wwPDB EM Validation Summary Report ⓘ

Nov 23, 2022 – 10:02 AM JST

PDB ID	:	7VD6
EMDB ID	:	EMD-31906
Title	:	Structure of S1M1-type FCPII complex from diatom
Authors	:	Nagao, R.; Kato, K.; Akita, F.; Miyazaki, N.; Shen, J.R.
Deposited on	:	2021-09-06
Resolution	:	2.80 Å(reported)
Based on initial model	:	6J40

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

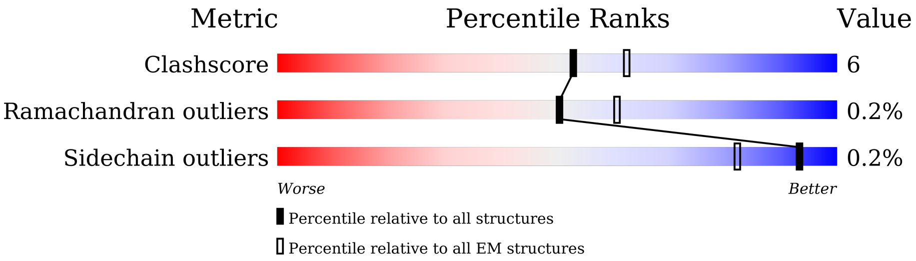
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 2.80 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	11	207	
1	13	207	
1	14	207	
1	15	207	
1	18	207	
2	12	207	
3	16	210	
4	17	207	

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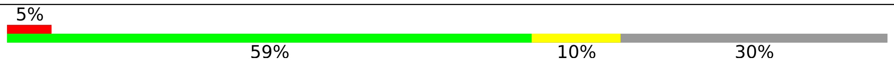
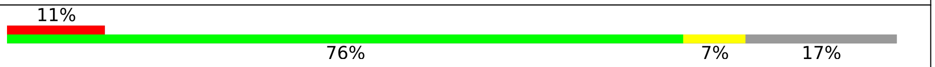
Mol	Chain	Length	Quality of chain
5	19	271	
6	20	223	
7	21	195	

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
8	CLA	11	303	X	-	-	-
8	CLA	11	305	X	-	-	-
8	CLA	11	309	X	-	-	-
8	CLA	12	301	X	-	-	-
8	CLA	12	303	X	-	-	-
8	CLA	12	304	X	-	-	-
8	CLA	12	305	X	-	-	-
8	CLA	12	309	X	-	-	-
8	CLA	12	311	X	-	-	-
8	CLA	13	304	X	-	-	-
8	CLA	13	306	X	-	-	-
8	CLA	13	308	X	-	-	-
8	CLA	14	302	X	-	-	-
8	CLA	14	305	X	-	-	-
8	CLA	14	307	X	-	-	-
8	CLA	14	308	X	-	-	-
8	CLA	14	310	X	-	-	-
8	CLA	15	303	X	-	-	-
8	CLA	15	305	X	-	-	-
8	CLA	15	307	X	-	-	-
8	CLA	15	308	X	-	-	-
8	CLA	15	310	X	-	-	-
8	CLA	16	303	X	-	-	-
8	CLA	16	306	X	-	-	-
8	CLA	16	307	X	-	-	-
8	CLA	16	309	X	-	-	-
8	CLA	17	304	X	-	-	-
8	CLA	17	307	X	-	-	-
8	CLA	17	308	X	-	-	-
8	CLA	17	310	X	-	-	-
8	CLA	18	302	X	-	-	-
8	CLA	18	303	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	CLA	18	305	X	-	-	-
8	CLA	18	307	X	-	-	-
8	CLA	18	308	X	-	-	-
8	CLA	19	301	X	-	-	-
8	CLA	19	302	X	-	-	-
8	CLA	19	303	X	-	-	-
8	CLA	19	304	X	-	-	-
8	CLA	19	305	X	-	-	-
8	CLA	19	306	X	-	-	-
8	CLA	19	307	X	-	-	-
8	CLA	19	309	X	-	-	-
8	CLA	19	310	X	-	-	-
8	CLA	20	304	X	-	-	-
8	CLA	20	307	X	-	-	-
8	CLA	20	308	X	-	-	-
8	CLA	20	309	X	-	-	-
8	CLA	20	310	X	-	-	-
8	CLA	21	202	X	-	-	-
8	CLA	21	204	X	-	-	-
8	CLA	21	205	X	-	-	-
8	CLA	21	206	X	-	-	-
8	CLA	21	208	X	-	-	-
8	CLA	21	209	X	-	-	-

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 23937 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 Chlorophyll a/b-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	11	176	1343	852	228	256	7	0	0
1	13	169	1296	823	220	246	7	0	0
1	14	172	1319	838	223	251	7	0	0
1	15	170	1307	832	221	247	7	0	0
1	18	168	1289	818	219	245	7	0	0

- Molecule 2 is a protein called Fcpb2, Fucoxanthin chlorophyll a/c-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	12	169	1302	828	222	244	8	0	0

- Molecule 3 is a protein called Fcpb3, Fucoxanthin chlorophyll a/c-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	16	179	1386	891	233	256	6	0	0

- Molecule 4 is a protein called Fcpb4, Fucoxanthin chlorophyll a/c-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	17	176	1353	862	227	258	6	0	0

- Molecule 5 is a protein called Fcpb5, Fucoxanthin chlorophyll a/c-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	19	220	1690	1088	283	314	5	0	0

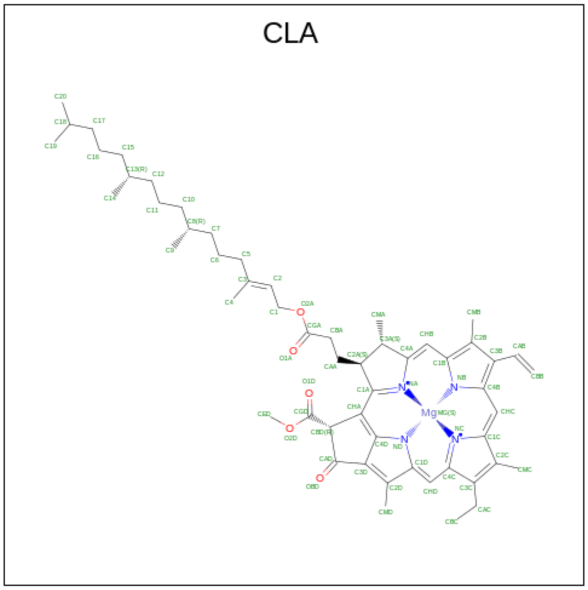
- Molecule 6 is a protein called Fcpb6, Fucoxanthin chlorophyll a/c-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	20	155	1198	773	202	215	8	0	0

- Molecule 7 is a protein called Fcpb7, Fucoxanthin chlorophyll a/c-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	21	162	1262	822	206	229	5	0	0

- Molecule 8 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
8	11	1	278	228	5	20	25	0
8	11	1	278	228	5	20	25	0
8	11	1	278	228	5	20	25	0
8	11	1	278	228	5	20	25	0

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Mol	Chain	Residues	Atoms	AltConf
8	11	1	Total C Mg N O 278 228 5 20 25	0
8	12	1	Total C Mg N O 407 337 7 28 35	0
8	12	1	Total C Mg N O 407 337 7 28 35	0
8	12	1	Total C Mg N O 407 337 7 28 35	0
8	12	1	Total C Mg N O 407 337 7 28 35	0
8	12	1	Total C Mg N O 407 337 7 28 35	0
8	12	1	Total C Mg N O 407 337 7 28 35	0
8	12	1	Total C Mg N O 407 337 7 28 35	0
8	13	1	Total C Mg N O 394 324 7 28 35	0
8	13	1	Total C Mg N O 394 324 7 28 35	0
8	13	1	Total C Mg N O 394 324 7 28 35	0
8	13	1	Total C Mg N O 394 324 7 28 35	0
8	13	1	Total C Mg N O 394 324 7 28 35	0
8	13	1	Total C Mg N O 394 324 7 28 35	0
8	13	1	Total C Mg N O 394 324 7 28 35	0
8	14	1	Total C Mg N O 394 324 7 28 35	0
8	14	1	Total C Mg N O 394 324 7 28 35	0
8	14	1	Total C Mg N O 394 324 7 28 35	0
8	14	1	Total C Mg N O 394 324 7 28 35	0
8	14	1	Total C Mg N O 394 324 7 28 35	0
8	14	1	Total C Mg N O 394 324 7 28 35	0

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Mol	Chain	Residues	Atoms					AltConf
8	14	1	Total 394	C 324	Mg 7	N 28	O 35	0
8	15	1	Total 329	C 269	Mg 6	N 24	O 30	0
8	15	1	Total 329	C 269	Mg 6	N 24	O 30	0
8	15	1	Total 329	C 269	Mg 6	N 24	O 30	0
8	15	1	Total 329	C 269	Mg 6	N 24	O 30	0
8	15	1	Total 329	C 269	Mg 6	N 24	O 30	0
8	15	1	Total 329	C 269	Mg 6	N 24	O 30	0
8	16	1	Total 293	C 243	Mg 5	N 20	O 25	0
8	16	1	Total 293	C 243	Mg 5	N 20	O 25	0
8	16	1	Total 293	C 243	Mg 5	N 20	O 25	0
8	16	1	Total 293	C 243	Mg 5	N 20	O 25	0
8	16	1	Total 293	C 243	Mg 5	N 20	O 25	0
8	17	1	Total 303	C 253	Mg 5	N 20	O 25	0
8	17	1	Total 303	C 253	Mg 5	N 20	O 25	0
8	17	1	Total 303	C 253	Mg 5	N 20	O 25	0
8	17	1	Total 303	C 253	Mg 5	N 20	O 25	0
8	17	1	Total 303	C 253	Mg 5	N 20	O 25	0
8	18	1	Total 394	C 324	Mg 7	N 28	O 35	0
8	18	1	Total 394	C 324	Mg 7	N 28	O 35	0
8	18	1	Total 394	C 324	Mg 7	N 28	O 35	0
8	18	1	Total 394	C 324	Mg 7	N 28	O 35	0

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Mol	Chain	Residues	Atoms	AltConf
8	18	1	Total C Mg N O 394 324 7 28 35	0
8	18	1	Total C Mg N O 394 324 7 28 35	0
8	18	1	Total C Mg N O 394 324 7 28 35	0
8	19	1	Total C Mg N O 531 441 9 36 45	0
8	19	1	Total C Mg N O 531 441 9 36 45	0
8	19	1	Total C Mg N O 531 441 9 36 45	0
8	19	1	Total C Mg N O 531 441 9 36 45	0
8	19	1	Total C Mg N O 531 441 9 36 45	0
8	19	1	Total C Mg N O 531 441 9 36 45	0
8	19	1	Total C Mg N O 531 441 9 36 45	0
8	19	1	Total C Mg N O 531 441 9 36 45	0
8	19	1	Total C Mg N O 531 441 9 36 45	0
8	20	1	Total C Mg N O 299 239 6 24 30	0
8	20	1	Total C Mg N O 299 239 6 24 30	0
8	20	1	Total C Mg N O 299 239 6 24 30	0
8	20	1	Total C Mg N O 299 239 6 24 30	0
8	20	1	Total C Mg N O 299 239 6 24 30	0
8	20	1	Total C Mg N O 299 239 6 24 30	0
8	21	1	Total C Mg N O 380 310 7 28 35	0
8	21	1	Total C Mg N O 380 310 7 28 35	0
8	21	1	Total C Mg N O 380 310 7 28 35	0

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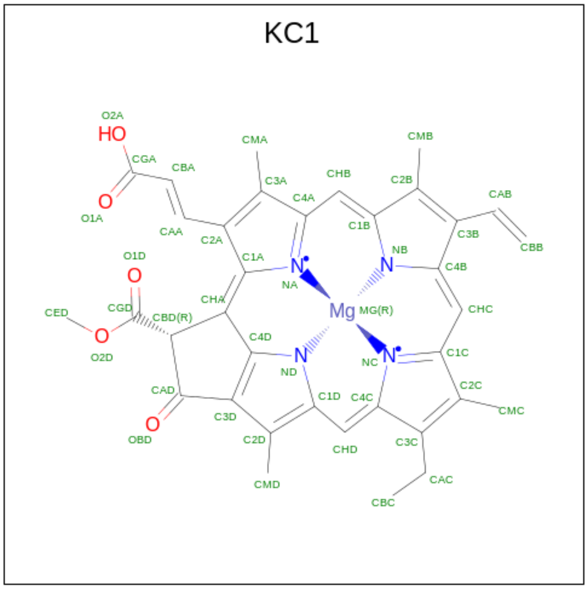
Mol	Chain	Residues	Atoms					AltConf
8	21	1	Total 380	C 310	Mg 7	N 28	O 35	0
8	21	1	Total 380	C 310	Mg 7	N 28	O 35	0
8	21	1	Total 380	C 310	Mg 7	N 28	O 35	0
8	21	1	Total 380	C 310	Mg 7	N 28	O 35	0

- Molecule 9 is Chlorophyll c1 (three-letter code: KC1) (formula: $C_{35}H_{30}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
9	11	1	Total 180	C 140	Mg 4	N 16	O 20	0
9	11	1	Total 180	C 140	Mg 4	N 16	O 20	0
9	11	1	Total 180	C 140	Mg 4	N 16	O 20	0
9	11	1	Total 180	C 140	Mg 4	N 16	O 20	0
9	12	1	Total 135	C 105	Mg 3	N 12	O 15	0
9	12	1	Total 135	C 105	Mg 3	N 12	O 15	0
9	12	1	Total 135	C 105	Mg 3	N 12	O 15	0

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Mol	Chain	Residues	Atoms					AltConf
9	13	1	Total 180	C 140	Mg 4	N 16	O 20	0
9	13	1	Total 180	C 140	Mg 4	N 16	O 20	0
9	13	1	Total 180	C 140	Mg 4	N 16	O 20	0
9	13	1	Total 180	C 140	Mg 4	N 16	O 20	0
9	14	1	Total 135	C 105	Mg 3	N 12	O 15	0
9	14	1	Total 135	C 105	Mg 3	N 12	O 15	0
9	14	1	Total 135	C 105	Mg 3	N 12	O 15	0
9	15	1	Total 180	C 140	Mg 4	N 16	O 20	0
9	15	1	Total 180	C 140	Mg 4	N 16	O 20	0
9	15	1	Total 180	C 140	Mg 4	N 16	O 20	0
9	15	1	Total 180	C 140	Mg 4	N 16	O 20	0
9	16	1	Total 180	C 140	Mg 4	N 16	O 20	0
9	16	1	Total 180	C 140	Mg 4	N 16	O 20	0
9	16	1	Total 180	C 140	Mg 4	N 16	O 20	0
9	16	1	Total 180	C 140	Mg 4	N 16	O 20	0
9	17	1	Total 180	C 140	Mg 4	N 16	O 20	0
9	17	1	Total 180	C 140	Mg 4	N 16	O 20	0
9	17	1	Total 180	C 140	Mg 4	N 16	O 20	0
9	17	1	Total 180	C 140	Mg 4	N 16	O 20	0
9	18	1	Total 135	C 105	Mg 3	N 12	O 15	0
9	18	1	Total 135	C 105	Mg 3	N 12	O 15	0

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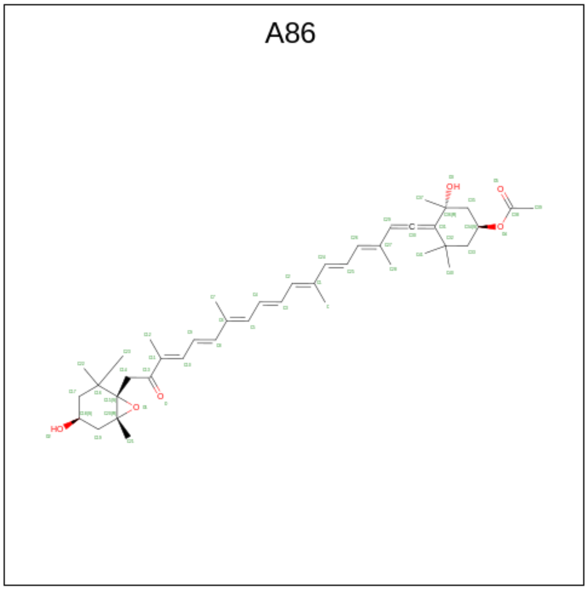
Mol	Chain	Residues	Atoms	AltConf
9	18	1	Total C Mg N O 135 105 3 12 15	0
9	19	1	Total C Mg N O 45 35 1 4 5	0
9	20	1	Total C Mg N O 135 105 3 12 15	0
9	20	1	Total C Mg N O 135 105 3 12 15	0
9	20	1	Total C Mg N O 135 105 3 12 15	0
9	21	1	Total C Mg N O 90 70 2 8 10	0
9	21	1	Total C Mg N O 90 70 2 8 10	0

- Molecule 10 is (3S,3'S,5R,5'R,6S,6'R,8'R)-3,5'-dihydroxy-8-oxo-6',7'-didehydro-5,5',6,6',7,8-hexahydro-5,6-epoxy-beta,beta-caroten-3'- yl acetate (three-letter code: A86) (formula: $C_{42}H_{58}O_6$).



Mol	Chain	Residues	Atoms	AltConf
10	11	1	Total C O 288 252 36	0
10	11	1	Total C O 288 252 36	0
10	11	1	Total C O 288 252 36	0

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Mol	Chain	Residues	Atoms	AltConf
10	11	1	Total C O 288 252 36	0
10	11	1	Total C O 288 252 36	0
10	11	1	Total C O 288 252 36	0
10	12	1	Total C O 336 294 42	0
10	12	1	Total C O 336 294 42	0
10	12	1	Total C O 336 294 42	0
10	12	1	Total C O 336 294 42	0
10	12	1	Total C O 336 294 42	0
10	12	1	Total C O 336 294 42	0
10	12	1	Total C O 336 294 42	0
10	13	1	Total C O 240 210 30	0
10	13	1	Total C O 240 210 30	0
10	13	1	Total C O 240 210 30	0
10	13	1	Total C O 240 210 30	0
10	13	1	Total C O 240 210 30	0
10	14	1	Total C O 288 252 36	0
10	14	1	Total C O 288 252 36	0
10	14	1	Total C O 288 252 36	0
10	14	1	Total C O 288 252 36	0
10	14	1	Total C O 288 252 36	0
10	14	1	Total C O 288 252 36	0

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Mol	Chain	Residues	Atoms	AltConf
10	15	1	Total C O 336 294 42	0
10	15	1	Total C O 336 294 42	0
10	15	1	Total C O 336 294 42	0
10	15	1	Total C O 336 294 42	0
10	15	1	Total C O 336 294 42	0
10	15	1	Total C O 336 294 42	0
10	15	1	Total C O 336 294 42	0
10	16	1	Total C O 144 126 18	0
10	16	1	Total C O 144 126 18	0
10	16	1	Total C O 144 126 18	0
10	17	1	Total C O 336 294 42	0
10	17	1	Total C O 336 294 42	0
10	17	1	Total C O 336 294 42	0
10	17	1	Total C O 336 294 42	0
10	17	1	Total C O 336 294 42	0
10	17	1	Total C O 336 294 42	0
10	17	1	Total C O 336 294 42	0
10	18	1	Total C O 192 168 24	0
10	18	1	Total C O 192 168 24	0
10	18	1	Total C O 192 168 24	0
10	18	1	Total C O 192 168 24	0

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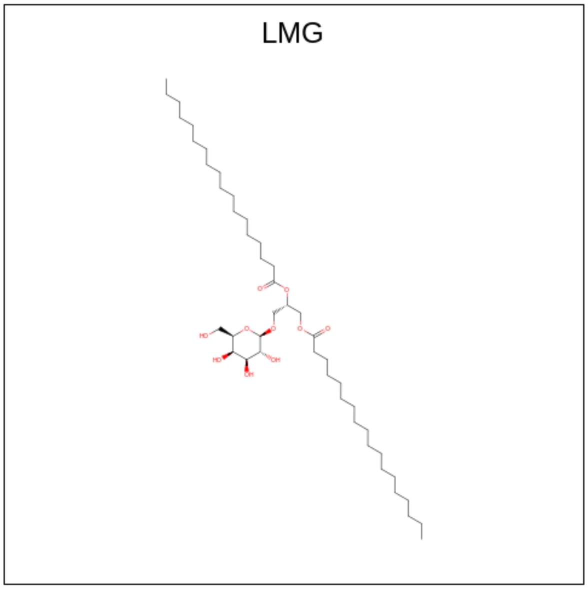
Mol	Chain	Residues	Atoms	AltConf
10	19	1	Total C O 96 84 12	0
10	19	1	Total C O 96 84 12	0
10	20	1	Total C O 144 126 18	0
10	20	1	Total C O 144 126 18	0
10	20	1	Total C O 144 126 18	0
10	21	1	Total C O 192 168 24	0
10	21	1	Total C O 192 168 24	0
10	21	1	Total C O 192 168 24	0
10	21	1	Total C O 192 168 24	0

- Molecule 11 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms	AltConf
11	11	1	Total C O 74 54 20	0
11	11	1	Total C O 74 54 20	0

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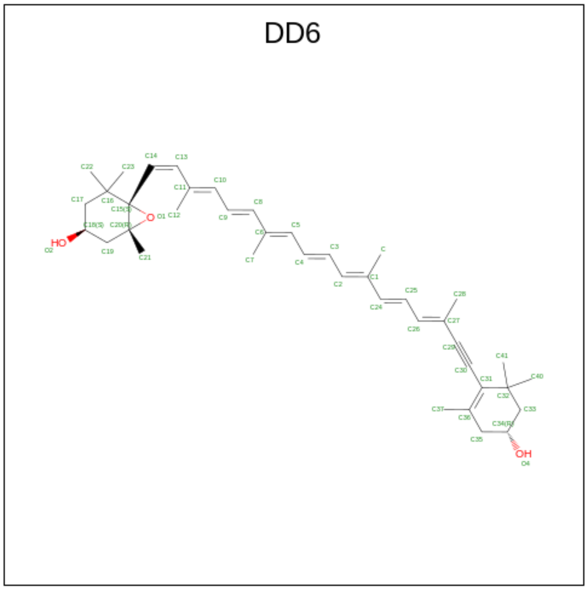
Mol	Chain	Residues	Atoms	AltConf
11	16	1	Total C O 36 26 10	0
11	17	1	Total C O 37 27 10	0

- Molecule 12 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

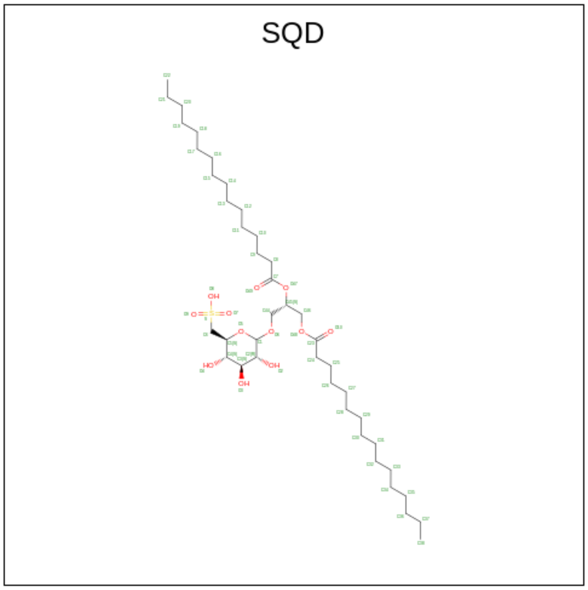
Mol	Chain	Residues	Atoms	AltConf
12	11	1	Total C O 19 17 2	0
12	12	2	Total C O 34 32 2	0
12	13	3	Total C O 49 47 2	0
12	14	1	Total C 16 16	0
12	15	2	Total C 28 28	0
12	16	2	Total C 24 24	0
12	17	3	Total C O 54 48 6	0
12	18	4	Total C 58 58	0
12	19	1	Total C 12 12	0

- Molecule 13 is (3S,3'R,5R,6S,7cis)-7',8'-didehydro-5,6-dihydro-5,6-epoxy-beta,beta-carotene-3,3'-diol (three-letter code: DD6) (formula: $C_{40}H_{54}O_3$).



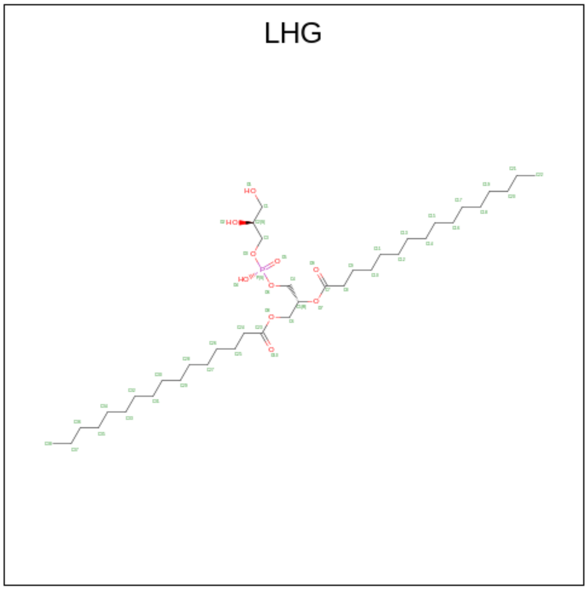
Mol	Chain	Residues	Atoms	AltConf
13	16	1	Total C O 43 40 3	0
13	19	1	Total C O 43 40 3	0
13	20	1	Total C O 86 80 6	0
13	20	1	Total C O 86 80 6	0
13	21	1	Total C O 86 80 6	0
13	21	1	Total C O 86 80 6	0

- Molecule 14 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: $C_{41}H_{78}O_{12}S$).



Mol	Chain	Residues	Atoms				AltConf
14	16	1	Total	C	O	S	0
			54	41	12	1	
14	17	1	Total	C	O	S	0
			49	36	12	1	

- Molecule 15 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms				AltConf
15	17	1	Total	C	O	P	0
			44	33	10	1	

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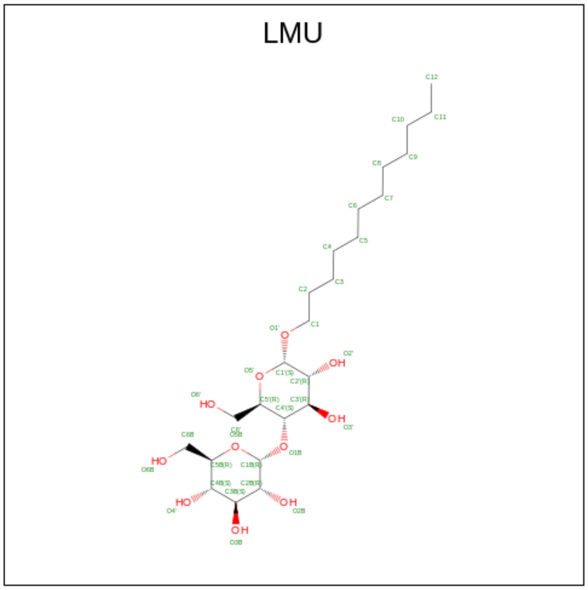
Mol	Chain	Residues	Atoms	AltConf
15	19	1	Total C O P 49 38 10 1	0
15	21	1	Total C O P 80 59 19 2	0
15	21	1	Total C O P 80 59 19 2	0

- Molecule 16 is DODECYL-ALPHA-D-MALTOSIDE (three-letter code: LMU) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms	AltConf
16	19	1	Total C O 35 24 11	0

- Molecule 17 is water.

Mol	Chain	Residues	Atoms	AltConf
17	11	3	Total O 3 3	0
17	12	1	Total O 1 1	0
17	13	2	Total O 2 2	0
17	14	1	Total O 1 1	0
17	15	1	Total O 1 1	0

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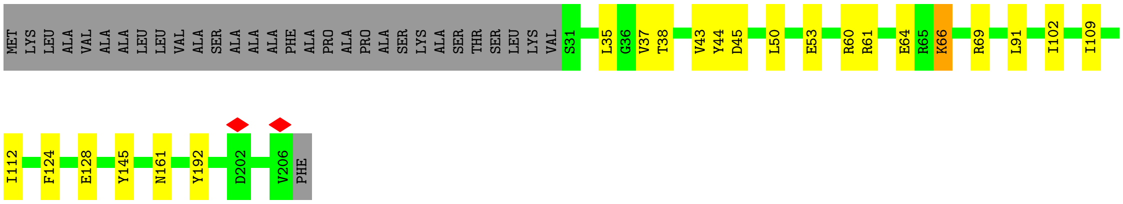
Mol	Chain	Residues	Atoms	AltConf
17	16	1	Total O 1 1	0
17	17	2	Total O 2 2	0
17	18	1	Total O 1 1	0
17	19	1	Total O 1 1	0

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.

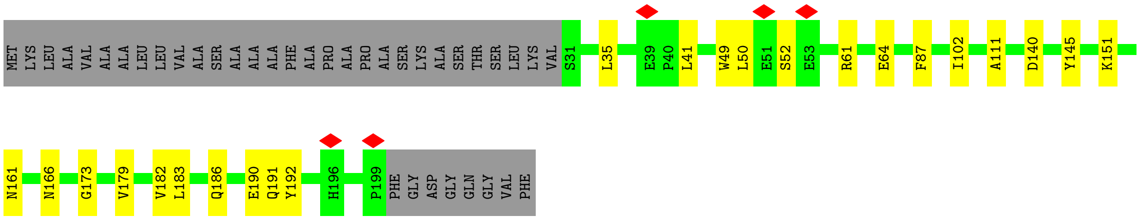
- Molecule 1: Chlorophyll a/b-binding protein

Chain 11:



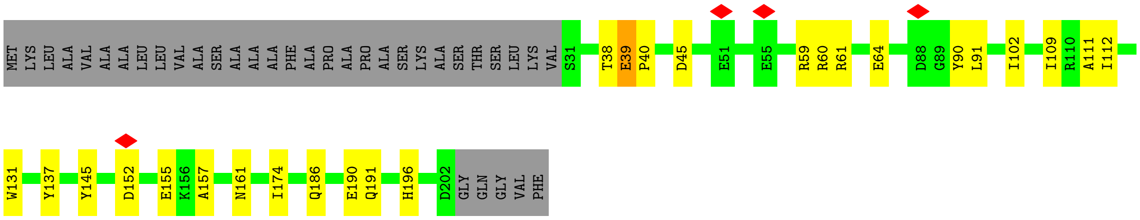
- Molecule 1: Chlorophyll a/b-binding protein

Chain 13:



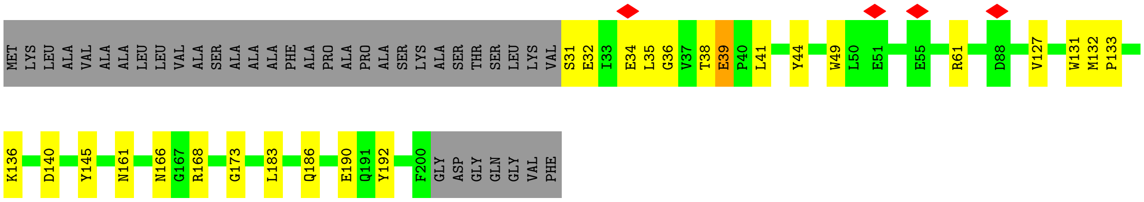
- Molecule 1: Chlorophyll a/b-binding protein

Chain 14:



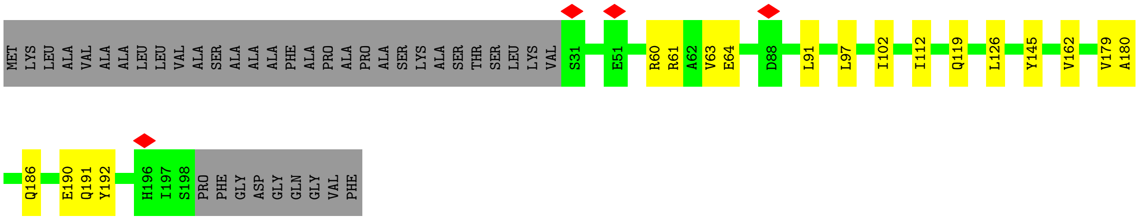
- Molecule 1: Chlorophyll a/b-binding protein

Chain 15:



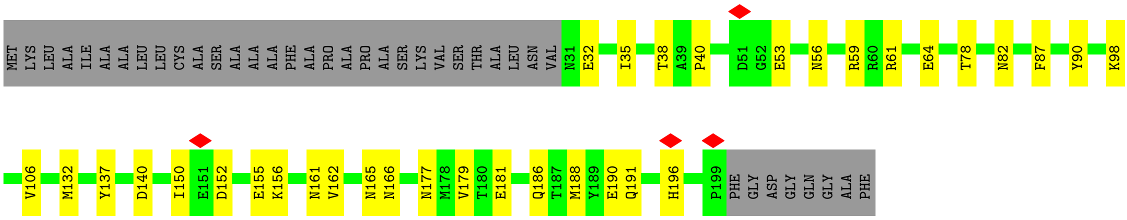
- Molecule 1: Chlorophyll a/b-binding protein

Chain 18:



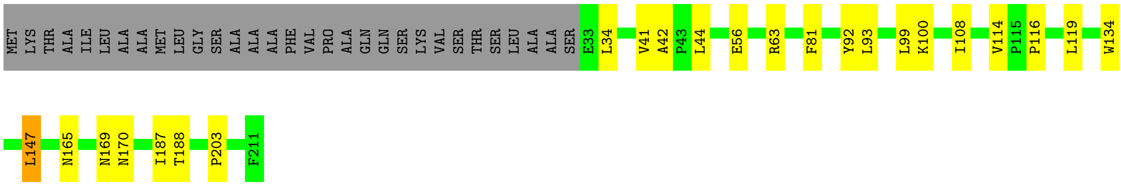
- Molecule 2: Fcpb2, Fucoxanthin chlorophyll a/c-binding protein

Chain 12:



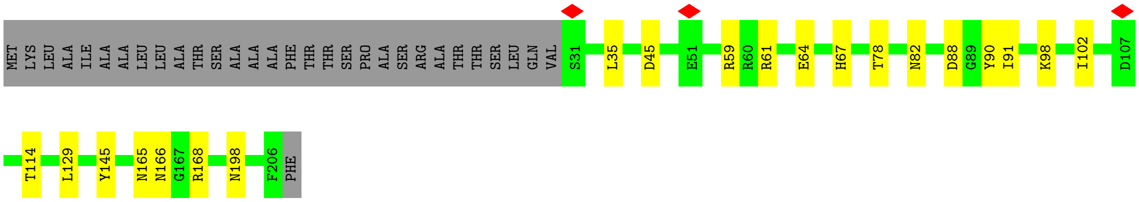
- Molecule 3: Fcpb3, Fucoxanthin chlorophyll a/c-binding protein

Chain 16:

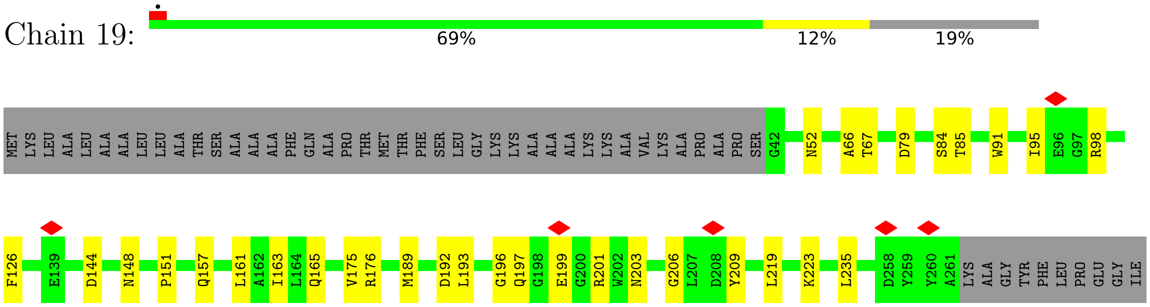


- Molecule 4: Fcpb4, Fucoxanthin chlorophyll a/c-binding protein

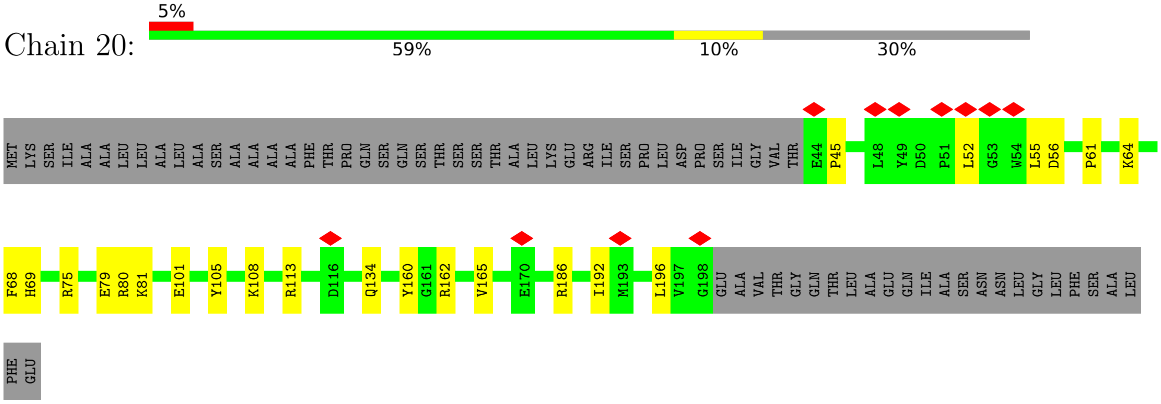
Chain 17:



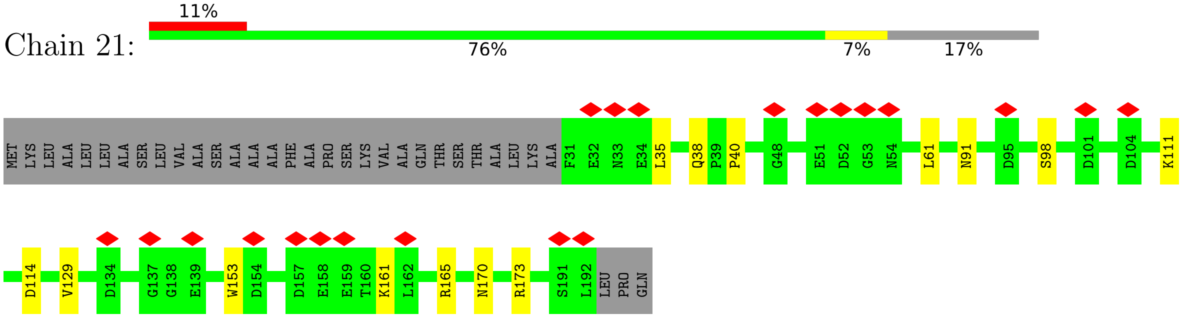
- Molecule 5: Fcpb5, Fucoxanthin chlorophyll a/c-binding protein



- Molecule 6: Fcpb6, Fucoxanthin chlorophyll a/c-binding protein



- Molecule 7: Fcpb7, Fucoxanthin chlorophyll a/c-binding protein



4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	373897	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	20	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.296	Depositor
Minimum map value	-0.107	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.055	Depositor
Map size (Å)	569.856, 569.856, 569.856	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.113, 1.113, 1.113	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: A86, UNL, SQD, LMG, DD6, LMU, CLA, LHG, KC1

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	11	0.40	0/1373	0.50	0/1861
1	13	0.34	0/1325	0.49	0/1797
1	14	0.34	0/1349	0.46	0/1829
1	15	0.33	0/1337	0.52	0/1813
1	18	0.34	0/1317	0.49	0/1785
2	12	0.36	0/1334	0.51	0/1810
3	16	0.37	0/1425	0.53	0/1930
4	17	0.38	0/1386	0.51	0/1879
5	19	0.35	0/1737	0.49	0/2365
6	20	0.34	0/1229	0.56	1/1662 (0.1%)
7	21	0.32	0/1290	0.51	0/1735
All	All	0.35	0/15102	0.51	1/20466 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	14	0	1
1	15	0	1
3	16	0	1
5	19	0	1
6	20	0	3
All	All	0	7

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	20	52	LEU	CA-CB-CG	5.28	127.43	115.30

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	14	39	GLU	Peptide
1	15	39	GLU	Peptide
3	16	147	LEU	Peptide
5	19	196	GLY	Peptide
6	20	55	LEU	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	11	1343	0	1306	18	0
1	13	1296	0	1267	18	0
1	14	1319	0	1283	18	0
1	15	1307	0	1275	21	0
1	18	1289	0	1260	14	0
2	12	1302	0	1257	25	0
3	16	1386	0	1314	19	0
4	17	1353	0	1291	17	0
5	19	1690	0	1627	22	0
6	20	1198	0	1180	13	0
7	21	1262	0	1247	9	0
8	11	278	0	261	6	0
8	12	407	0	403	13	0
8	13	394	0	378	13	0
8	14	394	0	378	7	0
8	15	329	0	304	14	0
8	16	293	0	291	8	0
8	17	303	0	310	7	0
8	18	394	0	376	12	0
8	19	531	0	537	13	0
8	20	299	0	242	4	0
8	21	380	0	342	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	11	180	0	0	1	0
9	12	135	0	0	0	0
9	13	180	0	0	0	0
9	14	135	0	0	0	0
9	15	180	0	0	0	0
9	16	180	0	0	0	0
9	17	180	0	0	2	0
9	18	135	0	0	1	0
9	19	45	0	0	0	0
9	20	135	0	0	0	0
9	21	90	0	0	0	0
10	11	288	0	0	3	0
10	12	336	0	0	0	0
10	13	240	0	0	1	0
10	14	288	0	0	2	0
10	15	336	0	0	1	0
10	16	144	0	0	0	0
10	17	336	0	0	0	0
10	18	192	0	0	2	0
10	19	96	0	0	0	0
10	20	144	0	0	0	0
10	21	192	0	0	0	0
11	11	74	0	88	0	0
11	16	36	0	42	1	0
11	17	37	0	44	0	0
12	11	19	0	0	0	0
12	12	34	0	0	0	0
12	13	49	0	0	0	0
12	14	16	0	0	0	0
12	15	28	0	0	0	0
12	16	24	0	0	0	0
12	17	54	0	0	0	0
12	18	58	0	0	0	0
12	19	12	0	0	0	0
13	16	43	0	0	0	0
13	19	43	0	0	2	0
13	20	86	0	0	2	0
13	21	86	0	0	0	0
14	16	54	0	77	2	0
14	17	49	0	65	3	0
15	17	44	0	61	1	0
15	19	49	0	74	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	21	80	0	102	4	0
16	19	35	0	46	1	0
17	11	3	0	0	0	0
17	12	1	0	0	0	0
17	13	2	0	0	0	0
17	14	1	0	0	0	0
17	15	1	0	0	0	0
17	16	1	0	0	0	0
17	17	2	0	0	0	0
17	18	1	0	0	0	0
17	19	1	0	0	0	0
All	All	23937	0	18728	237	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 6.

The worst 5 of 237 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:18:63:VAL:HG11	8:18:302:CLA:HAA2	1.79	0.65
8:19:302:CLA:H2	8:19:302:CLA:HED1	1.78	0.65
2:12:186:GLN:HB3	2:12:190:GLU:HB2	1.79	0.63
15:17:317:LHG:H121	5:19:175:VAL:HG22	1.81	0.62
1:18:145:TYR:HB2	8:18:307:CLA:HAA1	1.81	0.62

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	11	174/207 (84%)	166 (95%)	8 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	13	167/207 (81%)	161 (96%)	6 (4%)	0	100	100
1	14	170/207 (82%)	162 (95%)	6 (4%)	2 (1%)	13	39
1	15	168/207 (81%)	148 (88%)	19 (11%)	1 (1%)	25	56
1	18	166/207 (80%)	155 (93%)	11 (7%)	0	100	100
2	12	167/207 (81%)	163 (98%)	4 (2%)	0	100	100
3	16	177/210 (84%)	171 (97%)	6 (3%)	0	100	100
4	17	174/207 (84%)	169 (97%)	5 (3%)	0	100	100
5	19	218/271 (80%)	208 (95%)	10 (5%)	0	100	100
6	20	153/223 (69%)	135 (88%)	18 (12%)	0	100	100
7	21	160/195 (82%)	142 (89%)	18 (11%)	0	100	100
All	All	1894/2348 (81%)	1780 (94%)	111 (6%)	3 (0%)	50	78

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	14	39	GLU
1	15	39	GLU
1	14	40	PRO

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	11	138/158 (87%)	137 (99%)	1 (1%)	84	95
1	13	134/158 (85%)	134 (100%)	0	100	100
1	14	136/158 (86%)	136 (100%)	0	100	100
1	15	135/158 (85%)	135 (100%)	0	100	100
1	18	133/158 (84%)	133 (100%)	0	100	100
2	12	133/156 (85%)	133 (100%)	0	100	100
3	16	137/158 (87%)	136 (99%)	1 (1%)	84	95

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	17	137/159 (86%)	137 (100%)	0	100	100
5	19	169/202 (84%)	169 (100%)	0	100	100
6	20	122/174 (70%)	122 (100%)	0	100	100
7	21	129/152 (85%)	128 (99%)	1 (1%)	81	94
All	All	1503/1791 (84%)	1500 (100%)	3 (0%)	93	98

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

Mol	Chain	Res	Type
1	11	66	LYS
3	16	147	LEU
7	21	111	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	18	165	ASN
1	18	177	ASN
7	21	55	GLN
5	19	240	GLN
6	20	167	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 196 ligands modelled in this entry, 19 are unknown - leaving 177 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	$\#\|Z\| > 2$
9	KC1	16	304	3	48,53,53	3.41	23 (47%)	55,89,89	3.83	28 (50%)
10	A86	12	319	-	44,50,50	3.86	23 (52%)	51,76,76	7.96	22 (43%)
8	CLA	15	301	1	65,73,73	2.02	16 (24%)	76,113,113	2.76	23 (30%)
8	CLA	18	310	-	45,53,73	2.51	16 (35%)	52,89,113	3.16	23 (44%)
9	KC1	14	306	1	48,53,53	3.40	24 (50%)	55,89,89	3.73	30 (54%)
14	SQD	16	314	-	53,54,54	0.96	6 (11%)	62,65,65	1.61	10 (16%)
13	DD6	20	312	-	39,45,45	6.64	24 (61%)	52,67,67	7.39	27 (51%)
10	A86	15	314	-	44,50,50	4.20	23 (52%)	51,76,76	8.25	19 (37%)
8	CLA	16	301	3	65,73,73	1.95	18 (27%)	76,113,113	2.75	24 (31%)
11	LMG	11	315	-	42,42,55	1.07	3 (7%)	50,50,63	1.21	2 (4%)
10	A86	13	313	-	44,50,50	4.06	23 (52%)	51,76,76	7.97	17 (33%)
10	A86	15	311	-	44,50,50	3.95	23 (52%)	51,76,76	7.98	14 (27%)
8	CLA	21	206	7	65,73,73	2.00	15 (23%)	76,113,113	2.73	27 (35%)
8	CLA	14	310	-	45,53,73	2.46	16 (35%)	52,89,113	3.17	23 (44%)
10	A86	14	314	-	44,50,50	4.12	23 (52%)	51,76,76	8.42	20 (39%)
10	A86	21	213	-	44,50,50	4.20	22 (50%)	51,76,76	8.13	17 (33%)
8	CLA	12	307	17	50,58,73	2.32	17 (34%)	58,95,113	3.14	28 (48%)
11	LMG	16	315	-	36,36,55	0.98	1 (2%)	44,44,63	1.22	5 (11%)
8	CLA	14	308	17	65,73,73	2.00	16 (24%)	76,113,113	2.63	29 (38%)
13	DD6	21	212	-	39,45,45	6.69	22 (56%)	52,67,67	7.19	35 (67%)
8	CLA	19	305	5	51,59,73	2.20	15 (29%)	59,96,113	3.06	27 (45%)
10	A86	19	313	-	44,50,50	4.05	24 (54%)	51,76,76	8.71	21 (41%)
8	CLA	19	301	5	65,73,73	1.96	16 (24%)	76,113,113	2.73	29 (38%)
8	CLA	18	301	1	65,73,73	1.98	16 (24%)	76,113,113	2.73	27 (35%)
8	CLA	19	310	5	65,73,73	2.00	17 (26%)	76,113,113	2.61	27 (35%)
10	A86	17	311	-	44,50,50	3.97	23 (52%)	51,76,76	8.33	14 (27%)
15	LHG	21	201	-	34,34,48	0.75	1 (2%)	37,39,54	1.39	5 (13%)
8	CLA	18	302	-	65,73,73	2.02	15 (23%)	76,113,113	2.68	28 (36%)
10	A86	18	314	-	44,50,50	3.99	23 (52%)	51,76,76	7.77	17 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
9	KC1	17	303	-	48,53,53	3.44	23 (47%)	55,89,89	3.68	31 (56%)
10	A86	17	313	-	44,50,50	3.96	22 (50%)	51,76,76	7.34	20 (39%)
8	CLA	16	309	-	45,53,73	2.40	15 (33%)	52,89,113	3.31	26 (50%)
8	CLA	11	305	17	45,53,73	2.40	17 (37%)	52,89,113	3.18	25 (48%)
10	A86	19	311	-	44,50,50	3.92	22 (50%)	51,76,76	7.71	19 (37%)
8	CLA	20	307	6	50,58,73	2.28	16 (32%)	58,95,113	3.00	27 (46%)
8	CLA	20	309	-	47,55,73	2.36	16 (34%)	54,91,113	3.09	27 (50%)
9	KC1	13	303	-	48,53,53	3.47	25 (52%)	55,89,89	3.79	31 (56%)
9	KC1	15	306	1	48,53,53	3.42	24 (50%)	55,89,89	3.71	31 (56%)
10	A86	17	316	-	44,50,50	3.97	23 (52%)	51,76,76	7.80	19 (37%)
8	CLA	11	309	17	51,59,73	2.25	16 (31%)	59,96,113	3.01	25 (42%)
10	A86	18	312	-	44,50,50	4.02	23 (52%)	51,76,76	8.09	19 (37%)
10	A86	14	312	-	44,50,50	3.93	23 (52%)	51,76,76	7.97	23 (45%)
8	CLA	15	305	-	45,53,73	2.48	16 (35%)	52,89,113	3.19	25 (48%)
9	KC1	16	302	-	48,53,53	3.43	24 (50%)	55,89,89	3.53	31 (56%)
8	CLA	12	303	2	65,73,73	1.97	15 (23%)	76,113,113	2.65	26 (34%)
9	KC1	21	203	-	48,53,53	3.44	25 (52%)	55,89,89	3.87	28 (50%)
10	A86	11	311	-	44,50,50	3.87	22 (50%)	51,76,76	7.83	22 (43%)
8	CLA	13	301	17	65,73,73	2.01	17 (26%)	76,113,113	2.68	28 (36%)
9	KC1	14	309	1	48,53,53	3.37	23 (47%)	55,89,89	3.69	29 (52%)
8	CLA	12	309	2	52,60,73	2.24	17 (32%)	60,97,113	3.04	31 (51%)
8	CLA	18	308	17	65,73,73	1.99	18 (27%)	76,113,113	2.64	28 (36%)
9	KC1	11	308	1	48,53,53	3.39	23 (47%)	55,89,89	3.66	31 (56%)
9	KC1	17	306	4	48,53,53	3.38	23 (47%)	55,89,89	3.67	32 (58%)
10	A86	12	313	-	44,50,50	3.91	23 (52%)	51,76,76	7.91	18 (35%)
10	A86	13	314	-	44,50,50	4.14	24 (54%)	51,76,76	8.66	19 (37%)
10	A86	16	313	-	44,50,50	3.73	22 (50%)	51,76,76	7.57	16 (31%)
10	A86	17	312	-	44,50,50	3.92	23 (52%)	51,76,76	7.66	20 (39%)
8	CLA	13	302	1	65,73,73	2.02	15 (23%)	76,113,113	2.68	27 (35%)
10	A86	15	316	-	44,50,50	4.01	23 (52%)	51,76,76	7.73	19 (37%)
8	CLA	18	303	-	56,64,73	2.16	16 (28%)	65,102,113	2.96	31 (47%)
8	CLA	12	311	-	45,53,73	2.45	16 (35%)	52,89,113	3.20	25 (48%)
8	CLA	21	209	7	45,53,73	2.47	17 (37%)	52,89,113	3.17	24 (46%)
8	CLA	11	301	1	65,73,73	1.97	16 (24%)	76,113,113	2.72	28 (36%)
11	LMG	17	318	-	37,37,55	1.00	3 (8%)	45,45,63	1.27	5 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$\|Z\| > 2$	Counts	RMSZ	#$\|Z\| > 2$
8	CLA	17	310	17	65,73,73	2.05	17 (26%)	76,113,113	2.89	32 (42%)
8	CLA	17	302	4	65,73,73	2.03	16 (24%)	76,113,113	2.66	23 (30%)
10	A86	13	315	-	44,50,50	4.16	23 (52%)	51,76,76	8.63	19 (37%)
8	CLA	21	202	7	57,65,73	2.18	16 (28%)	66,103,113	2.89	26 (39%)
10	A86	11	314	-	44,50,50	3.91	23 (52%)	51,76,76	7.74	21 (41%)
8	CLA	20	302	6	56,64,73	2.19	16 (28%)	65,102,113	3.03	29 (44%)
8	CLA	19	304	5	45,53,73	2.40	17 (37%)	52,89,113	3.21	21 (40%)
10	A86	21	215	-	44,50,50	4.04	23 (52%)	51,76,76	7.91	16 (31%)
10	A86	15	312	-	44,50,50	4.03	23 (52%)	51,76,76	7.74	20 (39%)
9	KC1	19	308	-	48,53,53	3.37	24 (50%)	55,89,89	3.86	33 (60%)
8	CLA	13	306	-	45,53,73	2.50	17 (37%)	52,89,113	3.16	24 (46%)
8	CLA	13	311	-	45,53,73	2.49	18 (40%)	52,89,113	3.23	24 (46%)
8	CLA	14	305	-	45,53,73	2.45	17 (37%)	52,89,113	3.18	25 (48%)
9	KC1	14	304	1	48,53,53	3.44	25 (52%)	55,89,89	3.93	28 (50%)
9	KC1	13	305	1	48,53,53	3.43	24 (50%)	55,89,89	3.72	29 (52%)
8	CLA	19	309	5	45,53,73	2.41	17 (37%)	52,89,113	3.09	24 (46%)
10	A86	13	316	-	44,50,50	4.05	23 (52%)	51,76,76	7.68	19 (37%)
8	CLA	19	302	-	65,73,73	1.97	16 (24%)	76,113,113	2.80	26 (34%)
10	A86	16	310	-	44,50,50	3.79	21 (47%)	51,76,76	7.60	19 (37%)
9	KC1	17	305	4	48,53,53	3.40	24 (50%)	55,89,89	3.65	28 (50%)
9	KC1	18	309	1	48,53,53	3.40	24 (50%)	55,89,89	3.80	31 (56%)
8	CLA	18	307	-	53,61,73	2.23	17 (32%)	61,98,113	2.97	28 (45%)
10	A86	17	314	-	44,50,50	4.03	23 (52%)	51,76,76	8.33	20 (39%)
8	CLA	21	208	-	65,73,73	2.07	18 (27%)	76,113,113	2.65	27 (35%)
9	KC1	12	310	2	48,53,53	3.40	23 (47%)	55,89,89	3.66	32 (58%)
8	CLA	14	307	1	52,60,73	2.21	15 (28%)	60,97,113	2.89	30 (50%)
10	A86	13	312	-	44,50,50	3.94	23 (52%)	51,76,76	7.96	21 (41%)
10	A86	15	315	-	44,50,50	3.98	23 (52%)	51,76,76	7.76	18 (35%)
9	KC1	15	304	1	48,53,53	3.44	25 (52%)	55,89,89	3.89	30 (54%)
9	KC1	18	306	1	48,53,53	3.41	26 (54%)	55,89,89	3.77	35 (63%)
8	CLA	21	205	7	45,53,73	2.42	17 (37%)	52,89,113	3.18	25 (48%)
8	CLA	20	308	6	45,53,73	2.48	18 (40%)	52,89,113	3.17	25 (48%)
8	CLA	11	303	-	65,73,73	1.99	16 (24%)	76,113,113	2.81	31 (40%)
10	A86	11	318	-	44,50,50	3.89	23 (52%)	51,76,76	7.53	21 (41%)
9	KC1	11	302	-	48,53,53	3.42	23 (47%)	55,89,89	3.70	28 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
9	KC1	21	207	7	48,53,53	3.42	26 (54%)	55,89,89	3.94	31 (56%)
9	KC1	16	308	3	48,53,53	3.39	23 (47%)	55,89,89	3.65	29 (52%)
8	CLA	12	304	-	65,73,73	1.98	17 (26%)	76,113,113	2.64	26 (34%)
8	CLA	15	310	-	45,53,73	2.45	16 (35%)	52,89,113	3.23	24 (46%)
13	DD6	21	216	-	39,45,45	6.75	21 (53%)	52,67,67	7.23	30 (57%)
9	KC1	20	306	6	48,53,53	3.43	25 (52%)	55,89,89	3.79	29 (52%)
9	KC1	15	309	1	48,53,53	3.38	23 (47%)	55,89,89	3.64	30 (54%)
10	A86	21	214	-	44,50,50	4.11	23 (52%)	51,76,76	8.35	17 (33%)
16	LMU	19	315	-	36,36,36	1.15	2 (5%)	47,47,47	1.01	2 (4%)
15	LHG	21	217	-	44,44,48	0.63	0	47,50,54	1.22	4 (8%)
10	A86	12	316	-	44,50,50	4.00	24 (54%)	51,76,76	7.58	21 (41%)
10	A86	16	311	-	44,50,50	3.84	23 (52%)	51,76,76	7.71	23 (45%)
10	A86	11	312	-	44,50,50	4.00	22 (50%)	51,76,76	7.68	18 (35%)
8	CLA	19	303	17	65,73,73	1.98	16 (24%)	76,113,113	2.84	30 (39%)
8	CLA	13	309	17	65,73,73	2.02	17 (26%)	76,113,113	2.70	25 (32%)
10	A86	17	321	-	44,50,50	3.92	23 (52%)	51,76,76	7.77	18 (35%)
13	DD6	20	314	-	39,45,45	6.79	23 (58%)	52,67,67	6.81	31 (59%)
10	A86	18	313	-	44,50,50	4.12	23 (52%)	51,76,76	8.22	19 (37%)
11	LMG	11	316	-	32,32,55	0.99	0	40,40,63	1.20	4 (10%)
8	CLA	14	303	-	57,65,73	2.17	18 (31%)	66,103,113	3.07	30 (45%)
10	A86	20	311	-	44,50,50	4.09	24 (54%)	51,76,76	8.50	14 (27%)
8	CLA	12	305	-	65,73,73	1.99	17 (26%)	76,113,113	2.82	31 (40%)
8	CLA	19	306	5	65,73,73	1.93	16 (24%)	76,113,113	2.70	28 (36%)
8	CLA	21	210	-	45,53,73	2.46	16 (35%)	52,89,113	3.25	24 (46%)
10	A86	12	302	-	44,50,50	3.91	21 (47%)	51,76,76	7.71	19 (37%)
10	A86	21	211	-	44,50,50	4.13	22 (50%)	51,76,76	8.27	12 (23%)
14	SQD	17	301	-	48,49,54	0.99	5 (10%)	57,60,65	1.54	11 (19%)
8	CLA	13	304	-	57,65,73	2.16	16 (28%)	66,103,113	2.94	30 (45%)
10	A86	20	313	-	44,50,50	4.17	23 (52%)	51,76,76	8.68	17 (33%)
10	A86	14	315	-	44,50,50	3.96	23 (52%)	51,76,76	7.96	18 (35%)
8	CLA	14	301	1	65,73,73	1.98	16 (24%)	76,113,113	2.72	26 (34%)
8	CLA	15	303	-	57,65,73	2.16	17 (29%)	66,103,113	2.99	31 (46%)
8	CLA	17	307	4	52,60,73	2.25	16 (30%)	60,97,113	2.96	28 (46%)
8	CLA	15	308	17	65,73,73	1.99	17 (26%)	76,113,113	2.72	28 (36%)
8	CLA	18	305	-	45,53,73	2.44	17 (37%)	52,89,113	3.18	25 (48%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	KC1	17	309	4	48,53,53	3.41	23 (47%)	55,89,89	3.69	29 (52%)
10	A86	11	310	-	44,50,50	3.90	22 (50%)	51,76,76	7.57	19 (37%)
9	KC1	12	308	2	48,53,53	3.37	22 (45%)	55,89,89	3.62	29 (52%)
8	CLA	16	307	17	61,69,73	2.04	15 (24%)	71,108,113	2.73	27 (38%)
8	CLA	13	308	1	52,60,73	2.24	15 (28%)	60,97,113	2.91	30 (50%)
10	A86	15	313	-	44,50,50	4.05	22 (50%)	51,76,76	7.57	17 (33%)
10	A86	12	315	-	44,50,50	4.05	23 (52%)	51,76,76	8.27	19 (37%)
8	CLA	16	306	3	65,73,73	1.96	15 (23%)	76,113,113	2.62	27 (35%)
8	CLA	12	301	17	65,73,73	1.98	16 (24%)	76,113,113	2.69	29 (38%)
10	A86	11	313	-	44,50,50	3.98	23 (52%)	51,76,76	8.35	22 (43%)
10	A86	12	314	-	44,50,50	4.11	22 (50%)	51,76,76	8.11	14 (27%)
10	A86	15	319	-	44,50,50	3.92	23 (52%)	51,76,76	7.42	23 (45%)
8	CLA	14	302	-	65,73,73	2.01	16 (24%)	76,113,113	2.62	29 (38%)
13	DD6	16	312	-	39,45,45	6.69	23 (58%)	52,67,67	6.71	27 (51%)
8	CLA	17	304	-	56,64,73	2.19	16 (28%)	65,102,113	3.03	31 (47%)
10	A86	12	312	-	44,50,50	3.97	23 (52%)	51,76,76	8.12	21 (41%)
13	DD6	19	312	-	39,45,45	6.53	22 (56%)	52,67,67	6.55	32 (61%)
9	KC1	18	304	1	48,53,53	3.41	25 (52%)	55,89,89	3.69	27 (49%)
15	LHG	17	317	-	43,43,48	0.65	0	46,49,54	1.30	6 (13%)
8	CLA	15	307	1	52,60,73	2.24	15 (28%)	60,97,113	3.02	28 (46%)
8	CLA	17	308	17	65,73,73	2.00	17 (26%)	76,113,113	2.63	28 (36%)
8	CLA	20	310	6	45,53,73	2.46	17 (37%)	52,89,113	3.13	23 (44%)
9	KC1	11	306	1	48,53,53	3.38	23 (47%)	55,89,89	3.74	29 (52%)
10	A86	18	311	-	44,50,50	4.00	23 (52%)	51,76,76	8.19	19 (37%)
10	A86	20	301	-	44,50,50	4.03	23 (52%)	51,76,76	8.45	22 (43%)
9	KC1	13	310	1	48,53,53	3.41	24 (50%)	55,89,89	3.74	29 (52%)
10	A86	14	311	-	44,50,50	3.88	22 (50%)	51,76,76	8.29	22 (43%)
9	KC1	16	305	3	48,53,53	3.41	24 (50%)	55,89,89	3.70	27 (49%)
8	CLA	21	204	-	58,66,73	2.18	18 (31%)	67,104,113	3.02	32 (47%)
10	A86	14	313	-	44,50,50	4.10	24 (54%)	51,76,76	7.52	19 (37%)
8	CLA	16	303	-	57,65,73	2.13	16 (28%)	66,103,113	2.97	30 (45%)
9	KC1	20	303	-	48,53,53	3.41	23 (47%)	55,89,89	4.04	33 (60%)
9	KC1	20	305	6	48,53,53	3.45	25 (52%)	55,89,89	3.65	28 (50%)
9	KC1	12	306	2	48,53,53	3.36	22 (45%)	55,89,89	3.86	26 (47%)
8	CLA	11	307	1	52,60,73	2.23	17 (32%)	60,97,113	3.03	26 (43%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$\|Z\| > 2$	Counts	RMSZ	#$\|Z\| > 2$
9	KC1	11	304	1	48,53,53	3.43	25 (52%)	55,89,89	3.72	28 (50%)
10	A86	14	316	-	44,50,50	3.95	24 (54%)	51,76,76	7.55	21 (41%)
9	KC1	15	302	-	48,53,53	3.42	26 (54%)	55,89,89	3.76	30 (54%)
15	LHG	19	314	8	48,48,48	0.71	1 (2%)	51,54,54	1.22	6 (11%)
8	CLA	19	307	15	65,73,73	2.00	16 (24%)	76,113,113	2.68	27 (35%)
10	A86	17	315	-	44,50,50	3.88	22 (50%)	51,76,76	8.70	16 (31%)
8	CLA	20	304	-	56,64,73	2.13	17 (30%)	65,102,113	3.15	32 (49%)
9	KC1	13	307	1	48,53,53	3.39	24 (50%)	55,89,89	3.72	29 (52%)

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
9	KC1	16	304	3	-	6/15/71/71	-
10	A86	12	319	-	-	9/34/90/90	0/3/3/3
8	CLA	15	301	1	-	6/37/115/115	-
8	CLA	18	310	-	-	5/13/91/115	-
9	KC1	14	306	1	-	6/15/71/71	-
14	SQD	16	314	-	-	24/49/69/69	0/1/1/1
13	DD6	20	312	-	-	14/26/80/80	0/3/3/3
10	A86	15	314	-	-	13/34/90/90	0/3/3/3
8	CLA	16	301	3	-	9/37/115/115	-
11	LMG	11	315	-	-	19/37/57/70	0/1/1/1
10	A86	13	313	-	-	8/34/90/90	0/3/3/3
10	A86	15	311	-	-	6/34/90/90	0/3/3/3
8	CLA	21	206	7	1/1/15/20	15/37/115/115	-
8	CLA	14	310	-	1/1/11/20	2/13/91/115	-
10	A86	14	314	-	-	14/34/90/90	0/3/3/3
10	A86	21	213	-	-	8/34/90/90	0/3/3/3
8	CLA	12	307	17	-	0/19/97/115	-
11	LMG	16	315	-	-	14/31/51/70	0/1/1/1
8	CLA	14	308	17	1/1/15/20	13/37/115/115	-
13	DD6	21	212	-	-	13/26/80/80	0/3/3/3
8	CLA	19	305	5	1/1/12/20	6/21/99/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	A86	19	313	-	-	9/34/90/90	0/3/3/3
8	CLA	19	301	5	1/1/15/20	9/37/115/115	-
8	CLA	18	301	1	-	13/37/115/115	-
8	CLA	19	310	5	1/1/15/20	7/37/115/115	-
10	A86	17	311	-	-	11/34/90/90	0/3/3/3
15	LHG	21	201	-	-	19/38/38/53	-
8	CLA	18	302	-	1/1/15/20	8/37/115/115	-
10	A86	18	314	-	-	13/34/90/90	0/3/3/3
9	KC1	17	303	-	-	6/15/71/71	-
10	A86	17	313	-	-	7/34/90/90	0/3/3/3
8	CLA	16	309	-	1/1/11/20	6/13/91/115	-
8	CLA	11	305	17	1/1/11/20	2/13/91/115	-
10	A86	19	311	-	-	7/34/90/90	0/3/3/3
8	CLA	20	307	6	1/1/12/20	5/19/97/115	-
8	CLA	20	309	-	1/1/11/20	2/16/94/115	-
9	KC1	13	303	-	-	5/15/71/71	-
9	KC1	15	306	1	-	6/15/71/71	-
10	A86	17	316	-	-	14/34/90/90	0/3/3/3
8	CLA	11	309	17	1/1/12/20	6/21/99/115	-
10	A86	18	312	-	-	9/34/90/90	0/3/3/3
10	A86	14	312	-	-	6/34/90/90	0/3/3/3
8	CLA	15	305	-	1/1/11/20	3/13/91/115	-
9	KC1	16	302	-	-	2/15/71/71	-
8	CLA	12	303	2	1/1/15/20	13/37/115/115	-
9	KC1	21	203	-	-	4/15/71/71	-
10	A86	11	311	-	-	6/34/90/90	0/3/3/3
8	CLA	13	301	17	-	10/37/115/115	-
9	KC1	14	309	1	-	8/15/71/71	-
8	CLA	12	309	2	1/1/12/20	12/22/100/115	-
8	CLA	18	308	17	1/1/15/20	9/37/115/115	-
9	KC1	11	308	1	-	8/15/71/71	-
9	KC1	17	306	4	-	9/15/71/71	-
10	A86	12	313	-	-	4/34/90/90	0/3/3/3
10	A86	13	314	-	-	19/34/90/90	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	A86	16	313	-	-	8/34/90/90	0/3/3/3
10	A86	17	312	-	-	8/34/90/90	0/3/3/3
8	CLA	13	302	1	-	11/37/115/115	-
10	A86	15	316	-	-	14/34/90/90	0/3/3/3
8	CLA	18	303	-	1/1/13/20	9/27/105/115	-
8	CLA	12	311	-	1/1/11/20	7/13/91/115	-
8	CLA	21	209	7	1/1/11/20	7/13/91/115	-
8	CLA	11	301	1	-	9/37/115/115	-
11	LMG	17	318	-	-	13/32/52/70	0/1/1/1
8	CLA	17	310	17	1/1/15/20	9/37/115/115	-
8	CLA	17	302	4	-	12/37/115/115	-
10	A86	13	315	-	-	9/34/90/90	0/3/3/3
8	CLA	21	202	7	1/1/13/20	7/28/106/115	-
10	A86	11	314	-	-	6/34/90/90	0/3/3/3
8	CLA	20	302	6	-	11/27/105/115	-
8	CLA	19	304	5	1/1/11/20	3/13/91/115	-
10	A86	21	215	-	-	7/34/90/90	0/3/3/3
10	A86	15	312	-	-	8/34/90/90	0/3/3/3
9	KC1	19	308	-	-	3/15/71/71	-
8	CLA	13	306	-	1/1/11/20	3/13/91/115	-
8	CLA	13	311	-	-	2/13/91/115	-
8	CLA	14	305	-	1/1/11/20	3/13/91/115	-
9	KC1	14	304	1	-	4/15/71/71	-
9	KC1	13	305	1	-	7/15/71/71	-
8	CLA	19	309	5	1/1/11/20	3/13/91/115	-
10	A86	13	316	-	-	10/34/90/90	0/3/3/3
8	CLA	19	302	-	1/1/15/20	12/37/115/115	-
10	A86	16	310	-	-	5/34/90/90	0/3/3/3
9	KC1	17	305	4	-	6/15/71/71	-
9	KC1	18	309	1	-	6/15/71/71	-
8	CLA	18	307	-	1/1/12/20	8/23/101/115	-
10	A86	17	314	-	-	8/34/90/90	0/3/3/3
8	CLA	21	208	-	1/1/15/20	13/37/115/115	-
9	KC1	12	310	2	-	7/15/71/71	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	CLA	14	307	1	1/1/12/20	11/22/100/115	-
10	A86	13	312	-	-	6/34/90/90	0/3/3/3
10	A86	15	315	-	-	8/34/90/90	0/3/3/3
9	KC1	15	304	1	-	6/15/71/71	-
9	KC1	18	306	1	-	5/15/71/71	-
8	CLA	21	205	7	1/1/11/20	7/13/91/115	-
8	CLA	20	308	6	1/1/11/20	6/13/91/115	-
8	CLA	11	303	-	1/1/15/20	7/37/115/115	-
10	A86	11	318	-	-	7/34/90/90	0/3/3/3
9	KC1	11	302	-	-	2/15/71/71	-
9	KC1	21	207	7	-	6/15/71/71	-
9	KC1	16	308	3	-	5/15/71/71	-
8	CLA	12	304	-	1/1/15/20	9/37/115/115	-
8	CLA	15	310	-	1/1/11/20	2/13/91/115	-
13	DD6	21	216	-	-	15/26/80/80	0/3/3/3
9	KC1	20	306	6	-	9/15/71/71	-
9	KC1	15	309	1	-	6/15/71/71	-
10	A86	21	214	-	-	6/34/90/90	0/3/3/3
16	LMU	19	315	-	-	6/21/61/61	0/2/2/2
15	LHG	21	217	-	-	28/49/49/53	-
10	A86	12	316	-	-	14/34/90/90	0/3/3/3
10	A86	16	311	-	-	7/34/90/90	0/3/3/3
10	A86	11	312	-	-	9/34/90/90	0/3/3/3
8	CLA	19	303	17	1/1/15/20	15/37/115/115	-
8	CLA	13	309	17	-	11/37/115/115	-
10	A86	17	321	-	-	7/34/90/90	0/3/3/3
13	DD6	20	314	-	-	12/26/80/80	0/3/3/3
10	A86	18	313	-	-	13/34/90/90	0/3/3/3
11	LMG	11	316	-	-	13/27/47/70	0/1/1/1
8	CLA	14	303	-	-	5/28/106/115	-
10	A86	20	311	-	-	6/34/90/90	0/3/3/3
8	CLA	12	305	-	1/1/15/20	10/37/115/115	-
8	CLA	19	306	5	1/1/15/20	7/37/115/115	-
8	CLA	21	210	-	-	4/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	A86	12	302	-	-	13/34/90/90	0/3/3/3
10	A86	21	211	-	-	9/34/90/90	0/3/3/3
14	SQD	17	301	-	-	25/44/64/69	0/1/1/1
8	CLA	13	304	-	1/1/13/20	14/28/106/115	-
10	A86	20	313	-	-	15/34/90/90	0/3/3/3
10	A86	14	315	-	-	6/34/90/90	0/3/3/3
8	CLA	14	301	1	-	13/37/115/115	-
8	CLA	15	303	-	1/1/13/20	8/28/106/115	-
8	CLA	17	307	4	1/1/12/20	8/22/100/115	-
8	CLA	15	308	17	1/1/15/20	10/37/115/115	-
8	CLA	18	305	-	1/1/11/20	4/13/91/115	-
9	KC1	17	309	4	-	7/15/71/71	-
10	A86	11	310	-	-	7/34/90/90	0/3/3/3
9	KC1	12	308	2	-	6/15/71/71	-
8	CLA	16	307	17	1/1/14/20	13/33/111/115	-
8	CLA	13	308	1	1/1/12/20	12/22/100/115	-
10	A86	15	313	-	-	9/34/90/90	0/3/3/3
10	A86	12	315	-	-	10/34/90/90	0/3/3/3
8	CLA	16	306	3	1/1/15/20	15/37/115/115	-
8	CLA	12	301	17	1/1/15/20	15/37/115/115	-
10	A86	11	313	-	-	10/34/90/90	0/3/3/3
10	A86	12	314	-	-	13/34/90/90	0/3/3/3
10	A86	15	319	-	-	8/34/90/90	0/3/3/3
8	CLA	14	302	-	1/1/15/20	17/37/115/115	-
13	DD6	16	312	-	-	11/26/80/80	0/3/3/3
8	CLA	17	304	-	1/1/13/20	9/27/105/115	-
10	A86	12	312	-	-	5/34/90/90	0/3/3/3
13	DD6	19	312	-	-	12/26/80/80	0/3/3/3
9	KC1	18	304	1	-	7/15/71/71	-
15	LHG	17	317	-	-	27/48/48/53	-
8	CLA	15	307	1	1/1/12/20	12/22/100/115	-
8	CLA	17	308	17	1/1/15/20	7/37/115/115	-
8	CLA	20	310	6	1/1/11/20	3/13/91/115	-
9	KC1	11	306	1	-	8/15/71/71	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	A86	18	311	-	-	6/34/90/90	0/3/3/3
10	A86	20	301	-	-	14/34/90/90	0/3/3/3
9	KC1	13	310	1	-	7/15/71/71	-
10	A86	14	311	-	-	5/34/90/90	0/3/3/3
9	KC1	16	305	3	-	6/15/71/71	-
8	CLA	21	204	-	1/1/13/20	11/29/107/115	-
10	A86	14	313	-	-	12/34/90/90	0/3/3/3
8	CLA	16	303	-	1/1/13/20	9/28/106/115	-
9	KC1	20	303	-	-	7/15/71/71	-
9	KC1	20	305	6	-	7/15/71/71	-
9	KC1	12	306	2	-	6/15/71/71	-
8	CLA	11	307	1	-	6/22/100/115	-
9	KC1	11	304	1	-	4/15/71/71	-
10	A86	14	316	-	-	15/34/90/90	0/3/3/3
9	KC1	15	302	-	-	6/15/71/71	-
15	LHG	19	314	8	-	26/53/53/53	-
8	CLA	19	307	15	1/1/15/20	8/37/115/115	-
10	A86	17	315	-	-	9/34/90/90	0/3/3/3
8	CLA	20	304	-	1/1/13/20	10/27/105/115	-
9	KC1	13	307	1	-	5/15/71/71	-

The worst 5 of 3389 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	20	314	DD6	C10-C11	25.45	1.69	1.35
13	21	212	DD6	C10-C11	25.38	1.69	1.35
13	21	216	DD6	C10-C11	25.33	1.69	1.35
13	19	312	DD6	C10-C11	25.25	1.69	1.35
13	20	312	DD6	C10-C11	25.24	1.69	1.35

The worst 5 of 4223 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	17	315	A86	O1-C20-C19	57.91	156.89	113.38
10	20	313	A86	O1-C20-C19	57.24	156.38	113.38
10	19	313	A86	O1-C20-C19	56.80	156.05	113.38
10	13	314	A86	O1-C20-C19	56.48	155.81	113.38
10	20	311	A86	O1-C20-C19	56.44	155.78	113.38

5 of 55 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
8	11	303	CLA	ND
8	11	305	CLA	ND
8	11	309	CLA	ND
8	12	301	CLA	ND
8	12	303	CLA	ND

5 of 1582 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	11	301	CLA	C1A-C2A-CAA-CBA
8	11	301	CLA	C3A-C2A-CAA-CBA
8	11	303	CLA	C1A-C2A-CAA-CBA
8	11	309	CLA	CBD-CGD-O2D-CED
8	12	301	CLA	CHA-CBD-CGD-O1D

There are no ring outliers.

75 monomers are involved in 128 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	15	301	CLA	6	0
8	18	310	CLA	1	0
14	16	314	SQD	2	0
8	16	301	CLA	2	0
10	15	311	A86	1	0
8	21	206	CLA	3	0
10	14	314	A86	1	0
8	12	307	CLA	1	0
11	16	315	LMG	1	0
8	14	308	CLA	1	0
8	19	305	CLA	2	0
8	19	301	CLA	2	0
8	18	301	CLA	1	0
8	19	310	CLA	2	0
8	18	302	CLA	4	0
9	17	303	KC1	2	0
8	16	309	CLA	1	0
8	11	305	CLA	1	0
8	20	307	CLA	1	0
8	20	309	CLA	1	0
8	12	303	CLA	3	0
10	11	311	A86	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	13	301	CLA	2	0
8	12	309	CLA	1	0
8	18	308	CLA	3	0
8	13	302	CLA	2	0
8	18	303	CLA	1	0
8	12	311	CLA	1	0
8	11	301	CLA	2	0
8	17	310	CLA	1	0
8	17	302	CLA	1	0
8	21	202	CLA	2	0
8	20	302	CLA	2	0
8	19	304	CLA	1	0
8	13	311	CLA	3	0
8	19	309	CLA	1	0
8	19	302	CLA	3	0
8	18	307	CLA	2	0
8	21	208	CLA	1	0
8	14	307	CLA	1	0
10	13	312	A86	1	0
8	11	303	CLA	1	0
10	11	318	A86	1	0
8	12	304	CLA	1	0
8	15	310	CLA	1	0
16	19	315	LMU	1	0
15	21	217	LHG	4	0
8	13	309	CLA	4	0
13	20	314	DD6	2	0
10	18	313	A86	1	0
8	14	303	CLA	1	0
8	12	305	CLA	2	0
8	19	306	CLA	1	0
14	17	301	SQD	3	0
8	13	304	CLA	1	0
10	14	315	A86	1	0
8	14	301	CLA	2	0
8	17	307	CLA	1	0
8	15	308	CLA	6	0
10	11	310	A86	1	0
8	16	307	CLA	4	0
8	13	308	CLA	1	0
8	16	306	CLA	1	0
8	12	301	CLA	4	0

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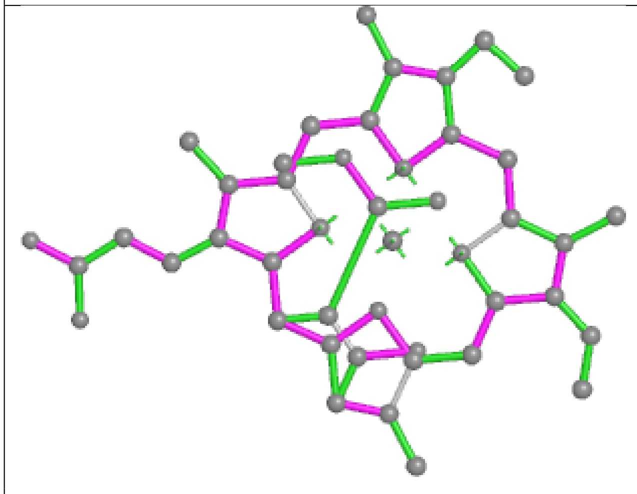
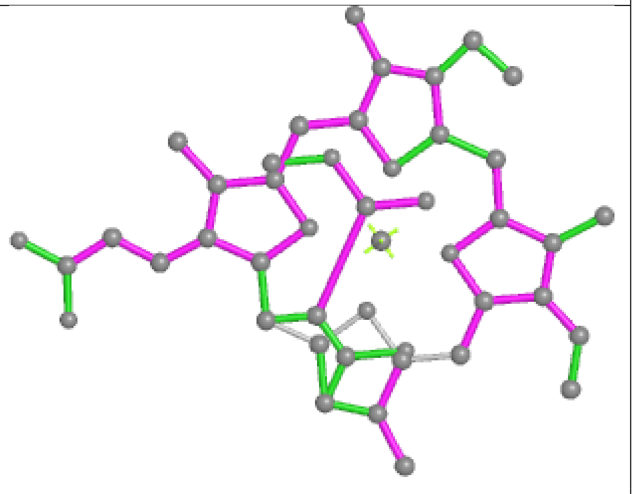
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	14	302	CLA	2	0
13	19	312	DD6	2	0
9	18	304	KC1	1	0
15	17	317	LHG	1	0
8	15	307	CLA	1	0
8	17	308	CLA	4	0
9	11	306	KC1	1	0
10	18	311	A86	1	0
8	11	307	CLA	2	0
15	19	314	LHG	2	0
8	19	307	CLA	2	0

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

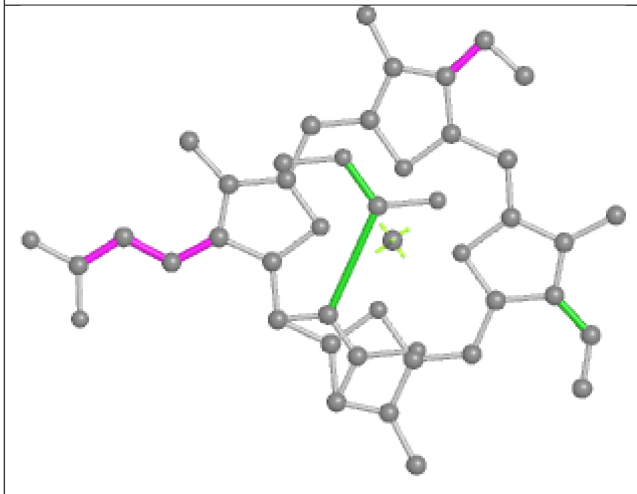
Ligand KC1 16 304



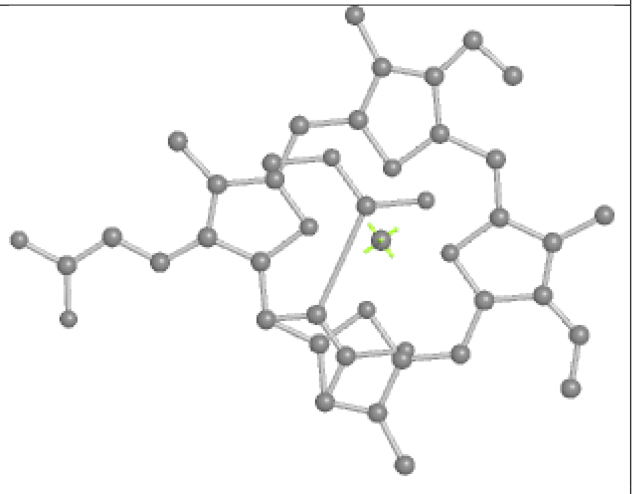
Bond lengths



Bond angles

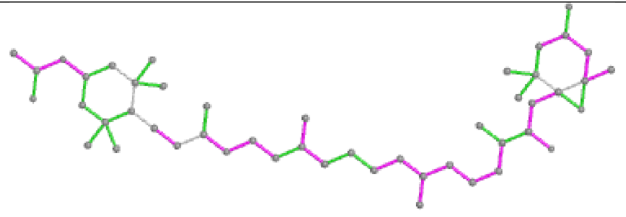


Torsions

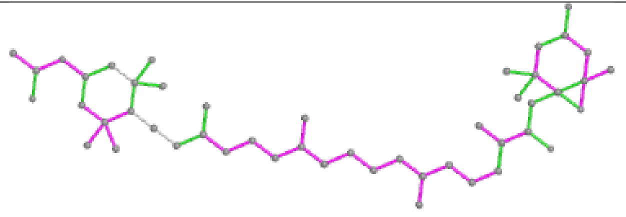


Rings

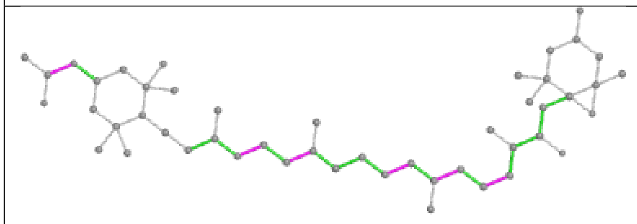
Ligand A86 12 319



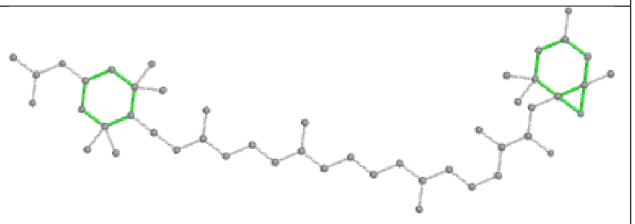
Bond lengths



Bond angles

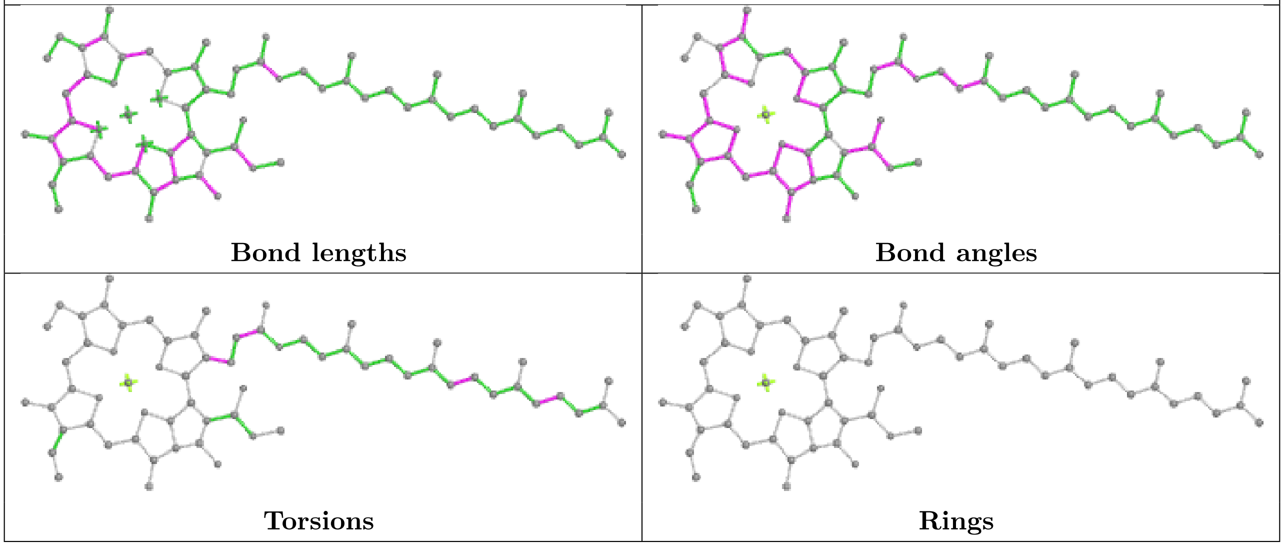


Torsions

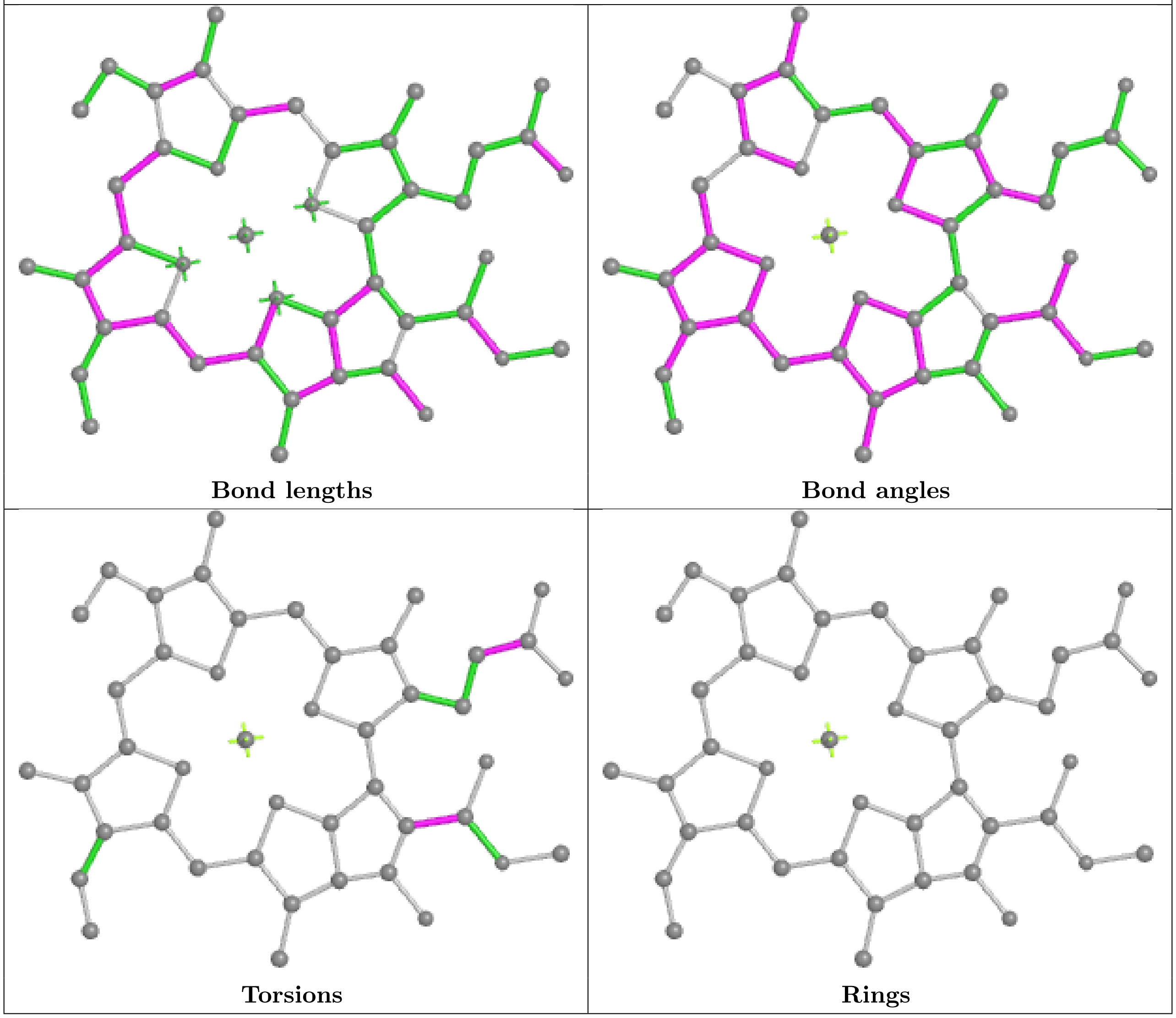


Rings

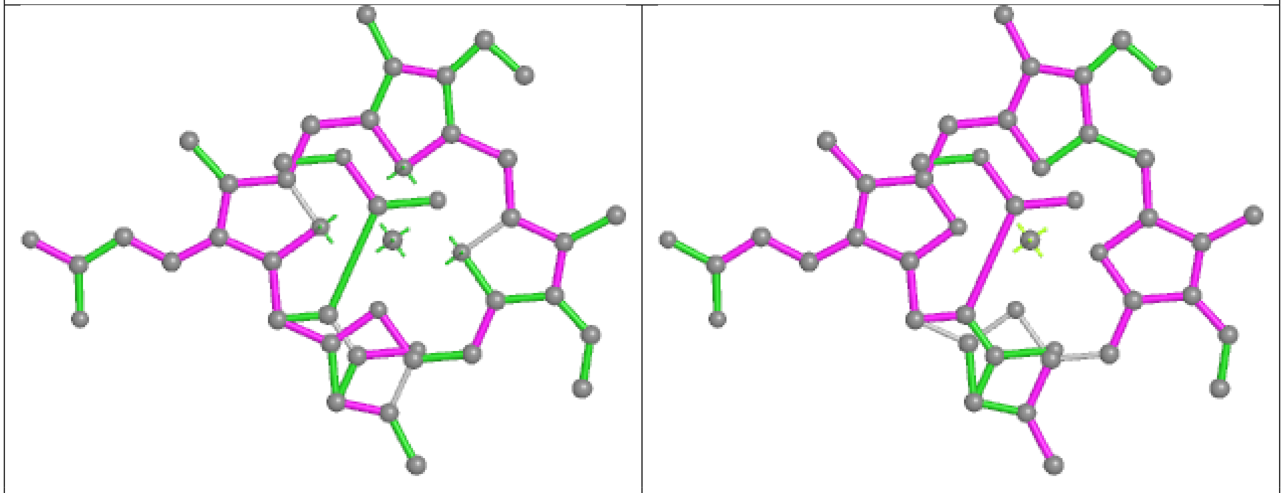
Ligand CLA 15 301


Bond lengths
Bond angles
Torsions
Rings

Ligand CLA 18 310

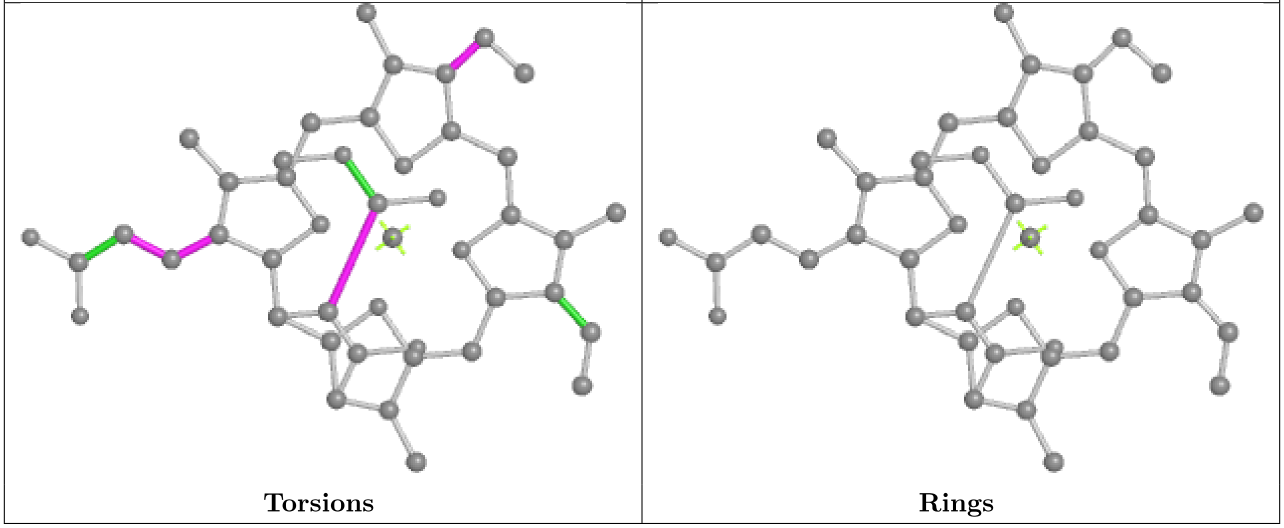

Bond lengths
Bond angles
Torsions
Rings

Ligand KC1 14 306



Bond lengths

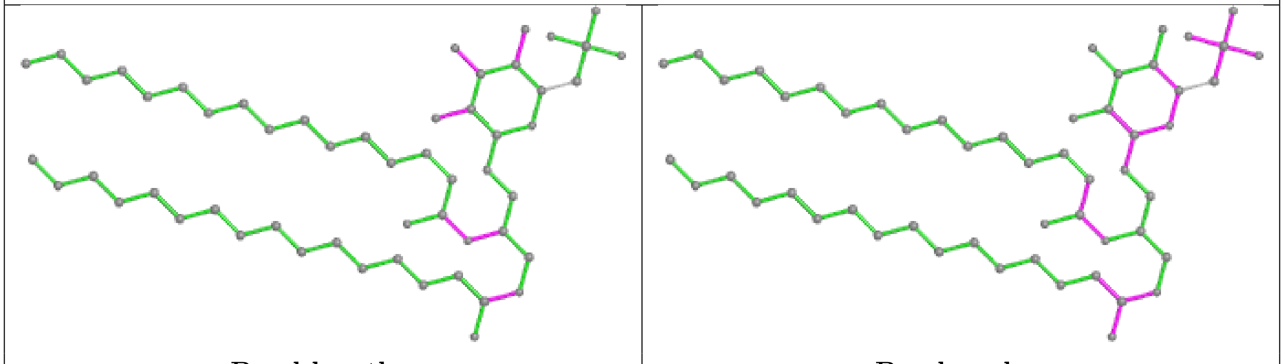
Bond angles



Torsions

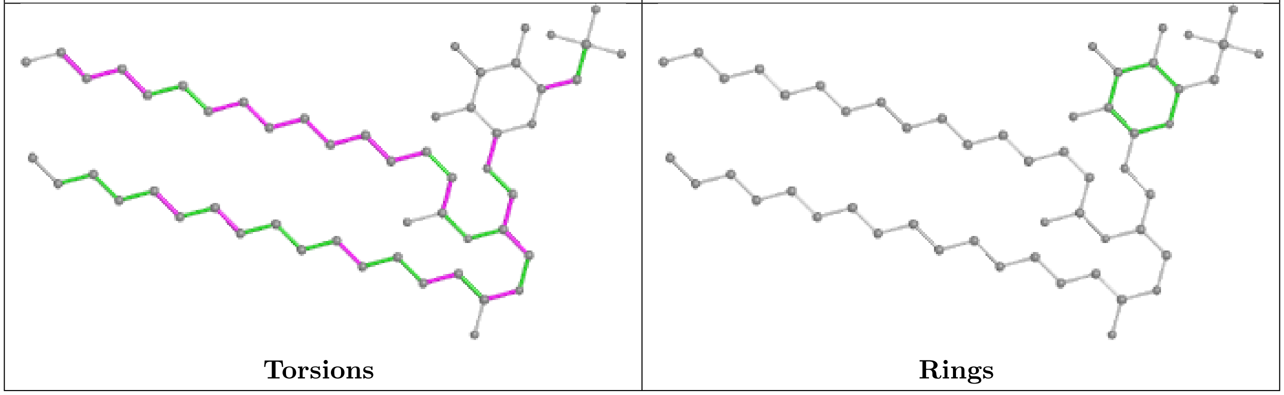
Rings

Ligand SQD 16 314



Bond lengths

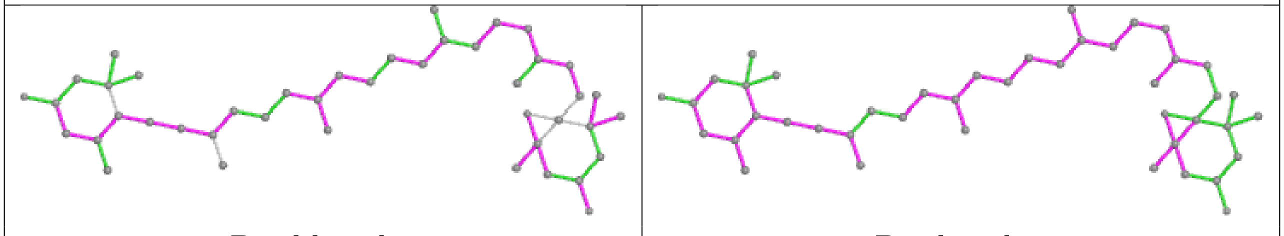
Bond angles



Torsions

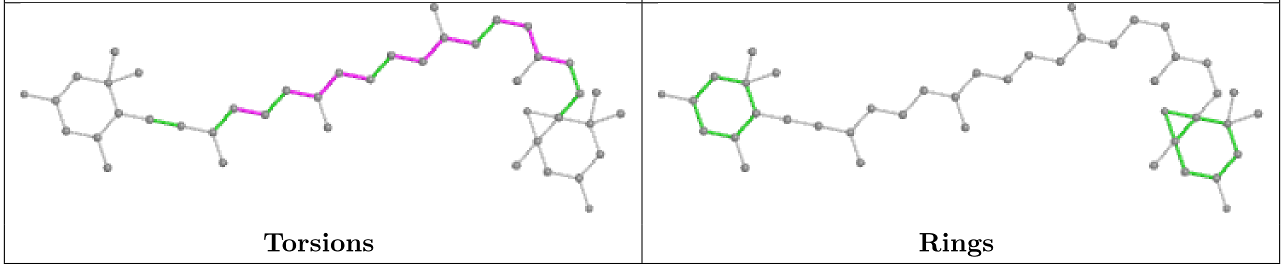
Rings

Ligand DD6 20 312



Bond lengths

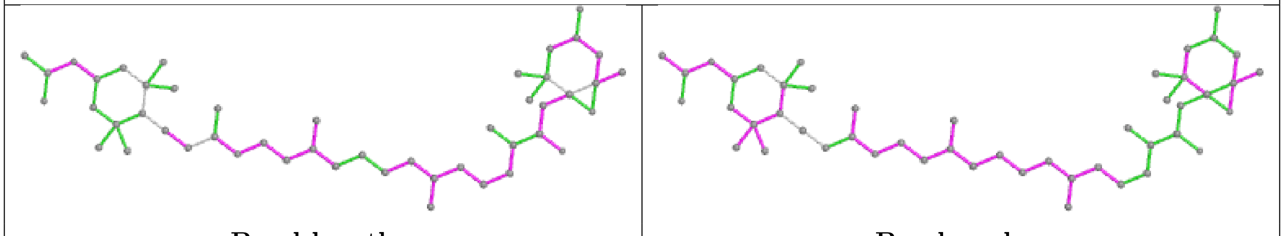
Bond angles



Torsions

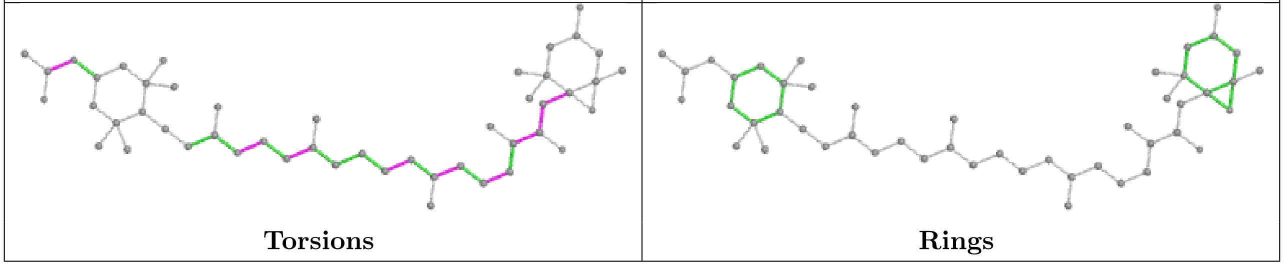
Rings

Ligand A86 15 314



Bond lengths

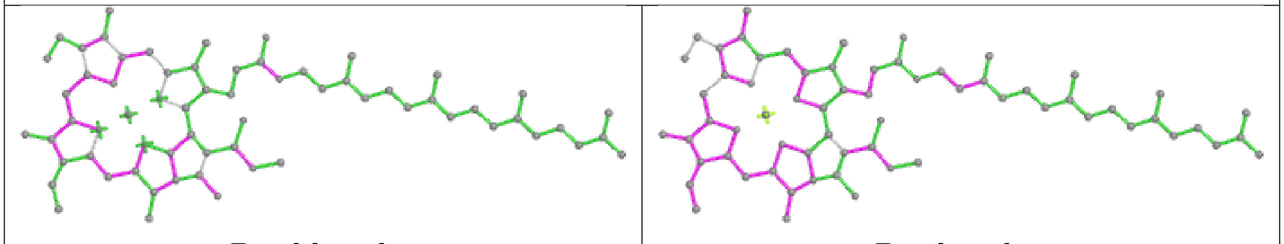
Bond angles



Torsions

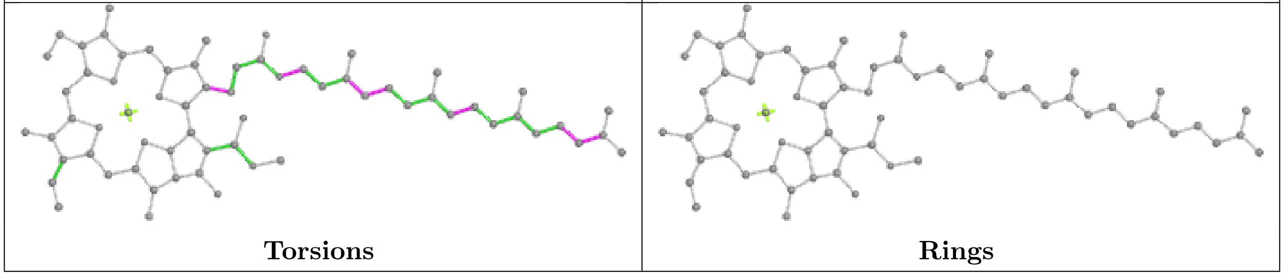
Rings

Ligand CLA 16 301



Bond lengths

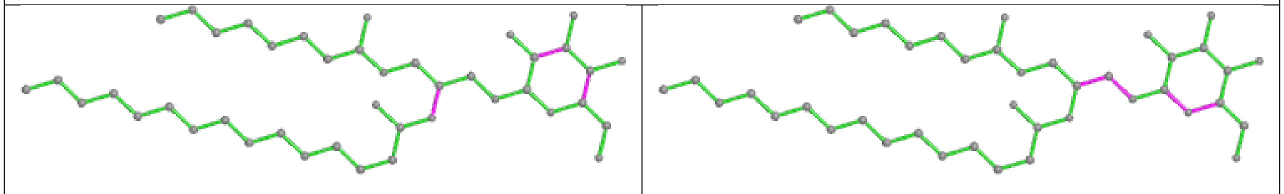
Bond angles



Torsions

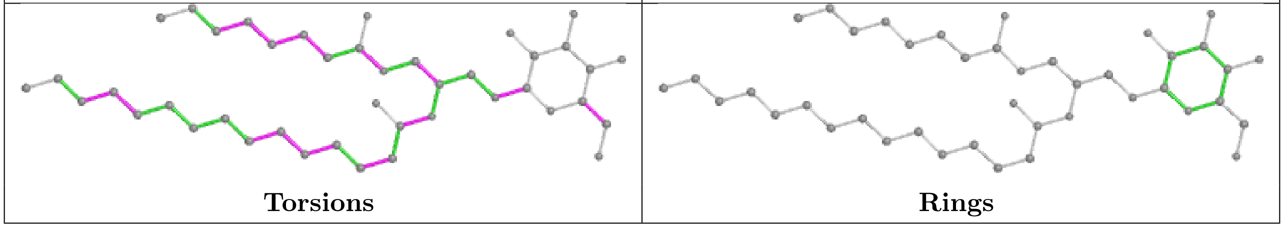
Rings

Ligand LMG 11 315



Bond lengths

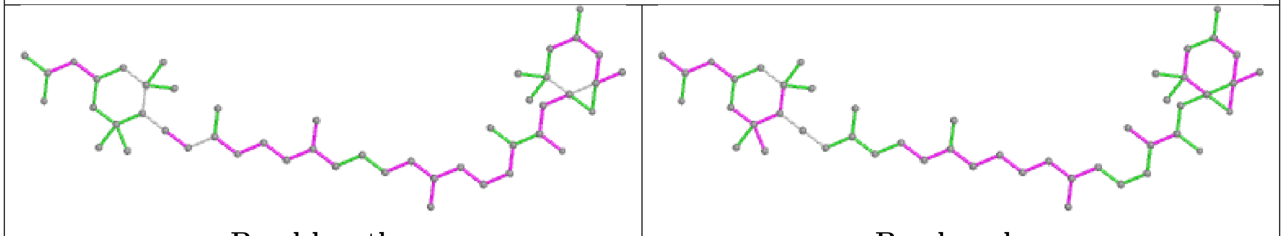
Bond angles



Torsions

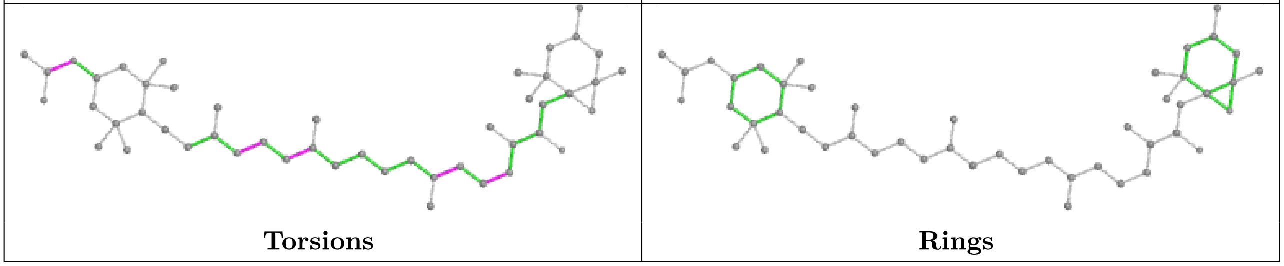
Rings

Ligand A86 13 313



Bond lengths

Bond angles



Torsions

Rings

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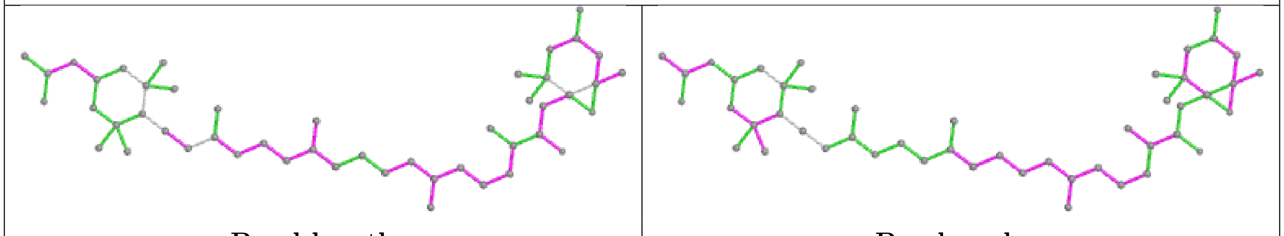
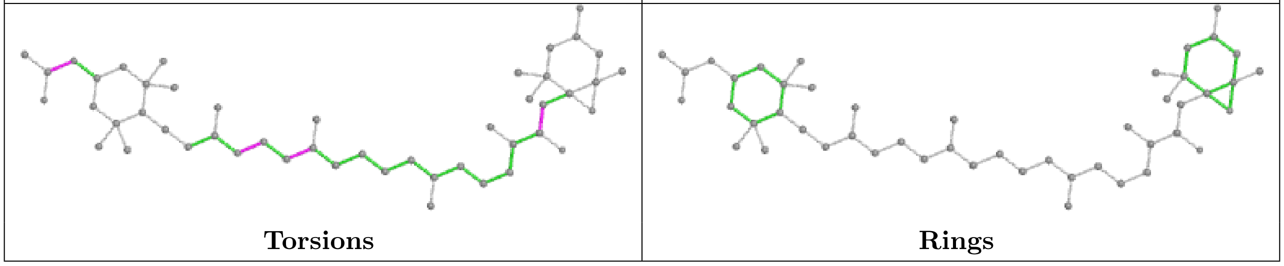


Bond lengths

Bond angles



Torsions

Rings

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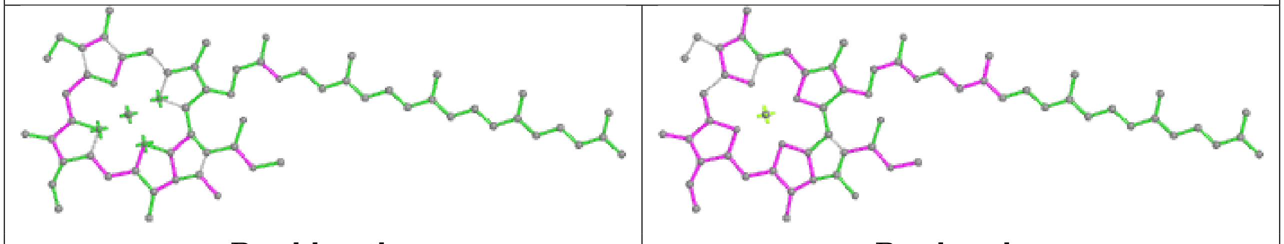
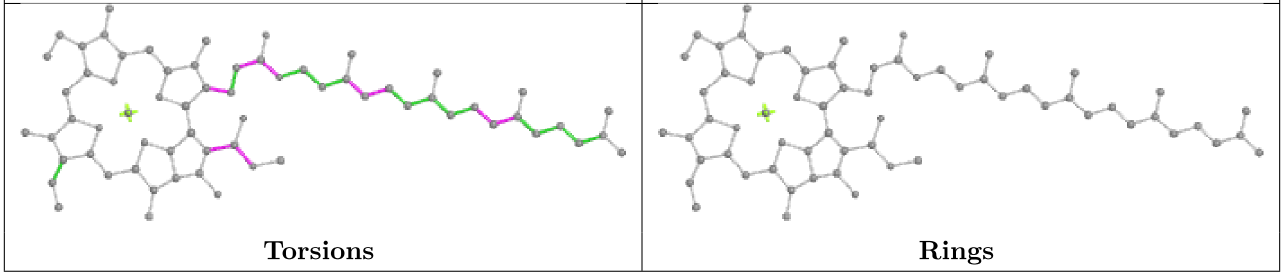


Bond lengths

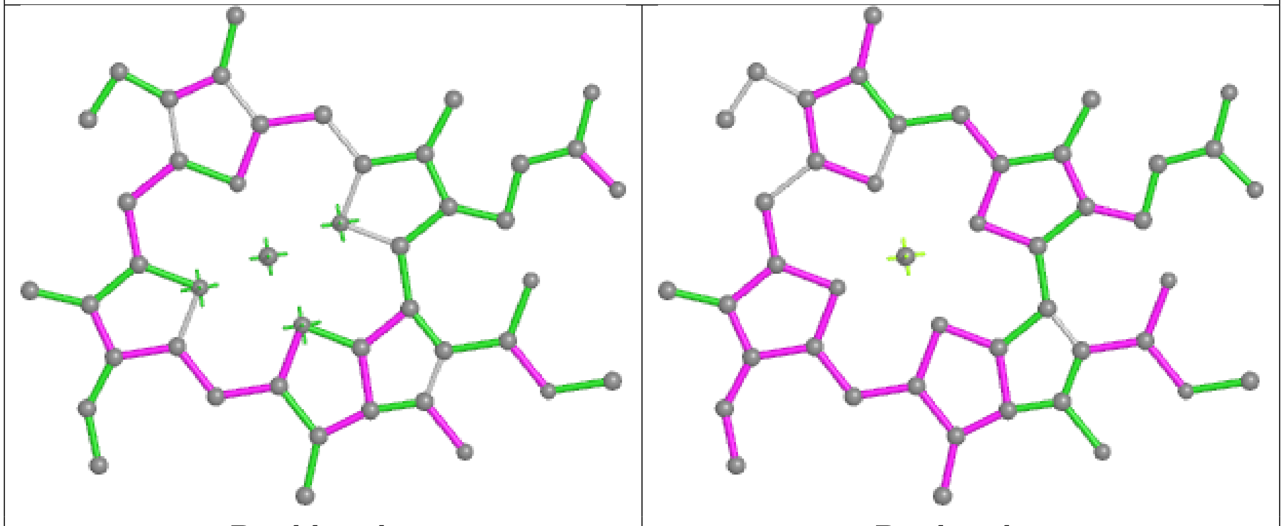
Bond angles



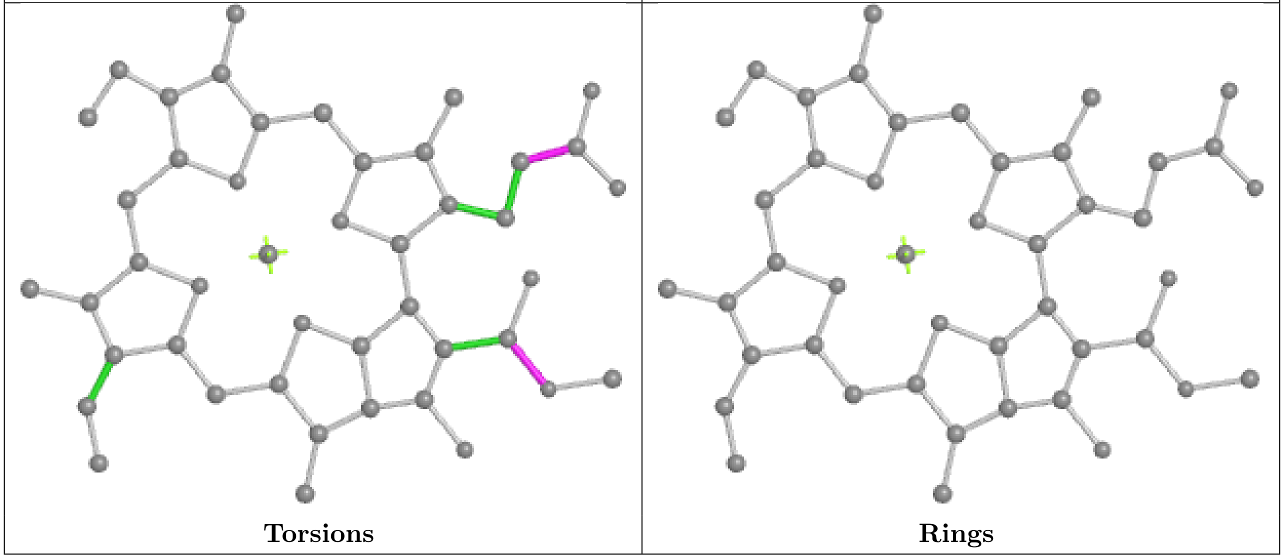
Torsions

Rings

Ligand CLA 14 310

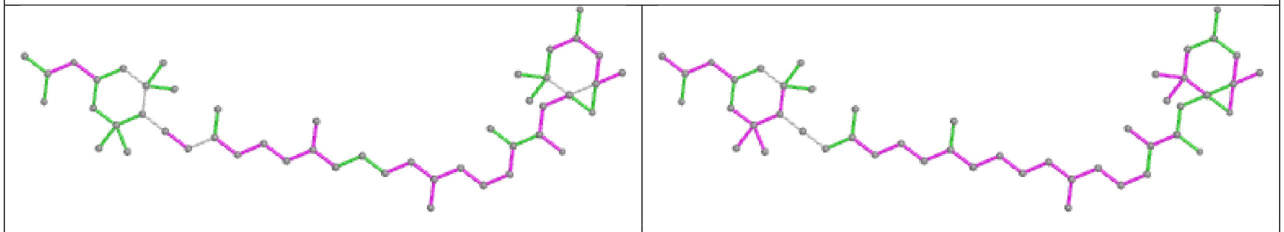


Bond lengths Bond angles

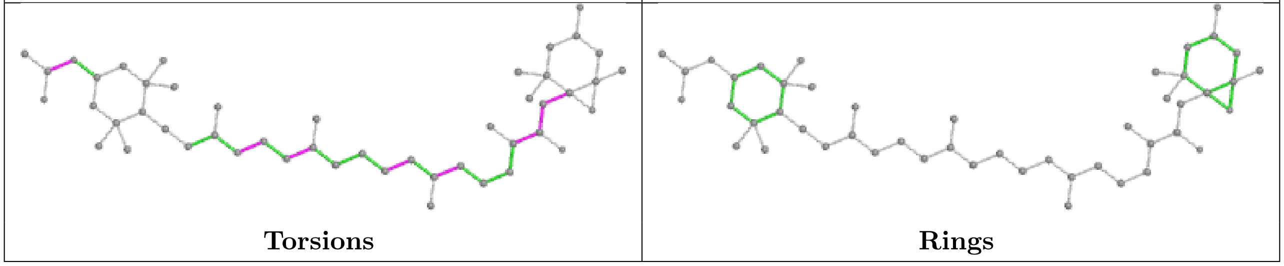


Torsions Rings

Ligand A86 14 314

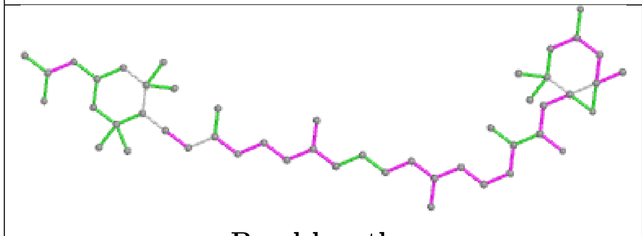


Bond lengths Bond angles



Torsions Rings

Ligand A86 21 213



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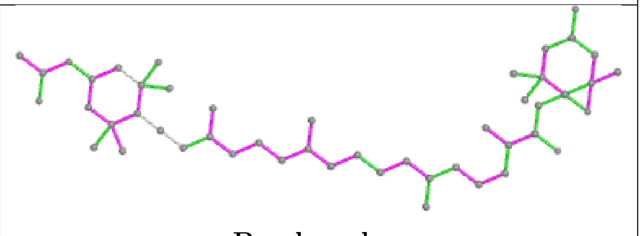
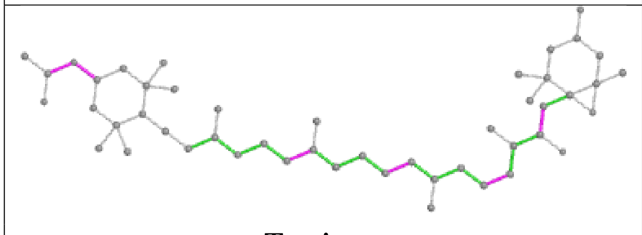
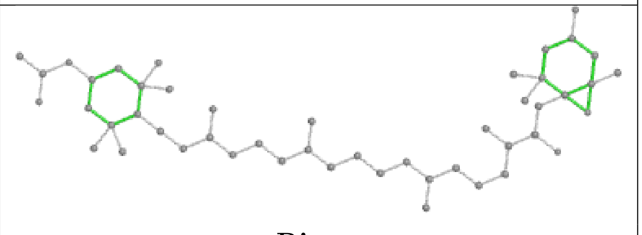


Bond angles

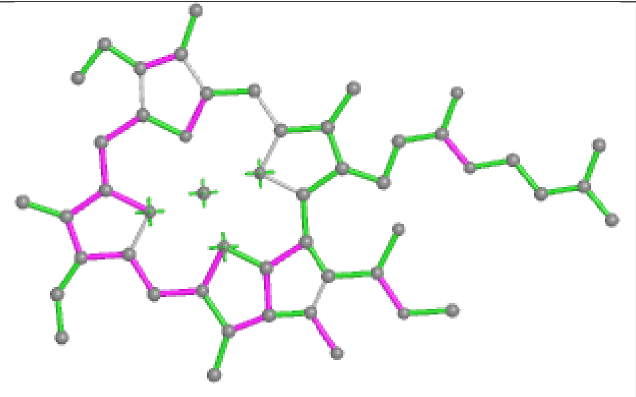


Torsions



Rings

Ligand CLA 12 307



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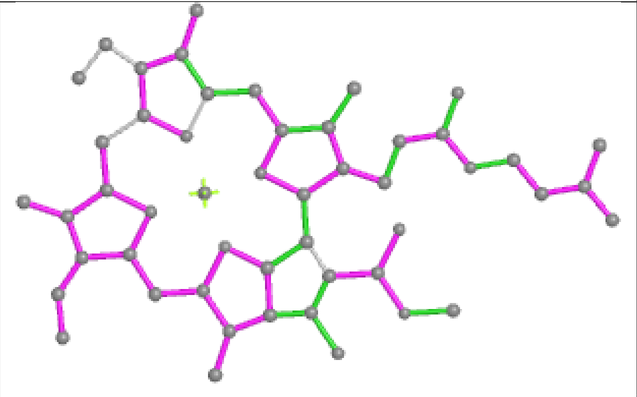
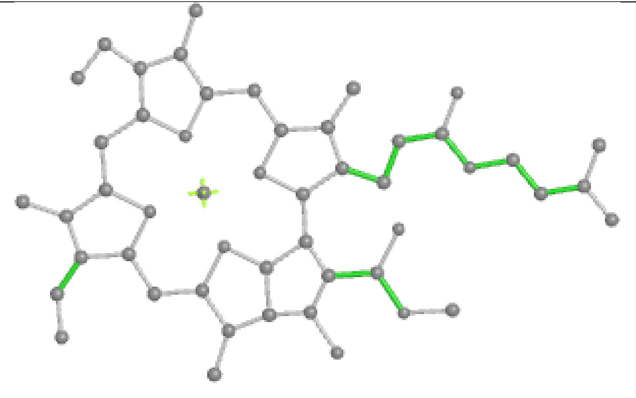


Bond angles



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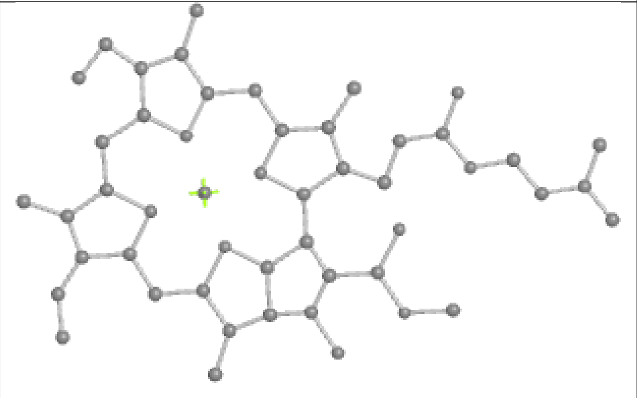
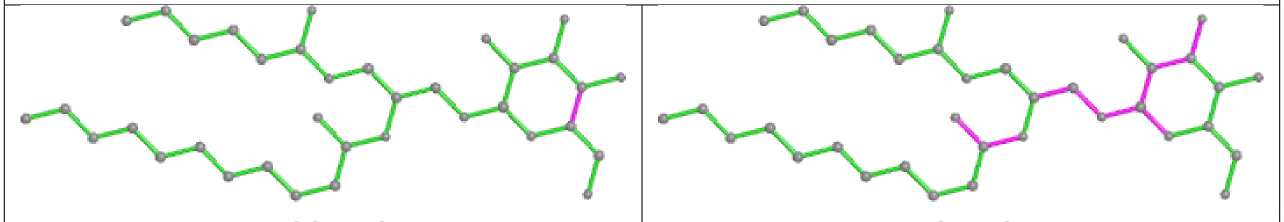


Rings

Ligand LMG 16 315



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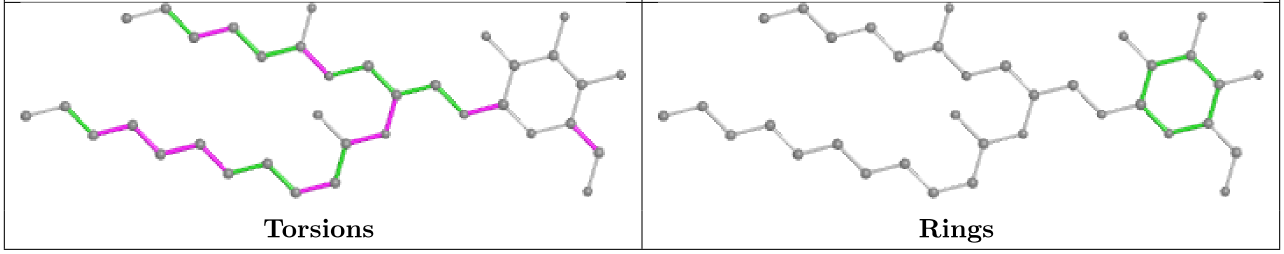
Bond angles



Torsions

Rings

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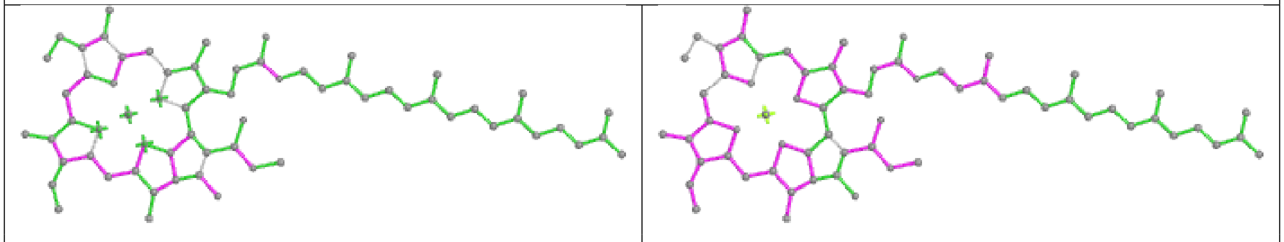

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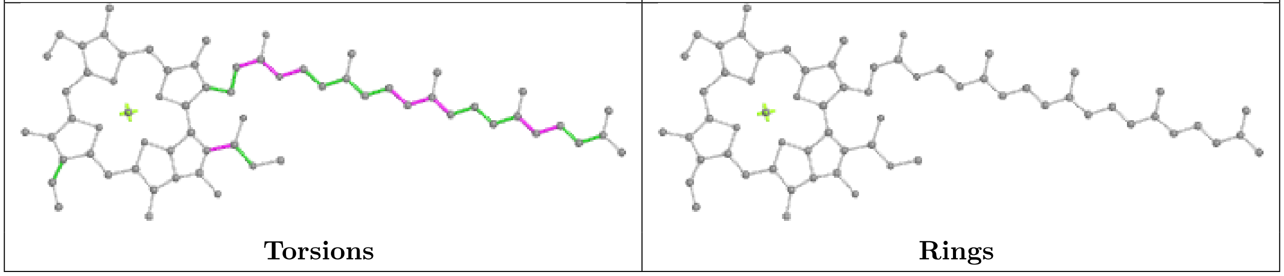
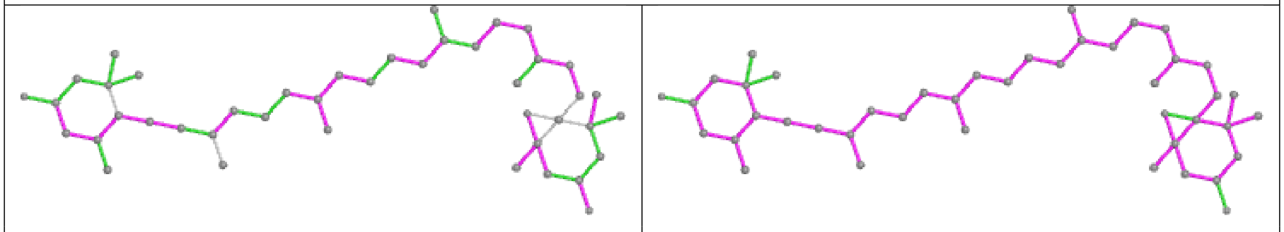
Bond angles



Torsions

Rings

Ligand DD6 21 212



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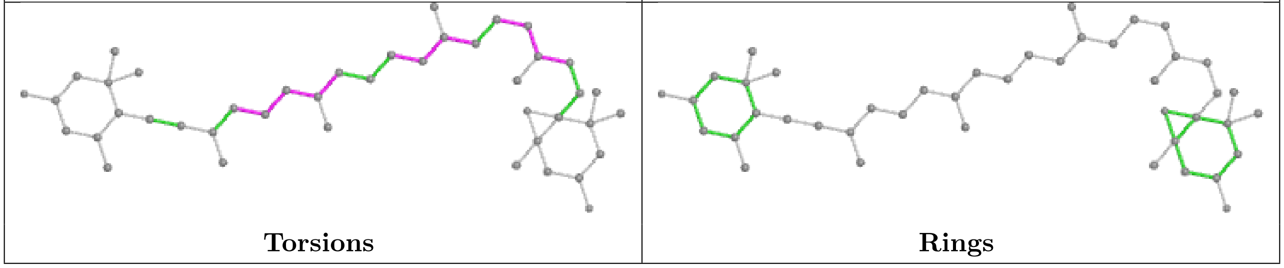
Bond angles



Torsions

Rings

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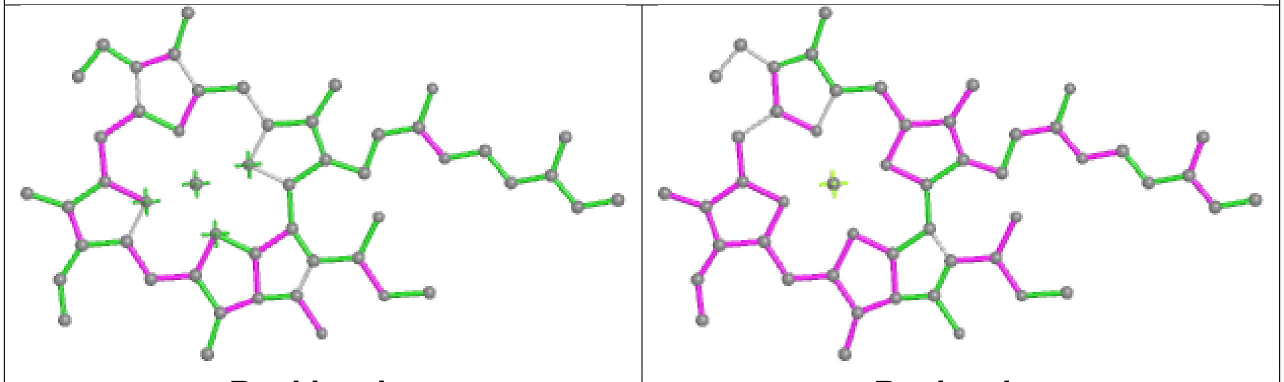
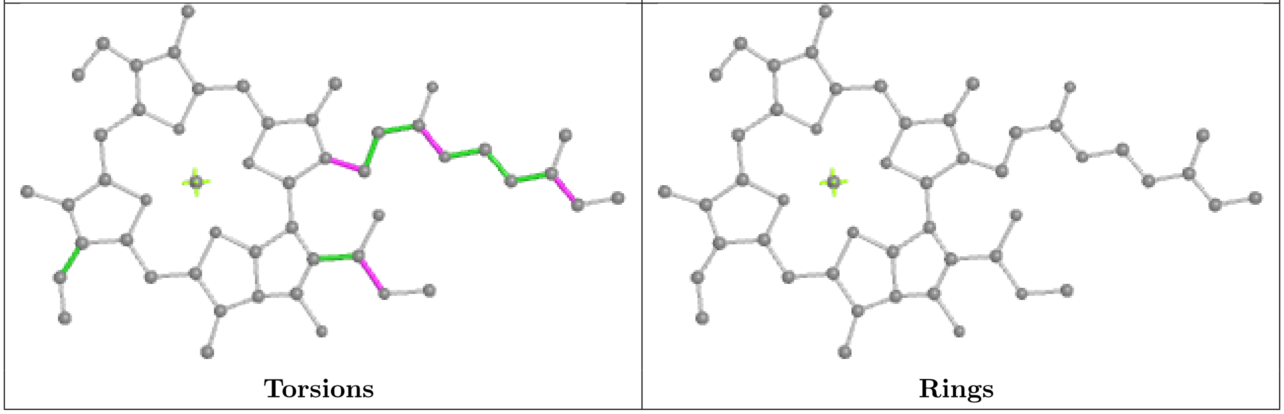


Bond lengths

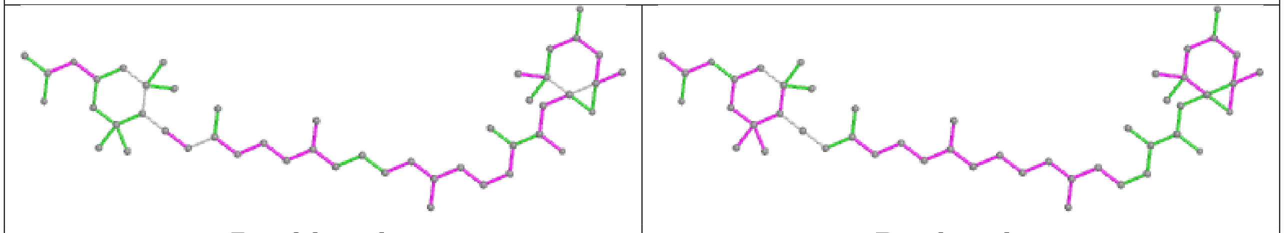
Bond angles



Torsions

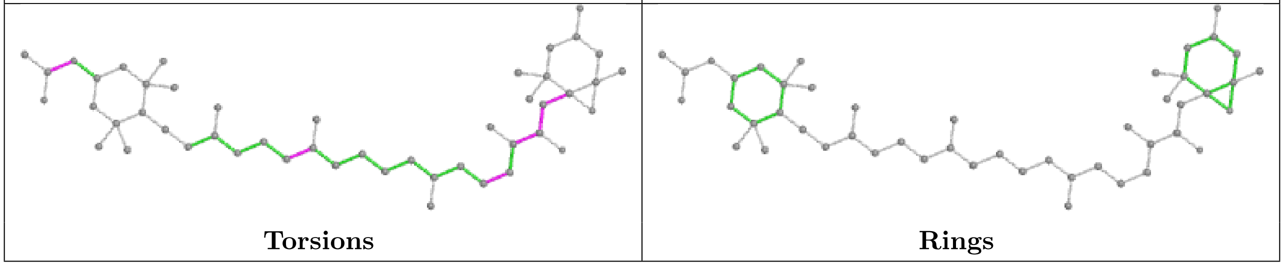
Rings

Ligand A86 19 313



Bond lengths

Bond angles



Torsions

Rings

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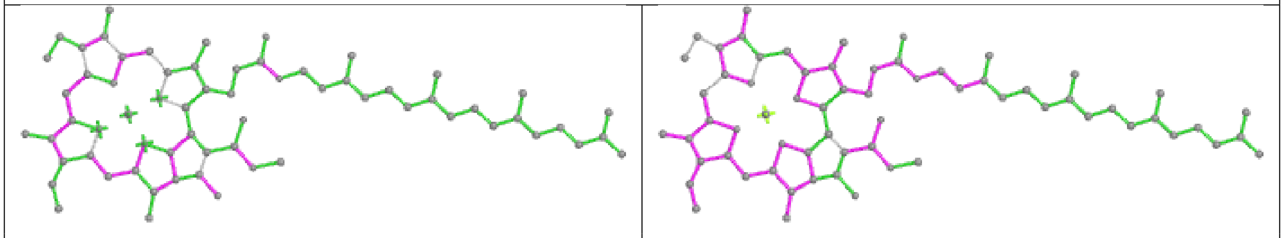
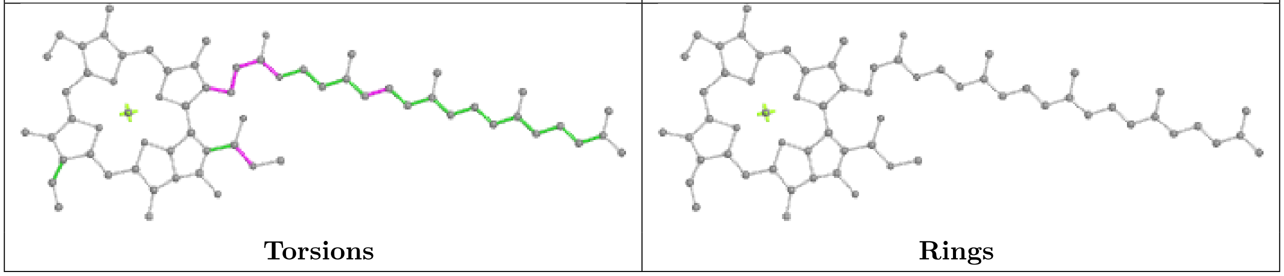

Bond lengths

Bond angles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Rings

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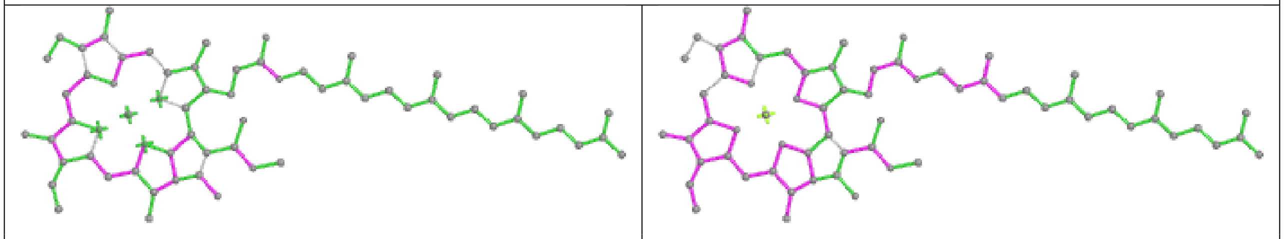
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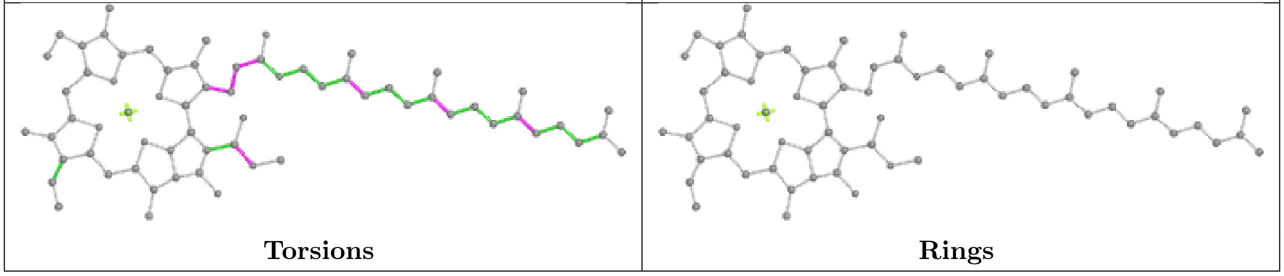
Bond angles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Rings

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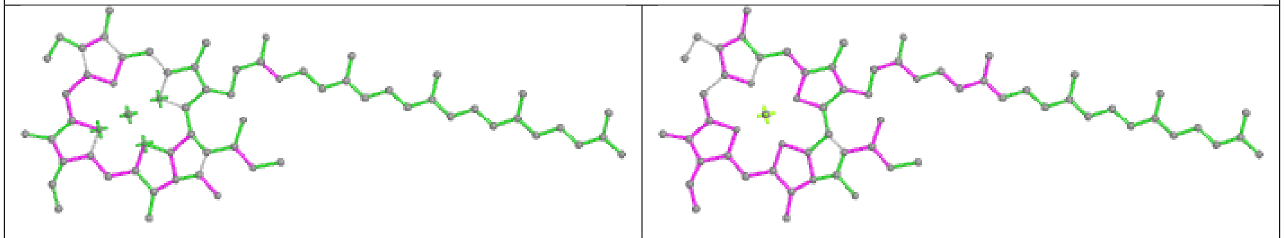
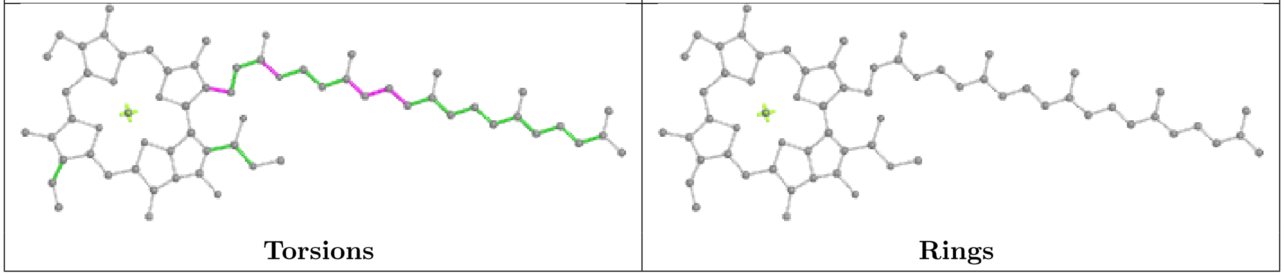

Bond lengths

Bond angles


Torsions

Rings

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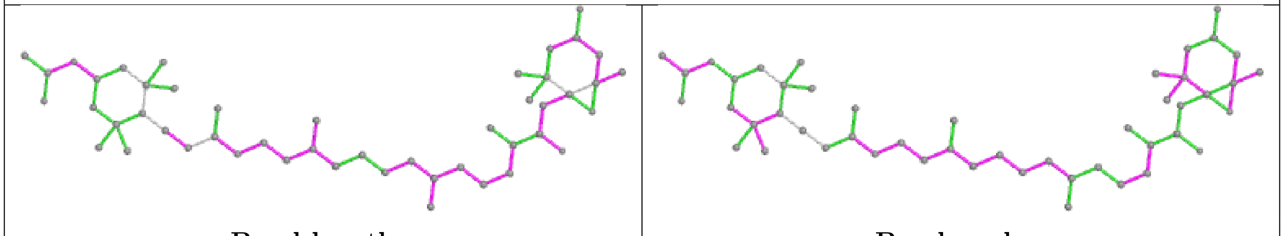
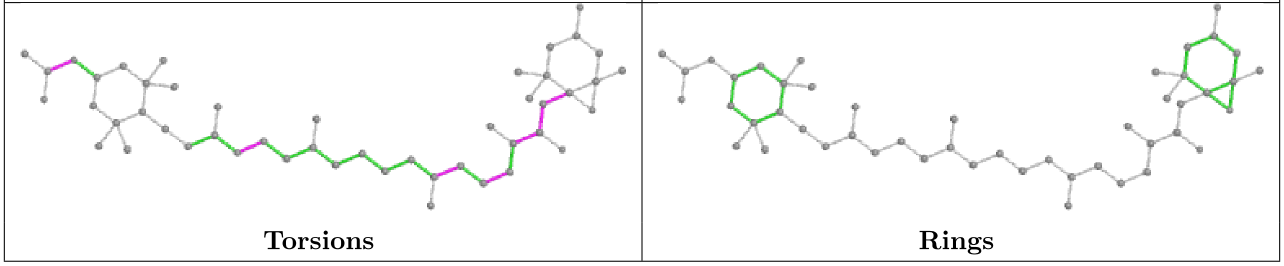


Bond lengths Bond angles



Torsions Rings

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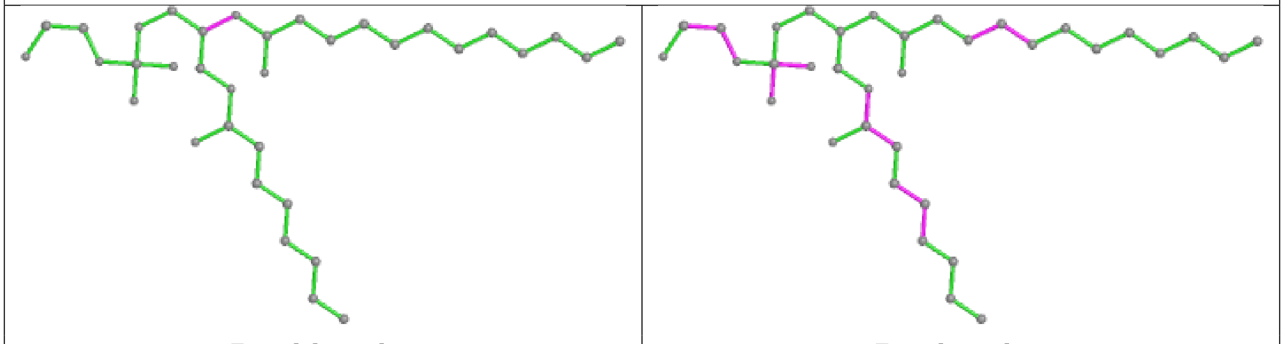
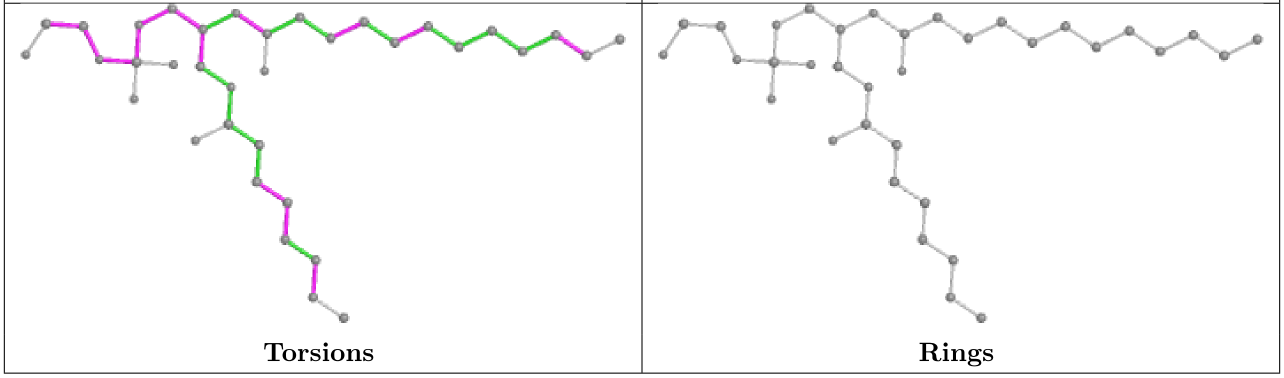


Bond lengths Bond angles



Torsions Rings

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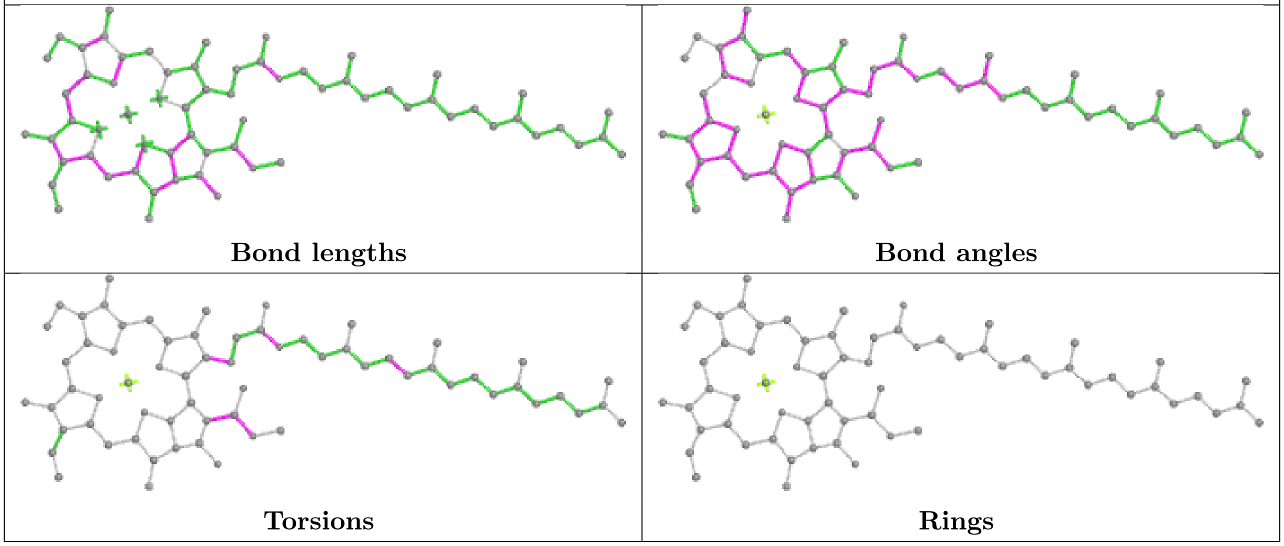

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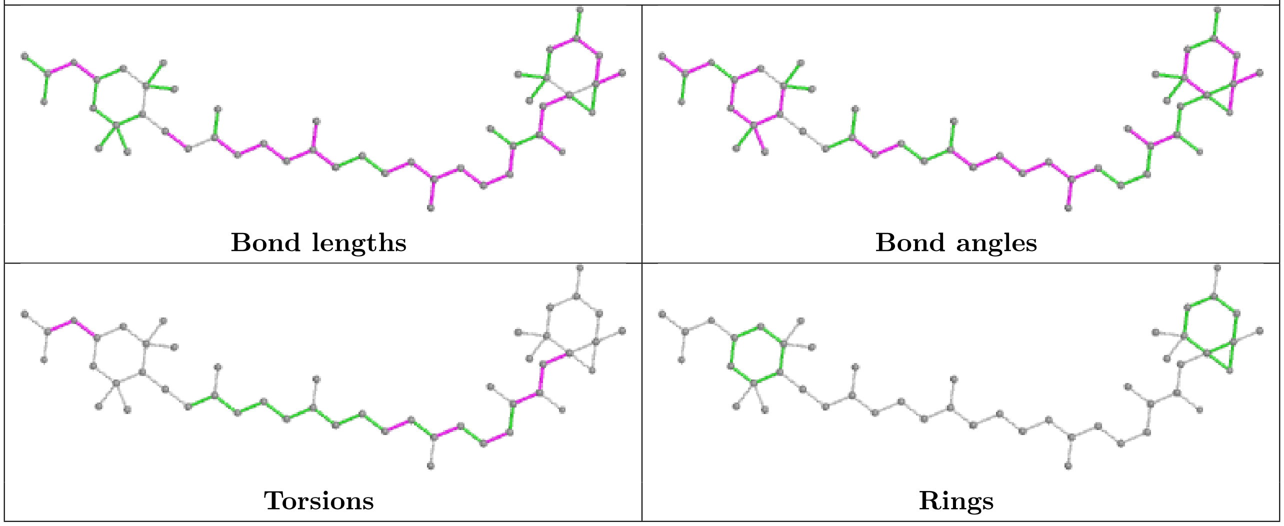
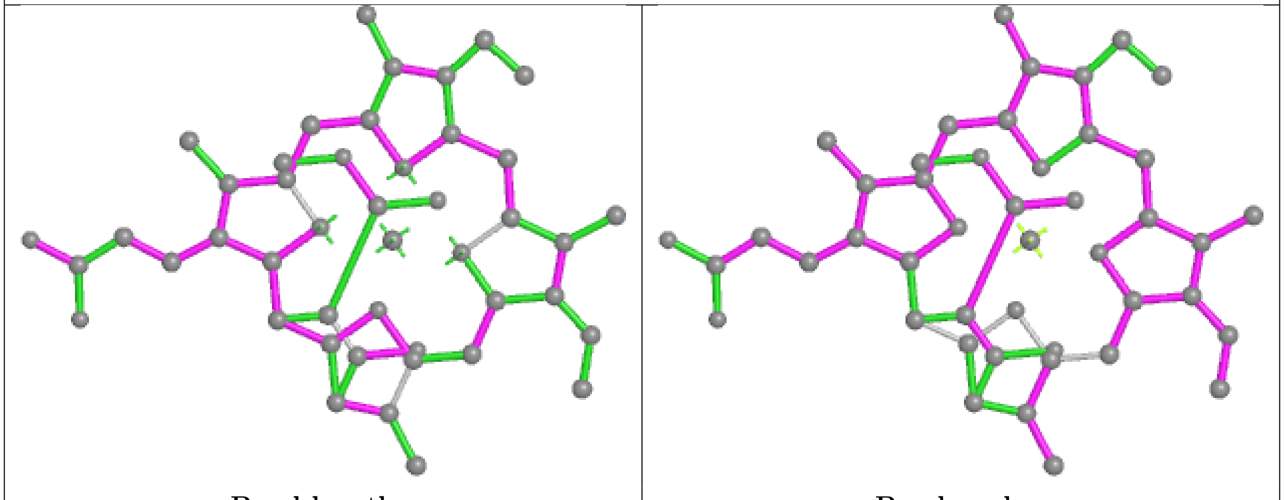


Ligand KC1 17 303



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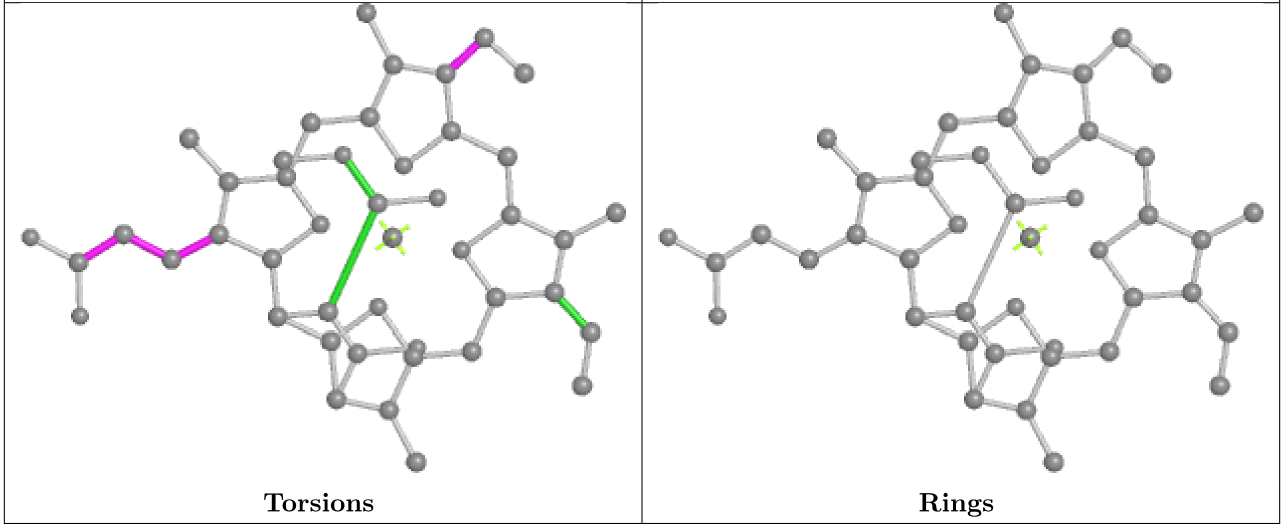
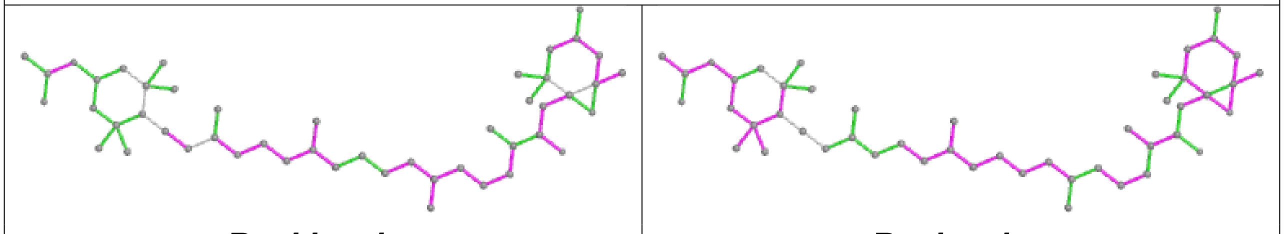


Torsions Rings

Ligand A86 17 313



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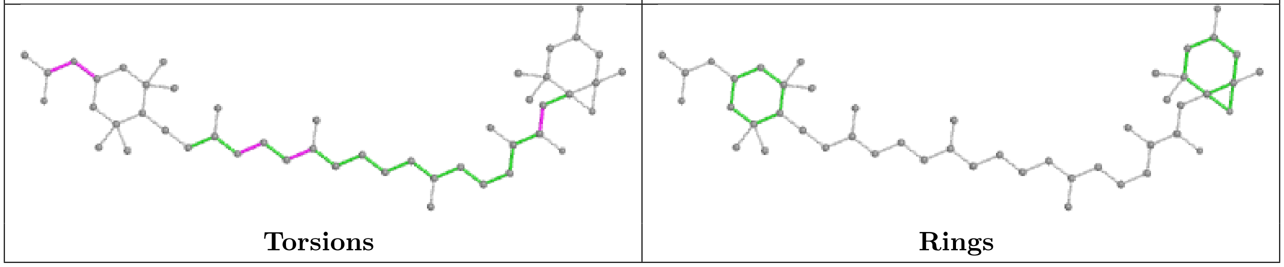

Torsions Rings

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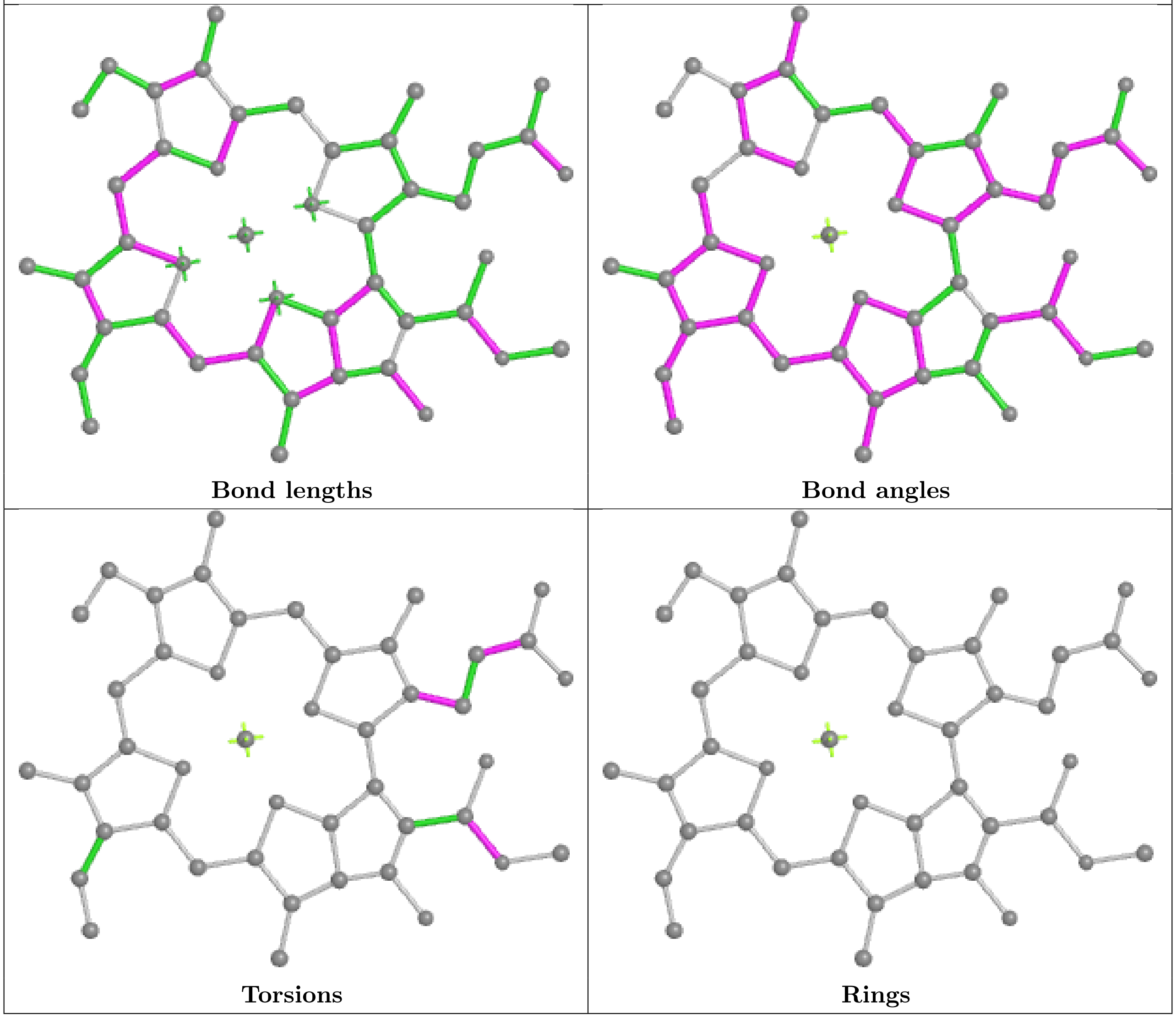


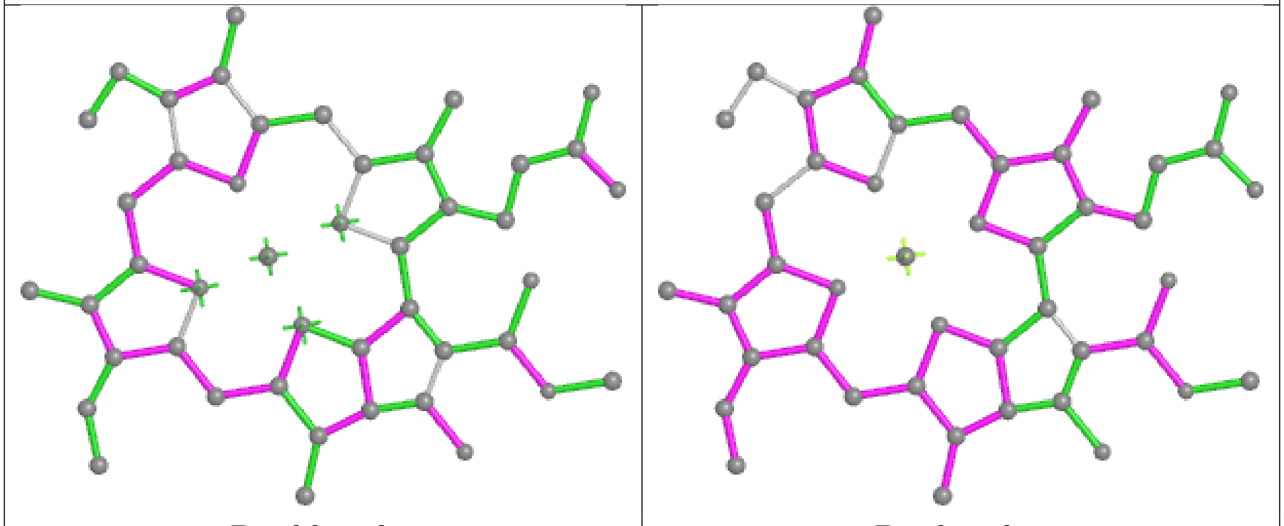
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA 11 305



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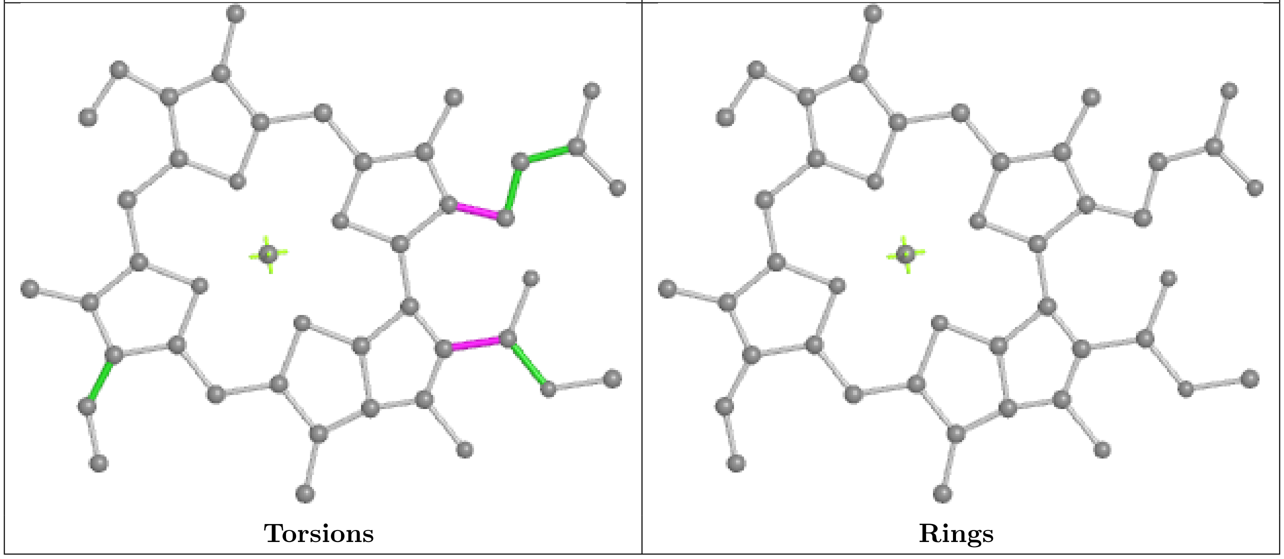
Bond angles



Torsions

Rings

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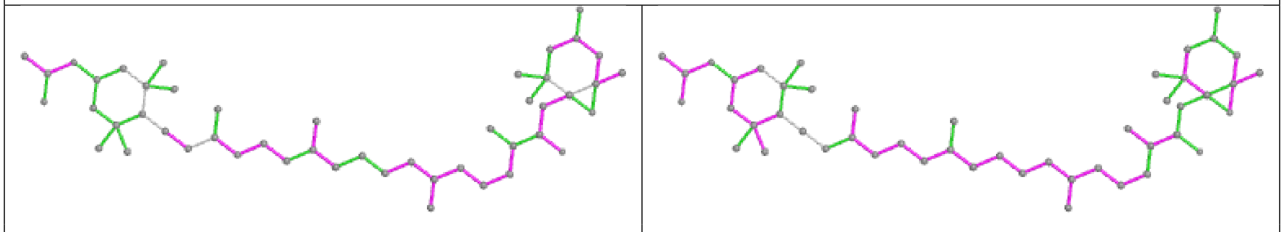
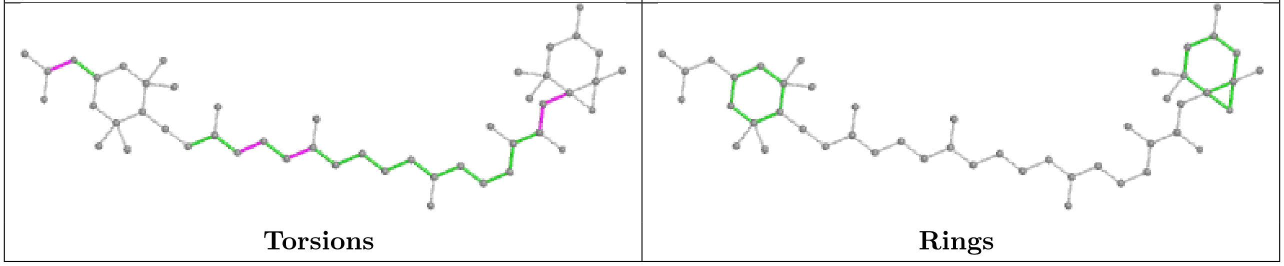


Bond lengths

Bond angles



Torsions

Rings

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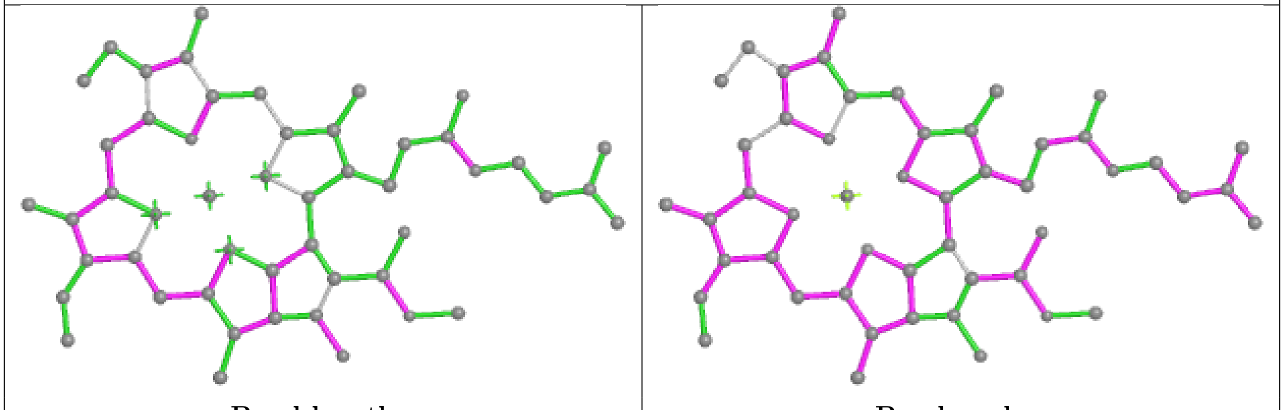
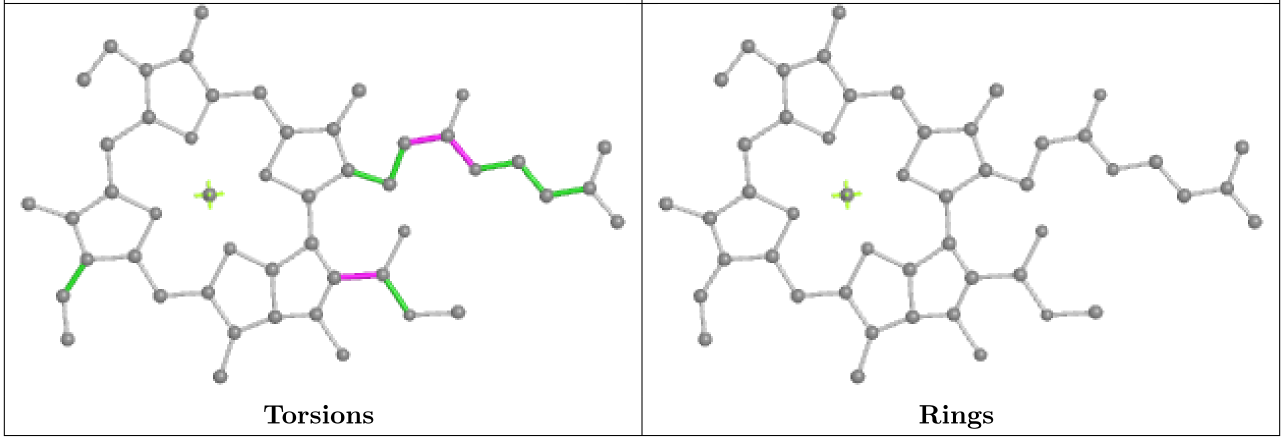


Bond lengths

Bond angles



Torsions

Rings

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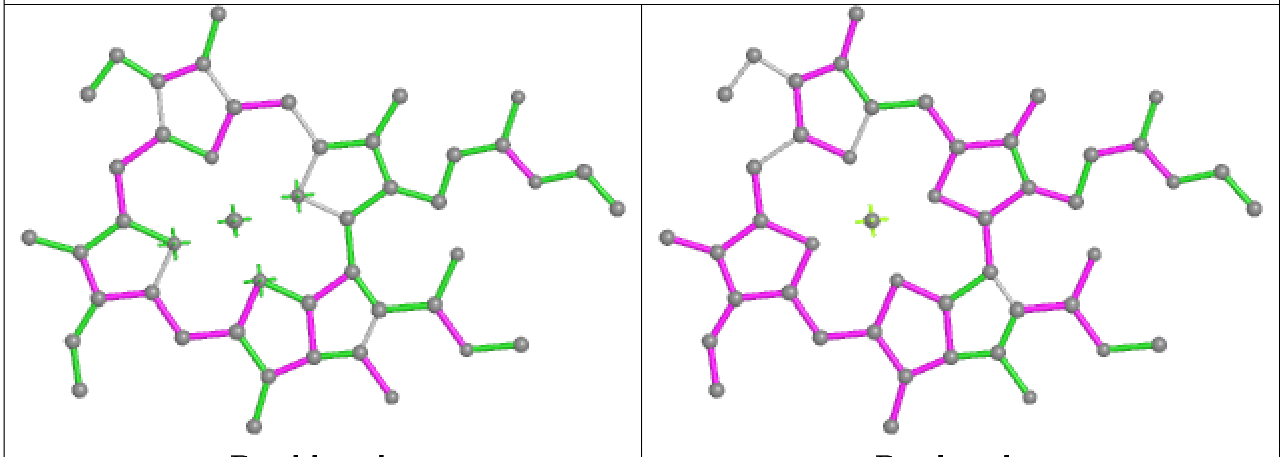
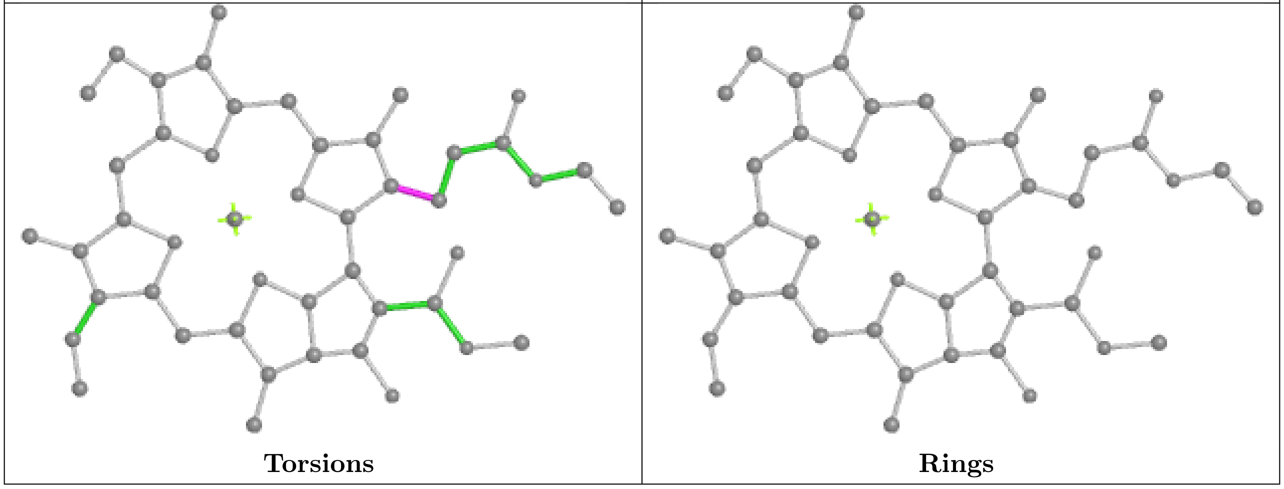
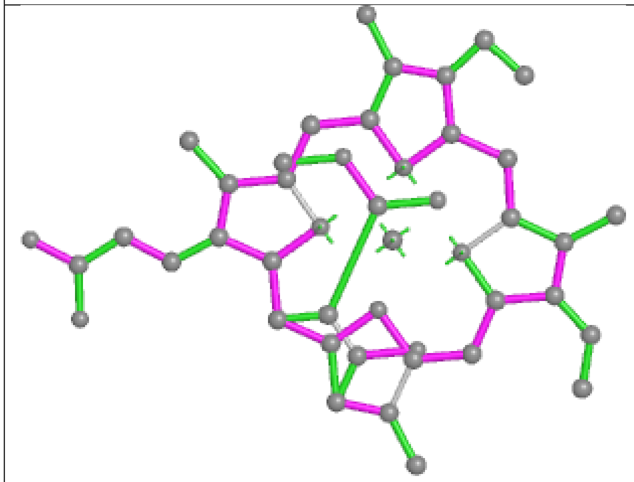


Bond lengths **Bond angles**



Torsions **Rings**

Ligand KC1 13 303



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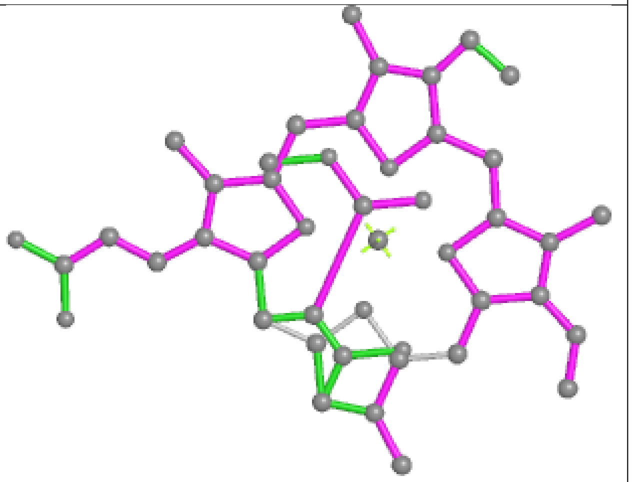
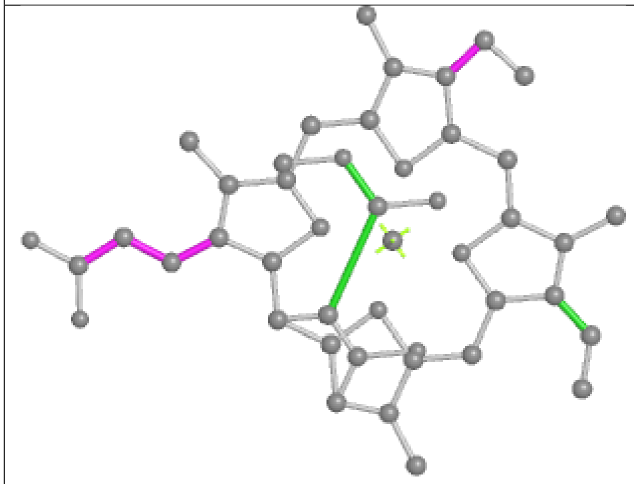


Bond angles



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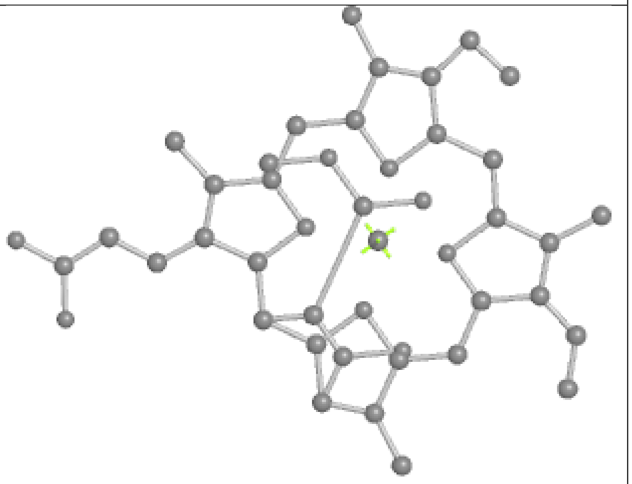

Rings

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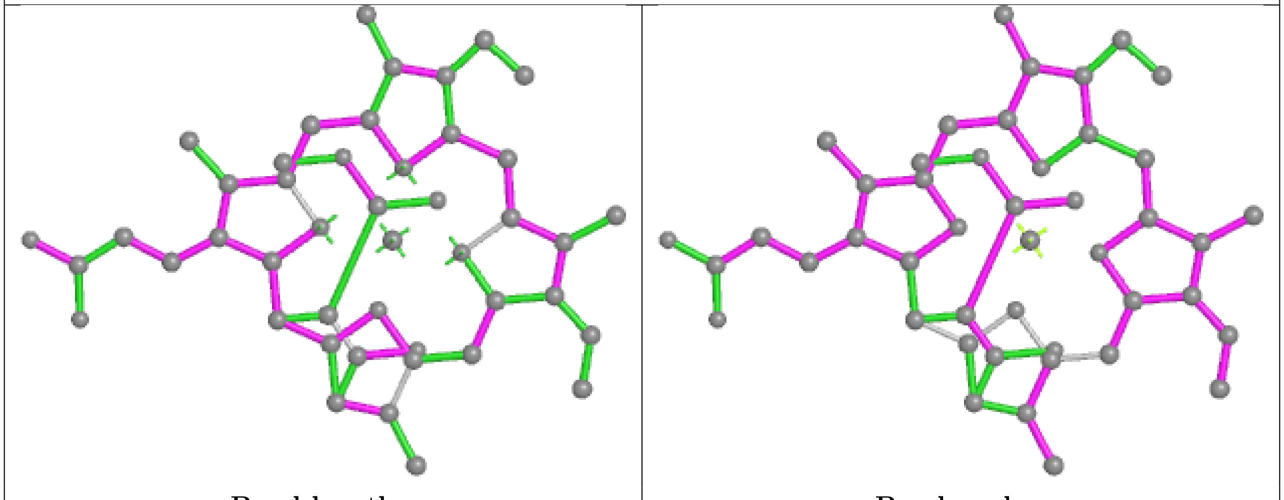
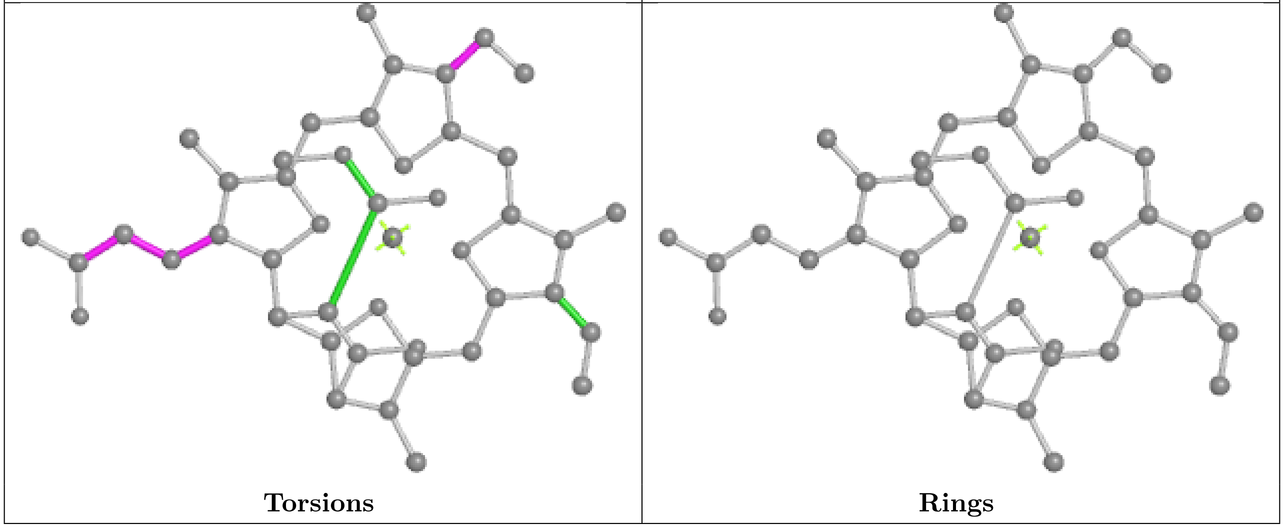


Bond lengths

Bond angles



Torsions

Rings

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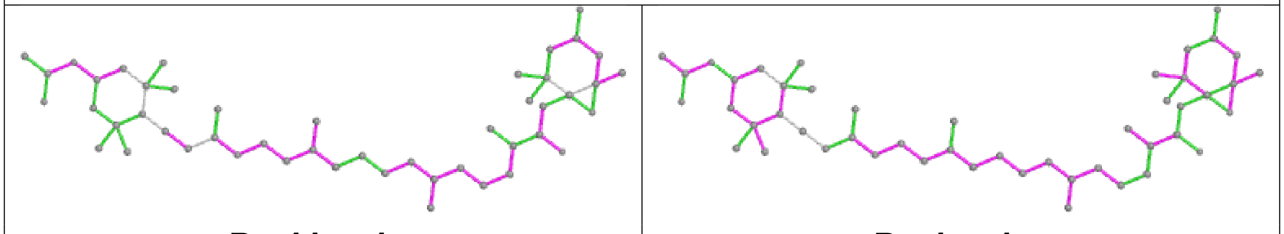
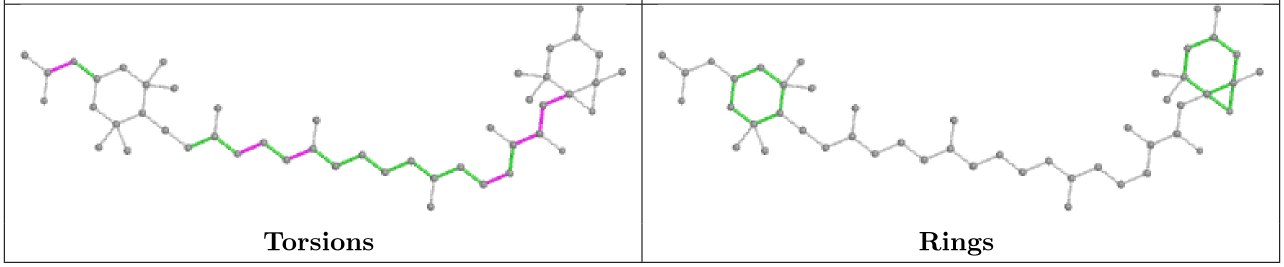


Bond lengths

Bond angles



Torsions

Rings

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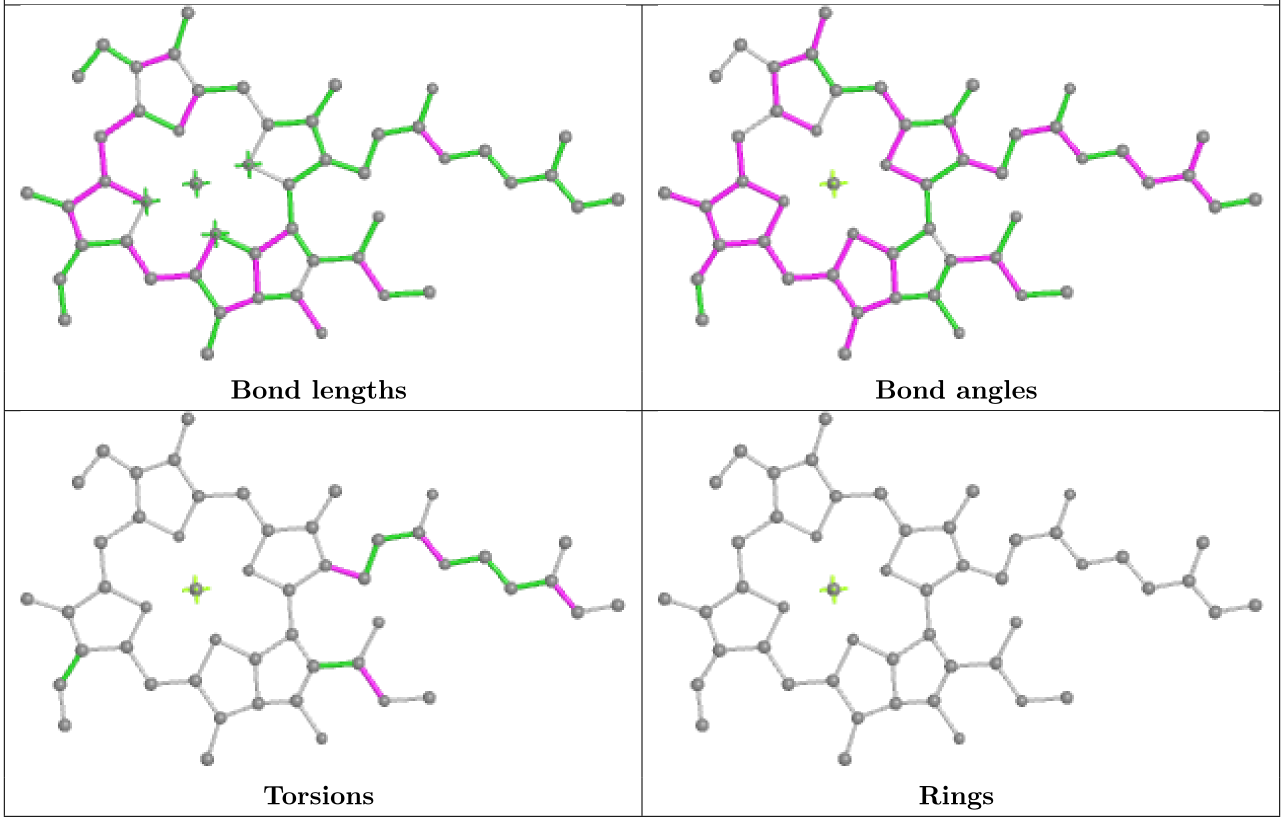


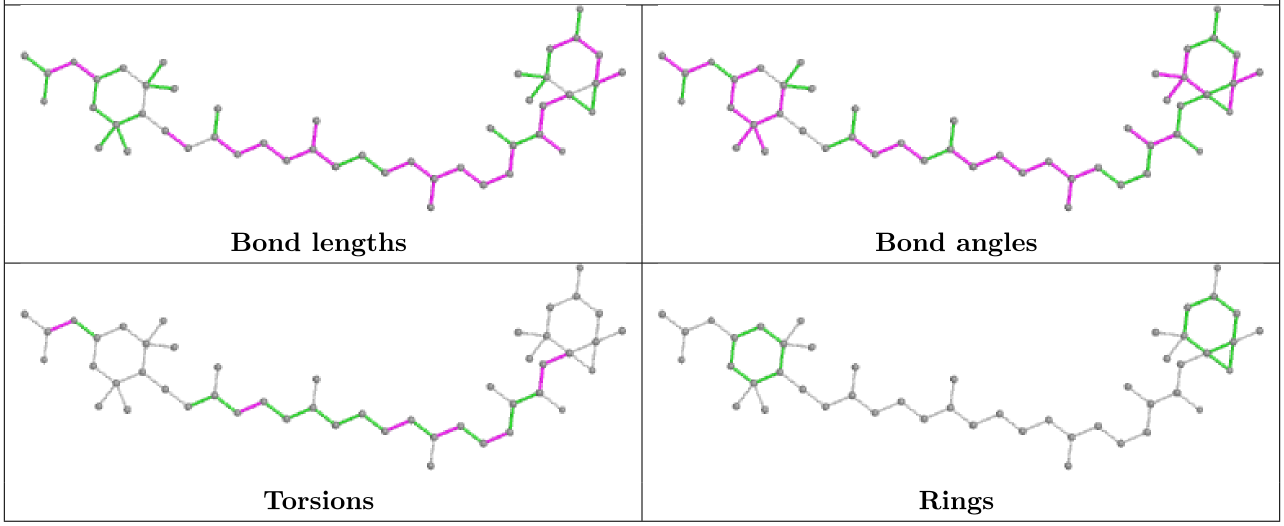
Bond lengths

Bond angles

Torsions

Rings

Ligand A86 18 312



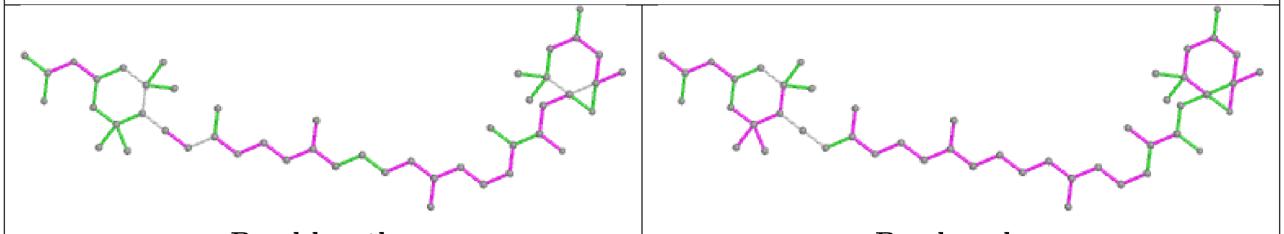
Bond lengths

Bond angles

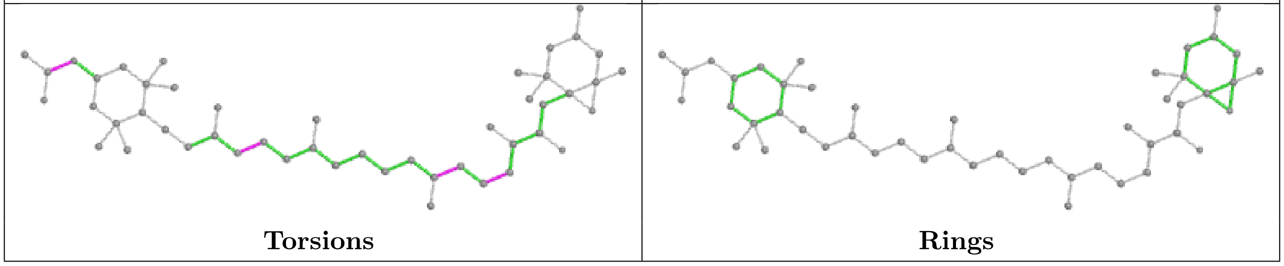
Torsions

Rings

Ligand A86 14 312

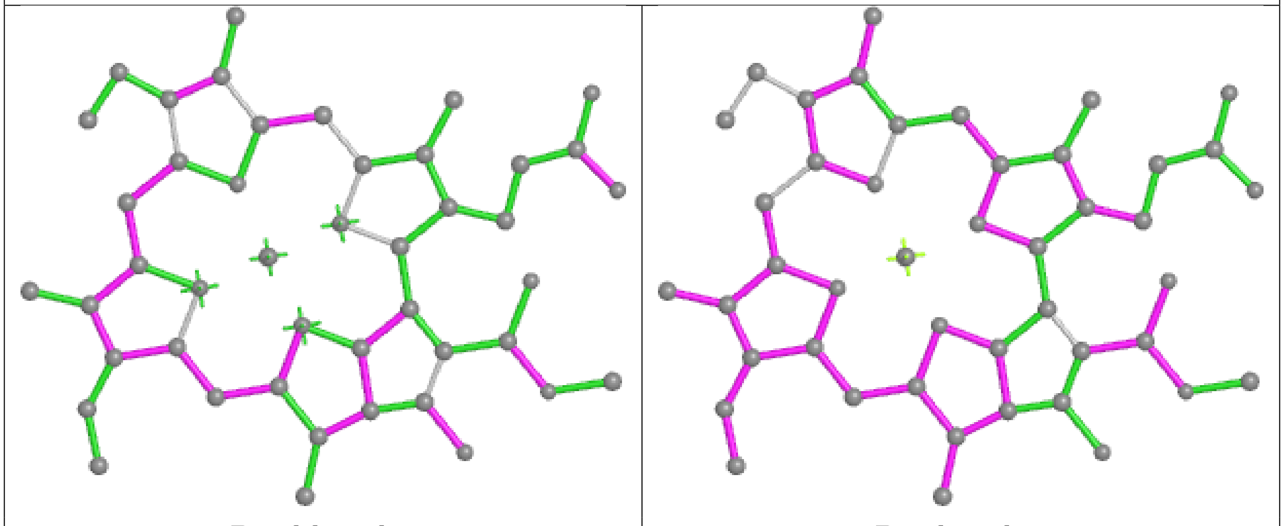


Bond lengths **Bond angles**

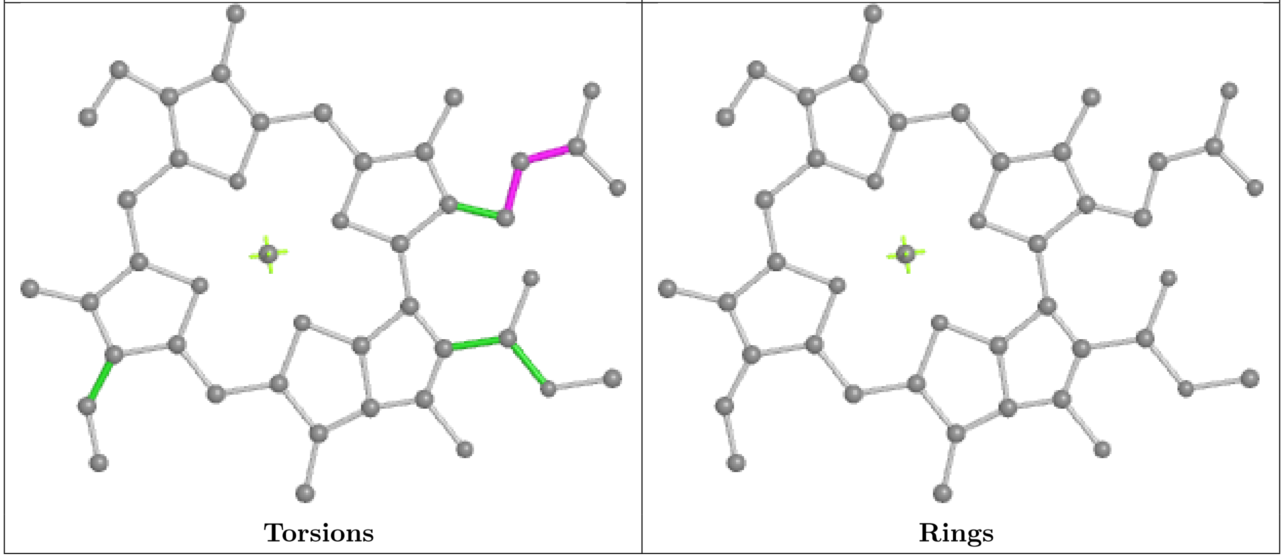


Torsions **Rings**

Ligand CLA 15 305

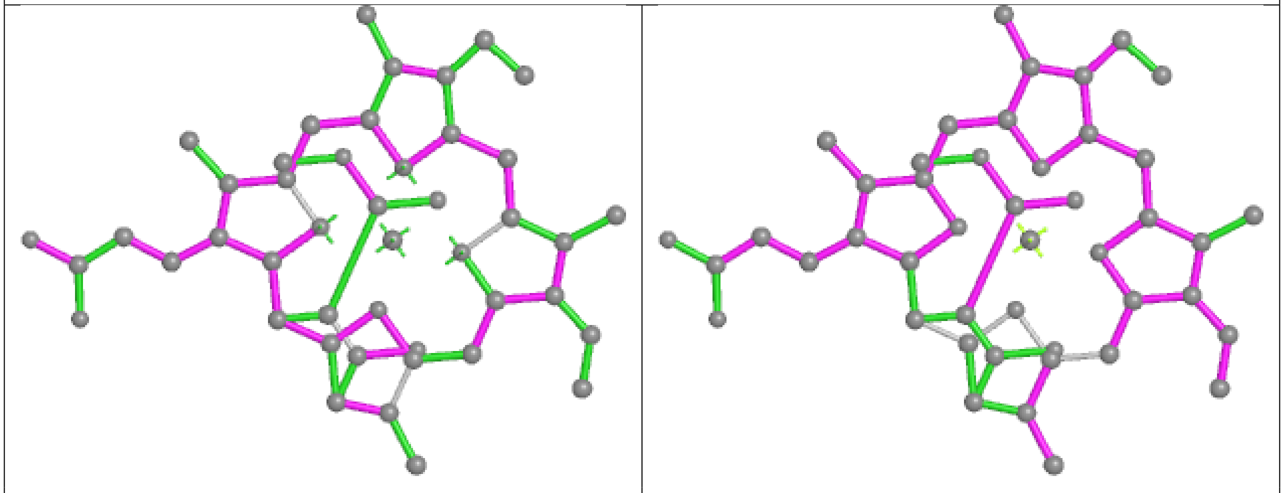


Bond lengths **Bond angles**

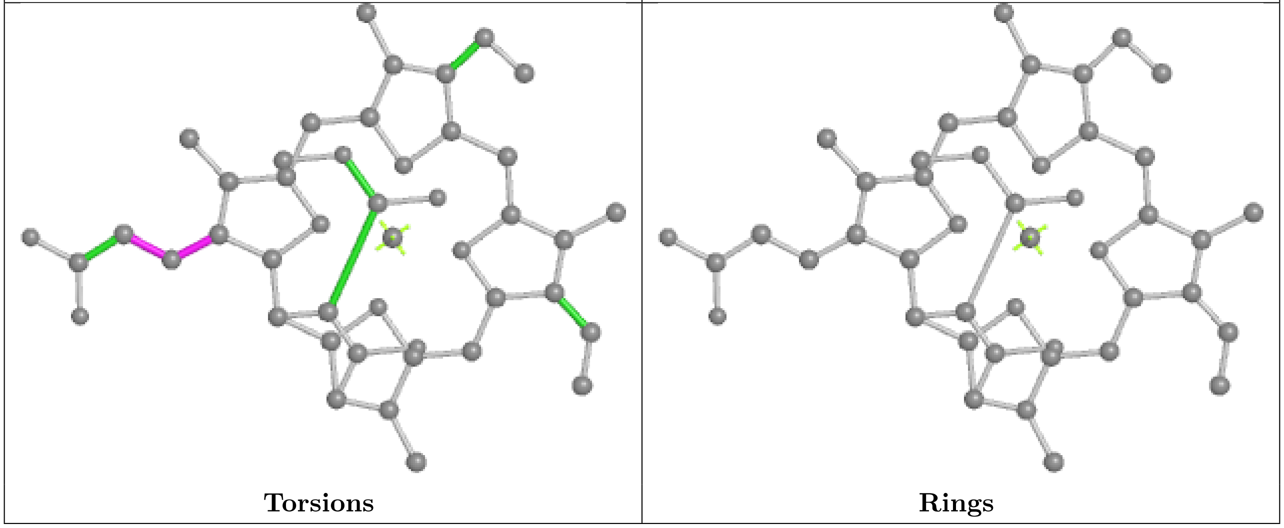


Torsions **Rings**

Ligand KC1 16 302

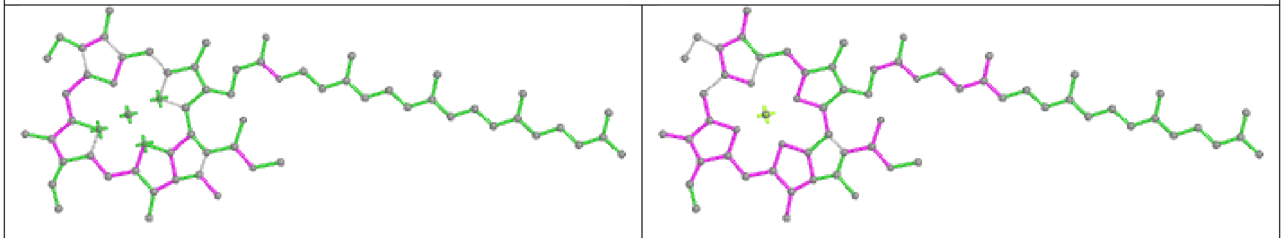


Bond lengths **Bond angles**

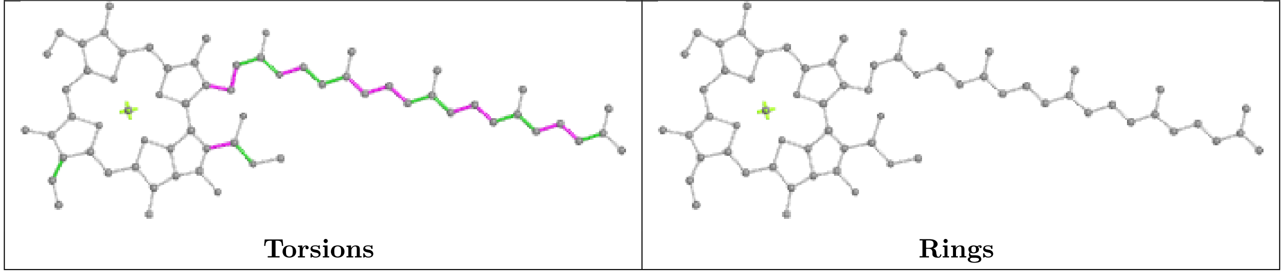


Torsions **Rings**

Ligand CLA 12 303

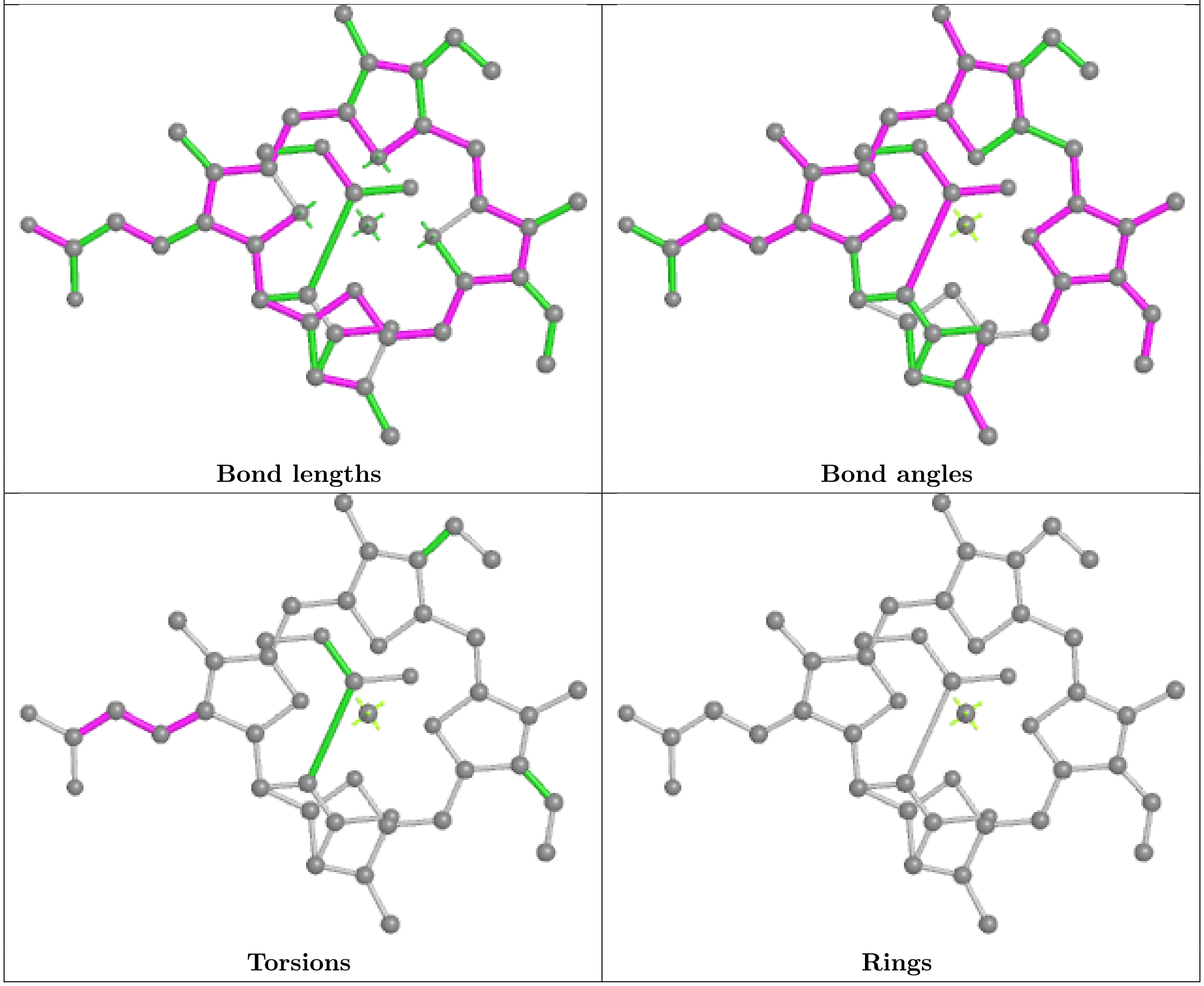


Bond lengths **Bond angles**



Torsions **Rings**

Ligand KC1 21 203



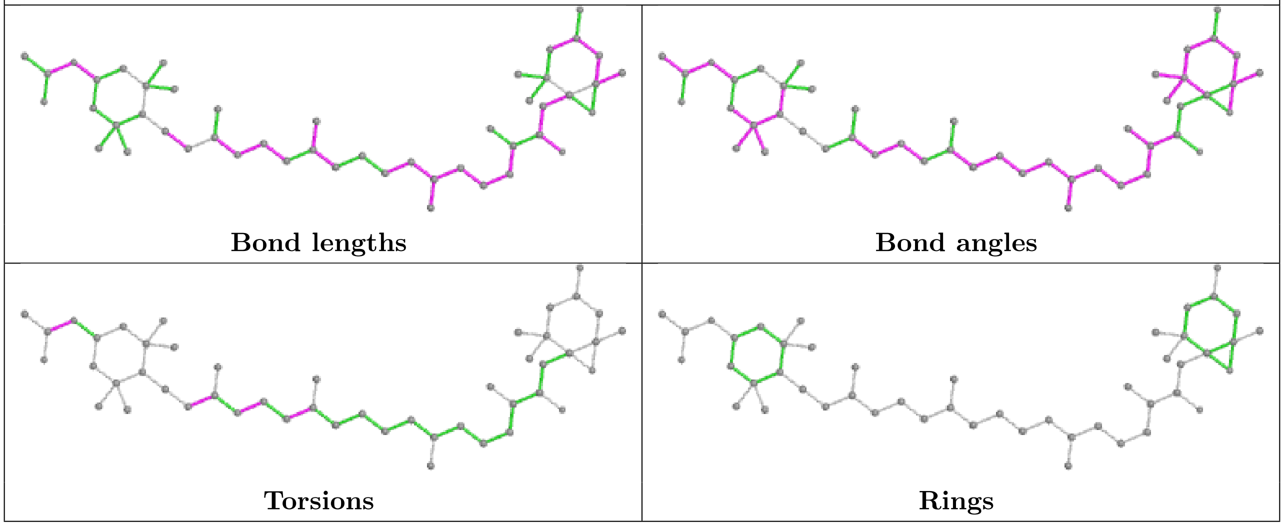
Bond lengths

Bond angles

Torsions

Rings

Ligand A86 11 311



Bond lengths

Bond angles

Torsions

Rings

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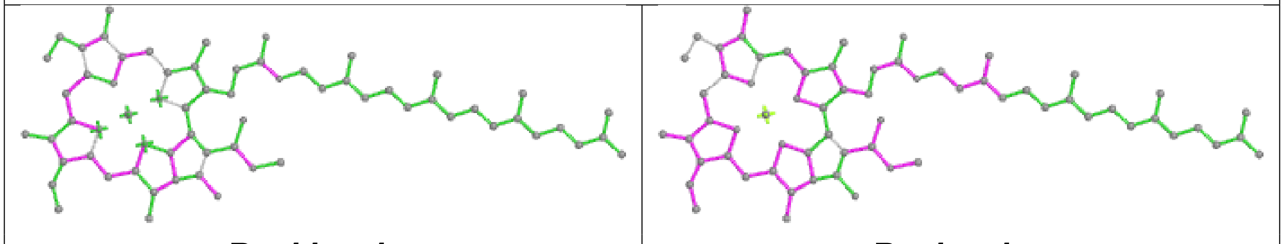
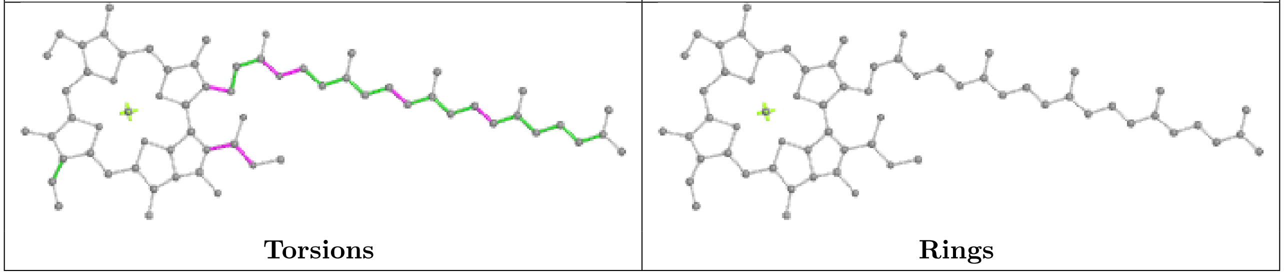
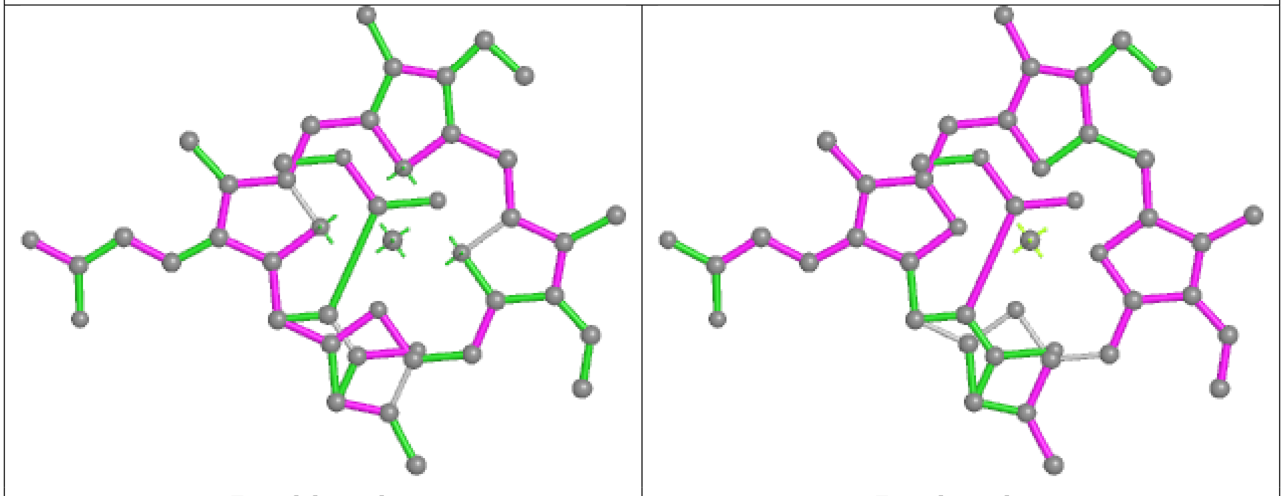


Bond lengths **Bond angles**

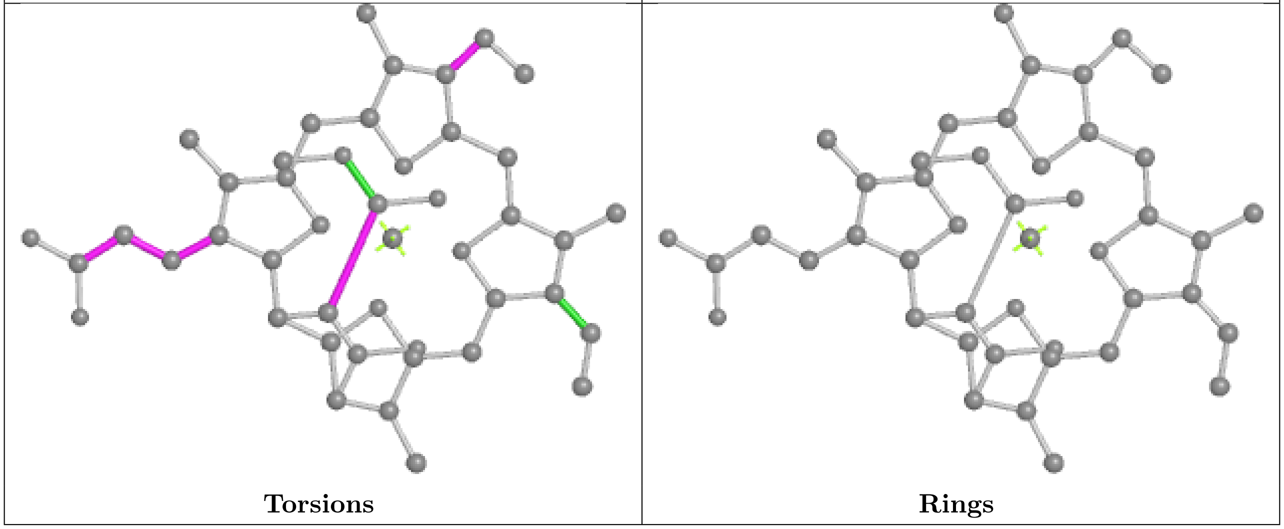


Torsions **Rings**

Ligand KC1 14 309

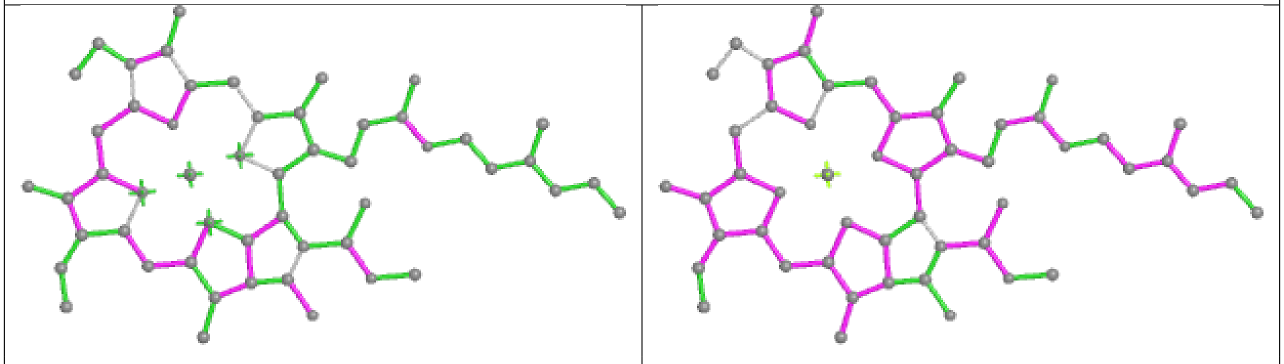


Bond lengths **Bond angles**

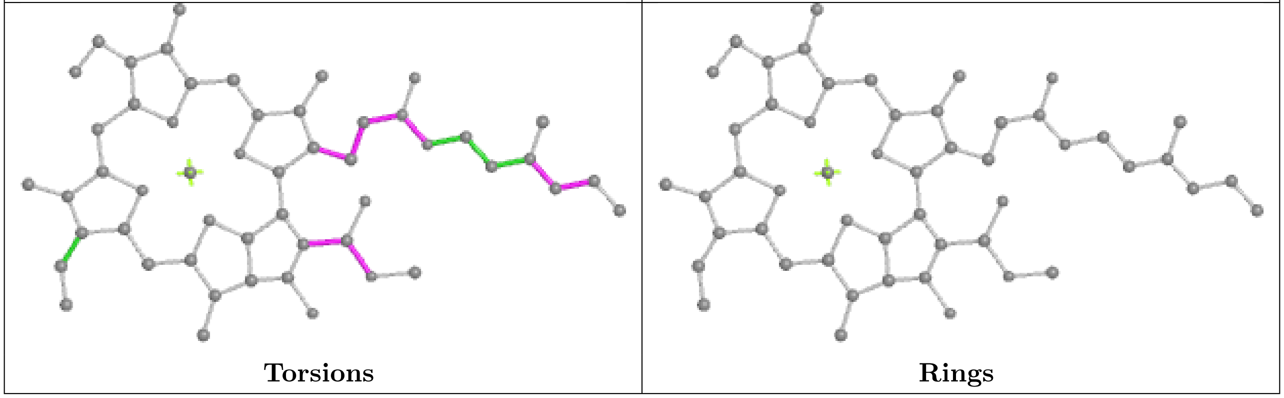


Torsions **Rings**

Ligand CLA 12 309

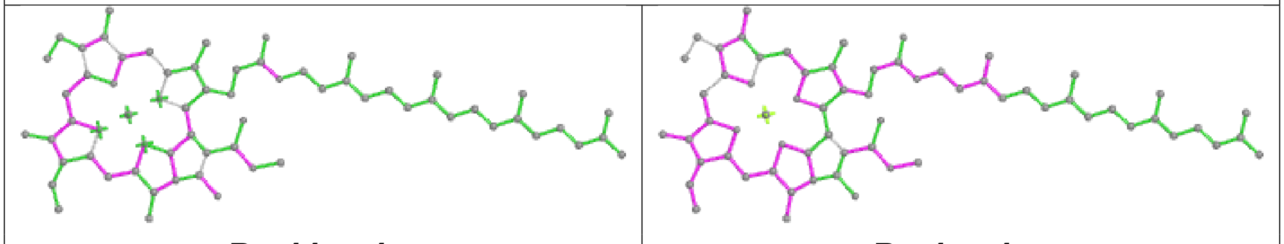


Bond lengths Bond angles

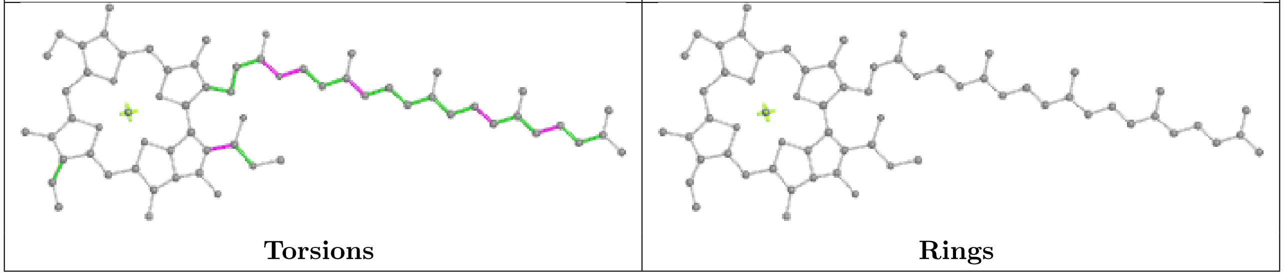


Torsions Rings

Ligand CLA 18 308

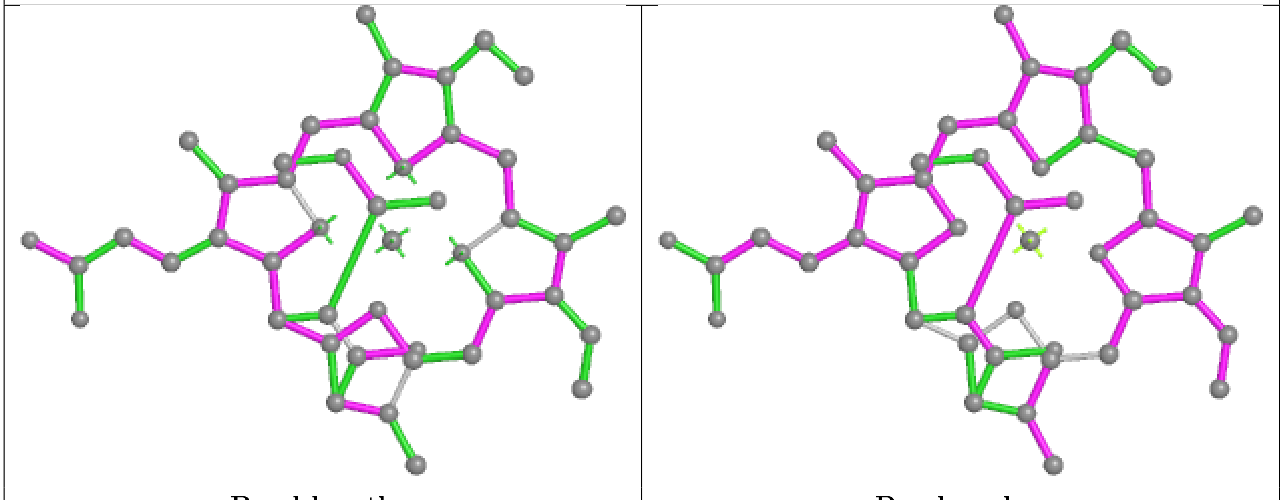


Bond lengths Bond angles



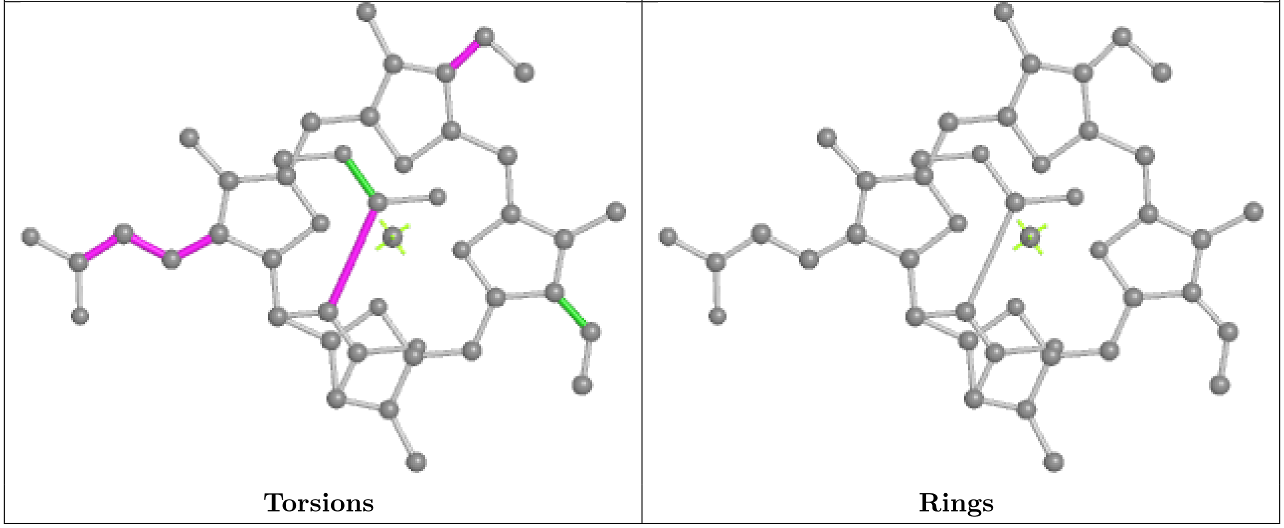
Torsions Rings

Ligand KC1 11 308



Bond lengths

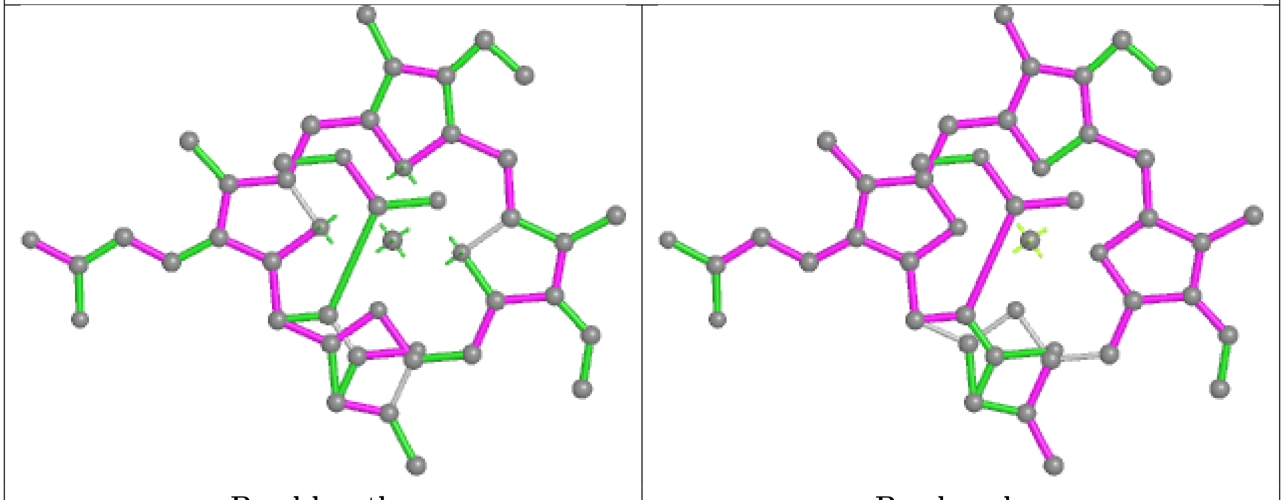
Bond angles



Torsions

Rings

Ligand KC1 17 306



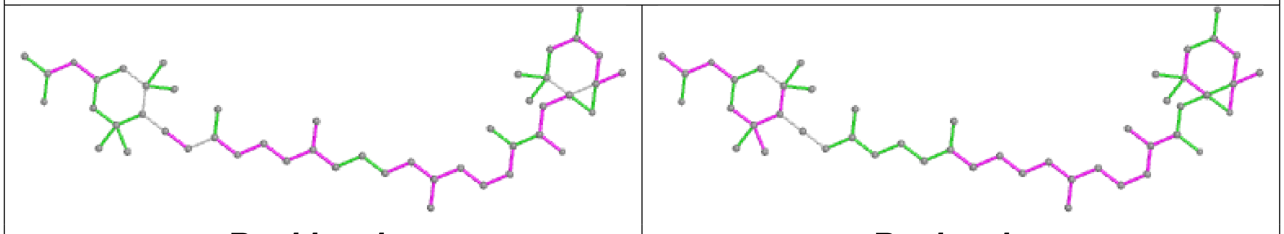
Bond lengths

Bond angles

Torsions

Rings

Ligand A86 12 313



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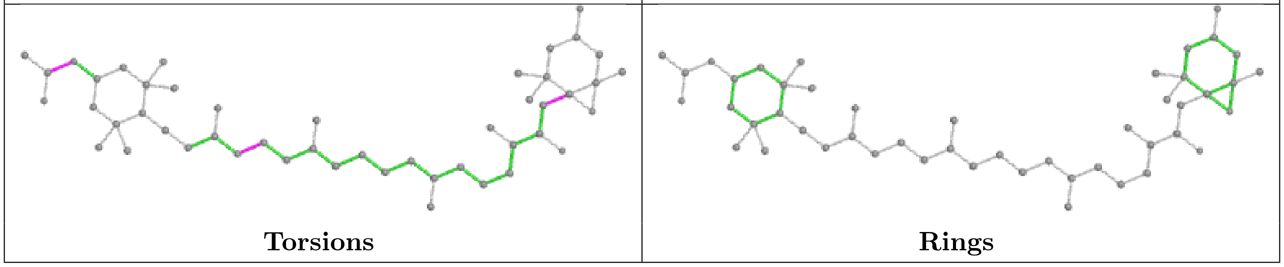
Bond angles



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Rings

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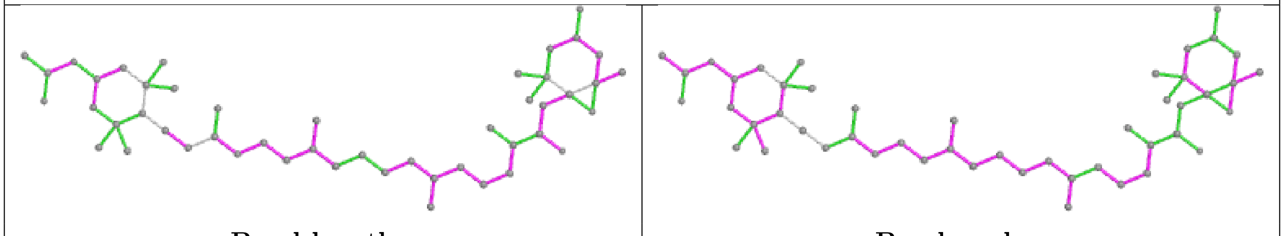
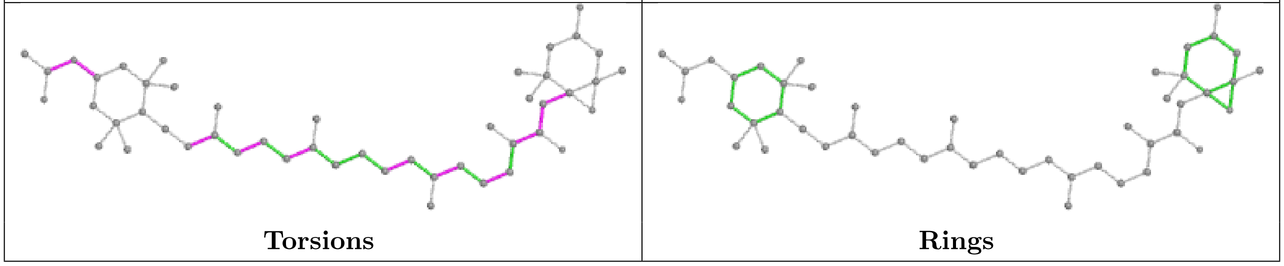
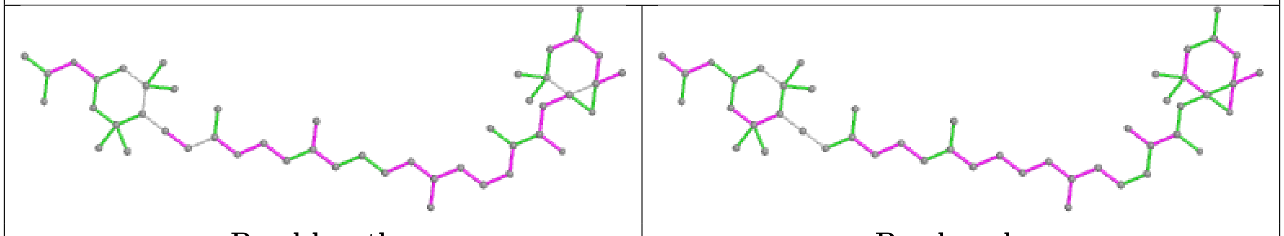


Bond lengths Bond angles

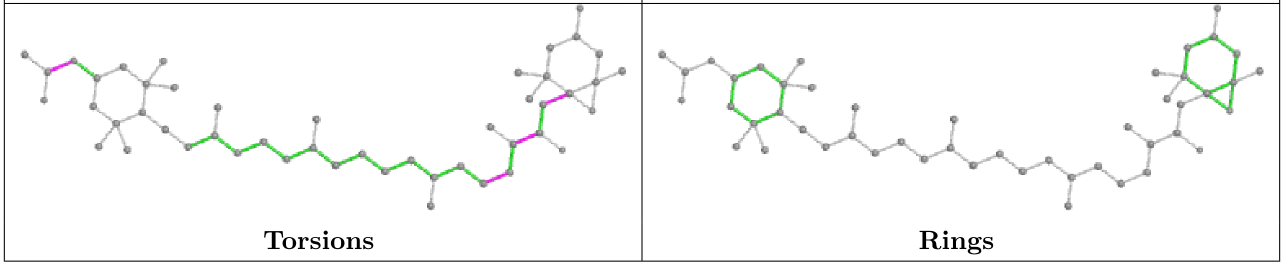


Torsions Rings

Ligand A86 16 313

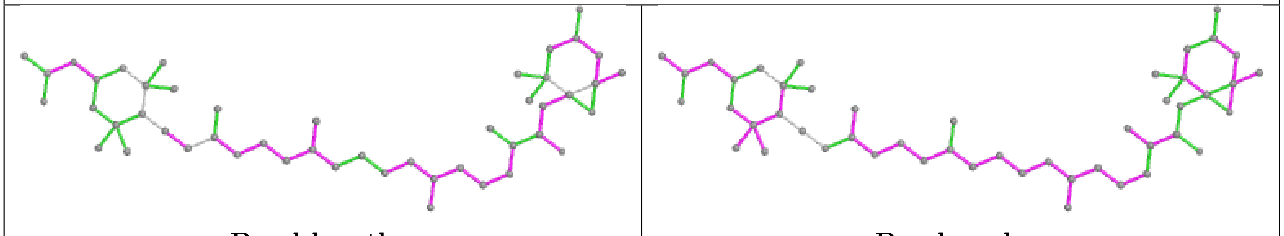


Bond lengths Bond angles

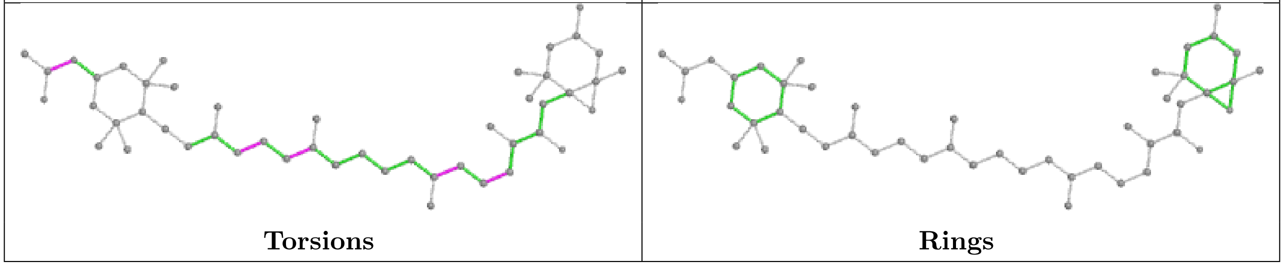


Torsions Rings

Ligand A86 17 312

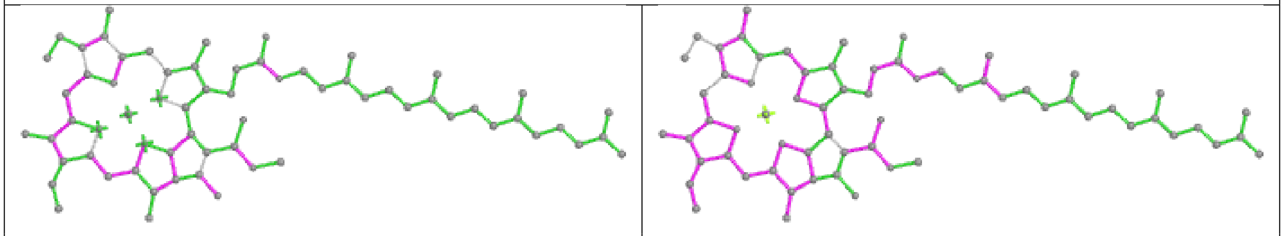


Bond lengths Bond angles



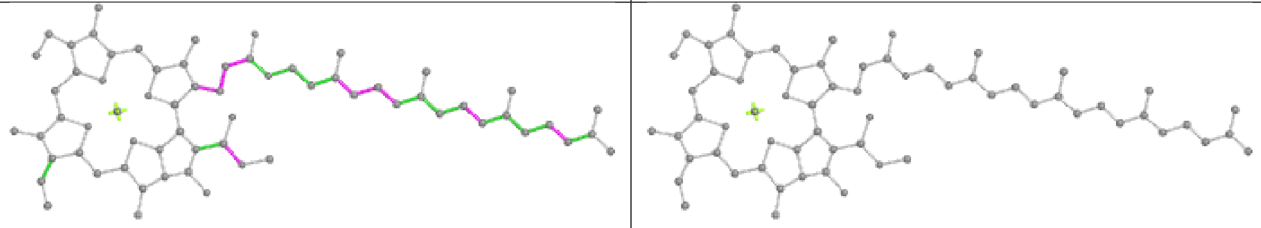
Torsions Rings

Ligand CLA 13 302



Bond lengths

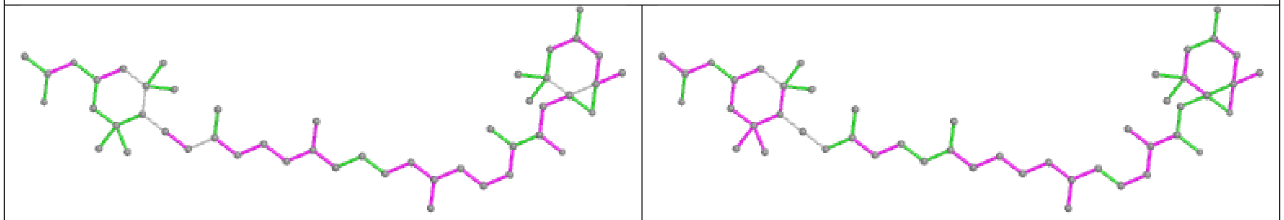
Bond angles



Torsions

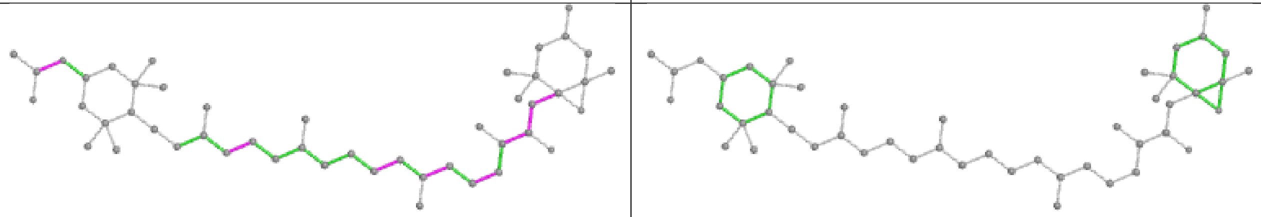
Rings

Ligand A86 15 316



Bond lengths

Bond angles



Torsions

Rings

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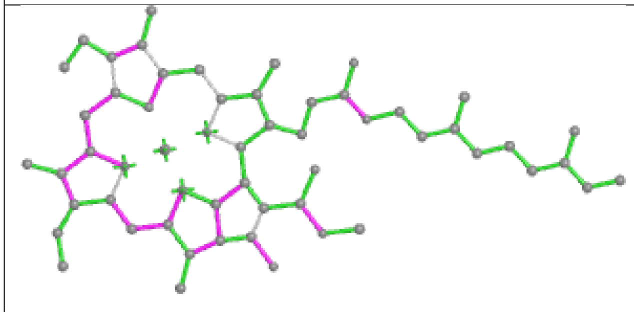
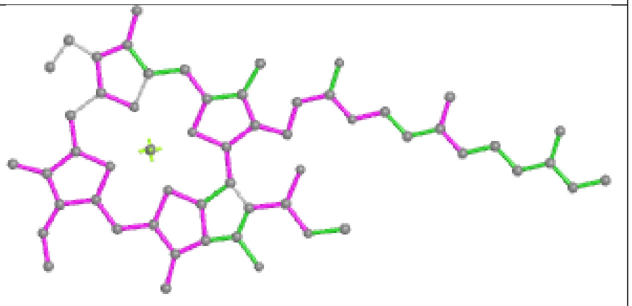
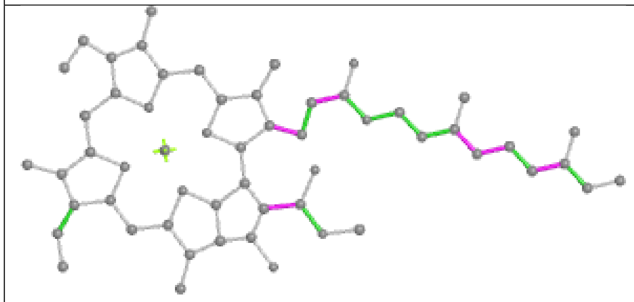
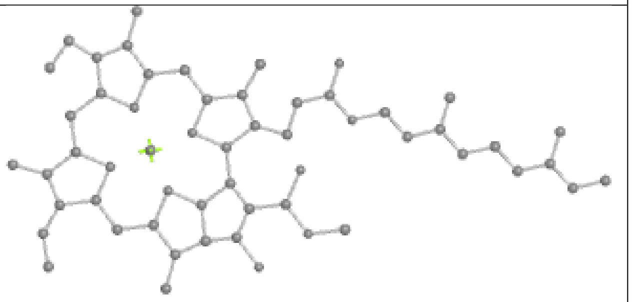
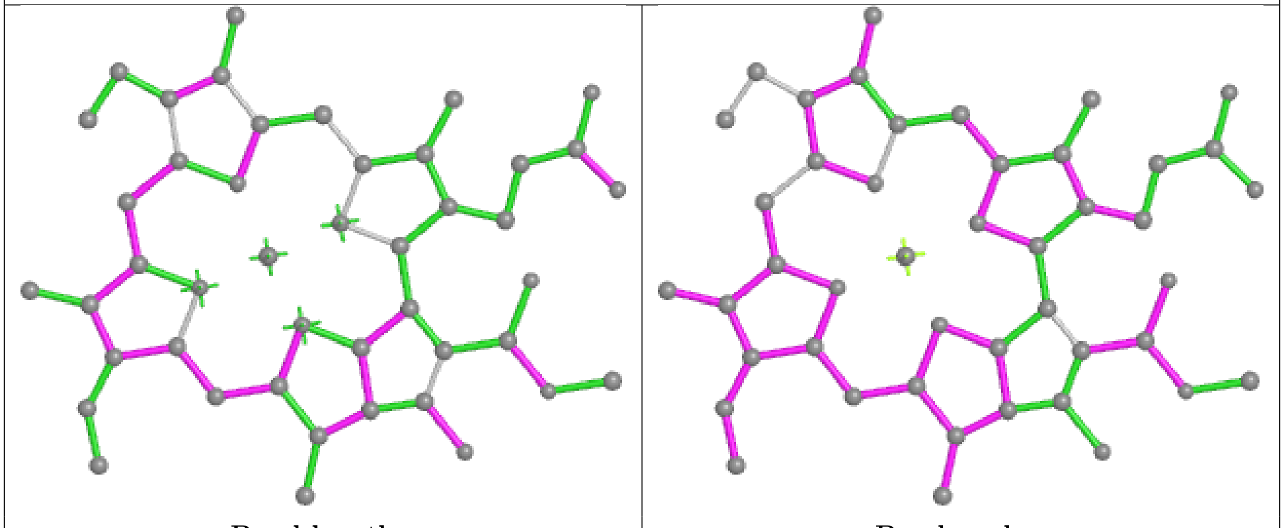
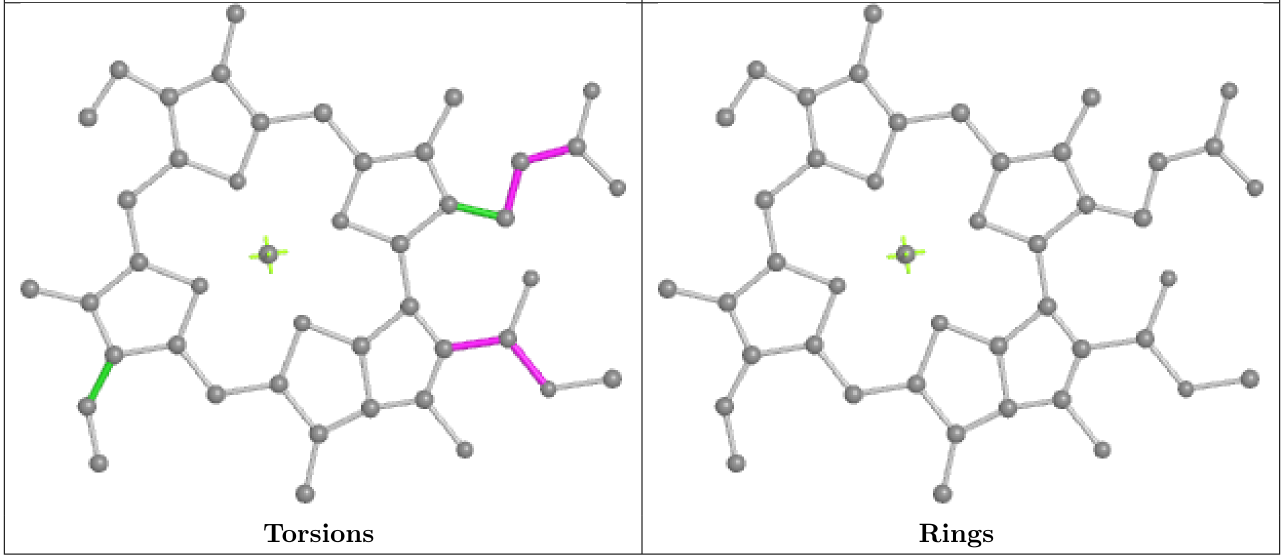
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

Ligand CLA 12 311

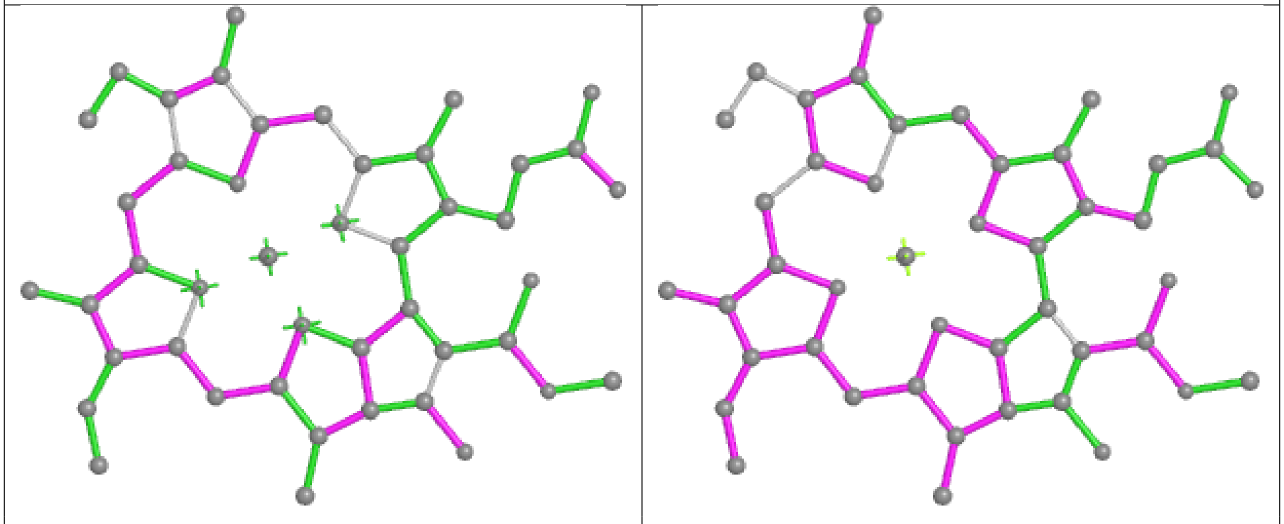


Bond lengths **Bond angles**



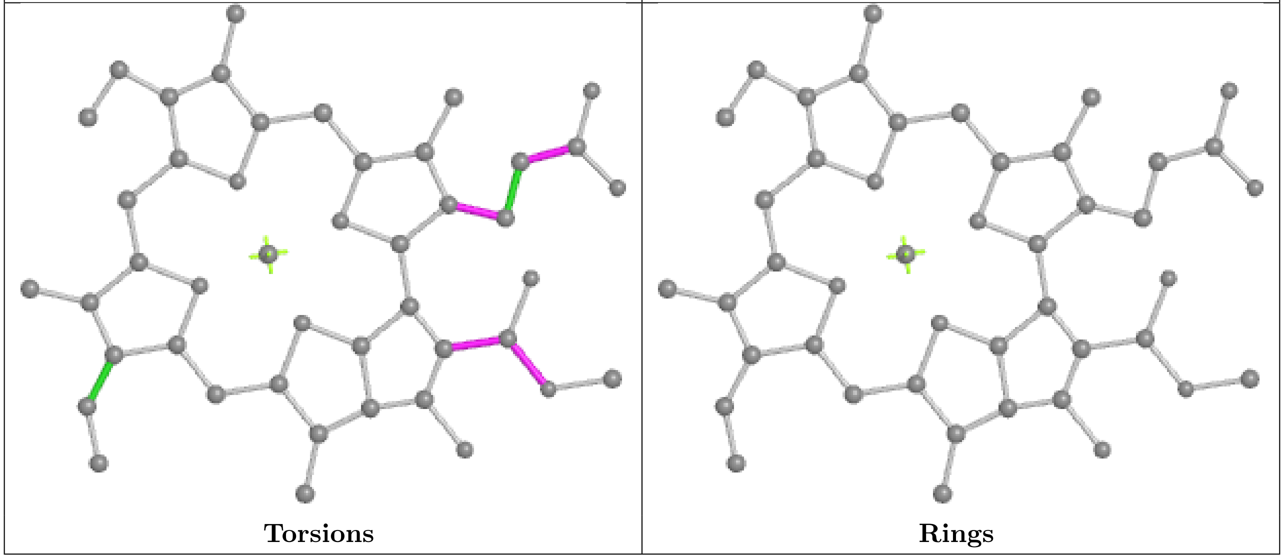
Torsions **Rings**

Ligand CLA 21 209



Bond lengths

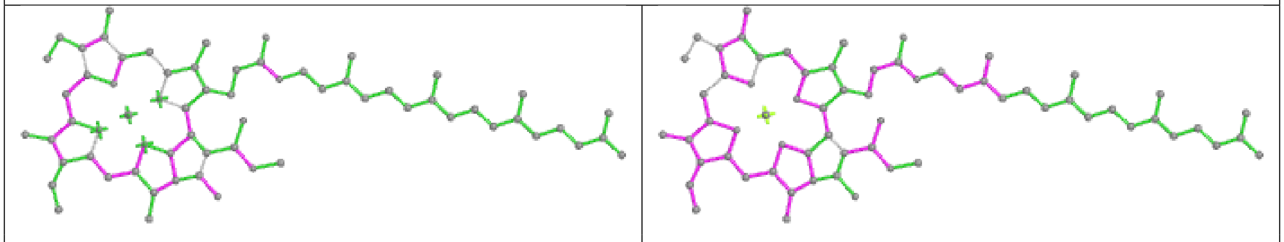
Bond angles



Torsions

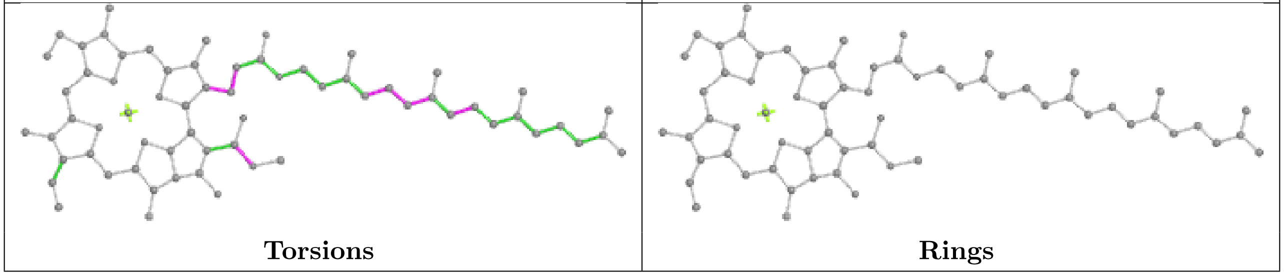
Rings

Ligand CLA 11 301



Bond lengths

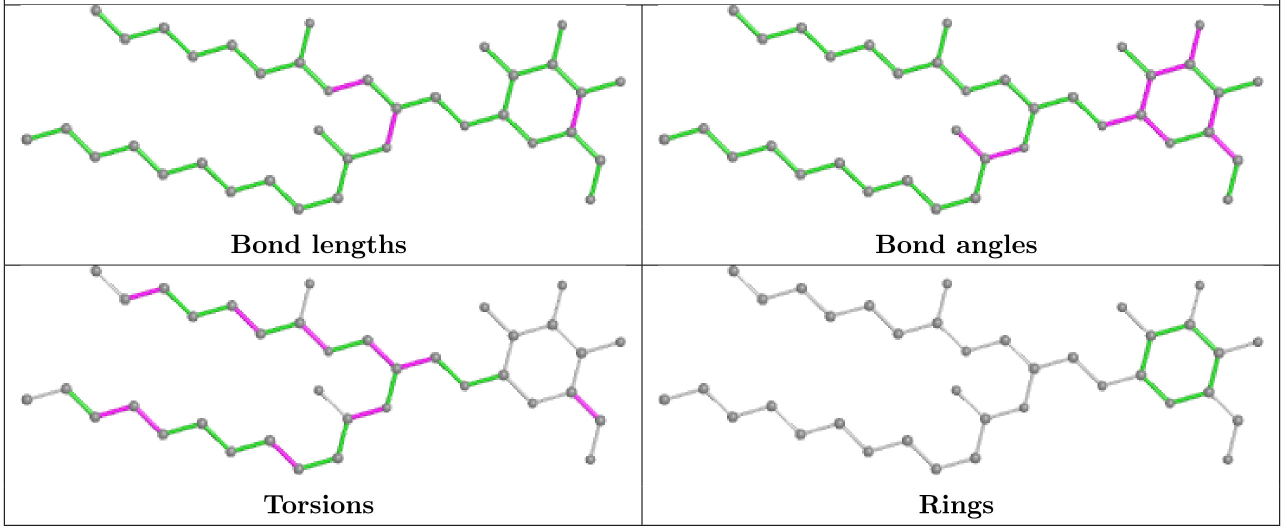
Bond angles



Torsions

Rings

Ligand LMG 17 318



Bond lengths

Bond angles

Torsions

Rings

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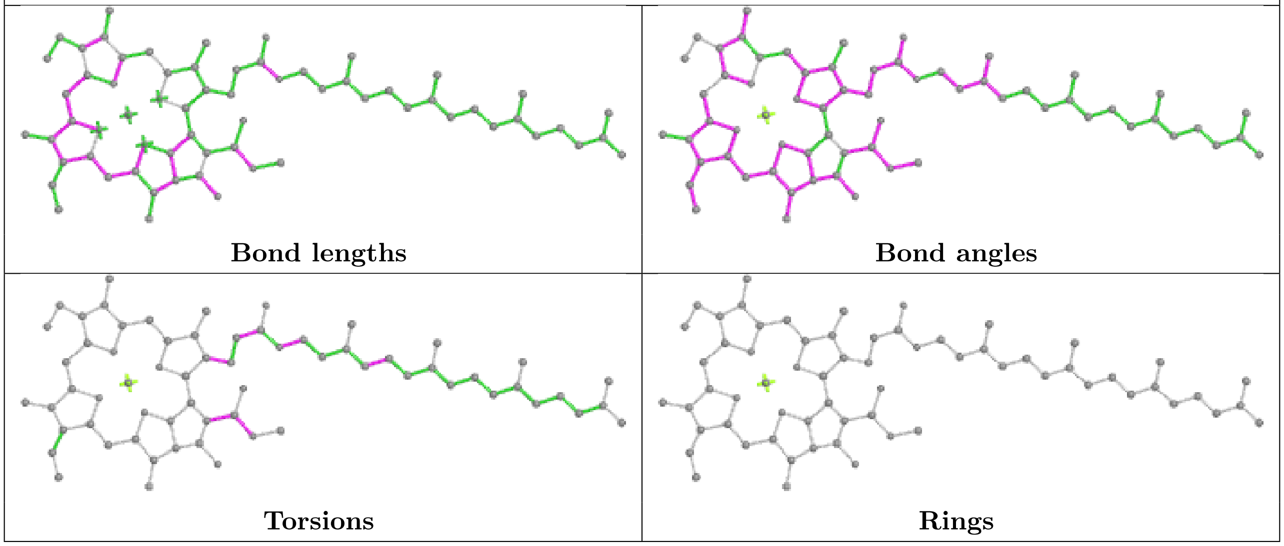


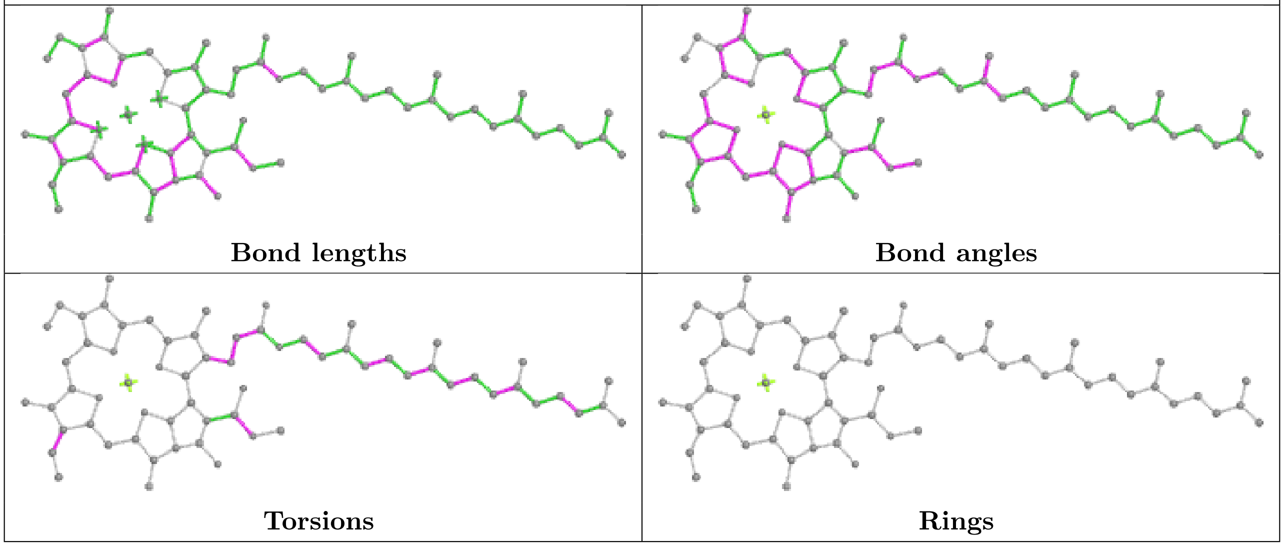
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA 17 302



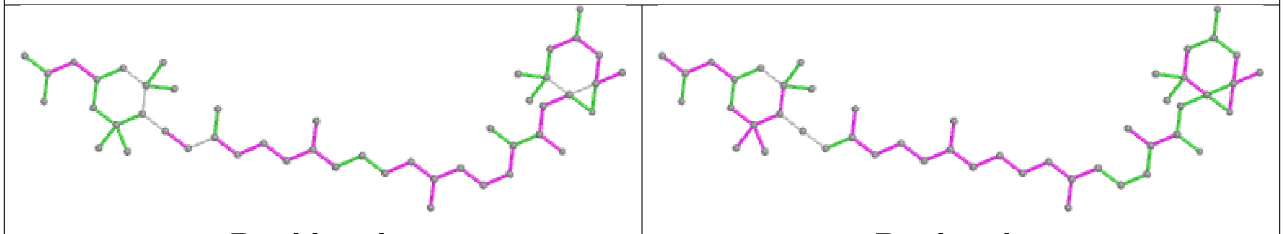
Bond lengths

Bond angles

Torsions

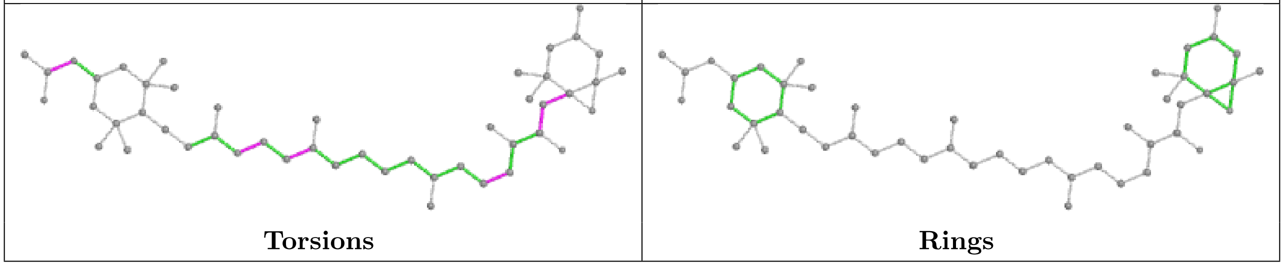
Rings

Ligand A86 13 315



Bond lengths

Bond angles



Torsions

Rings

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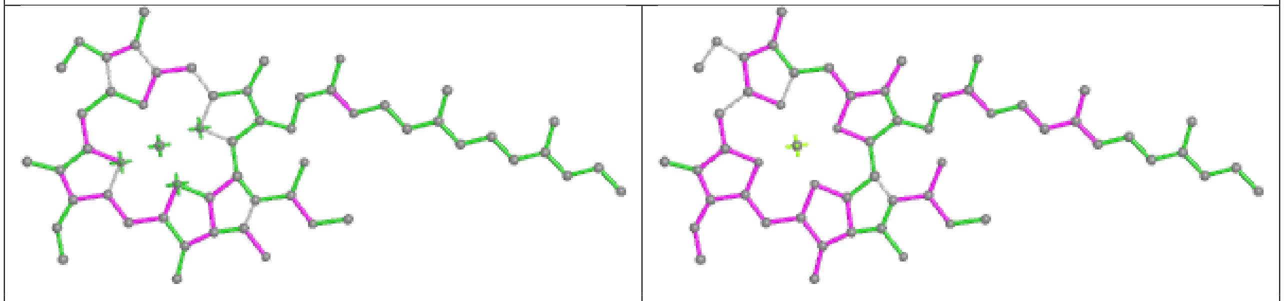
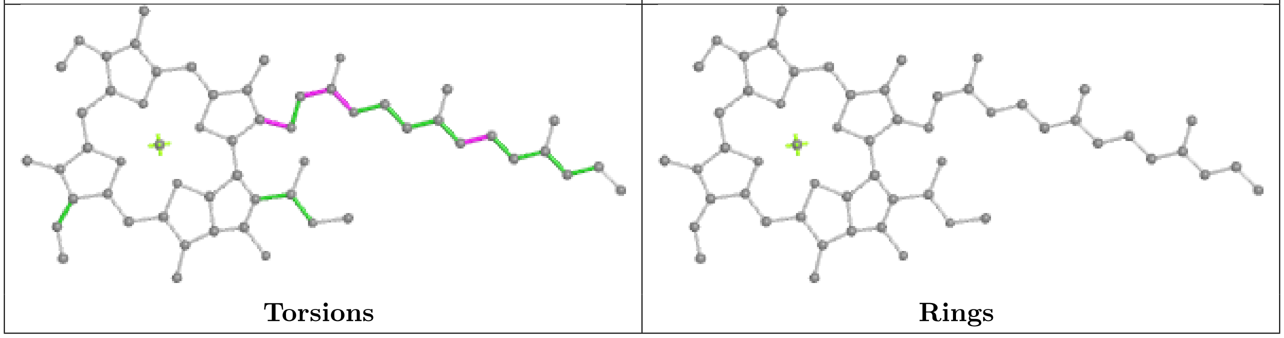


Bond lengths

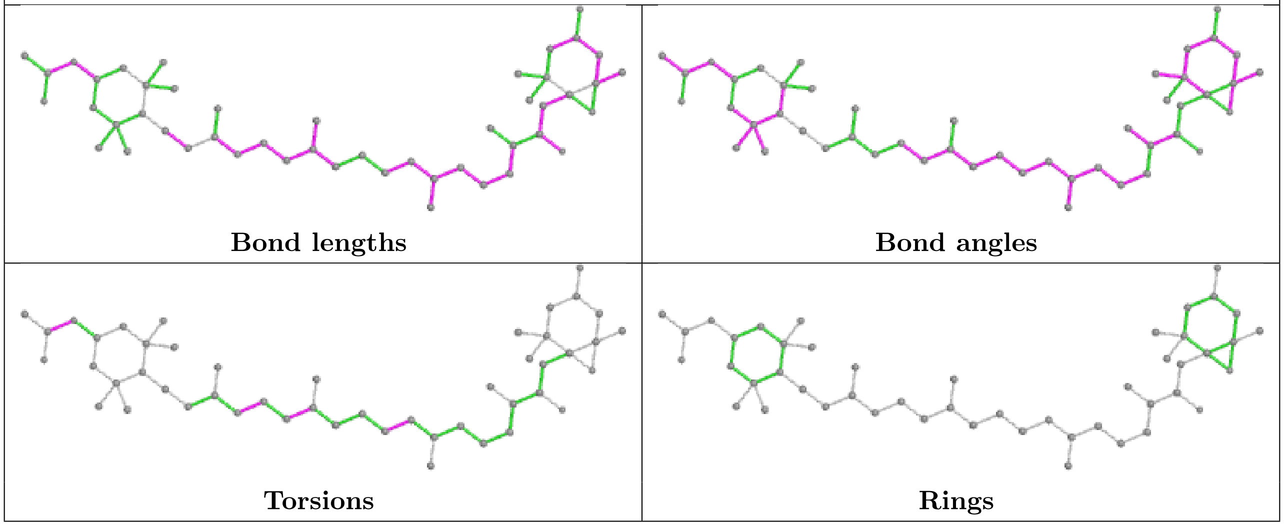
Bond angles



Torsions

Rings

Ligand A86 11 314



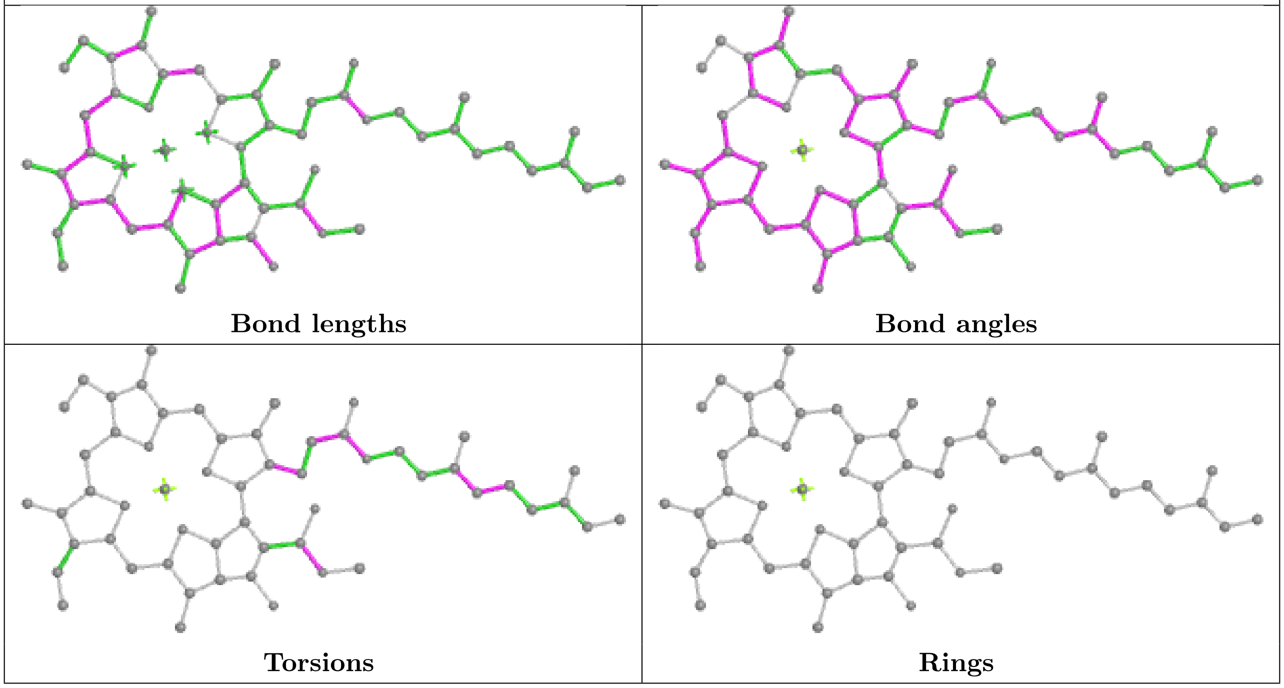
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA 20 302



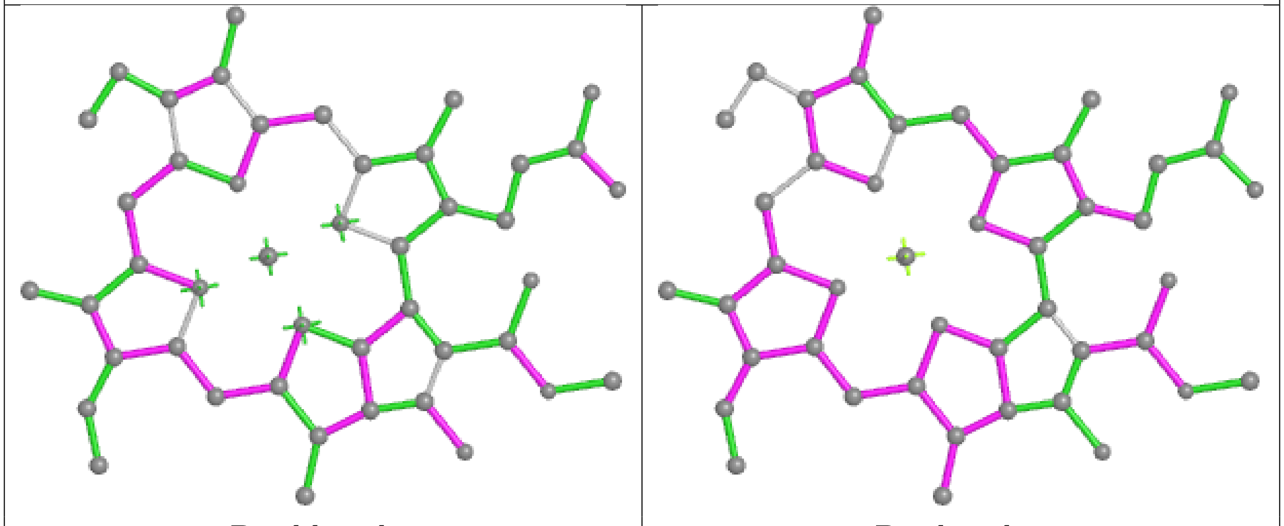
Bond lengths

Bond angles

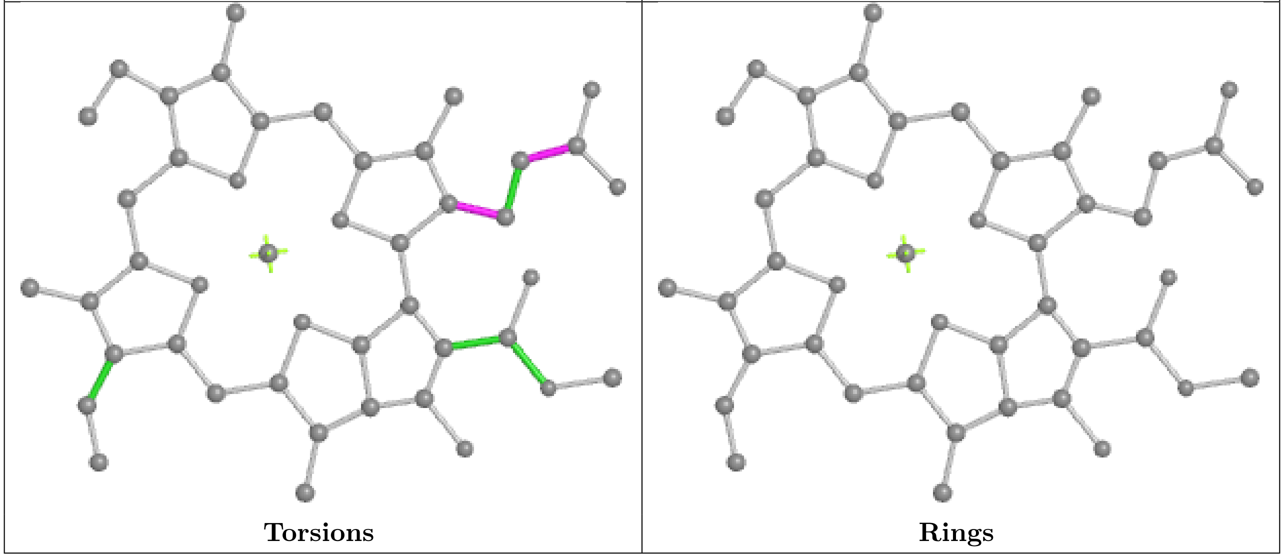
Torsions

Rings

Ligand CLA 19 304

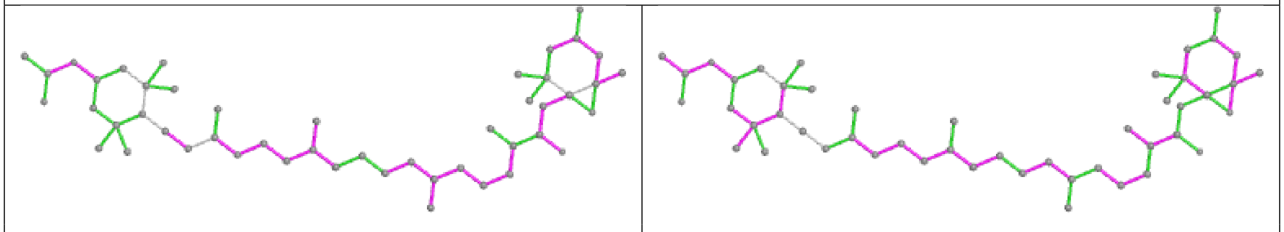


Bond lengths Bond angles

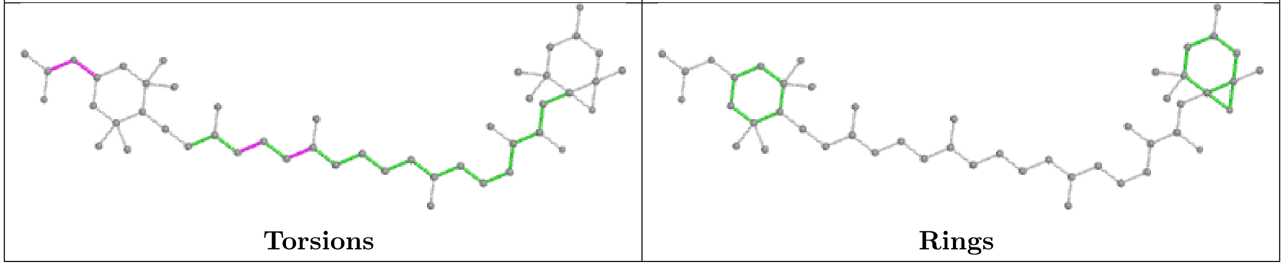


Torsions Rings

Ligand A86 21 215

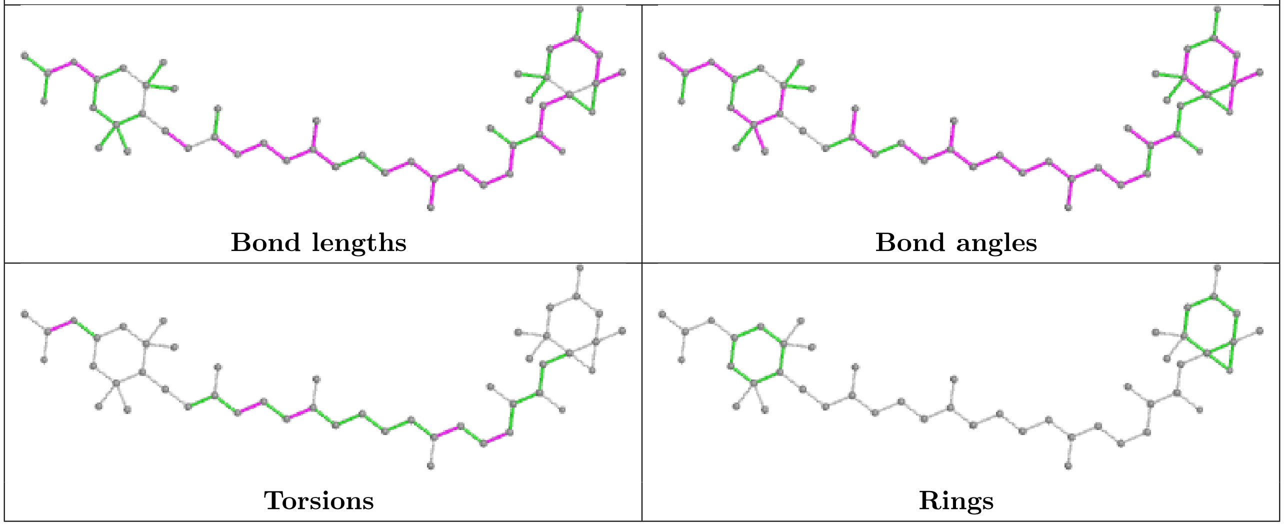


Bond lengths Bond angles



Torsions Rings

Ligand A86 15 312



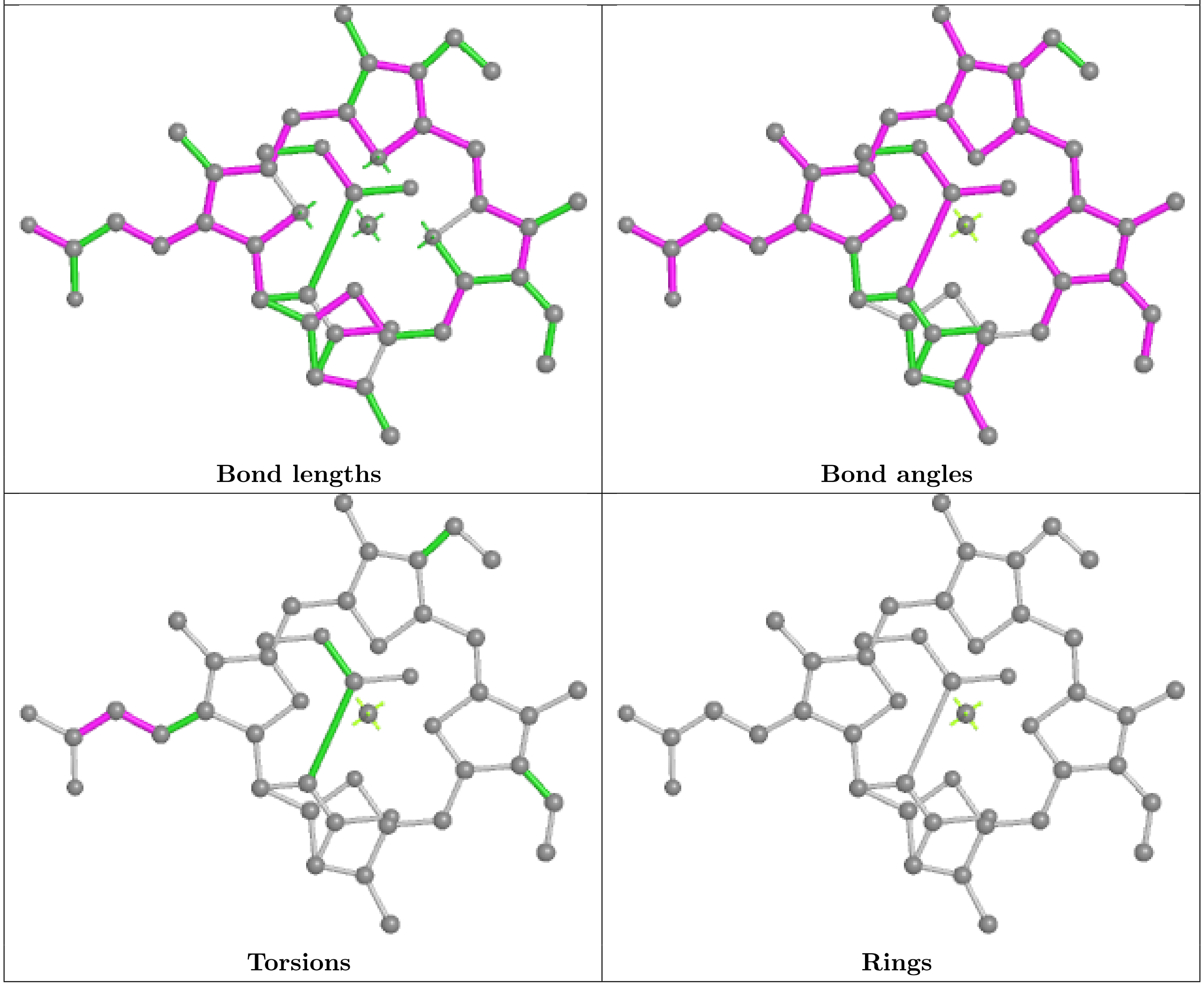
Bond lengths

Bond angles

Torsions

Rings

Ligand KC1 19 308



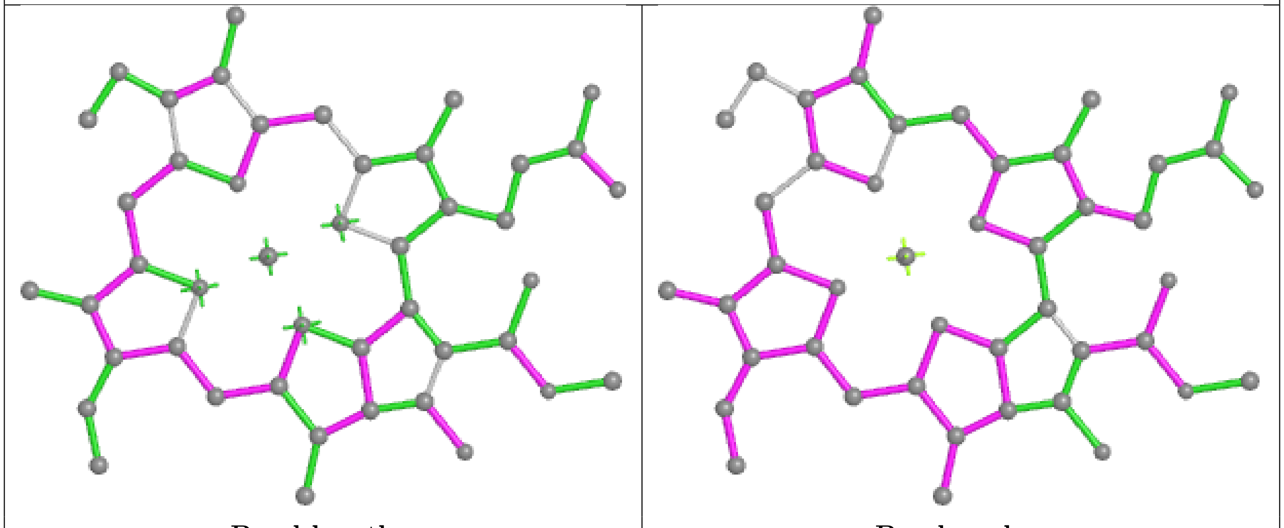
Bond lengths

Bond angles

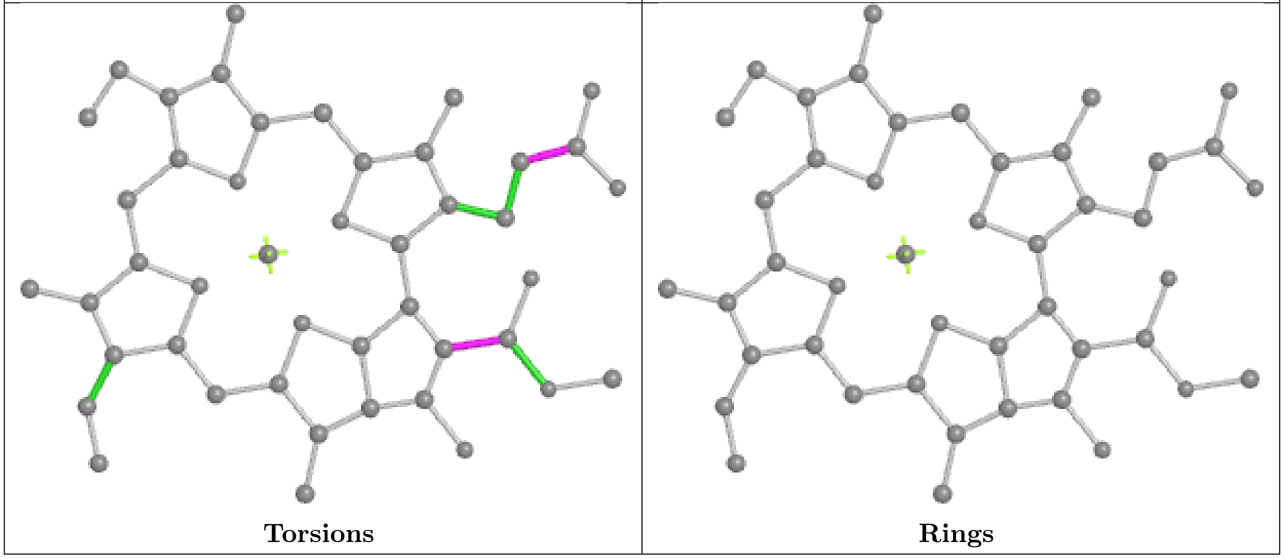
Torsions

Rings

Ligand CLA 13 306



Bond lengths **Bond angles**



Torsions **Rings**

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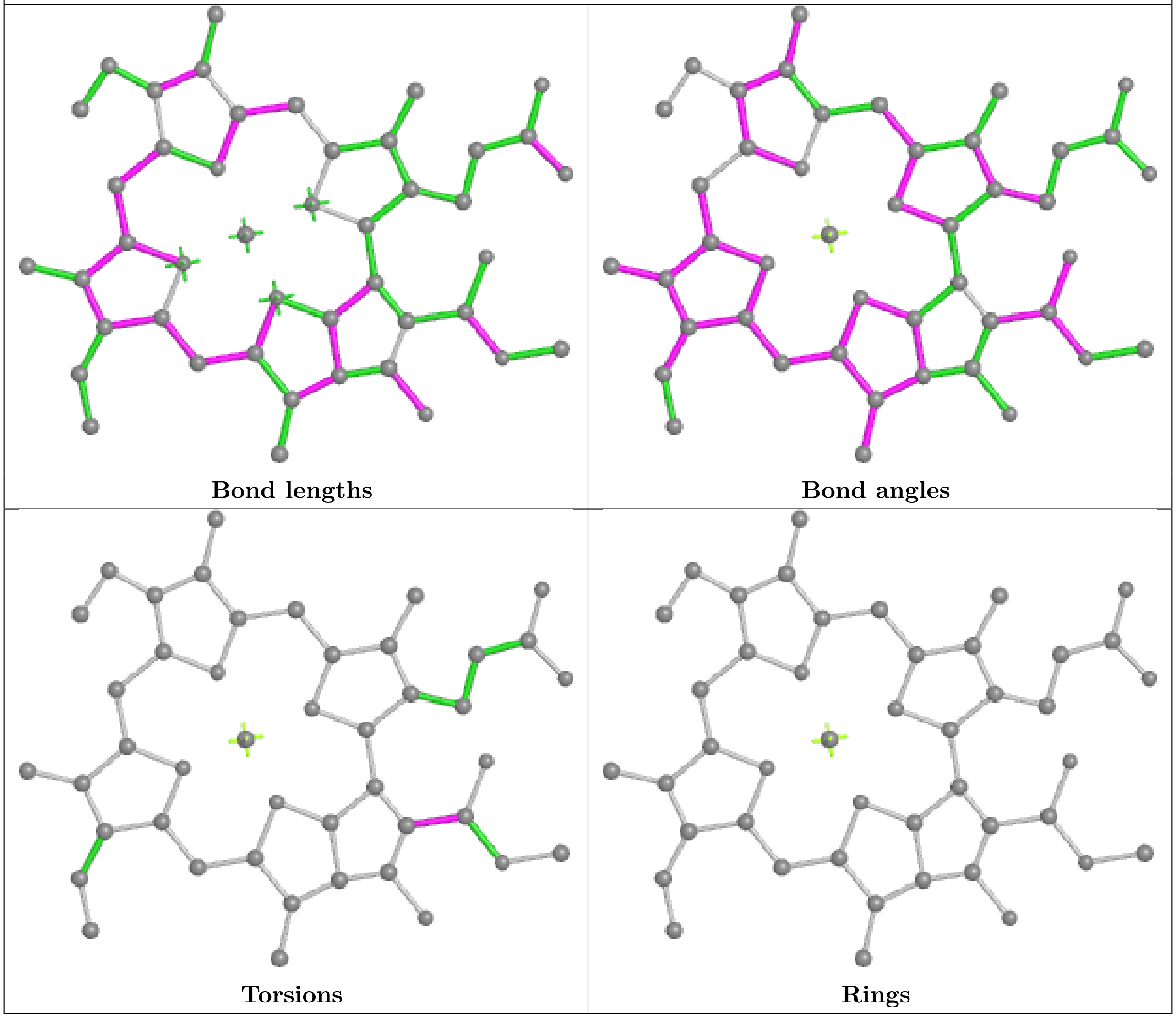


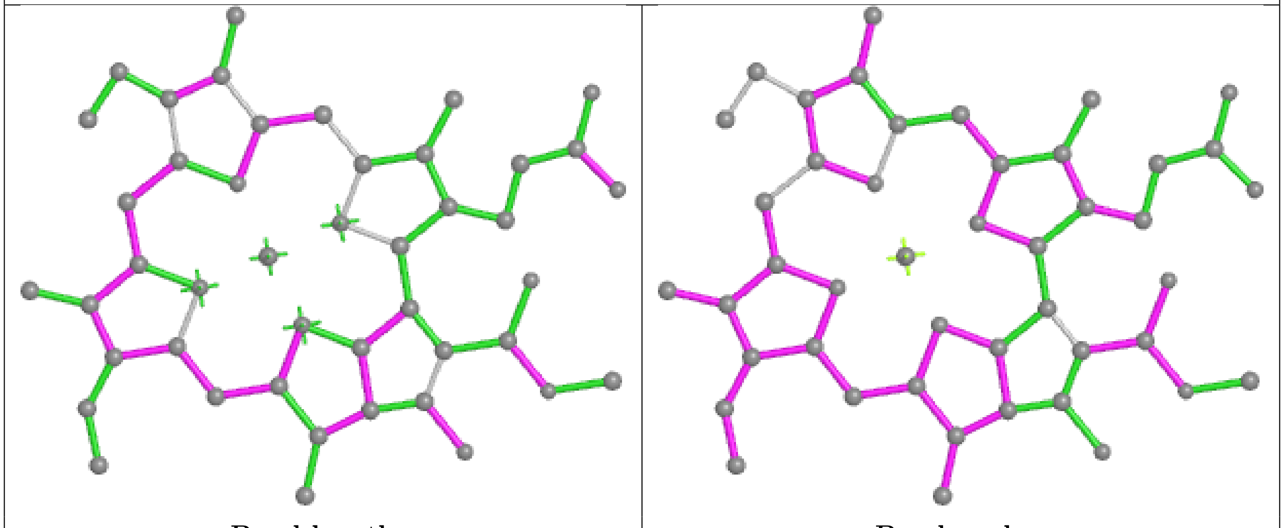
Bond lengths

Bond angles

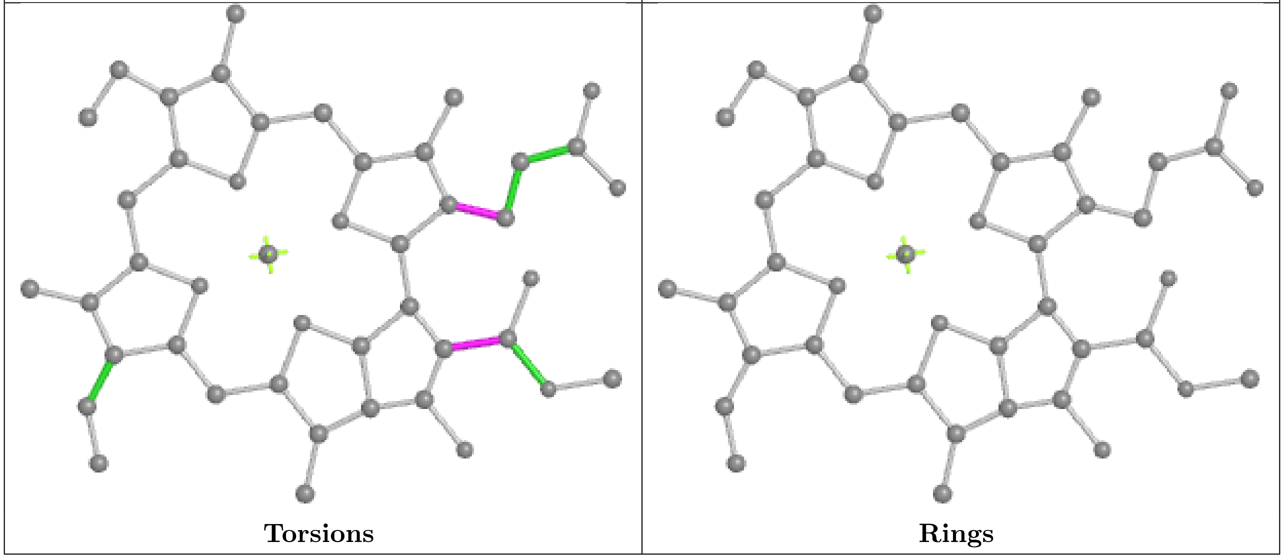
Torsions

Rings

Ligand CLA 14 305

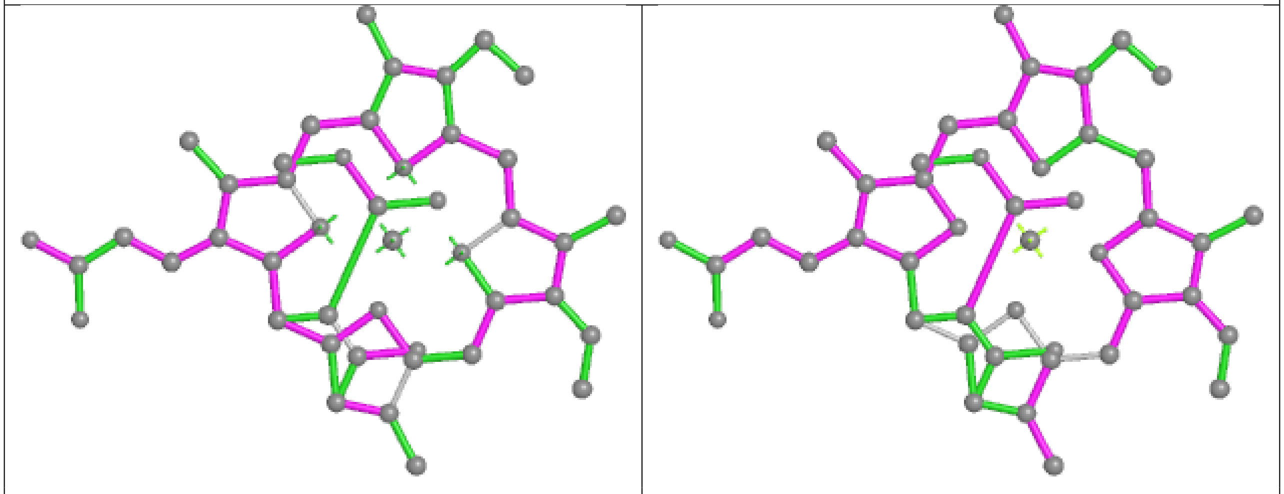


Bond lengths **Bond angles**



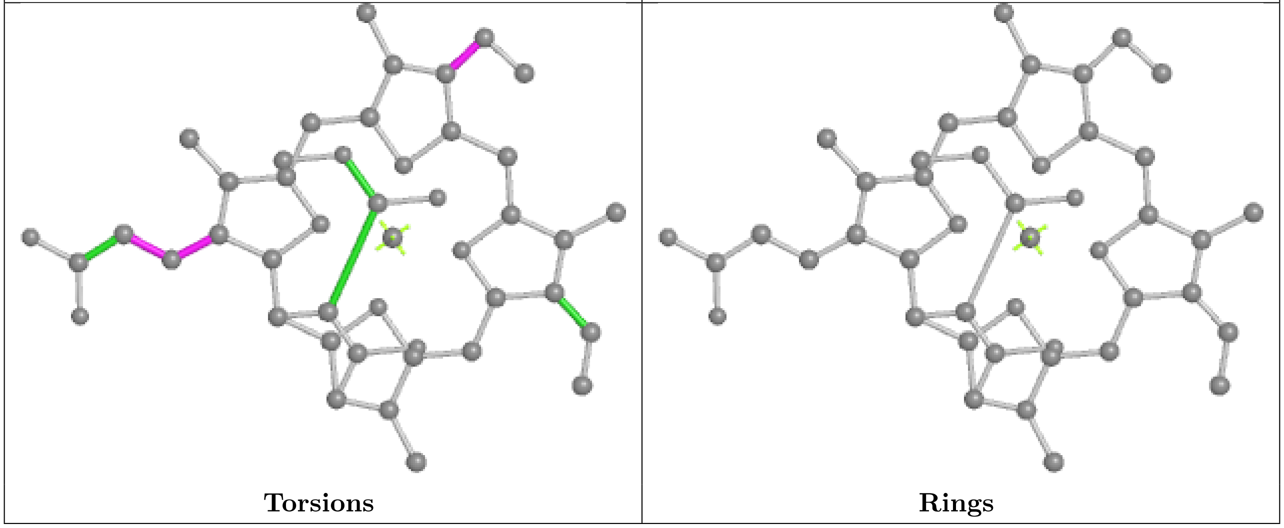
Torsions **Rings**

Ligand KC1 14 304



Bond lengths

Bond angles



Torsions

Rings

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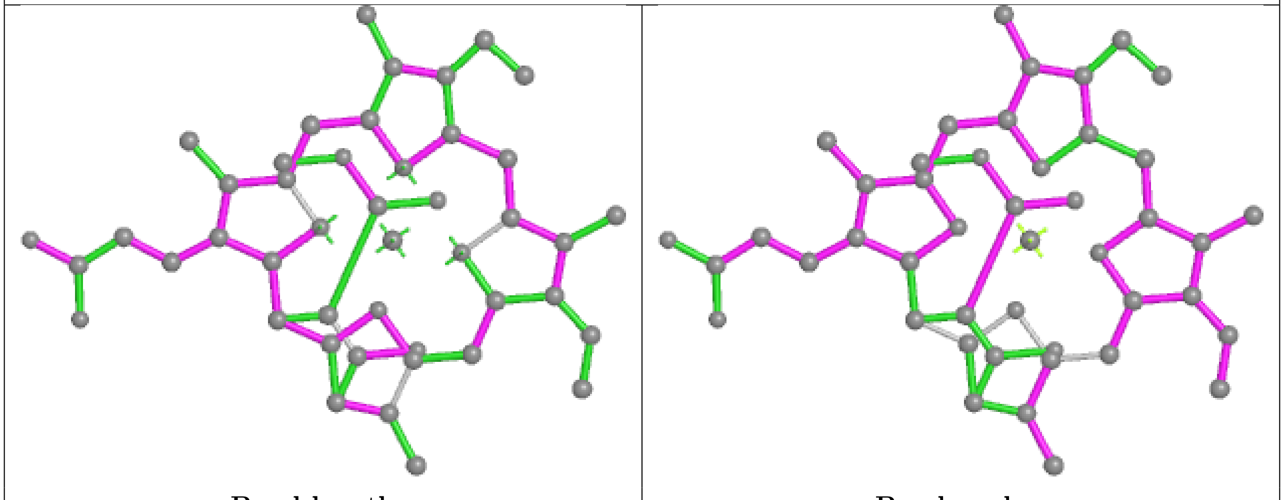
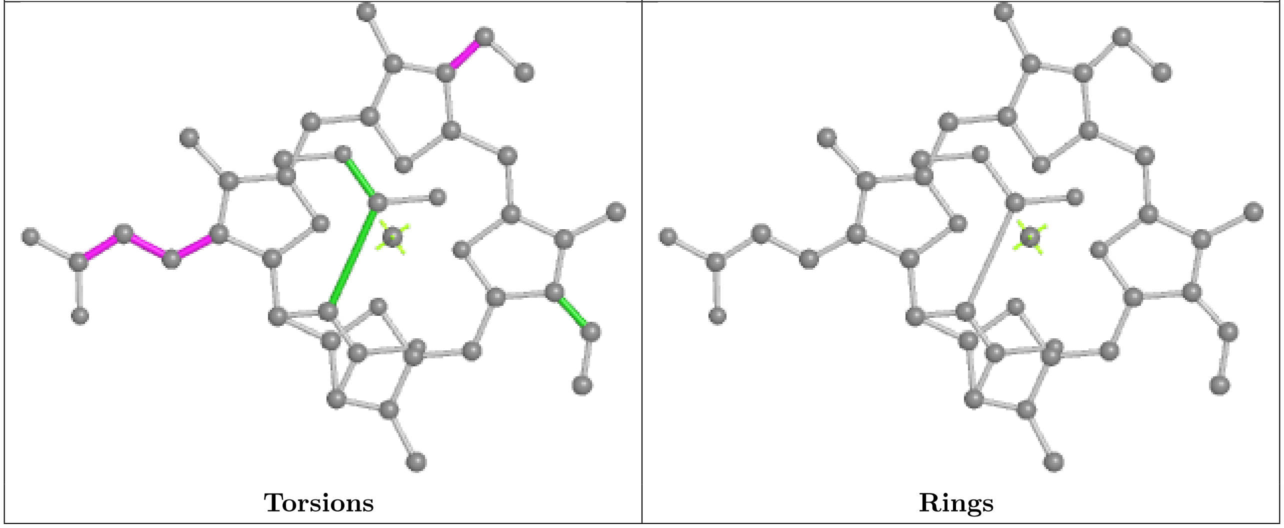


Bond lengths

Bond angles



Torsions

Rings

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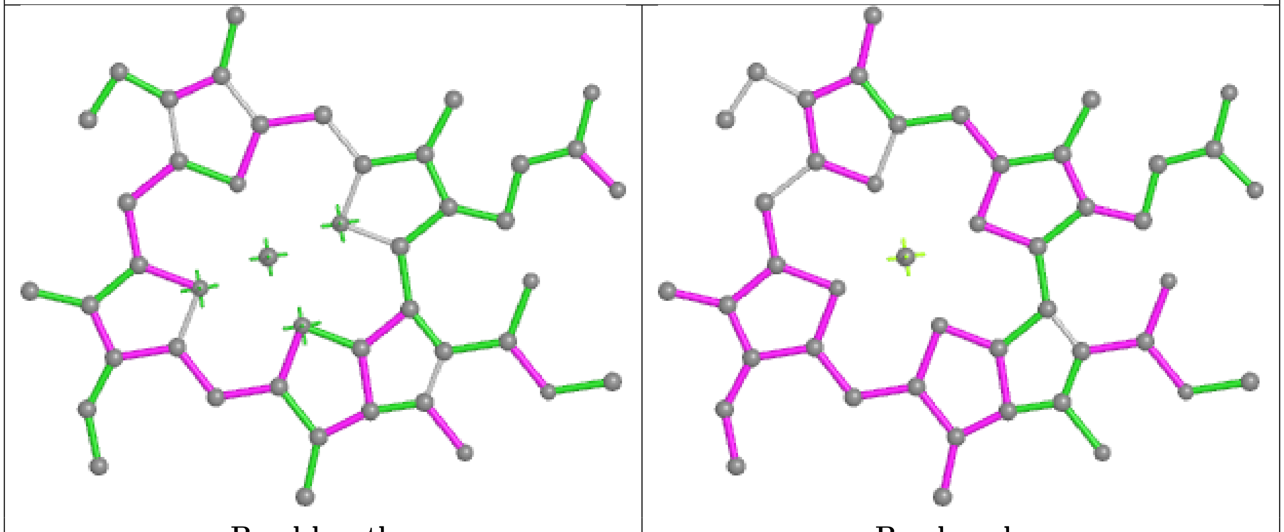
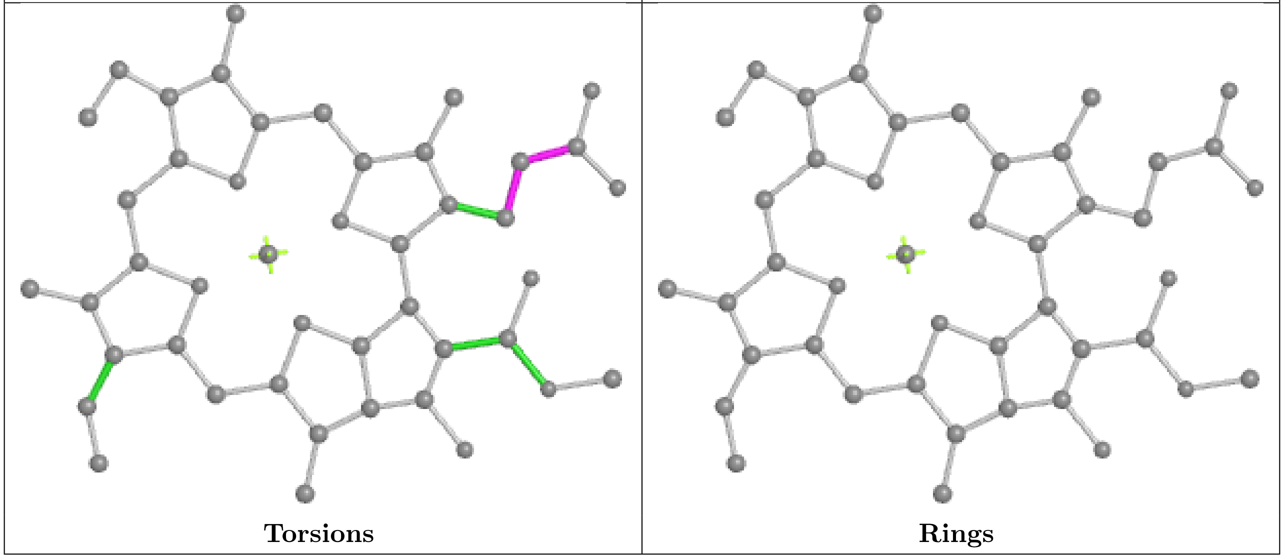


Bond lengths

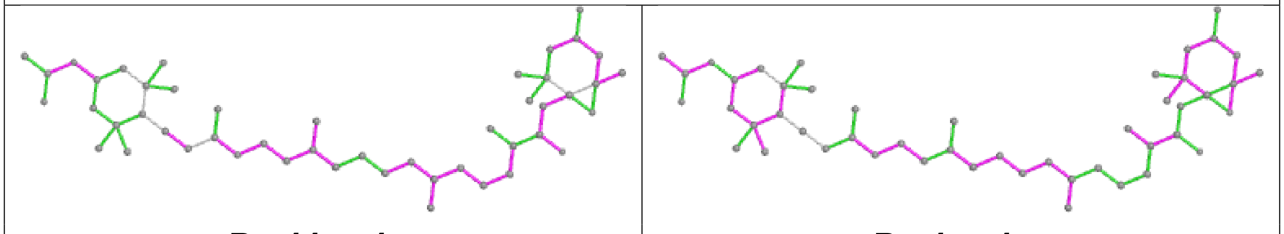
Bond angles



Torsions

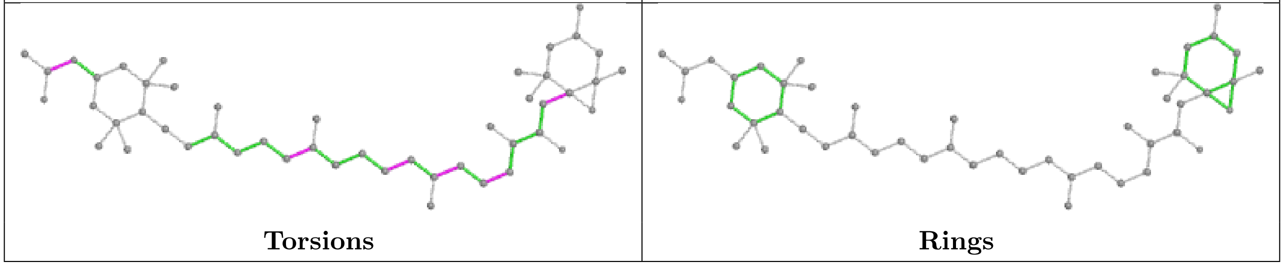
Rings

Ligand A86 13 316



Bond lengths

Bond angles



Torsions

Rings

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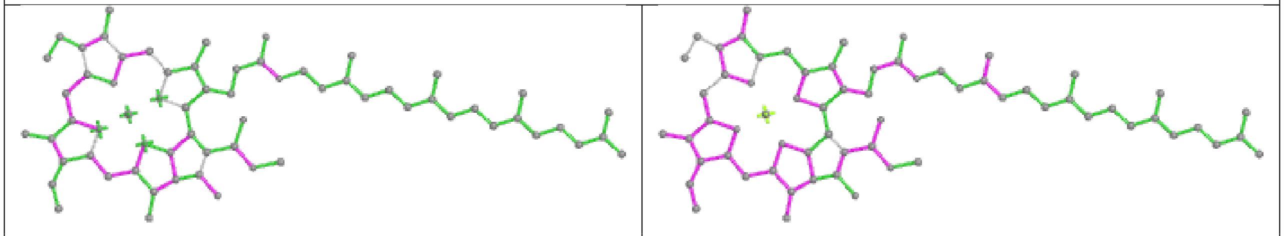
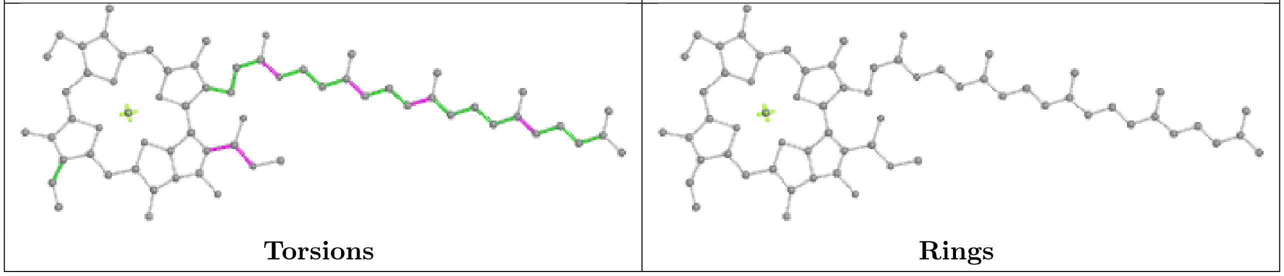


Bond lengths

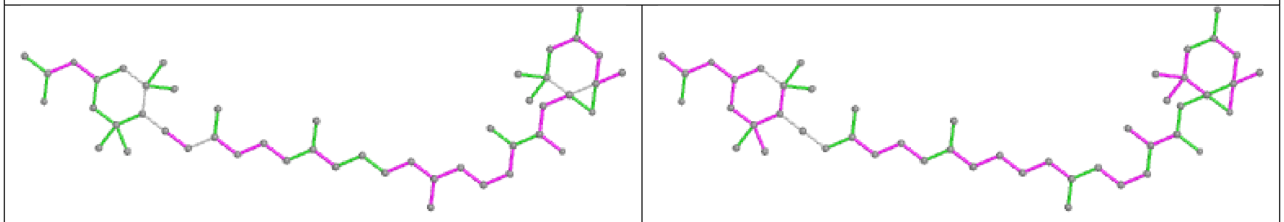
Bond angles



Torsions

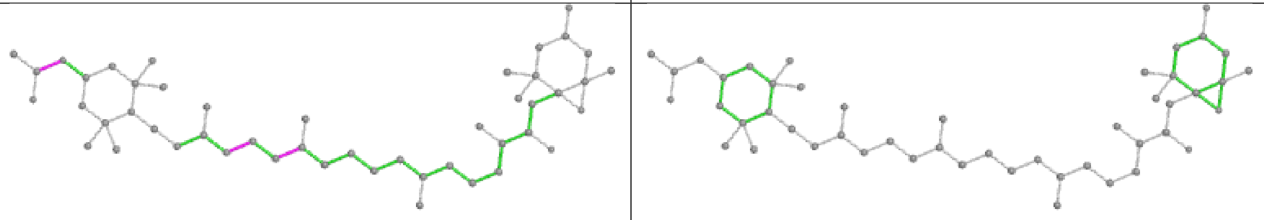
Rings

Ligand A86 16 310



Bond lengths

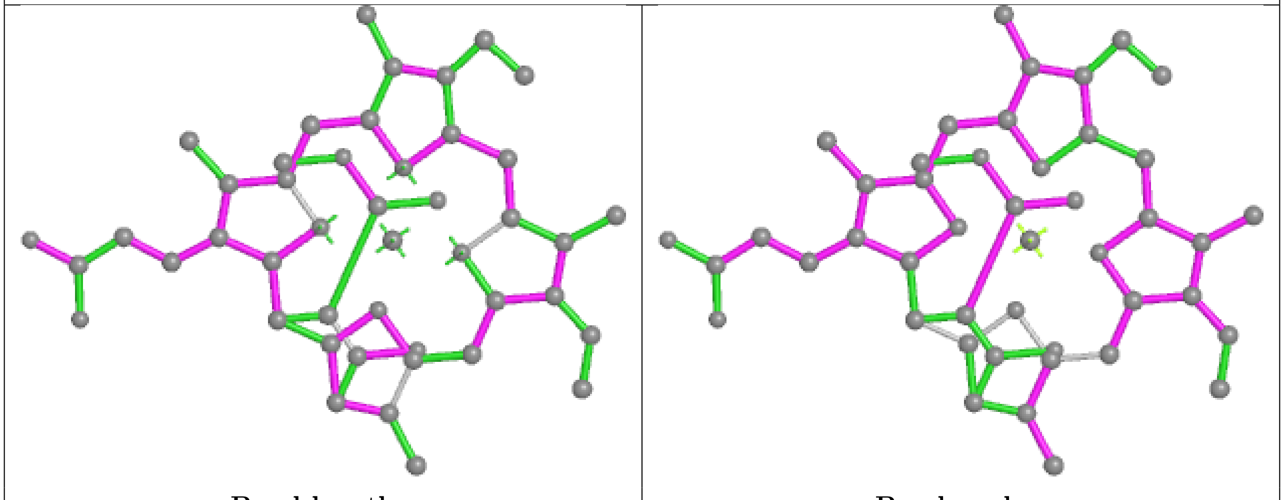
Bond angles



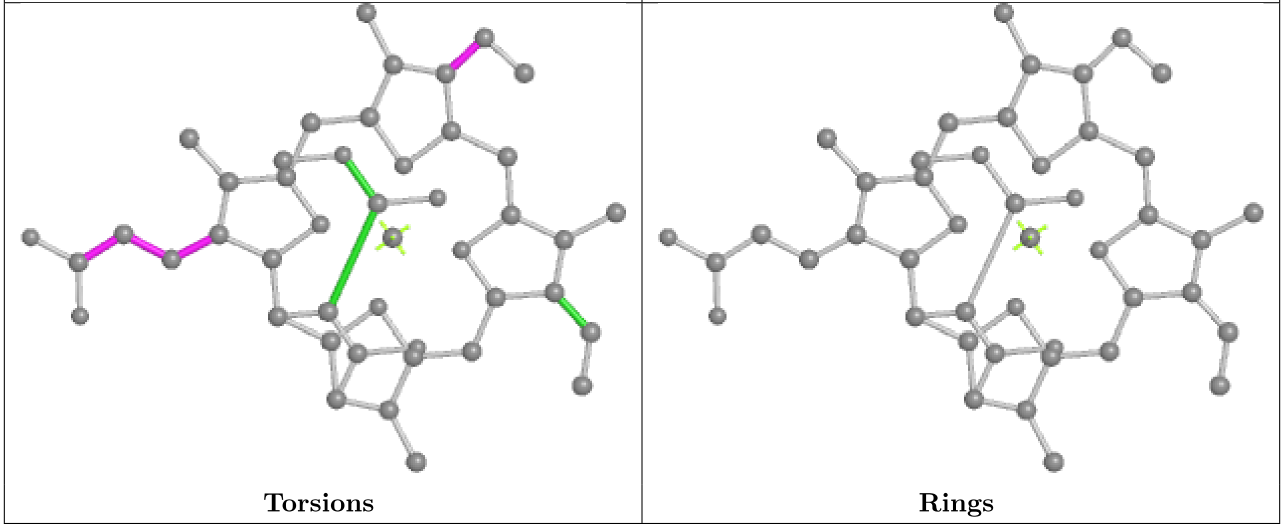
Torsions

Rings

Ligand KC1 17 305

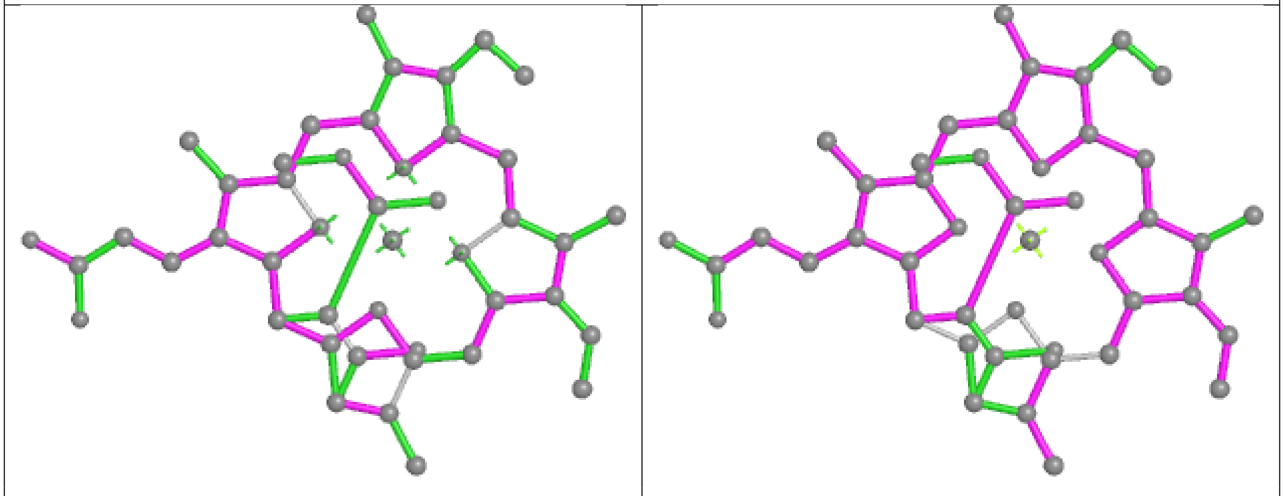


Bond lengths **Bond angles**



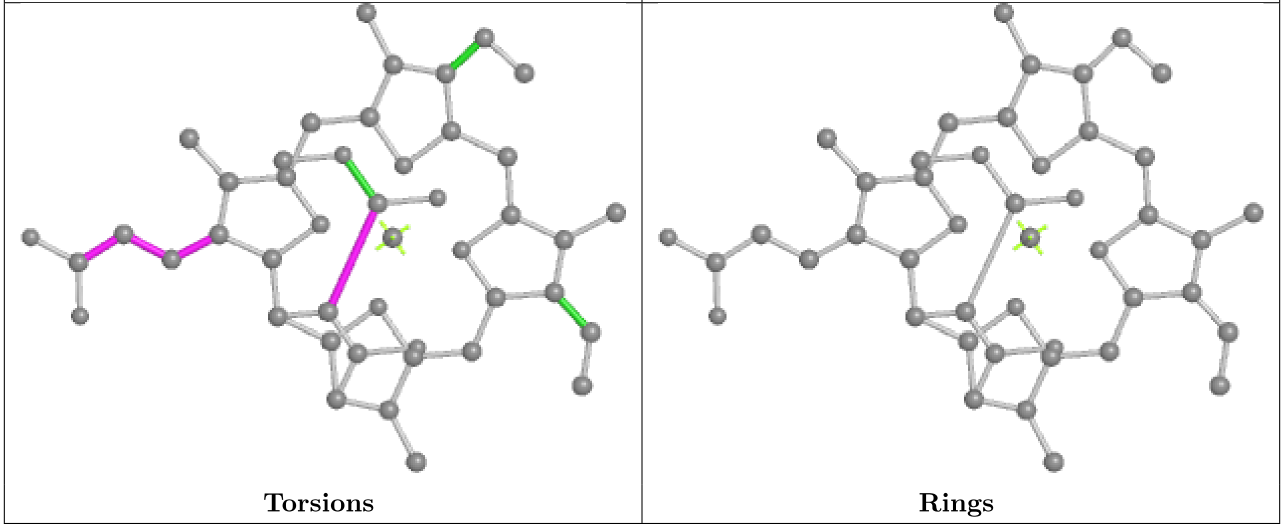
Torsions **Rings**

Ligand KC1 18 309



Bond lengths

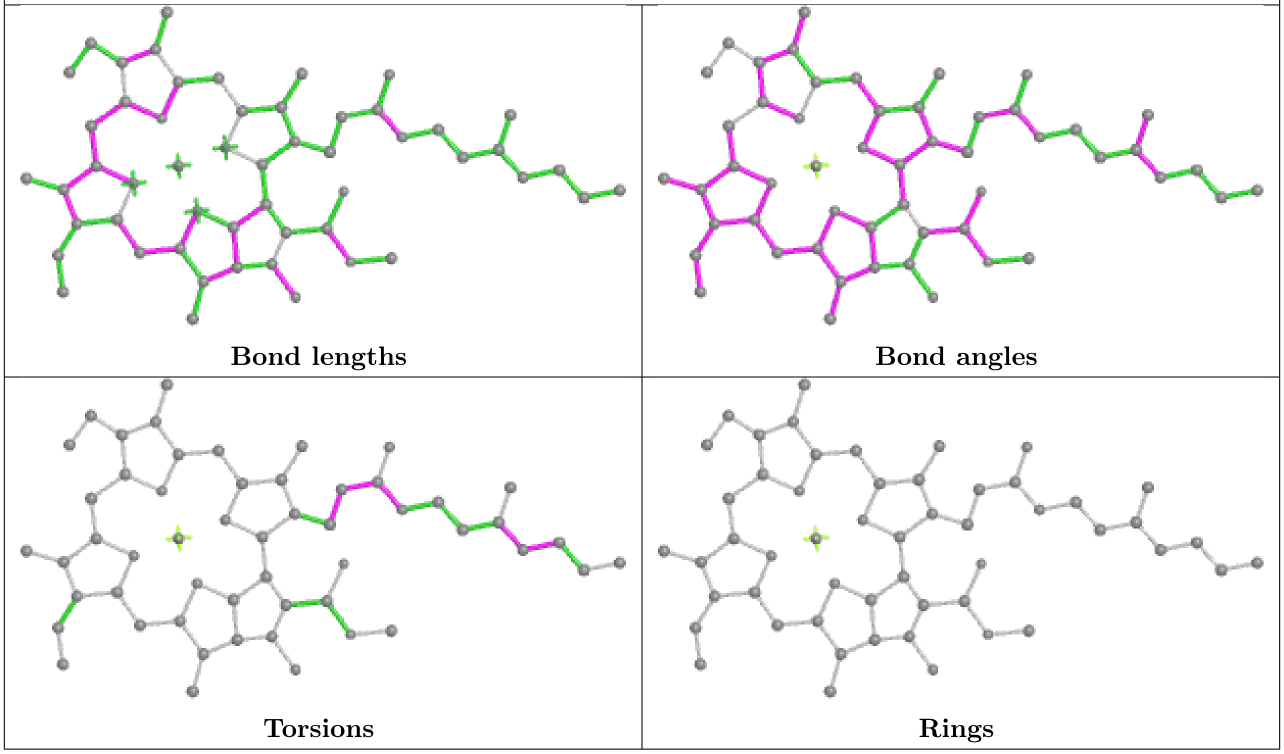
Bond angles



Torsions

Rings

Ligand CLA 18 307



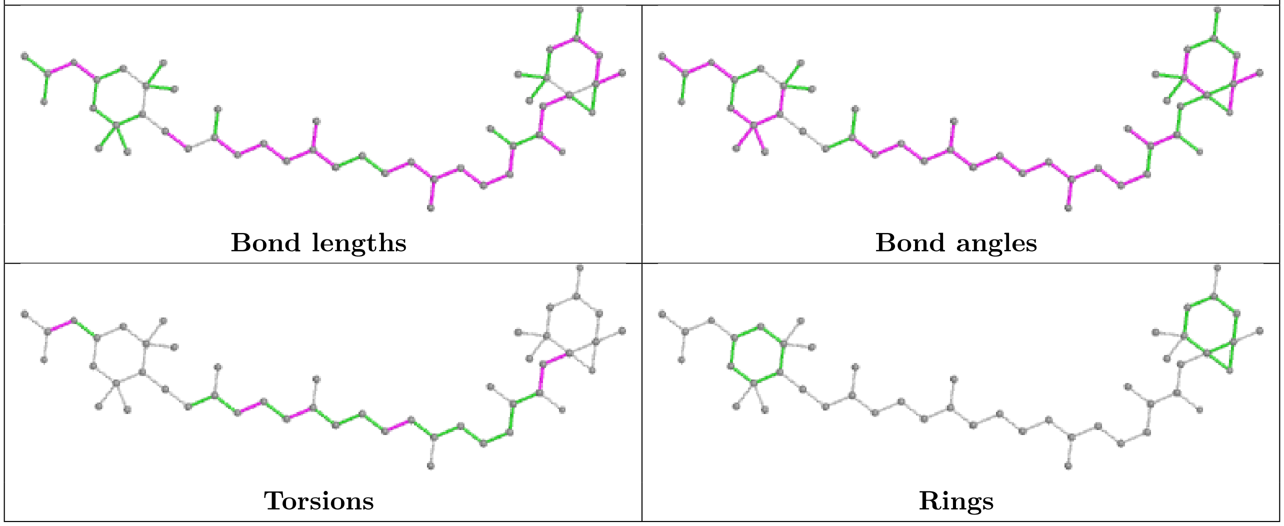
Bond lengths

Bond angles

Torsions

Rings

Ligand A86 17 314



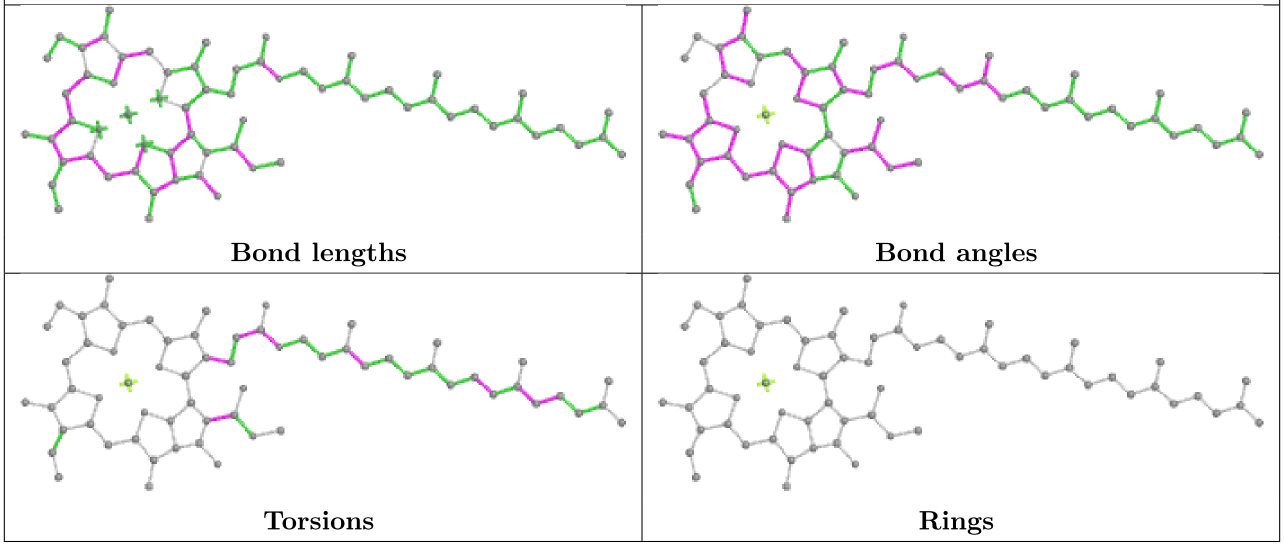
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA 21 208



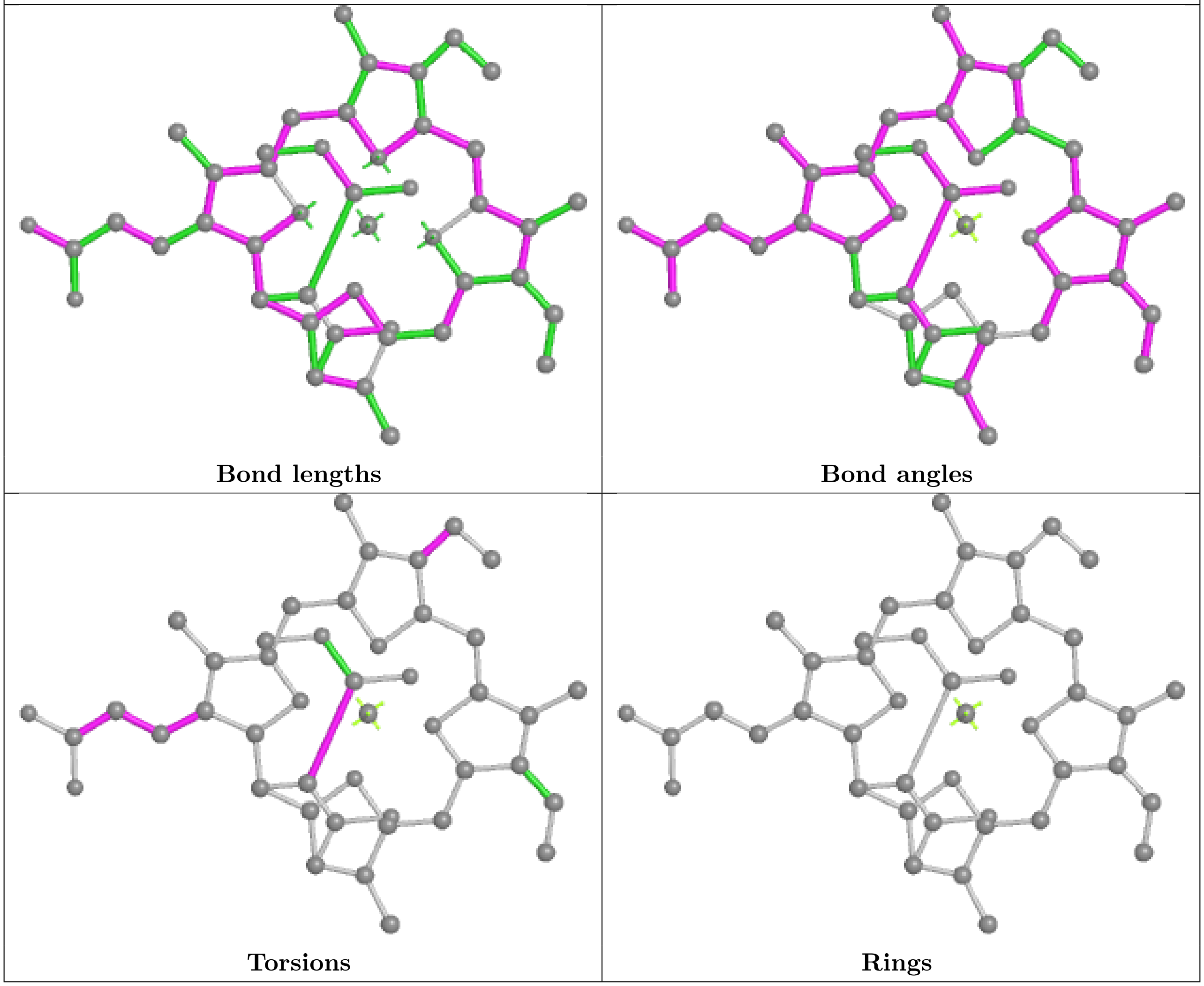
Bond lengths

Bond angles

Torsions

Rings

Ligand KC1 12 310



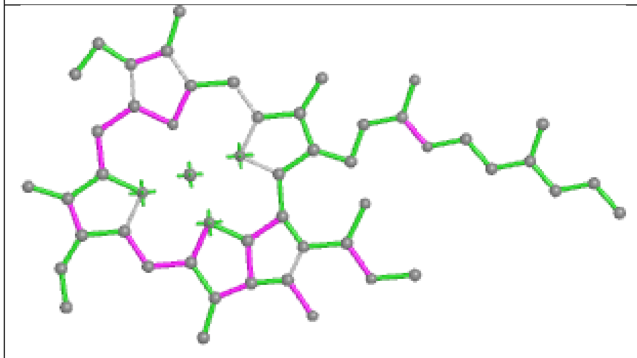
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA 14 307



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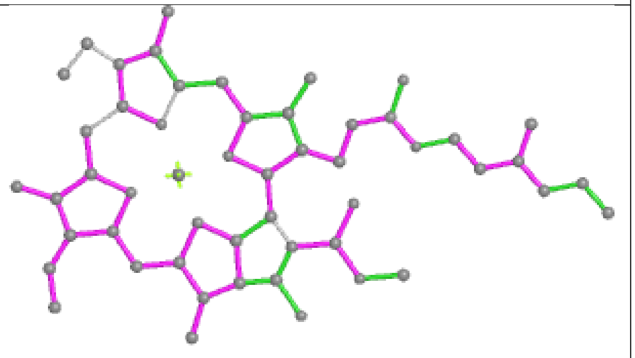
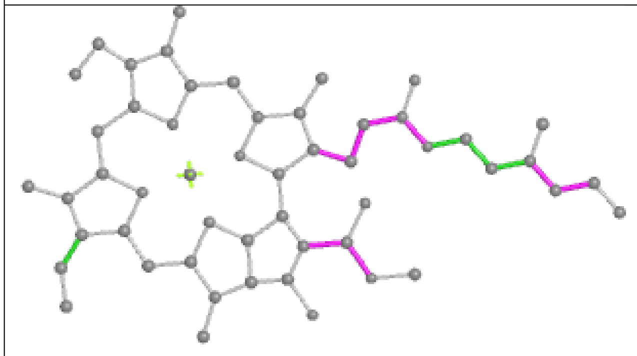
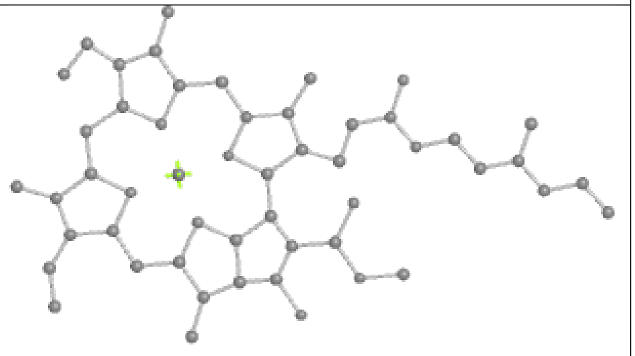


Bond angles

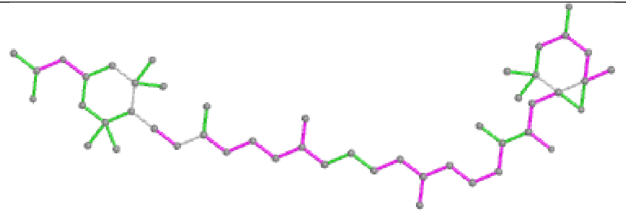


Torsions

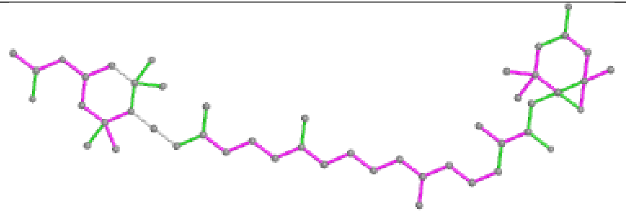


Rings

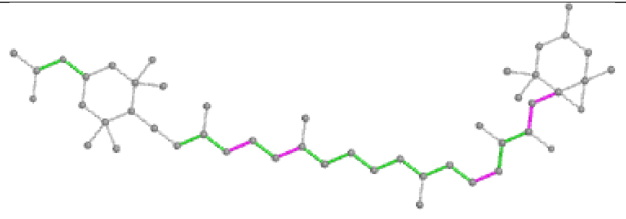
Ligand A86 13 312



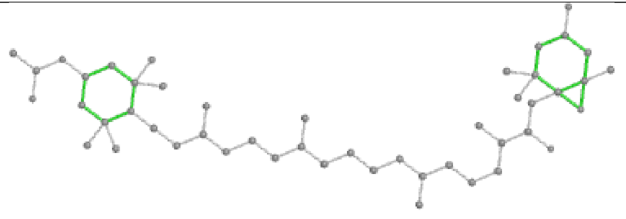
Bond lengths



Bond angles

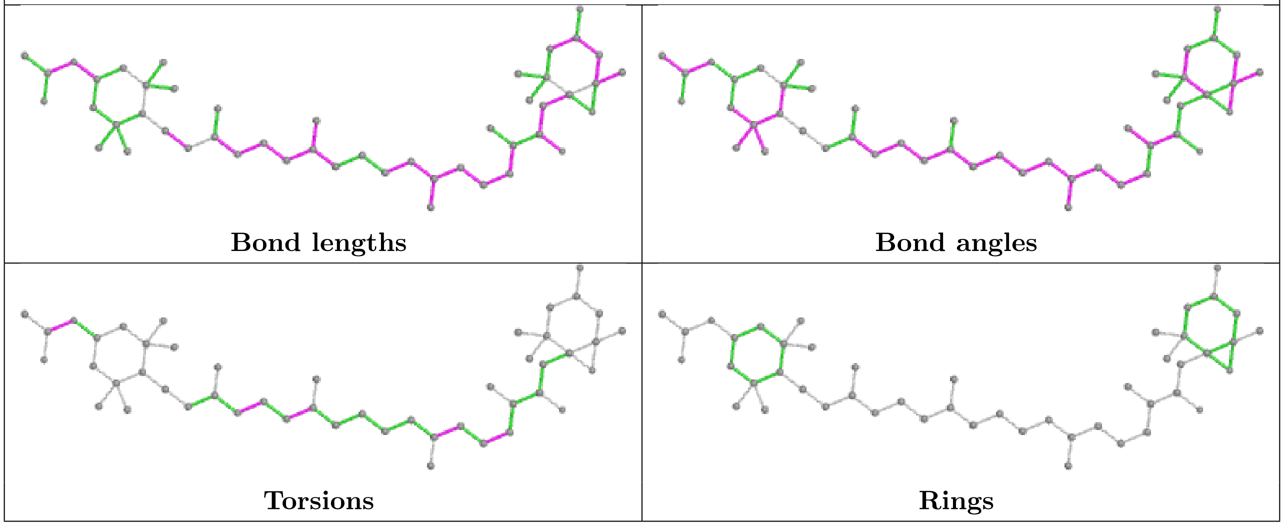


Torsions



Rings

Ligand A86 15 315



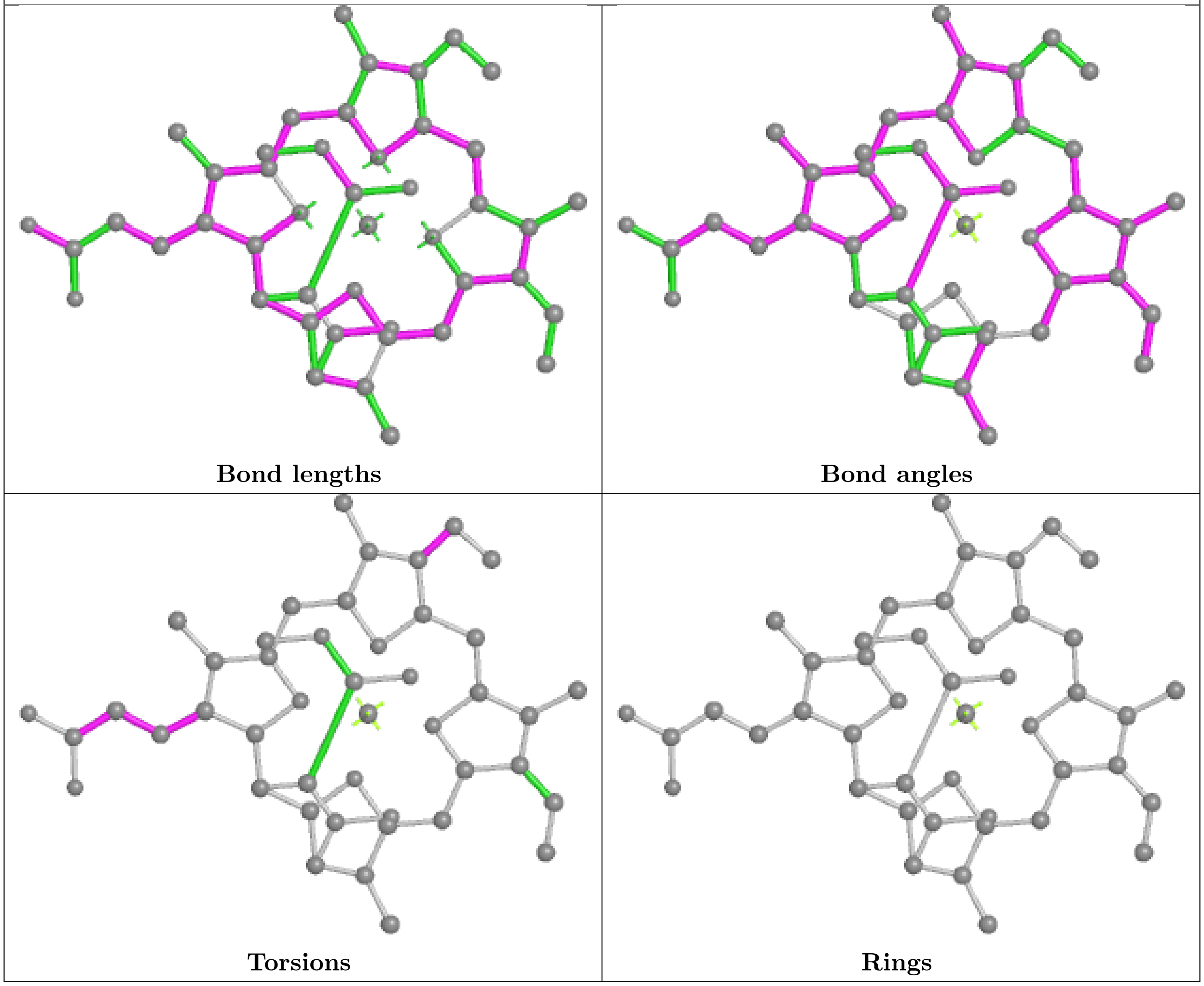
Bond lengths

Bond angles

Torsions

Rings

Ligand KC1 15 304



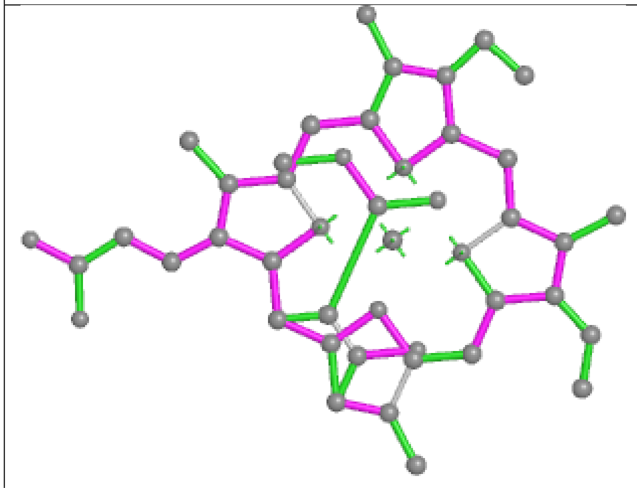
Bond lengths

Bond angles

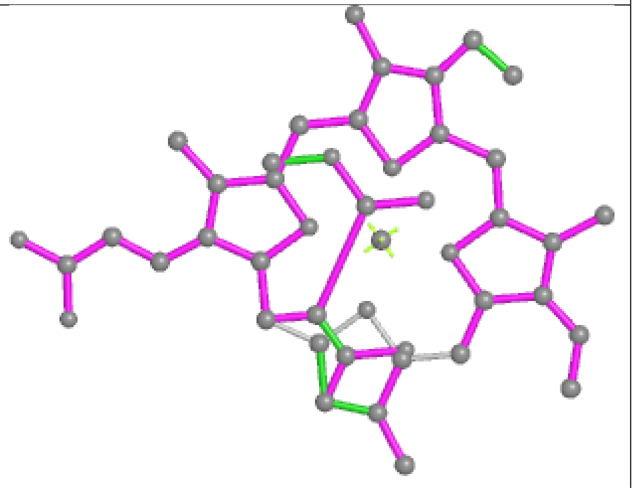
Torsions

Rings

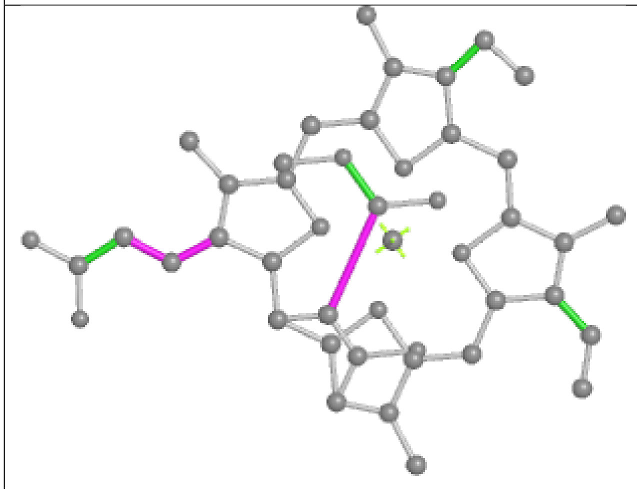
Ligand KC1 18 306



Bond lengths



Bond angles



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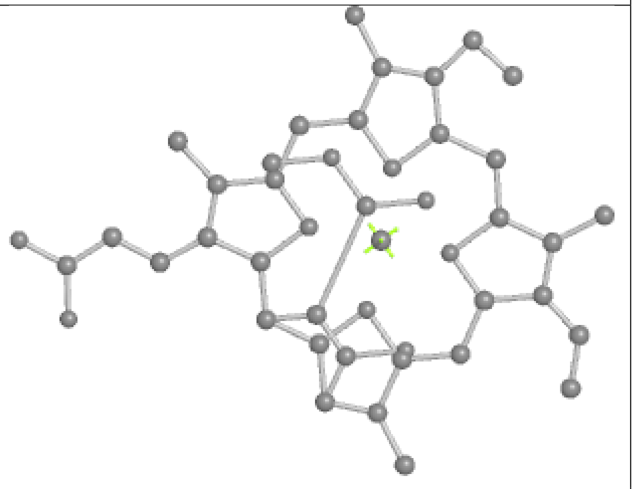
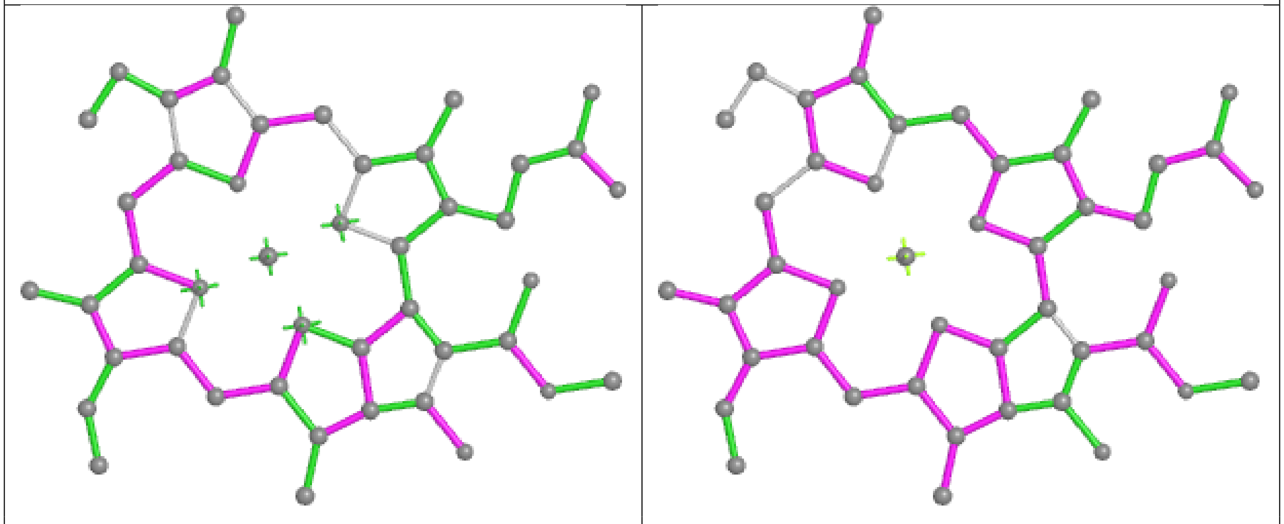


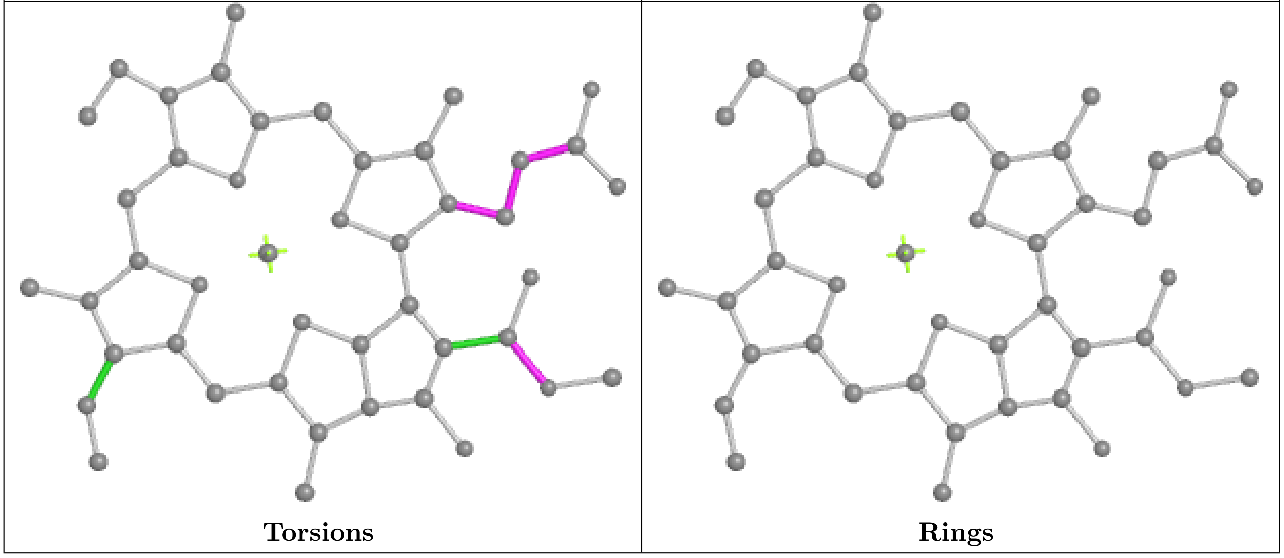
Rings

Ligand CLA 21 205



Bond lengths

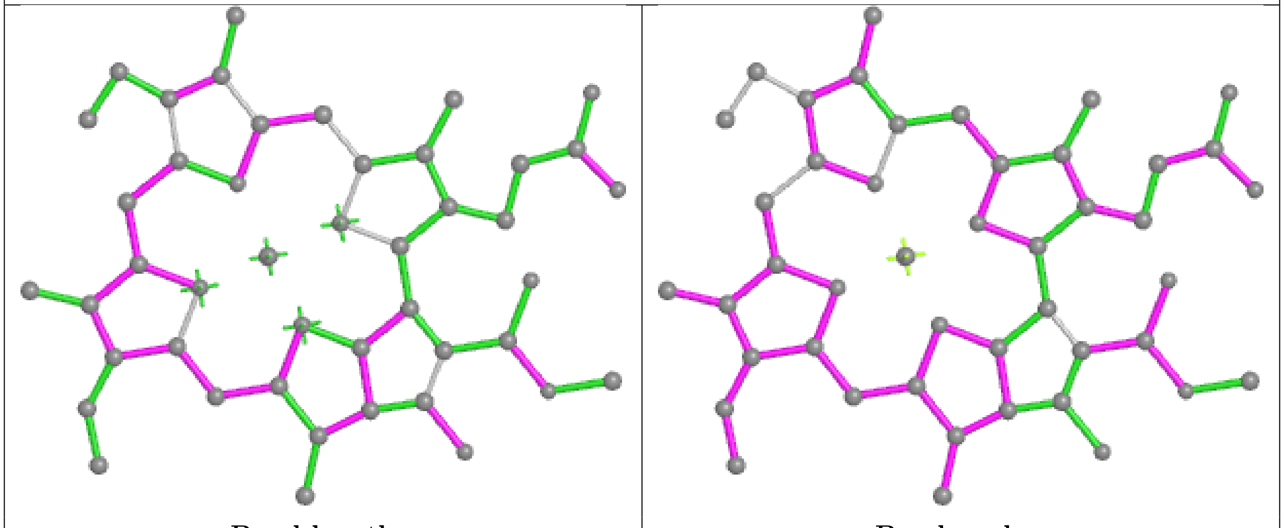
Bond angles



Torsions

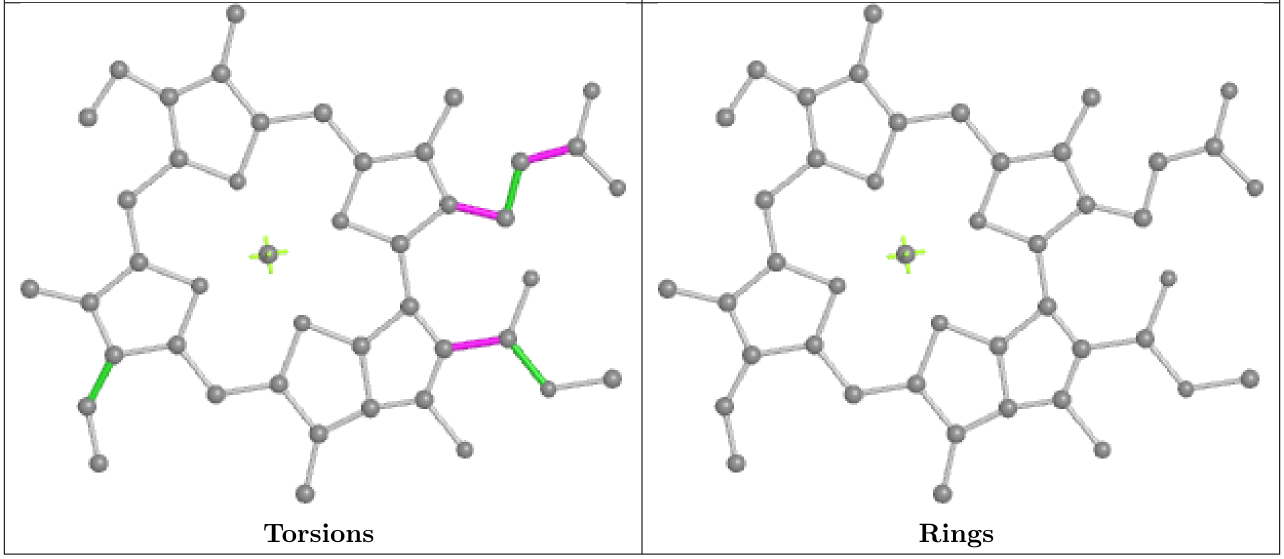
Rings

Ligand CLA 20 308



Bond lengths

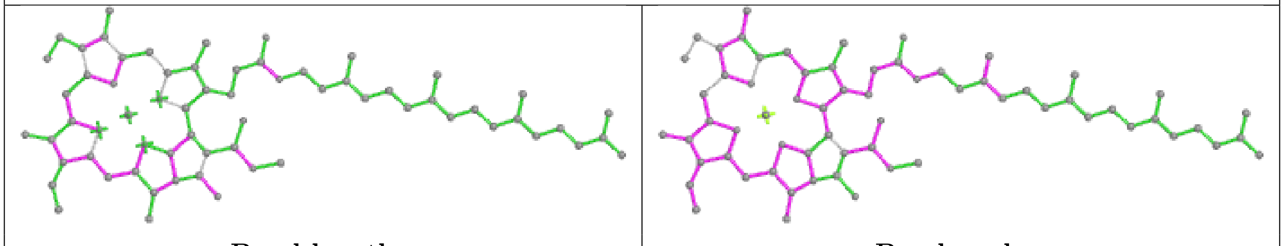
Bond angles



Torsions

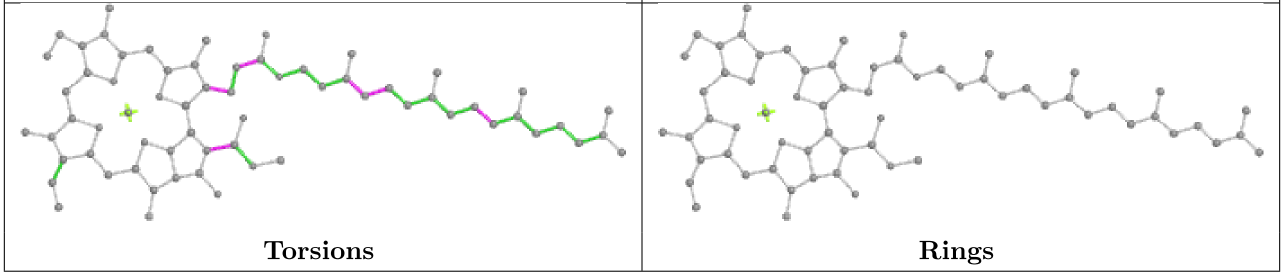
Rings

Ligand CLA 11 303



Bond lengths

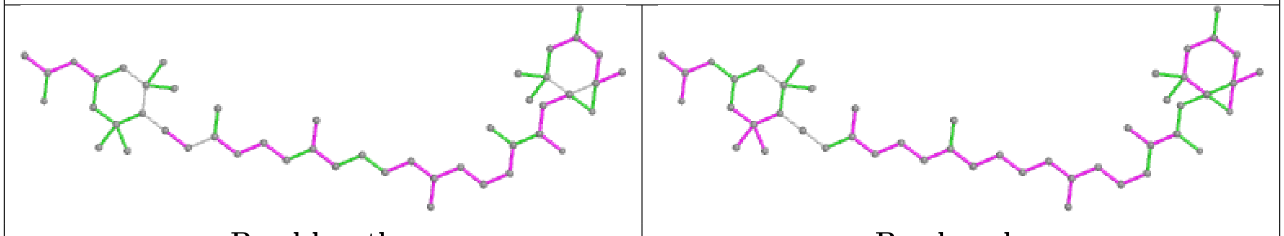
Bond angles



Torsions

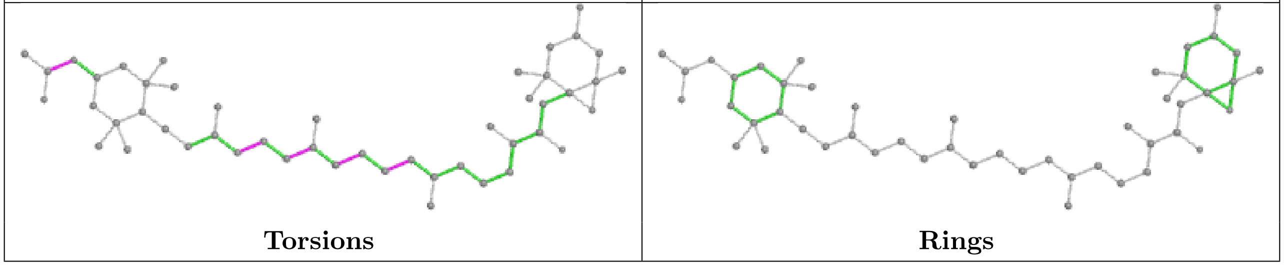
Rings

Ligand A86 11 318



Bond lengths

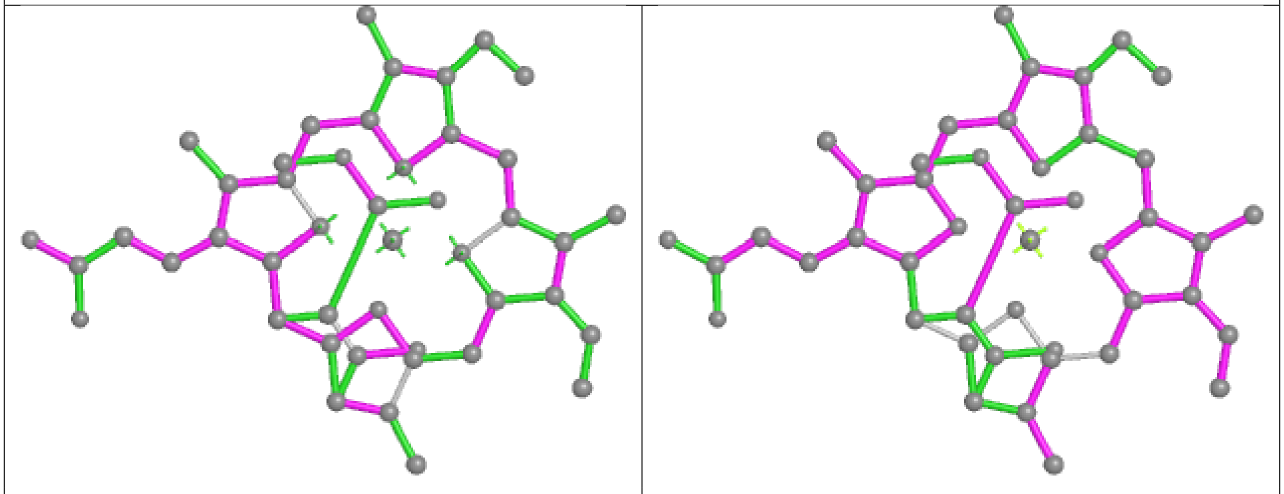
Bond angles



Torsions

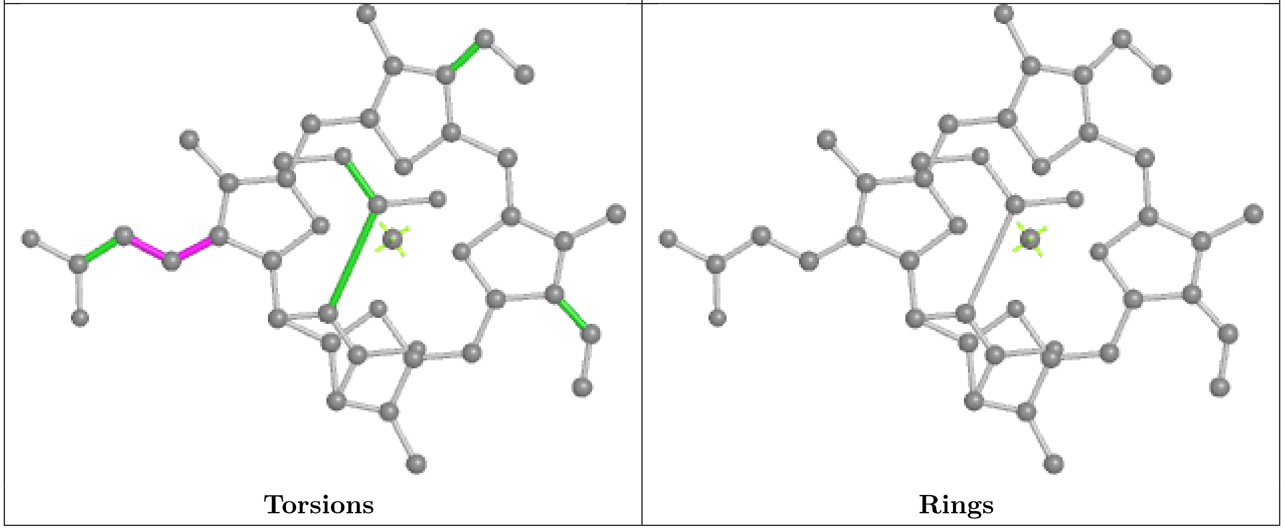
Rings

Ligand KC1 11 302



Bond lengths

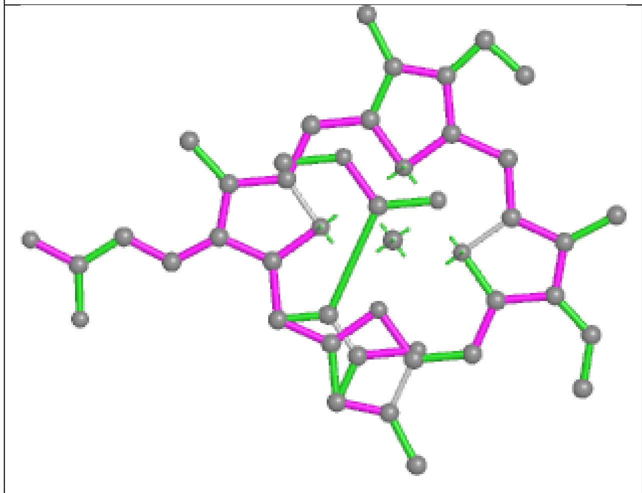
Bond angles



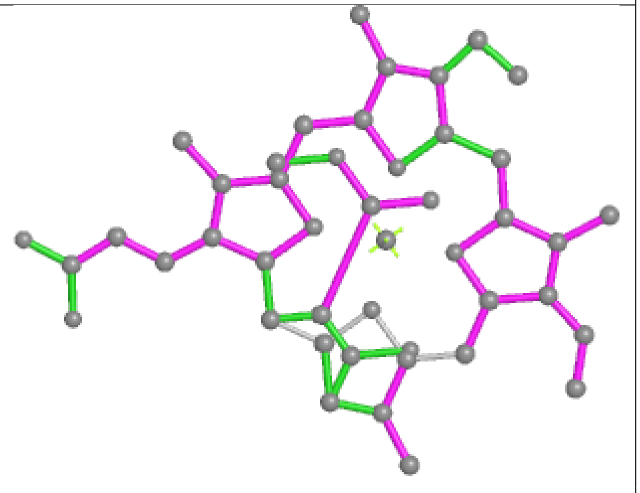
Torsions

Rings

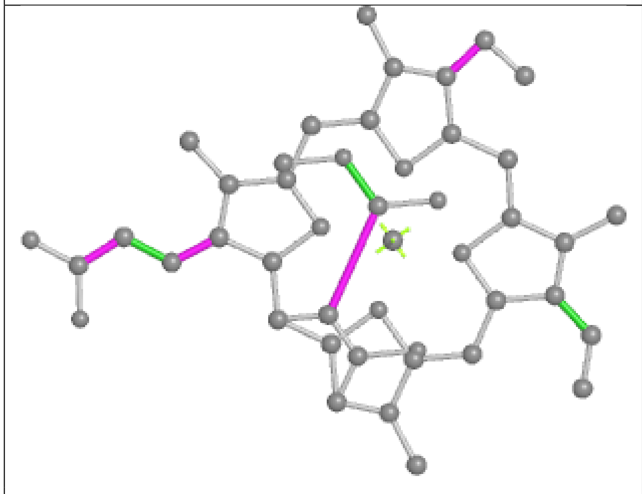
Ligand KC1 21 207



Bond lengths



Bond angles



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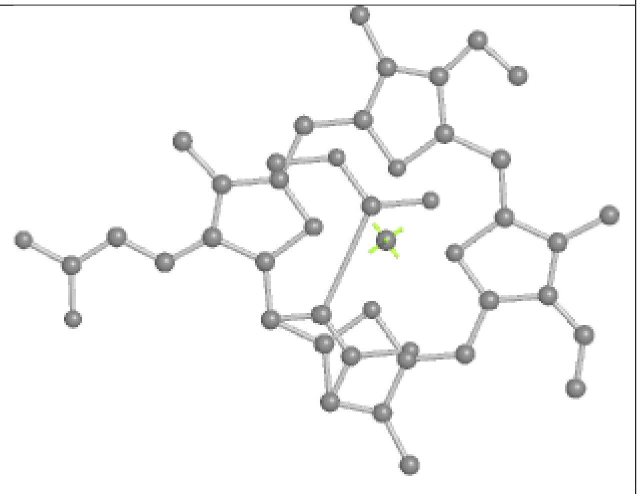
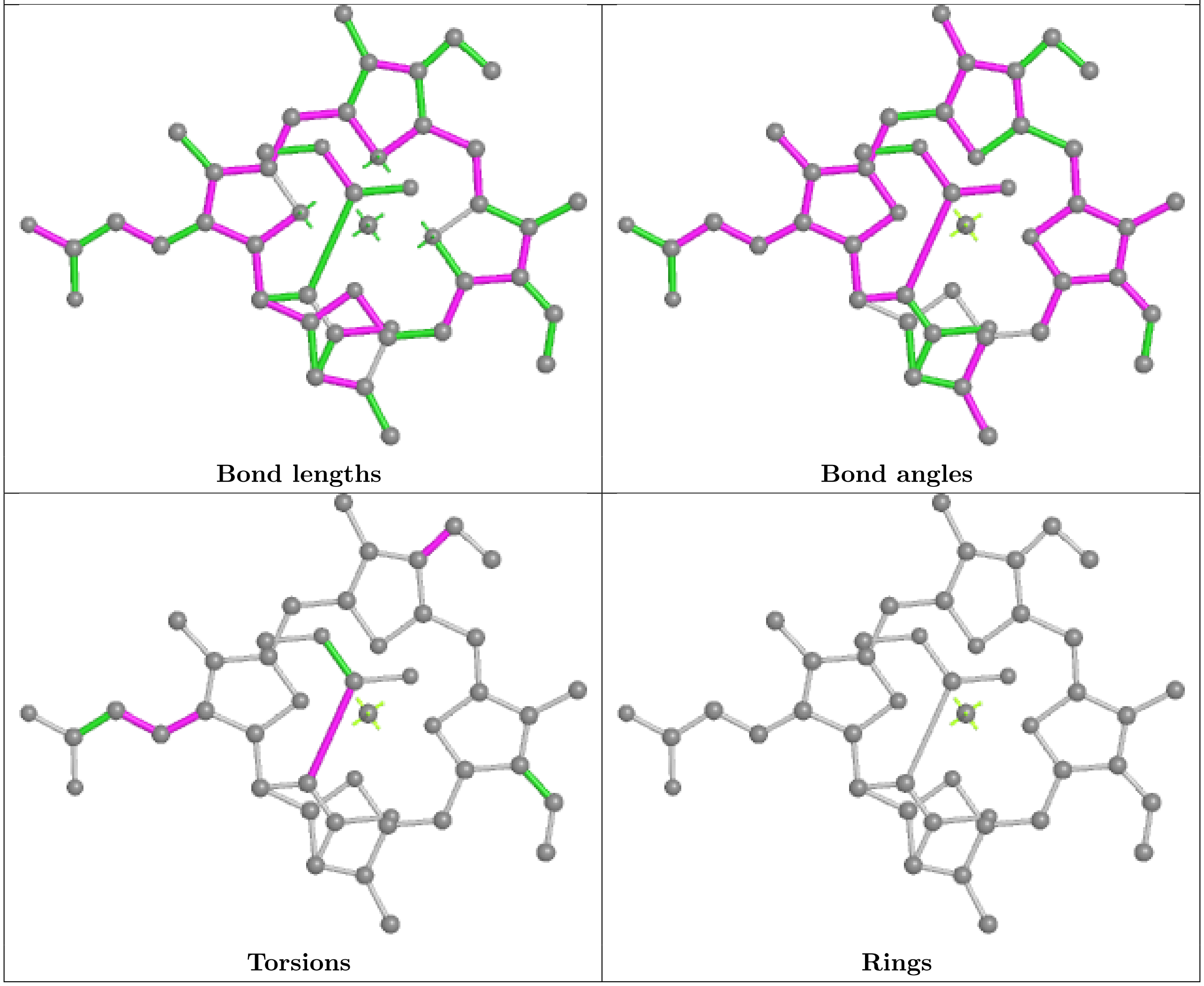


Rings

Ligand KC1 16 308



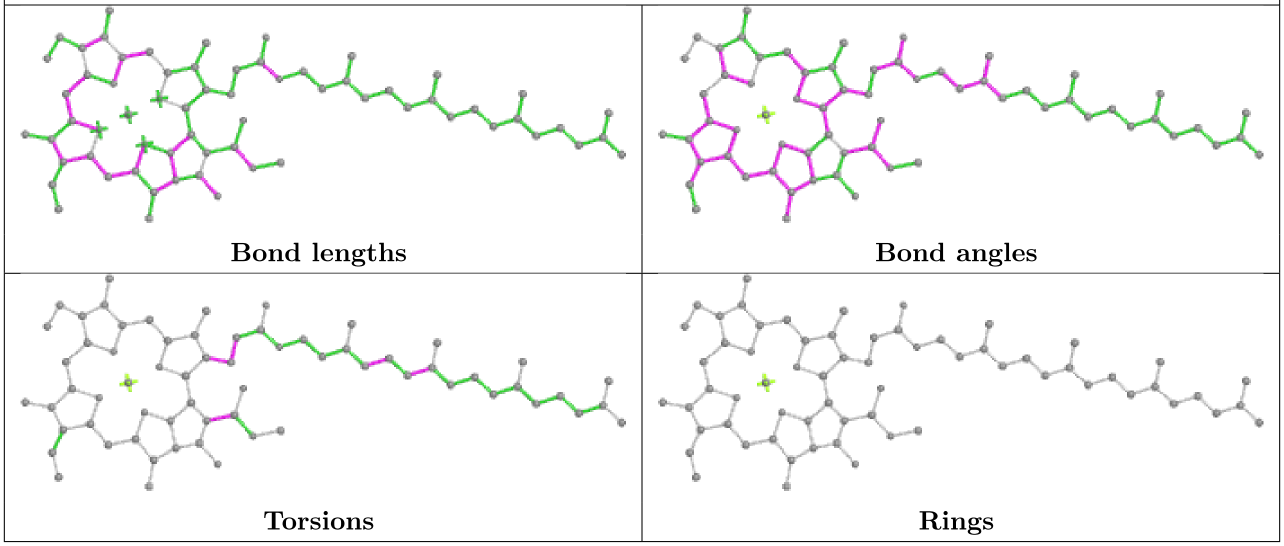
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA 12 304



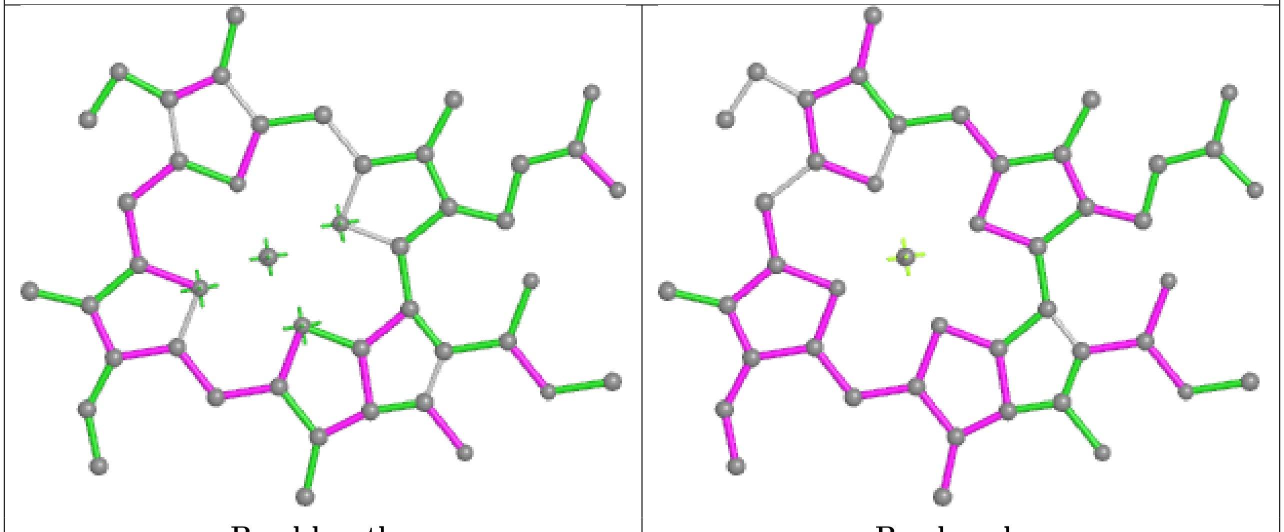
Bond lengths

Bond angles

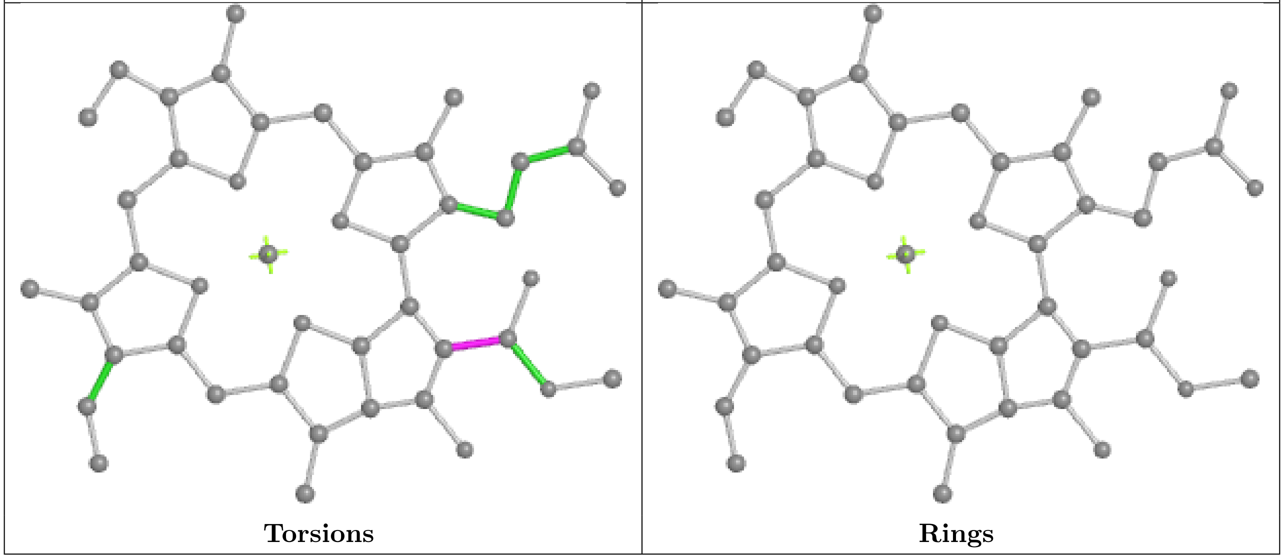
Torsions

Rings

Ligand CLA 15 310

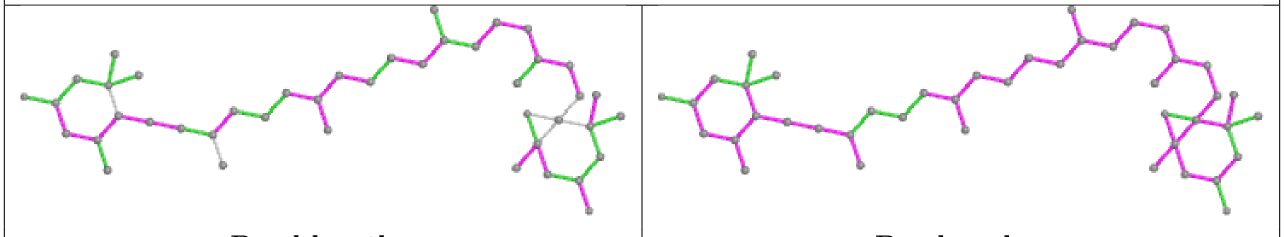


Bond lengths **Bond angles**

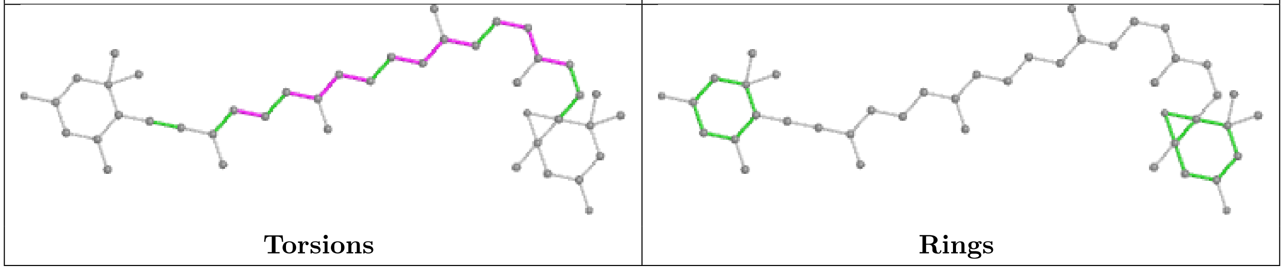


Torsions **Rings**

Ligand DD6 21 216

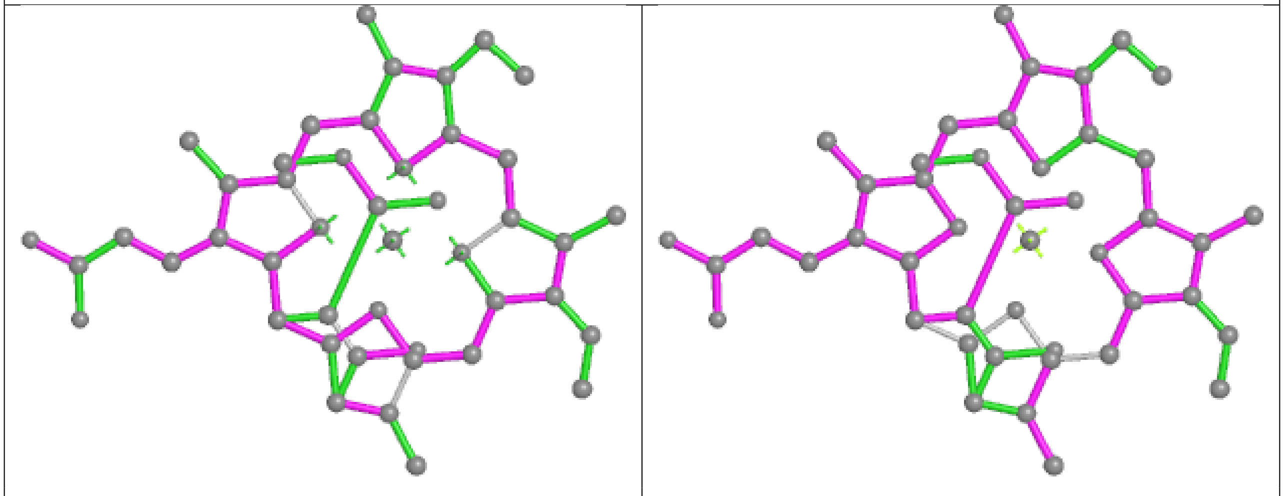


Bond lengths **Bond angles**



Torsions **Rings**

Ligand KC1 20 306



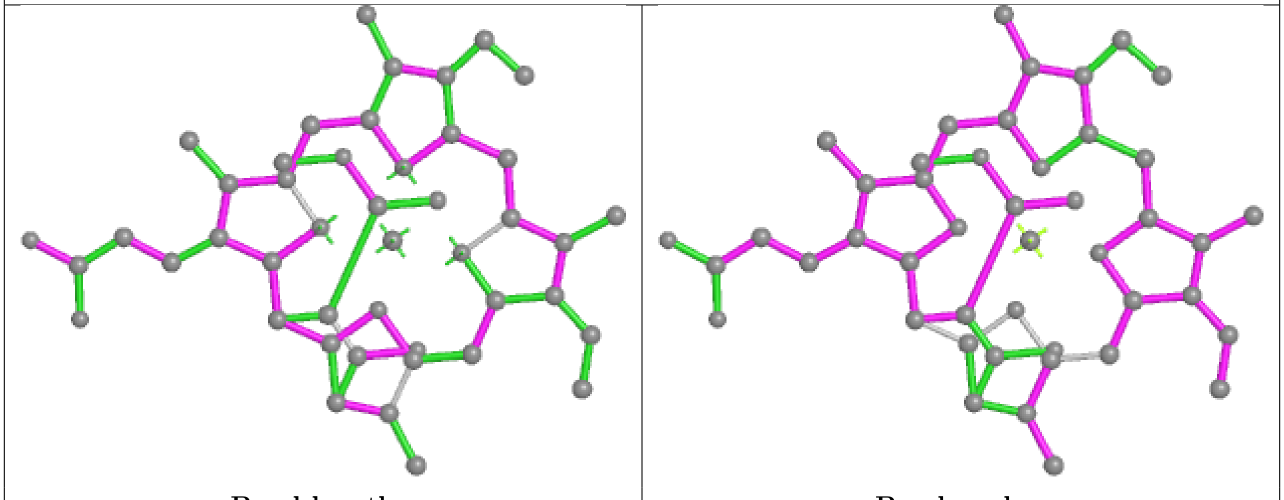
Bond lengths

Bond angles

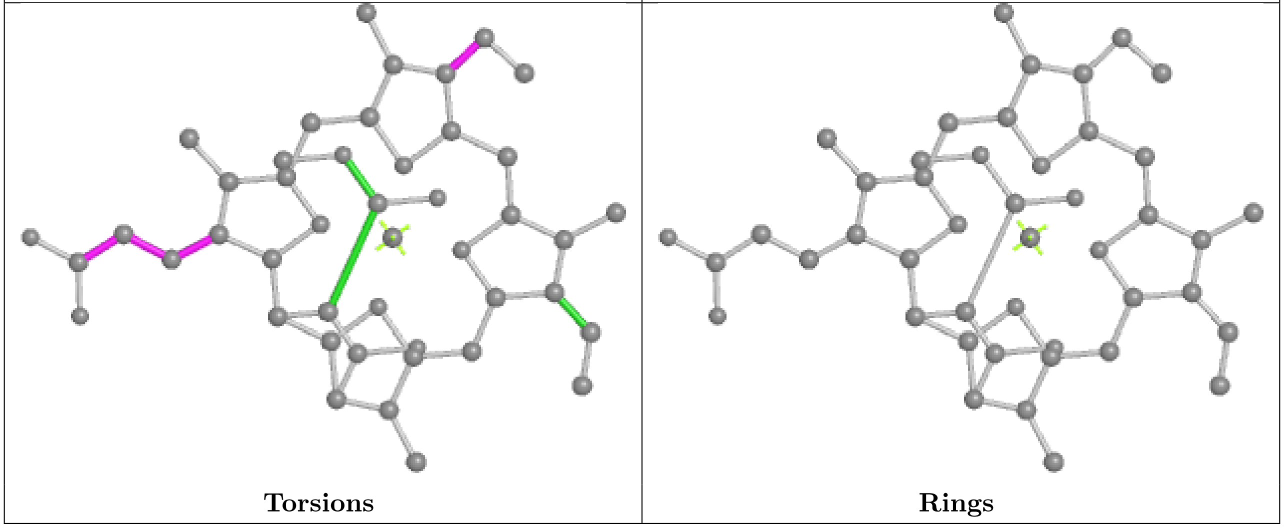
Torsions

Rings

Ligand KC1 15 309

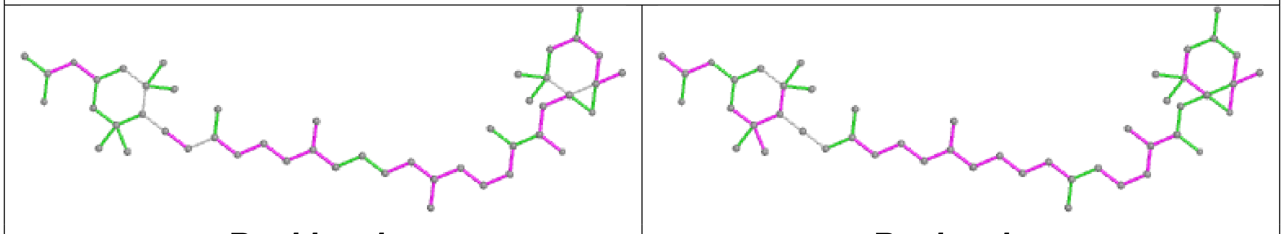


Bond lengths **Bond angles**

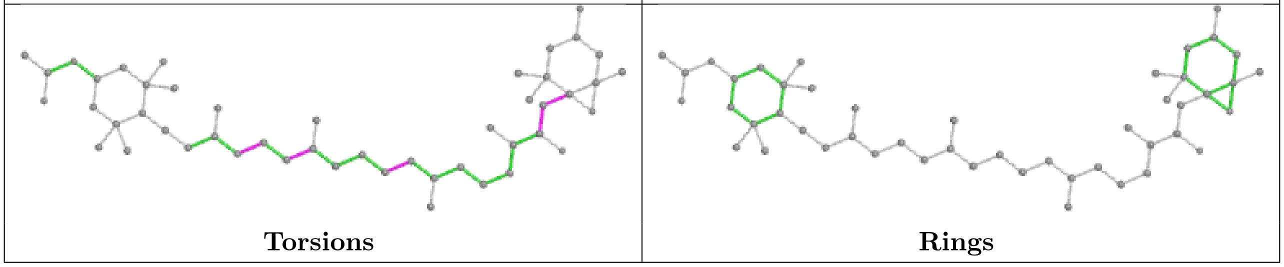


Torsions **Rings**

Ligand A86 21 214

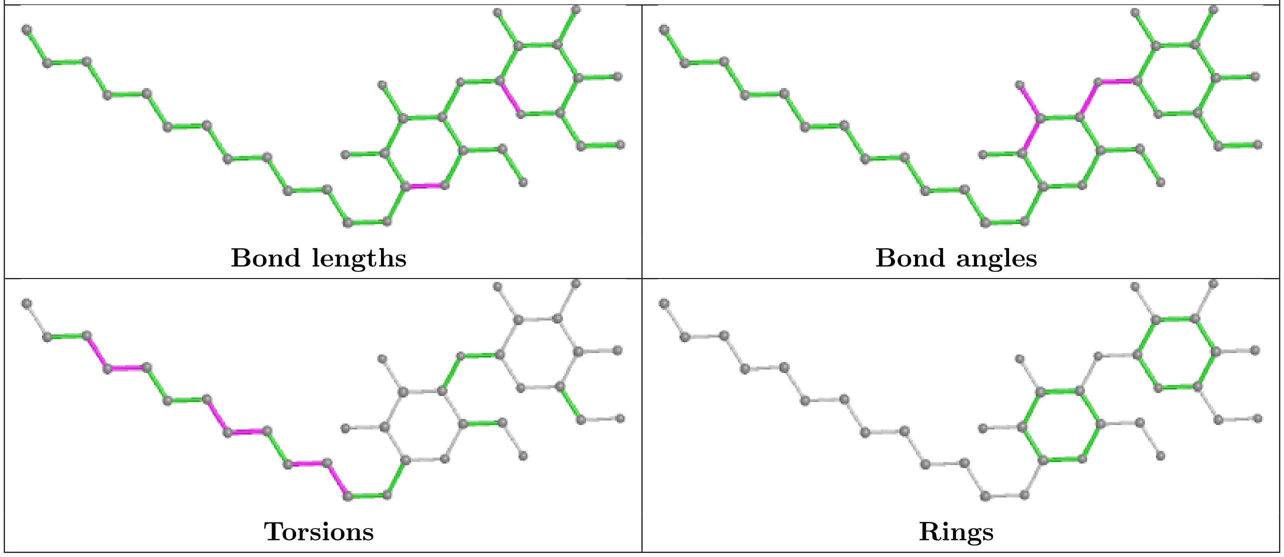


Bond lengths **Bond angles**



Torsions **Rings**

Ligand LMU 19 315



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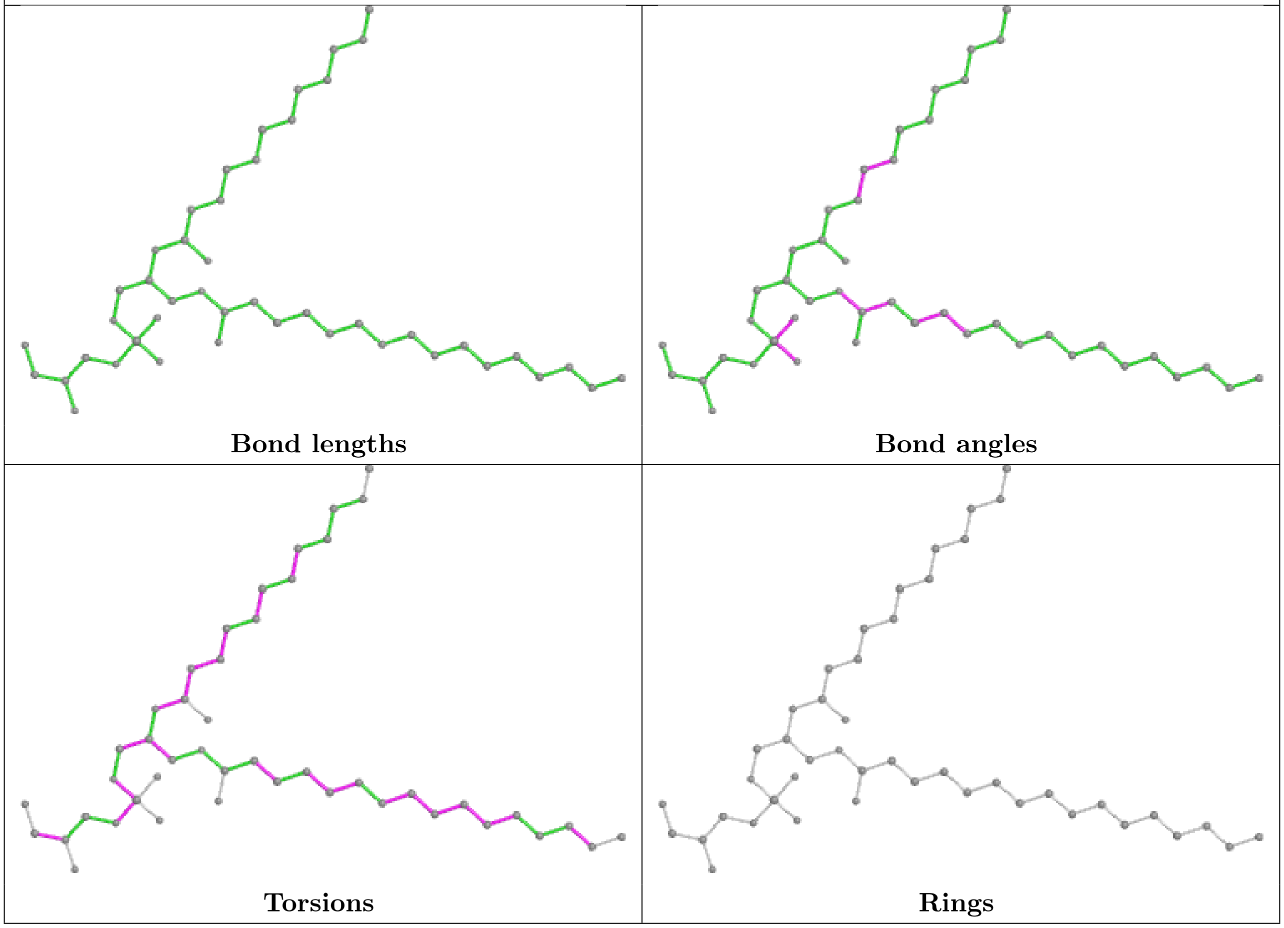
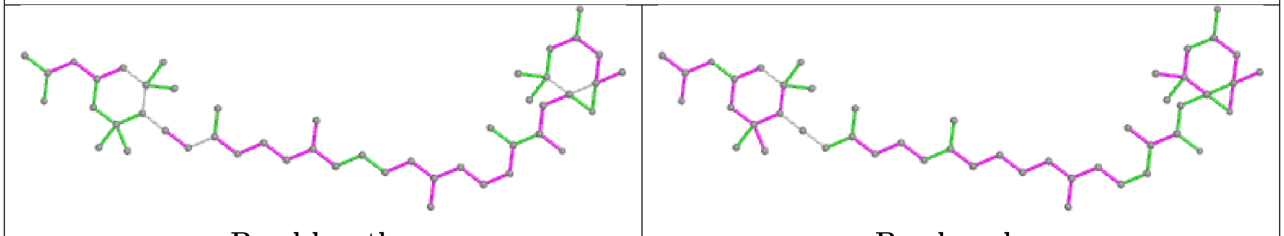
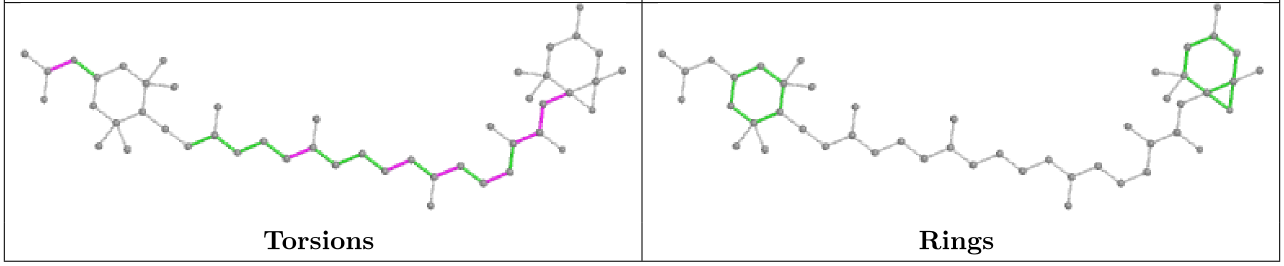


Ligand A86 12 316

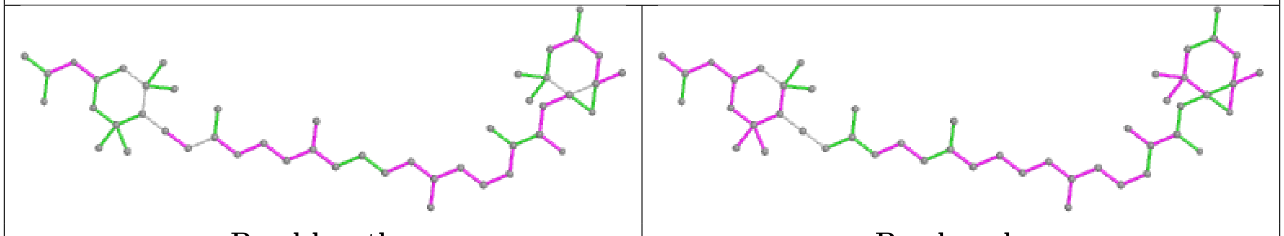


Bond lengths Bond angles

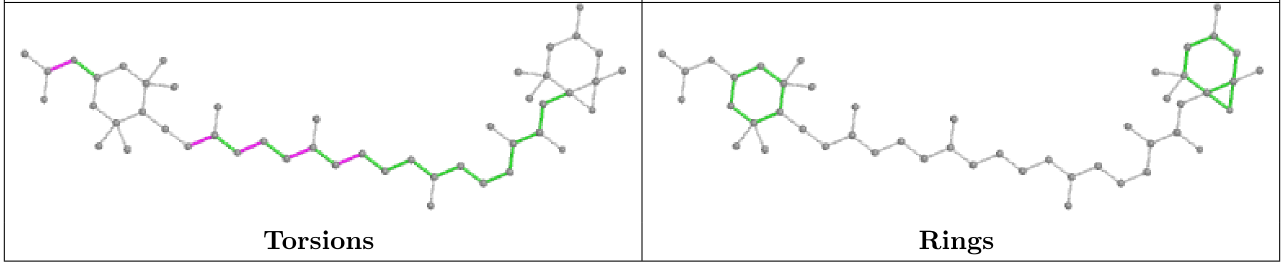


Torsions Rings

Ligand A86 16 311

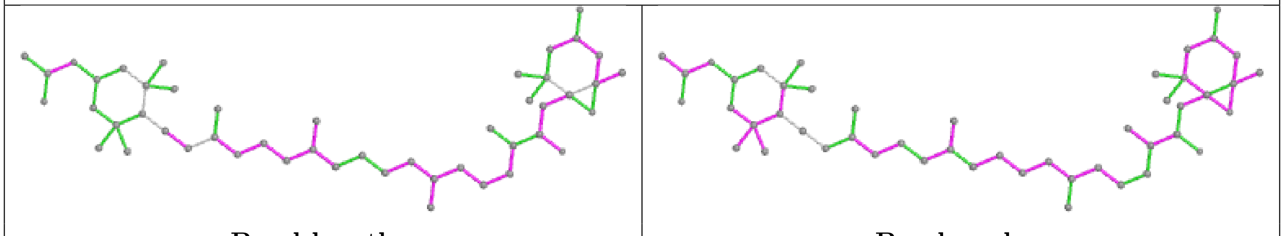


Bond lengths Bond angles

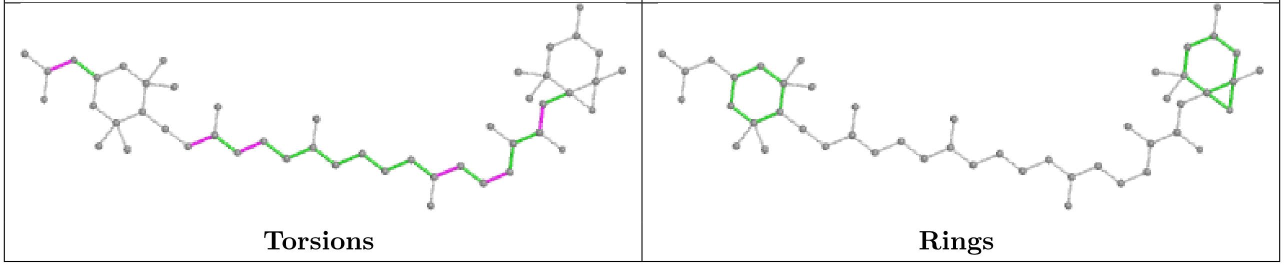


Torsions Rings

Ligand A86 11 312

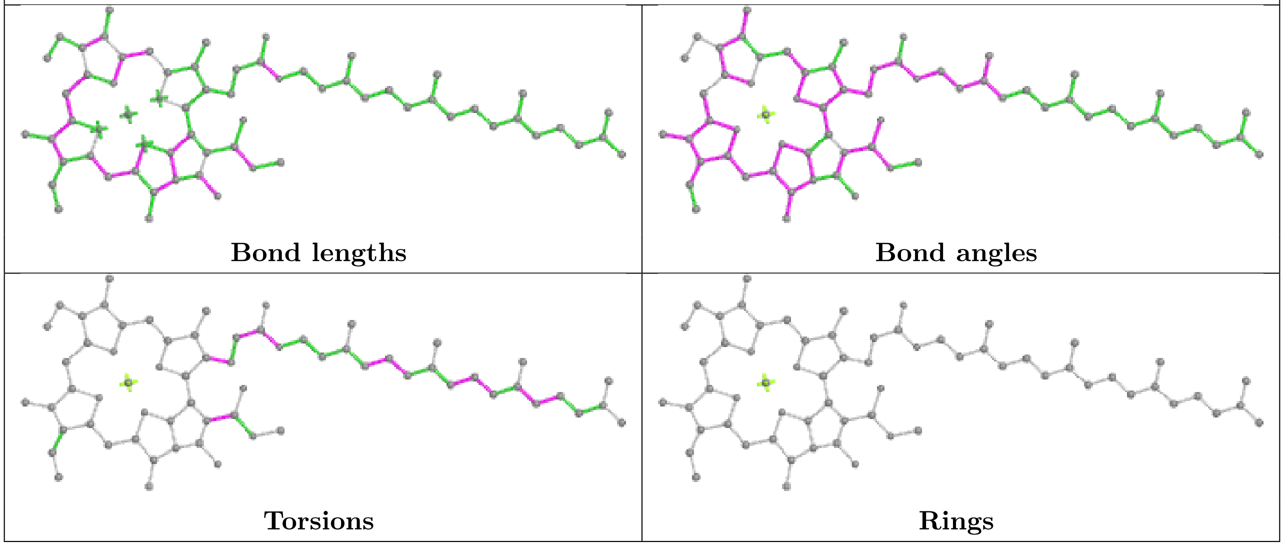


Bond lengths Bond angles

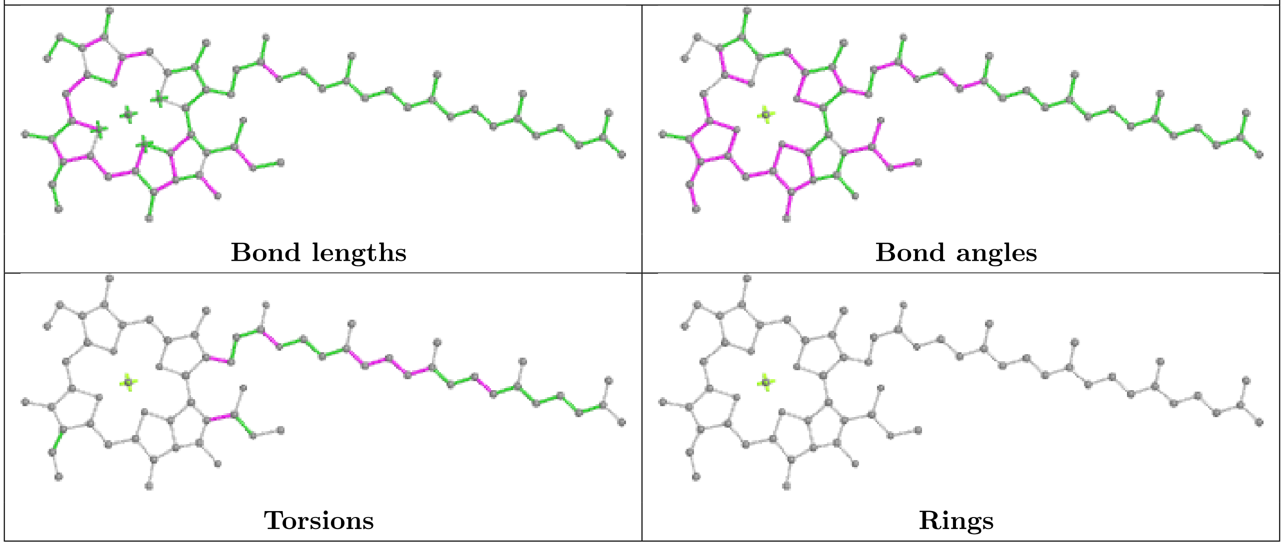


Torsions Rings

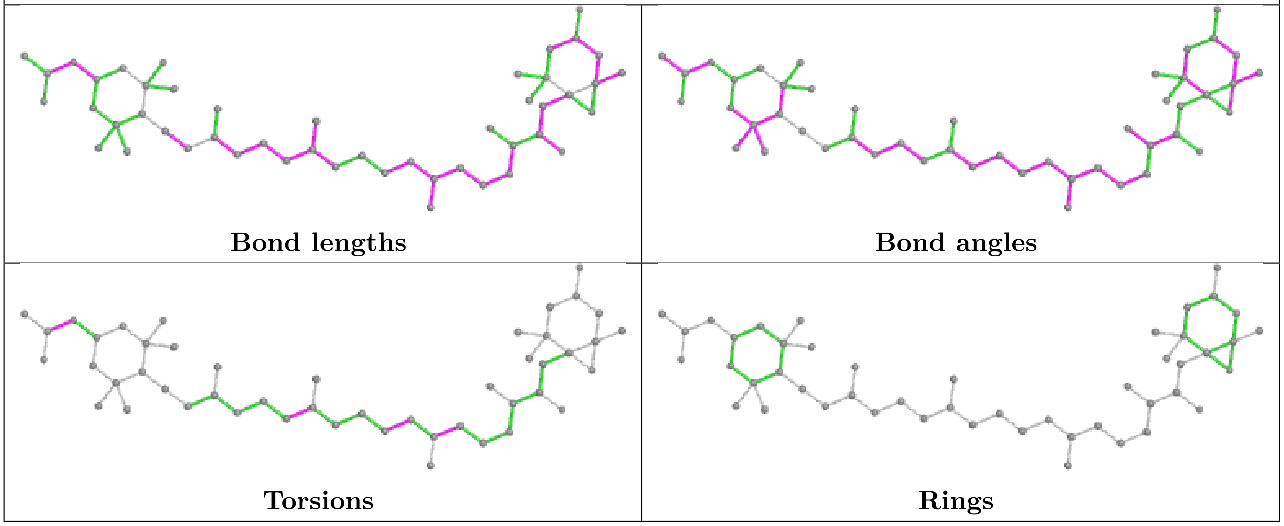
Ligand CLA 19 303


Bond lengths
Bond angles
Torsions
Rings

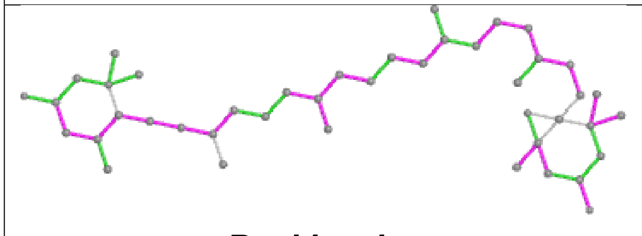
Ligand CLA 13 309


Bond lengths
Bond angles
Torsions
Rings

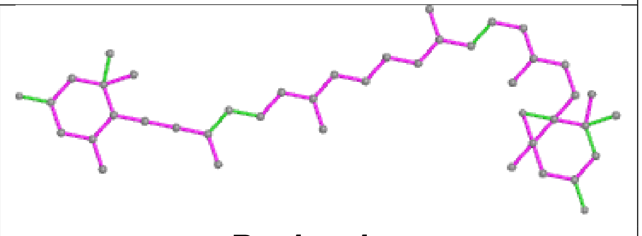
Ligand A86 17 321


Bond lengths
Bond angles
Torsions
Rings

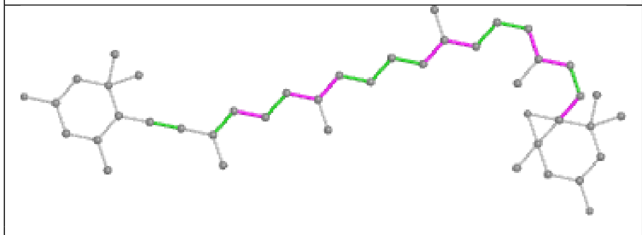
Ligand DD6 20 314



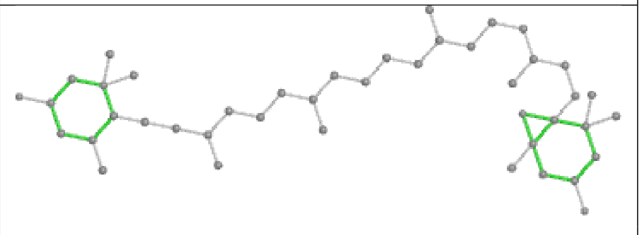
Bond lengths



Bond angles

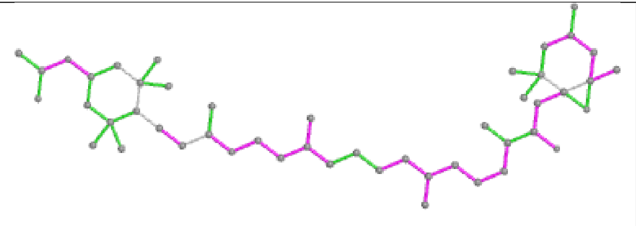


Torsions

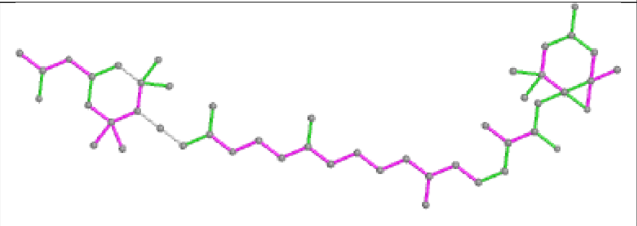


Rings

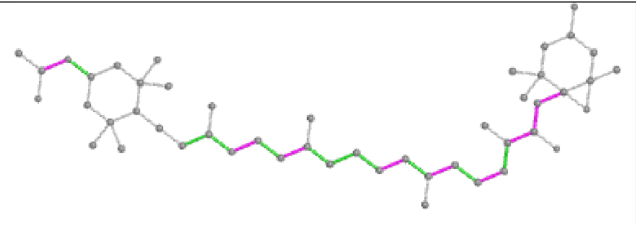
Ligand A86 18 313



Bond lengths



Bond angles



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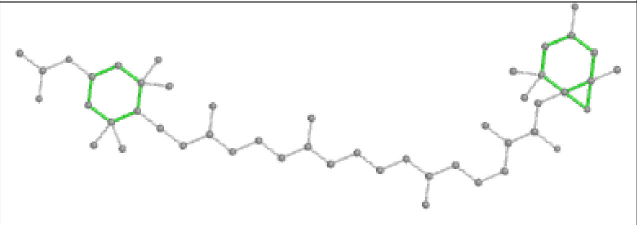
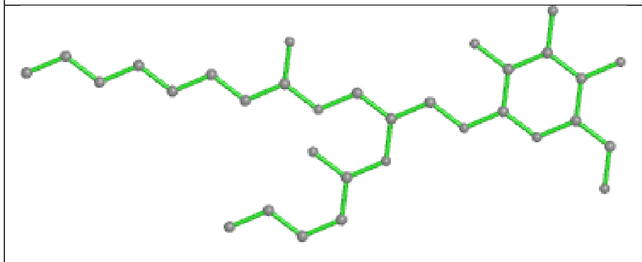
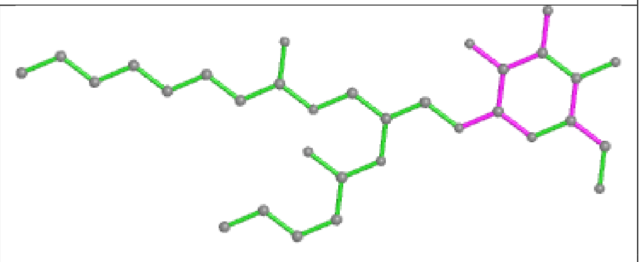


Rings

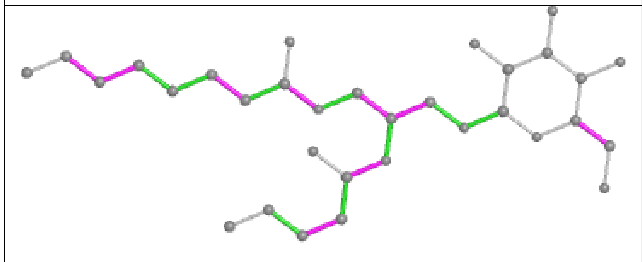
Ligand LMG 11 316



Bond lengths



Bond angles



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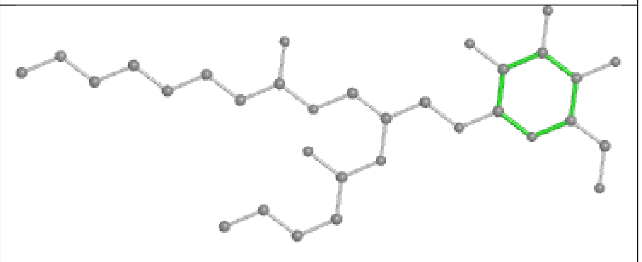
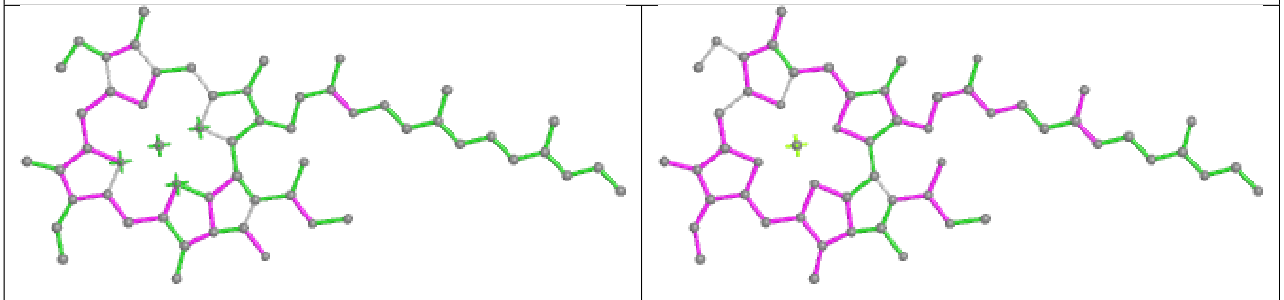
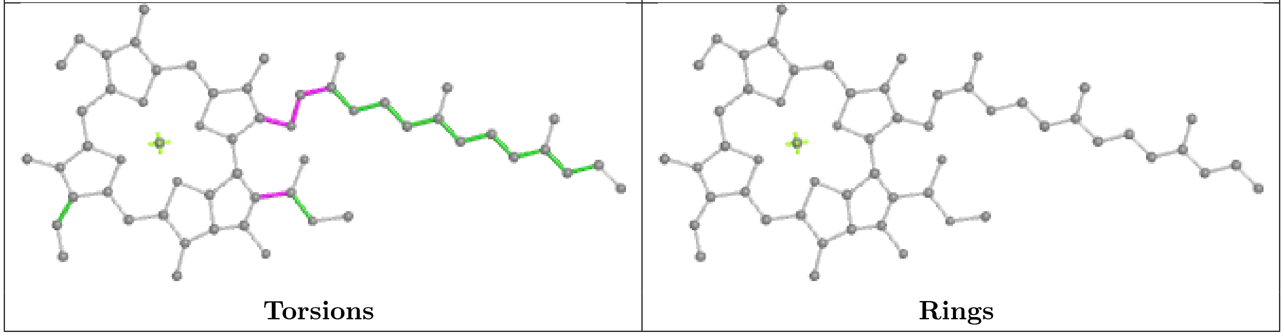


Rings

Ligand CLA 14 303

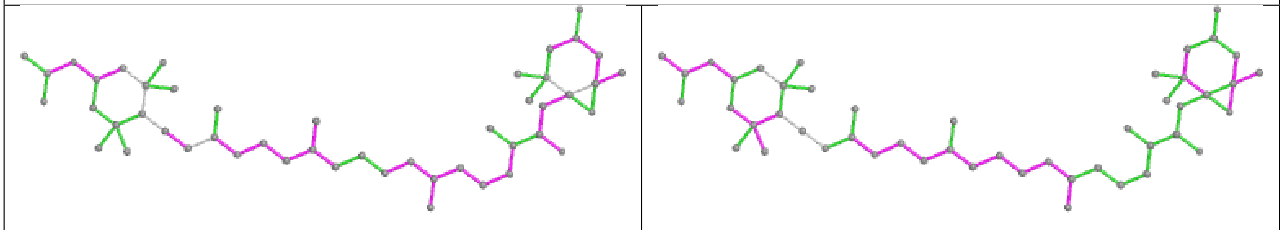


Bond lengths Bond angles

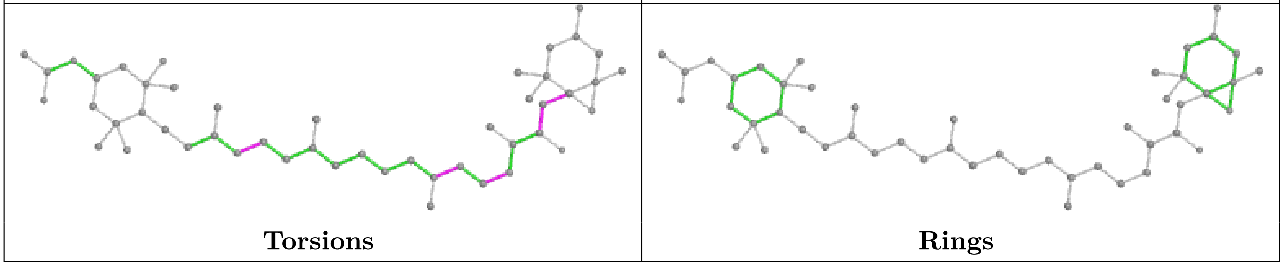


Torsions Rings

Ligand A86 20 311

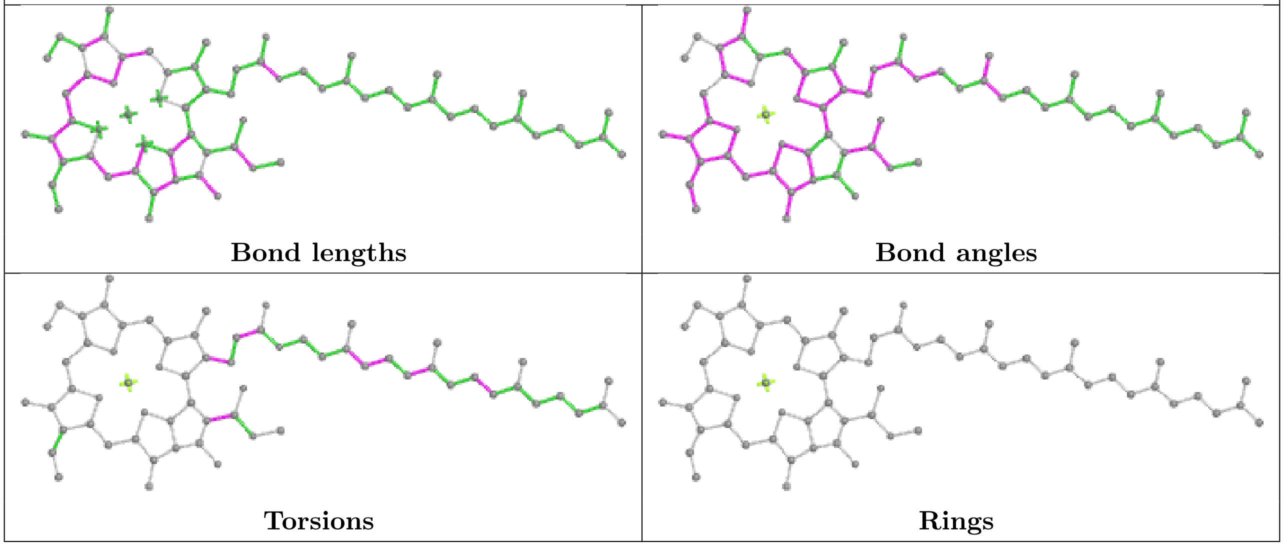


Bond lengths Bond angles



Torsions Rings

Ligand CLA 12 305



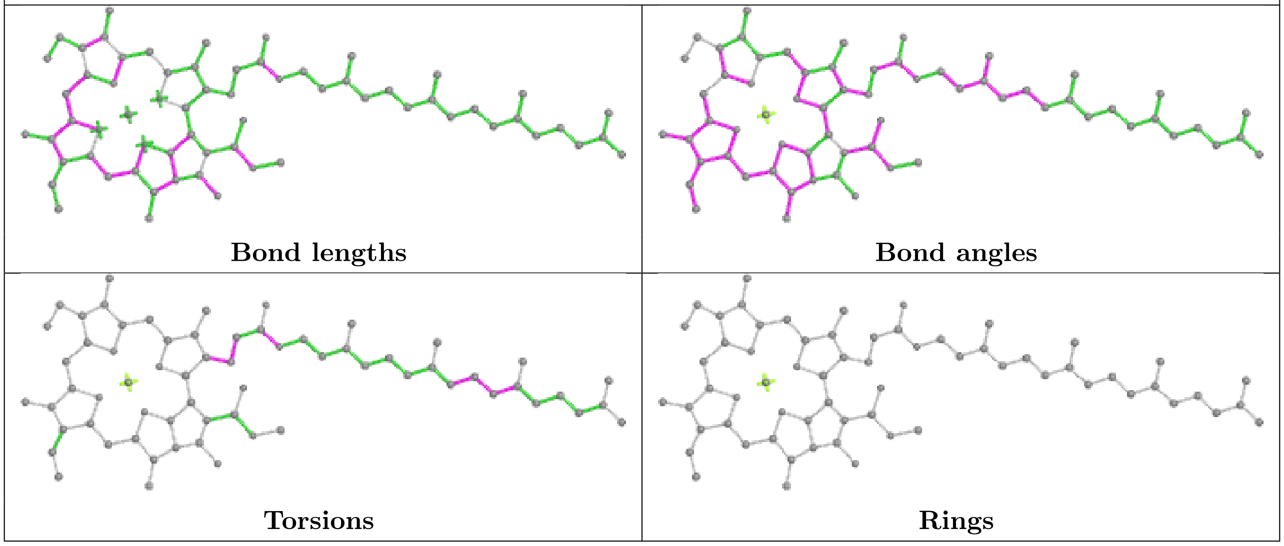
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA 19 306



Bond lengths

Bond angles

Torsions

Rings

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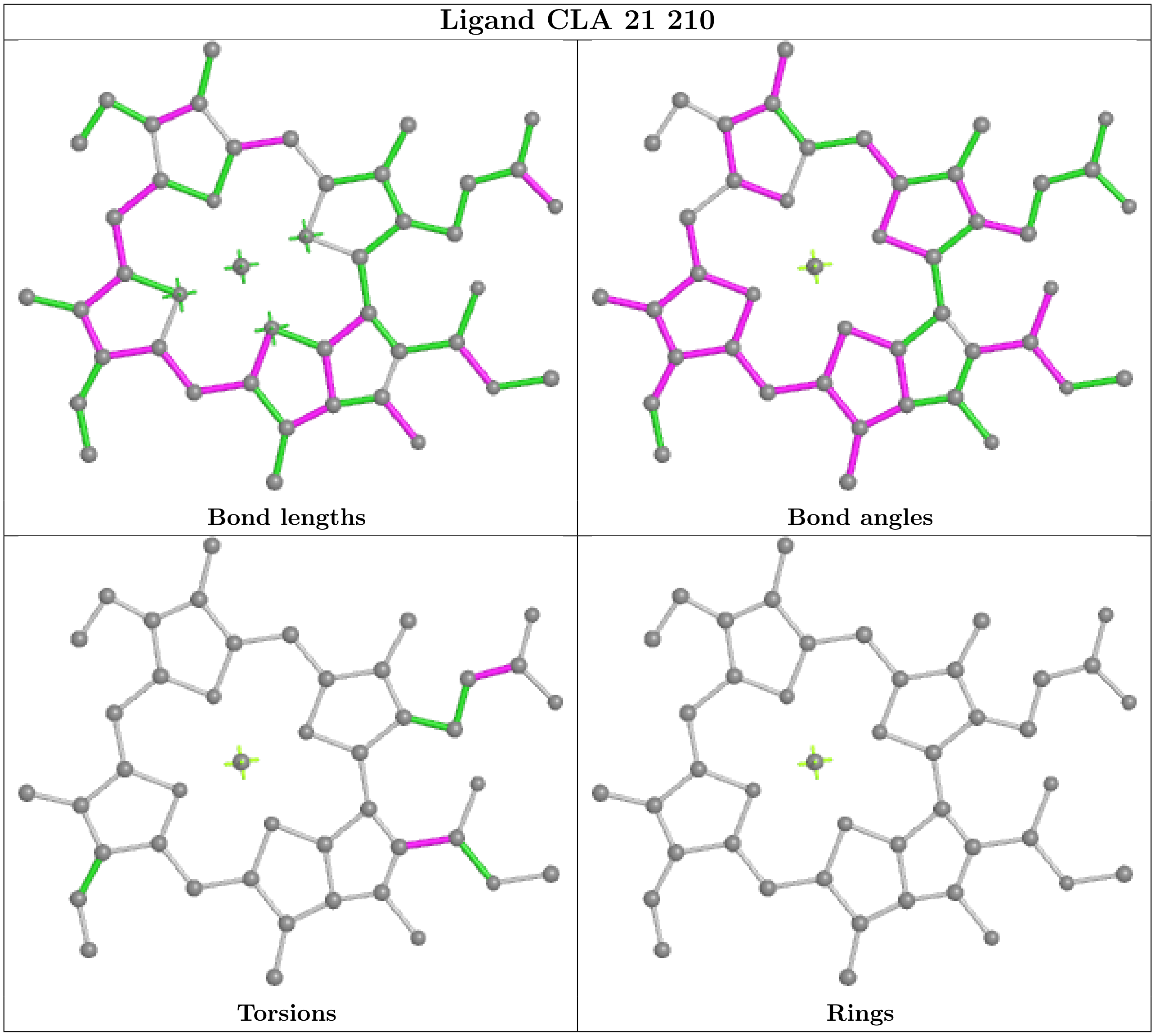

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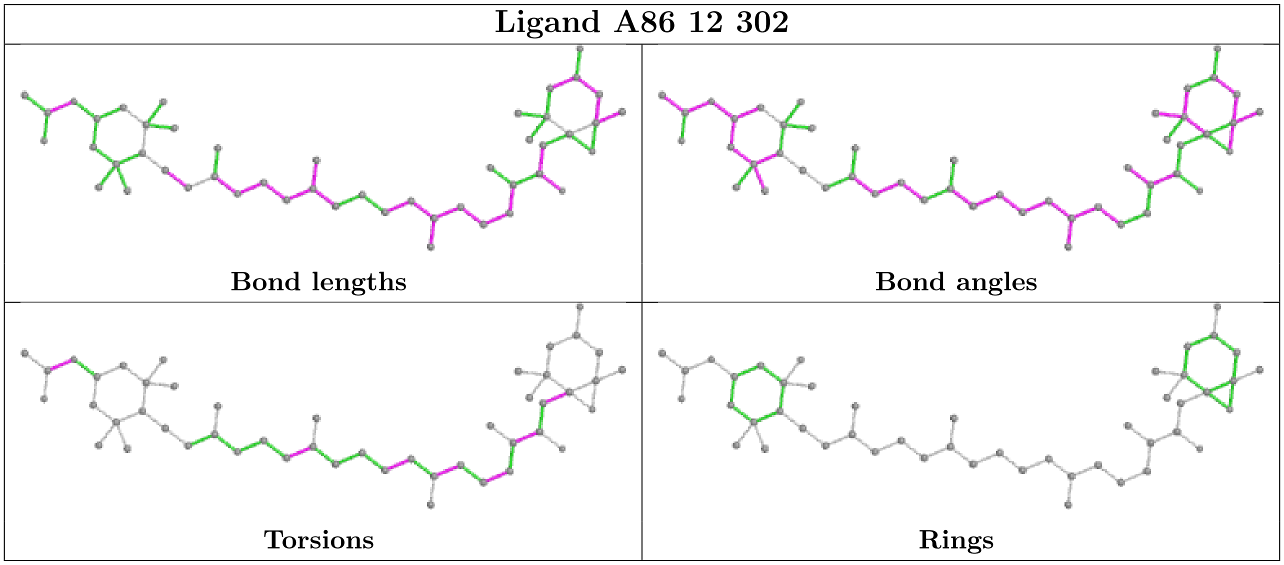

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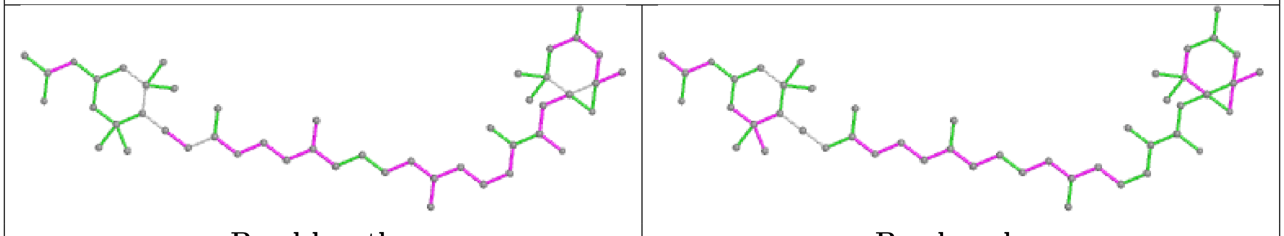
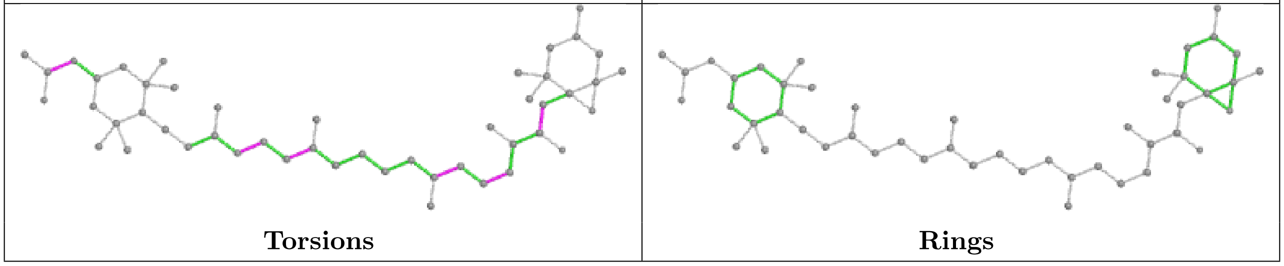


Bond lengths

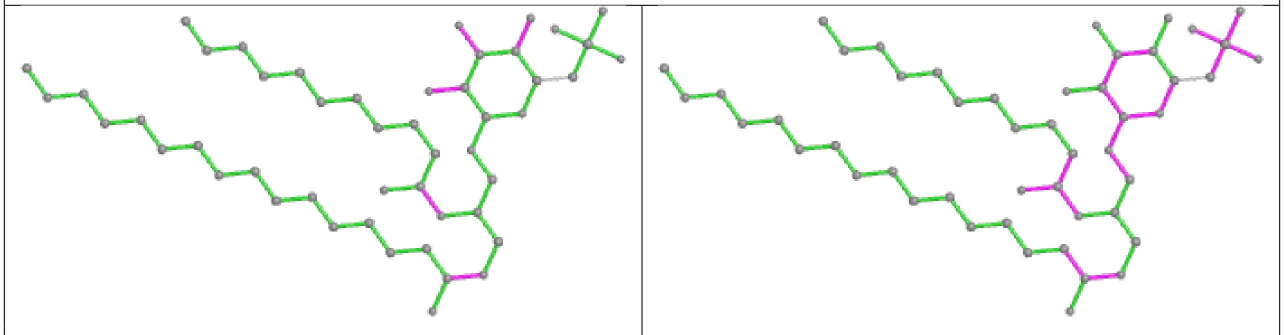
Bond angles



Torsions

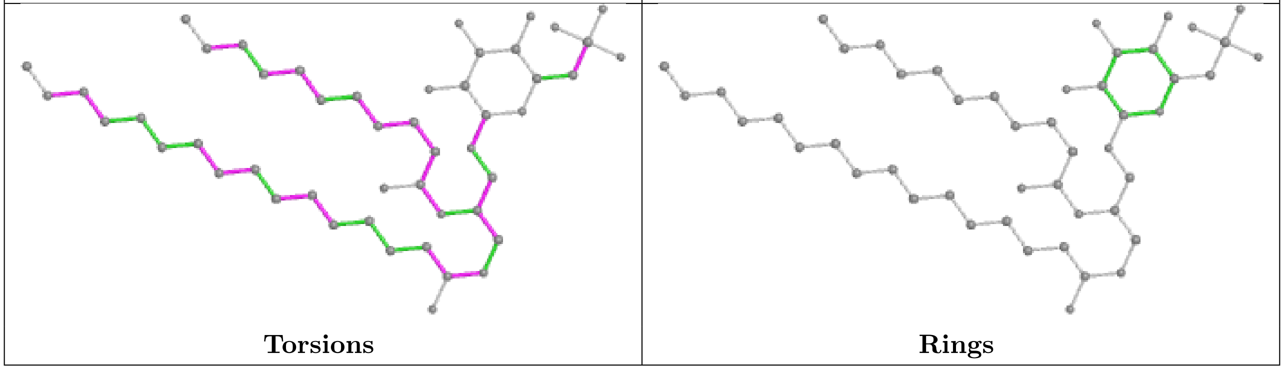
Rings

Ligand SQD 17 301



Bond lengths

Bond angles



Torsions

Rings

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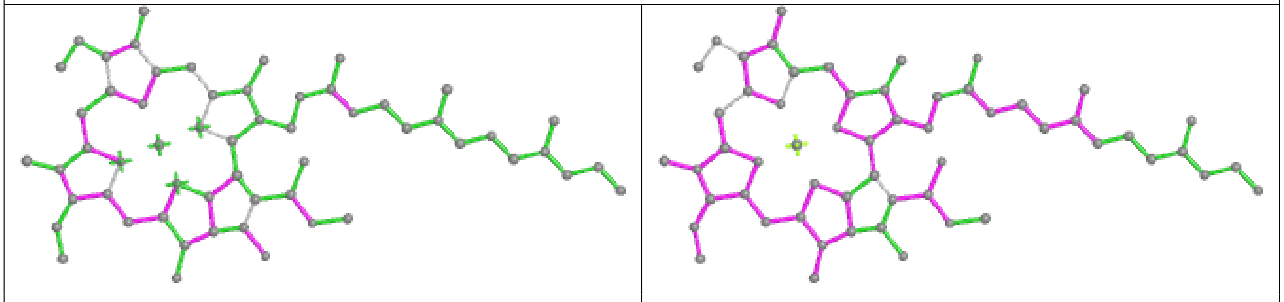
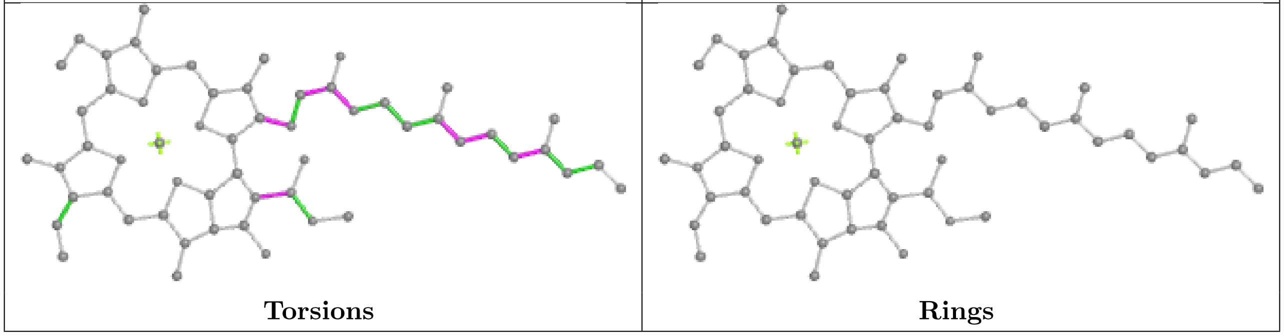


Bond lengths

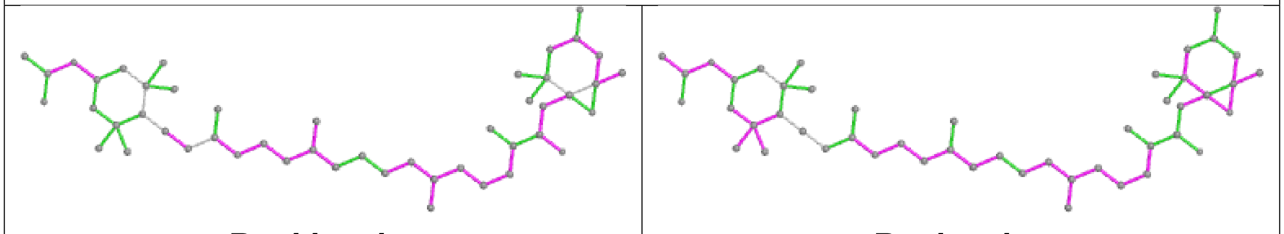
Bond angles



Torsions

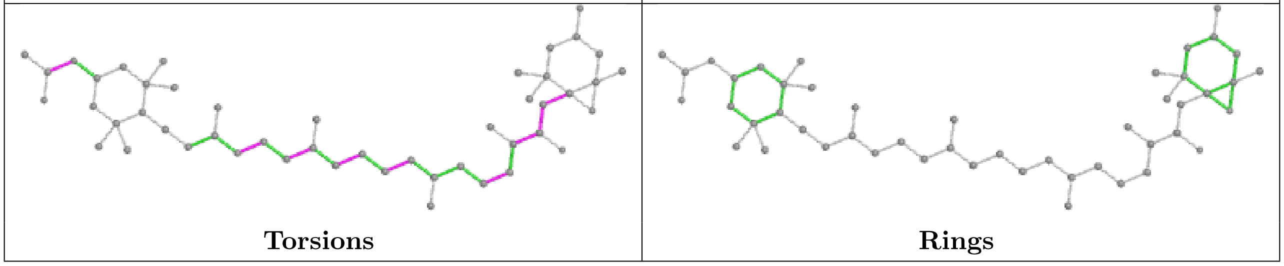
Rings

Ligand A86 20 313



Bond lengths

Bond angles



Torsions

Rings

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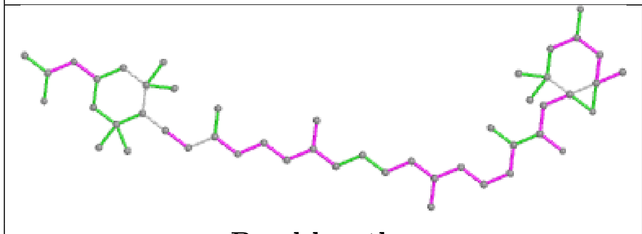
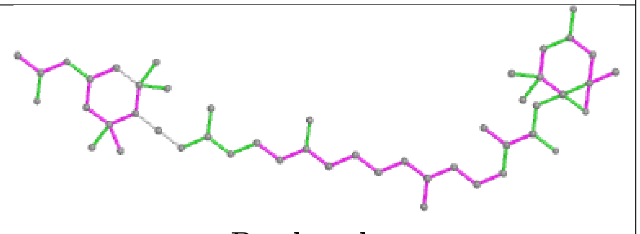
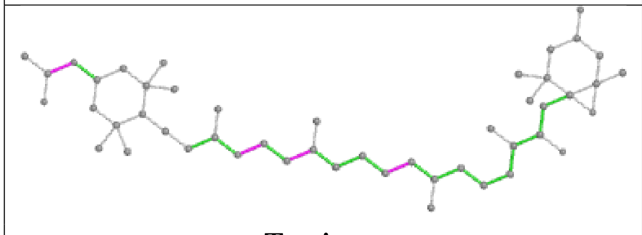

Bond lengths


Bond angles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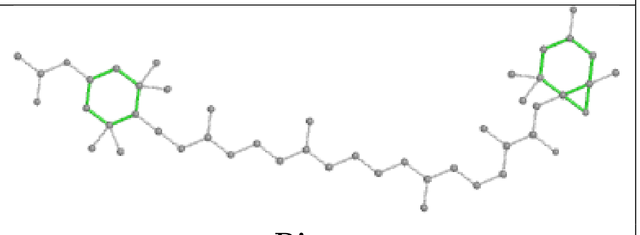
Rings

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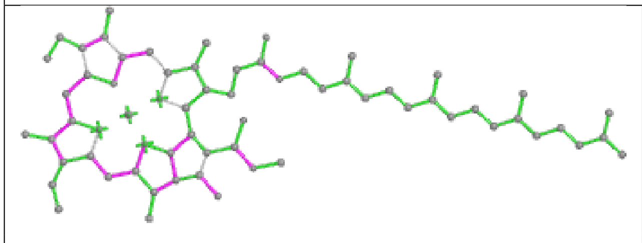
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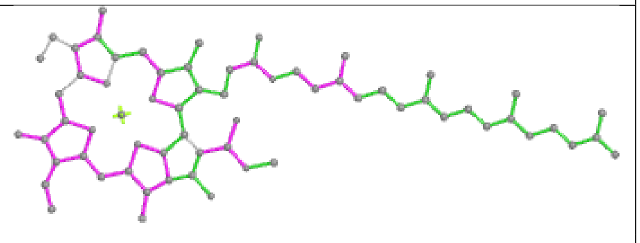
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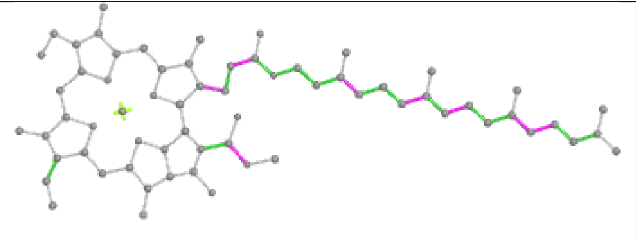
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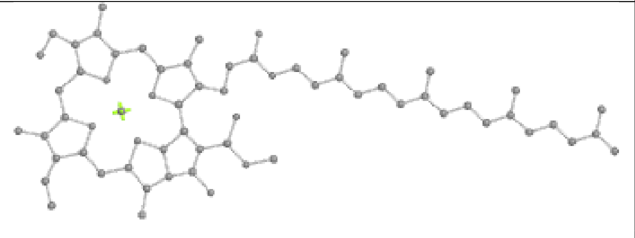
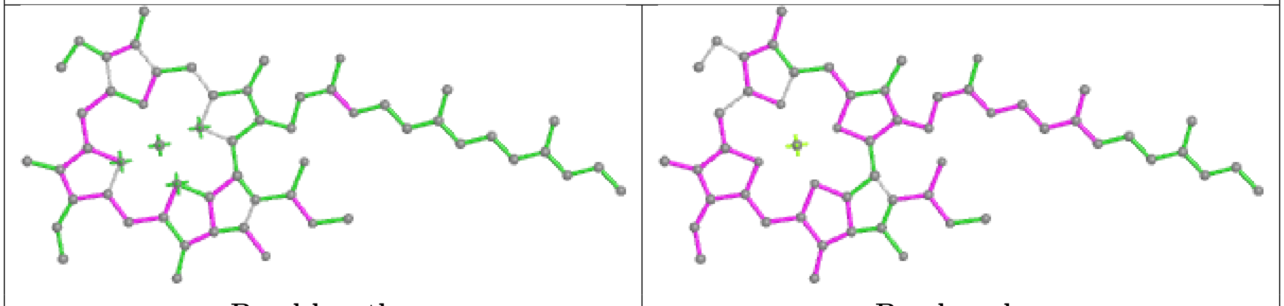
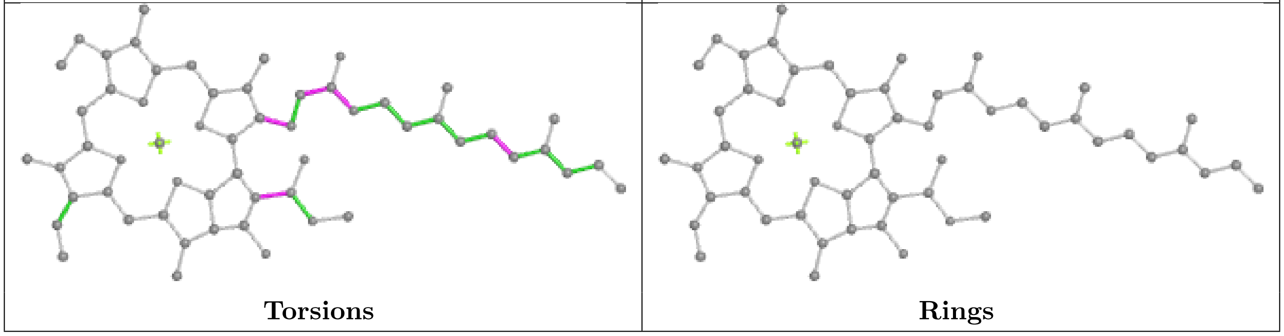

Rings

Ligand CLA 15 303



Bond lengths

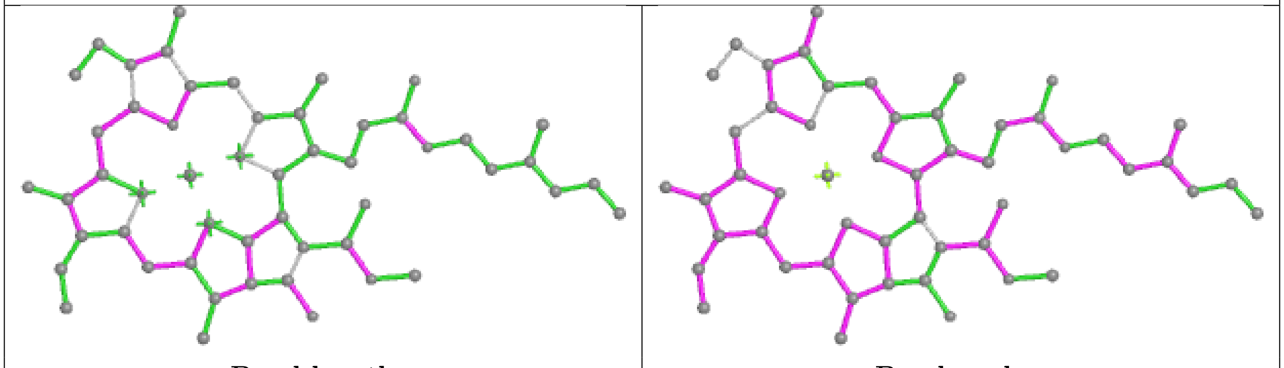
Bond angles



Torsions

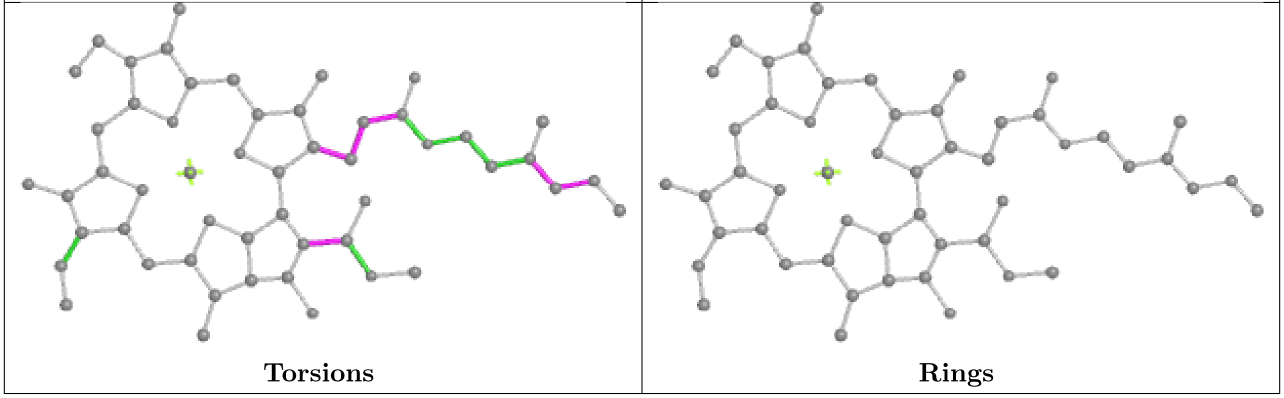
Rings

Ligand CLA 17 307



Bond lengths

Bond angles



Torsions

Rings

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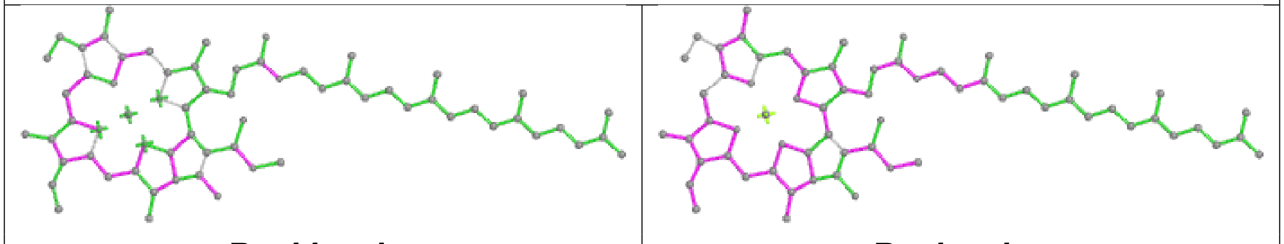
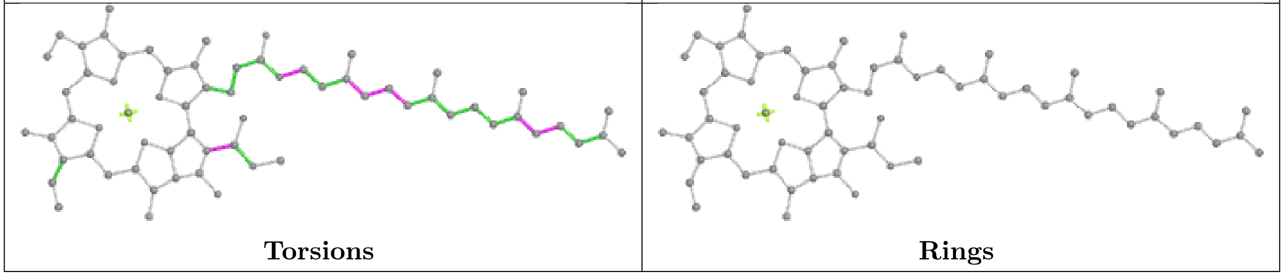


Bond lengths

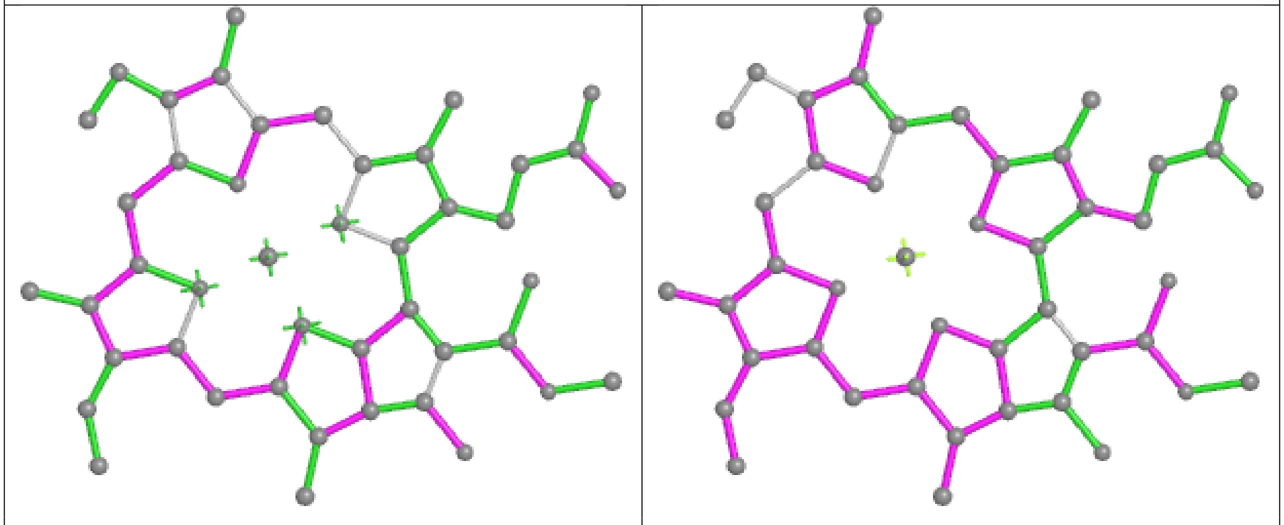
Bond angles



Torsions

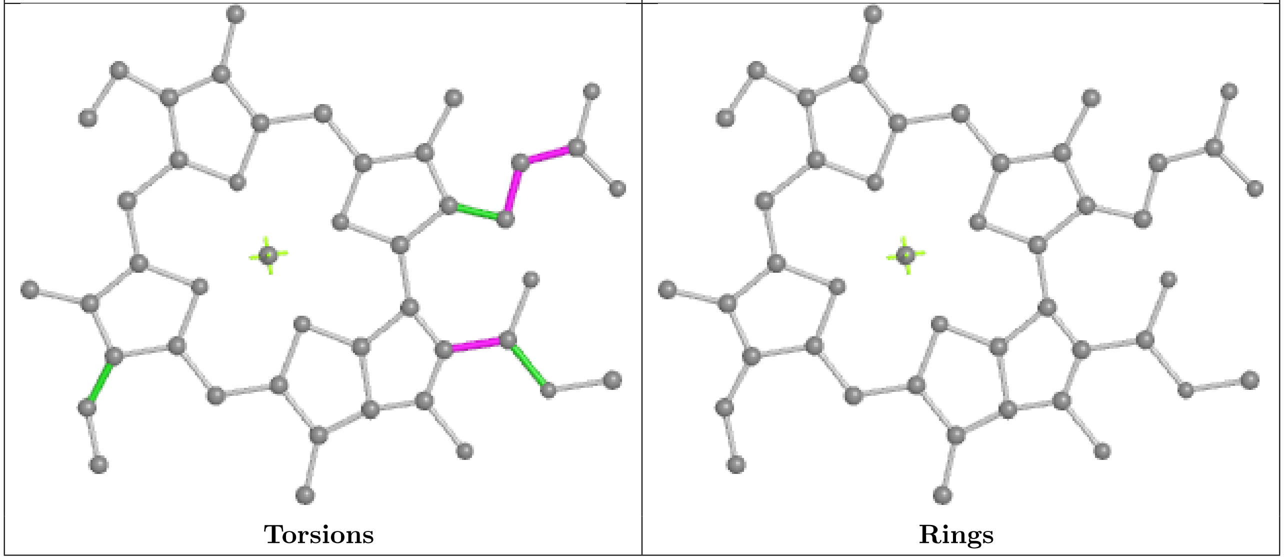
Rings

Ligand CLA 18 305



Bond lengths

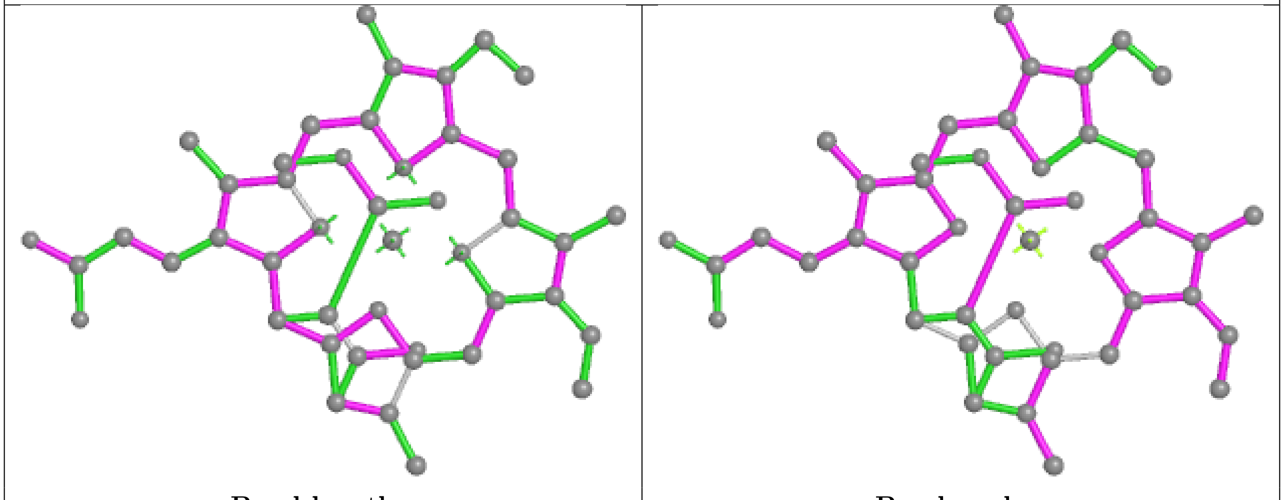
Bond angles



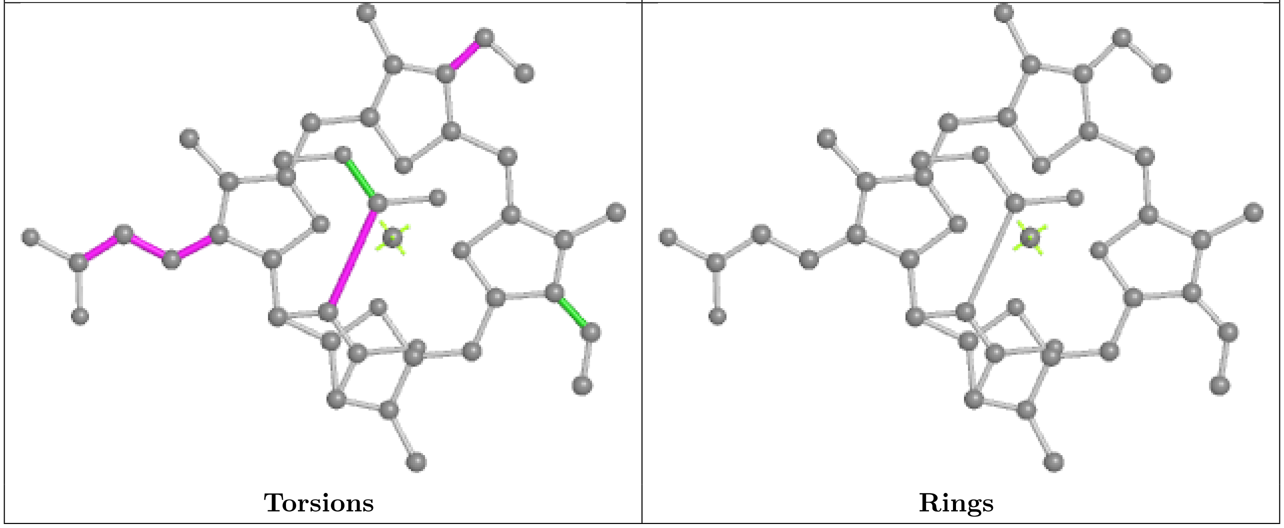
Torsions

Rings

Ligand KC1 17 309

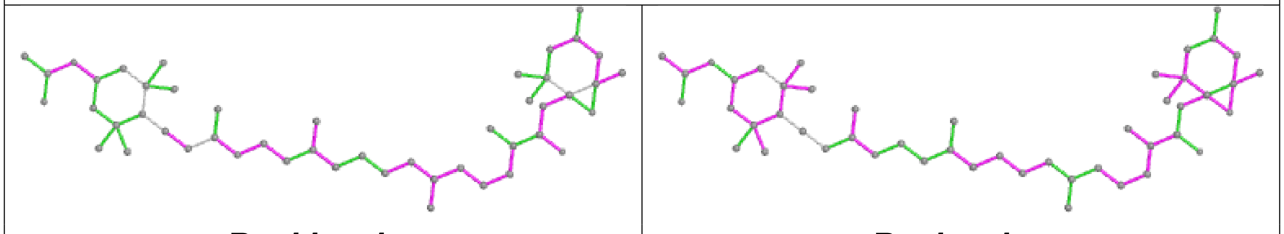


Bond lengths **Bond angles**

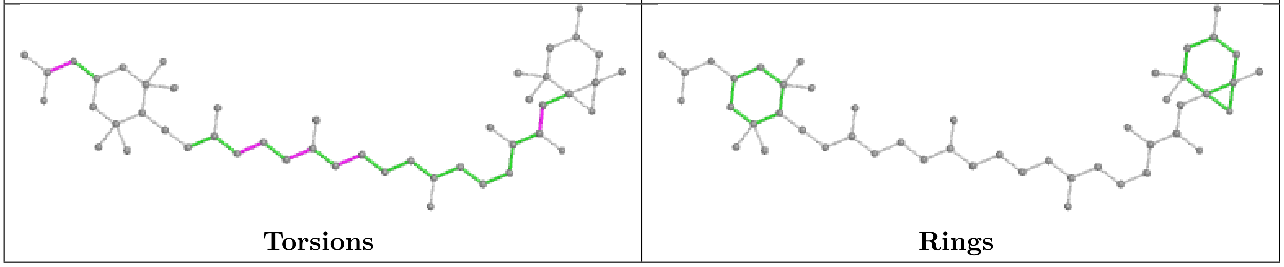


Torsions **Rings**

Ligand A86 11 310



Bond lengths **Bond angles**



Torsions **Rings**

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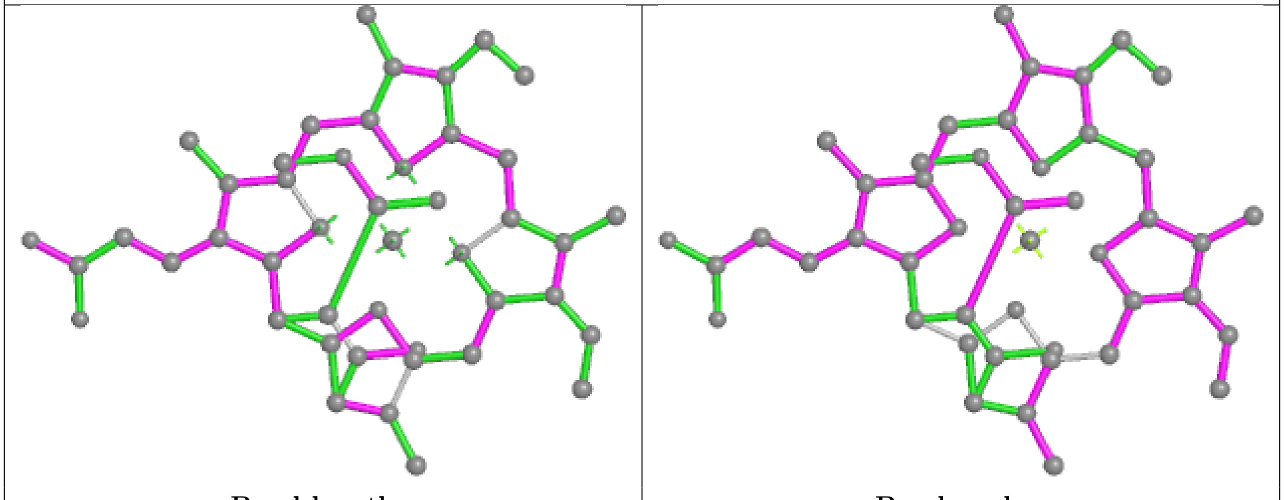
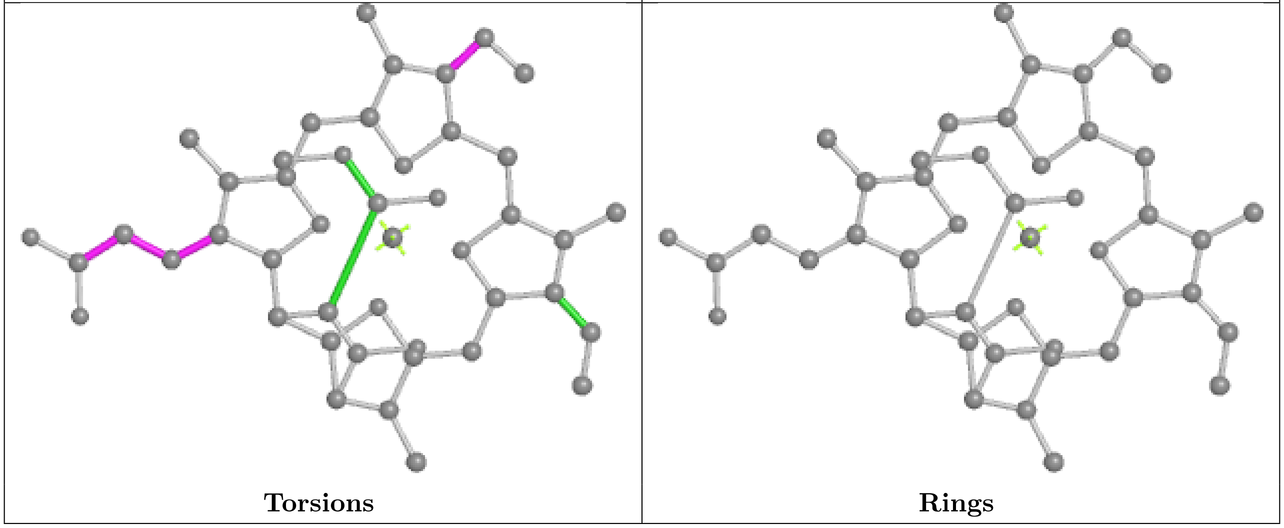
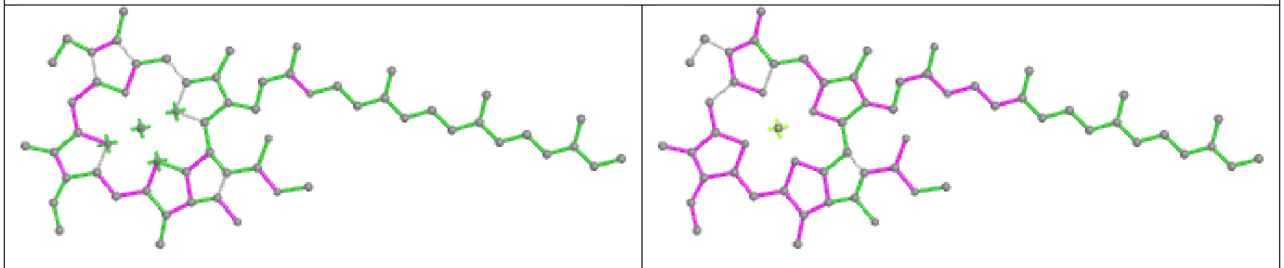


Bond lengths Bond angles

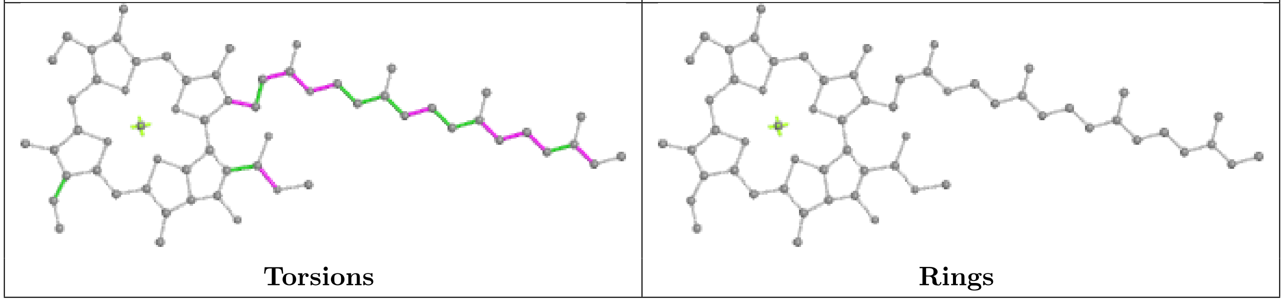


Torsions Rings

Ligand CLA 16 307

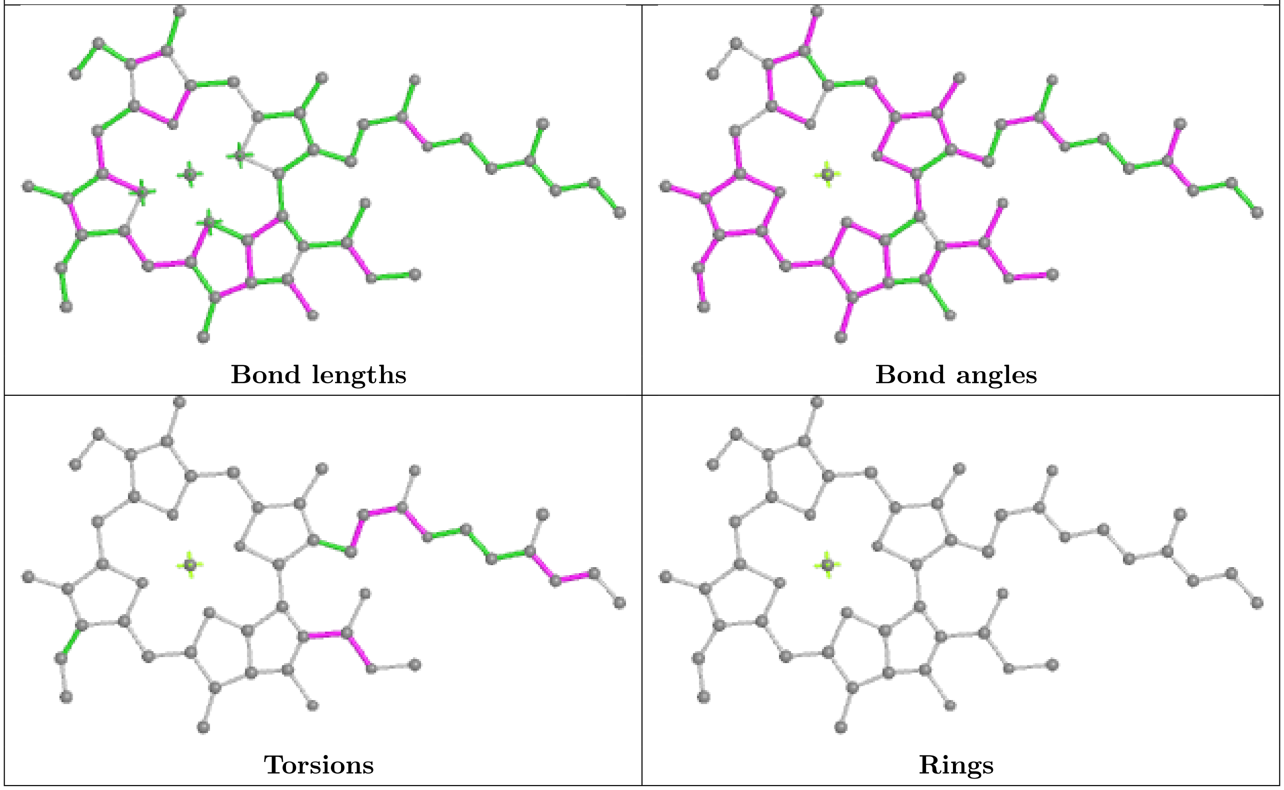


Bond lengths Bond angles



Torsions Rings

Ligand CLA 13 308



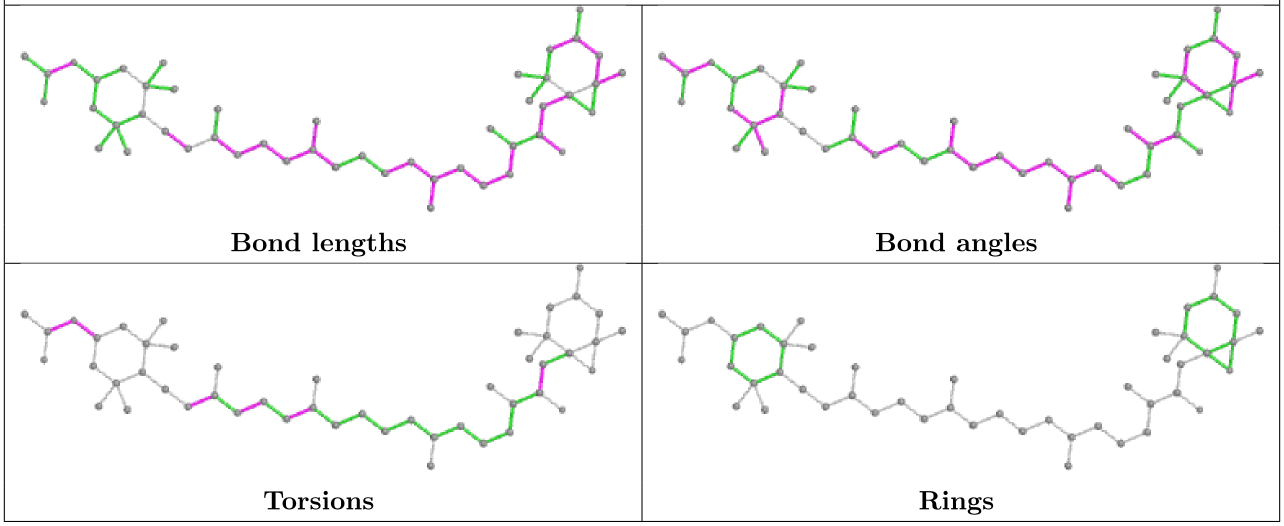
Bond lengths

Bond angles

Torsions

Rings

Ligand A86 15 313



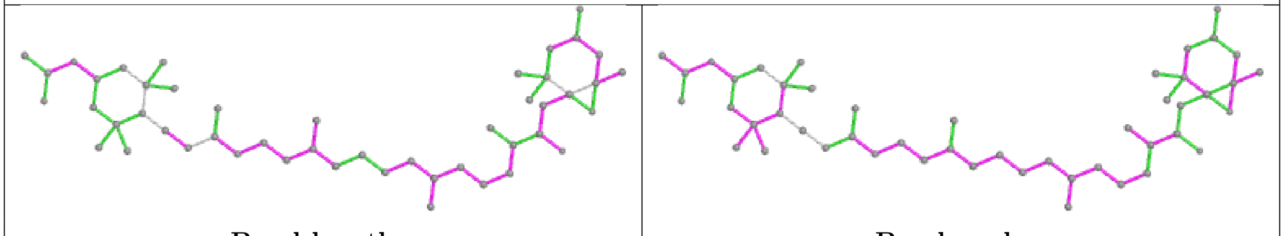
Bond lengths

Bond angles

Torsions

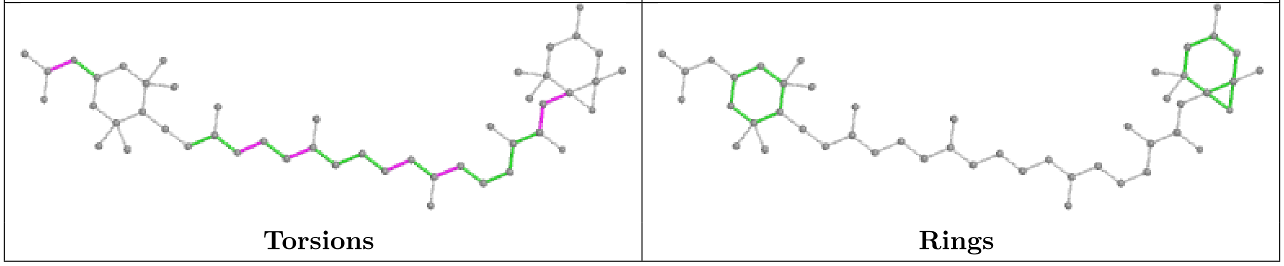
Rings

Ligand A86 12 315



Bond lengths

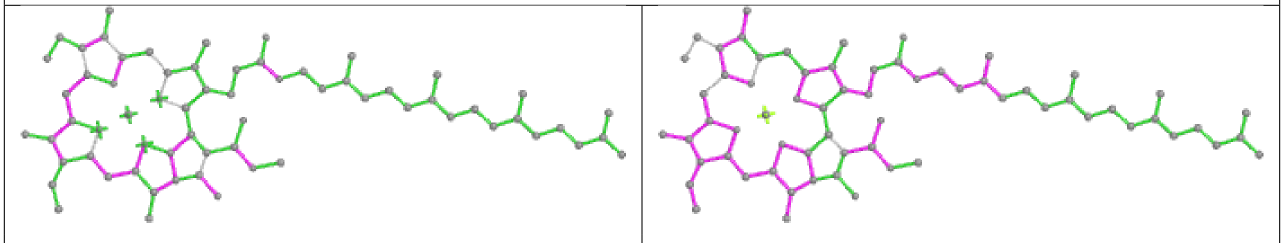
Bond angles



Torsions

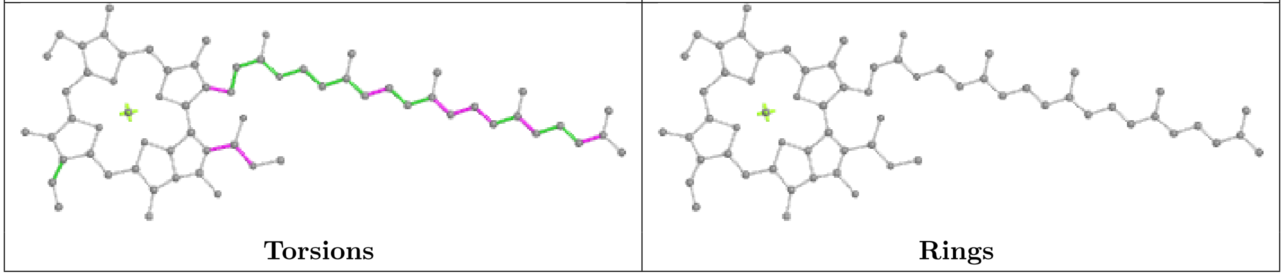
Rings

Ligand CLA 16 306



Bond lengths

Bond angles



Torsions

Rings

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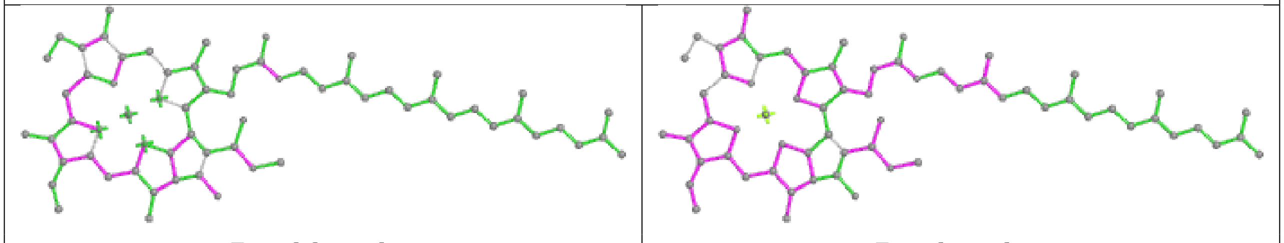
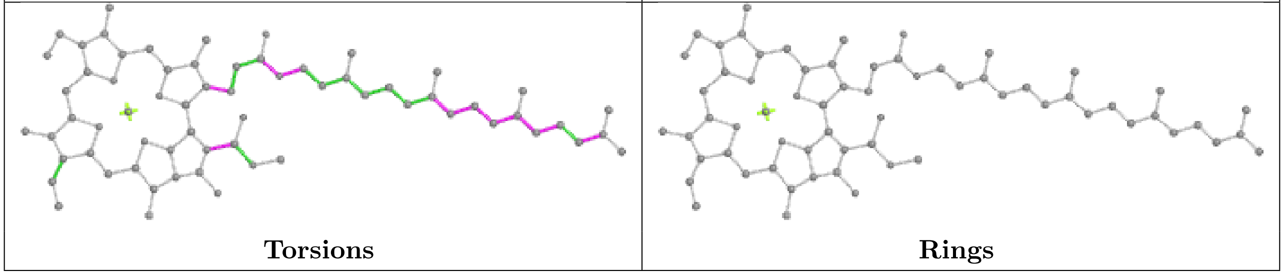


Bond lengths

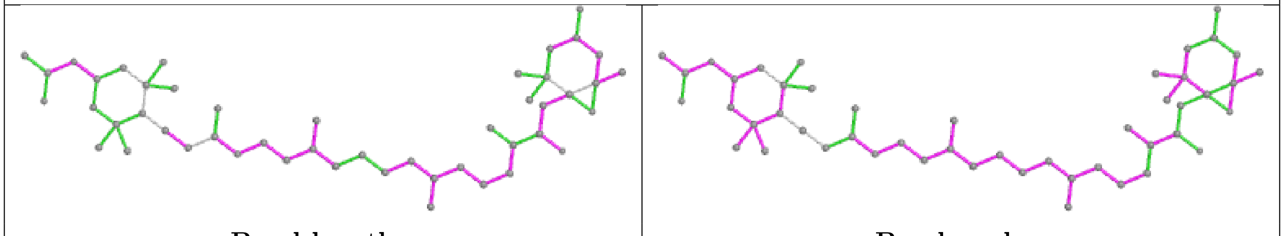
Bond angles



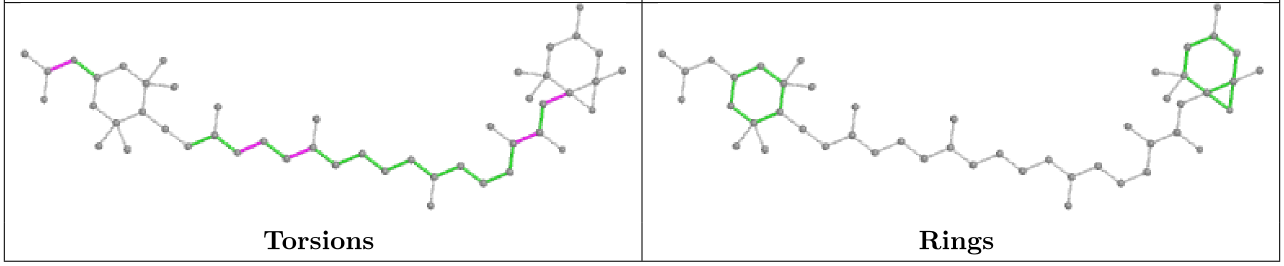
Torsions

Rings

Ligand A86 11 313



Bond lengths Bond angles



Torsions Rings

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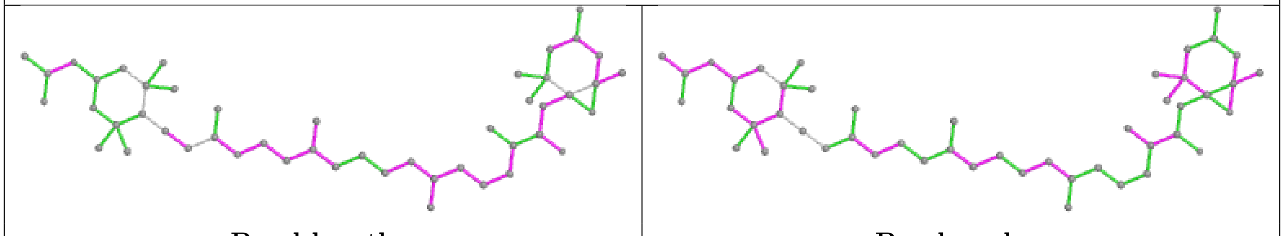
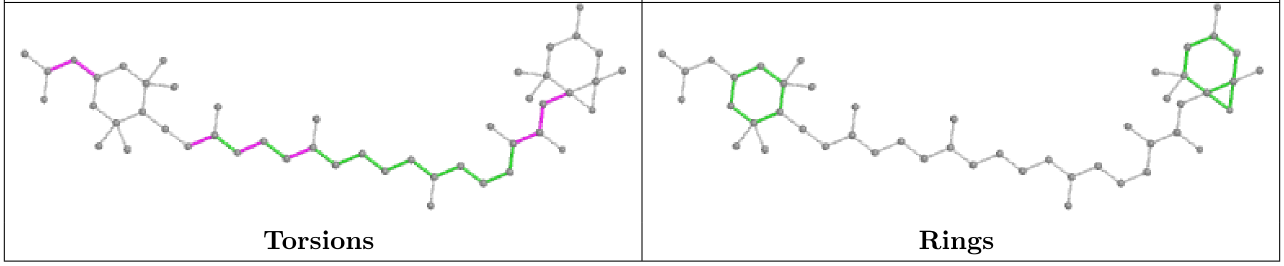


Bond lengths Bond angles



Torsions Rings

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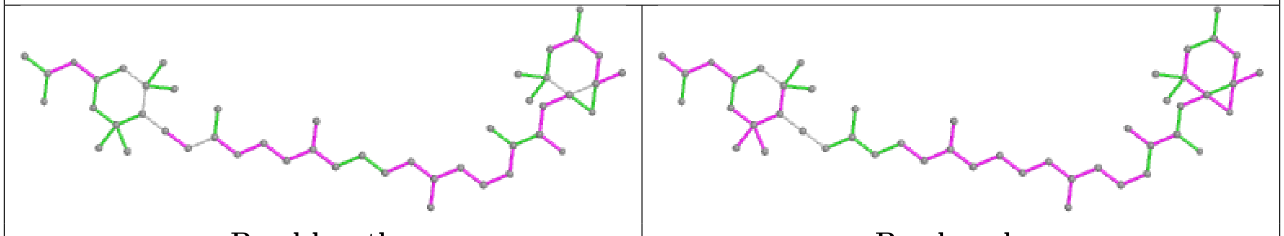
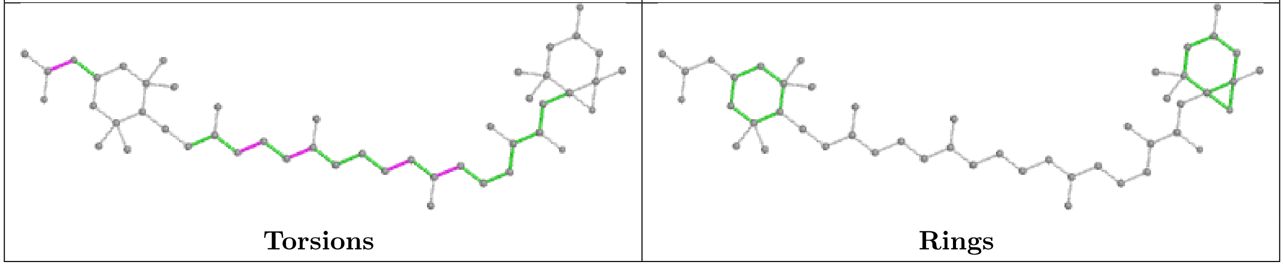


Bond lengths Bond angles



Torsions Rings

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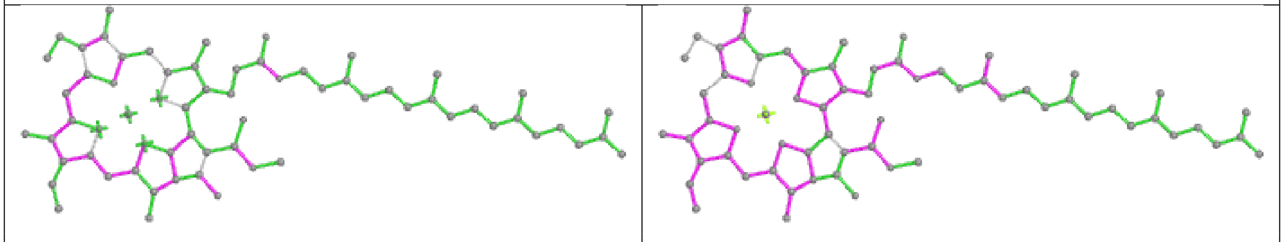
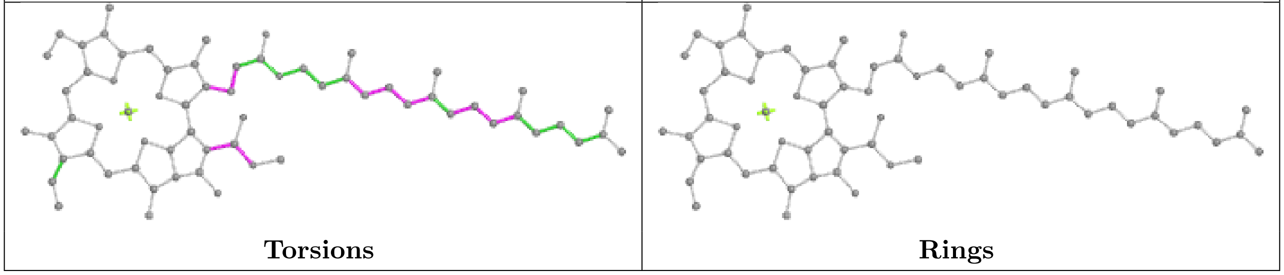


Bond lengths

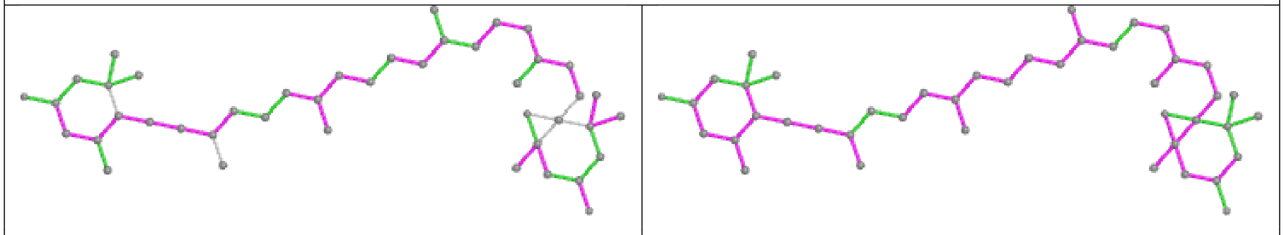
Bond angles



Torsions

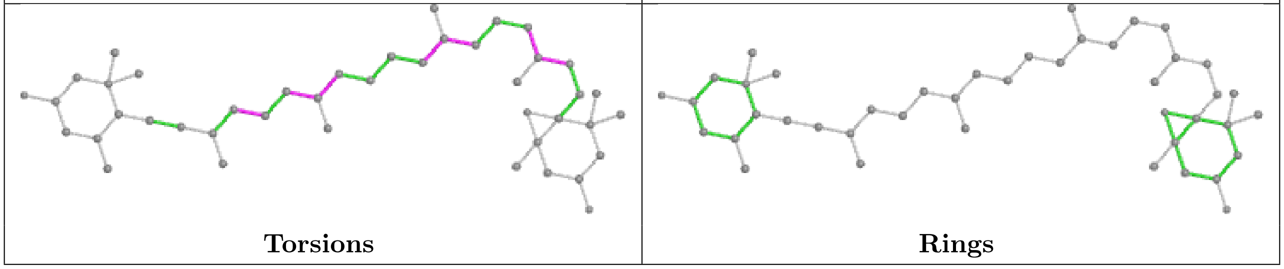
Rings

Ligand DD6 16 312



Bond lengths

Bond angles



Torsions

Rings

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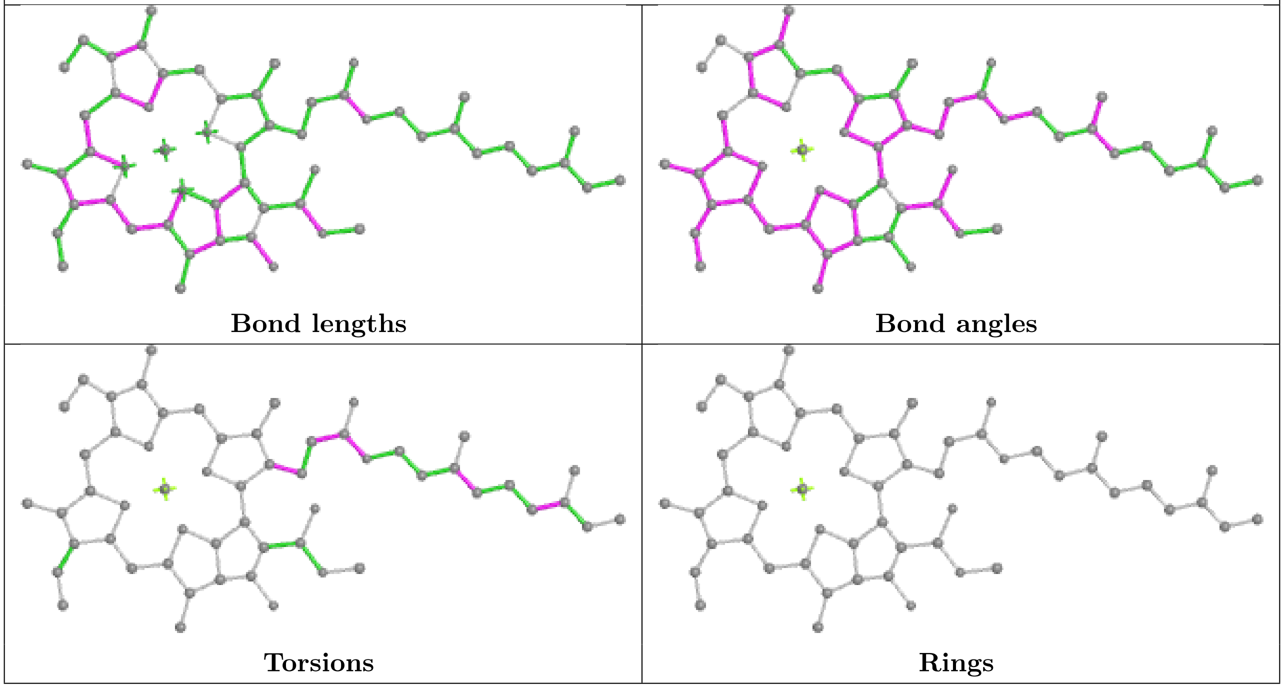
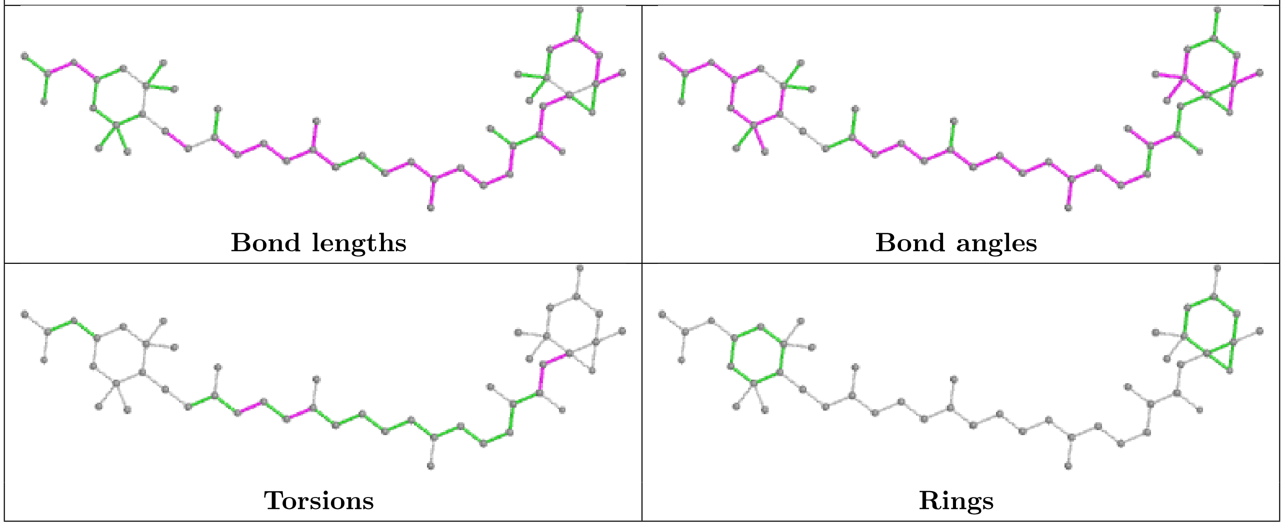

Bond lengths
Bond angles
Torsions
Rings

Ligand A86 12 312


Bond lengths
Bond angles
Torsions
Rings

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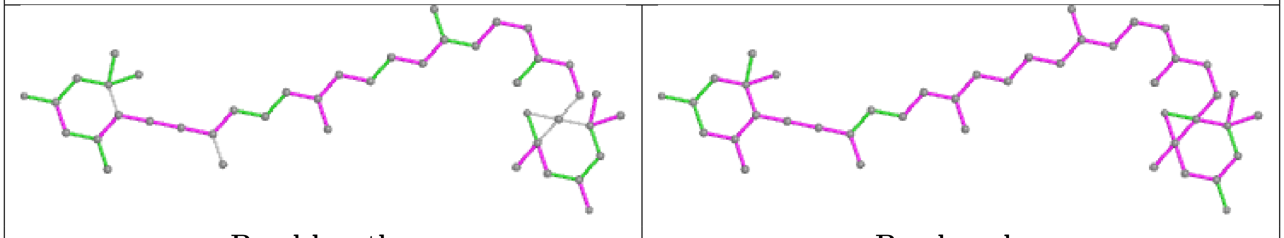
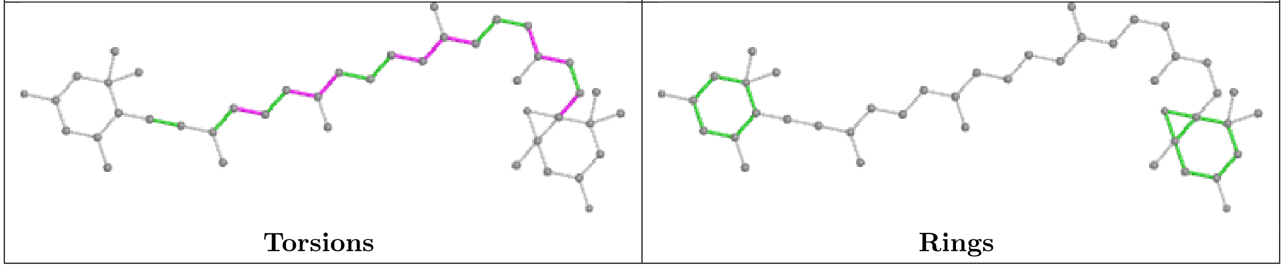
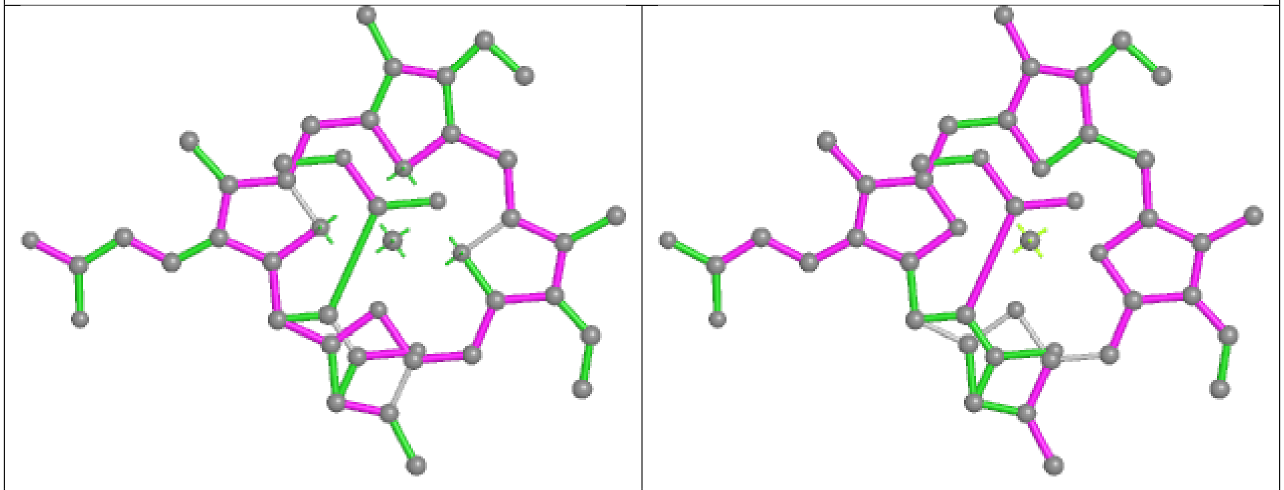


Bond lengths Bond angles

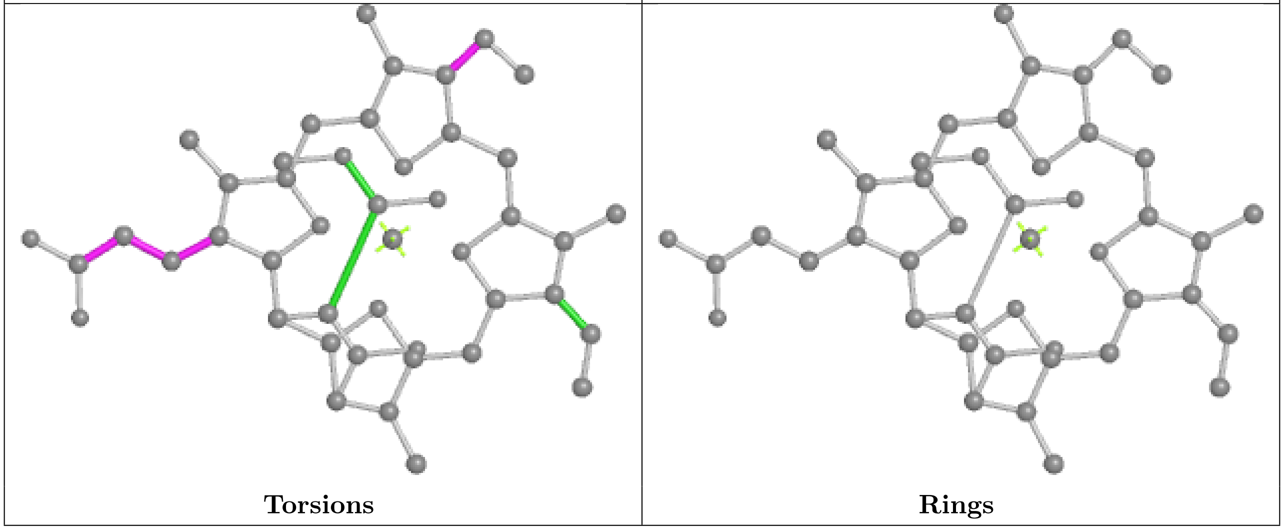


Torsions Rings

Ligand KC1 18 304



Bond lengths Bond angles



Torsions Rings

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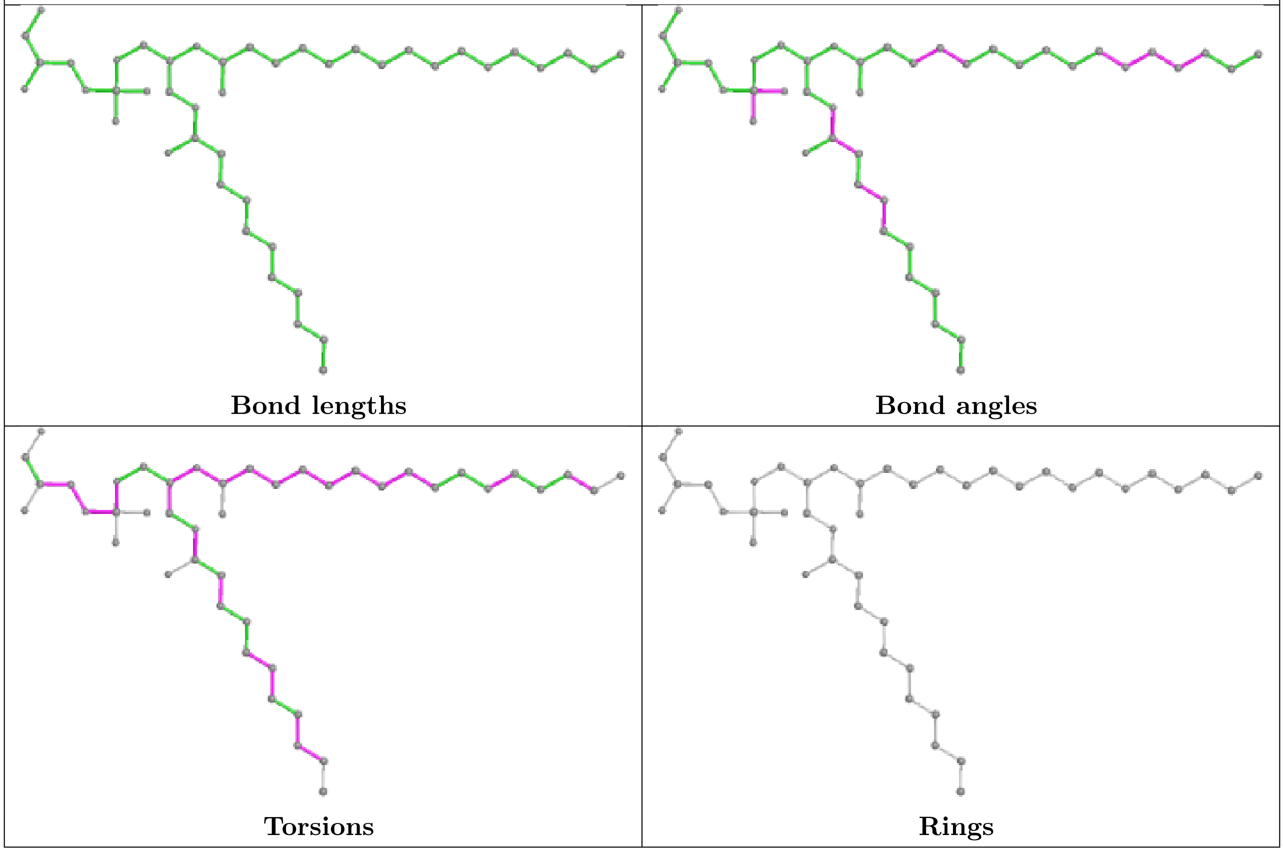

Bond lengths

Bond angles

Torsions

Rings

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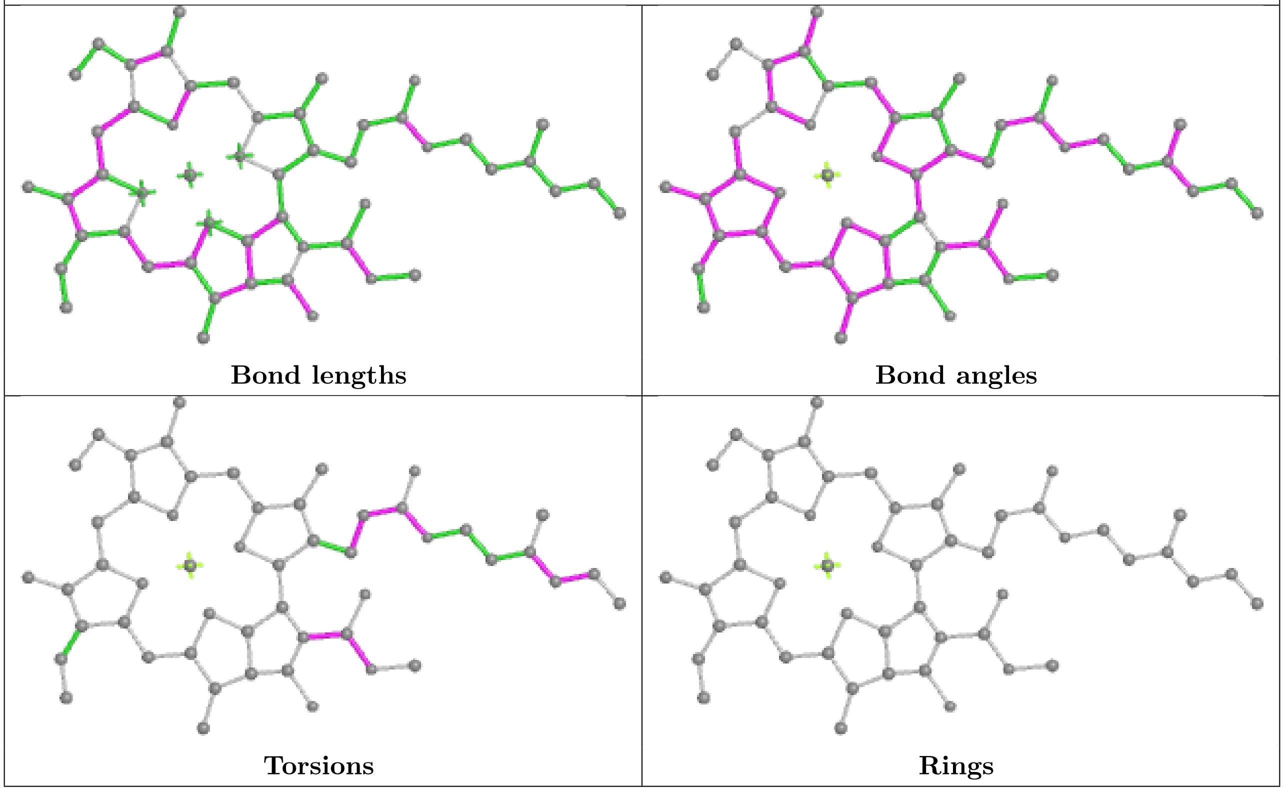


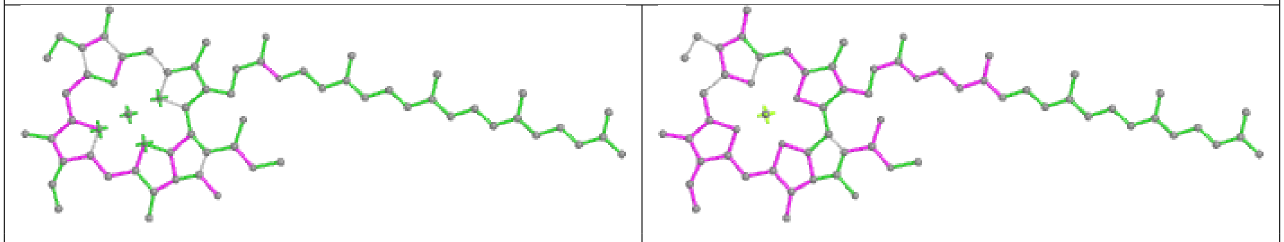
Bond lengths

Bond angles

Torsions

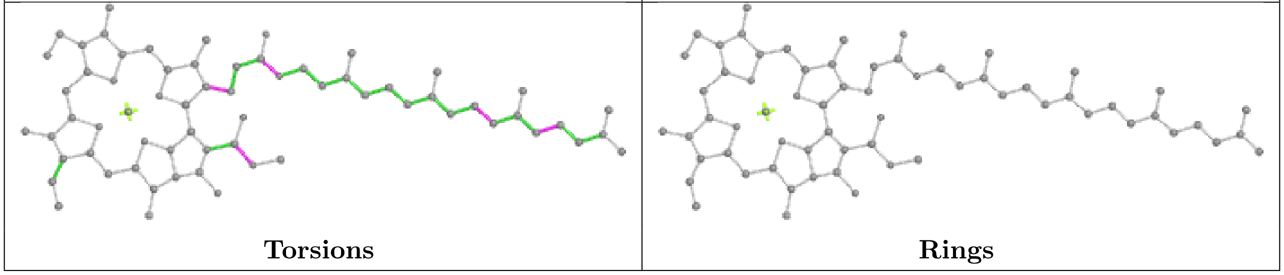
Rings

Ligand CLA 17 308



Bond lengths

Bond angles



Torsions

Rings

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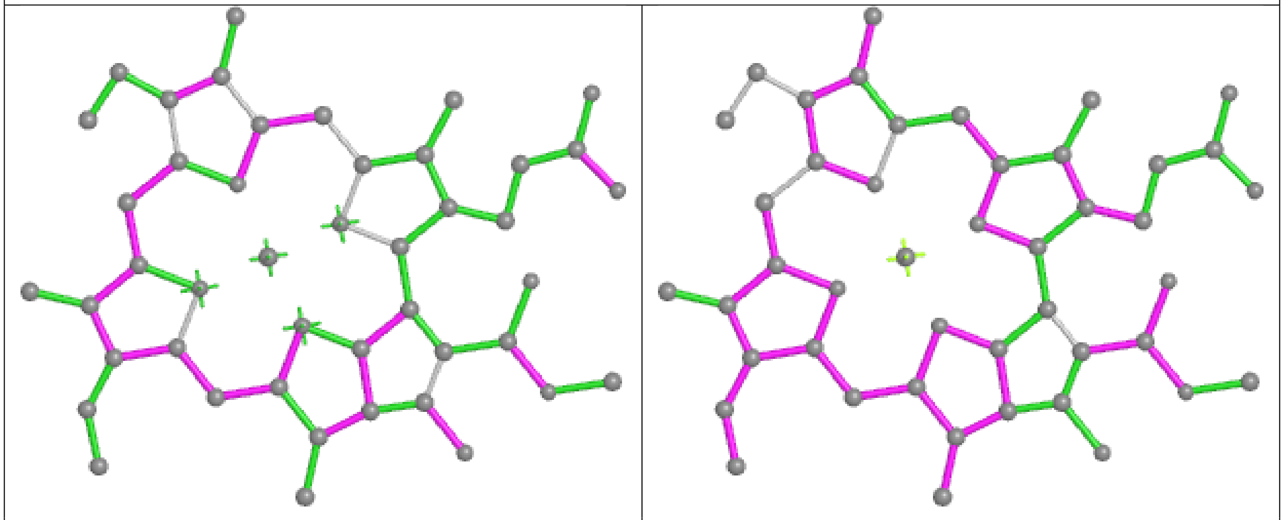
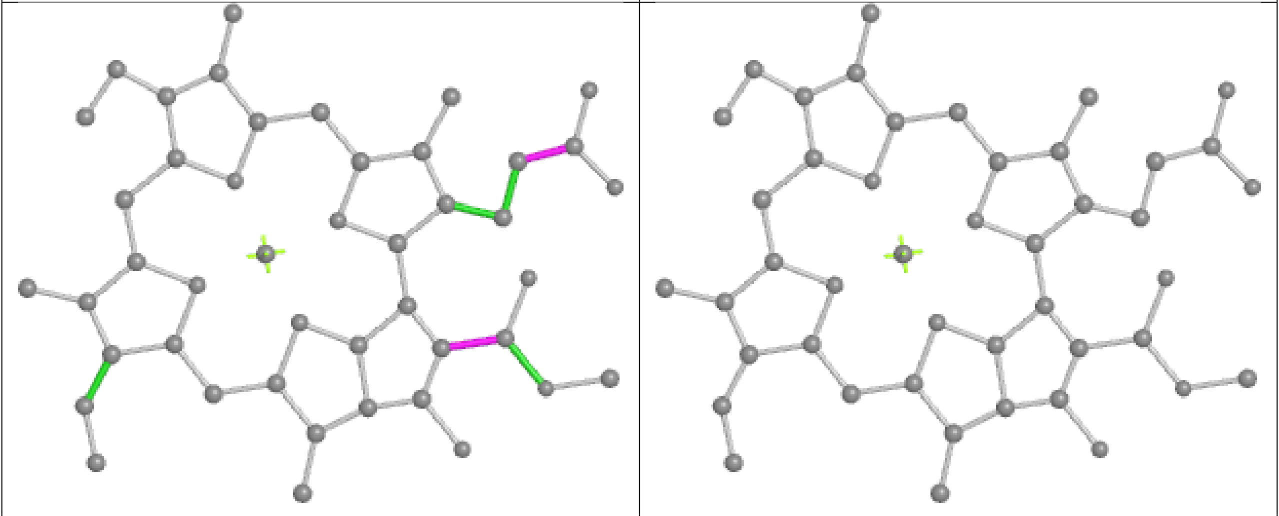


Bond lengths

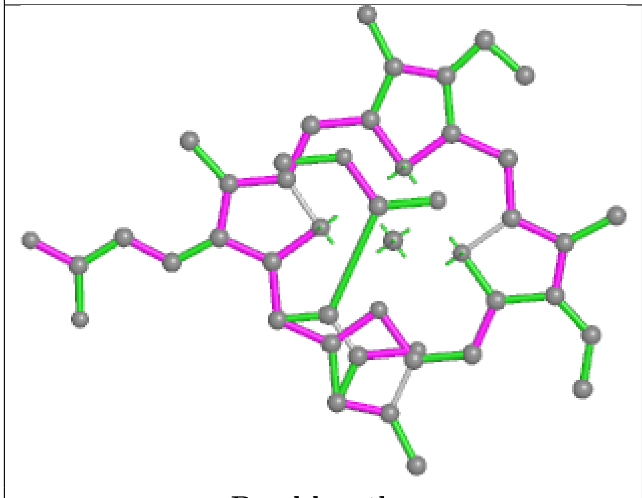
Bond angles



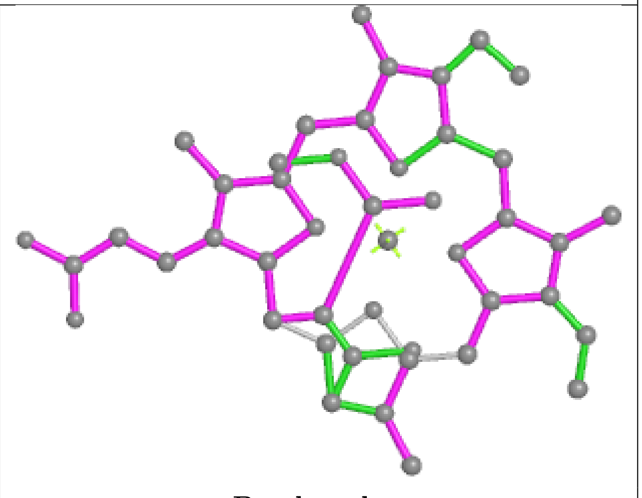
Torsions

Rings

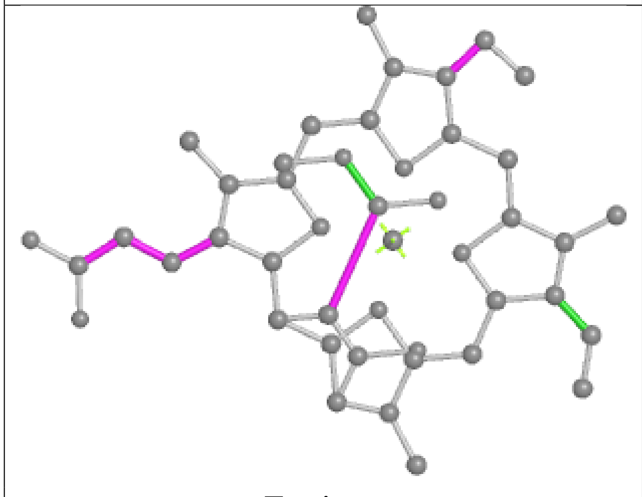
Ligand KC1 11 306



Bond lengths



Bond angles



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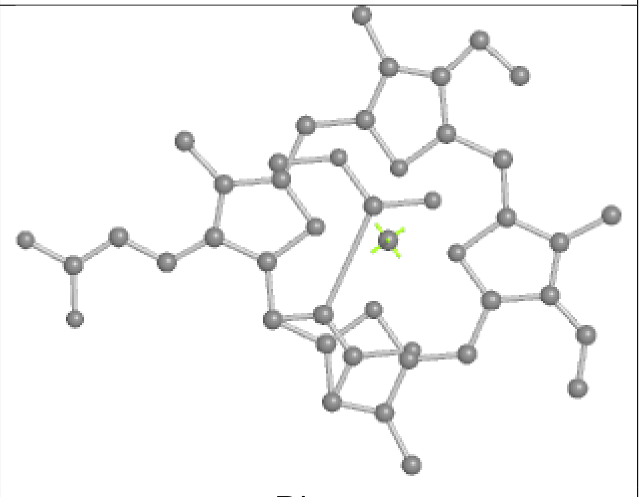
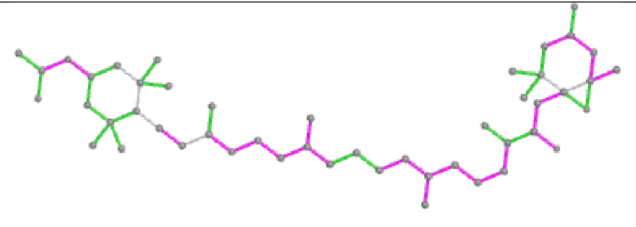


Rings

Ligand A86 18 311



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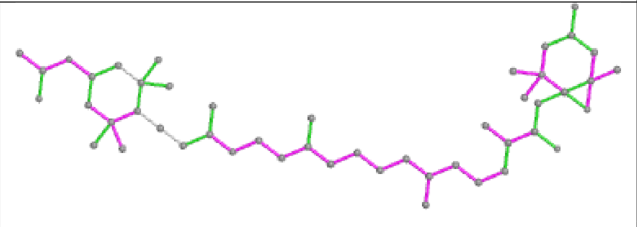
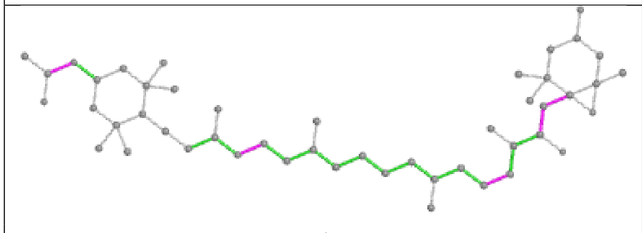


Bond angles



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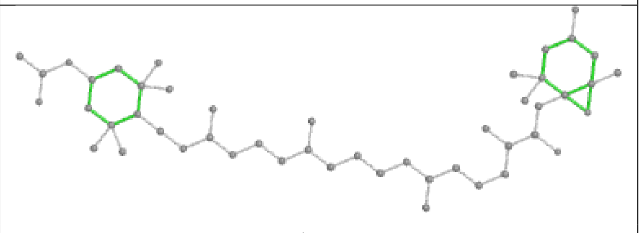
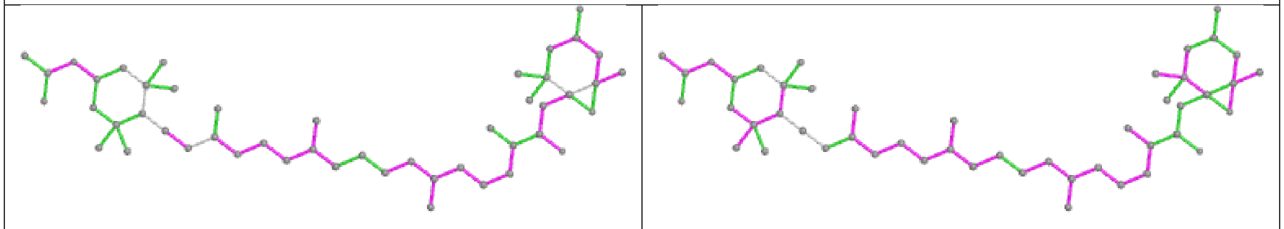


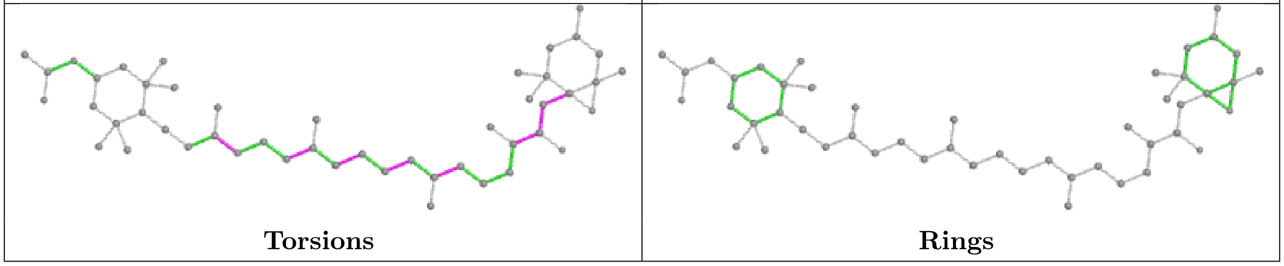
Rings

Ligand A86 20 301



Bond lengths

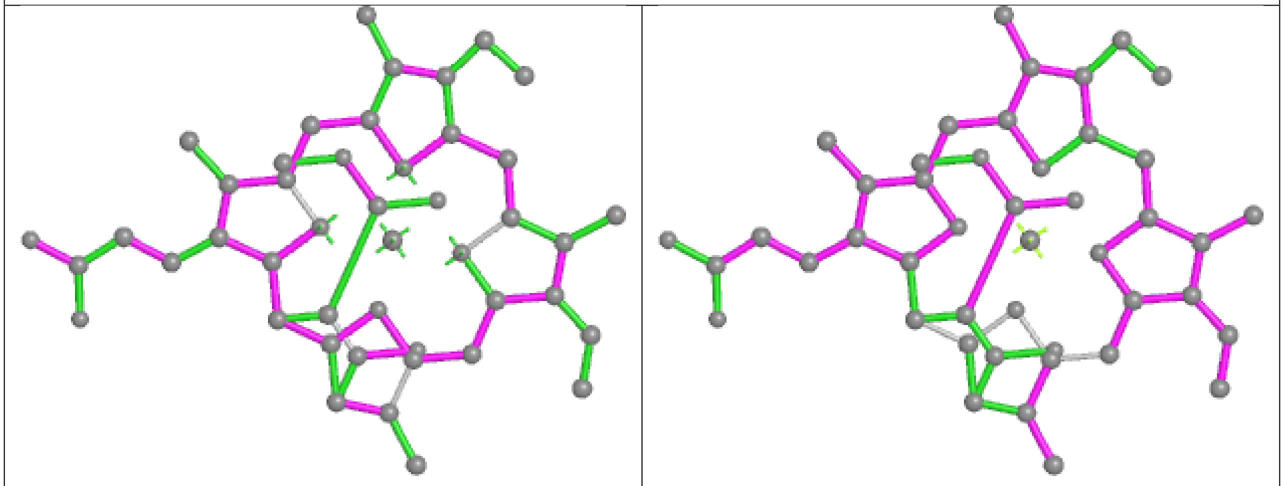
Bond angles



Torsions

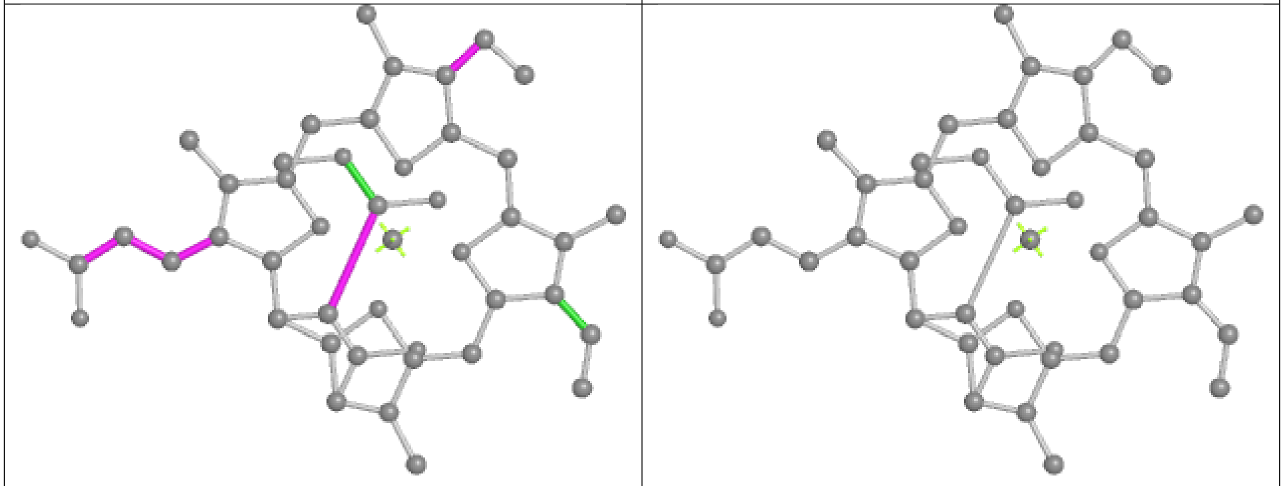
Rings

Ligand KC1 13 310



Bond lengths

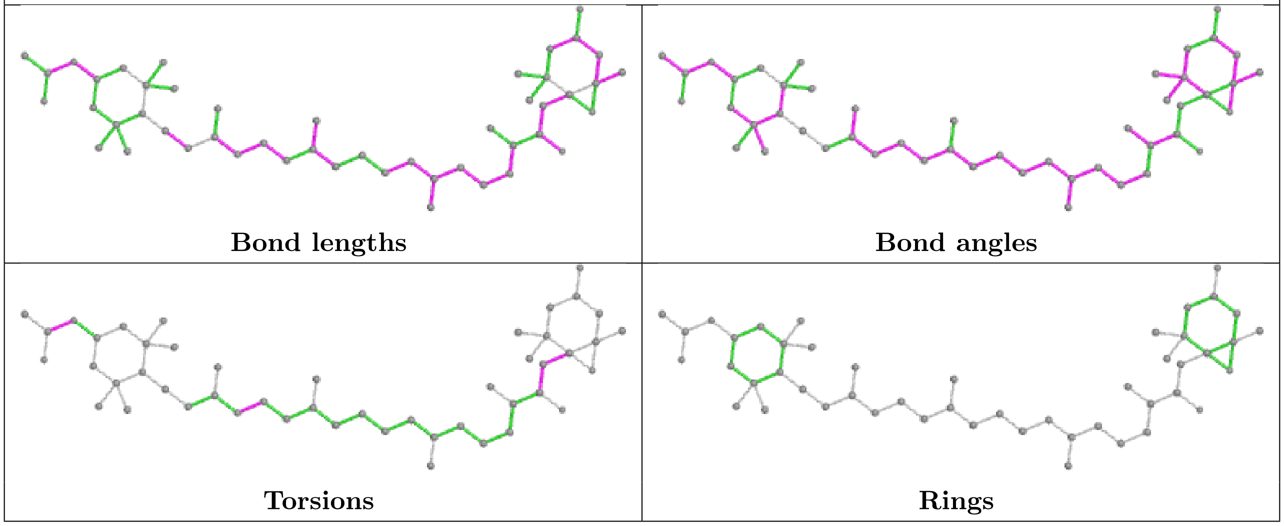
Bond angles



Torsions

Rings

Ligand A86 14 311



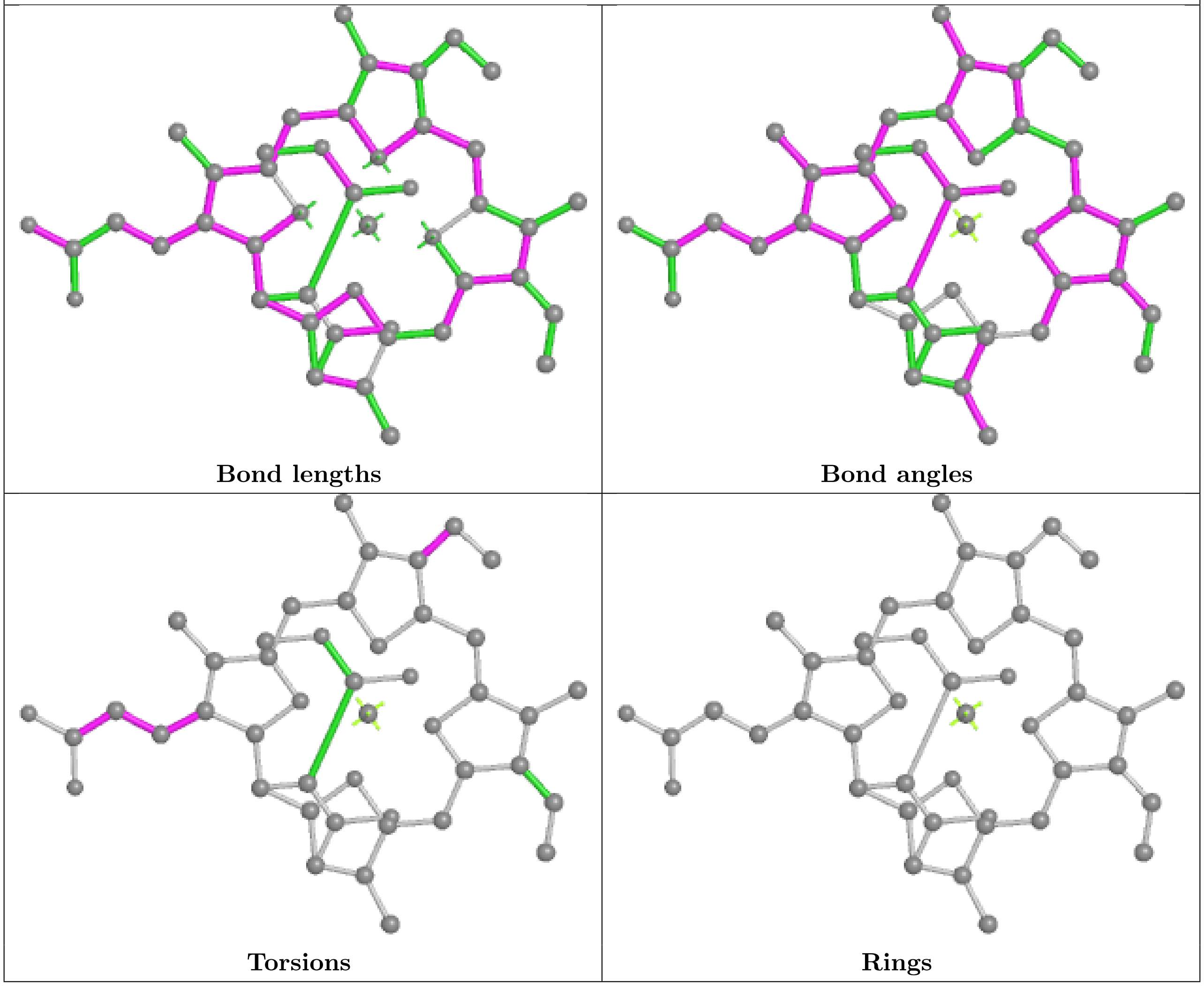
Bond lengths

Bond angles

Torsions

Rings

Ligand KC1 16 305



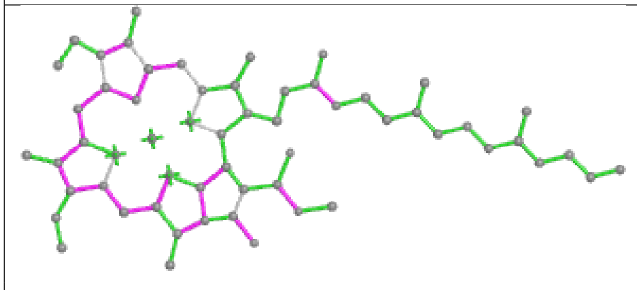
Bond lengths

Bond angles

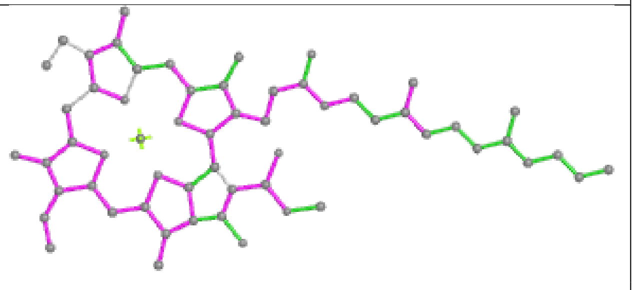
Torsions

Rings

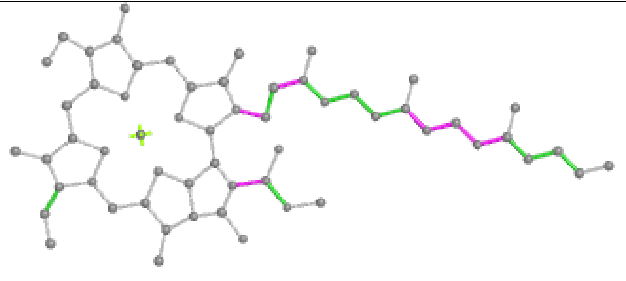
Ligand CLA 21 204



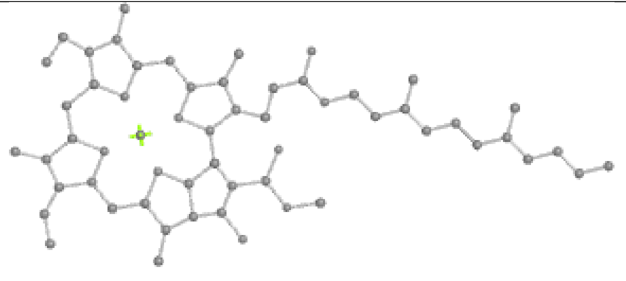
Bond lengths



Bond angles

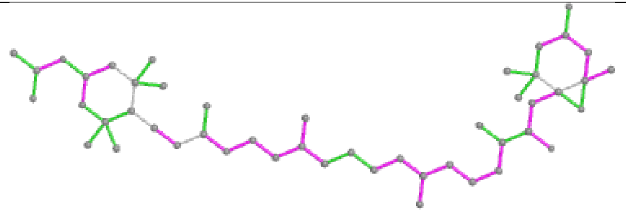


Torsions

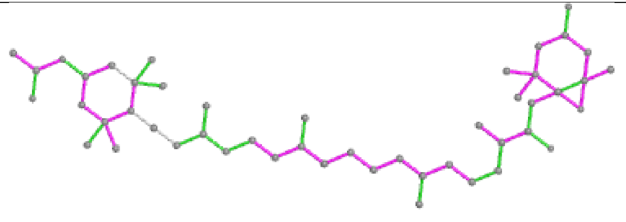


Rings

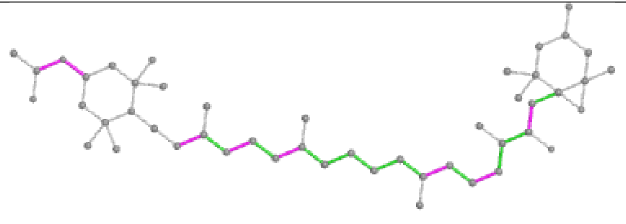
Ligand A86 14 313



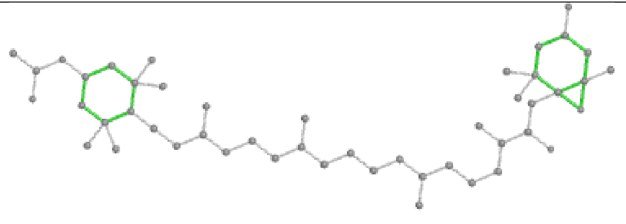
Bond lengths



Bond angles

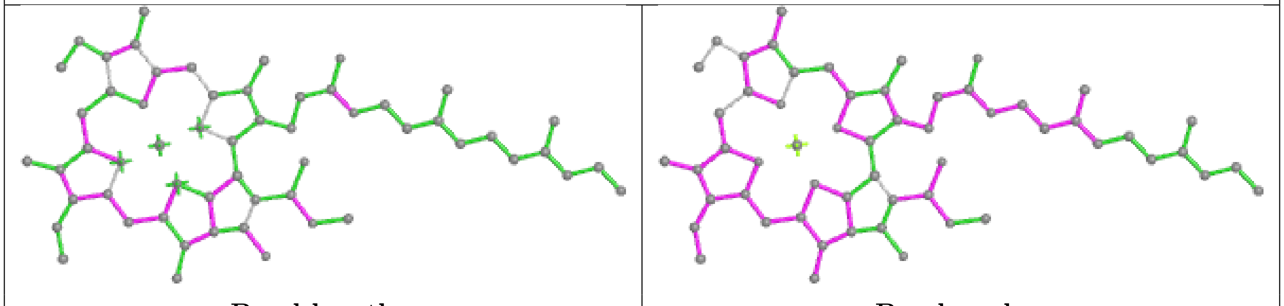


Torsions



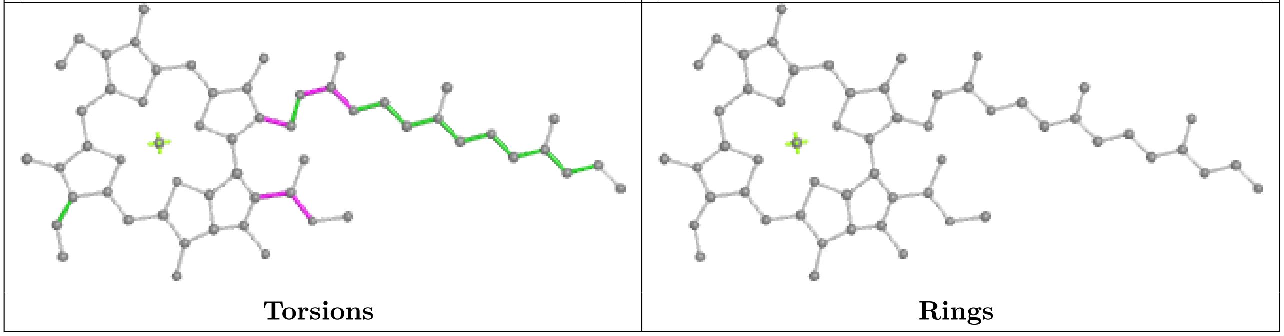
Rings

Ligand CLA 16 303



Bond lengths

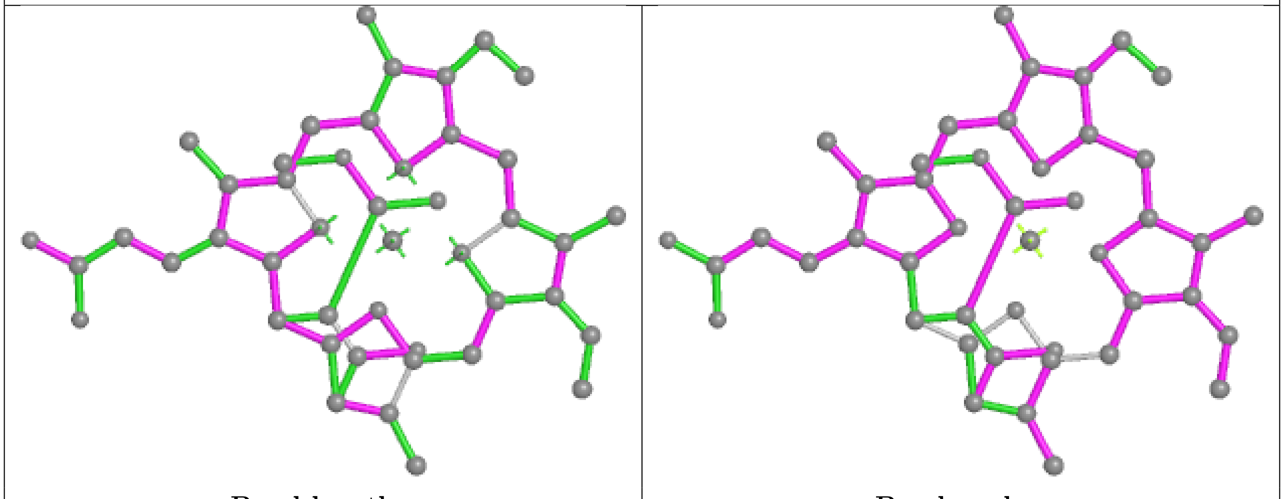
Bond angles



Torsions

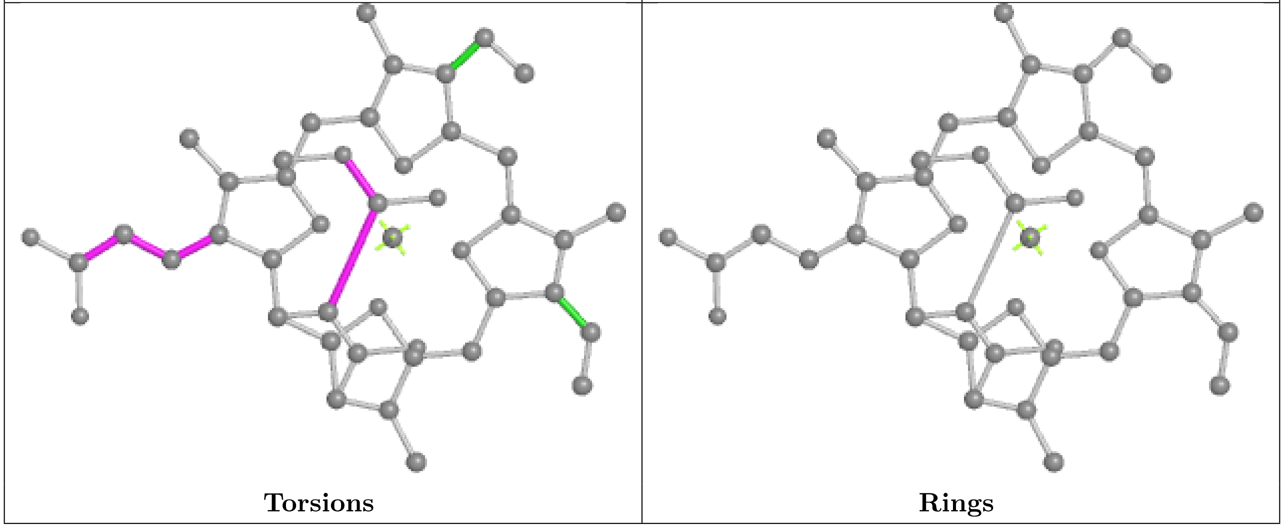
Rings

Ligand KC1 20 303



Bond lengths

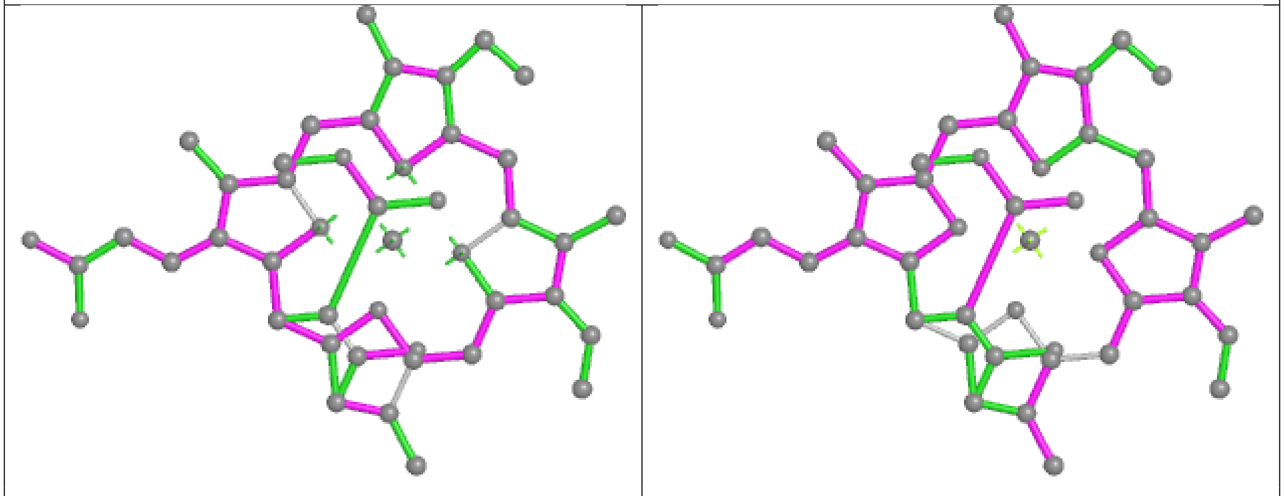
Bond angles



Torsions

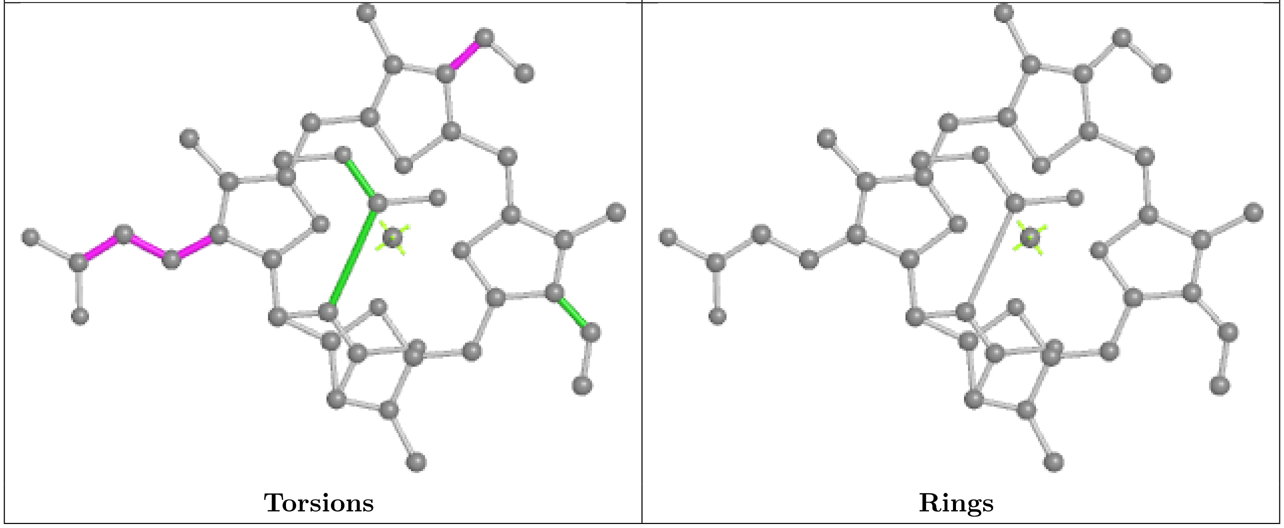
Rings

Ligand KC1 20 305



Bond lengths

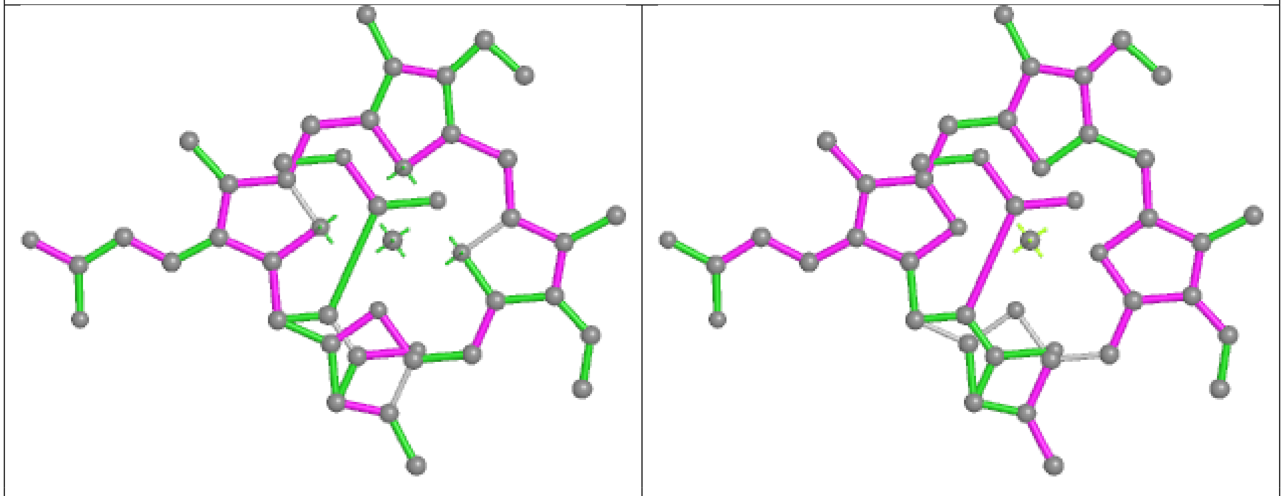
Bond angles



Torsions

Rings

Ligand KC1 12 306



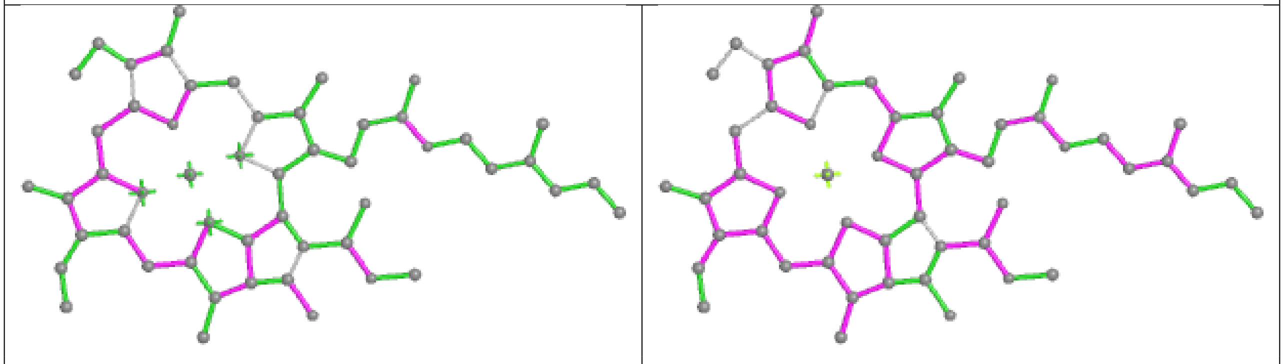
Bond lengths

Bond angles

Torsions

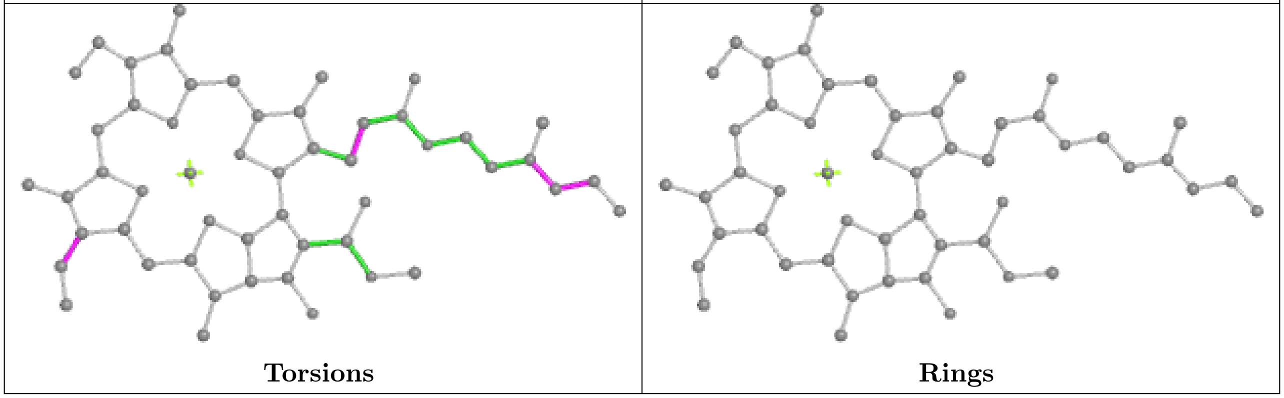
Rings

Ligand CLA 11 307



Bond lengths

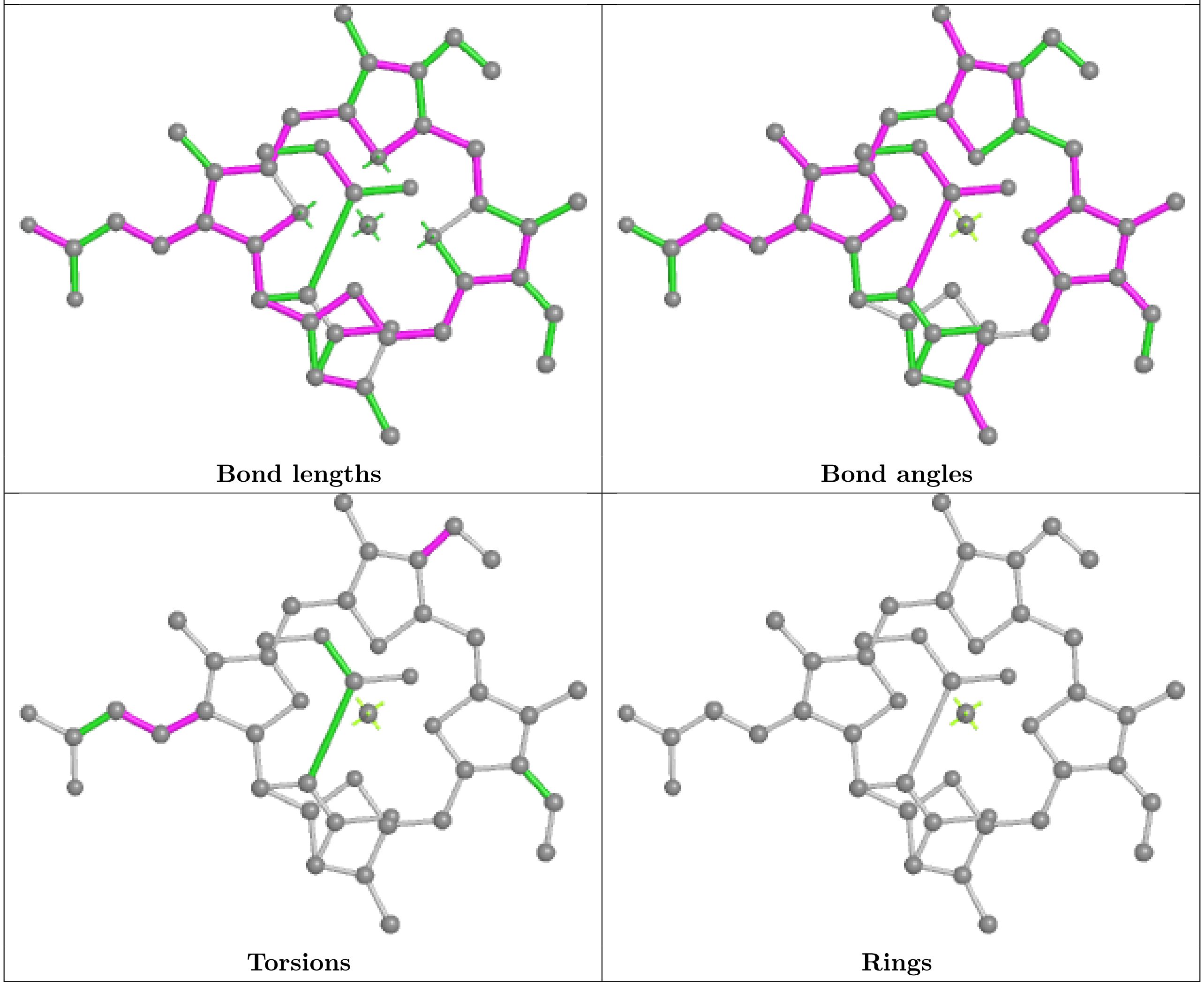
Bond angles



Torsions

Rings

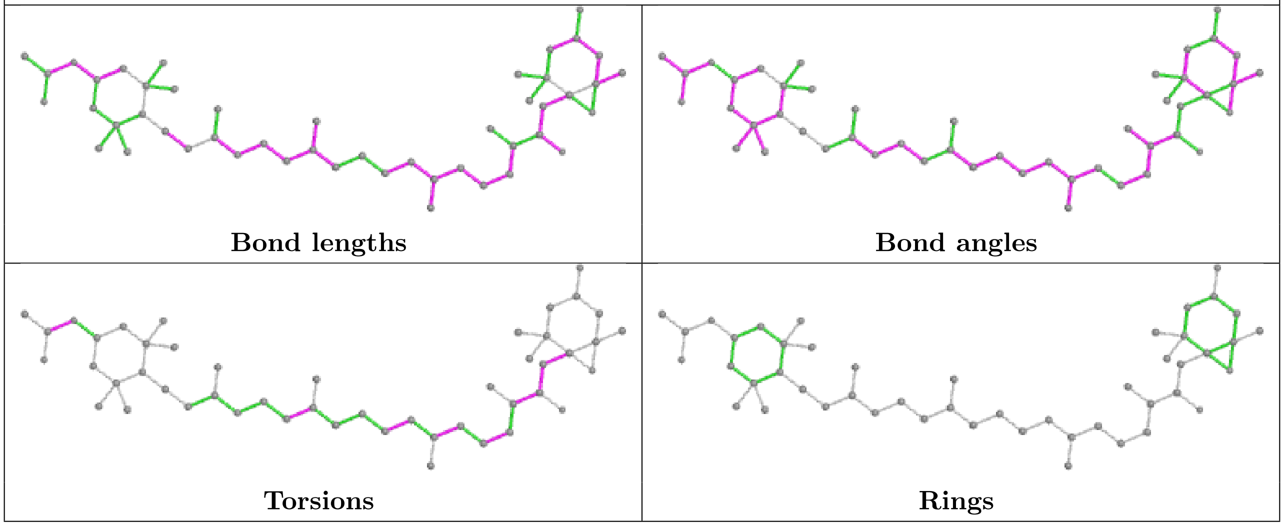
Ligand KC1 11 304



Bond lengths **Bond angles**

Torsions **Rings**

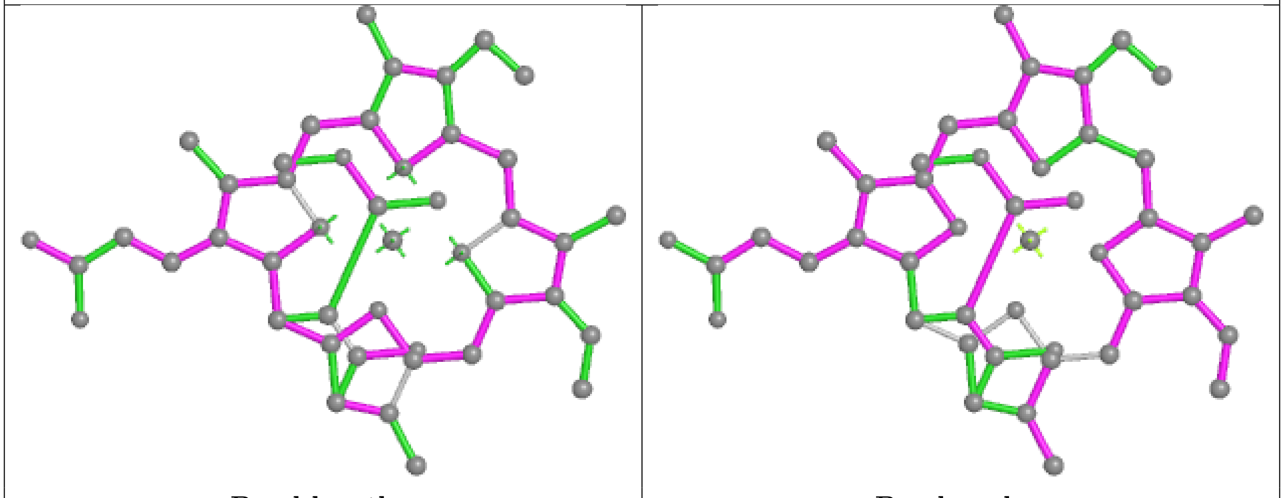
Ligand A86 14 316



Bond lengths **Bond angles**

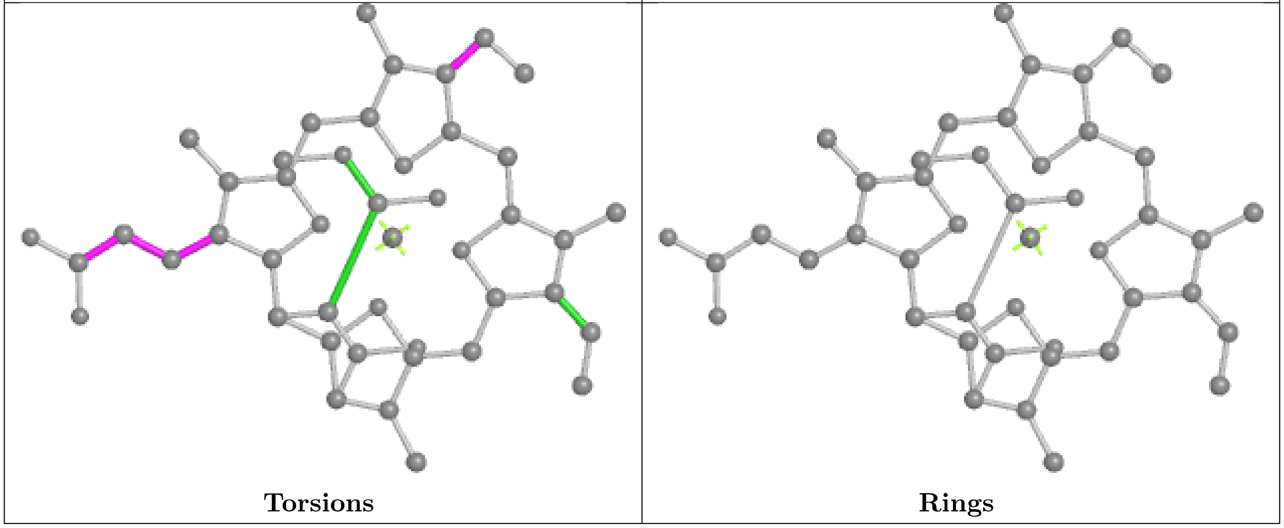
Torsions **Rings**

Ligand KC1 15 302



Bond lengths

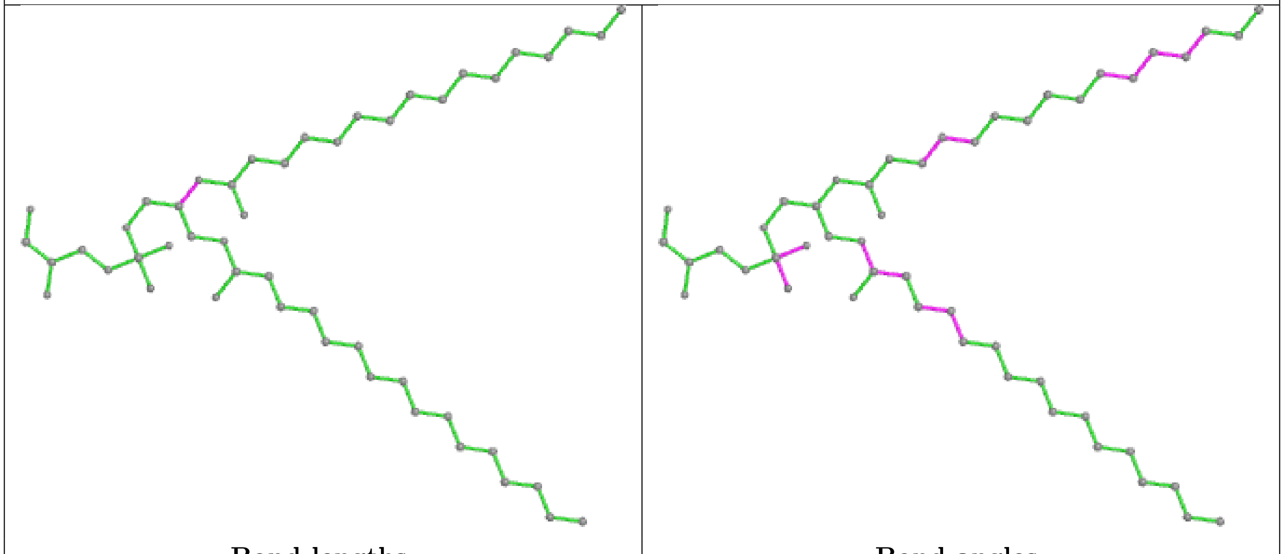
Bond angles



Torsions

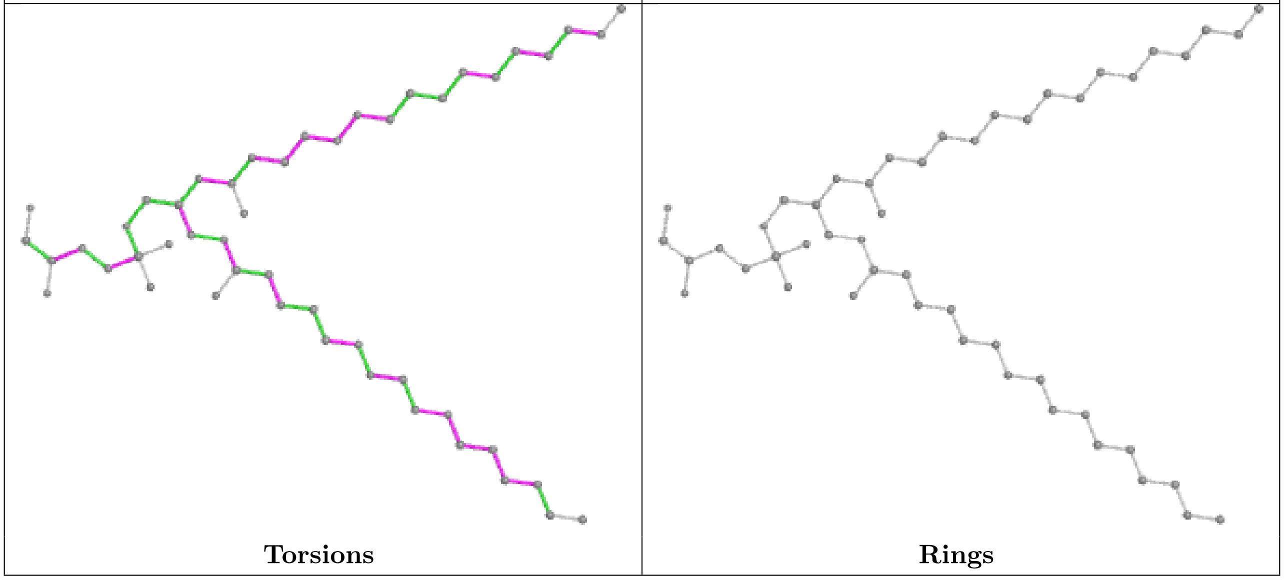
Rings

Ligand LHG 19 314



Bond lengths

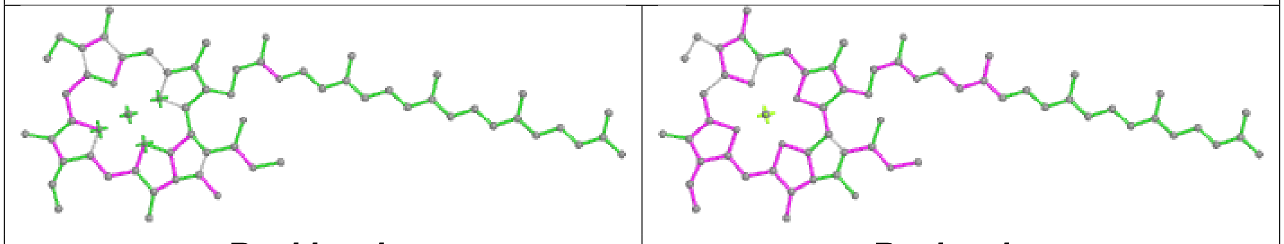
Bond angles



Torsions

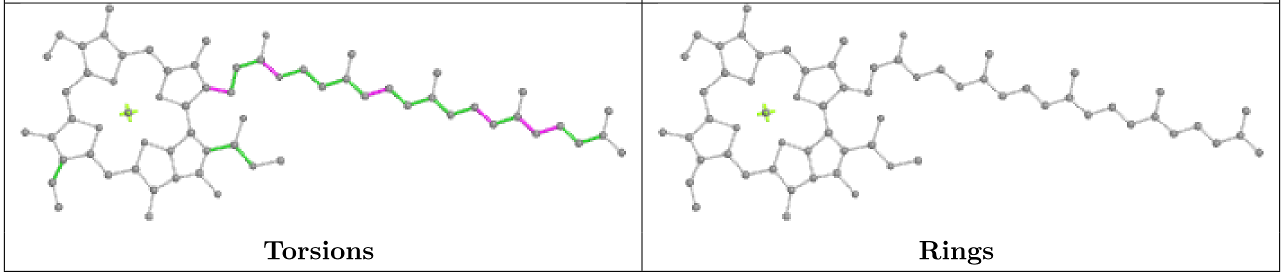
Rings

Ligand CLA 19 307



Bond lengths

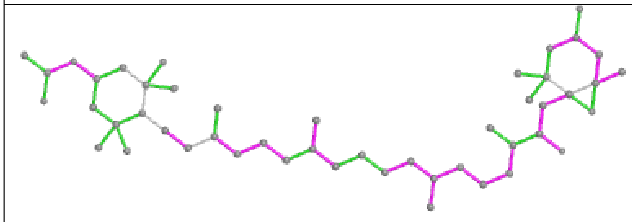
Bond angles



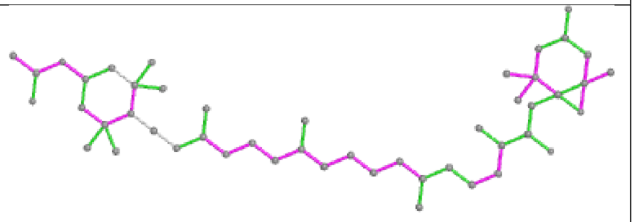
Torsions

Rings

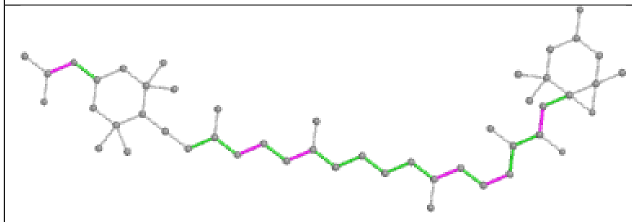
Ligand A86 17 315



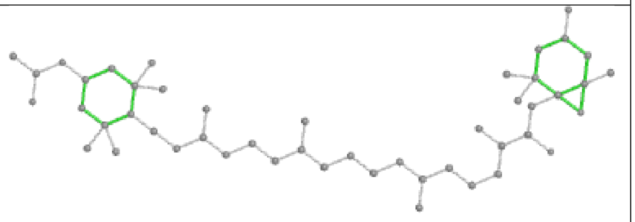
Bond lengths



Bond angles

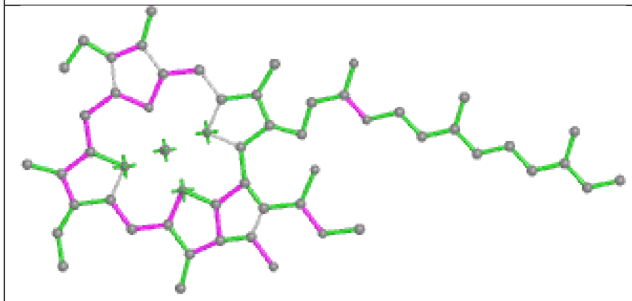


Torsions

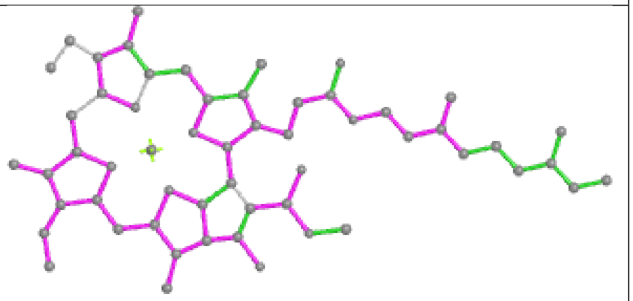


Rings

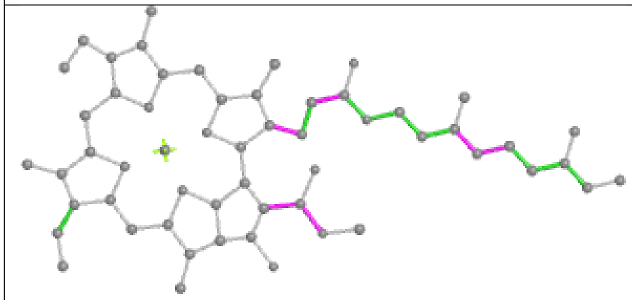
Ligand CLA 20 304



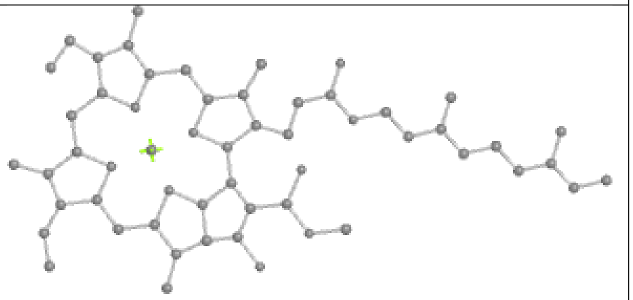
Bond lengths



Bond angles

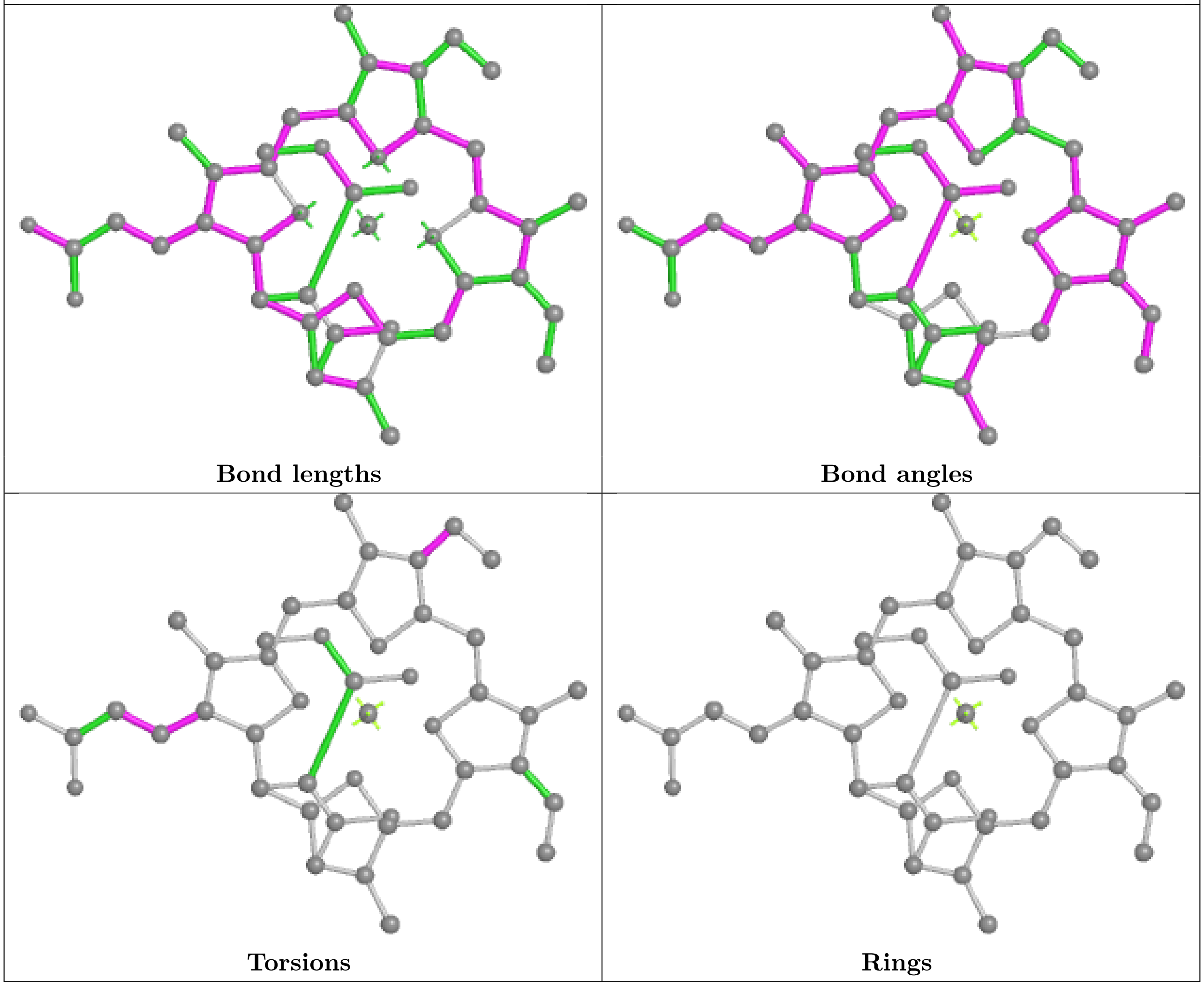


Torsions



Rings

Ligand KC1 13 307



Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Map visualisation ⓘ

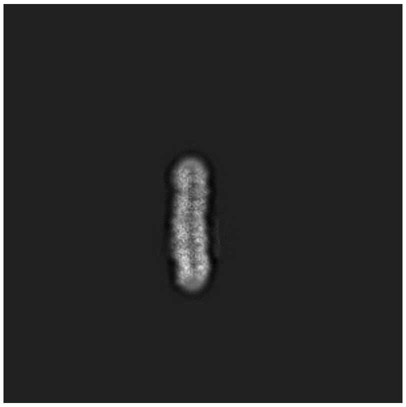
This section contains visualisations of the EMDB entry EMD-31906. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

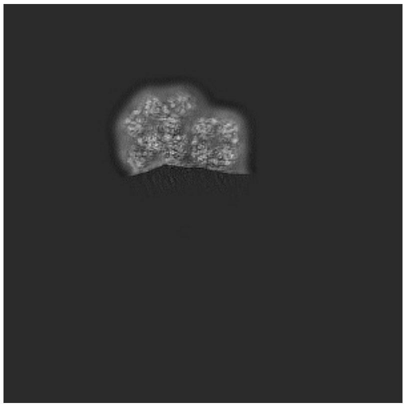
6.1 Orthogonal projections ⓘ

6.1.1 Primary map

X



Y

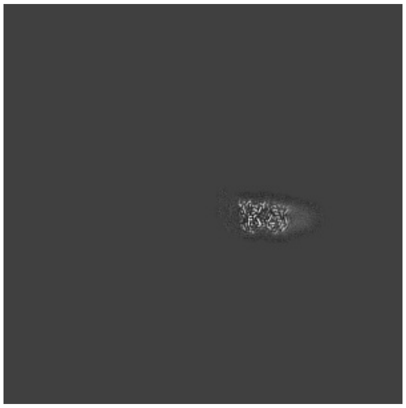


Z

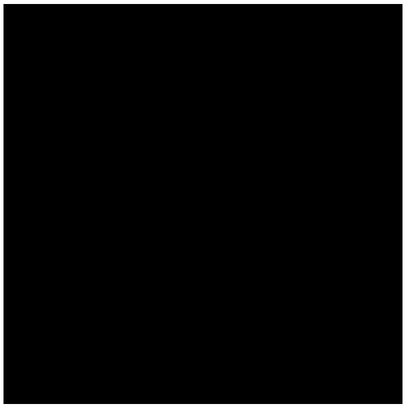
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ

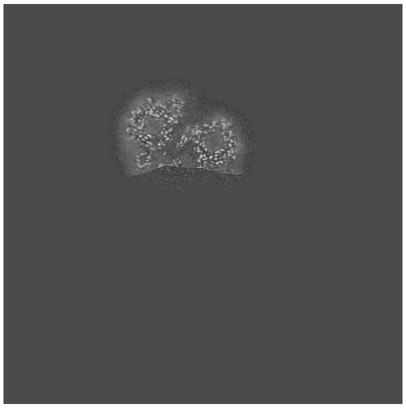
6.2.1 Primary map



X Index: 256



Y Index: 256



Z Index: 256

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

6.3 Largest variance slices

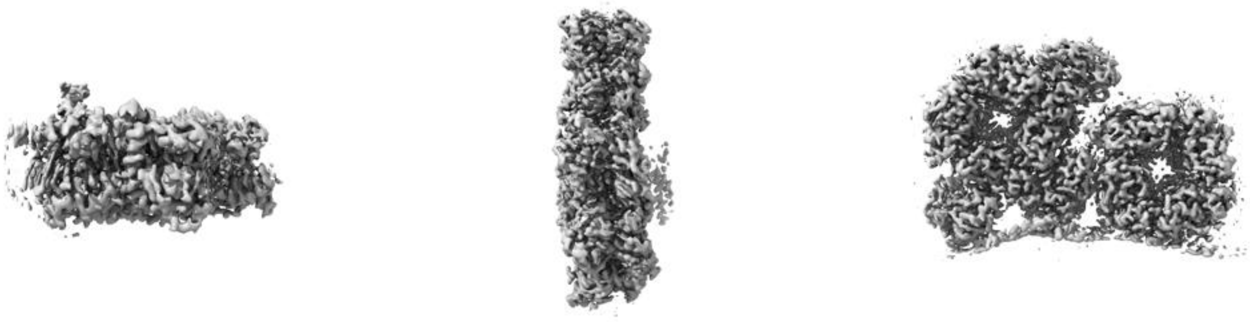
6.3.1 Primary map

X Index: 216 Y Index: 321 Z Index: 234

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

6.4 Orthogonal surface views

6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.055. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

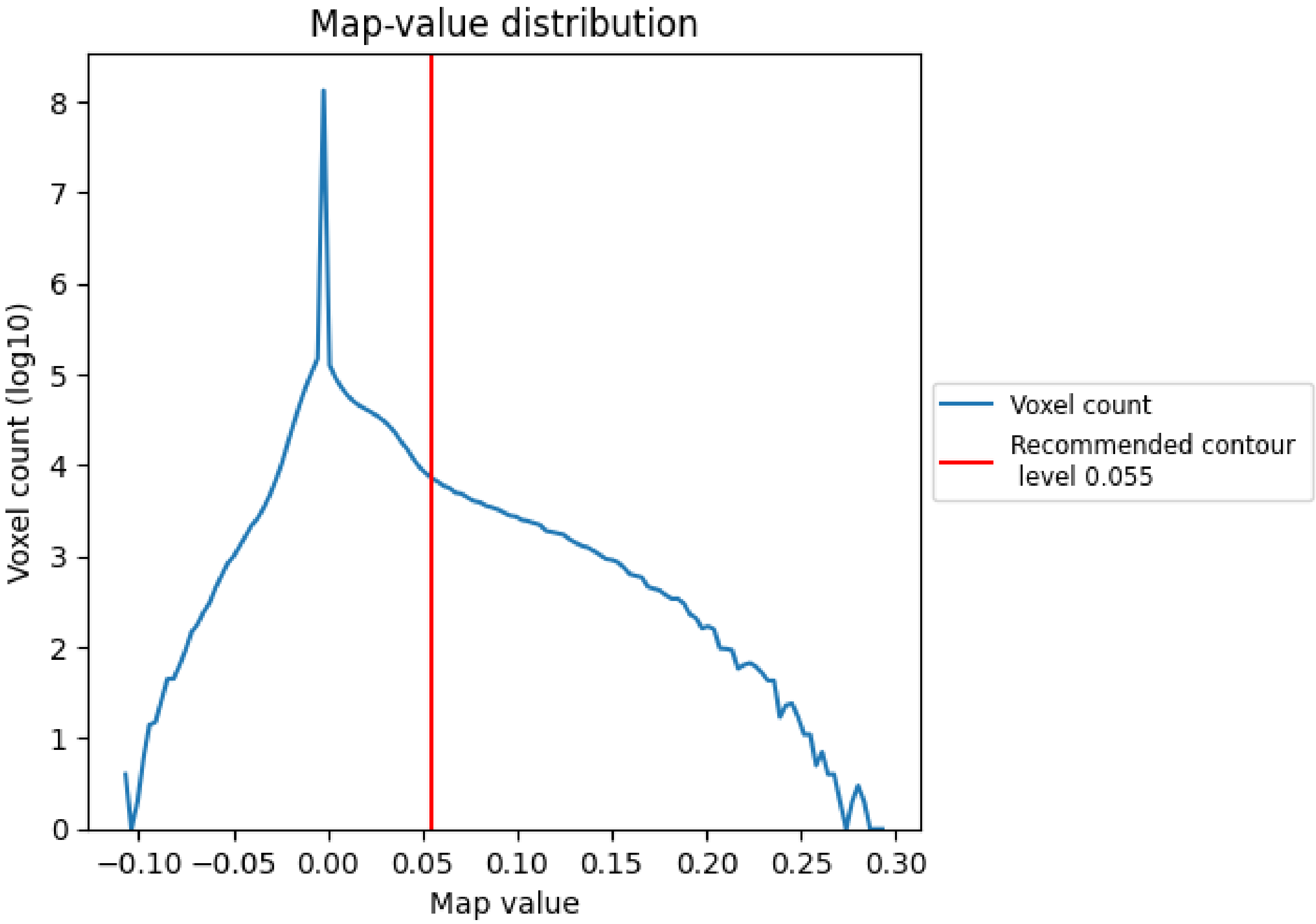
6.5 Mask visualisation ⓘ

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

7 Map analysis (i)

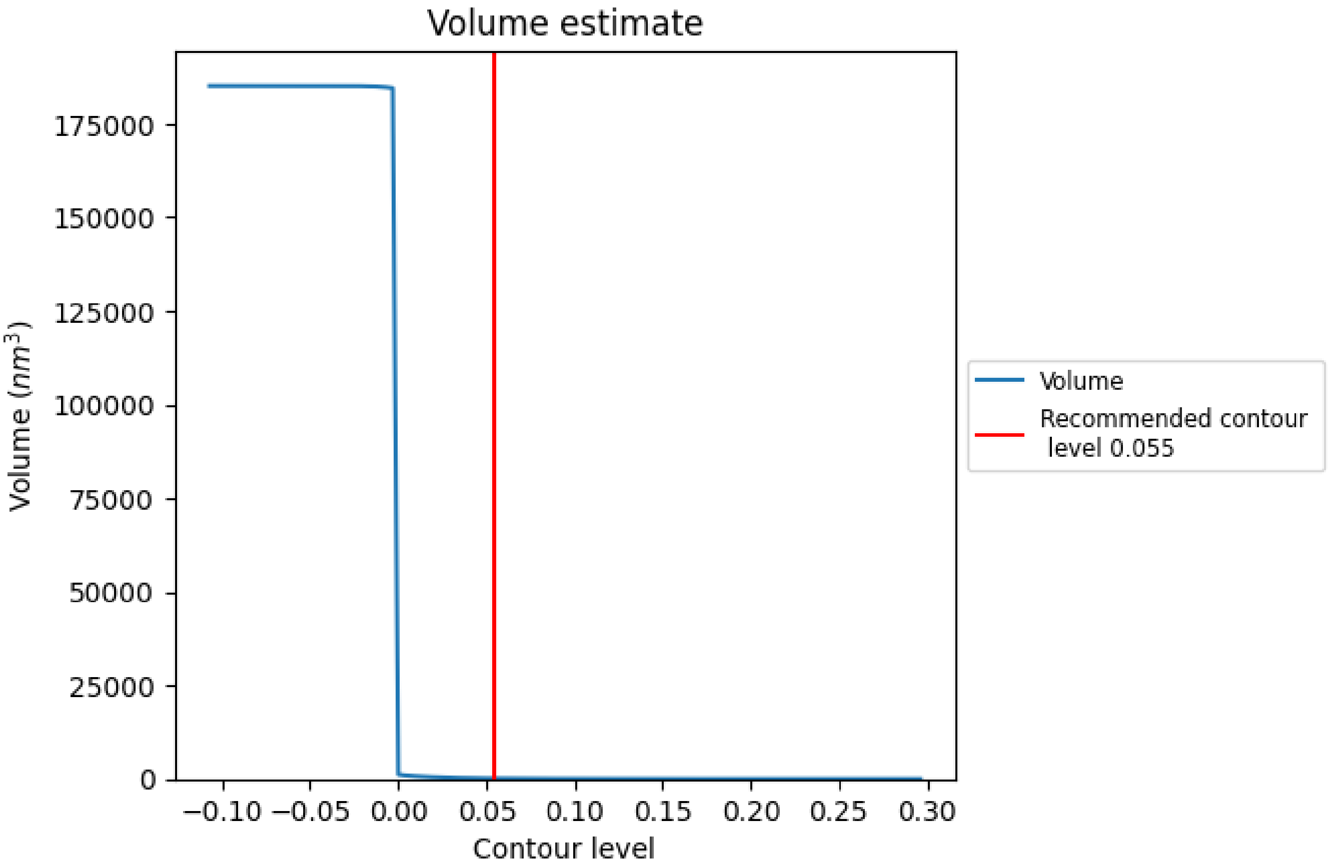
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

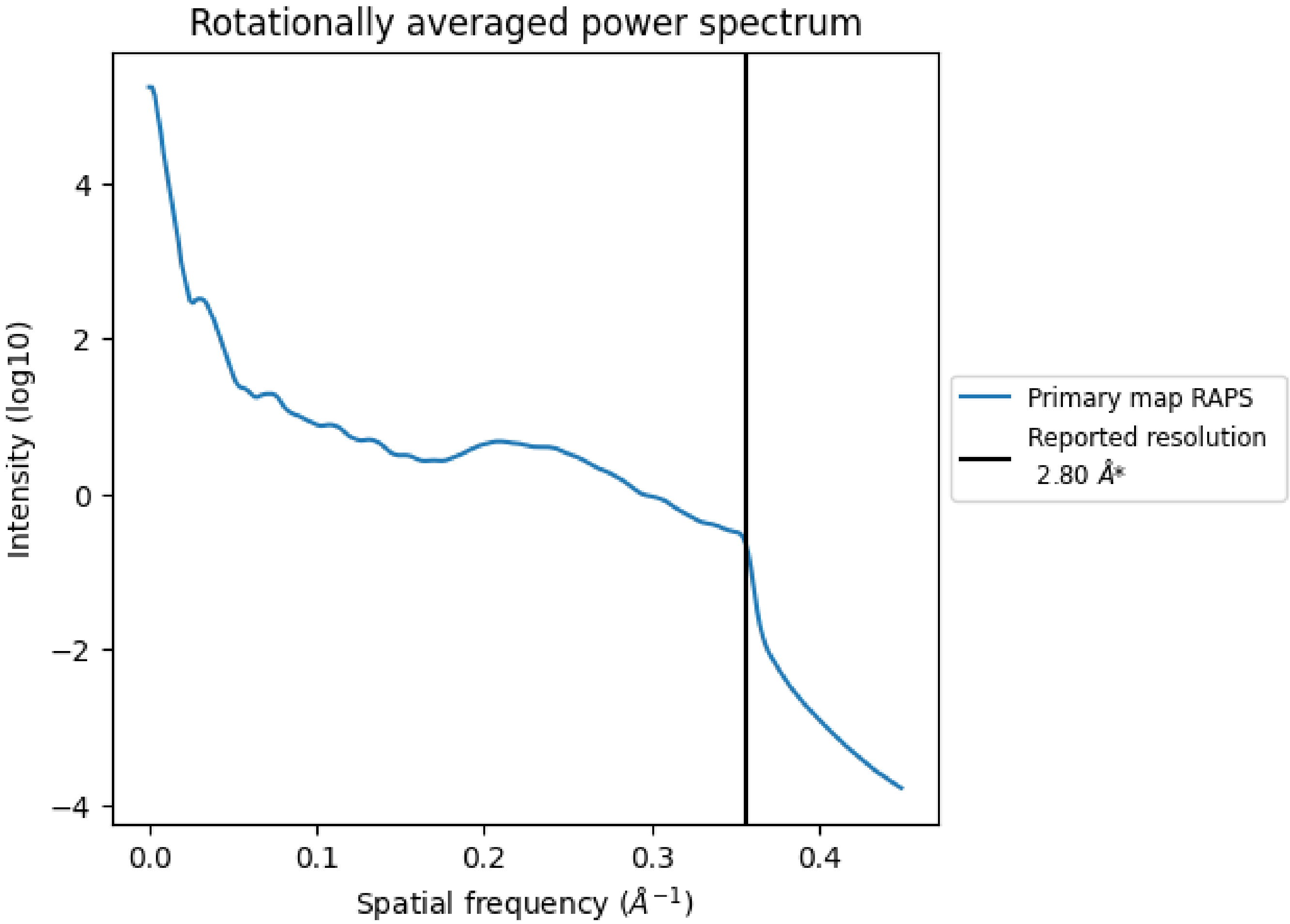
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 139 nm^3; this corresponds to an approximate mass of 126 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 ⓘ

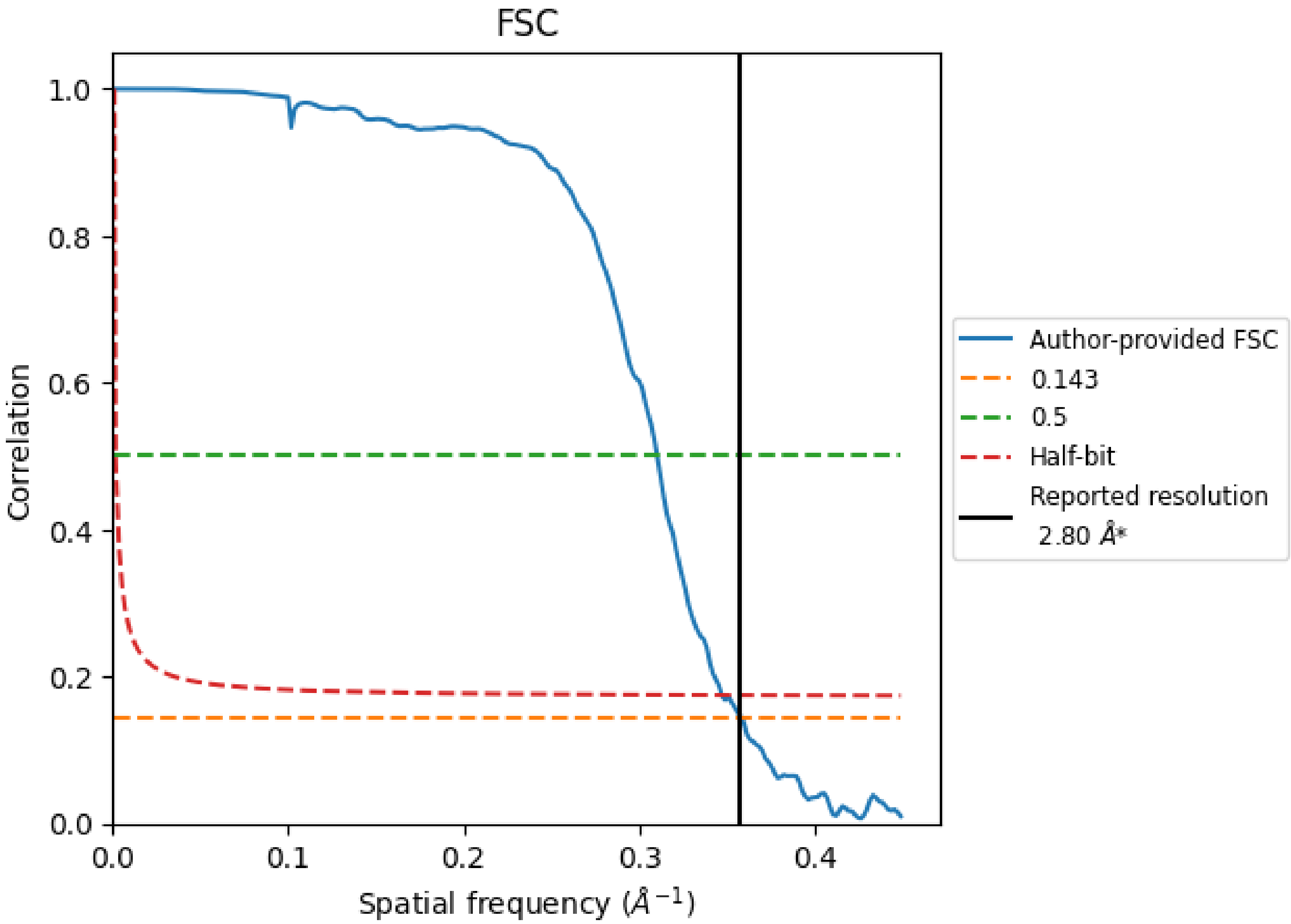


*Reported resolution corresponds to spatial frequency of 0.357 $Å^{-1}$

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 0.357 $Å^{-1}$

8.2 Resolution estimates (i)

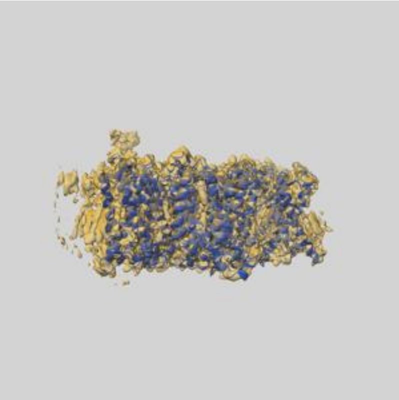
Resolution estimate (Å)	**Estimation criterion (FSC cut-off)**		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	2.79	3.22	2.88
Unmasked-calculated*	-	-	-

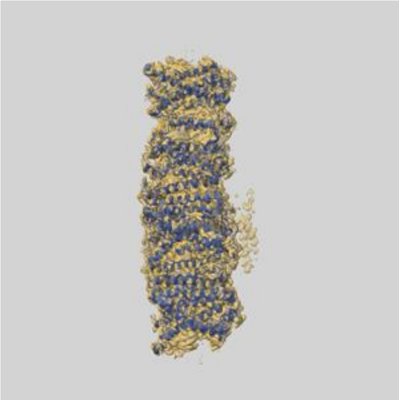
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

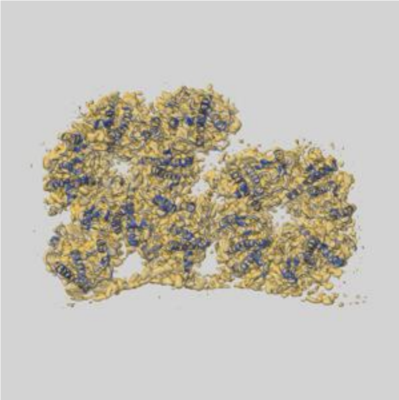
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-31906 and PDB model 7VD6. Per-residue inclusion information can be found in section 3 on page 21.

9.1 Map-model overlay (i)

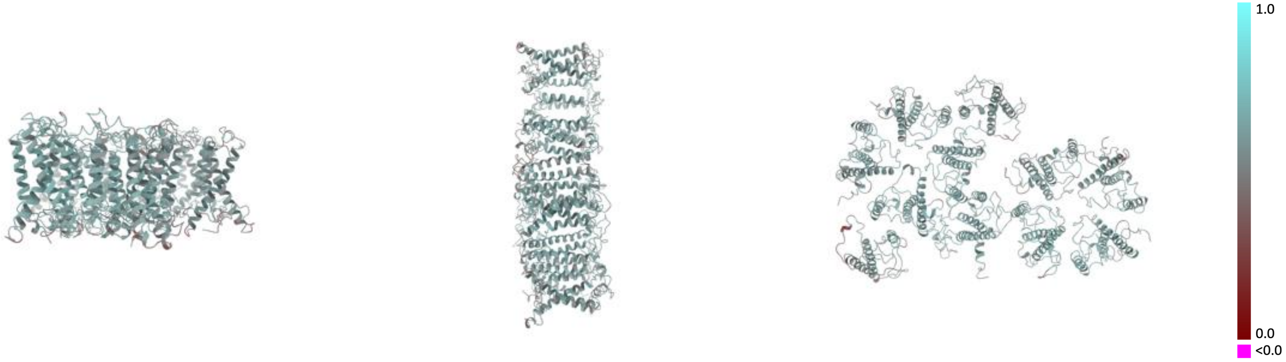

X


Y


Z

The images above show the 3D surface view of the map at the recommended contour level 0.055 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.

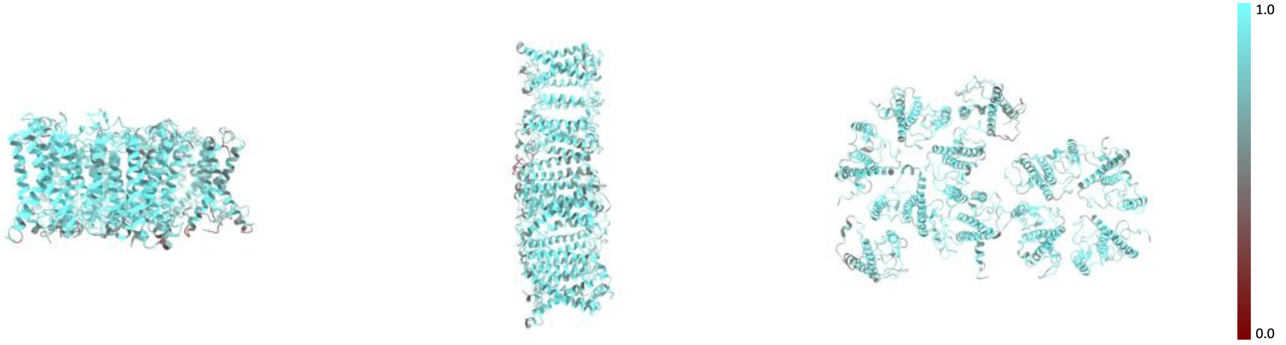
9.2 Q-score mapped to coordinate model



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.

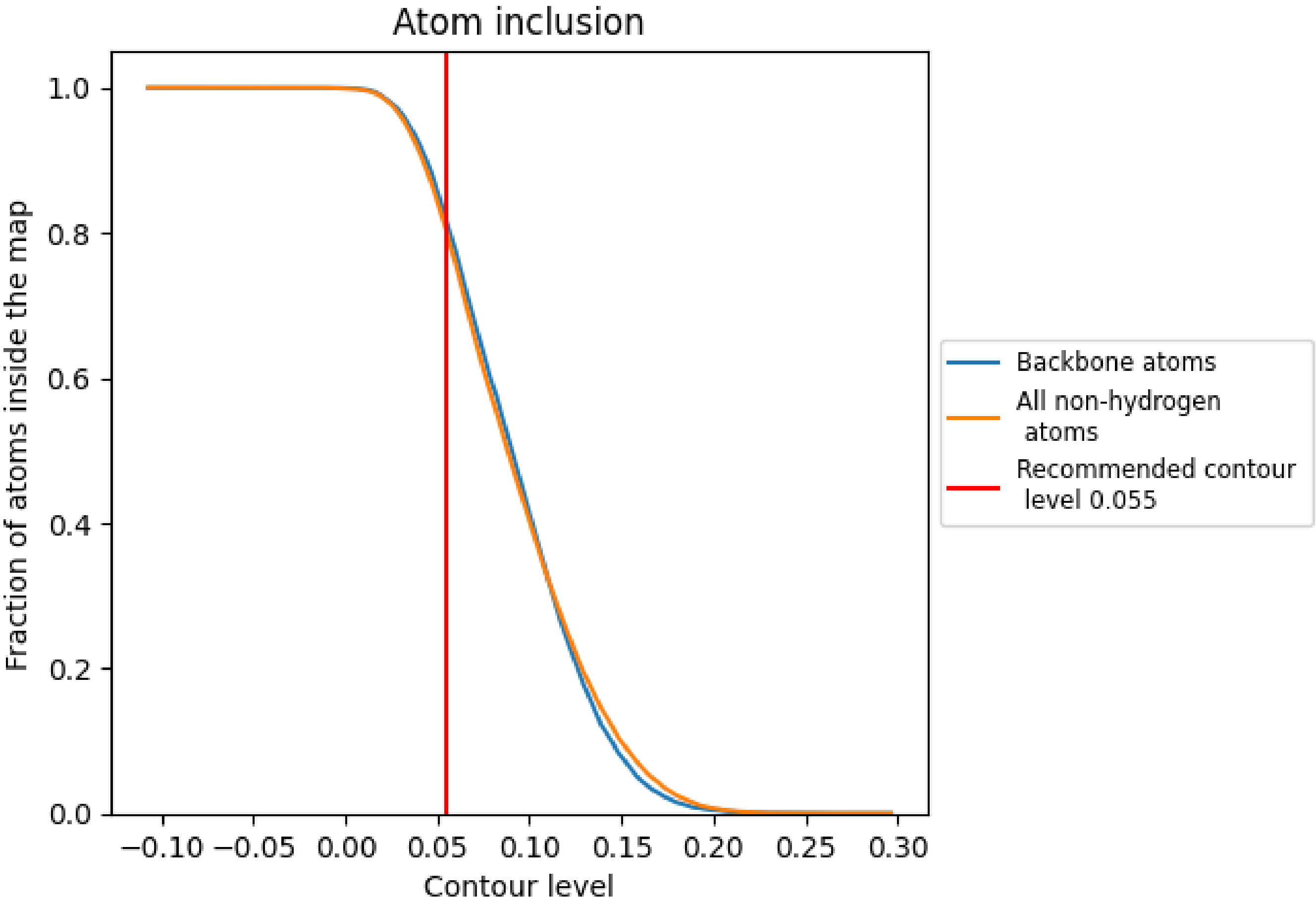
9.3 Atom inclusion mapped to coordinate model



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 (0.055).

9.4 Atom inclusion ⓘ



At the recommended contour level, 82% of all backbone atoms, 80% 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 (0.055) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8020	0.5650
11	0.8416	0.5920
12	0.8241	0.5710
13	0.7785	0.5400
14	0.7925	0.5550
15	0.7754	0.5530
16	0.8742	0.6000
17	0.8464	0.5940
18	0.7983	0.5550
19	0.8541	0.5990
20	0.7469	0.5190
21	0.6503	0.5210