wwPDB EM Validation Summary Report ⓘ

Dec 19, 2022 – 02:05 am GMT

PDB ID : 7BLZ
EMDB ID : EMD-12228
Title : Red alga C.merolae Photosystem I
Authors : Nelson, N.; Klaiman, D.; Hippler, M.
Deposited on : 2021-01-19
Resolution : 3.10 Å(reported)

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

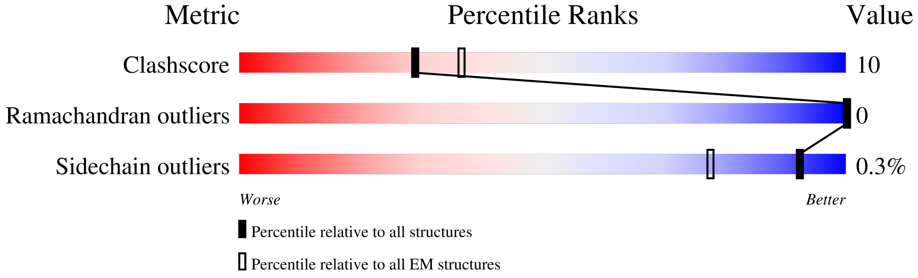
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

1 Overall quality at a glance

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

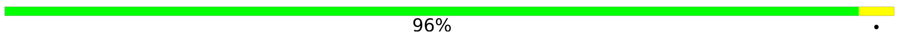
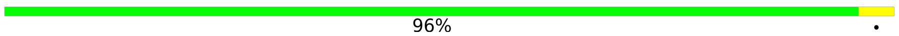
The reported resolution of this entry is 3.10 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	1	173	
2	2	179	
3	3	174	
4	A	743	
5	B	731	
6	C	80	
7	D	138	
8	E	61	

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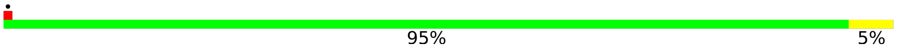
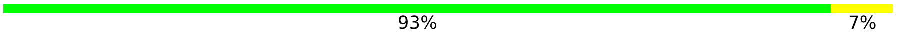
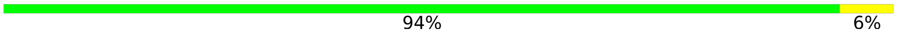
Mol	Chain	Length	Quality of chain
9	F	155	 95% 5%
10	I	31	 87% 13%
11	J	38	 89% 11%
12	K	54	 81% 19%
13	L	136	 88% 11%
14	M	27	 93% 7%
15	O	97	 94% 6%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
16	CLA	1	601	X	-	-	-
16	CLA	1	602	X	-	-	-
16	CLA	1	603	X	-	-	-
16	CLA	1	604	X	-	-	-
16	CLA	1	605	X	-	-	-
16	CLA	1	606	X	-	-	-
16	CLA	1	607	X	-	-	-
16	CLA	1	608	X	-	-	-
16	CLA	1	609	X	-	-	-
16	CLA	1	610	X	-	-	-
16	CLA	1	611	X	-	-	-
16	CLA	2	601	X	-	-	-
16	CLA	2	602	X	-	-	-
16	CLA	2	603	X	-	-	-
16	CLA	2	604	X	-	-	-
16	CLA	2	605	X	-	-	-
16	CLA	2	606	X	-	-	-
16	CLA	2	607	X	-	-	-
16	CLA	2	608	X	-	-	-
16	CLA	2	609	X	-	-	-
16	CLA	2	610	X	-	-	-
16	CLA	2	611	X	-	-	-
16	CLA	2	612	X	-	-	-
16	CLA	2	613	X	-	-	-
16	CLA	3	203	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
16	CLA	3	204	X	-	-	-
16	CLA	3	205	X	-	-	-
16	CLA	3	206	X	-	-	-
16	CLA	3	207	X	-	-	-
16	CLA	3	208	X	-	-	-
16	CLA	3	209	X	-	-	-
16	CLA	3	210	X	-	-	-
16	CLA	3	211	X	-	-	-
16	CLA	3	212	X	-	-	-
16	CLA	3	213	X	-	-	-
16	CLA	3	214	X	-	-	-
16	CLA	A	802	X	-	-	-
16	CLA	A	803	X	-	-	-
16	CLA	A	804	X	-	-	-
16	CLA	A	805	X	-	-	-
16	CLA	A	806	X	-	-	-
16	CLA	A	807	X	-	-	-
16	CLA	A	808	X	-	-	-
16	CLA	A	809	X	-	-	-
16	CLA	A	810	X	-	-	-
16	CLA	A	811	X	-	-	-
16	CLA	A	812	X	-	-	-
16	CLA	A	813	X	-	-	-
16	CLA	A	814	X	-	-	-
16	CLA	A	815	X	-	-	-
16	CLA	A	816	X	-	-	-
16	CLA	A	817	X	-	-	-
16	CLA	A	818	X	-	-	-
16	CLA	A	819	X	-	-	-
16	CLA	A	820	X	-	-	-
16	CLA	A	821	X	-	-	-
16	CLA	A	822	X	-	-	-
16	CLA	A	823	X	-	-	-
16	CLA	A	824	X	-	-	-
16	CLA	A	825	X	-	-	-
16	CLA	A	826	X	-	-	-
16	CLA	A	827	X	-	-	-
16	CLA	A	828	X	-	-	-
16	CLA	A	829	X	-	-	-
16	CLA	A	830	X	-	-	-
16	CLA	A	831	X	-	-	-
16	CLA	A	832	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
16	CLA	A	833	X	-	-	-
16	CLA	A	834	X	-	-	-
16	CLA	A	835	X	-	-	-
16	CLA	A	836	X	-	-	-
16	CLA	A	837	X	-	-	-
16	CLA	A	838	X	-	-	-
16	CLA	A	839	X	-	-	-
16	CLA	A	854	X	-	-	-
16	CLA	A	855	X	-	-	-
16	CLA	A	856	X	-	-	-
16	CLA	B	801	X	-	-	-
16	CLA	B	802	X	-	-	-
16	CLA	B	803	X	-	-	-
16	CLA	B	804	X	-	-	-
16	CLA	B	805	X	-	-	-
16	CLA	B	806	X	-	-	-
16	CLA	B	807	X	-	-	-
16	CLA	B	808	X	-	-	-
16	CLA	B	809	X	-	-	-
16	CLA	B	810	X	-	-	-
16	CLA	B	811	X	-	-	-
16	CLA	B	812	X	-	-	-
16	CLA	B	813	X	-	-	-
16	CLA	B	814	X	-	-	-
16	CLA	B	815	X	-	-	-
16	CLA	B	816	X	-	-	-
16	CLA	B	817	X	-	-	-
16	CLA	B	818	X	-	-	-
16	CLA	B	819	X	-	-	-
16	CLA	B	820	X	-	-	-
16	CLA	B	821	X	-	-	-
16	CLA	B	822	X	-	-	-
16	CLA	B	823	X	-	-	-
16	CLA	B	824	X	-	-	-
16	CLA	B	825	X	-	-	-
16	CLA	B	826	X	-	-	-
16	CLA	B	827	X	-	-	-
16	CLA	B	828	X	-	-	-
16	CLA	B	829	X	-	-	-
16	CLA	B	830	X	-	-	-
16	CLA	B	831	X	-	-	-
16	CLA	B	832	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
16	CLA	B	833	X	-	-	-
16	CLA	B	834	X	-	-	-
16	CLA	B	835	X	-	-	-
16	CLA	B	836	X	-	-	-
16	CLA	B	837	X	-	-	-
16	CLA	B	838	X	-	-	-
16	CLA	F	201	X	-	-	-
16	CLA	F	202	X	-	-	-
16	CLA	F	204	X	-	-	-
16	CLA	F	205	X	-	-	-
16	CLA	I	101	X	-	-	-
16	CLA	I	102	X	-	-	-
16	CLA	J	102	X	-	-	-
16	CLA	K	101	X	-	-	-
16	CLA	K	102	X	-	-	-
16	CLA	L	201	X	-	-	-
16	CLA	L	203	X	-	-	-
16	CLA	L	204	X	-	-	-
16	CLA	L	205	X	-	-	-
16	CLA	O	201	X	-	-	-
16	CLA	O	202	X	-	-	-
16	CLA	O	203	X	-	-	-
16	CLA	O	204	X	-	-	-
17	C7Z	1	612	X	-	-	-
17	C7Z	1	614	X	-	-	-
17	C7Z	1	615	X	-	-	-
17	C7Z	1	616	X	-	-	-
17	C7Z	2	614	X	-	-	-
17	C7Z	2	615	X	-	-	-
17	C7Z	3	201	X	-	-	-
17	C7Z	3	215	X	-	-	-
17	C7Z	3	216	X	-	-	-
17	C7Z	3	217	X	-	-	-
17	C7Z	3	218	X	-	-	-
17	C7Z	A	843	X	-	-	-
17	C7Z	J	104	X	-	-	-
18	RRX	1	613	X	-	-	-
18	RRX	2	616	X	-	-	-
18	RRX	A	847	X	-	-	-
18	RRX	J	103	X	X	-	-
18	RRX	K	103	X	-	-	-
20	ERG	1	618	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	ERG	2	618	X	-	-	-
20	ERG	2	621	X	-	-	-
22	PGT	2	619	X	-	-	-
22	PGT	B	848	X	-	-	-
26	CL0	A	801	X	-	-	-

2 Entry composition (i)

There are 33 unique types of molecules in this entry. The entry contains 68571 atoms, of which 34687 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 Similar to light harvesting protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	1	173	2734	906	1353	232	235	8	0	0

- Molecule 2 is a protein called Similar to chlorophyll a/b-binding protein, CP24.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	2	179	2780	906	1385	237	244	8	0	0

- Molecule 3 is a protein called Lhcr3.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	3	174	2689	871	1348	226	237	7	0	0

- Molecule 4 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
4	A	743	11555	3802	5740	999	987	27	0	0

- Molecule 5 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
5	B	731	11464	3827	5645	982	991	19	0	0

- Molecule 6 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
6	C	80	1173	367	576	104	114	12	0	0

- Molecule 7 is a protein called Photosystem I p700 chlorophyll A apoprotein A2.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
7	D	138	2187	694	1093	192	203	5	0	0

- Molecule 8 is a protein called Photosystem I iron-sulfur center subunit VII.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
8	E	61	1002	322	509	79	92	0	0

- Molecule 9 is a protein called PSI-F.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
9	F	155	2513	816	1243	215	235	4	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
10	I	31	483	158	253	32	39	1	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
11	J	38	639	214	327	46	51	1	0	0

- Molecule 12 is a protein called PSI-K.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
12	K	54	809	253	419	65	68	4	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
13	L	136	2096	682	1057	170	185	2	0	0

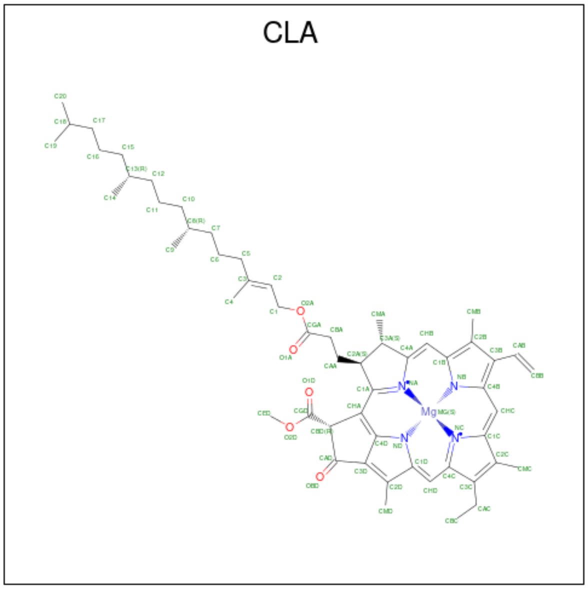
- Molecule 14 is a protein called Photosystem I reaction center subunit XII.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
14	M	27	430	136	226	32	34	2	0	0

- Molecule 15 is a protein called PsaO.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
15	O	97	1489	505	742	113	129	0	0

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



Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	Mg	N	O	
16	1	1	1474	594	770	11	44	55	0
16	1	1	1474	594	770	11	44	55	0
16	1	1	1474	594	770	11	44	55	0
16	1	1	1474	594	770	11	44	55	0
16	1	1	1474	594	770	11	44	55	0
16	1	1	1474	594	770	11	44	55	0
16	1	1	1474	594	770	11	44	55	0
16	1	1	1474	594	770	11	44	55	0

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Mol	Chain	Residues	Atoms	AltConf
16	1	1	Total C H Mg N O 1474 594 770 11 44 55	0
16	1	1	Total C H Mg N O 1474 594 770 11 44 55	0
16	1	1	Total C H Mg N O 1474 594 770 11 44 55	0
16	2	1	Total C H Mg N O 1781 713 938 13 52 65	0
16	2	1	Total C H Mg N O 1781 713 938 13 52 65	0
16	2	1	Total C H Mg N O 1781 713 938 13 52 65	0
16	2	1	Total C H Mg N O 1781 713 938 13 52 65	0
16	2	1	Total C H Mg N O 1781 713 938 13 52 65	0
16	2	1	Total C H Mg N O 1781 713 938 13 52 65	0
16	2	1	Total C H Mg N O 1781 713 938 13 52 65	0
16	2	1	Total C H Mg N O 1781 713 938 13 52 65	0
16	2	1	Total C H Mg N O 1781 713 938 13 52 65	0
16	2	1	Total C H Mg N O 1781 713 938 13 52 65	0
16	2	1	Total C H Mg N O 1781 713 938 13 52 65	0
16	2	1	Total C H Mg N O 1781 713 938 13 52 65	0
16	2	1	Total C H Mg N O 1781 713 938 13 52 65	0
16	3	1	Total C H Mg N O 1547 629 798 12 48 60	0
16	3	1	Total C H Mg N O 1547 629 798 12 48 60	0
16	3	1	Total C H Mg N O 1547 629 798 12 48 60	0
16	3	1	Total C H Mg N O 1547 629 798 12 48 60	0
16	3	1	Total C H Mg N O 1547 629 798 12 48 60	0

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Mol	Chain	Residues	Atoms	AltConf
16	3	1	Total C H Mg N O 1547 629 798 12 48 60	0
16	3	1	Total C H Mg N O 1547 629 798 12 48 60	0
16	3	1	Total C H Mg N O 1547 629 798 12 48 60	0
16	3	1	Total C H Mg N O 1547 629 798 12 48 60	0
16	3	1	Total C H Mg N O 1547 629 798 12 48 60	0
16	3	1	Total C H Mg N O 1547 629 798 12 48 60	0
16	3	1	Total C H Mg N O 1547 629 798 12 48 60	0
16	A	1	Total C H Mg N O 5649 2255 2984 41 164 205	0
16	A	1	Total C H Mg N O 5649 2255 2984 41 164 205	0
16	A	1	Total C H Mg N O 5649 2255 2984 41 164 205	0
16	A	1	Total C H Mg N O 5649 2255 2984 41 164 205	0
16	A	1	Total C H Mg N O 5649 2255 2984 41 164 205	0
16	A	1	Total C H Mg N O 5649 2255 2984 41 164 205	0
16	A	1	Total C H Mg N O 5649 2255 2984 41 164 205	0
16	A	1	Total C H Mg N O 5649 2255 2984 41 164 205	0
16	A	1	Total C H Mg N O 5649 2255 2984 41 164 205	0
16	A	1	Total C H Mg N O 5649 2255 2984 41 164 205	0
16	A	1	Total C H Mg N O 5649 2255 2984 41 164 205	0
16	A	1	Total C H Mg N O 5649 2255 2984 41 164 205	0
16	A	1	Total C H Mg N O 5649 2255 2984 41 164 205	0
16	A	1	Total C H Mg N O 5649 2255 2984 41 164 205	0

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Mol	Chain	Residues	Atoms	AltConf
16	A	1	Total C H Mg N O 5649 2255 2984 41 164 205	0
16	A	1	Total C H Mg N O 5649 2255 2984 41 164 205	0
16	A	1	Total C H Mg N O 5649 2255 2984 41 164 205	0
16	A	1	Total C H Mg N O 5649 2255 2984 41 164 205	0
16	A	1	Total C H Mg N O 5649 2255 2984 41 164 205	0
16	A	1	Total C H Mg N O 5649 2255 2984 41 164 205	0
16	A	1	Total C H Mg N O 5649 2255 2984 41 164 205	0
16	A	1	Total C H Mg N O 5649 2255 2984 41 164 205	0
16	A	1	Total C H Mg N O 5649 2255 2984 41 164 205	0
16	A	1	Total C H Mg N O 5649 2255 2984 41 164 205	0
16	A	1	Total C H Mg N O 5649 2255 2984 41 164 205	0
16	A	1	Total C H Mg N O 5649 2255 2984 41 164 205	0
16	A	1	Total C H Mg N O 5649 2255 2984 41 164 205	0
16	A	1	Total C H Mg N O 5649 2255 2984 41 164 205	0
16	A	1	Total C H Mg N O 5649 2255 2984 41 164 205	0
16	A	1	Total C H Mg N O 5649 2255 2984 41 164 205	0
16	A	1	Total C H Mg N O 5649 2255 2984 41 164 205	0
16	A	1	Total C H Mg N O 5649 2255 2984 41 164 205	0
16	A	1	Total C H Mg N O 5649 2255 2984 41 164 205	0
16	A	1	Total C H Mg N O 5649 2255 2984 41 164 205	0
16	A	1	Total C H Mg N O 5649 2255 2984 41 164 205	0

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Mol	Chain	Residues	Atoms	AltConf
16	A	1	Total C H Mg N O 5649 2255 2984 41 164 205	0
16	A	1	Total C H Mg N O 5649 2255 2984 41 164 205	0
16	A	1	Total C H Mg N O 5649 2255 2984 41 164 205	0
16	A	1	Total C H Mg N O 5649 2255 2984 41 164 205	0
16	A	1	Total C H Mg N O 5649 2255 2984 41 164 205	0
16	A	1	Total C H Mg N O 5649 2255 2984 41 164 205	0
16	B	1	Total C H Mg N O 5202 2080 2742 38 152 190	0
16	B	1	Total C H Mg N O 5202 2080 2742 38 152 190	0
16	B	1	Total C H Mg N O 5202 2080 2742 38 152 190	0
16	B	1	Total C H Mg N O 5202 2080 2742 38 152 190	0
16	B	1	Total C H Mg N O 5202 2080 2742 38 152 190	0
16	B	1	Total C H Mg N O 5202 2080 2742 38 152 190	0
16	B	1	Total C H Mg N O 5202 2080 2742 38 152 190	0
16	B	1	Total C H Mg N O 5202 2080 2742 38 152 190	0
16	B	1	Total C H Mg N O 5202 2080 2742 38 152 190	0
16	B	1	Total C H Mg N O 5202 2080 2742 38 152 190	0
16	B	1	Total C H Mg N O 5202 2080 2742 38 152 190	0
16	B	1	Total C H Mg N O 5202 2080 2742 38 152 190	0
16	B	1	Total C H Mg N O 5202 2080 2742 38 152 190	0
16	B	1	Total C H Mg N O 5202 2080 2742 38 152 190	0
16	B	1	Total C H Mg N O 5202 2080 2742 38 152 190	0

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Mol	Chain	Residues	Atoms						AltConf
16	B	1	Total 5202	C 2080	H 2742	Mg 38	N 152	O 190	0
16	B	1	Total 5202	C 2080	H 2742	Mg 38	N 152	O 190	0
16	B	1	Total 5202	C 2080	H 2742	Mg 38	N 152	O 190	0
16	B	1	Total 5202	C 2080	H 2742	Mg 38	N 152	O 190	0
16	B	1	Total 5202	C 2080	H 2742	Mg 38	N 152	O 190	0
16	B	1	Total 5202	C 2080	H 2742	Mg 38	N 152	O 190	0
16	B	1	Total 5202	C 2080	H 2742	Mg 38	N 152	O 190	0
16	B	1	Total 5202	C 2080	H 2742	Mg 38	N 152	O 190	0
16	B	1	Total 5202	C 2080	H 2742	Mg 38	N 152	O 190	0
16	B	1	Total 5202	C 2080	H 2742	Mg 38	N 152	O 190	0
16	B	1	Total 5202	C 2080	H 2742	Mg 38	N 152	O 190	0
16	B	1	Total 5202	C 2080	H 2742	Mg 38	N 152	O 190	0
16	B	1	Total 5202	C 2080	H 2742	Mg 38	N 152	O 190	0
16	B	1	Total 5202	C 2080	H 2742	Mg 38	N 152	O 190	0
16	B	1	Total 5202	C 2080	H 2742	Mg 38	N 152	O 190	0
16	B	1	Total 5202	C 2080	H 2742	Mg 38	N 152	O 190	0
16	B	1	Total 5202	C 2080	H 2742	Mg 38	N 152	O 190	0
16	B	1	Total 5202	C 2080	H 2742	Mg 38	N 152	O 190	0
16	B	1	Total 5202	C 2080	H 2742	Mg 38	N 152	O 190	0
16	B	1	Total 5202	C 2080	H 2742	Mg 38	N 152	O 190	0
16	B	1	Total 5202	C 2080	H 2742	Mg 38	N 152	O 190	0

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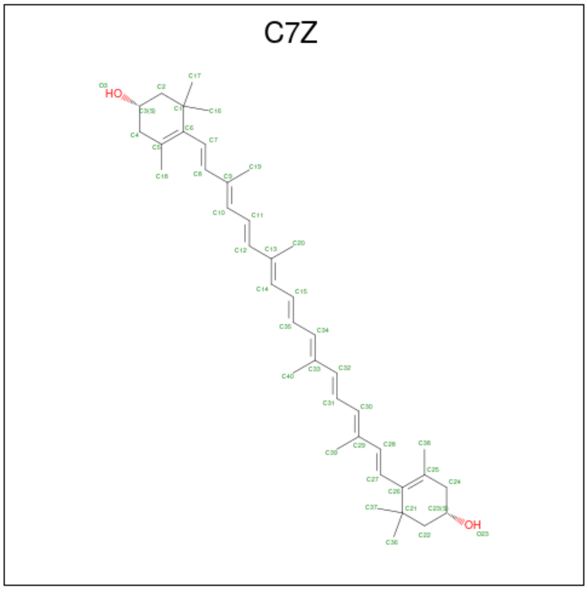
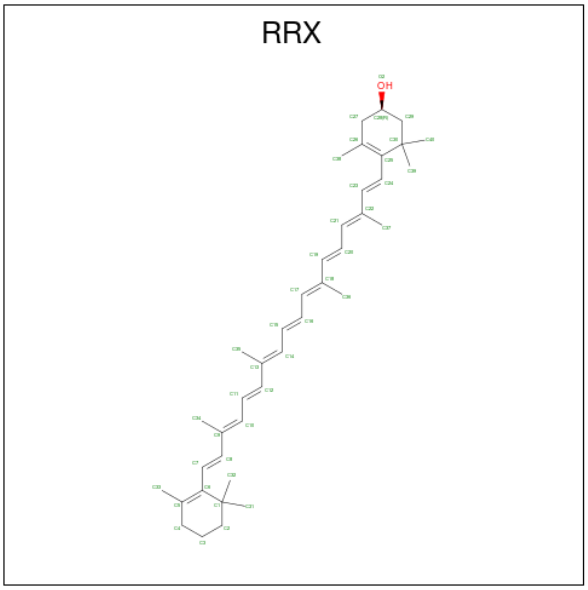
Mol	Chain	Residues	Atoms	AltConf
16	B	1	Total C H Mg N O 5202 2080 2742 38 152 190	0
16	B	1	Total C H Mg N O 5202 2080 2742 38 152 190	0
16	F	1	Total C H Mg N O 536 216 280 4 16 20	0
16	F	1	Total C H Mg N O 536 216 280 4 16 20	0
16	F	1	Total C H Mg N O 536 216 280 4 16 20	0
16	F	1	Total C H Mg N O 536 216 280 4 16 20	0
16	I	1	Total C H Mg N O 276 110 146 2 8 10	0
16	I	1	Total C H Mg N O 276 110 146 2 8 10	0
16	J	1	Total C H Mg N O 138 55 73 1 4 5	0
16	K	1	Total C H Mg N O 275 110 145 2 8 10	0
16	K	1	Total C H Mg N O 275 110 145 2 8 10	0
16	L	1	Total C H Mg N O 551 220 291 4 16 20	0
16	L	1	Total C H Mg N O 551 220 291 4 16 20	0
16	L	1	Total C H Mg N O 551 220 291 4 16 20	0
16	L	1	Total C H Mg N O 551 220 291 4 16 20	0
16	O	1	Total C H Mg N O 548 220 288 4 16 20	0
16	O	1	Total C H Mg N O 548 220 288 4 16 20	0
16	O	1	Total C H Mg N O 548 220 288 4 16 20	0
16	O	1	Total C H Mg N O 548 220 288 4 16 20	0

- Molecule 17 is (1 {S})-3,5,5-trimethyl-4-[(1 {E},3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E},17 {E})-3,7,12,16-tetramethyl-18-[(4 {S})-2,6,6-trimethyl-4-oxidanyl-cyclohexen-1-yl]octadeca-1,3,5,7,9,11,13,15,17-nonaenyl]cyclohex-3-en-1-ol (three-letter code: C7Z) (formula: $C_{40}H_{56}O_2$).



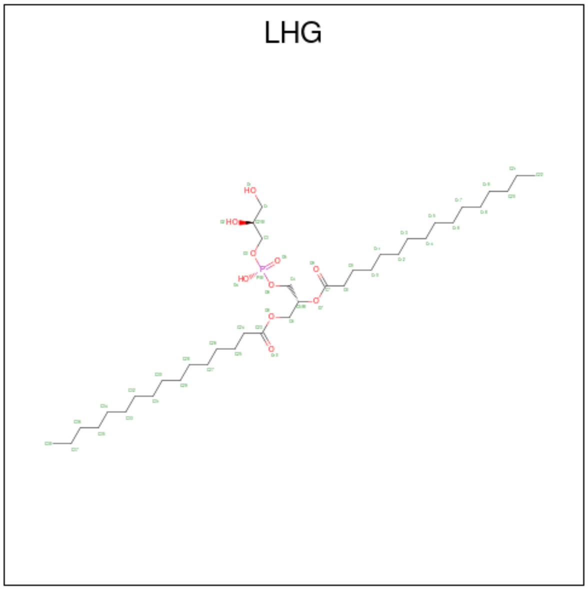
Mol	Chain	Residues	Atoms	AltConf
17	1	1	Total C O 168 160 8	0
17	1	1	Total C O 168 160 8	0
17	1	1	Total C O 168 160 8	0
17	1	1	Total C O 168 160 8	0
17	2	1	Total C O 84 80 4	0
17	2	1	Total C O 84 80 4	0
17	3	1	Total C O 210 200 10	0
17	3	1	Total C O 210 200 10	0
17	3	1	Total C O 210 200 10	0
17	3	1	Total C O 210 200 10	0
17	3	1	Total C O 210 200 10	0
17	A	1	Total C O 42 40 2	0
17	J	1	Total C O 42 40 2	0

- Molecule 18 is (3R)-beta,beta-caroten-3-ol (three-letter code: RRX) (formula: $C_{40}H_{56}O$).



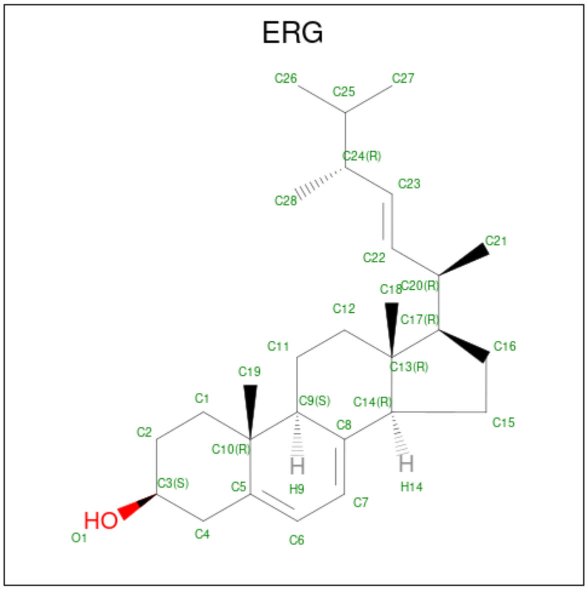
Mol	Chain	Residues	Atoms	AltConf
18	1	1	Total C H O 97 40 56 1	0
18	2	1	Total C H O 97 40 56 1	0
18	A	1	Total C H O 96 40 55 1	0
18	J	1	Total C H O 97 40 56 1	0
18	K	1	Total C H O 97 40 56 1	0

- Molecule 19 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



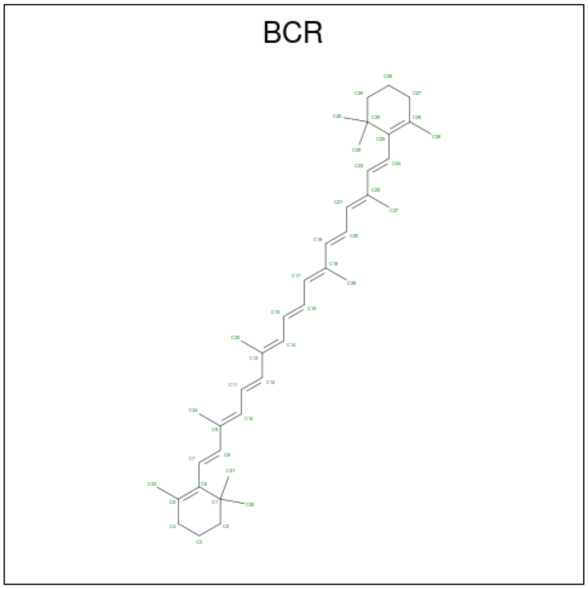
Mol	Chain	Residues	Atoms	AltConf
19	1	1	Total C H O P 123 38 74 10 1	0
19	2	1	Total C H O P 123 38 74 10 1	0
19	3	1	Total C H O P 123 38 74 10 1	0
19	A	1	Total C H O P 246 76 148 20 2	0
19	A	1	Total C H O P 246 76 148 20 2	0
19	B	1	Total C H O P 108 34 63 10 1	0

- Molecule 20 is ERGOSTEROL (three-letter code: ERG) (formula: $C_{28}H_{44}O$).



Mol	Chain	Residues	Atoms				AltConf
20	1	1	Total 67	C 28	H 38	O 1	0
20	2	1	Total 134	C 56	H 76	O 2	0
20	2	1	Total 134	C 56	H 76	O 2	0

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



Mol	Chain	Residues	Atoms			AltConf
21	2	1	Total 93	C 40	H 53	0

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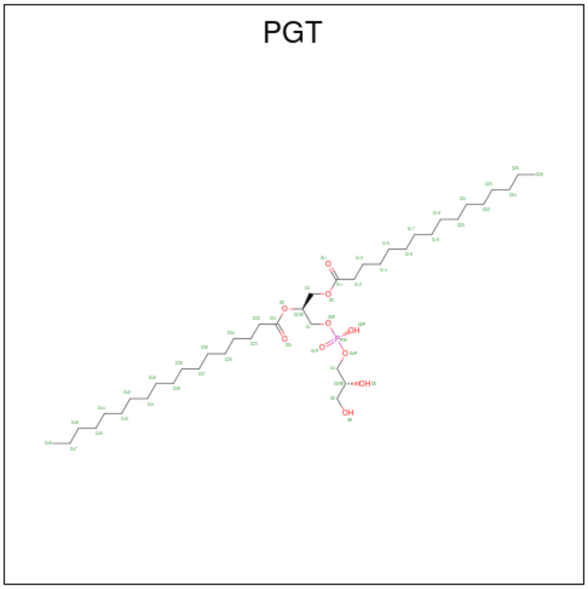
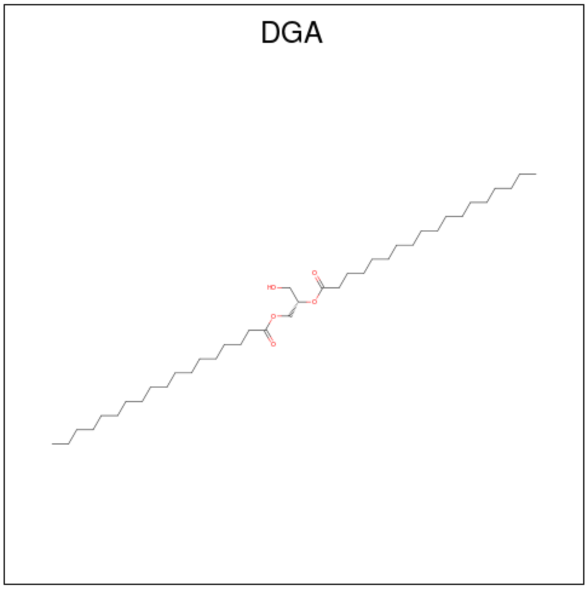
Mol	Chain	Residues	Atoms	AltConf
21	A	1	Total C H 460 200 260	0
21	A	1	Total C H 460 200 260	0
21	A	1	Total C H 460 200 260	0
21	A	1	Total C H 460 200 260	0
21	A	1	Total C H 460 200 260	0
21	B	1	Total C H 733 320 413	0
21	B	1	Total C H 733 320 413	0
21	B	1	Total C H 733 320 413	0
21	B	1	Total C H 733 320 413	0
21	B	1	Total C H 733 320 413	0
21	B	1	Total C H 733 320 413	0
21	B	1	Total C H 733 320 413	0
21	B	1	Total C H 733 320 413	0
21	F	1	Total C H 184 80 104	0
21	F	1	Total C H 184 80 104	0
21	I	1	Total C H 91 40 51	0
21	K	1	Total C H 91 40 51	0
21	L	1	Total C H 276 120 156	0
21	L	1	Total C H 276 120 156	0
21	L	1	Total C H 276 120 156	0
21	O	1	Total C H 92 40 52	0

- Molecule 22 is (1S)-2-{[{[(2R)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL STEARATE (three-letter code: PGT) (formula: $C_{40}H_{79}O_{10}P$).



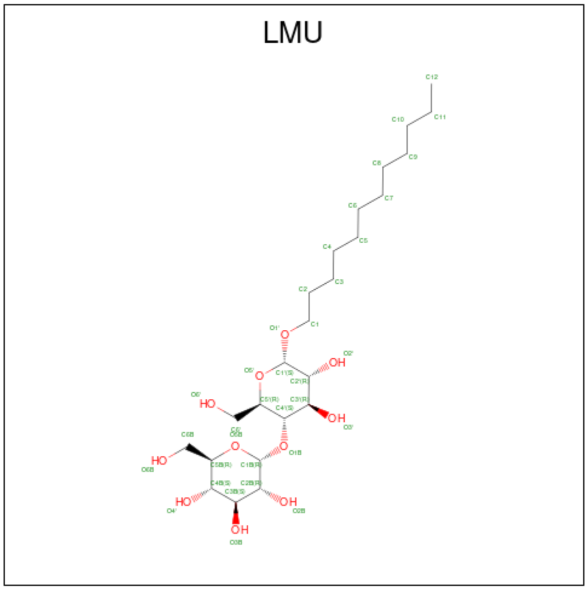
Mol	Chain	Residues	Atoms					AltConf
			Total	C	H	O	P	
22	2	1	81	24	46	10	1	0
22	B	1	81	24	46	10	1	0

- Molecule 23 is DIACYL GLYCEROL (three-letter code: DGA) (formula: $C_{39}H_{76}O_5$).



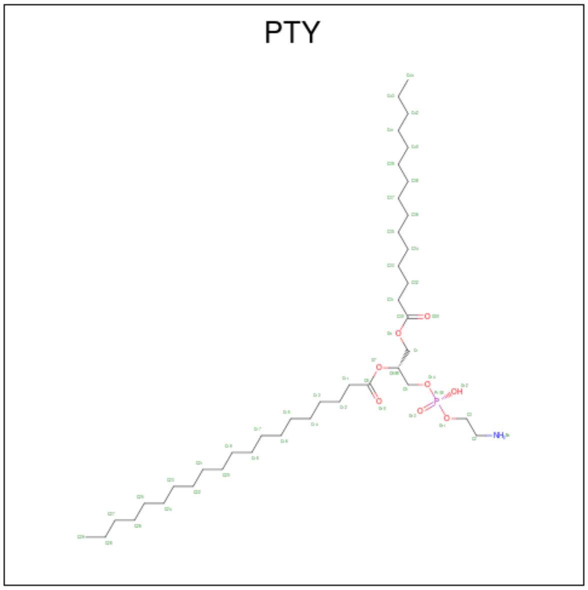
Mol	Chain	Residues	Atoms				AltConf
23	2	1	Total	C	H	O	0
			120	39	76	5	
23	J	1	Total	C	H	O	0
			120	39	76	5	

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



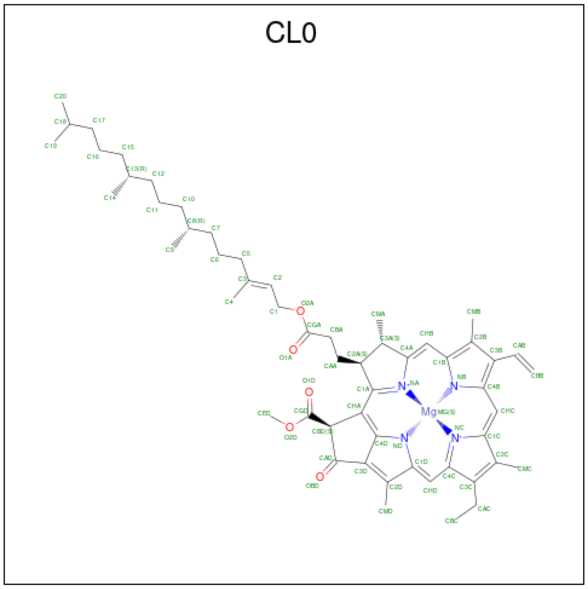
Mol	Chain	Residues	Atoms				AltConf
24	3	1	Total	C	H	O	0
			81	24	46	11	
24	A	1	Total	C	H	O	0
			81	24	46	11	

- Molecule 25 is PHOSPHATIDYLETHANOLAMINE (three-letter code: PTY) (formula: $C_{40}H_{80}NO_8P$).



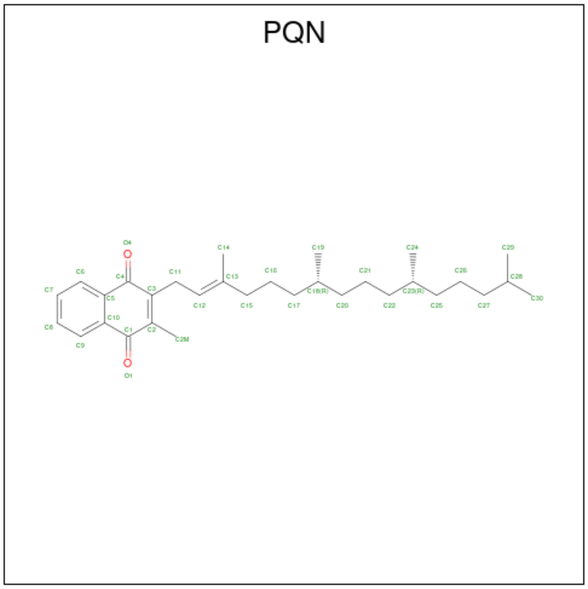
Mol	Chain	Residues	Atoms	AltConf
25	3	1	Total C H N O P 258 80 158 2 16 2	0
25	3	1	Total C H N O P 258 80 158 2 16 2	0
25	A	1	Total C H N O P 113 37 66 1 8 1	0
25	L	1	Total C H N O P 129 40 79 1 8 1	0

- Molecule 26 is CHLOROPHYLL A ISOMER (three-letter code: CL0) (formula: $C_{55}H_{72}MgN_4O_5$).



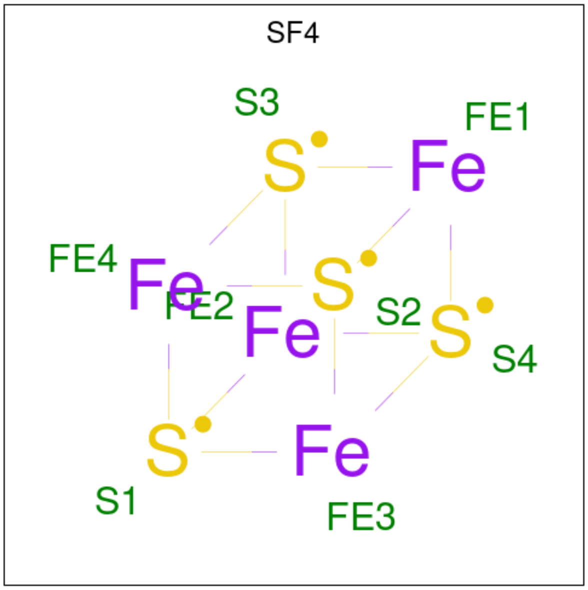
Mol	Chain	Residues	Atoms						AltConf
26	A	1	Total 138	C 55	H 73	Mg 1	N 4	O 5	0

- Molecule 27 is PHYLLOQUINONE (three-letter code: PQN) (formula: $C_{31}H_{46}O_2$).



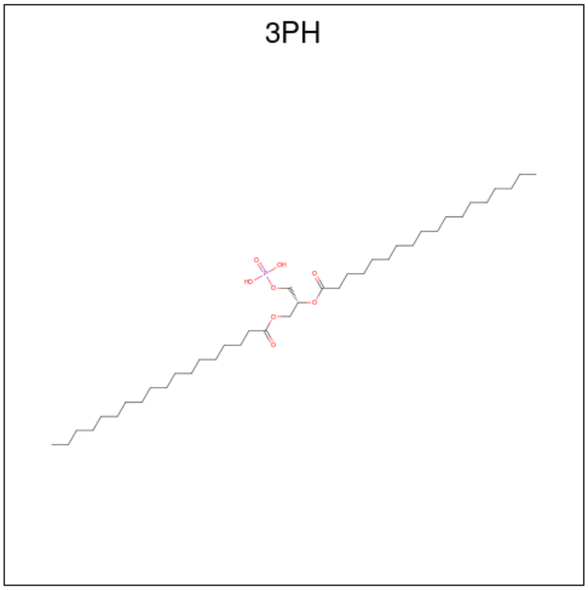
Mol	Chain	Residues	Atoms				AltConf
27	A	1	Total 79	C 31	H 46	O 2	0
27	B	1	Total 79	C 31	H 46	O 2	0

- Molecule 28 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



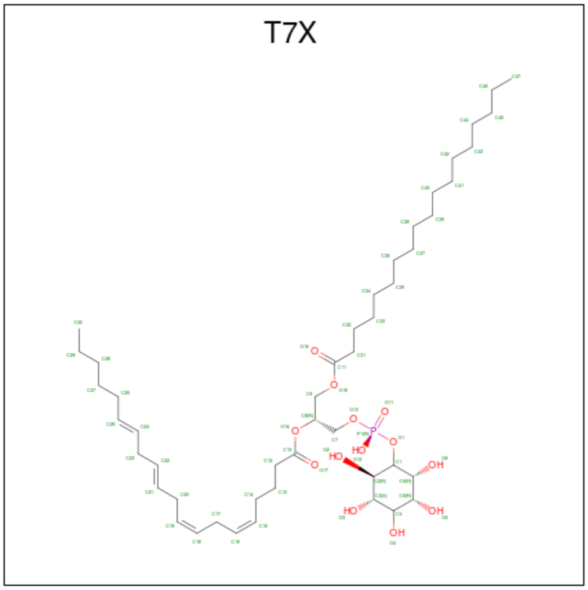
Mol	Chain	Residues	Atoms			AltConf
28	A	1	Total 8	Fe 4	S 4	0
28	C	1	Total 16	Fe 8	S 8	0
28	C	1	Total 16	Fe 8	S 8	0

- Molecule 29 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (three-letter code: 3PH) (formula: $C_{39}H_{77}O_8P$).



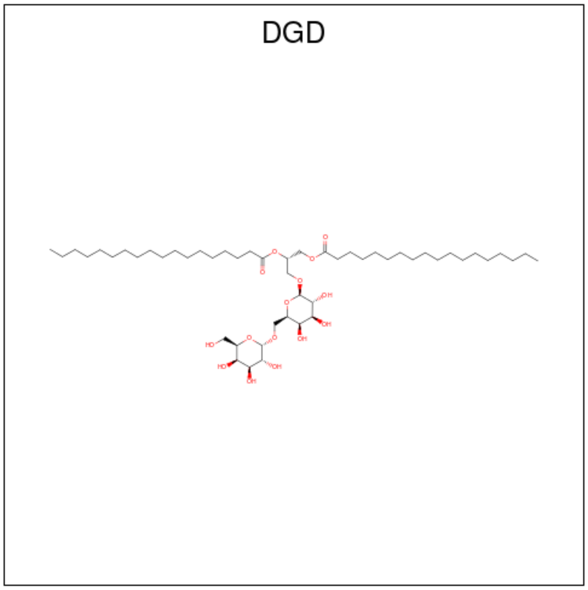
Mol	Chain	Residues	Atoms					AltConf
29	A	1	Total 123	C 39	H 75	O 8	P 1	0
29	B	1	Total 123	C 39	H 75	O 8	P 1	0
29	J	1	Total 123	C 39	H 75	O 8	P 1	0

- Molecule 30 is Phosphatidylinositol (three-letter code: T7X) (formula: $C_{47}H_{83}O_{13}P$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	H	O	P	
30	A	1	123	40	69	13	1	0

- Molecule 31 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	H	O	
31	B	1	450	153	252	45	0
31	B	1	450	153	252	45	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	H	O	
31	B	1	450	153	252	45	0

- Molecule 32 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
			Total	Ca	
32	B	2	2	2	0

- Molecule 33 is water.

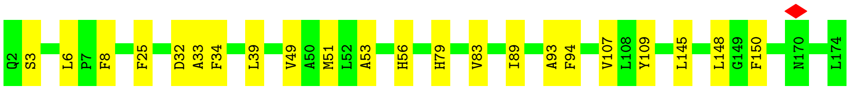
Mol	Chain	Residues	Atoms		AltConf
			Total	O	
33	1	15	15	15	0
33	2	8	8	8	0
33	3	6	6	6	0
33	A	79	79	79	0
33	B	68	68	68	0
33	C	24	24	24	0
33	D	14	14	14	0
33	E	11	11	11	0
33	F	11	11	11	0
33	J	2	2	2	0
33	K	2	2	2	0
33	L	2	2	2	0
33	M	2	2	2	0
33	O	5	5	5	0

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.

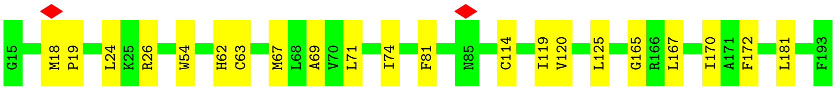
- Molecule 1: Similar to light harvesting protein

Chain 1:



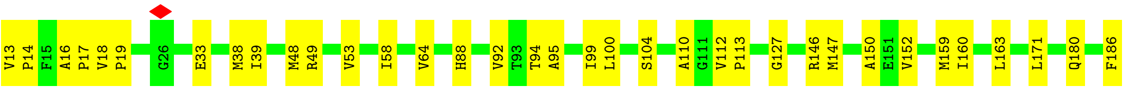
- Molecule 2: Similar to chlorophyll a/b-binding protein, CP24

Chain 2:



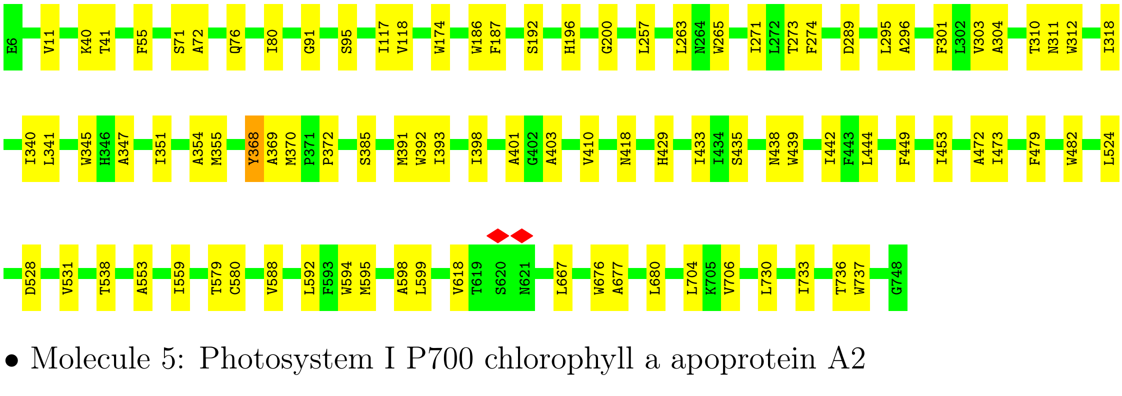
- Molecule 3: Lhcr3

Chain 3:



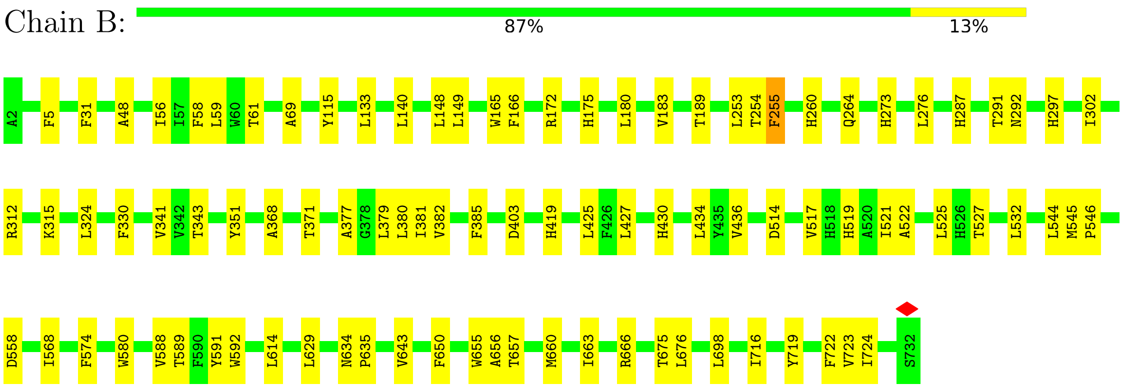
- Molecule 4: Photosystem I P700 chlorophyll a apoprotein A1

Chain A:



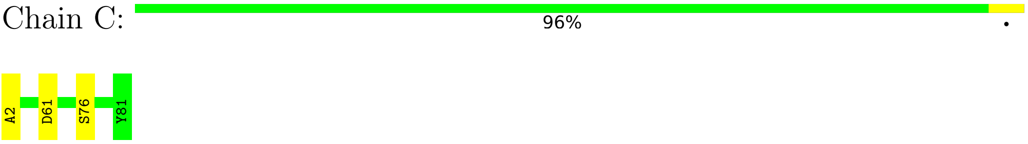
- Molecule 5: Photosystem I P700 chlorophyll a apoprotein A2

Chain B:



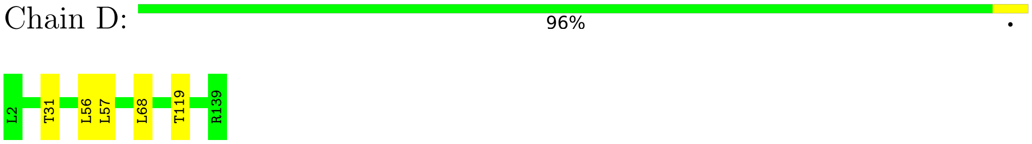
- Molecule 6: Photosystem I iron-sulfur center

Chain C:



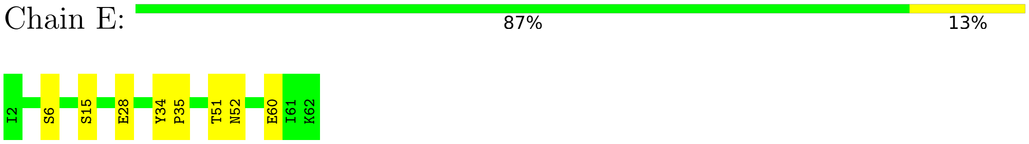
- Molecule 7: Photosystem I p700 chlorophyll A apoprotein A2

Chain D:



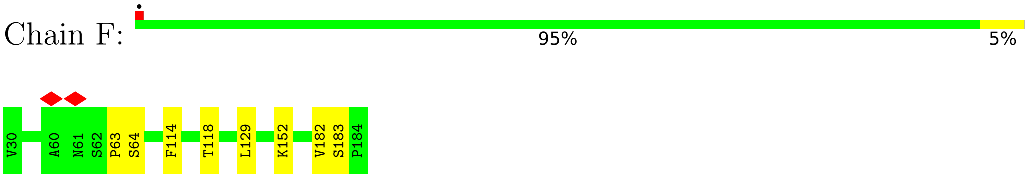
- Molecule 8: Photosystem I iron-sulfur center subunit VII

Chain E:



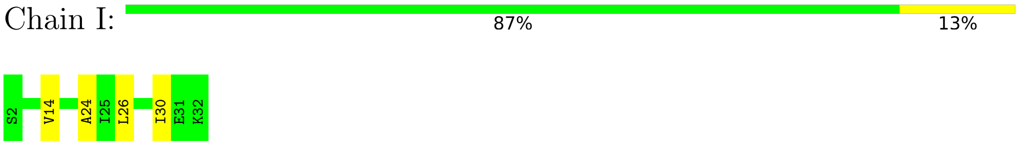
- Molecule 9: PSI-F

Chain F:



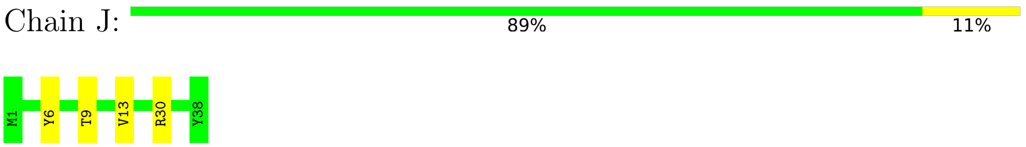
- Molecule 10: Photosystem I reaction center subunit VIII

Chain I:



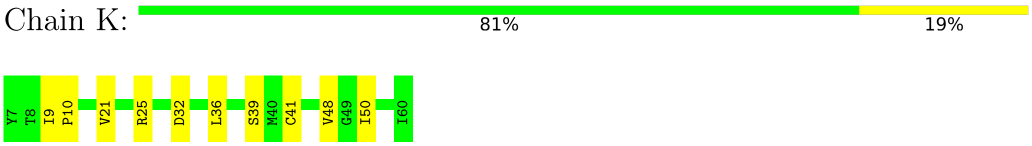
- Molecule 11: Photosystem I reaction center subunit IX

Chain J:



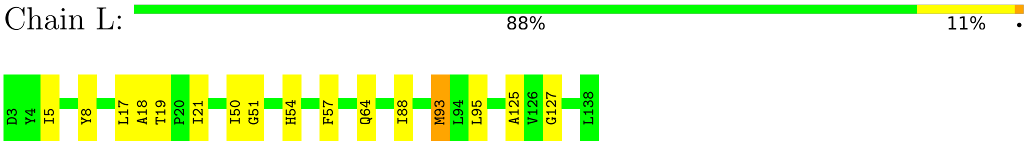
- Molecule 12: PSI-K

Chain K:



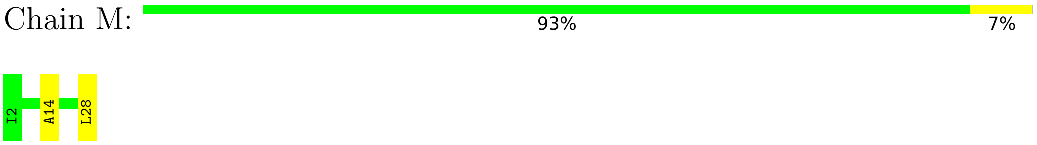
- Molecule 13: Photosystem I reaction center subunit XI

Chain L:



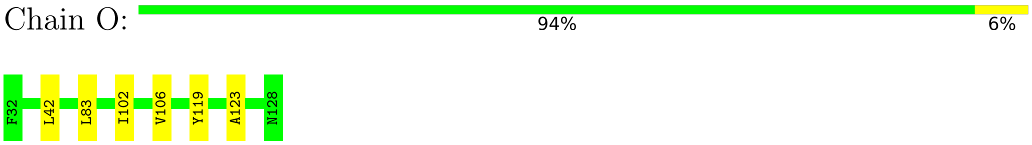
- Molecule 14: Photosystem I reaction center subunit XII

Chain M:



- Molecule 15: PsaO

Chain O:



4 Experimental information ⓘ

Property	**Value**	**Source**
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	128943	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{Å}^2$)	40.0	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.163	Depositor
Minimum map value	-0.074	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.0186	Depositor
Map size (Å)	315.59998, 315.59998, 315.59998	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0519999, 1.0519999, 1.0519999	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: BCR, CLA, CL0, PTY, PGT, ERG, PQN, CA, 3PH, T7X, C7Z, DGA, DGD, SF4, RRX, LHG, LMU

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	1	0.28	0/1426	0.52	0/1927
2	2	0.27	0/1431	0.50	0/1931
3	3	0.25	0/1376	0.52	0/1867
4	A	0.26	0/6002	0.49	0/8179
5	B	0.25	0/6028	0.47	0/8236
6	C	0.24	0/607	0.53	0/822
7	D	0.25	0/1118	0.53	0/1509
8	E	0.24	0/502	0.50	0/680
9	F	0.25	0/1304	0.51	0/1772
10	I	0.25	0/235	0.44	0/321
11	J	0.26	0/321	0.47	0/437
12	K	0.25	0/394	0.46	0/534
13	L	0.26	0/1064	0.53	1/1448 (0.1%)
14	M	0.25	0/205	0.38	0/277
15	O	0.27	0/773	0.45	0/1061
All	All	0.26	0/22786	0.49	1/31001 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	L	93	MET	CG-SD-CE	-6.72	89.44	100.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1381	1353	1353	21	0
2	2	1395	1385	1385	21	0
3	3	1341	1348	1348	38	0
4	A	5815	5740	5740	88	0
5	B	5819	5645	5645	85	0
6	C	597	576	576	2	0
7	D	1094	1093	1093	3	0
8	E	493	509	509	6	0
9	F	1270	1243	1243	9	0
10	I	230	253	253	4	0
11	J	312	327	327	3	0
12	K	390	419	419	8	0
13	L	1039	1057	1057	15	0
14	M	204	226	226	2	0
15	O	747	742	742	8	0
16	1	704	770	759	36	0
16	2	843	938	928	42	0
16	3	749	798	786	49	0
16	A	2665	2984	2944	151	0
16	B	2460	2742	2705	132	0
16	F	256	280	276	13	0
16	I	130	146	144	9	0
16	J	65	73	71	3	0
16	K	130	145	144	6	0
16	L	260	291	287	14	0
16	O	260	288	284	13	0
17	1	168	0	0	7	0
17	2	84	0	0	0	0
17	3	210	0	0	11	0
17	A	42	0	0	0	0
17	J	42	0	0	0	0
18	1	41	56	56	10	0
18	2	41	56	56	2	0
18	A	41	55	56	2	0
18	J	41	56	56	2	0
18	K	41	56	56	4	0
19	1	49	74	74	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	2	49	74	74	1	0
19	3	49	74	74	2	0
19	A	98	148	148	1	0
19	B	45	63	63	0	0
20	1	29	38	38	4	0
20	2	58	76	76	9	0
21	2	40	53	54	10	0
21	A	200	260	260	43	0
21	B	320	413	415	47	0
21	F	80	104	105	9	0
21	I	40	51	53	3	0
21	K	40	51	54	5	0
21	L	120	156	156	20	0
21	O	40	52	52	9	0
22	2	35	46	40	0	0
22	B	35	46	40	0	0
23	2	44	76	76	0	0
23	J	44	76	76	1	0
24	3	35	46	46	1	0
24	A	35	46	46	0	0
25	3	100	158	158	0	0
25	A	47	66	66	3	0
25	L	50	79	79	0	0
26	A	65	73	72	5	0
27	A	33	46	46	0	0
27	B	33	46	46	4	0
28	A	8	0	0	0	0
28	C	16	0	0	0	0
29	A	48	75	75	0	0
29	B	48	75	75	0	0
29	J	48	75	75	0	0
30	A	54	69	0	1	0
31	B	198	252	288	9	0
32	B	2	0	0	0	0
33	1	15	0	0	0	0
33	2	8	0	0	0	0
33	3	6	0	0	0	0
33	A	79	0	0	0	0
33	B	68	0	0	0	0
33	C	24	0	0	0	0
33	D	14	0	0	0	0
33	E	11	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	F	11	0	0	0	0
33	J	2	0	0	0	0
33	K	2	0	0	0	0
33	L	2	0	0	0	0
33	M	2	0	0	0	0
33	O	5	0	0	0	0
All	All	33884	34687	34524	699	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 10.

The worst 5 of 699 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)
20:2:621:ERG:C3	20:2:621:ERG:O1	1.70	1.39
20:2:618:ERG:O1	20:2:618:ERG:C3	1.70	1.37
20:1:618:ERG:C3	20:1:618:ERG:O1	1.70	1.36
16:A:854:CLA:HBB1	16:A:854:CLA:HMB1	1.36	1.04
16:A:828:CLA:HBB1	16:A:828:CLA:HMB1	1.37	1.01

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	171/173 (99%)	163 (95%)	8 (5%)	0	100	100
2	2	177/179 (99%)	167 (94%)	10 (6%)	0	100	100
3	3	172/174 (99%)	160 (93%)	12 (7%)	0	100	100
4	A	741/743 (100%)	714 (96%)	27 (4%)	0	100	100
5	B	729/731 (100%)	703 (96%)	26 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	C	78/80 (98%)	75 (96%)	3 (4%)	0	100	100
7	D	136/138 (99%)	128 (94%)	8 (6%)	0	100	100
8	E	59/61 (97%)	56 (95%)	3 (5%)	0	100	100
9	F	153/155 (99%)	144 (94%)	9 (6%)	0	100	100
10	I	29/31 (94%)	27 (93%)	2 (7%)	0	100	100
11	J	36/38 (95%)	36 (100%)	0	0	100	100
12	K	52/54 (96%)	52 (100%)	0	0	100	100
13	L	134/136 (98%)	126 (94%)	8 (6%)	0	100	100
14	M	25/27 (93%)	25 (100%)	0	0	100	100
15	O	95/97 (98%)	92 (97%)	3 (3%)	0	100	100
All	All	2787/2817 (99%)	2668 (96%)	119 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	143/143 (100%)	143 (100%)	0	100	100
2	2	144/144 (100%)	144 (100%)	0	100	100
3	3	136/136 (100%)	136 (100%)	0	100	100
4	A	600/600 (100%)	597 (100%)	3 (0%)	88	94
5	B	598/598 (100%)	595 (100%)	3 (0%)	88	94
6	C	66/66 (100%)	66 (100%)	0	100	100
7	D	117/117 (100%)	117 (100%)	0	100	100
8	E	58/58 (100%)	58 (100%)	0	100	100
9	F	137/137 (100%)	137 (100%)	0	100	100
10	I	26/26 (100%)	26 (100%)	0	100	100
11	J	34/34 (100%)	34 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	K	43/43 (100%)	42 (98%)	1 (2%)	50	77
13	L	109/109 (100%)	109 (100%)	0	100	100
14	M	22/22 (100%)	22 (100%)	0	100	100
15	O	75/75 (100%)	75 (100%)	0	100	100
All	All	2308/2308 (100%)	2301 (100%)	7 (0%)	92	96

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	B	255	PHE
5	B	351	TYR
12	K	25	ARG
5	B	514	ASP
4	A	368	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	56	HIS
2	2	130	ASN
4	A	533	HIS
5	B	437	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 206 ligands modelled in this entry, 2 are monoatomic - leaving 204 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	$\#\|Z\| > 2$
16	CLA	1	604	-	65,73,73	1.38	8 (12%)	76,113,113	1.90	15 (19%)
16	CLA	A	833	-	65,73,73	1.37	9 (13%)	76,113,113	1.91	16 (21%)
16	CLA	B	802	-	65,73,73	1.38	9 (13%)	76,113,113	1.92	14 (18%)
17	C7Z	J	104	-	43,43,43	5.40	26 (60%)	58,60,60	2.55	23 (39%)
16	CLA	F	205	9	65,73,73	1.38	8 (12%)	76,113,113	1.94	14 (18%)
21	BCR	2	617	-	41,41,41	1.90	5 (12%)	56,56,56	4.54	20 (35%)
21	BCR	L	207	-	41,41,41	1.85	4 (9%)	56,56,56	4.57	23 (41%)
16	CLA	3	204	3	63,71,73	1.39	9 (14%)	73,110,113	1.90	12 (16%)
16	CLA	L	204	-	65,73,73	1.38	9 (13%)	76,113,113	1.83	15 (19%)
16	CLA	A	831	-	65,73,73	1.38	9 (13%)	76,113,113	1.83	14 (18%)
16	CLA	1	610	-	65,73,73	1.36	9 (13%)	76,113,113	1.98	15 (19%)
17	C7Z	3	201	-	43,43,43	5.42	26 (60%)	58,60,60	2.37	20 (34%)
17	C7Z	3	217	-	43,43,43	5.36	25 (58%)	58,60,60	2.58	22 (37%)
16	CLA	3	209	3	65,73,73	1.37	10 (15%)	76,113,113	1.91	15 (19%)
16	CLA	A	836	-	65,73,73	1.37	9 (13%)	76,113,113	1.95	17 (22%)
16	CLA	B	810	-	65,73,73	1.36	8 (12%)	76,113,113	1.87	15 (19%)
16	CLA	I	101	-	65,73,73	1.35	8 (12%)	76,113,113	1.91	14 (18%)
16	CLA	A	807	-	65,73,73	1.36	8 (12%)	76,113,113	1.92	15 (19%)
16	CLA	2	609	-	65,73,73	1.36	9 (13%)	76,113,113	1.91	15 (19%)
16	CLA	B	805	-	65,73,73	1.36	9 (13%)	76,113,113	1.90	15 (19%)
16	CLA	B	831	33	65,73,73	1.36	8 (12%)	76,113,113	1.90	14 (18%)
16	CLA	B	820	-	65,73,73	1.37	9 (13%)	76,113,113	1.96	15 (19%)
21	BCR	F	206	-	41,41,41	1.86	4 (9%)	56,56,56	4.22	23 (41%)
16	CLA	3	211	-	65,73,73	1.37	9 (13%)	76,113,113	1.96	16 (21%)
21	BCR	A	844	-	41,41,41	1.86	4 (9%)	56,56,56	4.26	21 (37%)
16	CLA	A	827	-	65,73,73	1.36	9 (13%)	76,113,113	1.89	14 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
31	DGD	B	846	-	67,67,67	1.19	7 (10%)	81,81,81	1.03	3 (3%)
19	LHG	2	622	16	48,48,48	0.40	0	51,54,54	1.06	4 (7%)
31	DGD	B	849	-	67,67,67	1.20	8 (11%)	81,81,81	1.04	5 (6%)
16	CLA	A	856	-	65,73,73	1.35	8 (12%)	76,113,113	1.92	16 (21%)
16	CLA	B	833	-	65,73,73	1.36	9 (13%)	76,113,113	1.86	18 (23%)
16	CLA	A	839	33	65,73,73	1.38	9 (13%)	76,113,113	1.87	12 (15%)
16	CLA	2	606	-	65,73,73	1.36	9 (13%)	76,113,113	1.96	14 (18%)
16	CLA	A	826	-	65,73,73	1.36	9 (13%)	76,113,113	1.89	12 (15%)
21	BCR	B	847	-	41,41,41	1.88	4 (9%)	56,56,56	4.87	26 (46%)
16	CLA	B	826	-	65,73,73	1.37	9 (13%)	76,113,113	1.88	14 (18%)
30	T7X	A	851	-	54,54,61	0.88	4 (7%)	64,66,73	1.00	3 (4%)
17	C7Z	1	612	-	43,43,43	5.41	25 (58%)	58,60,60	2.10	16 (27%)
25	PTY	3	221	-	49,49,49	0.89	4 (8%)	52,54,54	0.98	2 (3%)
16	CLA	F	204	-	65,73,73	1.37	9 (13%)	76,113,113	1.82	14 (18%)
23	DGA	2	620	-	43,43,43	1.17	3 (6%)	45,45,45	1.16	3 (6%)
21	BCR	L	206	-	41,41,41	1.82	5 (12%)	56,56,56	4.49	19 (33%)
16	CLA	3	213	-	46,54,73	1.61	9 (19%)	53,90,113	2.17	13 (24%)
16	CLA	A	814	-	65,73,73	1.35	9 (13%)	76,113,113	1.97	17 (22%)
16	CLA	B	813	-	65,73,73	1.35	8 (12%)	76,113,113	1.88	15 (19%)
16	CLA	2	612	-	65,73,73	1.38	9 (13%)	76,113,113	1.85	15 (19%)
16	CLA	3	210	3	65,73,73	1.35	8 (12%)	76,113,113	2.17	18 (23%)
16	CLA	A	817	-	65,73,73	1.37	8 (12%)	76,113,113	1.87	16 (21%)
26	CL0	A	801	-	65,73,73	2.35	19 (29%)	76,113,113	2.48	23 (30%)
16	CLA	A	804	-	65,73,73	1.39	11 (16%)	76,113,113	1.91	18 (23%)
16	CLA	F	201	-	61,69,73	1.41	9 (14%)	71,108,113	1.81	14 (19%)
24	LMU	3	202	-	36,36,36	0.46	0	47,47,47	0.74	0
16	CLA	A	802	-	65,73,73	1.37	9 (13%)	76,113,113	2.00	14 (18%)
16	CLA	A	855	33	65,73,73	1.39	8 (12%)	76,113,113	1.76	13 (17%)
16	CLA	A	822	-	65,73,73	1.36	8 (12%)	76,113,113	1.89	16 (21%)
16	CLA	O	201	-	65,73,73	1.33	8 (12%)	76,113,113	2.01	17 (22%)
16	CLA	B	832	-	65,73,73	1.38	9 (13%)	76,113,113	1.92	16 (21%)
16	CLA	1	603	-	65,73,73	1.38	9 (13%)	76,113,113	1.92	18 (23%)
16	CLA	F	202	-	65,73,73	1.37	9 (13%)	76,113,113	2.12	20 (26%)
16	CLA	1	609	-	65,73,73	1.40	8 (12%)	76,113,113	1.81	14 (18%)
19	LHG	A	842	-	48,48,48	0.40	0	51,54,54	0.93	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$\|Z\| > 2$	Counts	RMSZ	#$\|Z\| > 2$
25	PTY	A	852	-	45,45,49	0.92	4 (8%)	47,49,54	1.01	2 (4%)
21	BCR	B	841	-	41,41,41	1.79	4 (9%)	56,56,56	4.44	26 (46%)
16	CLA	2	610	19	65,73,73	1.38	9 (13%)	76,113,113	2.00	17 (22%)
17	C7Z	2	615	-	43,43,43	5.41	26 (60%)	58,60,60	2.57	22 (37%)
21	BCR	F	203	-	41,41,41	1.83	4 (9%)	56,56,56	4.72	22 (39%)
16	CLA	2	603	-	65,73,73	1.37	11 (16%)	76,113,113	1.85	15 (19%)
16	CLA	A	805	-	65,73,73	1.34	8 (12%)	76,113,113	1.91	14 (18%)
16	CLA	A	820	33	65,73,73	1.38	10 (15%)	76,113,113	1.84	13 (17%)
21	BCR	A	857	-	41,41,41	1.85	4 (9%)	56,56,56	4.85	26 (46%)
16	CLA	3	203	-	65,73,73	1.37	9 (13%)	76,113,113	2.01	16 (21%)
16	CLA	O	203	-	65,73,73	1.39	9 (13%)	76,113,113	1.89	14 (18%)
16	CLA	1	606	-	65,73,73	1.35	9 (13%)	76,113,113	2.10	18 (23%)
16	CLA	L	205	-	65,73,73	1.35	9 (13%)	76,113,113	1.97	14 (18%)
28	SF4	C	102	6	0,12,12	-	-	-		
16	CLA	B	817	-	65,73,73	1.36	9 (13%)	76,113,113	1.84	13 (17%)
16	CLA	A	824	33	65,73,73	1.38	10 (15%)	76,113,113	1.89	14 (18%)
16	CLA	B	824	-	65,73,73	1.34	7 (10%)	76,113,113	1.90	17 (22%)
19	LHG	3	219	-	48,48,48	0.41	0	51,54,54	0.93	3 (5%)
16	CLA	A	811	-	65,73,73	1.36	9 (13%)	76,113,113	1.88	15 (19%)
16	CLA	2	607	-	65,73,73	1.38	9 (13%)	76,113,113	1.82	11 (14%)
21	BCR	B	845	-	41,41,41	1.84	4 (9%)	56,56,56	4.44	19 (33%)
16	CLA	A	828	-	65,73,73	1.37	9 (13%)	76,113,113	1.80	14 (18%)
16	CLA	3	212	-	58,66,73	1.44	9 (15%)	67,104,113	2.09	17 (25%)
16	CLA	A	832	-	65,73,73	1.37	10 (15%)	76,113,113	1.88	15 (19%)
16	CLA	B	829	-	65,73,73	1.37	10 (15%)	76,113,113	1.88	14 (18%)
24	LMU	A	853	-	36,36,36	0.44	0	47,47,47	0.75	0
16	CLA	B	830	-	65,73,73	1.35	9 (13%)	76,113,113	1.83	15 (19%)
16	CLA	B	806	-	65,73,73	1.35	9 (13%)	76,113,113	1.89	16 (21%)
16	CLA	1	601	-	65,73,73	1.37	8 (12%)	76,113,113	1.87	15 (19%)
16	CLA	K	102	-	65,73,73	1.37	8 (12%)	76,113,113	1.85	13 (17%)
16	CLA	B	812	-	65,73,73	1.37	9 (13%)	76,113,113	1.92	17 (22%)
20	ERG	2	621	-	31,32,32	8.27	19 (61%)	47,50,50	2.95	18 (38%)
16	CLA	L	203	13	65,73,73	1.37	9 (13%)	76,113,113	1.86	15 (19%)
16	CLA	2	604	-	65,73,73	1.35	9 (13%)	76,113,113	1.99	17 (22%)
16	CLA	B	838	22	65,73,73	1.36	9 (13%)	76,113,113	1.93	17 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
16	CLA	B	814	-	65,73,73	1.36	10 (15%)	76,113,113	1.88	14 (18%)
16	CLA	A	821	-	65,73,73	1.36	9 (13%)	76,113,113	1.98	19 (25%)
16	CLA	1	607	1	60,68,73	1.41	8 (13%)	70,107,113	1.95	14 (20%)
16	CLA	A	809	-	65,73,73	1.38	9 (13%)	76,113,113	1.80	14 (18%)
16	CLA	B	835	-	65,73,73	1.37	9 (13%)	76,113,113	1.87	16 (21%)
16	CLA	B	809	5	65,73,73	1.35	9 (13%)	76,113,113	2.07	19 (25%)
28	SF4	C	101	6	0,12,12	-	-	-		
16	CLA	1	611	-	65,73,73	1.38	9 (13%)	76,113,113	1.84	13 (17%)
23	DGA	J	101	-	43,43,43	1.15	3 (6%)	45,45,45	1.16	3 (6%)
17	C7Z	1	615	-	43,43,43	5.38	26 (60%)	58,60,60	2.45	19 (32%)
16	CLA	B	828	-	65,73,73	1.38	9 (13%)	76,113,113	1.83	13 (17%)
16	CLA	3	214	-	65,73,73	1.38	9 (13%)	76,113,113	1.92	15 (19%)
19	LHG	B	851	-	44,44,48	0.42	0	47,50,54	0.95	3 (6%)
16	CLA	2	608	-	65,73,73	1.39	8 (12%)	76,113,113	1.98	18 (23%)
16	CLA	A	808	4	65,73,73	1.38	9 (13%)	76,113,113	1.93	18 (23%)
16	CLA	A	823	-	65,73,73	1.36	8 (12%)	76,113,113	1.83	15 (19%)
20	ERG	2	618	-	31,32,32	8.30	18 (58%)	47,50,50	3.52	22 (46%)
27	PQN	B	839	-	34,34,34	0.46	0	42,45,45	1.00	2 (4%)
16	CLA	B	823	-	65,73,73	1.36	8 (12%)	76,113,113	1.83	14 (18%)
16	CLA	2	611	2	65,73,73	1.38	9 (13%)	76,113,113	1.91	16 (21%)
18	RRX	J	103	-	42,42,42	4.92	24 (57%)	57,58,58	3.14	30 (52%)
16	CLA	B	819	-	65,73,73	1.39	9 (13%)	76,113,113	1.93	14 (18%)
25	PTY	3	220	-	49,49,49	0.89	4 (8%)	52,54,54	1.06	2 (3%)
16	CLA	1	602	1	59,67,73	1.42	8 (13%)	68,105,113	2.07	16 (23%)
29	3PH	A	849	-	47,47,47	0.86	4 (8%)	51,52,52	1.07	2 (3%)
16	CLA	2	605	-	65,73,73	1.36	8 (12%)	76,113,113	1.88	16 (21%)
16	CLA	L	201	-	65,73,73	1.39	9 (13%)	76,113,113	1.83	16 (21%)
22	PGT	2	619	-	34,34,50	1.45	6 (17%)	37,40,56	1.03	2 (5%)
16	CLA	J	102	11	65,73,73	1.37	9 (13%)	76,113,113	2.06	17 (22%)
16	CLA	B	803	33	65,73,73	1.40	9 (13%)	76,113,113	1.79	15 (19%)
17	C7Z	2	614	-	43,43,43	5.39	26 (60%)	58,60,60	2.31	17 (29%)
21	BCR	B	843	-	41,41,41	1.84	4 (9%)	56,56,56	4.82	27 (48%)
18	RRX	A	847	-	42,42,42	4.98	25 (59%)	57,58,58	2.92	26 (45%)
18	RRX	1	613	-	42,42,42	4.96	25 (59%)	57,58,58	2.41	20 (35%)
16	CLA	B	821	-	65,73,73	1.39	9 (13%)	76,113,113	2.09	17 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
16	CLA	I	102	-	65,73,73	1.36	8 (12%)	76,113,113	1.83	14 (18%)
18	RRX	K	103	-	42,42,42	4.99	26 (61%)	57,58,58	2.35	22 (38%)
16	CLA	1	605	-	65,73,73	1.37	9 (13%)	76,113,113	1.88	15 (19%)
31	DGD	B	850	-	67,67,67	1.18	7 (10%)	81,81,81	1.04	3 (3%)
21	BCR	A	845	-	41,41,41	1.82	4 (9%)	56,56,56	5.62	29 (51%)
16	CLA	A	810	16	65,73,73	1.37	9 (13%)	76,113,113	1.99	16 (21%)
17	C7Z	3	215	-	43,43,43	5.42	26 (60%)	58,60,60	2.20	14 (24%)
16	CLA	O	204	-	65,73,73	1.37	9 (13%)	76,113,113	1.94	16 (21%)
16	CLA	A	829	-	65,73,73	1.37	8 (12%)	76,113,113	1.83	12 (15%)
16	CLA	A	816	-	65,73,73	1.40	8 (12%)	76,113,113	1.90	16 (21%)
16	CLA	A	830	-	65,73,73	1.40	9 (13%)	76,113,113	1.86	14 (18%)
16	CLA	B	808	-	65,73,73	1.37	10 (15%)	76,113,113	1.92	15 (19%)
21	BCR	I	103	-	41,41,41	1.81	4 (9%)	56,56,56	5.34	25 (44%)
16	CLA	A	806	-	65,73,73	1.37	8 (12%)	76,113,113	1.93	14 (18%)
16	CLA	B	816	-	65,73,73	1.39	10 (15%)	76,113,113	1.85	16 (21%)
16	CLA	A	815	-	65,73,73	1.37	9 (13%)	76,113,113	2.05	17 (22%)
16	CLA	1	608	19	65,73,73	1.38	8 (12%)	76,113,113	1.84	15 (19%)
16	CLA	3	206	-	65,73,73	1.36	9 (13%)	76,113,113	1.88	16 (21%)
16	CLA	A	812	-	65,73,73	1.35	8 (12%)	76,113,113	1.89	14 (18%)
16	CLA	B	815	-	55,63,73	1.48	9 (16%)	64,101,113	1.97	14 (21%)
21	BCR	B	855	-	41,41,41	1.85	4 (9%)	56,56,56	4.67	28 (50%)
17	C7Z	3	216	-	43,43,43	5.39	27 (62%)	58,60,60	3.47	24 (41%)
16	CLA	A	838	-	65,73,73	1.38	8 (12%)	76,113,113	1.88	16 (21%)
17	C7Z	3	218	-	43,43,43	5.38	26 (60%)	58,60,60	2.50	25 (43%)
21	BCR	B	840	-	41,41,41	1.83	4 (9%)	56,56,56	4.56	18 (32%)
16	CLA	B	825	-	65,73,73	1.38	9 (13%)	76,113,113	1.92	13 (17%)
21	BCR	O	205	-	41,41,41	1.83	4 (9%)	56,56,56	4.44	16 (28%)
25	PTY	L	208	-	49,49,49	0.89	4 (8%)	52,54,54	1.03	2 (3%)
16	CLA	A	835	-	65,73,73	1.36	8 (12%)	76,113,113	2.03	16 (21%)
16	CLA	2	613	-	65,73,73	1.38	9 (13%)	76,113,113	1.96	15 (19%)
16	CLA	B	801	-	65,73,73	1.36	8 (12%)	76,113,113	1.84	15 (19%)
16	CLA	3	205	-	65,73,73	1.35	7 (10%)	76,113,113	2.21	22 (28%)
21	BCR	A	850	-	41,41,41	1.88	4 (9%)	56,56,56	4.87	23 (41%)
17	C7Z	A	843	-	43,43,43	5.41	26 (60%)	58,60,60	2.24	18 (31%)
22	PGT	B	848	16	34,34,50	1.54	7 (20%)	37,40,56	1.06	2 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
16	CLA	B	836	-	65,73,73	1.39	9 (13%)	76,113,113	1.87	13 (17%)
16	CLA	A	813	-	65,73,73	1.38	9 (13%)	76,113,113	1.87	14 (18%)
16	CLA	2	602	2	64,71,73	1.50	10 (15%)	74,110,113	1.89	15 (20%)
16	CLA	B	834	-	65,73,73	1.36	9 (13%)	76,113,113	1.99	18 (23%)
16	CLA	O	202	-	65,73,73	1.36	8 (12%)	76,113,113	1.88	13 (17%)
16	CLA	A	819	-	65,73,73	1.37	10 (15%)	76,113,113	1.96	16 (21%)
20	ERG	1	618	-	31,32,32	8.17	18 (58%)	47,50,50	4.76	19 (40%)
21	BCR	B	844	-	41,41,41	1.82	4 (9%)	56,56,56	4.48	21 (37%)
27	PQN	A	840	-	34,34,34	0.44	0	42,45,45	1.30	4 (9%)
16	CLA	B	827	-	65,73,73	1.37	10 (15%)	76,113,113	1.80	15 (19%)
28	SF4	A	848	4,5	0,12,12	-	-	-		
21	BCR	K	104	-	41,41,41	1.82	4 (9%)	56,56,56	4.15	26 (46%)
16	CLA	A	803	16	65,73,73	1.35	8 (12%)	76,113,113	1.99	16 (21%)
16	CLA	K	101	-	65,73,73	1.38	10 (15%)	76,113,113	1.88	17 (22%)
19	LHG	1	617	16	48,48,48	0.42	0	51,54,54	0.94	3 (5%)
16	CLA	3	208	-	65,73,73	1.36	8 (12%)	76,113,113	1.93	16 (21%)
29	3PH	B	854	-	47,47,47	0.87	4 (8%)	51,52,52	1.02	2 (3%)
29	3PH	J	105	-	47,47,47	0.88	3 (6%)	51,52,52	0.96	2 (3%)
16	CLA	B	837	-	65,73,73	1.37	8 (12%)	76,113,113	2.08	17 (22%)
16	CLA	A	837	-	65,73,73	1.37	9 (13%)	76,113,113	1.88	16 (21%)
17	C7Z	1	614	-	43,43,43	5.41	26 (60%)	58,60,60	2.32	17 (29%)
21	BCR	A	846	-	41,41,41	1.80	4 (9%)	56,56,56	4.48	25 (44%)
19	LHG	A	841	-	48,48,48	0.41	0	51,54,54	0.90	2 (3%)
16	CLA	B	818	33	65,73,73	1.38	9 (13%)	76,113,113	1.97	13 (17%)
16	CLA	3	207	-	62,70,73	1.39	8 (12%)	72,109,113	1.93	15 (20%)
21	BCR	B	842	-	41,41,41	1.87	4 (9%)	56,56,56	4.46	21 (37%)
16	CLA	2	601	-	65,73,73	1.38	9 (13%)	76,113,113	1.95	14 (18%)
16	CLA	B	807	-	65,73,73	1.33	7 (10%)	76,113,113	1.88	13 (17%)
16	CLA	A	825	-	65,73,73	1.39	9 (13%)	76,113,113	1.88	16 (21%)
21	BCR	L	202	-	41,41,41	1.75	4 (9%)	56,56,56	4.40	19 (33%)
16	CLA	B	822	-	65,73,73	1.40	8 (12%)	76,113,113	1.82	15 (19%)
17	C7Z	1	616	-	43,43,43	5.38	26 (60%)	58,60,60	2.79	22 (37%)
16	CLA	A	834	4	65,73,73	1.36	8 (12%)	76,113,113	1.88	16 (21%)
18	RRX	2	616	-	42,42,42	5.00	25 (59%)	57,58,58	2.37	24 (42%)
16	CLA	B	811	-	65,73,73	1.38	9 (13%)	76,113,113	1.85	14 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$\|Z\|>2$	Counts	RMSZ	#$\|Z\|>2$
16	CLA	B	804	-	65,73,73	1.35	8 (12%)	76,113,113	1.92	16 (21%)
16	CLA	A	818	-	65,73,73	1.35	9 (13%)	76,113,113	2.17	18 (23%)
16	CLA	A	854	-	65,73,73	1.34	8 (12%)	76,113,113	1.79	13 (17%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	1	604	-	1/1/19/20	11/37/115/115	-
16	CLA	A	833	-	1/1/19/20	15/37/115/115	-
16	CLA	B	802	-	1/1/19/20	12/37/115/115	-
17	C7Z	J	104	-	1/1/12/26	6/29/67/67	0/2/2/2
16	CLA	F	205	9	1/1/19/20	17/37/115/115	-
21	BCR	2	617	-	-	8/29/63/63	0/2/2/2
21	BCR	L	207	-	-	8/29/63/63	0/2/2/2
16	CLA	3	204	3	1/1/18/20	8/35/113/115	-
16	CLA	L	204	-	1/1/19/20	21/37/115/115	-
16	CLA	A	831	-	1/1/19/20	13/37/115/115	-
16	CLA	1	610	-	1/1/19/20	11/37/115/115	-
17	C7Z	3	201	-	1/1/12/26	10/29/67/67	0/2/2/2
17	C7Z	3	217	-	1/1/12/26	11/29/67/67	0/2/2/2
16	CLA	3	209	3	1/1/19/20	17/37/115/115	-
16	CLA	A	836	-	1/1/19/20	9/37/115/115	-
16	CLA	B	810	-	1/1/19/20	11/37/115/115	-
16	CLA	I	101	-	1/1/19/20	12/37/115/115	-
16	CLA	A	807	-	1/1/19/20	14/37/115/115	-
16	CLA	2	609	-	1/1/19/20	17/37/115/115	-
16	CLA	B	805	-	1/1/19/20	14/37/115/115	-
16	CLA	B	831	33	1/1/19/20	15/37/115/115	-
16	CLA	B	820	-	1/1/19/20	14/37/115/115	-
21	BCR	F	206	-	-	10/29/63/63	0/2/2/2
16	CLA	3	211	-	1/1/19/20	17/37/115/115	-
21	BCR	A	844	-	-	6/29/63/63	0/2/2/2
16	CLA	A	827	-	1/1/19/20	15/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	DGD	B	846	-	-	20/55/95/95	0/2/2/2
19	LHG	2	622	16	-	30/53/53/53	-
31	DGD	B	849	-	-	16/55/95/95	0/2/2/2
16	CLA	A	856	-	1/1/19/20	13/37/115/115	-
16	CLA	B	833	-	1/1/19/20	15/37/115/115	-
16	CLA	A	839	33	1/1/19/20	12/37/115/115	-
16	CLA	2	606	-	1/1/19/20	15/37/115/115	-
16	CLA	A	826	-	1/1/19/20	13/37/115/115	-
21	BCR	B	847	-	-	15/29/63/63	0/2/2/2
16	CLA	B	826	-	1/1/19/20	17/37/115/115	-
30	T7X	A	851	-	-	19/49/73/80	0/1/1/1
17	C7Z	1	612	-	1/1/12/26	11/29/67/67	0/2/2/2
25	PTY	3	221	-	-	18/53/53/53	-
16	CLA	F	204	-	1/1/19/20	11/37/115/115	-
23	DGA	2	620	-	-	21/45/45/45	-
21	BCR	L	206	-	-	8/29/63/63	0/2/2/2
16	CLA	3	213	-	1/1/14/20	9/15/93/115	-
16	CLA	A	814	-	1/1/19/20	20/37/115/115	-
16	CLA	B	813	-	1/1/19/20	12/37/115/115	-
16	CLA	2	612	-	1/1/19/20	14/37/115/115	-
16	CLA	3	210	3	1/1/19/20	15/37/115/115	-
16	CLA	A	817	-	1/1/19/20	15/37/115/115	-
26	CL0	A	801	-	3/3/24/25	15/37/135/135	-
16	CLA	A	804	-	1/1/19/20	14/37/115/115	-
16	CLA	F	201	-	1/1/18/20	15/33/111/115	-
24	LMU	3	202	-	-	13/21/61/61	0/2/2/2
16	CLA	A	802	-	1/1/19/20	17/37/115/115	-
16	CLA	A	855	33	1/1/19/20	10/37/115/115	-
16	CLA	A	822	-	1/1/19/20	13/37/115/115	-
16	CLA	O	201	-	1/1/19/20	12/37/115/115	-
16	CLA	B	832	-	1/1/19/20	15/37/115/115	-
16	CLA	1	603	-	1/1/19/20	11/37/115/115	-
16	CLA	F	202	-	2/2/19/20	15/37/115/115	-
16	CLA	1	609	-	1/1/19/20	13/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	LHG	A	842	-	-	28/53/53/53	-
25	PTY	A	852	-	-	23/48/48/53	-
21	BCR	B	841	-	-	10/29/63/63	0/2/2/2
16	CLA	2	610	19	1/1/19/20	16/37/115/115	-
17	C7Z	2	615	-	1/1/12/26	8/29/67/67	0/2/2/2
21	BCR	F	203	-	-	8/29/63/63	0/2/2/2
16	CLA	2	603	-	1/1/19/20	9/37/115/115	-
16	CLA	A	805	-	1/1/19/20	18/37/115/115	-
16	CLA	A	820	33	1/1/19/20	13/37/115/115	-
21	BCR	A	857	-	-	9/29/63/63	0/2/2/2
16	CLA	3	203	-	1/1/19/20	15/37/115/115	-
16	CLA	O	203	-	1/1/19/20	17/37/115/115	-
16	CLA	1	606	-	1/1/19/20	17/37/115/115	-
16	CLA	L	205	-	1/1/19/20	13/37/115/115	-
28	SF4	C	102	6	-	-	0/6/5/5
16	CLA	B	817	-	1/1/19/20	7/37/115/115	-
16	CLA	A	824	33	1/1/19/20	14/37/115/115	-
16	CLA	B	824	-	1/1/19/20	15/37/115/115	-
19	LHG	3	219	-	-	32/53/53/53	-
16	CLA	A	811	-	1/1/19/20	10/37/115/115	-
16	CLA	2	607	-	1/1/19/20	12/37/115/115	-
21	BCR	B	845	-	-	12/29/63/63	0/2/2/2
16	CLA	A	828	-	1/1/19/20	7/37/115/115	-
16	CLA	3	212	-	1/1/17/20	12/29/107/115	-
16	CLA	A	832	-	1/1/19/20	10/37/115/115	-
16	CLA	B	829	-	1/1/19/20	12/37/115/115	-
24	LMU	A	853	-	-	7/21/61/61	0/2/2/2
16	CLA	B	830	-	1/1/19/20	14/37/115/115	-
16	CLA	B	806	-	1/1/19/20	11/37/115/115	-
16	CLA	1	601	-	1/1/19/20	16/37/115/115	-
16	CLA	K	102	-	1/1/19/20	15/37/115/115	-
16	CLA	B	812	-	1/1/19/20	20/37/115/115	-
20	ERG	2	621	-	5/5/15/15	4/13/71/71	0/4/4/4
16	CLA	L	203	13	1/1/19/20	12/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	2	604	-	1/1/19/20	10/37/115/115	-
16	CLA	B	838	22	1/1/19/20	13/37/115/115	-
16	CLA	B	814	-	1/1/19/20	12/37/115/115	-
16	CLA	A	821	-	1/1/19/20	13/37/115/115	-
16	CLA	1	607	1	1/1/18/20	12/31/109/115	-
16	CLA	A	809	-	1/1/19/20	17/37/115/115	-
16	CLA	B	835	-	1/1/19/20	14/37/115/115	-
16	CLA	B	809	5	1/1/19/20	17/37/115/115	-
28	SF4	C	101	6	-	-	0/6/5/5
16	CLA	1	611	-	1/1/19/20	13/37/115/115	-
23	DGA	J	101	-	-	17/45/45/45	-
17	C7Z	1	615	-	1/1/12/26	11/29/67/67	0/2/2/2
16	CLA	B	828	-	1/1/19/20	7/37/115/115	-
16	CLA	3	214	-	1/1/19/20	16/37/115/115	-
19	LHG	B	851	-	-	24/49/49/53	-
16	CLA	2	608	-	1/1/19/20	21/37/115/115	-
16	CLA	A	808	4	1/1/19/20	14/37/115/115	-
16	CLA	A	823	-	1/1/19/20	11/37/115/115	-
20	ERG	2	618	-	4/4/15/15	10/13/71/71	0/4/4/4
27	PQN	B	839	-	-	9/23/43/43	0/2/2/2
16	CLA	B	823	-	1/1/19/20	15/37/115/115	-
16	CLA	2	611	2	1/1/19/20	15/37/115/115	-
18	RRX	J	103	-	1/1/25/25	16/29/65/65	0/2/2/2
16	CLA	B	819	-	1/1/19/20	14/37/115/115	-
25	PTY	3	220	-	-	19/53/53/53	-
16	CLA	1	602	1	1/1/17/20	8/30/108/115	-
29	3PH	A	849	-	-	19/49/49/49	-
16	CLA	2	605	-	1/1/19/20	16/37/115/115	-
16	CLA	L	201	-	1/1/19/20	8/37/115/115	-
22	PGT	2	619	-	1/1/5/5	20/38/38/55	-
16	CLA	J	102	11	2/2/19/20	18/37/115/115	-
16	CLA	B	803	33	1/1/19/20	9/37/115/115	-
17	C7Z	2	614	-	1/1/12/26	10/29/67/67	0/2/2/2
21	BCR	B	843	-	-	9/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	RRX	A	847	-	1/1/24/25	13/29/65/65	0/2/2/2
18	RRX	1	613	-	1/1/25/25	20/29/65/65	0/2/2/2
16	CLA	B	821	-	2/2/19/20	13/37/115/115	-
16	CLA	I	102	-	1/1/19/20	14/37/115/115	-
18	RRX	K	103	-	1/1/25/25	16/29/65/65	0/2/2/2
16	CLA	1	605	-	1/1/19/20	14/37/115/115	-
31	DGD	B	850	-	-	18/55/95/95	0/2/2/2
21	BCR	A	845	-	-	11/29/63/63	0/2/2/2
16	CLA	A	810	16	1/1/19/20	11/37/115/115	-
17	C7Z	3	215	-	1/1/12/26	9/29/67/67	0/2/2/2
16	CLA	O	204	-	1/1/19/20	10/37/115/115	-
16	CLA	A	829	-	1/1/19/20	13/37/115/115	-
16	CLA	A	816	-	1/1/19/20	14/37/115/115	-
16	CLA	A	830	-	1/1/19/20	13/37/115/115	-
16	CLA	B	808	-	1/1/19/20	11/37/115/115	-
21	BCR	I	103	-	-	10/29/63/63	0/2/2/2
16	CLA	A	806	-	1/1/19/20	11/37/115/115	-
16	CLA	B	816	-	1/1/19/20	11/37/115/115	-
16	CLA	A	815	-	1/1/19/20	21/37/115/115	-
16	CLA	1	608	19	1/1/19/20	14/37/115/115	-
16	CLA	3	206	-	1/1/19/20	11/37/115/115	-
16	CLA	A	812	-	1/1/19/20	14/37/115/115	-
16	CLA	B	815	-	1/1/17/20	9/25/103/115	-
21	BCR	B	855	-	-	9/29/63/63	0/2/2/2
17	C7Z	3	216	-	1/1/12/26	9/29/67/67	0/2/2/2
16	CLA	A	838	-	1/1/19/20	6/37/115/115	-
17	C7Z	3	218	-	1/1/12/26	8/29/67/67	0/2/2/2
21	BCR	B	840	-	-	8/29/63/63	0/2/2/2
16	CLA	B	825	-	1/1/19/20	12/37/115/115	-
21	BCR	O	205	-	-	11/29/63/63	0/2/2/2
25	PTY	L	208	-	-	23/53/53/53	-
16	CLA	A	835	-	1/1/19/20	13/37/115/115	-
16	CLA	2	613	-	1/1/19/20	18/37/115/115	-
16	CLA	B	801	-	1/1/19/20	16/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	3	205	-	1/1/19/20	11/37/115/115	-
21	BCR	A	850	-	-	14/29/63/63	0/2/2/2
17	C7Z	A	843	-	1/1/12/26	12/29/67/67	0/2/2/2
22	PGT	B	848	16	1/1/5/5	21/38/38/55	-
16	CLA	B	836	-	1/1/19/20	13/37/115/115	-
16	CLA	A	813	-	1/1/19/20	16/37/115/115	-
16	CLA	2	602	2	1/1/19/20	13/35/113/115	-
16	CLA	B	834	-	1/1/19/20	14/37/115/115	-
16	CLA	O	202	-	1/1/19/20	11/37/115/115	-
16	CLA	A	819	-	1/1/19/20	17/37/115/115	-
20	ERG	1	618	-	6/6/15/15	3/13/71/71	0/4/4/4
21	BCR	B	844	-	-	7/29/63/63	0/2/2/2
27	PQN	A	840	-	-	10/23/43/43	0/2/2/2
16	CLA	B	827	-	1/1/19/20	12/37/115/115	-
28	SF4	A	848	4,5	-	-	0/6/5/5
21	BCR	K	104	-	-	14/29/63/63	0/2/2/2
16	CLA	A	803	16	1/1/19/20	13/37/115/115	-
16	CLA	K	101	-	1/1/19/20	16/37/115/115	-
19	LHG	1	617	16	-	29/53/53/53	-
16	CLA	3	208	-	1/1/19/20	14/37/115/115	-
29	3PH	B	854	-	-	28/49/49/49	-
29	3PH	J	105	-	-	20/49/49/49	-
16	CLA	B	837	-	1/1/19/20	15/37/115/115	-
16	CLA	A	837	-	1/1/19/20	17/37/115/115	-
17	C7Z	1	614	-	1/1/12/26	13/29/67/67	0/2/2/2
21	BCR	A	846	-	-	6/29/63/63	0/2/2/2
19	LHG	A	841	-	-	35/53/53/53	-
16	CLA	B	818	33	1/1/19/20	15/37/115/115	-
16	CLA	3	207	-	1/1/18/20	14/34/112/115	-
21	BCR	B	842	-	-	6/29/63/63	0/2/2/2
16	CLA	2	601	-	1/1/19/20	20/37/115/115	-
16	CLA	B	807	-	1/1/19/20	11/37/115/115	-
16	CLA	A	825	-	1/1/19/20	15/37/115/115	-
21	BCR	L	202	-	-	8/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	B	822	-	1/1/19/20	6/37/115/115	-
17	C7Z	1	616	-	1/1/12/26	7/29/67/67	0/2/2/2
16	CLA	A	834	4	1/1/19/20	14/37/115/115	-
18	RRX	2	616	-	1/1/25/25	13/29/65/65	0/2/2/2
16	CLA	B	811	-	1/1/19/20	8/37/115/115	-
16	CLA	B	804	-	1/1/19/20	13/37/115/115	-
16	CLA	A	818	-	1/1/19/20	14/37/115/115	-
16	CLA	A	854	-	1/1/19/20	11/37/115/115	-

The worst 5 of 1855 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	2	621	ERG	C1-C10	-24.95	1.06	1.54
20	2	618	ERG	C1-C10	-24.94	1.06	1.54
20	1	618	ERG	C1-C10	-24.51	1.07	1.54
20	2	618	ERG	C10-C9	-22.33	1.26	1.55
20	2	621	ERG	C10-C9	-21.86	1.26	1.55

The worst 5 of 3037 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	K	104	BCR	C10-C11-C12	18.18	179.96	123.22
20	1	618	ERG	C18-C13-C12	-18.17	81.89	110.59
21	B	842	BCR	C10-C11-C12	17.98	179.32	123.22
21	O	205	BCR	C10-C11-C12	17.86	178.94	123.22
21	L	202	BCR	C10-C11-C12	17.78	178.71	123.22

5 of 173 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
16	1	601	CLA	ND
16	1	602	CLA	ND
16	1	603	CLA	ND
16	1	604	CLA	ND
16	1	605	CLA	ND

5 of 2730 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	1	601	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
16	1	601	CLA	CHA-CBD-CGD-O2D
16	1	601	CLA	CBD-CGD-O2D-CED
16	1	604	CLA	CHA-CBD-CGD-O1D
16	1	604	CLA	CHA-CBD-CGD-O2D

There are no ring outliers.

181 monomers are involved in 586 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	1	604	CLA	2	0
16	A	833	CLA	1	0
16	B	802	CLA	4	0
16	F	205	CLA	1	0
21	2	617	BCR	10	0
21	L	207	BCR	4	0
16	3	204	CLA	4	0
16	L	204	CLA	2	0
16	1	610	CLA	4	0
17	3	201	C7Z	2	0
17	3	217	C7Z	2	0
16	3	209	CLA	8	0
16	A	836	CLA	3	0
16	B	810	CLA	4	0
16	I	101	CLA	6	0
16	A	807	CLA	4	0
16	2	609	CLA	3	0
16	B	805	CLA	2	0
16	B	831	CLA	5	0
21	F	206	BCR	5	0
16	3	211	CLA	3	0
21	A	844	BCR	8	0
16	A	827	CLA	8	0
31	B	846	DGD	4	0
19	2	622	LHG	1	0
31	B	849	DGD	2	0
16	A	856	CLA	3	0
16	B	833	CLA	4	0
16	A	839	CLA	4	0
16	2	606	CLA	4	0
16	A	826	CLA	5	0
21	B	847	BCR	4	0
16	B	826	CLA	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	A	851	T7X	1	0
17	1	612	C7Z	2	0
16	F	204	CLA	2	0
21	L	206	BCR	6	0
16	3	213	CLA	9	0
16	A	814	CLA	5	0
16	B	813	CLA	2	0
16	2	612	CLA	4	0
16	3	210	CLA	3	0
16	A	817	CLA	4	0
26	A	801	CL0	5	0
16	A	804	CLA	3	0
16	F	201	CLA	4	0
24	3	202	LMU	1	0
16	A	802	CLA	2	0
16	A	855	CLA	6	0
16	A	822	CLA	4	0
16	O	201	CLA	4	0
16	B	832	CLA	4	0
16	1	603	CLA	4	0
16	F	202	CLA	6	0
16	1	609	CLA	5	0
19	A	842	LHG	1	0
25	A	852	PTY	3	0
21	B	841	BCR	3	0
16	2	610	CLA	2	0
21	F	203	BCR	4	0
16	2	603	CLA	1	0
16	A	805	CLA	4	0
16	A	820	CLA	3	0
21	A	857	BCR	7	0
16	3	203	CLA	3	0
16	O	203	CLA	5	0
16	1	606	CLA	4	0
16	L	205	CLA	2	0
16	B	817	CLA	4	0
16	A	824	CLA	5	0
16	B	824	CLA	1	0
19	3	219	LHG	2	0
16	A	811	CLA	3	0
16	2	607	CLA	6	0
21	B	845	BCR	8	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	A	828	CLA	7	0
16	3	212	CLA	3	0
16	A	832	CLA	5	0
16	B	829	CLA	5	0
16	B	830	CLA	5	0
16	B	806	CLA	4	0
16	1	601	CLA	5	0
16	K	102	CLA	3	0
16	B	812	CLA	5	0
20	2	621	ERG	5	0
16	L	203	CLA	3	0
16	2	604	CLA	1	0
16	B	838	CLA	4	0
16	B	814	CLA	2	0
16	A	821	CLA	6	0
16	1	607	CLA	5	0
16	A	809	CLA	5	0
16	B	835	CLA	5	0
16	B	809	CLA	4	0
16	1	611	CLA	2	0
23	J	101	DGA	1	0
17	1	615	C7Z	1	0
16	B	828	CLA	3	0
16	3	214	CLA	3	0
16	2	608	CLA	4	0
16	A	808	CLA	3	0
16	A	823	CLA	5	0
20	2	618	ERG	4	0
27	B	839	PQN	4	0
16	B	823	CLA	1	0
16	2	611	CLA	3	0
18	J	103	RRX	2	0
16	B	819	CLA	4	0
16	1	602	CLA	6	0
16	2	605	CLA	6	0
16	L	201	CLA	7	0
16	J	102	CLA	3	0
16	B	803	CLA	7	0
21	B	843	BCR	5	0
18	A	847	RRX	2	0
18	1	613	RRX	10	0
16	B	821	CLA	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	I	102	CLA	3	0
18	K	103	RRX	4	0
16	1	605	CLA	1	0
31	B	850	DGD	3	0
21	A	845	BCR	9	0
16	A	810	CLA	3	0
17	3	215	C7Z	3	0
16	O	204	CLA	1	0
16	A	829	CLA	3	0
16	A	816	CLA	4	0
16	A	830	CLA	7	0
16	B	808	CLA	7	0
21	I	103	BCR	3	0
16	A	806	CLA	2	0
16	B	816	CLA	6	0
16	A	815	CLA	2	0
16	1	608	CLA	3	0
16	3	206	CLA	1	0
16	A	812	CLA	5	0
16	B	815	CLA	1	0
21	B	855	BCR	10	0
17	3	216	C7Z	3	0
16	A	838	CLA	2	0
17	3	218	C7Z	1	0
21	B	840	BCR	5	0
16	B	825	CLA	5	0
21	O	205	BCR	9	0
16	A	835	CLA	2	0
16	2	613	CLA	3	0
16	B	801	CLA	7	0
16	3	205	CLA	6	0
21	A	850	BCR	5	0
16	B	836	CLA	1	0
16	A	813	CLA	1	0
16	2	602	CLA	4	0
16	B	834	CLA	8	0
16	O	202	CLA	3	0
16	A	819	CLA	6	0
20	1	618	ERG	4	0
21	B	844	BCR	9	0
16	B	827	CLA	4	0
21	K	104	BCR	5	0

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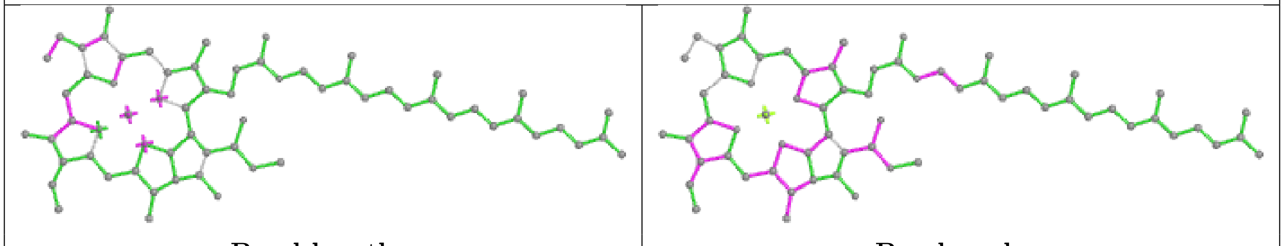
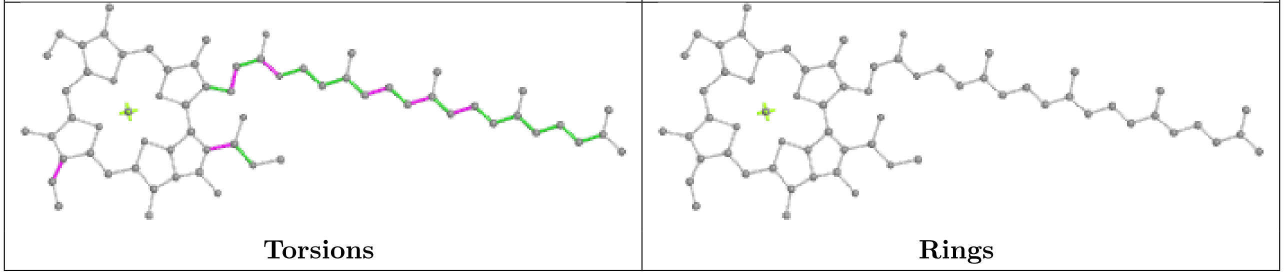
Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	A	803	CLA	1	0
16	K	101	CLA	3	0
19	1	617	LHG	1	0
16	3	208	CLA	4	0
16	B	837	CLA	5	0
16	A	837	CLA	8	0
17	1	614	C7Z	3	0
21	A	846	BCR	14	0
16	B	818	CLA	3	0
16	3	207	CLA	8	0
21	B	842	BCR	3	0
16	2	601	CLA	5	0
16	A	825	CLA	7	0
21	L	202	BCR	10	0
16	B	822	CLA	4	0
17	1	616	C7Z	1	0
16	A	834	CLA	1	0
18	2	616	RRX	2	0
16	B	811	CLA	4	0
16	B	804	CLA	8	0
16	A	818	CLA	5	0
16	A	854	CLA	10	0

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

Ligand CLA 1 604

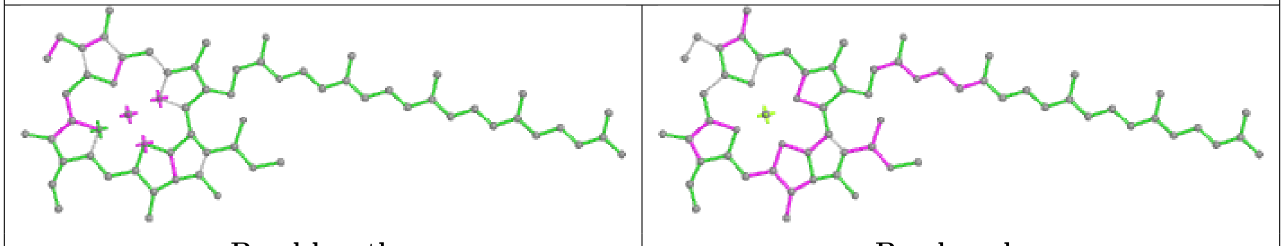


Bond lengths Bond angles

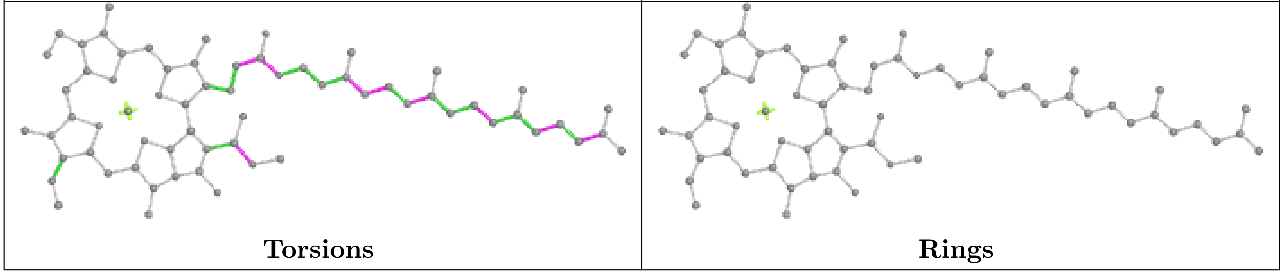


Torsions Rings

Ligand CLA A 833

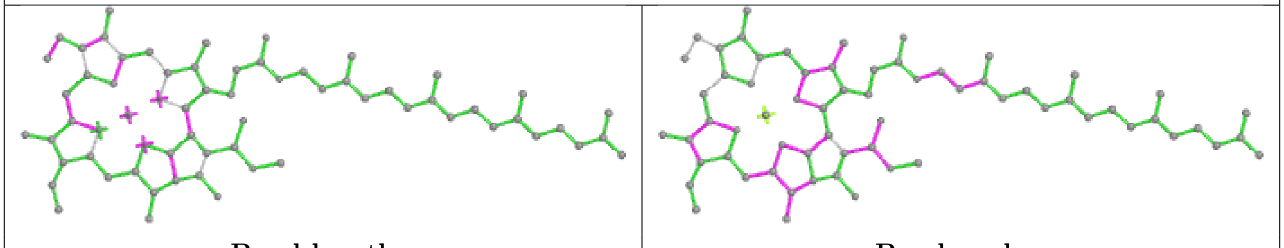


Bond lengths Bond angles

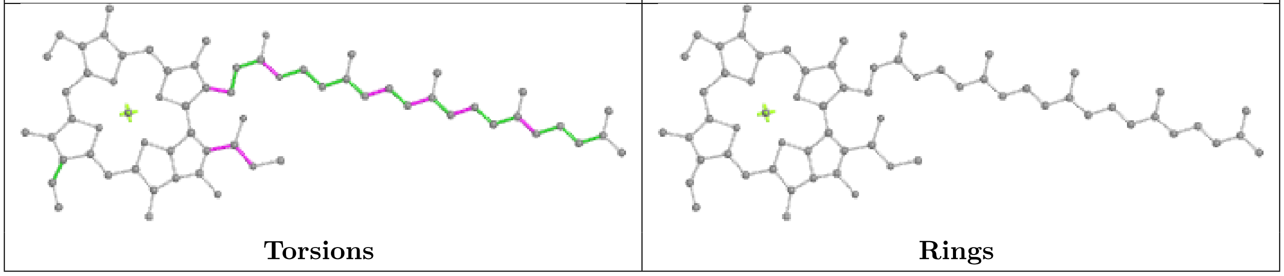


Torsions Rings

Ligand CLA B 802

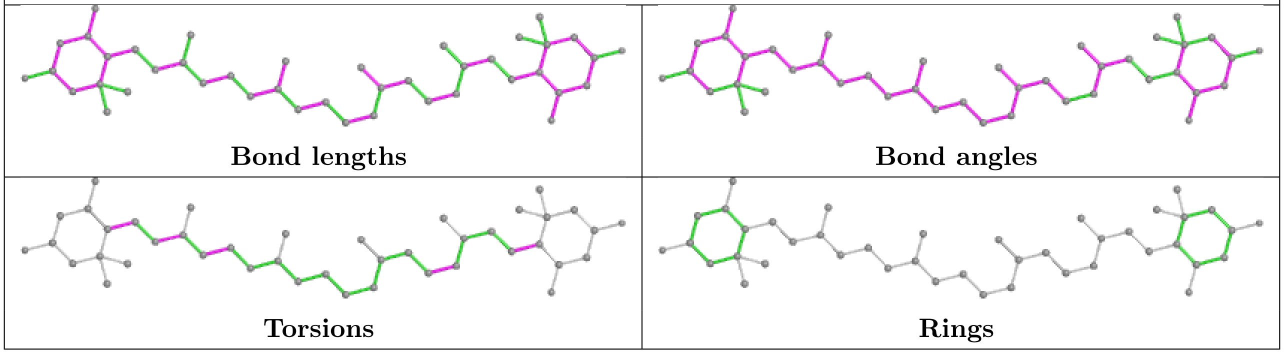


Bond lengths Bond angles



Torsions Rings

Ligand C7Z J 104



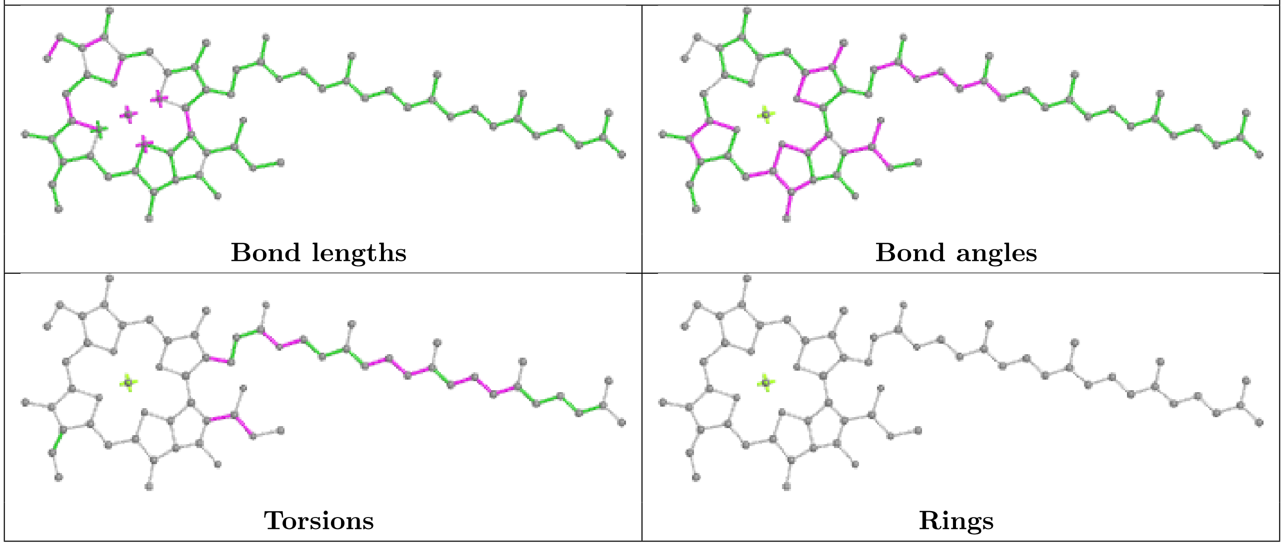
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA F 205



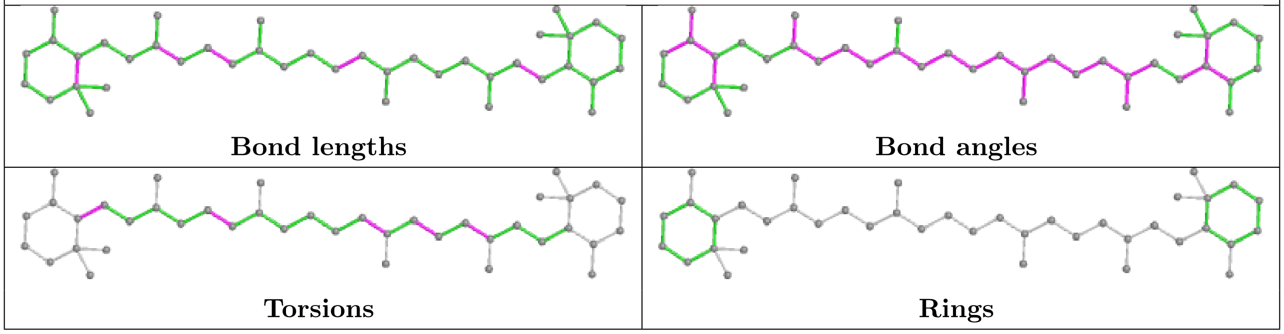
Bond lengths

Bond angles

Torsions

Rings

Ligand BCR 2 617



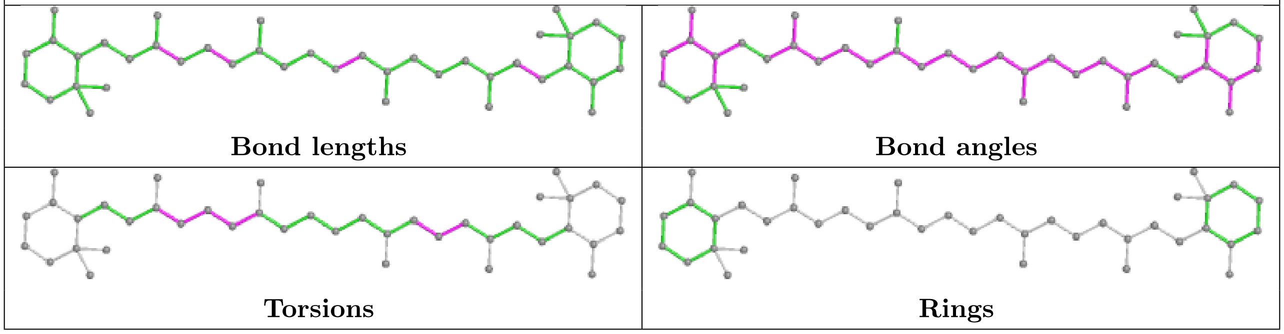
Bond lengths

Bond angles

Torsions

Rings

Ligand BCR L 207



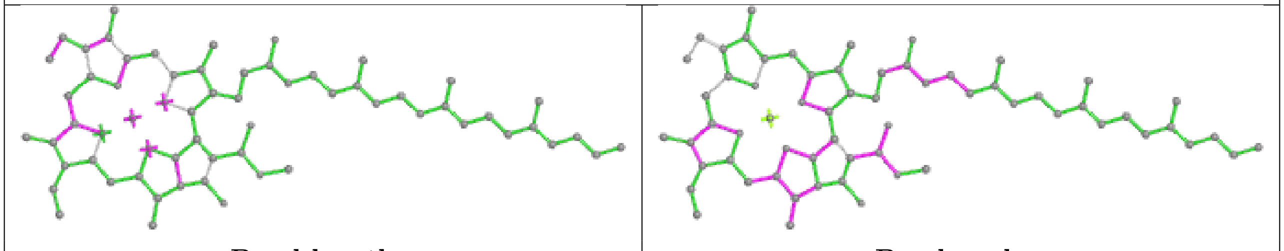
Bond lengths

Bond angles

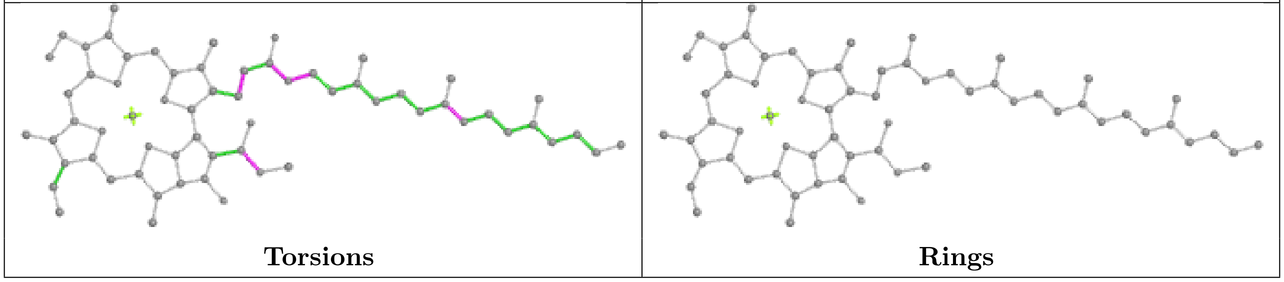
Torsions

Rings

Ligand CLA 3 204

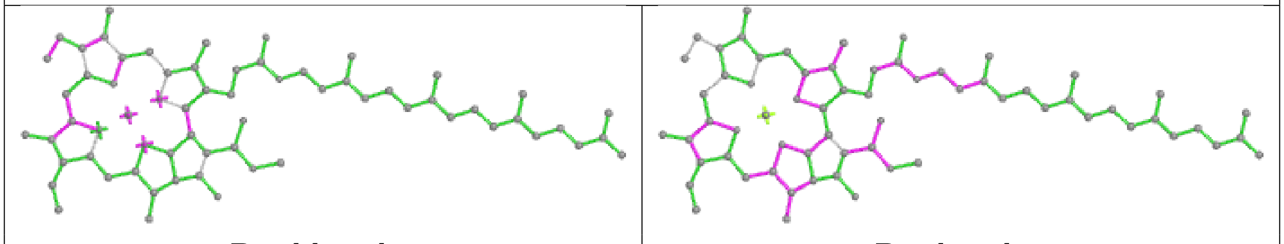


Bond lengths Bond angles

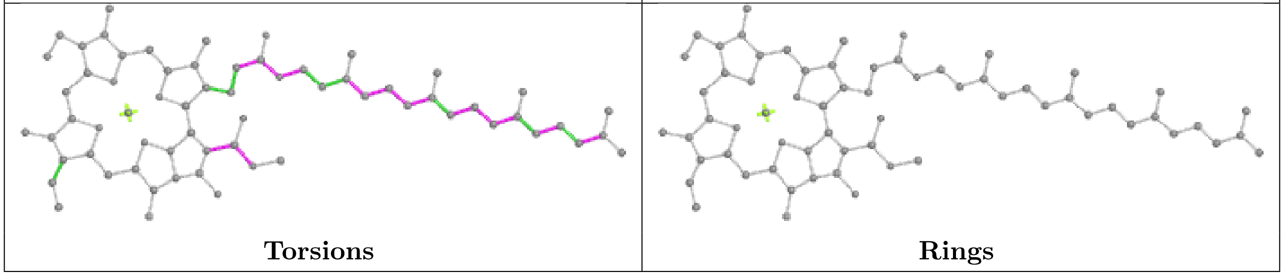


Torsions Rings

Ligand CLA L 204

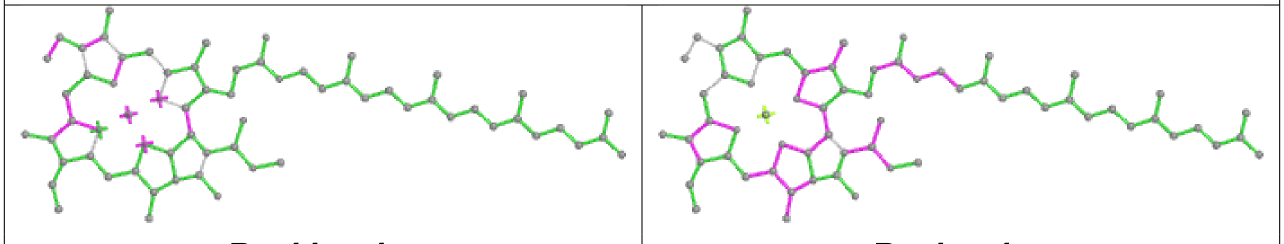


Bond lengths Bond angles

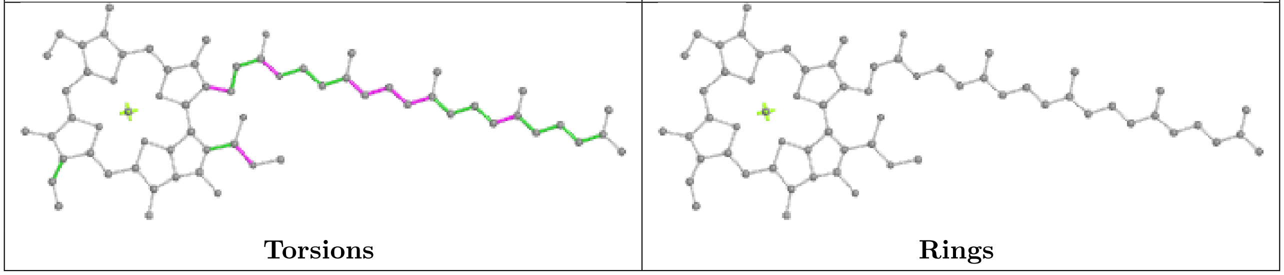


Torsions Rings

Ligand CLA A 831

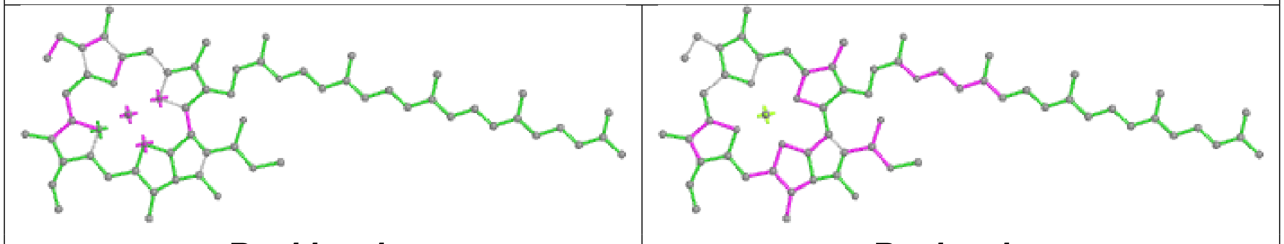


Bond lengths Bond angles

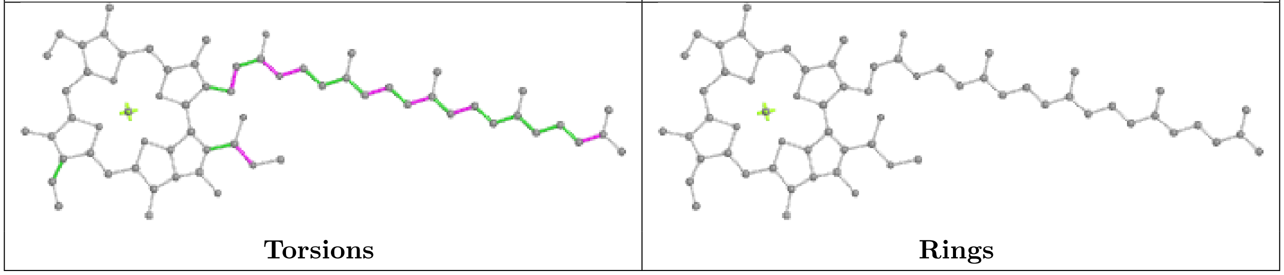


Torsions Rings

Ligand CLA 1 610

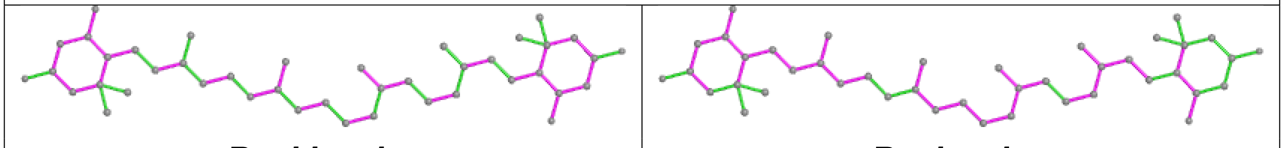


Bond lengths Bond angles

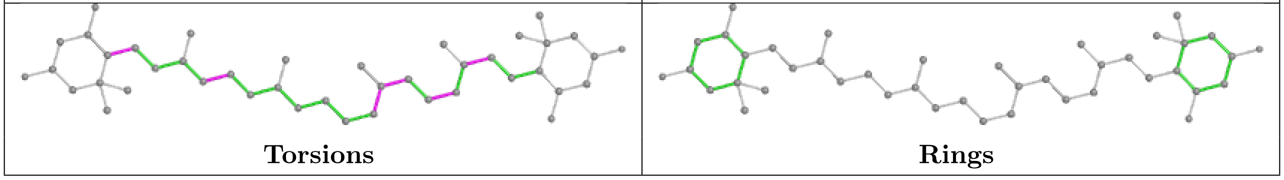


Torsions Rings

Ligand C7Z 3 201

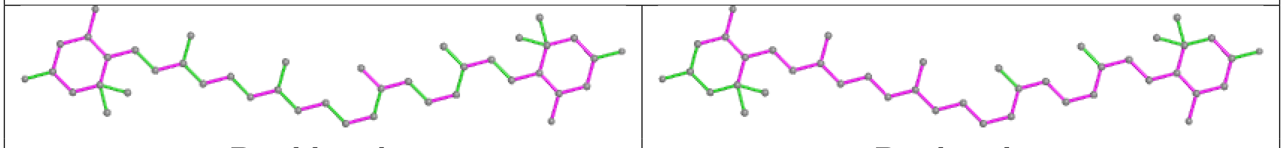


Bond lengths Bond angles

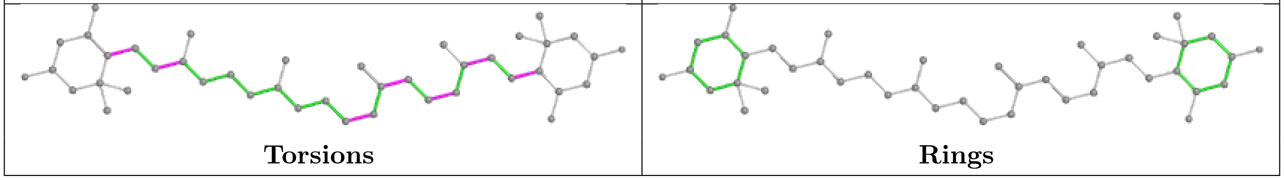


Torsions Rings

Ligand C7Z 3 217

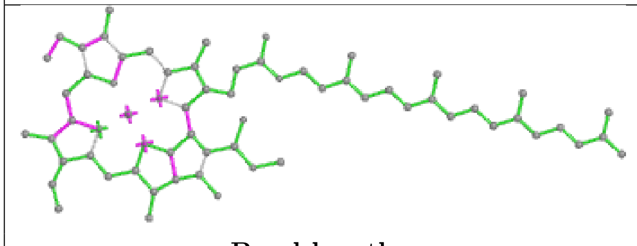
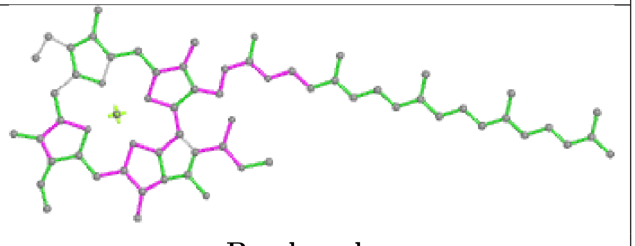
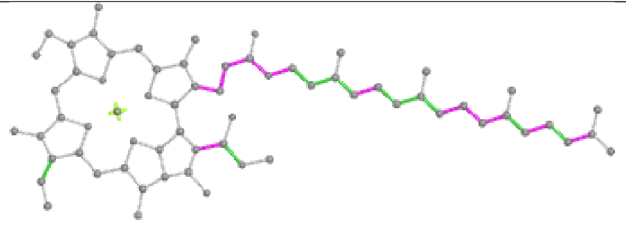
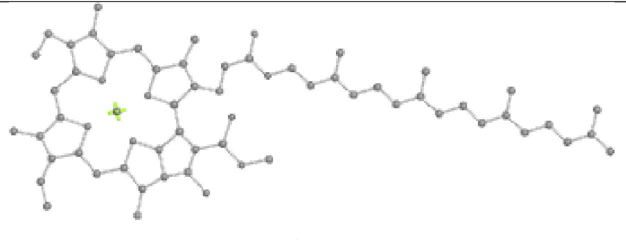


Bond lengths Bond angles

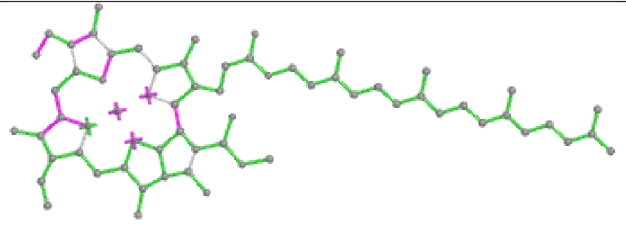
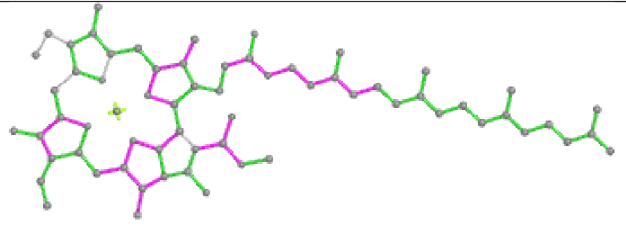
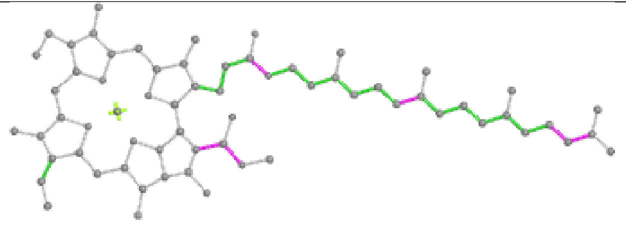
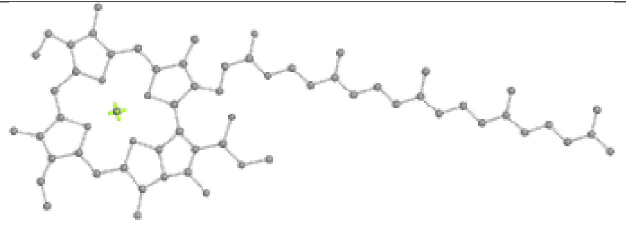


Torsions Rings

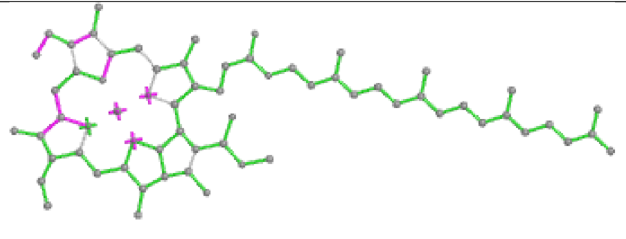
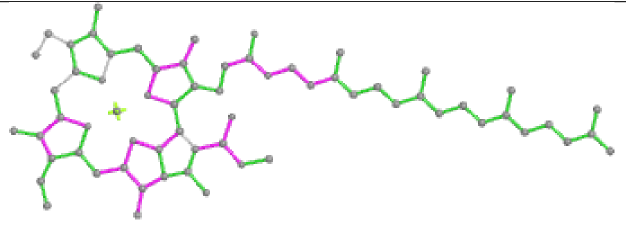
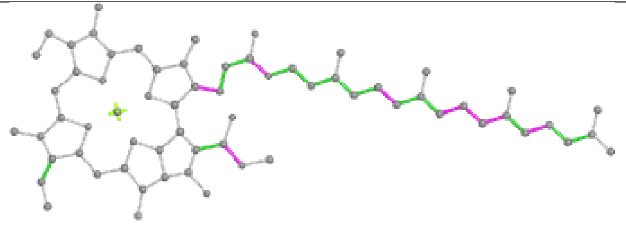
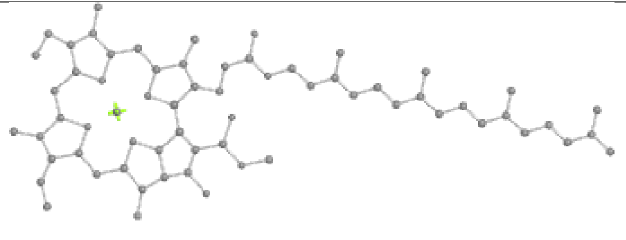
Ligand CLA 3 209

 Bond lengths	 Bond angles
 Torsions	 Rings

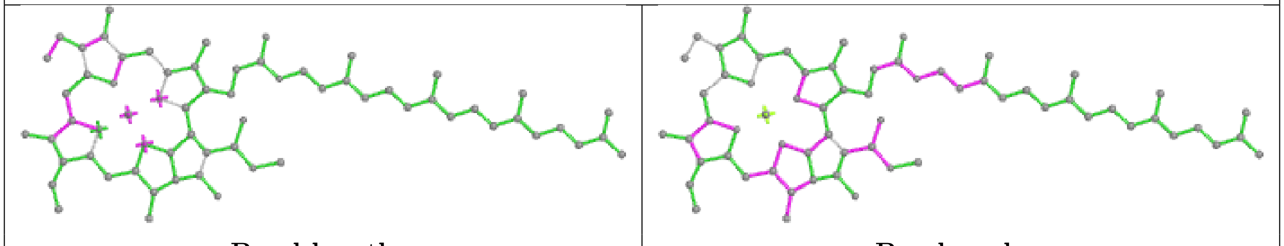
Ligand CLA A 836

 Bond lengths	 Bond angles
 Torsions	 Rings

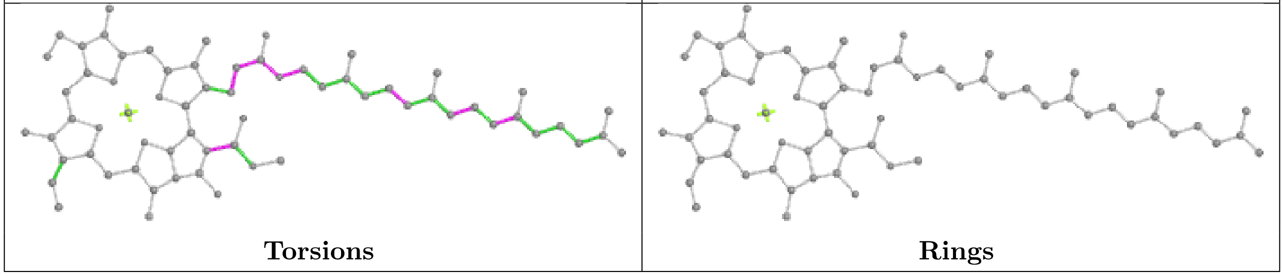
Ligand CLA B 810

 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA I 101

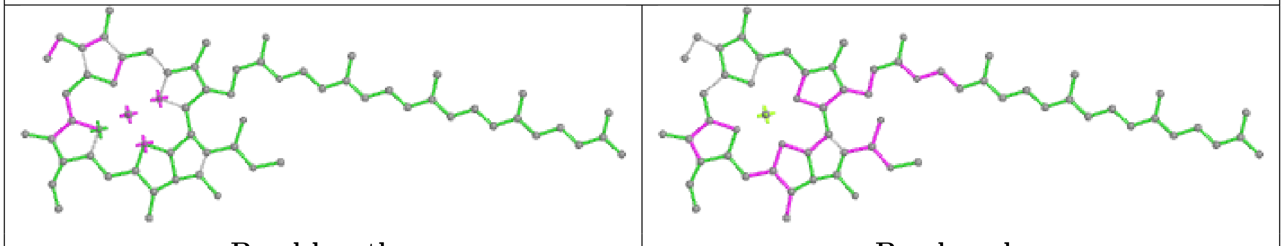


Bond lengths Bond angles

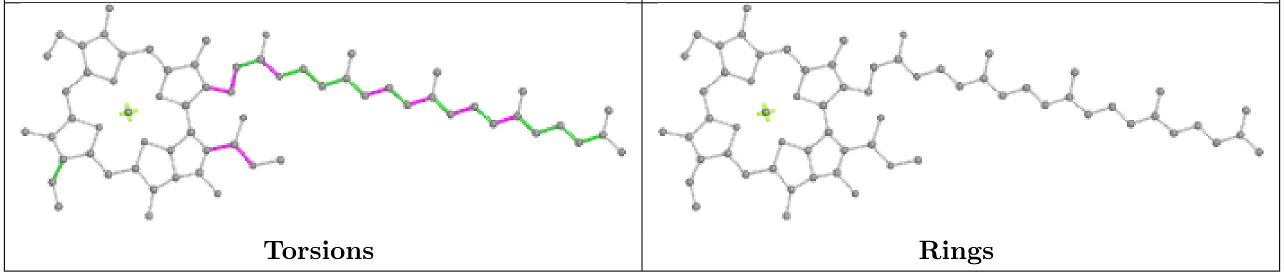


Torsions Rings

Ligand CLA A 807

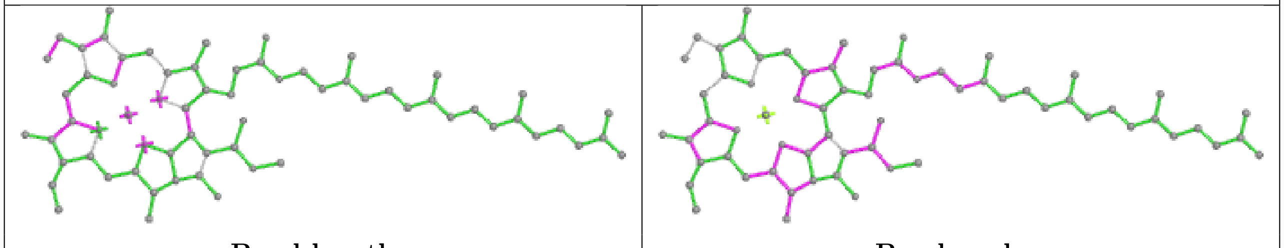


Bond lengths Bond angles

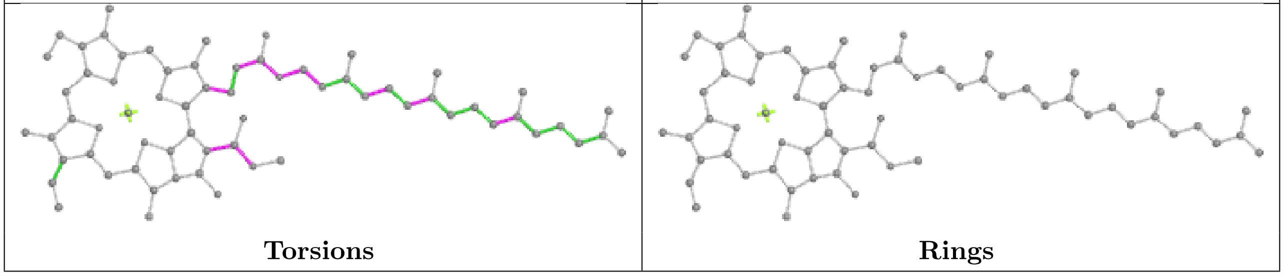


Torsions Rings

Ligand CLA 2 609



Bond lengths Bond angles



Torsions Rings

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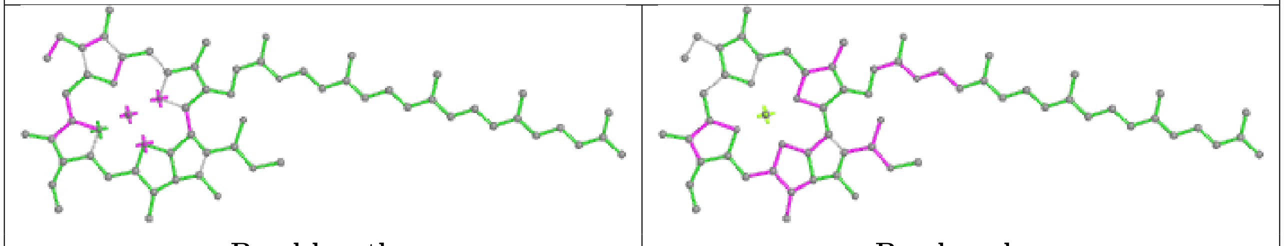
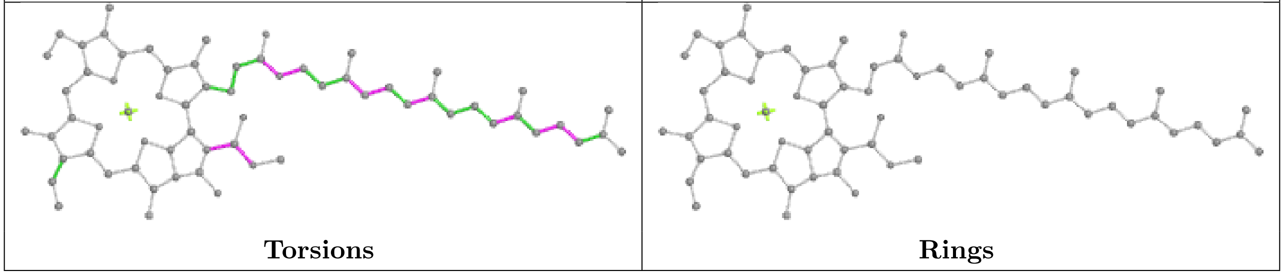

Bond lengths Bond angles


Torsions Rings

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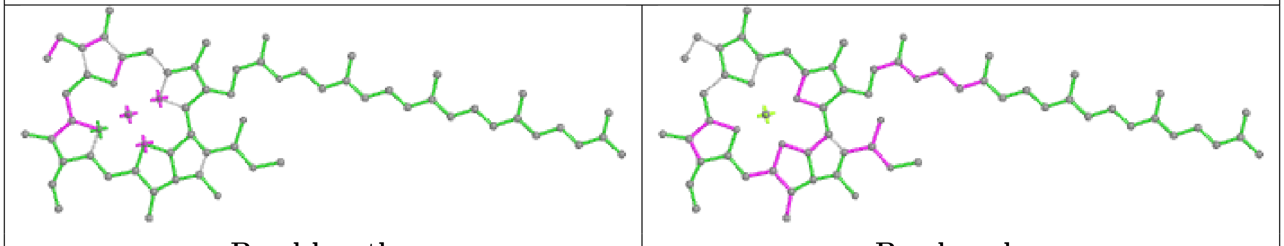
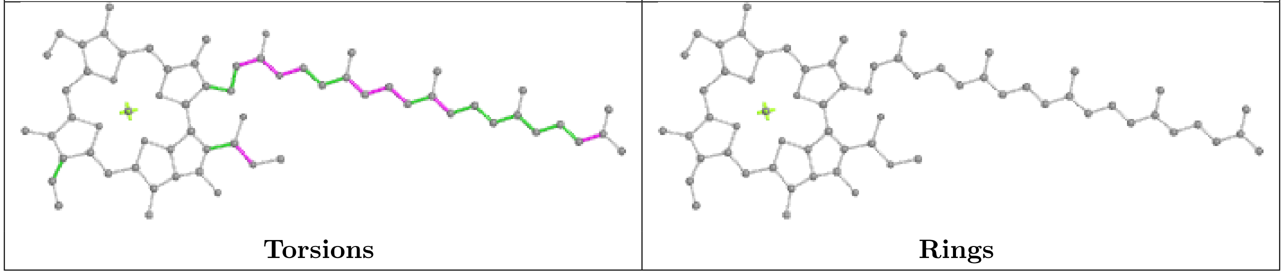

Bond lengths Bond angles


Torsions Rings

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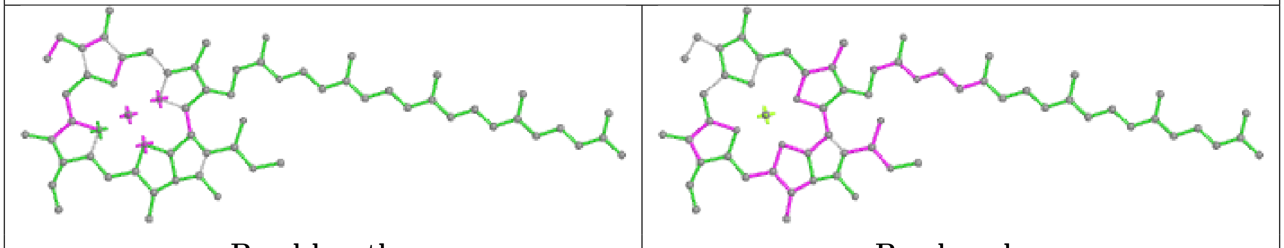
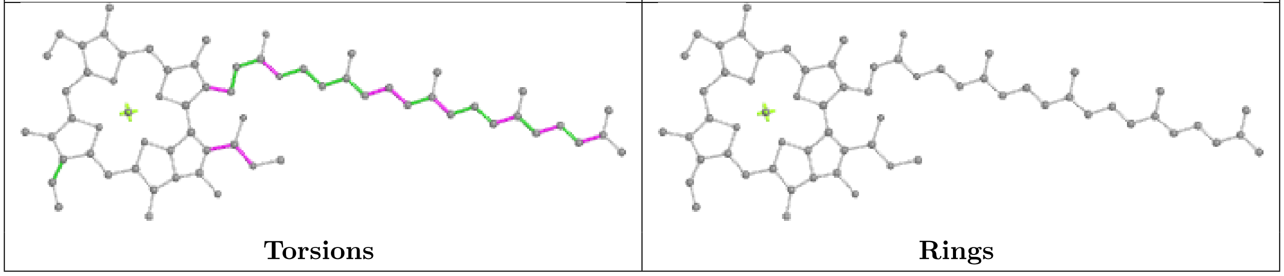
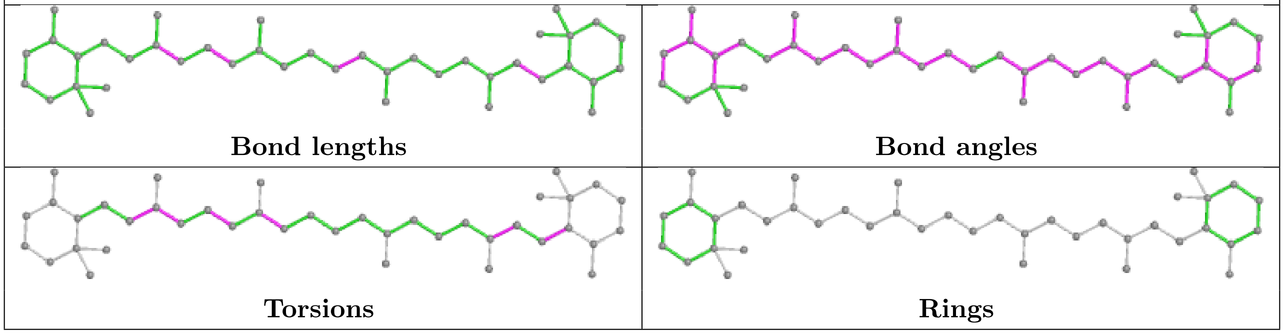

Bond lengths Bond angles


Torsions Rings

Ligand BCR F 206



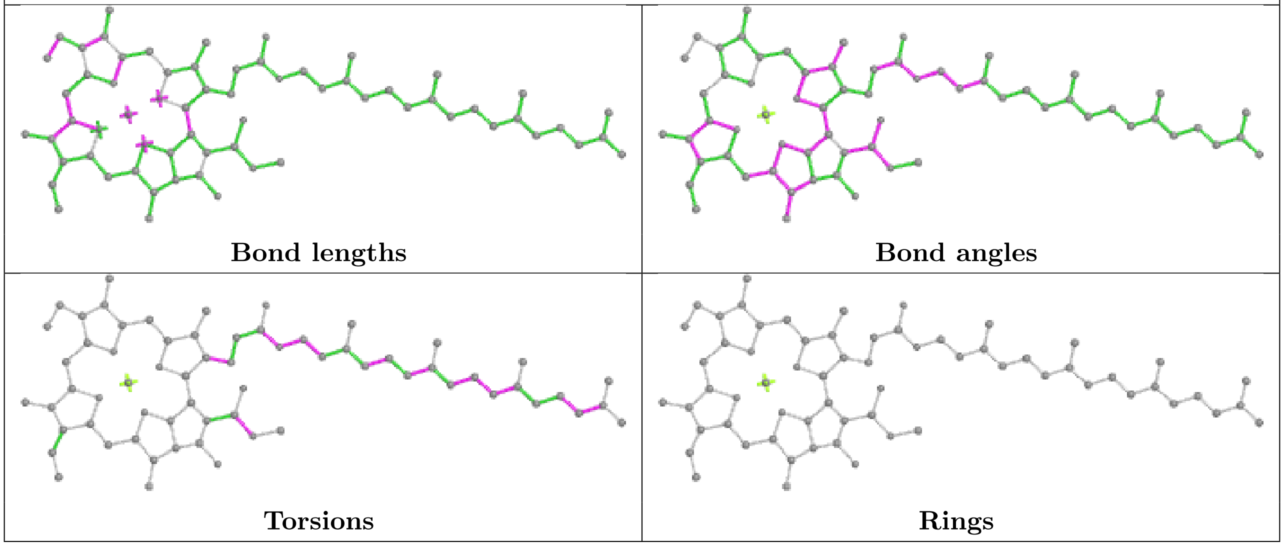
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA 3 211



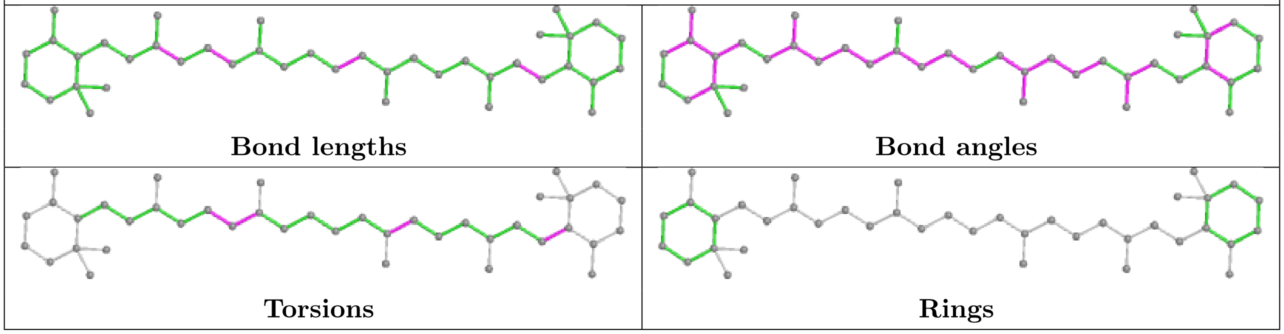
Bond lengths

Bond angles

Torsions

Rings

Ligand BCR A 844



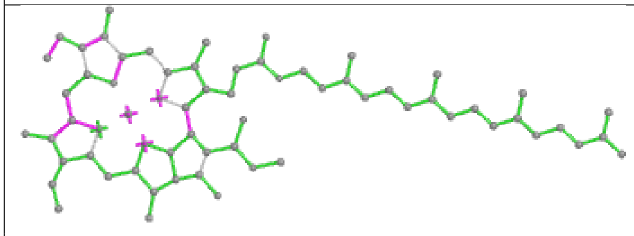
Bond lengths

Bond angles

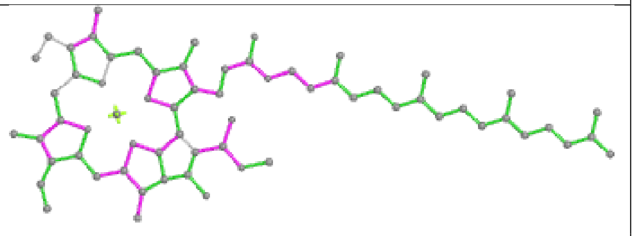
Torsions

Rings

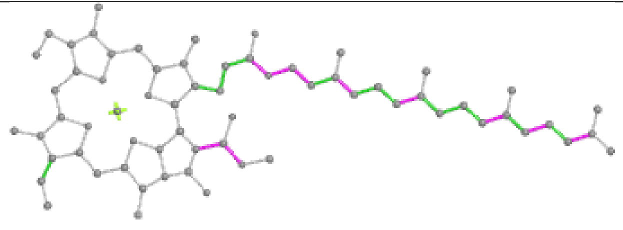
Ligand CLA A 827



Bond lengths



Bond angles



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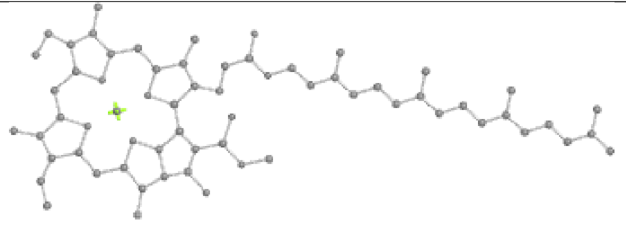
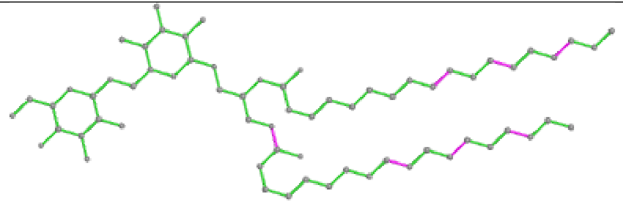
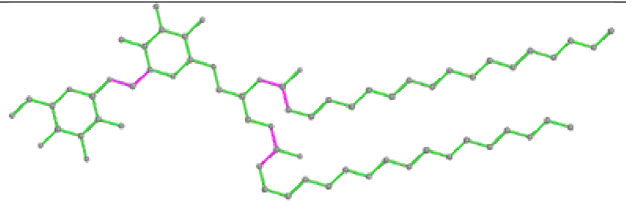


Rings

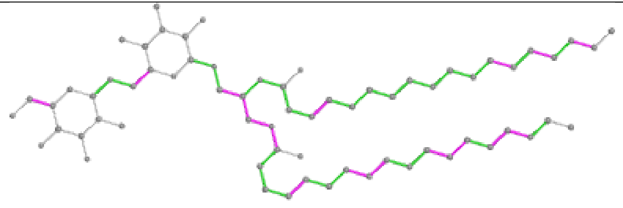
Ligand DGD B 846



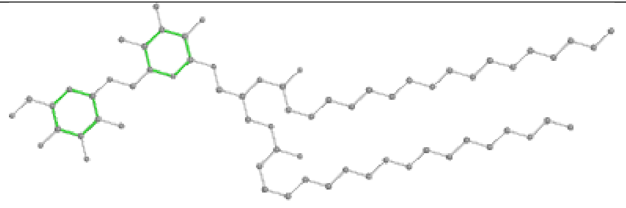
Bond lengths



Bond angles

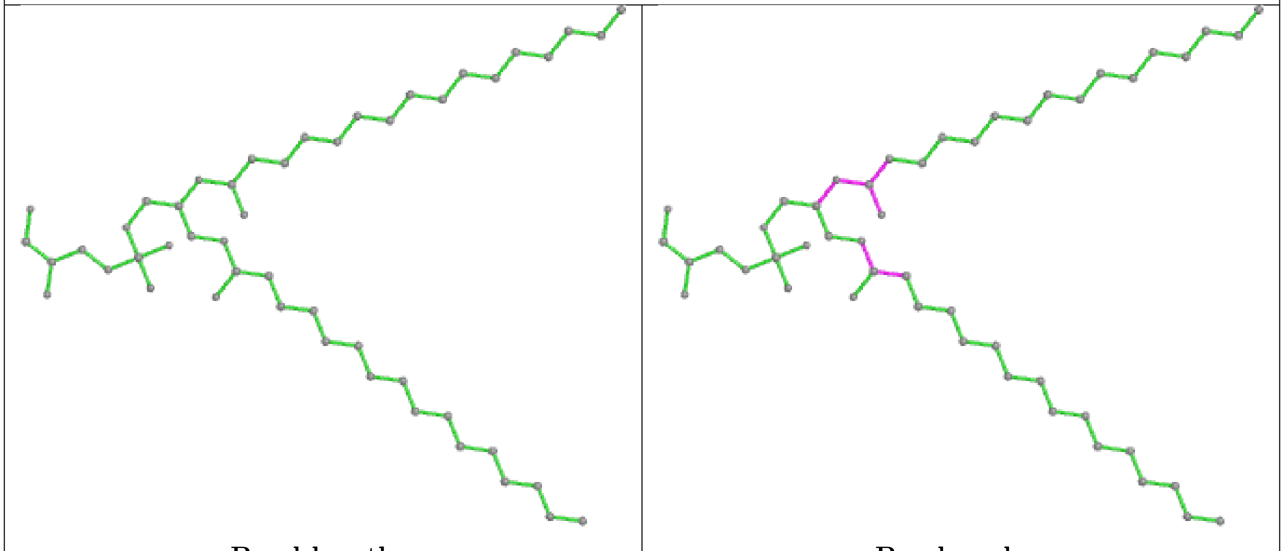


Torsions



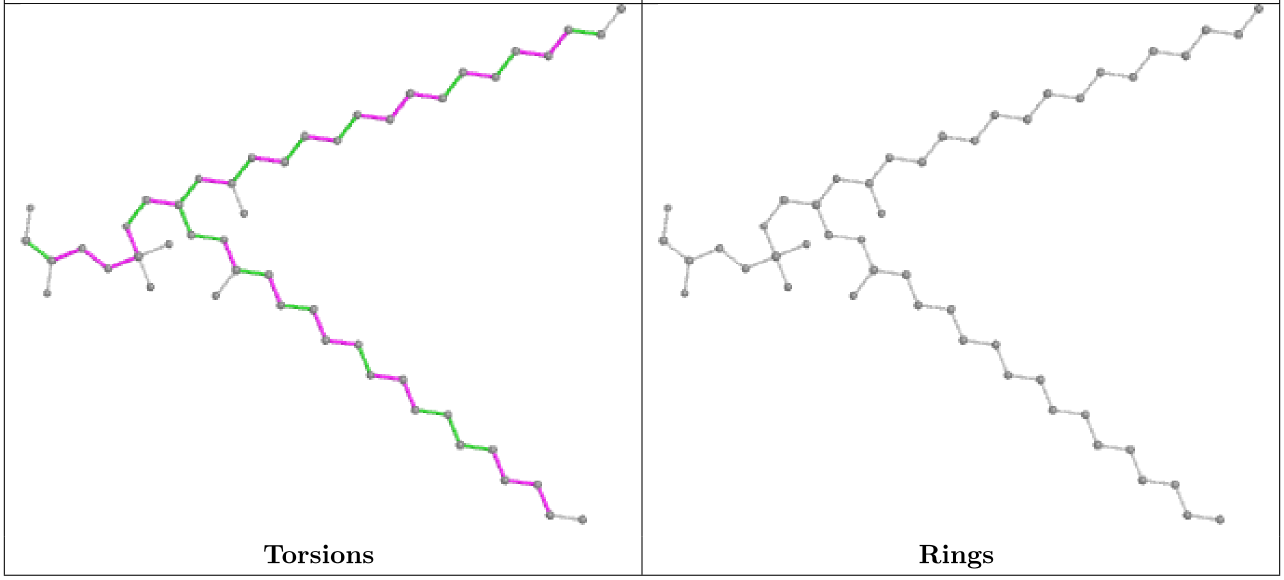
Rings

Ligand LHG 2 622



Bond lengths

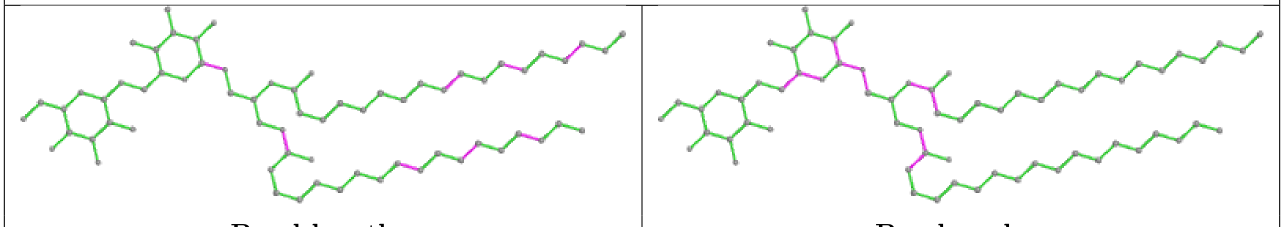
Bond angles



Torsions

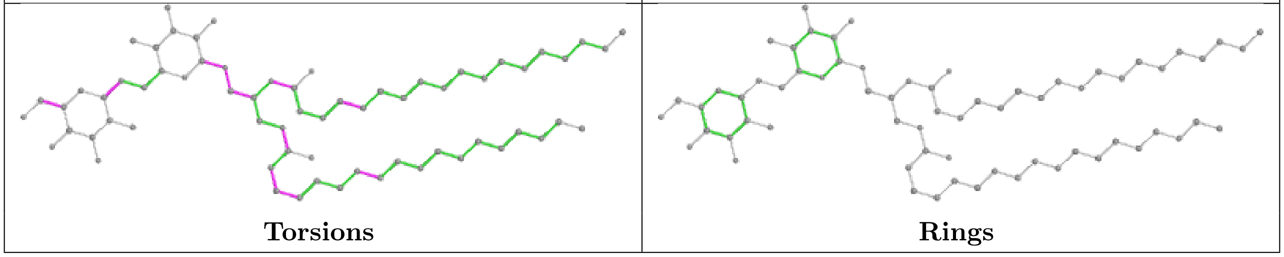
Rings

Ligand DGD B 849



Bond lengths

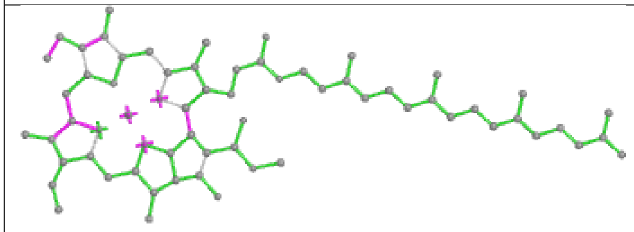
Bond angles



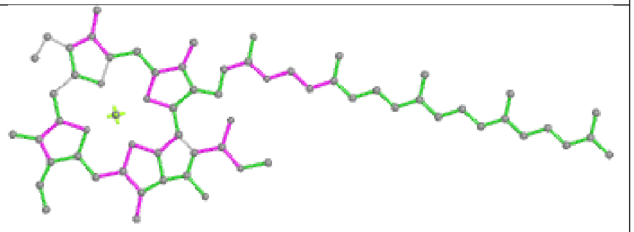
Torsions

Rings

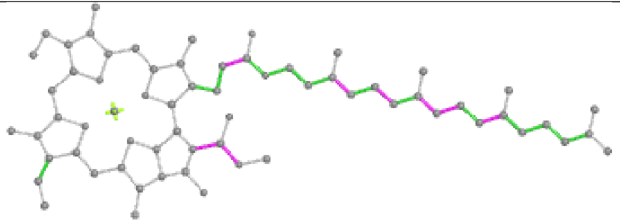
Ligand CLA A 856



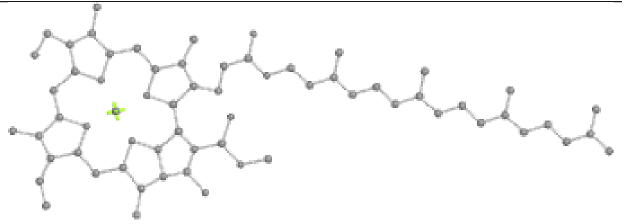
Bond lengths



Bond angles

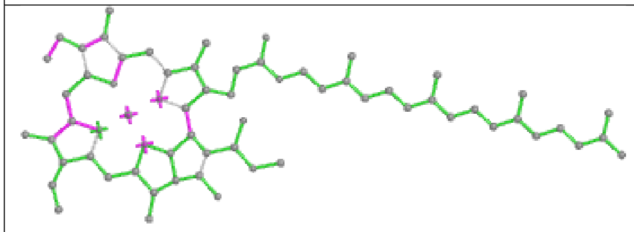


Torsions

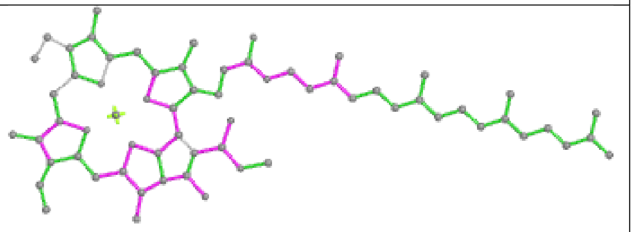


Rings

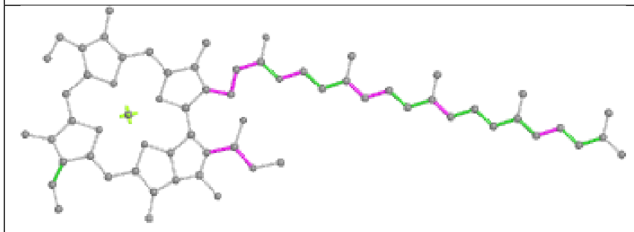
Ligand CLA B 833



Bond lengths



Bond angles



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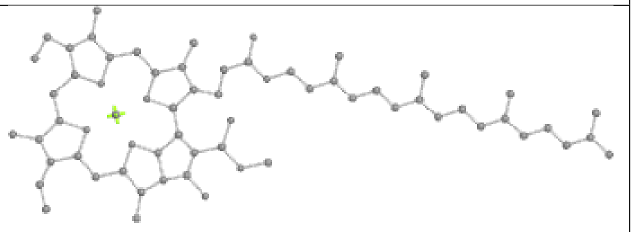
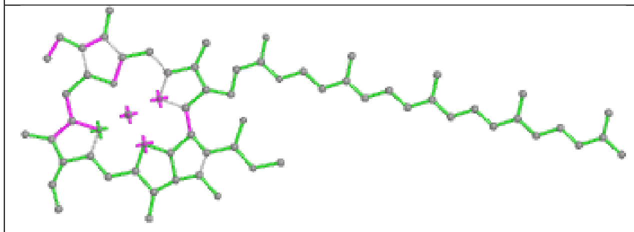
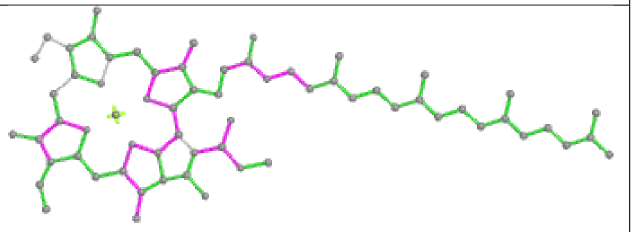


Rings

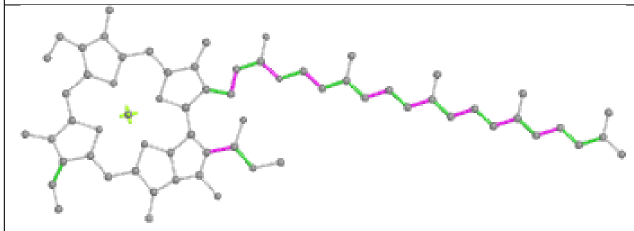
Ligand CLA A 839



Bond lengths



Bond angles



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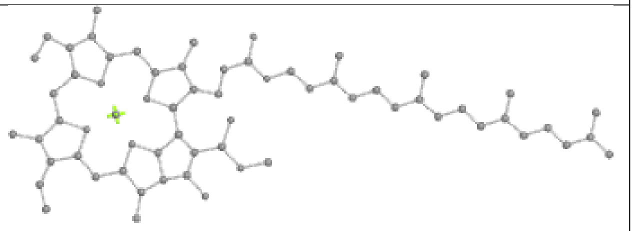
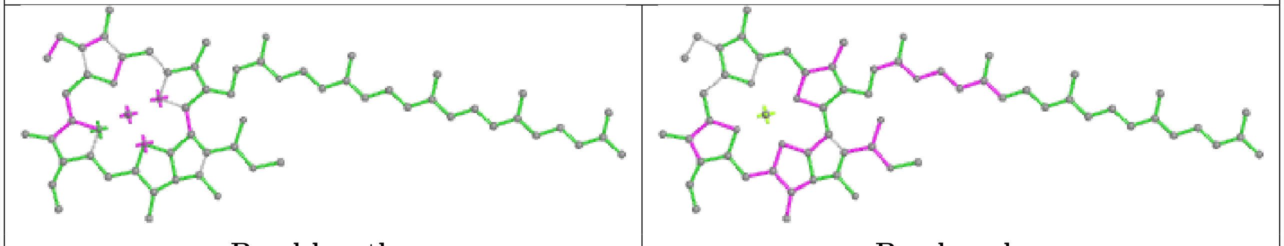
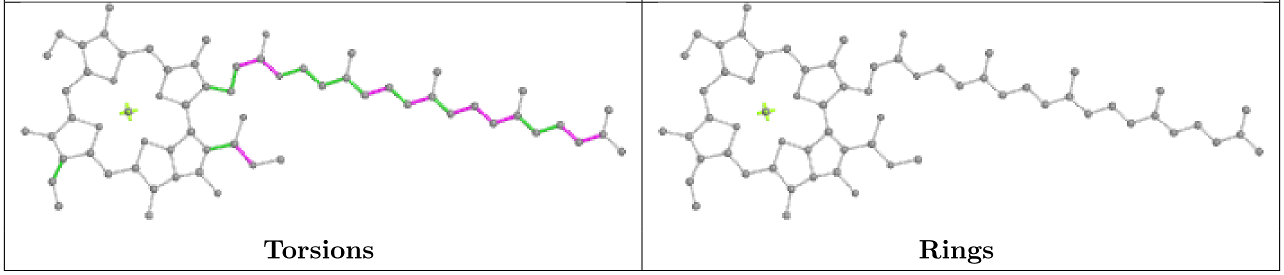


Rings

Ligand CLA 2 606

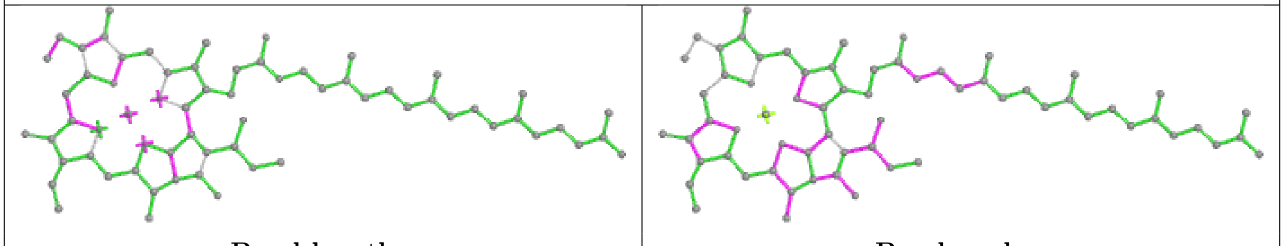


Bond lengths Bond angles

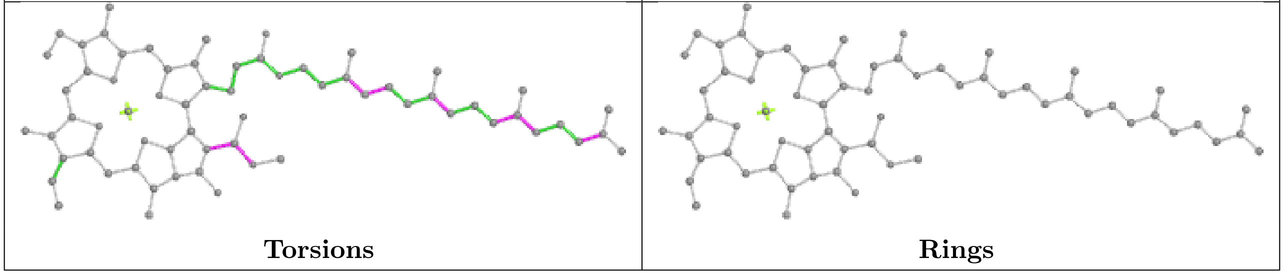


Torsions Rings

Ligand CLA A 826

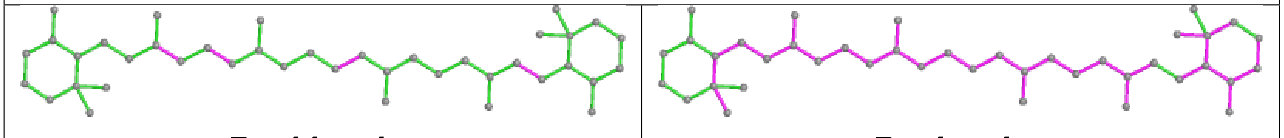


Bond lengths Bond angles

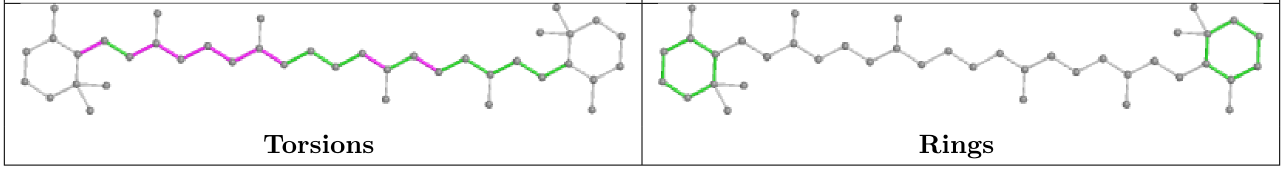


Torsions Rings

Ligand BCR B 847

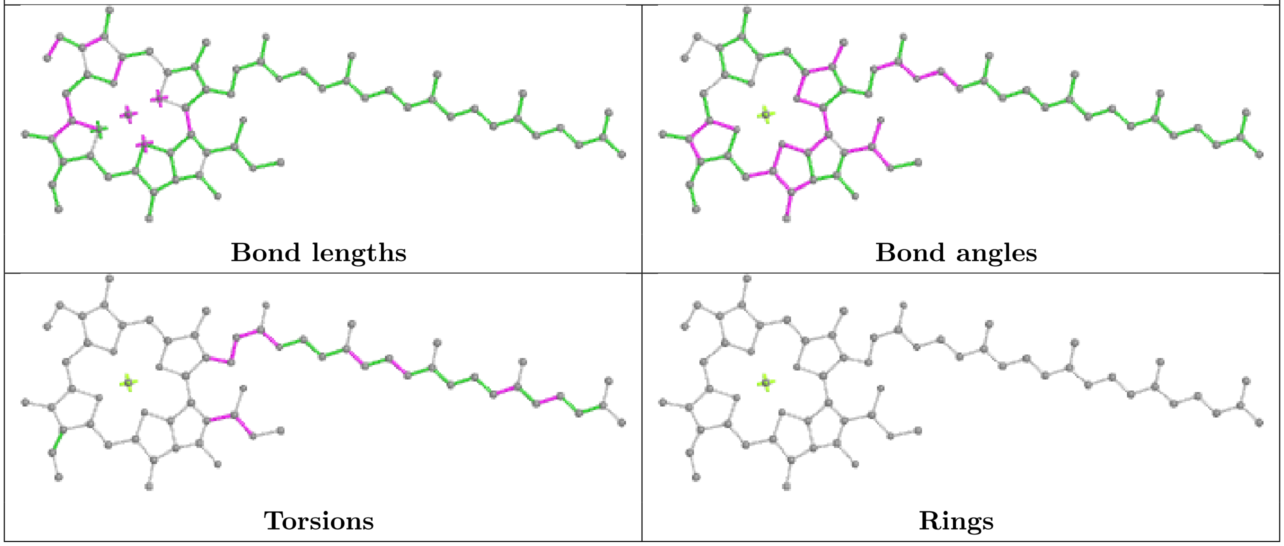


Bond lengths Bond angles



Torsions Rings

Ligand CLA B 826



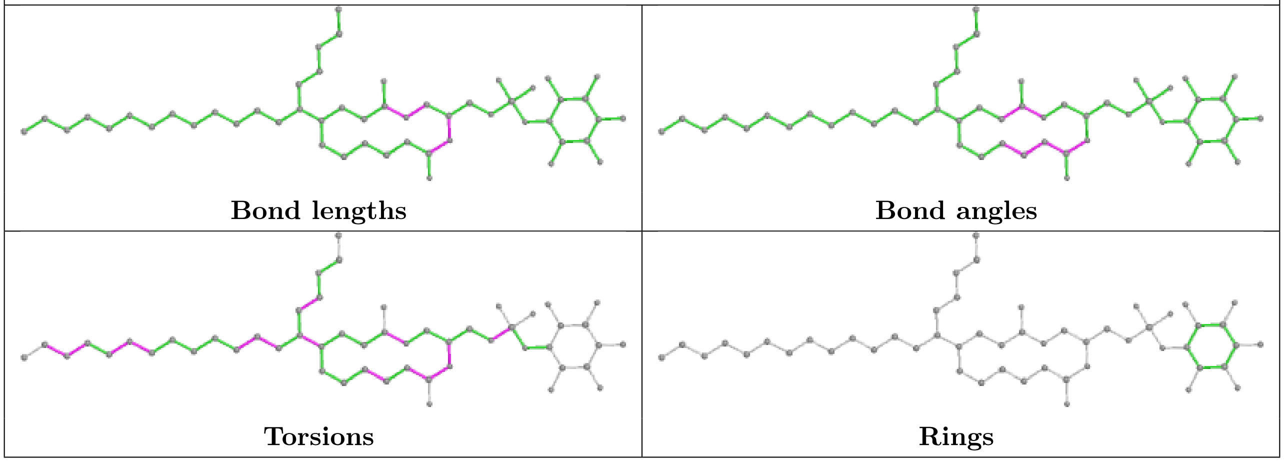
Bond lengths

Bond angles

Torsions

Rings

Ligand T7X A 851



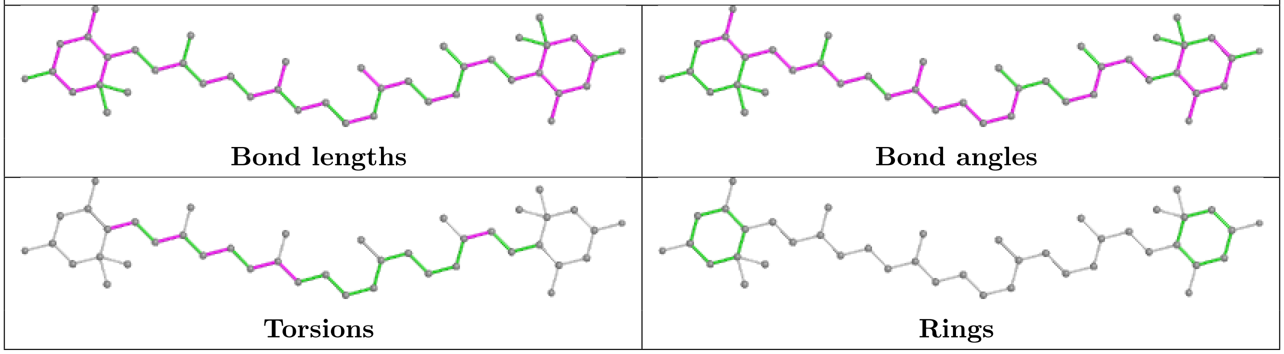
Bond lengths

Bond angles

Torsions

Rings

Ligand C7Z 1 612



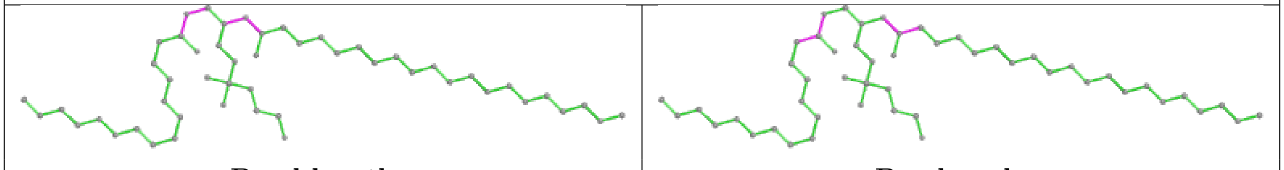
Bond lengths

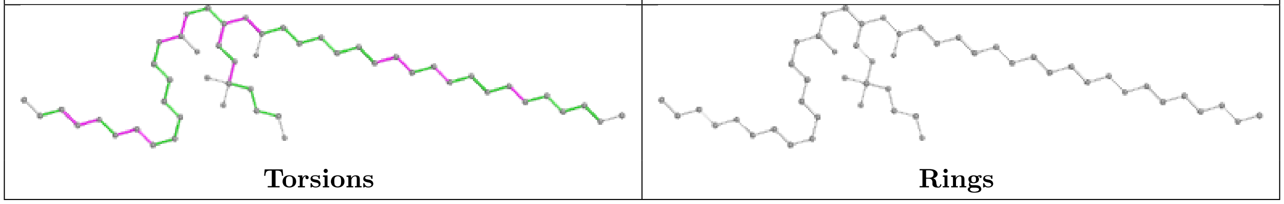
Bond angles

Torsions

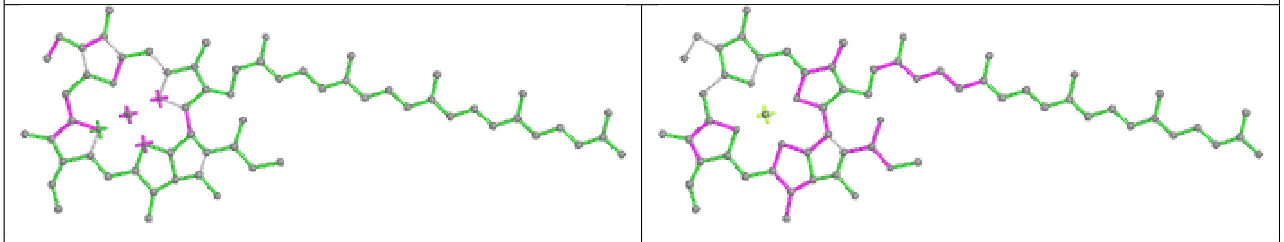
Rings

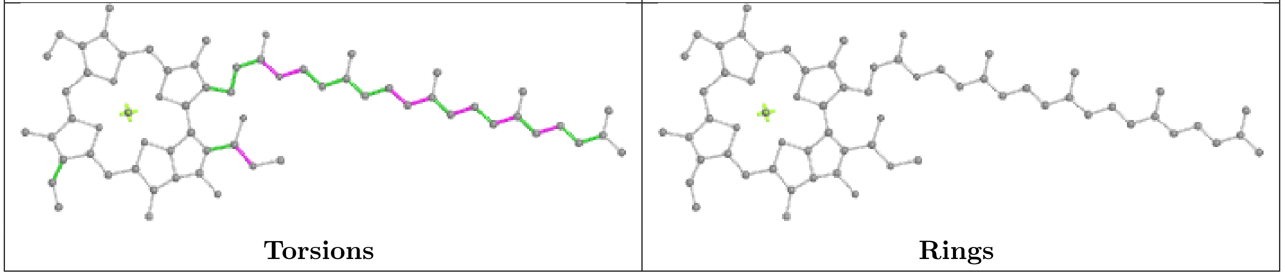
Ligand PTY 3 221


Bond lengths Bond angles

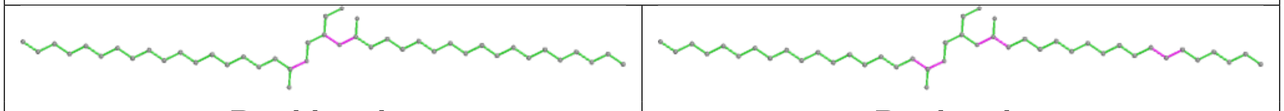

Torsions Rings

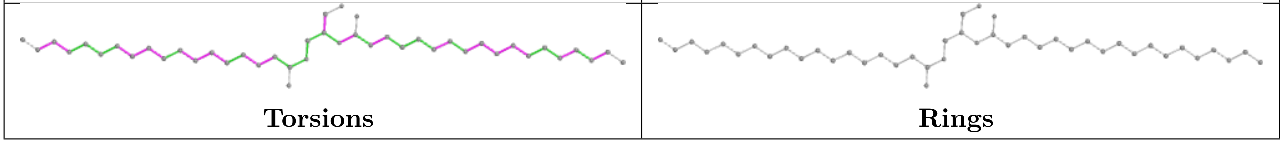
Ligand CLA F 204


Bond lengths Bond angles

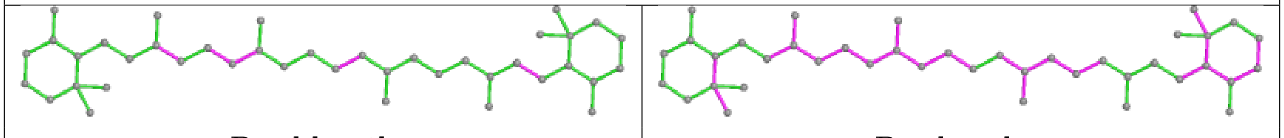

Torsions Rings

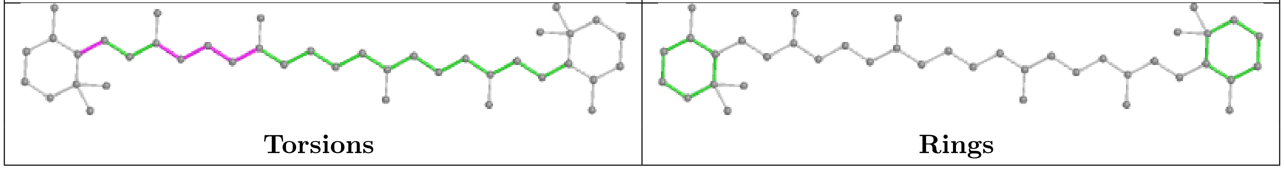
Ligand DGA 2 620


Bond lengths Bond angles

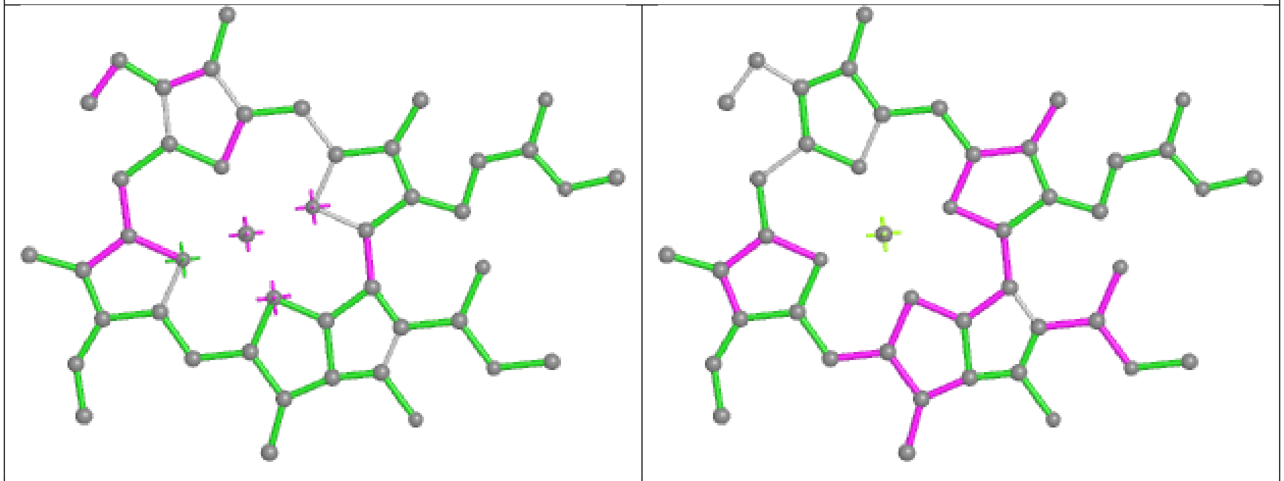

Torsions Rings

Ligand BCR L 206


Bond lengths Bond angles

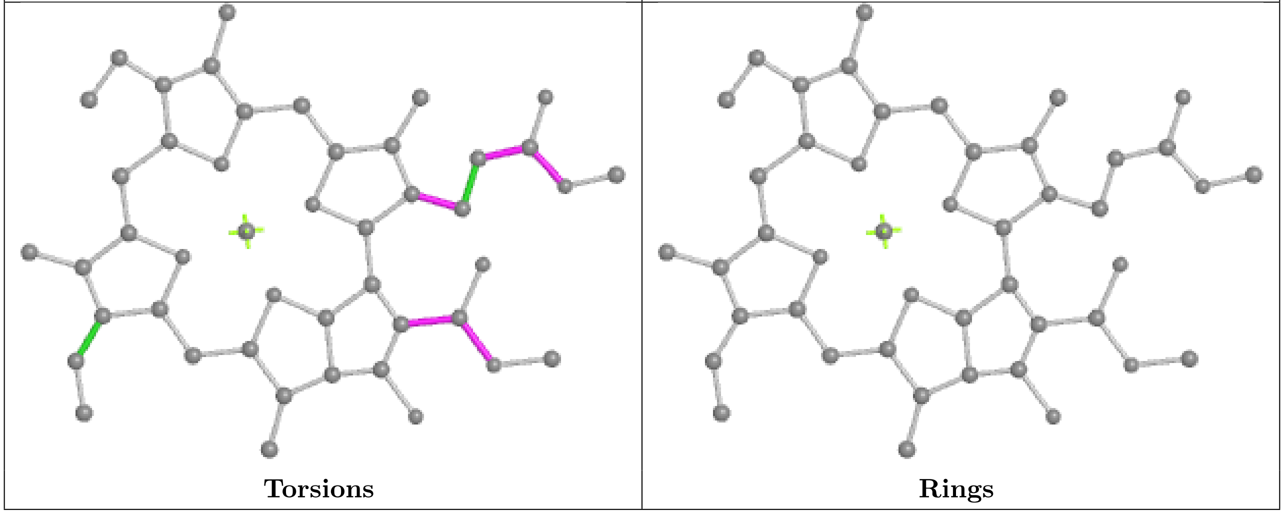

Torsions Rings

Ligand CLA 3 213



Bond lengths

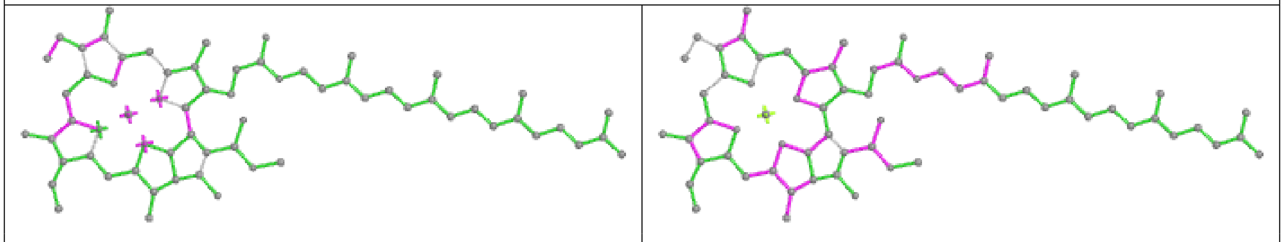
Bond angles



Torsions

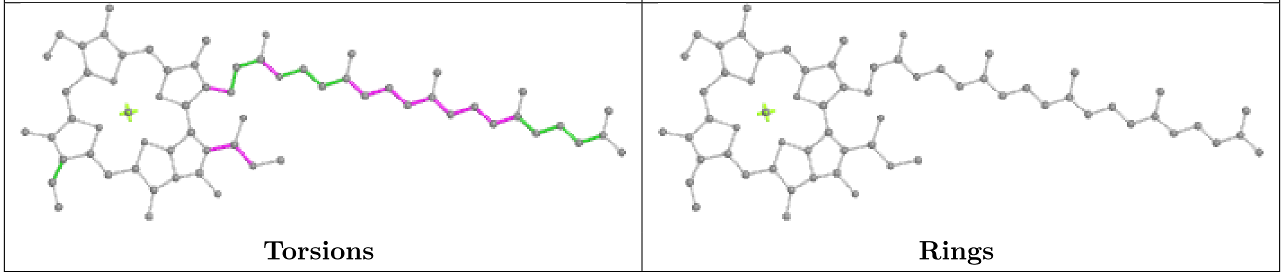
Rings

Ligand CLA A 814



Bond lengths

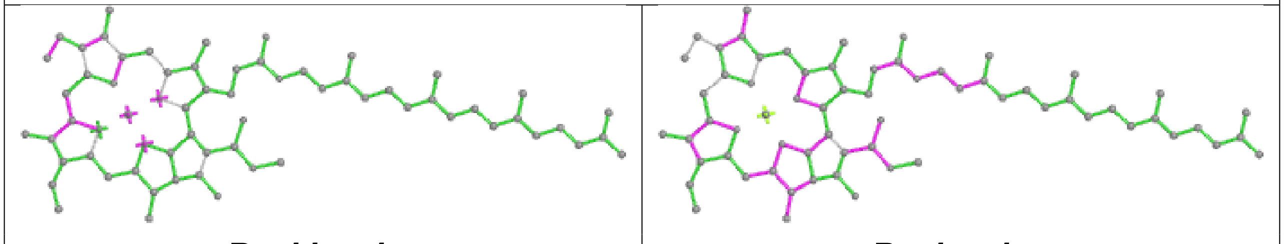
Bond angles



Torsions

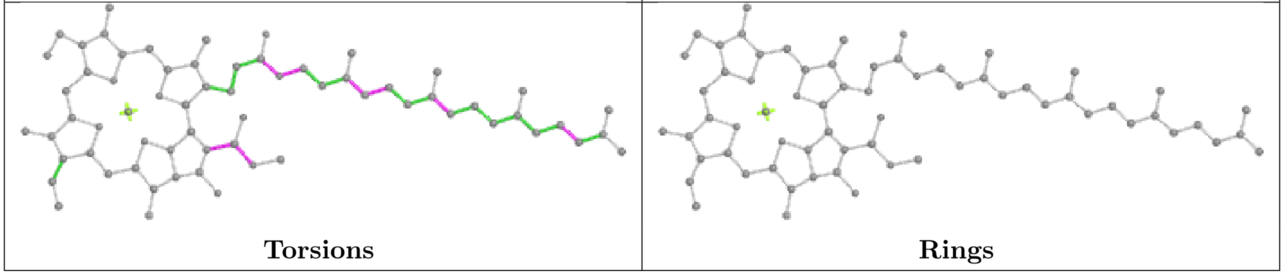
Rings

Ligand CLA B 813



Bond lengths

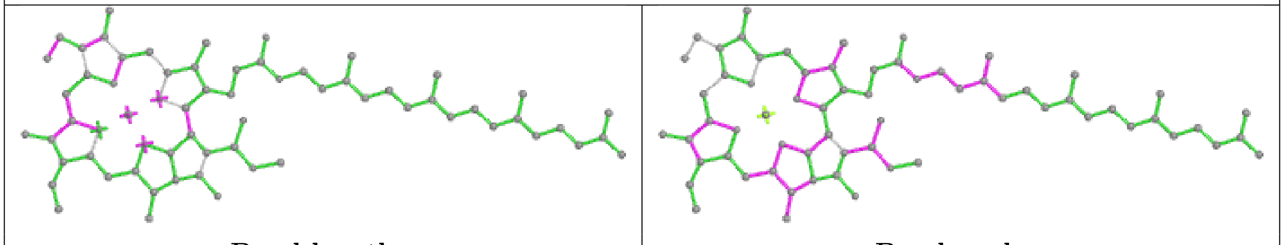
Bond angles



Torsions

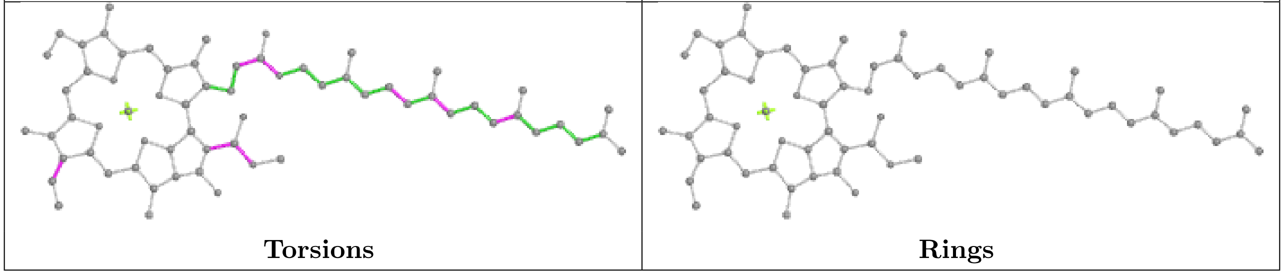
Rings

Ligand CLA 2 612



Bond lengths

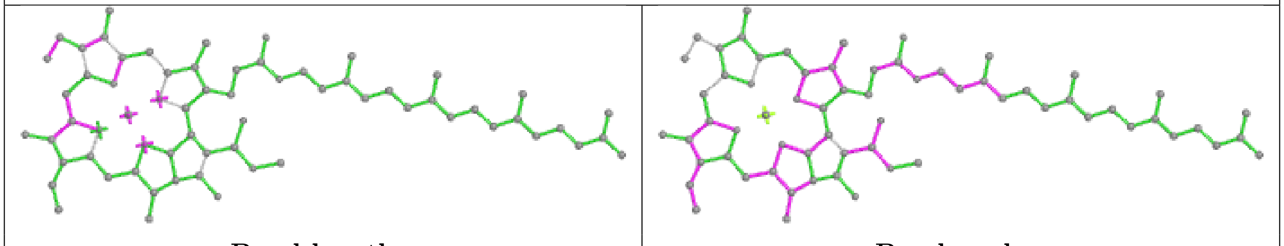
Bond angles



Torsions

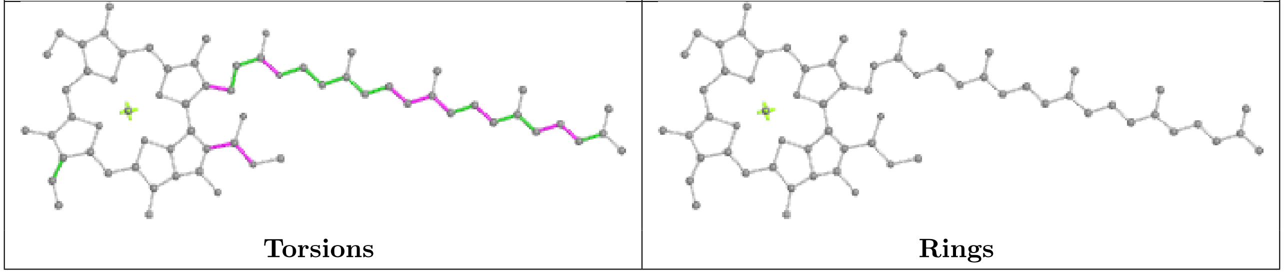
Rings

Ligand CLA 3 210



Bond lengths

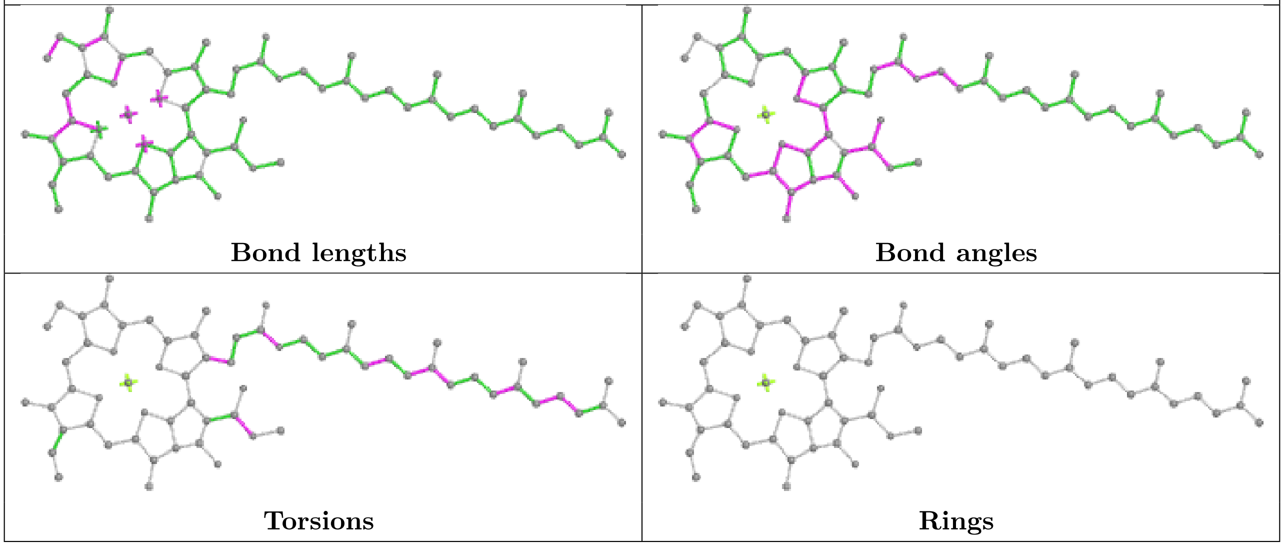
Bond angles



Torsions

Rings

Ligand CLA A 817



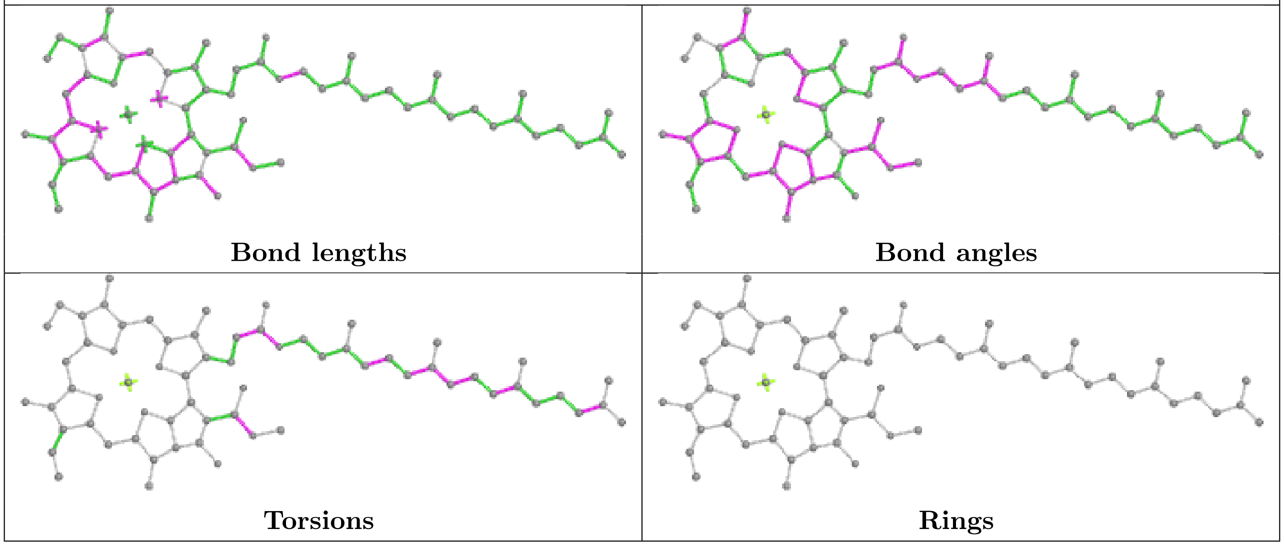
Bond lengths

Bond angles

Torsions

Rings

Ligand CL0 A 801



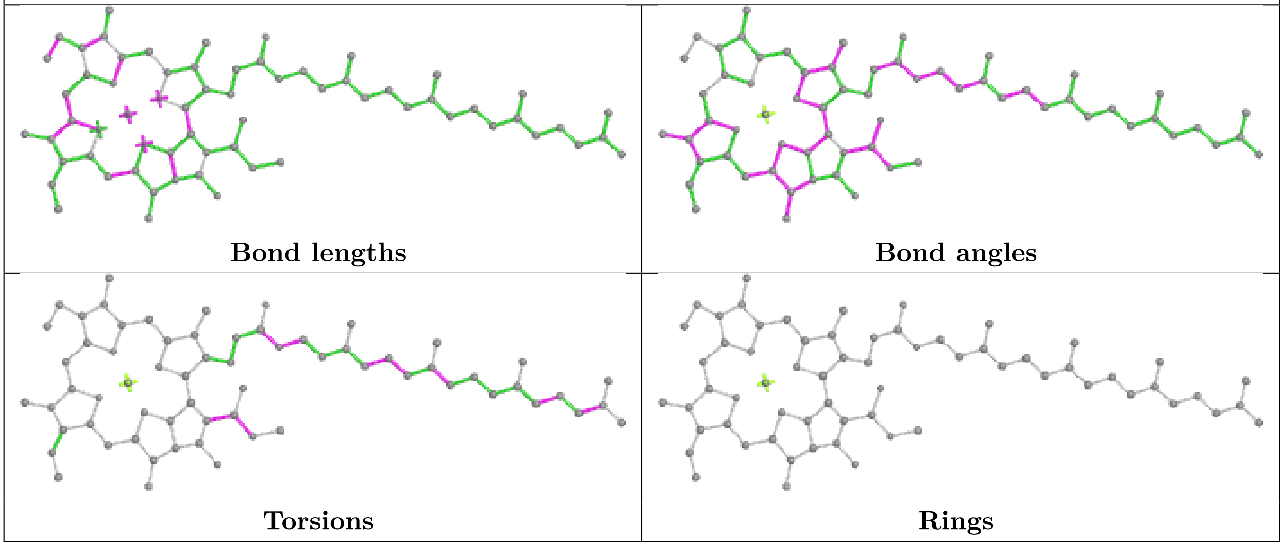
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA A 804



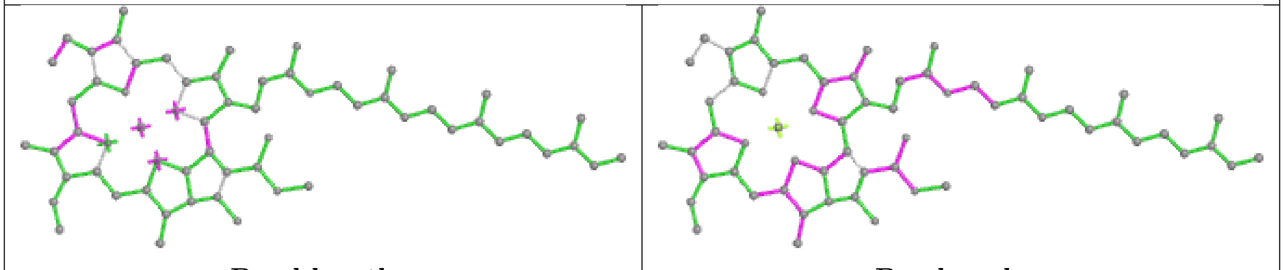
Bond lengths

Bond angles

Torsions

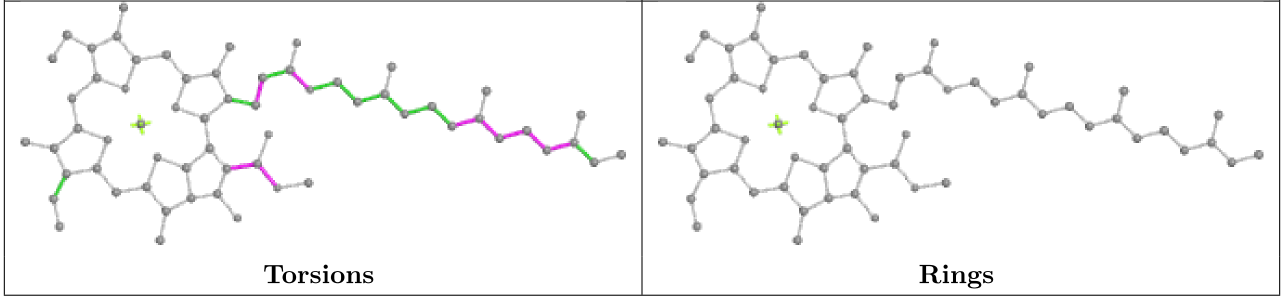
Rings

Ligand CLA F 201



Bond lengths

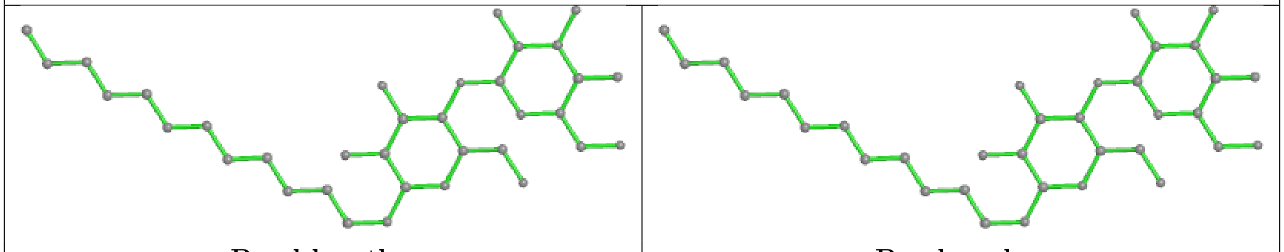
Bond angles



Torsions

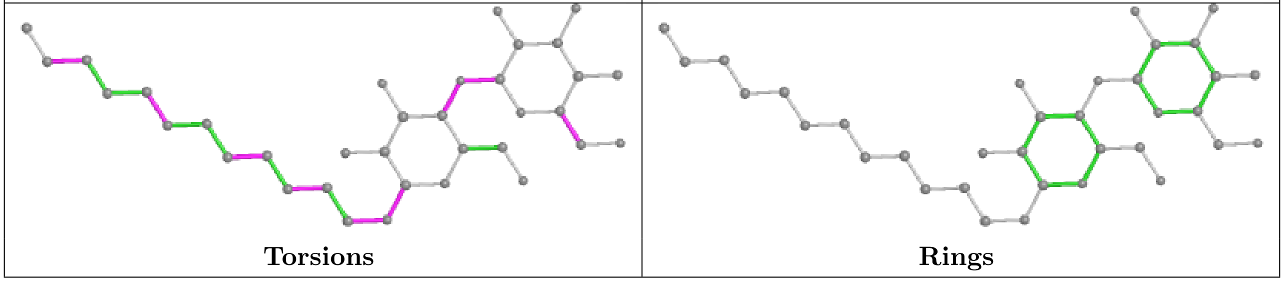
Rings

Ligand LMU 3 202



Bond lengths

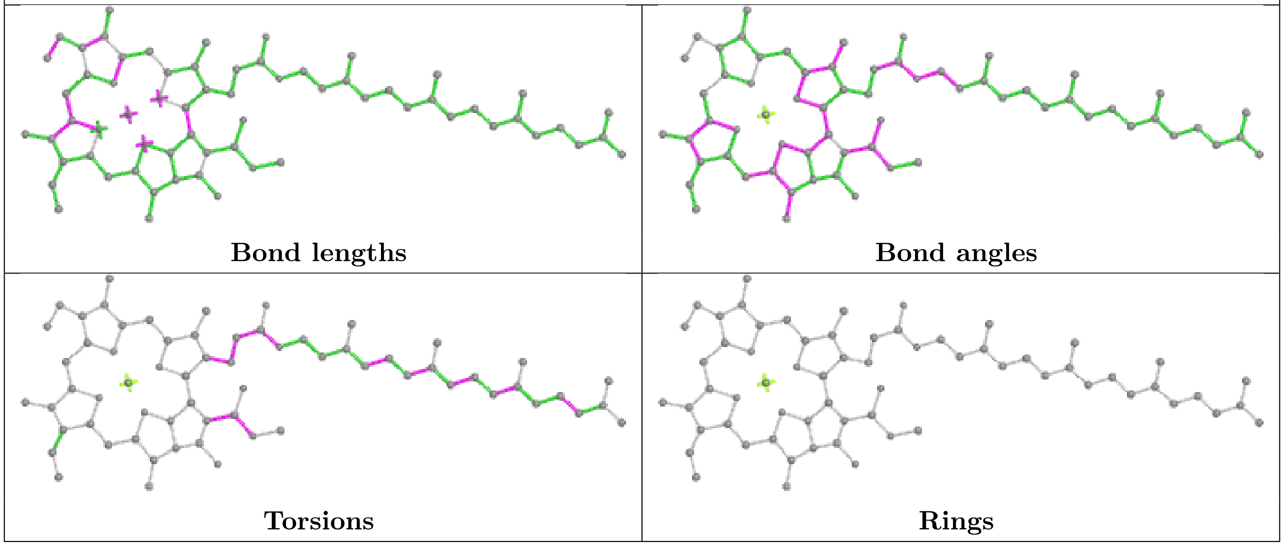
Bond angles



Torsions

Rings

Ligand CLA A 802



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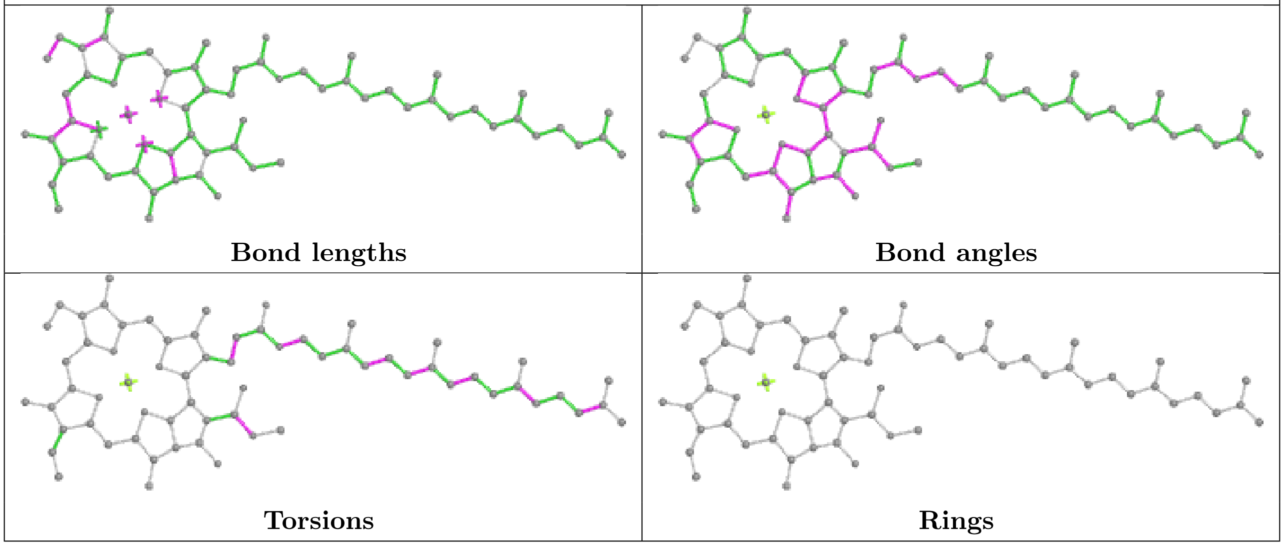

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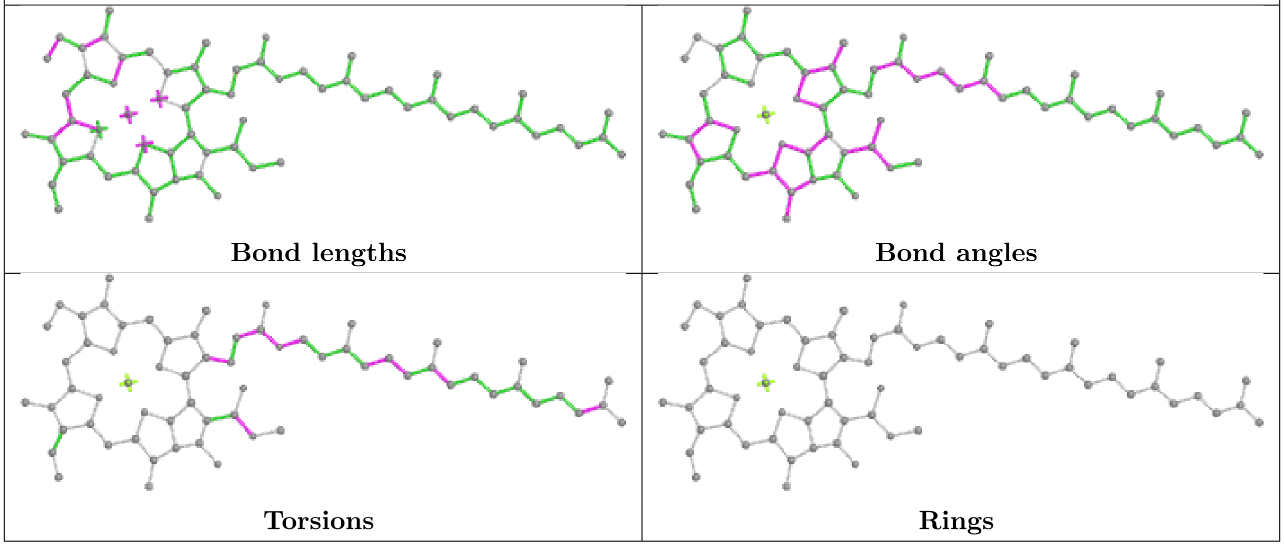
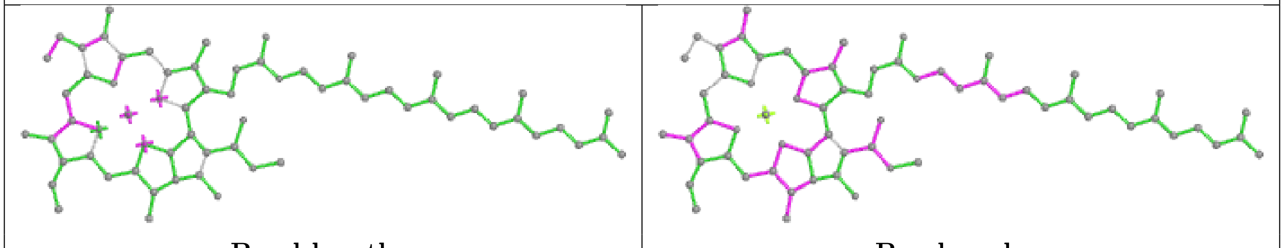
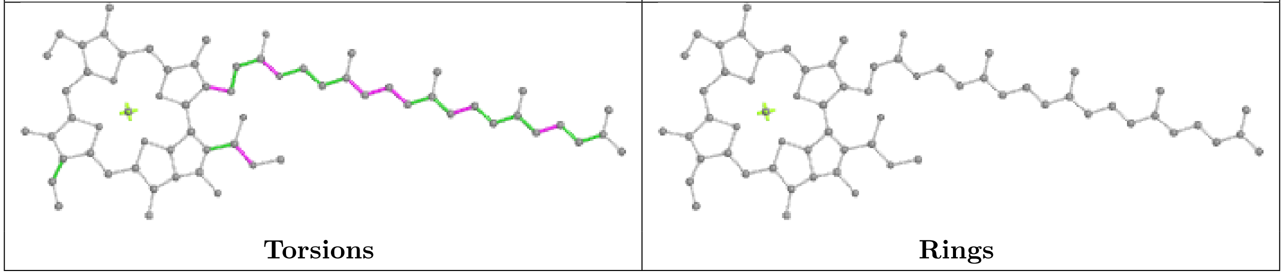


Ligand CLA O 201

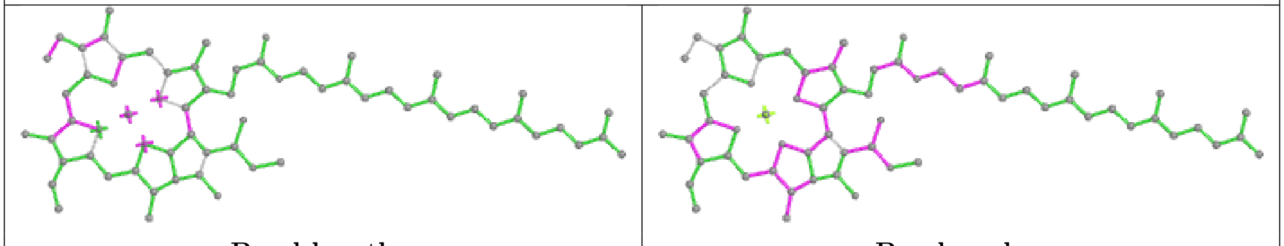


Bond lengths Bond angles

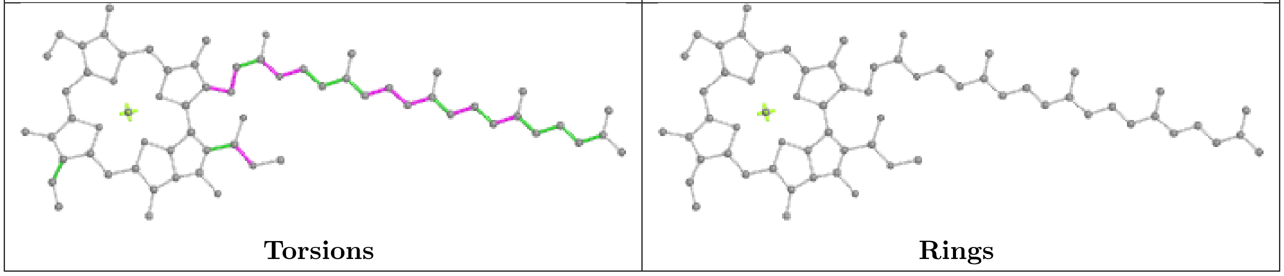


Torsions Rings

Ligand CLA B 832

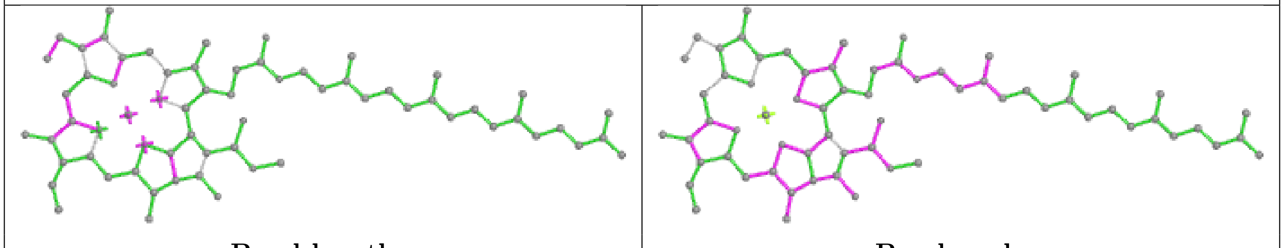


Bond lengths Bond angles

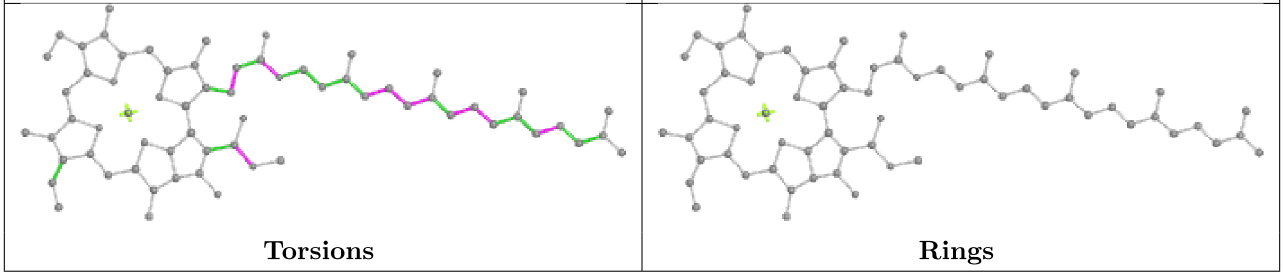


Torsions Rings

Ligand CLA 1 603



Bond lengths Bond angles



Torsions Rings

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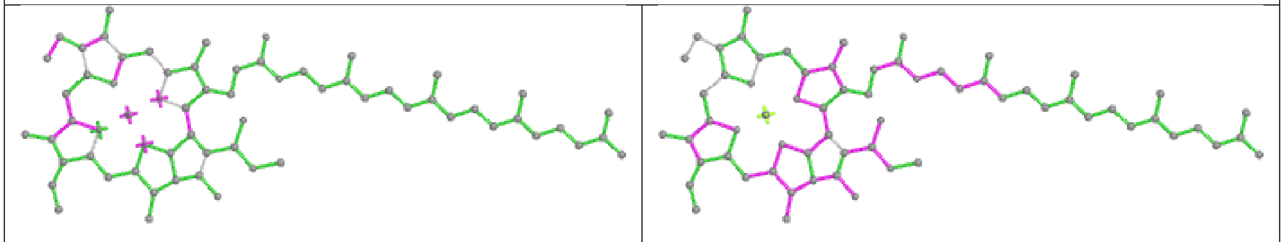
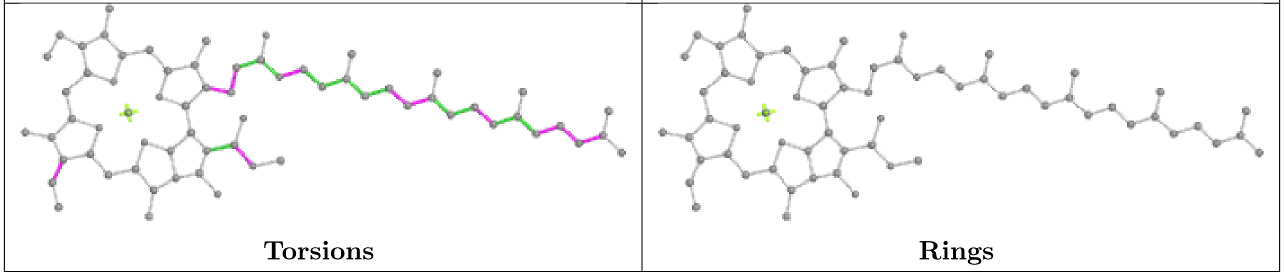
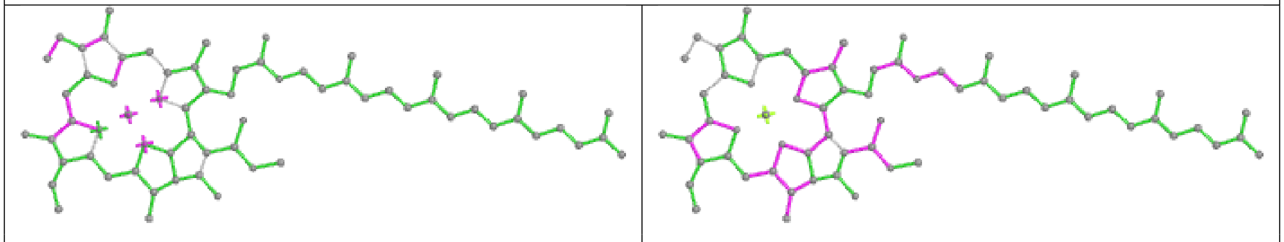


Bond lengths Bond angles

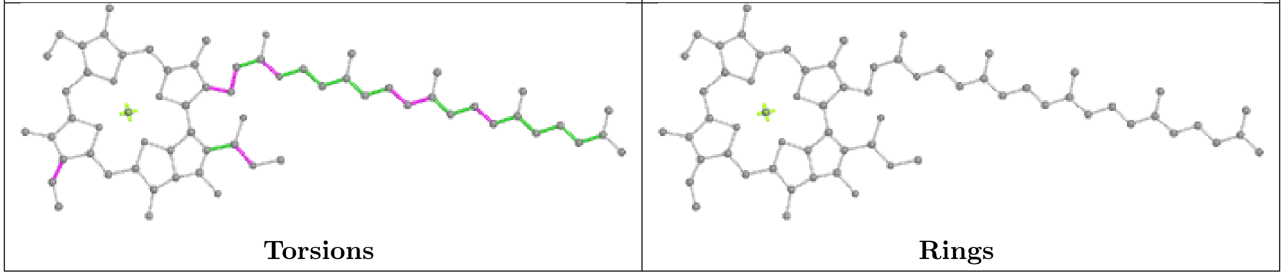


Torsions Rings

Ligand CLA 1 609

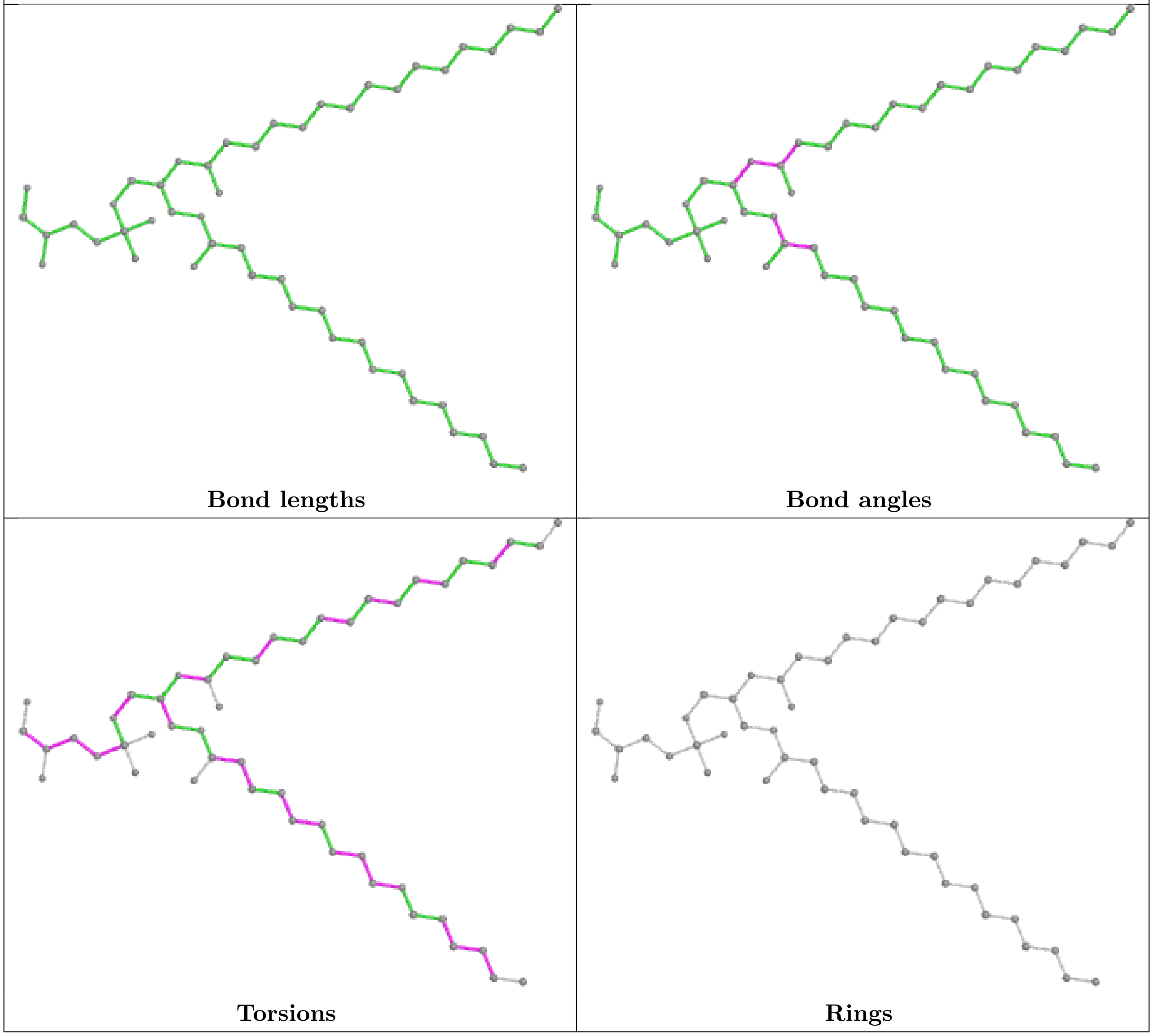


Bond lengths Bond angles



Torsions Rings

Ligand LHG A 842



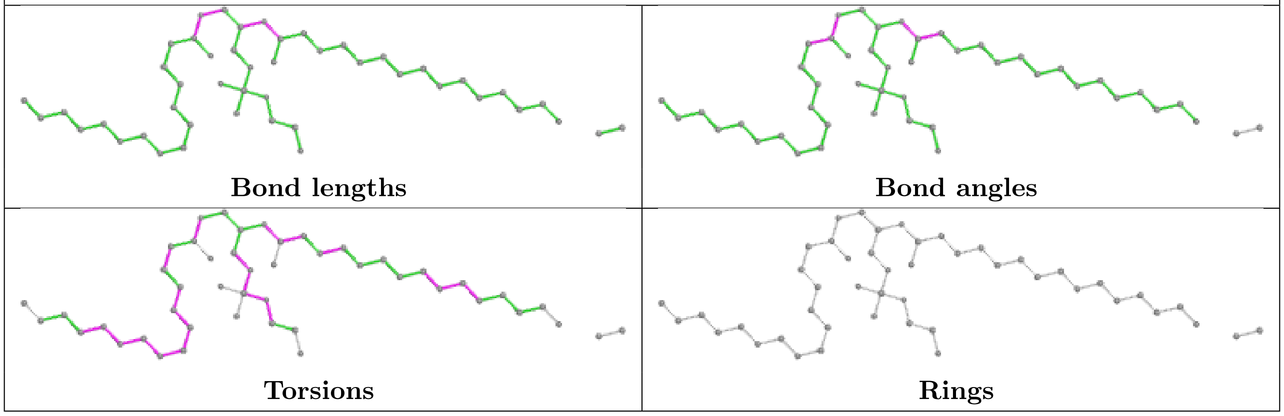
Bond lengths

Bond angles

Torsions

Rings

Ligand PTY A 852



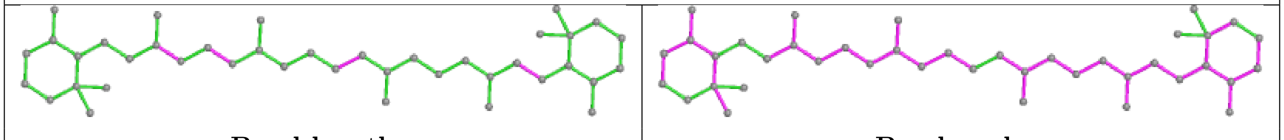
Bond lengths

Bond angles

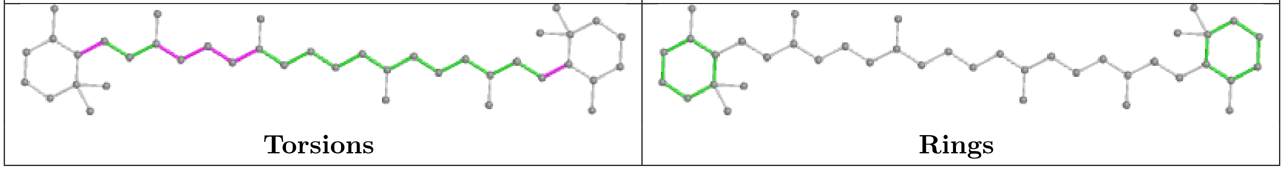
Torsions

Rings

Ligand BCR B 841

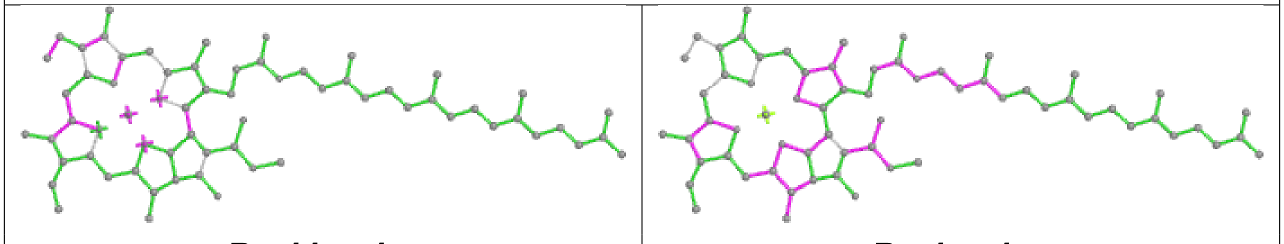


Bond lengths **Bond angles**

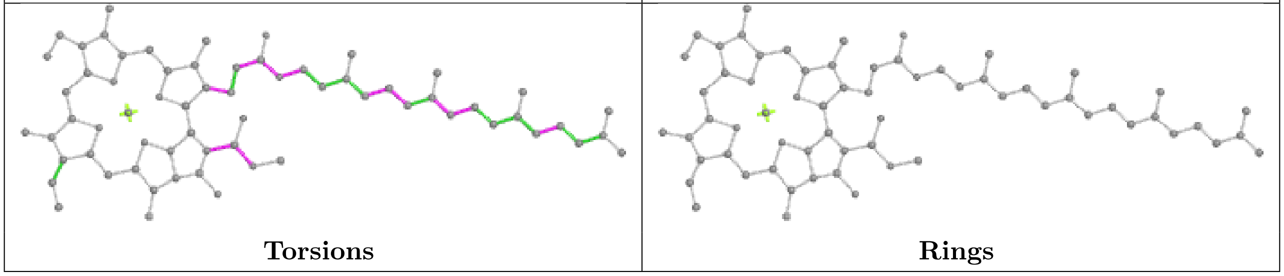


Torsions **Rings**

Ligand CLA 2 610

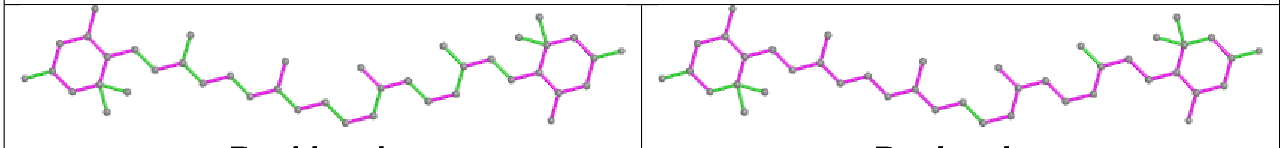


Bond lengths **Bond angles**

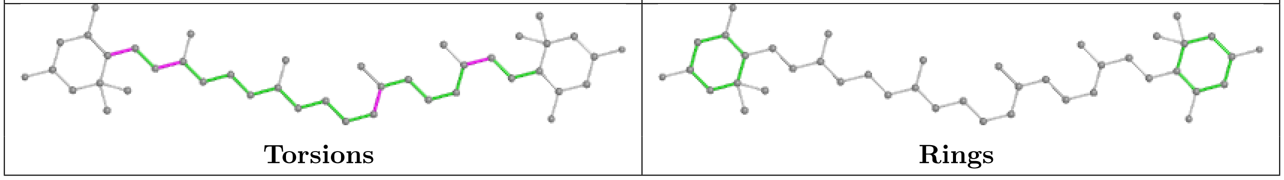


Torsions **Rings**

Ligand C7Z 2 615

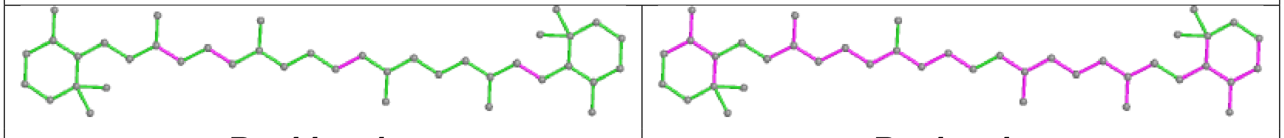


Bond lengths **Bond angles**

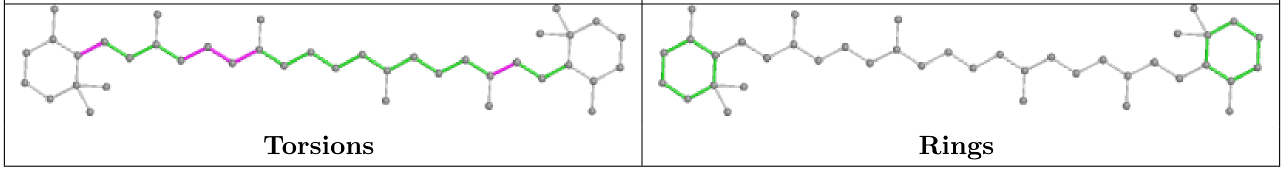


Torsions **Rings**

Ligand BCR F 203

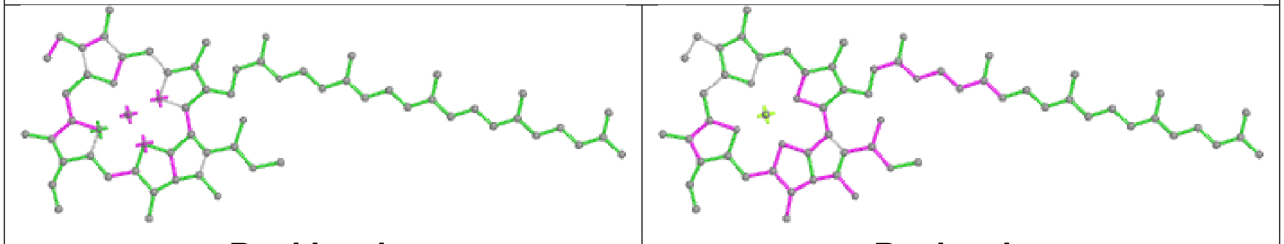


Bond lengths **Bond angles**

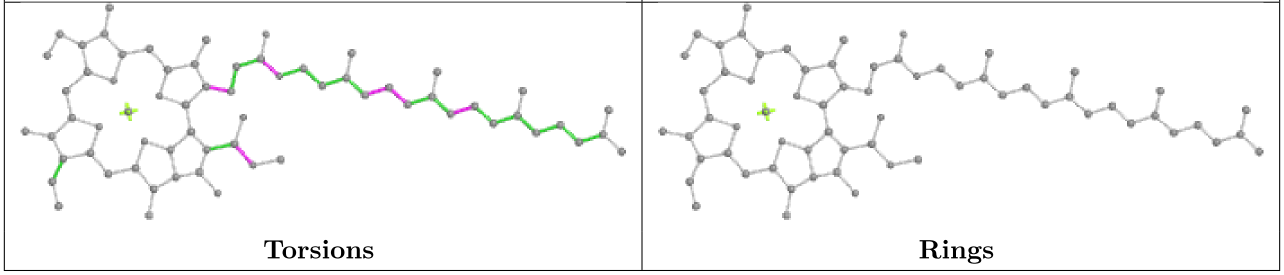


Torsions **Rings**

Ligand CLA 2 603

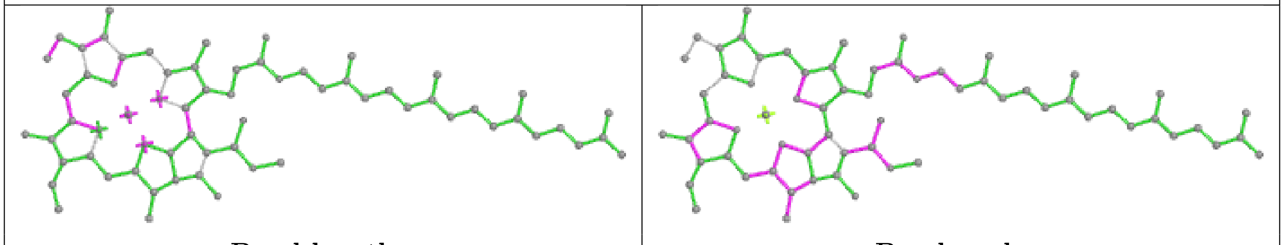


Bond lengths Bond angles

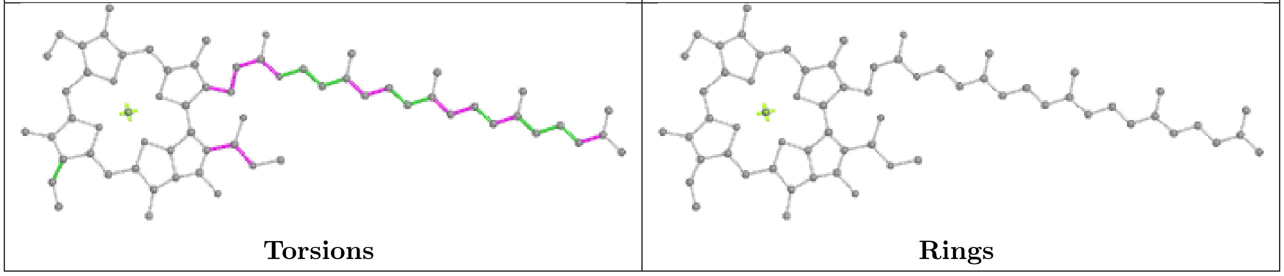


Torsions Rings

Ligand CLA A 805

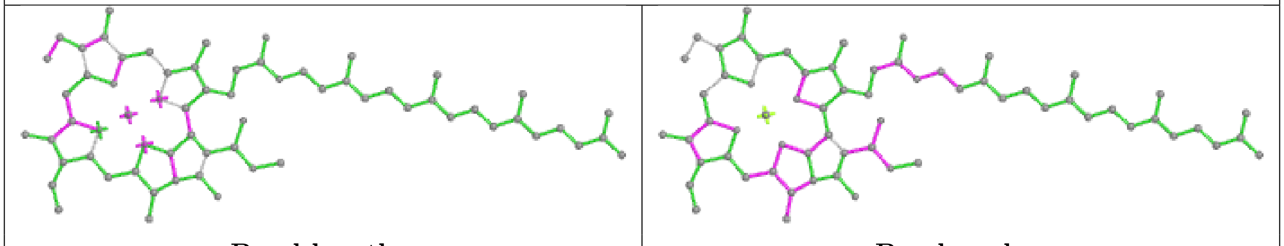


Bond lengths Bond angles

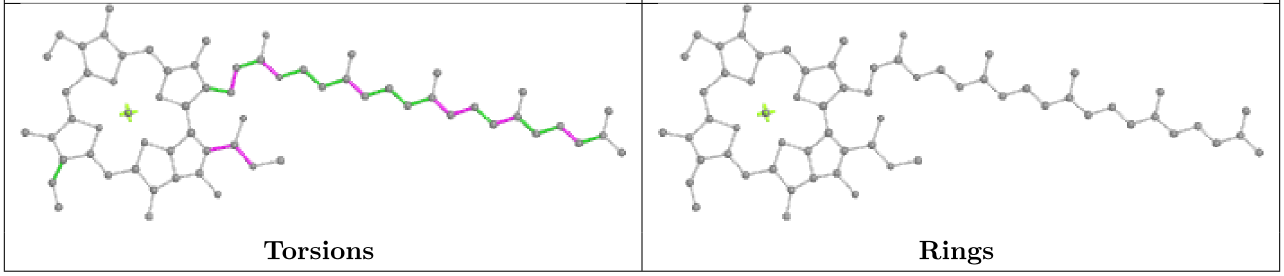


Torsions Rings

Ligand CLA A 820

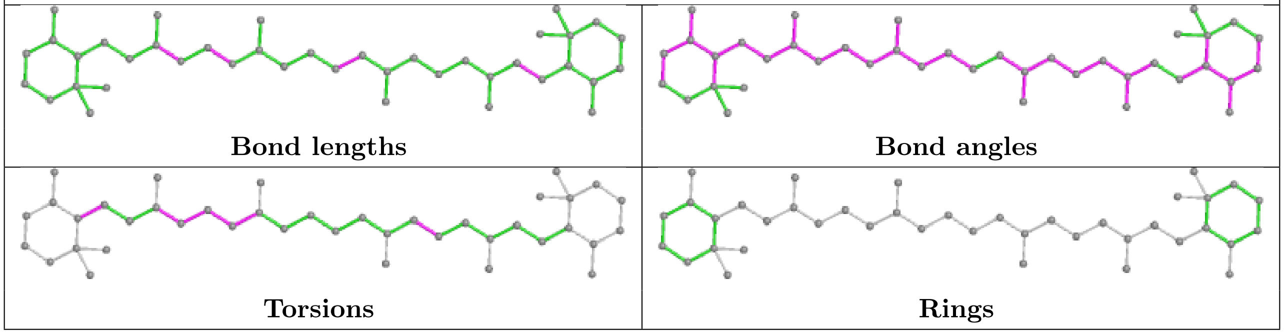


Bond lengths Bond angles

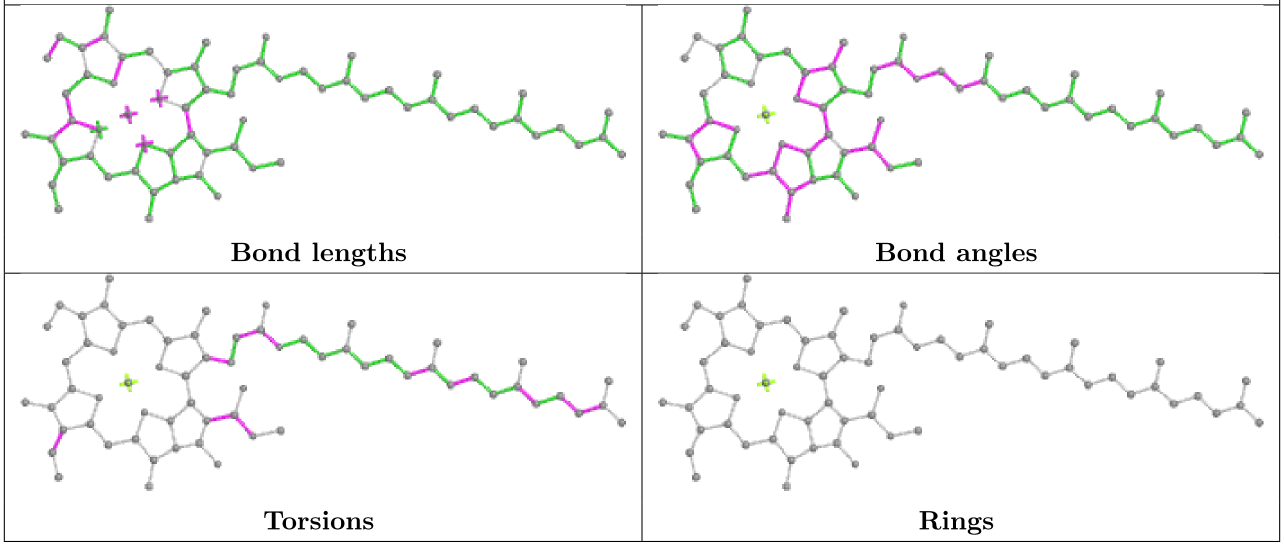


Torsions Rings

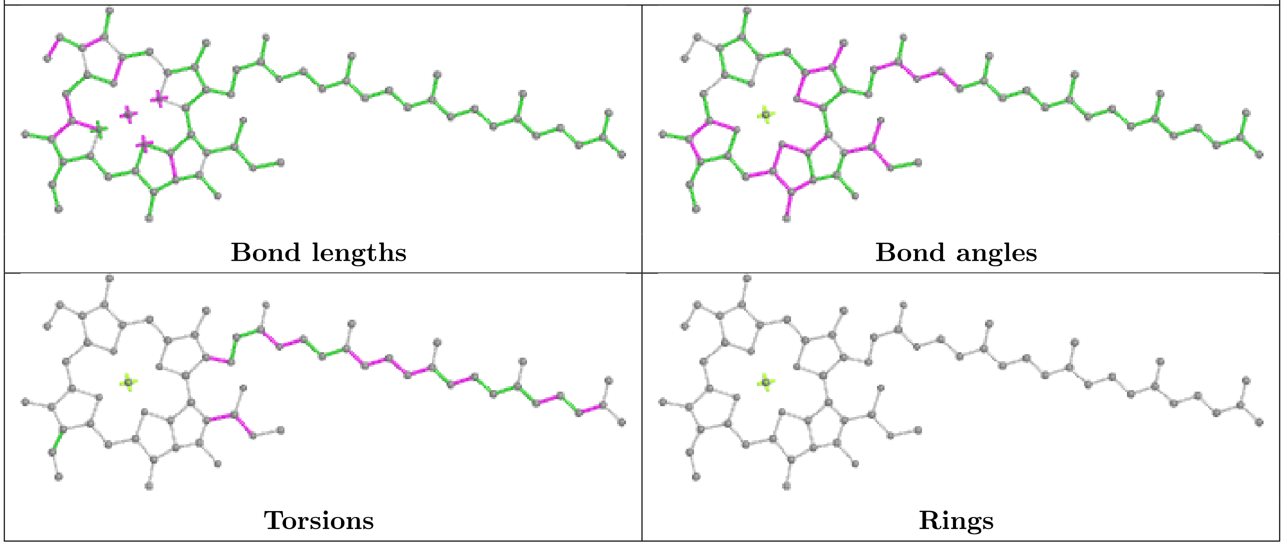
Ligand BCR A 857



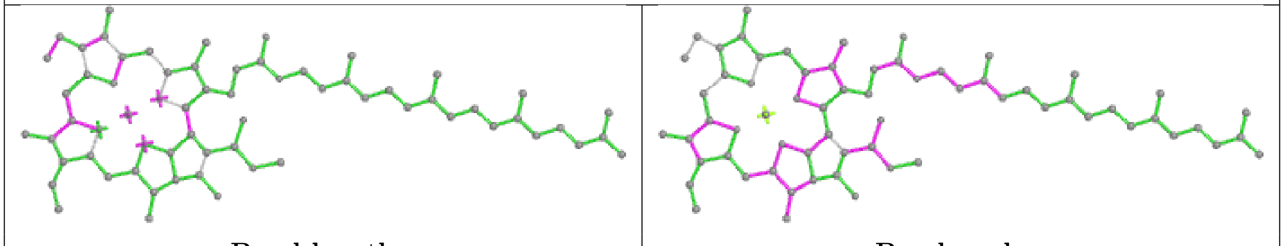
Ligand CLA 3 203



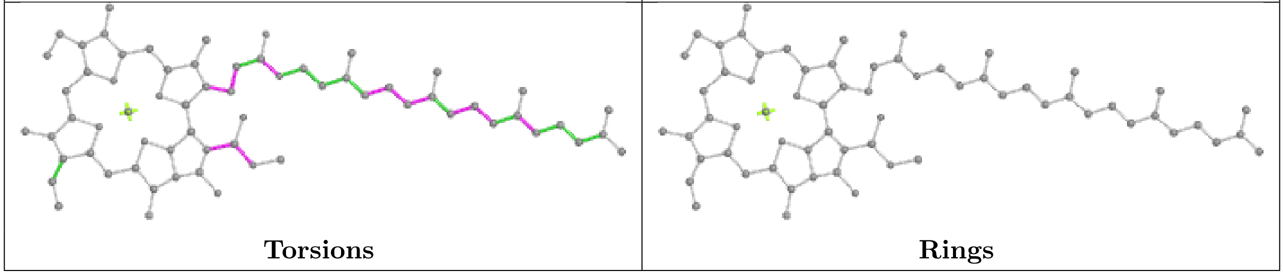
Ligand CLA O 203



Ligand CLA 1 606

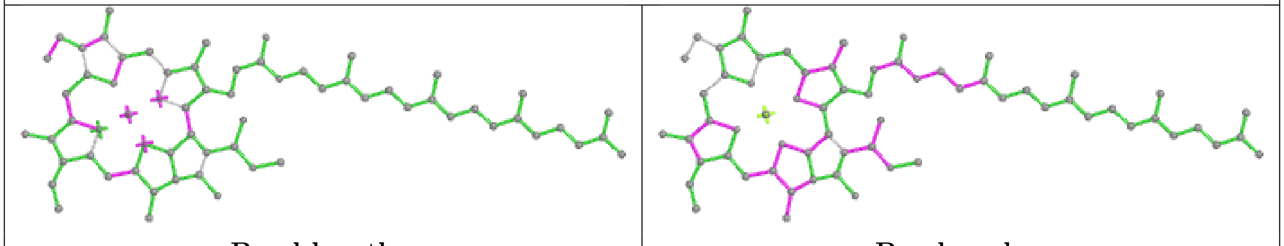


Bond lengths Bond angles

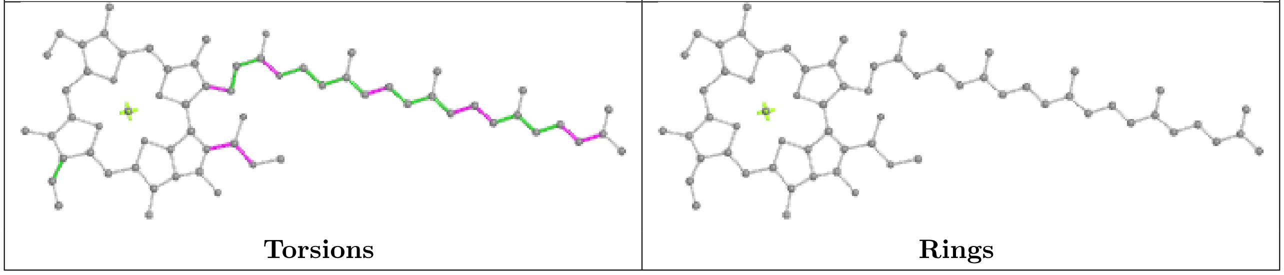


Torsions Rings

Ligand CLA L 205

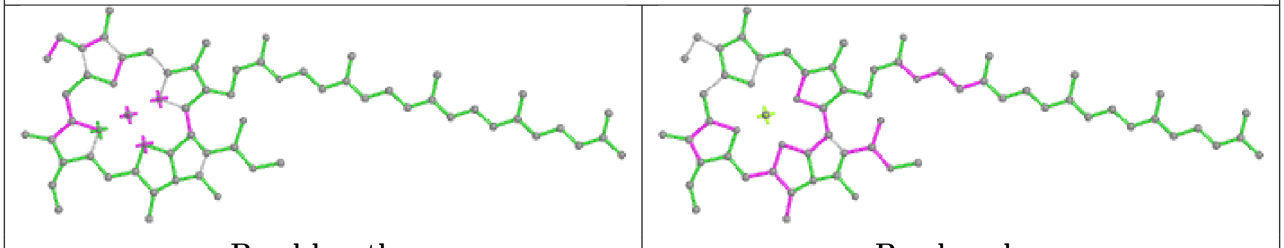


Bond lengths Bond angles

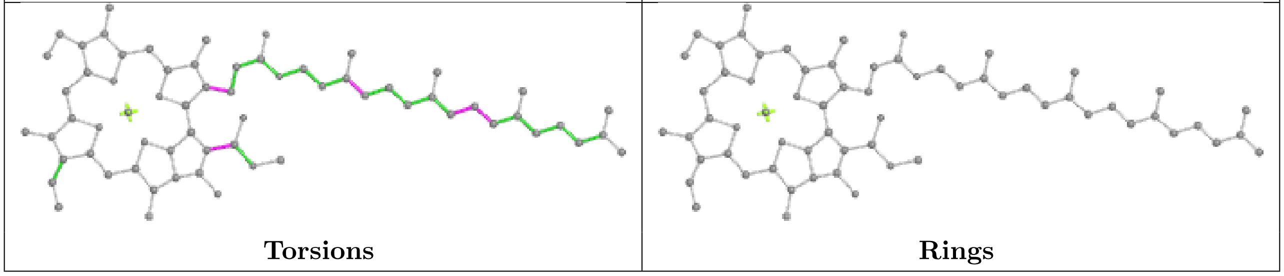


Torsions Rings

Ligand CLA B 817

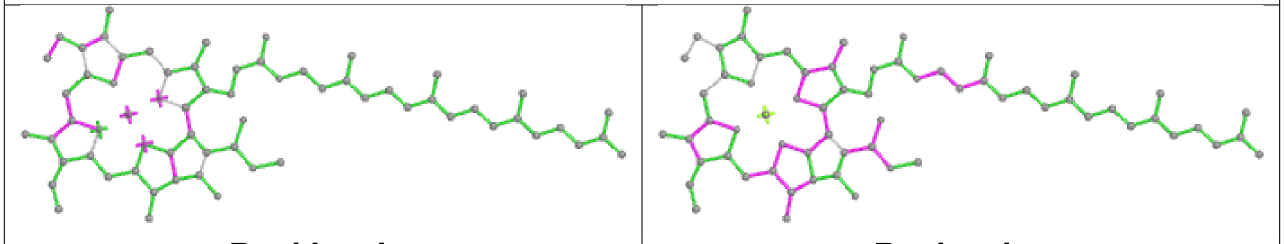


Bond lengths Bond angles



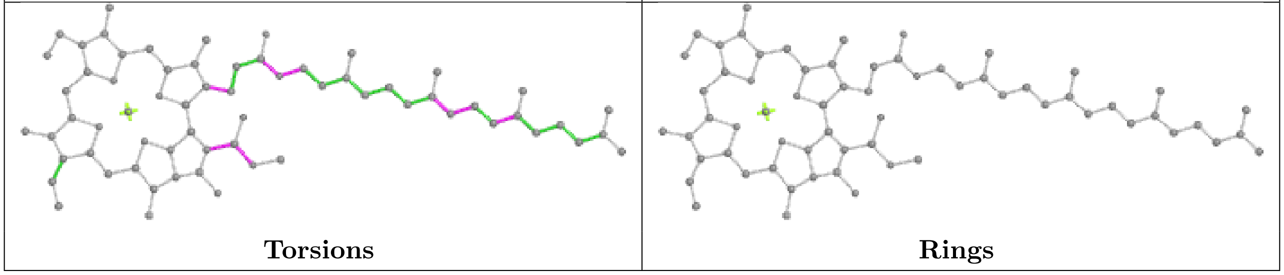
Torsions Rings

Ligand CLA A 824



Bond lengths

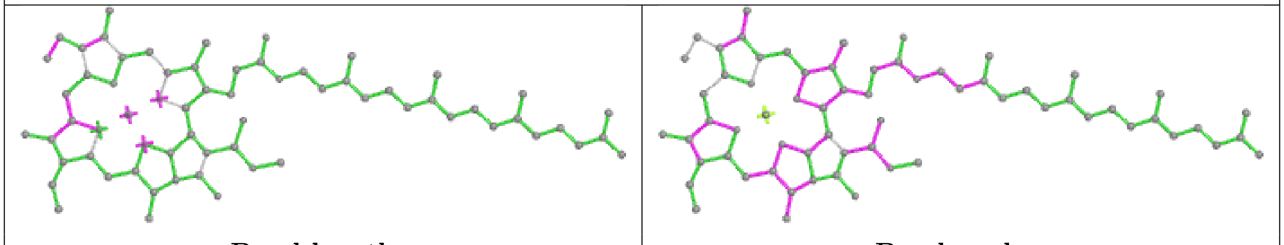
Bond angles



Torsions

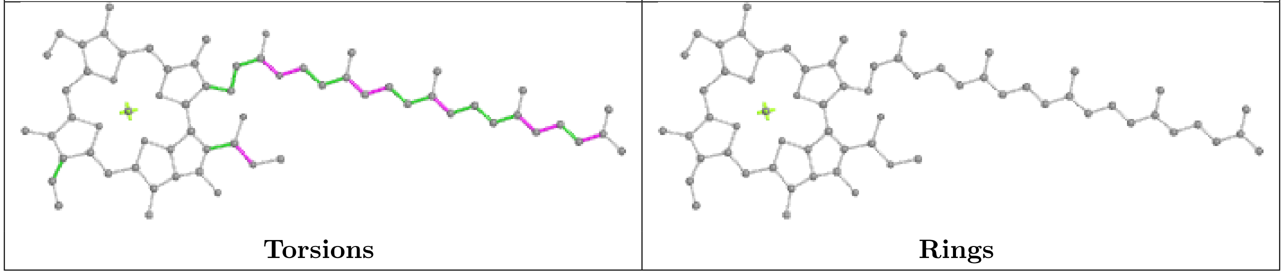
Rings

Ligand CLA B 824



Bond lengths

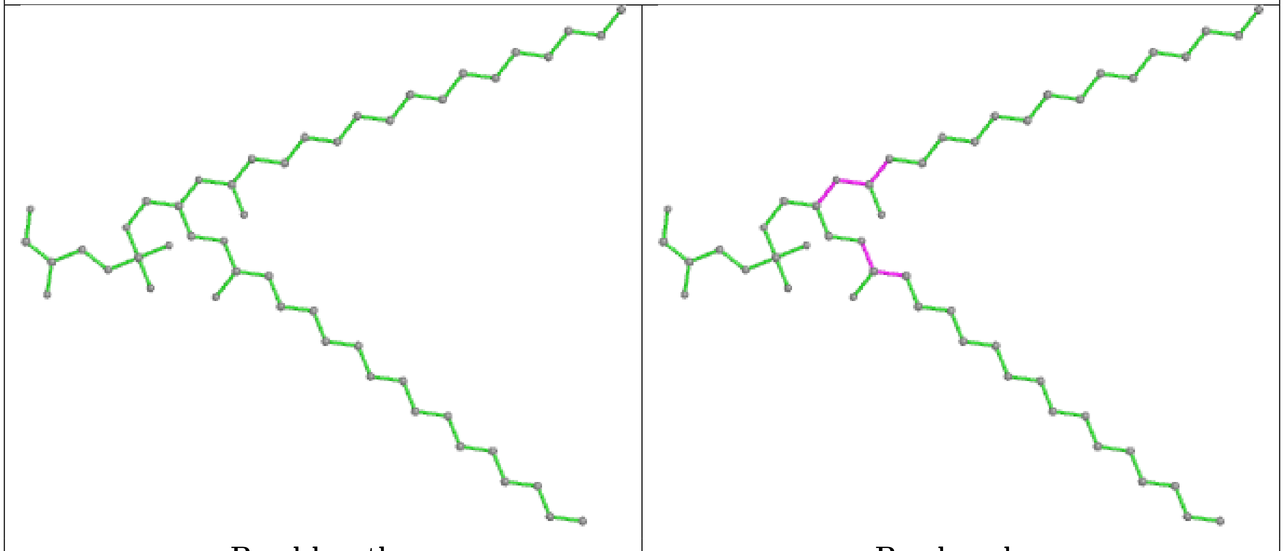
Bond angles



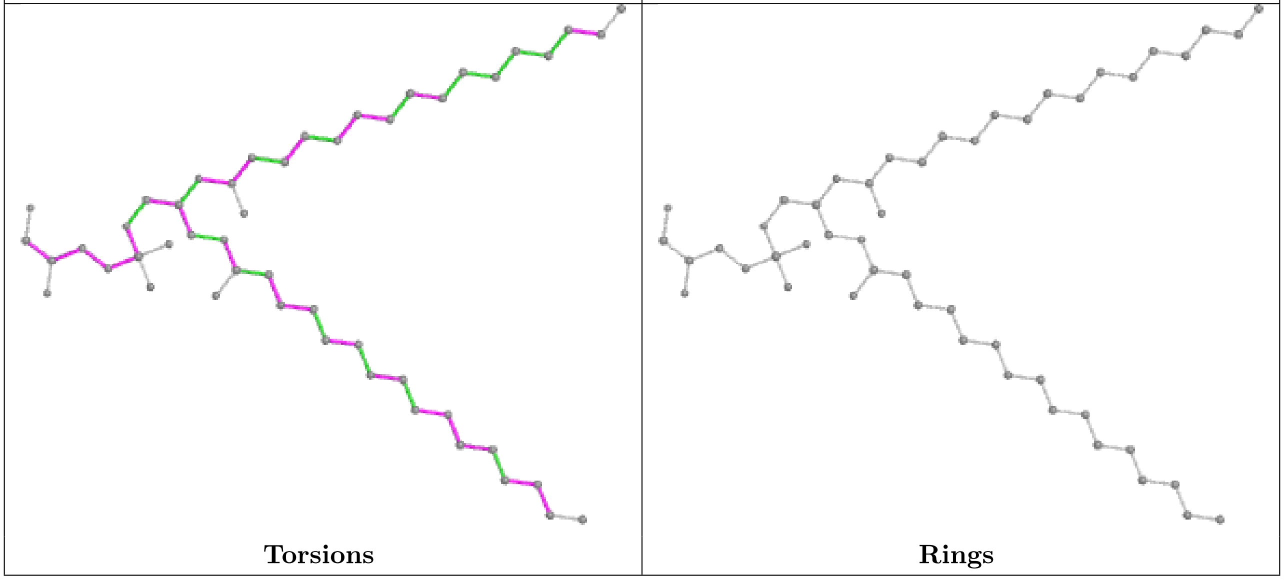
Torsions

Rings

Ligand LHG 3 219

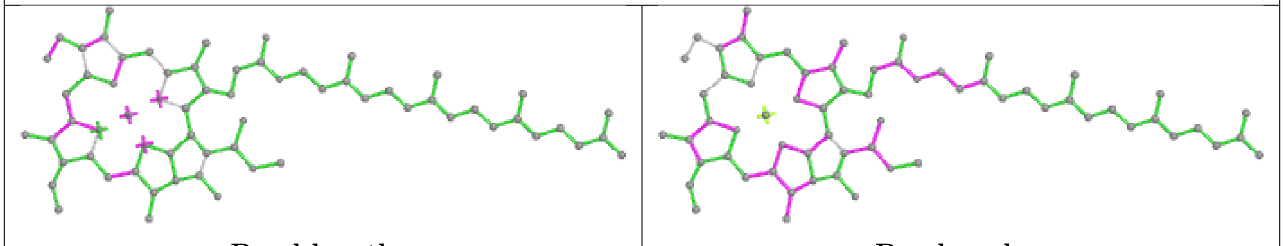


Bond lengths Bond angles

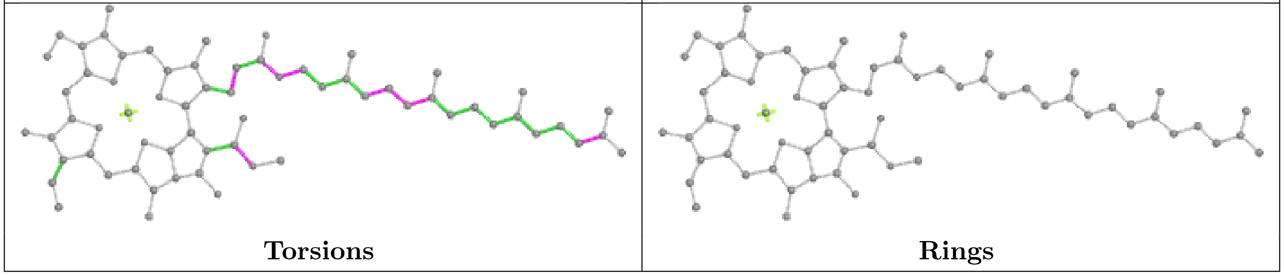


Torsions Rings

Ligand CLA A 811

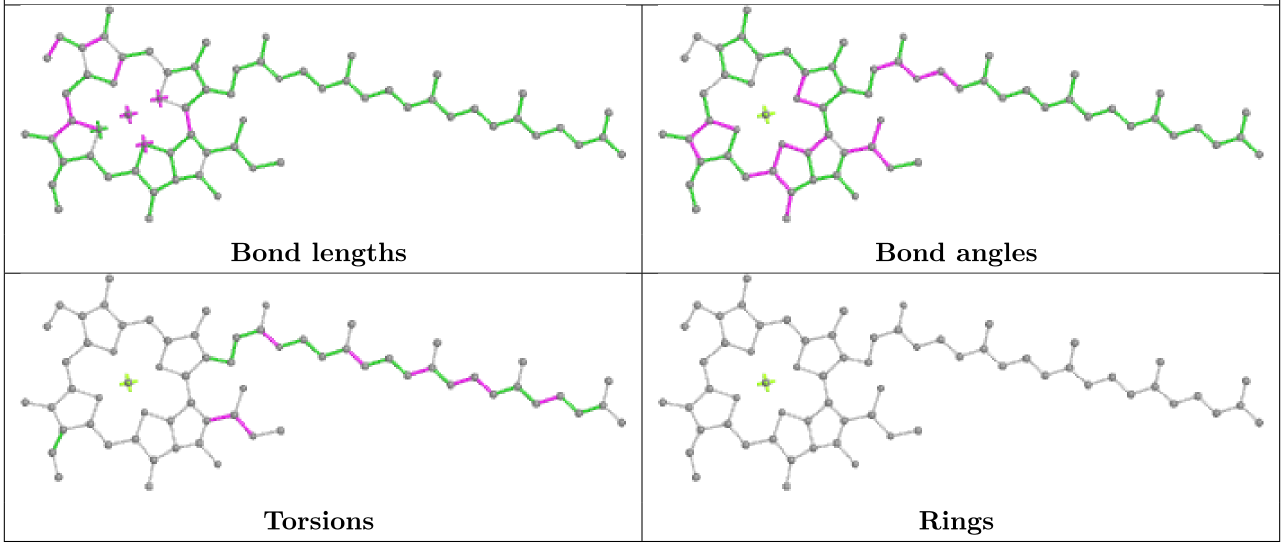


Bond lengths Bond angles



Torsions Rings

Ligand CLA 2 607



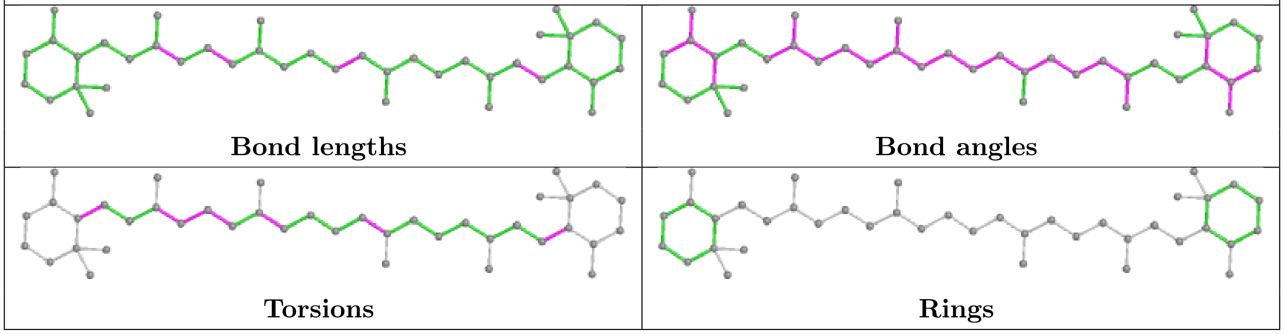
Bond lengths

Bond angles

Torsions

Rings

Ligand BCR B 845



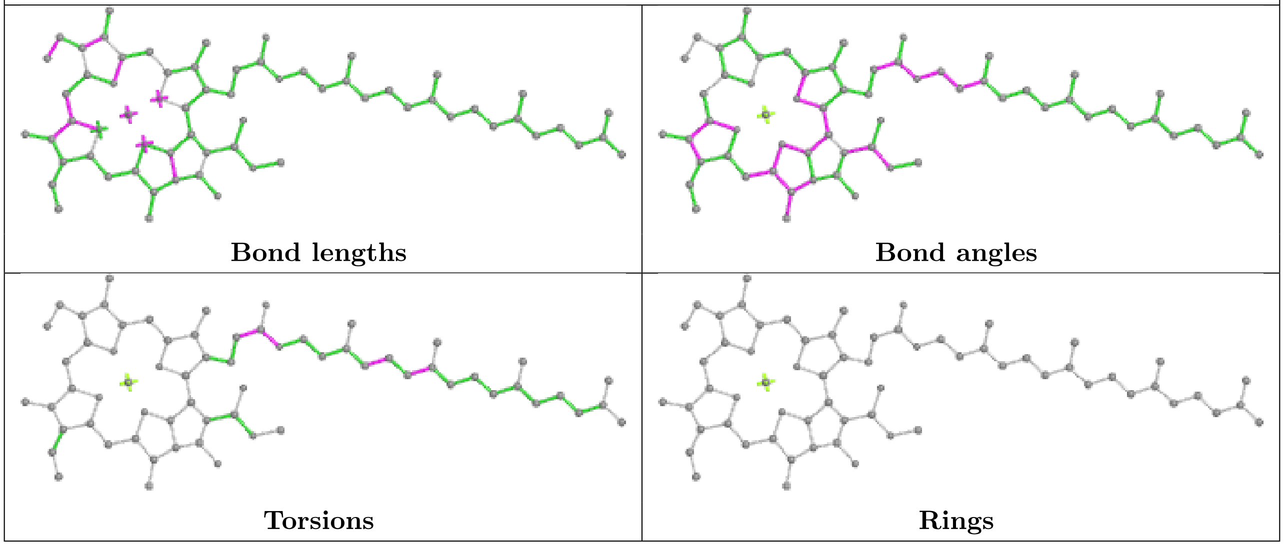
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA A 828



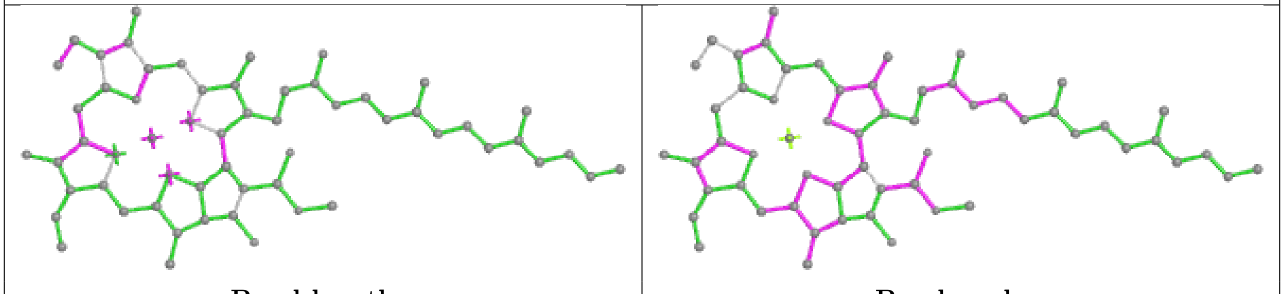
Bond lengths

Bond angles

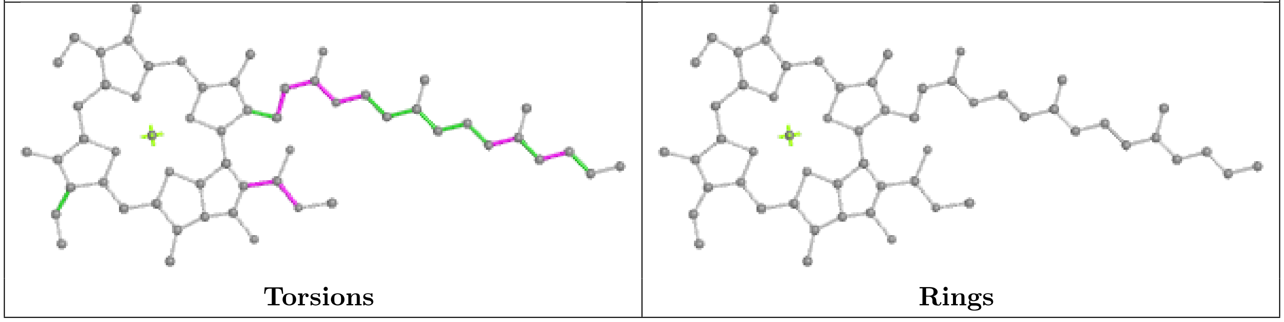
Torsions

Rings

Ligand CLA 3 212

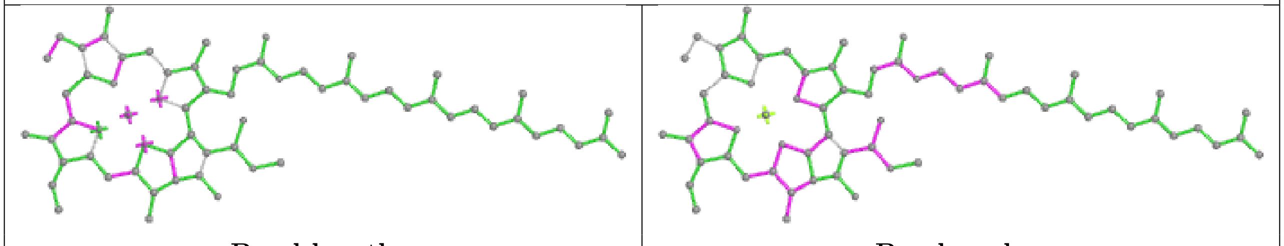


Bond lengths Bond angles

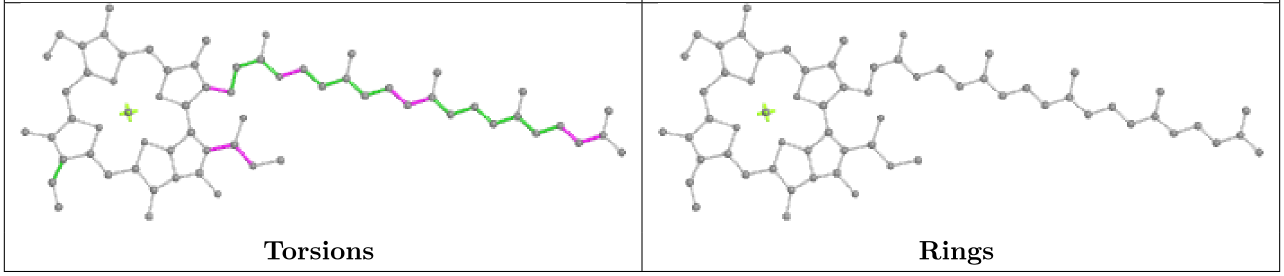


Torsions Rings

Ligand CLA A 832

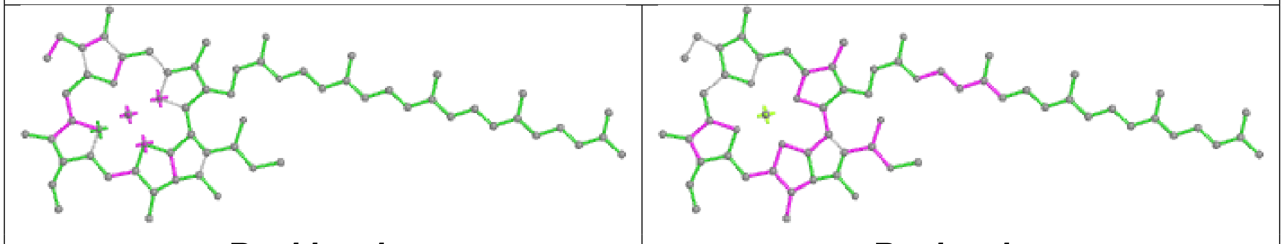


Bond lengths Bond angles

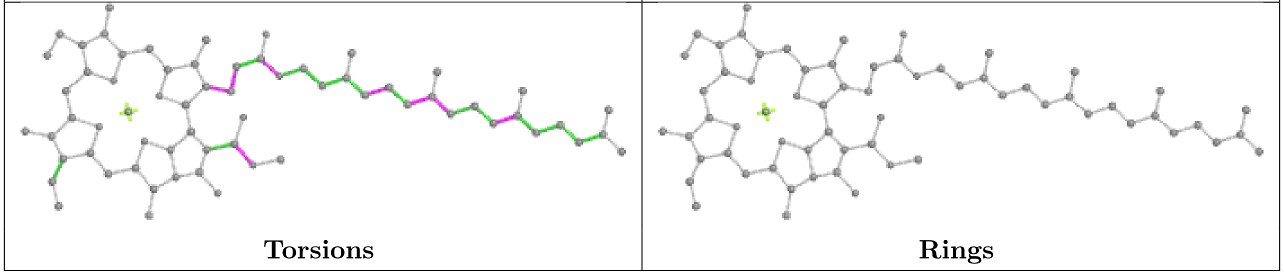


Torsions Rings

Ligand CLA B 829

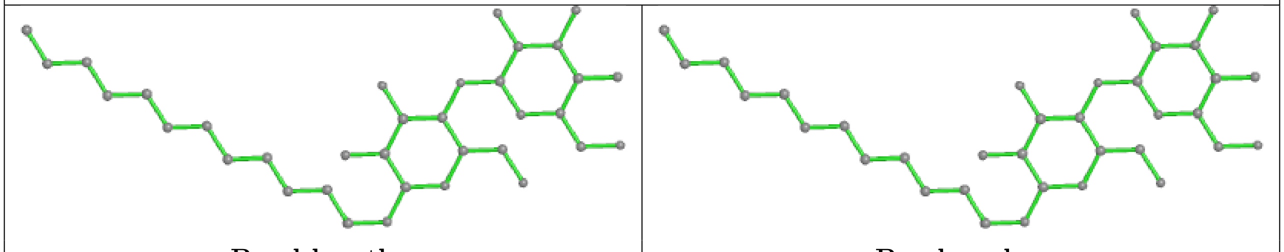


Bond lengths Bond angles

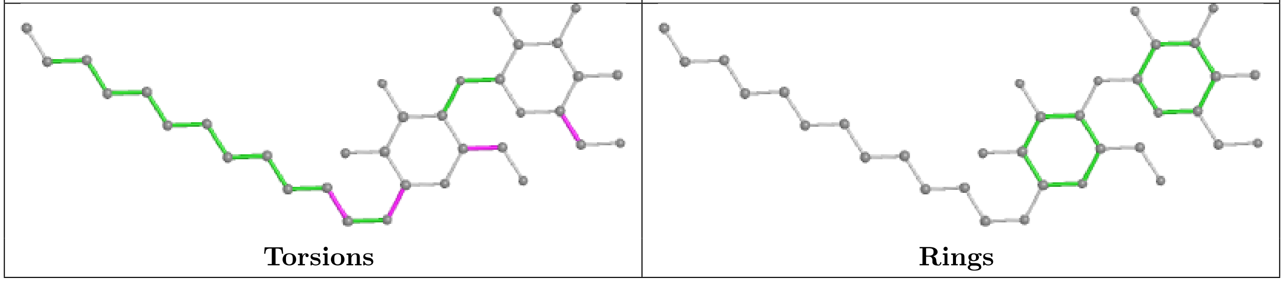


Torsions Rings

Ligand LMU A 853



Bond lengths Bond angles



Torsions Rings

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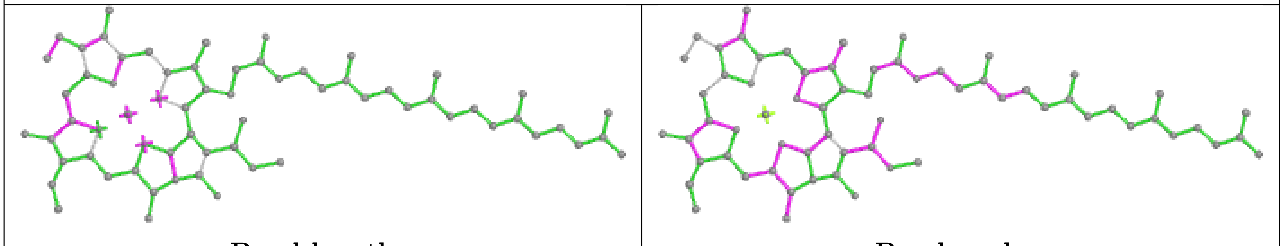
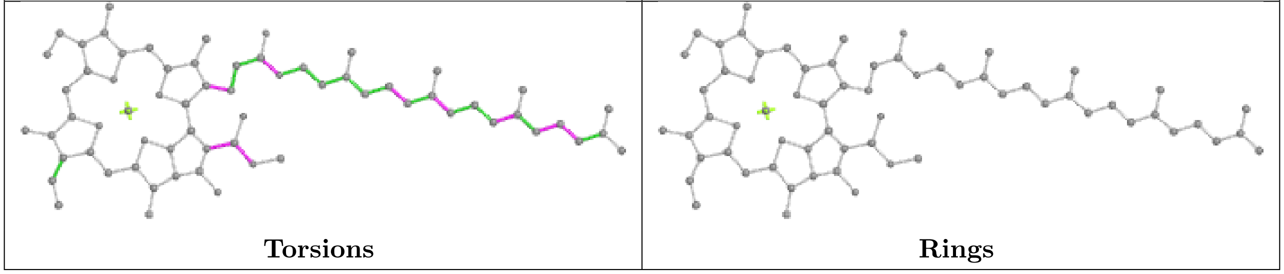
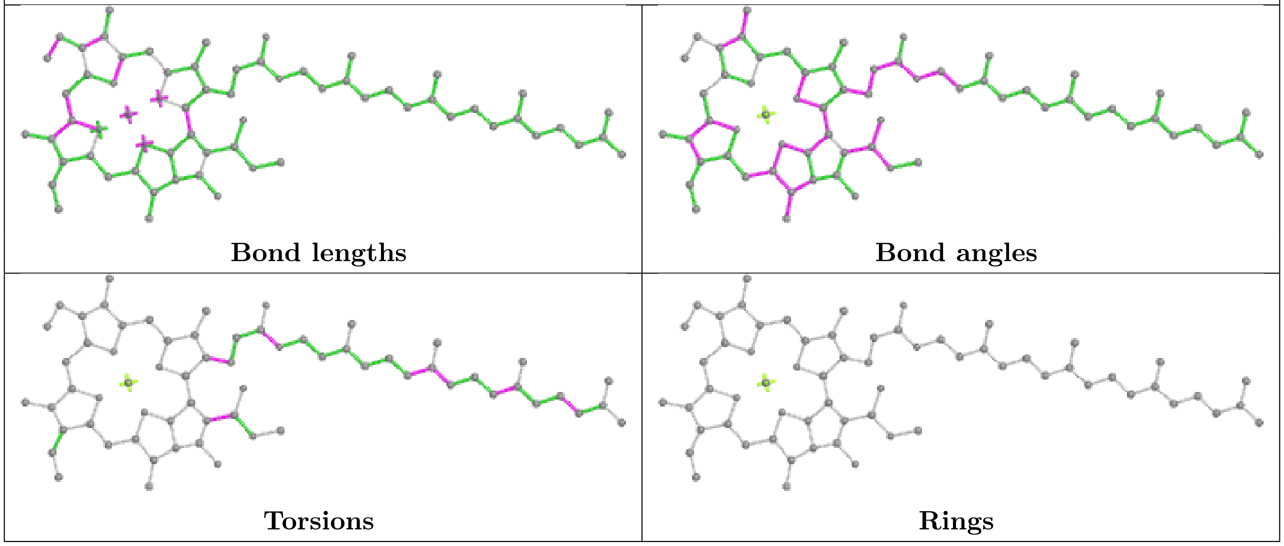


Bond lengths Bond angles

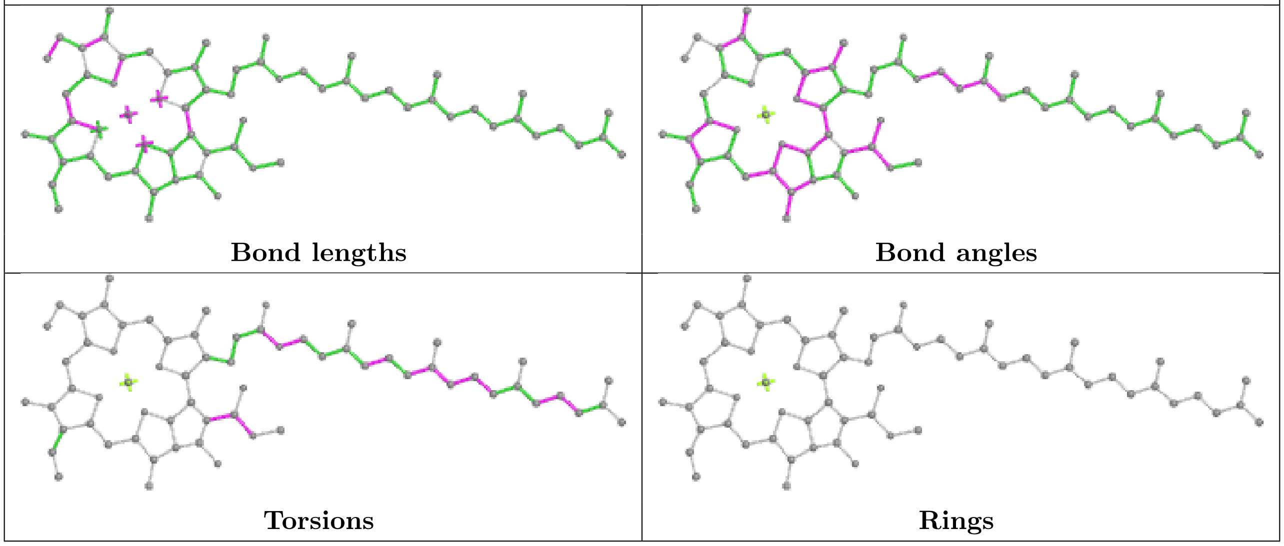


Torsions Rings

Ligand CLA B 806



Ligand CLA 1 601



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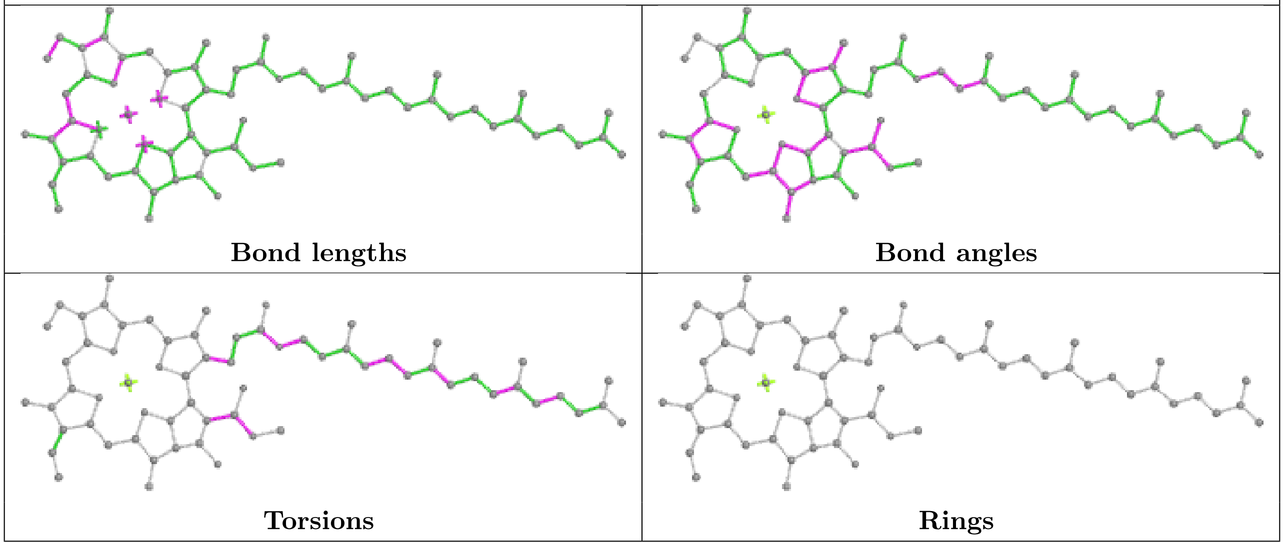

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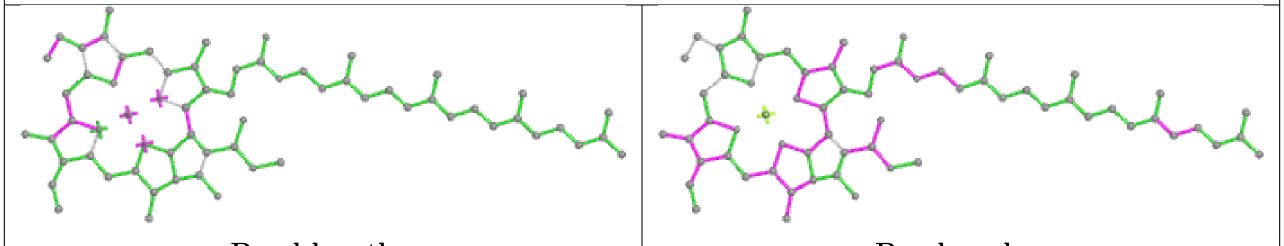
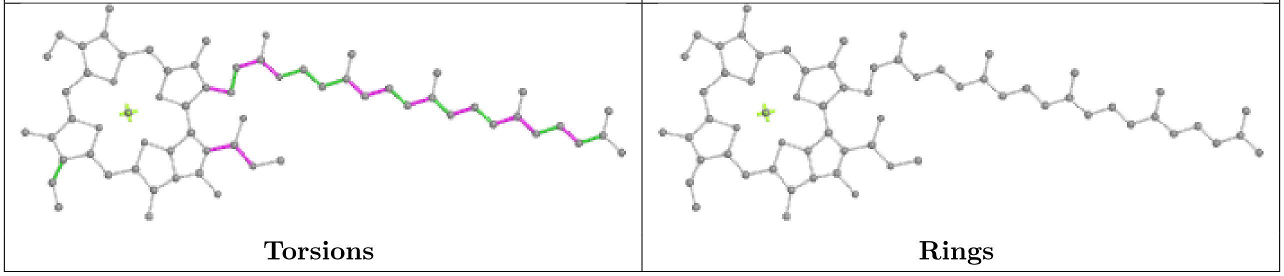
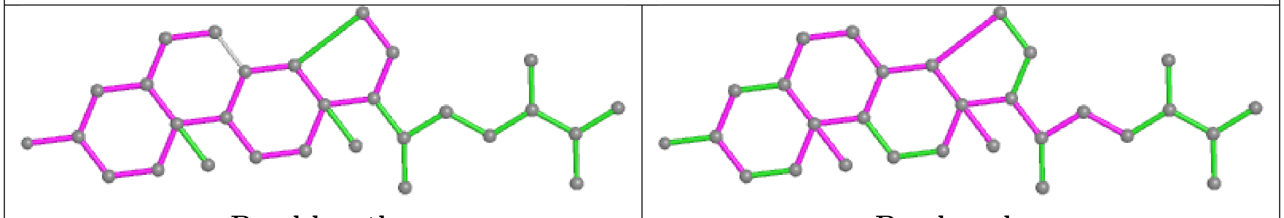


Bond lengths Bond angles

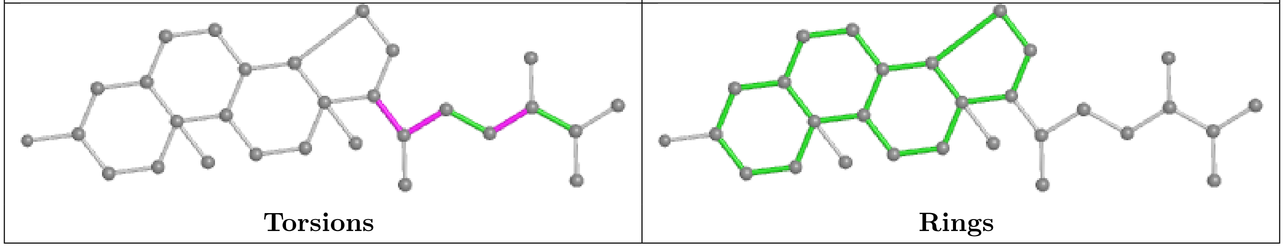


Torsions Rings

Ligand ERG 2 621

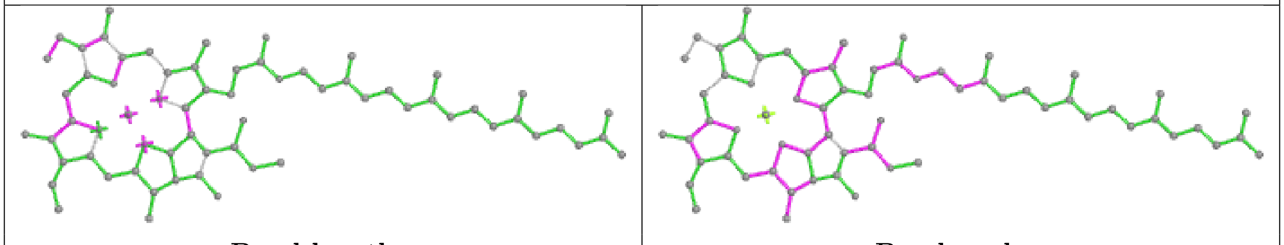


Bond lengths Bond angles

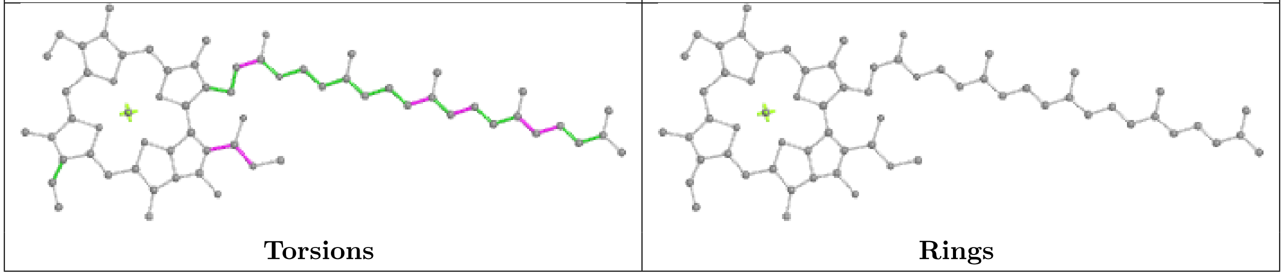


Torsions Rings

Ligand CLA L 203

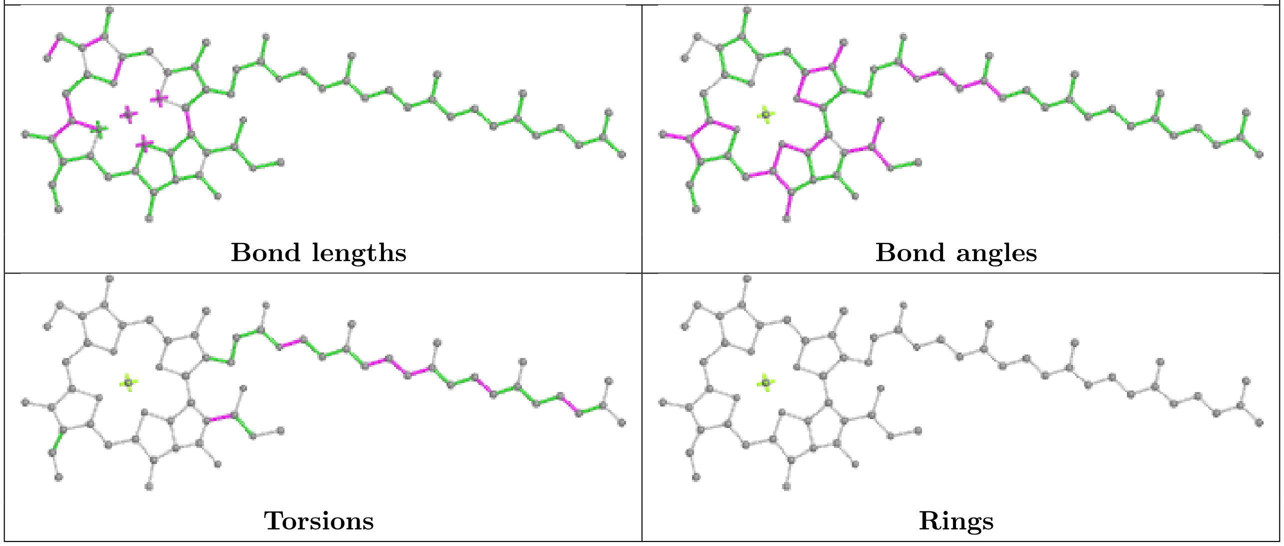


Bond lengths Bond angles



Torsions Rings

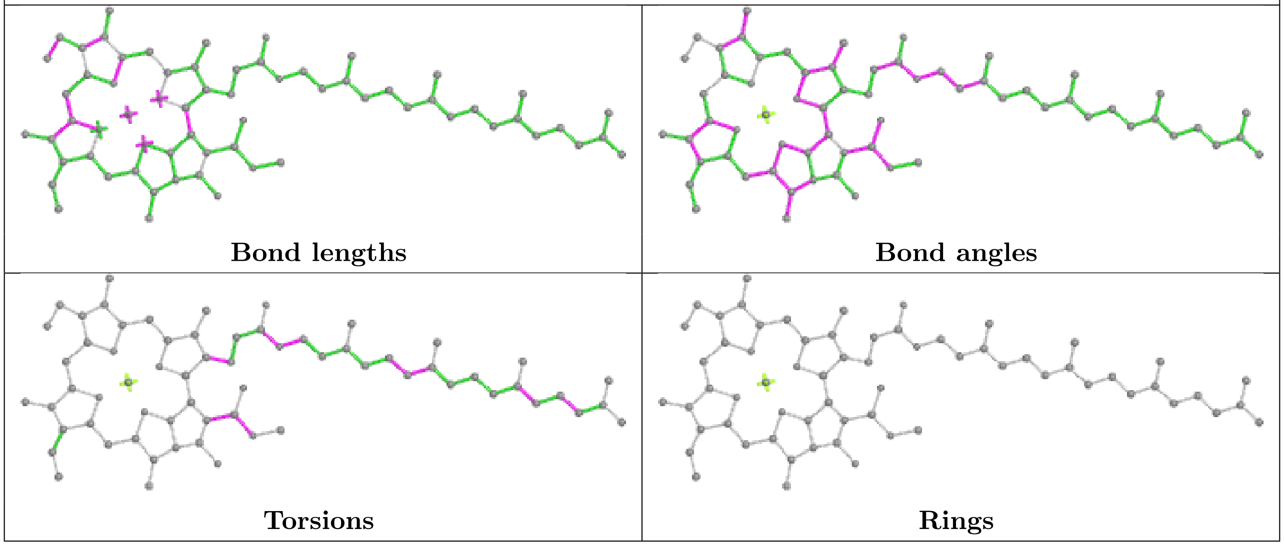
Ligand CLA 2 604



Bond lengths Bond angles

Torsions Rings

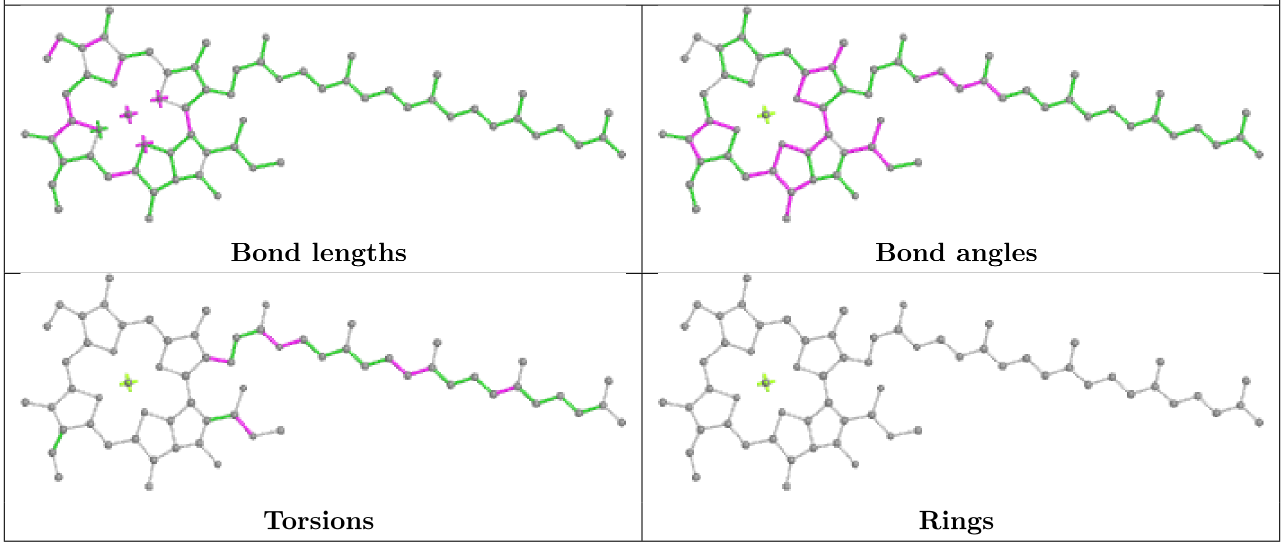
Ligand CLA B 838



Bond lengths Bond angles

Torsions Rings

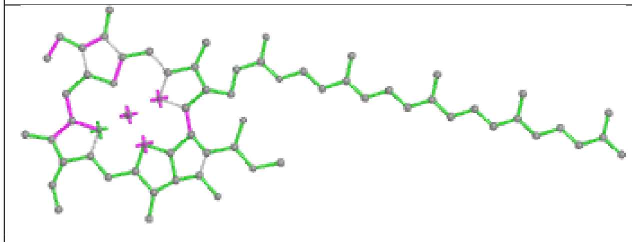
Ligand CLA B 814



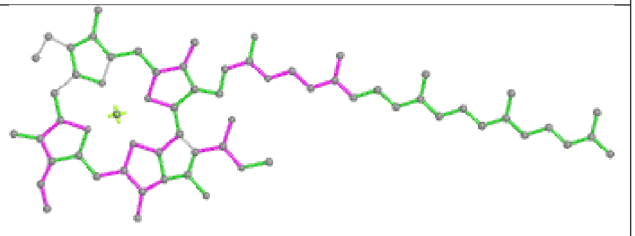
Bond lengths Bond angles

Torsions Rings

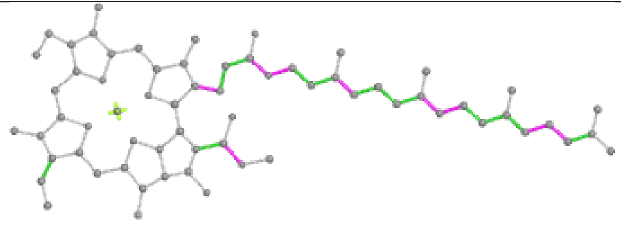
Ligand CLA A 821



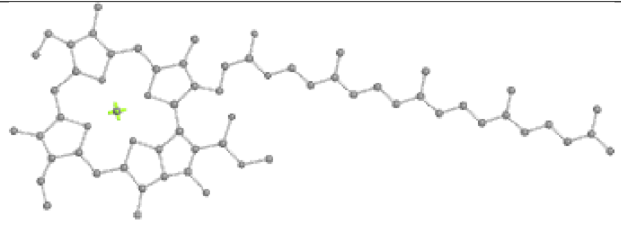
Bond lengths



Bond angles

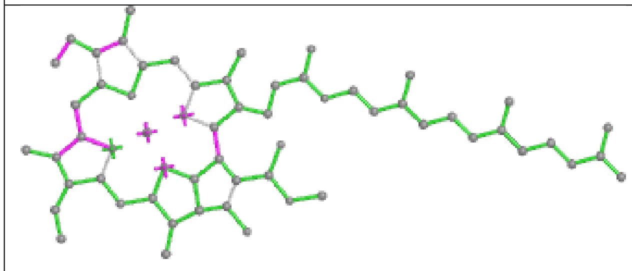


Torsions

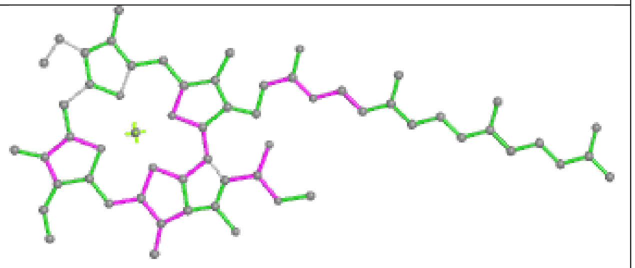


Rings

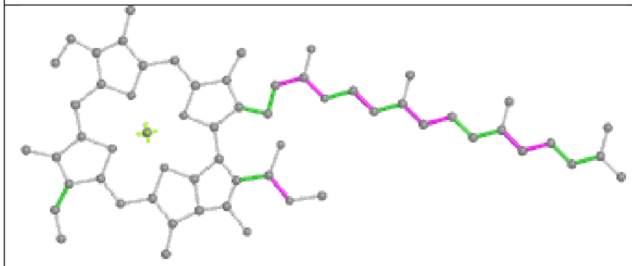
Ligand CLA 1 607



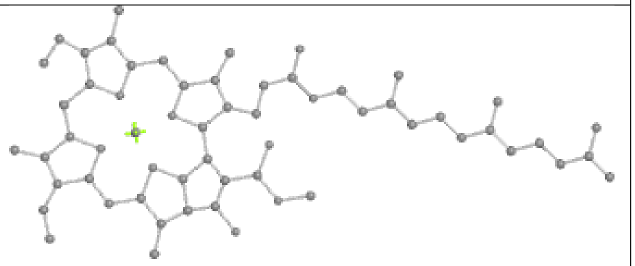
Bond lengths



Bond angles

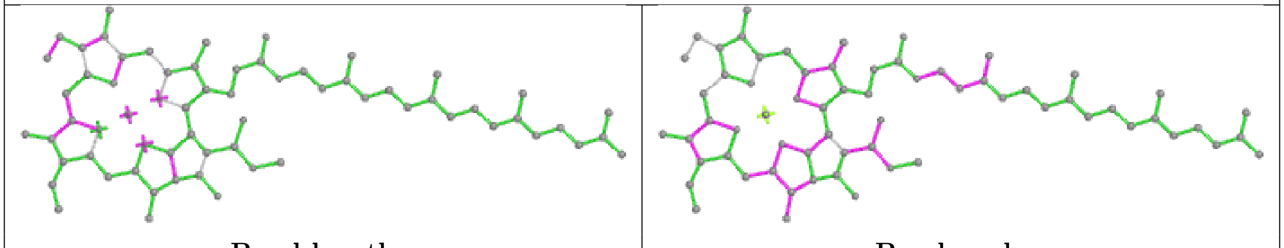


Torsions

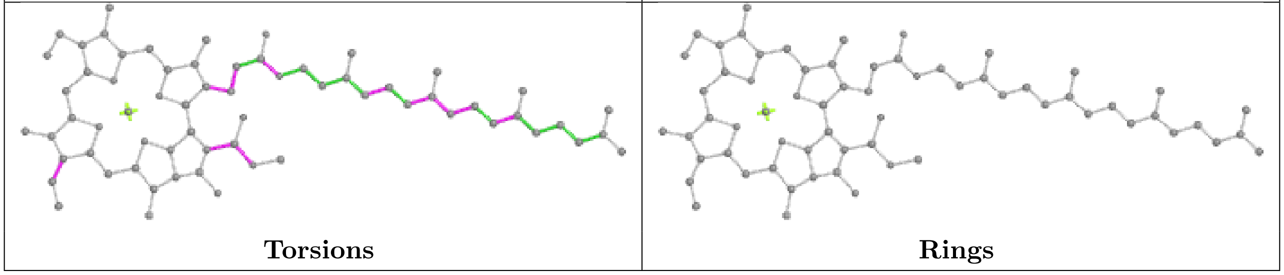


Rings

Ligand CLA A 809

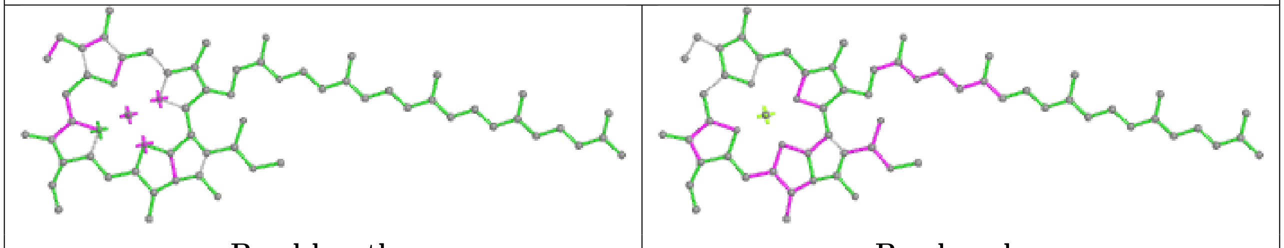


Bond lengths Bond angles

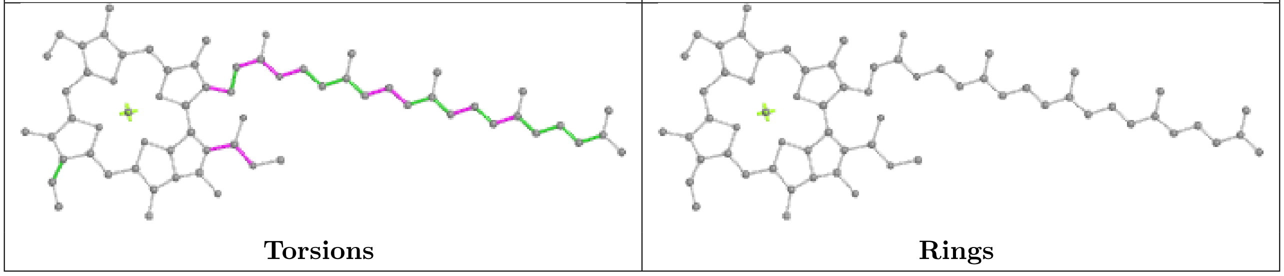


Torsions Rings

Ligand CLA B 835



Bond lengths Bond angles



Torsions Rings

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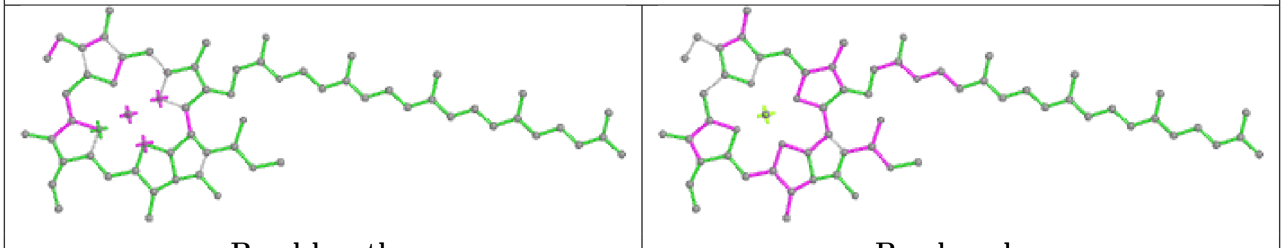
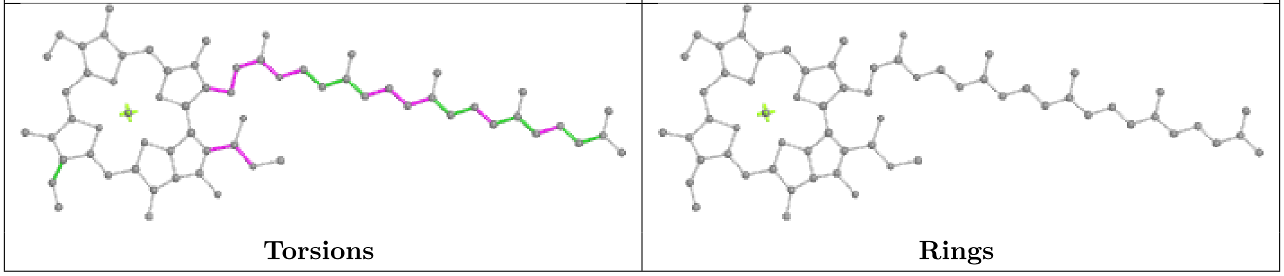
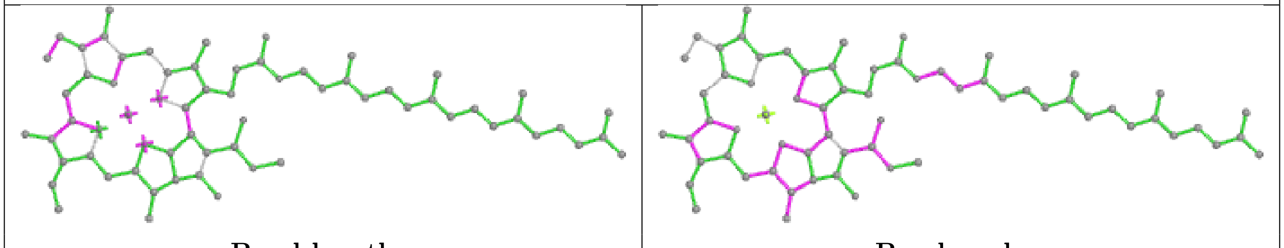


Bond lengths Bond angles



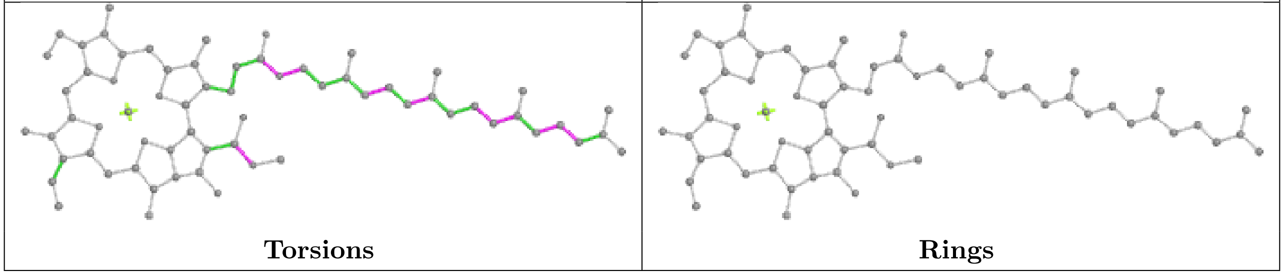
Torsions Rings

Ligand CLA 1 611



Bond lengths

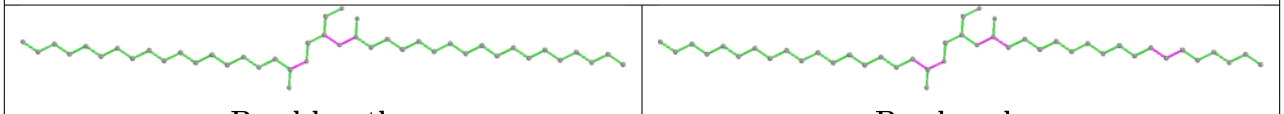
Bond angles



Torsions

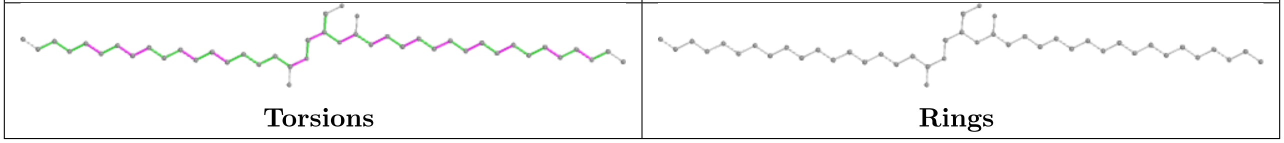
Rings

Ligand DGA J 101



Bond lengths

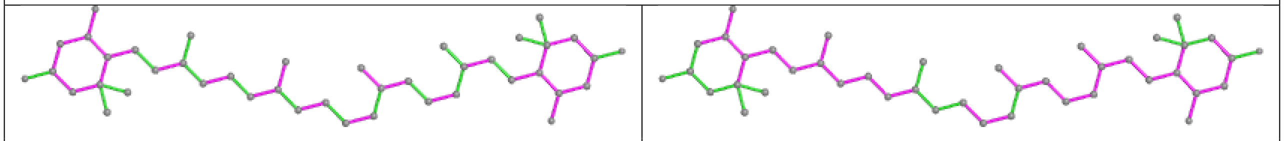
Bond angles



Torsions

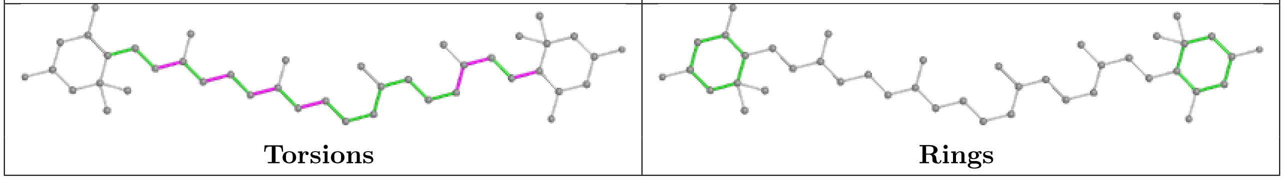
Rings

Ligand C7Z 1 615



Bond lengths

Bond angles



Torsions

Rings

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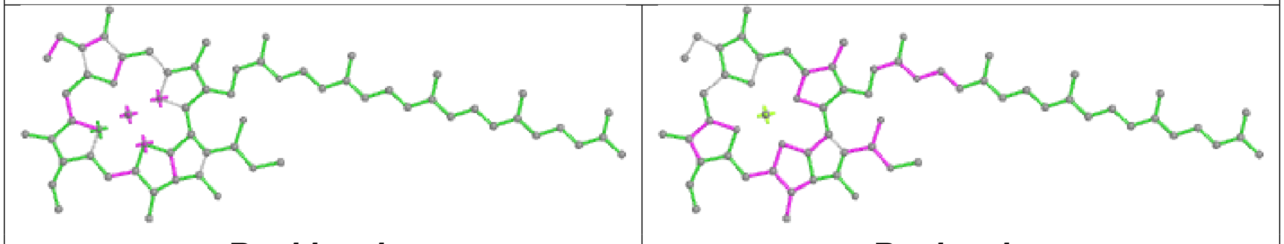
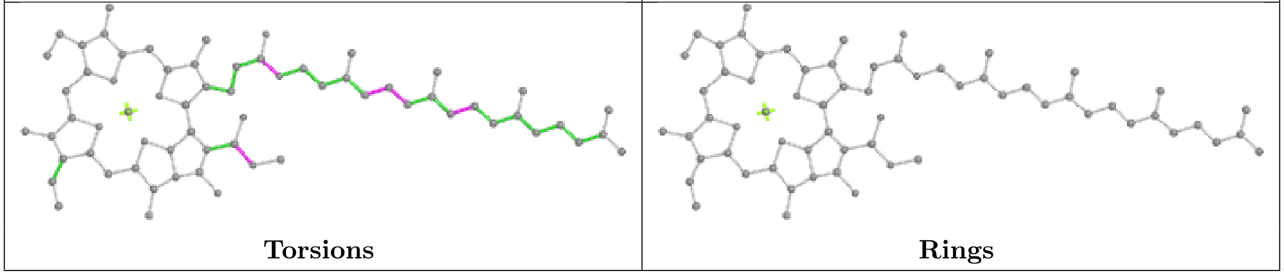


Bond lengths

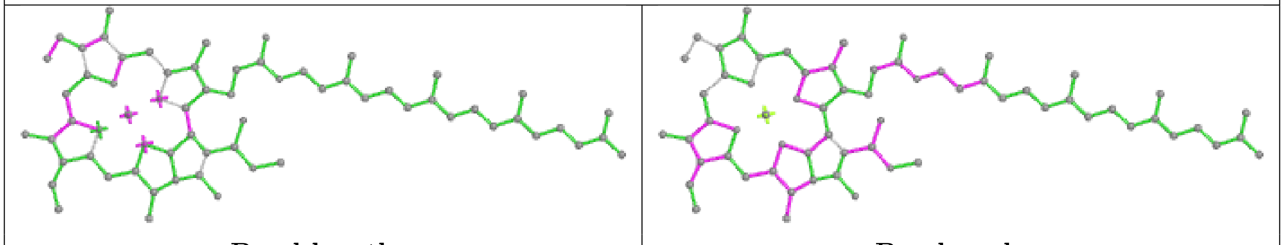
Bond angles



Torsions

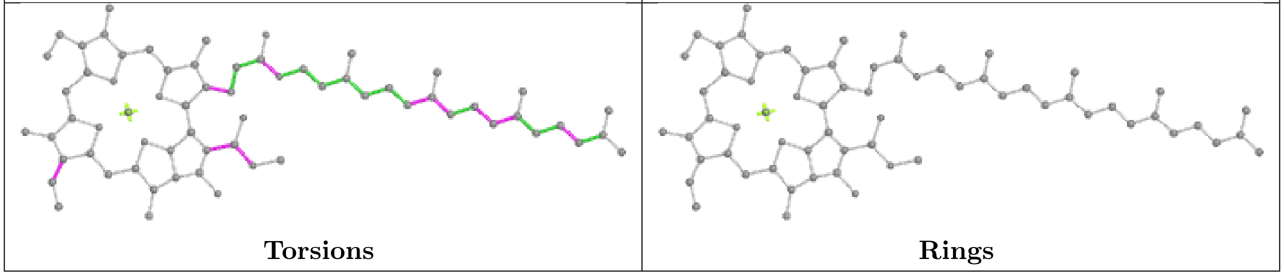
Rings

Ligand CLA 3 214



Bond lengths

Bond angles



Torsions

Rings

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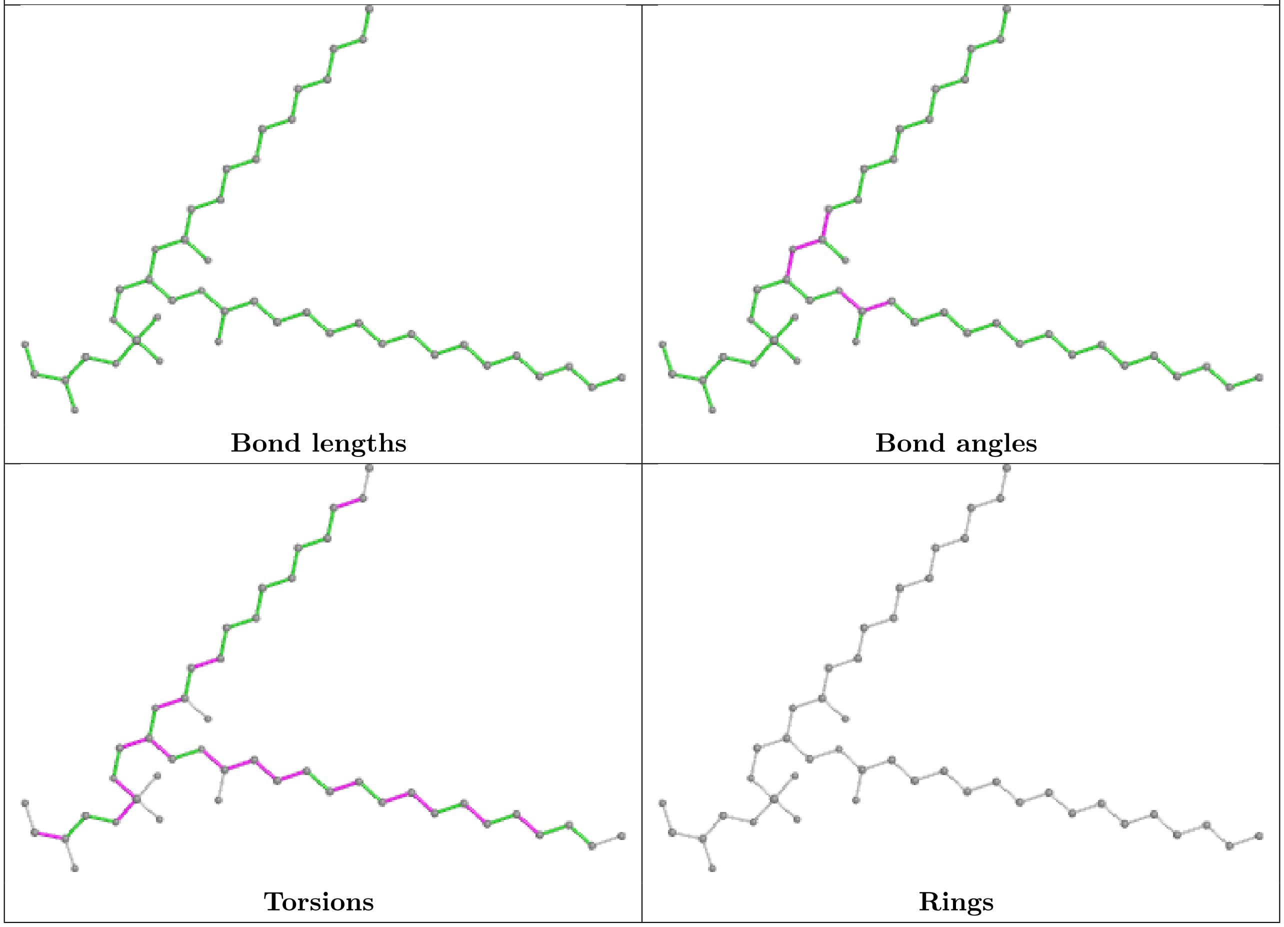


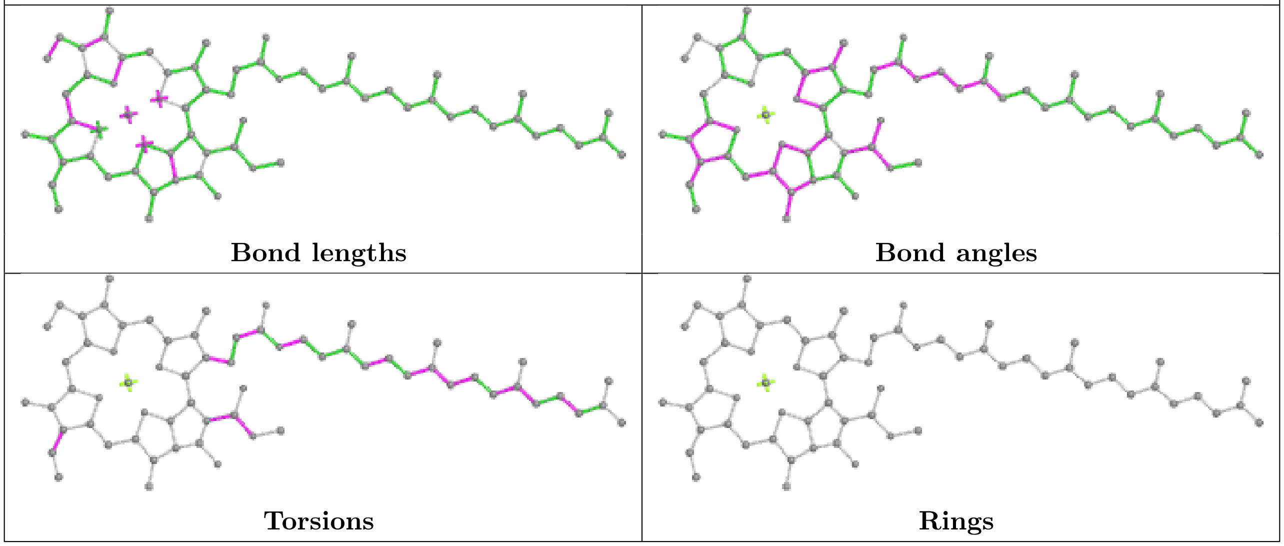
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA 2 608



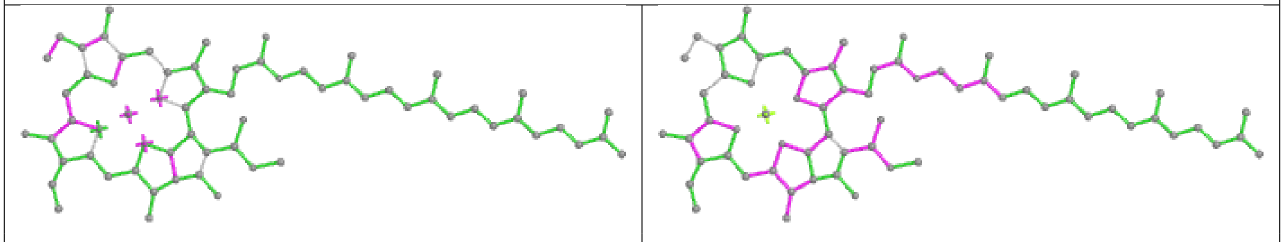
Bond lengths

Bond angles

Torsions

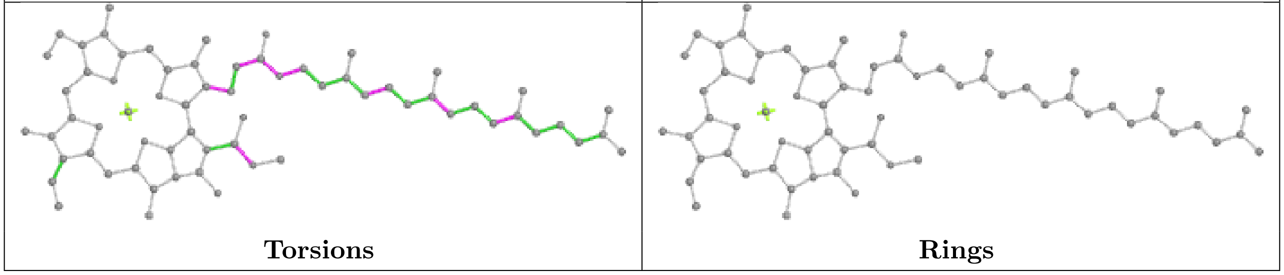
Rings

Ligand CLA A 808



Bond lengths

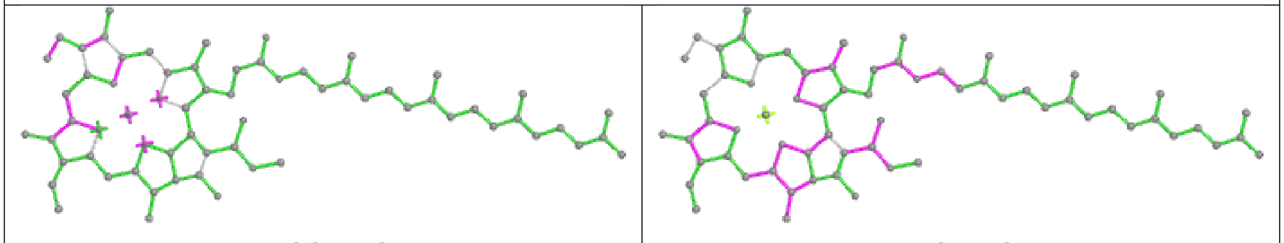
Bond angles



Torsions

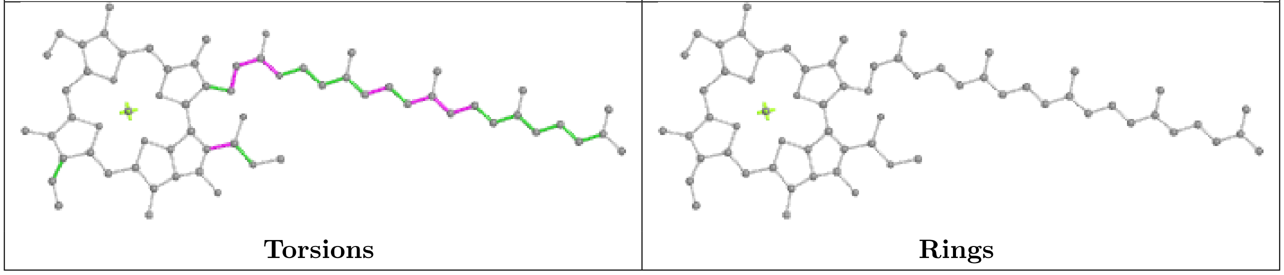
Rings

Ligand CLA A 823



Bond lengths

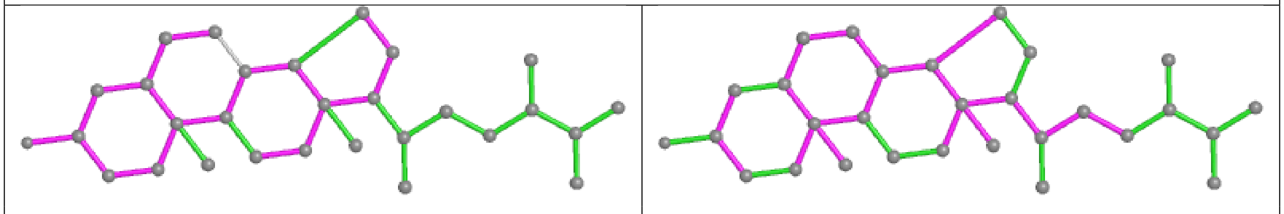
Bond angles



Torsions

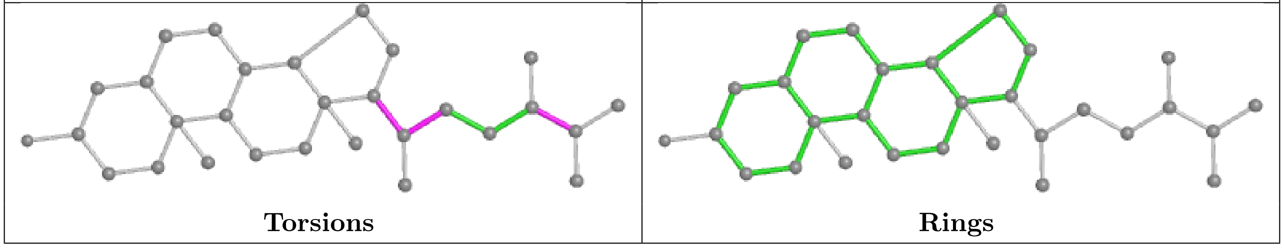
Rings

Ligand ERG 2 618



Bond lengths

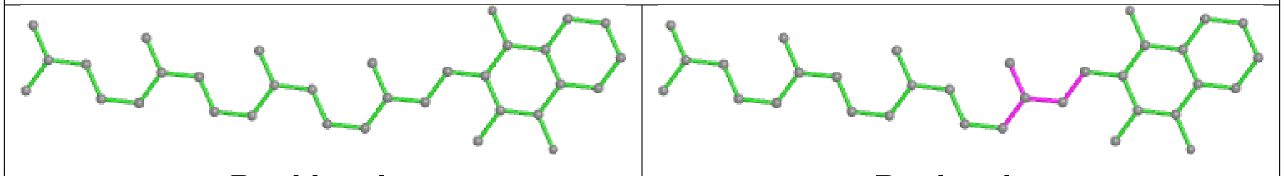
Bond angles



Torsions

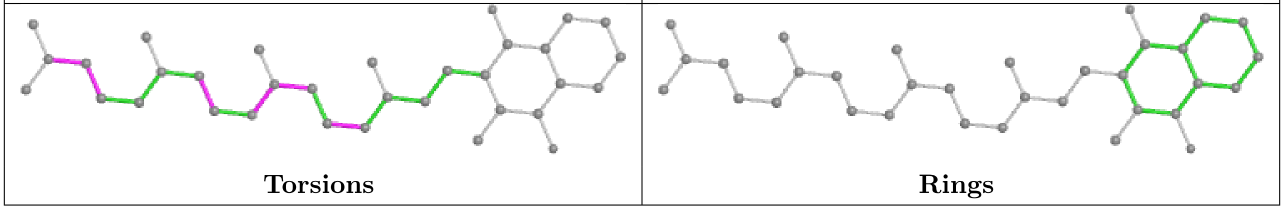
Rings

Ligand PQN B 839



Bond lengths

Bond angles



Torsions

Rings

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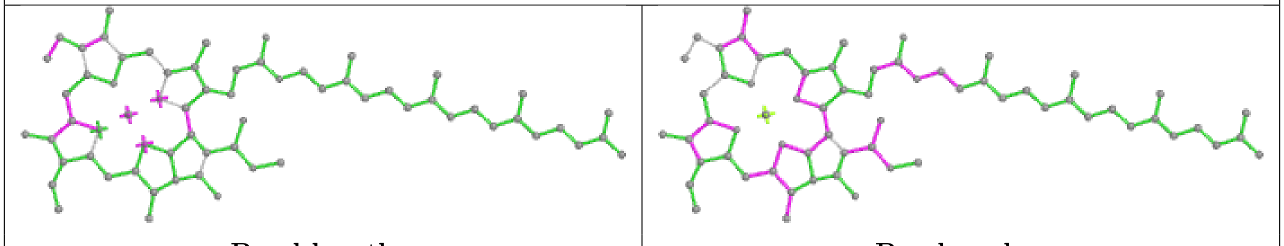
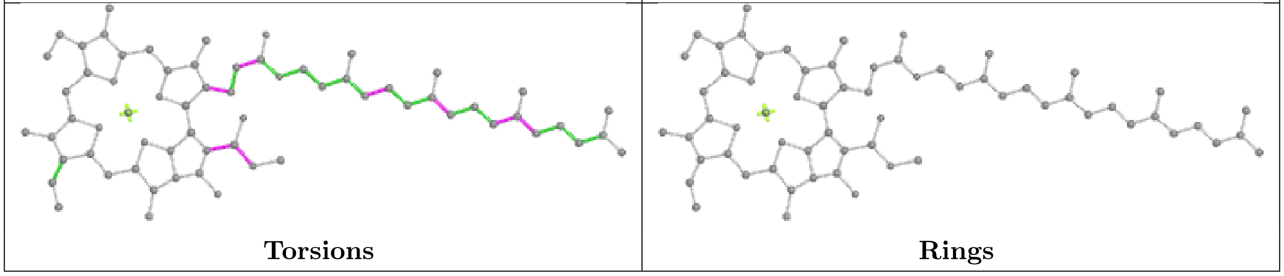


Bond lengths

Bond angles



Torsions

Rings

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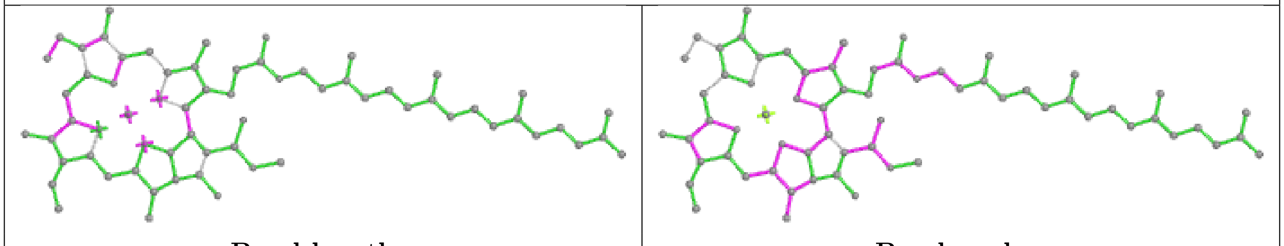
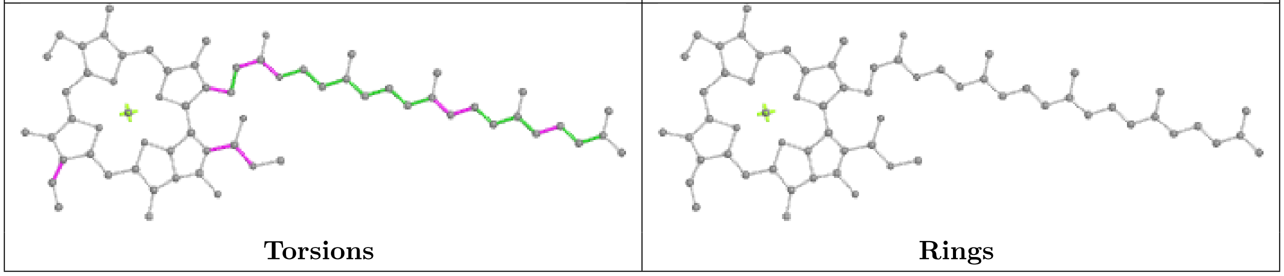


Bond lengths

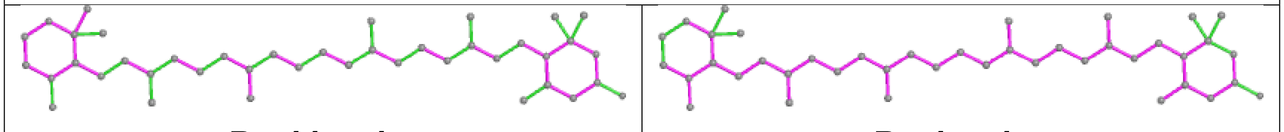
Bond angles



Torsions

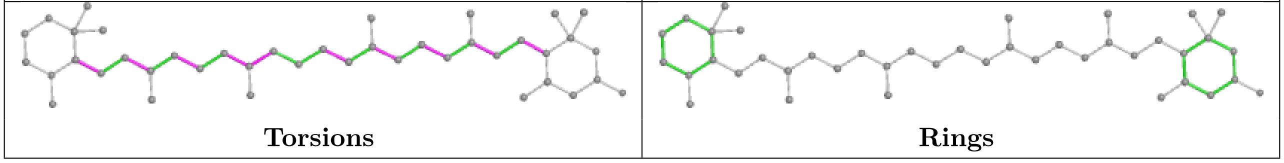
Rings

Ligand RRX J 103



Bond lengths

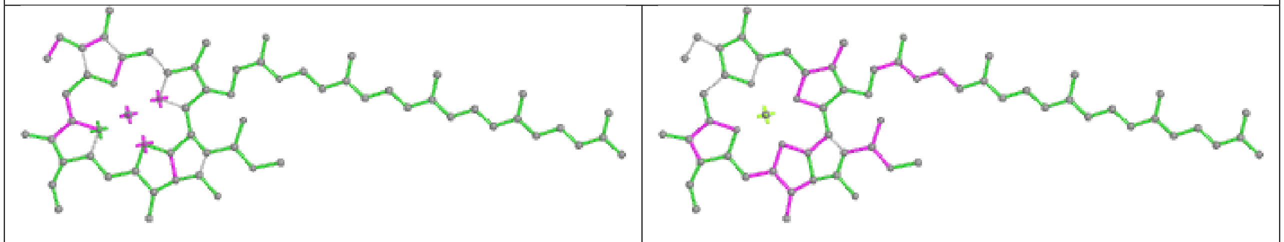
Bond angles



Torsions

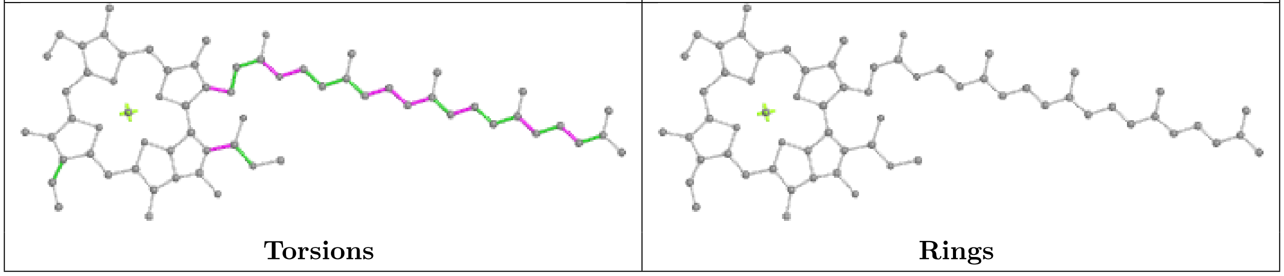
Rings

Ligand CLA B 819



Bond lengths

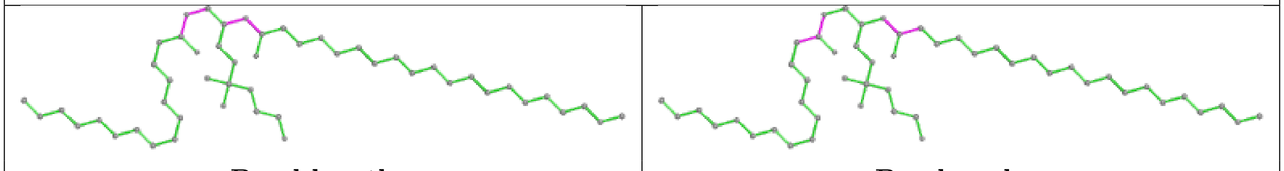
Bond angles



Torsions

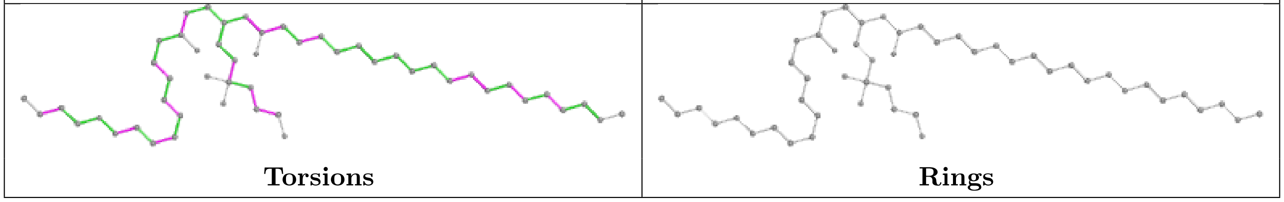
Rings

Ligand PTY 3 220



Bond lengths

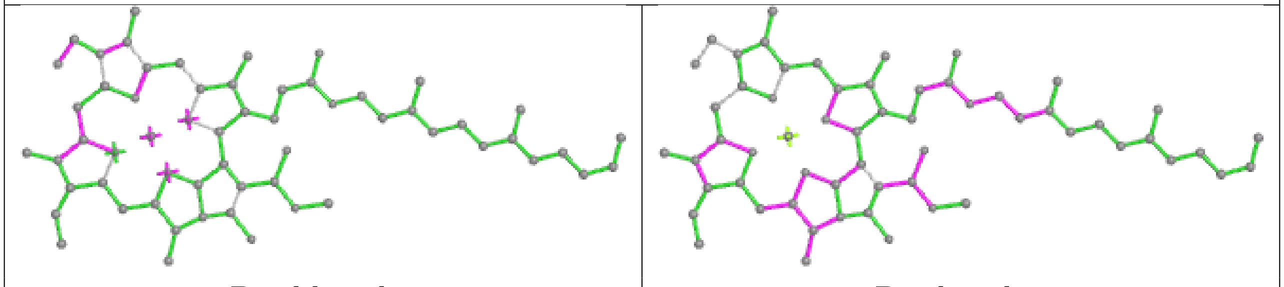
Bond angles



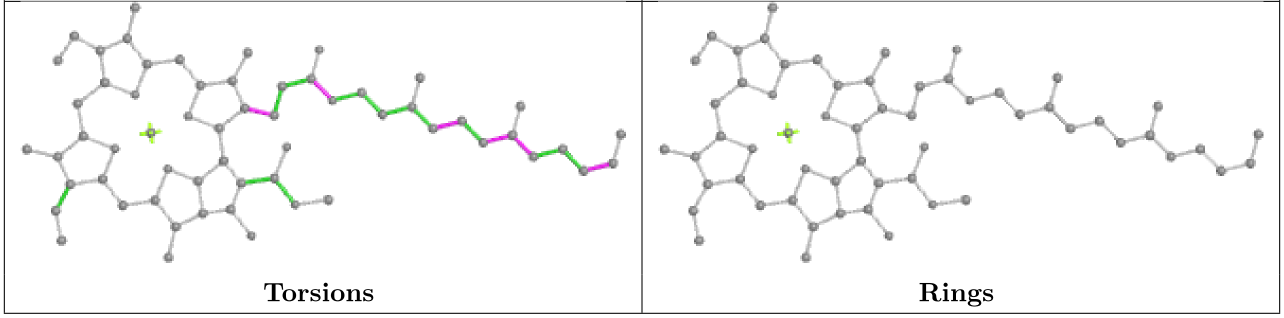
Torsions

Rings

Ligand CLA 1 602

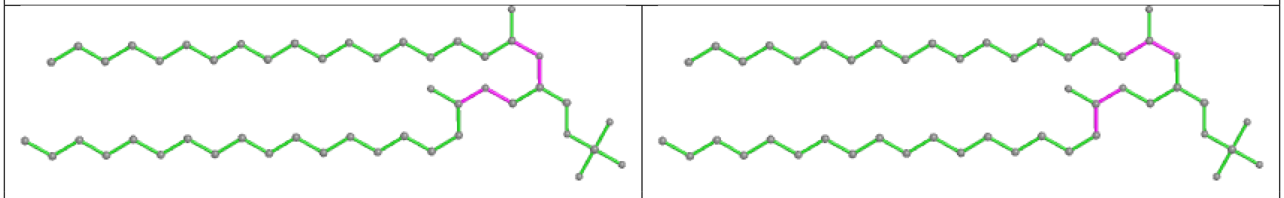


Bond lengths Bond angles

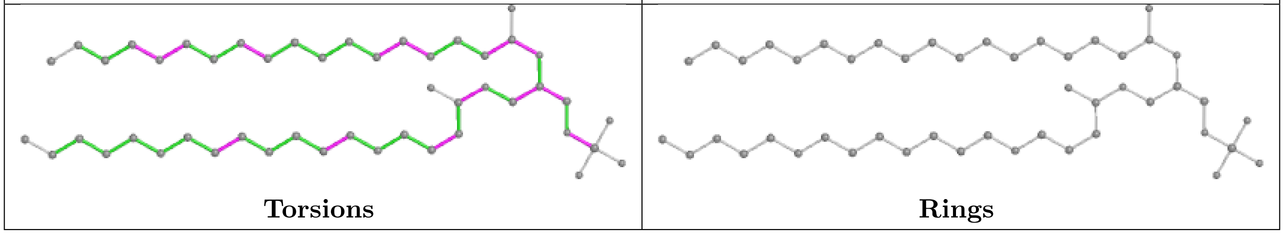


Torsions Rings

Ligand 3PH A 849

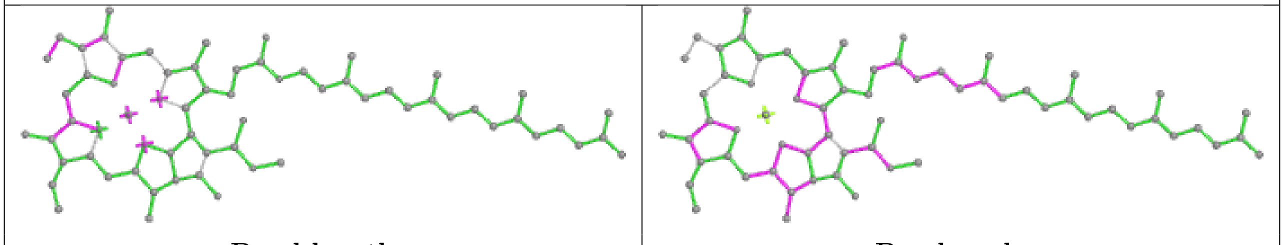


Bond lengths Bond angles

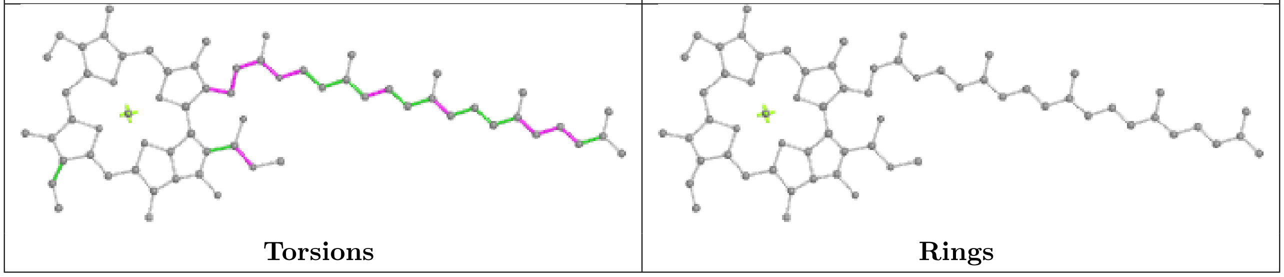


Torsions Rings

Ligand CLA 2 605

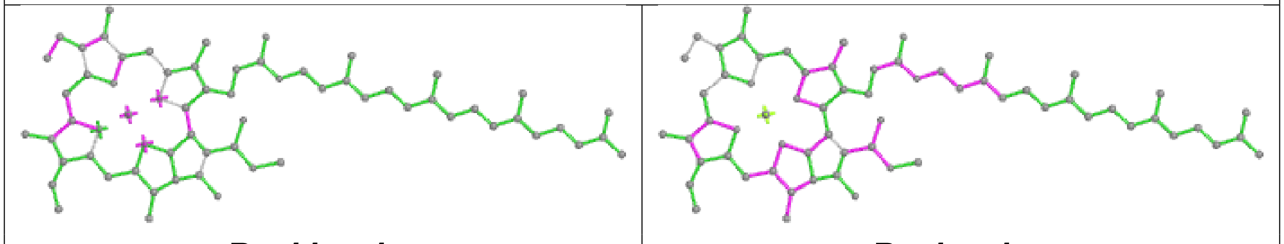


Bond lengths Bond angles



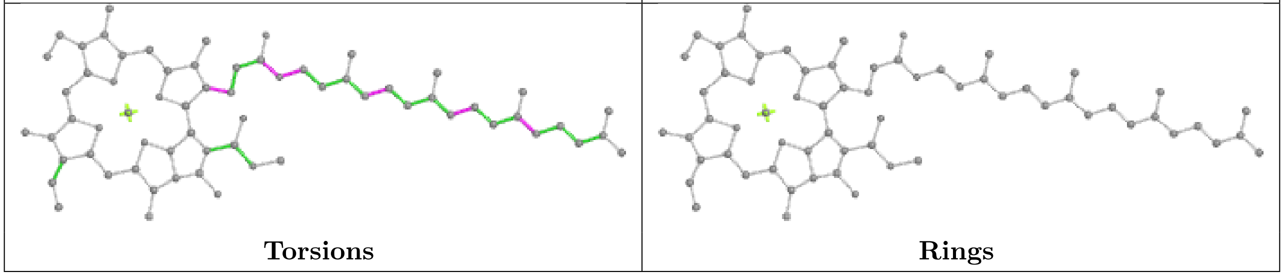
Torsions Rings

Ligand CLA L 201



Bond lengths

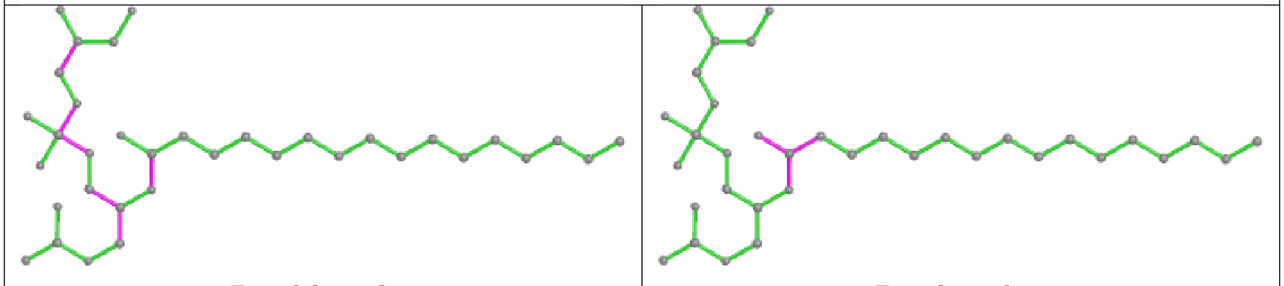
Bond angles



Torsions

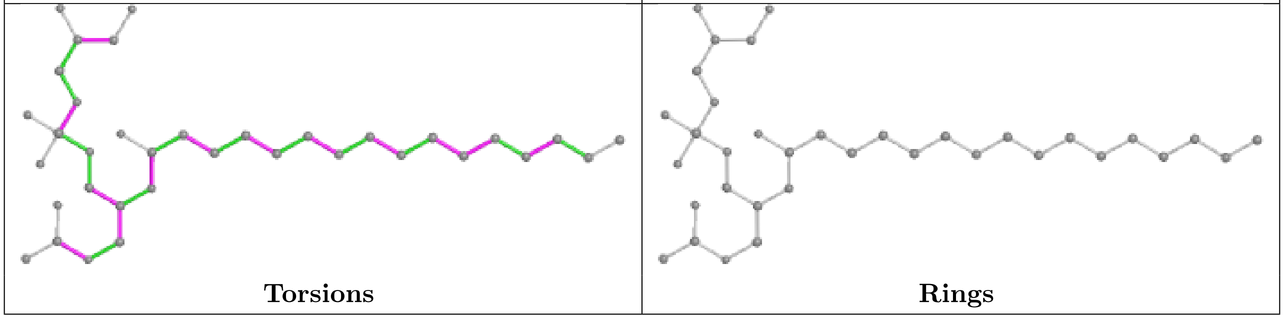
Rings

Ligand PGT 2 619



Bond lengths

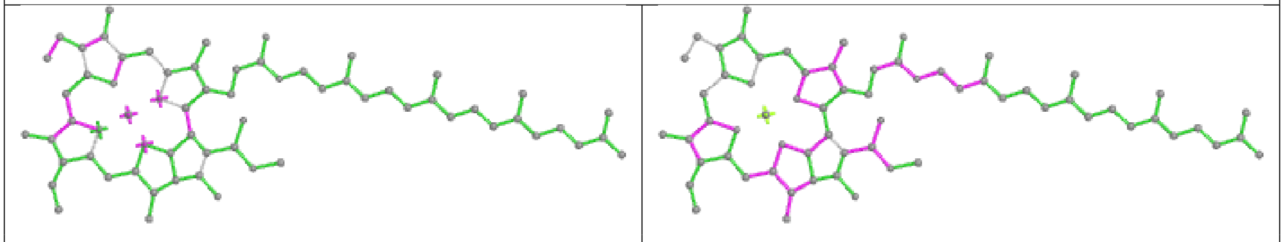
Bond angles



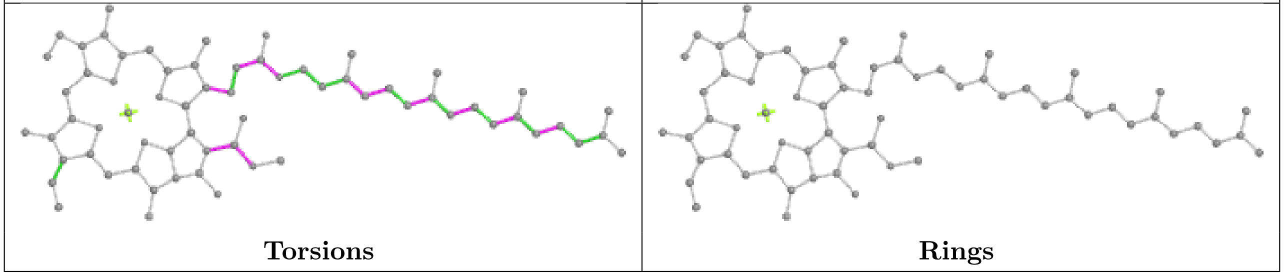
Torsions

Rings

Ligand CLA J 102

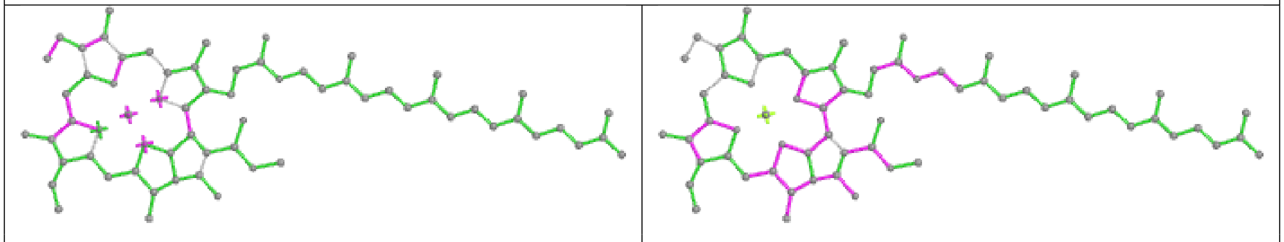


Bond lengths Bond angles

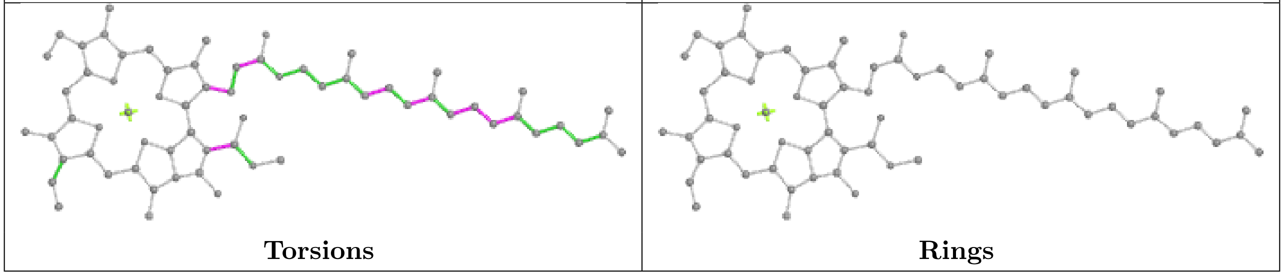


Torsions Rings

Ligand CLA B 803

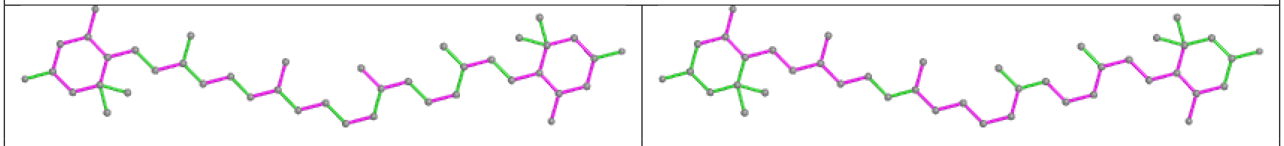


Bond lengths Bond angles

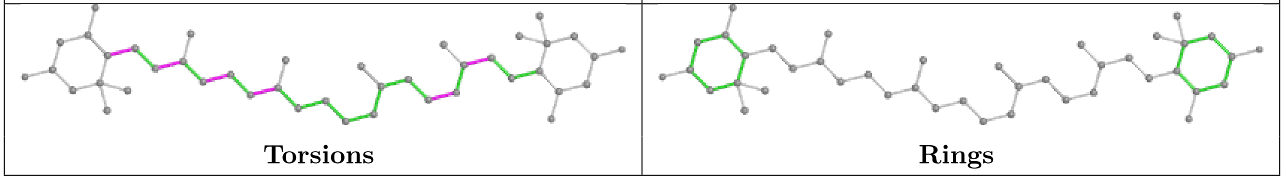


Torsions Rings

Ligand C7Z 2 614

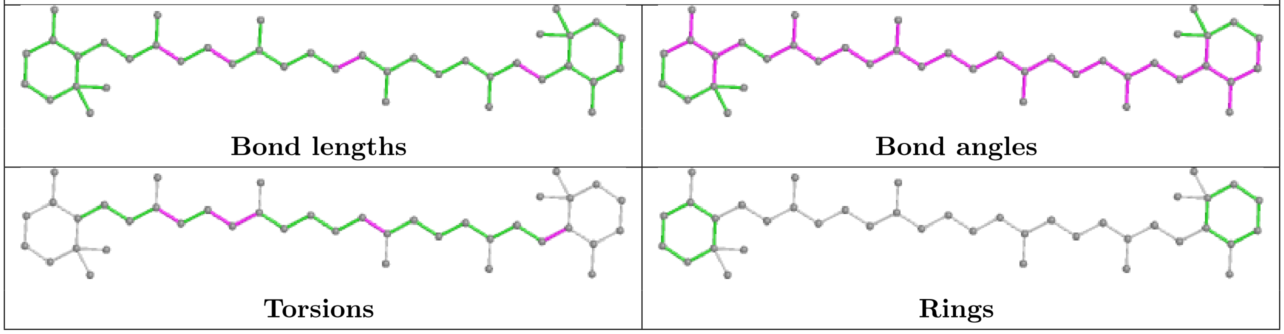


Bond lengths Bond angles



Torsions Rings

Ligand BCR B 843



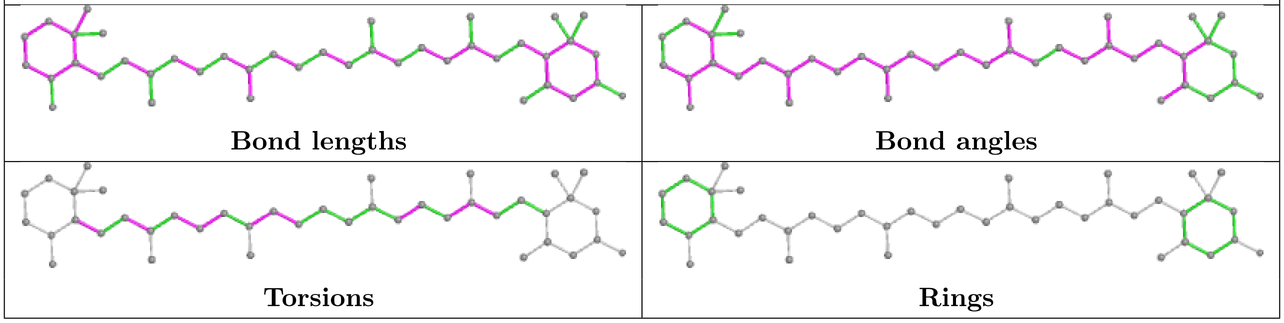
Bond lengths

Bond angles

Torsions

Rings

Ligand RRX A 847



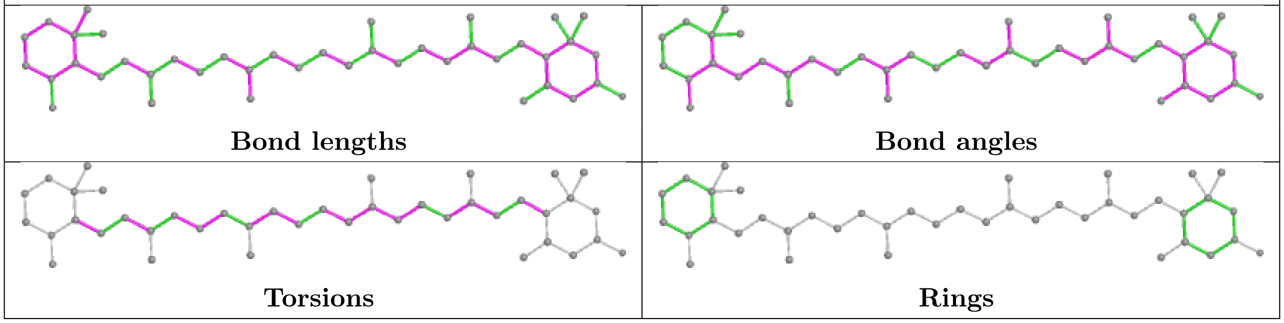
Bond lengths

Bond angles

Torsions

Rings

Ligand RRX 1 613



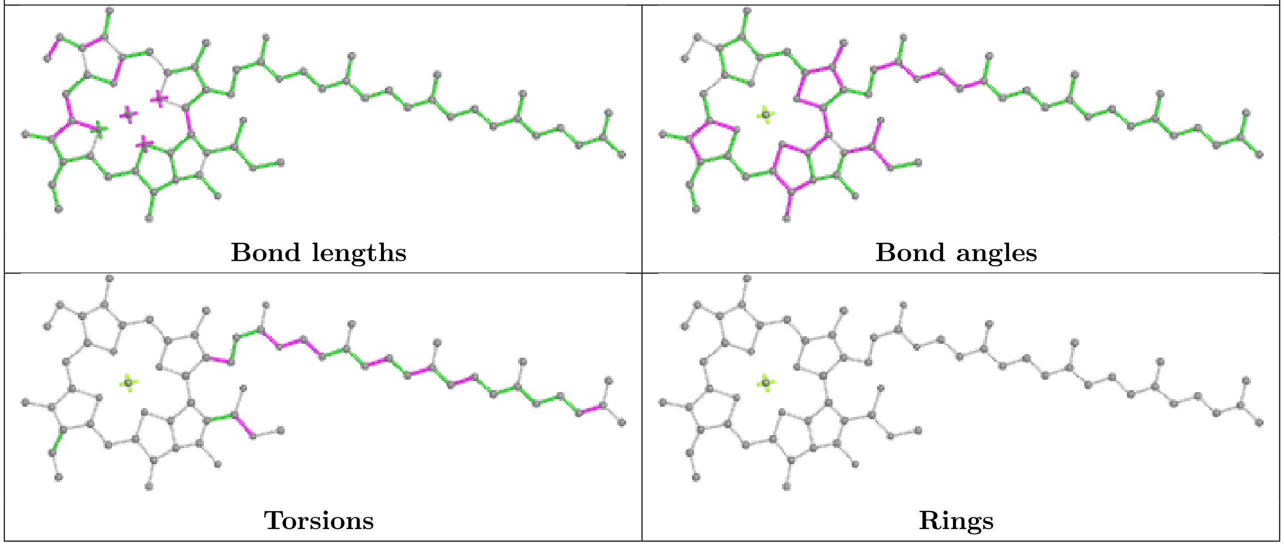
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA B 821



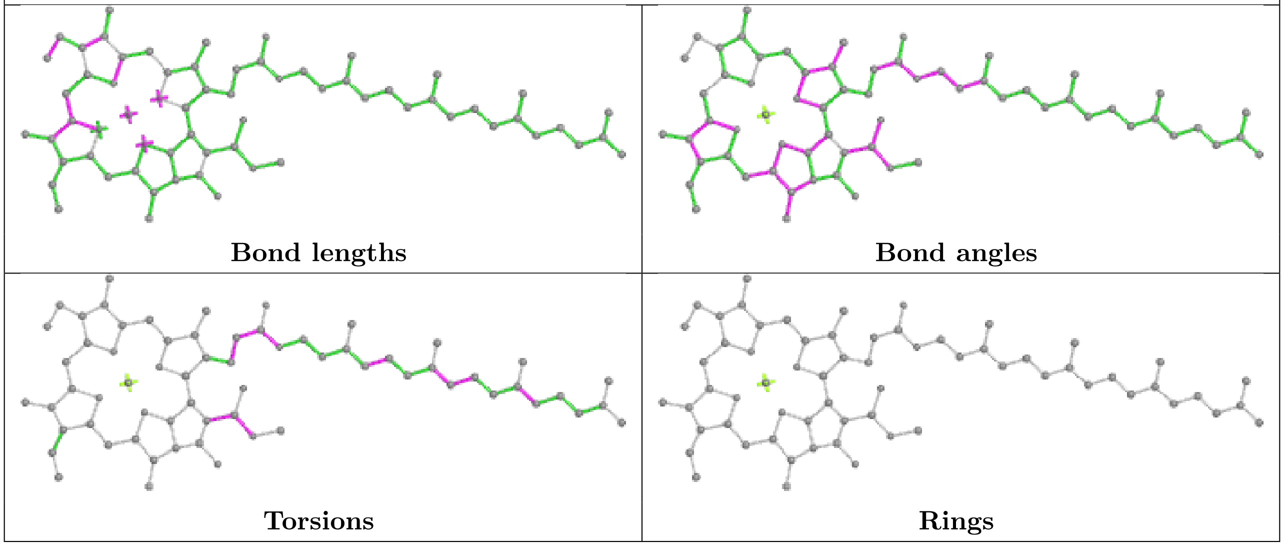
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA I 102



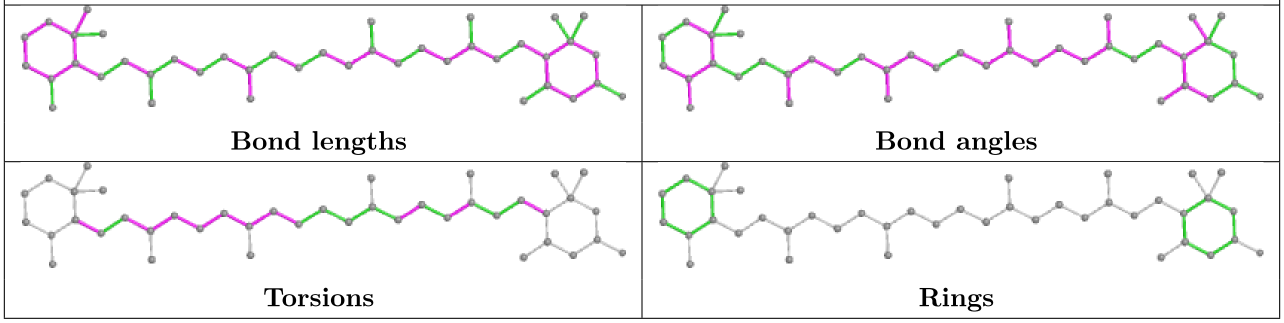
Bond lengths

Bond angles

Torsions

Rings

Ligand RRX K 103



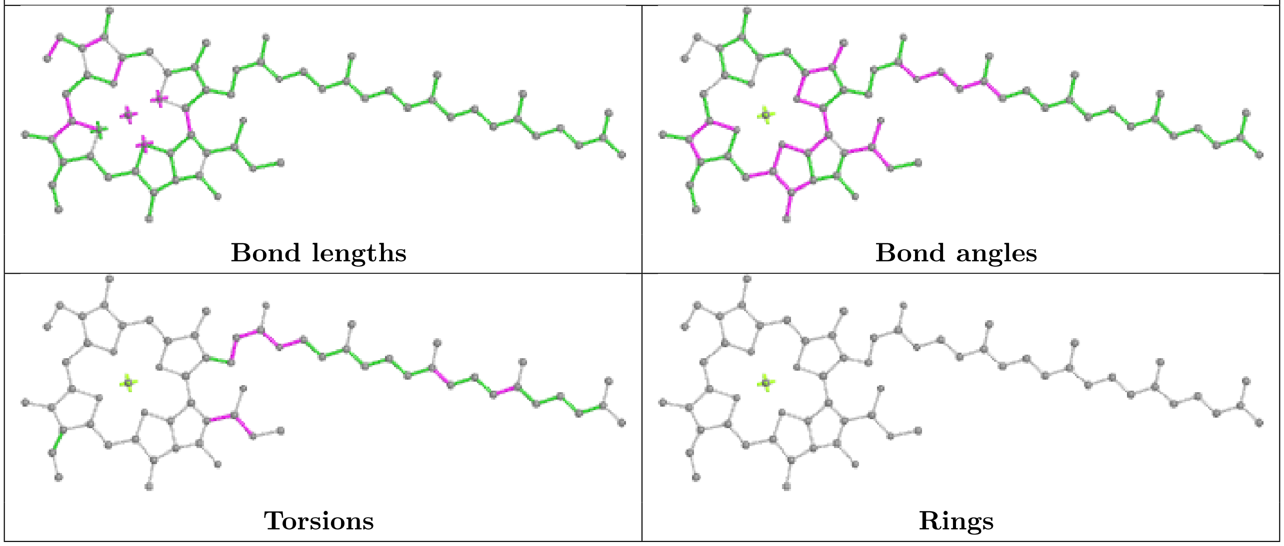
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA 1 605



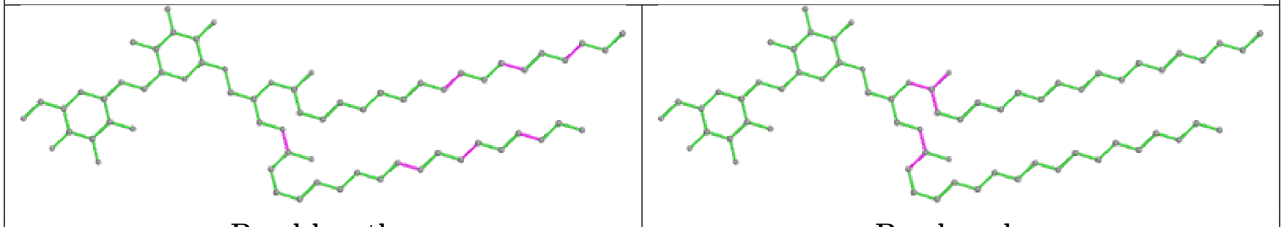
Bond lengths

Bond angles

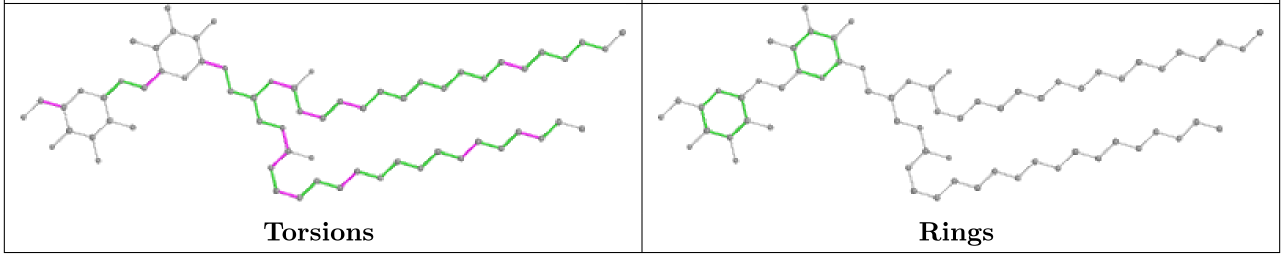
Torsions

Rings

Ligand DGD B 850

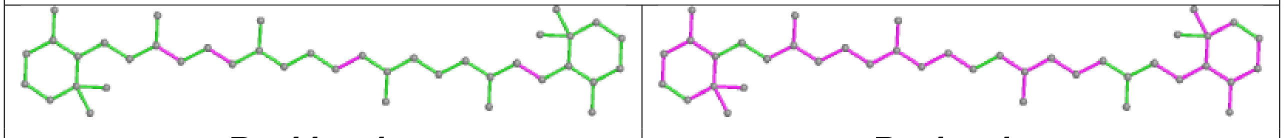


Bond lengths Bond angles

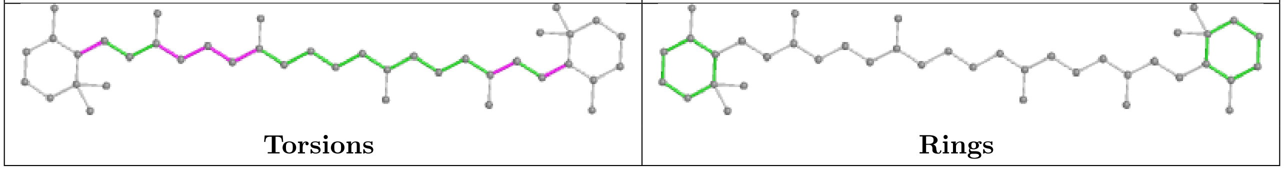


Torsions Rings

Ligand BCR A 845

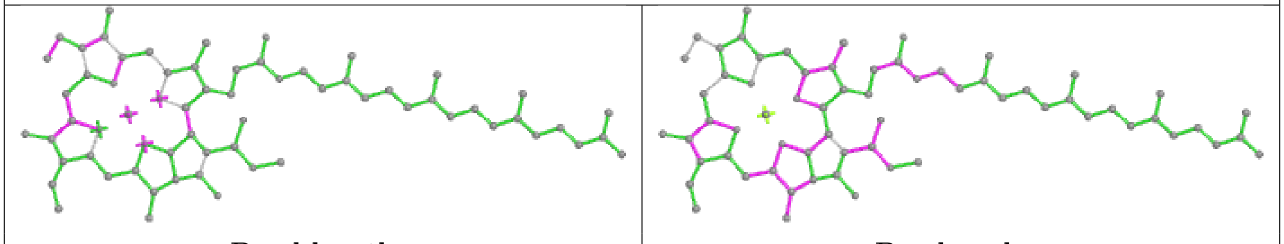


Bond lengths Bond angles

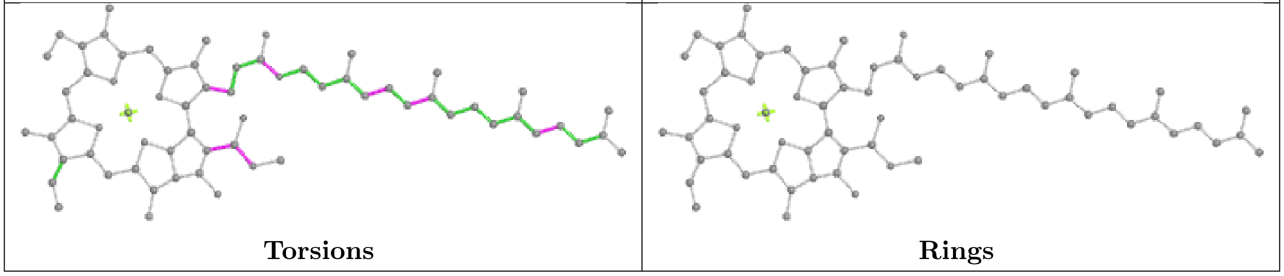


Torsions Rings

Ligand CLA A 810

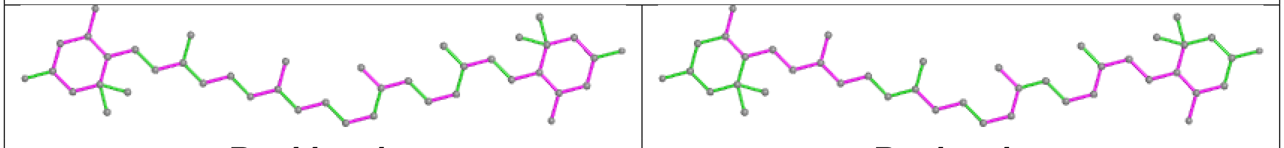


Bond lengths Bond angles

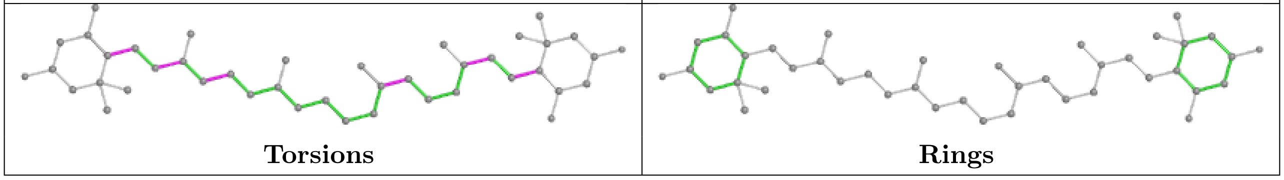


Torsions Rings

Ligand C7Z 3 215

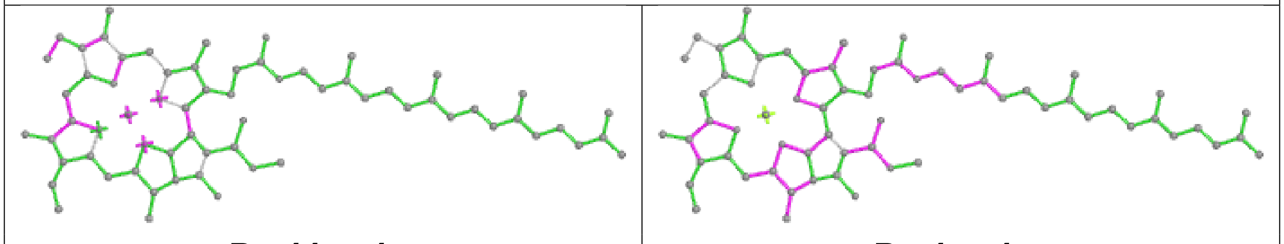


Bond lengths **Bond angles**

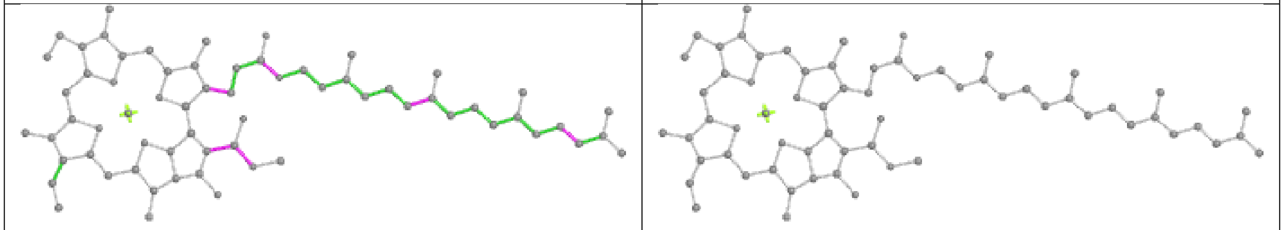


Torsions **Rings**

Ligand CLA O 204

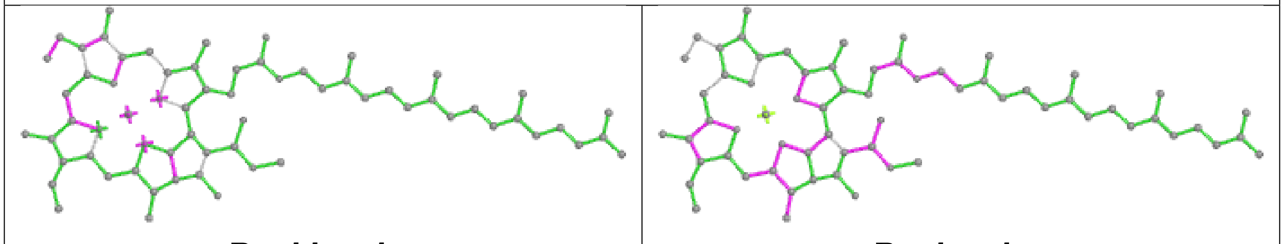


Bond lengths **Bond angles**

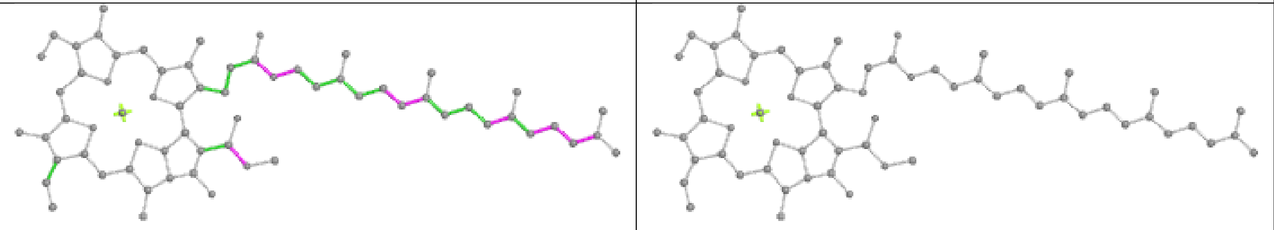


Torsions **Rings**

Ligand CLA A 829

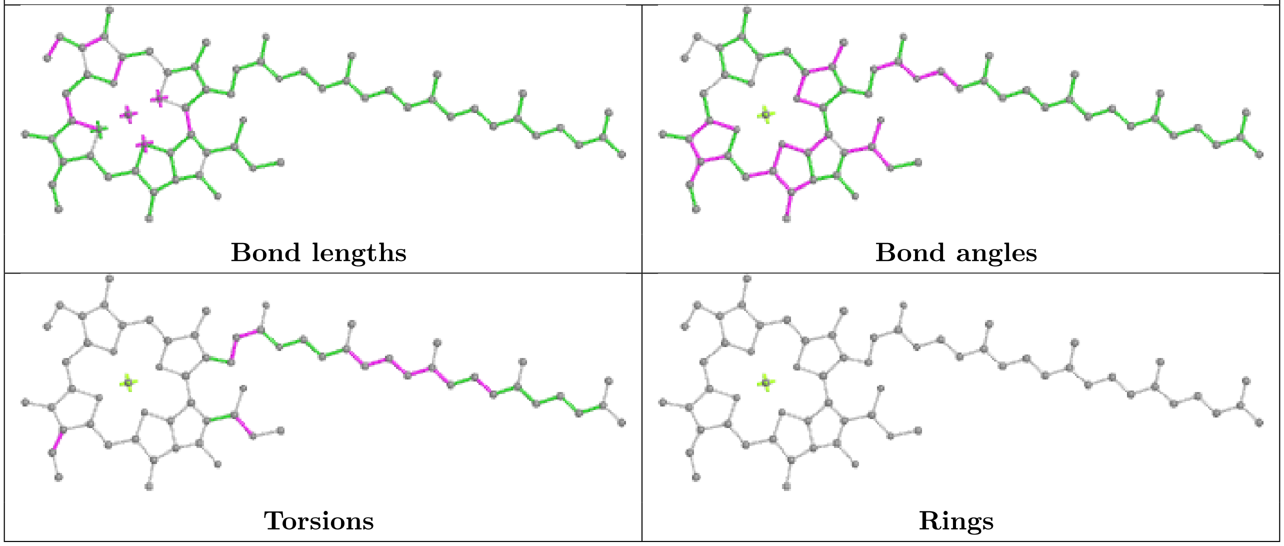


Bond lengths **Bond angles**



Torsions **Rings**

Ligand CLA A 816



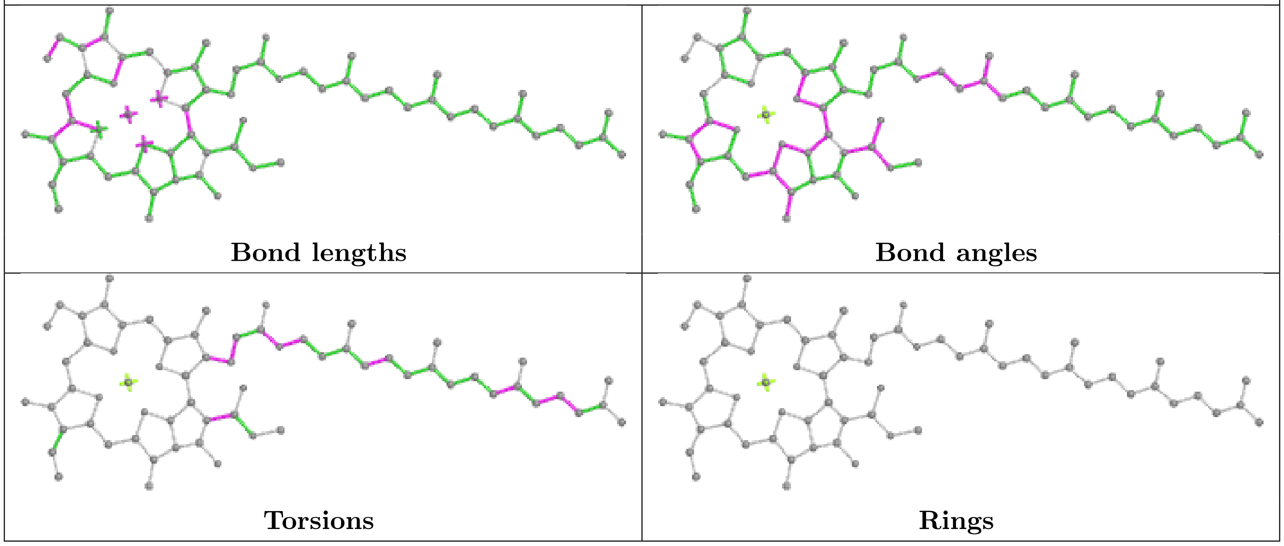
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA A 830



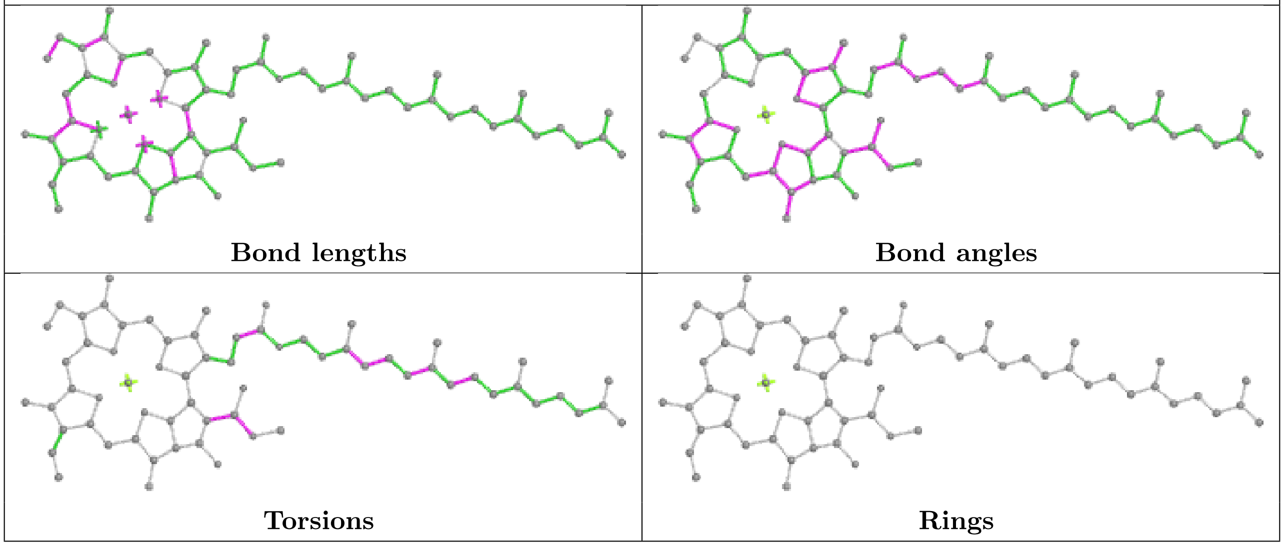
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA B 808



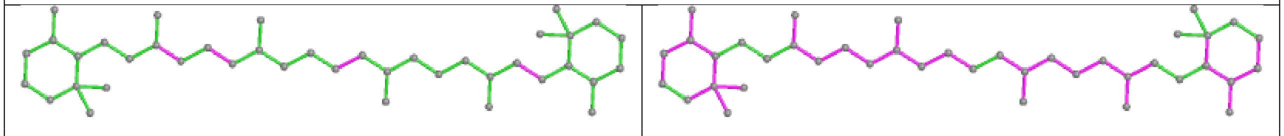
Bond lengths

Bond angles

Torsions

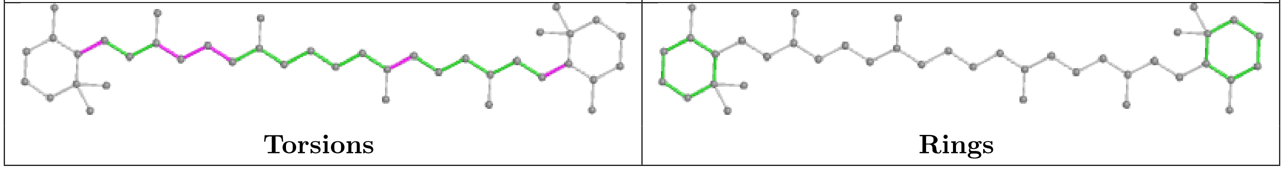
Rings

Ligand BCR I 103



Bond lengths

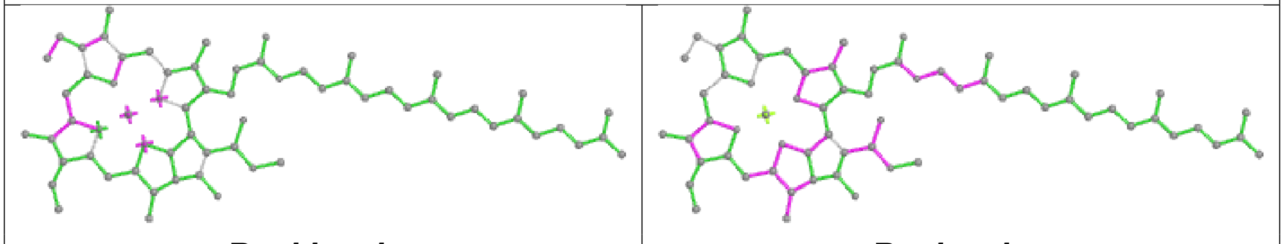
Bond angles



Torsions

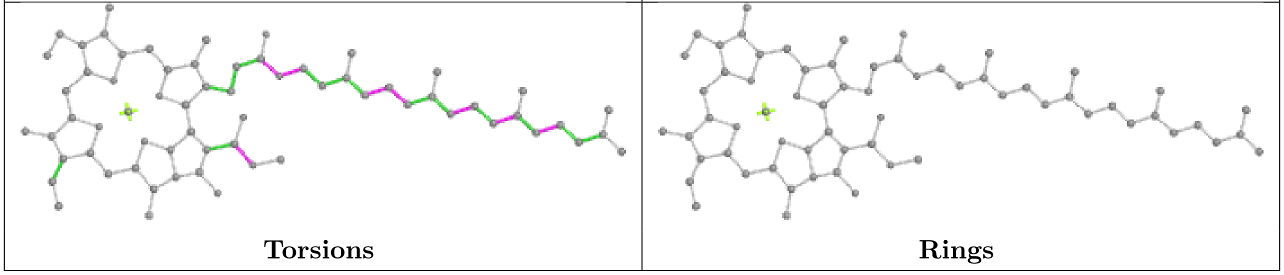
Rings

Ligand CLA A 806



Bond lengths

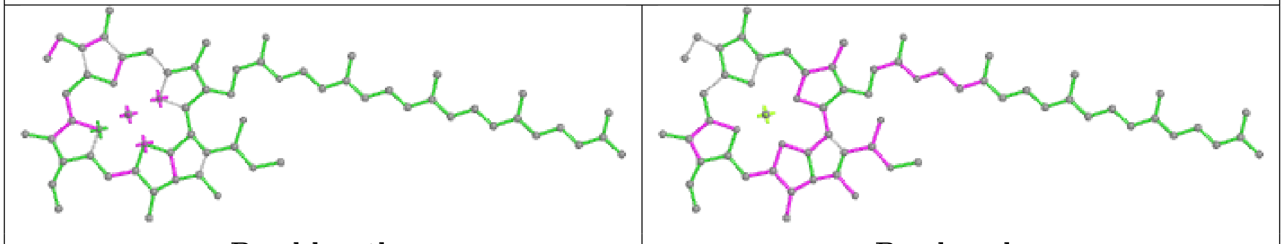
Bond angles



Torsions

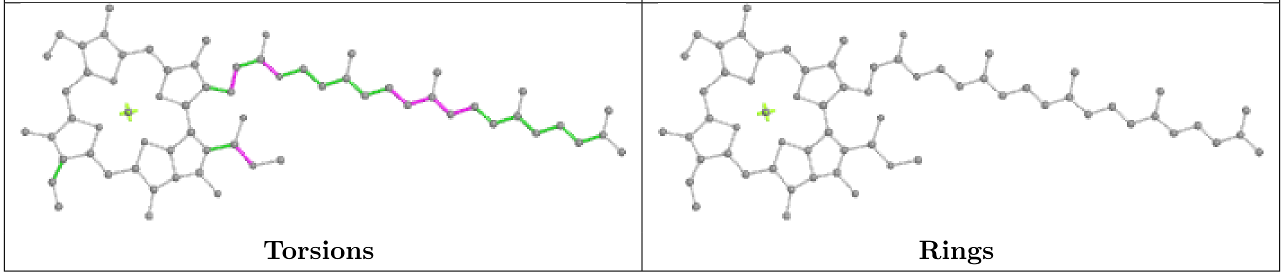
Rings

Ligand CLA B 816



Bond lengths

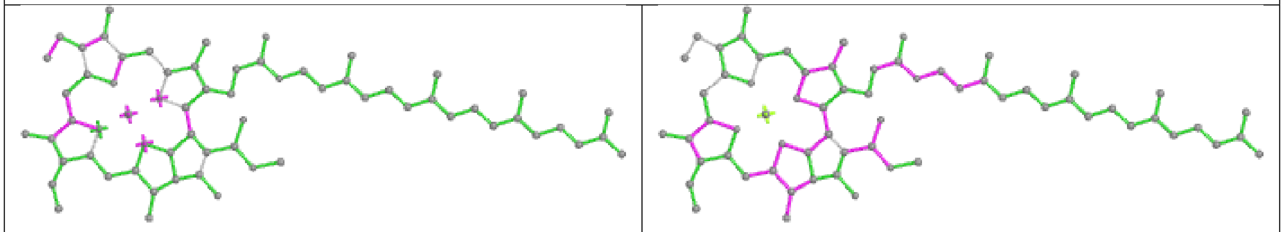
Bond angles



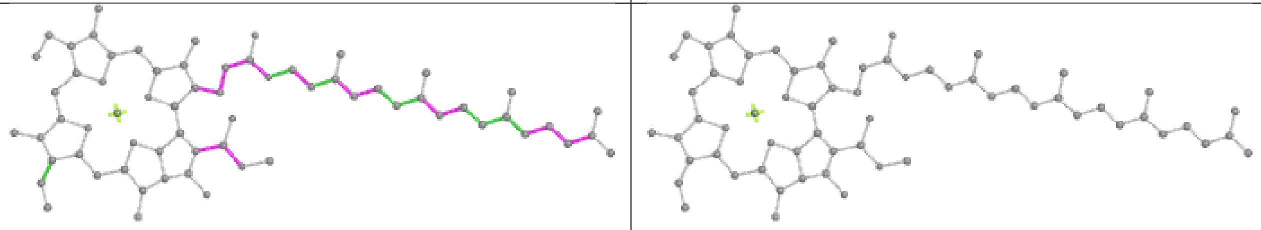
Torsions

Rings

Ligand CLA A 815

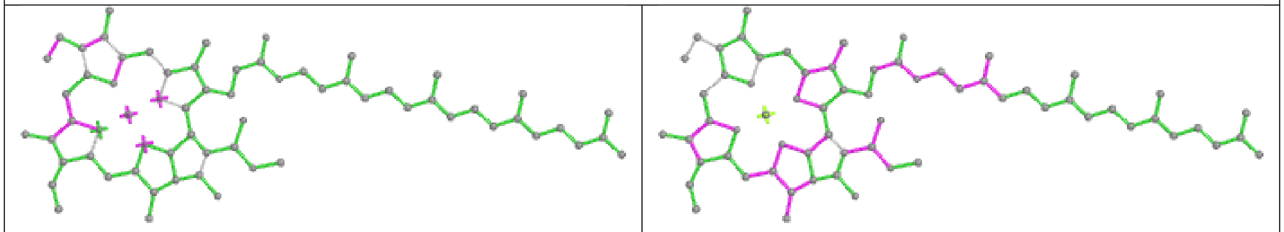


Bond lengths Bond angles

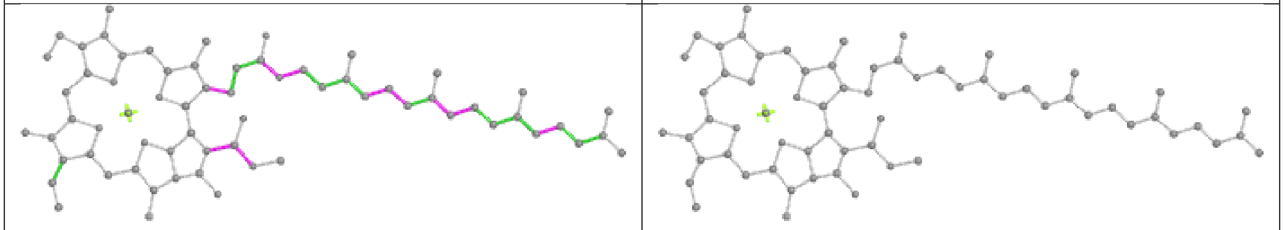


Torsions Rings

Ligand CLA 1 608

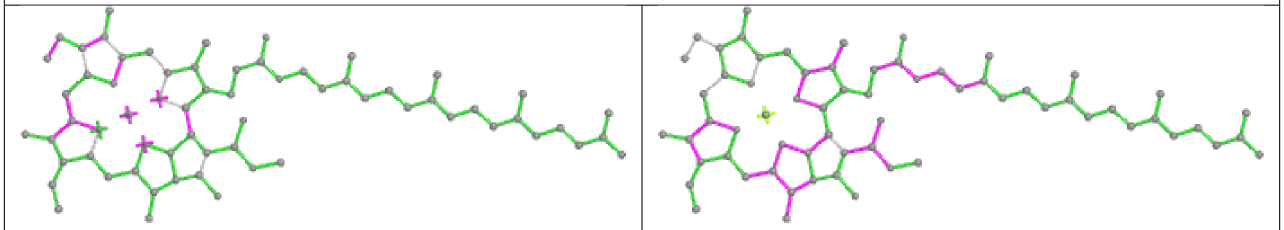


Bond lengths Bond angles

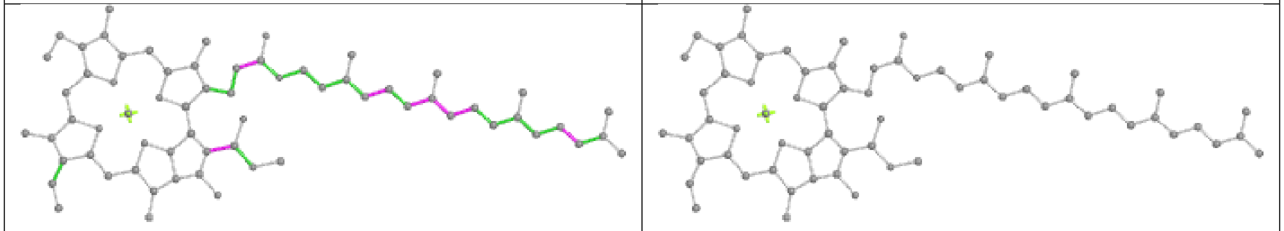


Torsions Rings

Ligand CLA 3 206

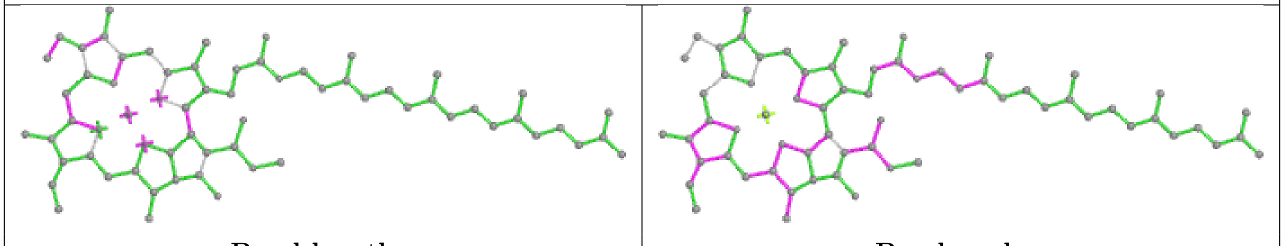


Bond lengths Bond angles

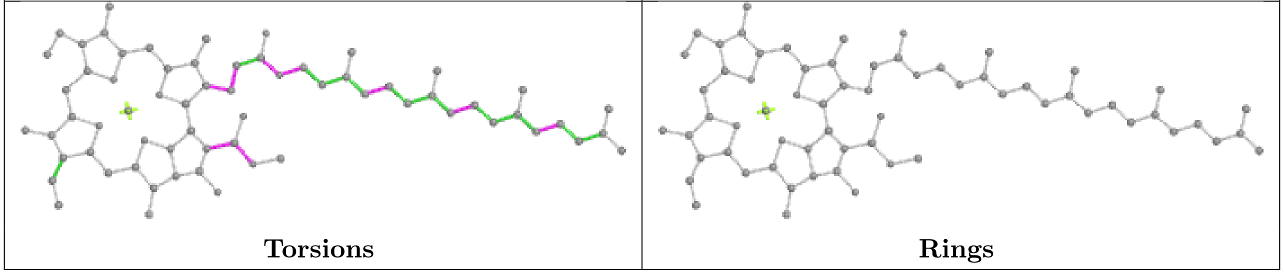


Torsions Rings

Ligand CLA A 812

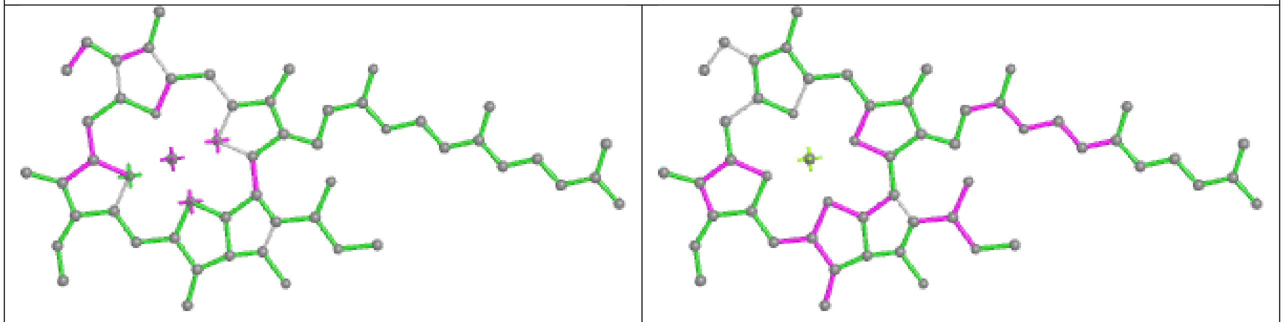


Bond lengths Bond angles

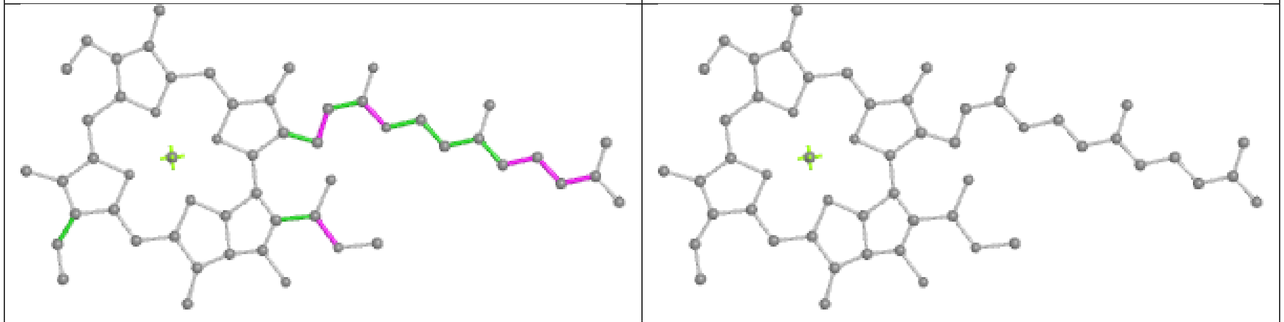


Torsions Rings

Ligand CLA B 815

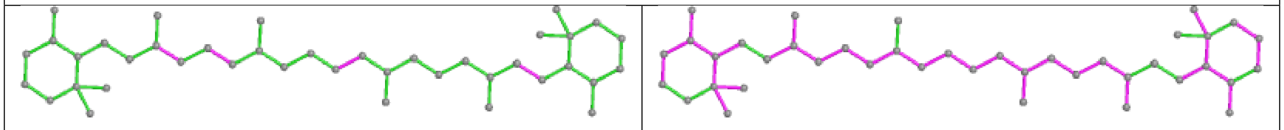


Bond lengths Bond angles

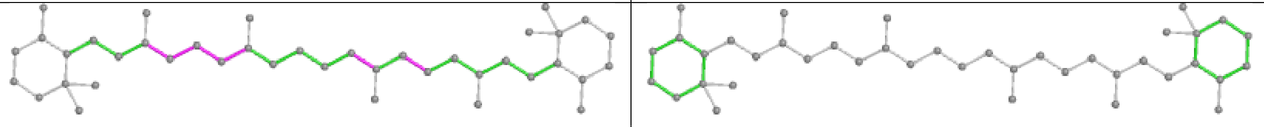


Torsions Rings

Ligand BCR B 855

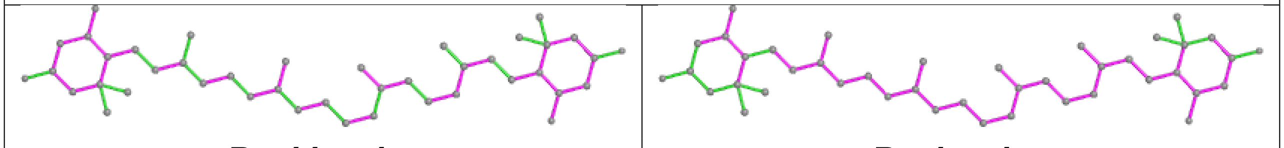


Bond lengths Bond angles



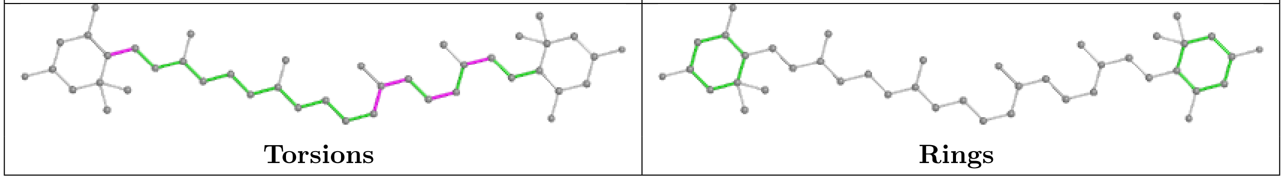
Torsions Rings

Ligand C7Z 3 216



Bond lengths

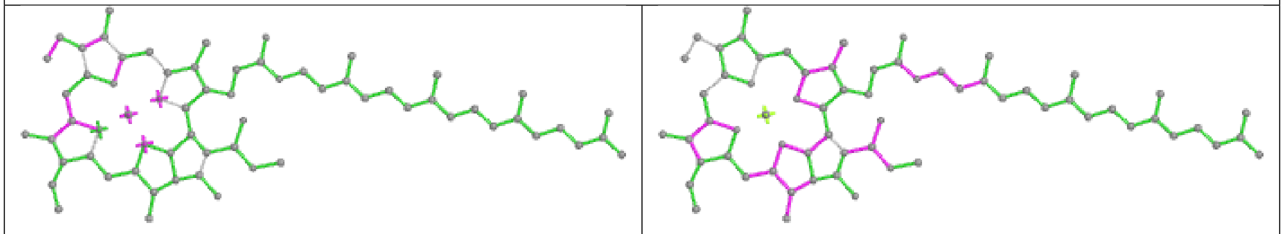
Bond angles



Torsions

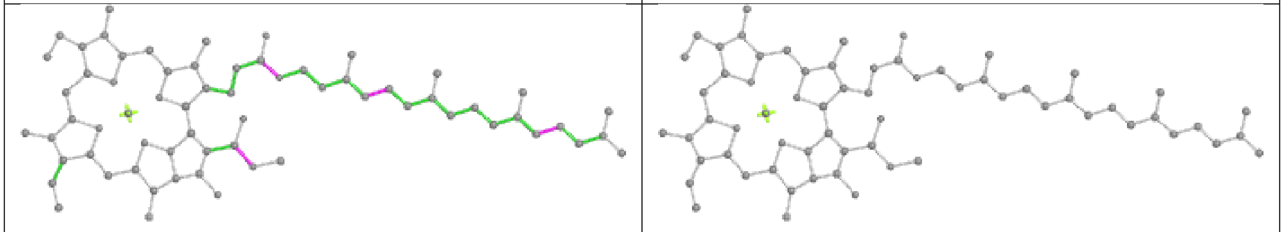
Rings

Ligand CLA A 838



Bond lengths

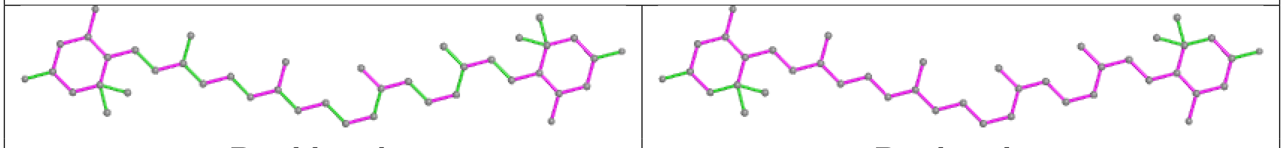
Bond angles



Torsions

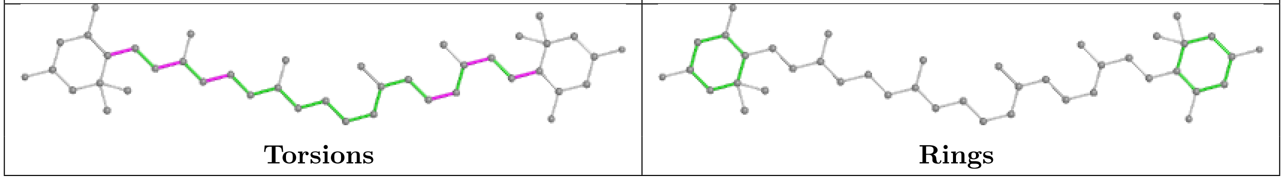
Rings

Ligand C7Z 3 218



Bond lengths

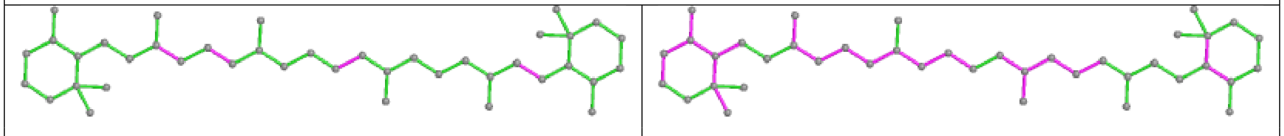
Bond angles



Torsions

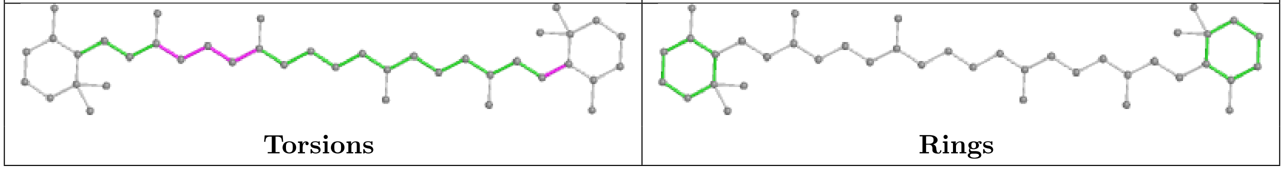
Rings

Ligand BCR B 840



Bond lengths

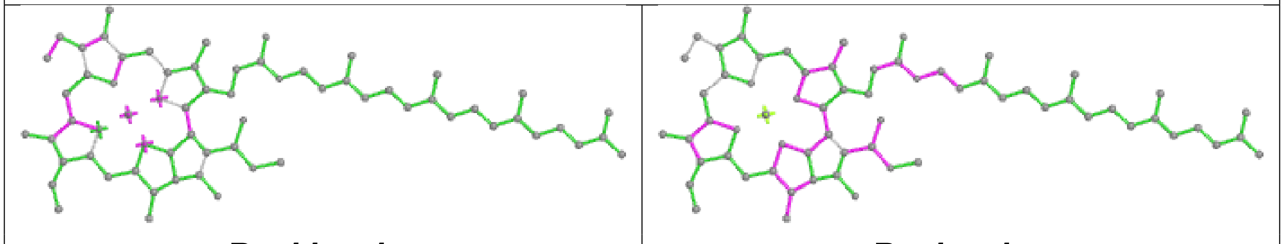
Bond angles



Torsions

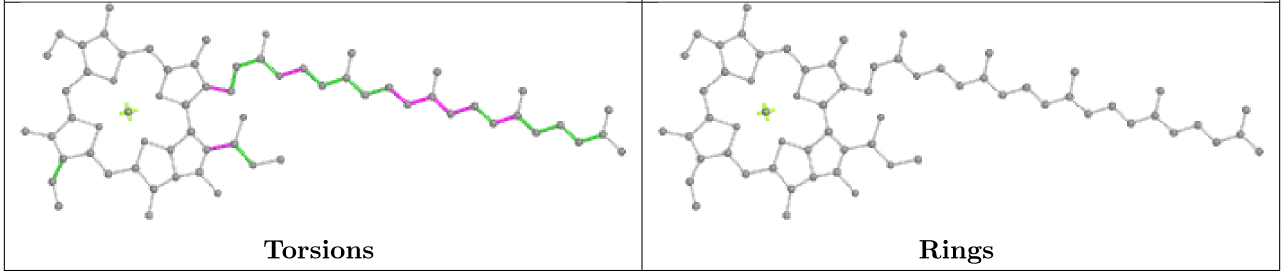
Rings

Ligand CLA B 825



Bond lengths

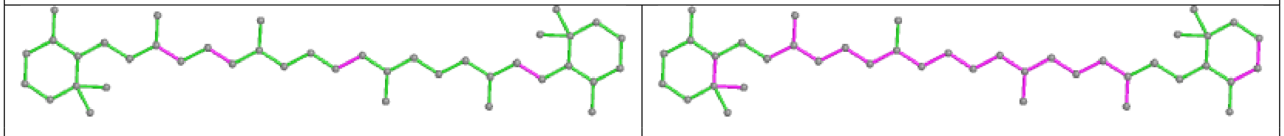
Bond angles



Torsions

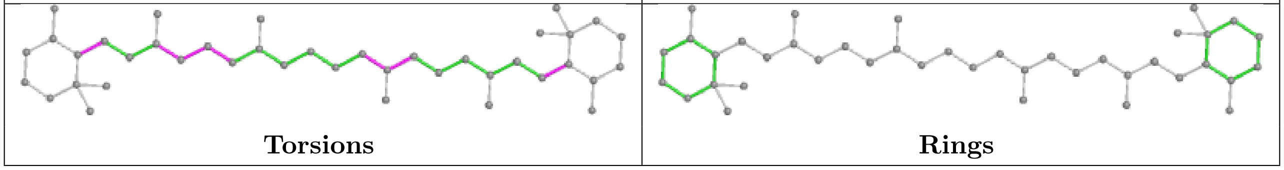
Rings

Ligand BCR O 205



Bond lengths

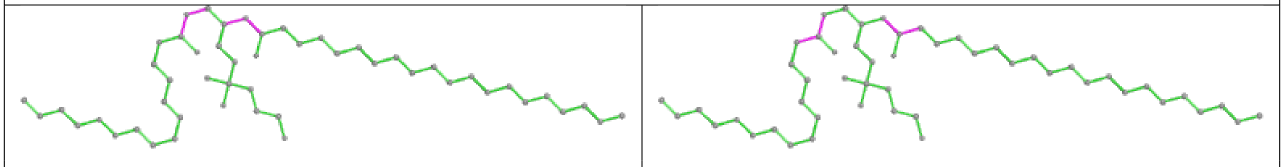
Bond angles



Torsions

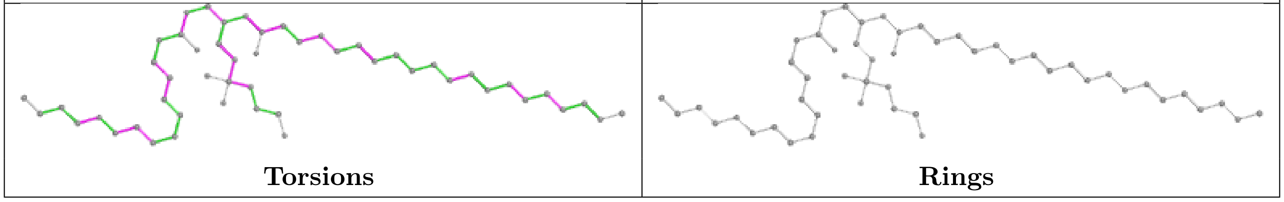
Rings

Ligand PTY L 208



Bond lengths

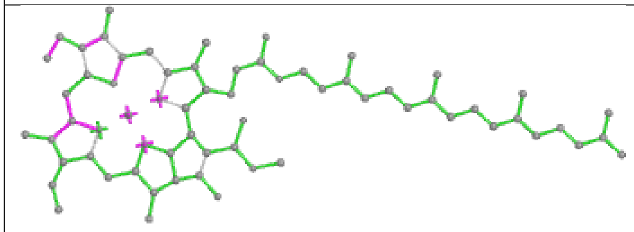
Bond angles



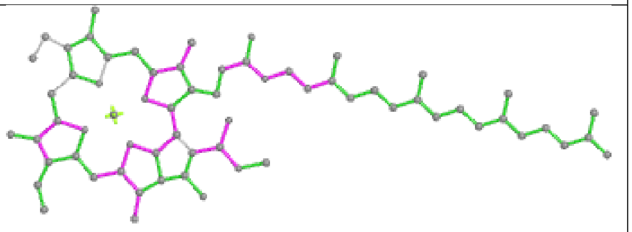
Torsions

Rings

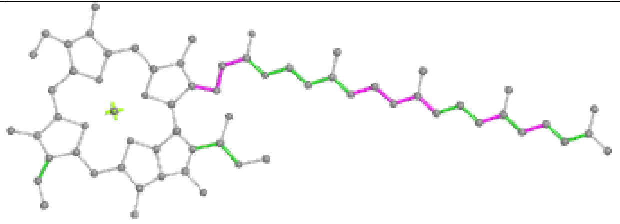
Ligand CLA A 835



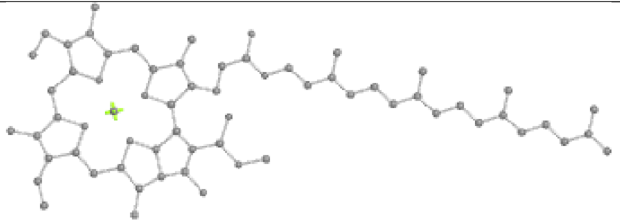
Bond lengths



Bond angles

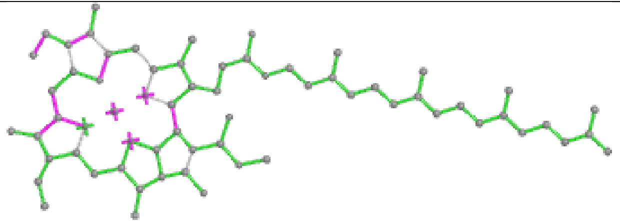


Torsions

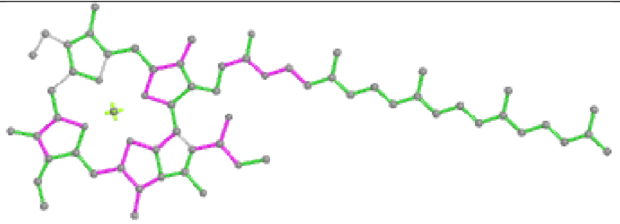


Rings

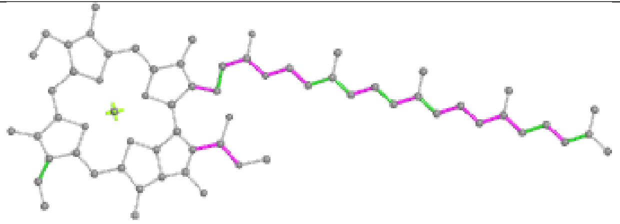
Ligand CLA 2 613



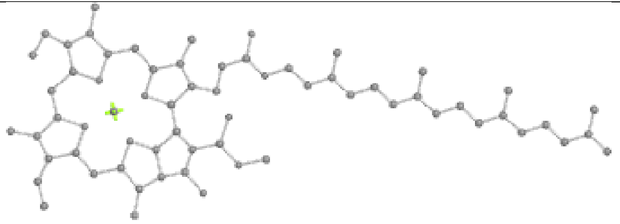
Bond lengths



Bond angles

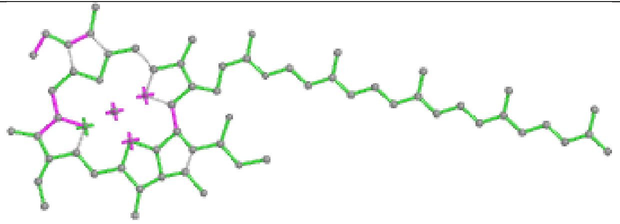


Torsions

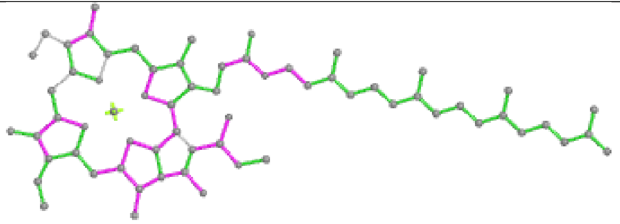


Rings

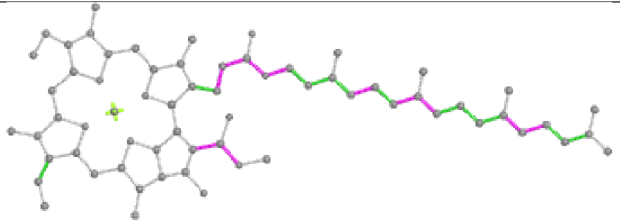
Ligand CLA B 801



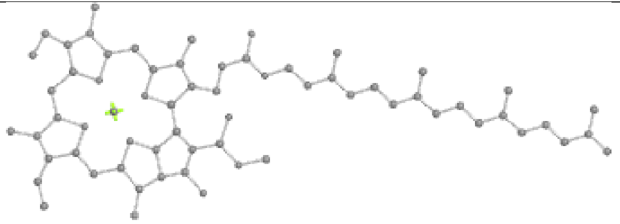
Bond lengths



Bond angles

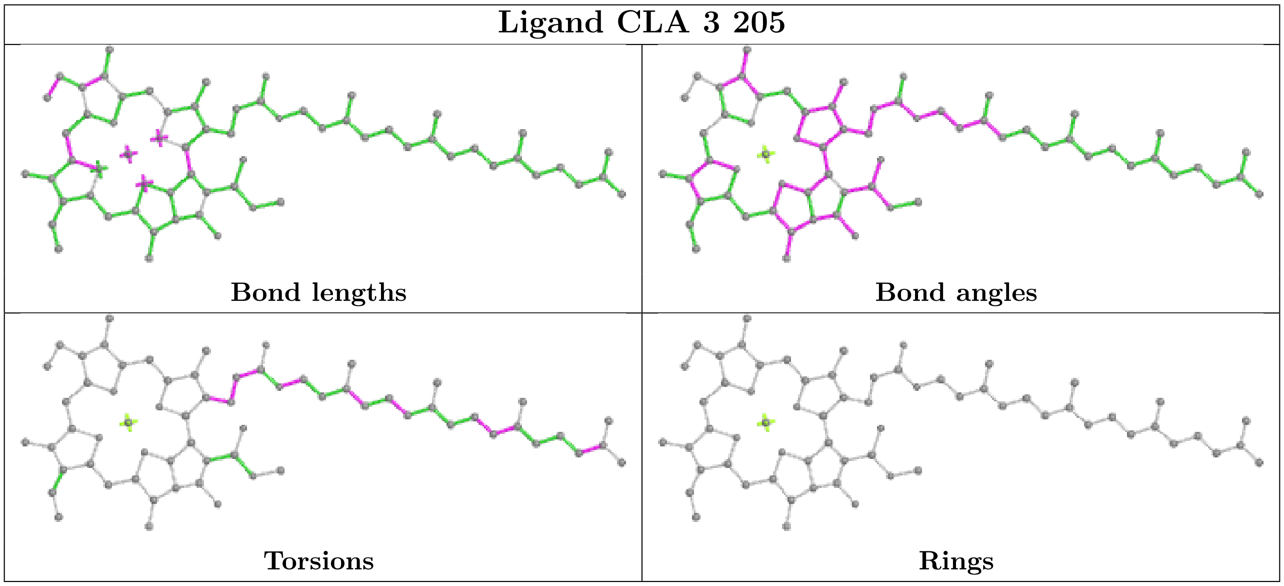


Torsions



Rings

Ligand CLA 3 205



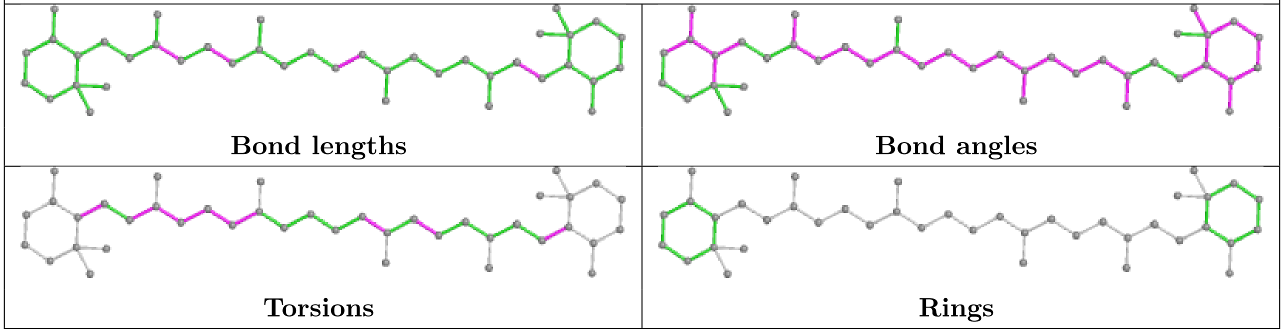
Bond lengths

Bond angles

Torsions

Rings

Ligand BCR A 850



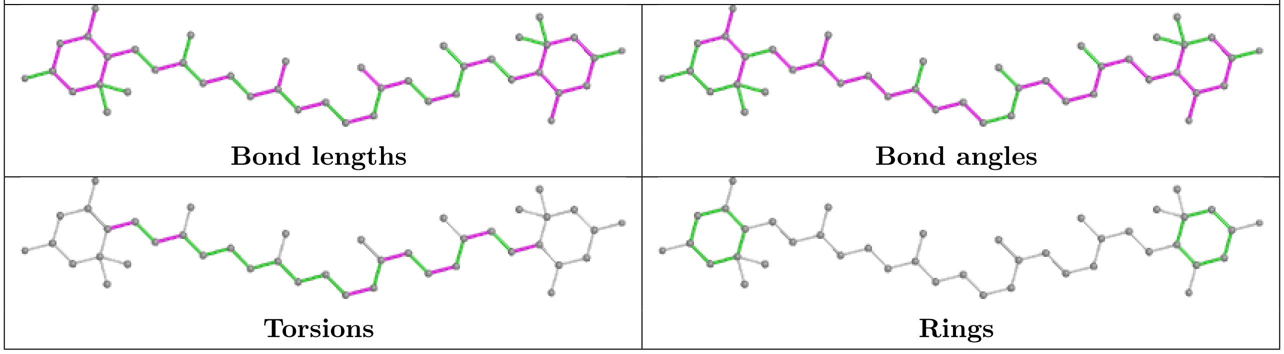
Bond lengths

Bond angles

Torsions

Rings

Ligand C7Z A 843



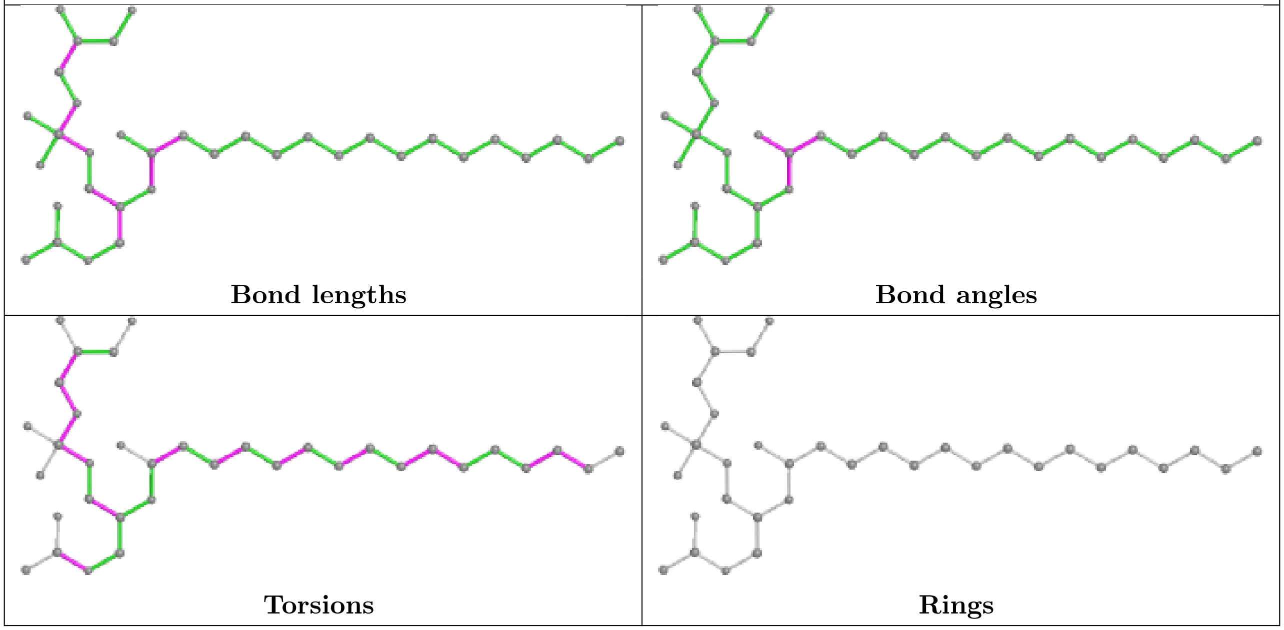
Bond lengths

Bond angles

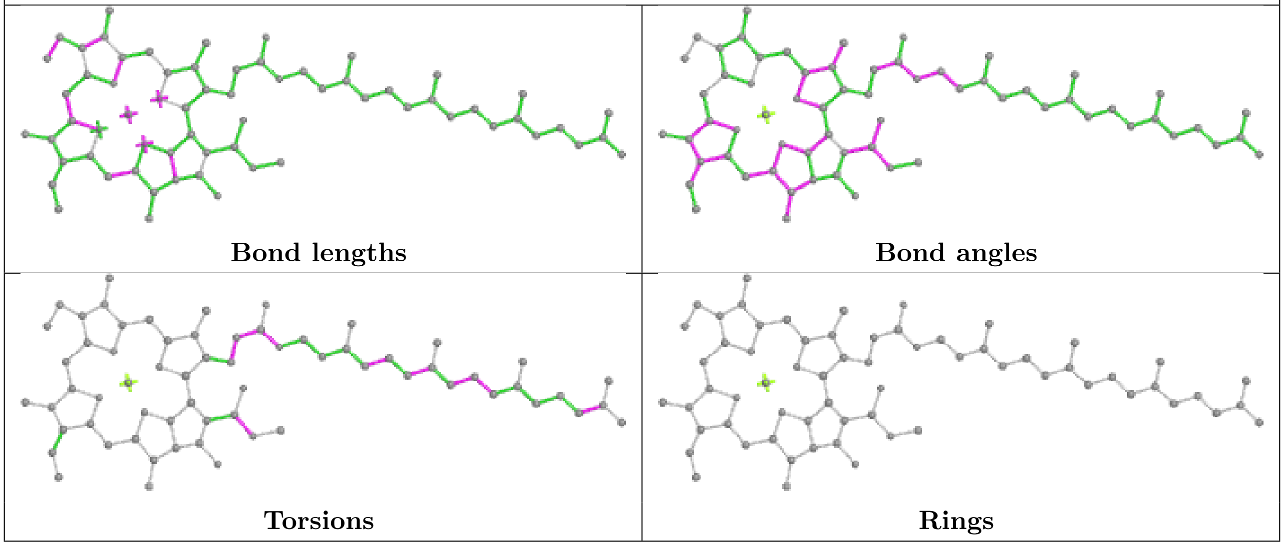
Torsions

Rings

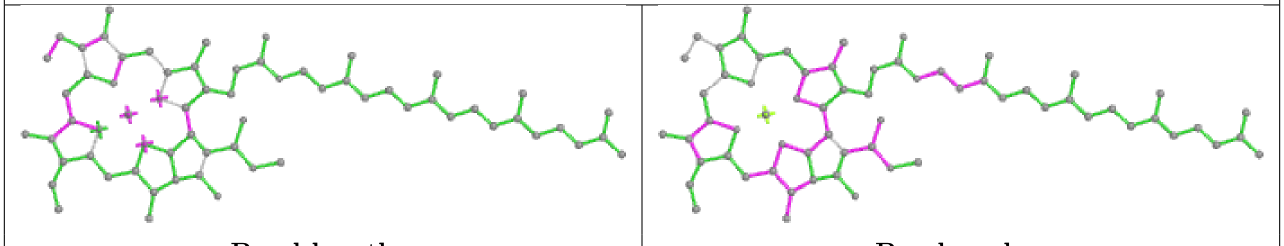
Ligand PGT B 848

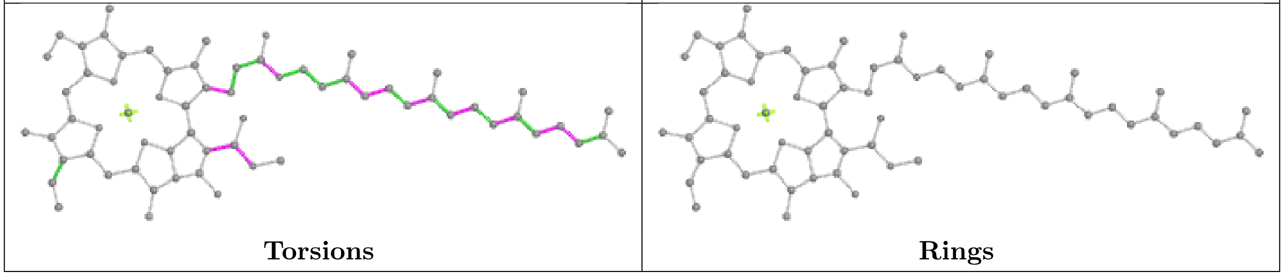


Ligand CLA B 836

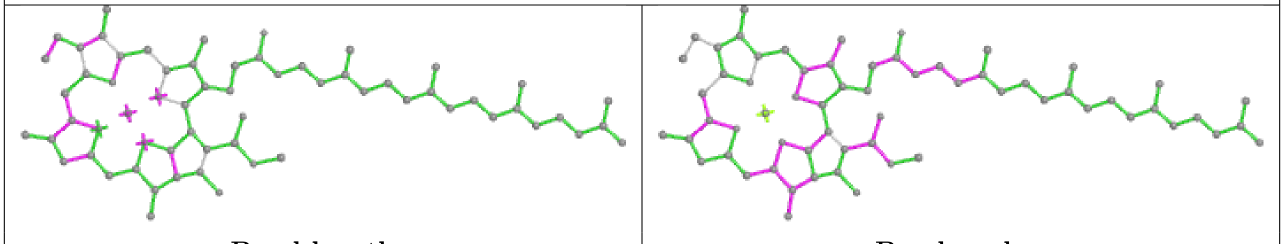


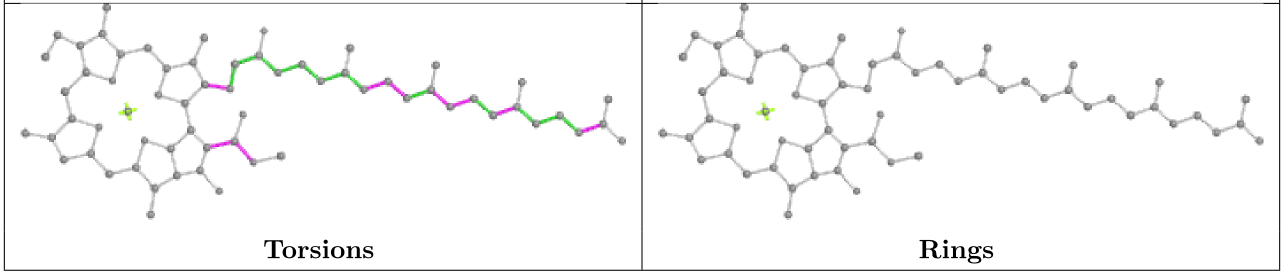
Ligand CLA A 813


Bond lengths Bond angles

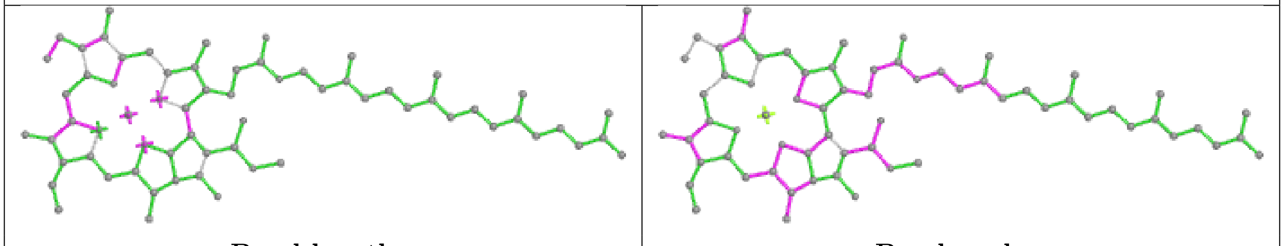

Torsions Rings

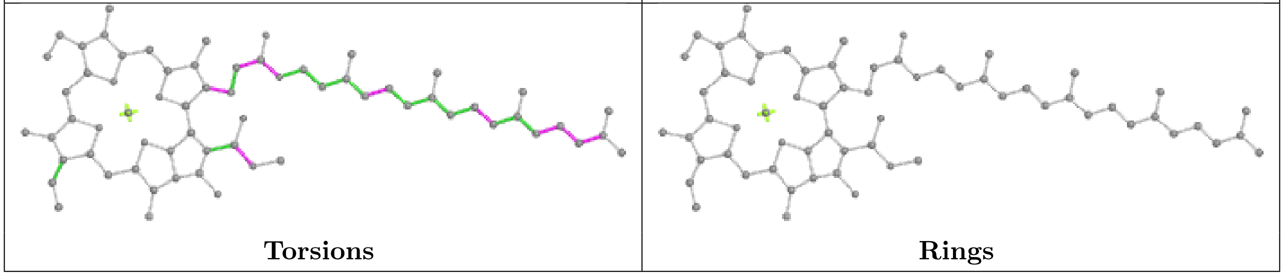
Ligand CLA 2 602


Bond lengths Bond angles

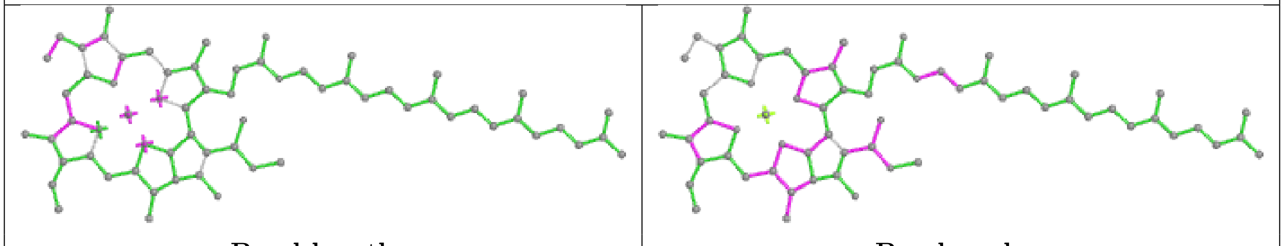

Torsions Rings

Ligand CLA B 834


Bond lengths Bond angles

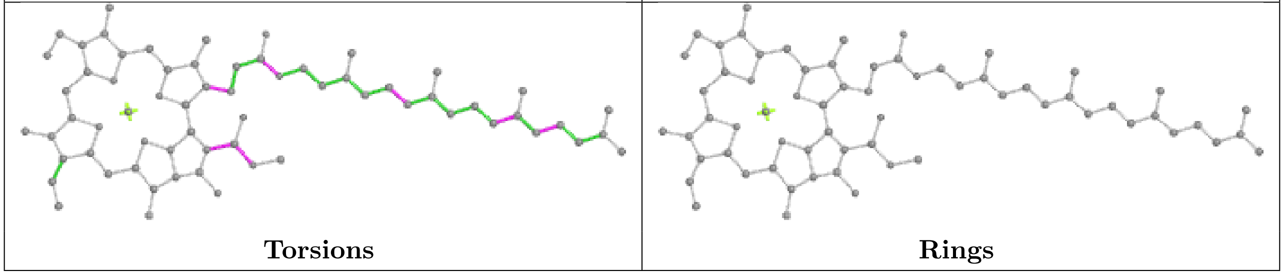

Torsions Rings

Ligand CLA O 202



Bond lengths

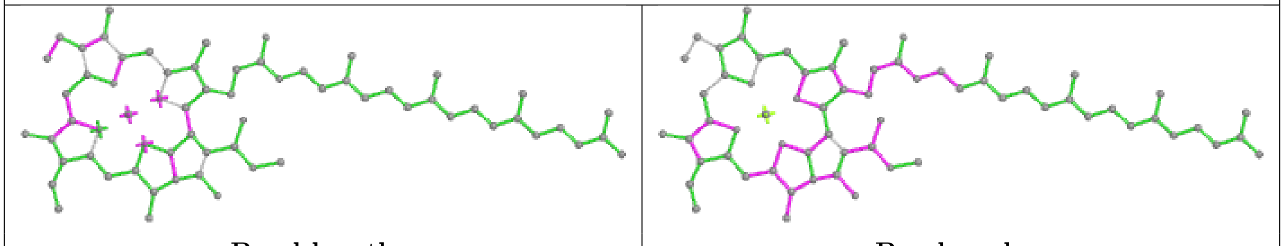
Bond angles



Torsions

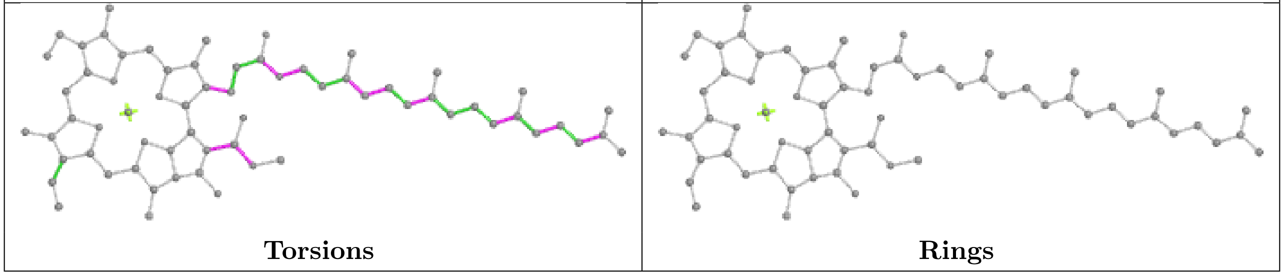
Rings

Ligand CLA A 819



Bond lengths

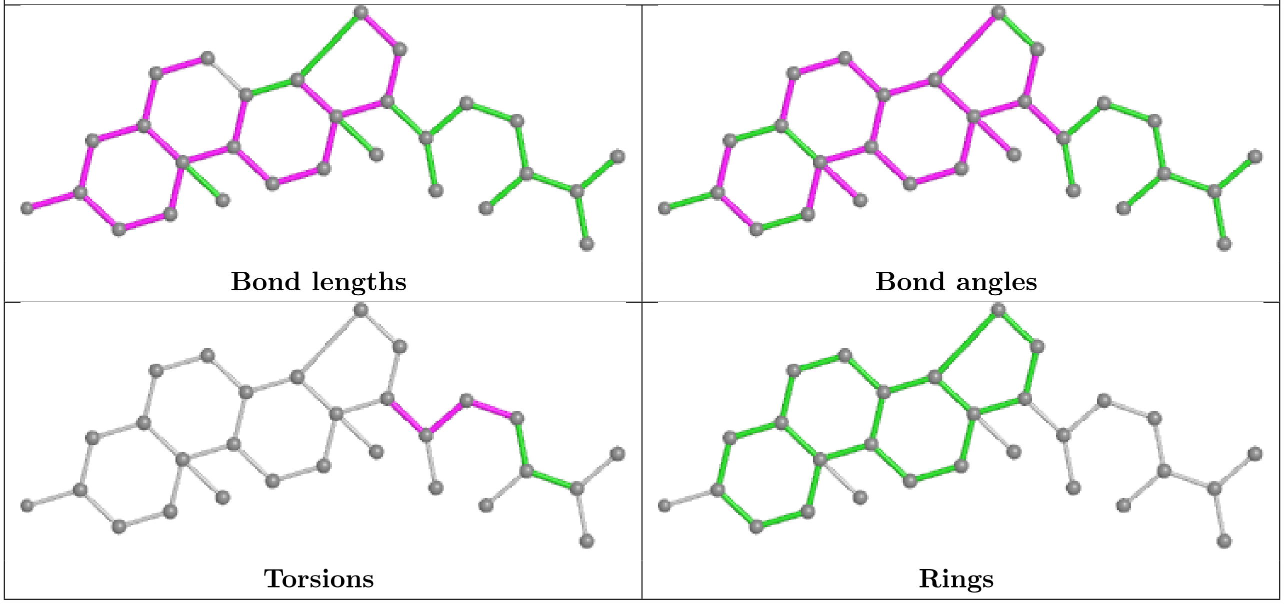
Bond angles



Torsions

Rings

Ligand ERG 1 618



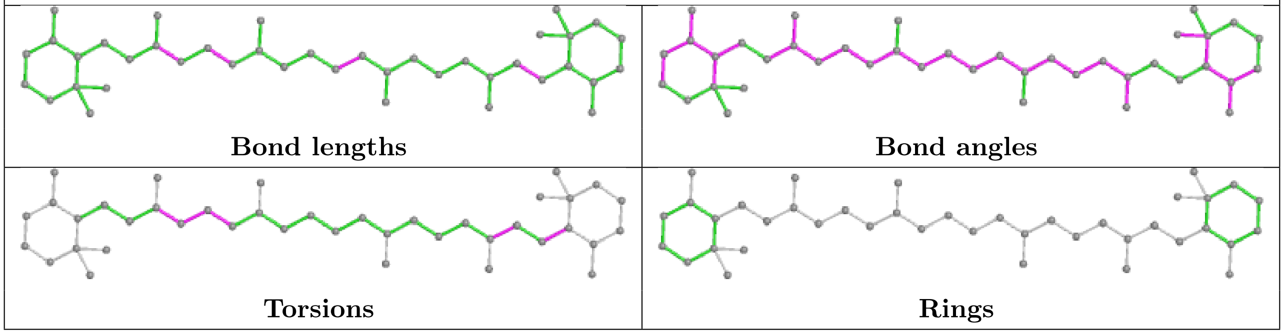
Bond lengths

Bond angles

Torsions

Rings

Ligand BCR B 844



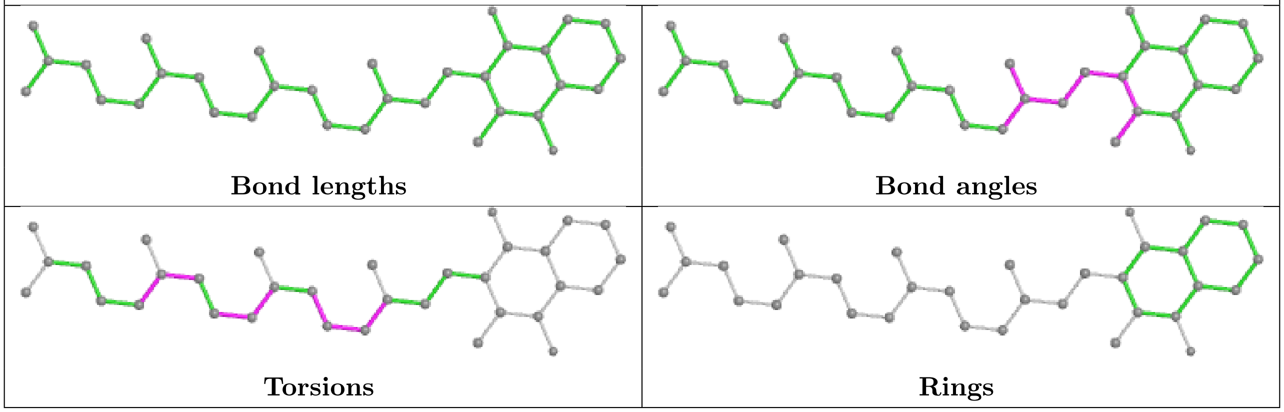
Bond lengths

Bond angles

Torsions

Rings

Ligand PQN A 840



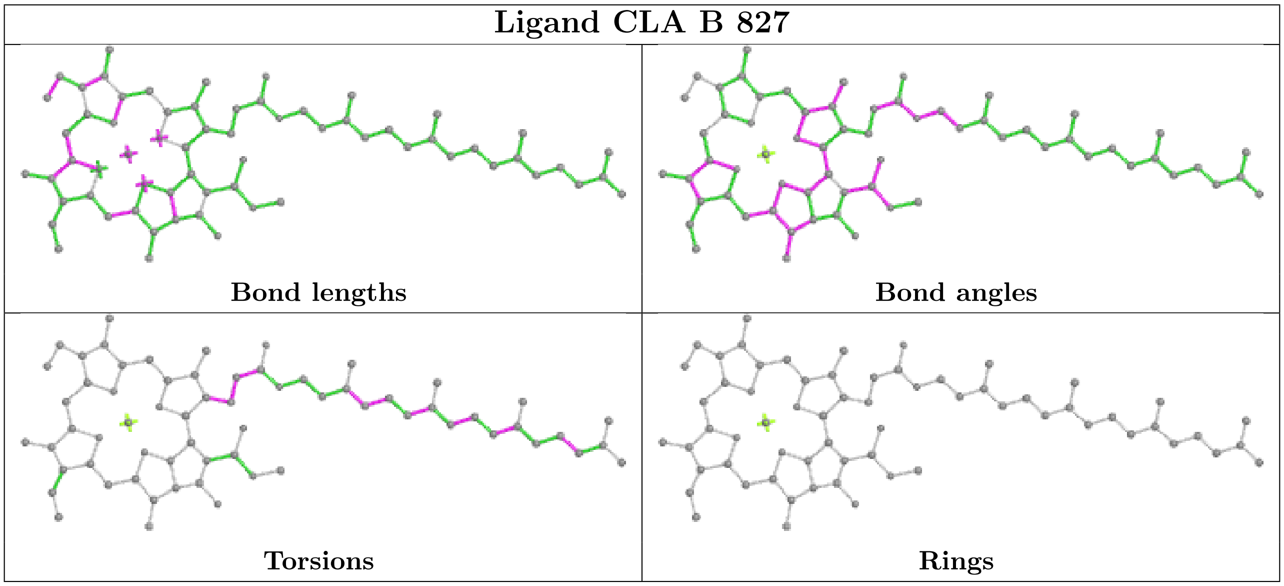
Bond lengths

Bond angles

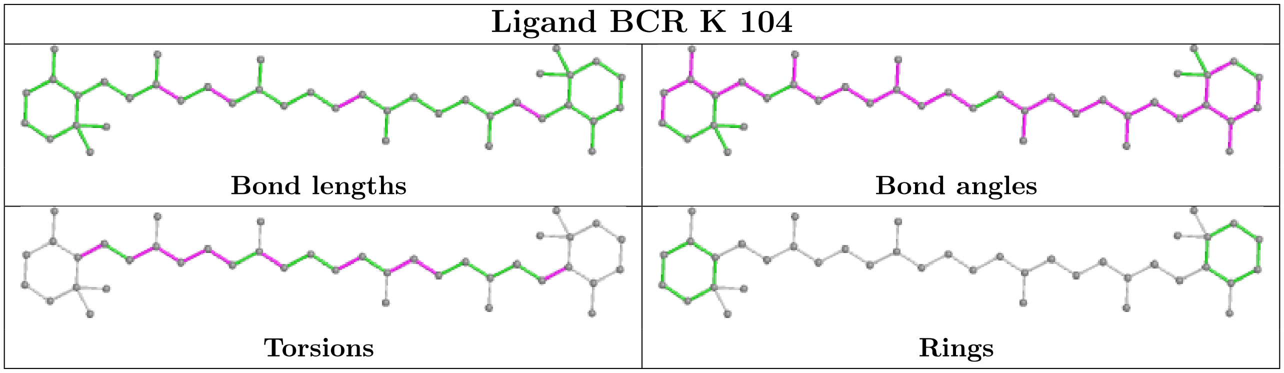
Torsions

Rings

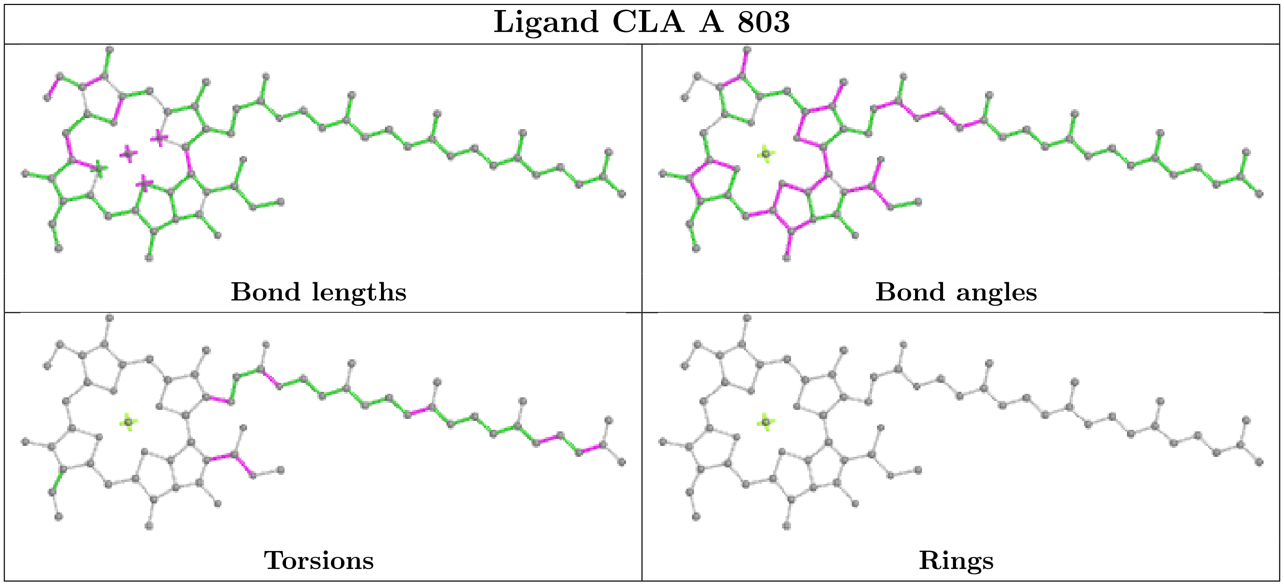
Ligand CLA B 827



Ligand BCR K 104



Ligand CLA A 803



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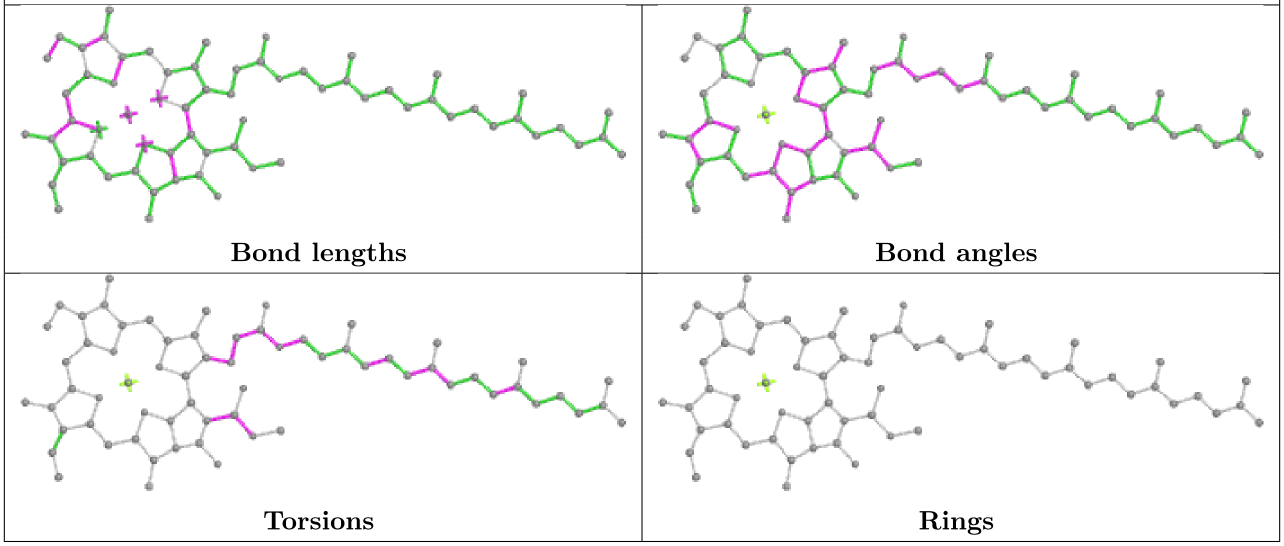
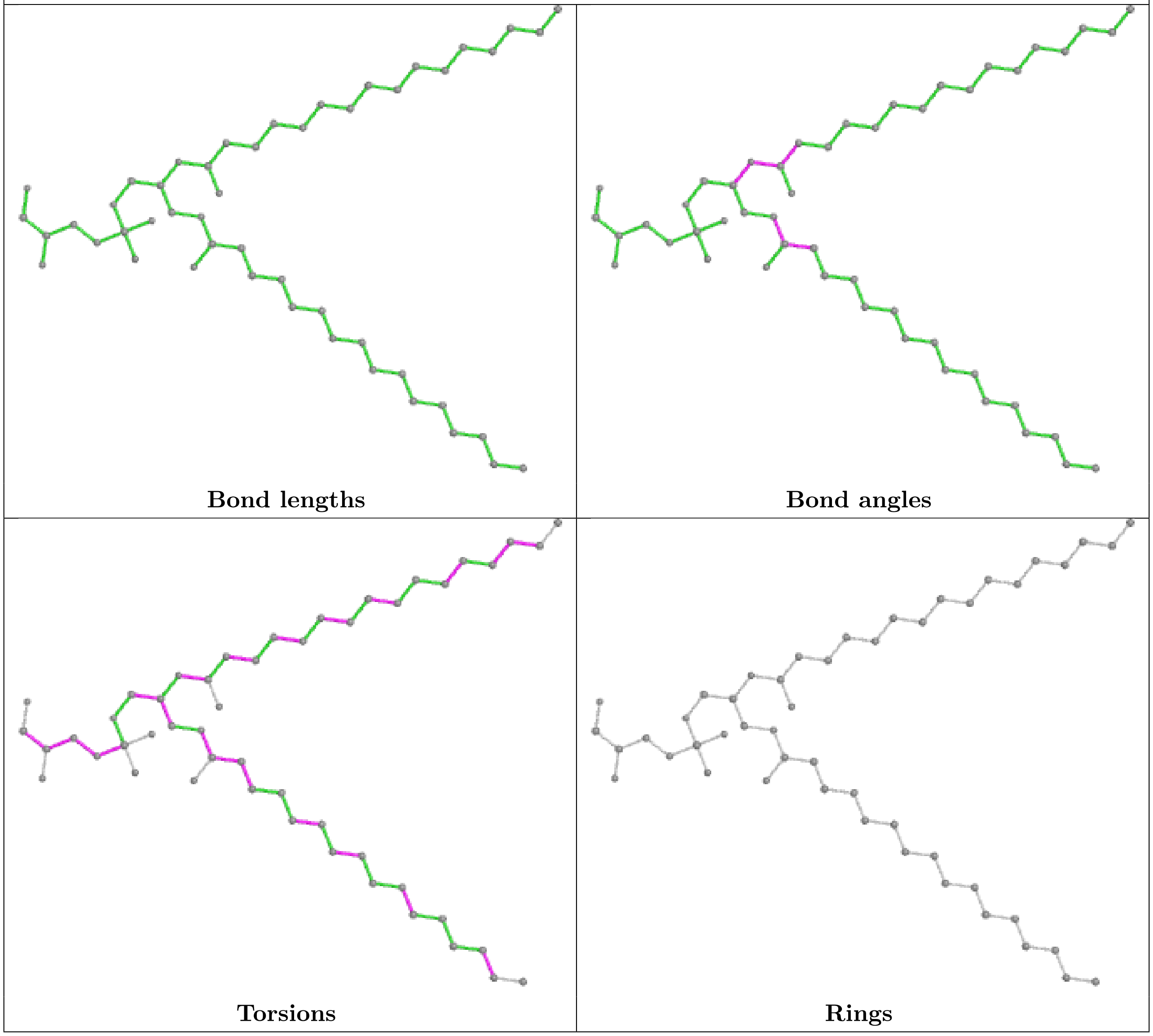
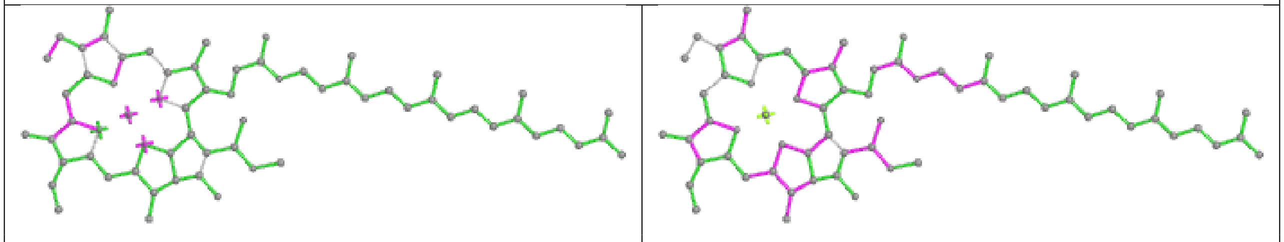


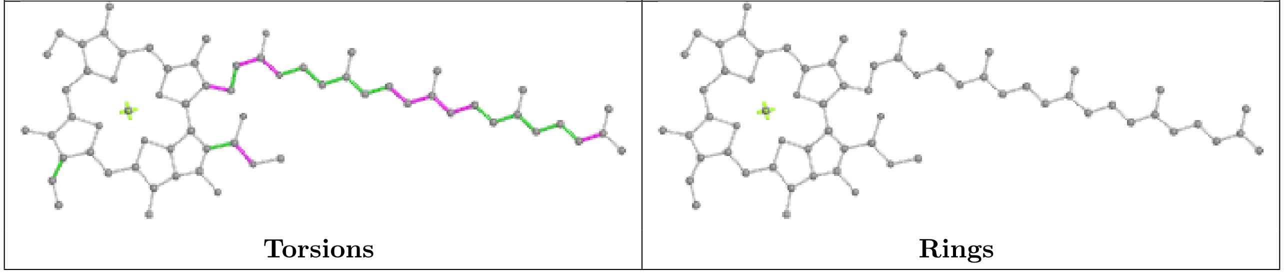
Ligand LHG 1 617



Ligand CLA 3 208

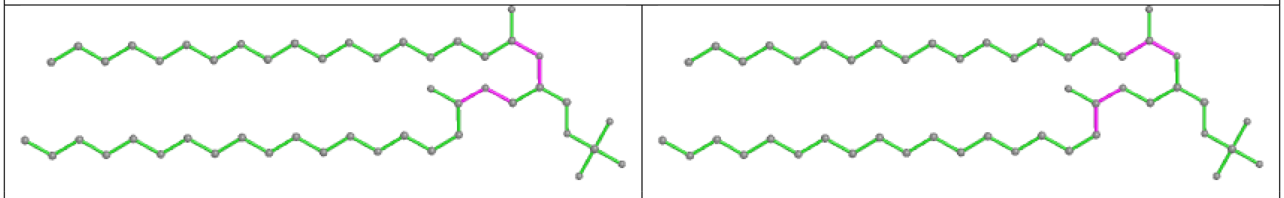


Bond lengths Bond angles

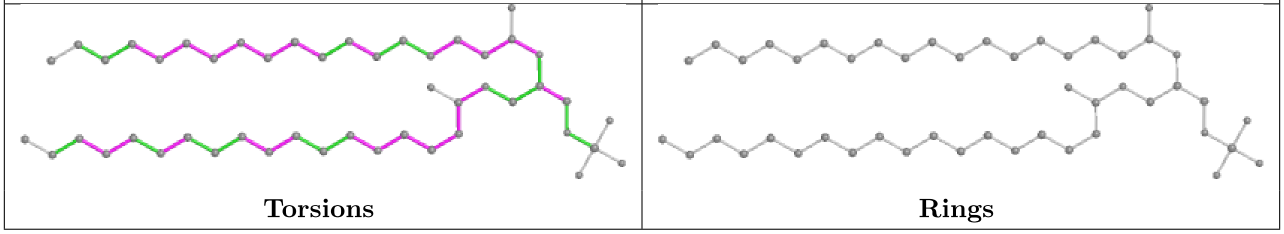


Torsions Rings

Ligand 3PH B 854

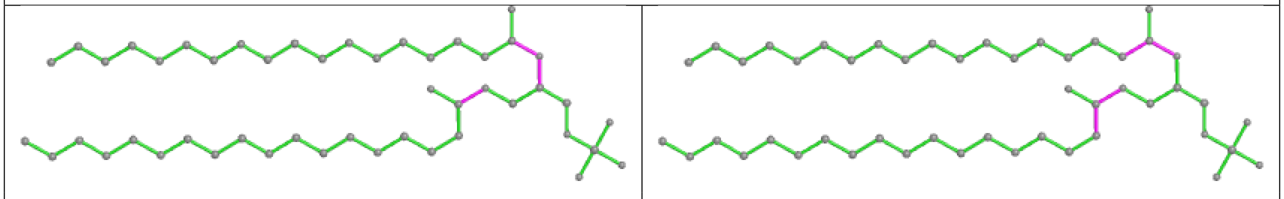


Bond lengths Bond angles

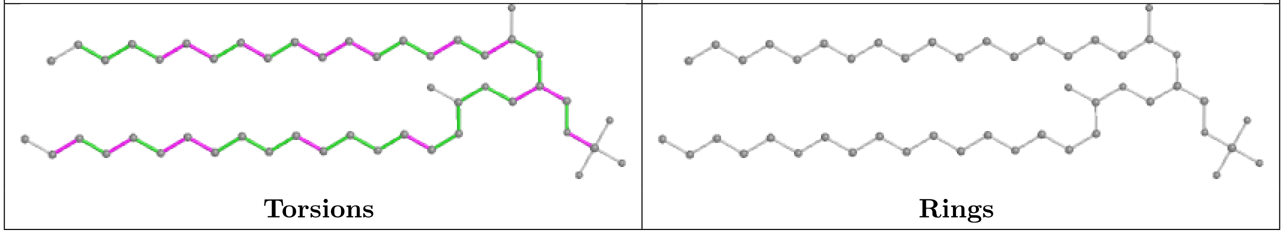


Torsions Rings

Ligand 3PH J 105

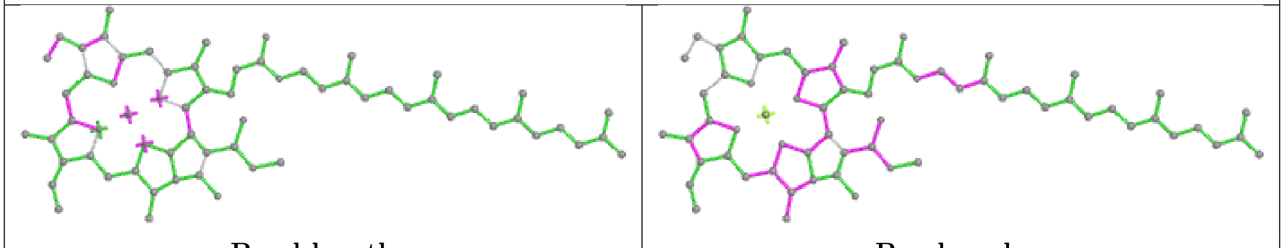


Bond lengths Bond angles



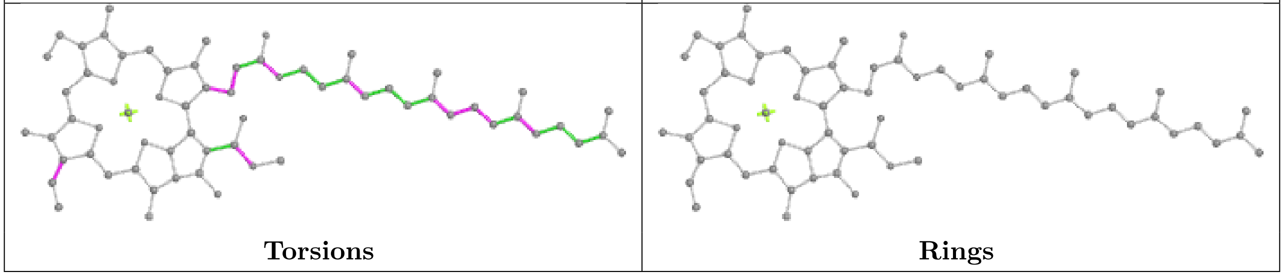
Torsions Rings

Ligand CLA B 837



Bond lengths

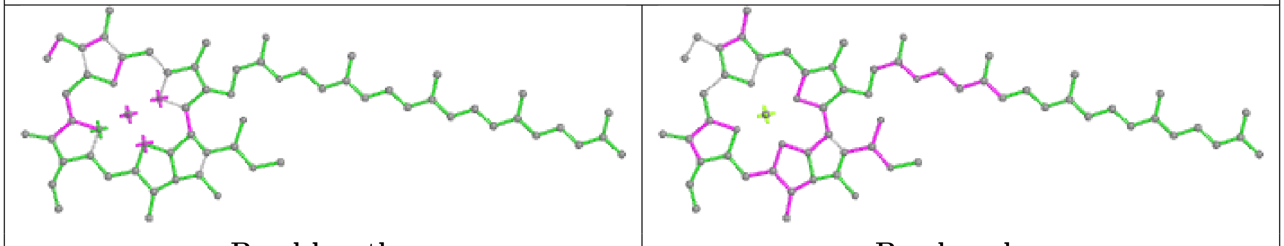
Bond angles



Torsions

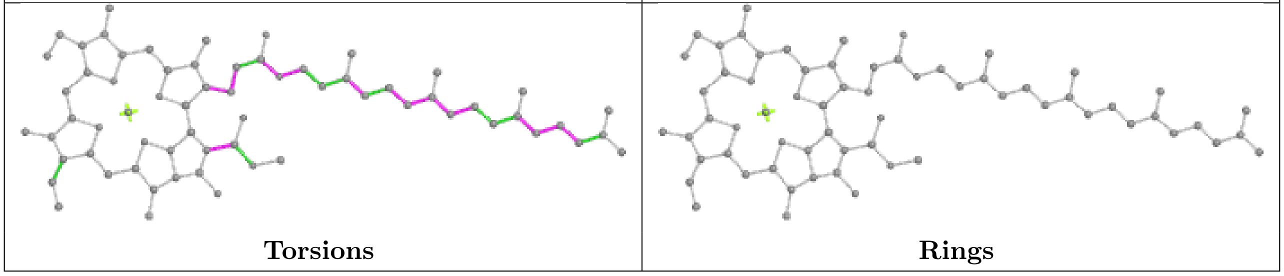
Rings

Ligand CLA A 837



Bond lengths

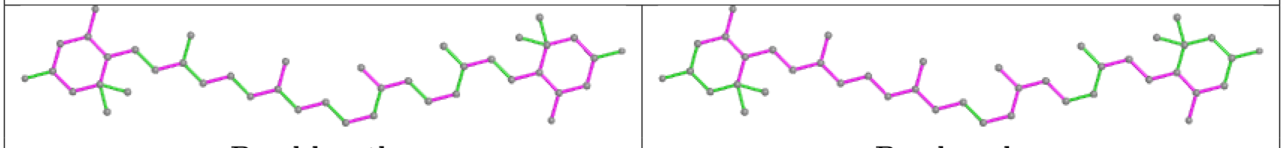
Bond angles



Torsions

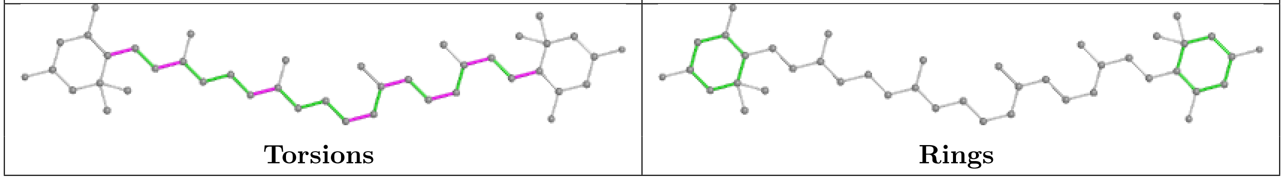
Rings

Ligand C7Z 1 614



Bond lengths

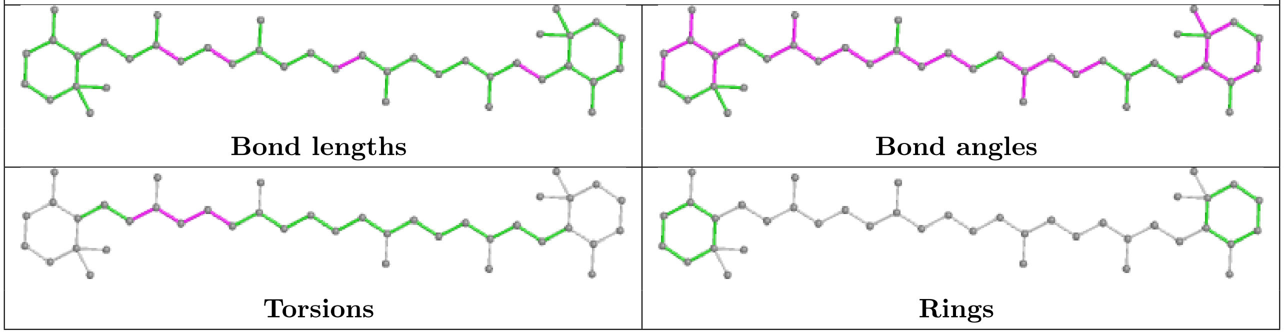
Bond angles



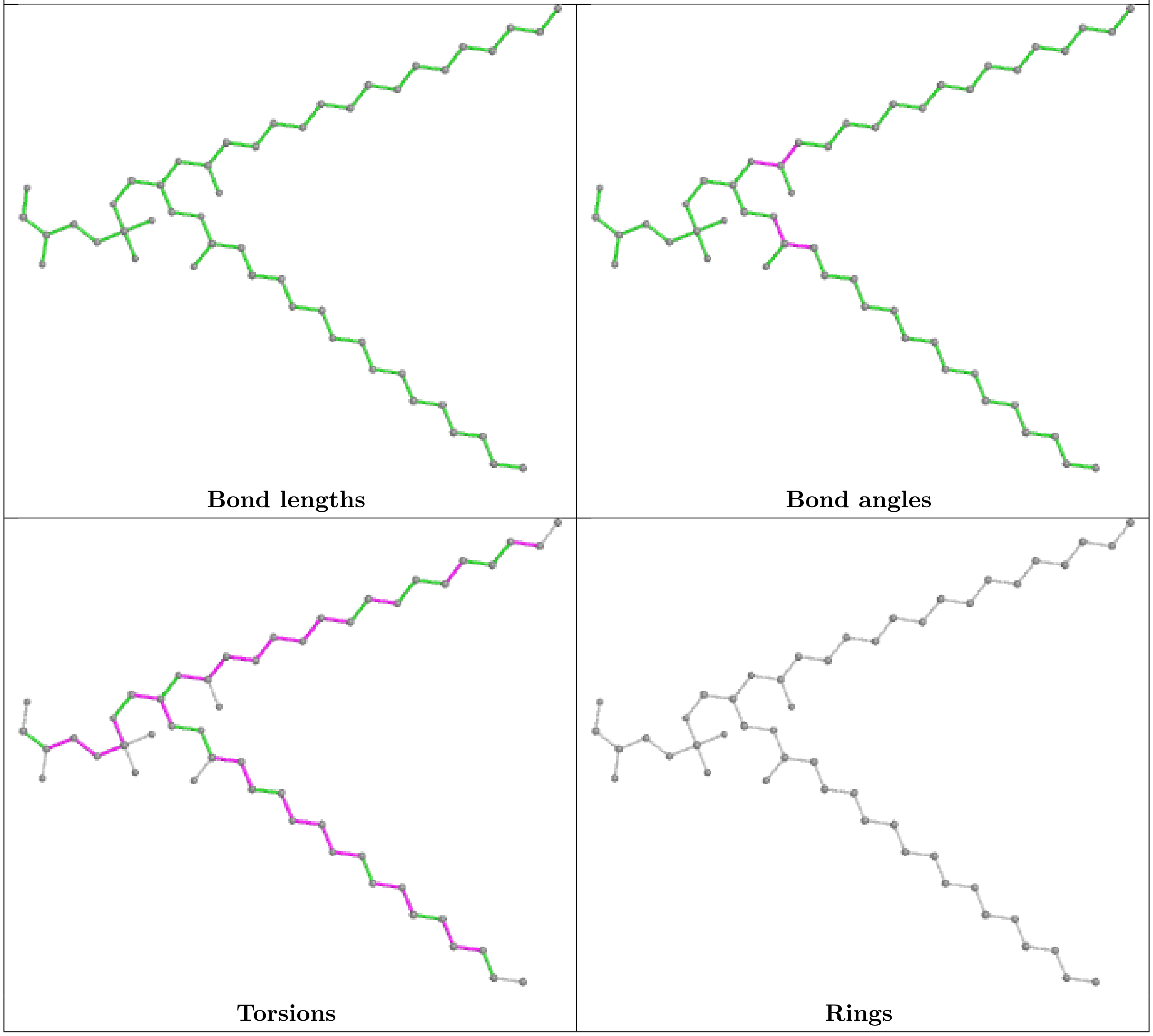
Torsions

Rings

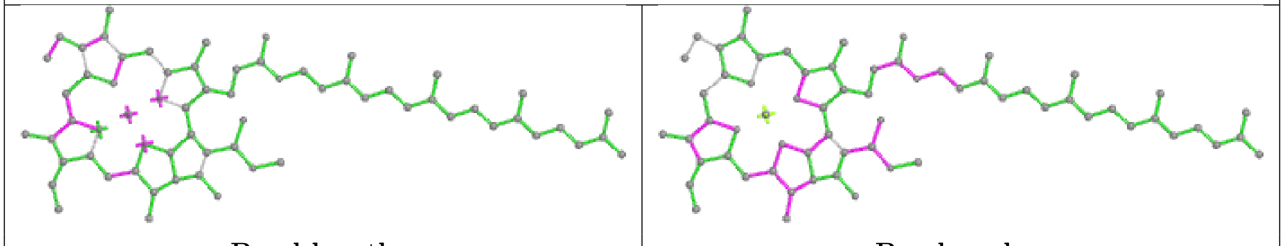
Ligand BCR A 846



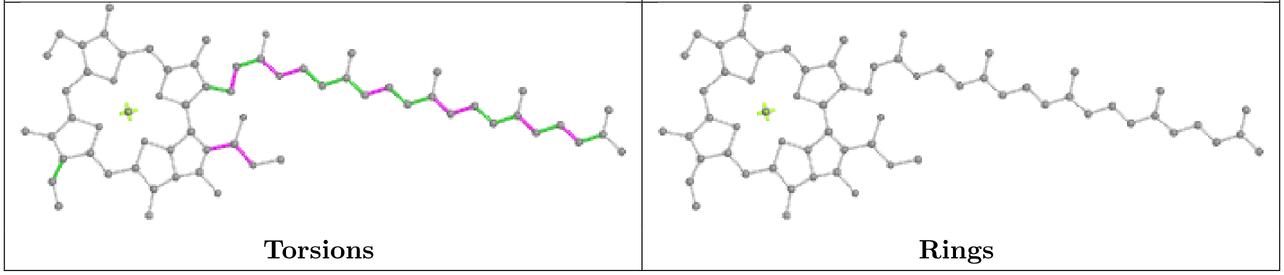
Ligand LHG A 841



Ligand CLA B 818

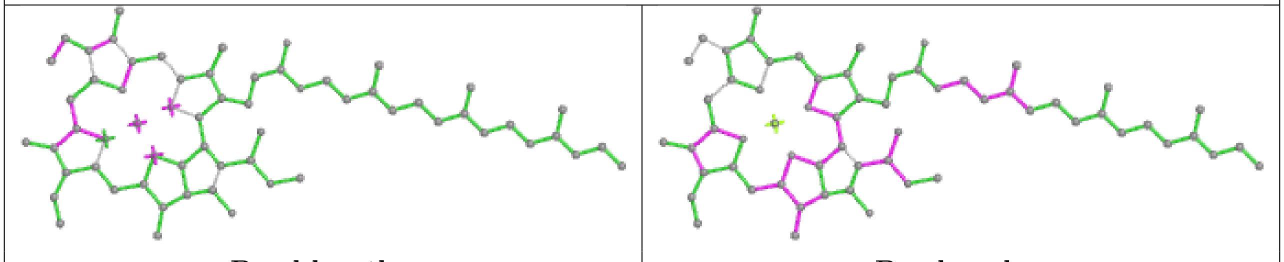

Bond lengths

Bond angles

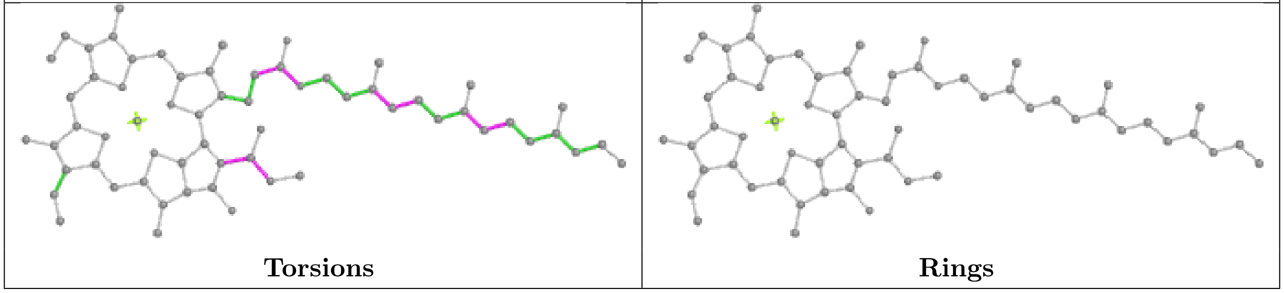

Torsions

Rings

Ligand CLA 3 207

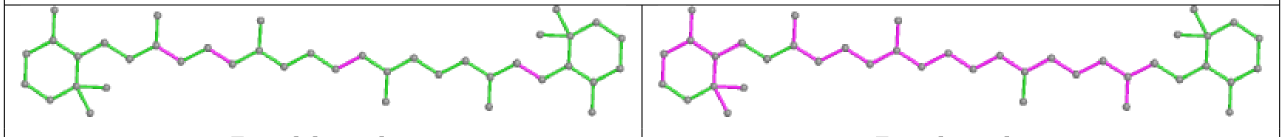

Bond lengths

Bond angles

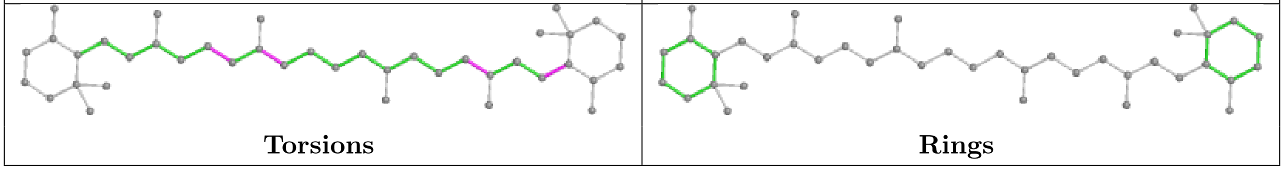

Torsions

Rings

Ligand BCR B 842

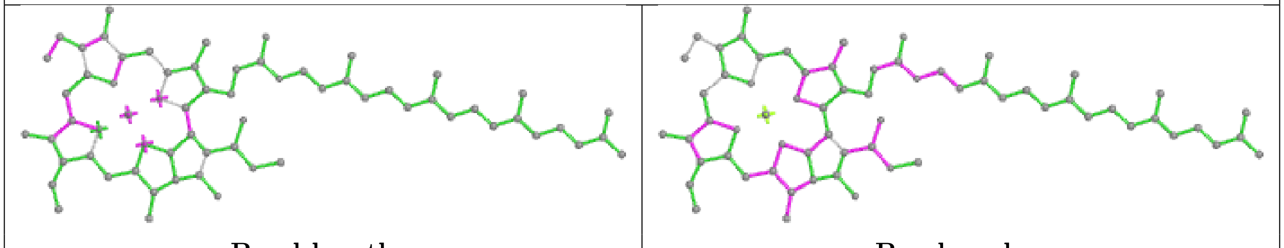

Bond lengths

Bond angles

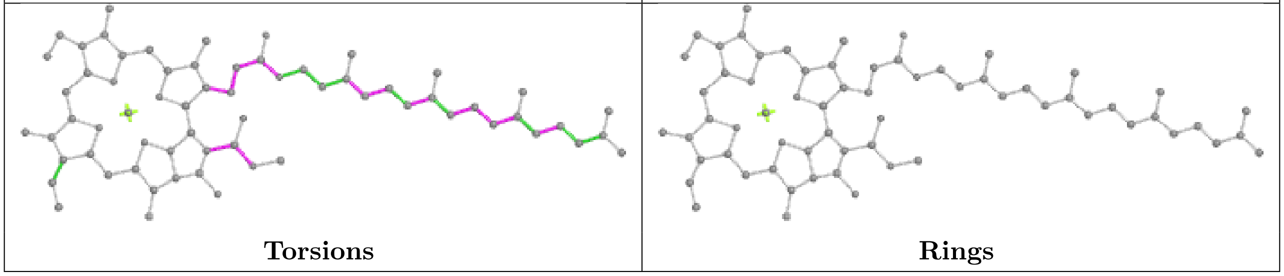

Torsions

Rings

Ligand CLA 2 601

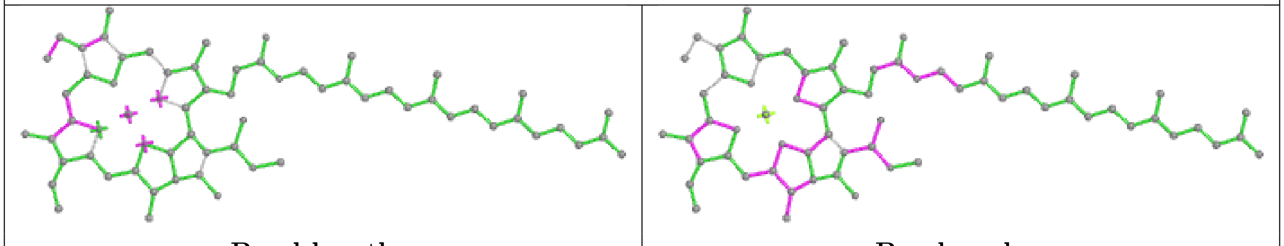


Bond lengths **Bond angles**

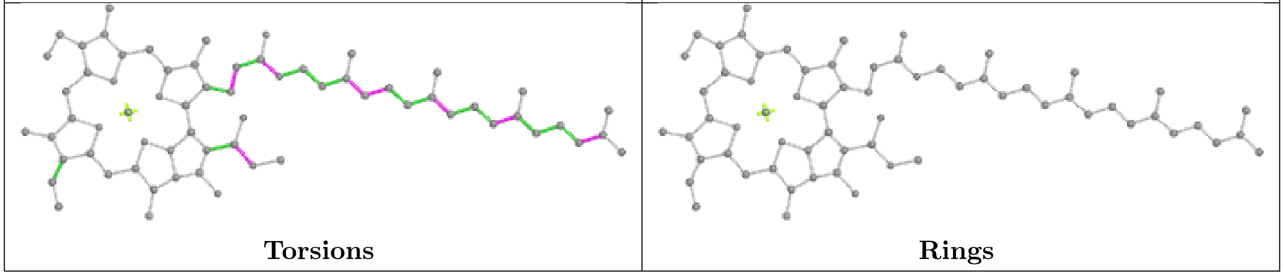


Torsions **Rings**

Ligand CLA B 807

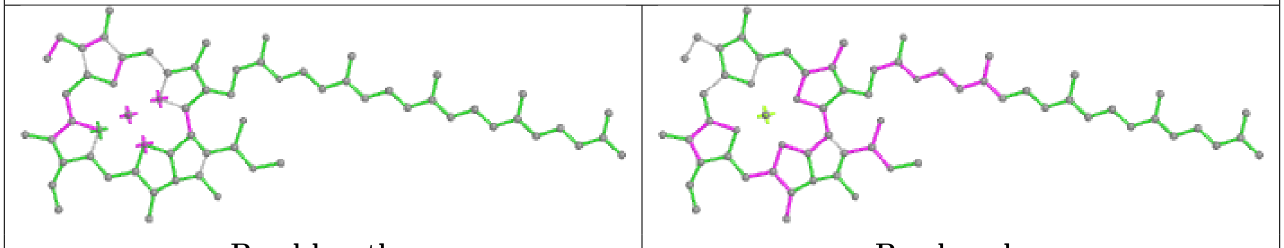


Bond lengths **Bond angles**

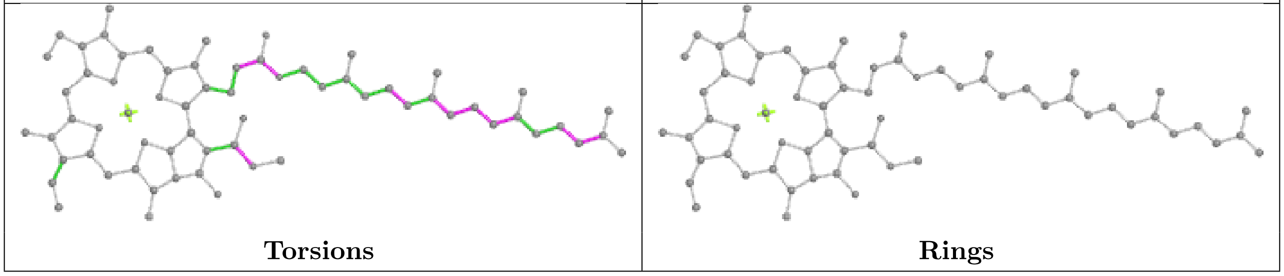


Torsions **Rings**

Ligand CLA A 825

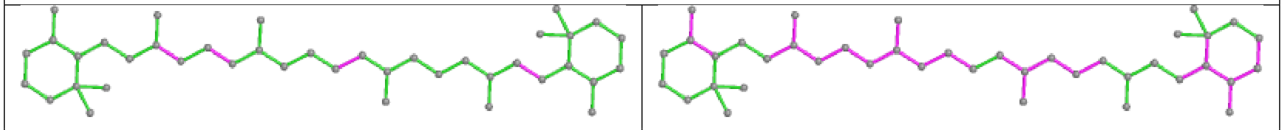


Bond lengths **Bond angles**



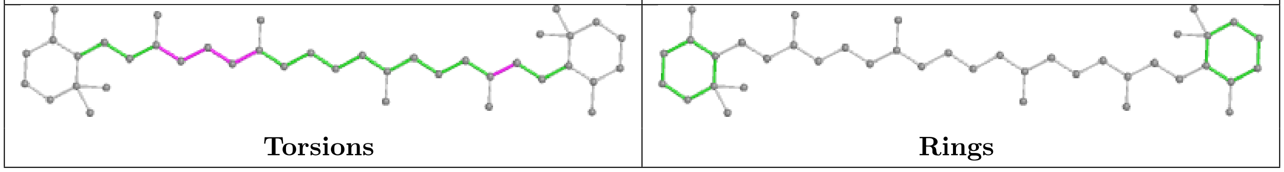
Torsions **Rings**

Ligand BCR L 202



Bond lengths

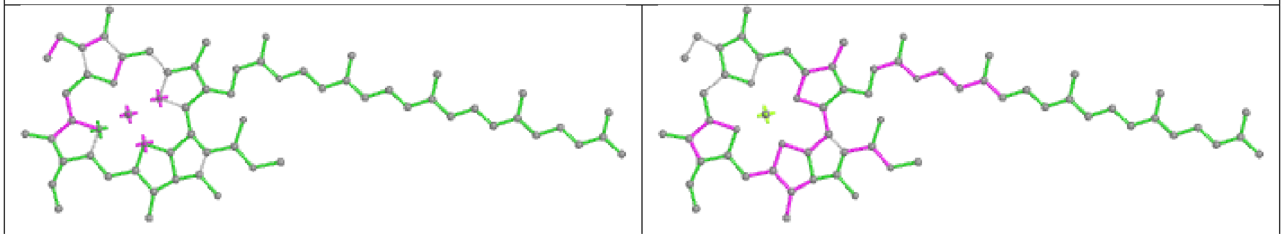
Bond angles



Torsions

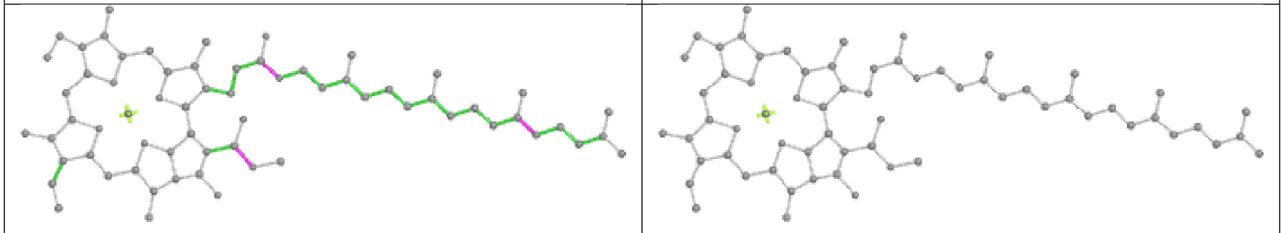
Rings

Ligand CLA B 822



Bond lengths

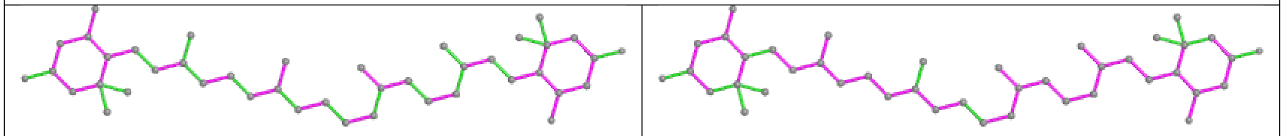
Bond angles



Torsions

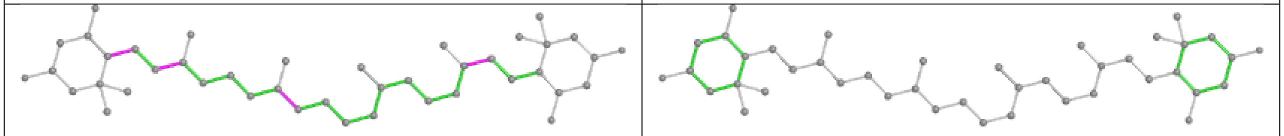
Rings

Ligand C7Z 1 616



Bond lengths

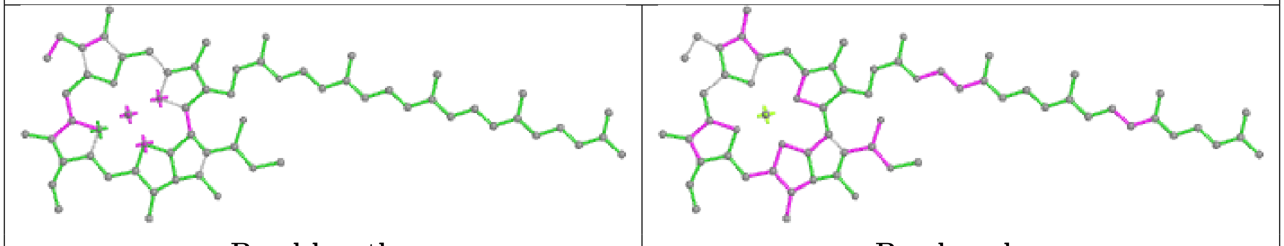
Bond angles

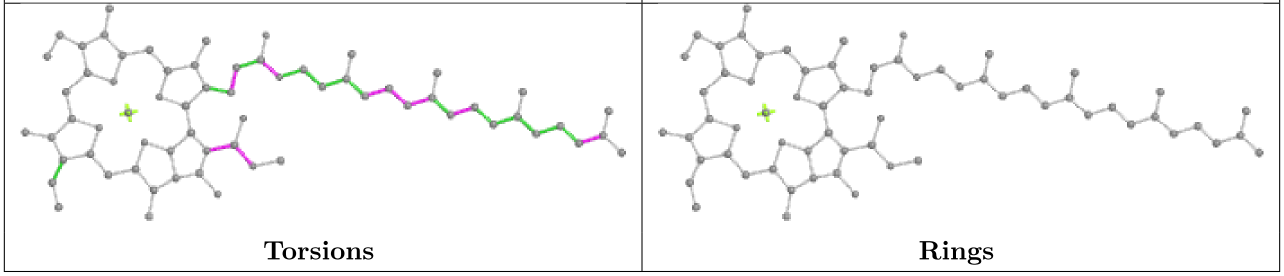


Torsions

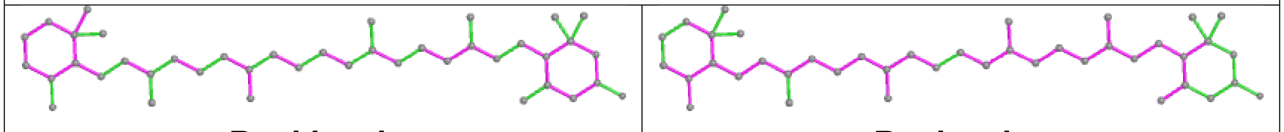
Rings

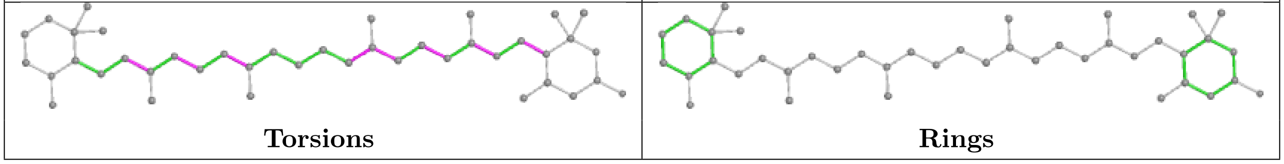
Ligand CLA A 834


Bond lengths Bond angles

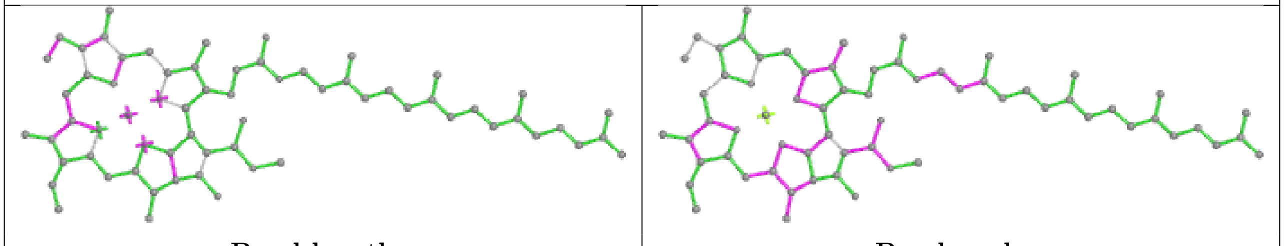

Torsions Rings

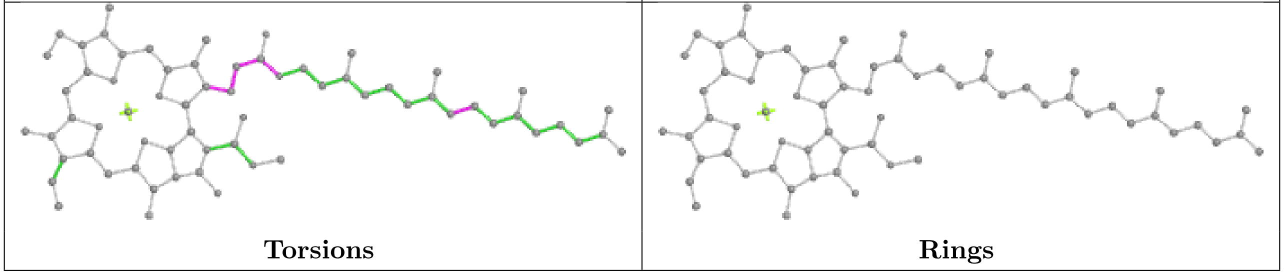
Ligand RRX 2 616


Bond lengths Bond angles

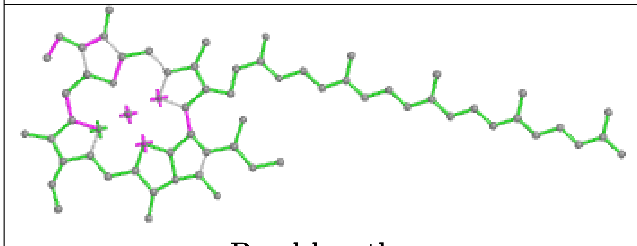

Torsions Rings

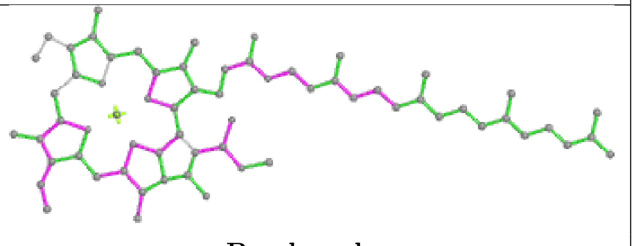
Ligand CLA B 811

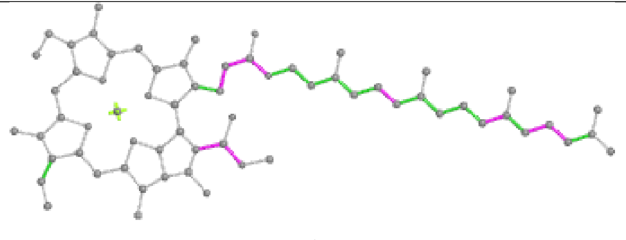

Bond lengths Bond angles

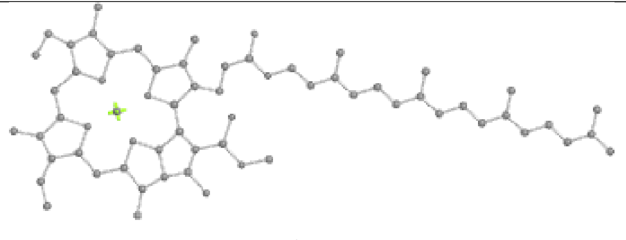

Torsions Rings

Ligand CLA B 804

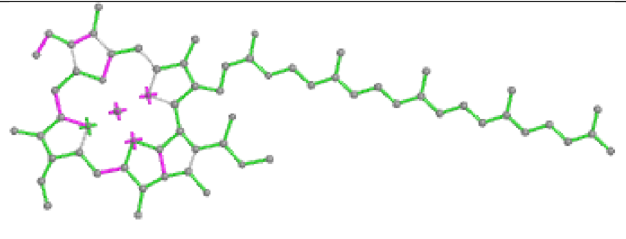

Bond lengths

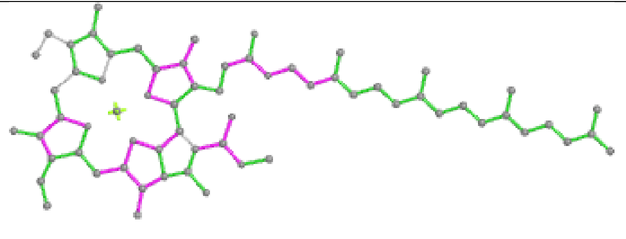

Bond angles

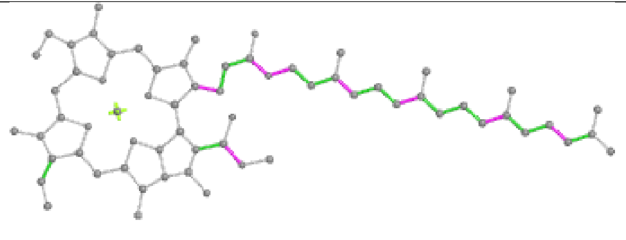

Torsions

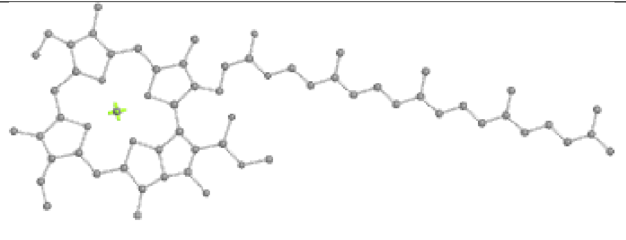

Rings

Ligand CLA A 818

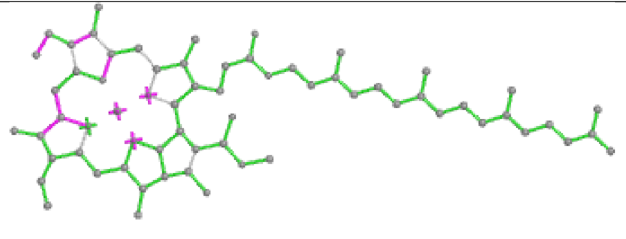

Bond lengths

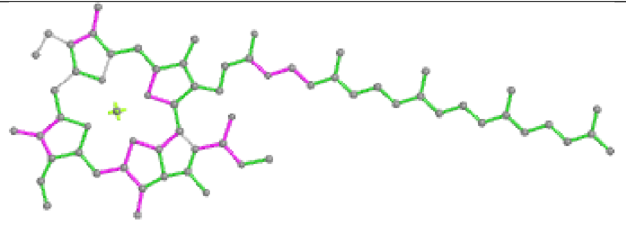

Bond angles

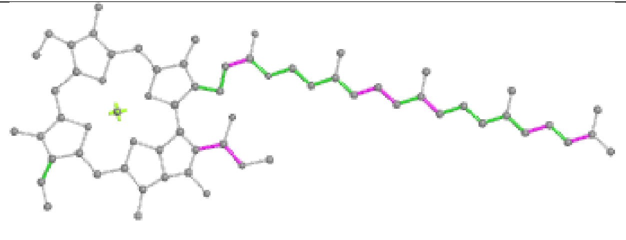

Torsions

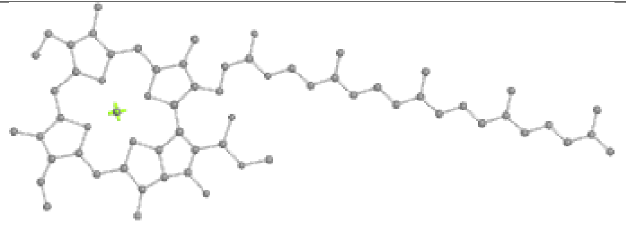

Rings

Ligand CLA A 854


Bond lengths


Bond angles


Torsions


Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

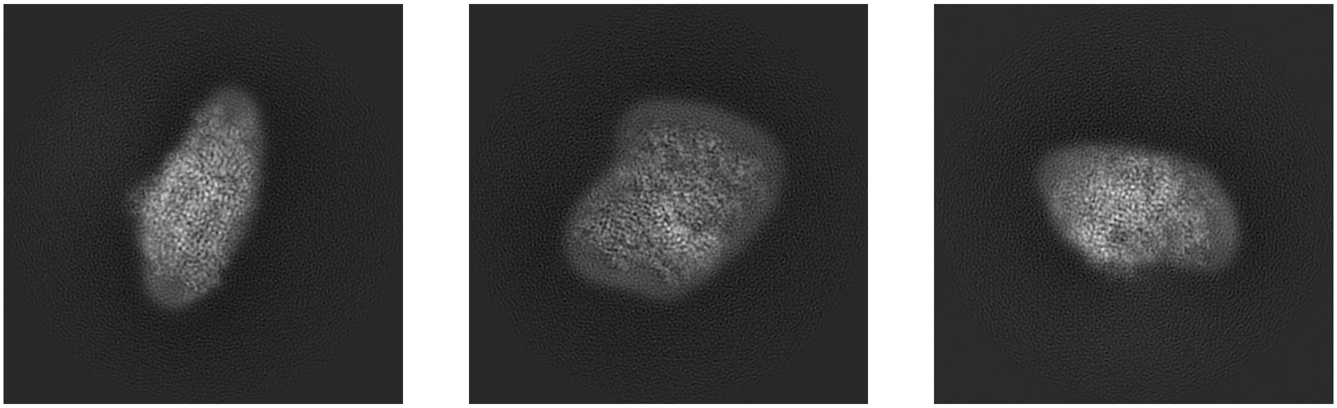
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-12228. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

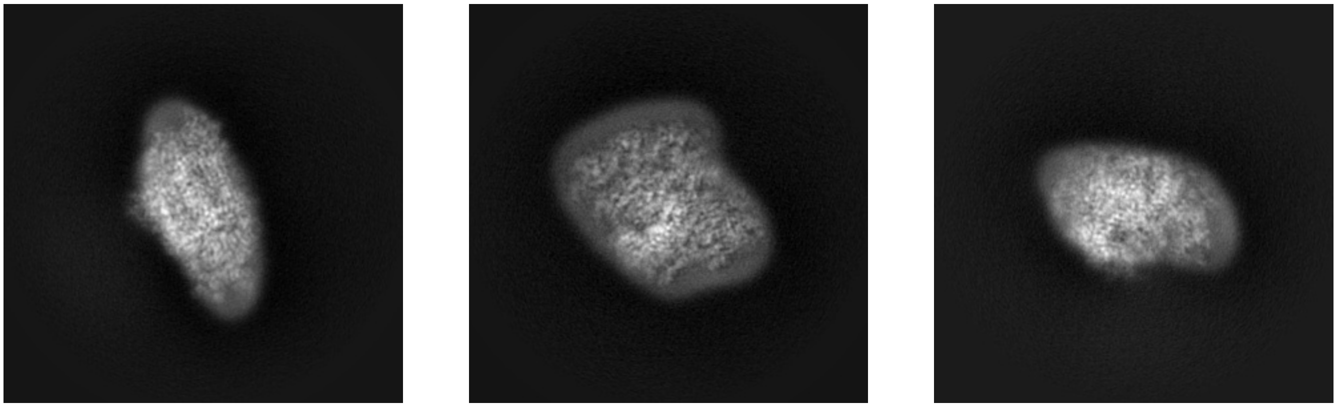
6.1 Orthogonal projections

6.1.1 Primary map



X Y Z

6.1.2 Raw map

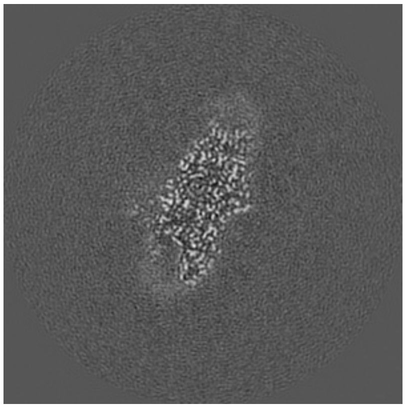


X Y Z

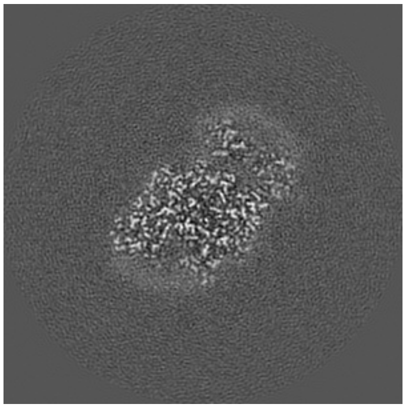
The images above show the map projected in three orthogonal directions.

6.2 Central slices

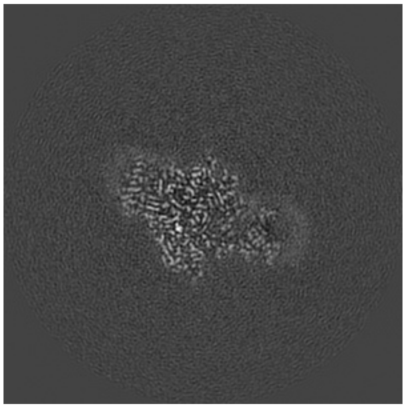
6.2.1 Primary map



X Index: 150

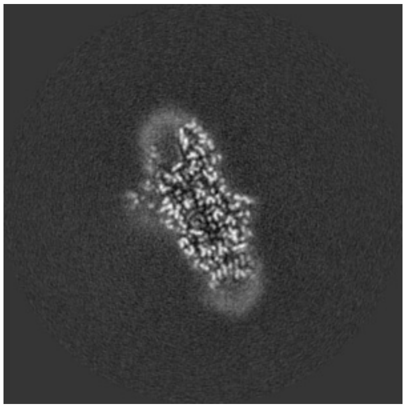


Y Index: 150

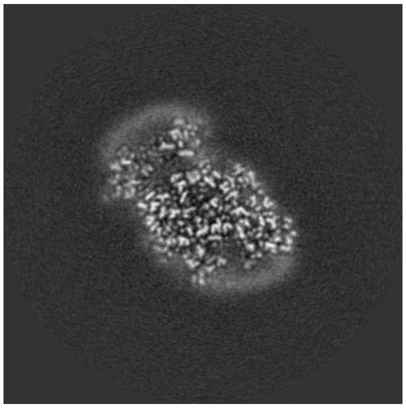


Z Index: 150

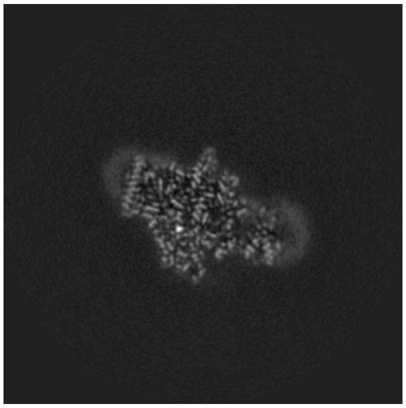
6.2.2 Raw map



X Index: 150



Y Index: 150

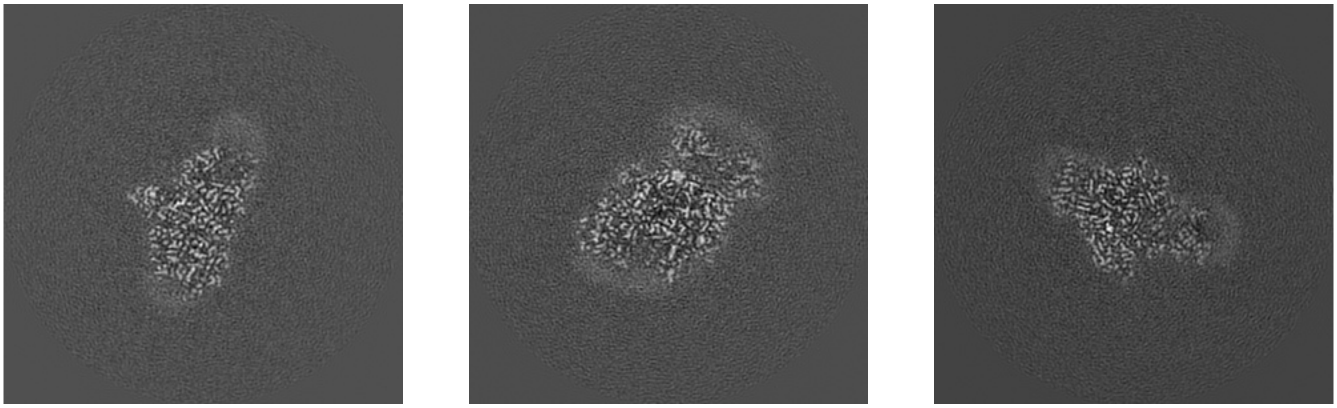


Z Index: 150

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

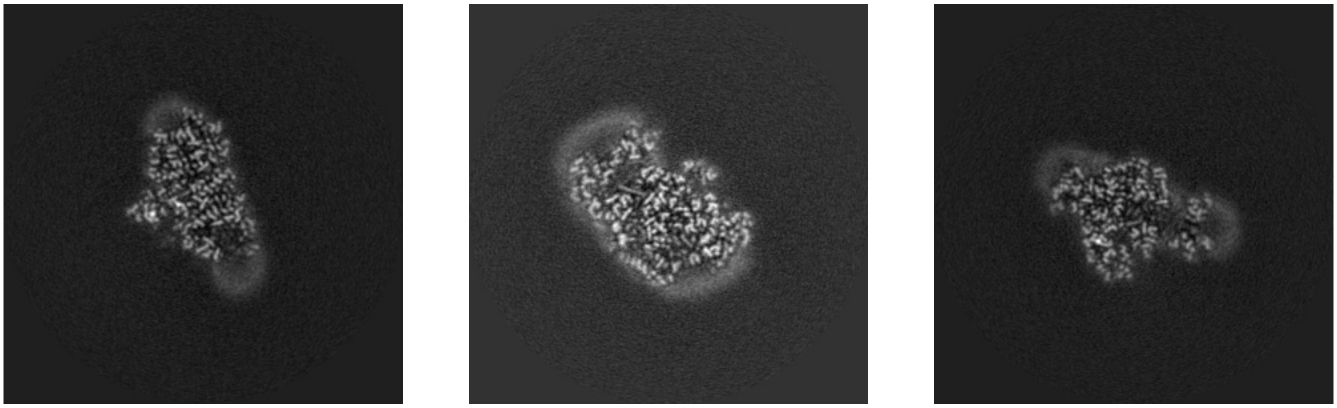
6.3 Largest variance slices

6.3.1 Primary map



X Index: 130 Y Index: 151 Z Index: 150

6.3.2 Raw map



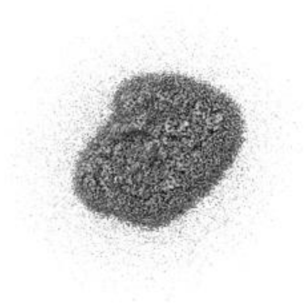
X Index: 130 Y Index: 158 Z Index: 144

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X



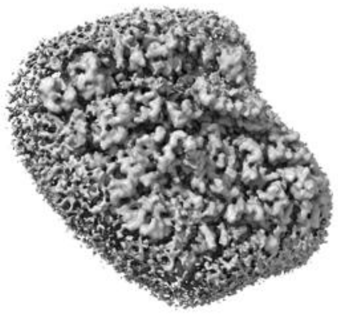
Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.0186. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map

X



Y

Z

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

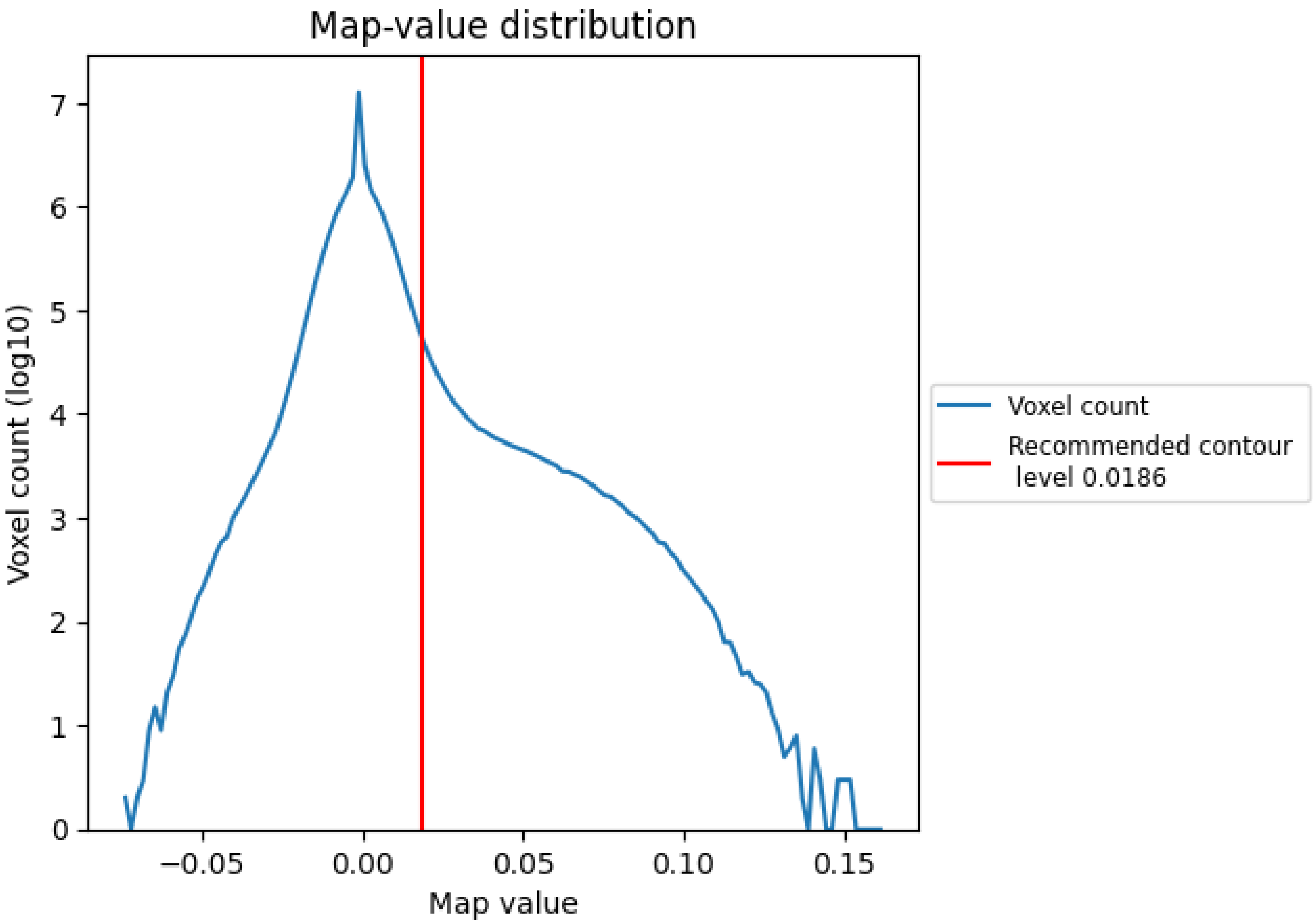
6.5 Mask visualisation (i)

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

7 Map analysis ⓘ

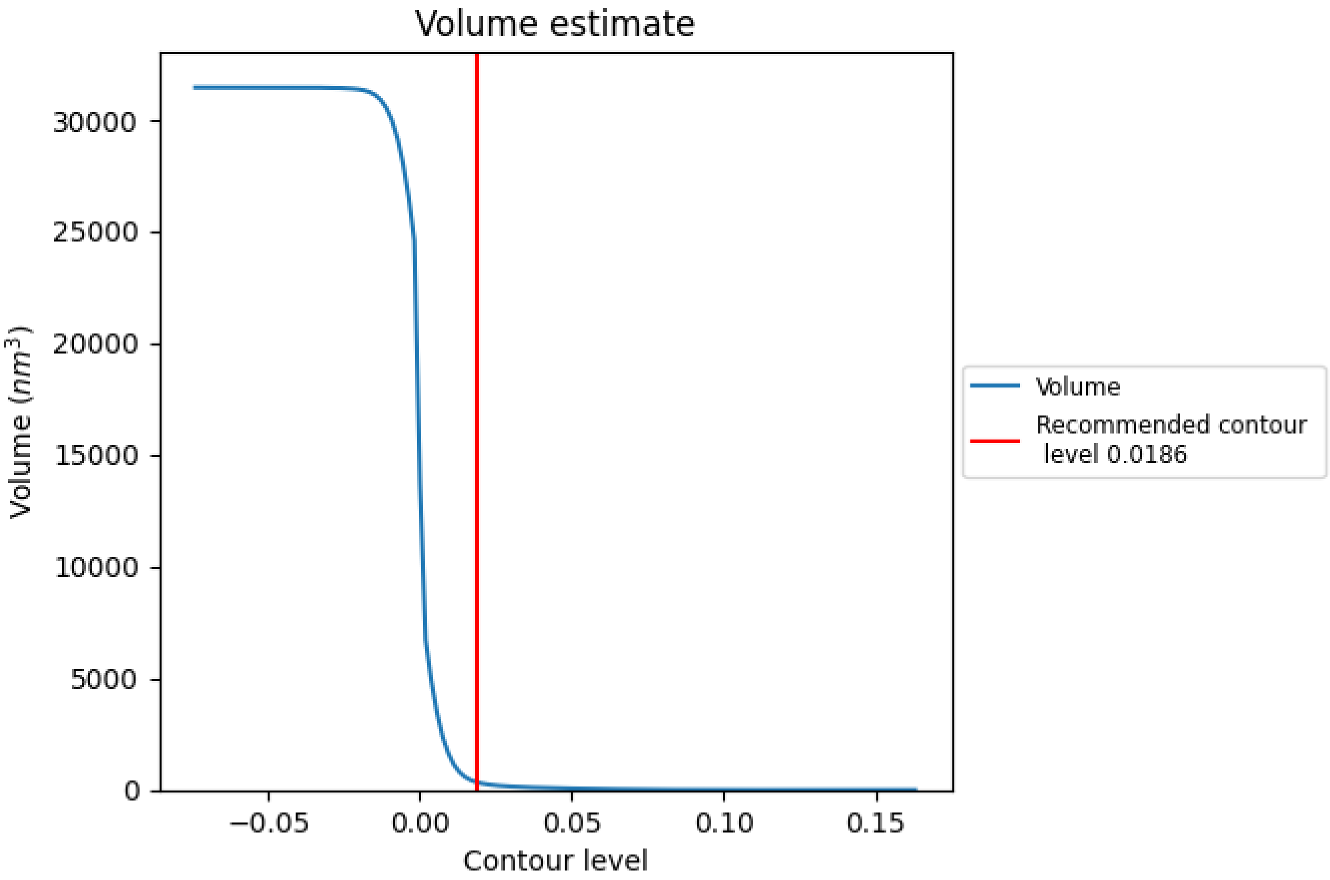
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ



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

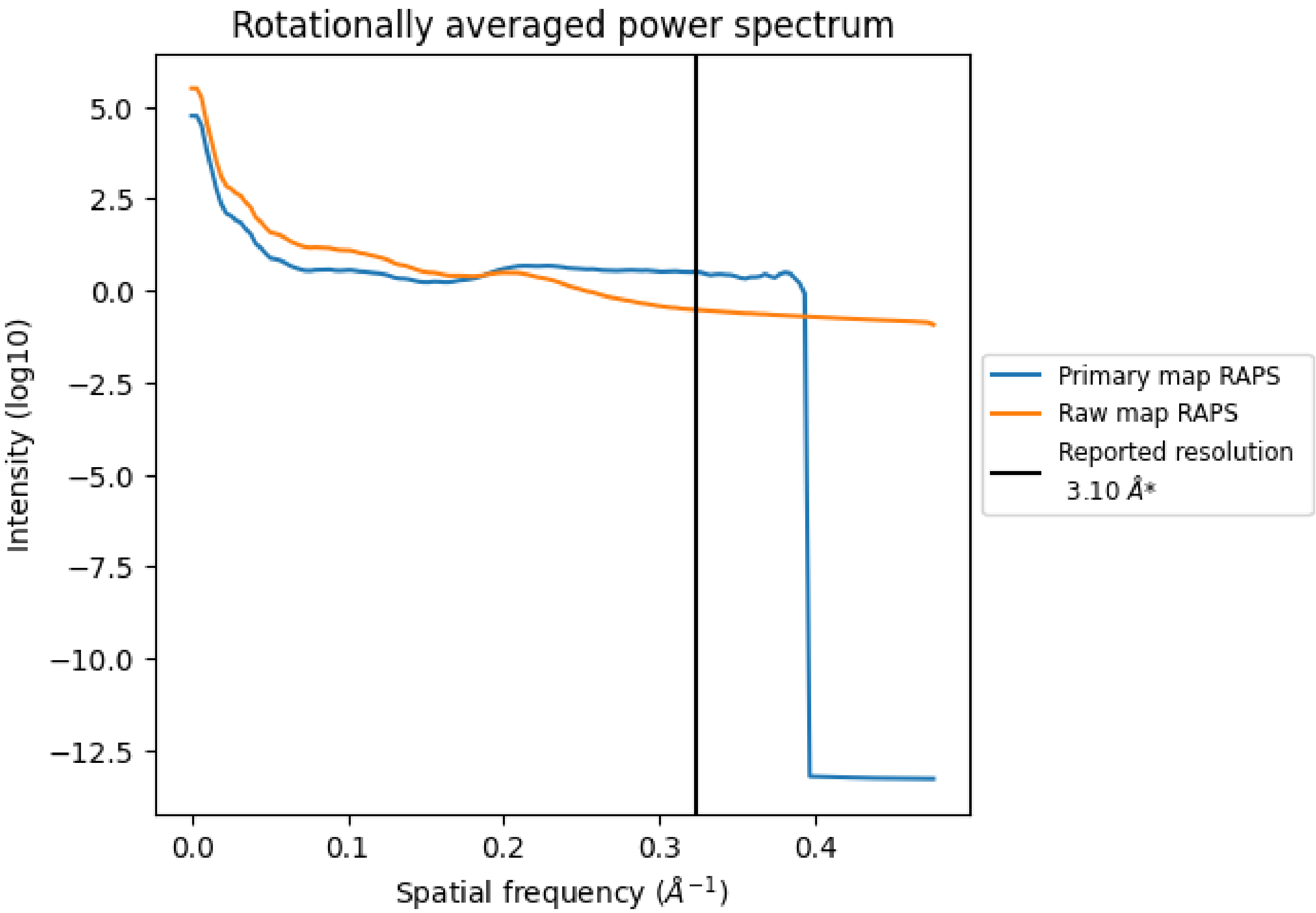
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 355 nm^3; this corresponds to an approximate mass of 321 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

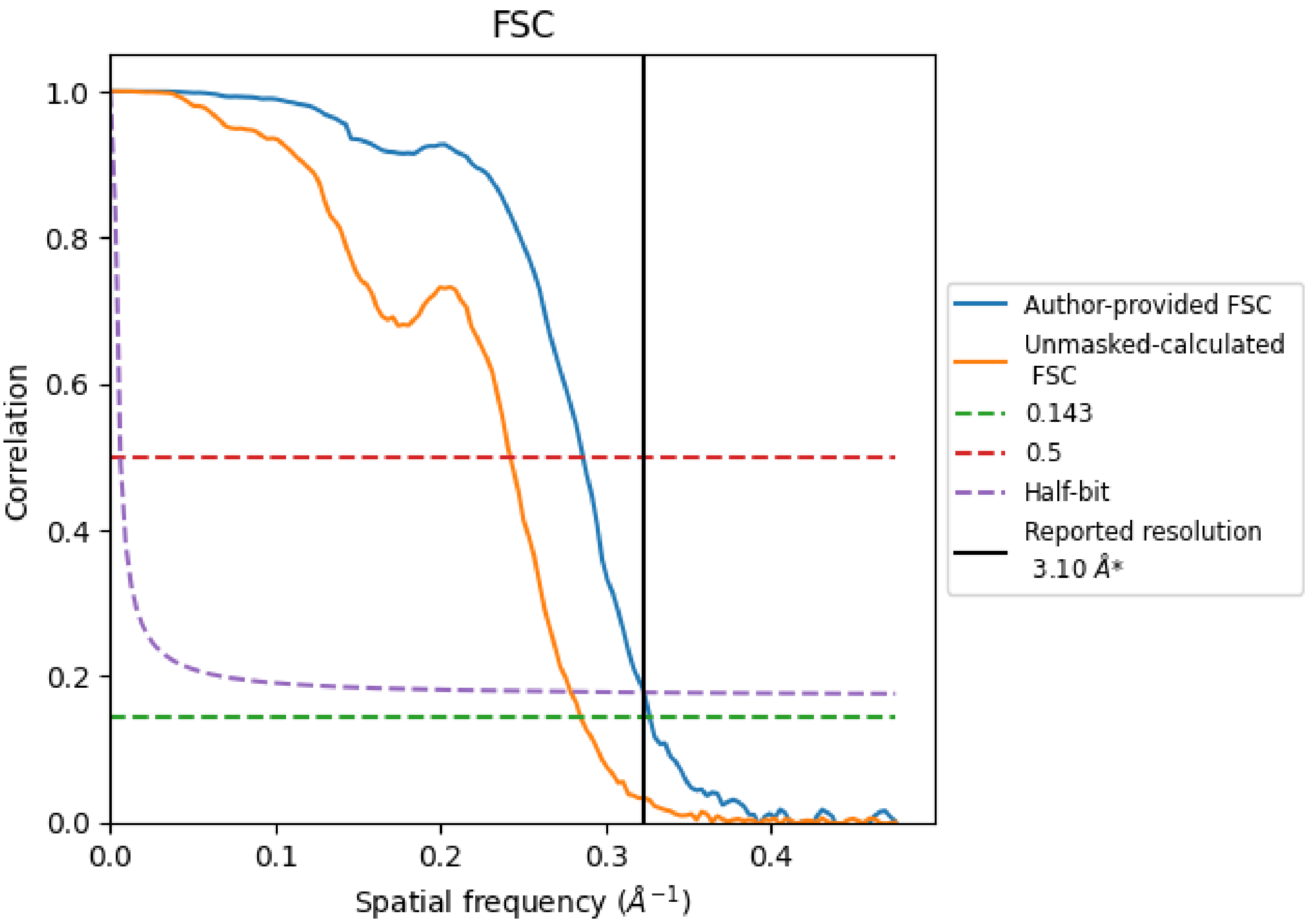


*Reported resolution corresponds to spatial frequency of 0.323 $Å^{-1}$

8 Fourier-Shell correlation ⓘ

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

8.1 FSC ⓘ



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

8.2 Resolution estimates

Resolution estimate (Å)	**Estimation criterion (FSC cut-off)**		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.06	3.50	3.09
Unmasked-calculated*	3.51	4.13	3.59

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.51 differs from the reported value 3.1 by more than 10 %

9 Map-model fit (i)

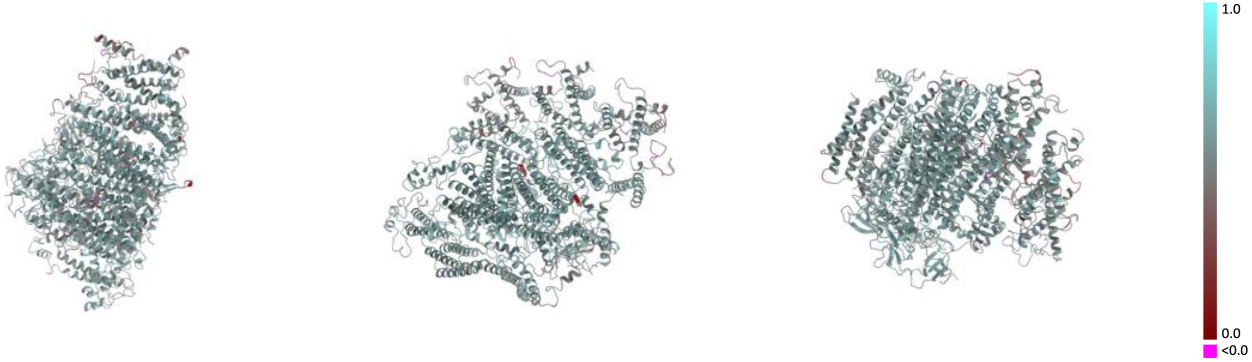
This section contains information regarding the fit between EMDB map EMD-12228 and PDB model 7BLZ. Per-residue inclusion information can be found in section 3 on page 29.

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 0.0186 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.

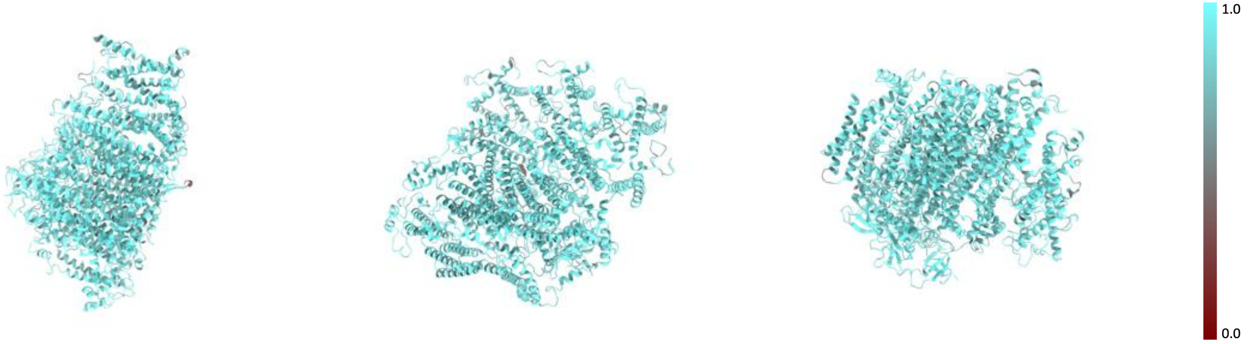
9.2 Q-score mapped to coordinate model ⓘ



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.

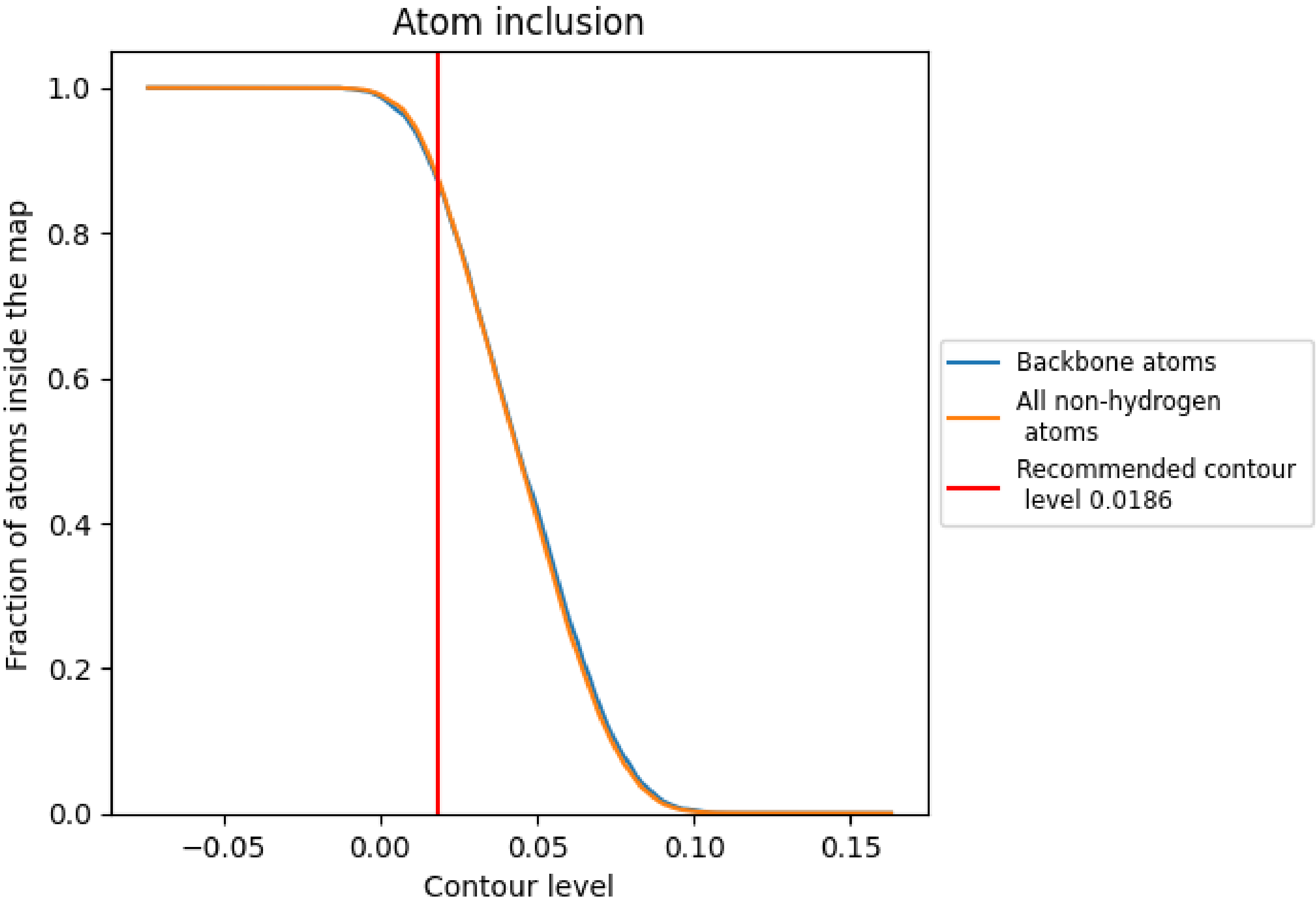
9.3 Atom inclusion mapped to coordinate model ⓘ



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 (0.0186).

9.4 Atom inclusion ⓘ



At the recommended contour level, 87% of all backbone atoms, 87% 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 (0.0186) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8740	0.5470
1	0.8140	0.4800
2	0.8132	0.4930
3	0.7951	0.4820
A	0.9136	0.5800
B	0.9075	0.5710
C	0.9566	0.5860
D	0.9216	0.5680
E	0.9134	0.5640
F	0.8732	0.5450
I	0.8772	0.5500
J	0.8237	0.5150
K	0.8228	0.5260
L	0.8478	0.5200
M	0.8719	0.5430
O	0.8451	0.5130