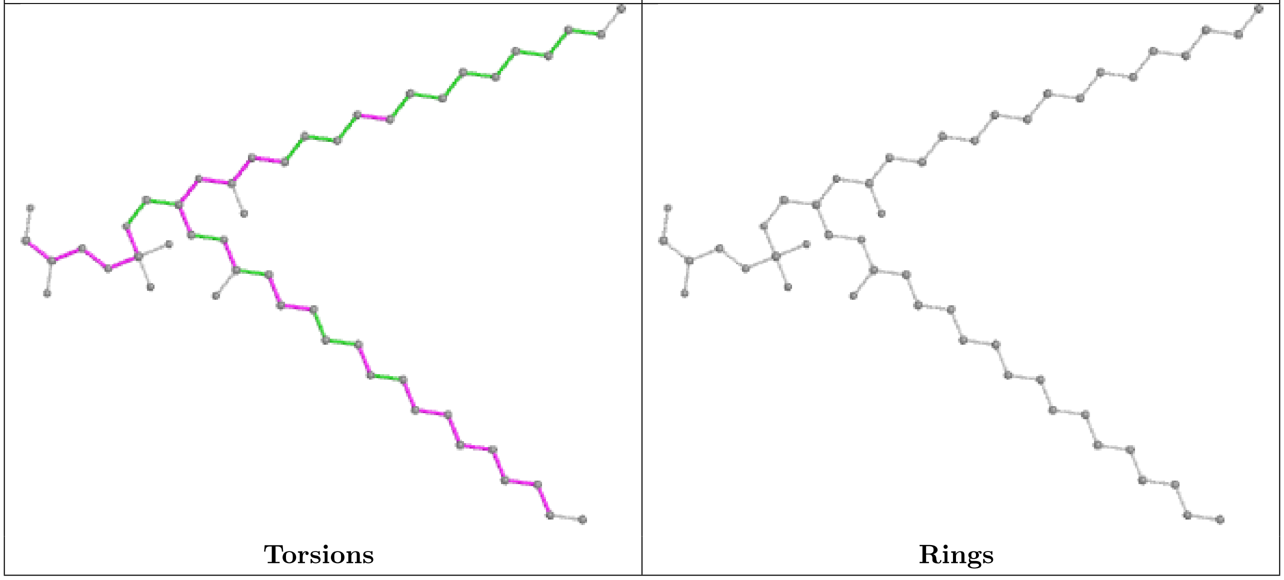
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

Ligand LHG f 206



Bond lengths

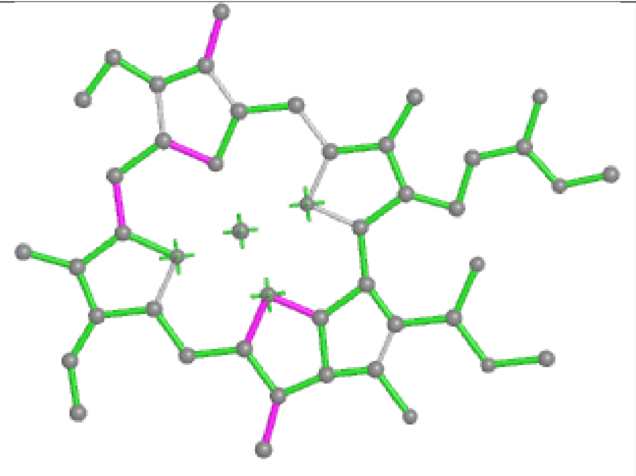
Bond angles



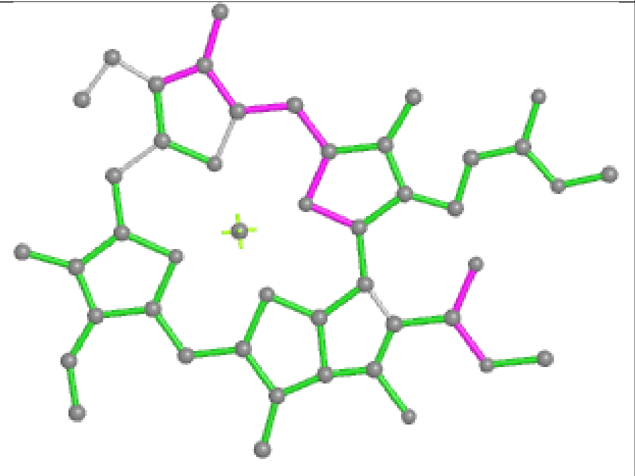
Torsions

Rings

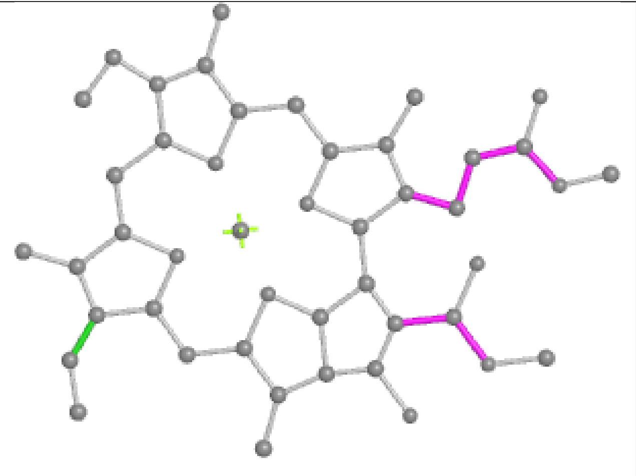
Ligand CLA k 101



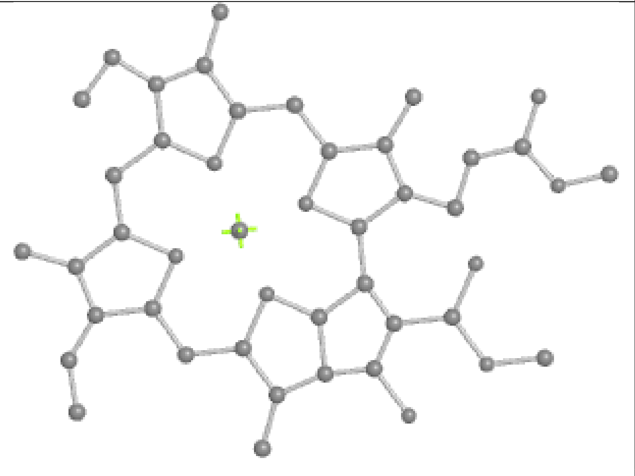
Bond lengths



Bond angles

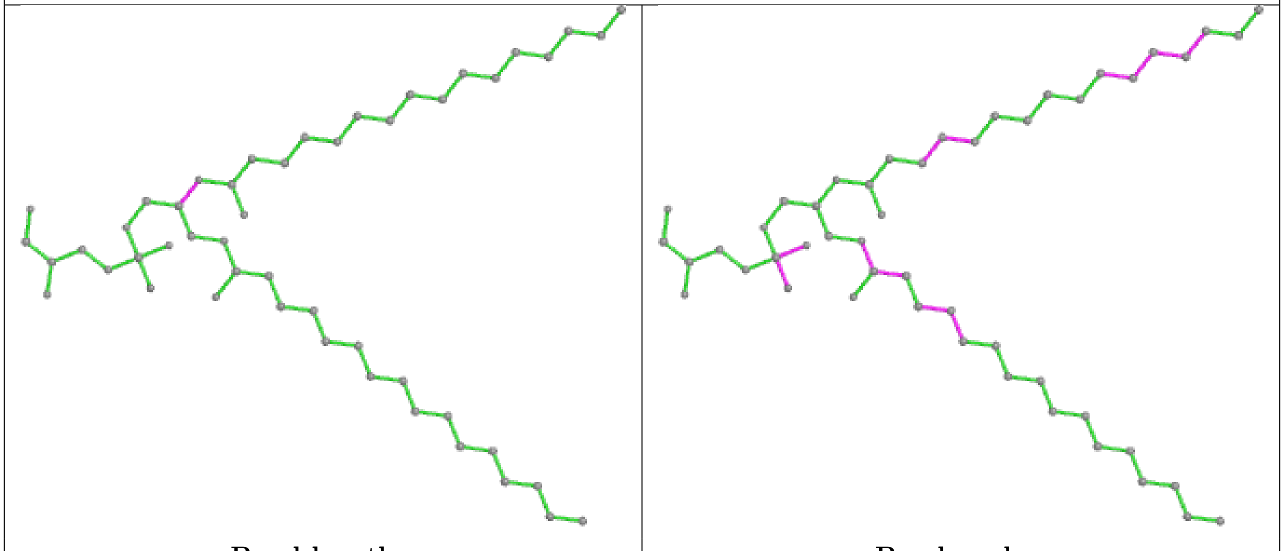


Torsions

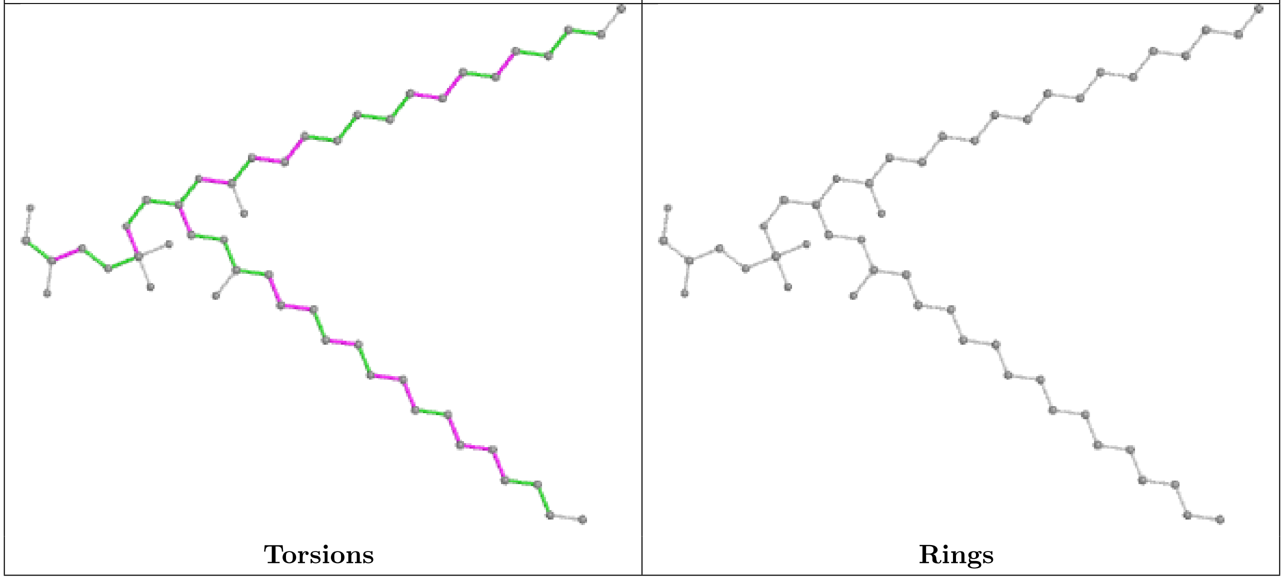


Rings

Ligand LHG a 855

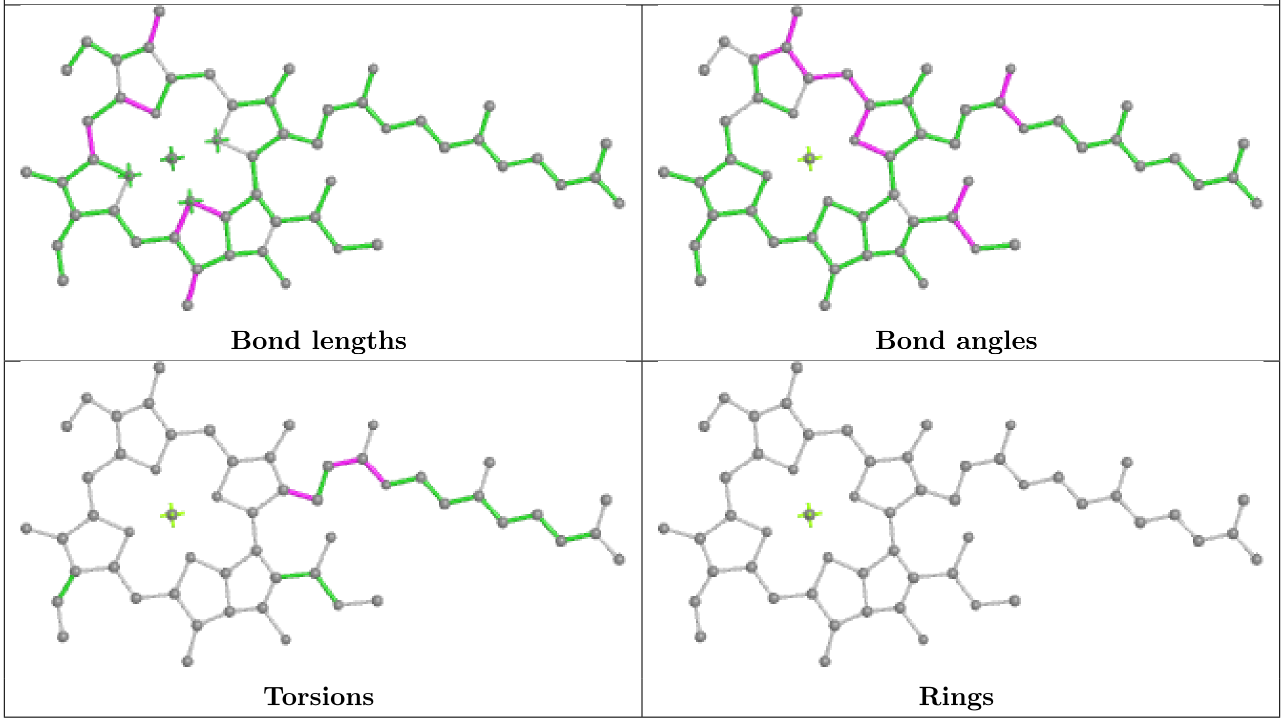


Bond lengths **Bond angles**



Torsions **Rings**

Ligand CLA b 824



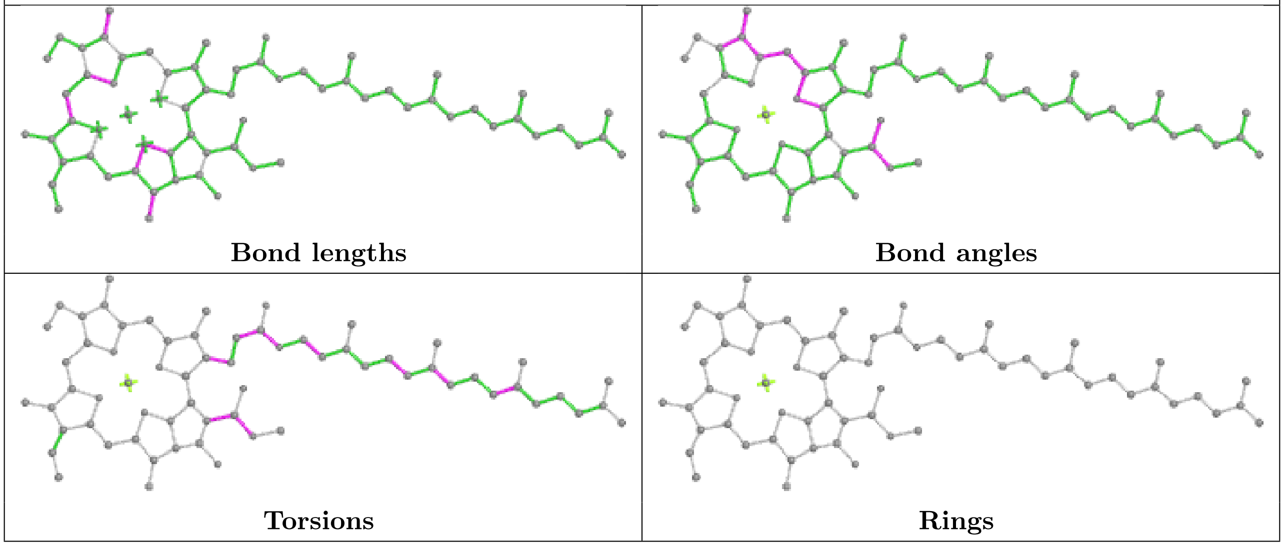
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA A 407



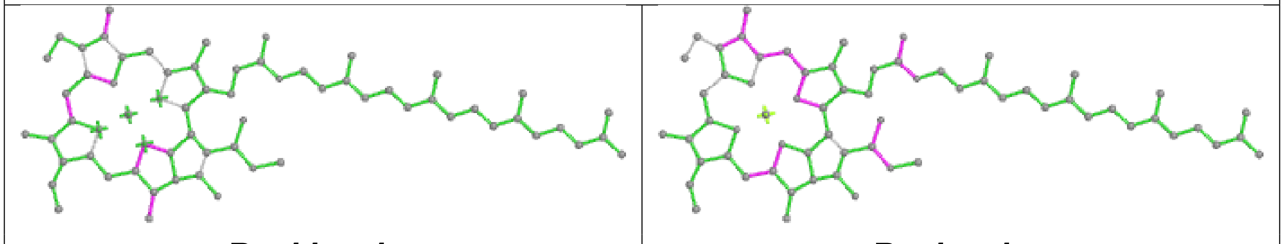
Bond lengths

Bond angles

Torsions

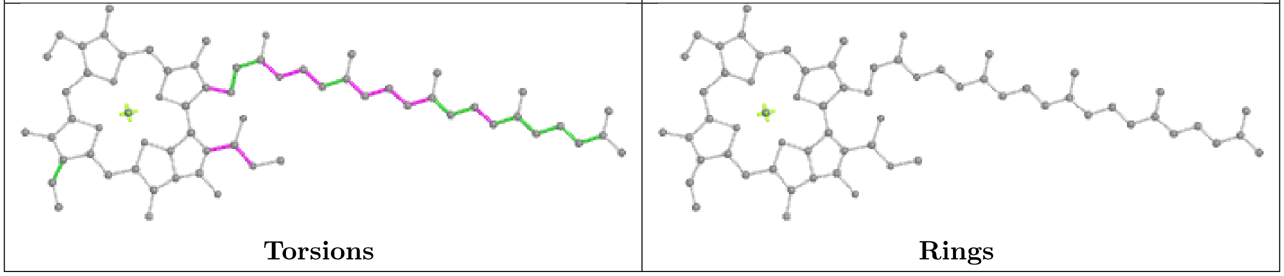
Rings

Ligand CLA b 836



Bond lengths

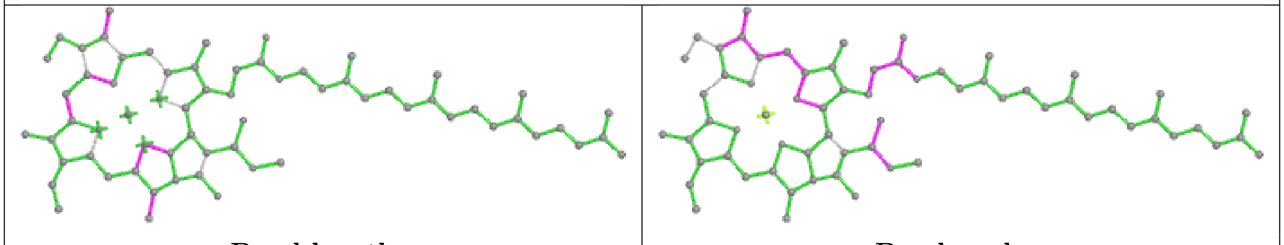
Bond angles



Torsions

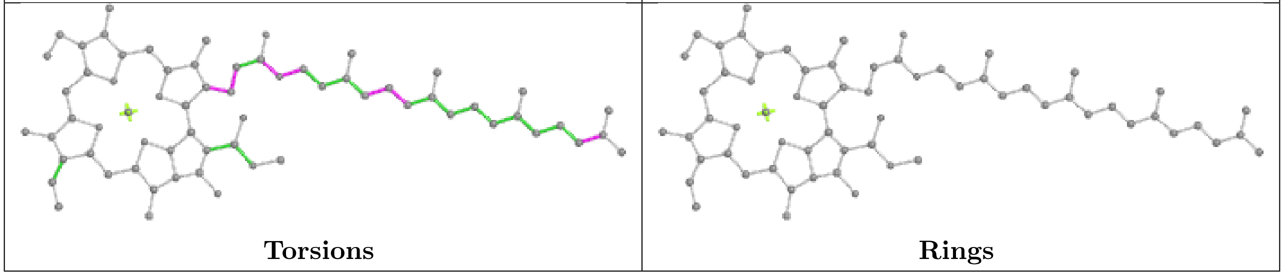
Rings

Ligand CL0 a 801



Bond lengths

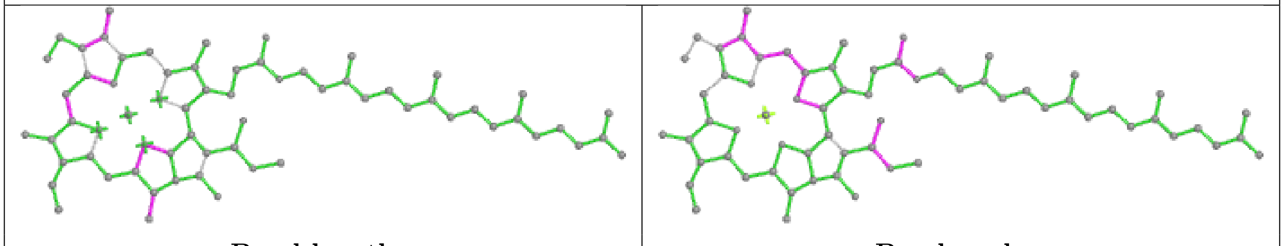
Bond angles



Torsions

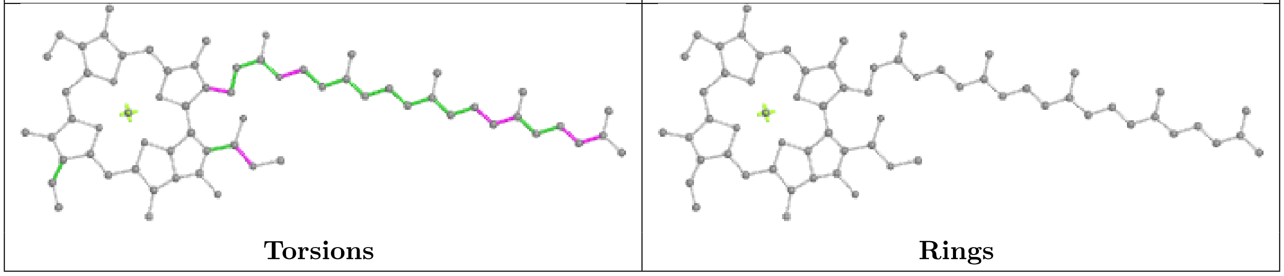
Rings

Ligand CLA b 839



Bond lengths

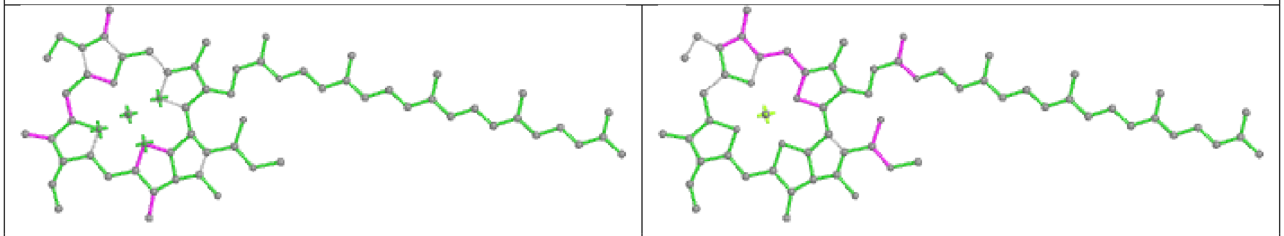
Bond angles



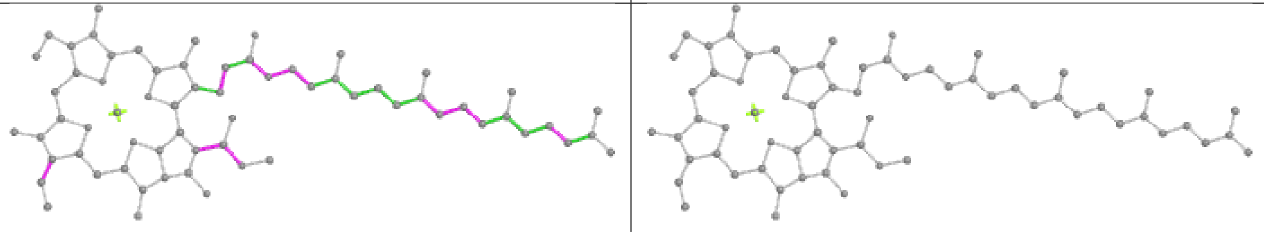
Torsions

Rings

Ligand CLA b 802

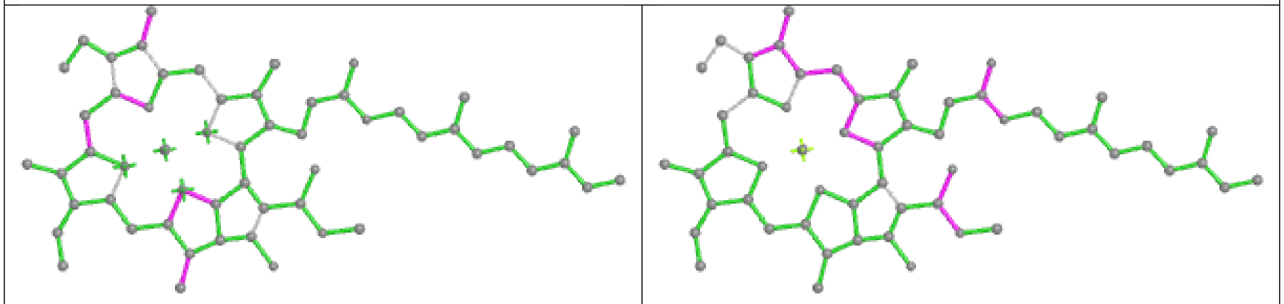


Bond lengths Bond angles

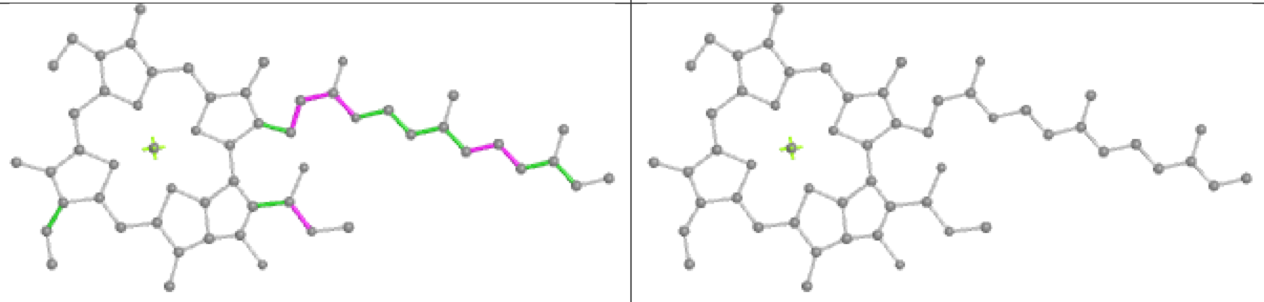


Torsions Rings

Ligand CLA b 809

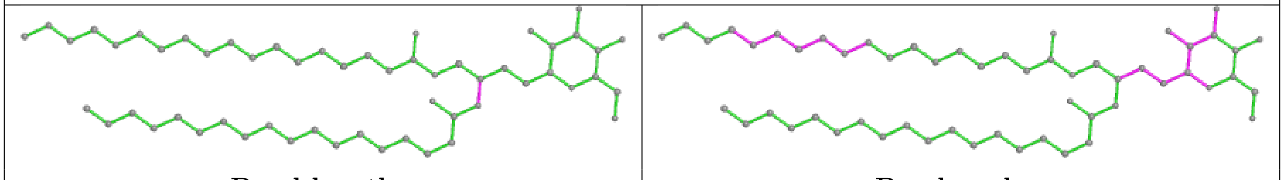


Bond lengths Bond angles

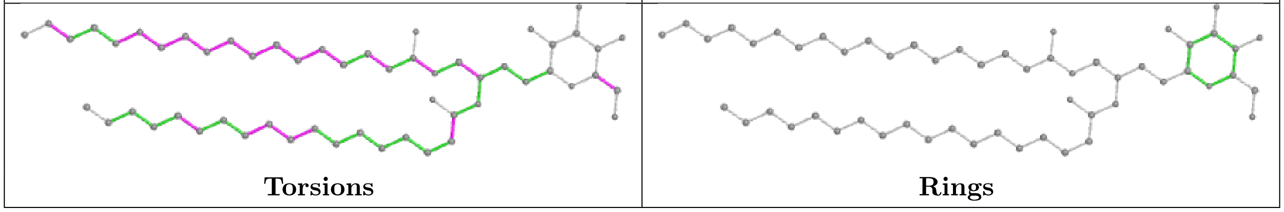


Torsions Rings

Ligand LMG b 848

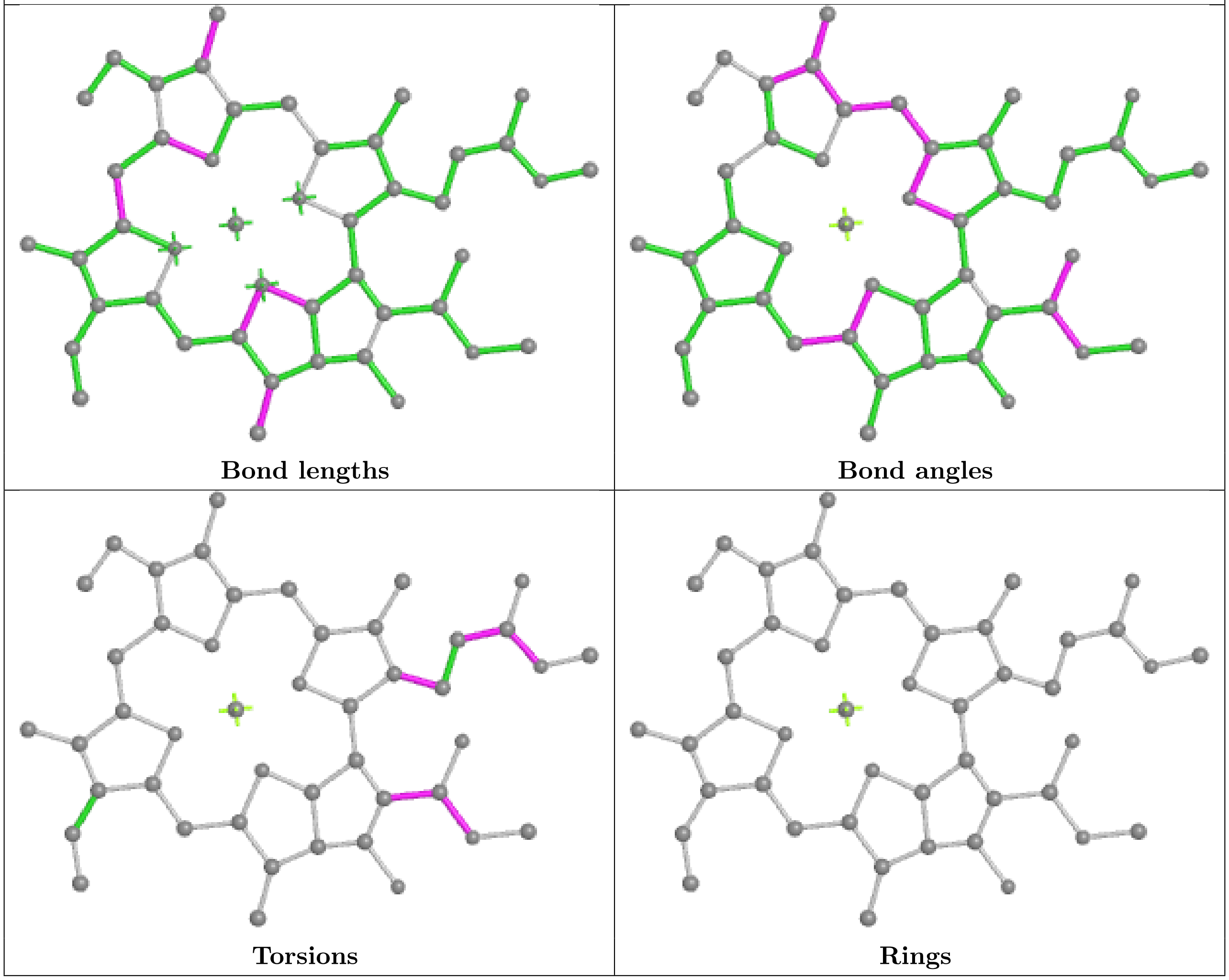


Bond lengths Bond angles



Torsions Rings

Ligand CLA A 403



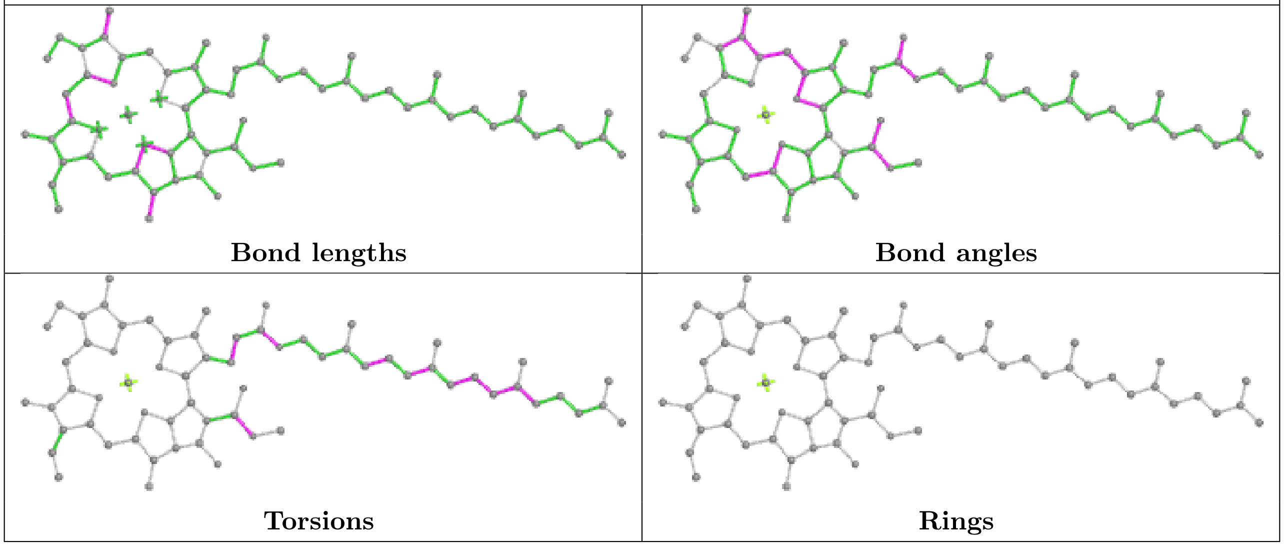
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA b 803



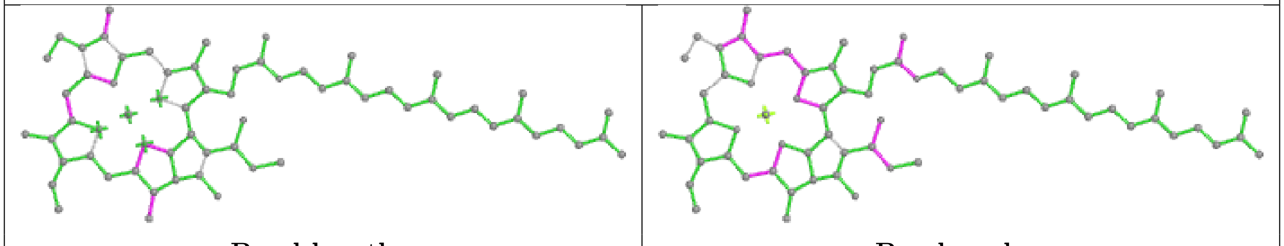
Bond lengths

Bond angles

Torsions

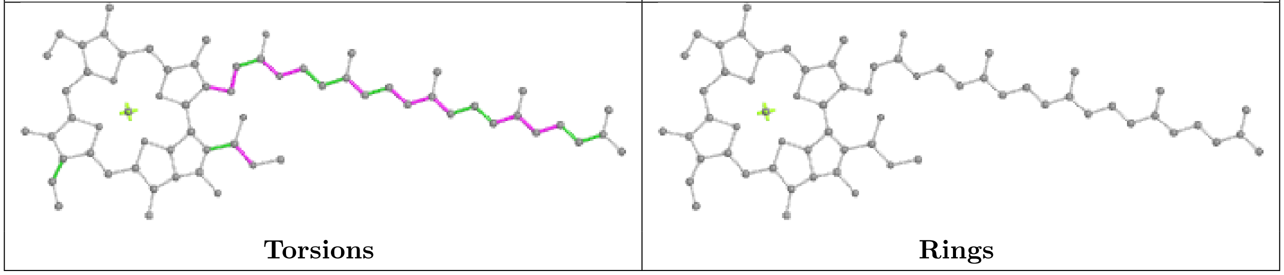
Rings

Ligand CLA b 833



Bond lengths

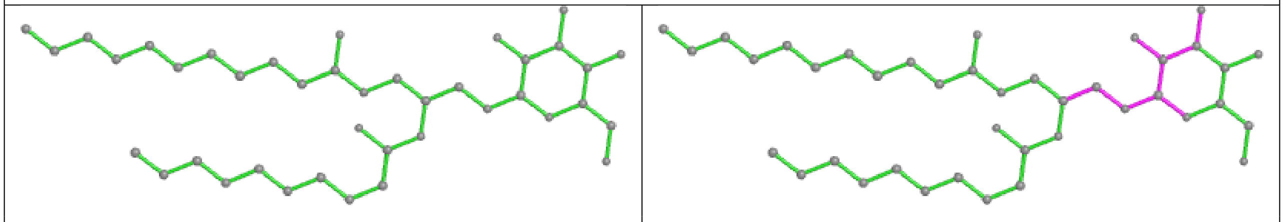
Bond angles



Torsions

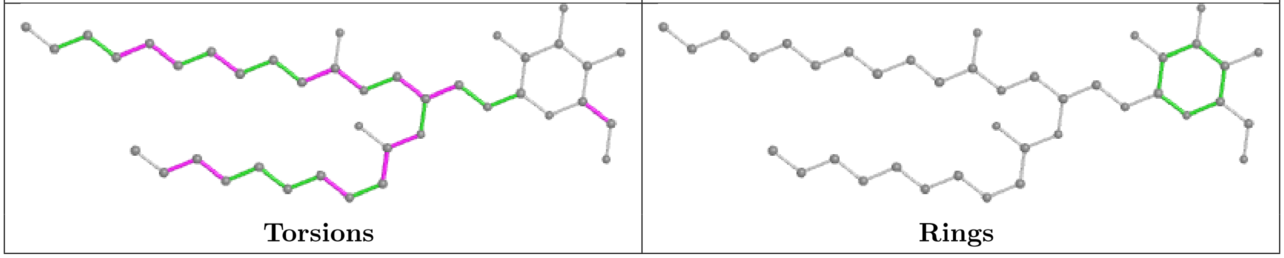
Rings

Ligand LMG a 854



Bond lengths

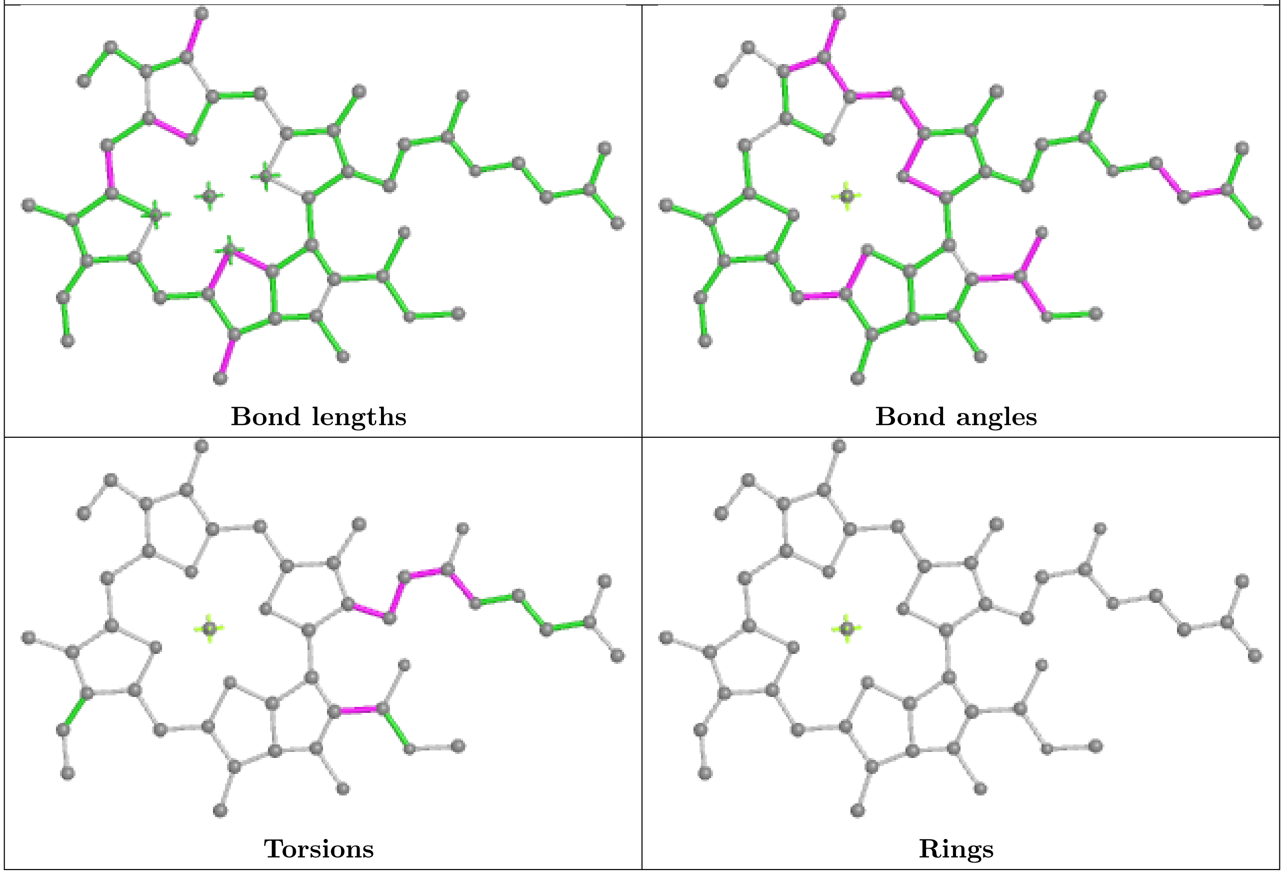
Bond angles



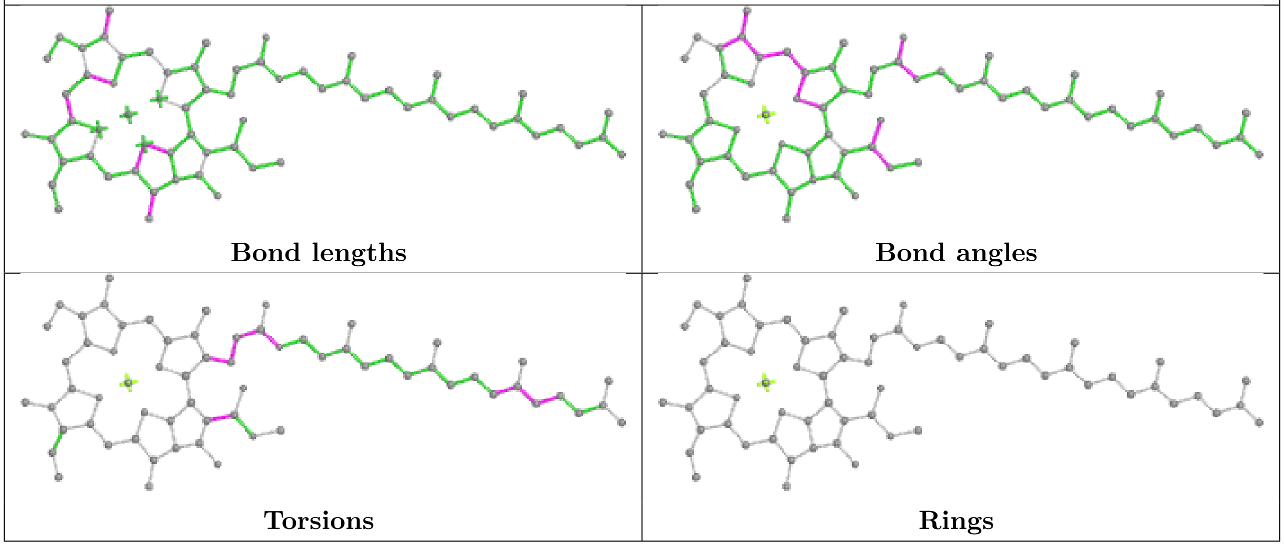
Torsions

Rings

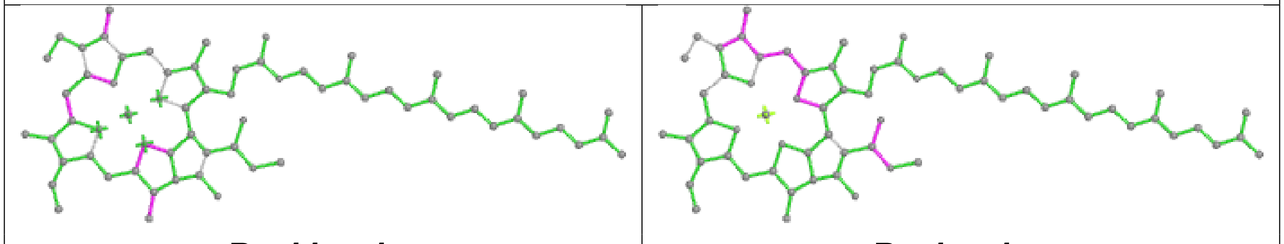
Ligand CLA A 405



Ligand CLA a 812

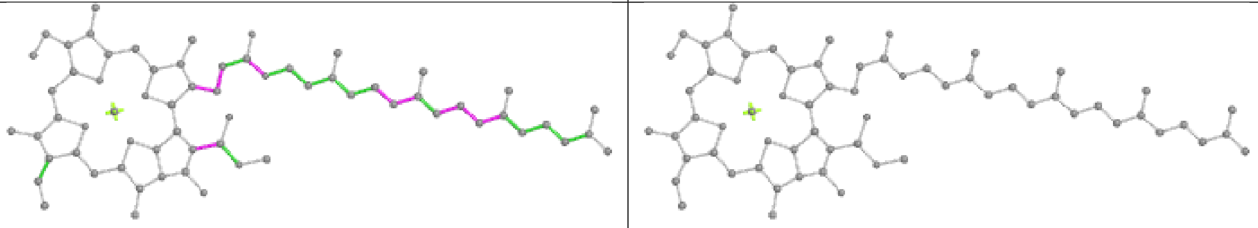


Ligand CLA a 842



Bond lengths

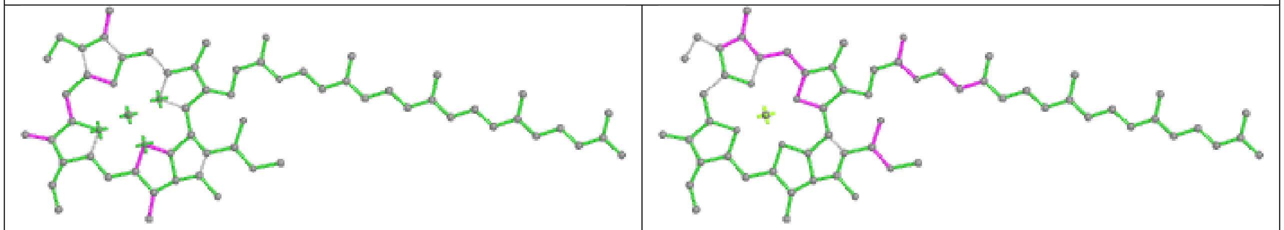
Bond angles



Torsions

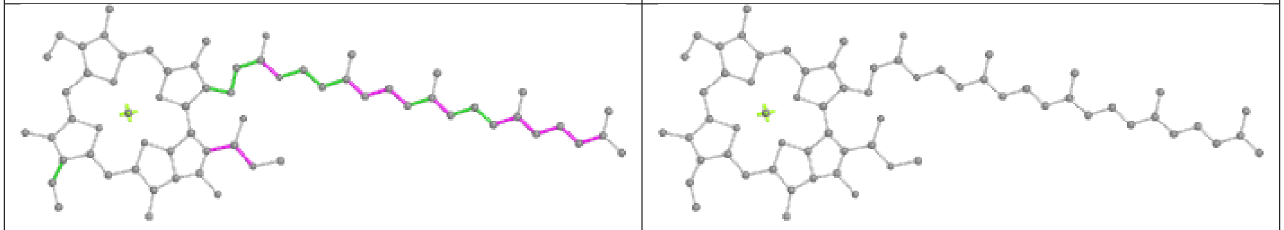
Rings

Ligand CLA b 805



Bond lengths

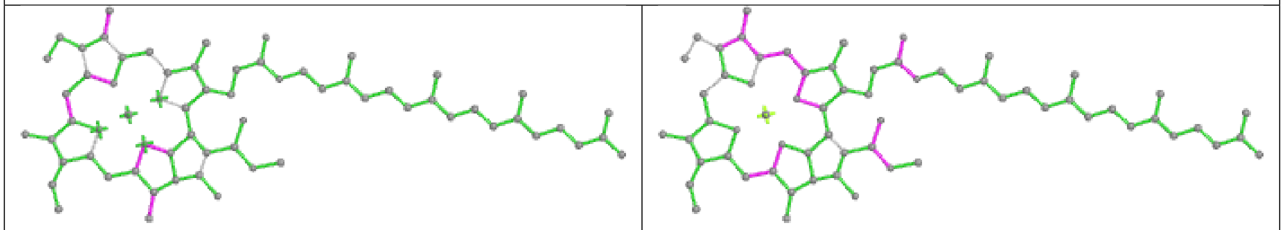
Bond angles



Torsions

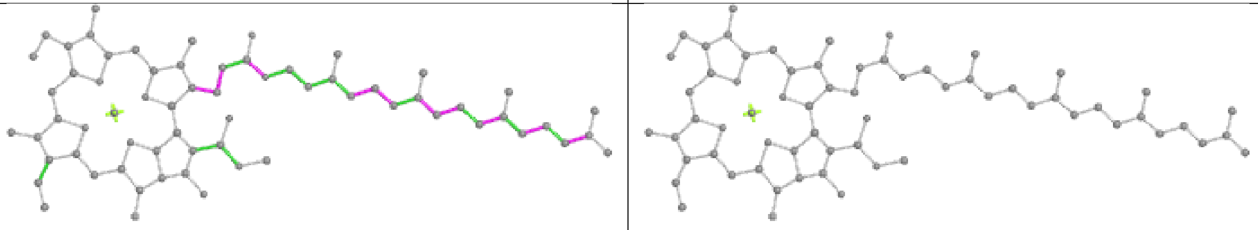
Rings

Ligand CLA a 808



Bond lengths

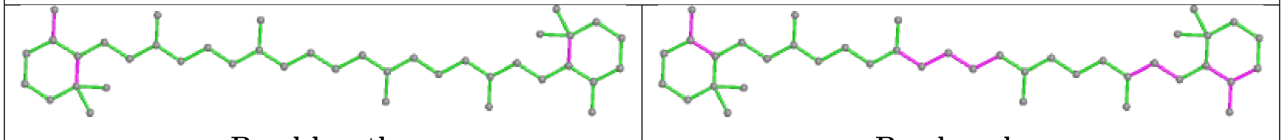
Bond angles



Torsions

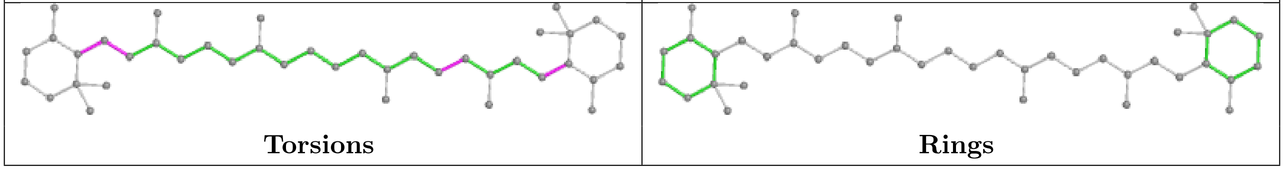
Rings

Ligand BCR a 859



Bond lengths

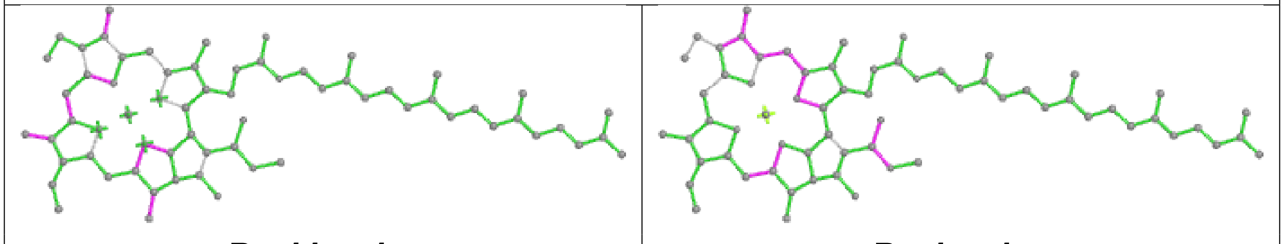
Bond angles



Torsions

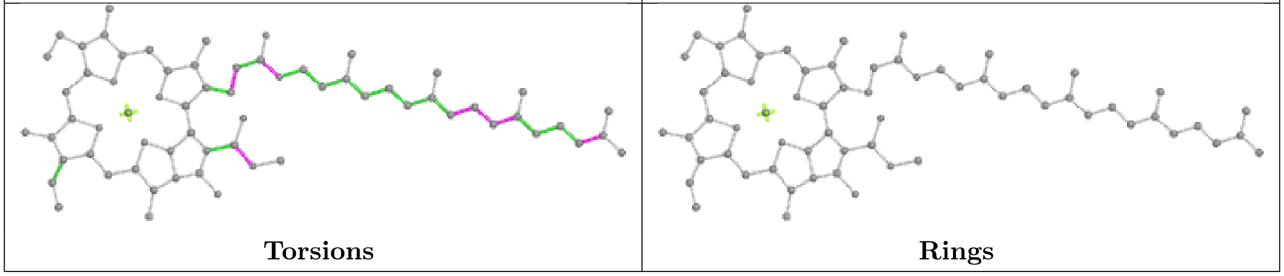
Rings

Ligand CLA b 827



Bond lengths

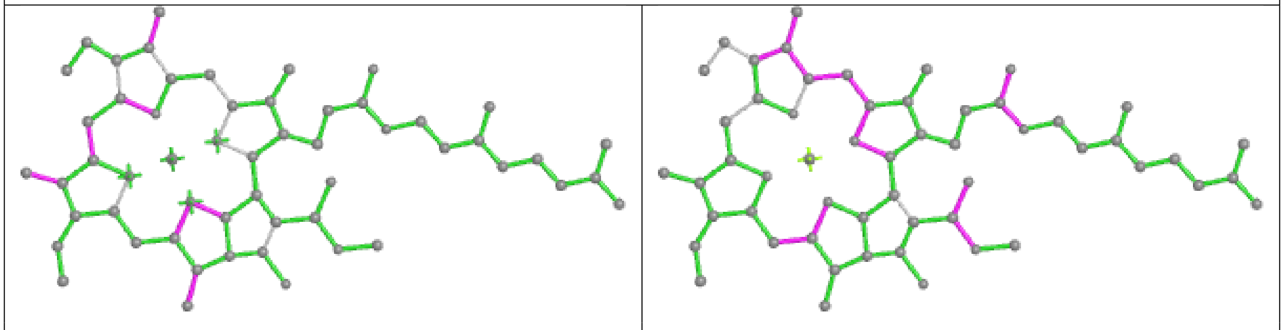
Bond angles



Torsions

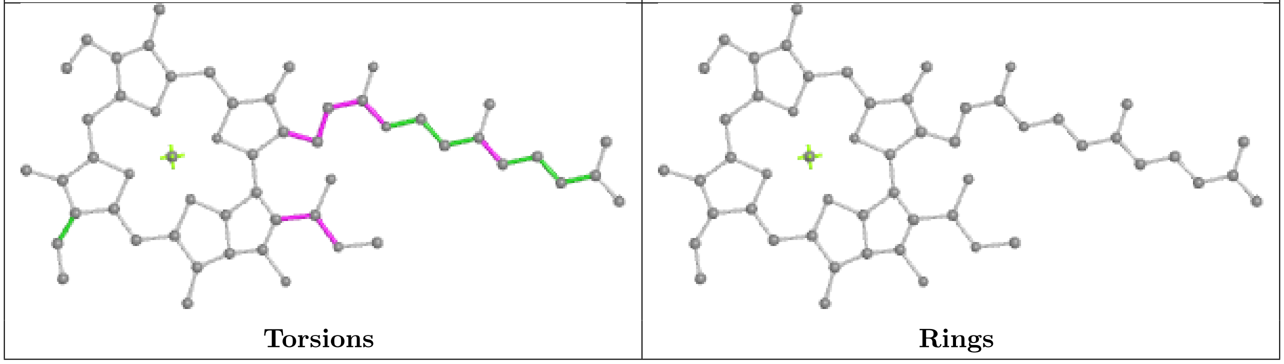
Rings

Ligand CLA D 402



Bond lengths

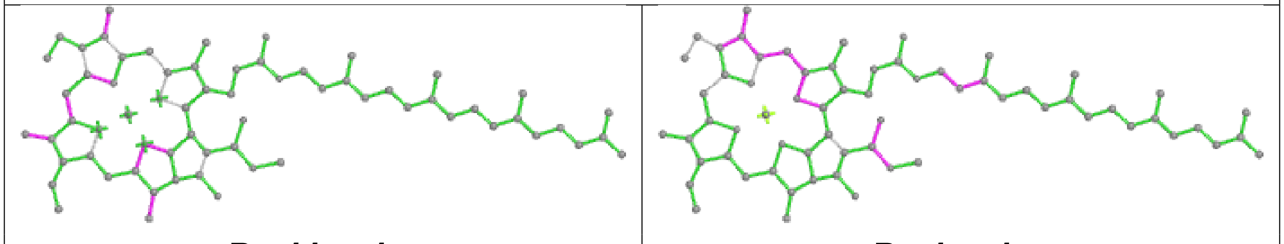
Bond angles



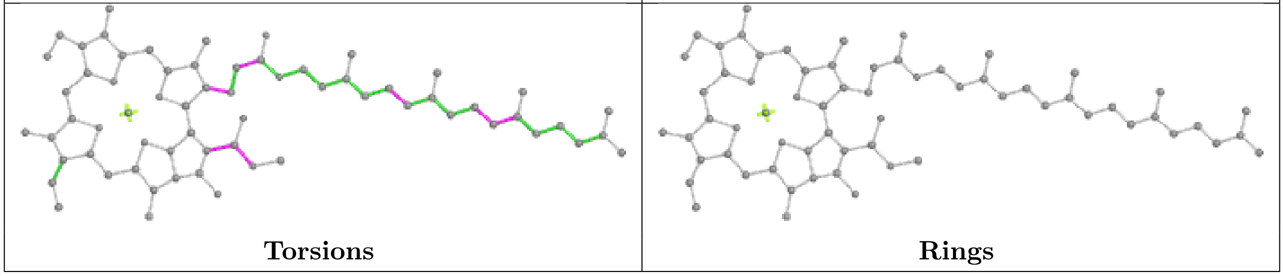
Torsions

Rings

Ligand CLA a 806

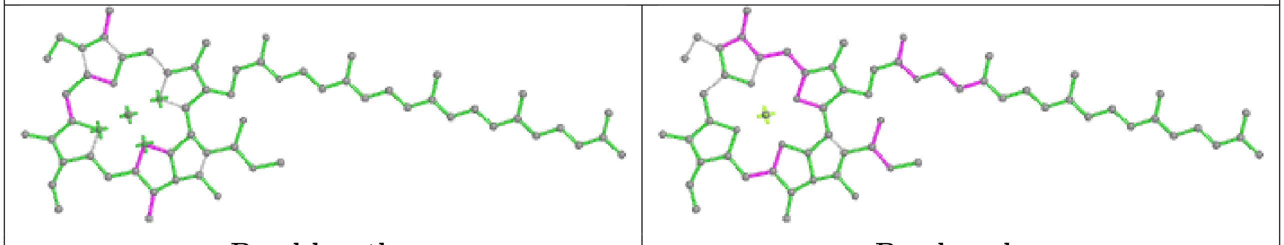


Bond lengths Bond angles

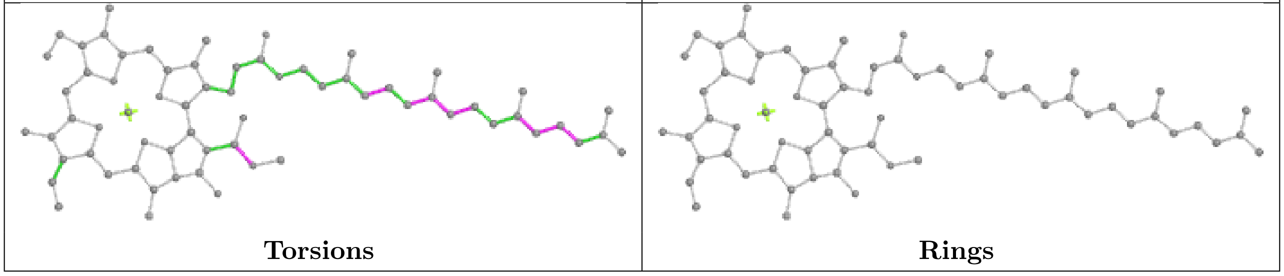


Torsions Rings

Ligand CLA b 813

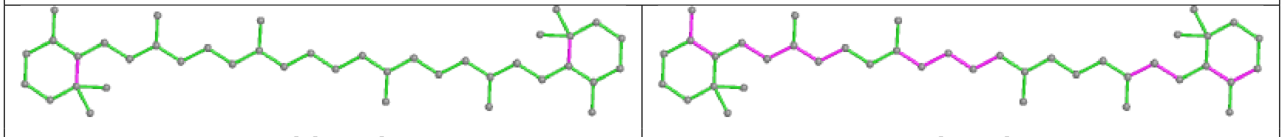


Bond lengths Bond angles

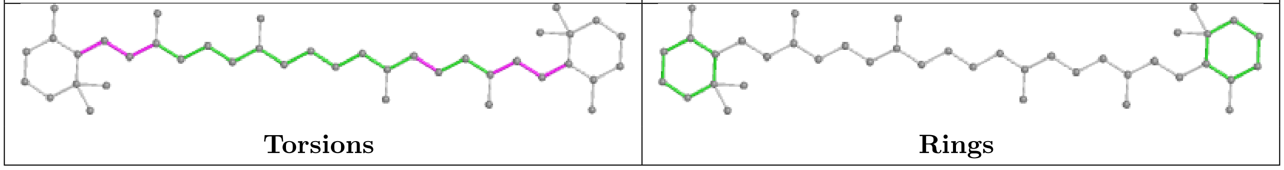


Torsions Rings

Ligand BCR b 842

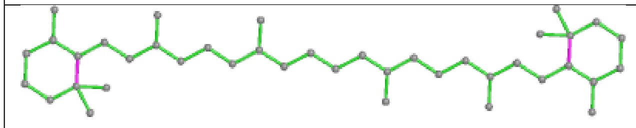


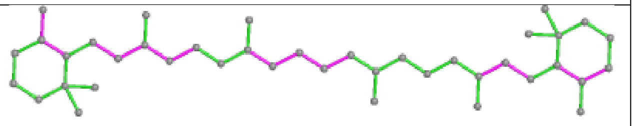
Bond lengths Bond angles

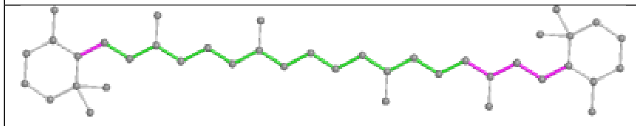


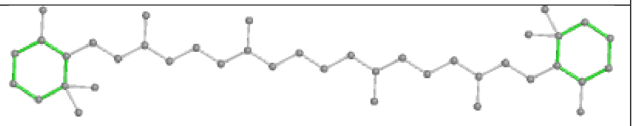
Torsions Rings

Ligand BCR a 849

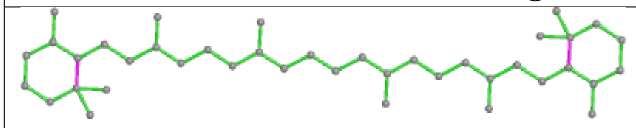

Bond lengths

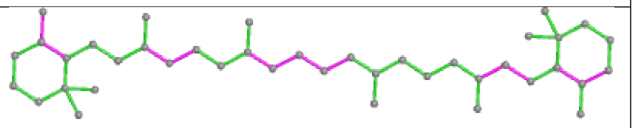

Bond angles

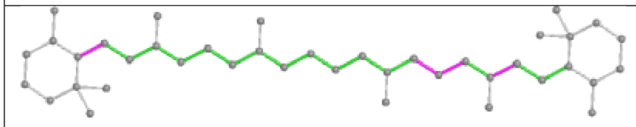

Torsions

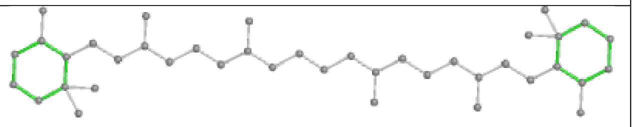

Rings

Ligand BCR b 843

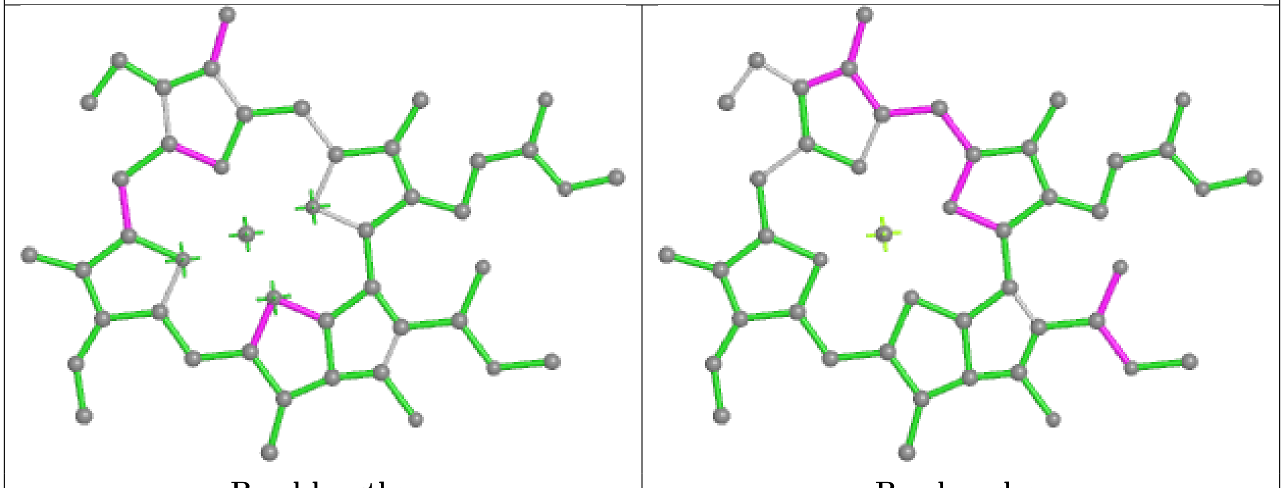

Bond lengths


Bond angles

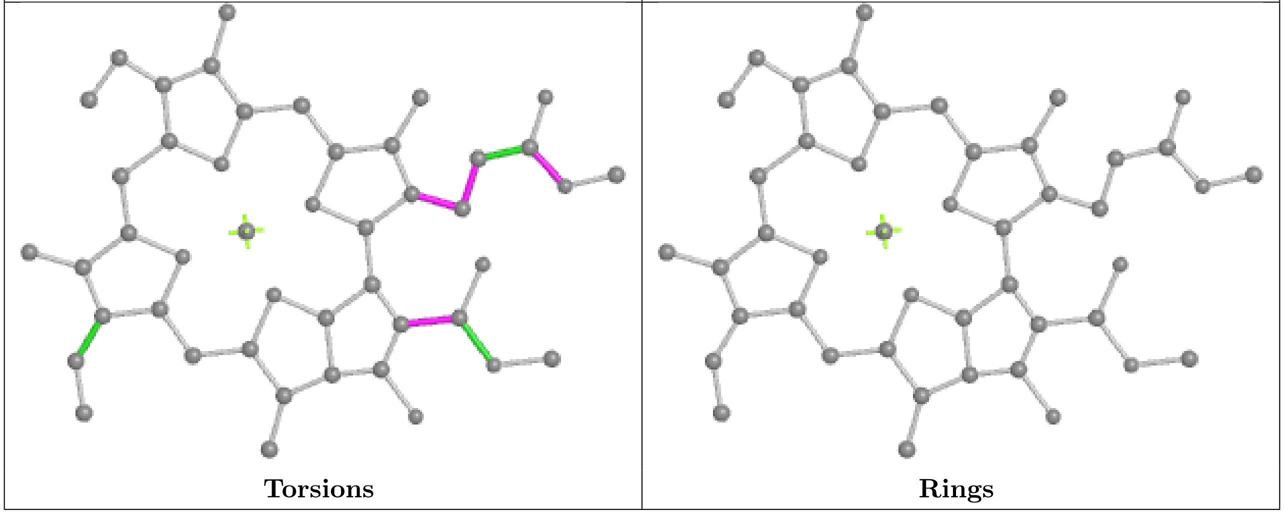

Torsions


Rings

Ligand CLA b 840

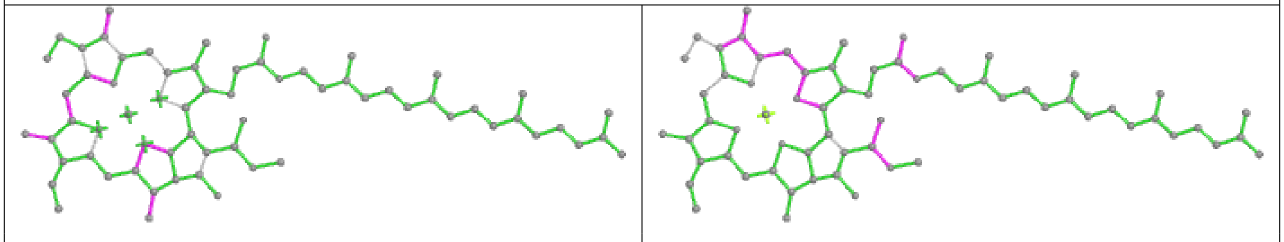


Bond lengths Bond angles

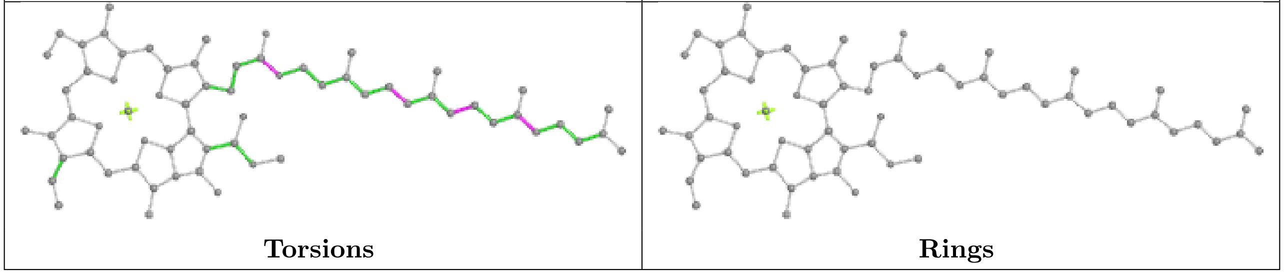


Torsions Rings

Ligand CLA b 825

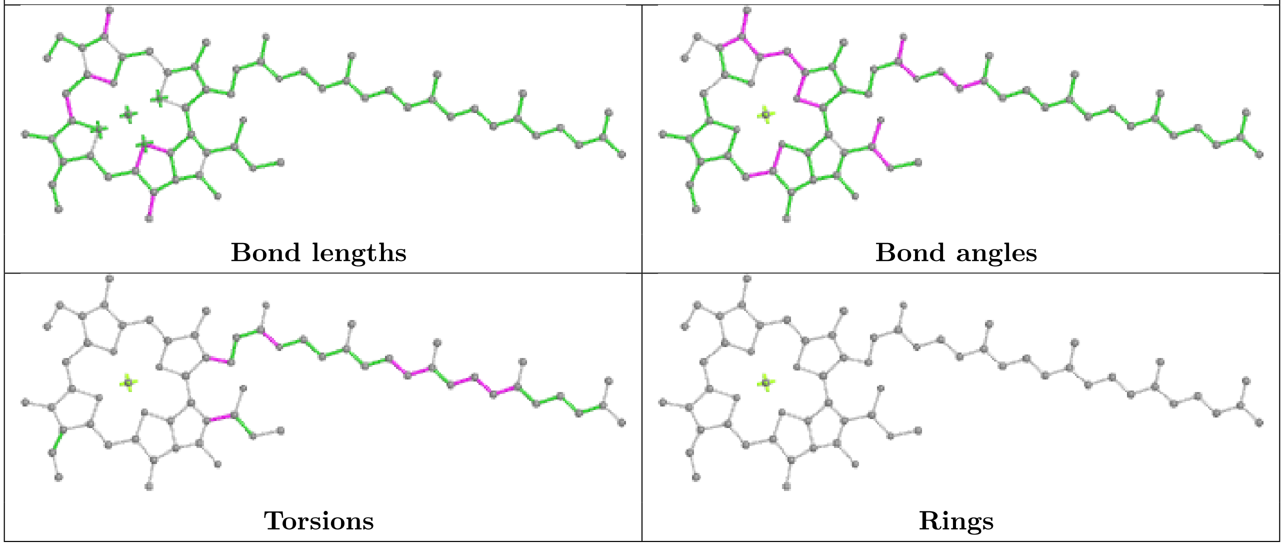


Bond lengths Bond angles

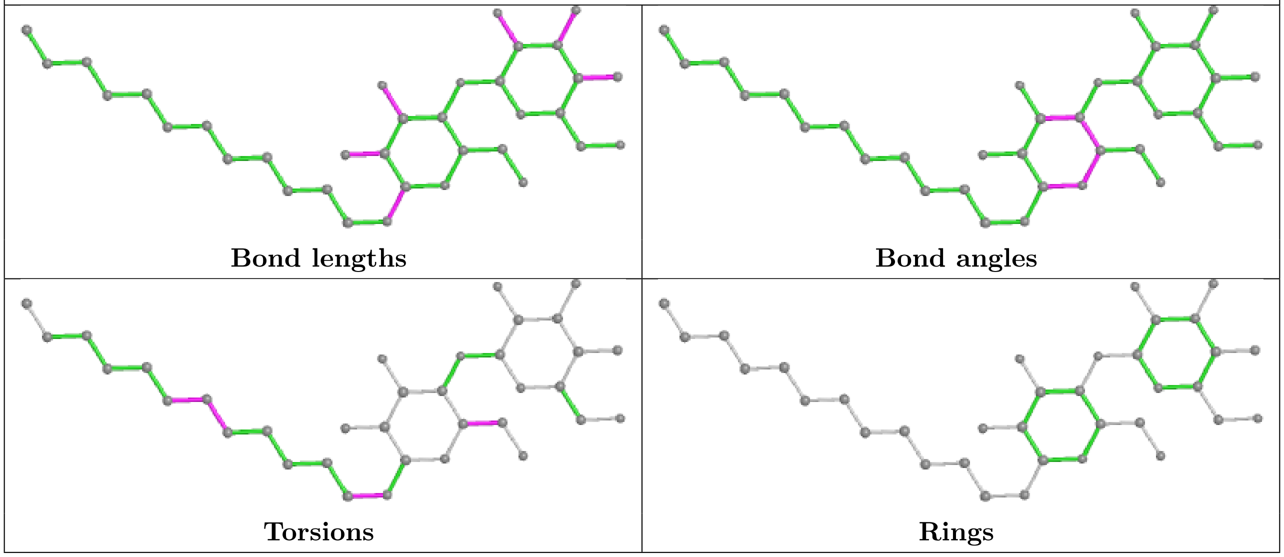


Torsions Rings

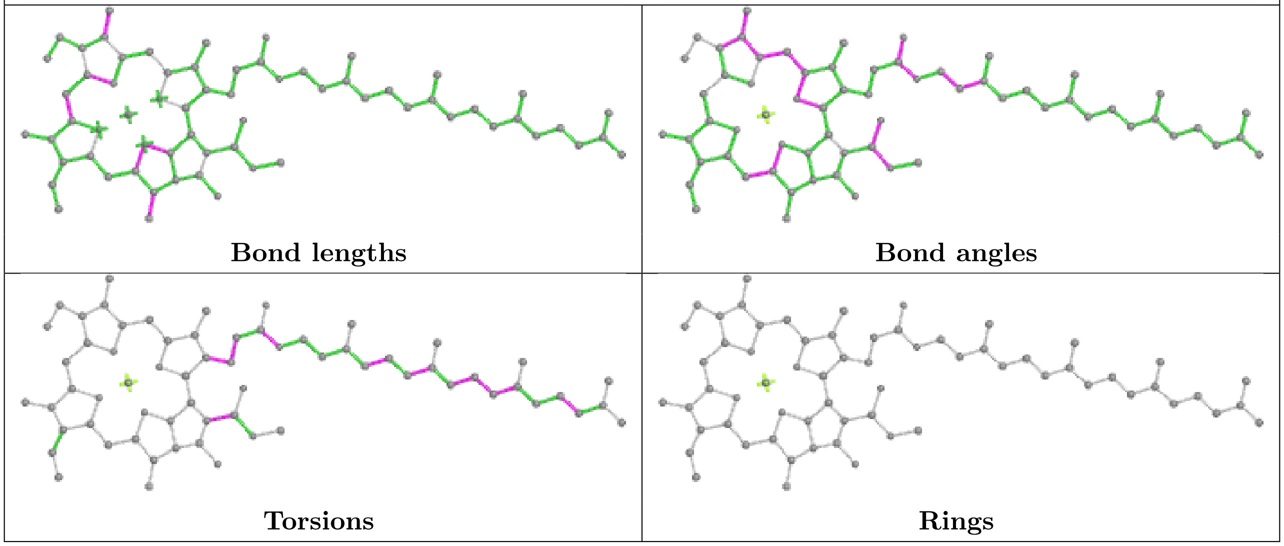
Ligand CLA b 838

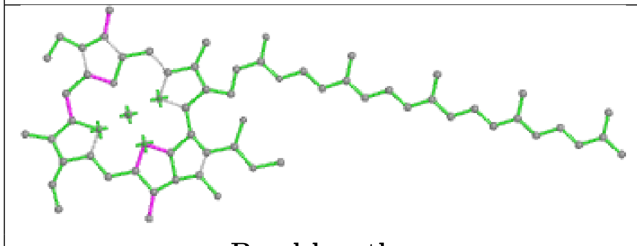
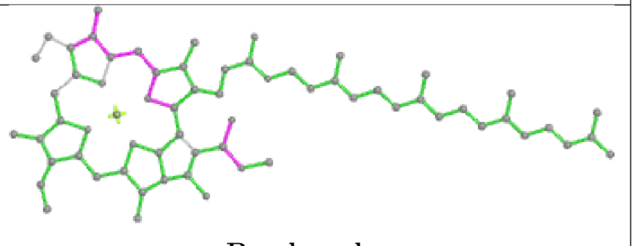
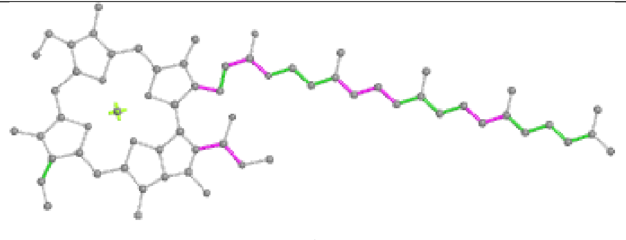
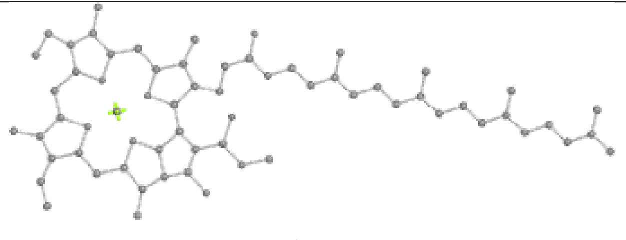

Bond lengths
Bond angles
Torsions
Rings

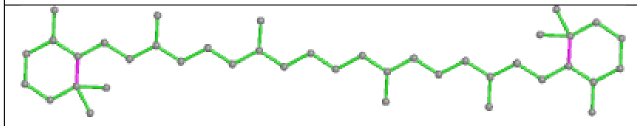
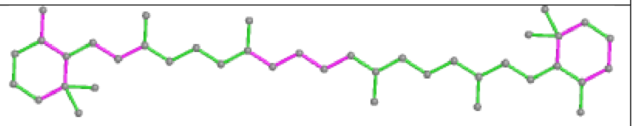
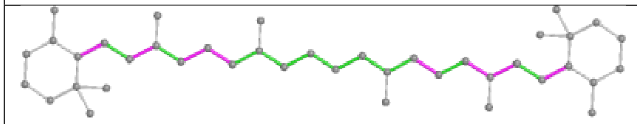
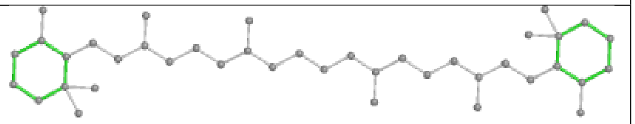
Ligand LMT j 102


Bond lengths
Bond angles
Torsions
Rings

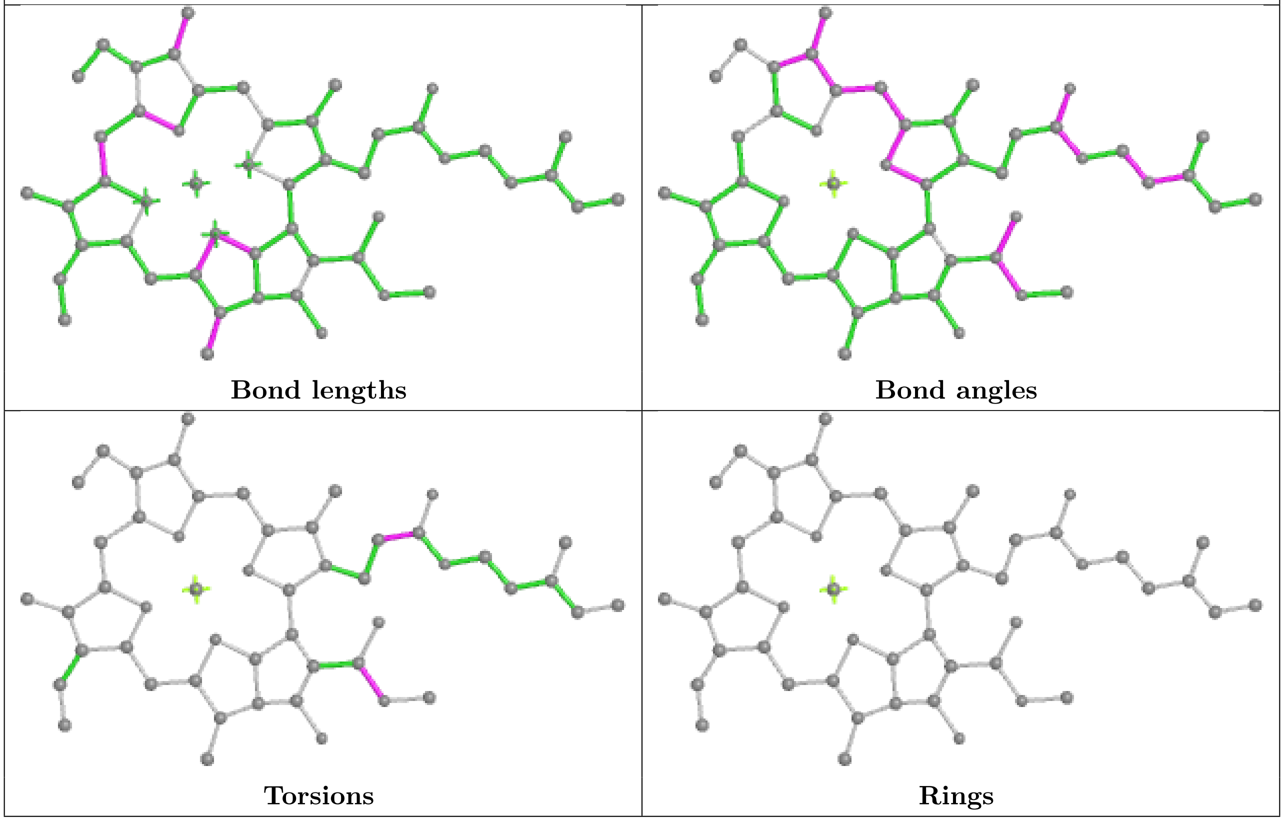
Ligand CLA a 809


Bond lengths
Bond angles
Torsions
Rings

Ligand CLA b 828	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR i 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA a 810



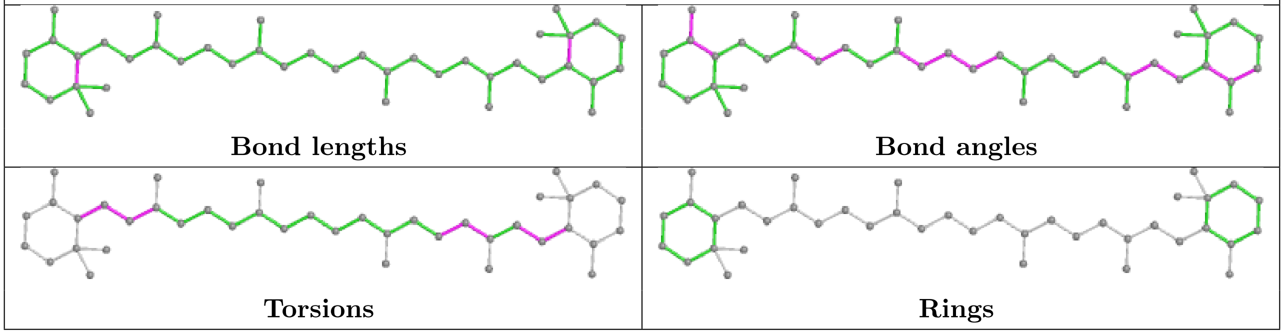
Bond lengths

Bond angles

Torsions

Rings

Ligand BCR A 406



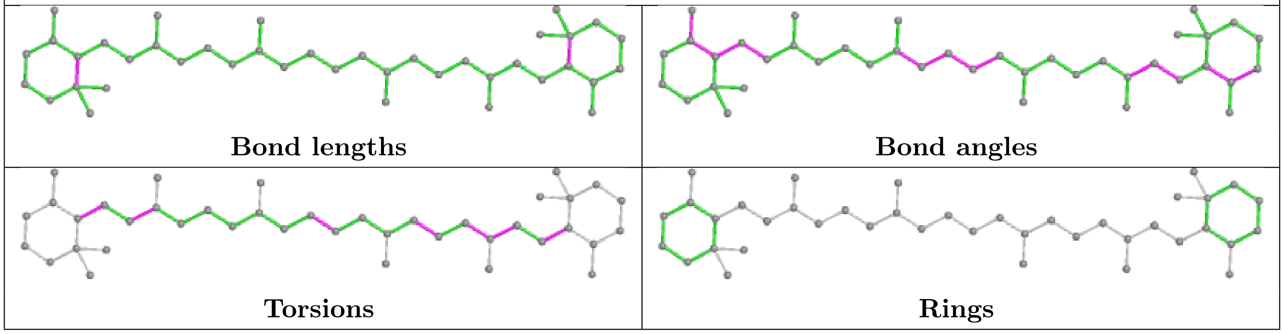
Bond lengths

Bond angles

Torsions

Rings

Ligand BCR a 850



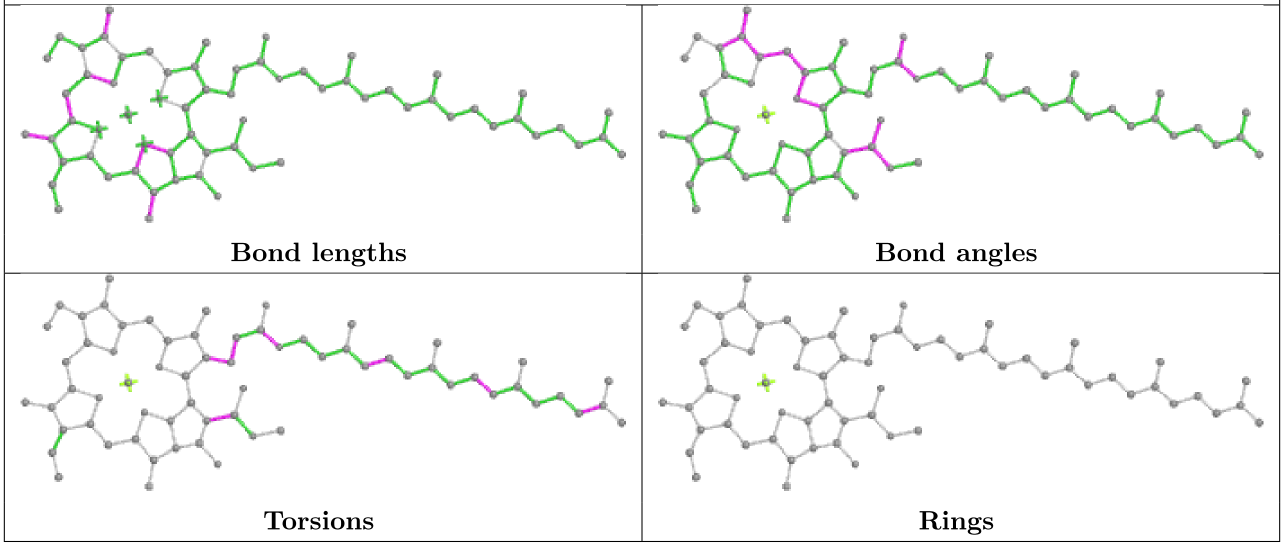
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA a 803



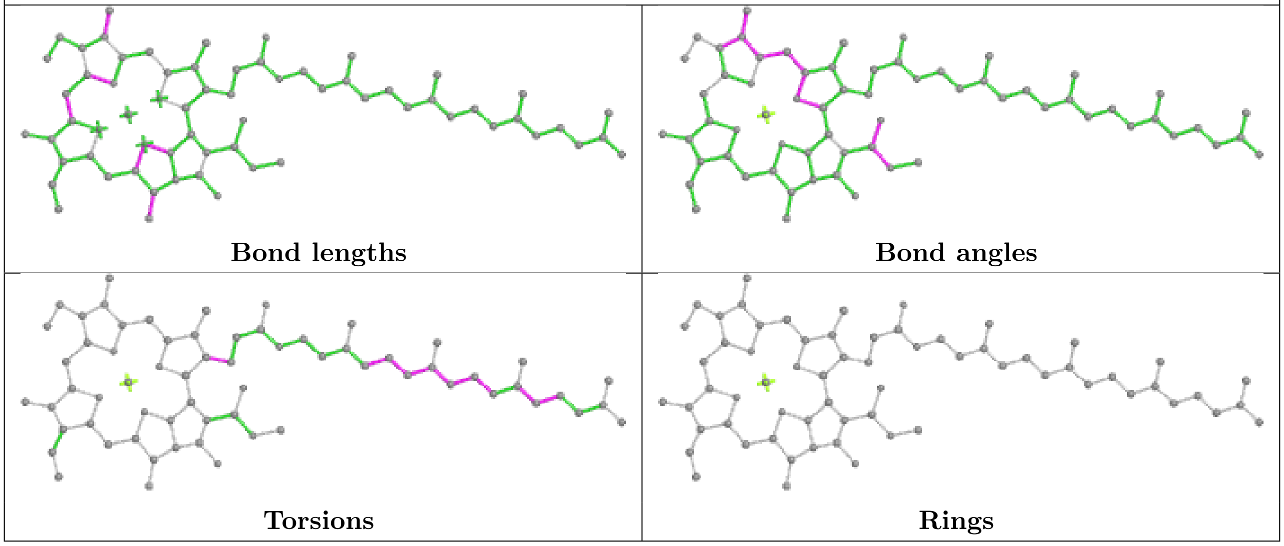
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA b 817



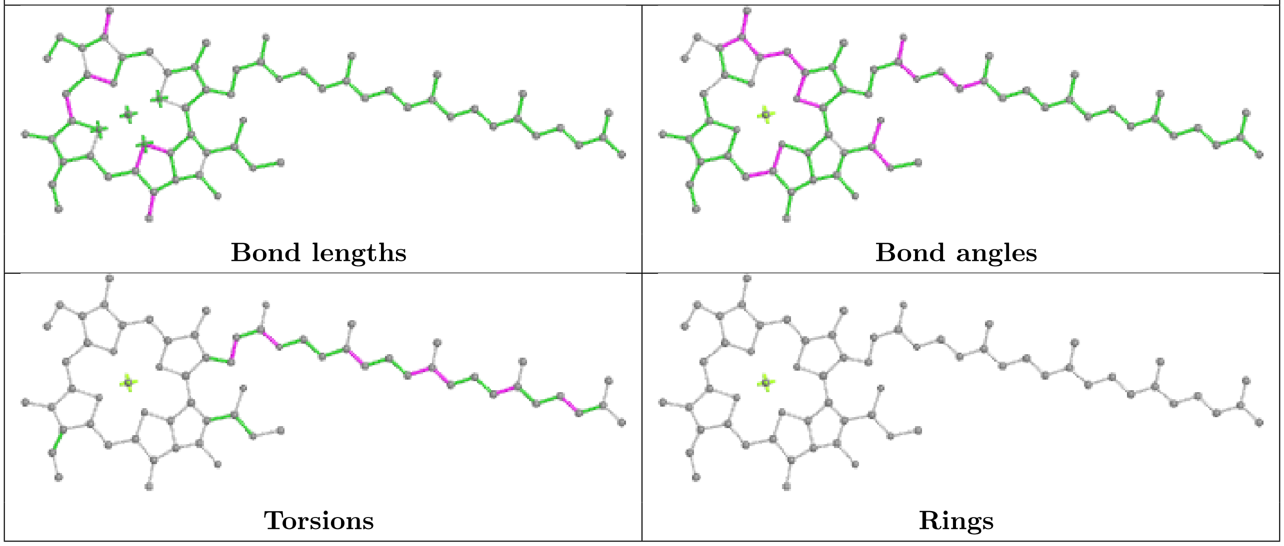
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA b 816



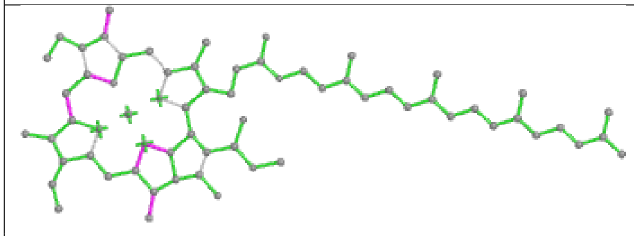
Bond lengths

Bond angles

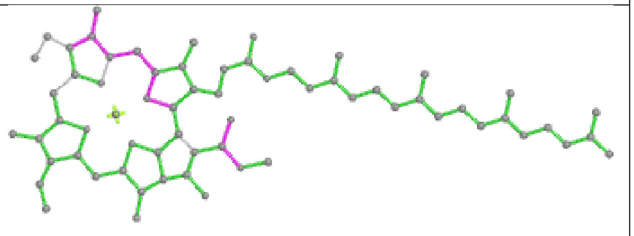
Torsions

Rings

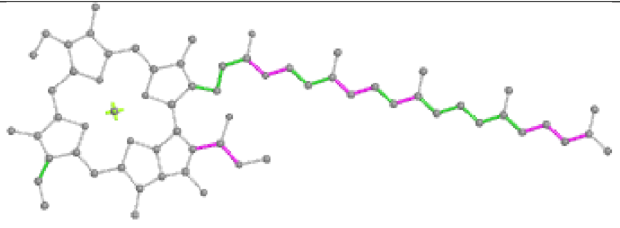
Ligand CLA f 201



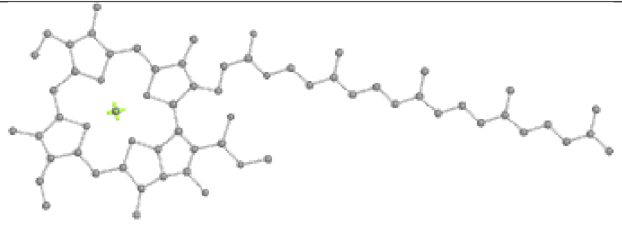
Bond lengths



Bond angles

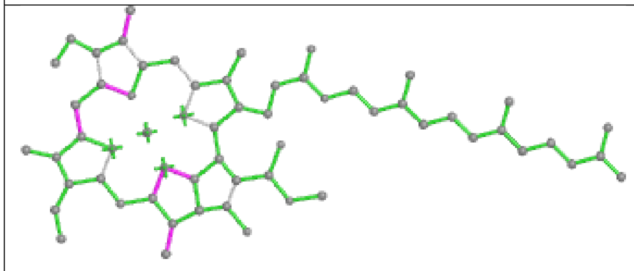


Torsions

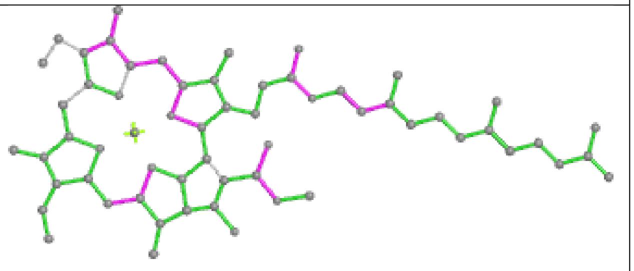


Rings

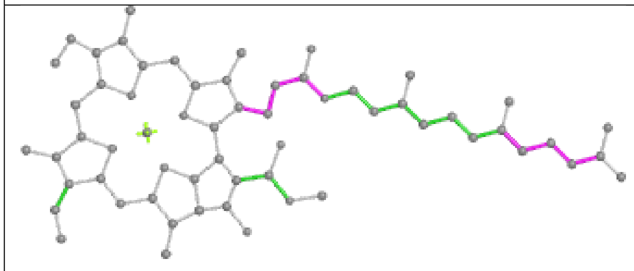
Ligand CLA a 833



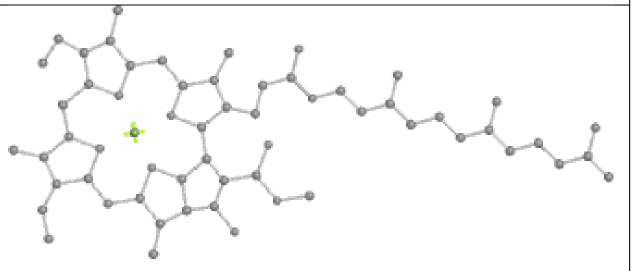
Bond lengths



Bond angles

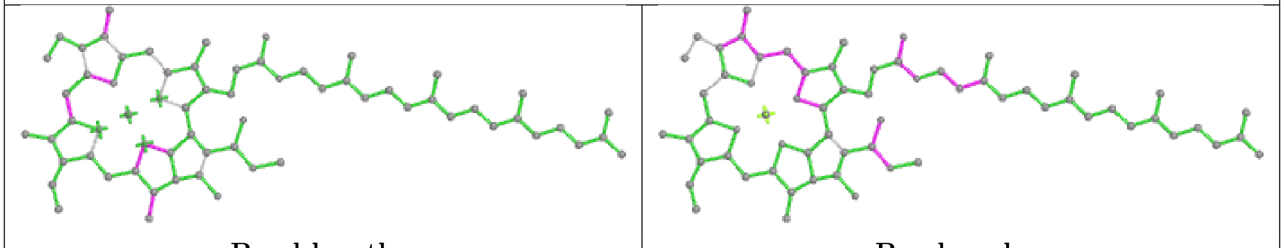


Torsions



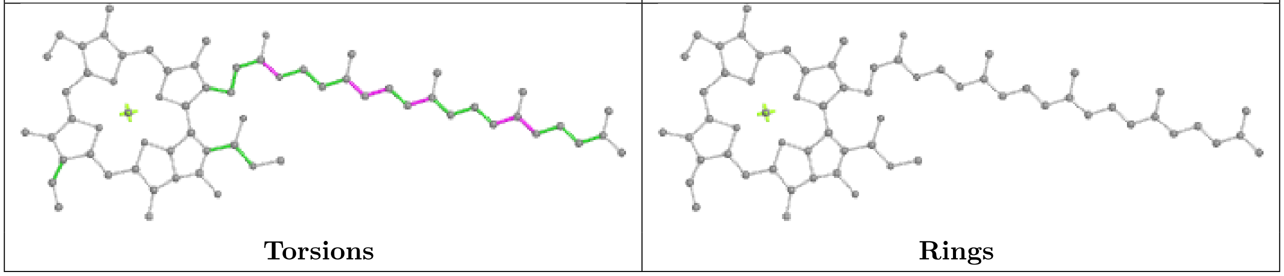
Rings

Ligand CLA a 836



Bond lengths

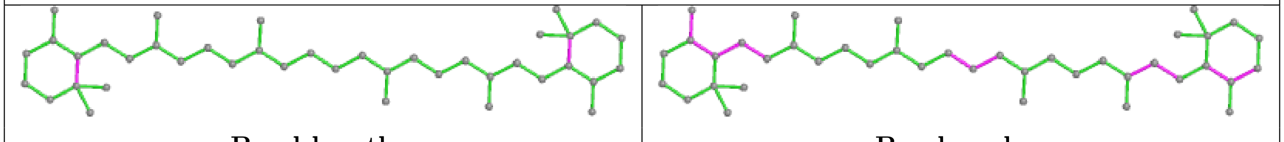
Bond angles



Torsions

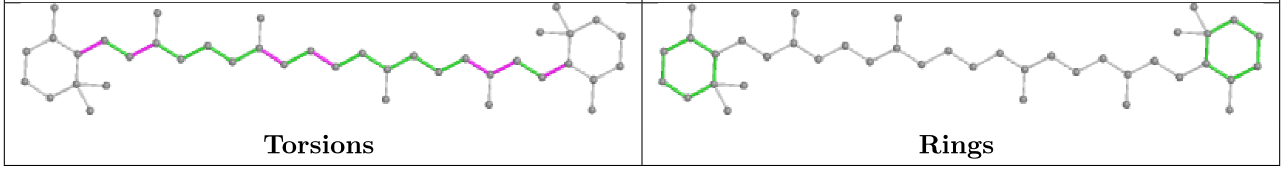
Rings

Ligand BCR f 202



Bond lengths

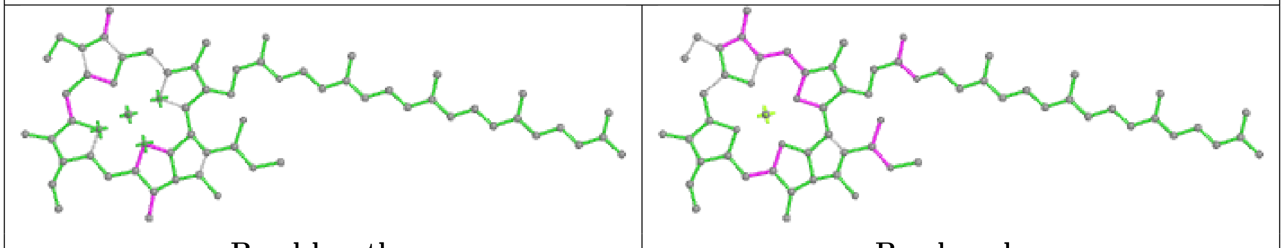
Bond angles



Torsions

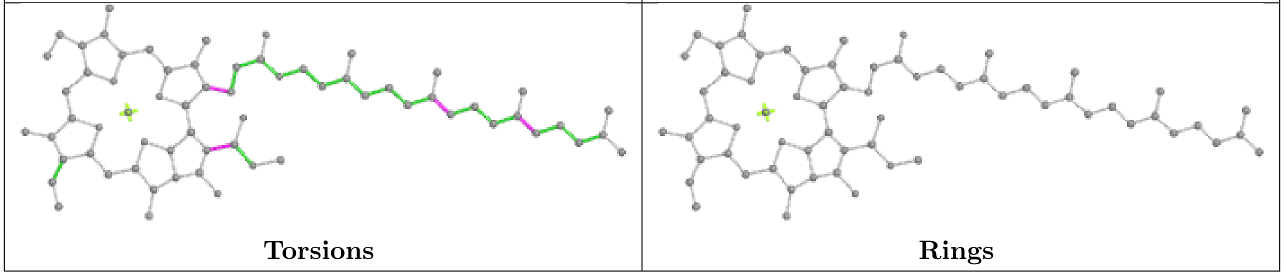
Rings

Ligand CLA a 827



Bond lengths

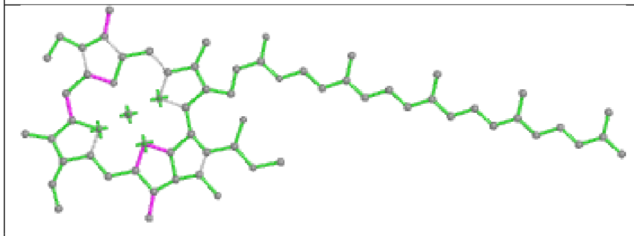
Bond angles



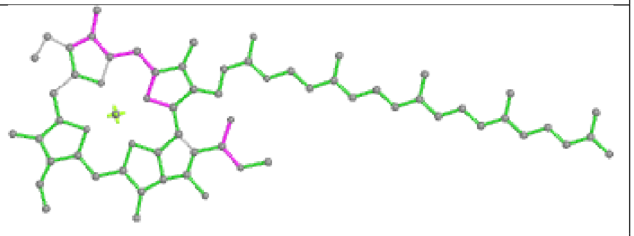
Torsions

Rings

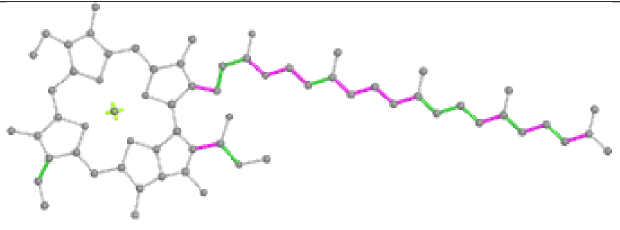
Ligand CLA a 857



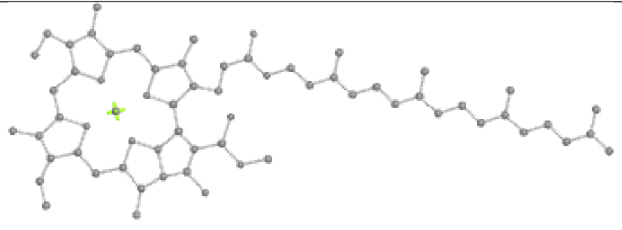
Bond lengths



Bond angles

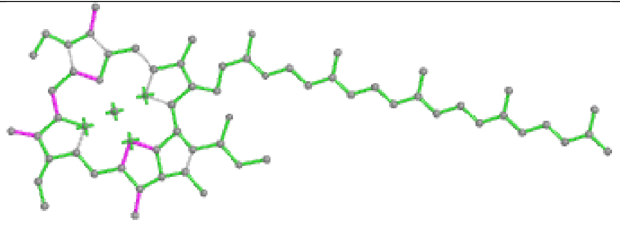


Torsions

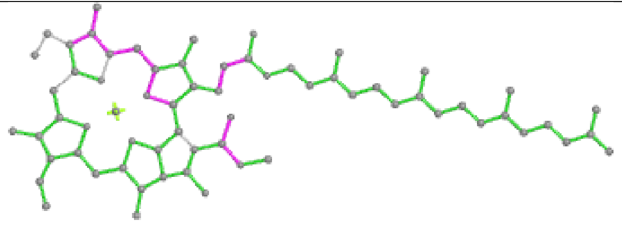


Rings

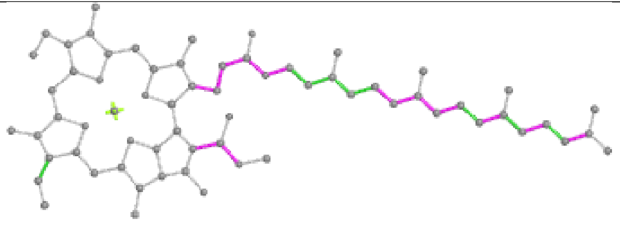
Ligand CLA a 821



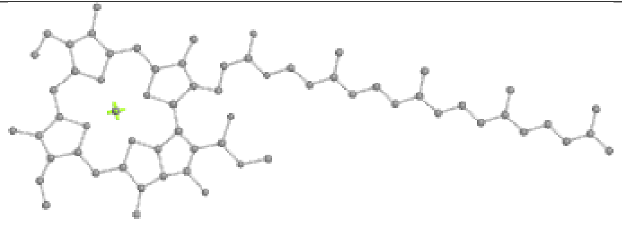
Bond lengths



Bond angles

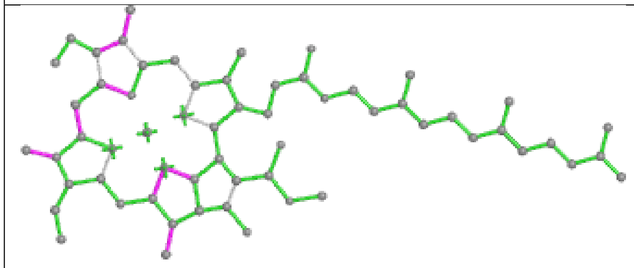


Torsions

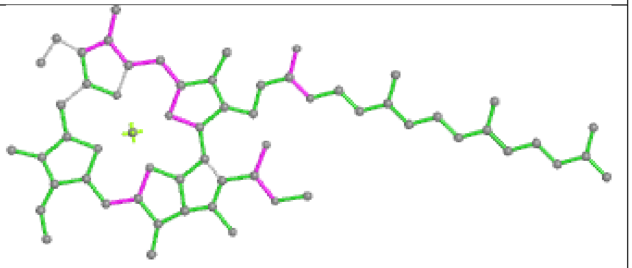


Rings

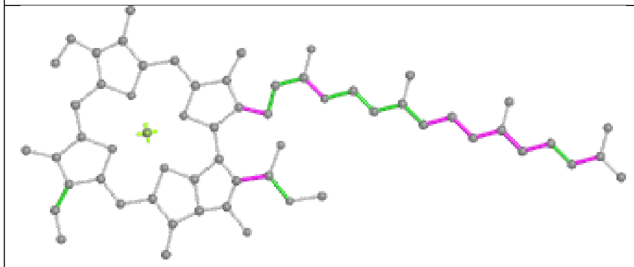
Ligand CLA a 813



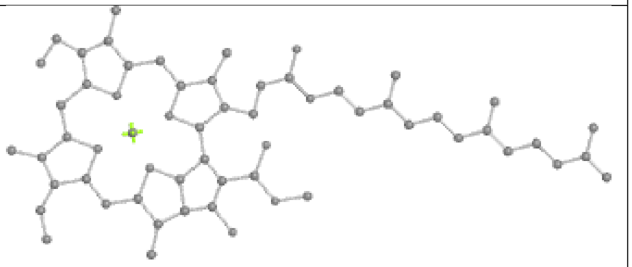
Bond lengths



Bond angles

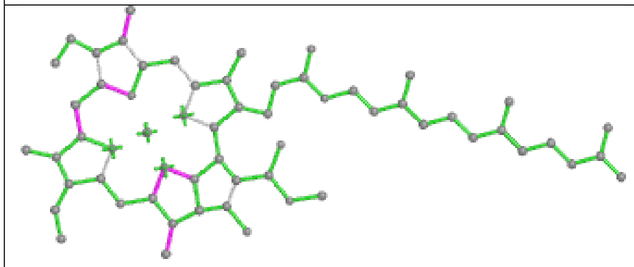


Torsions

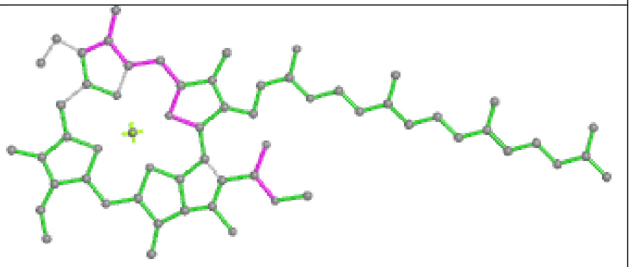


Rings

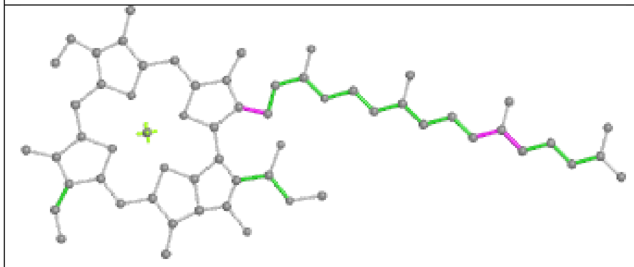
Ligand CLA b 818



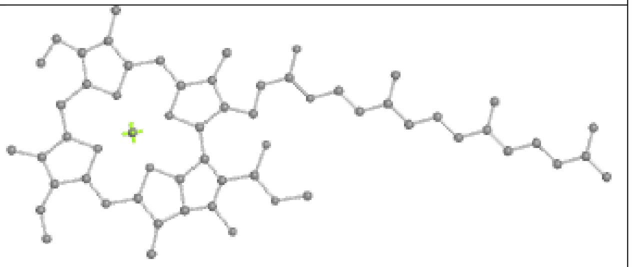
Bond lengths



Bond angles

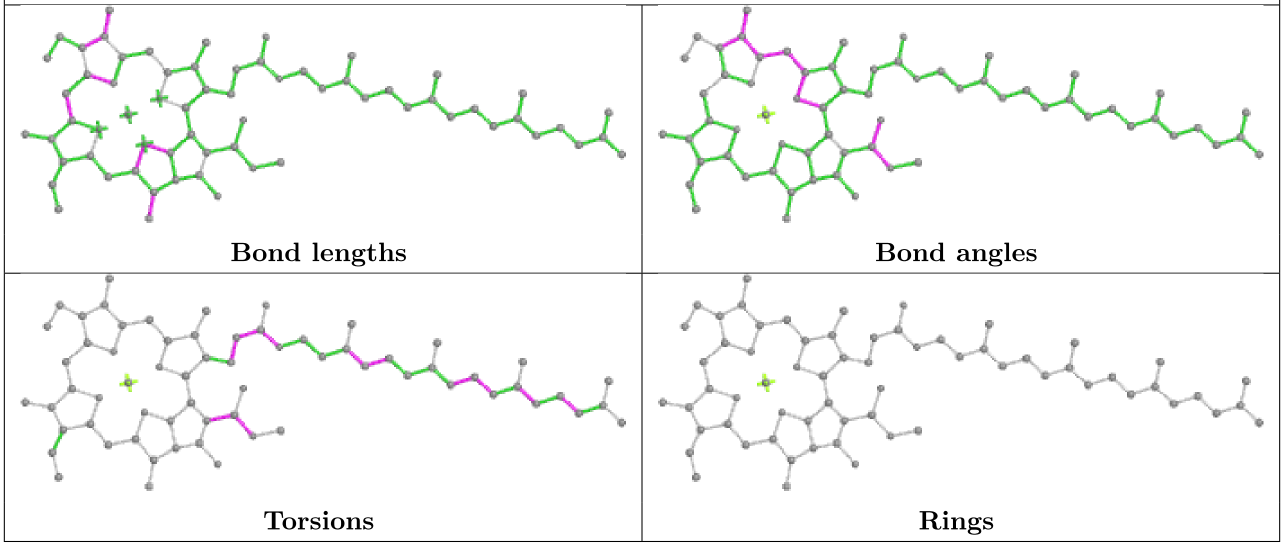


Torsions



Rings

Ligand CLA a 840



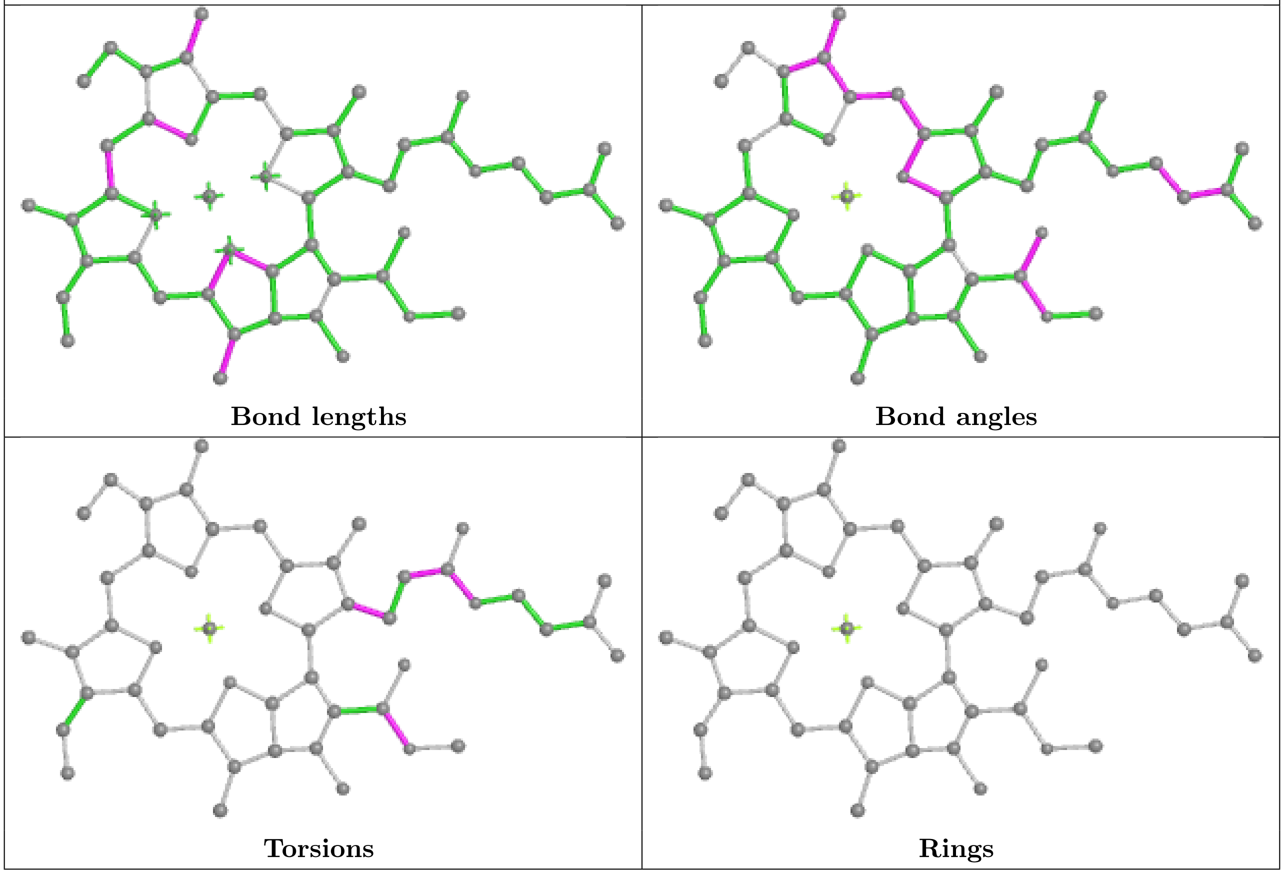
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA b 834



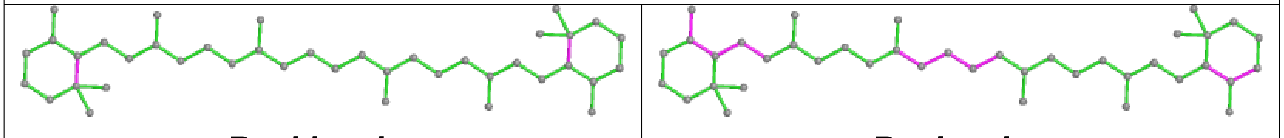
Bond lengths

Bond angles

Torsions

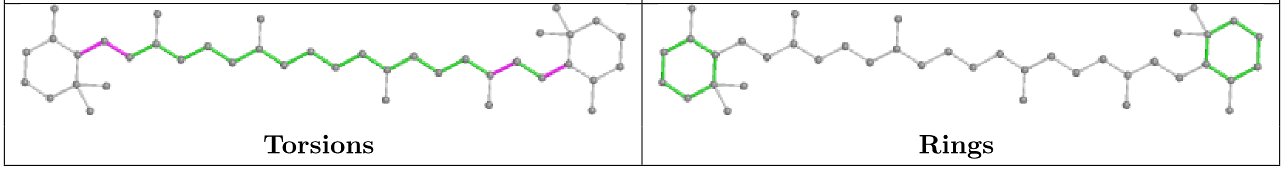
Rings

Ligand BCR a 848



Bond lengths

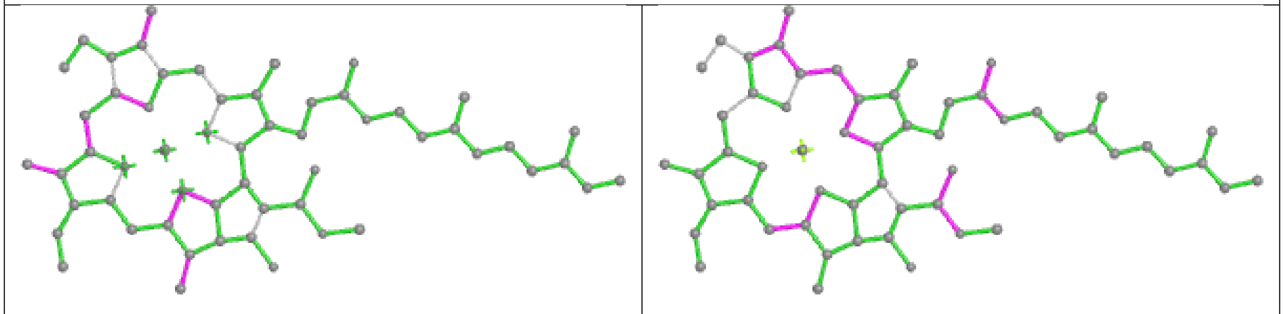
Bond angles



Torsions

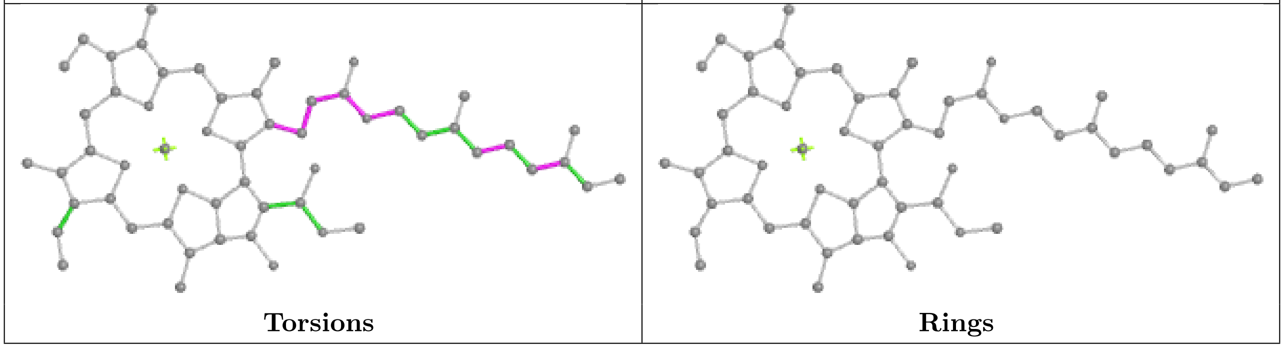
Rings

Ligand CLA a 843



Bond lengths

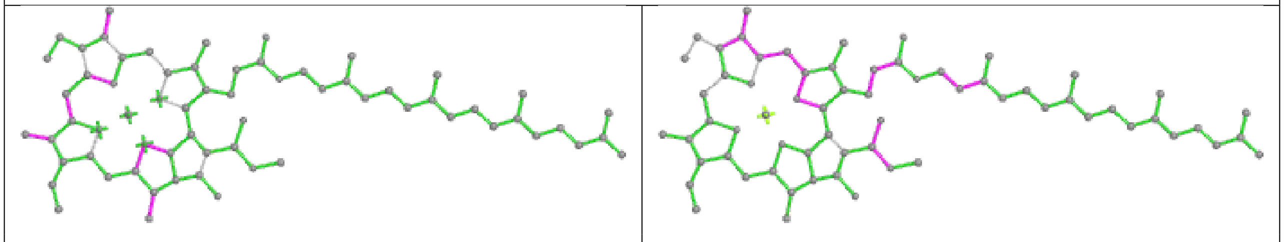
Bond angles



Torsions

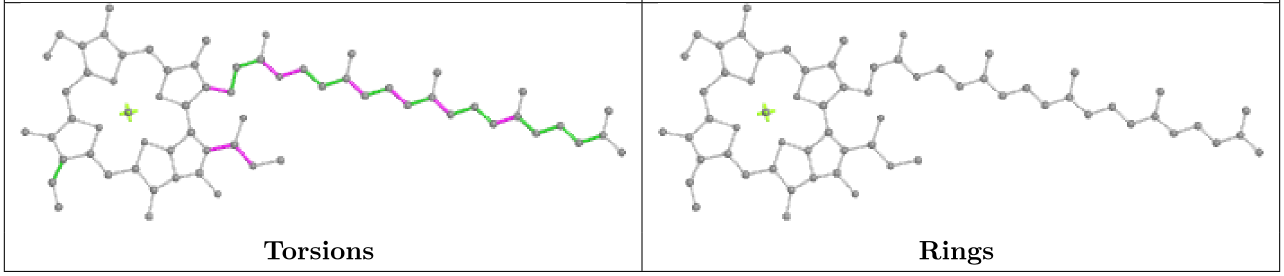
Rings

Ligand CLA b 801



Bond lengths

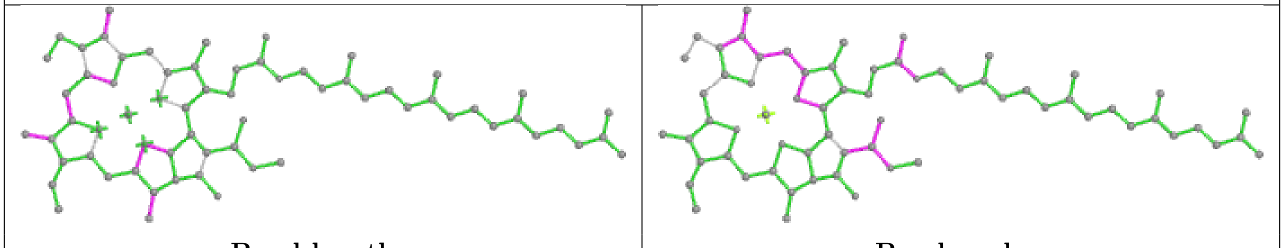
Bond angles



Torsions

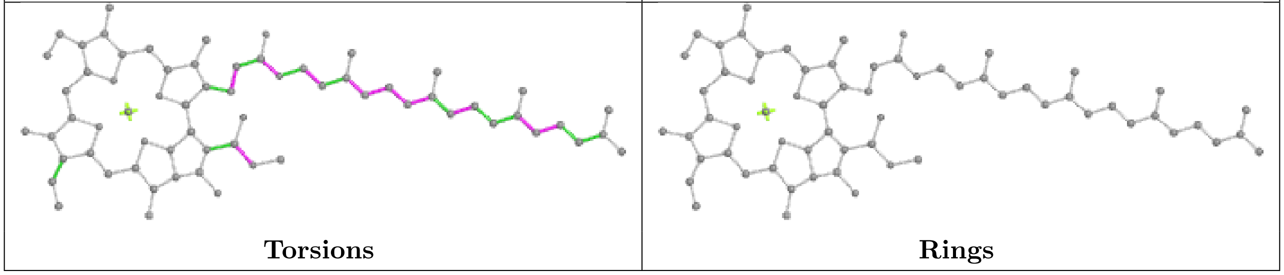
Rings

Ligand CLA b 812



Bond lengths

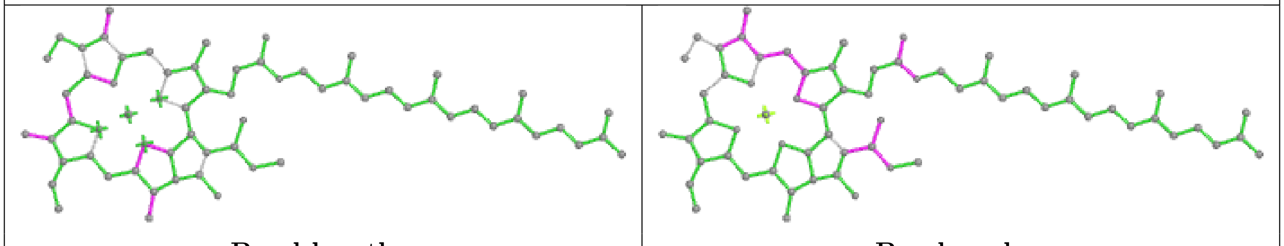
Bond angles



Torsions

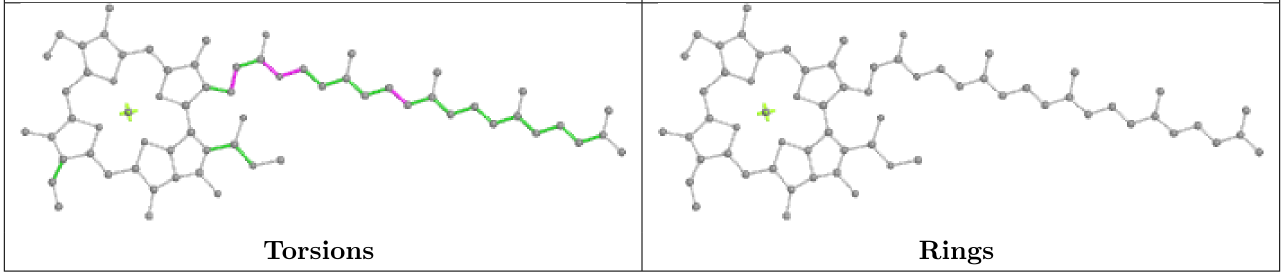
Rings

Ligand CLA a 856



Bond lengths

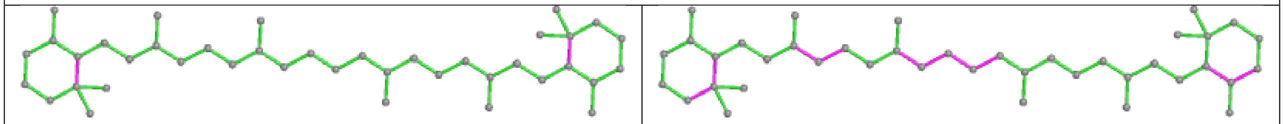
Bond angles



Torsions

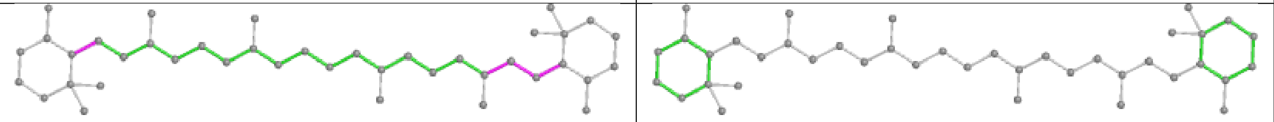
Rings

Ligand BCR b 845



Bond lengths

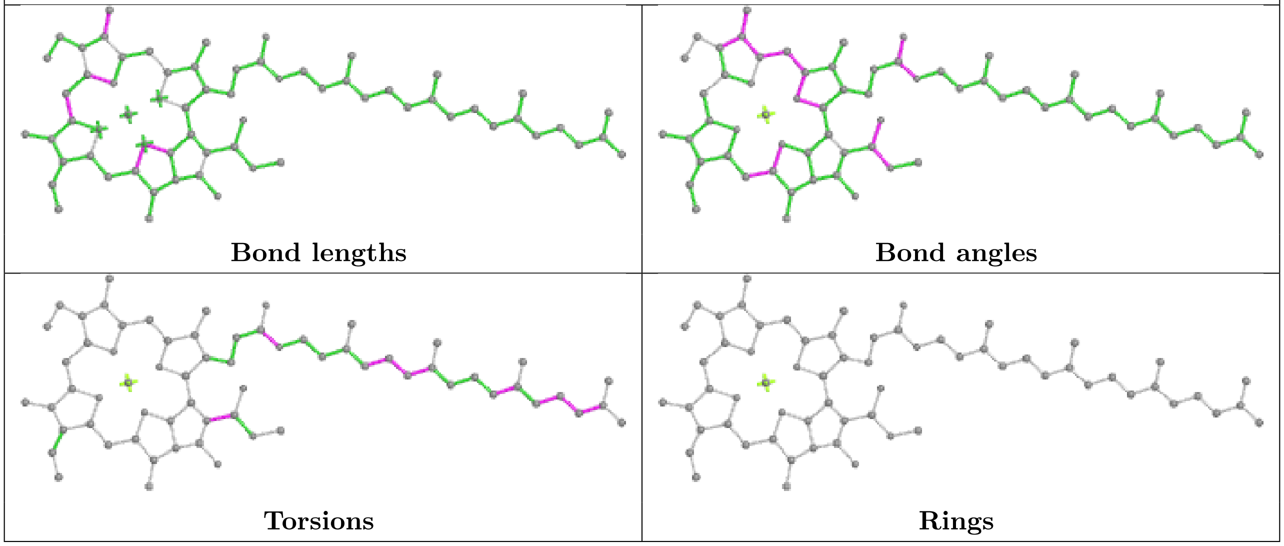
Bond angles



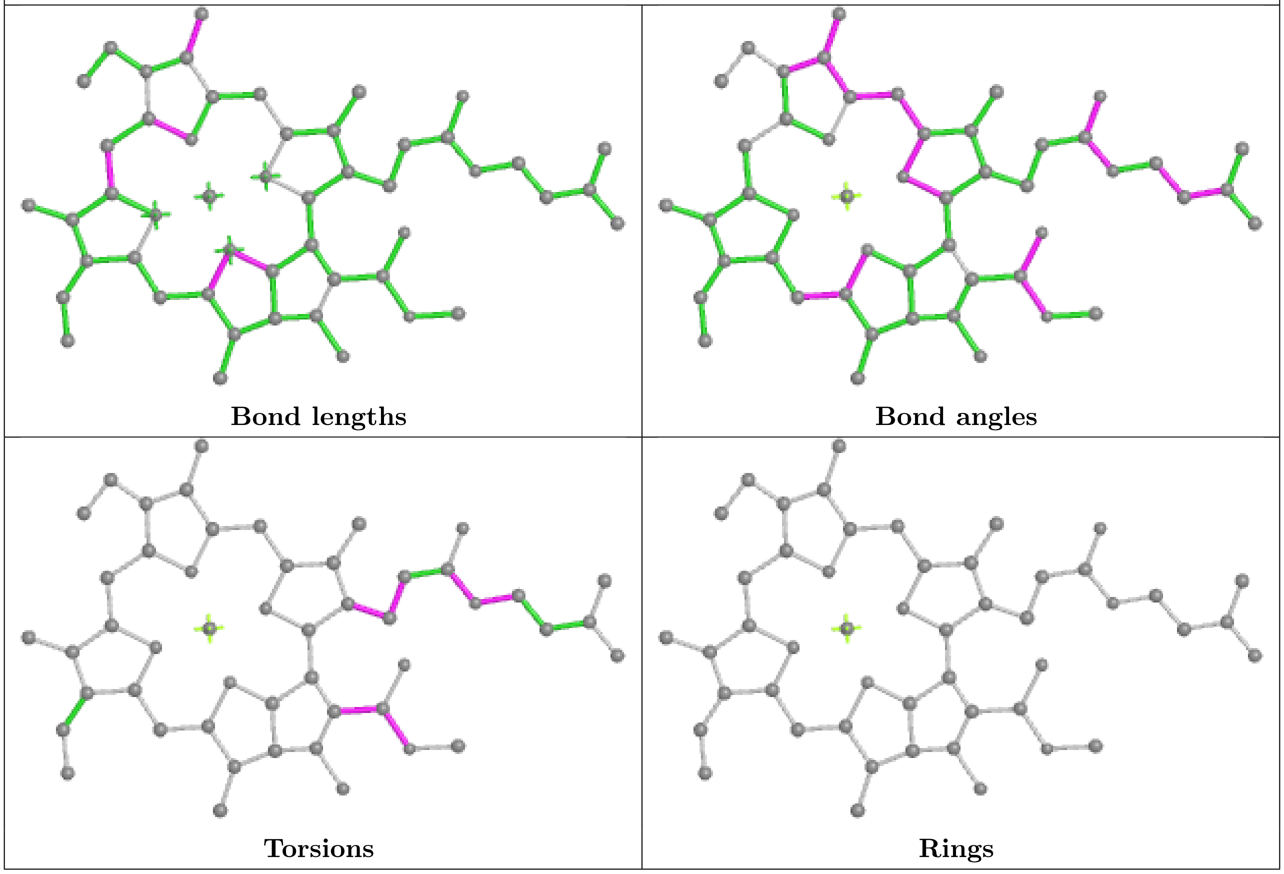
Torsions

Rings

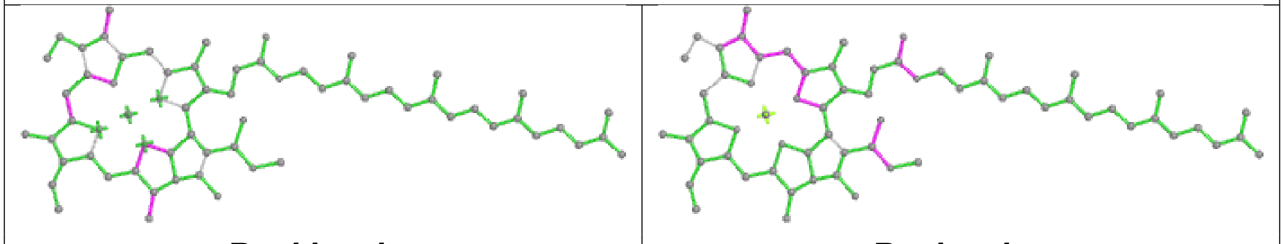
Ligand CLA a 860



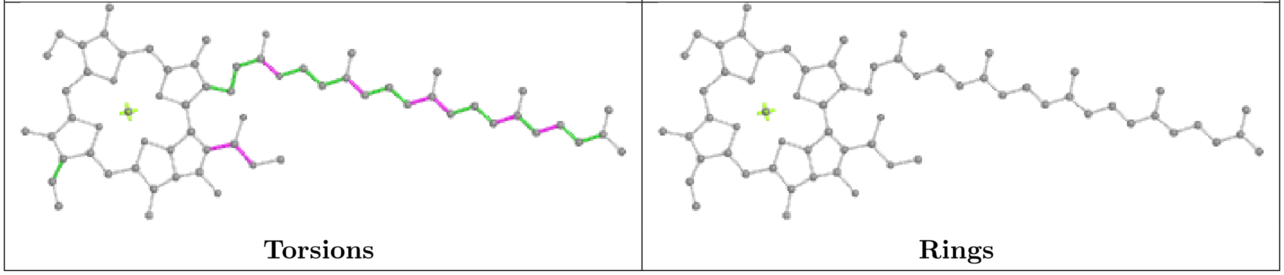
Ligand CLA l 202



Ligand CLA a 834

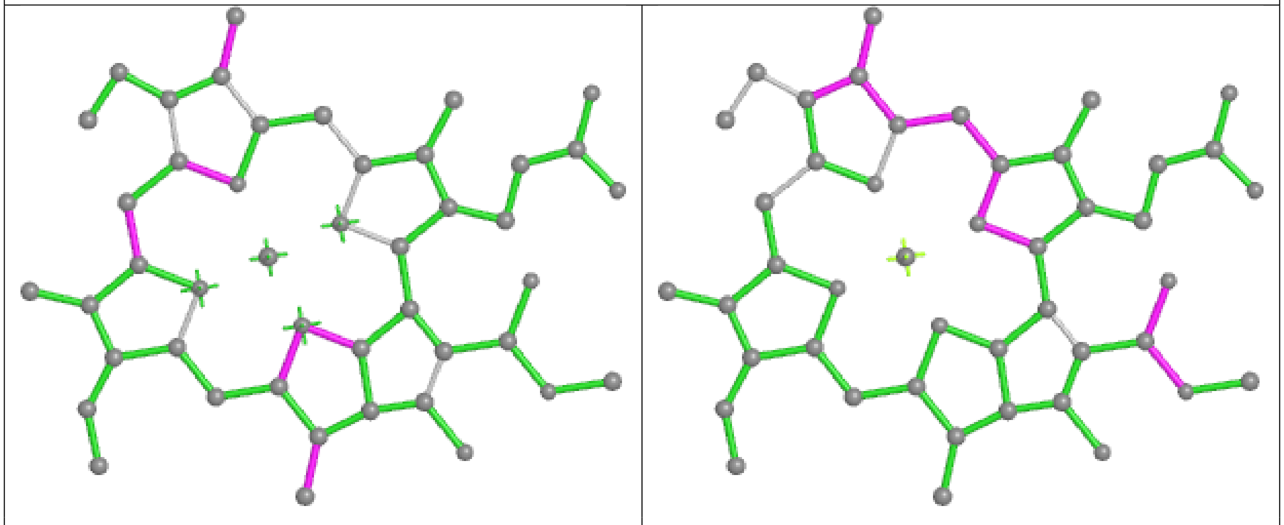


Bond lengths Bond angles

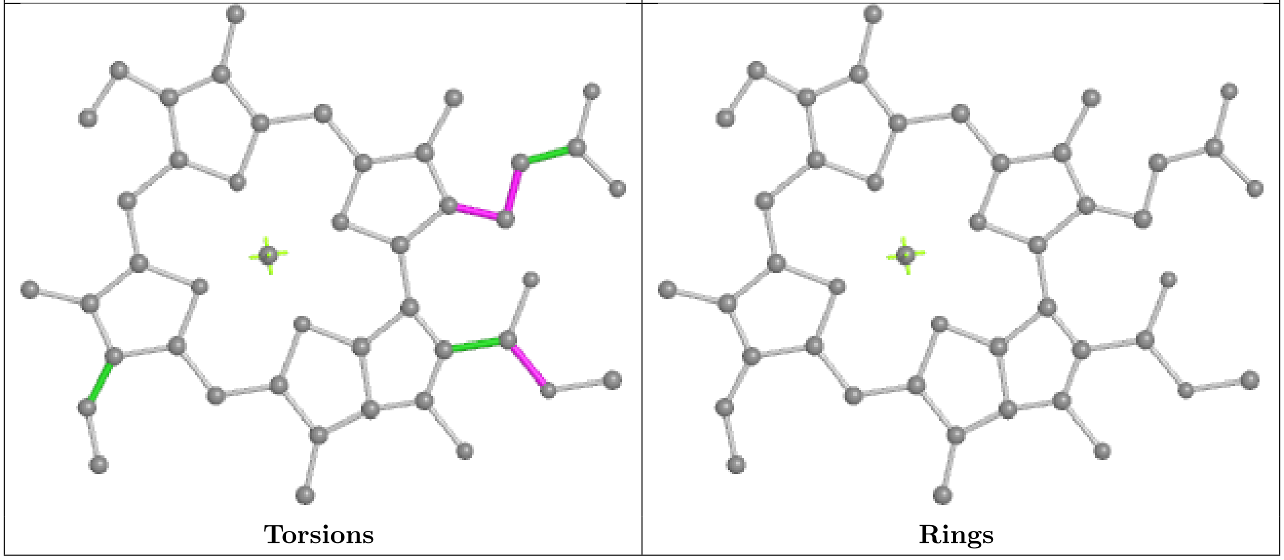


Torsions Rings

Ligand CLA k 102

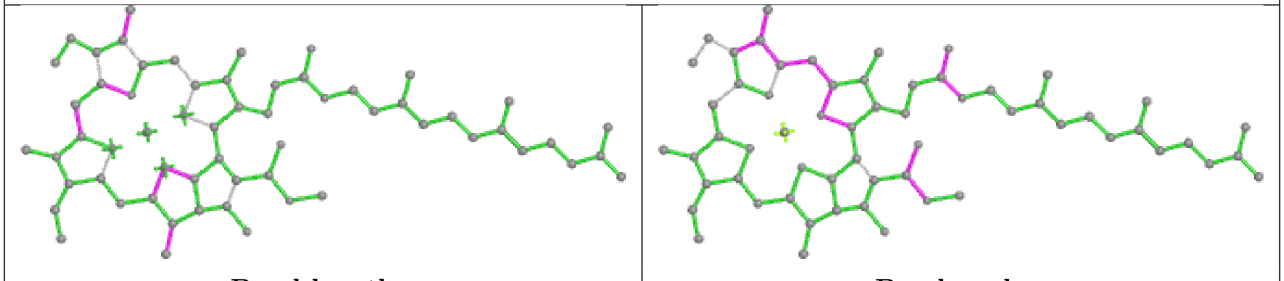


Bond lengths Bond angles



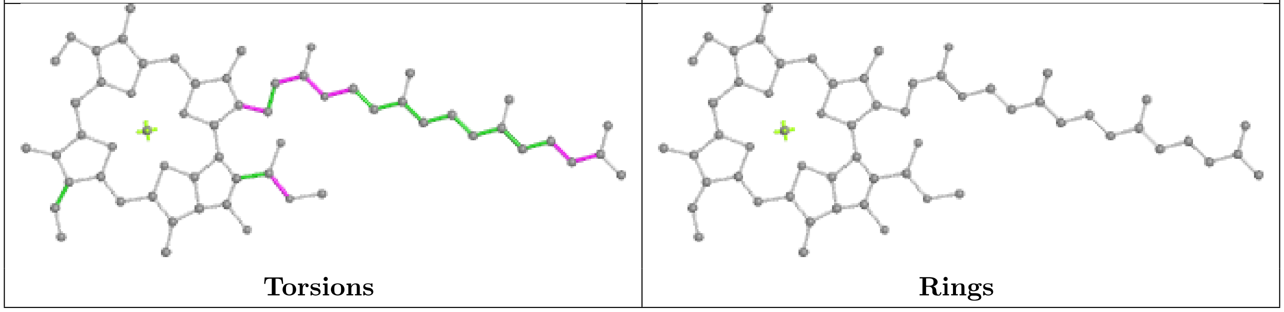
Torsions Rings

Ligand CLA b 820



Bond lengths

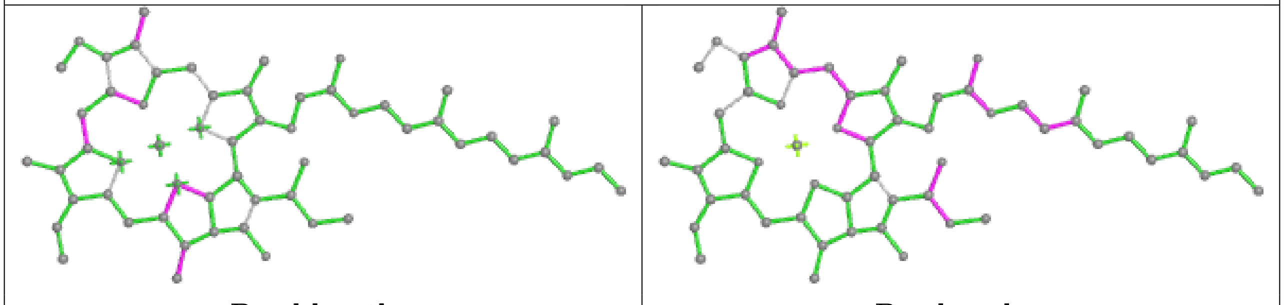
Bond angles



Torsions

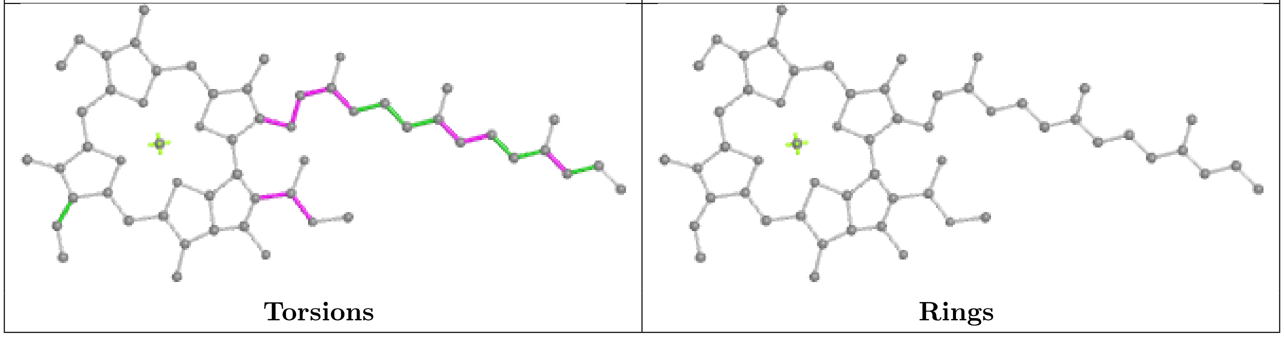
Rings

Ligand CLA b 822



Bond lengths

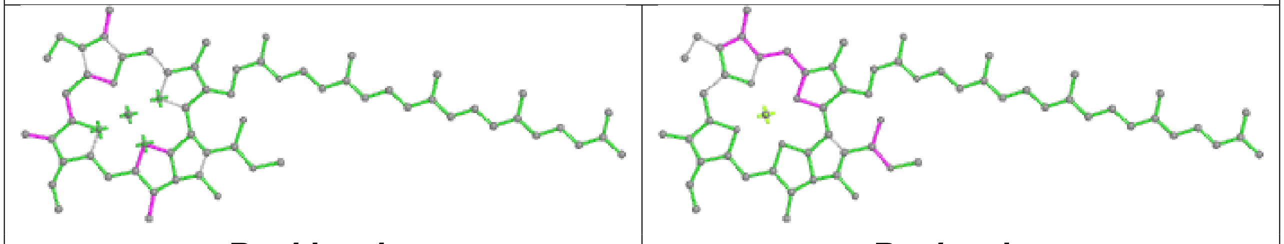
Bond angles



Torsions

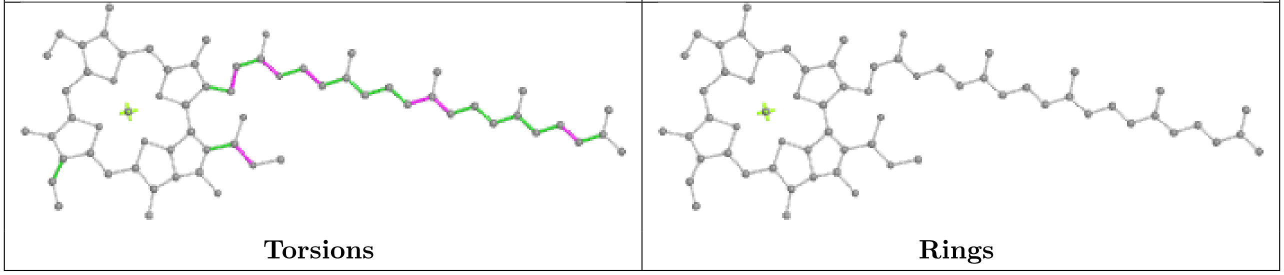
Rings

Ligand CLA A 402



Bond lengths

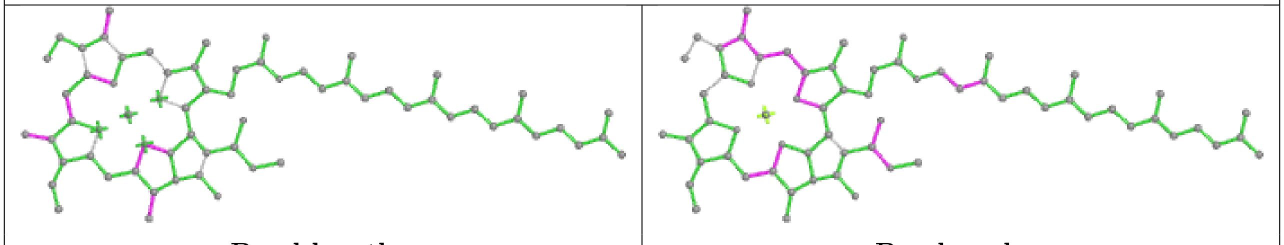
Bond angles



Torsions

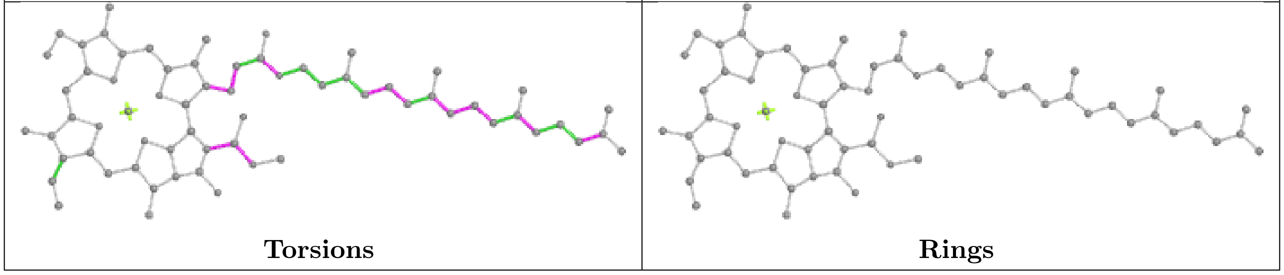
Rings

Ligand CLA b 832



Bond lengths

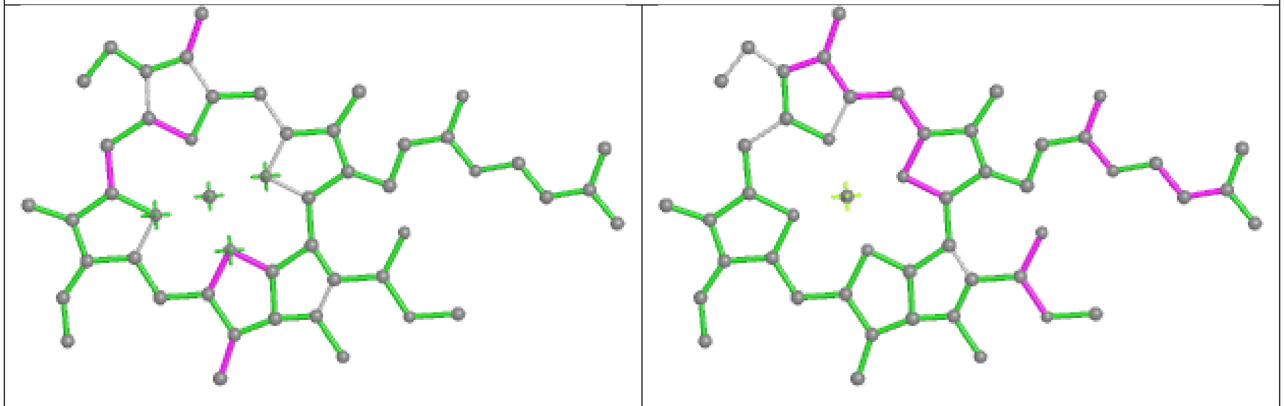
Bond angles



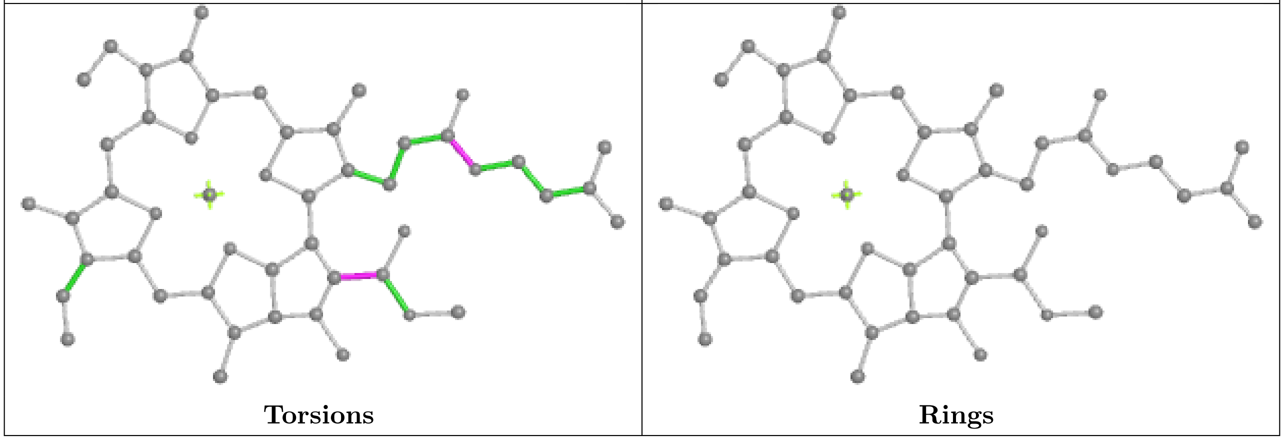
Torsions

Rings

Ligand CLA f 203

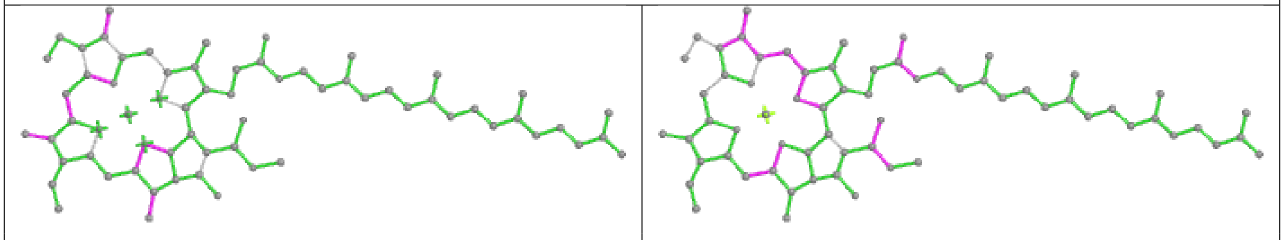


Bond lengths **Bond angles**

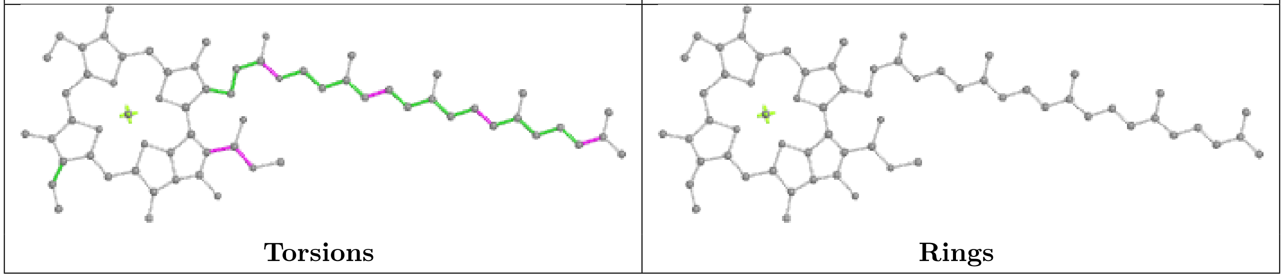


Torsions **Rings**

Ligand CLA b 807

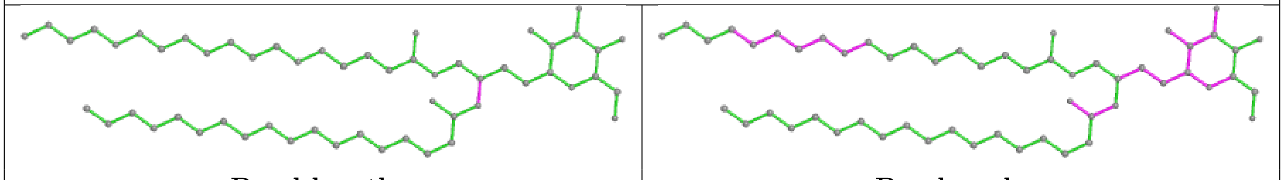


Bond lengths **Bond angles**

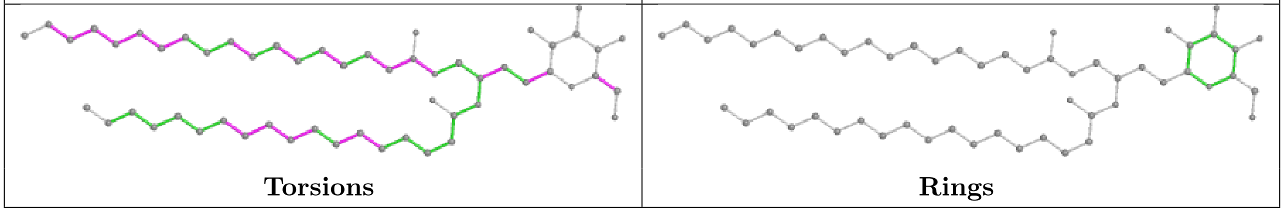


Torsions **Rings**

Ligand LMG b 850

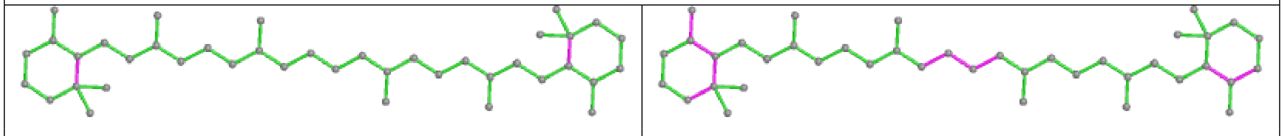


Bond lengths Bond angles

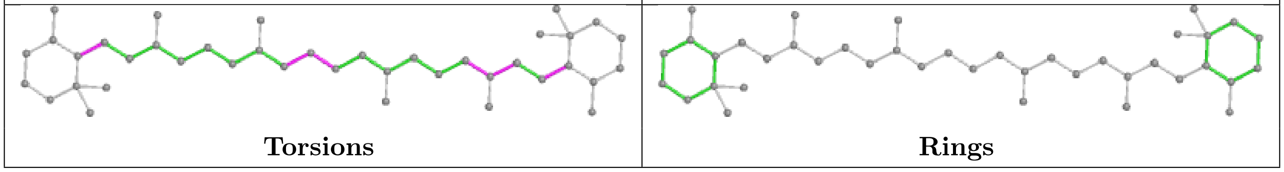


Torsions Rings

Ligand BCR i 101

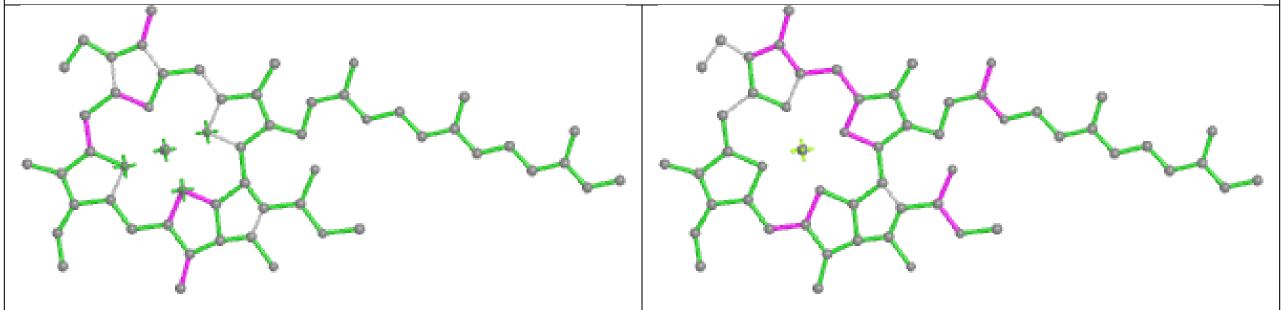


Bond lengths Bond angles

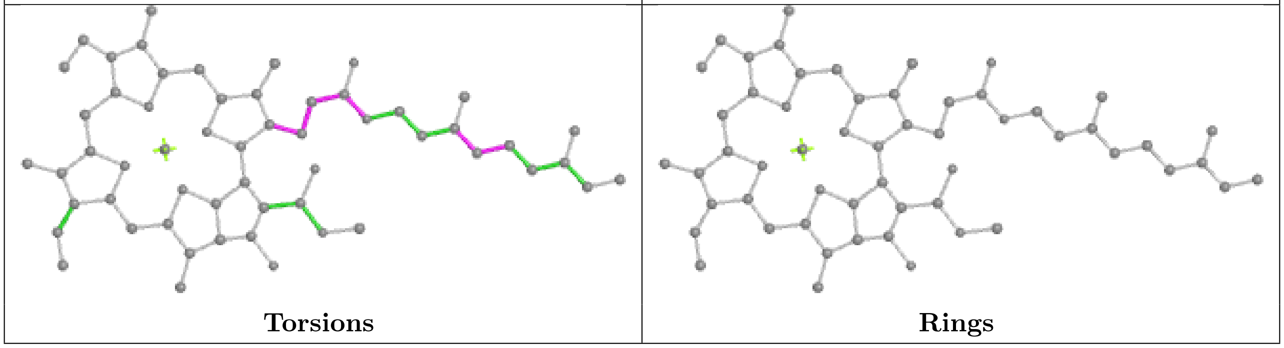


Torsions Rings

Ligand CLA a 832

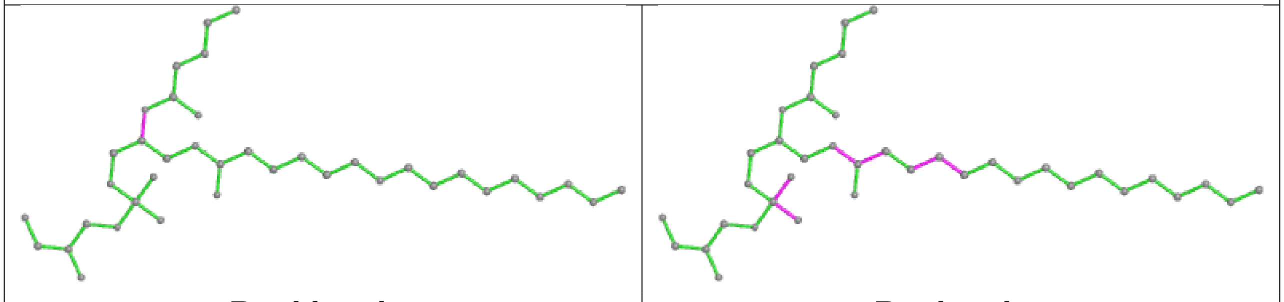


Bond lengths Bond angles



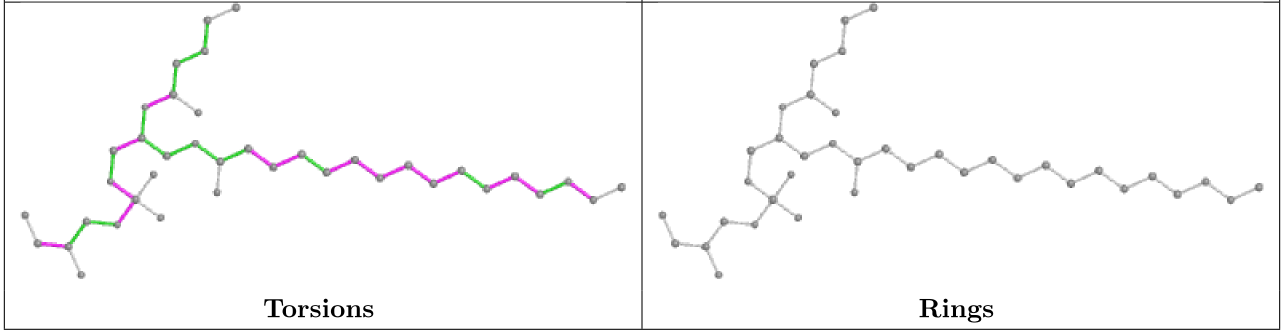
Torsions Rings

Ligand LHG b 849



Bond lengths

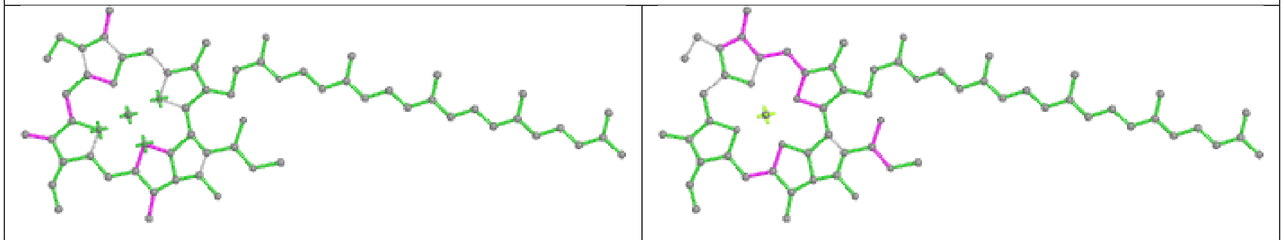
Bond angles



Torsions

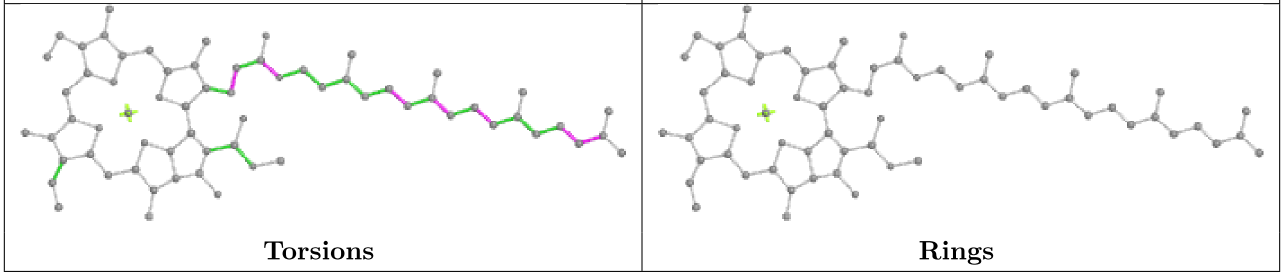
Rings

Ligand CLA a 804



Bond lengths

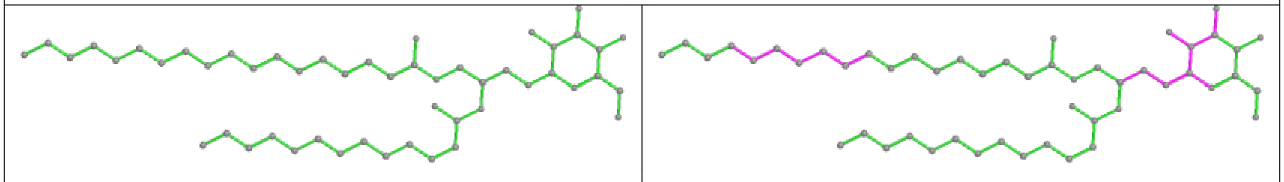
Bond angles



Torsions

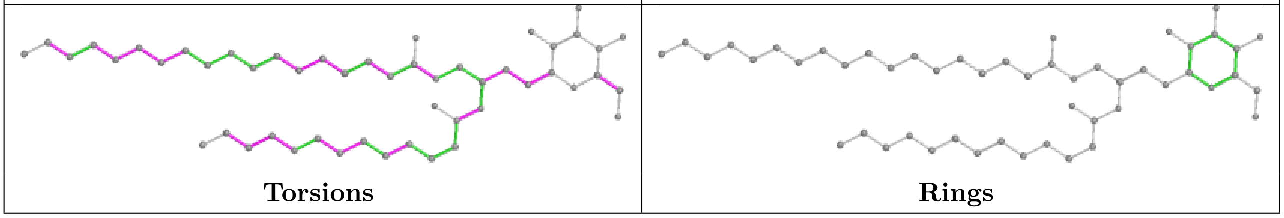
Rings

Ligand LMG l 201



Bond lengths

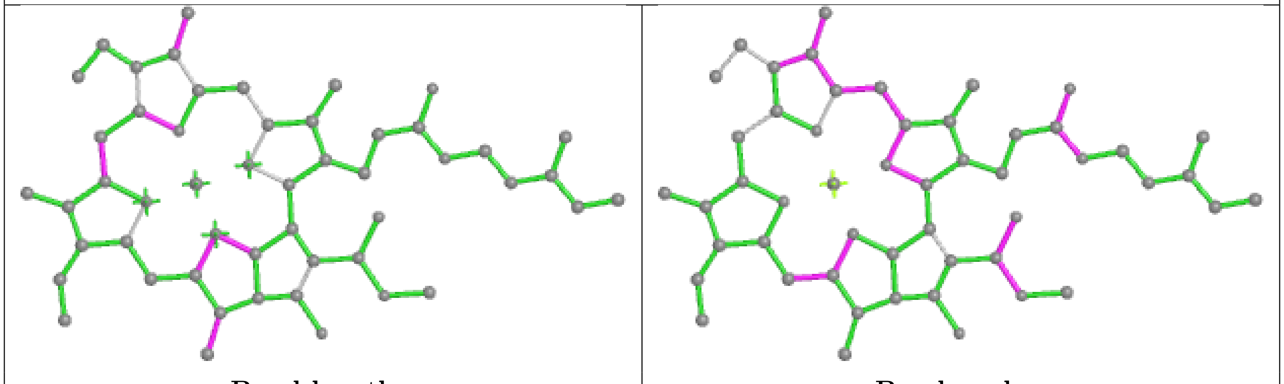
Bond angles



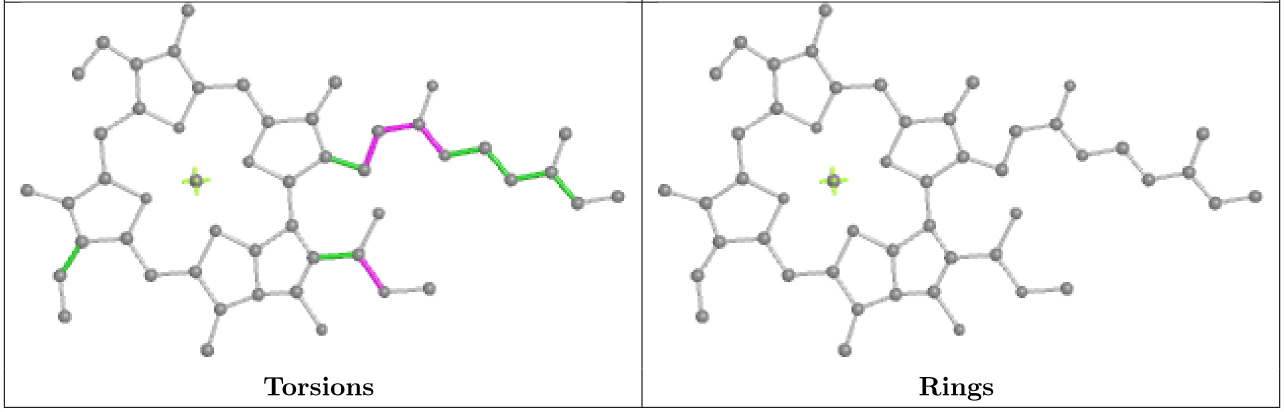
Torsions

Rings

Ligand CLA b 829

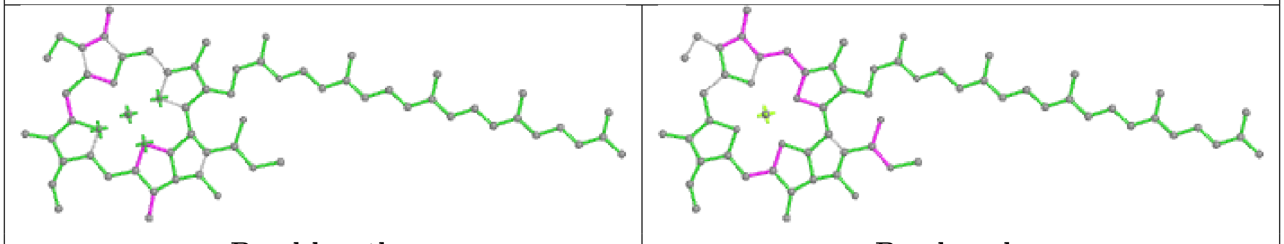


Bond lengths Bond angles

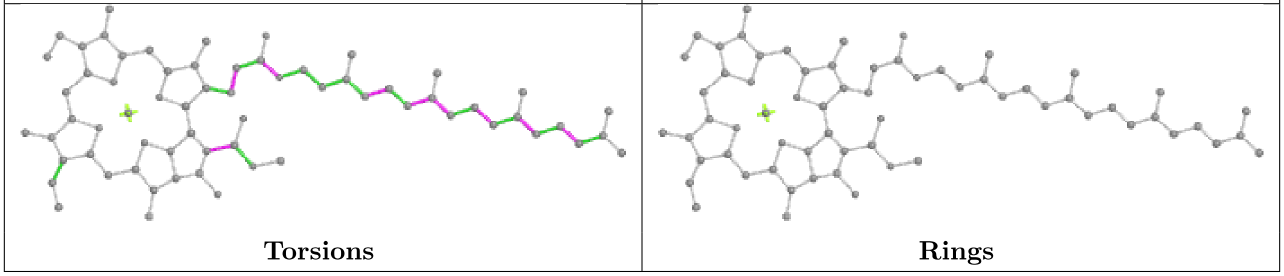


Torsions Rings

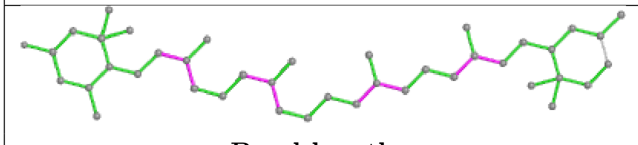
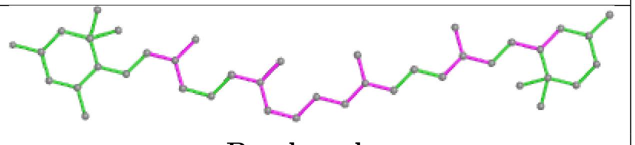
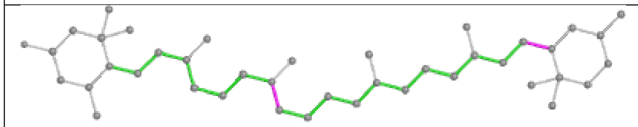
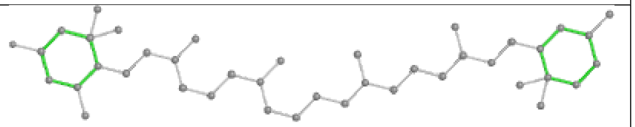
Ligand CLA b 831

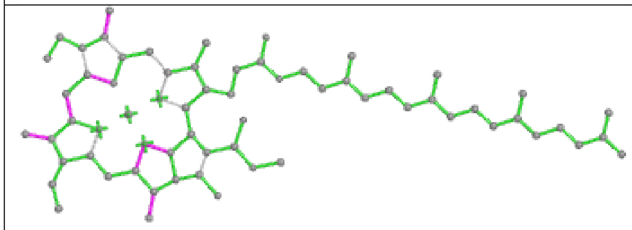
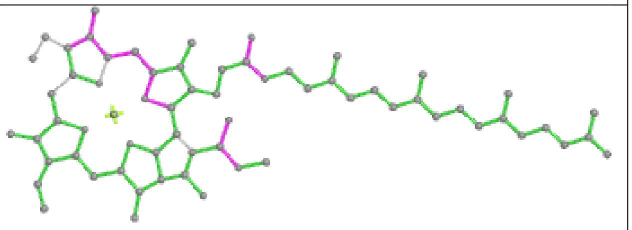
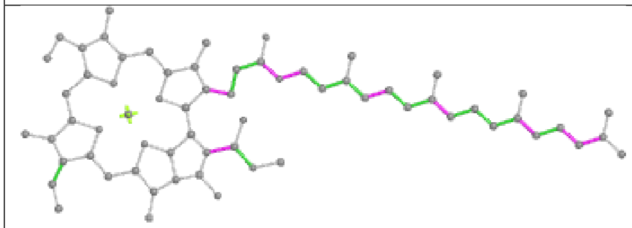
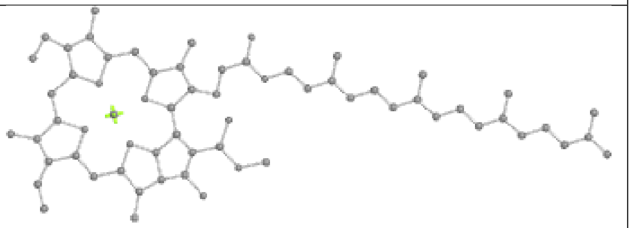


Bond lengths Bond angles

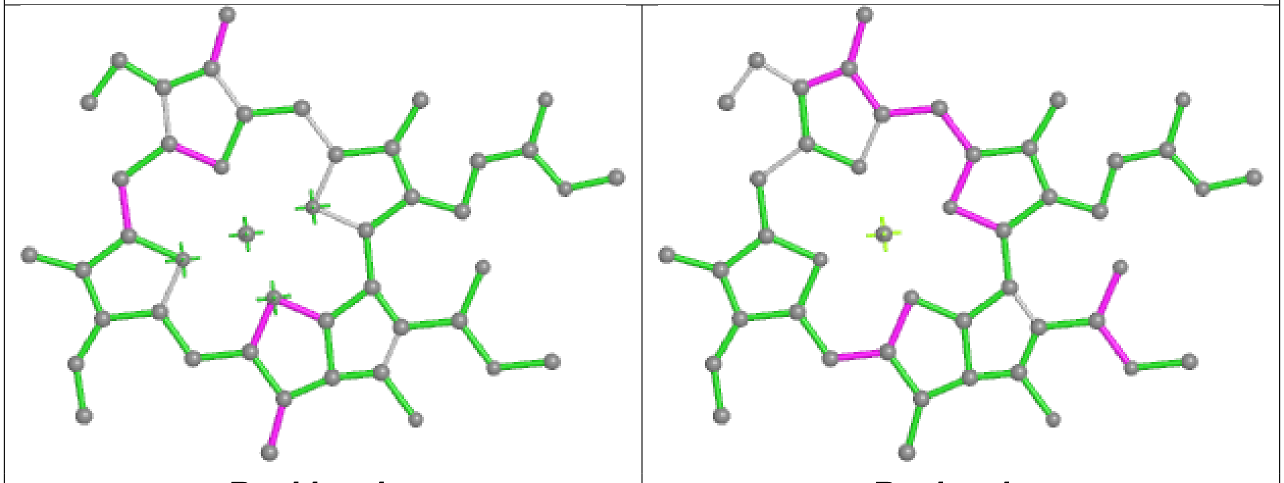


Torsions Rings

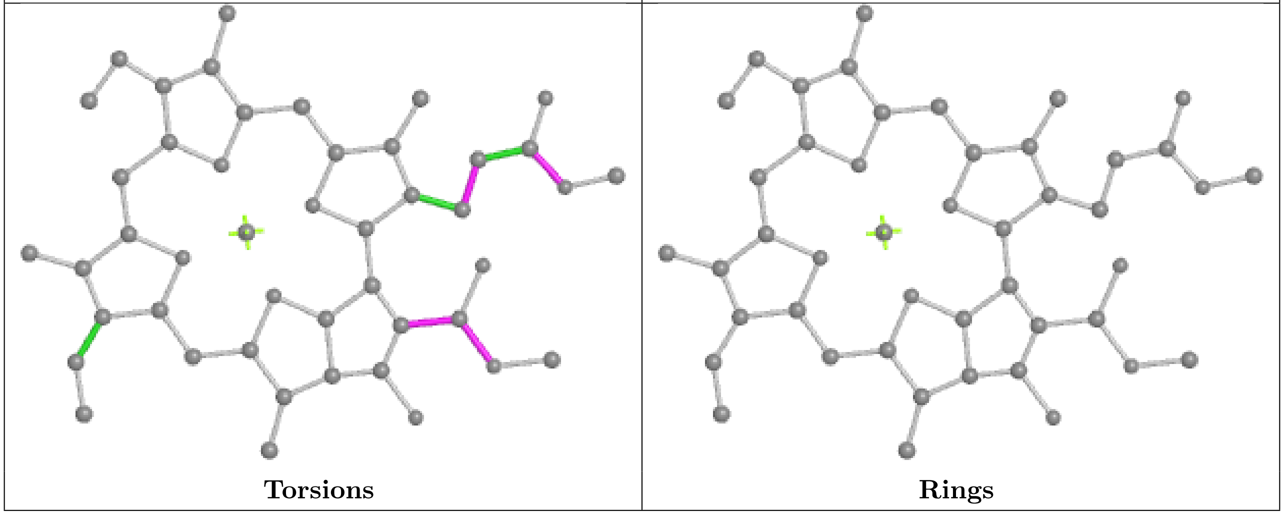
Ligand ZEX f 205	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA a 818	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA j 104

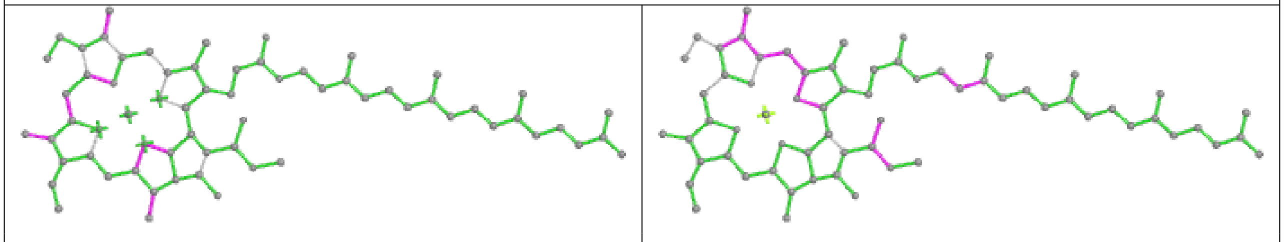


Bond lengths Bond angles

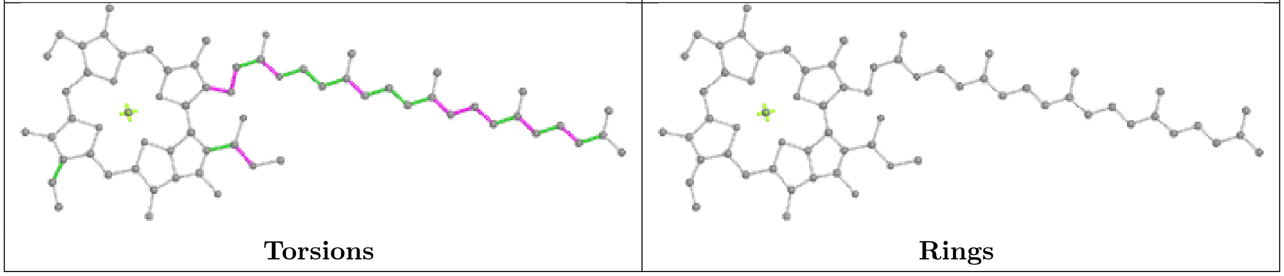


Torsions Rings

Ligand CLA a 828

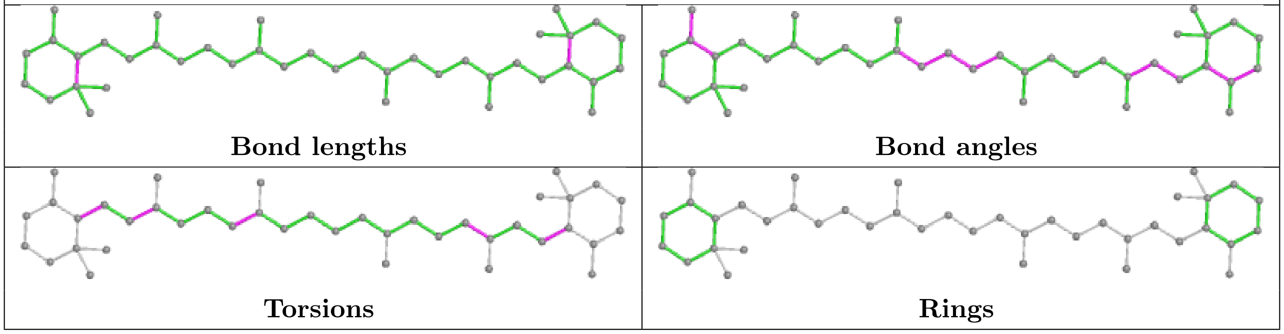


Bond lengths Bond angles



Torsions Rings

Ligand BCR a 847



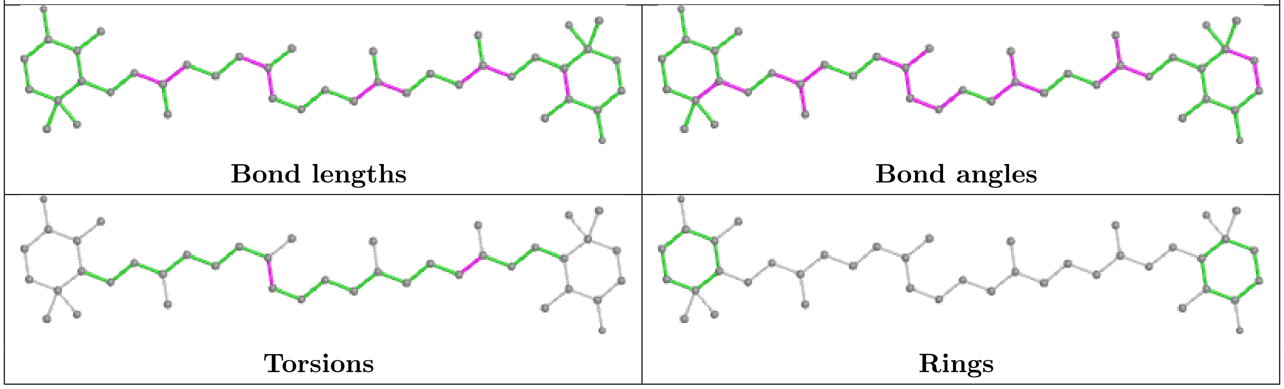
Bond lengths

Bond angles

Torsions

Rings

Ligand 45D a 858



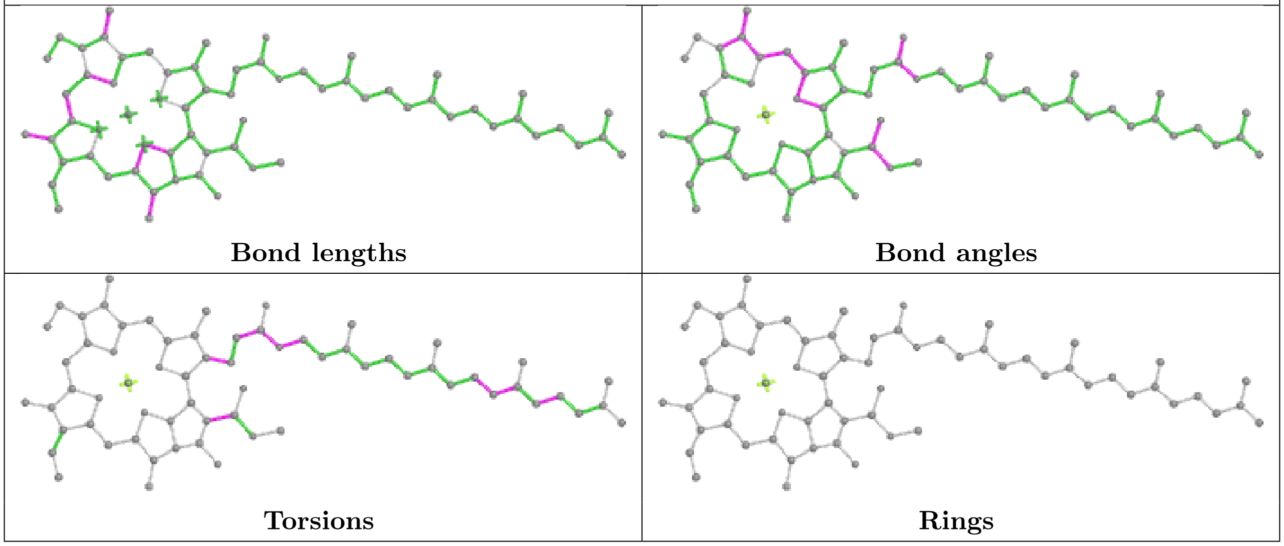
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA l 203



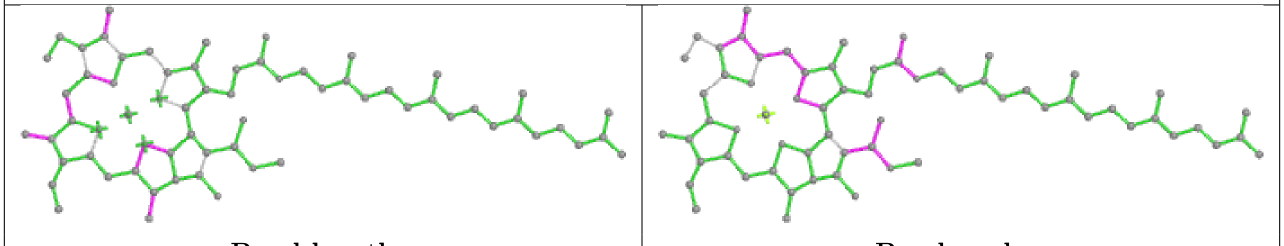
Bond lengths

Bond angles

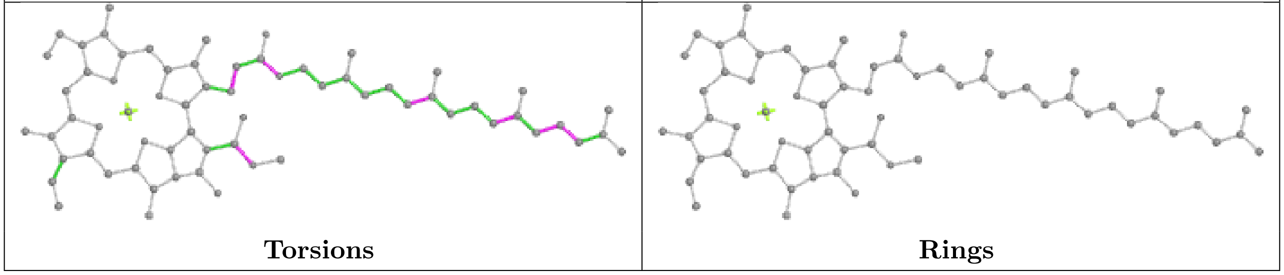
Torsions

Rings

Ligand CLA a 814

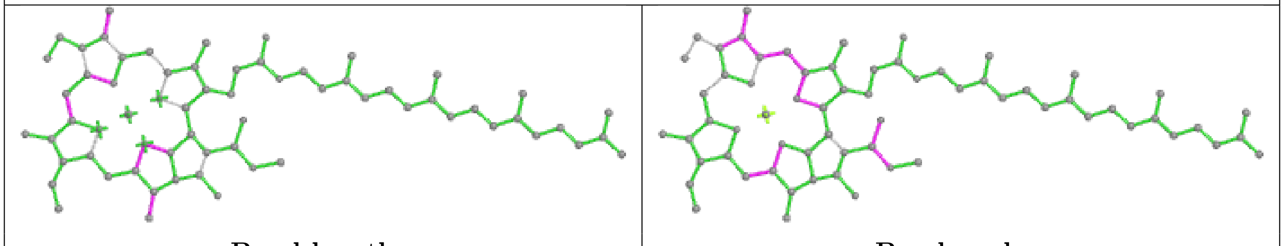


Bond lengths Bond angles

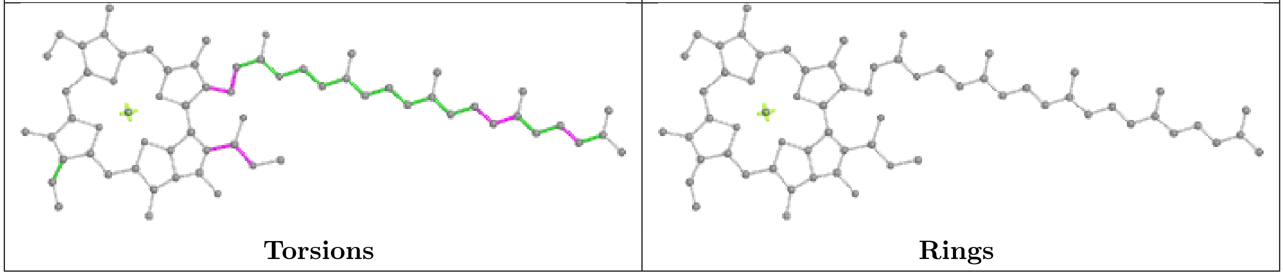


Torsions Rings

Ligand CLA a 829

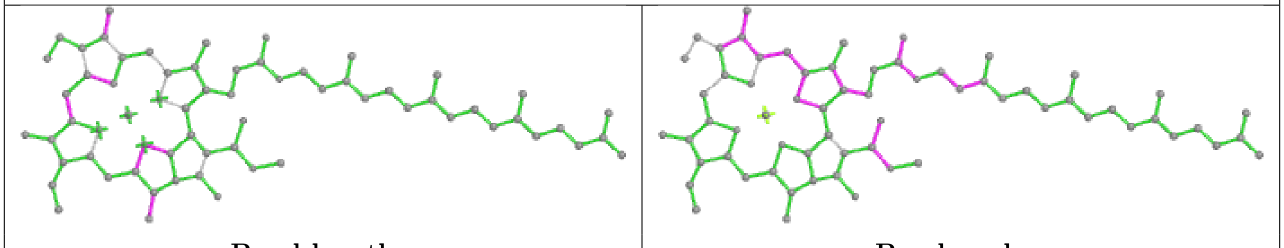


Bond lengths Bond angles

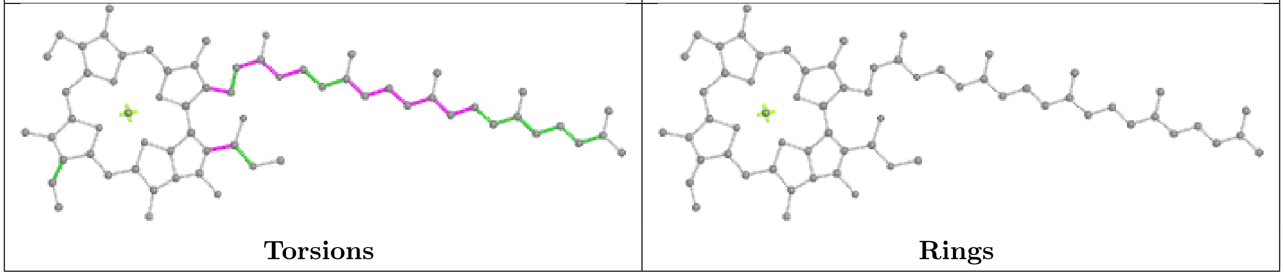


Torsions Rings

Ligand CLA a 824

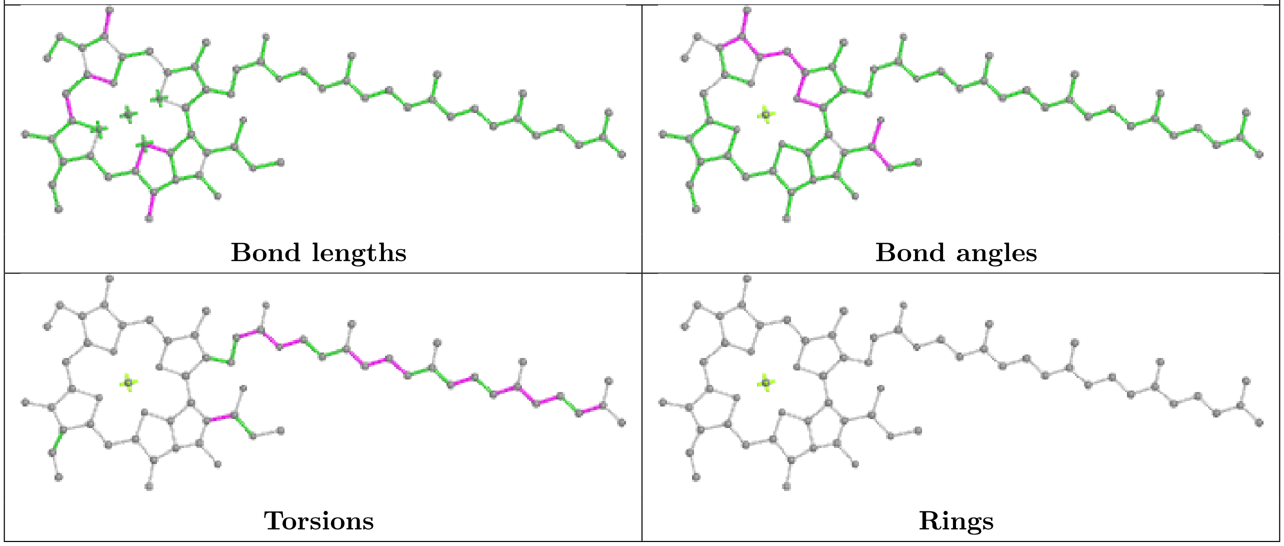


Bond lengths Bond angles



Torsions Rings

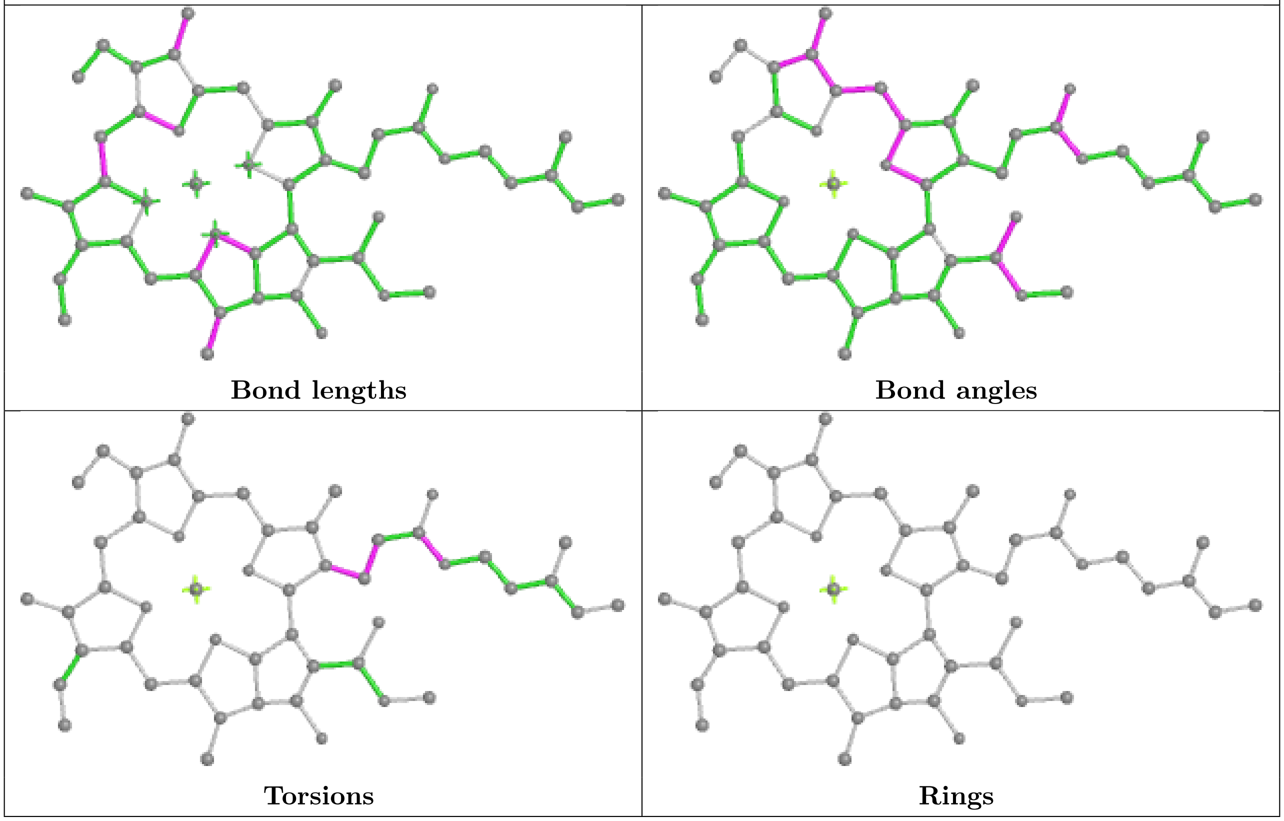
Ligand CLA a 830



Bond lengths Bond angles

Torsions Rings

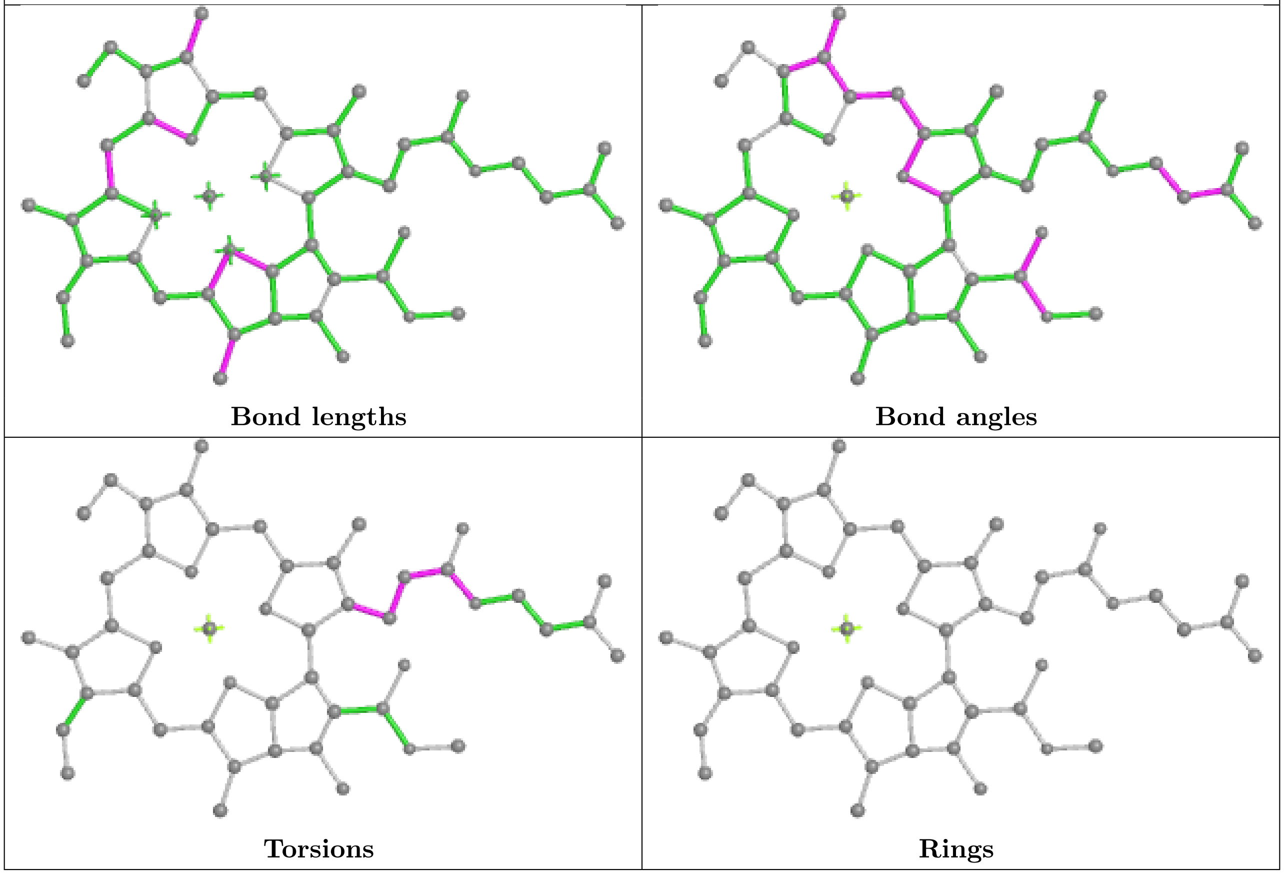
Ligand CLA a 838



Bond lengths Bond angles

Torsions Rings

Ligand CLA b 811



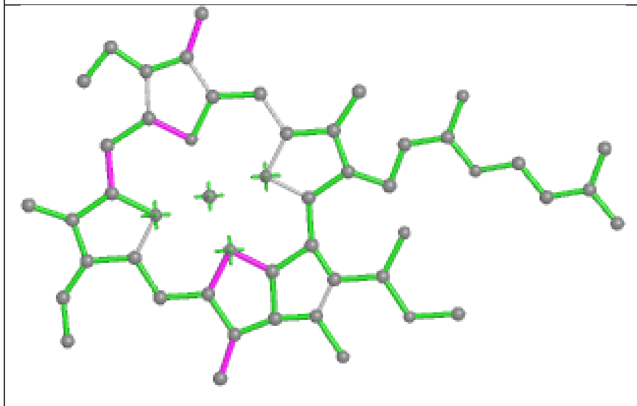
Bond lengths

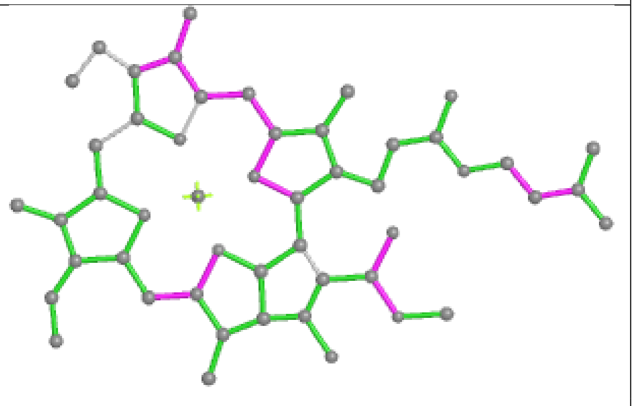
Bond angles

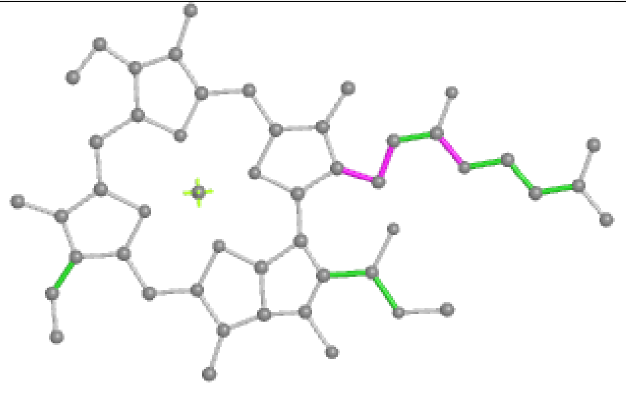
Torsions

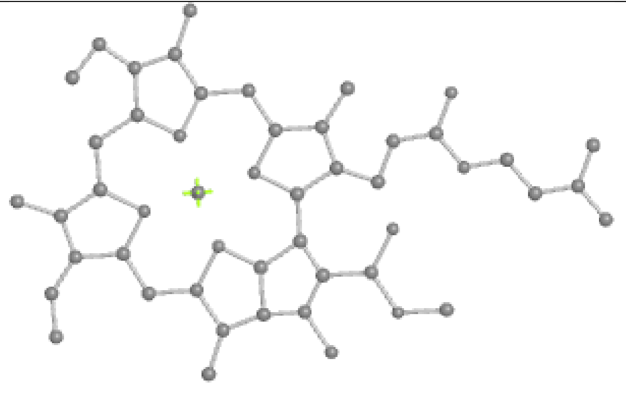
Rings

Ligand CLA b 830

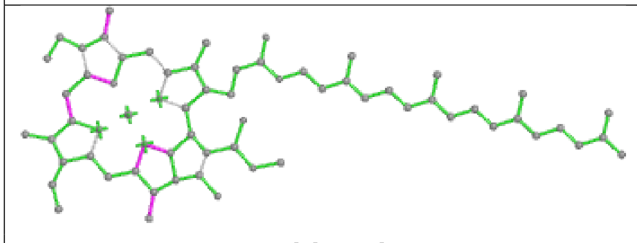

Bond lengths

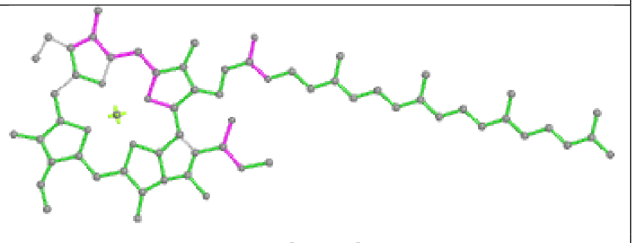

Bond angles

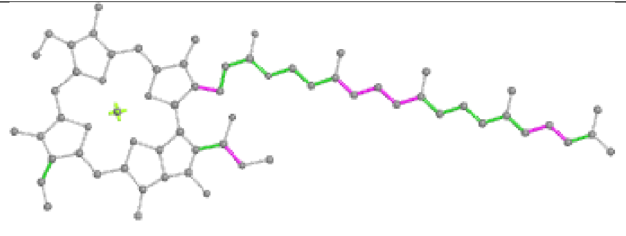

Torsions

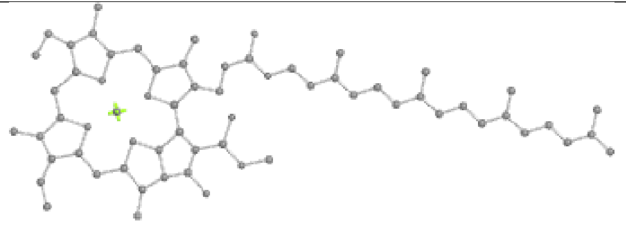

Rings

Ligand CLA b 819

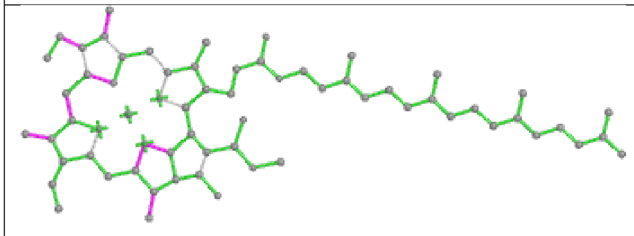

Bond lengths


Bond angles

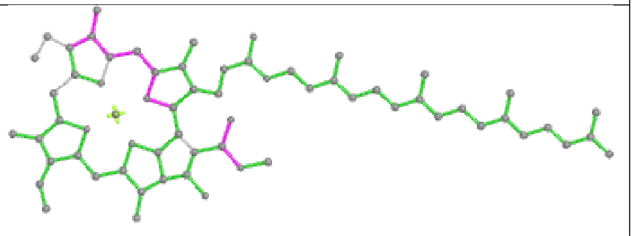

Torsions


Rings

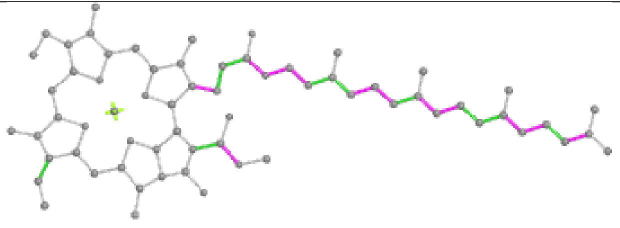
Ligand CLA a 819



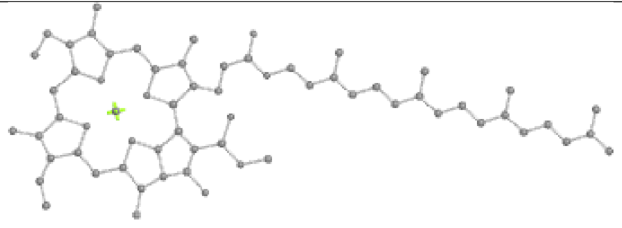
Bond lengths



Bond angles

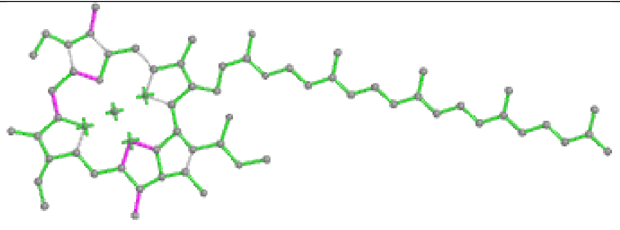


Torsions

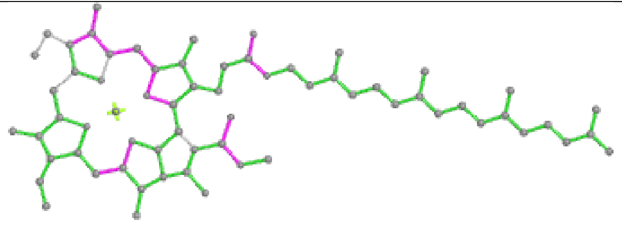


Rings

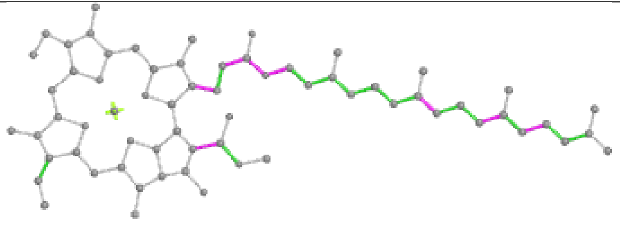
Ligand CLA a 839



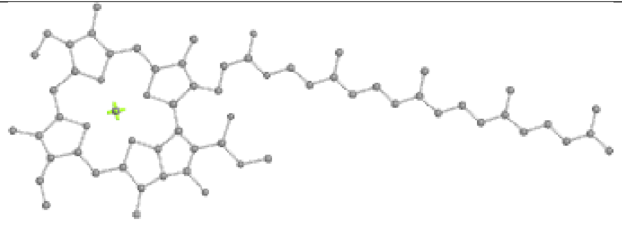
Bond lengths



Bond angles

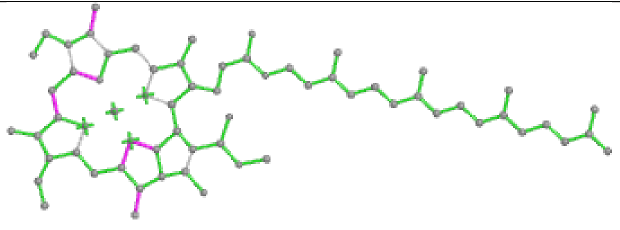


Torsions

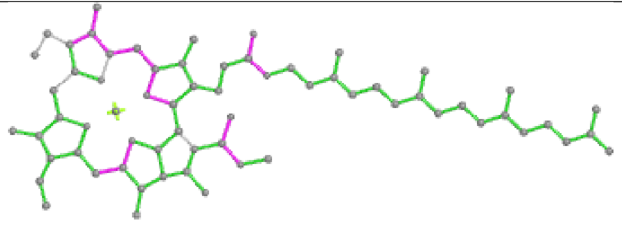


Rings

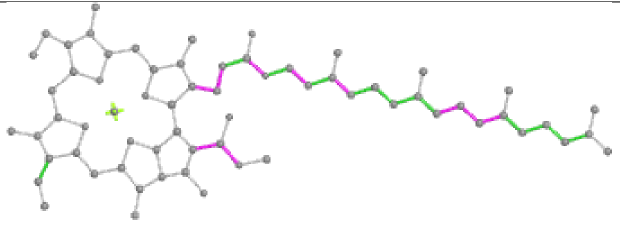
Ligand CLA b 826



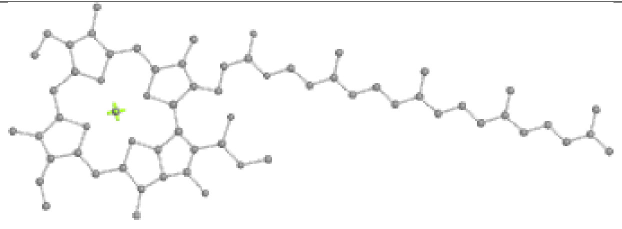
Bond lengths



Bond angles

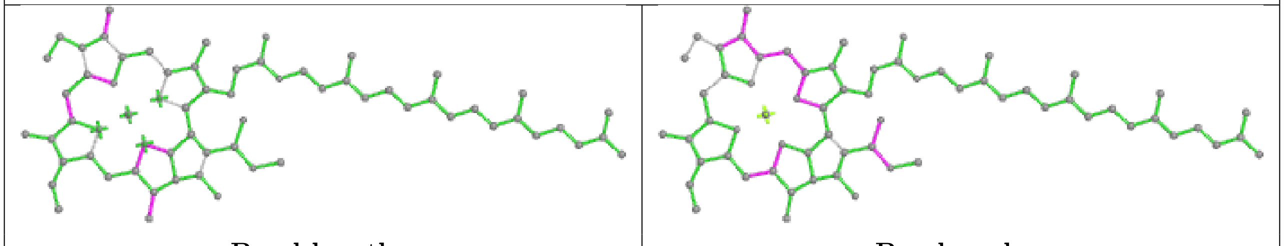


Torsions

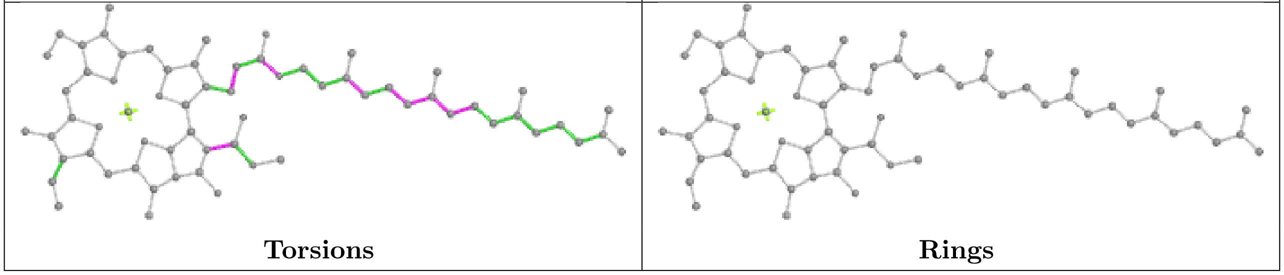


Rings

Ligand CLA a 837

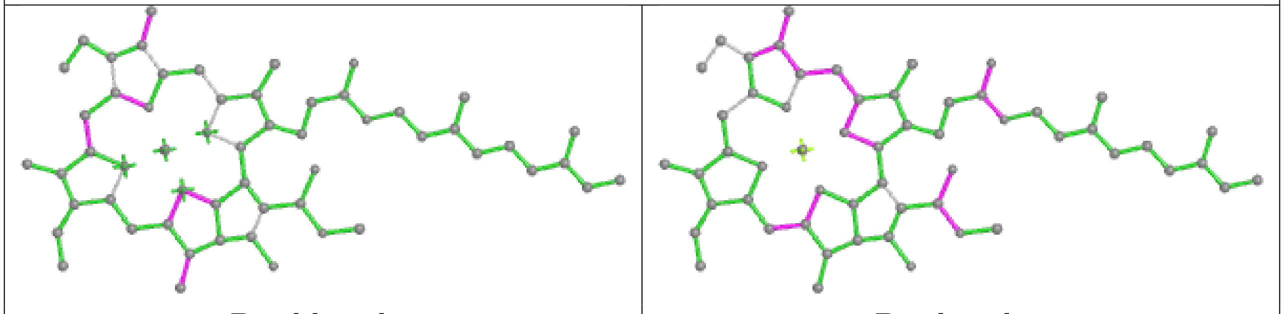


Bond lengths Bond angles

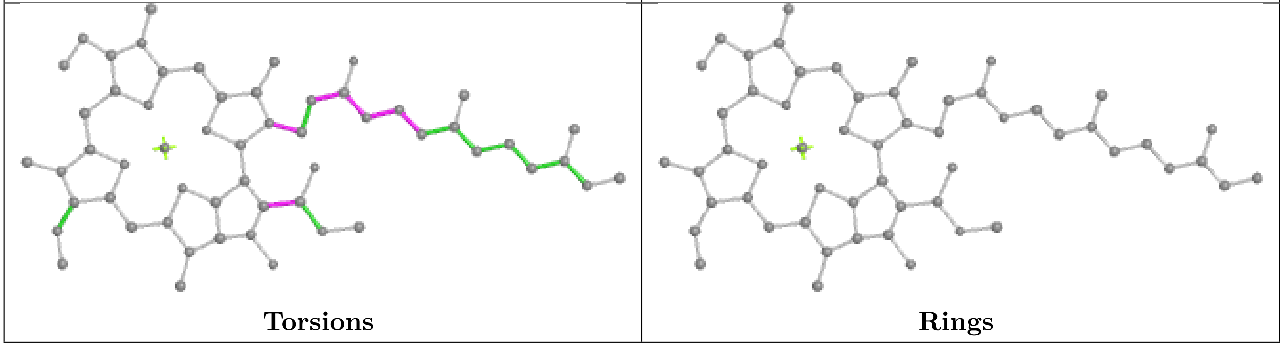


Torsions Rings

Ligand CLA b 815

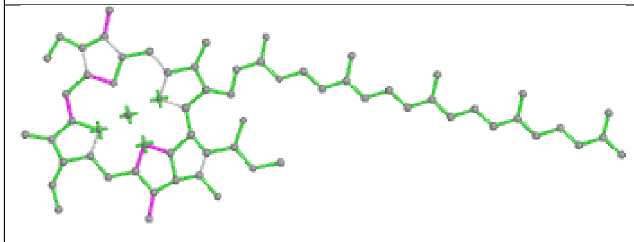


Bond lengths Bond angles

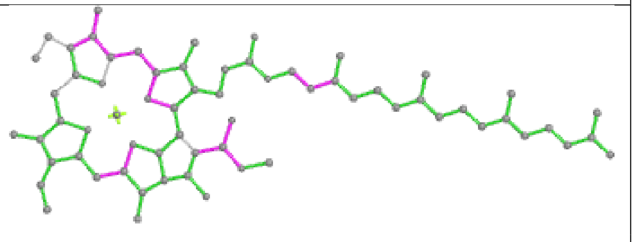


Torsions Rings

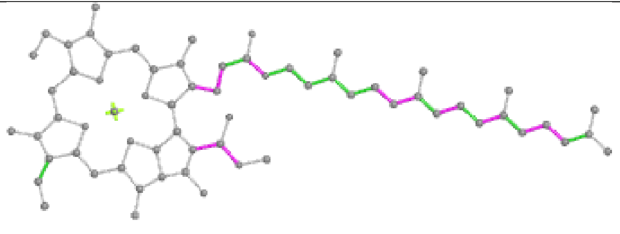
Ligand CLA a 815



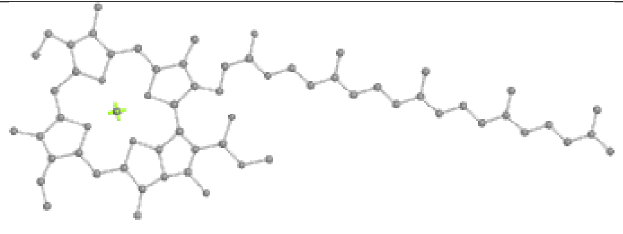
Bond lengths



Bond angles

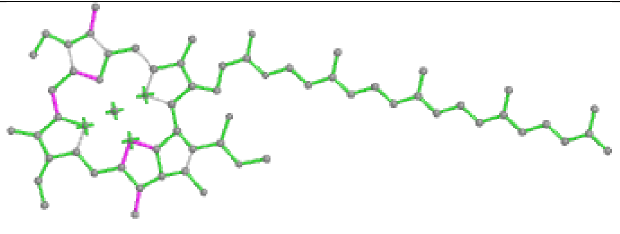


Torsions

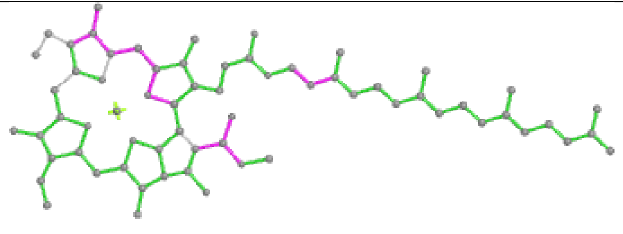


Rings

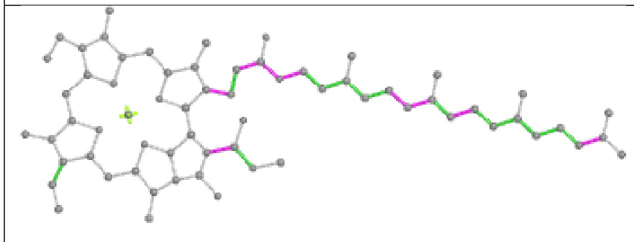
Ligand CLA a 835



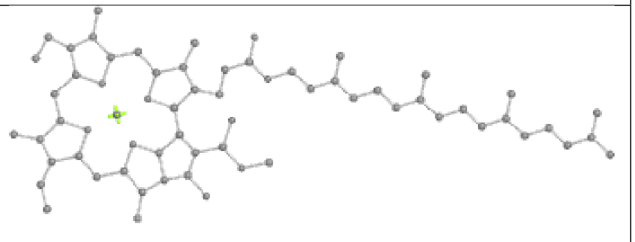
Bond lengths



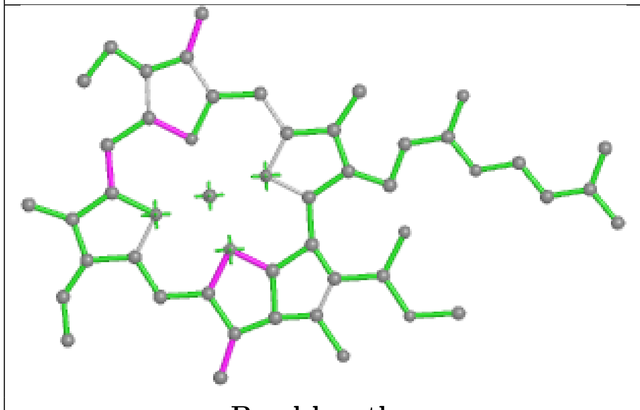
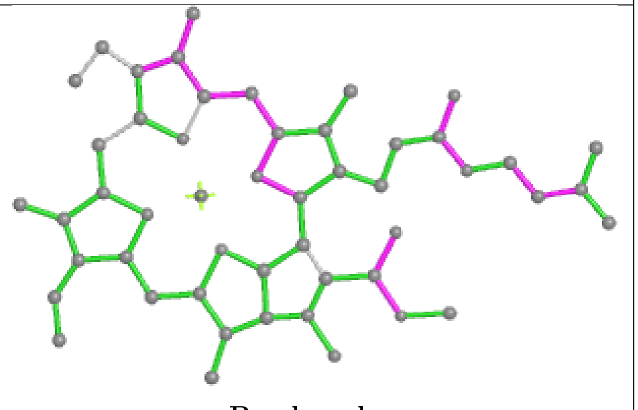
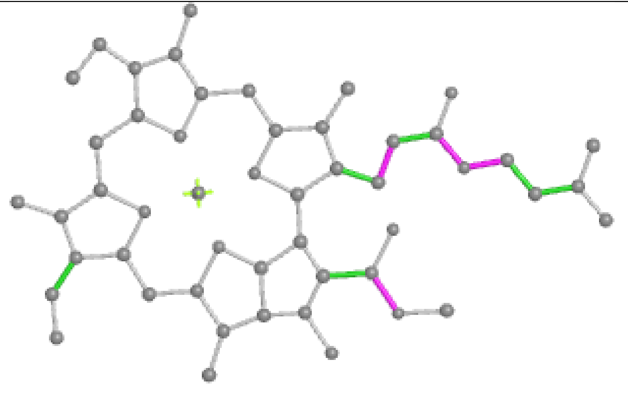
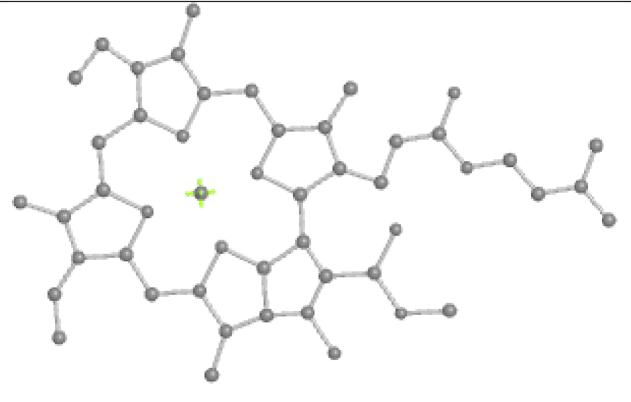
Bond angles

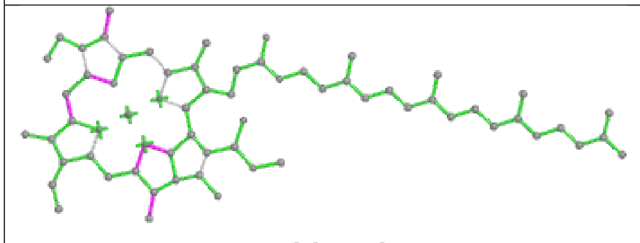
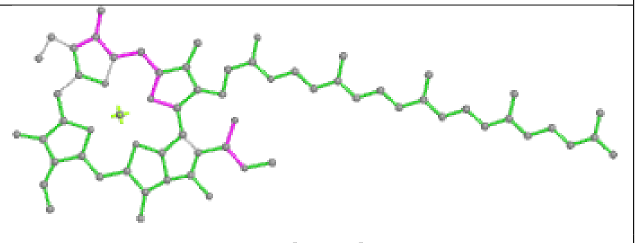
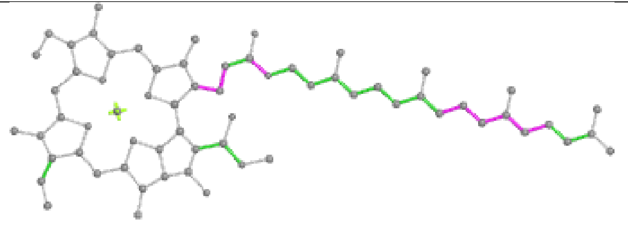
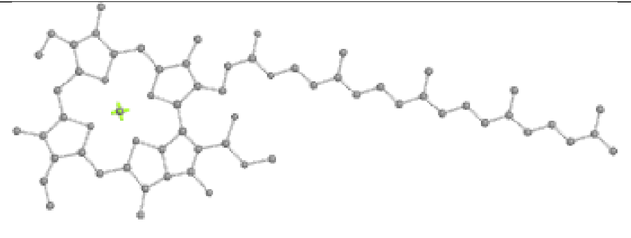


Torsions

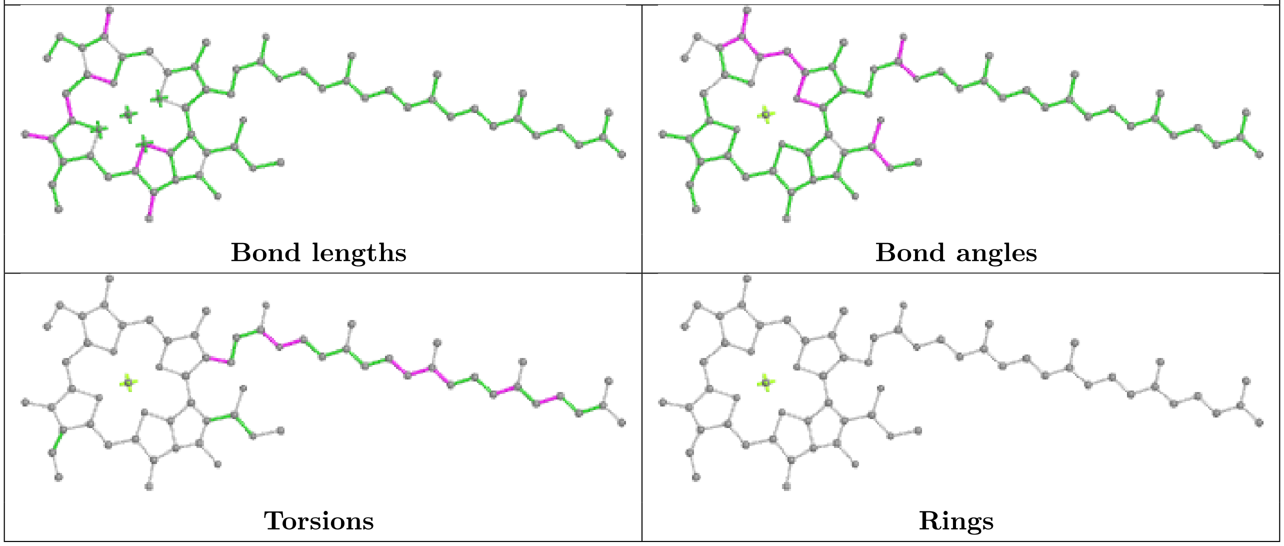


Rings

Ligand CLA a 811	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA a 822	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA b 823



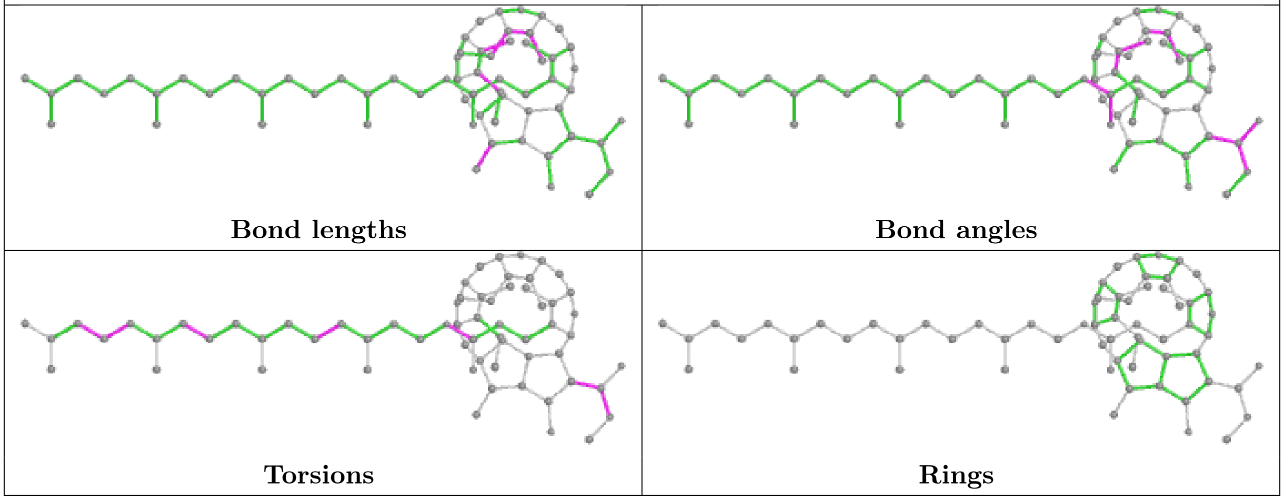
Bond lengths

Bond angles

Torsions

Rings

Ligand PHO D 401



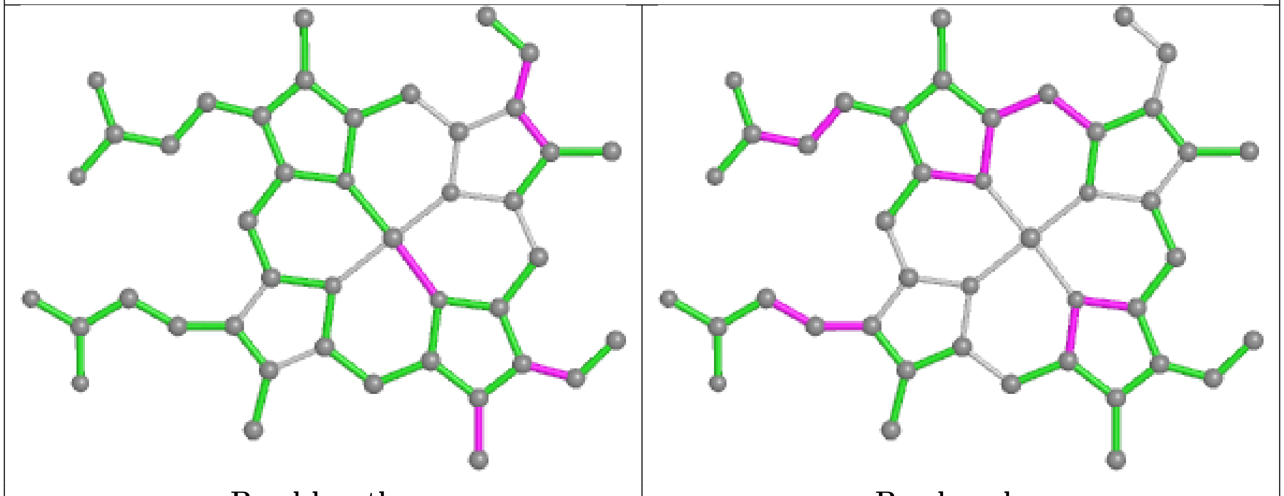
Bond lengths

Bond angles

Torsions

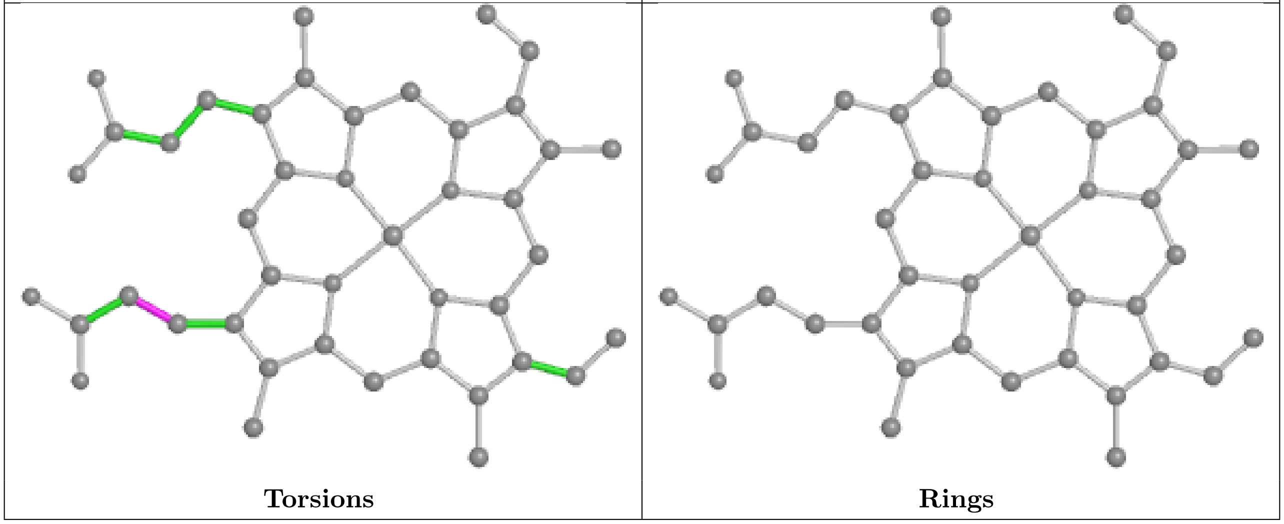
Rings

Ligand HEM E 101



Bond lengths

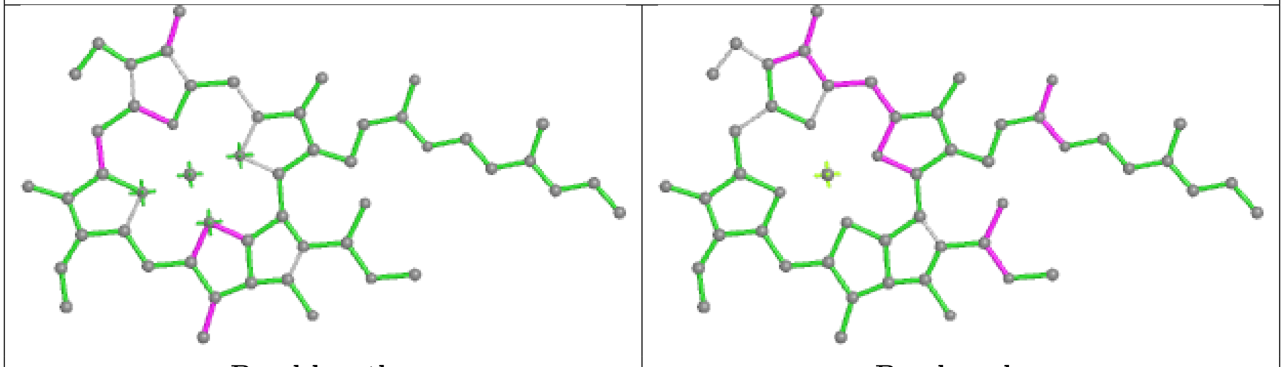
Bond angles



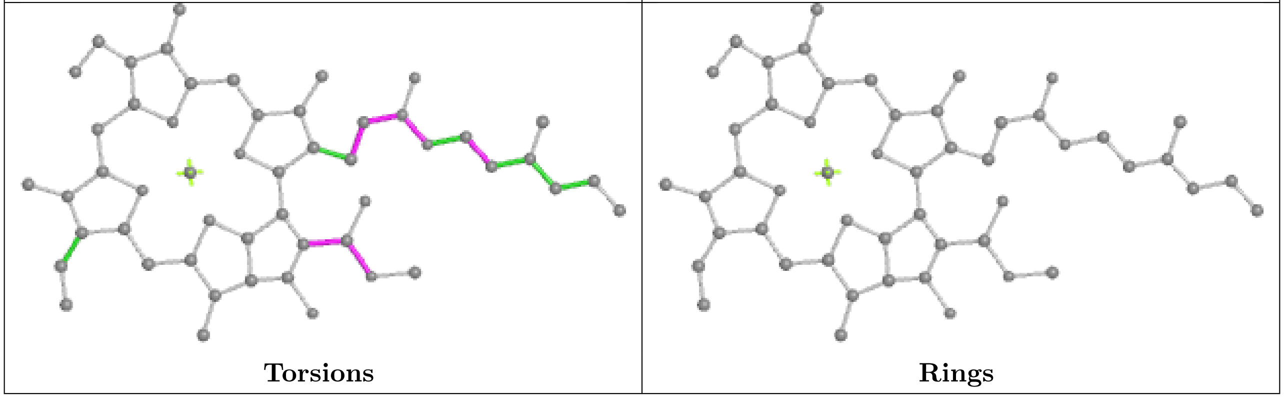
Torsions

Rings

Ligand CLA l 204

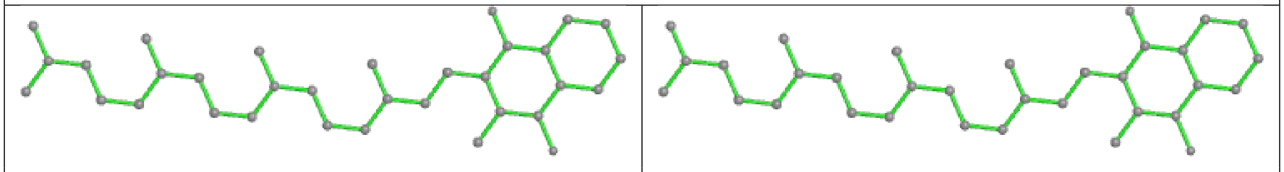


Bond lengths Bond angles

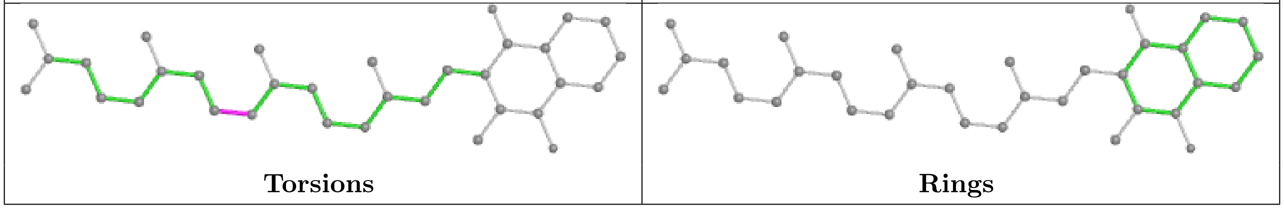


Torsions Rings

Ligand PQN a 844

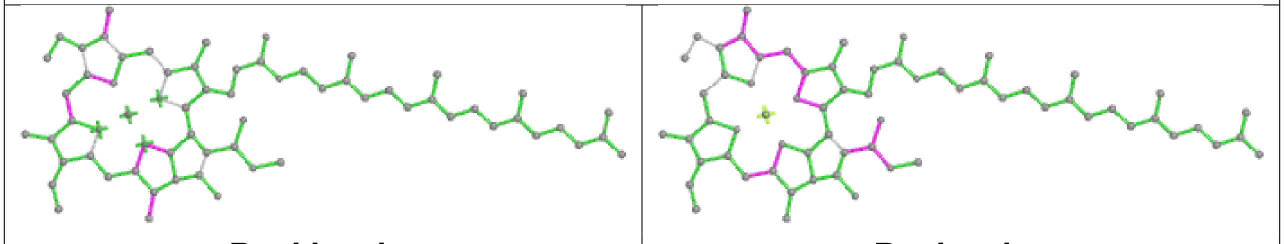


Bond lengths Bond angles

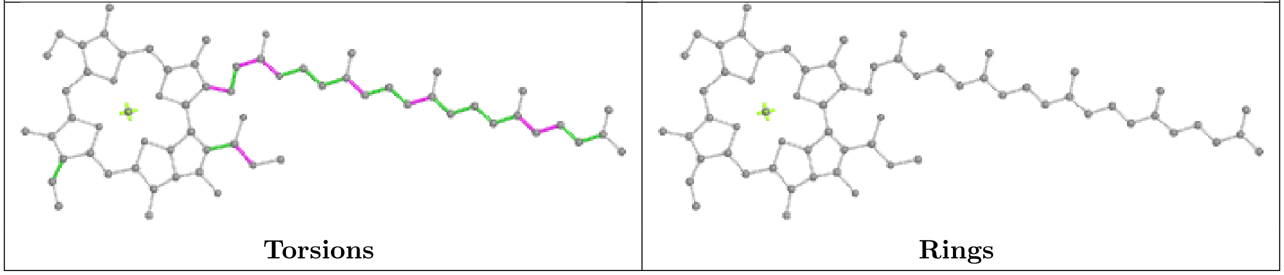


Torsions Rings

Ligand CLA b 804

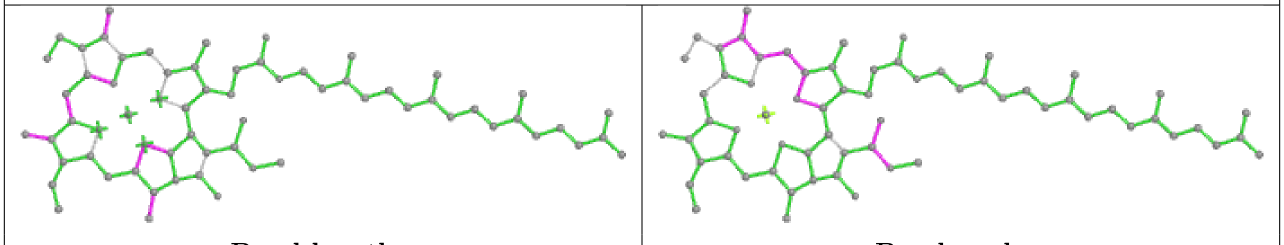


Bond lengths Bond angles

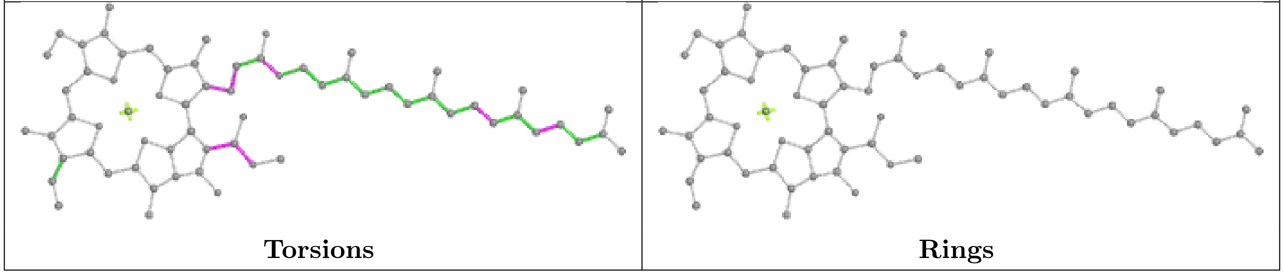


Torsions Rings

Ligand CLA a 805

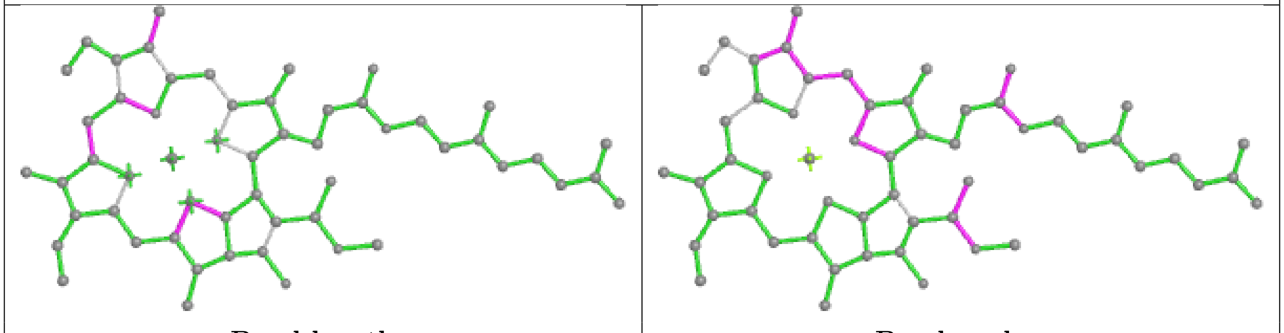


Bond lengths Bond angles



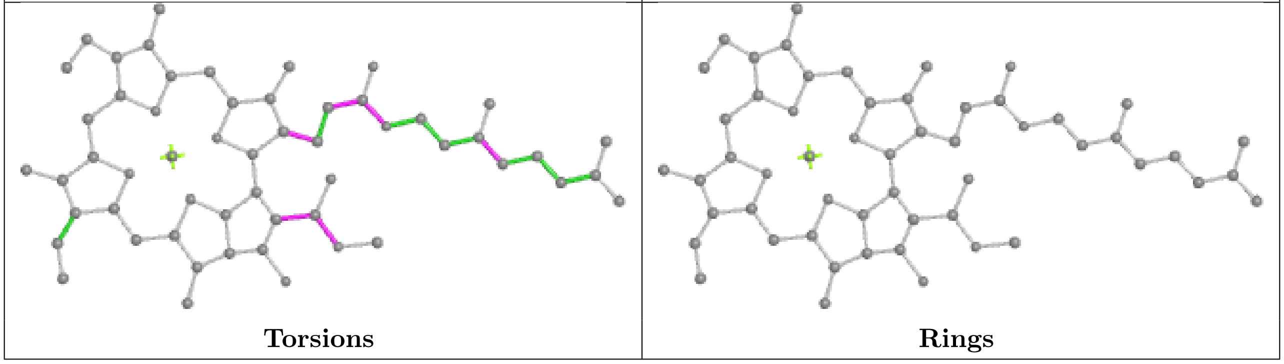
Torsions Rings

Ligand CLA j 103



Bond lengths

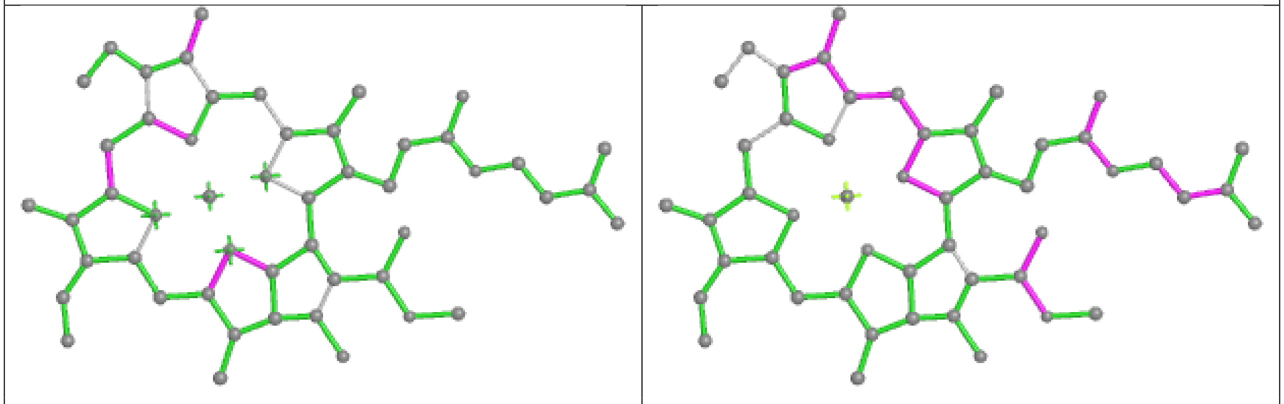
Bond angles



Torsions

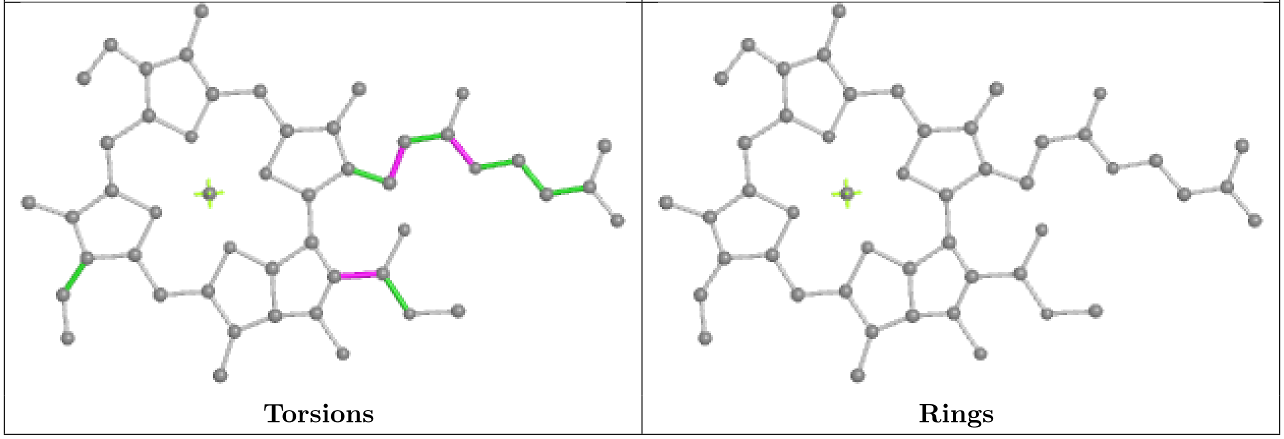
Rings

Ligand CLA f 204



Bond lengths

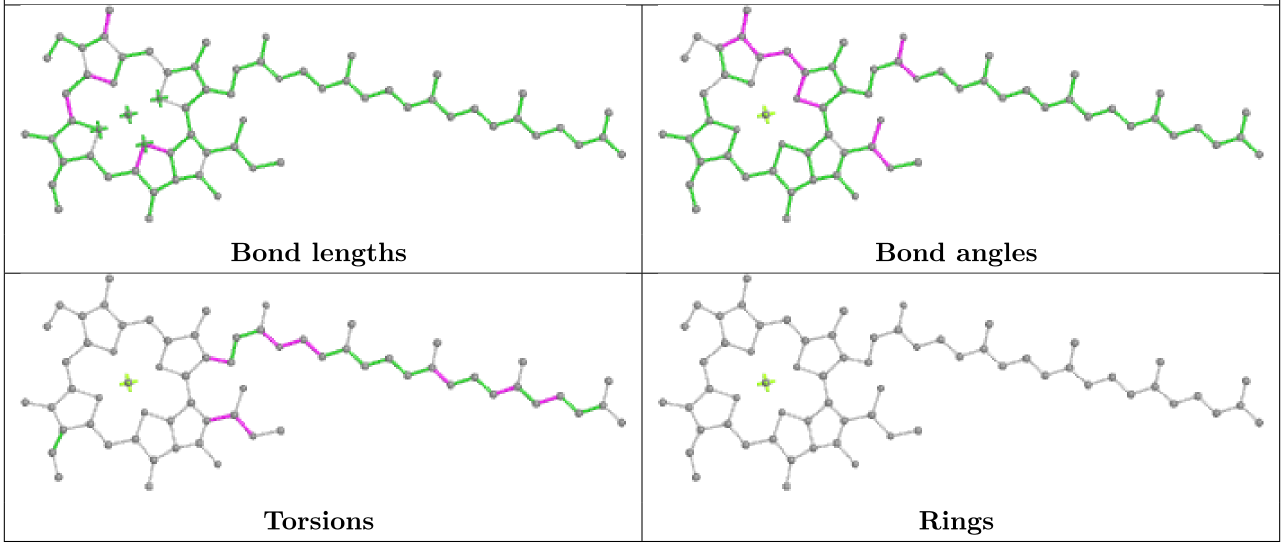
Bond angles



Torsions

Rings

Ligand CLA a 823



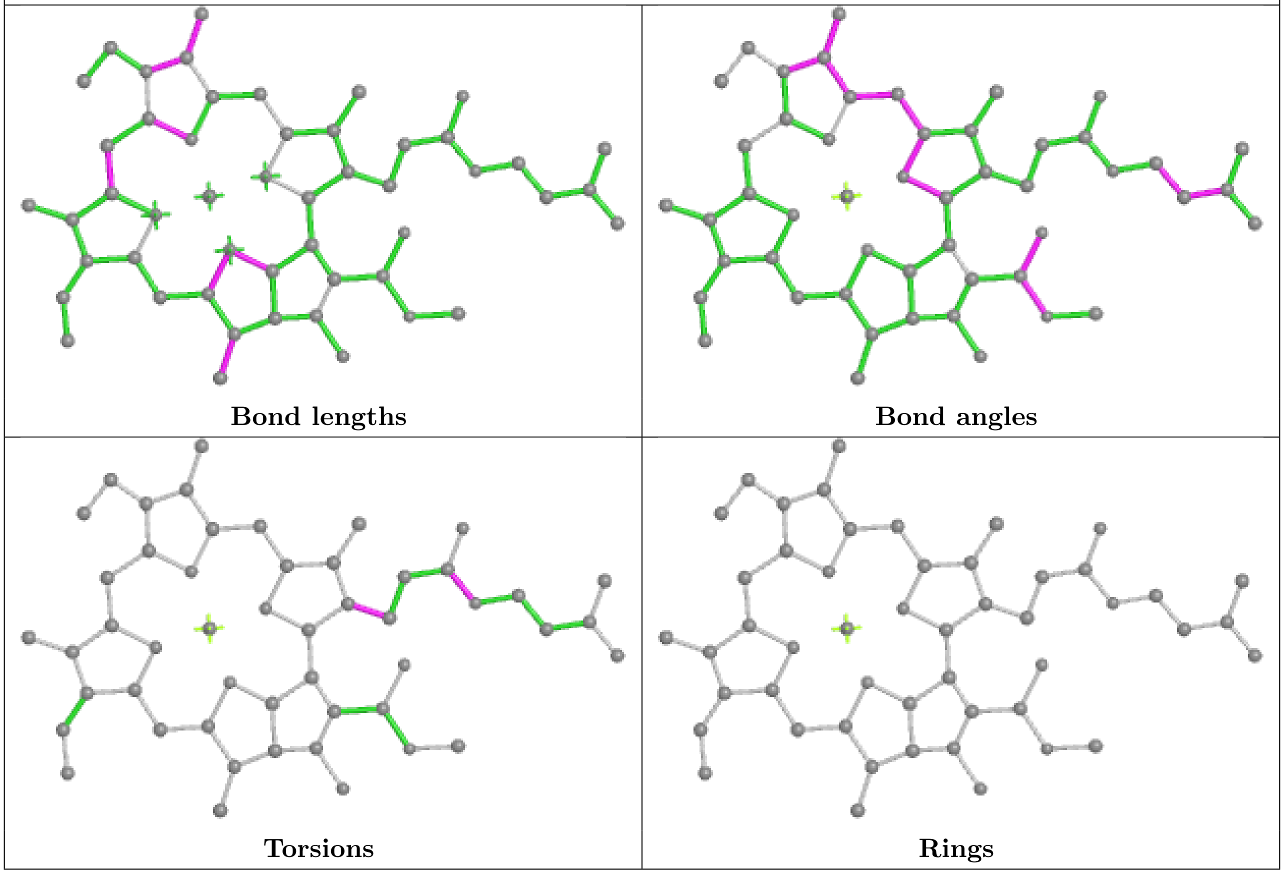
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA b 837



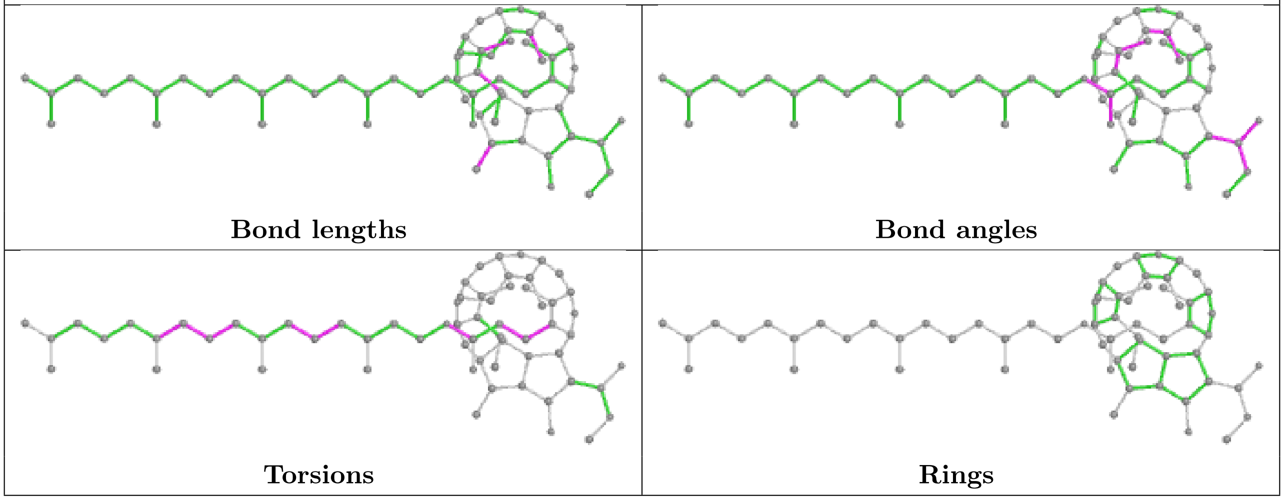
Bond lengths

Bond angles

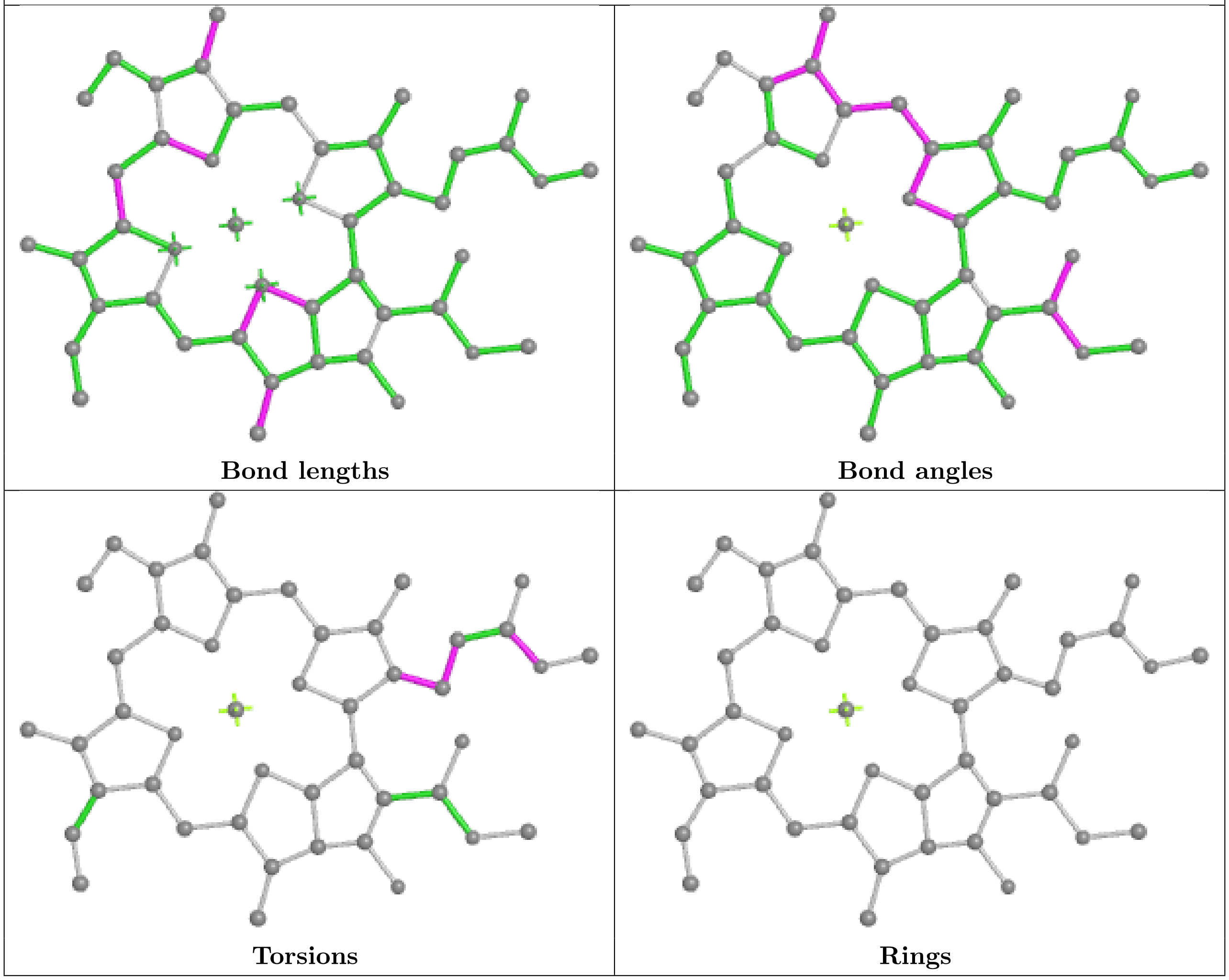
Torsions

Rings

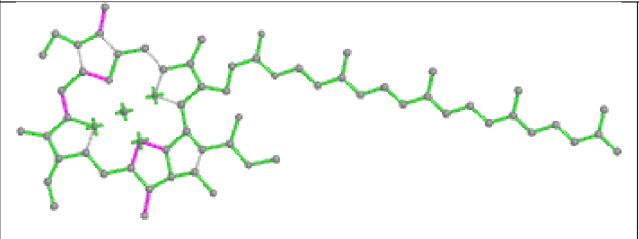
Ligand PHO A 404


Bond lengths
Bond angles
Torsions
Rings

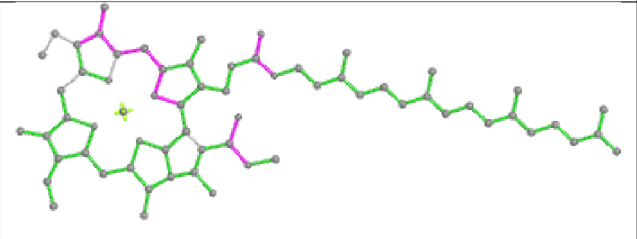
Ligand CLA a 817


Bond lengths
Bond angles
Torsions
Rings

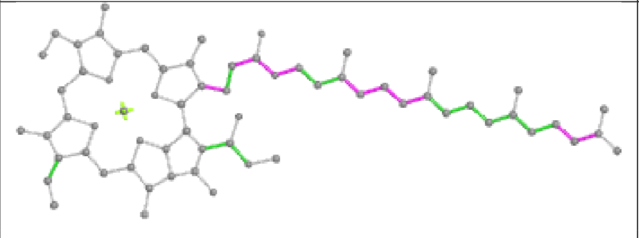
Ligand CLA b 806



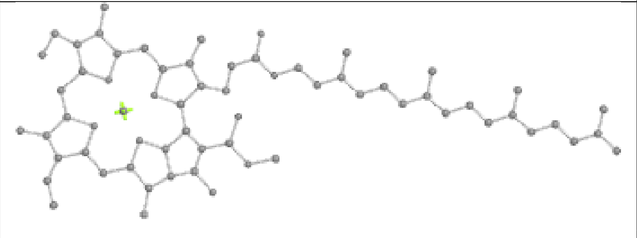
Bond lengths



Bond angles

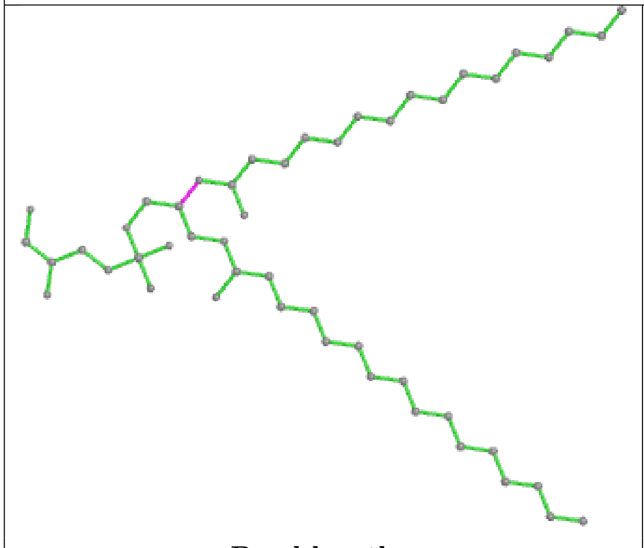


Torsions

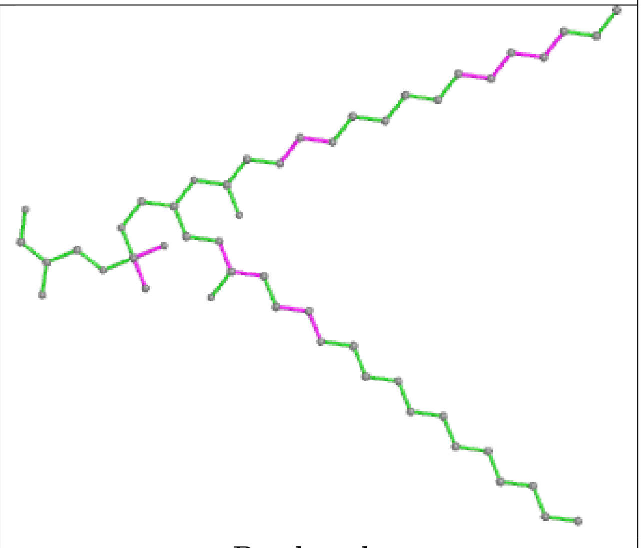


Rings

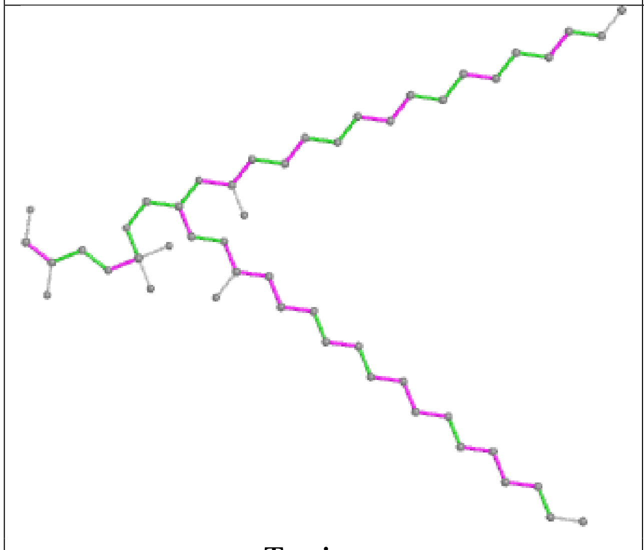
Ligand LHG a 852



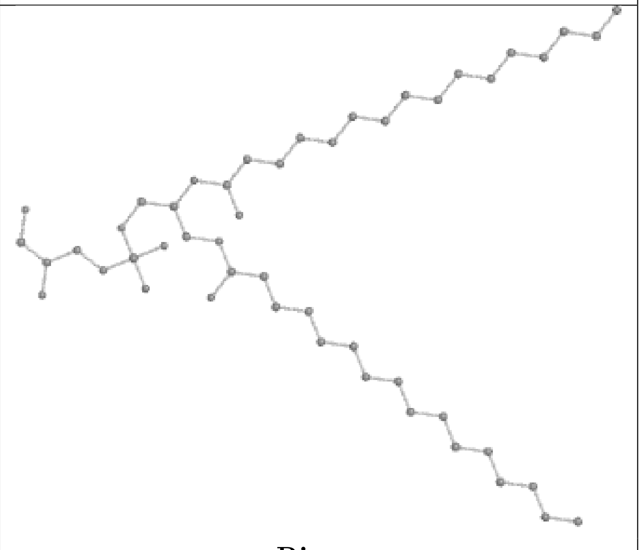
Bond lengths



Bond angles

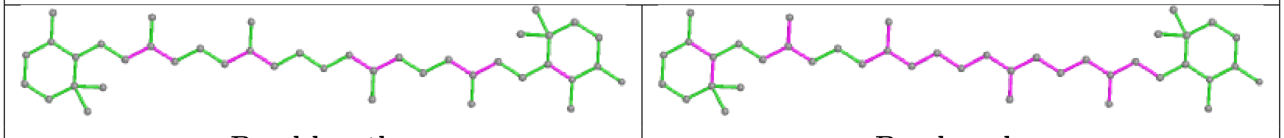


Torsions



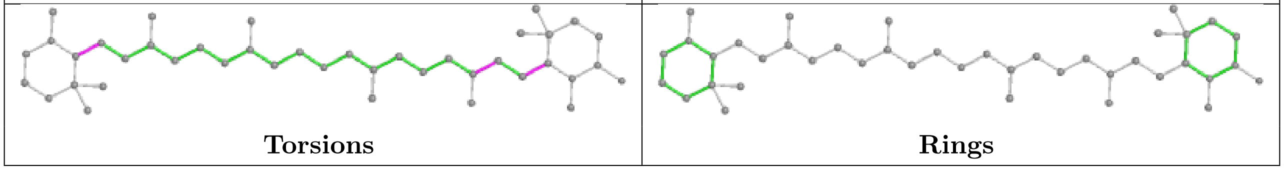
Rings

Ligand ECH m 101



Bond lengths

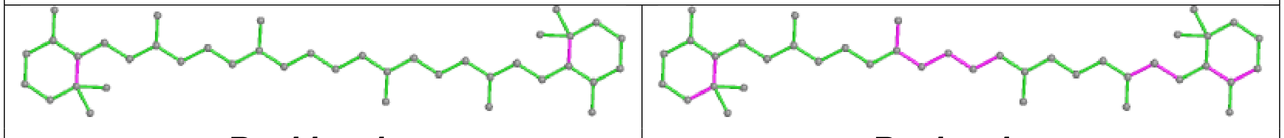
Bond angles



Torsions

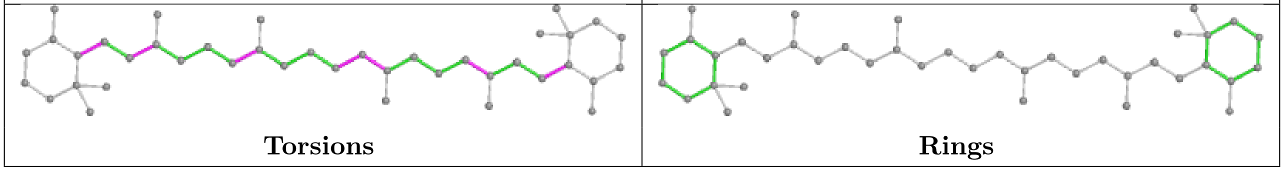
Rings

Ligand BCR k 103



Bond lengths

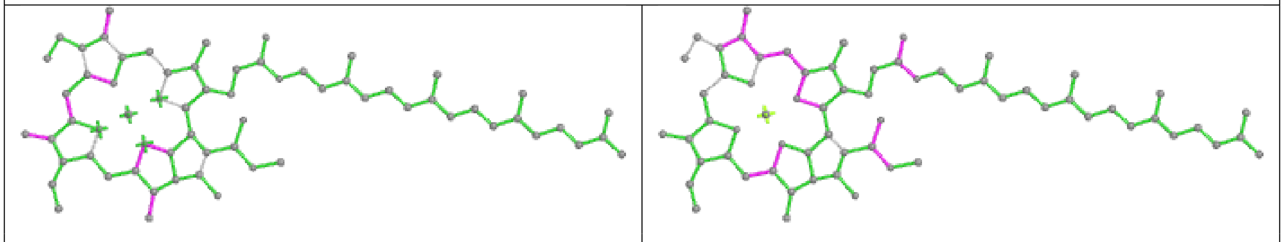
Bond angles



Torsions

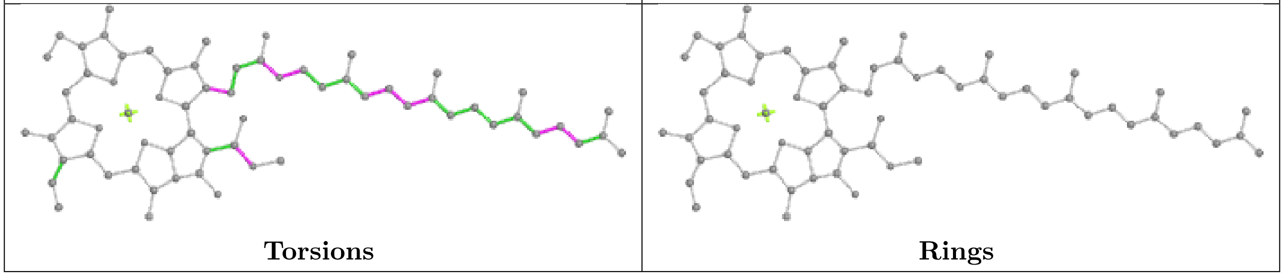
Rings

Ligand CLA a 841



Bond lengths

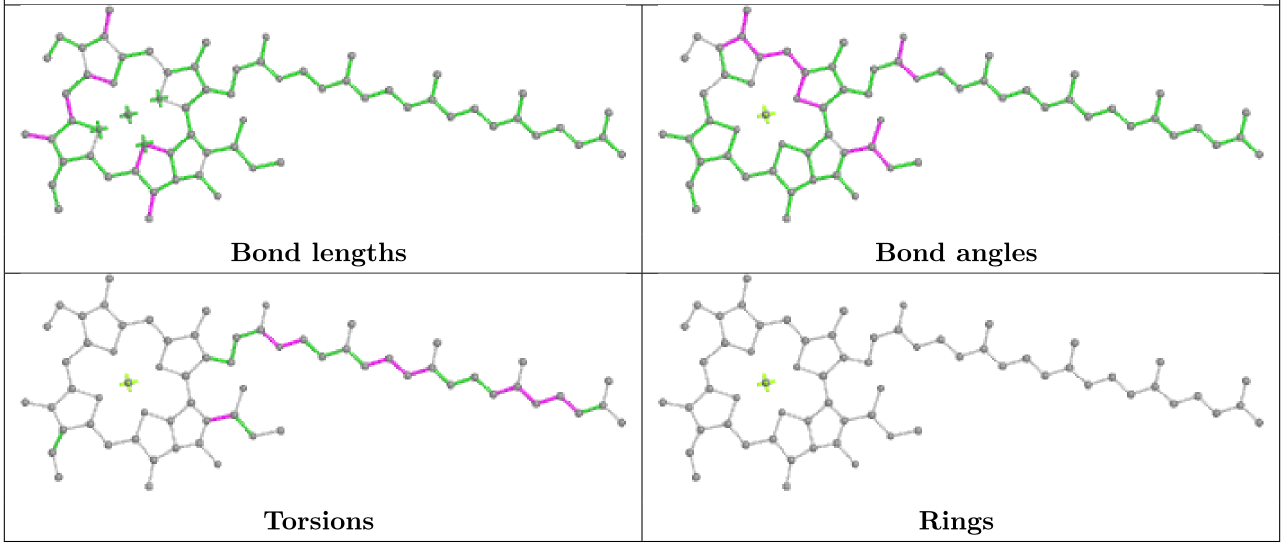
Bond angles



Torsions

Rings

Ligand CLA a 826



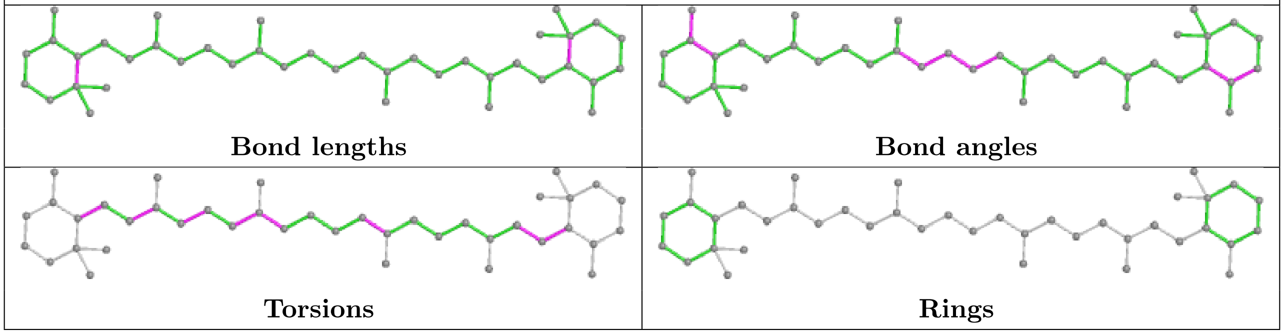
Bond lengths

Bond angles

Torsions

Rings

Ligand BCR l 205



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.

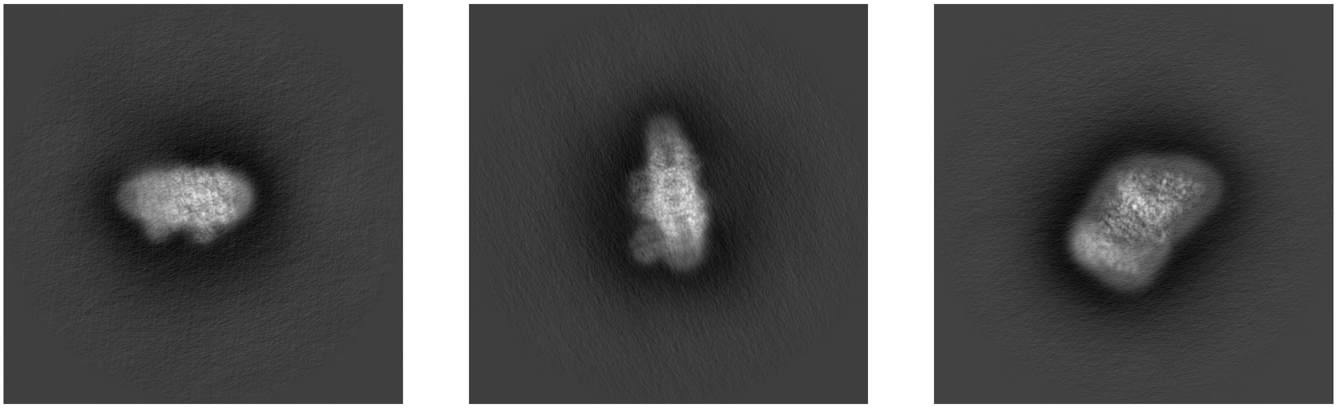
6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-15522. 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.

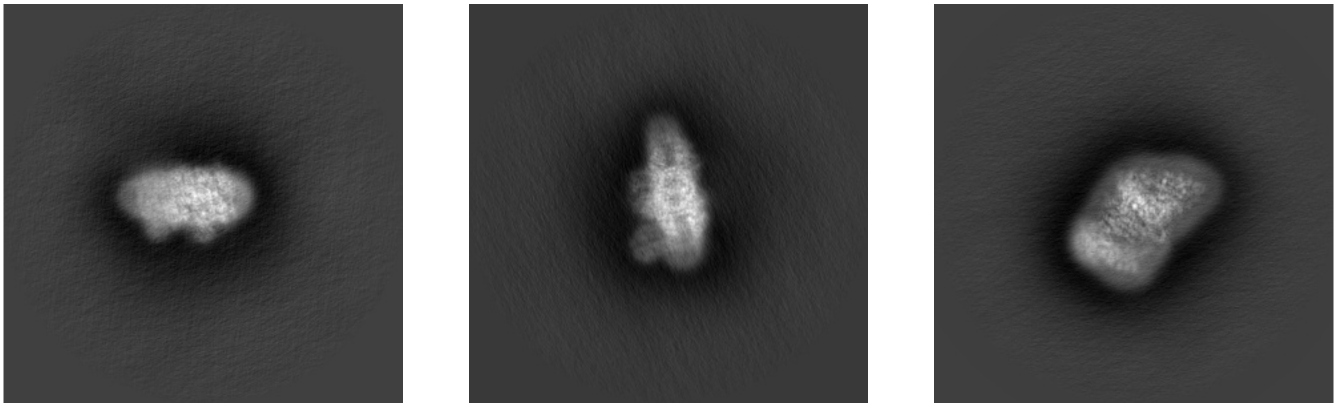
6.1 Orthogonal projections ⓘ

6.1.1 Primary map



X Y Z

6.1.2 Raw map

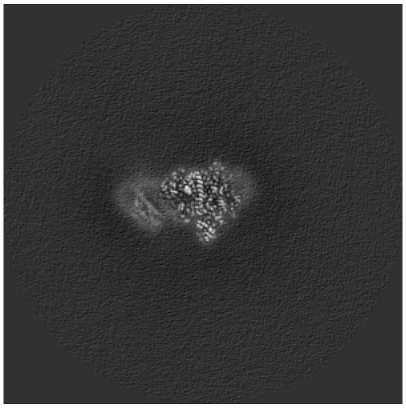


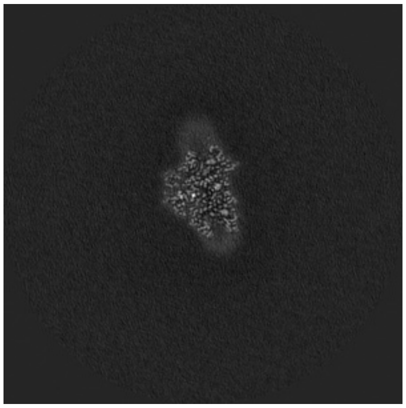
X Y Z

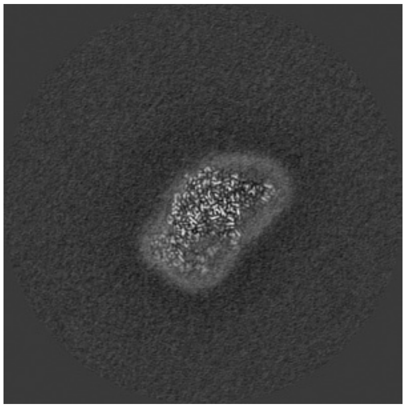
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ

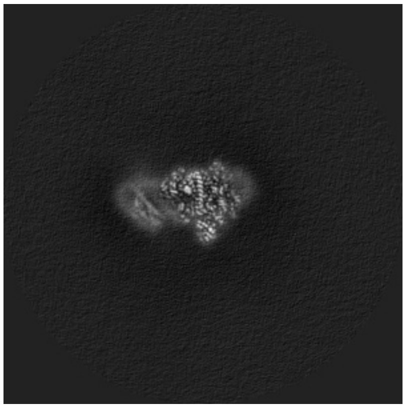
6.2.1 Primary map

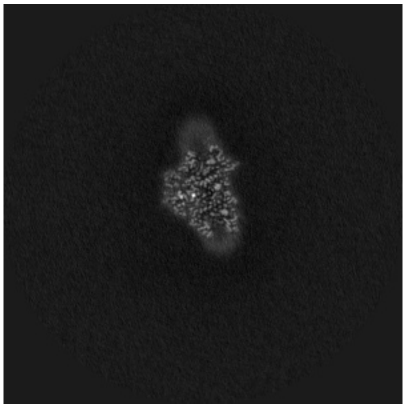

X Index: 200

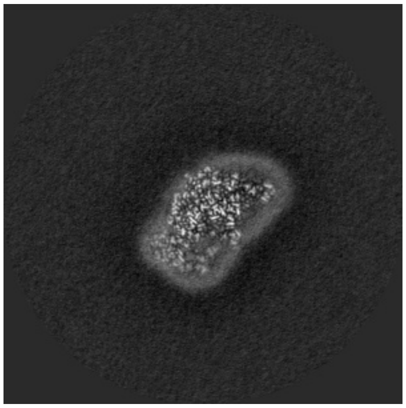

Y Index: 200


Z Index: 200

6.2.2 Raw map


X Index: 200

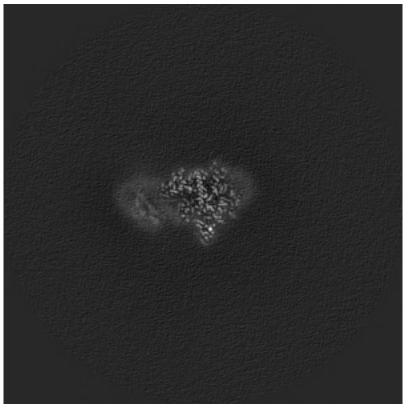

Y Index: 200


Z Index: 200

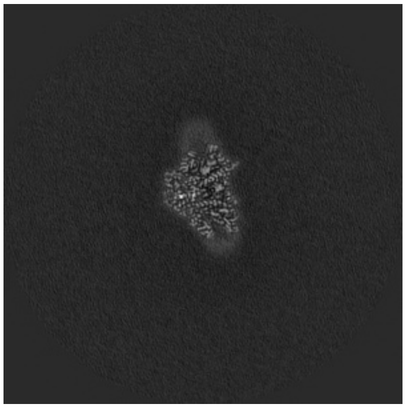
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices

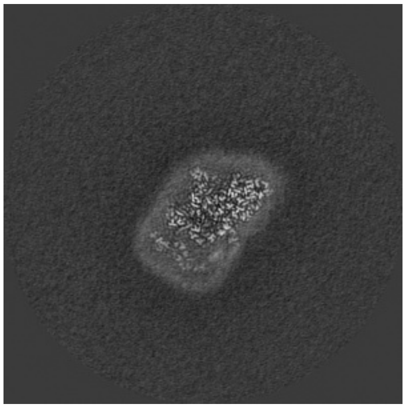
6.3.1 Primary map



X Index: 201

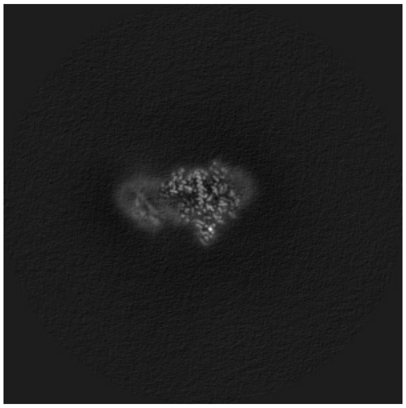


Y Index: 199

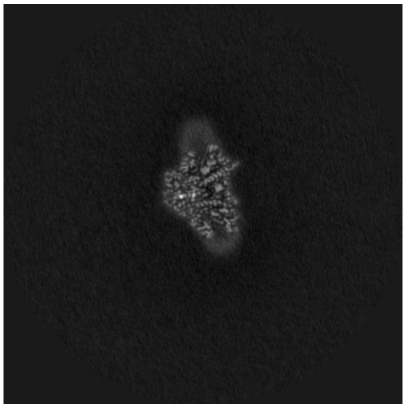


Z Index: 210

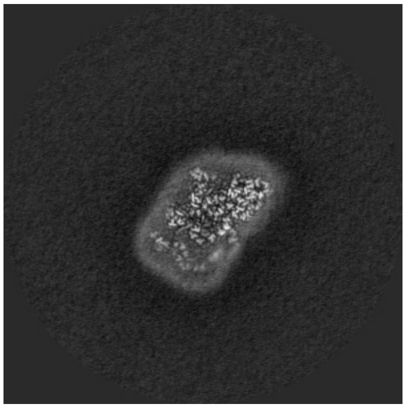
6.3.2 Raw map



X Index: 201



Y Index: 199

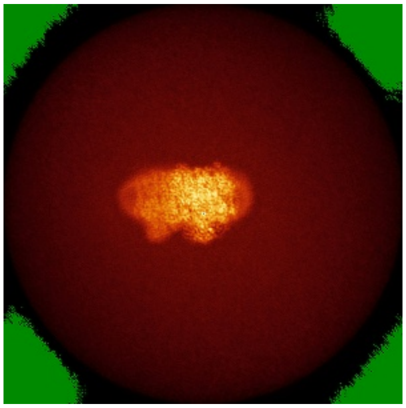


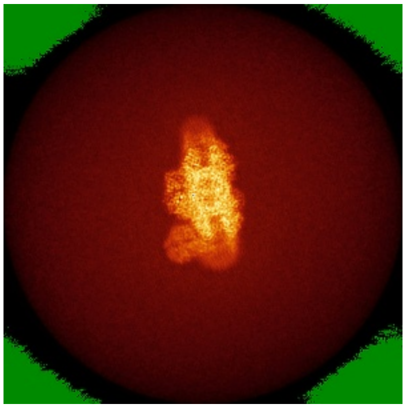
Z Index: 210

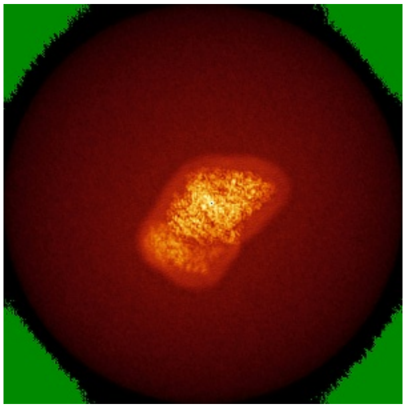
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color)

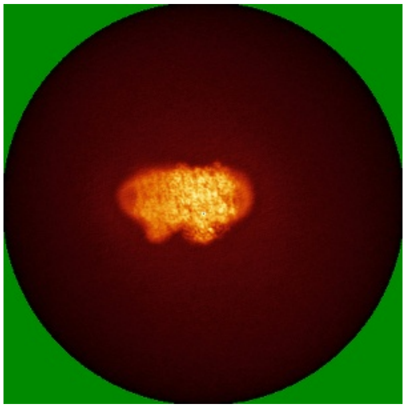
6.4.1 Primary map

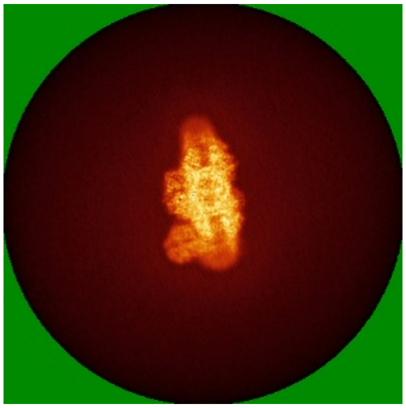

X

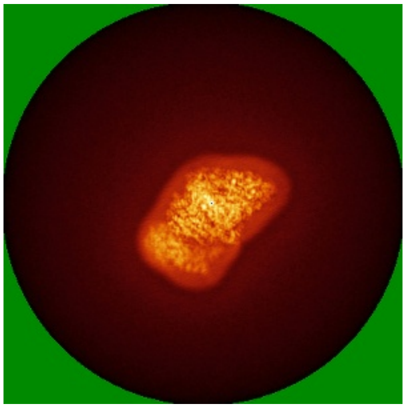

Y


Z

6.4.2 Raw map


X

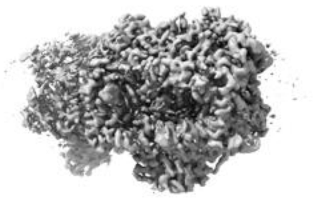

Y


Z

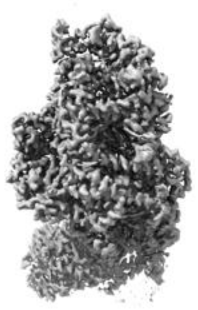
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views

6.5.1 Primary map



X

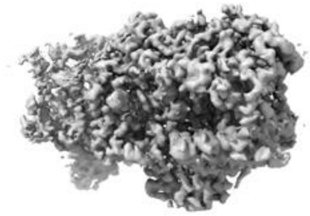


Y

Z

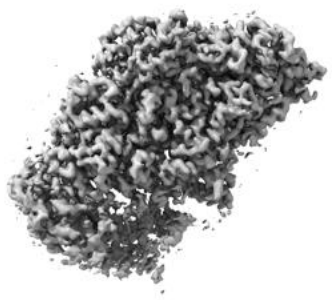
The images above show the 3D surface view of the map at the recommended contour level 0.0845. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

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.

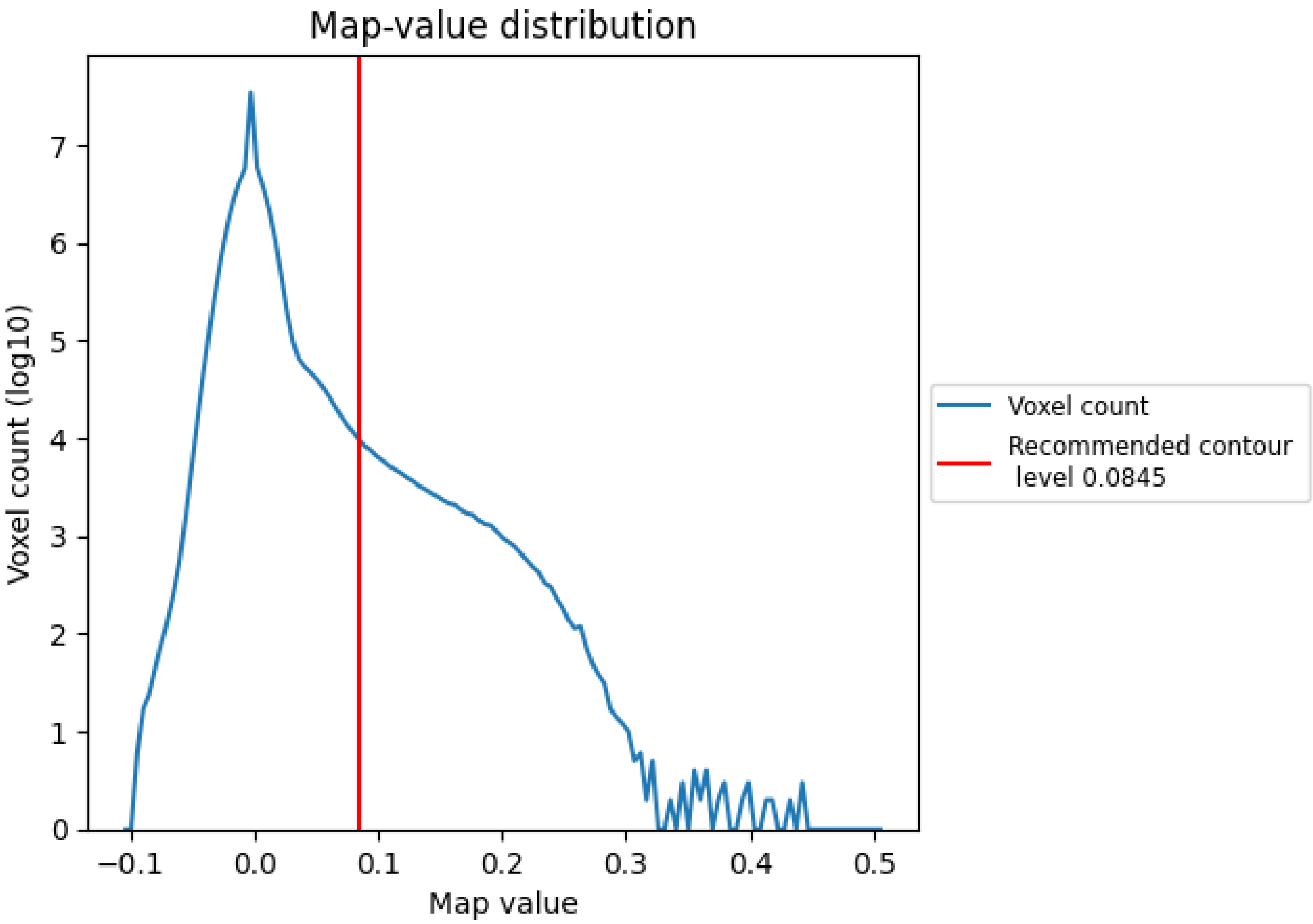
6.6 Mask visualisation

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

7 Map analysis ⓘ

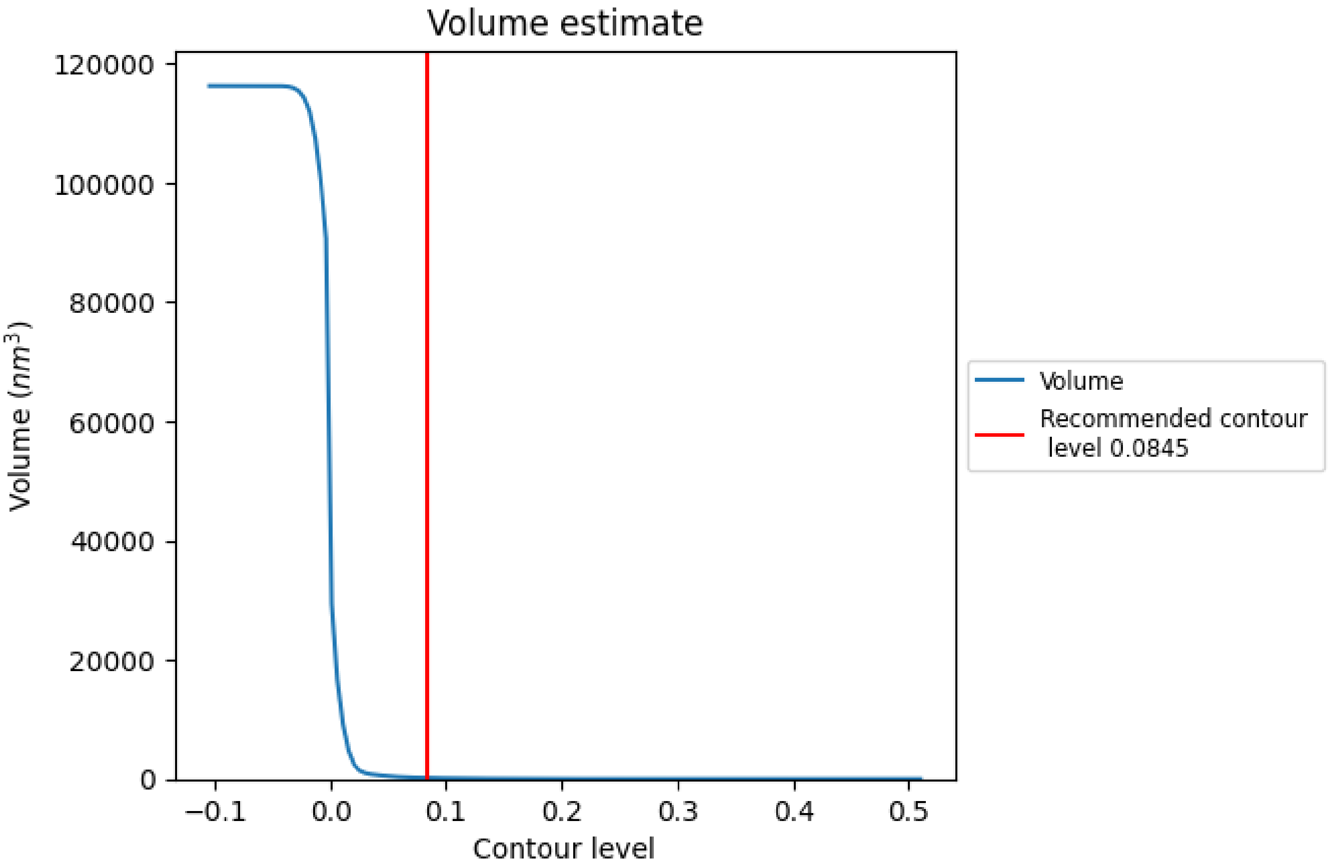
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

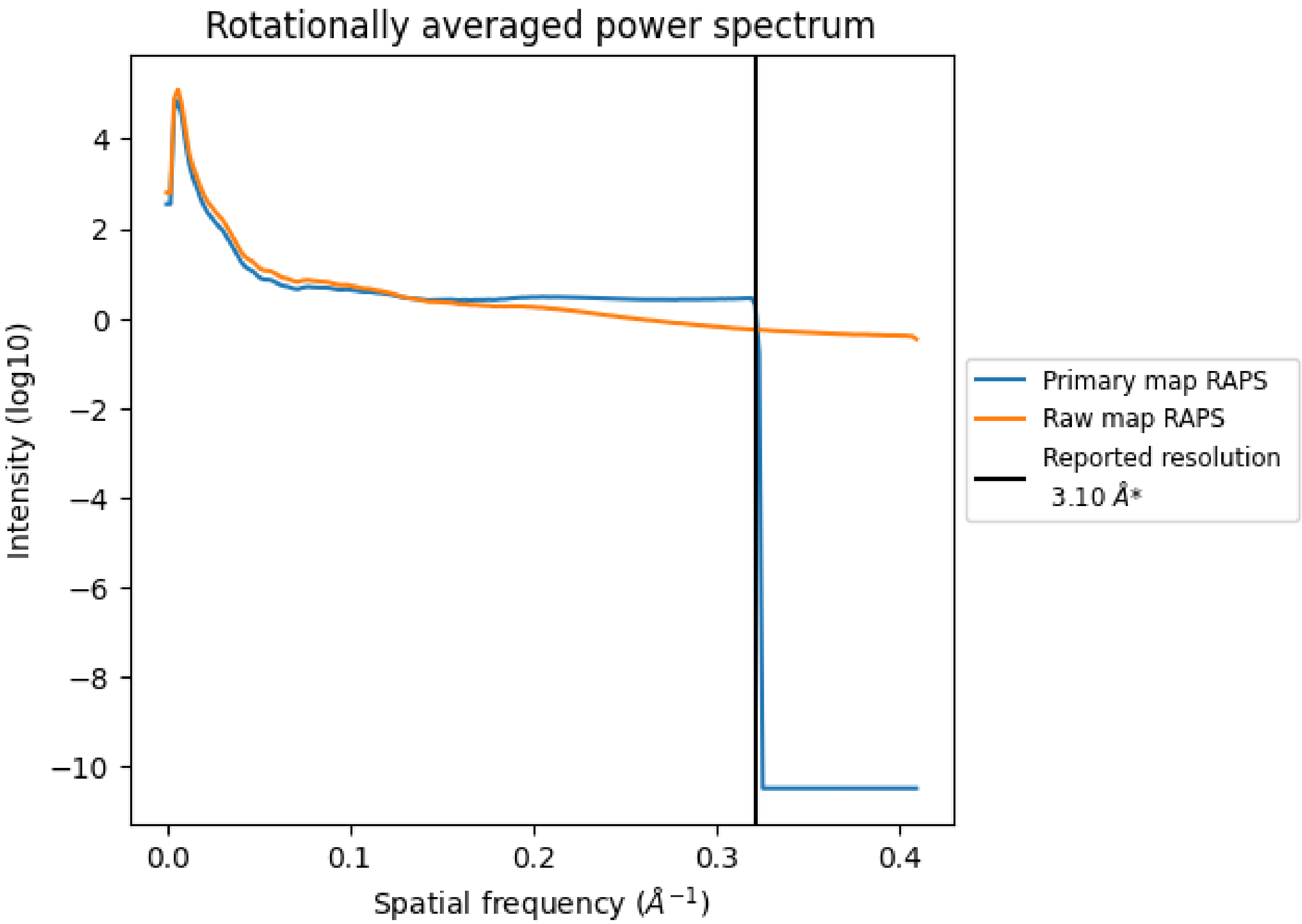
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 173 nm^3; this corresponds to an approximate mass of 156 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

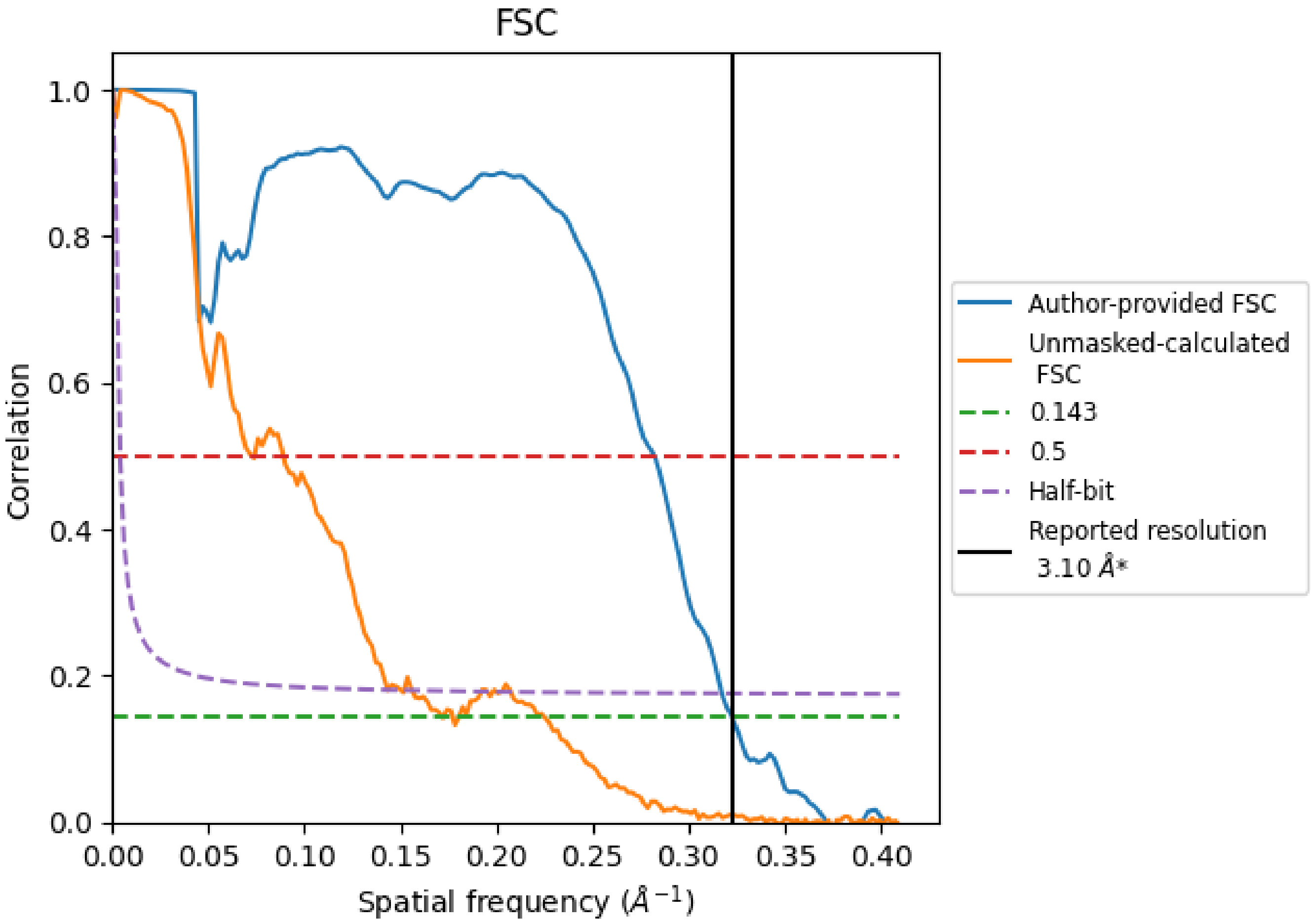


*Reported resolution corresponds to spatial frequency of 0.323 Å^{-1}

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 0.323 Å^{-1}

8.2 Resolution estimates ⓘ

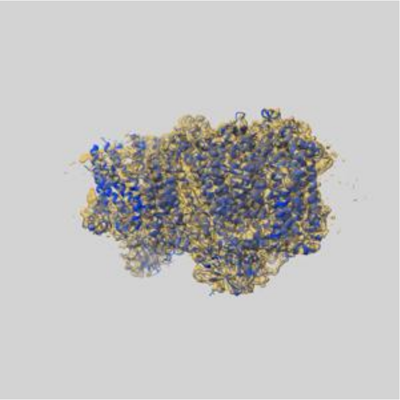
Resolution estimate (Å)	**Estimation criterion (FSC cut-off)**		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.10	3.55	3.15
Unmasked-calculated*	5.82	13.79	6.97

*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 5.82 differs from the reported value 3.1 by more than 10 %

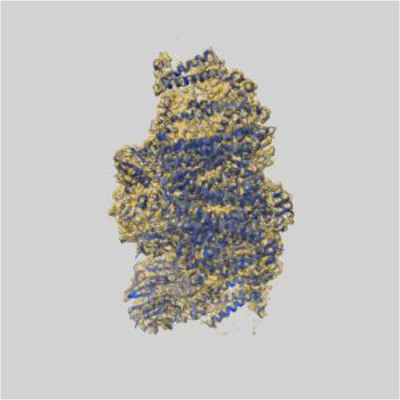
9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-15522 and PDB model 8AM5. Per-residue inclusion information can be found in section 3 on page 23.

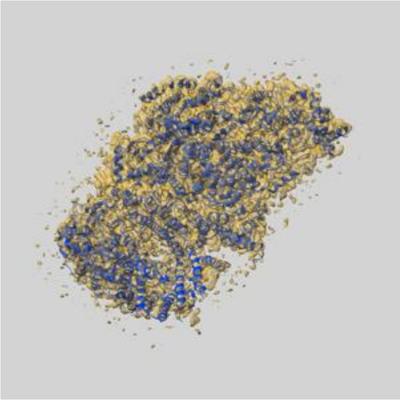
9.1 Map-model overlay ⓘ



X



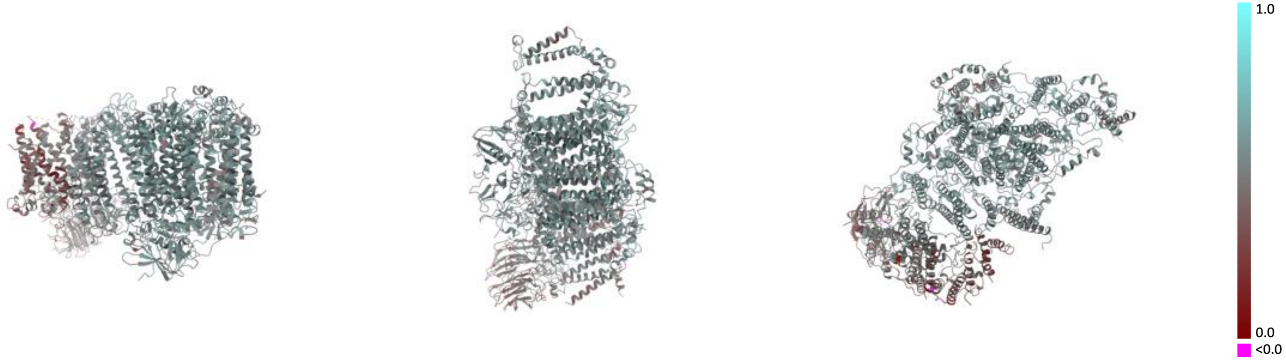
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0845 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.

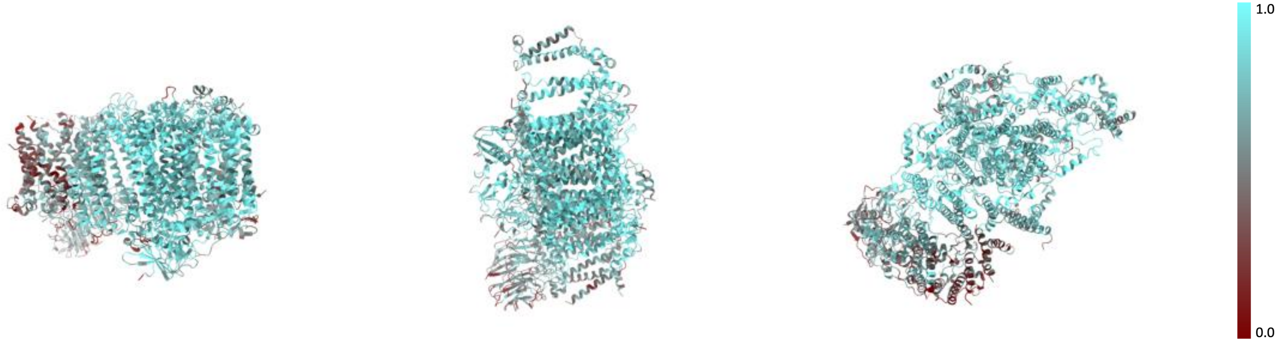
9.2 Q-score mapped to coordinate model ⓘ



X Y Z

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.

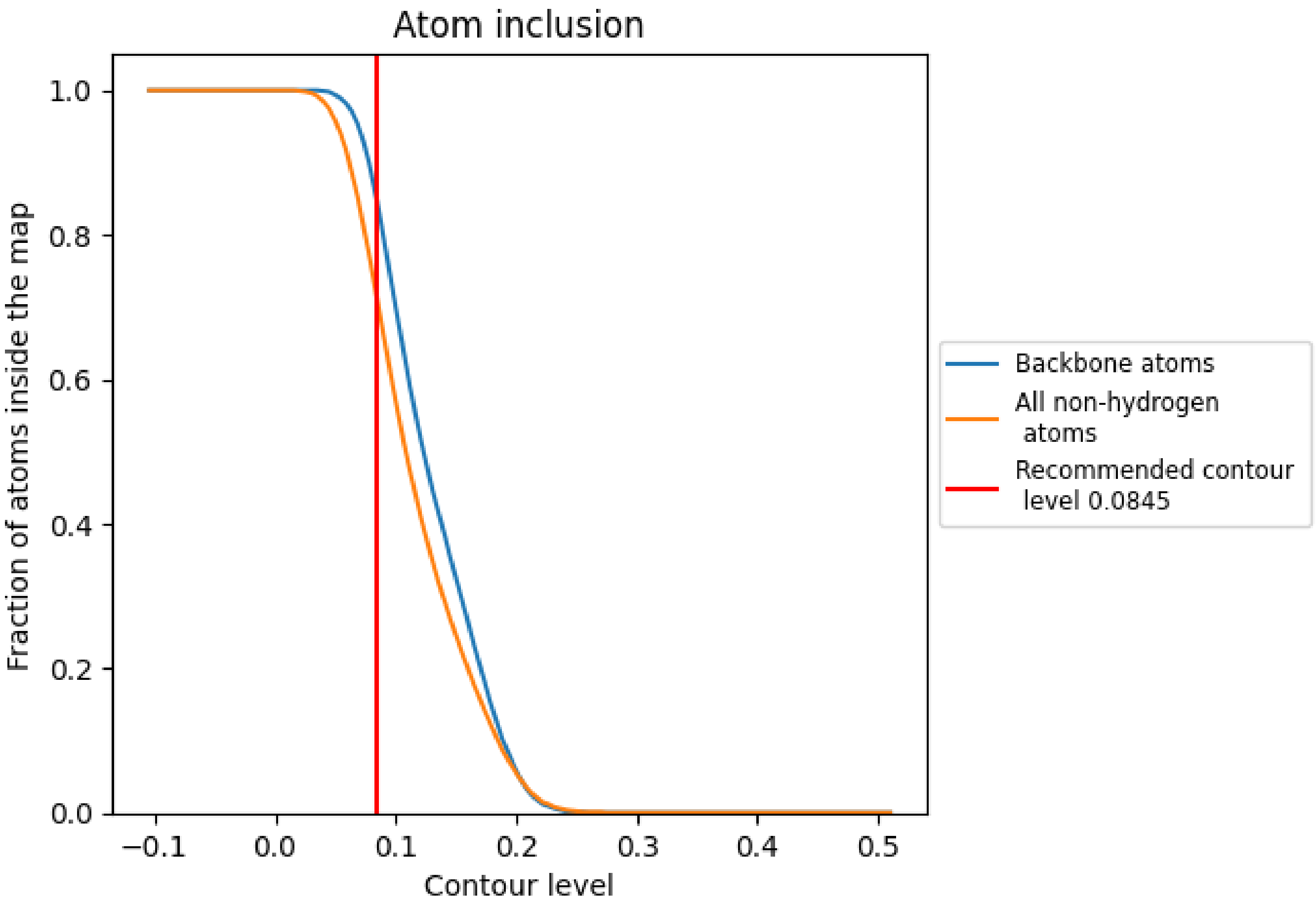
9.3 Atom inclusion mapped to coordinate model ⓘ



X Y Z

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 (0.0845).

9.4 Atom inclusion ⓘ



At the recommended contour level, 85% of all backbone atoms, 71% 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 (0.0845) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7120	0.5200
A	0.6090	0.4720
D	0.4770	0.4120
E	0.4100	0.3530
F	0.3460	0.3150
I	0.4820	0.4130
S	0.4850	0.4110
a	0.7970	0.5600
b	0.8220	0.5610
c	0.8970	0.5540
d	0.7830	0.5440
e	0.7480	0.5360
f	0.6720	0.5250
i	0.7080	0.5450
j	0.5850	0.5060
k	0.5770	0.4970
l	0.6190	0.4990
m	0.6920	0.5460