wwPDB EM Validation Summary Report (i)

Nov 21, 2022 – 03:25 PM JST

PDB ID	:	7D1U
EMDB ID	:	EMD-30548
Title	:	Cryo-EM Structure of PSII at 2.08 angstrom resolution
Authors	:	Kato, K.; Miyazaki, N.; Hamaguchi, T.; Nakajima, Y.; Akita, F.; Yonekura, K.; Shen, J.R.
Deposited on	:	2020-09-15
Resolution	:	2.08 Å(reported)
Based on initial model	:	3WU2

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

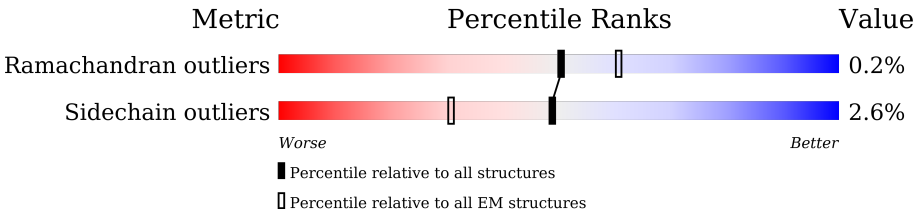
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.08 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)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	334	100%
1	a	334	100%
2	B	505	98%
2	b	505	98%
3	C	451	99%
3	c	451	99%
4	D	342	99%
4	d	342	99%
5	E	81	6% 95% 5%

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Mol	Chain	Length	Quality of chain
5	e	81	6% 95% 5%
6	F	34	100%
6	f	34	100%
7	H	63	92% 8%
7	h	63	92% 8%
8	I	36	6% 92% 8%
8	i	36	6% 92% 8%
9	J	37	8% 97%
9	j	37	8% 97%
10	K	37	100%
10	k	37	100%
11	L	37	5% 97%
11	l	37	5% 97%
12	M	34	97%
12	m	34	97%
13	O	244	23% 94% 6%
13	o	244	23% 94% 6%
14	T	31	10% 90% 6%
14	t	31	10% 90% 6%
15	U	97	7% 96%
15	u	97	7% 96%
16	V	137	5% 97%
16	v	137	5% 97%
17	Y	30	30% 83% 7% 10%
17	y	30	30% 83% 7% 10%

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Mol	Chain	Length	Quality of chain
18	X	40	5% 95% 5%
18	x	40	5% 95% 5%
19	Z	62	45% 89% 11%
19	z	62	45% 89% 11%
20	R	34	100% 94% 6%
20	r	34	100% 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
24	CLA	A	405	X	-	-	-
24	CLA	A	408	X	-	-	-
24	CLA	B	601	X	-	-	-
24	CLA	B	602	X	-	-	-
24	CLA	B	603	X	-	-	-
24	CLA	B	604	X	-	-	-
24	CLA	B	605	X	-	-	-
24	CLA	B	606	X	-	-	-
24	CLA	B	607	X	-	-	-
24	CLA	B	609	X	-	-	-
24	CLA	B	610	X	-	-	-
24	CLA	B	611	X	-	-	-
24	CLA	B	612	X	-	-	-
24	CLA	B	613	X	-	-	-
24	CLA	B	614	X	-	-	-
24	CLA	B	615	X	-	-	-
24	CLA	B	616	X	-	-	-
24	CLA	C	502	X	-	-	-
24	CLA	C	504	X	-	-	-
24	CLA	C	505	X	-	-	-
24	CLA	C	506	X	-	-	-
24	CLA	C	507	X	-	-	-
24	CLA	C	508	X	-	-	-
24	CLA	C	509	X	-	-	-
24	CLA	C	510	X	-	-	-
24	CLA	C	511	X	-	-	-
24	CLA	C	512	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	C	513	X	-	-	-
24	CLA	D	401	X	-	-	-
24	CLA	D	403	X	-	-	-
24	CLA	D	404	X	-	-	-
24	CLA	a	405	X	-	-	-
24	CLA	a	408	X	-	-	-
24	CLA	b	603	X	-	-	-
24	CLA	b	604	X	-	-	-
24	CLA	b	605	X	-	-	-
24	CLA	b	606	X	-	-	-
24	CLA	b	607	X	-	-	-
24	CLA	b	608	X	-	-	-
24	CLA	b	609	X	-	-	-
24	CLA	b	611	X	-	-	-
24	CLA	b	613	X	-	-	-
24	CLA	b	614	X	-	-	-
24	CLA	b	615	X	-	-	-
24	CLA	b	616	X	-	-	-
24	CLA	b	617	X	-	-	-
24	CLA	b	618	X	-	-	-
24	CLA	c	502	X	-	-	-
24	CLA	c	504	X	-	-	-
24	CLA	c	505	X	-	-	-
24	CLA	c	506	X	-	-	-
24	CLA	c	507	X	-	-	-
24	CLA	c	508	X	-	-	-
24	CLA	c	509	X	-	-	-
24	CLA	c	510	X	-	-	-
24	CLA	c	511	X	-	-	-
24	CLA	c	512	X	-	-	-
24	CLA	c	513	X	-	-	-
24	CLA	d	401	X	-	-	-
24	CLA	d	403	X	-	-	-
24	CLA	d	404	X	-	-	-

2 Entry composition (i)

There are 39 unique types of molecules in this entry. The entry contains 52655 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Photosystem II protein D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	334	Total	C	N	O	S	0	0
			2620	1716	431	458	15		
1	a	334	Total	C	N	O	S	0	0
			2620	1716	431	458	15		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	279	PRO	ARG	conflict	UNP P51765
a	279	PRO	ARG	conflict	UNP P51765

- Molecule 2 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	504	Total	C	N	O	S	0	0
			3969	2605	661	690	13		
2	b	504	Total	C	N	O	S	0	0
			3969	2605	661	690	13		

- Molecule 3 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	451	Total	C	N	O	S	0	0
			3486	2281	584	608	13		
3	c	451	Total	C	N	O	S	0	0
			3486	2281	584	608	13		

- Molecule 4 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	341	Total	C	N	O	S	0	0
			2718	1800	444	462	12		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	d	341	Total 2718	C 1800	N 444	O 462	S 12	0	0

- Molecule 5 is a protein called Cytochrome b559 subunit alpha.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	81	Total 661	C 432	N 107	O 122	0	0
5	e	81	Total 661	C 432	N 107	O 122	0	0

- Molecule 6 is a protein called Cytochrome b559 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	34	Total 275	C 187	N 45	O 42	S 1	0	0
6	f	34	Total 275	C 187	N 45	O 42	S 1	0	0

- Molecule 7 is a protein called Photosystem II reaction center protein H.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	63	Total 498	C 333	N 80	O 83	S 2	0	0
7	h	63	Total 498	C 333	N 80	O 83	S 2	0	0

- Molecule 8 is a protein called Photosystem II reaction center protein I.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	36	Total 296	C 200	N 46	O 49	S 1	0	0
8	i	36	Total 296	C 200	N 46	O 49	S 1	0	0

- Molecule 9 is a protein called Photosystem II reaction center protein J.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	36	Total 257	C 174	N 40	O 42	S 1	0	0
9	j	36	Total 257	C 174	N 40	O 42	S 1	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
10	K	37	Total 293	C 204	N 43	O 46	0	0
10	k	37	Total 293	C 204	N 43	O 46	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	33	LEU	PHE	conflict	UNP P19054
K	39	TRP	VAL	conflict	UNP P19054
k	33	LEU	PHE	conflict	UNP P19054
k	39	TRP	VAL	conflict	UNP P19054

- Molecule 11 is a protein called Photosystem II reaction center protein L.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	37	Total 304	C 202	N 48	O 53	S 1	0	0
11	l	37	Total 304	C 202	N 48	O 53	S 1	0	0

- Molecule 12 is a protein called Photosystem II reaction center protein M.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	33	Total 260	C 173	N 38	O 48	S 1	0	0
12	m	33	Total 260	C 173	N 38	O 48	S 1	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	8	LEU	PHE	conflict	UNP P12312
m	8	LEU	PHE	conflict	UNP P12312

- Molecule 13 is a protein called Photosystem II manganese-stabilizing polypeptide.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	O	244	Total 1874	C 1170	N 317	O 383	S 4	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
13	o	244	Total	C	N	O	S	0	0
			1874	1170	317	383	4		

- Molecule 14 is a protein called Photosystem II reaction center protein T.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	T	30	Total	C	N	O	S	0	0
			258	181	36	39	2		
14	t	30	Total	C	N	O	S	0	0
			258	181	36	39	2		

- Molecule 15 is a protein called Photosystem II 12 kDa extrinsic protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	U	97	Total	C	N	O	0	0
			774	491	129	154		
15	u	97	Total	C	N	O	0	0
			774	491	129	154		

- Molecule 16 is a protein called Cytochrome c-550.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	V	137	Total	C	N	O	S	0	0
			1064	675	177	208	4		
16	v	137	Total	C	N	O	S	0	0
			1064	675	177	208	4		

- Molecule 17 is a protein called Photosystem II reaction center protein Ycf12.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Y	27	Total	C	N	O	S	0	0
			200	131	35	31	3		
17	y	27	Total	C	N	O	S	0	0
			200	131	35	31	3		

- Molecule 18 is a protein called Photosystem II reaction center protein X.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	X	38	Total	C	N	O	0	0
			281	188	45	48		
18	x	38	Total	C	N	O	0	0
			281	188	45	48		

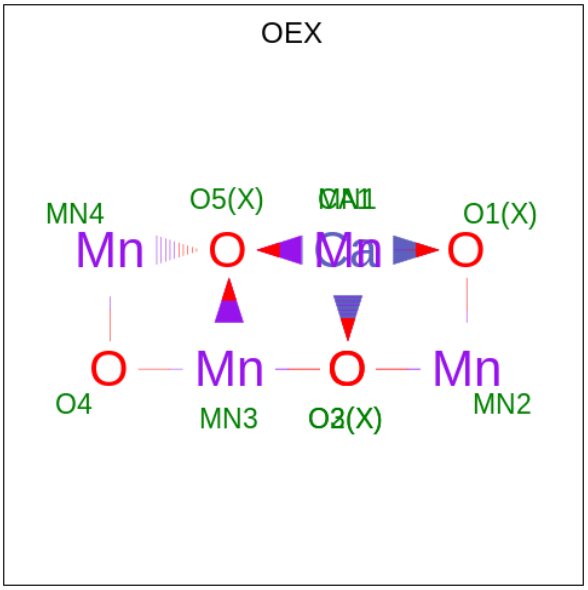
- Molecule 19 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Z	62	Total	C	N	O	S	0	0
			479	328	72	77	2		
19	z	62	Total	C	N	O	S	0	0
			479	328	72	77	2		

- Molecule 20 is a protein called Photosystem II protein Y.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	R	34	Total	C	N	O	0	0
			273	186	47	40		
20	r	34	Total	C	N	O	0	0
			273	186	47	40		

- Molecule 21 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula: $CaMn_4O_5$).



Mol	Chain	Residues	Atoms				AltConf
21	A	1	Total	Ca	Mn	O	0
			10	1	4	5	
21	a	1	Total	Ca	Mn	O	0
			10	1	4	5	

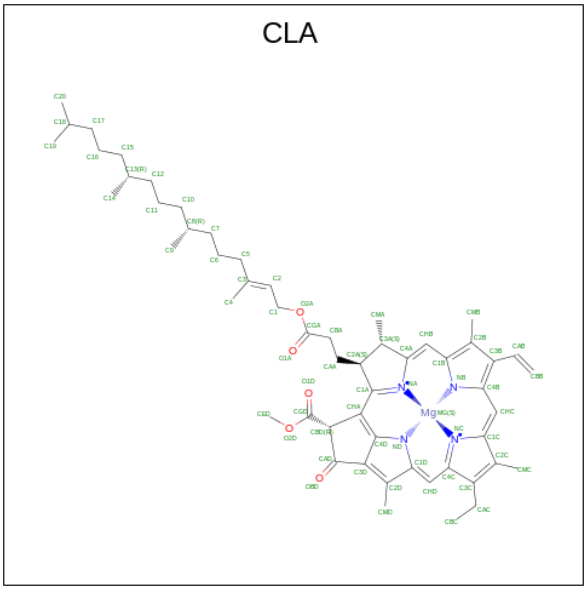
- Molecule 22 is FE (II) ION (three-letter code: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms	AltConf
22	A	1	Total Fe 1 1	0
22	a	1	Total Fe 1 1	0

- Molecule 23 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	AltConf
23	A	2	Total Cl 2 2	0
23	a	2	Total Cl 2 2	0

- Molecule 24 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms	AltConf
24	A	1	Total C Mg N O 195 165 3 12 15	0
24	A	1	Total C Mg N O 195 165 3 12 15	0
24	A	1	Total C Mg N O 195 165 3 12 15	0
24	B	1	Total C Mg N O 1040 880 16 64 80	0
24	B	1	Total C Mg N O 1040 880 16 64 80	0
24	B	1	Total C Mg N O 1040 880 16 64 80	0

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Mol	Chain	Residues	Atoms					AltConf
24	B	1	Total 1040	C 880	Mg 16	N 64	O 80	0
24	B	1	Total 1040	C 880	Mg 16	N 64	O 80	0
24	B	1	Total 1040	C 880	Mg 16	N 64	O 80	0
24	B	1	Total 1040	C 880	Mg 16	N 64	O 80	0
24	B	1	Total 1040	C 880	Mg 16	N 64	O 80	0
24	B	1	Total 1040	C 880	Mg 16	N 64	O 80	0
24	B	1	Total 1040	C 880	Mg 16	N 64	O 80	0
24	B	1	Total 1040	C 880	Mg 16	N 64	O 80	0
24	B	1	Total 1040	C 880	Mg 16	N 64	O 80	0
24	B	1	Total 1040	C 880	Mg 16	N 64	O 80	0
24	B	1	Total 1040	C 880	Mg 16	N 64	O 80	0
24	B	1	Total 1040	C 880	Mg 16	N 64	O 80	0
24	B	1	Total 1040	C 880	Mg 16	N 64	O 80	0
24	C	1	Total 845	C 715	Mg 13	N 52	O 65	0
24	C	1	Total 845	C 715	Mg 13	N 52	O 65	0
24	C	1	Total 845	C 715	Mg 13	N 52	O 65	0
24	C	1	Total 845	C 715	Mg 13	N 52	O 65	0
24	C	1	Total 845	C 715	Mg 13	N 52	O 65	0
24	C	1	Total 845	C 715	Mg 13	N 52	O 65	0
24	C	1	Total 845	C 715	Mg 13	N 52	O 65	0
24	C	1	Total 845	C 715	Mg 13	N 52	O 65	0

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Mol	Chain	Residues	Atoms					AltConf
24	C	1	Total 845	C 715	Mg 13	N 52	O 65	0
24	C	1	Total 845	C 715	Mg 13	N 52	O 65	0
24	C	1	Total 845	C 715	Mg 13	N 52	O 65	0
24	C	1	Total 845	C 715	Mg 13	N 52	O 65	0
24	C	1	Total 845	C 715	Mg 13	N 52	O 65	0
24	D	1	Total 195	C 165	Mg 3	N 12	O 15	0
24	D	1	Total 195	C 165	Mg 3	N 12	O 15	0
24	D	1	Total 195	C 165	Mg 3	N 12	O 15	0
24	a	1	Total 195	C 165	Mg 3	N 12	O 15	0
24	a	1	Total 195	C 165	Mg 3	N 12	O 15	0
24	a	1	Total 195	C 165	Mg 3	N 12	O 15	0
24	b	1	Total 1040	C 880	Mg 16	N 64	O 80	0
24	b	1	Total 1040	C 880	Mg 16	N 64	O 80	0
24	b	1	Total 1040	C 880	Mg 16	N 64	O 80	0
24	b	1	Total 1040	C 880	Mg 16	N 64	O 80	0
24	b	1	Total 1040	C 880	Mg 16	N 64	O 80	0
24	b	1	Total 1040	C 880	Mg 16	N 64	O 80	0
24	b	1	Total 1040	C 880	Mg 16	N 64	O 80	0
24	b	1	Total 1040	C 880	Mg 16	N 64	O 80	0
24	b	1	Total 1040	C 880	Mg 16	N 64	O 80	0
24	b	1	Total 1040	C 880	Mg 16	N 64	O 80	0

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Mol	Chain	Residues	Atoms					AltConf
24	b	1	Total 1040	C 880	Mg 16	N 64	O 80	0
24	b	1	Total 1040	C 880	Mg 16	N 64	O 80	0
24	b	1	Total 1040	C 880	Mg 16	N 64	O 80	0
24	b	1	Total 1040	C 880	Mg 16	N 64	O 80	0
24	b	1	Total 1040	C 880	Mg 16	N 64	O 80	0
24	b	1	Total 1040	C 880	Mg 16	N 64	O 80	0
24	c	1	Total 845	C 715	Mg 13	N 52	O 65	0
24	c	1	Total 845	C 715	Mg 13	N 52	O 65	0
24	c	1	Total 845	C 715	Mg 13	N 52	O 65	0
24	c	1	Total 845	C 715	Mg 13	N 52	O 65	0
24	c	1	Total 845	C 715	Mg 13	N 52	O 65	0
24	c	1	Total 845	C 715	Mg 13	N 52	O 65	0
24	c	1	Total 845	C 715	Mg 13	N 52	O 65	0
24	c	1	Total 845	C 715	Mg 13	N 52	O 65	0
24	c	1	Total 845	C 715	Mg 13	N 52	O 65	0
24	c	1	Total 845	C 715	Mg 13	N 52	O 65	0
24	c	1	Total 845	C 715	Mg 13	N 52	O 65	0
24	c	1	Total 845	C 715	Mg 13	N 52	O 65	0
24	c	1	Total 845	C 715	Mg 13	N 52	O 65	0
24	d	1	Total 195	C 165	Mg 3	N 12	O 15	0
24	d	1	Total 195	C 165	Mg 3	N 12	O 15	0

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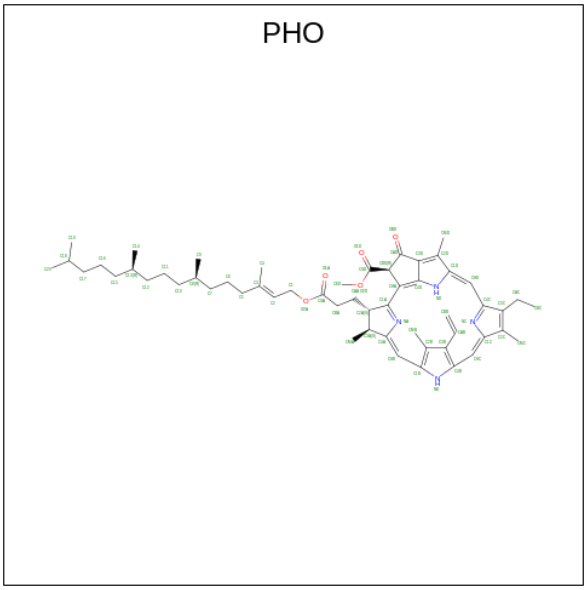
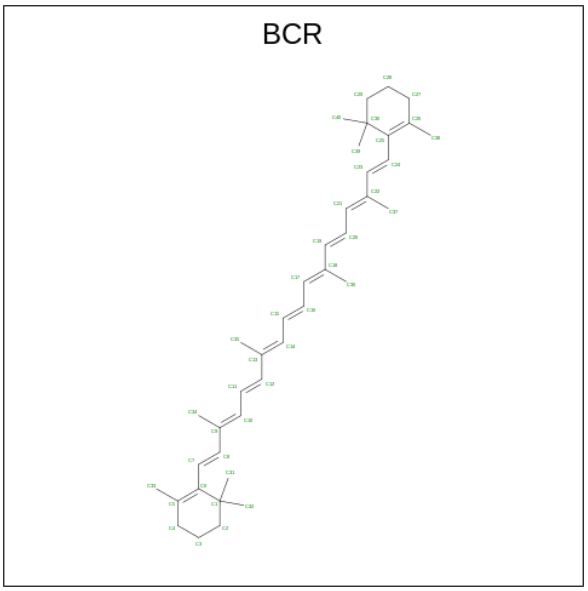
Mol	Chain	Residues	Atoms					AltConf
24	d	1	Total	C	Mg	N	O	0
			195	165	3	12	15	

- Molecule 25 is PHEOPHYTIN A (three-letter code: PHO) (formula: $C_{55}H_{74}N_4O_5$).



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

- Molecule 26 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms	AltConf
26	A	1	Total C 40 40	0
26	B	1	Total C 160 160	0
26	B	1	Total C 160 160	0
26	B	1	Total C 160 160	0
26	B	1	Total C 160 160	0
26	C	1	Total C 120 120	0
26	C	1	Total C 120 120	0
26	C	1	Total C 120 120	0
26	D	1	Total C 40 40	0
26	T	1	Total C 40 40	0
26	Y	1	Total C 40 40	0
26	a	1	Total C 40 40	0
26	b	1	Total C 120 120	0
26	b	1	Total C 120 120	0

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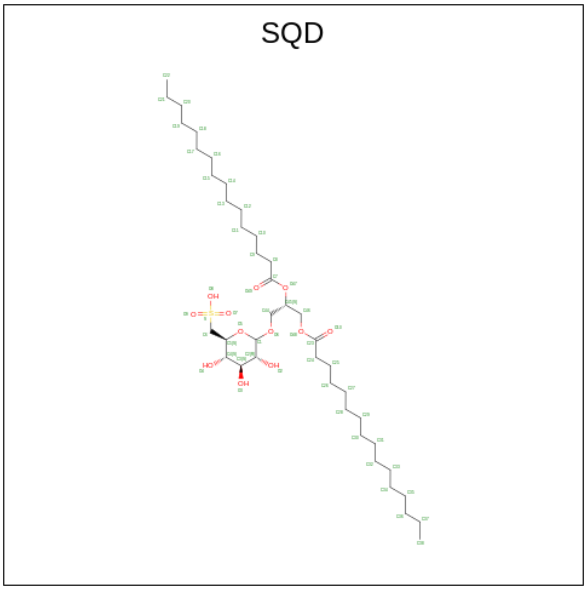
Mol	Chain	Residues	Atoms	AltConf
26	b	1	Total C 120 120	0
26	c	1	Total C 120 120	0
26	c	1	Total C 120 120	0
26	c	1	Total C 120 120	0
26	d	1	Total C 40 40	0
26	y	1	Total C 40 40	0

- Molecule 27 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: $C_{41}H_{78}O_{12}S$).



Mol	Chain	Residues	Atoms	AltConf
27	A	1	Total C O S 108 82 24 2	0
27	A	1	Total C O S 108 82 24 2	0
27	D	1	Total C O S 45 32 12 1	0
27	L	1	Total C O S 54 41 12 1	0
27	a	1	Total C O S 108 82 24 2	0

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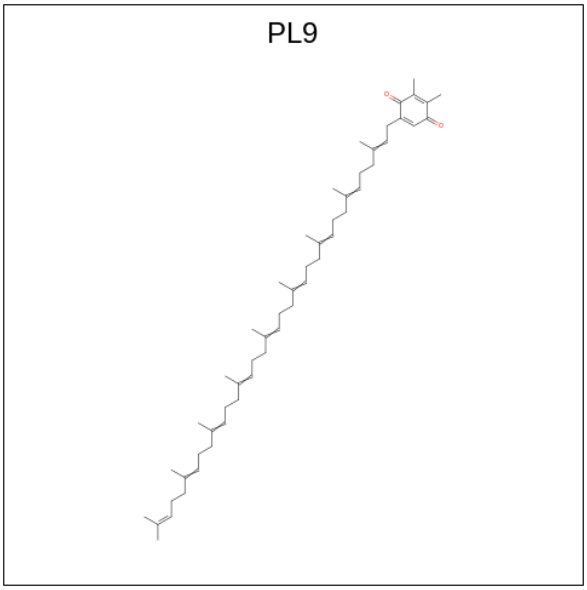
Mol	Chain	Residues	Atoms				AltConf
27	a	1	Total	C	O	S	0
			108	82	24	2	
27	d	1	Total	C	O	S	0
			45	32	12	1	
27	l	1	Total	C	O	S	0
			54	41	12	1	

- Molecule 28 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (three-letter code: PL9) (formula: $C_{53}H_{80}O_2$).



Mol	Chain	Residues	Atoms			AltConf
28	A	1	Total	C	O	0
			55	53	2	
28	D	1	Total	C	O	0
			55	53	2	
28	a	1	Total	C	O	0
			55	53	2	
28	d	1	Total	C	O	0
			55	53	2	

- Molecule 29 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

Mol	Chain	Residues	Atoms			AltConf
29	A	1	Total	C	O	0
			36	31	5	

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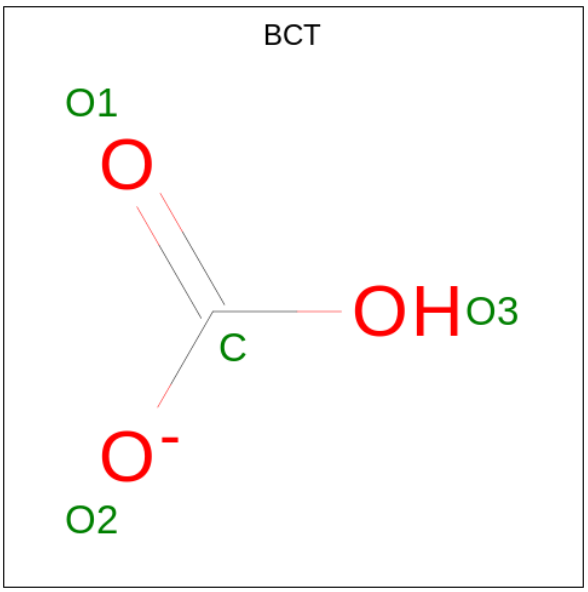
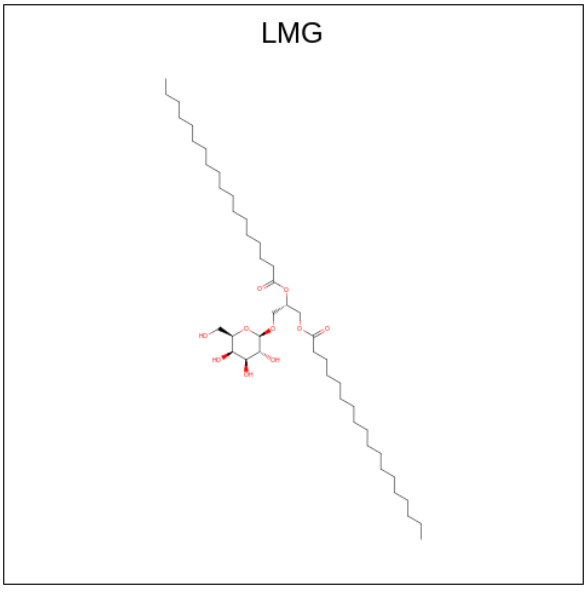
Mol	Chain	Residues	Atoms	AltConf
29	B	6	Total C O 85 80 5	0
29	C	1	Total C 10 10	0
29	D	1	Total C O 40 35 5	0
29	E	1	Total C 10 10	0
29	I	2	Total C 17 17	0
29	J	1	Total C 10 10	0
29	K	1	Total C O 34 29 5	0
29	M	1	Total C 10 10	0
29	T	2	Total C 26 26	0
29	X	1	Total C 10 10	0
29	a	1	Total C O 36 31 5	0
29	b	6	Total C O 85 80 5	0
29	c	1	Total C 10 10	0
29	d	1	Total C O 40 35 5	0
29	e	1	Total C 10 10	0
29	i	2	Total C 17 17	0
29	j	1	Total C 10 10	0
29	k	1	Total C O 34 29 5	0
29	m	1	Total C 10 10	0
29	t	2	Total C 26 26	0
29	x	1	Total C 10 10	0

- Molecule 30 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



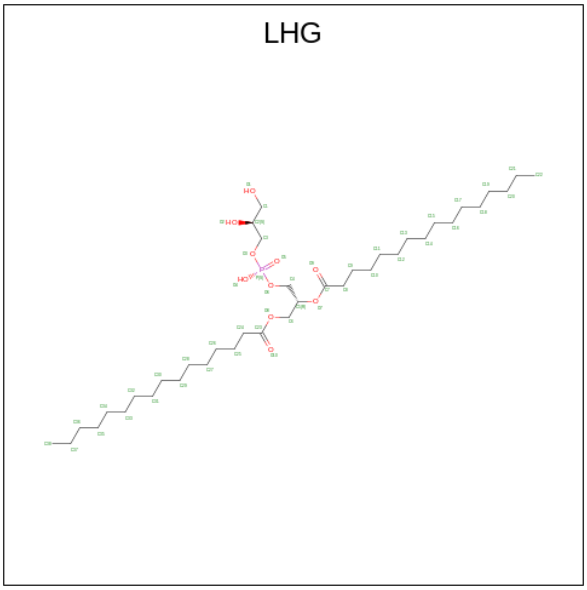
Mol	Chain	Residues	Atoms			AltConf
30	A	1	Total	C	O	0
			4	1	3	
30	a	1	Total	C	O	0
			4	1	3	

- Molecule 31 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms	AltConf
31	B	1	Total C O 51 41 10	0
31	C	1	Total C O 153 123 30	0
31	C	1	Total C O 153 123 30	0
31	C	1	Total C O 153 123 30	0
31	D	1	Total C O 51 41 10	0
31	b	1	Total C O 51 41 10	0
31	c	1	Total C O 153 123 30	0
31	c	1	Total C O 153 123 30	0
31	c	1	Total C O 153 123 30	0
31	d	1	Total C O 51 41 10	0

- Molecule 32 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms	AltConf
32	B	1	Total C O P 49 38 10 1	0

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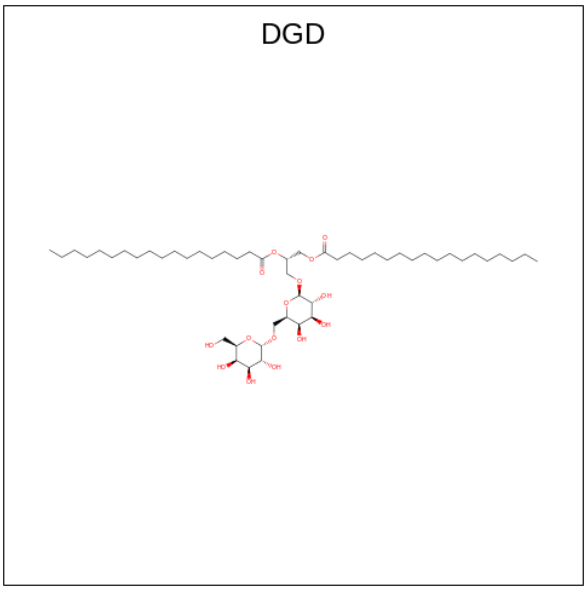
Mol	Chain	Residues	Atoms				AltConf
32	D	1	Total	C	O	P	0
			144	111	30	3	
32	D	1	Total	C	O	P	0
			144	111	30	3	
32	D	1	Total	C	O	P	0
			144	111	30	3	
32	E	1	Total	C	O	P	0
			49	38	10	1	
32	b	1	Total	C	O	P	0
			49	38	10	1	
32	d	1	Total	C	O	P	0
			144	111	30	3	
32	d	1	Total	C	O	P	0
			144	111	30	3	
32	d	1	Total	C	O	P	0
			144	111	30	3	
32	e	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 33 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



Mol	Chain	Residues	Atoms			AltConf
33	C	1	Total	C	O	0
			186	141	45	
33	C	1	Total	C	O	0
			186	141	45	

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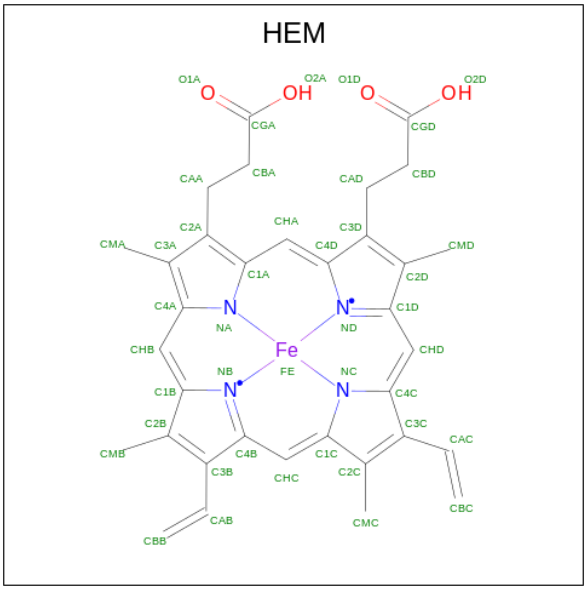
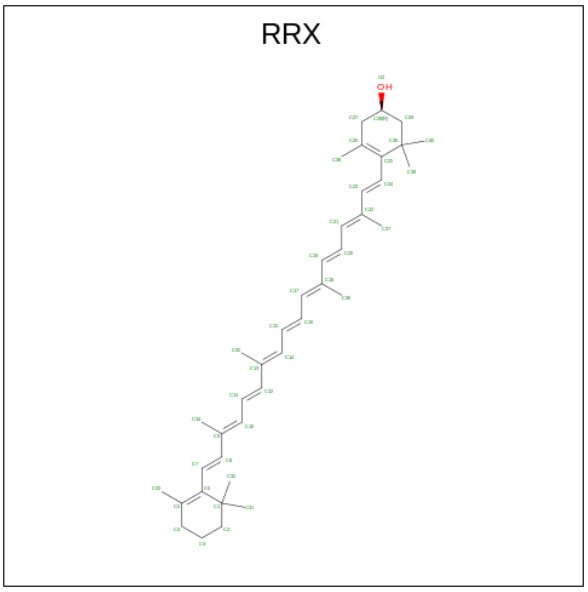
Mol	Chain	Residues	Atoms	AltConf
33	C	1	Total C O 186 141 45	0
33	H	1	Total C O 62 47 15	0
33	c	1	Total C O 186 141 45	0
33	c	1	Total C O 186 141 45	0
33	c	1	Total C O 186 141 45	0
33	h	1	Total C O 62 47 15	0

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



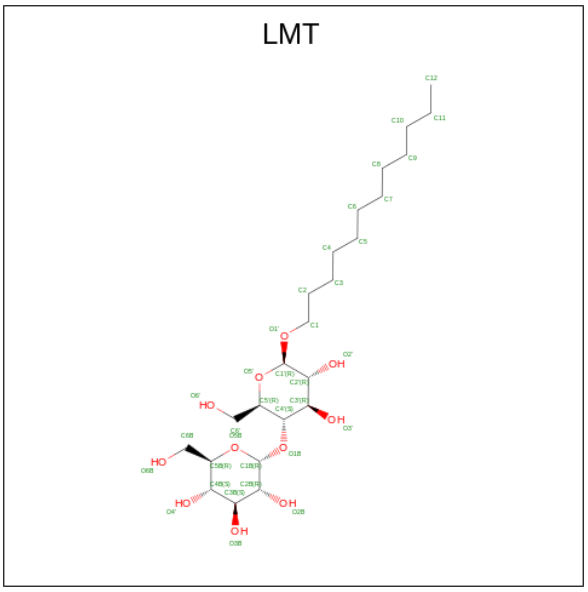
Mol	Chain	Residues	Atoms	AltConf
34	E	1	Total C Fe N O 43 34 1 4 4	0
34	e	1	Total C Fe N O 43 34 1 4 4	0

- Molecule 35 is (3R)-beta,beta-caroten-3-ol (three-letter code: RRX) (formula: $C_{40}H_{56}O$).



Mol	Chain	Residues	Atoms	AltConf
35	H	1	Total C O 41 40 1	0
35	h	1	Total C O 41 40 1	0

- Molecule 36 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms	AltConf
36	I	1	Total C O 35 24 11	0

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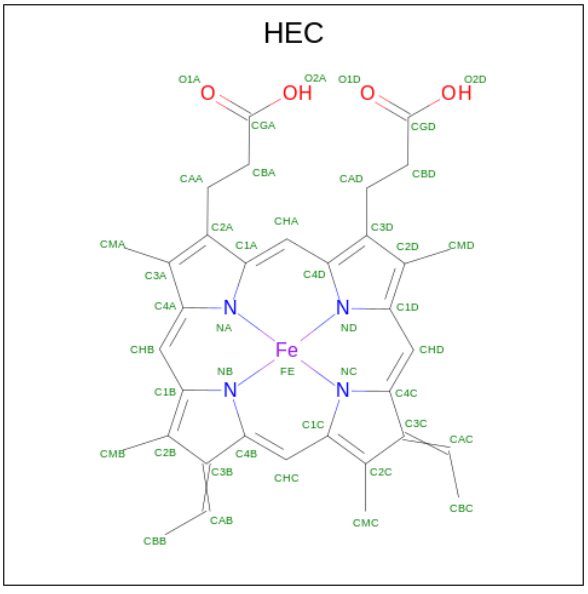
Mol	Chain	Residues	Atoms	AltConf
36	J	1	Total C O 24 18 6	0
36	M	1	Total C O 35 24 11	0
36	Z	1	Total C O 35 24 11	0
36	i	1	Total C O 35 24 11	0
36	j	1	Total C O 24 18 6	0
36	m	1	Total C O 35 24 11	0
36	z	1	Total C O 35 24 11	0

- Molecule 37 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
37	J	1	Total Mg 1 1	0
37	j	1	Total Mg 1 1	0

- Molecule 38 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



Mol	Chain	Residues	Atoms					AltConf
38	V	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
38	v	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 39 is water.

Mol	Chain	Residues	Atoms		AltConf
39	A	142	Total	O	0
			142	142	
39	B	252	Total	O	0
			252	252	
39	C	184	Total	O	0
			184	184	
39	D	145	Total	O	0
			145	145	
39	E	21	Total	O	0
			21	21	
39	F	2	Total	O	0
			2	2	
39	H	34	Total	O	0
			34	34	
39	I	13	Total	O	0
			13	13	
39	J	5	Total	O	0
			5	5	
39	K	3	Total	O	0
			3	3	
39	L	15	Total	O	0
			15	15	
39	M	6	Total	O	0
			6	6	
39	O	104	Total	O	0
			104	104	
39	T	9	Total	O	0
			9	9	
39	U	56	Total	O	0
			56	56	
39	V	63	Total	O	0
			63	63	
39	X	6	Total	O	0
			6	6	
39	a	141	Total	O	0
			141	141	

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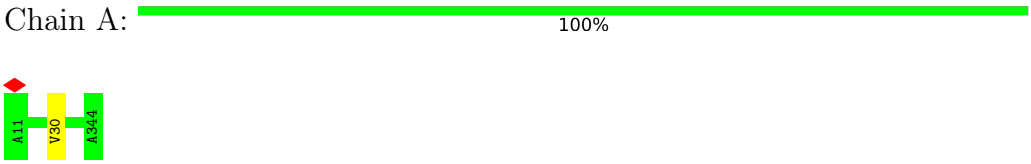
Mol	Chain	Residues	Atoms	AltConf
39	b	253	Total O 253 253	0
39	c	184	Total O 184 184	0
39	d	145	Total O 145 145	0
39	e	21	Total O 21 21	0
39	f	2	Total O 2 2	0
39	h	34	Total O 34 34	0
39	i	13	Total O 13 13	0
39	j	5	Total O 5 5	0
39	k	3	Total O 3 3	0
39	l	15	Total O 15 15	0
39	m	6	Total O 6 6	0
39	o	105	Total O 105 105	0
39	t	9	Total O 9 9	0
39	u	56	Total O 56 56	0
39	v	63	Total O 63 63	0
39	x	6	Total O 6 6	0

3 Residue-property plots (i)

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

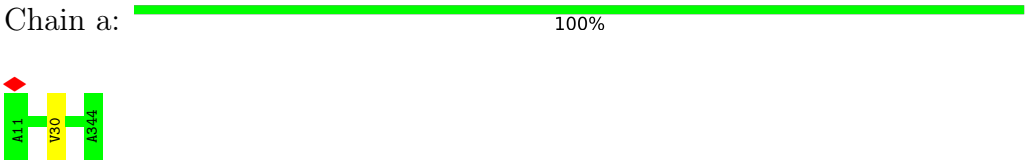
• Molecule 1: Photosystem II protein D1

Chain A:



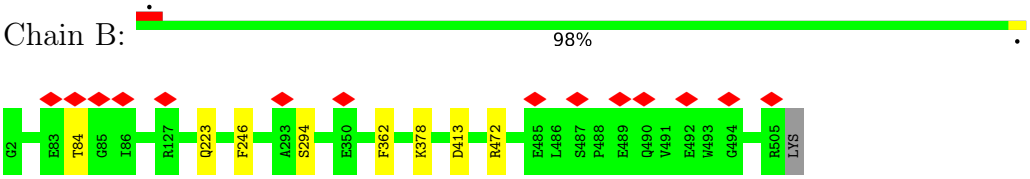
• Molecule 1: Photosystem II protein D1

Chain a:



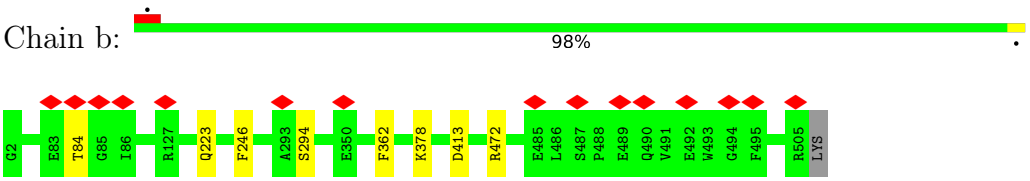
• Molecule 2: Photosystem II CP47 reaction center protein

Chain B:



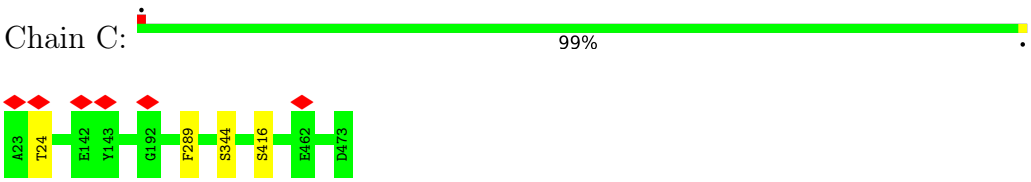
• Molecule 2: Photosystem II CP47 reaction center protein

Chain b:



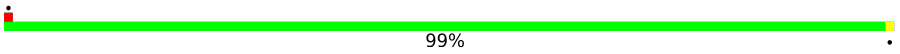
• Molecule 3: Photosystem II CP43 reaction center protein

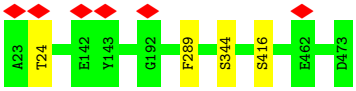
Chain C:



• Molecule 3: Photosystem II CP43 reaction center protein

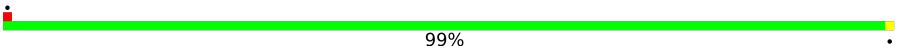
Chain c:

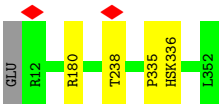




• Molecule 4: Photosystem II D2 protein

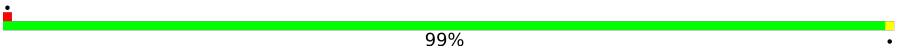
Chain D:

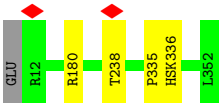




• Molecule 4: Photosystem II D2 protein

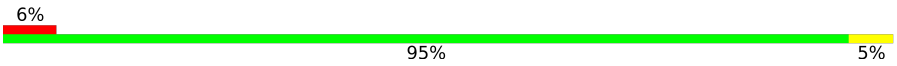
Chain d:

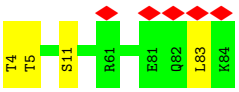




• Molecule 5: Cytochrome b559 subunit alpha

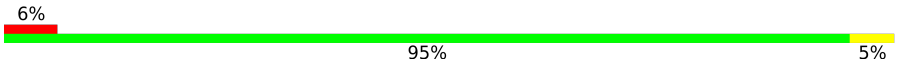
Chain E:

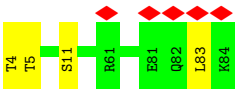




• Molecule 5: Cytochrome b559 subunit alpha

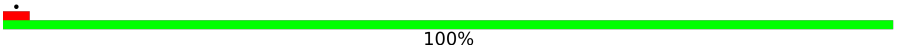
Chain e:





• Molecule 6: Cytochrome b559 subunit beta

Chain F:

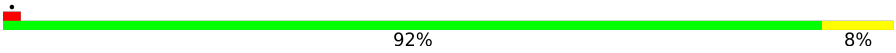


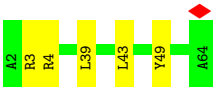
• Molecule 6: Cytochrome b559 subunit beta

Chain f:

• Molecule 7: Photosystem II reaction center protein H

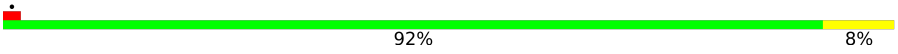
Chain H:

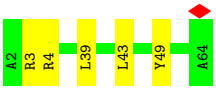




• Molecule 7: Photosystem II reaction center protein H

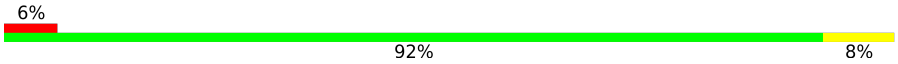
Chain h:

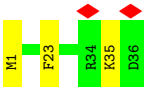




• Molecule 8: Photosystem II reaction center protein I

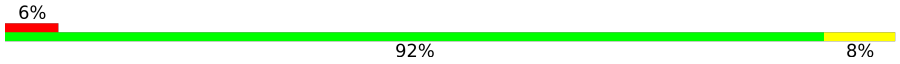
Chain I:

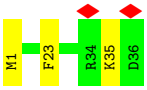




• Molecule 8: Photosystem II reaction center protein I

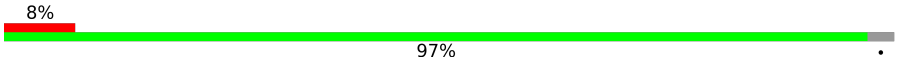
Chain i:

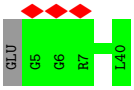




• Molecule 9: Photosystem II reaction center protein J

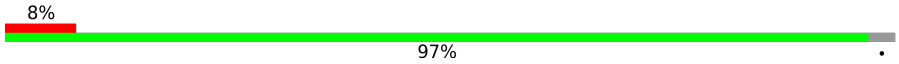
Chain J:

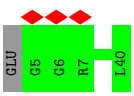




• Molecule 9: Photosystem II reaction center protein J

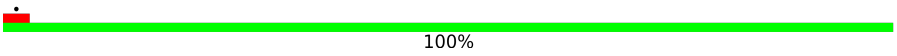
Chain j:





• Molecule 10: Photosystem II reaction center protein K

Chain K:

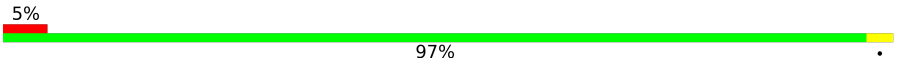


• Molecule 10: Photosystem II reaction center protein K

Chain k:

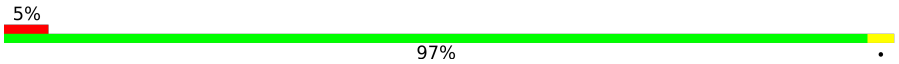
• Molecule 11: Photosystem II reaction center protein L

Chain L:



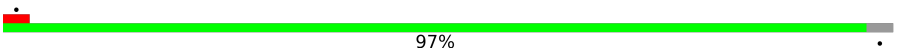
• Molecule 11: Photosystem II reaction center protein L

Chain l:



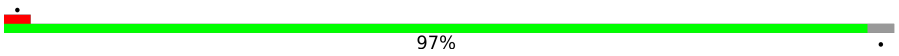
• Molecule 12: Photosystem II reaction center protein M

Chain M:



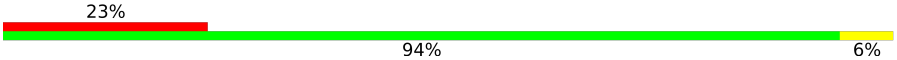
• Molecule 12: Photosystem II reaction center protein M

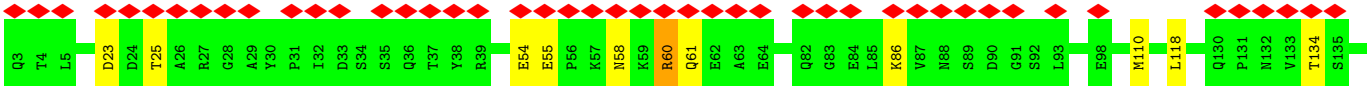
Chain m:

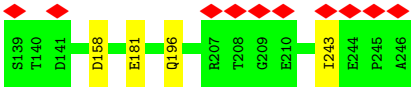


• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:

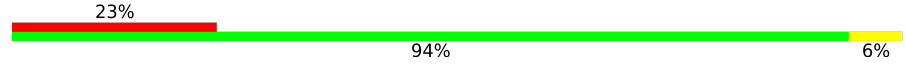


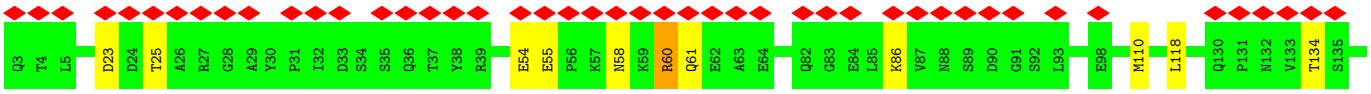


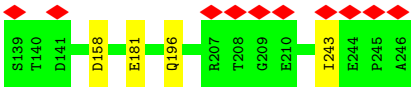


• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:

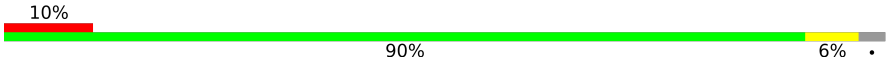


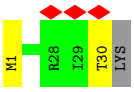




• Molecule 14: Photosystem II reaction center protein T

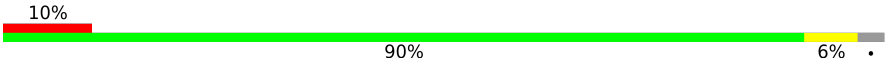
Chain T:

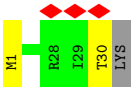




• Molecule 14: Photosystem II reaction center protein T

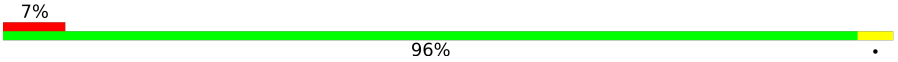
Chain t:

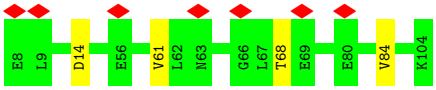




• Molecule 15: Photosystem II 12 kDa extrinsic protein

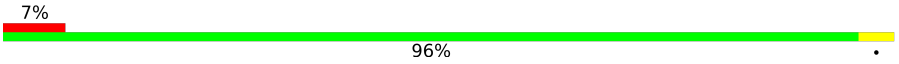
Chain U:

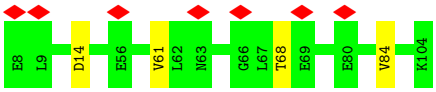




• Molecule 15: Photosystem II 12 kDa extrinsic protein

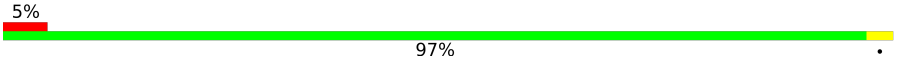
Chain u:





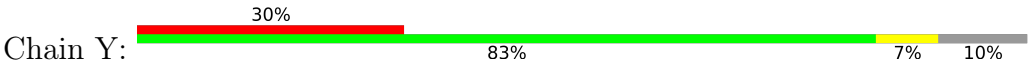
• Molecule 16: Cytochrome c-550

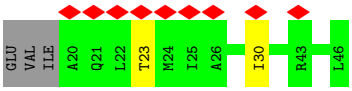
Chain V:



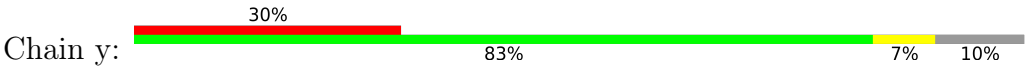
• Molecule 16: Cytochrome c-550

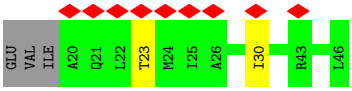
• Molecule 17: Photosystem II reaction center protein Ycf12



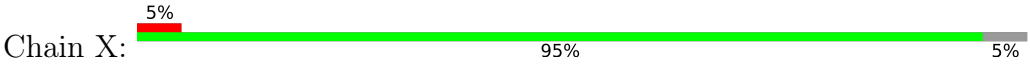


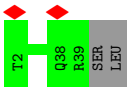
• Molecule 17: Photosystem II reaction center protein Ycf12



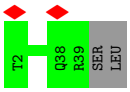


• Molecule 18: Photosystem II reaction center protein X

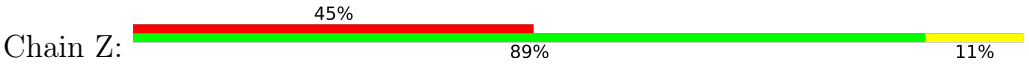


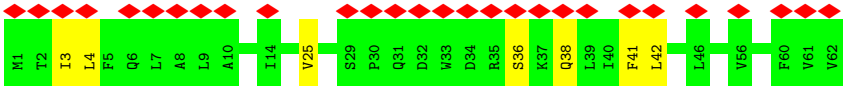


• Molecule 18: Photosystem II reaction center protein X



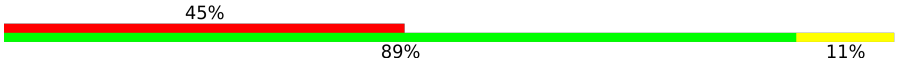
• Molecule 19: Photosystem II reaction center protein Z

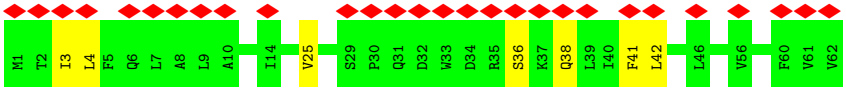




• Molecule 19: Photosystem II reaction center protein Z

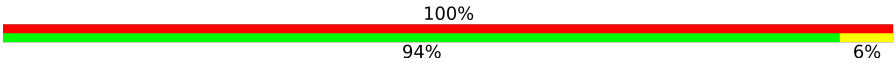
Chain z:

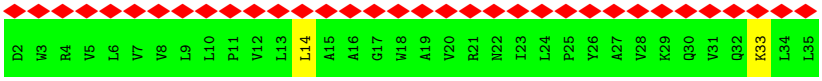




• Molecule 20: Photosystem II protein Y

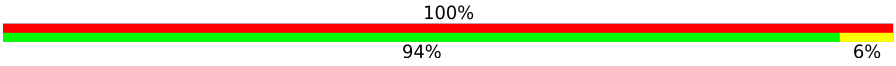
Chain R:

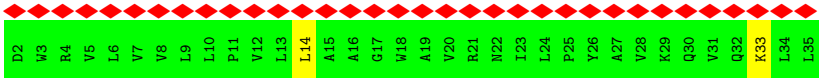




• Molecule 20: Photosystem II protein Y

Chain r:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	174099	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL CRYO ARM 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	83	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.057	Depositor
Minimum map value	-0.030	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	328.80002, 328.80002, 328.80002	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.822, 0.822, 0.822	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: HEC, OEX, BCR, DGD, SQD, PHO, LMG, CLA, MG, UNL, LHG, FME, RRX, FE2, HEM, CL, HSK, LMT, PL9, BCT

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.43	0/2705	0.59	0/3689
1	a	0.43	0/2705	0.59	0/3689
2	B	0.43	0/4109	0.57	0/5600
2	b	0.43	0/4109	0.57	0/5600
3	C	0.41	0/3599	0.56	0/4900
3	c	0.41	0/3599	0.56	0/4900
4	D	0.44	0/2800	0.60	0/3814
4	d	0.44	0/2800	0.60	0/3814
5	E	0.40	0/680	0.54	0/928
5	e	0.40	0/680	0.54	0/928
6	F	0.40	0/284	0.52	0/387
6	f	0.40	0/284	0.52	0/387
7	H	0.43	0/511	0.59	0/697
7	h	0.43	0/511	0.59	0/697
8	I	0.40	0/293	0.55	0/396
8	i	0.40	0/293	0.55	0/396
9	J	0.37	0/263	0.50	0/356
9	j	0.37	0/263	0.50	0/356
10	K	0.40	0/303	0.59	0/416
10	k	0.40	0/303	0.59	0/416
11	L	0.41	0/311	0.56	0/422
11	l	0.41	0/311	0.56	0/422
12	M	0.41	0/253	0.55	0/346
12	m	0.41	0/253	0.56	0/346
13	O	0.37	0/1905	0.63	2/2583 (0.1%)
13	o	0.37	0/1905	0.63	2/2583 (0.1%)
14	T	0.45	0/257	0.53	0/349
14	t	0.45	0/257	0.53	0/349
15	U	0.40	0/785	0.59	0/1064
15	u	0.40	0/785	0.59	0/1064
16	V	0.40	0/1085	0.57	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
16	v	0.40	0/1085	0.57	0/1473
17	Y	0.32	0/201	0.59	0/268
17	y	0.32	0/201	0.59	0/268
18	X	0.33	0/284	0.55	0/384
18	x	0.33	0/284	0.55	0/384
19	Z	0.35	0/490	0.61	0/669
19	z	0.35	0/490	0.61	0/669
20	R	0.31	0/279	0.59	0/383
20	r	0.31	0/279	0.59	0/383
All	All	0.41	0/42794	0.58	4/58248 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
4	D	0	1
4	d	0	1
All	All	0	2

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	O	158	ASP	CB-CG-OD1	5.43	123.19	118.30
13	o	158	ASP	CB-CG-OD1	5.41	123.17	118.30
13	o	158	ASP	CB-CA-C	5.15	120.71	110.40
13	O	158	ASP	CB-CA-C	5.13	120.67	110.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	335	PRO	Mainchain
4	d	335	PRO	Mainchain

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	332/334 (99%)	326 (98%)	5 (2%)	1 (0%)	41	39
1	a	332/334 (99%)	326 (98%)	5 (2%)	1 (0%)	41	39
2	B	502/505 (99%)	498 (99%)	4 (1%)	0	100	100
2	b	502/505 (99%)	498 (99%)	4 (1%)	0	100	100
3	C	449/451 (100%)	439 (98%)	9 (2%)	1 (0%)	47	47
3	c	449/451 (100%)	439 (98%)	9 (2%)	1 (0%)	47	47
4	D	338/342 (99%)	329 (97%)	9 (3%)	0	100	100
4	d	338/342 (99%)	329 (97%)	9 (3%)	0	100	100
5	E	79/81 (98%)	79 (100%)	0	0	100	100
5	e	79/81 (98%)	79 (100%)	0	0	100	100
6	F	32/34 (94%)	32 (100%)	0	0	100	100
6	f	32/34 (94%)	32 (100%)	0	0	100	100
7	H	61/63 (97%)	58 (95%)	3 (5%)	0	100	100
7	h	61/63 (97%)	58 (95%)	3 (5%)	0	100	100
8	I	34/36 (94%)	31 (91%)	3 (9%)	0	100	100
8	i	34/36 (94%)	31 (91%)	3 (9%)	0	100	100
9	J	34/37 (92%)	32 (94%)	2 (6%)	0	100	100
9	j	34/37 (92%)	32 (94%)	2 (6%)	0	100	100
10	K	35/37 (95%)	35 (100%)	0	0	100	100
10	k	35/37 (95%)	35 (100%)	0	0	100	100
11	L	35/37 (95%)	35 (100%)	0	0	100	100
11	l	35/37 (95%)	35 (100%)	0	0	100	100
12	M	31/34 (91%)	31 (100%)	0	0	100	100
12	m	31/34 (91%)	31 (100%)	0	0	100	100
13	O	242/244 (99%)	229 (95%)	11 (4%)	2 (1%)	19	14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	o	242/244 (99%)	229 (95%)	11 (4%)	2 (1%)	19	14
14	T	28/31 (90%)	28 (100%)	0	0	100	100
14	t	28/31 (90%)	28 (100%)	0	0	100	100
15	U	95/97 (98%)	92 (97%)	3 (3%)	0	100	100
15	u	95/97 (98%)	92 (97%)	3 (3%)	0	100	100
16	V	135/137 (98%)	130 (96%)	4 (3%)	1 (1%)	22	17
16	v	135/137 (98%)	130 (96%)	4 (3%)	1 (1%)	22	17
17	Y	25/30 (83%)	24 (96%)	1 (4%)	0	100	100
17	y	25/30 (83%)	24 (96%)	1 (4%)	0	100	100
18	X	36/40 (90%)	35 (97%)	1 (3%)	0	100	100
18	x	36/40 (90%)	35 (97%)	1 (3%)	0	100	100
19	Z	60/62 (97%)	56 (93%)	4 (7%)	0	100	100
19	z	60/62 (97%)	56 (93%)	4 (7%)	0	100	100
20	R	32/34 (94%)	32 (100%)	0	0	100	100
20	r	32/34 (94%)	32 (100%)	0	0	100	100
All	All	5230/5332 (98%)	5102 (98%)	118 (2%)	10 (0%)	50	47

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416	SER
13	O	58	ASN
3	c	416	SER
13	o	58	ASN
13	O	60	ARG

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	269/269 (100%)	269 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	a	269/269 (100%)	269 (100%)	0	100 100
2	B	402/403 (100%)	394 (98%)	8 (2%)	55 59
2	b	402/403 (100%)	394 (98%)	8 (2%)	55 59
3	C	352/352 (100%)	349 (99%)	3 (1%)	78 83
3	c	352/352 (100%)	349 (99%)	3 (1%)	78 83
4	D	275/276 (100%)	273 (99%)	2 (1%)	84 87
4	d	275/276 (100%)	273 (99%)	2 (1%)	84 87
5	E	72/72 (100%)	68 (94%)	4 (6%)	21 18
5	e	72/72 (100%)	68 (94%)	4 (6%)	21 18
6	F	28/28 (100%)	28 (100%)	0	100 100
6	f	28/28 (100%)	28 (100%)	0	100 100
7	H	53/53 (100%)	48 (91%)	5 (9%)	8 5
7	h	53/53 (100%)	48 (91%)	5 (9%)	8 5
8	I	32/32 (100%)	30 (94%)	2 (6%)	18 14
8	i	32/32 (100%)	30 (94%)	2 (6%)	18 14
9	J	24/25 (96%)	24 (100%)	0	100 100
9	j	24/25 (96%)	24 (100%)	0	100 100
10	K	30/30 (100%)	30 (100%)	0	100 100
10	k	30/30 (100%)	30 (100%)	0	100 100
11	L	35/35 (100%)	34 (97%)	1 (3%)	42 44
11	l	35/35 (100%)	34 (97%)	1 (3%)	42 44
12	M	29/30 (97%)	29 (100%)	0	100 100
12	m	29/30 (97%)	29 (100%)	0	100 100
13	O	207/207 (100%)	194 (94%)	13 (6%)	18 14
13	o	207/207 (100%)	194 (94%)	13 (6%)	18 14
14	T	26/27 (96%)	25 (96%)	1 (4%)	33 33
14	t	26/27 (96%)	25 (96%)	1 (4%)	33 33
15	U	84/84 (100%)	80 (95%)	4 (5%)	25 23
15	u	84/84 (100%)	80 (95%)	4 (5%)	25 23
16	V	117/117 (100%)	114 (97%)	3 (3%)	46 49
16	v	117/117 (100%)	114 (97%)	3 (3%)	46 49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
17	Y	20/23 (87%)	18 (90%)	2 (10%)	7 4
17	y	20/23 (87%)	18 (90%)	2 (10%)	7 4
18	X	31/33 (94%)	31 (100%)	0	100 100
18	x	31/33 (94%)	31 (100%)	0	100 100
19	Z	52/52 (100%)	45 (86%)	7 (14%)	4 1
19	z	52/52 (100%)	45 (86%)	7 (14%)	4 1
20	R	29/29 (100%)	27 (93%)	2 (7%)	15 12
20	r	29/29 (100%)	27 (93%)	2 (7%)	15 12
All	All	4334/4354 (100%)	4220 (97%)	114 (3%)	49 49

5 of 114 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	b	84	THR
19	z	41	PHE
5	e	5	THR
19	z	38	GLN
15	u	84	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 35 such sidechains are listed below:

Mol	Chain	Res	Type
13	o	36	GLN
13	o	88	ASN
16	v	25	GLN
13	O	147	ASN
13	O	88	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

8 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	HSK	d	336	4	7,11,12	1.43	1 (14%)	3,14,16	1.47	1 (33%)
8	FME	i	1	8	8,9,10	0.82	0	7,9,11	1.03	1 (14%)
14	FME	t	1	14	8,9,10	0.99	0	7,9,11	1.32	1 (14%)
8	FME	I	1	8	8,9,10	0.85	0	7,9,11	1.03	1 (14%)
12	FME	M	1	12	8,9,10	1.02	0	7,9,11	0.66	0
12	FME	m	1	12	8,9,10	1.01	0	7,9,11	0.66	0
4	HSK	D	336	4	7,11,12	1.42	1 (14%)	3,14,16	1.47	1 (33%)
14	FME	T	1	14	8,9,10	1.00	0	7,9,11	1.32	1 (14%)

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
4	HSK	d	336	4	-	1/5/6/8	0/1/1/1
8	FME	i	1	8	-	0/7/9/11	-
14	FME	t	1	14	-	3/7/9/11	-
8	FME	I	1	8	-	0/7/9/11	-
12	FME	M	1	12	-	1/7/9/11	-
12	FME	m	1	12	-	1/7/9/11	-
4	HSK	D	336	4	-	1/5/6/8	0/1/1/1
14	FME	T	1	14	-	3/7/9/11	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	d	336	HSK	CE1-ND1	2.71	1.40	1.36
4	D	336	HSK	CE1-ND1	2.61	1.39	1.36

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	t	1	FME	C-CA-N	2.94	115.04	109.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	T	1	FME	C-CA-N	2.93	115.01	109.73
4	D	336	HSK	CB-CA-C	-2.30	107.16	111.47
4	d	336	HSK	CB-CA-C	-2.30	107.17	111.47
8	I	1	FME	C-CA-N	2.27	113.83	109.73

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	336	HSK	OXT-C-CA-CB
12	M	1	FME	CB-CA-N-CN
4	d	336	HSK	OXT-C-CA-CB
12	m	1	FME	CB-CA-N-CN
14	T	1	FME	N-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 196 ligands modelled in this entry, 8 are monoatomic and 36 are unknown - leaving 152 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	$\#\|Z\| > 2$
24	CLA	B	610	39	65,73,73	1.98	17 (26%)	76,113,113	2.66	28 (36%)
24	CLA	c	510	-	65,73,73	2.04	16 (24%)	76,113,113	2.76	32 (42%)
21	OEX	A	401	39,1,3	0,15,15	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	CLA	B	608	-	65,73,73	1.94	17 (26%)	76,113,113	2.47	31 (40%)
26	BCR	C	516	-	41,41,41	1.02	2 (4%)	56,56,56	1.17	5 (8%)
32	LHG	e	101	-	48,48,48	0.68	0	51,54,54	1.20	6 (11%)
26	BCR	a	409	-	41,41,41	1.06	2 (4%)	56,56,56	1.27	7 (12%)
24	CLA	A	406	39	65,73,73	1.99	17 (26%)	76,113,113	2.66	28 (36%)
36	LMT	I	102	-	36,36,36	1.31	5 (13%)	47,47,47	1.24	3 (6%)
24	CLA	C	507	-	65,73,73	1.98	18 (27%)	76,113,113	2.65	27 (35%)
24	CLA	c	509	-	65,73,73	1.96	17 (26%)	76,113,113	2.70	24 (31%)
31	LMG	b	622	-	51,51,55	0.92	2 (3%)	59,59,63	1.27	7 (11%)
24	CLA	c	505	39	65,73,73	2.01	19 (29%)	76,113,113	2.84	29 (38%)
24	CLA	b	618	-	65,73,73	1.95	16 (24%)	76,113,113	2.70	28 (36%)
31	LMG	c	520	-	51,51,55	1.00	6 (11%)	59,59,63	1.41	8 (13%)
24	CLA	b	605	-	65,73,73	1.94	15 (23%)	76,113,113	2.73	28 (36%)
24	CLA	c	502	-	65,73,73	1.94	17 (26%)	76,113,113	2.70	24 (31%)
31	LMG	C	522	-	51,51,55	0.89	4 (7%)	59,59,63	1.46	7 (11%)
24	CLA	C	514	-	65,73,73	2.08	19 (29%)	76,113,113	2.84	32 (42%)
24	CLA	c	514	-	65,73,73	2.07	19 (29%)	76,113,113	2.84	32 (42%)
24	CLA	A	408	-	65,73,73	1.93	16 (24%)	76,113,113	2.69	27 (35%)
28	PL9	a	411	-	55,55,55	1.46	9 (16%)	68,69,69	1.53	13 (19%)
26	BCR	b	620	-	41,41,41	1.03	2 (4%)	56,56,56	1.25	7 (12%)
33	DGD	c	517	-	63,63,67	1.17	7 (11%)	77,77,81	1.38	7 (9%)
24	CLA	C	505	39	65,73,73	2.01	19 (29%)	76,113,113	2.84	29 (38%)
24	CLA	d	401	39	65,73,73	2.07	16 (24%)	76,113,113	2.77	29 (38%)
34	HEM	e	103	6,5	41,50,50	1.54	4 (9%)	45,82,82	1.53	6 (13%)
36	LMT	J	102	-	24,24,36	1.09	3 (12%)	29,29,47	1.15	2 (6%)
24	CLA	B	609	-	65,73,73	1.97	14 (21%)	76,113,113	2.72	28 (36%)
26	BCR	T	101	-	41,41,41	0.97	1 (2%)	56,56,56	1.30	8 (14%)
27	SQD	d	407	-	44,45,54	1.10	5 (11%)	53,56,65	1.96	13 (24%)
24	CLA	C	510	-	65,73,73	2.04	15 (23%)	76,113,113	2.76	31 (40%)
24	CLA	b	603	39	65,73,73	2.03	19 (29%)	76,113,113	2.70	27 (35%)
36	LMT	m	102	-	36,36,36	1.28	6 (16%)	47,47,47	0.95	1 (2%)
24	CLA	B	615	-	65,73,73	1.90	17 (26%)	76,113,113	2.67	26 (34%)
33	DGD	H	102	-	63,63,67	1.08	5 (7%)	77,77,81	1.16	5 (6%)
24	CLA	c	511	-	65,73,73	2.00	17 (26%)	76,113,113	2.59	28 (36%)
26	BCR	c	521	-	41,41,41	1.08	2 (4%)	56,56,56	1.15	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
28	PL9	D	406	-	55,55,55	1.44	7 (12%)	68,69,69	1.51	13 (19%)
25	PHO	d	402	-	51,69,69	1.06	5 (9%)	47,99,99	1.39	8 (17%)
24	CLA	C	511	-	65,73,73	2.00	17 (26%)	76,113,113	2.59	28 (36%)
24	CLA	B	616	-	65,73,73	1.95	16 (24%)	76,113,113	2.70	28 (36%)
24	CLA	b	616	-	65,73,73	1.95	17 (26%)	76,113,113	2.62	29 (38%)
24	CLA	D	404	-	65,73,73	2.04	16 (24%)	76,113,113	2.84	28 (36%)
27	SQD	A	410	-	53,54,54	0.95	6 (11%)	62,65,65	1.92	10 (16%)
28	PL9	d	406	-	55,55,55	1.45	7 (12%)	68,69,69	1.51	13 (19%)
24	CLA	c	513	-	65,73,73	1.98	18 (27%)	76,113,113	2.60	24 (31%)
32	LHG	D	410	-	45,45,48	0.77	1 (2%)	48,51,54	1.14	5 (10%)
26	BCR	b	619	-	41,41,41	1.00	1 (2%)	56,56,56	1.11	4 (7%)
24	CLA	b	613	-	65,73,73	1.93	17 (26%)	76,113,113	2.56	24 (31%)
24	CLA	C	502	-	65,73,73	1.94	17 (26%)	76,113,113	2.70	24 (31%)
31	LMG	d	411	37	51,51,55	0.98	5 (9%)	59,59,63	1.33	6 (10%)
26	BCR	B	617	-	41,41,41	1.00	1 (2%)	56,56,56	1.11	4 (7%)
32	LHG	d	408	-	48,48,48	0.80	1 (2%)	51,54,54	1.31	6 (11%)
24	CLA	b	606	-	65,73,73	1.91	16 (24%)	76,113,113	2.60	30 (39%)
24	CLA	c	503	-	65,73,73	1.92	19 (29%)	76,113,113	2.59	23 (30%)
24	CLA	C	509	-	65,73,73	1.96	17 (26%)	76,113,113	2.70	24 (31%)
24	CLA	D	403	-	65,73,73	1.86	18 (27%)	76,113,113	2.59	30 (39%)
33	DGD	c	518	-	63,63,67	1.21	9 (14%)	77,77,81	1.39	9 (11%)
34	HEM	E	103	6,5	41,50,50	1.54	4 (9%)	45,82,82	1.53	6 (13%)
24	CLA	b	610	-	65,73,73	1.94	17 (26%)	76,113,113	2.47	31 (40%)
24	CLA	B	612	-	65,73,73	1.86	17 (26%)	76,113,113	2.61	32 (42%)
24	CLA	D	401	39	65,73,73	2.06	15 (23%)	76,113,113	2.76	29 (38%)
26	BCR	b	621	-	41,41,41	1.05	2 (4%)	56,56,56	1.06	2 (3%)
24	CLA	b	615	-	65,73,73	1.97	19 (29%)	76,113,113	2.75	26 (34%)
27	SQD	D	407	-	44,45,54	1.10	5 (11%)	53,56,65	1.96	13 (24%)
26	BCR	d	405	-	41,41,41	1.12	3 (7%)	56,56,56	1.15	7 (12%)
24	CLA	b	609	39	65,73,73	1.91	16 (24%)	76,113,113	2.80	28 (36%)
24	CLA	B	603	-	65,73,73	1.94	15 (23%)	76,113,113	2.73	28 (36%)
24	CLA	b	604	-	65,73,73	1.99	15 (23%)	76,113,113	2.85	29 (38%)
26	BCR	c	516	-	41,41,41	1.03	2 (4%)	56,56,56	1.18	5 (8%)
30	BCT	a	414	22	2,3,3	1.32	0	2,3,3	4.48	2 (100%)
31	LMG	c	501	-	51,51,55	0.94	3 (5%)	59,59,63	1.35	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	CLA	B	605	-	65,73,73	1.85	15 (23%)	76,113,113	2.73	26 (34%)
24	CLA	C	512	3	65,73,73	1.95	17 (26%)	76,113,113	2.74	27 (35%)
24	CLA	a	408	-	65,73,73	1.93	16 (24%)	76,113,113	2.69	27 (35%)
32	LHG	d	410	-	45,45,48	0.77	1 (2%)	48,51,54	1.14	5 (10%)
31	LMG	D	411	37	51,51,55	0.97	5 (9%)	59,59,63	1.33	6 (10%)
24	CLA	B	613	-	65,73,73	1.97	19 (29%)	76,113,113	2.75	26 (34%)
27	SQD	a	412	-	53,54,54	0.94	4 (7%)	62,65,65	1.72	12 (19%)
24	CLA	c	512	3	65,73,73	1.95	17 (26%)	76,113,113	2.74	27 (35%)
31	LMG	c	522	-	51,51,55	0.89	4 (7%)	59,59,63	1.46	7 (11%)
26	BCR	B	627	-	41,41,41	0.98	1 (2%)	56,56,56	1.29	8 (14%)
28	PL9	A	411	-	55,55,55	1.47	9 (16%)	68,69,69	1.52	13 (19%)
33	DGD	C	517	-	63,63,67	1.17	7 (11%)	77,77,81	1.38	7 (9%)
24	CLA	b	608	-	65,73,73	1.99	18 (27%)	76,113,113	2.84	27 (35%)
24	CLA	b	614	-	65,73,73	1.85	17 (26%)	76,113,113	2.61	32 (42%)
32	LHG	B	625	-	48,48,48	0.76	1 (2%)	51,54,54	1.21	5 (9%)
26	BCR	Y	101	-	41,41,41	1.10	3 (7%)	56,56,56	1.21	7 (12%)
33	DGD	c	519	-	63,63,67	1.15	7 (11%)	77,77,81	1.26	7 (9%)
24	CLA	C	504	-	65,73,73	2.02	19 (29%)	76,113,113	2.64	23 (30%)
24	CLA	d	404	-	65,73,73	2.04	16 (24%)	76,113,113	2.84	28 (36%)
24	CLA	a	406	39	65,73,73	2.00	17 (26%)	76,113,113	2.67	28 (36%)
32	LHG	d	409	-	48,48,48	0.83	2 (4%)	51,54,54	1.16	6 (11%)
33	DGD	C	518	-	63,63,67	1.22	9 (14%)	77,77,81	1.39	9 (11%)
24	CLA	b	612	39	65,73,73	1.96	17 (26%)	76,113,113	2.75	26 (34%)
24	CLA	B	604	-	65,73,73	1.91	16 (24%)	76,113,113	2.60	31 (40%)
26	BCR	y	101	-	41,41,41	1.10	3 (7%)	56,56,56	1.21	7 (12%)
24	CLA	c	507	-	65,73,73	1.98	18 (27%)	76,113,113	2.65	27 (35%)
24	CLA	c	508	39	65,73,73	1.96	17 (26%)	76,113,113	2.73	27 (35%)
24	CLA	C	503	-	65,73,73	1.92	19 (29%)	76,113,113	2.59	23 (30%)
31	LMG	B	620	-	51,51,55	0.92	2 (3%)	59,59,63	1.27	7 (11%)
24	CLA	c	506	-	65,73,73	1.94	20 (30%)	76,113,113	2.58	26 (34%)
32	LHG	D	408	-	48,48,48	0.80	1 (2%)	51,54,54	1.31	6 (11%)
32	LHG	b	627	-	48,48,48	0.76	1 (2%)	51,54,54	1.21	5 (9%)
24	CLA	C	508	39	65,73,73	1.95	17 (26%)	76,113,113	2.73	27 (35%)
24	CLA	B	601	39	65,73,73	2.03	19 (29%)	76,113,113	2.70	27 (35%)
24	CLA	C	513	-	65,73,73	1.99	18 (27%)	76,113,113	2.61	24 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	CLA	B	602	-	65,73,73	2.00	15 (23%)	76,113,113	2.85	29 (38%)
36	LMT	Z	101	-	36,36,36	1.19	5 (13%)	47,47,47	1.01	3 (6%)
26	BCR	C	521	-	41,41,41	1.08	2 (4%)	56,56,56	1.15	6 (10%)
35	RRX	H	101	-	42,42,42	1.94	11 (26%)	57,58,58	1.99	15 (26%)
36	LMT	j	102	-	24,24,36	1.09	3 (12%)	29,29,47	1.15	2 (6%)
24	CLA	B	607	39	65,73,73	1.91	16 (24%)	76,113,113	2.80	28 (36%)
36	LMT	M	101	-	36,36,36	1.28	6 (16%)	47,47,47	0.95	1 (2%)
25	PHO	A	407	-	51,69,69	1.00	5 (9%)	47,99,99	1.30	7 (14%)
36	LMT	z	101	-	36,36,36	1.19	6 (16%)	47,47,47	1.01	3 (6%)
24	CLA	a	405	-	65,73,73	1.97	18 (27%)	76,113,113	2.51	26 (34%)
32	LHG	D	409	-	48,48,48	0.83	2 (4%)	51,54,54	1.16	6 (11%)
24	CLA	b	611	-	65,73,73	1.96	15 (23%)	76,113,113	2.72	28 (36%)
24	CLA	d	403	-	65,73,73	1.86	18 (27%)	76,113,113	2.59	30 (39%)
26	BCR	B	618	-	41,41,41	1.03	2 (4%)	56,56,56	1.24	7 (12%)
27	SQD	a	410	-	53,54,54	0.95	6 (11%)	62,65,65	1.92	10 (16%)
33	DGD	h	102	-	63,63,67	1.08	5 (7%)	77,77,81	1.17	5 (6%)
26	BCR	A	409	-	41,41,41	1.06	2 (4%)	56,56,56	1.27	7 (12%)
31	LMG	C	520	-	51,51,55	1.00	6 (11%)	59,59,63	1.41	6 (10%)
27	SQD	l	101	-	53,54,54	0.92	5 (9%)	62,65,65	2.00	12 (19%)
31	LMG	C	501	-	51,51,55	0.93	3 (5%)	59,59,63	1.35	6 (10%)
24	CLA	b	617	-	65,73,73	1.90	17 (26%)	76,113,113	2.67	26 (34%)
25	PHO	D	402	-	51,69,69	1.06	5 (9%)	47,99,99	1.38	8 (17%)
32	LHG	E	101	-	48,48,48	0.68	0	51,54,54	1.20	6 (11%)
24	CLA	b	607	-	65,73,73	1.86	15 (23%)	76,113,113	2.73	26 (34%)
38	HEC	v	201	16	32,50,50	2.12	4 (12%)	24,82,82	1.69	4 (16%)
24	CLA	c	504	-	65,73,73	2.03	19 (29%)	76,113,113	2.64	23 (30%)
26	BCR	B	619	-	41,41,41	1.05	2 (4%)	56,56,56	1.06	2 (3%)
35	RRX	h	101	-	42,42,42	1.94	11 (26%)	57,58,58	1.99	15 (26%)
26	BCR	c	515	-	41,41,41	1.11	3 (7%)	56,56,56	1.29	8 (14%)
27	SQD	A	412	-	53,54,54	0.95	5 (9%)	62,65,65	1.72	12 (19%)
24	CLA	B	606	-	65,73,73	1.99	18 (27%)	76,113,113	2.84	27 (35%)
25	PHO	a	407	-	51,69,69	1.01	5 (9%)	47,99,99	1.30	7 (14%)
26	BCR	C	515	-	41,41,41	1.11	3 (7%)	56,56,56	1.28	8 (14%)
24	CLA	B	611	-	65,73,73	1.93	16 (24%)	76,113,113	2.56	24 (31%)
24	CLA	A	405	-	65,73,73	1.98	18 (27%)	76,113,113	2.51	26 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
38	HEC	V	201	16	32,50,50	2.13	4 (12%)	24,82,82	1.69	4 (16%)
24	CLA	C	506	-	65,73,73	1.94	20 (30%)	76,113,113	2.58	26 (34%)
21	OEX	a	401	39,1,3	0,15,15	-	-	-		
27	SQD	L	101	-	53,54,54	0.93	5 (9%)	62,65,65	2.00	12 (19%)
30	BCT	A	414	22	2,3,3	1.32	0	2,3,3	4.47	2 (100%)
36	LMT	i	102	-	36,36,36	1.31	6 (16%)	47,47,47	1.25	3 (6%)
33	DGD	C	519	-	63,63,67	1.15	7 (11%)	77,77,81	1.26	7 (9%)
24	CLA	B	614	-	65,73,73	1.95	17 (26%)	76,113,113	2.62	29 (38%)
26	BCR	D	405	-	41,41,41	1.12	3 (7%)	56,56,56	1.15	7 (12%)

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
24	CLA	B	610	39	1/1/15/20	8/37/115/115	-
24	CLA	c	510	-	1/1/15/20	6/37/115/115	-
24	CLA	B	608	-	-	2/37/115/115	-
26	BCR	C	516	-	-	11/29/63/63	0/2/2/2
32	LHG	e	101	-	-	24/53/53/53	-
26	BCR	a	409	-	-	8/29/63/63	0/2/2/2
24	CLA	A	406	39	-	6/37/115/115	-
36	LMT	I	102	-	-	10/21/61/61	0/2/2/2
24	CLA	C	507	-	1/1/15/20	14/37/115/115	-
24	CLA	c	509	-	1/1/15/20	3/37/115/115	-
31	LMG	b	622	-	-	17/46/66/70	0/1/1/1
24	CLA	c	505	39	1/1/15/20	6/37/115/115	-
24	CLA	b	618	-	1/1/15/20	10/37/115/115	-
31	LMG	c	520	-	-	22/46/66/70	0/1/1/1
24	CLA	b	605	-	1/1/15/20	10/37/115/115	-
24	CLA	c	502	-	1/1/15/20	5/37/115/115	-
31	LMG	C	522	-	-	25/46/66/70	0/1/1/1
24	CLA	C	514	-	-	12/37/115/115	-
24	CLA	c	514	-	-	12/37/115/115	-
24	CLA	A	408	-	1/1/15/20	12/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	PL9	a	411	-	-	12/53/73/73	0/1/1/1
26	BCR	b	620	-	-	4/29/63/63	0/2/2/2
33	DGD	c	517	-	-	17/51/91/95	0/2/2/2
24	CLA	C	505	39	1/1/15/20	6/37/115/115	-
24	CLA	d	401	39	1/1/15/20	8/37/115/115	-
34	HEM	e	103	6,5	-	2/12/54/54	-
36	LMT	J	102	-	-	5/15/35/61	0/1/1/2
24	CLA	B	609	-	1/1/15/20	3/37/115/115	-
26	BCR	T	101	-	-	8/29/63/63	0/2/2/2
27	SQD	d	407	-	-	18/40/60/69	0/1/1/1
24	CLA	C	510	-	1/1/15/20	6/37/115/115	-
24	CLA	b	603	39	1/1/15/20	9/37/115/115	-
36	LMT	m	102	-	-	4/21/61/61	0/2/2/2
24	CLA	B	615	-	1/1/15/20	6/37/115/115	-
33	DGD	H	102	-	-	14/51/91/95	0/2/2/2
24	CLA	c	511	-	1/1/15/20	8/37/115/115	-
26	BCR	c	521	-	-	9/29/63/63	0/2/2/2
28	PL9	D	406	-	-	10/53/73/73	0/1/1/1
25	PHO	d	402	-	-	3/37/103/103	0/5/6/6
24	CLA	C	511	-	1/1/15/20	8/37/115/115	-
24	CLA	B	616	-	1/1/15/20	10/37/115/115	-
24	CLA	b	616	-	1/1/15/20	13/37/115/115	-
24	CLA	D	404	-	1/1/15/20	11/37/115/115	-
27	SQD	A	410	-	-	21/49/69/69	0/1/1/1
28	PL9	d	406	-	-	10/53/73/73	0/1/1/1
24	CLA	c	513	-	1/1/15/20	13/37/115/115	-
32	LHG	D	410	-	-	15/50/50/53	-
26	BCR	b	619	-	-	7/29/63/63	0/2/2/2
24	CLA	b	613	-	1/1/15/20	6/37/115/115	-
24	CLA	C	502	-	1/1/15/20	5/37/115/115	-
31	LMG	d	411	37	-	16/46/66/70	0/1/1/1
26	BCR	B	617	-	-	6/29/63/63	0/2/2/2
32	LHG	d	408	-	-	12/53/53/53	-
24	CLA	b	606	-	1/1/15/20	5/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	c	503	-	-	8/37/115/115	-
24	CLA	C	509	-	1/1/15/20	3/37/115/115	-
24	CLA	D	403	-	1/1/15/20	4/37/115/115	-
33	DGD	c	518	-	-	23/51/91/95	0/2/2/2
34	HEM	E	103	6,5	-	2/12/54/54	-
24	CLA	b	610	-	-	2/37/115/115	-
24	CLA	B	612	-	1/1/15/20	6/37/115/115	-
24	CLA	D	401	39	1/1/15/20	8/37/115/115	-
26	BCR	b	621	-	-	11/29/63/63	0/2/2/2
24	CLA	b	615	-	1/1/15/20	8/37/115/115	-
27	SQD	D	407	-	-	18/40/60/69	0/1/1/1
26	BCR	d	405	-	-	5/29/63/63	0/2/2/2
24	CLA	b	609	39	1/1/15/20	3/37/115/115	-
24	CLA	B	603	-	1/1/15/20	9/37/115/115	-
24	CLA	b	604	-	1/1/15/20	2/37/115/115	-
26	BCR	c	516	-	-	11/29/63/63	0/2/2/2
31	LMG	c	501	-	-	22/46/66/70	0/1/1/1
24	CLA	B	605	-	1/1/15/20	9/37/115/115	-
24	CLA	C	512	3	1/1/15/20	5/37/115/115	-
24	CLA	a	408	-	1/1/15/20	12/37/115/115	-
32	LHG	d	410	-	-	15/50/50/53	-
31	LMG	D	411	37	-	16/46/66/70	0/1/1/1
24	CLA	B	613	-	1/1/15/20	8/37/115/115	-
27	SQD	a	412	-	-	17/49/69/69	0/1/1/1
24	CLA	c	512	3	1/1/15/20	5/37/115/115	-
31	LMG	c	522	-	-	25/46/66/70	0/1/1/1
26	BCR	B	627	-	-	8/29/63/63	0/2/2/2
28	PL9	A	411	-	-	12/53/73/73	0/1/1/1
33	DGD	C	517	-	-	17/51/91/95	0/2/2/2
24	CLA	b	608	-	1/1/15/20	5/37/115/115	-
24	CLA	b	614	-	1/1/15/20	6/37/115/115	-
32	LHG	B	625	-	-	19/53/53/53	-
26	BCR	Y	101	-	-	5/29/63/63	0/2/2/2
33	DGD	c	519	-	-	16/51/91/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	C	504	-	1/1/15/20	7/37/115/115	-
24	CLA	d	404	-	1/1/15/20	11/37/115/115	-
24	CLA	a	406	39	-	6/37/115/115	-
32	LHG	d	409	-	-	18/53/53/53	-
33	DGD	C	518	-	-	23/51/91/95	0/2/2/2
24	CLA	b	612	39	-	8/37/115/115	-
24	CLA	B	604	-	1/1/15/20	5/37/115/115	-
26	BCR	y	101	-	-	5/29/63/63	0/2/2/2
24	CLA	c	507	-	1/1/15/20	14/37/115/115	-
24	CLA	c	508	39	1/1/15/20	10/37/115/115	-
24	CLA	C	503	-	-	8/37/115/115	-
31	LMG	B	620	-	-	17/46/66/70	0/1/1/1
24	CLA	c	506	-	1/1/15/20	9/37/115/115	-
32	LHG	D	408	-	-	12/53/53/53	-
32	LHG	b	627	-	-	19/53/53/53	-
24	CLA	C	508	39	1/1/15/20	10/37/115/115	-
24	CLA	B	601	39	1/1/15/20	9/37/115/115	-
24	CLA	C	513	-	1/1/15/20	13/37/115/115	-
24	CLA	B	602	-	1/1/15/20	2/37/115/115	-
36	LMT	Z	101	-	-	11/21/61/61	0/2/2/2
26	BCR	C	521	-	-	9/29/63/63	0/2/2/2
35	RRX	H	101	-	-	2/29/65/65	0/2/2/2
36	LMT	j	102	-	-	5/15/35/61	0/1/1/2
24	CLA	B	607	39	1/1/15/20	3/37/115/115	-
36	LMT	M	101	-	-	4/21/61/61	0/2/2/2
25	PHO	A	407	-	-	3/37/103/103	0/5/6/6
36	LMT	z	101	-	-	11/21/61/61	0/2/2/2
24	CLA	a	405	-	1/1/15/20	5/37/115/115	-
32	LHG	D	409	-	-	18/53/53/53	-
24	CLA	b	611	-	1/1/15/20	3/37/115/115	-
24	CLA	d	403	-	1/1/15/20	4/37/115/115	-
26	BCR	B	618	-	-	4/29/63/63	0/2/2/2
27	SQD	a	410	-	-	21/49/69/69	0/1/1/1
33	DGD	h	102	-	-	14/51/91/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	BCR	A	409	-	-	8/29/63/63	0/2/2/2
31	LMG	C	520	-	-	22/46/66/70	0/1/1/1
27	SQD	l	101	-	-	21/49/69/69	0/1/1/1
31	LMG	C	501	-	-	22/46/66/70	0/1/1/1
24	CLA	b	617	-	1/1/15/20	5/37/115/115	-
25	PHO	D	402	-	-	3/37/103/103	0/5/6/6
32	LHG	E	101	-	-	24/53/53/53	-
24	CLA	b	607	-	1/1/15/20	9/37/115/115	-
38	HEC	v	201	16	-	2/10/54/54	-
24	CLA	c	504	-	1/1/15/20	7/37/115/115	-
26	BCR	B	619	-	-	11/29/63/63	0/2/2/2
35	RRX	h	101	-	-	2/29/65/65	0/2/2/2
26	BCR	c	515	-	-	8/29/63/63	0/2/2/2
27	SQD	A	412	-	-	17/49/69/69	0/1/1/1
24	CLA	B	606	-	1/1/15/20	5/37/115/115	-
25	PHO	a	407	-	-	3/37/103/103	0/5/6/6
26	BCR	C	515	-	-	8/29/63/63	0/2/2/2
24	CLA	B	611	-	1/1/15/20	6/37/115/115	-
24	CLA	A	405	-	1/1/15/20	5/37/115/115	-
38	HEC	V	201	16	-	2/10/54/54	-
24	CLA	C	506	-	1/1/15/20	9/37/115/115	-
36	LMT	i	102	-	-	10/21/61/61	0/2/2/2
27	SQD	L	101	-	-	20/49/69/69	0/1/1/1
33	DGD	C	519	-	-	16/51/91/95	0/2/2/2
24	CLA	B	614	-	1/1/15/20	13/37/115/115	-
26	BCR	D	405	-	-	5/29/63/63	0/2/2/2

The worst 5 of 1515 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	V	201	HEC	C2B-C3B	-7.12	1.33	1.40
38	v	201	HEC	C2B-C3B	-7.12	1.33	1.40
24	C	513	CLA	C3B-C2B	6.49	1.49	1.40
24	c	513	CLA	C3B-C2B	6.48	1.49	1.40
24	D	404	CLA	C3B-C2B	6.45	1.49	1.40

The worst 5 of 2468 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	d	404	CLA	C1D-ND-C4D	-10.13	99.14	106.33
24	D	404	CLA	C1D-ND-C4D	-10.06	99.19	106.33
24	C	512	CLA	C1D-ND-C4D	-9.87	99.32	106.33
24	c	512	CLA	C1D-ND-C4D	-9.87	99.32	106.33
24	B	613	CLA	C1D-ND-C4D	-9.86	99.33	106.33

5 of 61 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
24	A	405	CLA	ND
24	A	408	CLA	ND
24	B	601	CLA	ND
24	B	602	CLA	ND
24	B	603	CLA	ND

5 of 1464 torsion outliers are listed below:

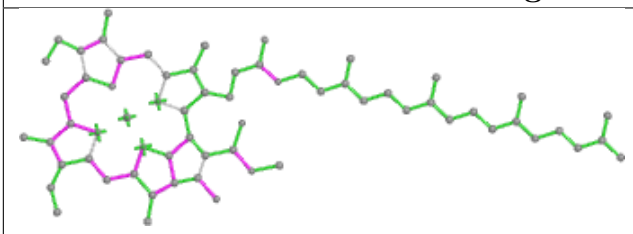
Mol	Chain	Res	Type	Atoms
24	B	603	CLA	C2-C3-C5-C6
24	B	603	CLA	C4-C3-C5-C6
24	B	605	CLA	C2-C3-C5-C6
24	B	605	CLA	C4-C3-C5-C6
24	B	606	CLA	CHA-CBD-CGD-O1D

There are no ring outliers.

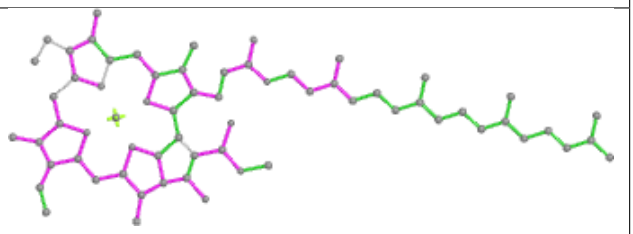
No monomer is involved in short contacts.

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

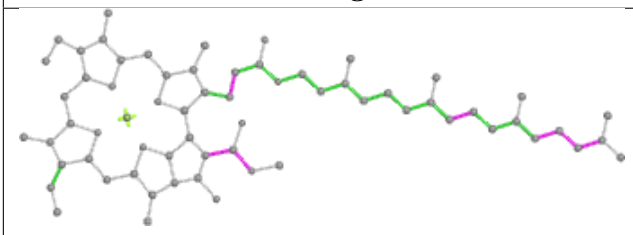
Ligand CLA B 610



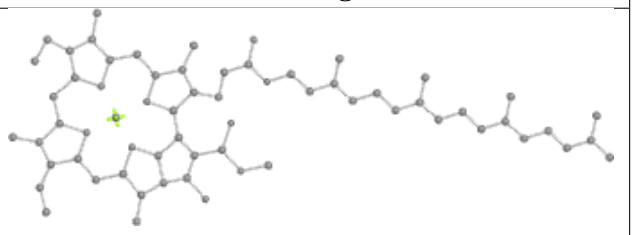
Bond lengths



Bond angles

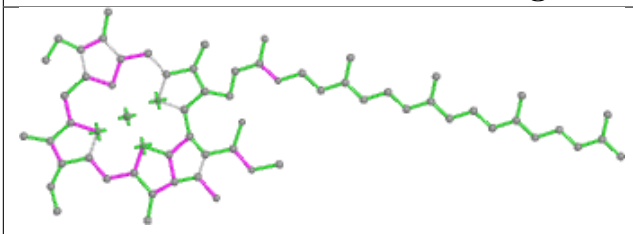


Torsions

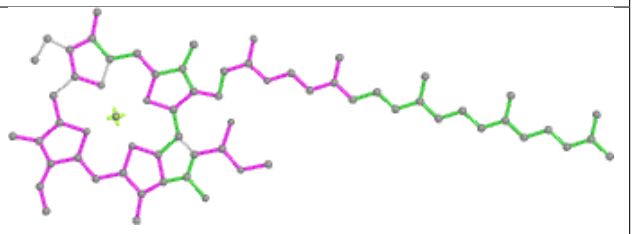


Rings

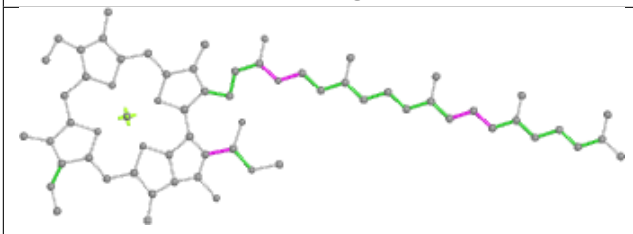
Ligand CLA c 510



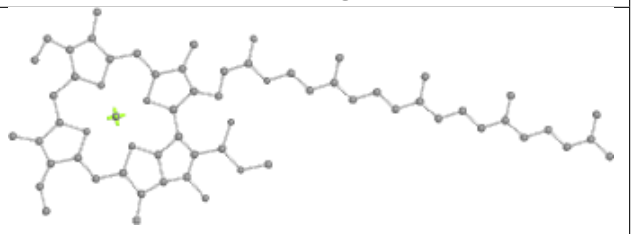
Bond lengths



Bond angles

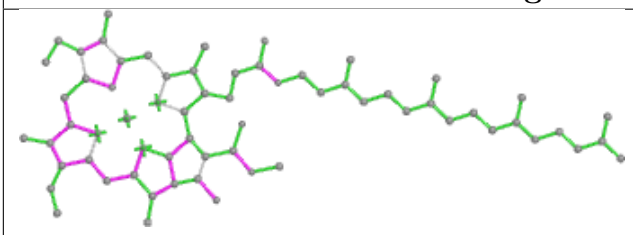


Torsions

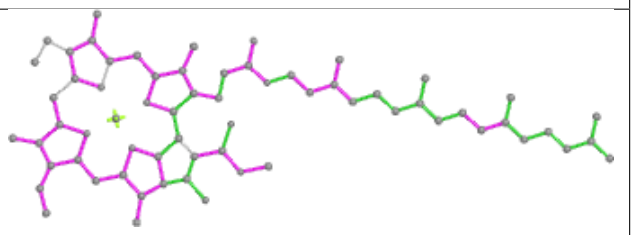


Rings

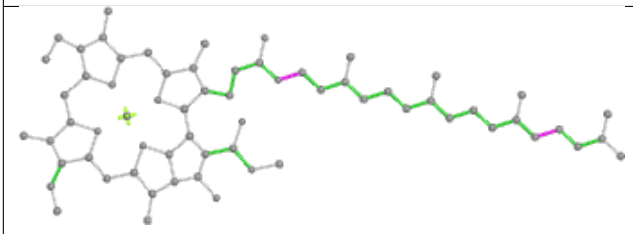
Ligand CLA B 608



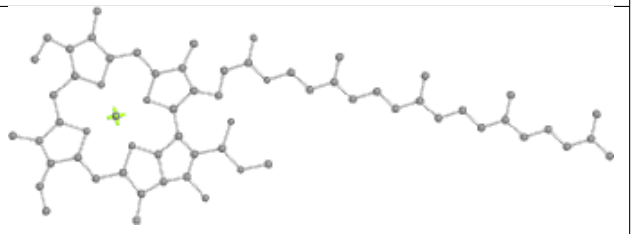
Bond lengths



Bond angles

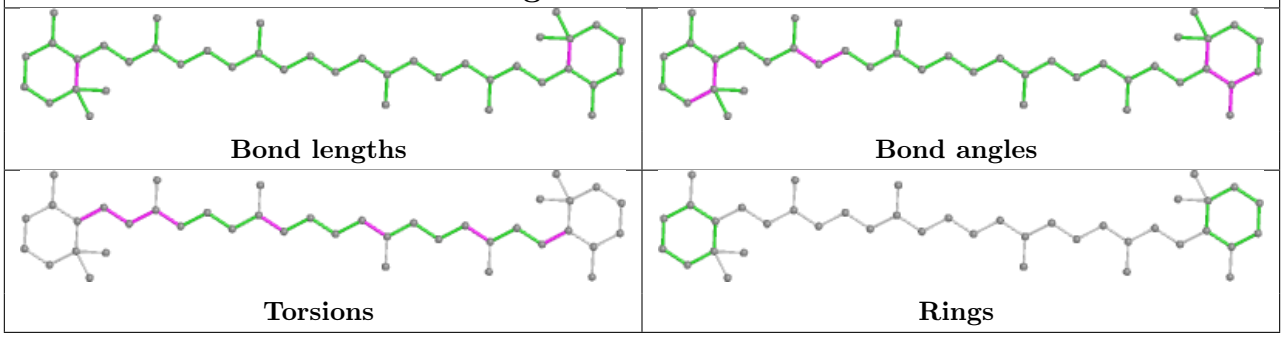


Torsions

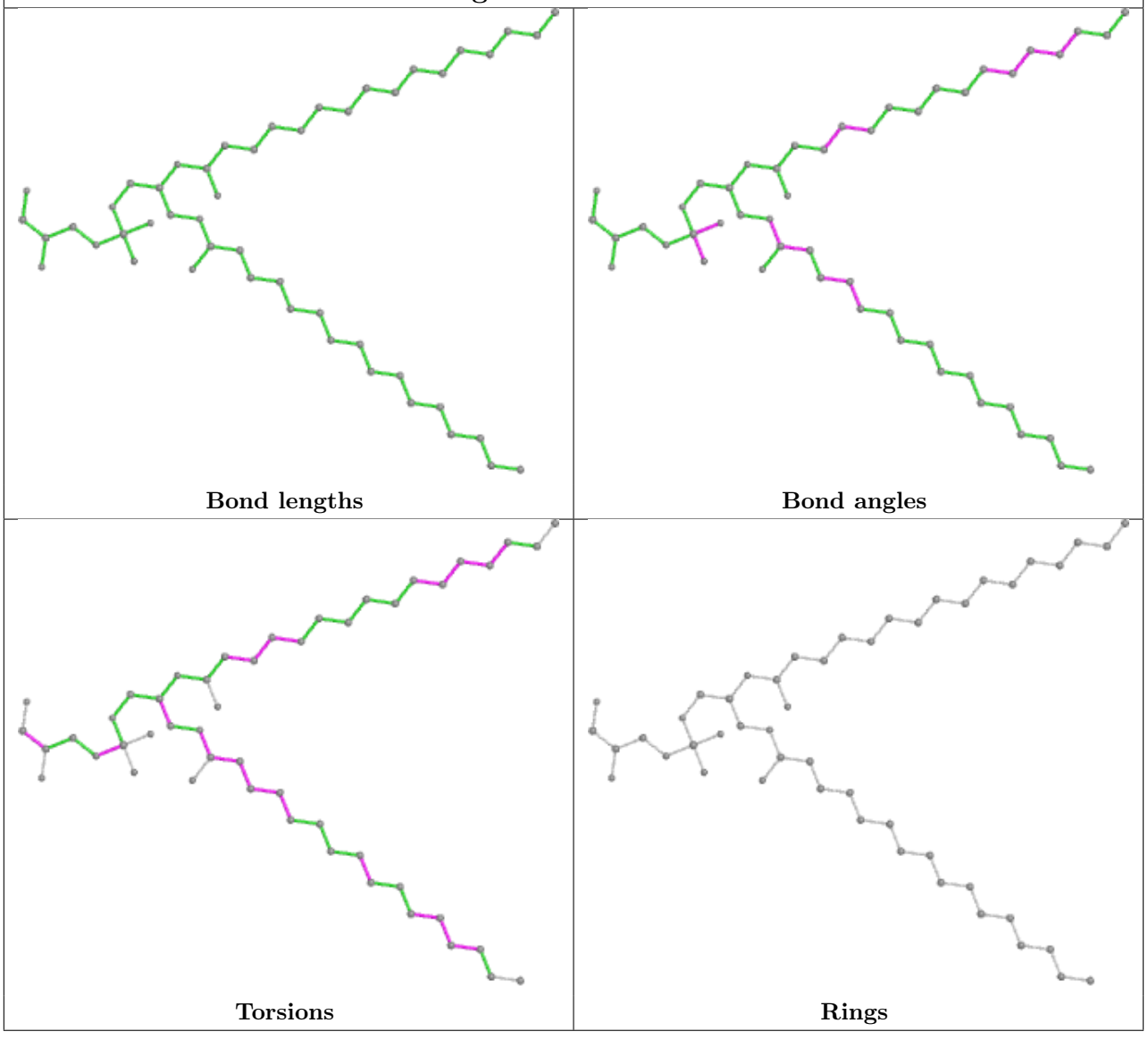


Rings

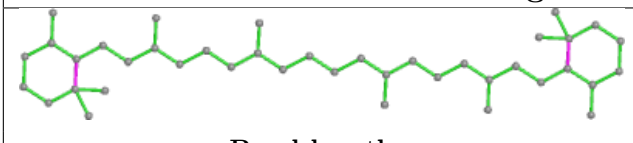
Ligand BCR C 516



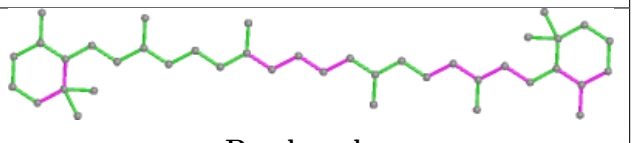
Ligand LHG e 101



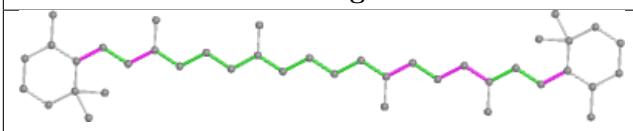
Ligand BCR a 409



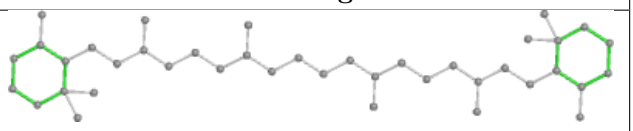
Bond lengths



Bond angles

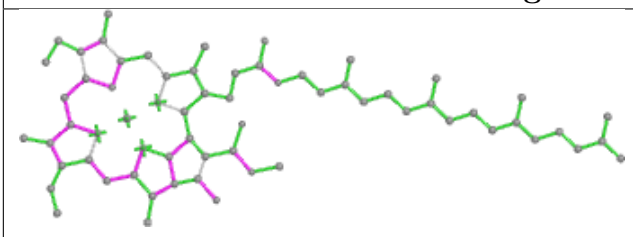


Torsions

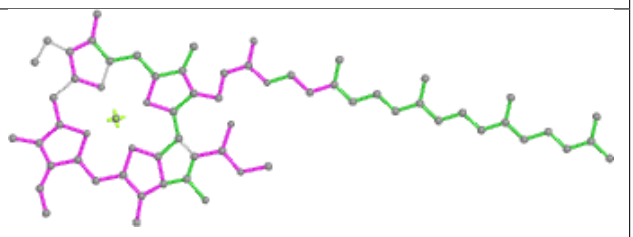


Rings

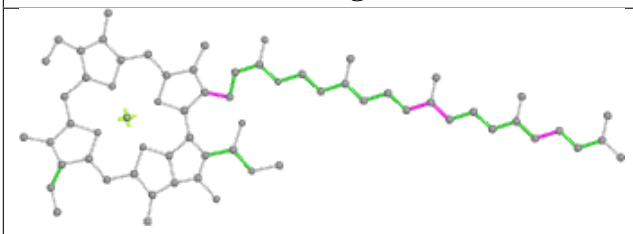
Ligand CLA A 406



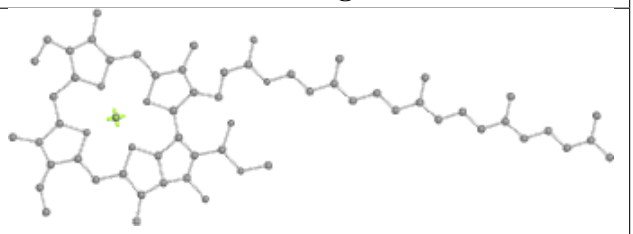
Bond lengths



Bond angles

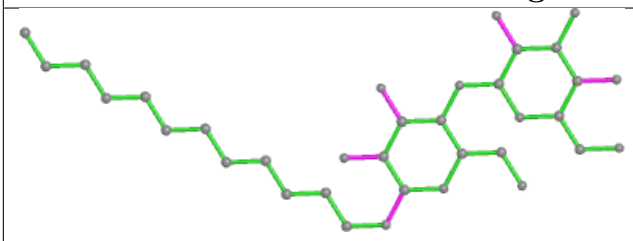


Torsions

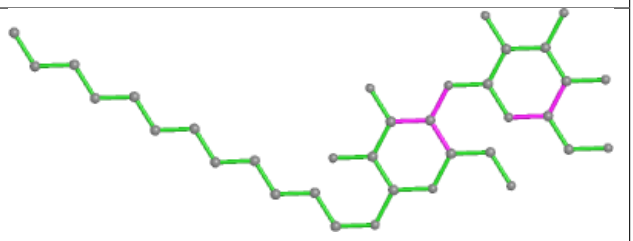


Rings

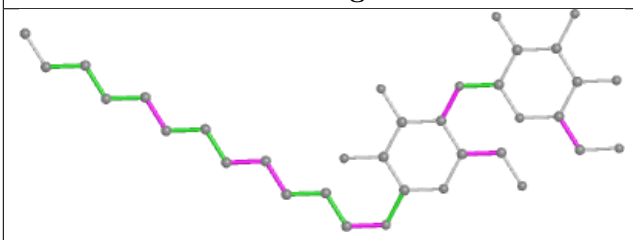
Ligand LMT I 102



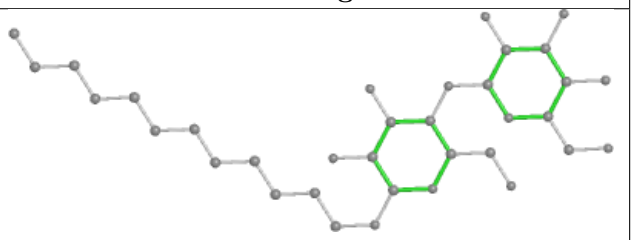
Bond lengths



Bond angles

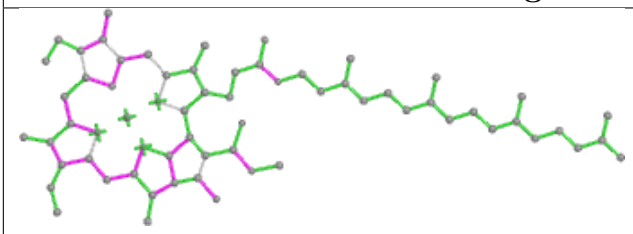


Torsions

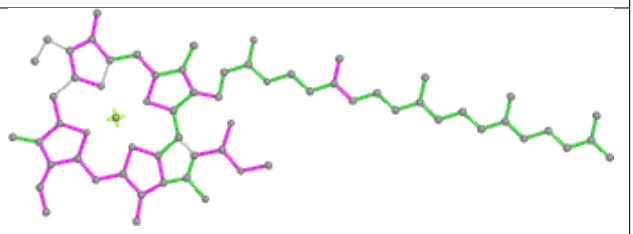


Rings

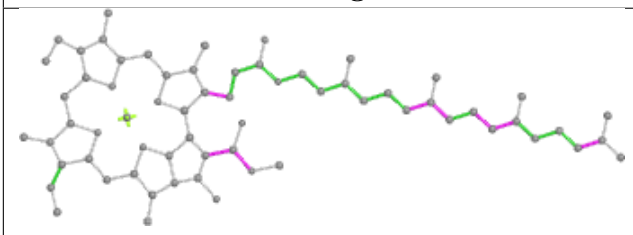
Ligand CLA C 507



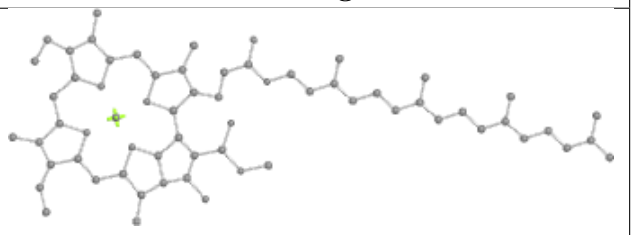
Bond lengths



Bond angles

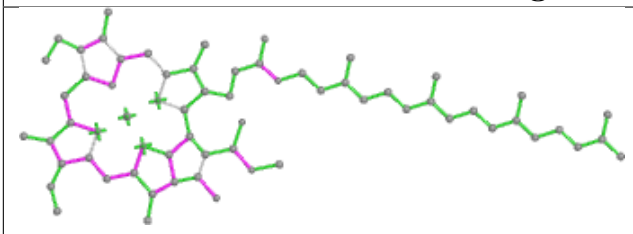


Torsions

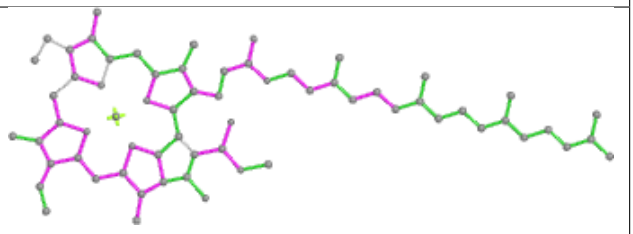


Rings

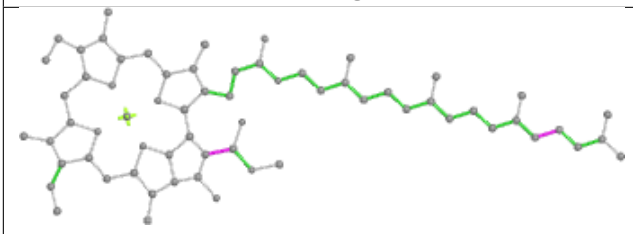
Ligand CLA c 509



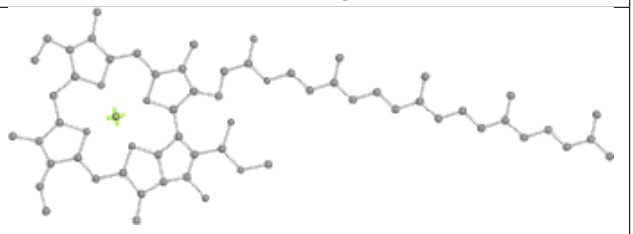
Bond lengths



Bond angles

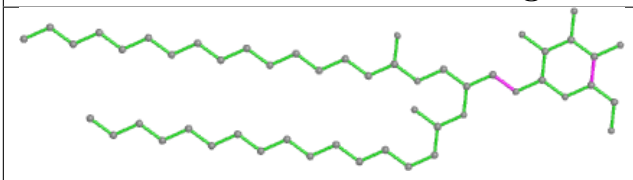


Torsions

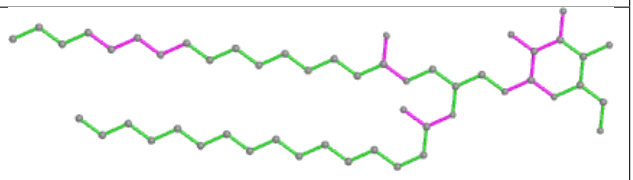


Rings

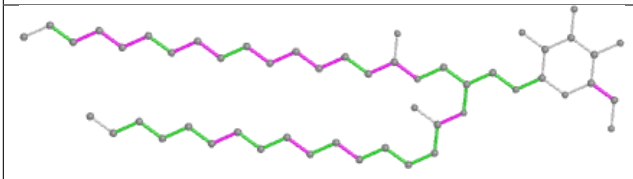
Ligand LMG b 622



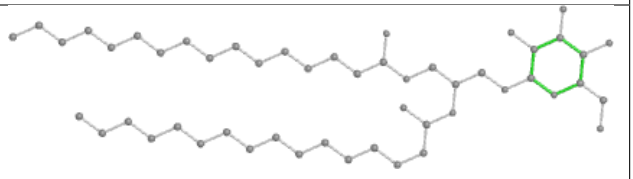
Bond lengths



Bond angles

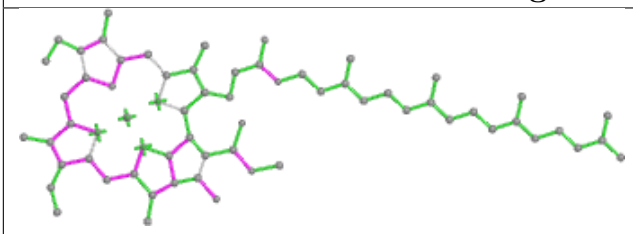


Torsions

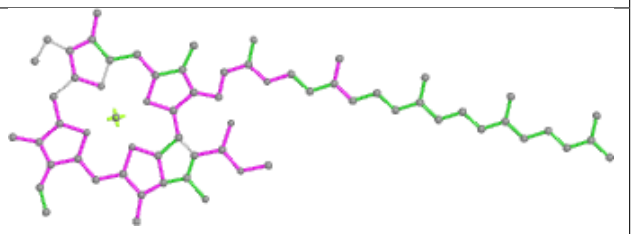


Rings

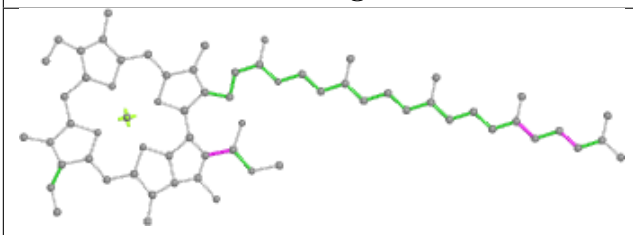
Ligand CLA c 505



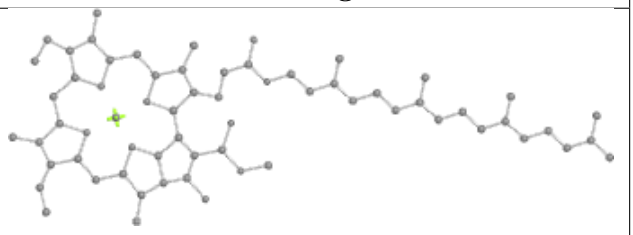
Bond lengths



Bond angles

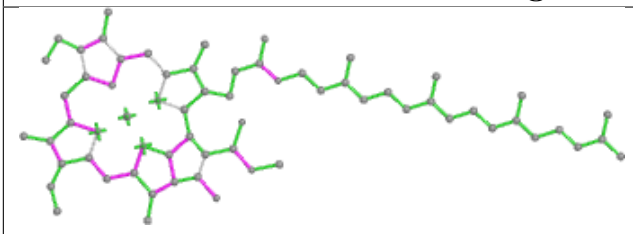


Torsions

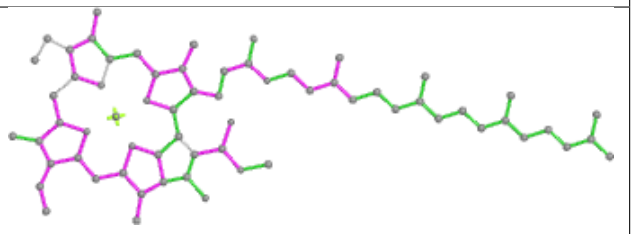


Rings

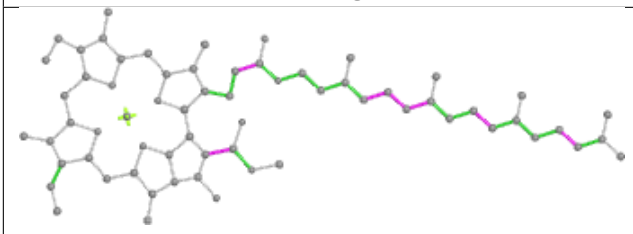
Ligand CLA b 618



Bond lengths



Bond angles



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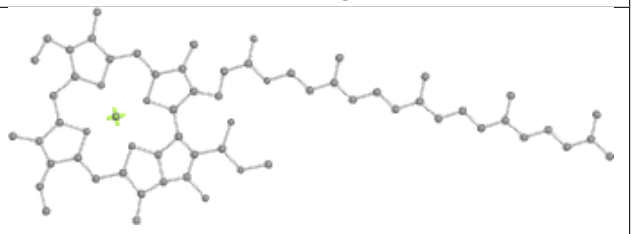
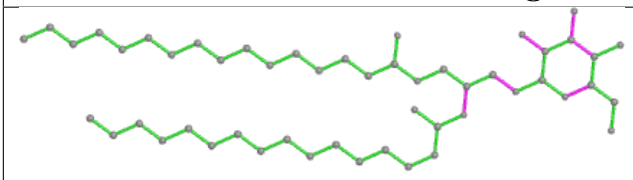


Rings

Ligand LMG c 520



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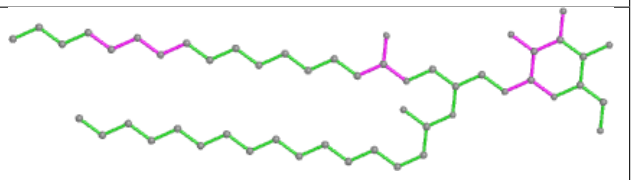
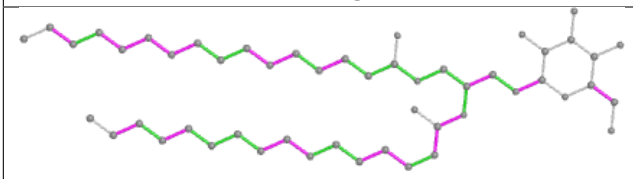
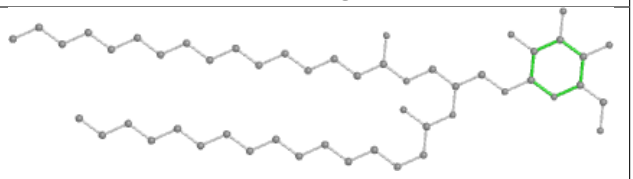


Bond angles

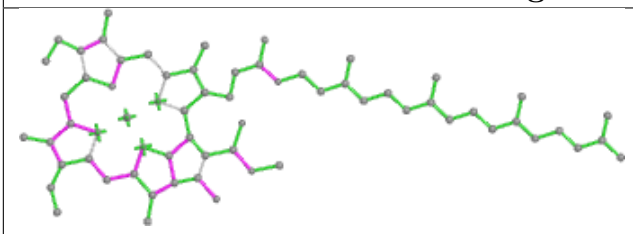


Torsions

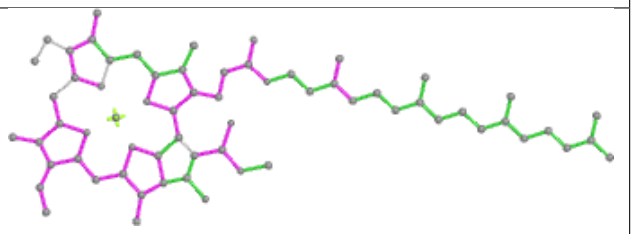


Rings

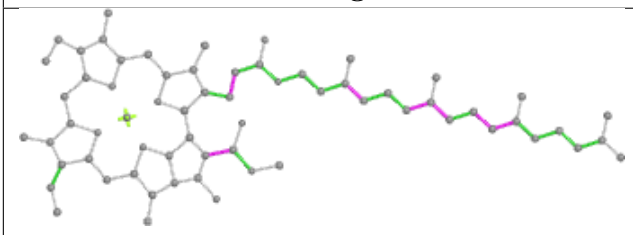
Ligand CLA b 605



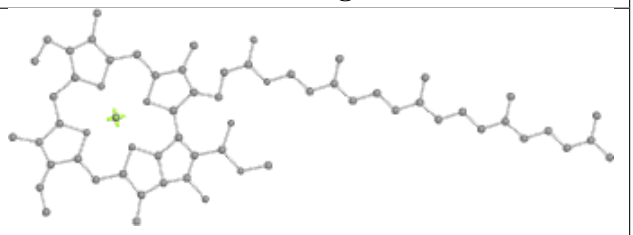
Bond lengths



Bond angles

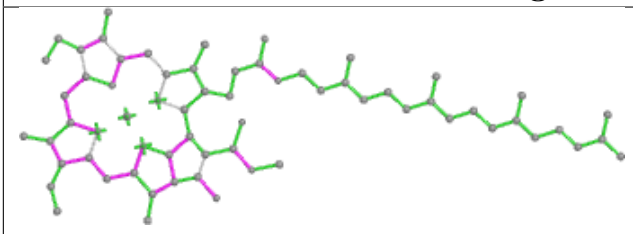


Torsions

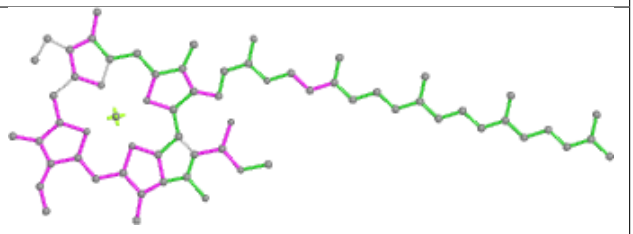


Rings

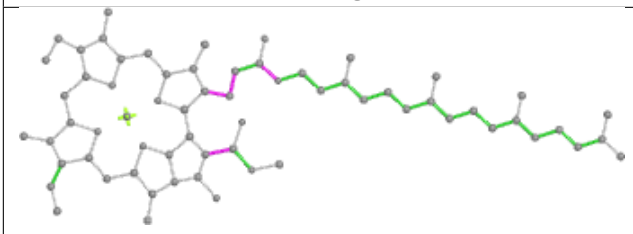
Ligand CLA c 502



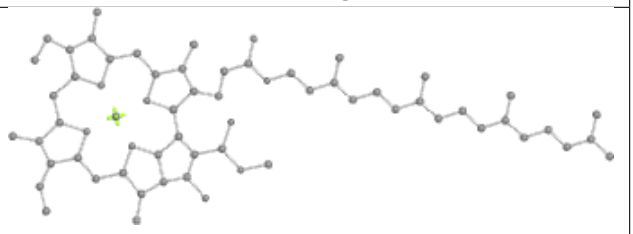
Bond lengths



Bond angles

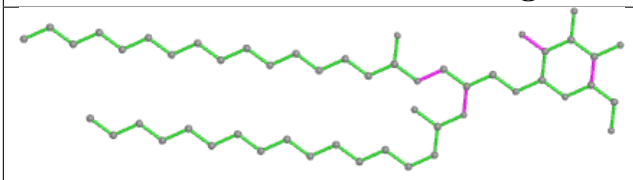


Torsions

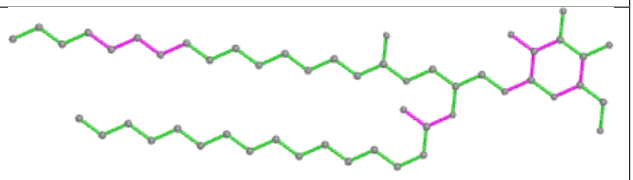


Rings

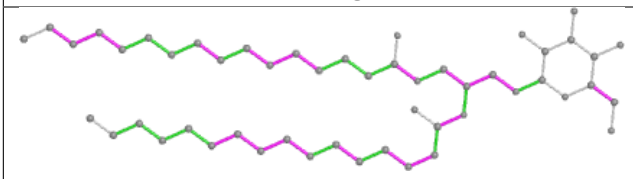
Ligand LMG C 522



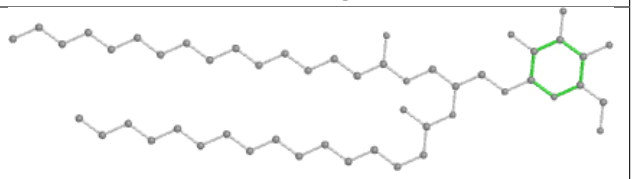
Bond lengths



Bond angles

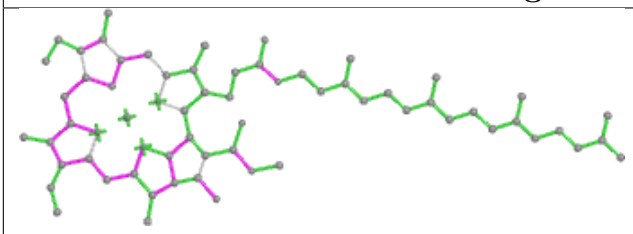


Torsions

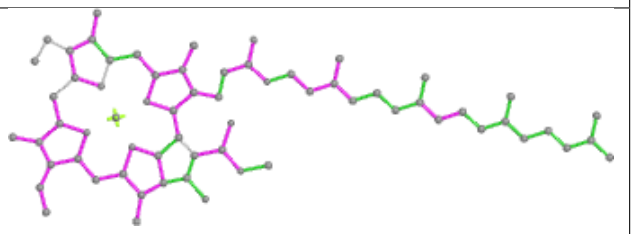


Rings

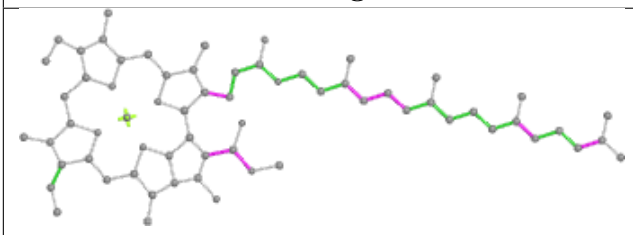
Ligand CLA C 514



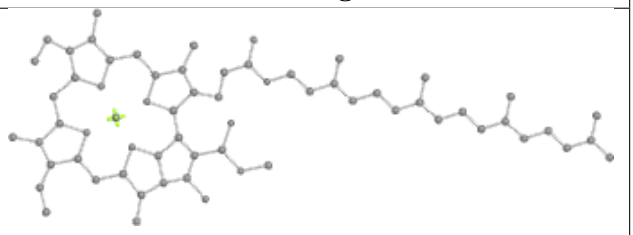
Bond lengths



Bond angles

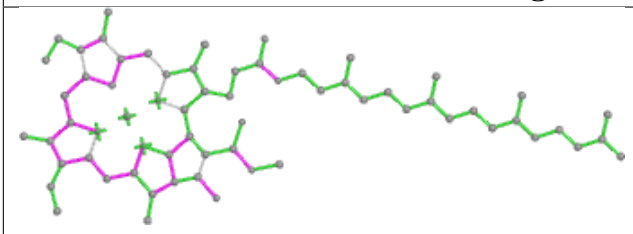


Torsions



Rings

Ligand CLA c 514



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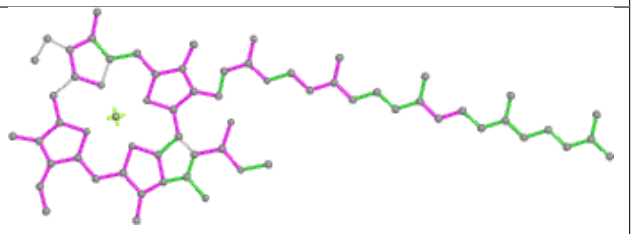
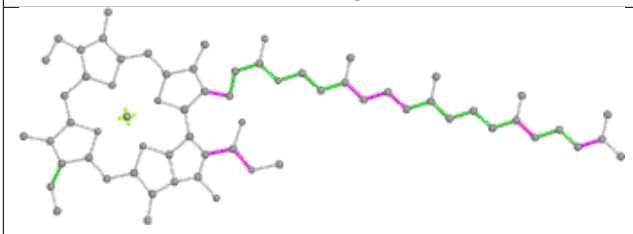
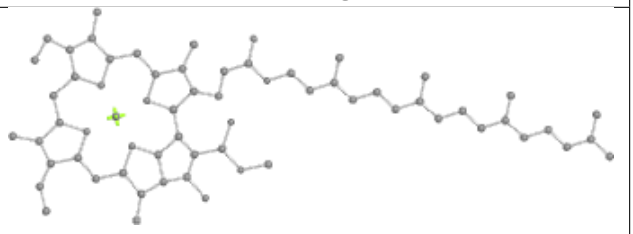


Bond angles

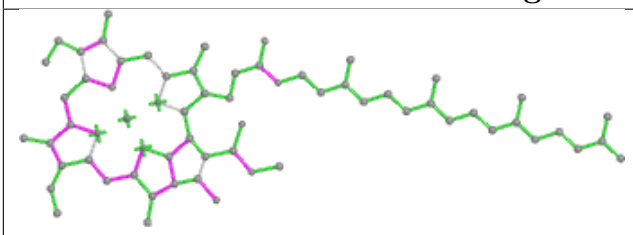


Torsions

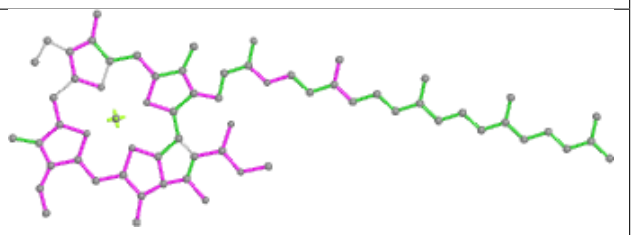


Rings

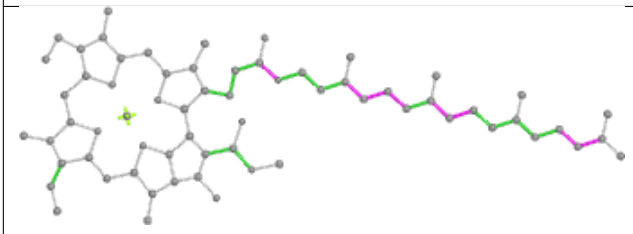
Ligand CLA A 408



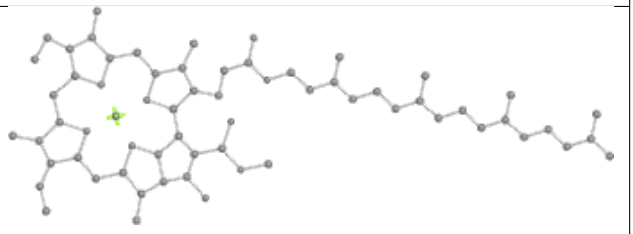
Bond lengths



Bond angles

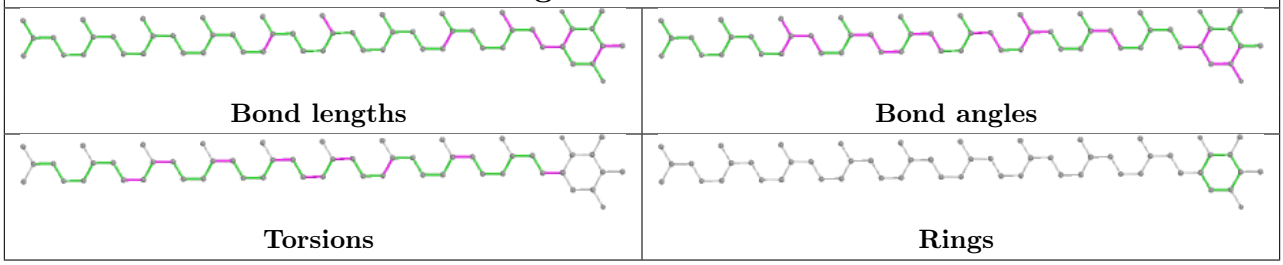


Torsions

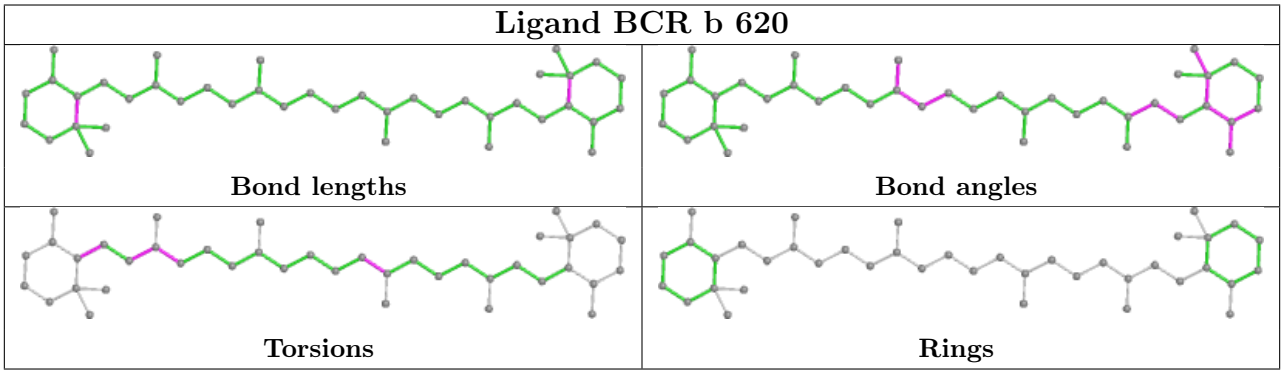


Rings

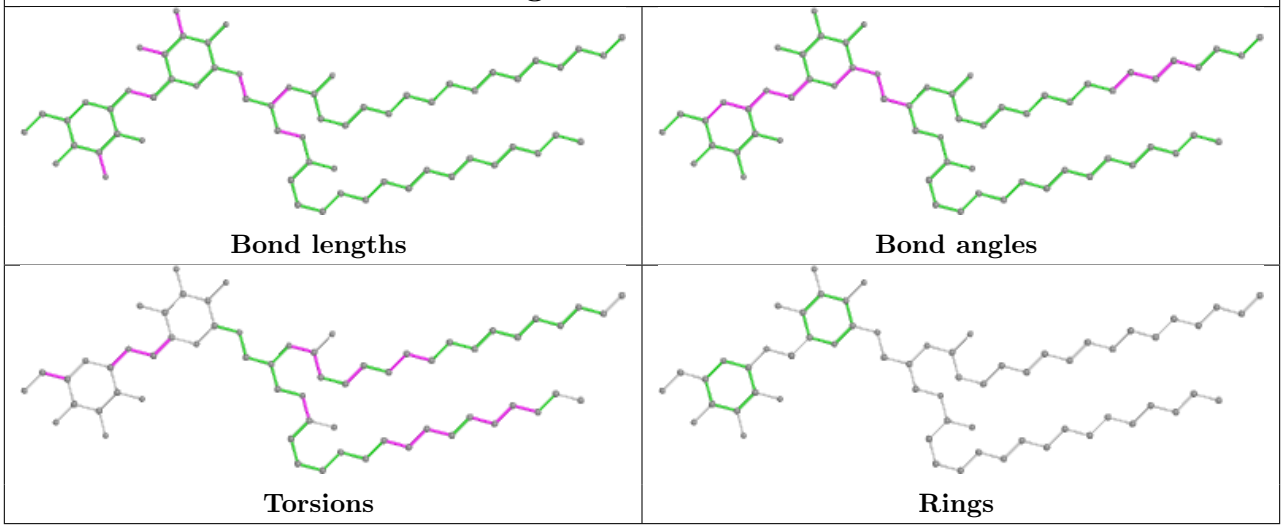
Ligand PL9 a 411



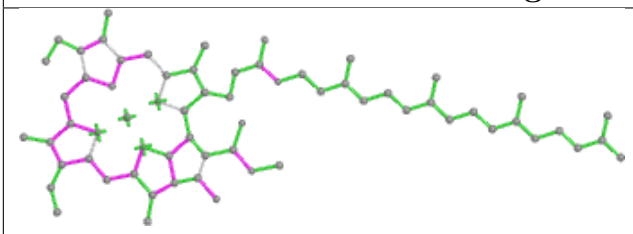
Ligand BCR b 620



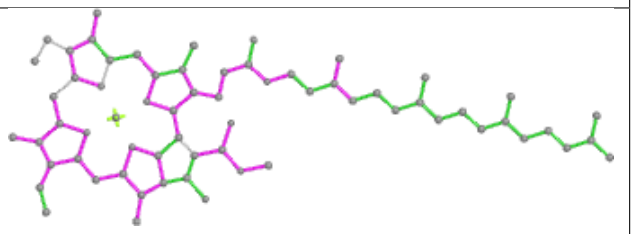
Ligand DGD c 517



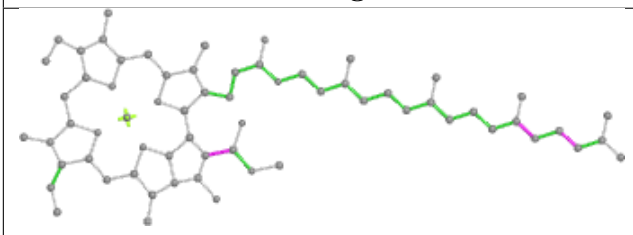
Ligand CLA C 505



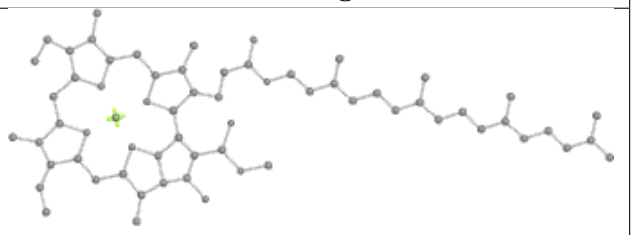
Bond lengths



Bond angles

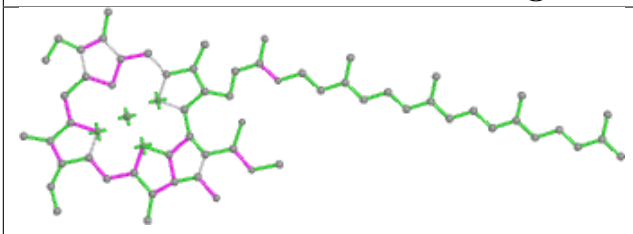


Torsions

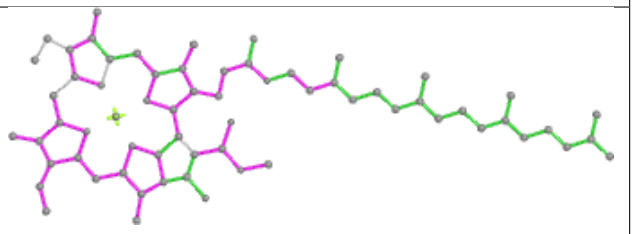


Rings

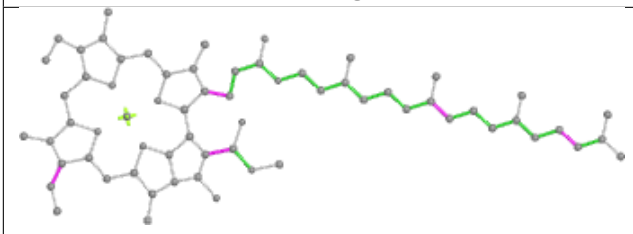
Ligand CLA d 401



Bond lengths



Bond angles



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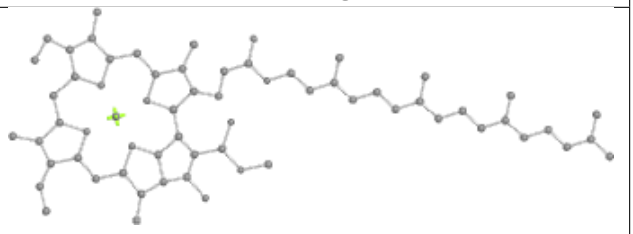
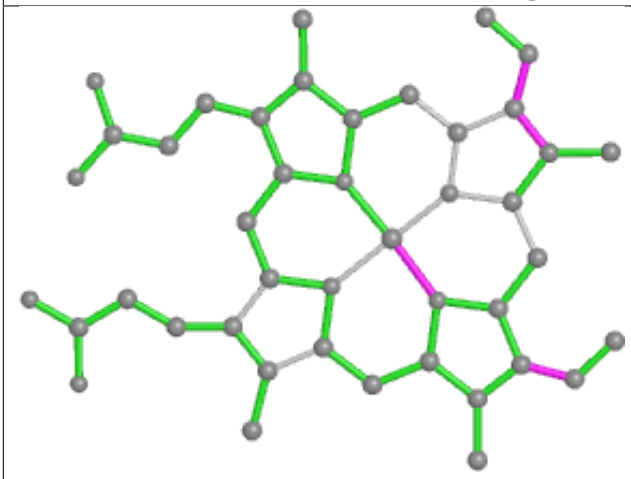
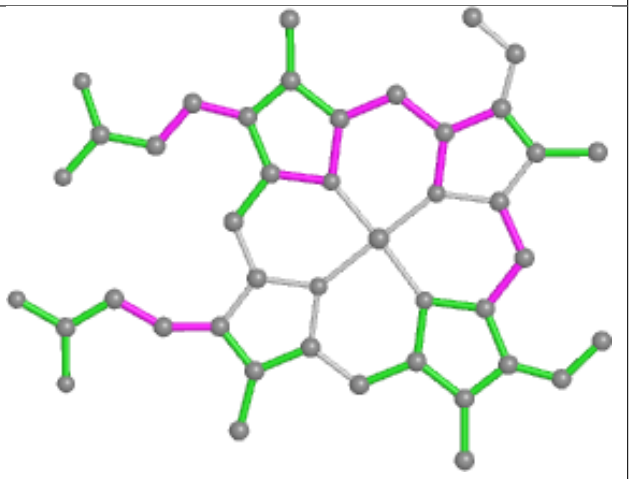


Rings

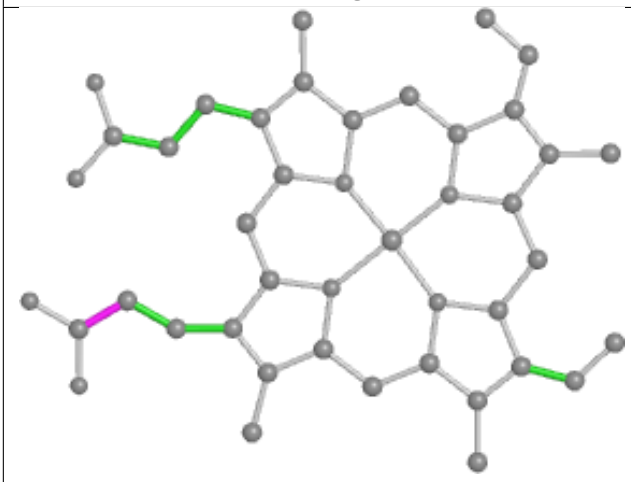
Ligand HEM e 103



Bond lengths



Bond angles



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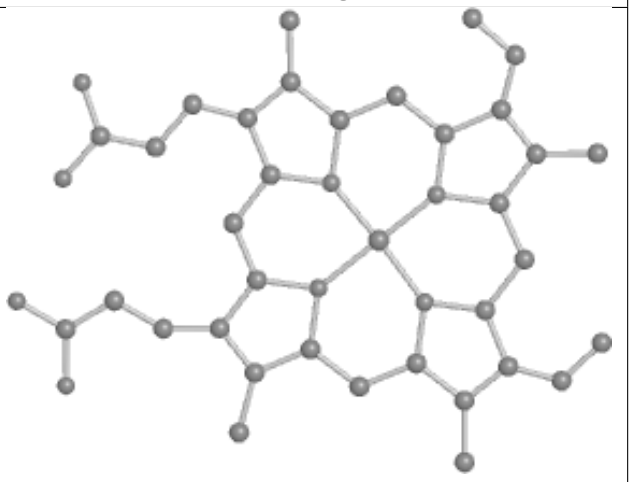
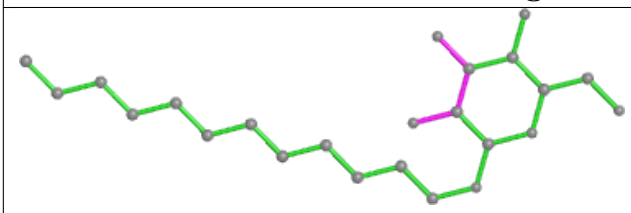
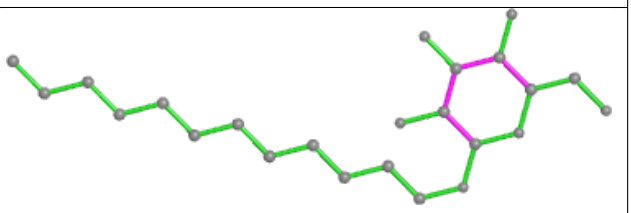


Rings

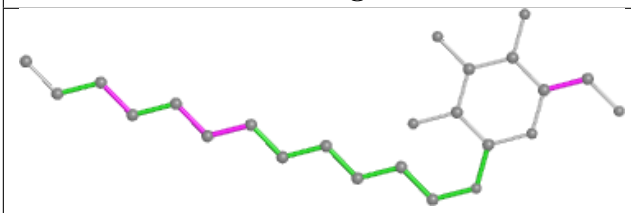
Ligand LMT J 102



Bond lengths



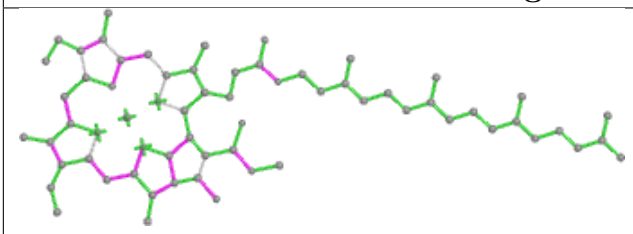
Bond angles



Torsions

Rings

Ligand CLA B 609



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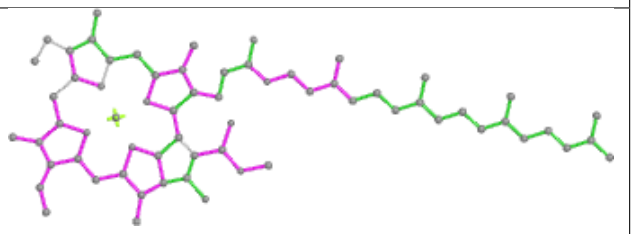
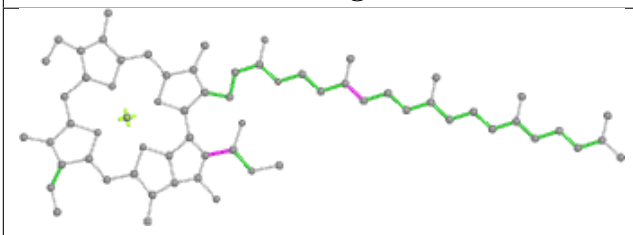


Bond angles



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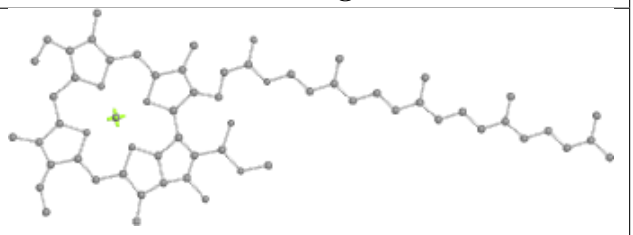
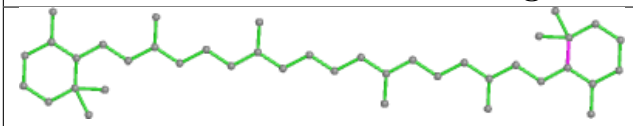
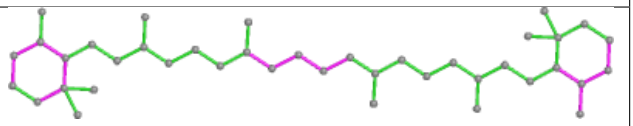


Rings

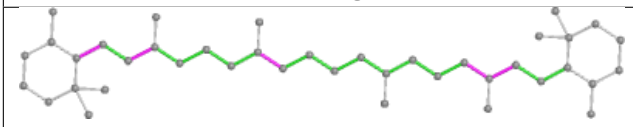
Ligand BCR T 101



Bond lengths



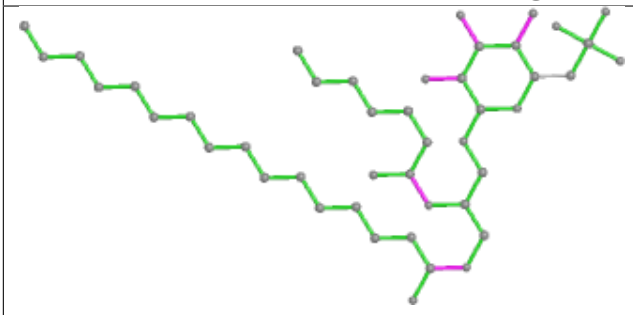
Bond angles



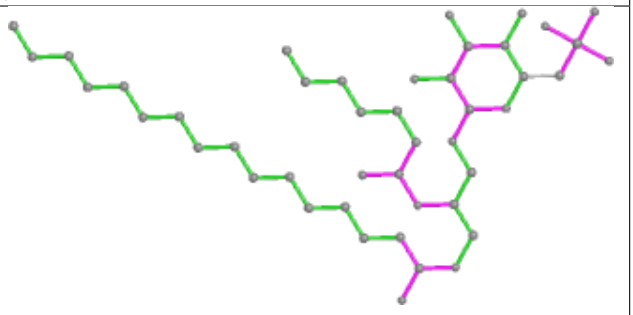
Torsions

Rings

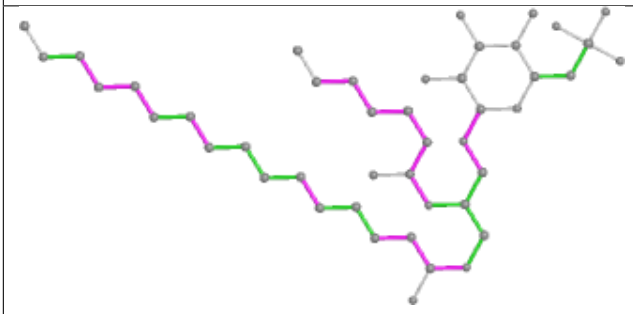
Ligand SQD d 407



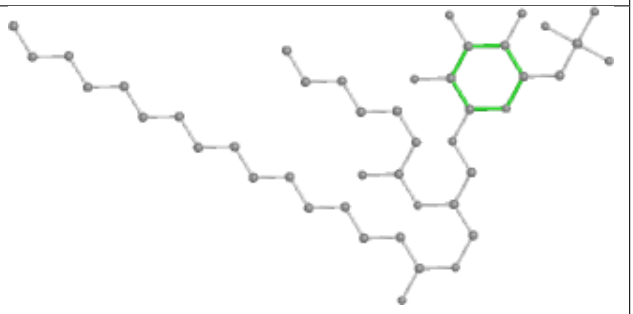
Bond lengths



Bond angles

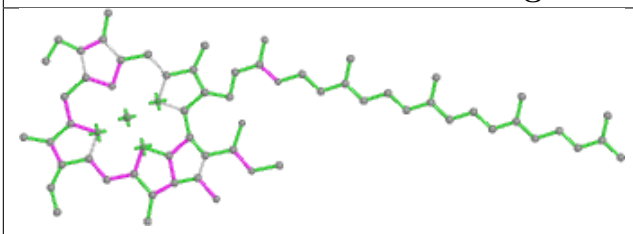


Torsions



Rings

Ligand CLA C 510



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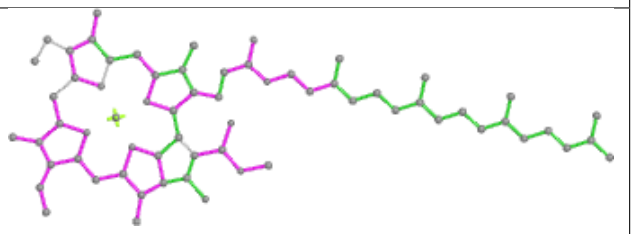
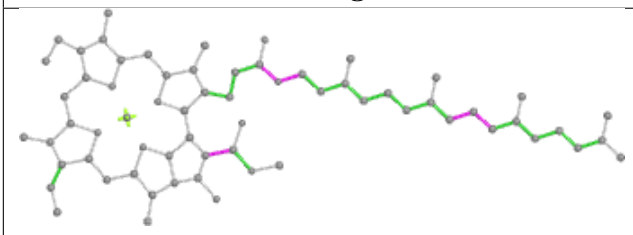
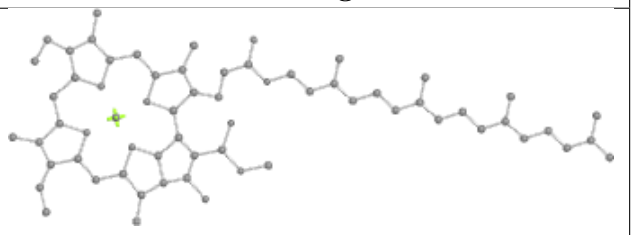


Bond angles

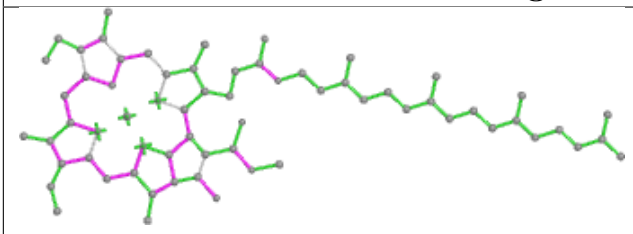


Torsions



Rings

Ligand CLA b 603



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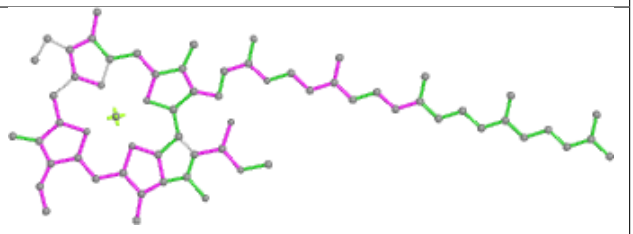
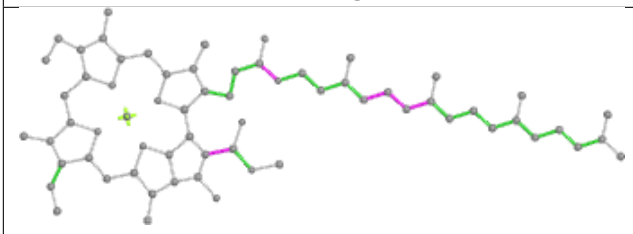
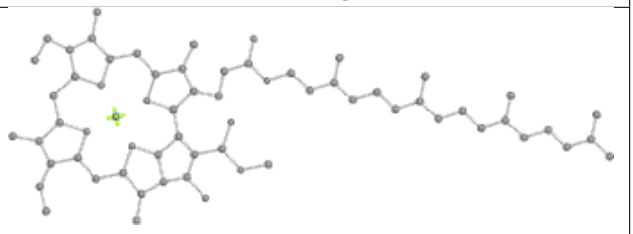


Bond angles

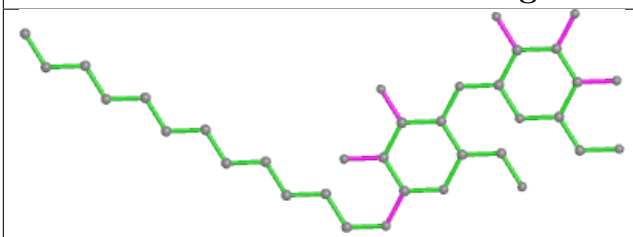


Torsions

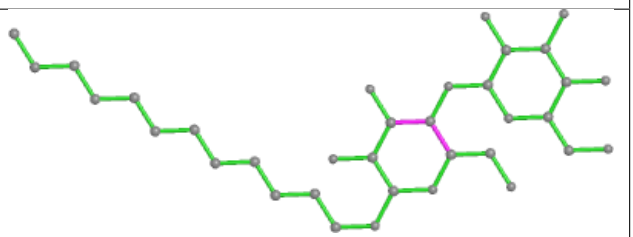


Rings

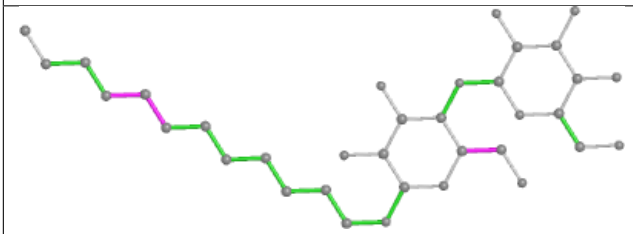
Ligand LMT m 102



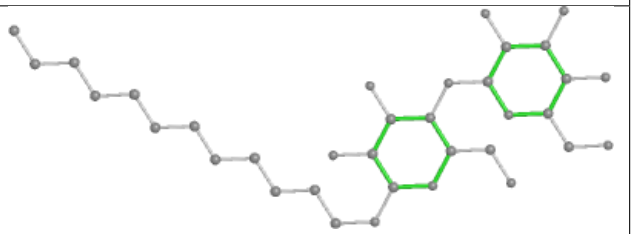
Bond lengths



Bond angles

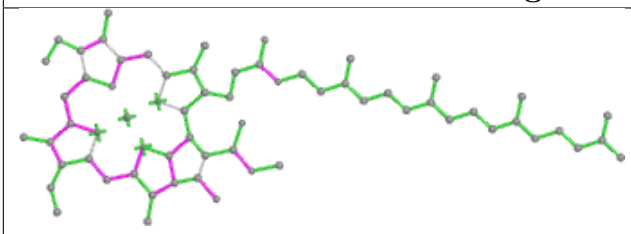


Torsions

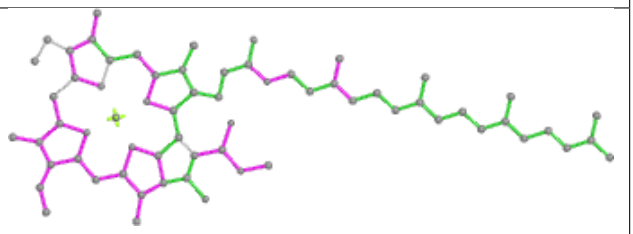


Rings

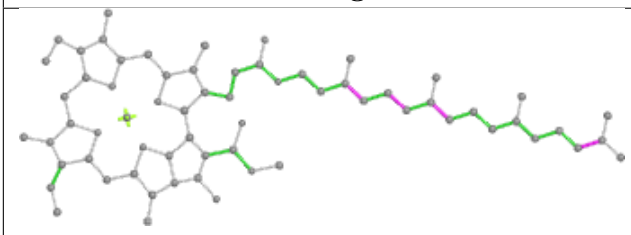
Ligand CLA B 615



Bond lengths



Bond angles



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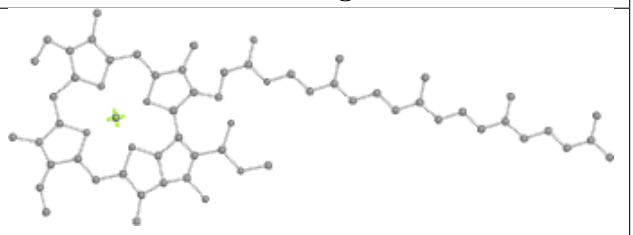
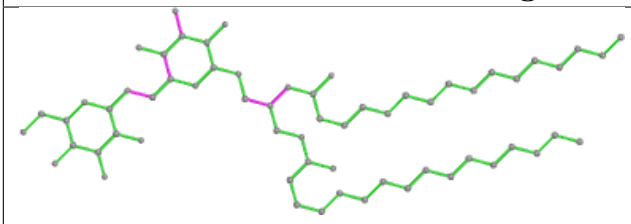
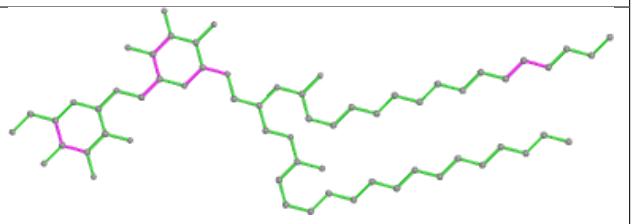


Rings

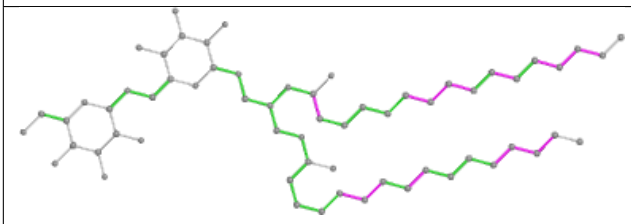
Ligand DGD H 102



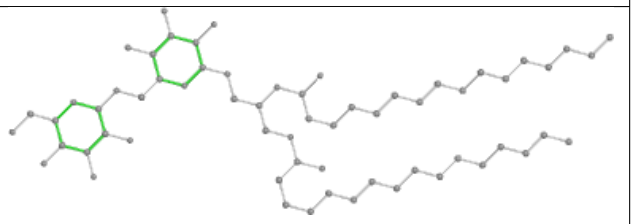
Bond lengths



Bond angles

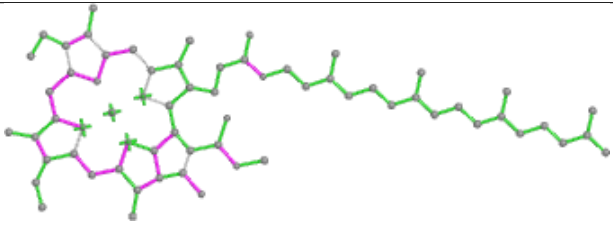


Torsions



Rings

Ligand CLA c 511



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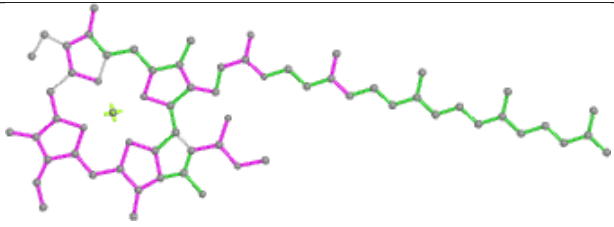
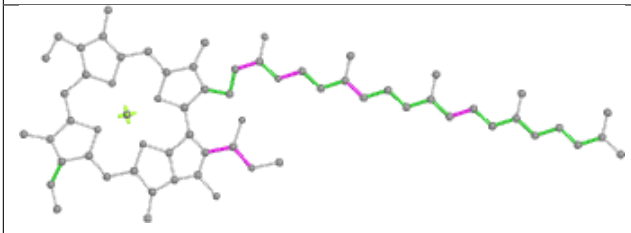
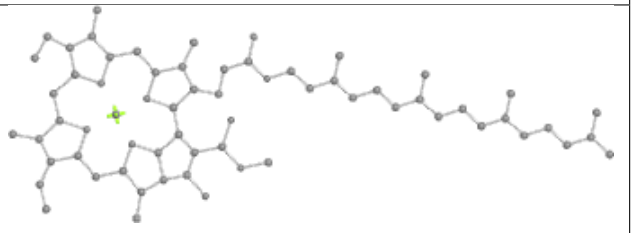


Bond angles

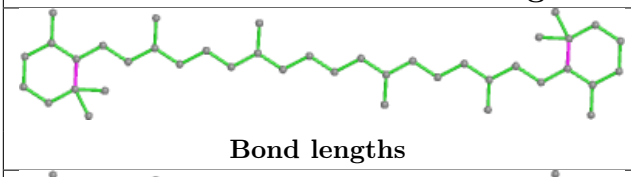


Torsions



Rings

Ligand BCR c 521



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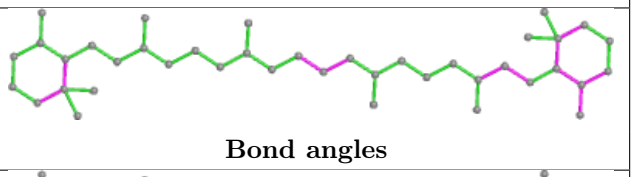
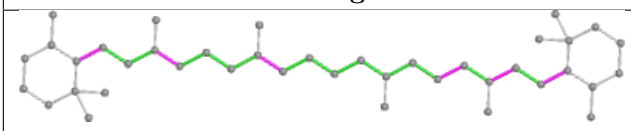


Bond angles



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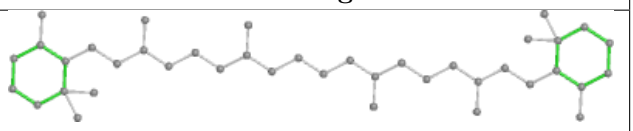
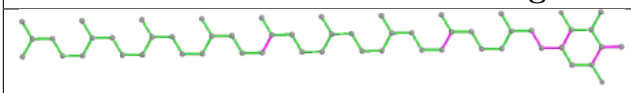


Rings

Ligand PL9 D 406



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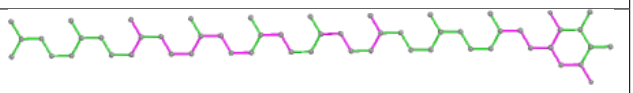
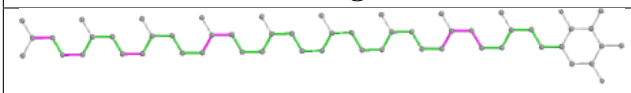
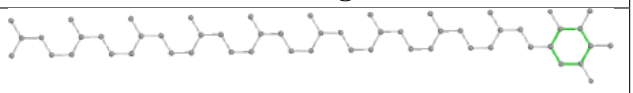


Bond angles

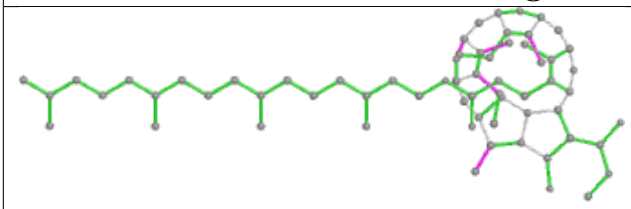


Torsions



Rings

Ligand PHO d 402



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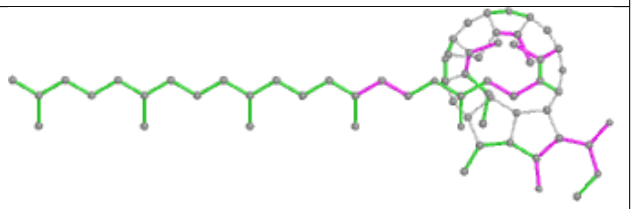
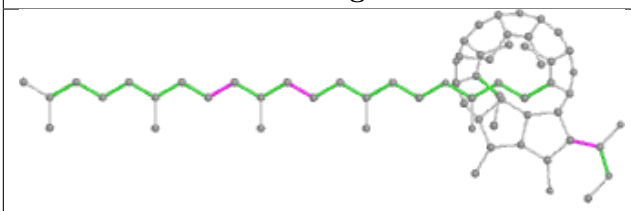
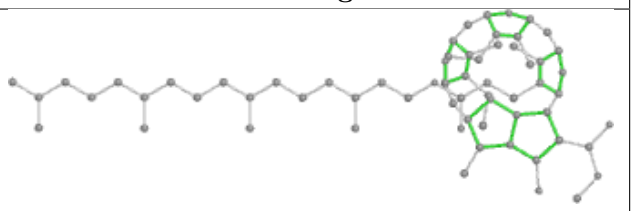


Bond angles

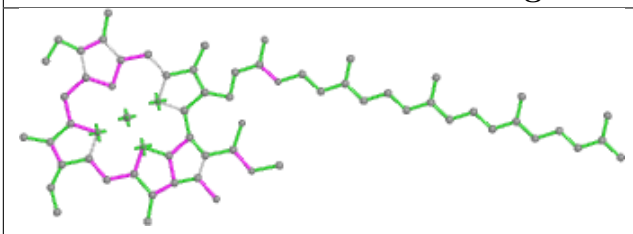


Torsions



Rings

Ligand CLA C 511



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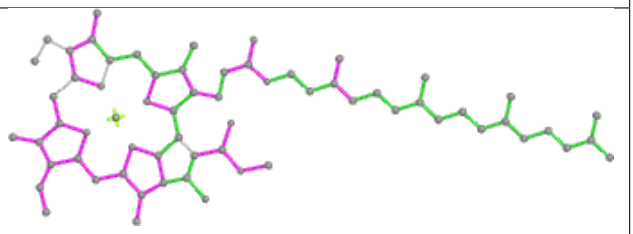
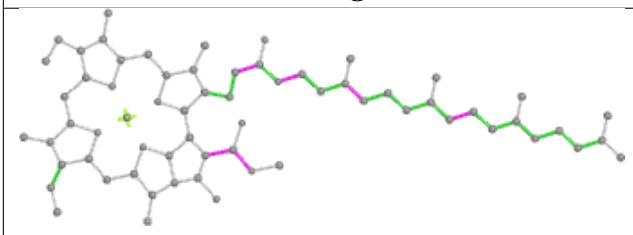


Bond angles



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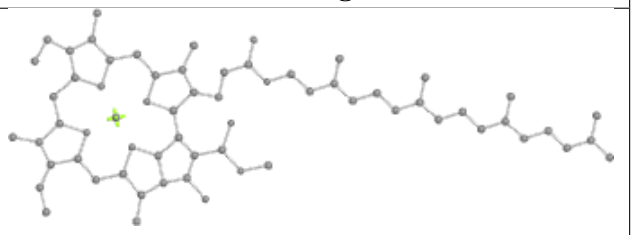
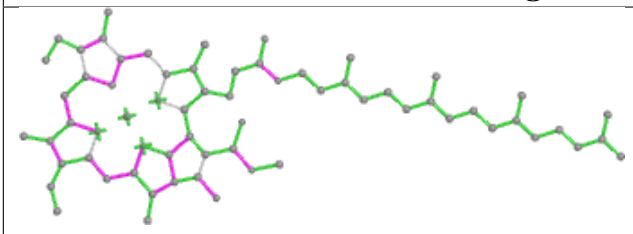


Rings

Ligand CLA B 616



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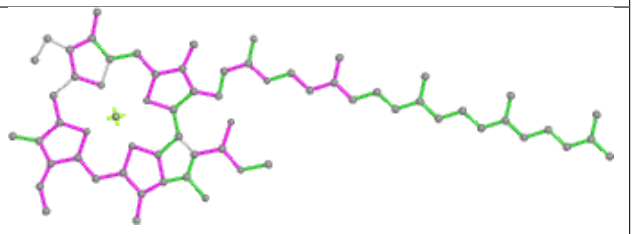
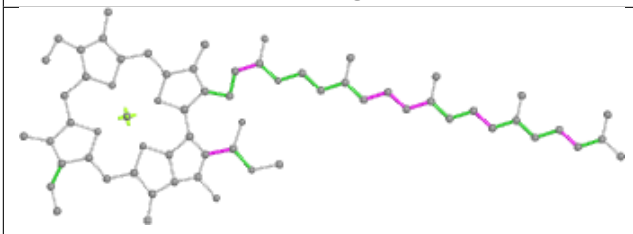
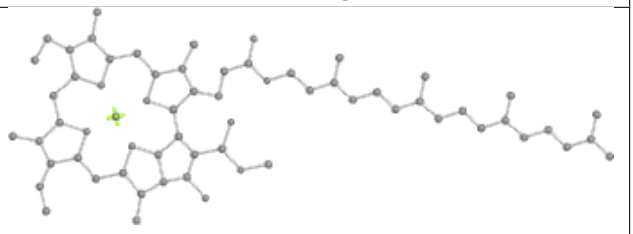


Bond angles

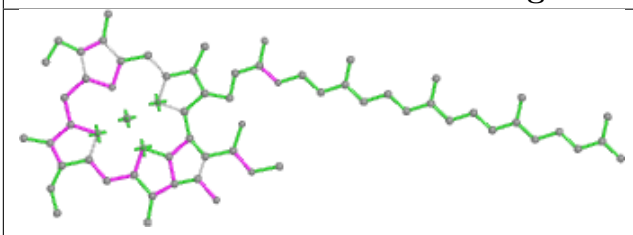


Torsions

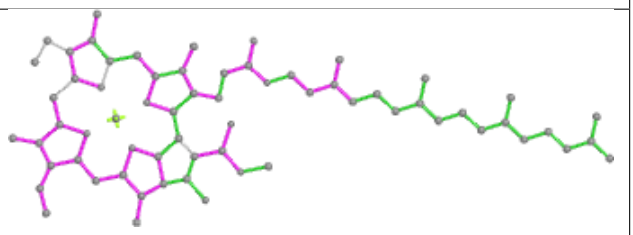


Rings

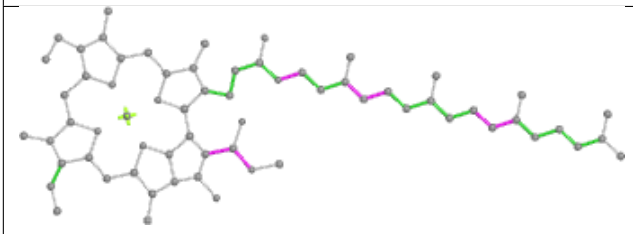
Ligand CLA b 616



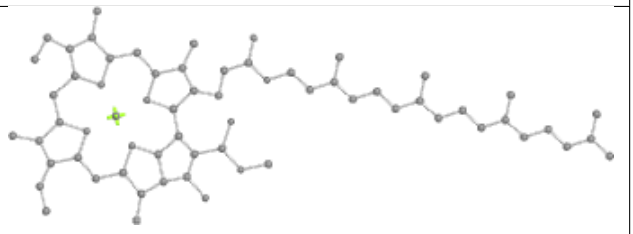
Bond lengths



Bond angles

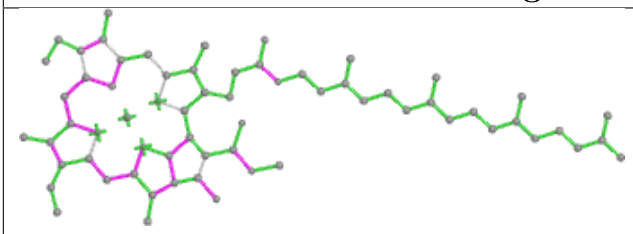


Torsions

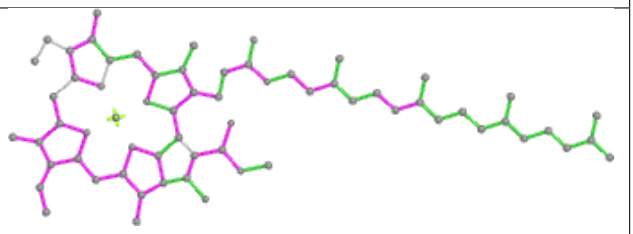


Rings

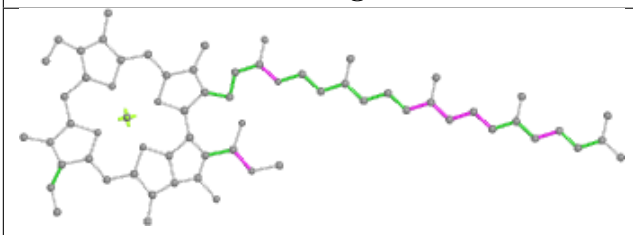
Ligand CLA D 404



Bond lengths



Bond angles



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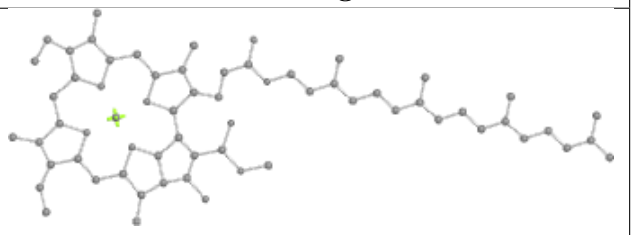
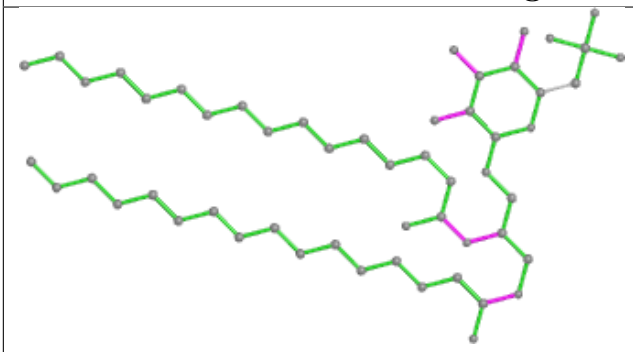


Rings

Ligand SQD A 410



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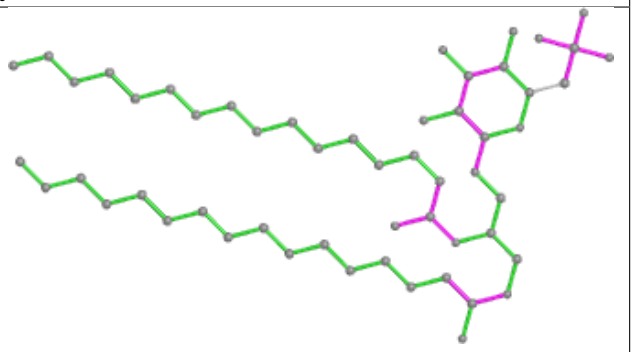
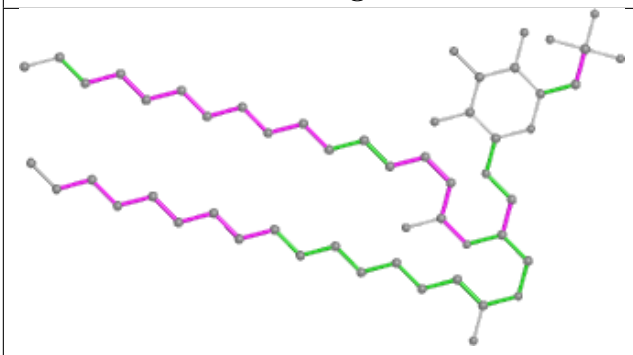
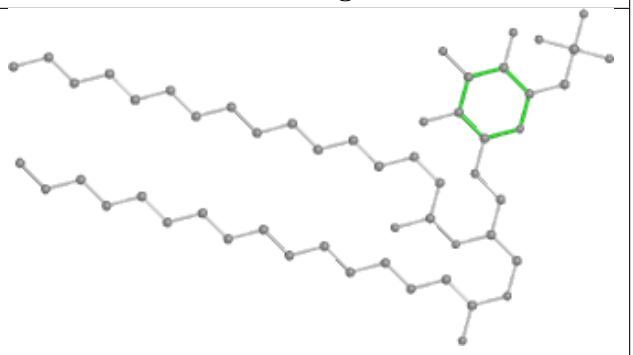


Bond angles

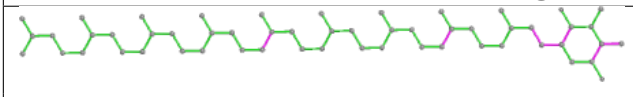


Torsions

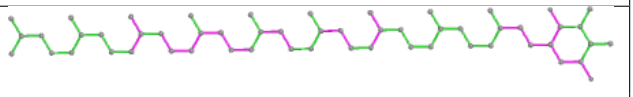


Rings

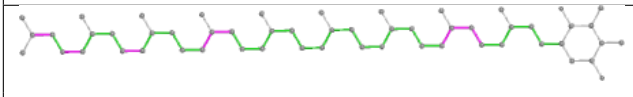
Ligand PL9 d 406



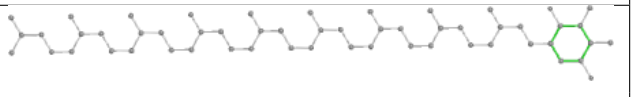
Bond lengths



Bond angles

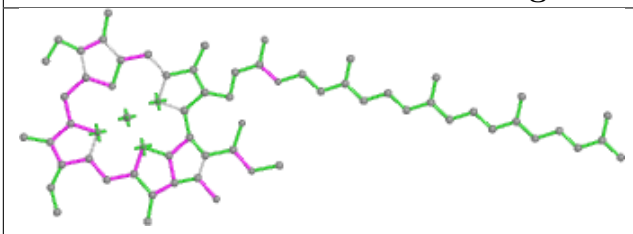


Torsions



Rings

Ligand CLA c 513



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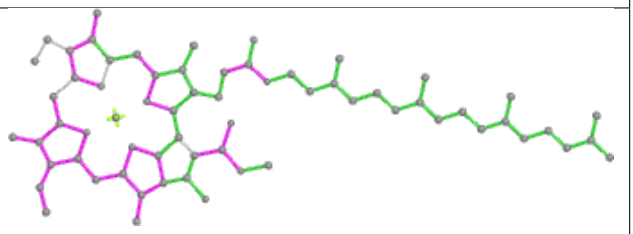
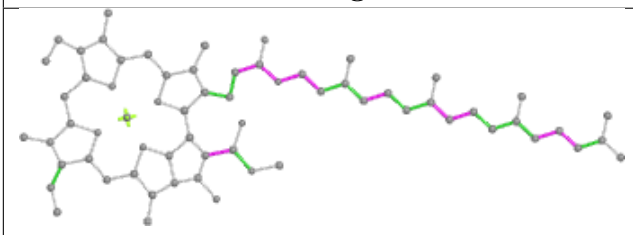
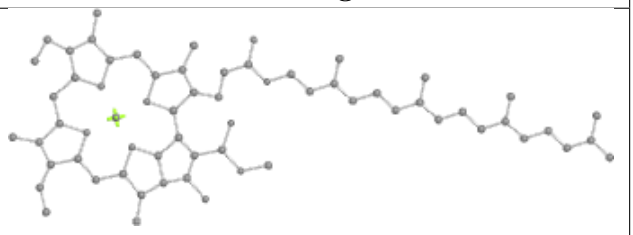


Bond angles

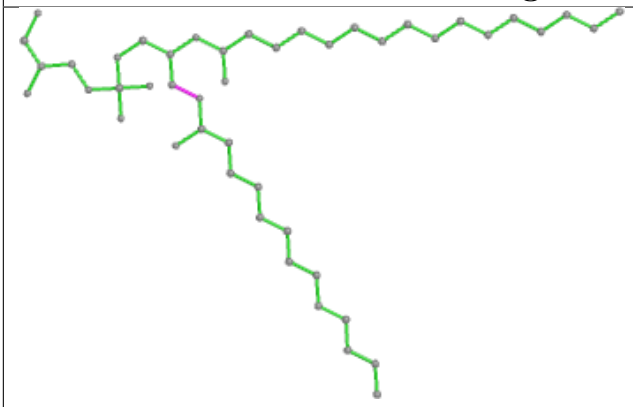


Torsions

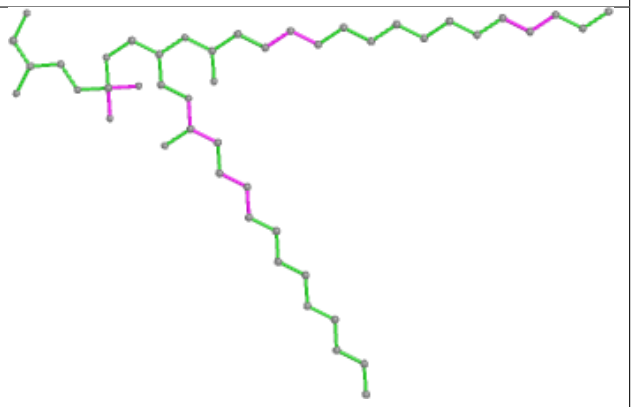


Rings

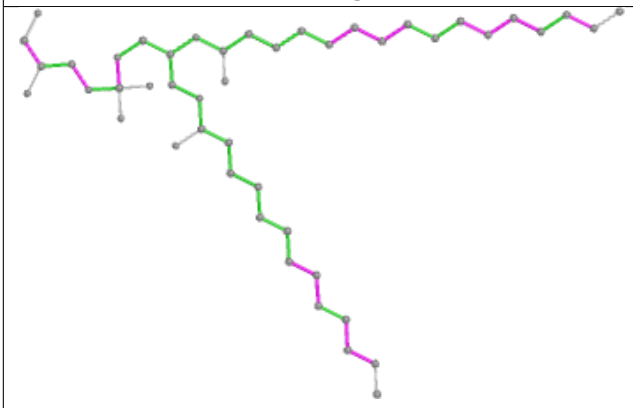
Ligand LHG D 410



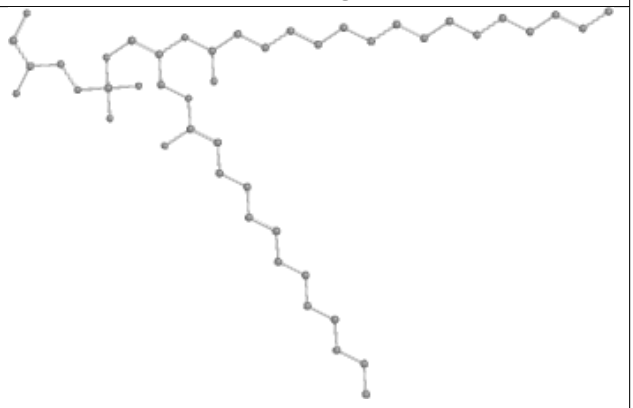
Bond lengths



Bond angles

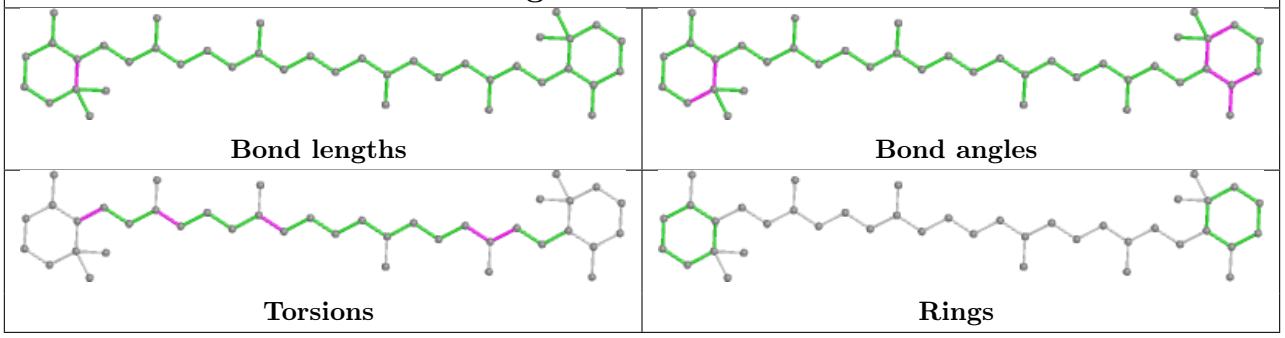


Torsions

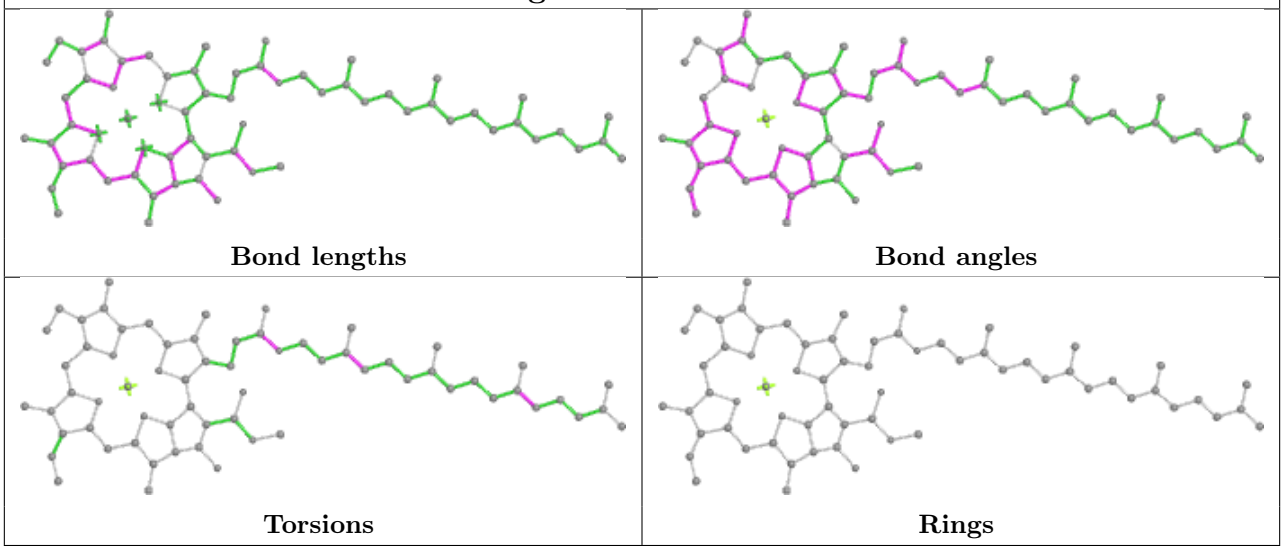


Rings

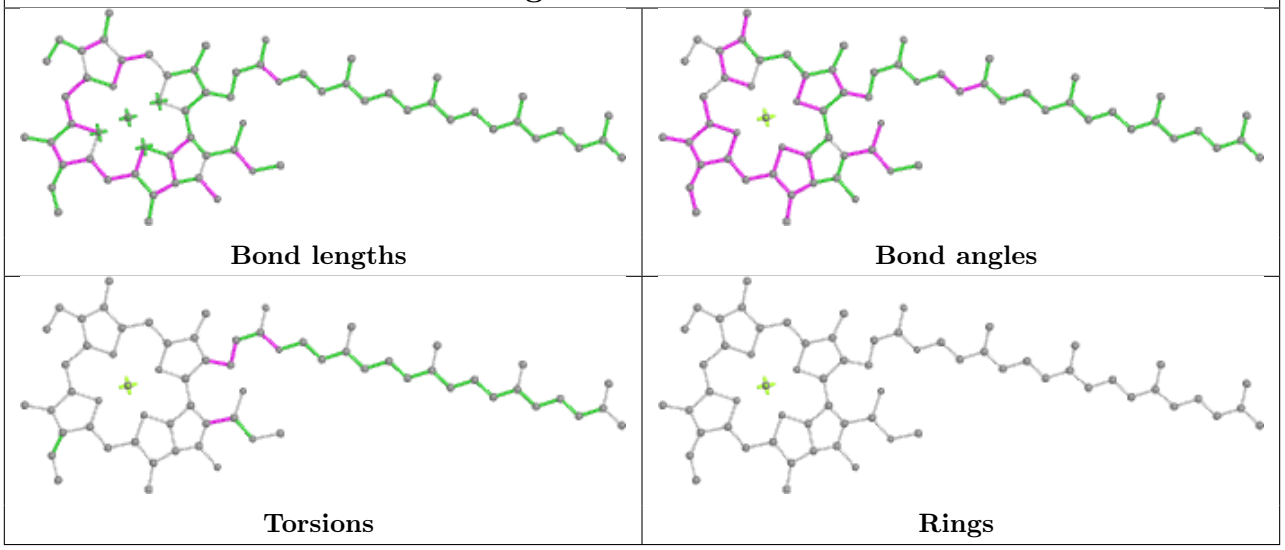
Ligand BCR b 619



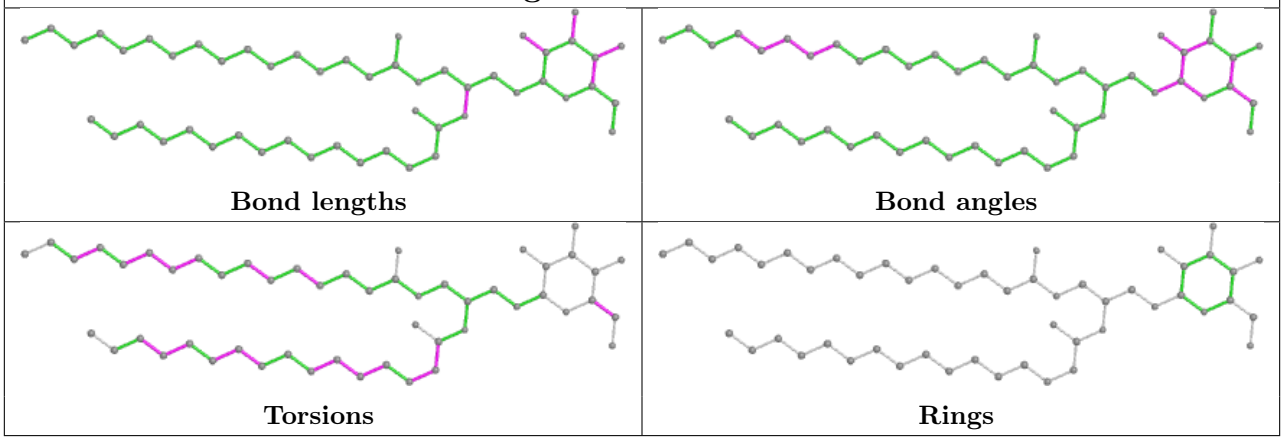
Ligand CLA b 613



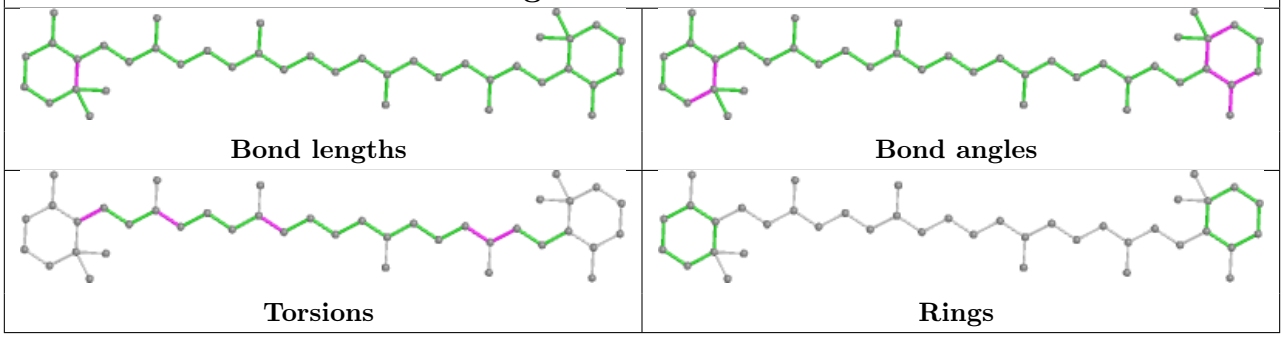
Ligand CLA C 502



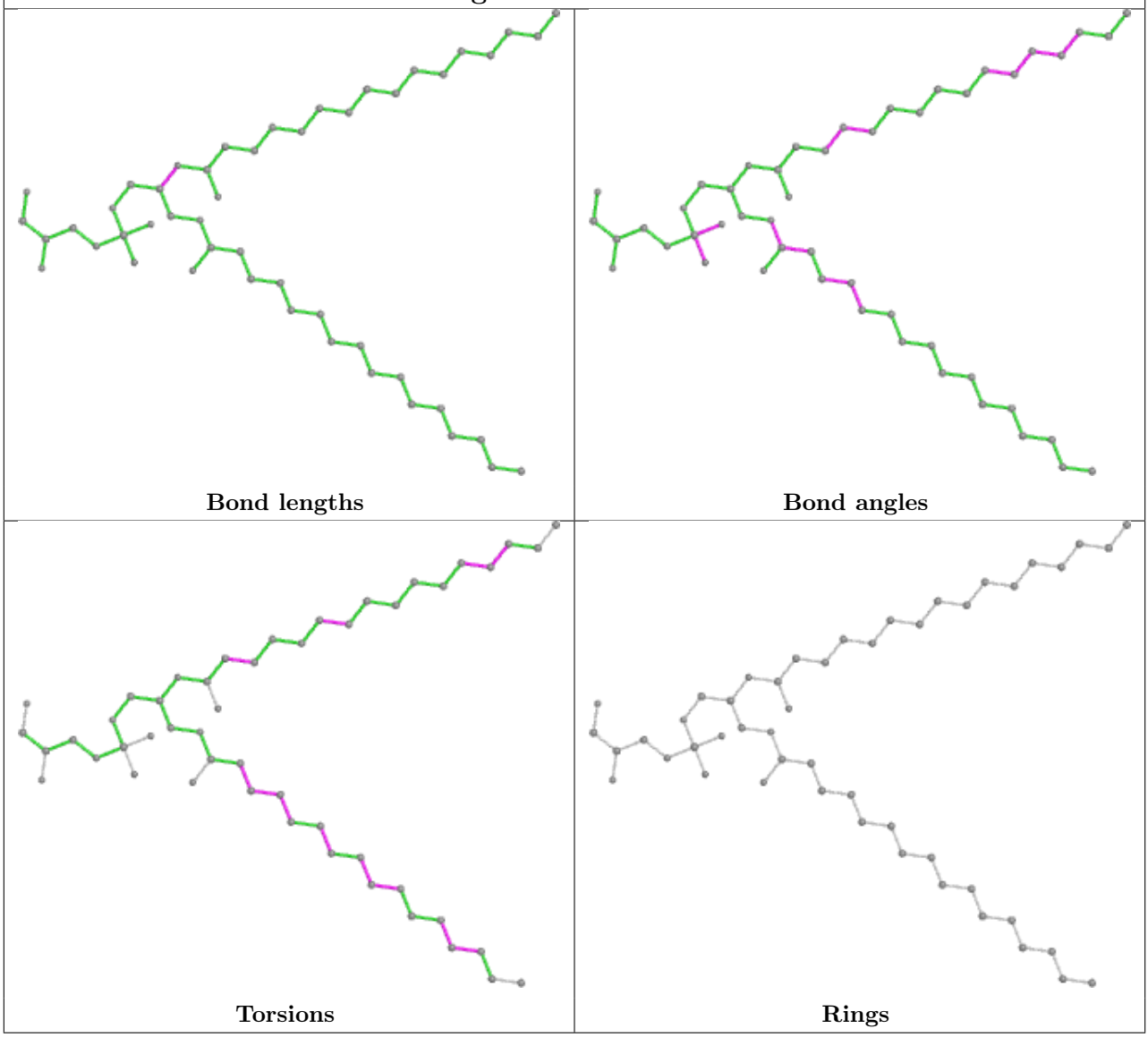
Ligand LMG d 411



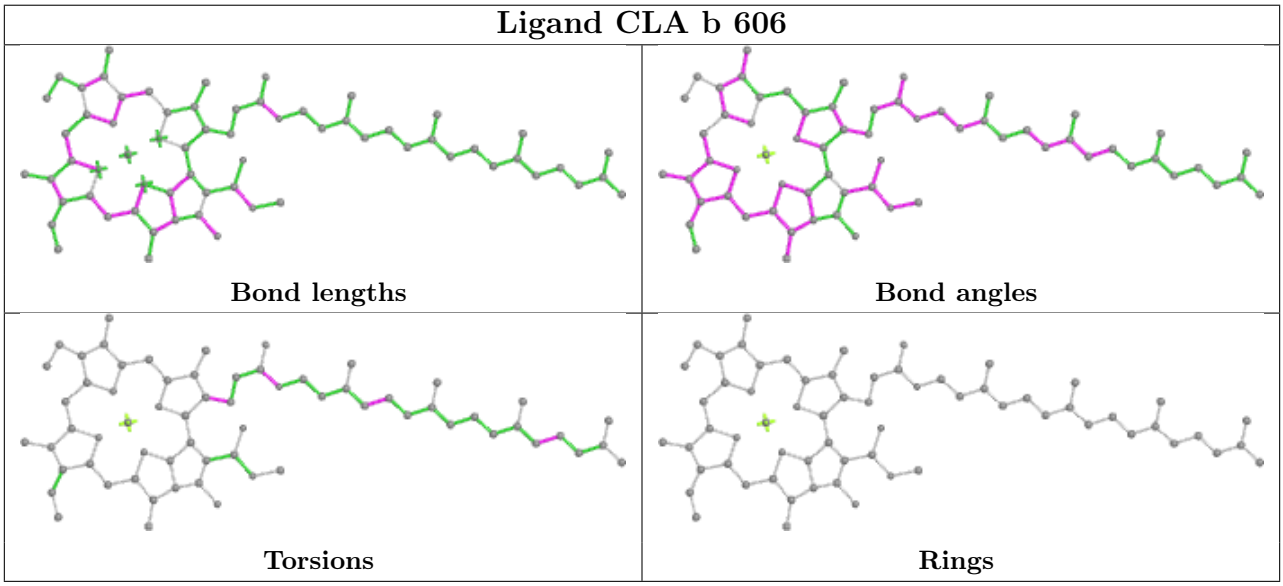
Ligand BCR B 617



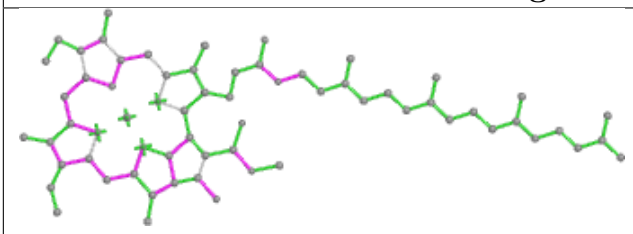
Ligand LHG d 408



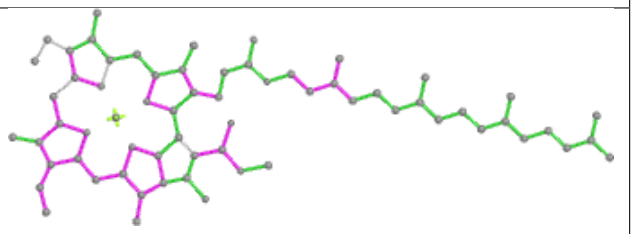
Ligand CLA b 606



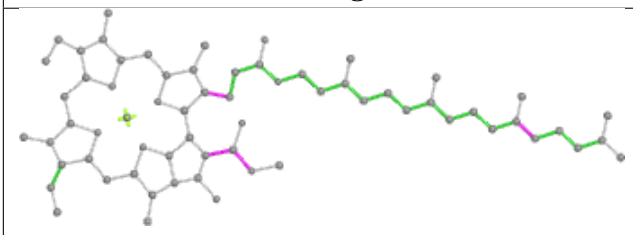
Ligand CLA c 503



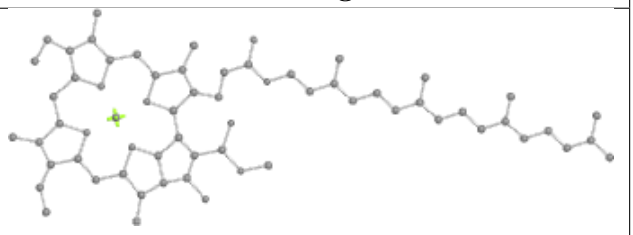
Bond lengths



Bond angles

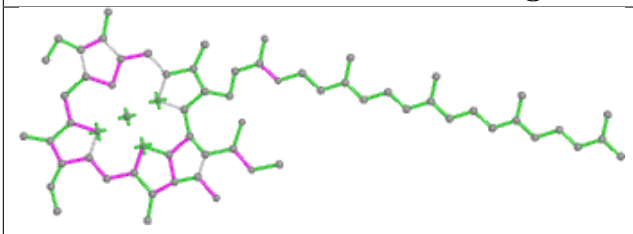


Torsions

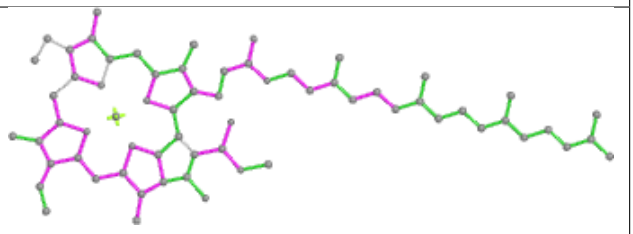


Rings

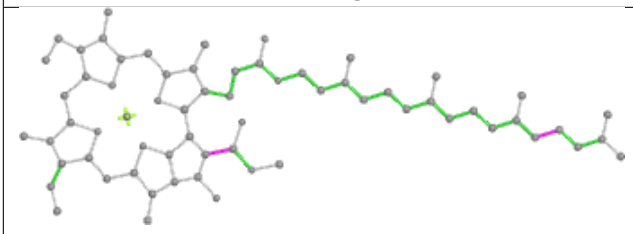
Ligand CLA C 509



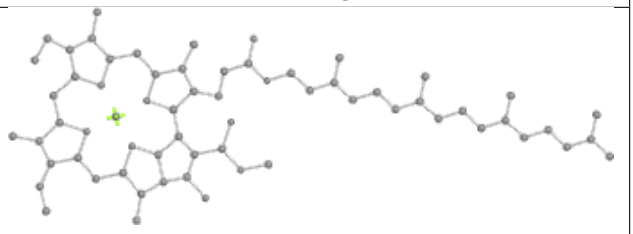
Bond lengths



Bond angles

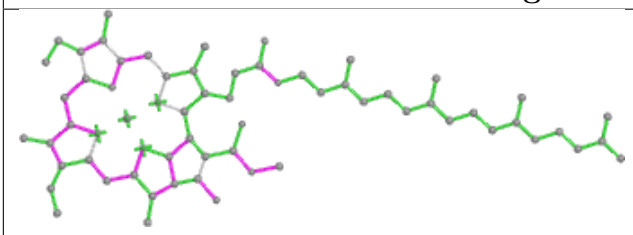


Torsions

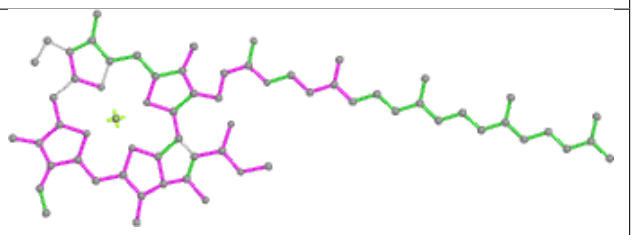


Rings

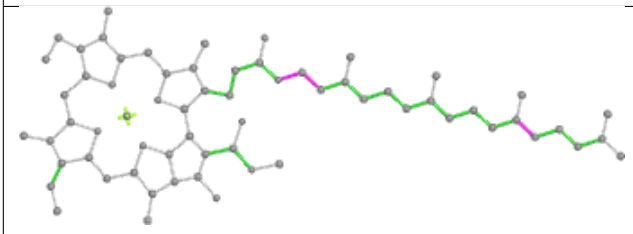
Ligand CLA D 403



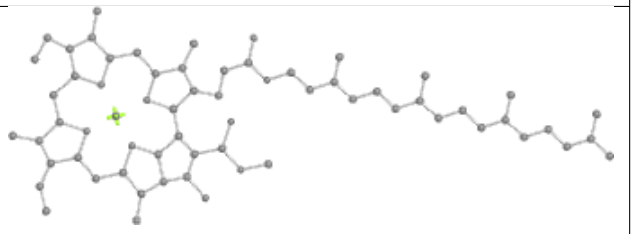
Bond lengths



Bond angles

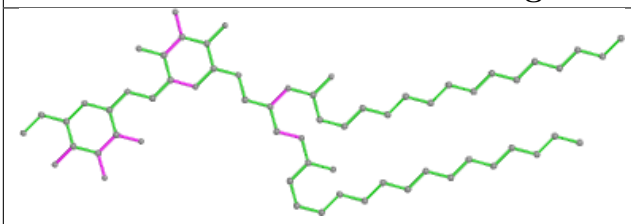


Torsions



Rings

Ligand DGD c 518



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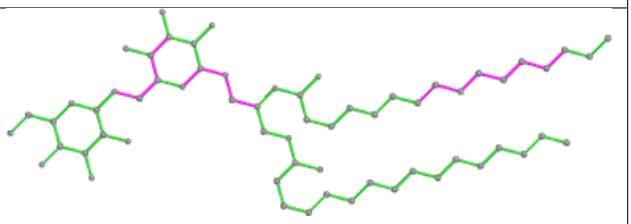
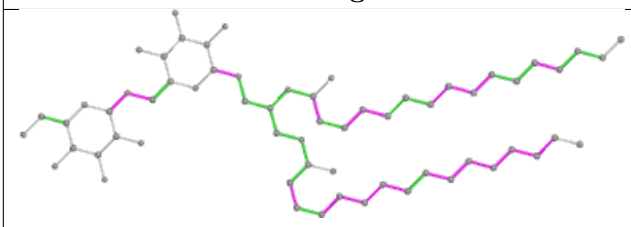
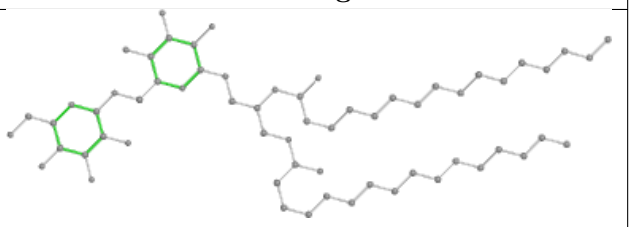


Bond angles

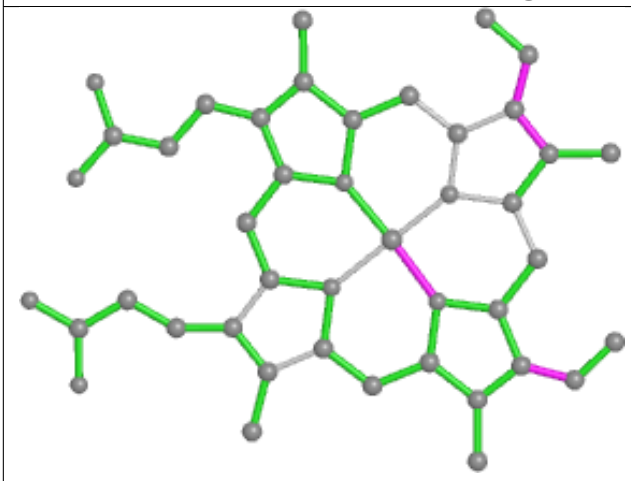


Torsions

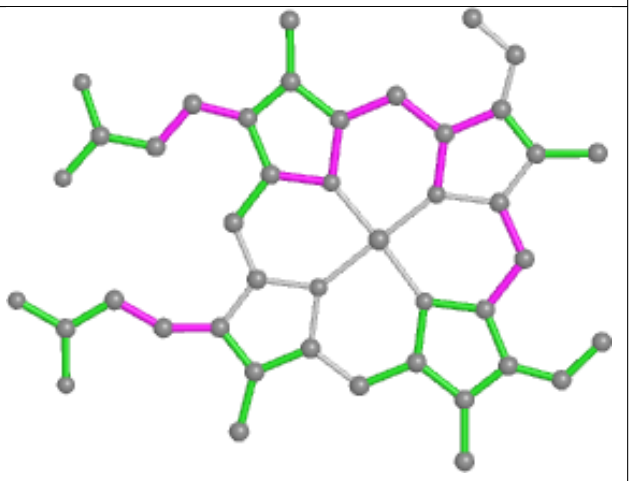


Rings

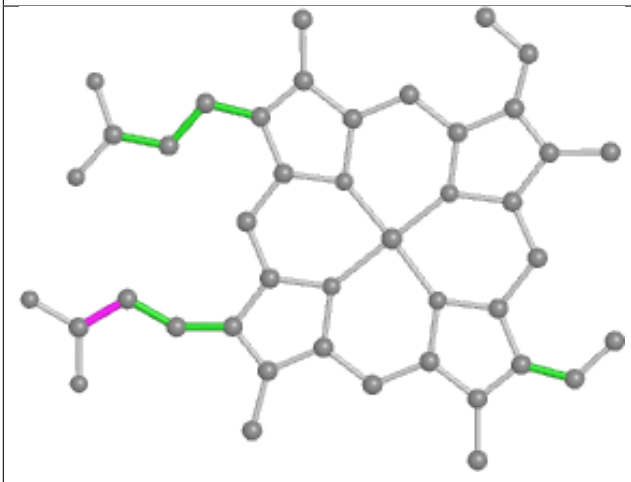
Ligand HEM E 103



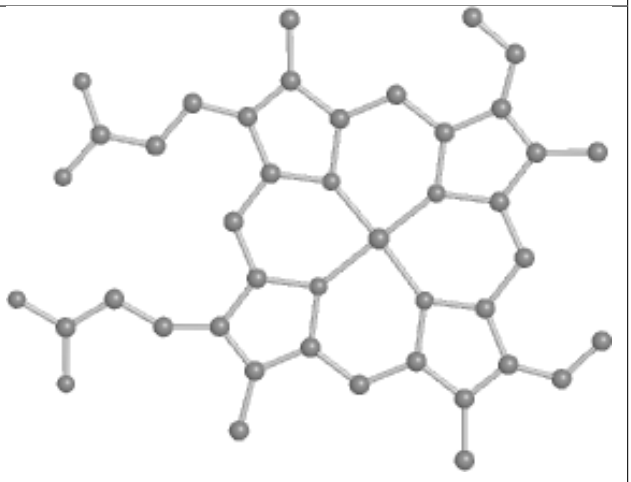
Bond lengths



Bond angles

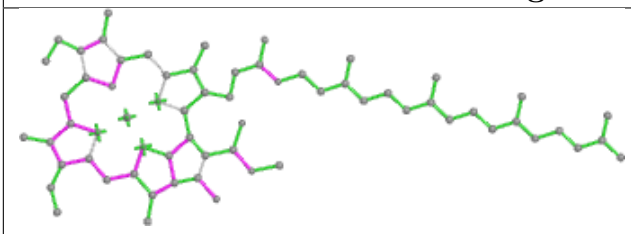


Torsions

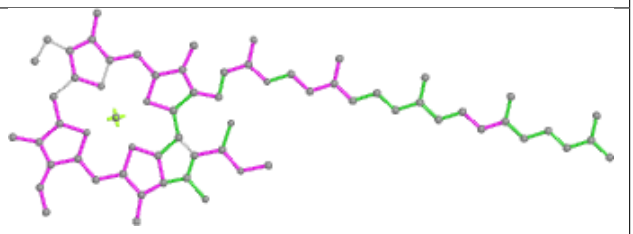


Rings

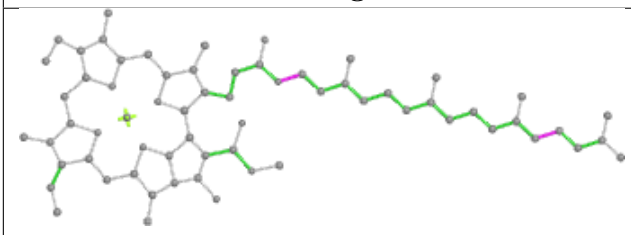
Ligand CLA b 610



Bond lengths



Bond angles



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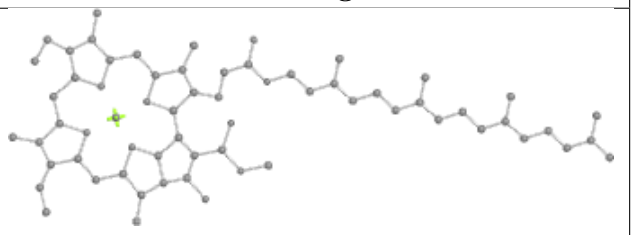
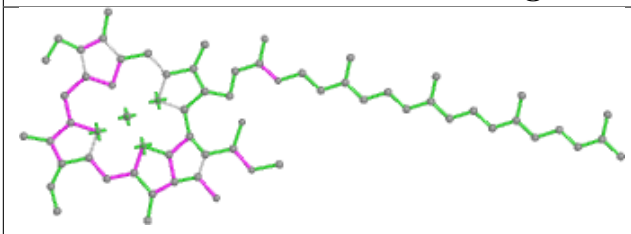


Rings

Ligand CLA B 612



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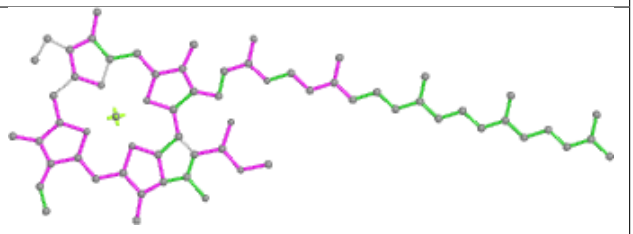
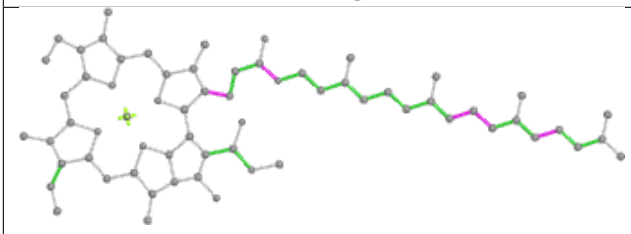
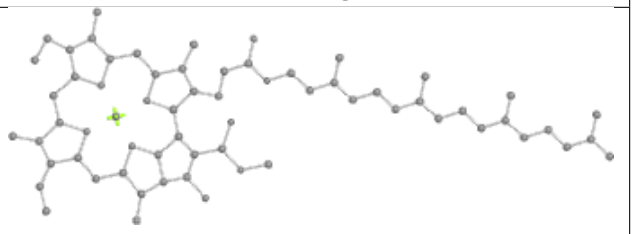


Bond angles

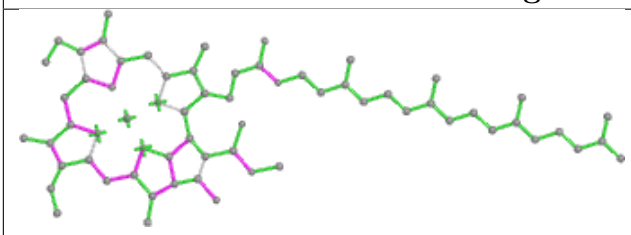


Torsions

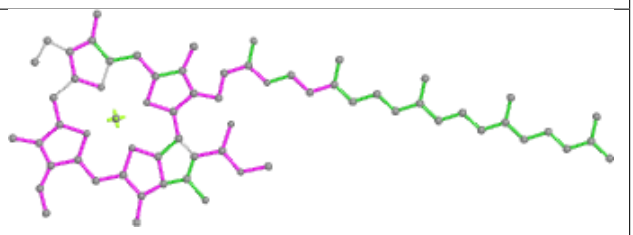


Rings

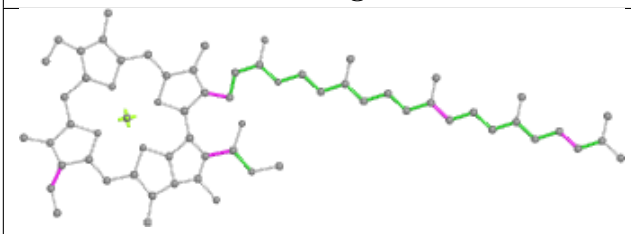
Ligand CLA D 401



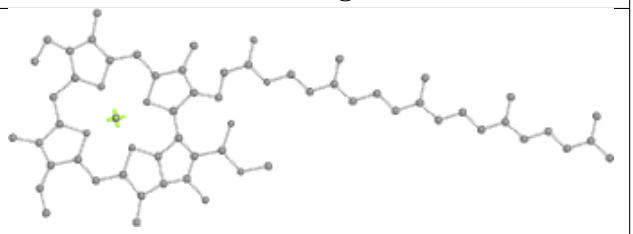
Bond lengths



Bond angles

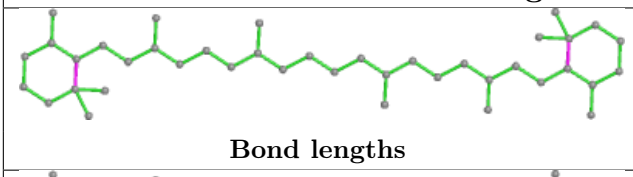


Torsions



Rings

Ligand BCR b 621



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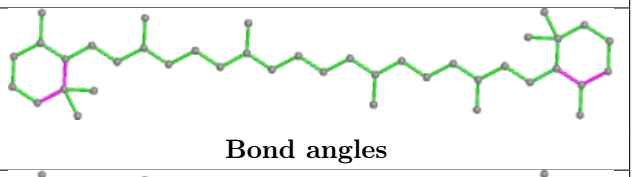
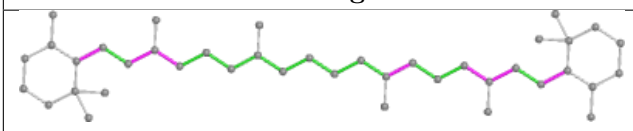
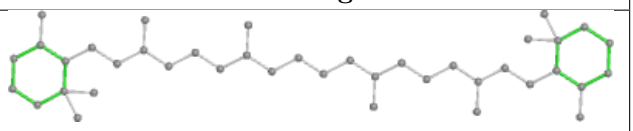


Bond angles

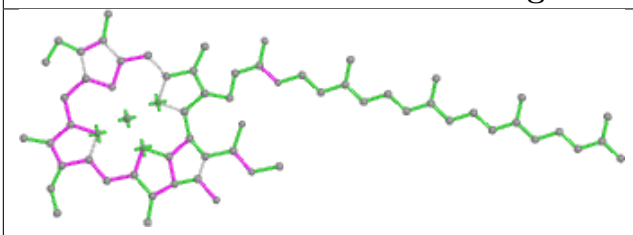


Torsions

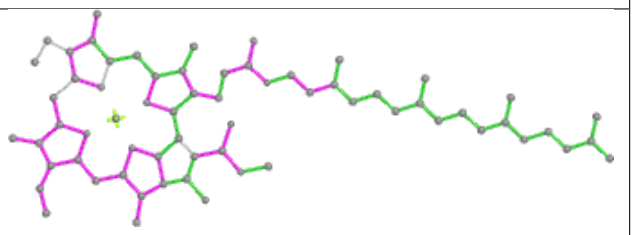


Rings

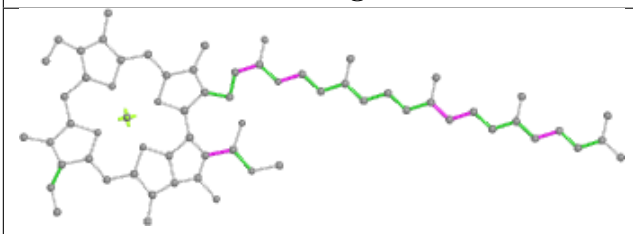
Ligand CLA b 615



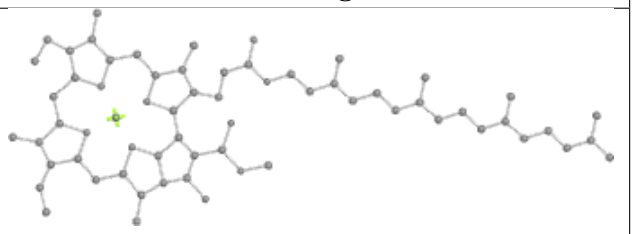
Bond lengths



Bond angles

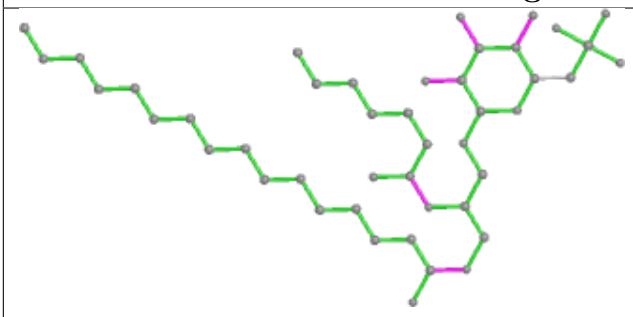


Torsions



Rings

Ligand SQD D 407



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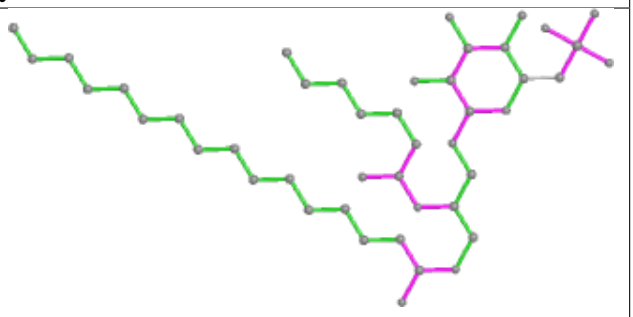
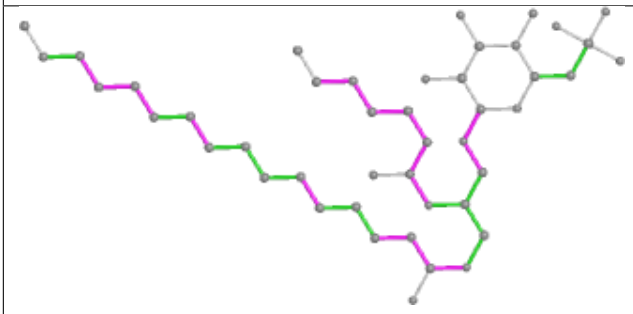
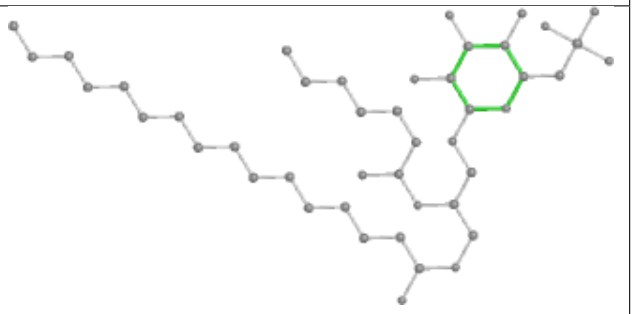


Bond angles

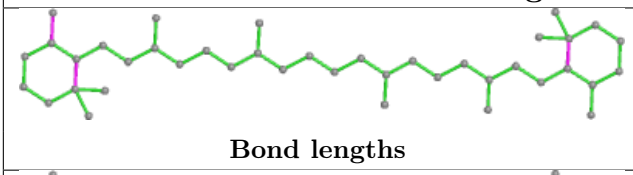


Torsions

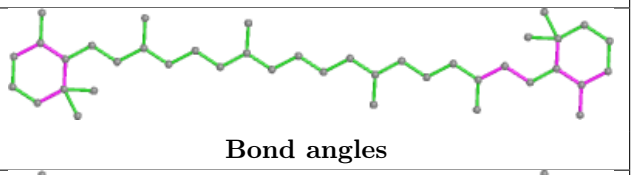


Rings

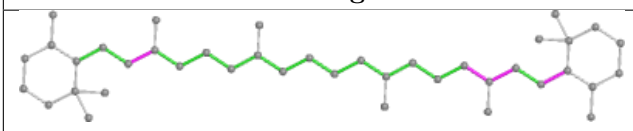
Ligand BCR d 405



Bond lengths



Bond angles



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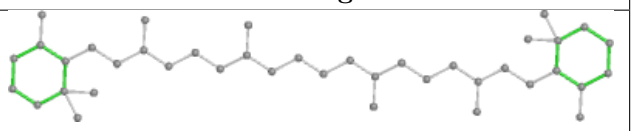
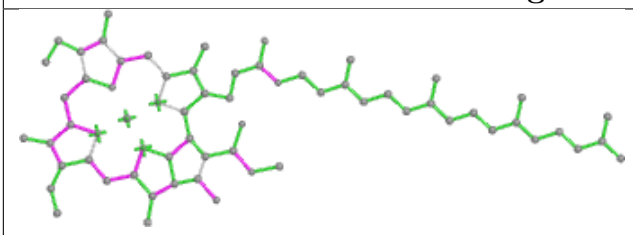
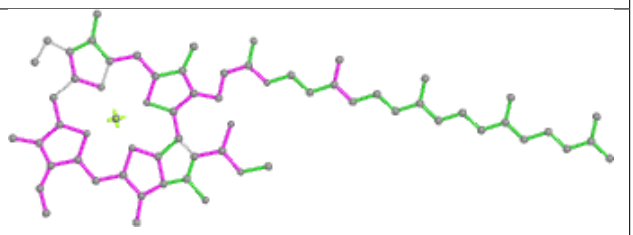


Rings

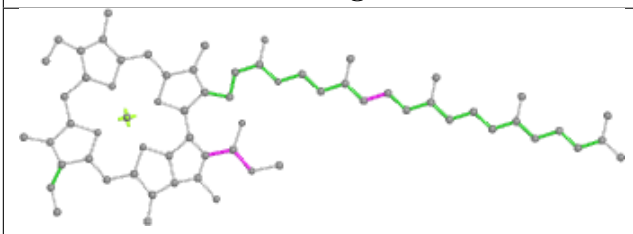
Ligand CLA b 609



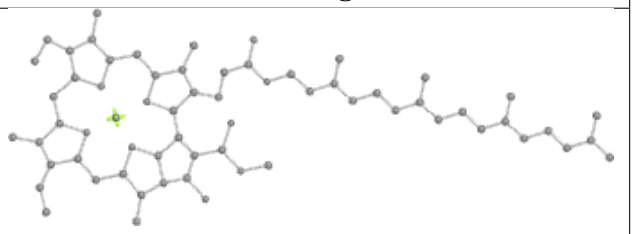
Bond lengths



Bond angles

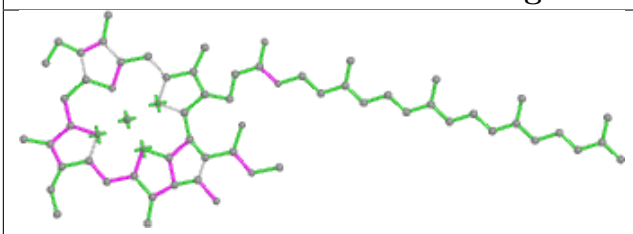


Torsions

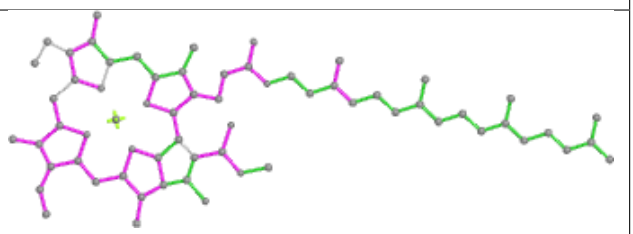


Rings

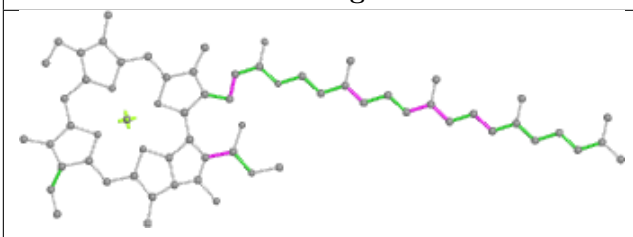
Ligand CLA B 603



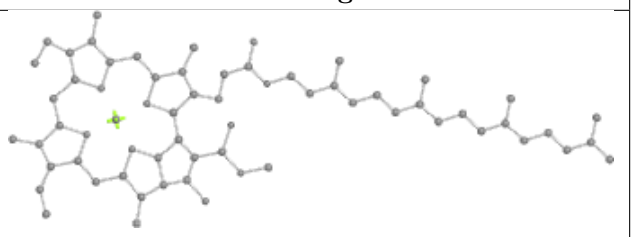
Bond lengths



Bond angles

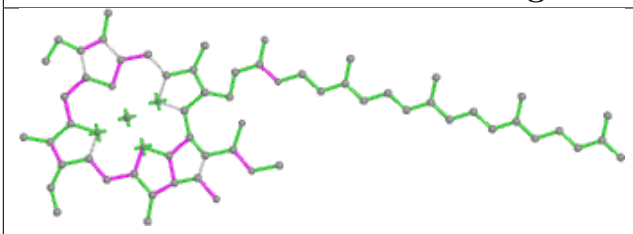


Torsions

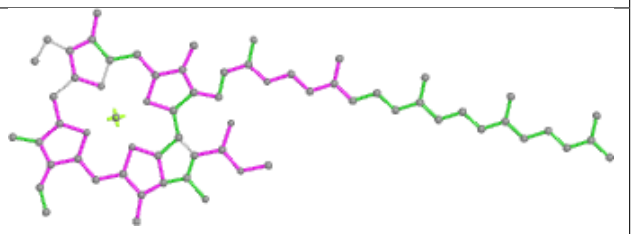


Rings

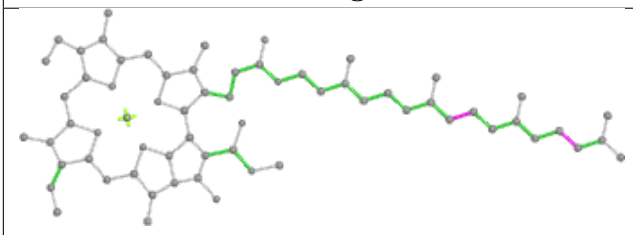
Ligand CLA b 604



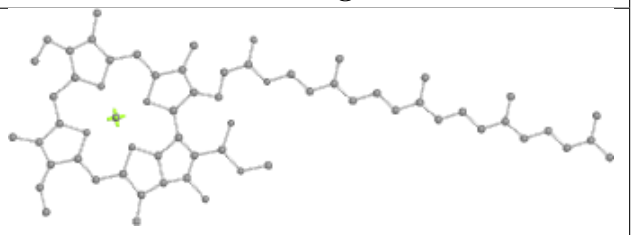
Bond lengths



Bond angles

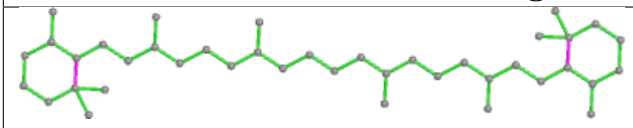


Torsions

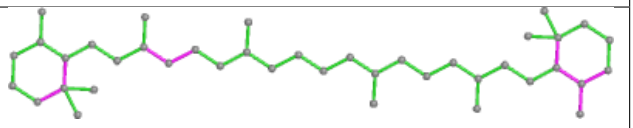


Rings

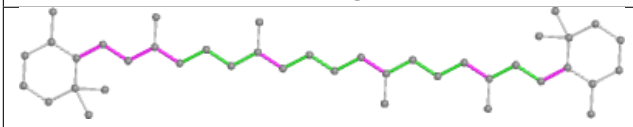
Ligand BCR c 516



Bond lengths



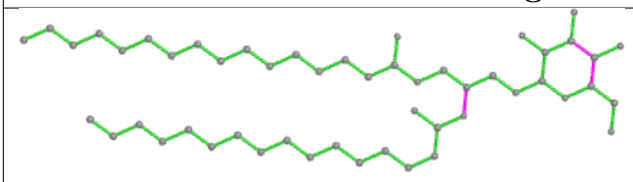
Bond angles



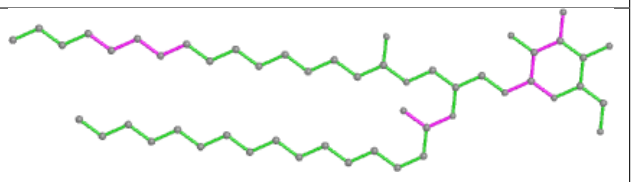
Torsions

Rings

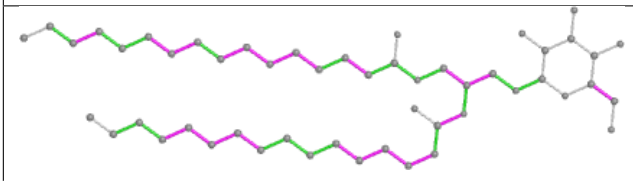
Ligand LMG c 501



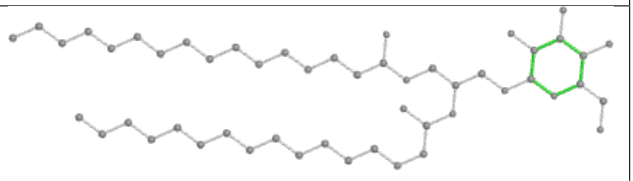
Bond lengths



Bond angles

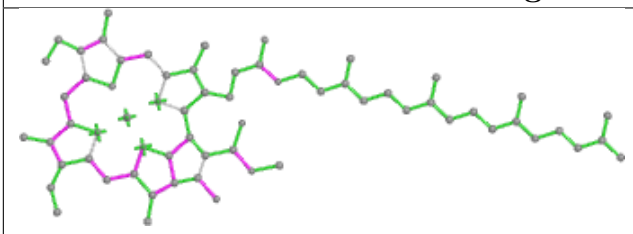


Torsions

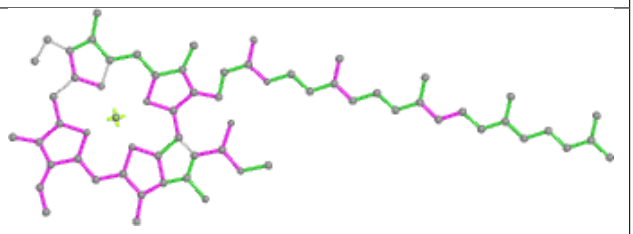


Rings

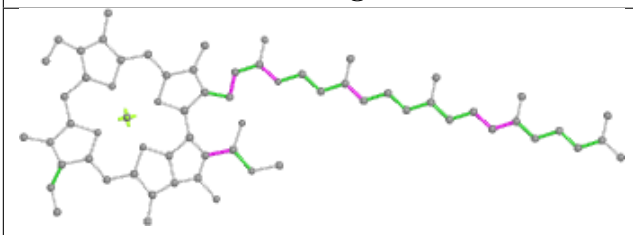
Ligand CLA B 605



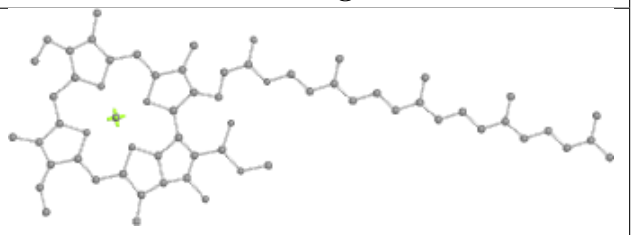
Bond lengths



Bond angles

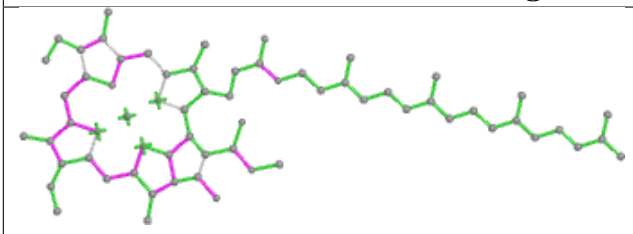


Torsions

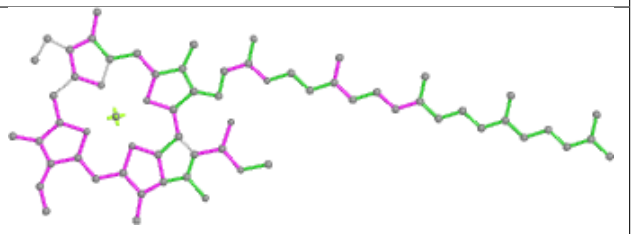


Rings

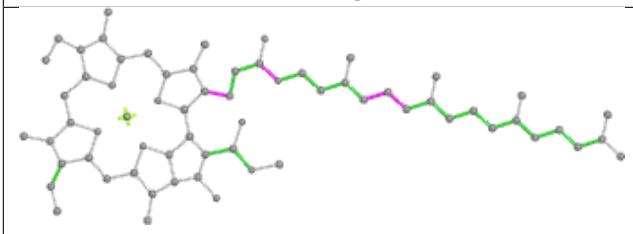
Ligand CLA C 512



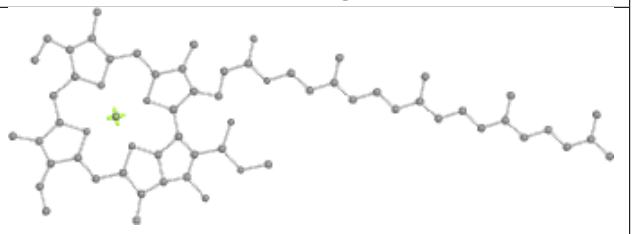
Bond lengths



Bond angles

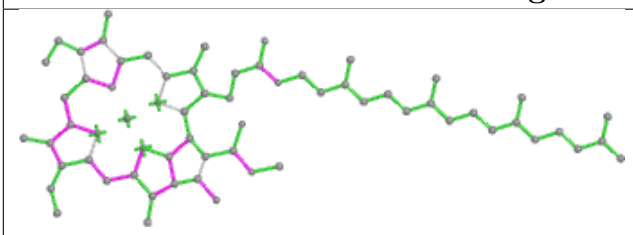


Torsions

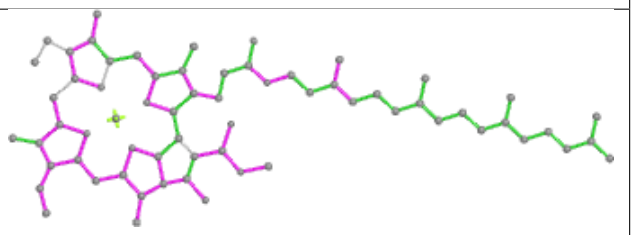


Rings

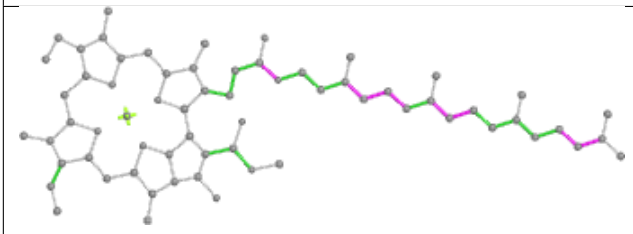
Ligand CLA a 408



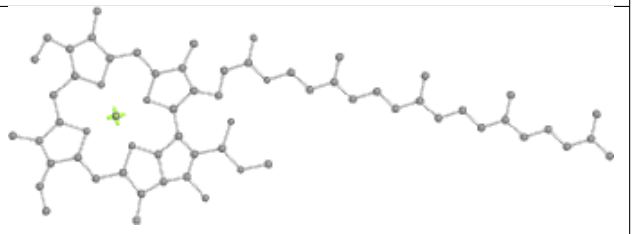
Bond lengths



Bond angles

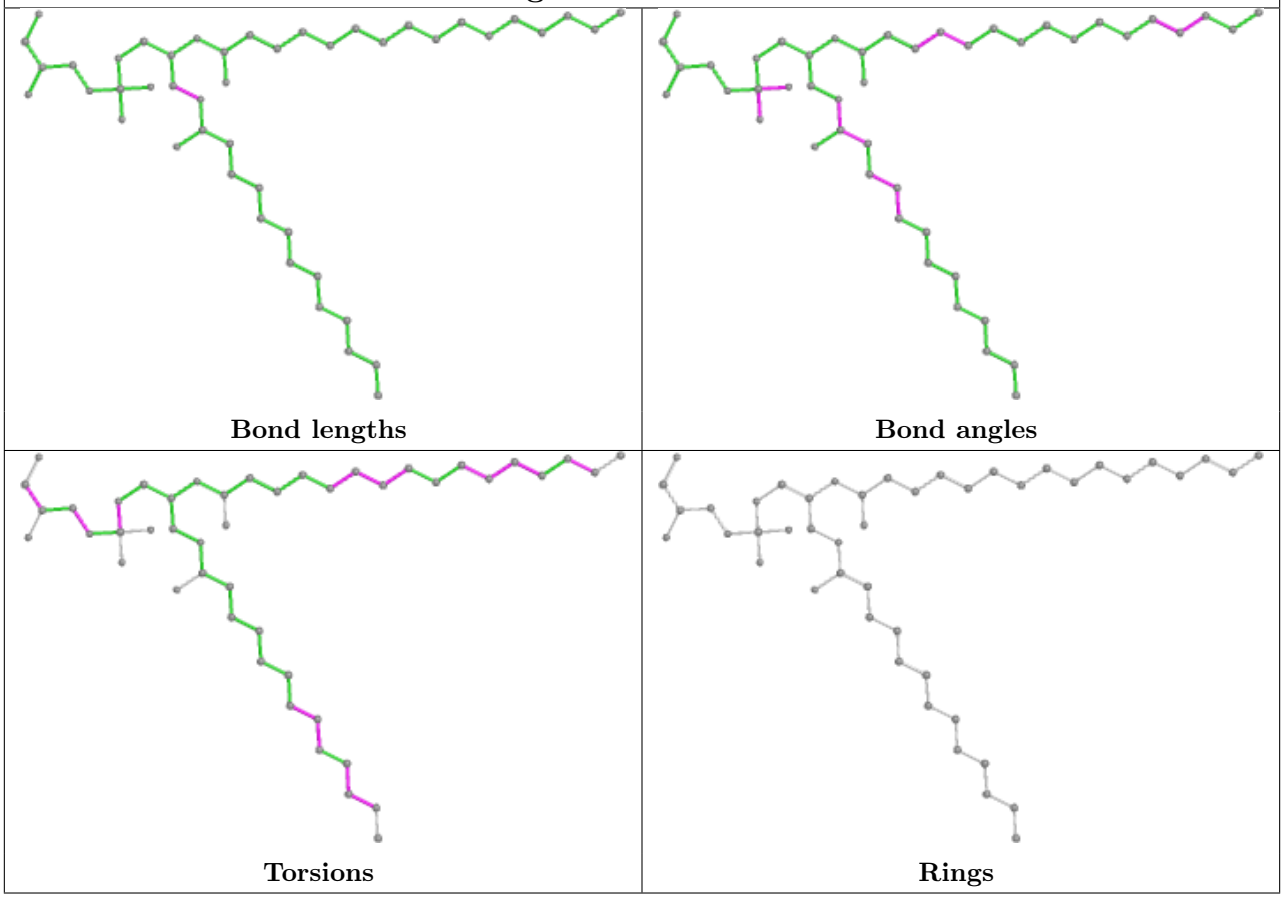


Torsions

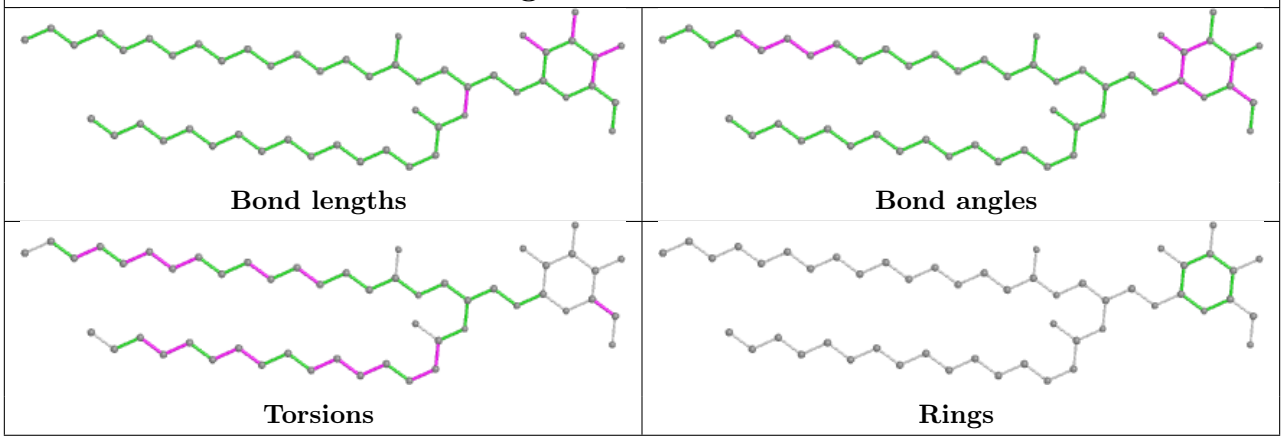


Rings

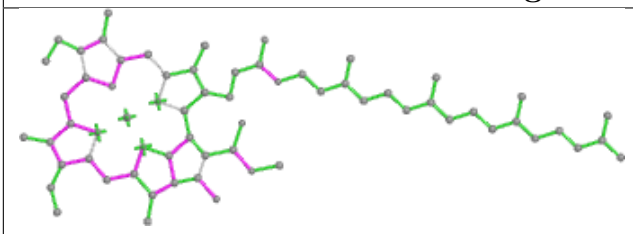
Ligand LHG d 410



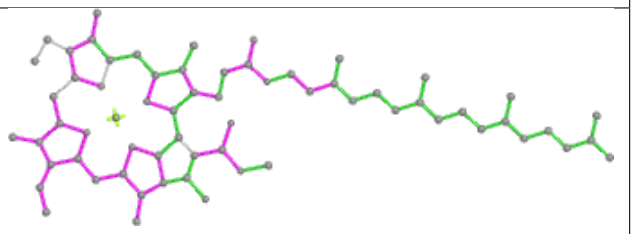
Ligand LMG D 411



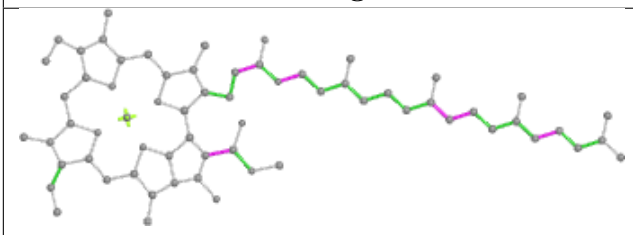
Ligand CLA B 613



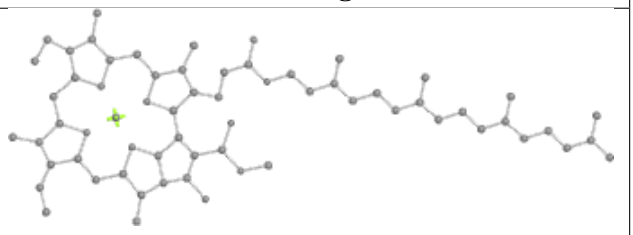
Bond lengths



Bond angles

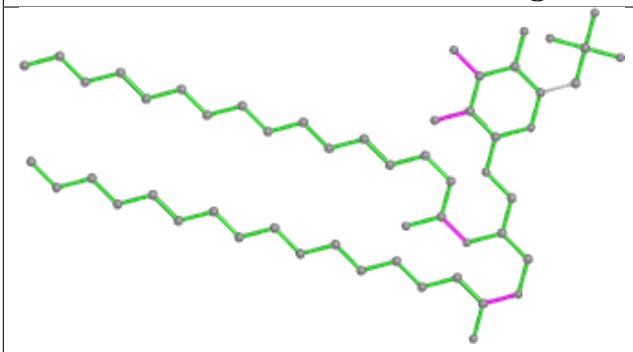


Torsions

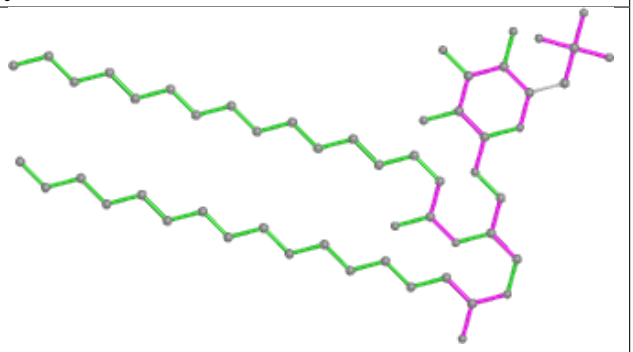


Rings

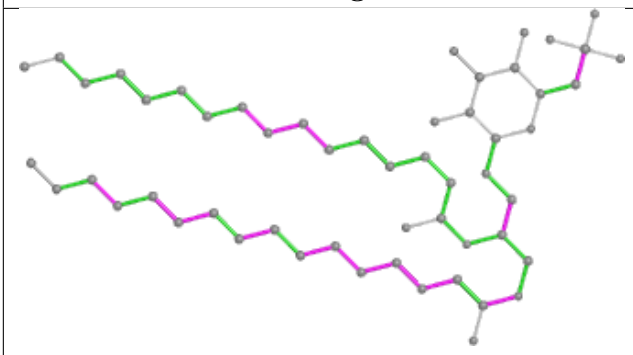
Ligand SQD a 412



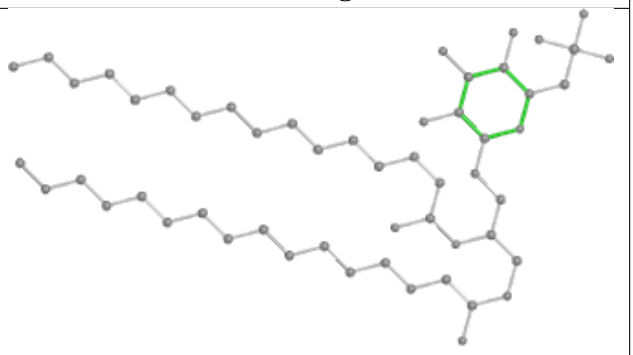
Bond lengths



Bond angles

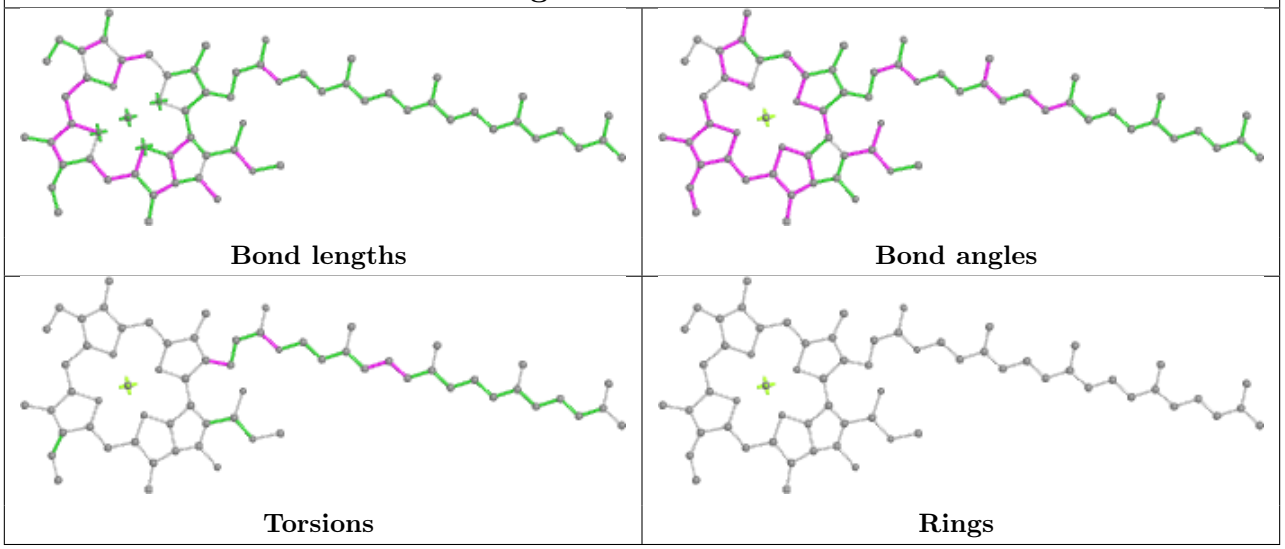


Torsions

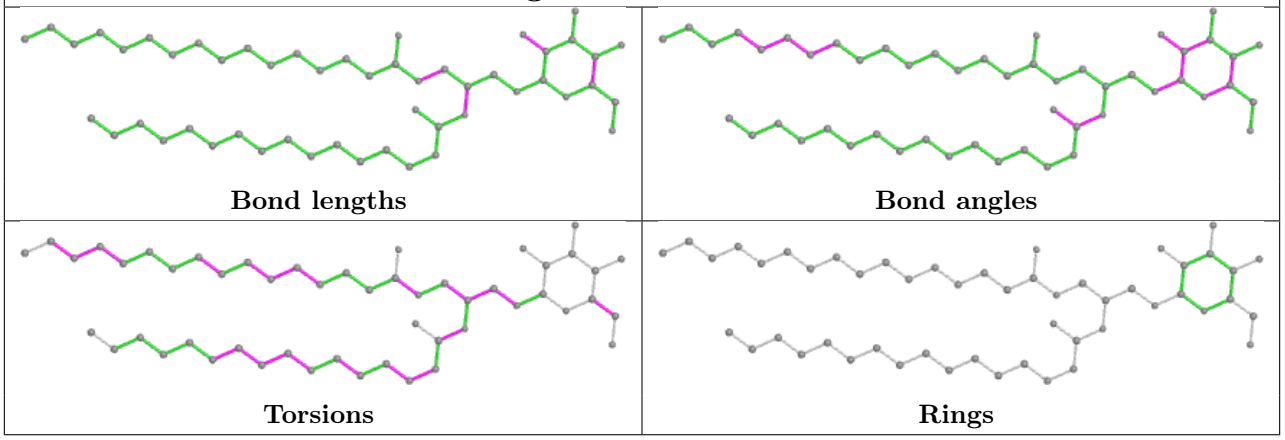


Rings

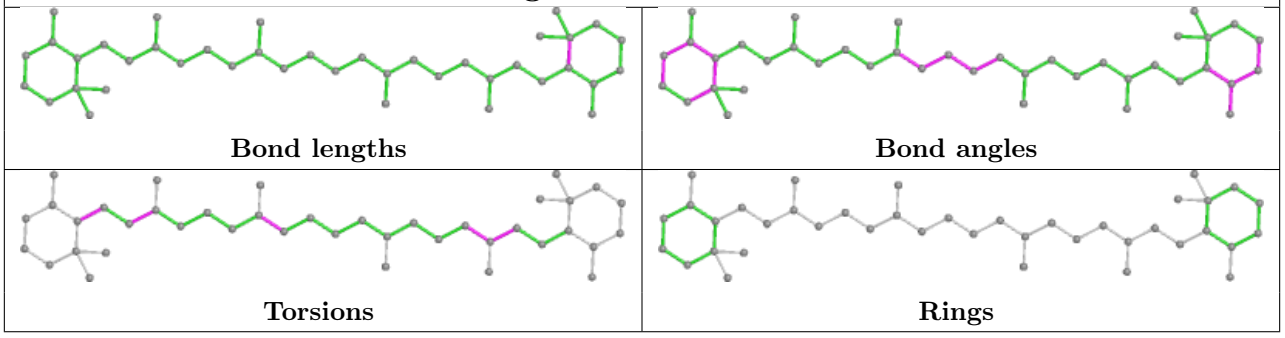
Ligand CLA c 512



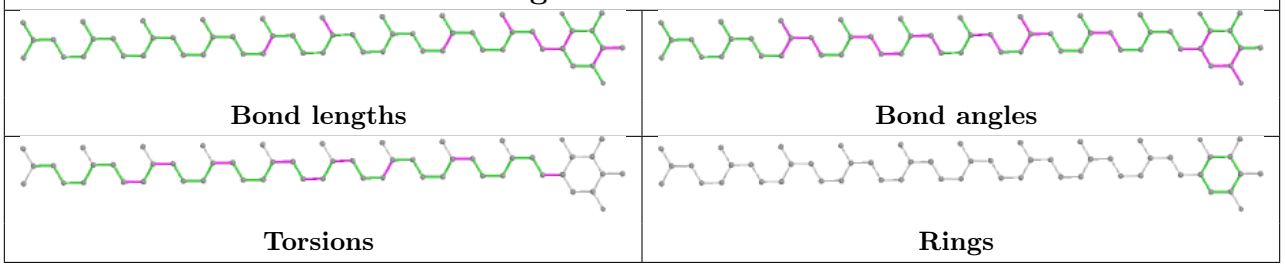
Ligand LMG c 522



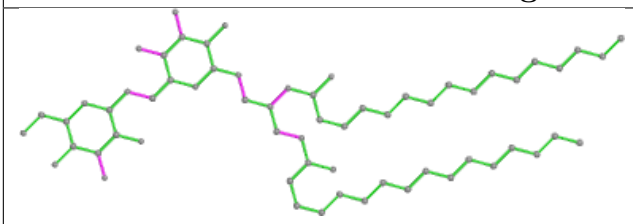
Ligand BCR B 627



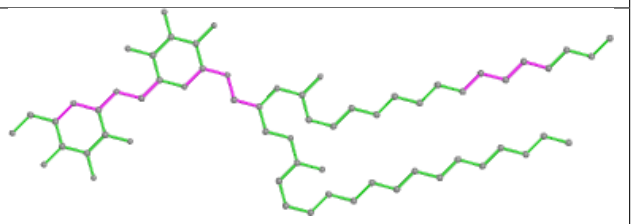
Ligand PL9 A 411



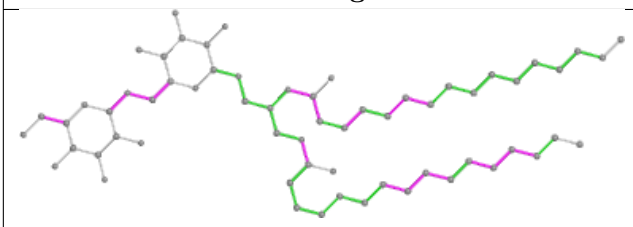
Ligand DGD C 517



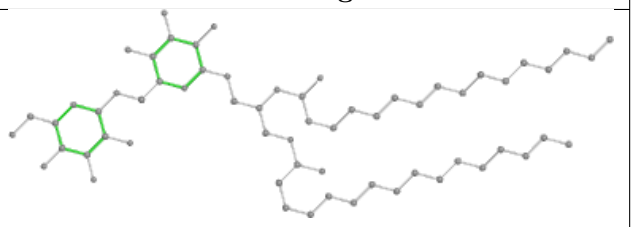
Bond lengths



Bond angles

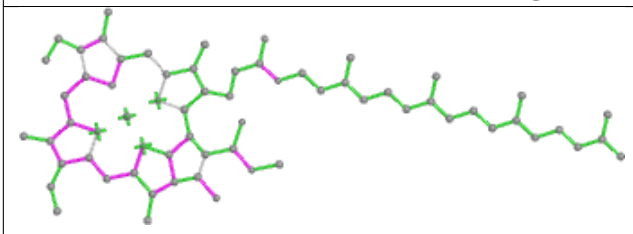


Torsions

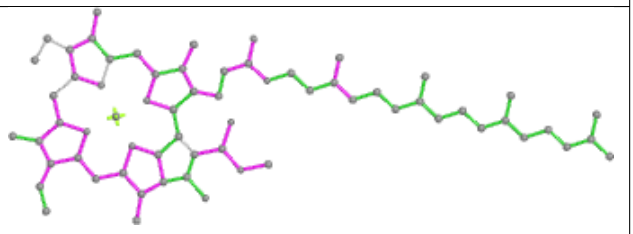


Rings

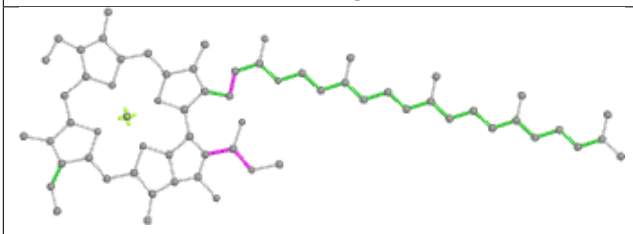
Ligand CLA b 608



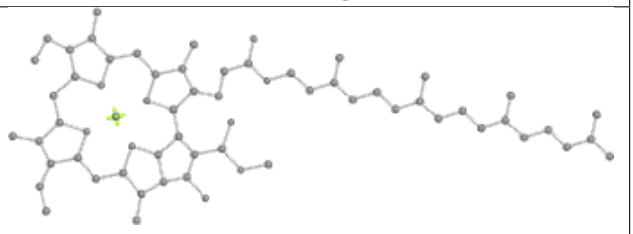
Bond lengths



Bond angles

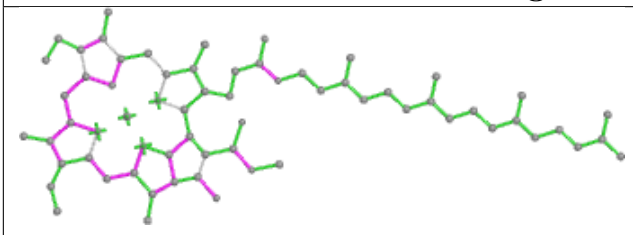


Torsions

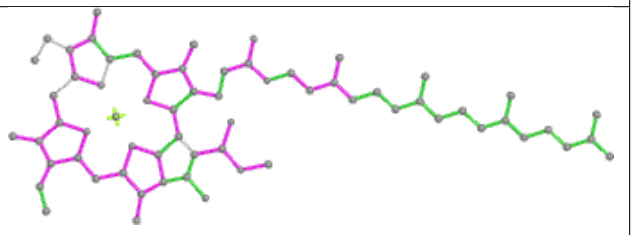


Rings

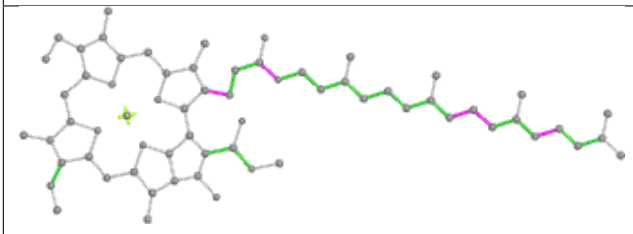
Ligand CLA b 614



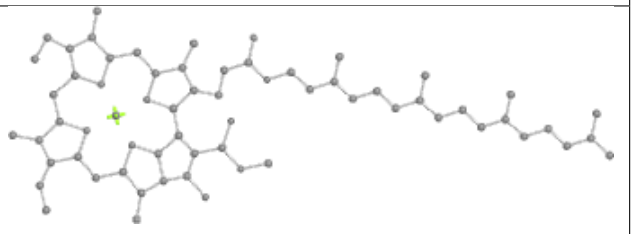
Bond lengths



Bond angles

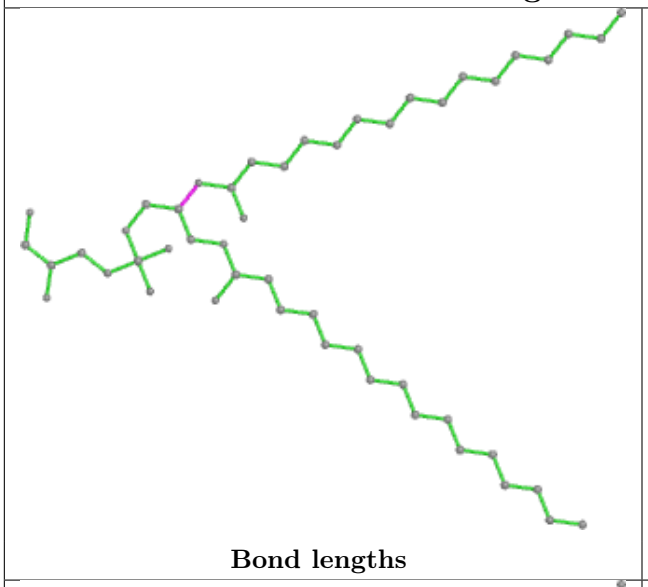


Torsions

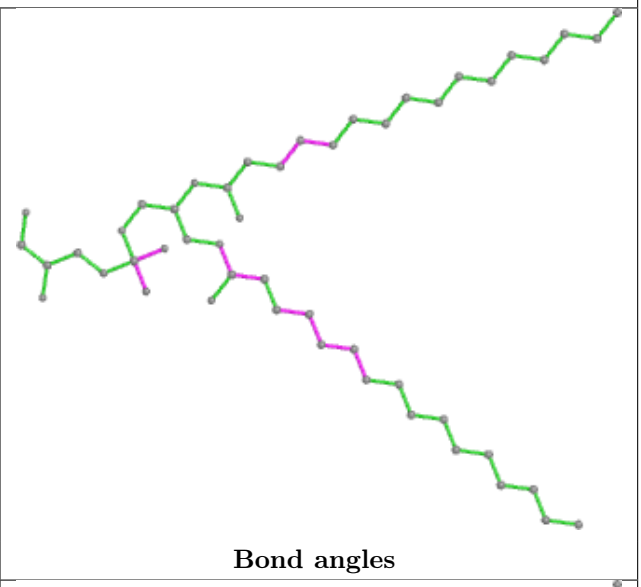


Rings

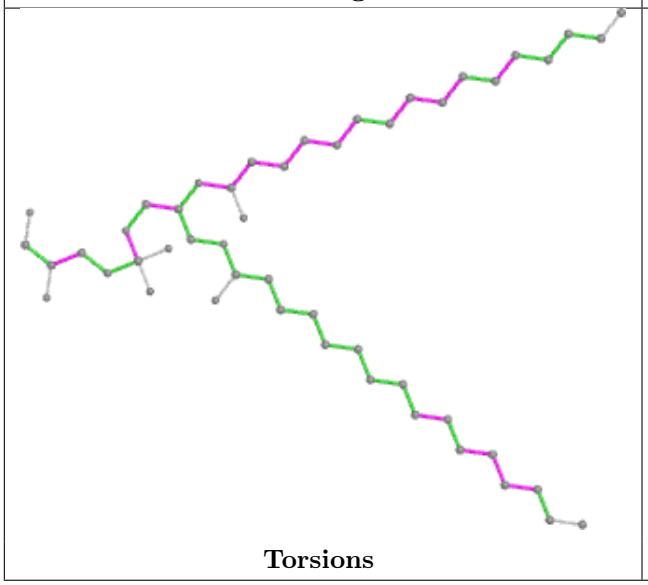
Ligand LHG B 625



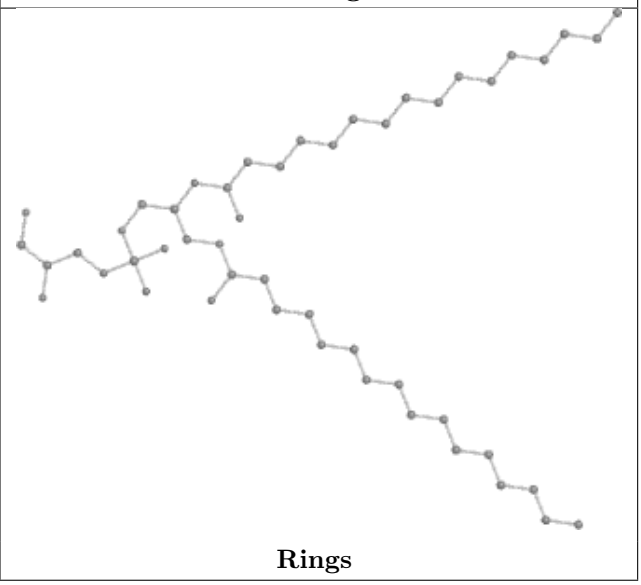
Bond lengths



Bond angles

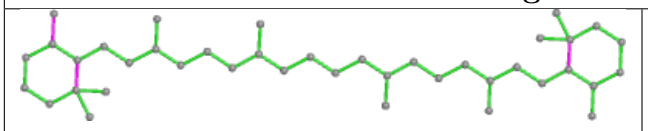


Torsions

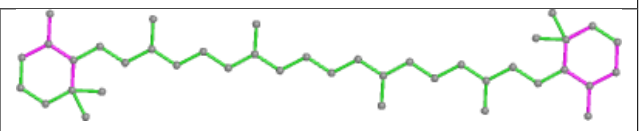


Rings

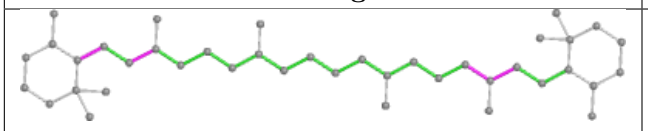
Ligand BCR Y 101



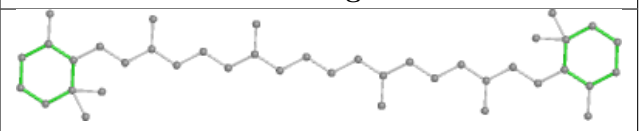
Bond lengths



Bond angles

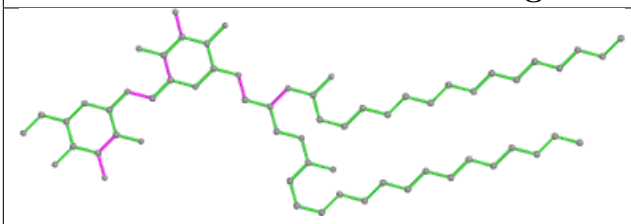


Torsions

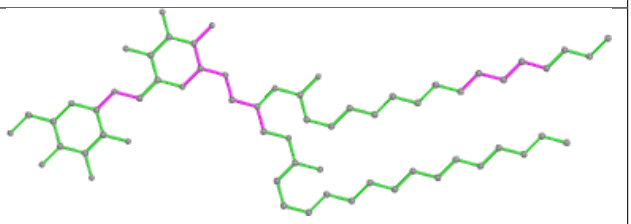


Rings

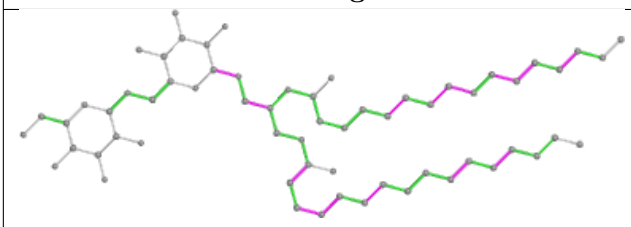
Ligand DGD c 519



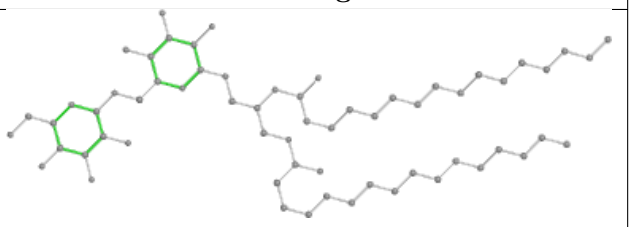
Bond lengths



Bond angles

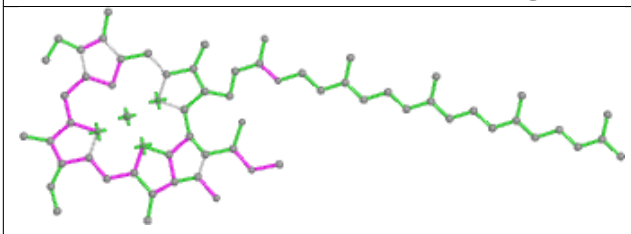


Torsions

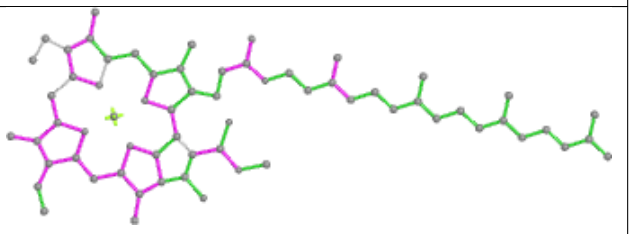


Rings

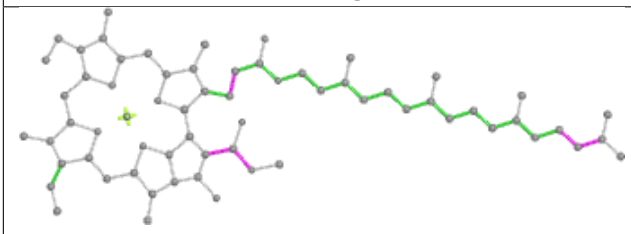
Ligand CLA C 504



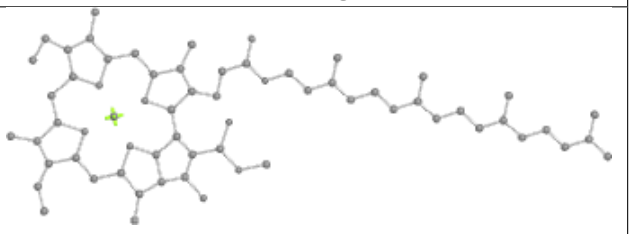
Bond lengths



Bond angles

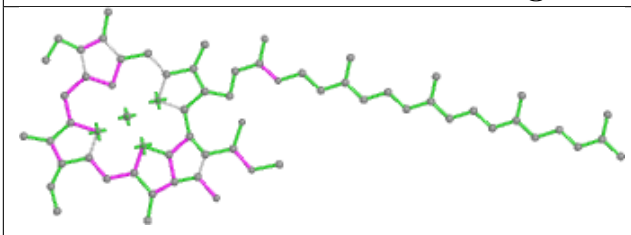


Torsions

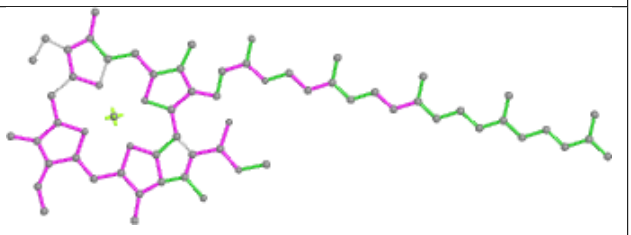


Rings

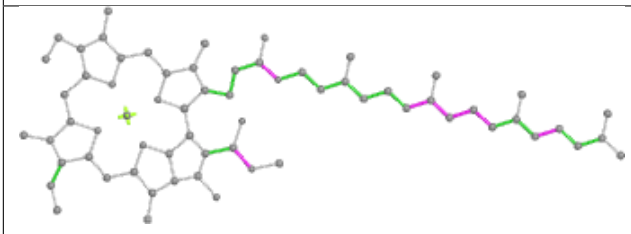
Ligand CLA d 404



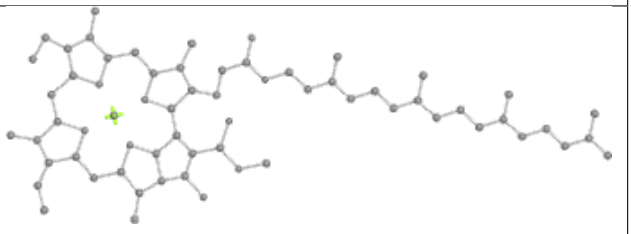
Bond lengths



Bond angles

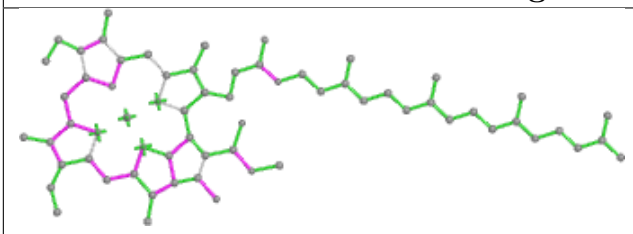


Torsions

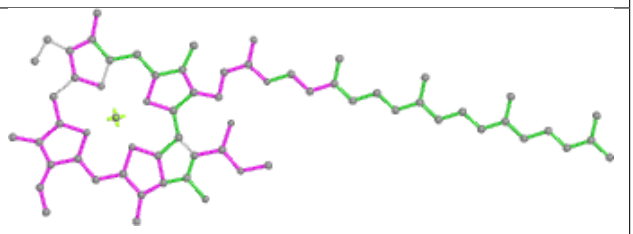


Rings

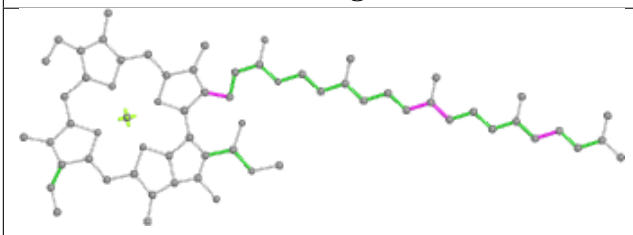
Ligand CLA a 406



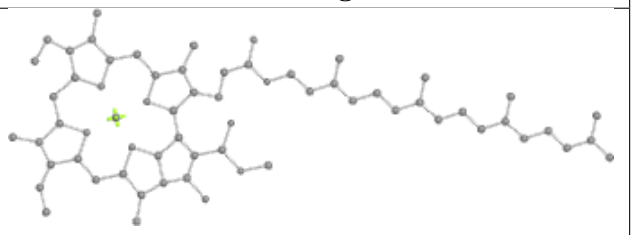
Bond lengths



Bond angles

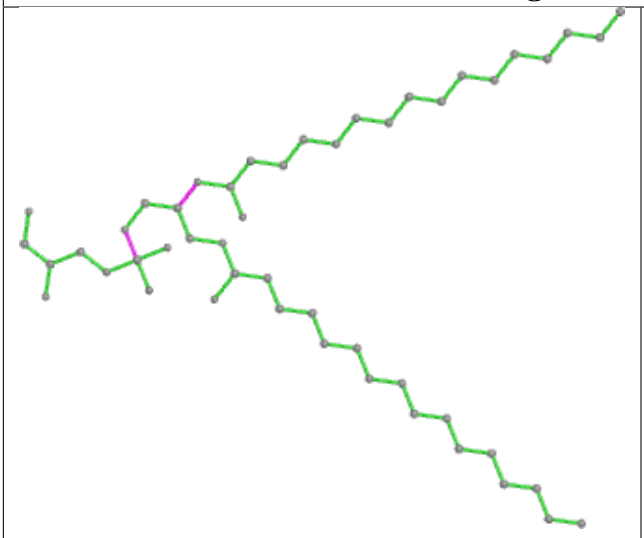


Torsions



Rings

Ligand LHG d 409



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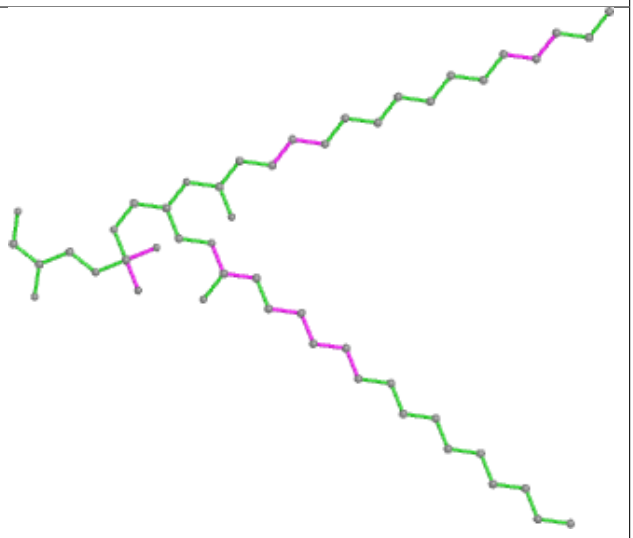
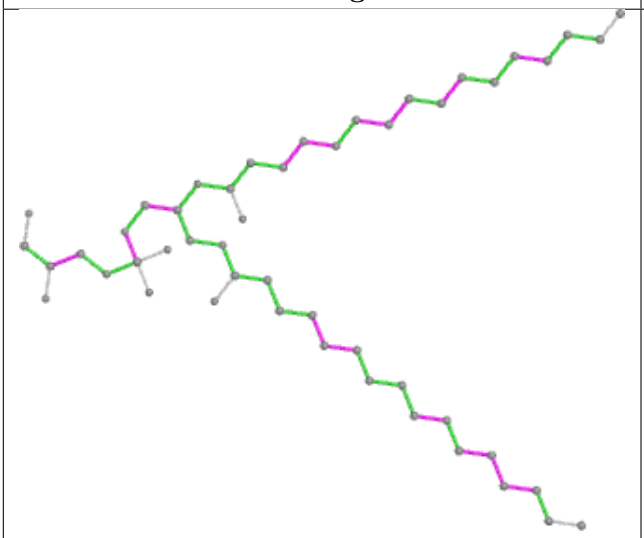
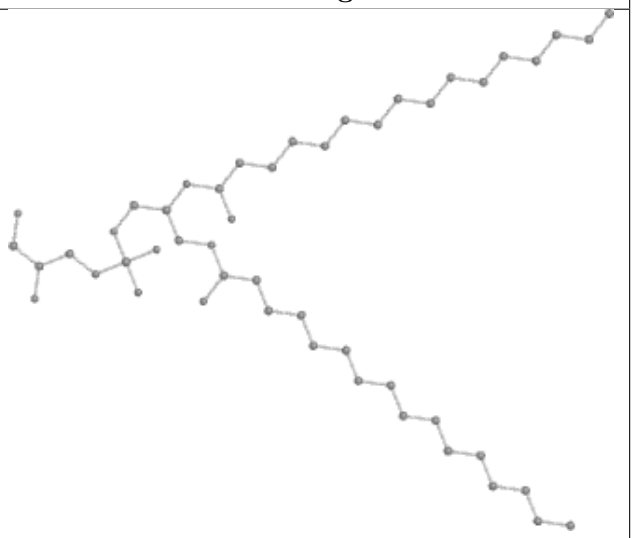


Bond angles

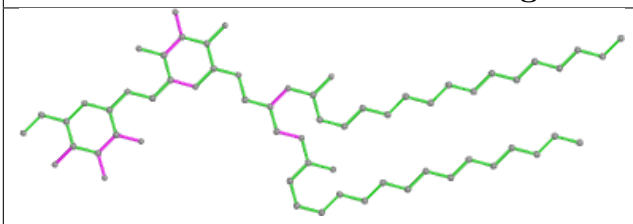


Torsions

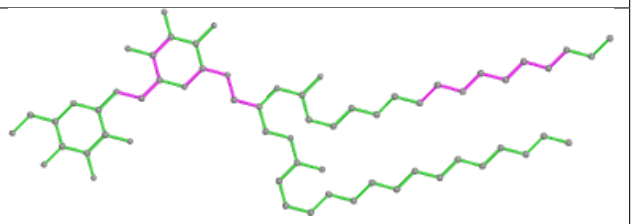


Rings

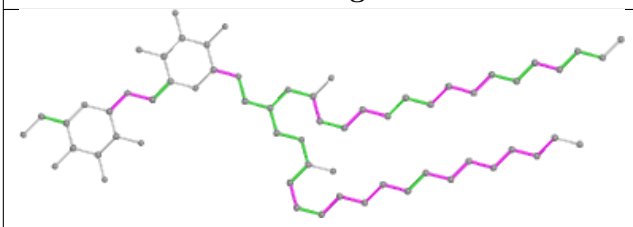
Ligand DGD C 518



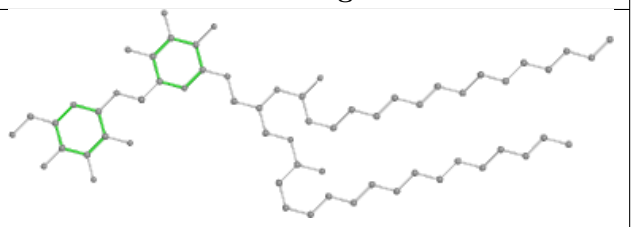
Bond lengths



Bond angles

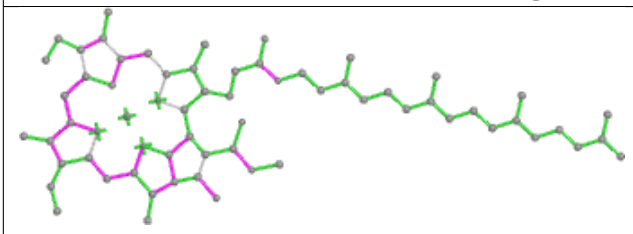


Torsions

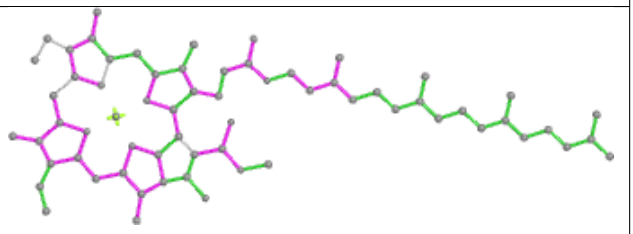


Rings

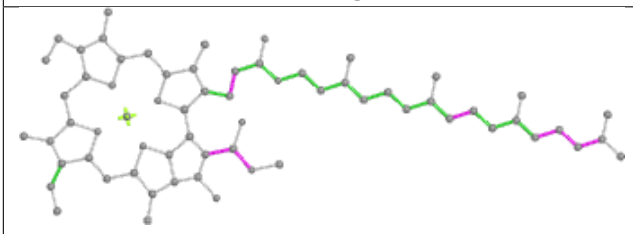
Ligand CLA b 612



Bond lengths



Bond angles



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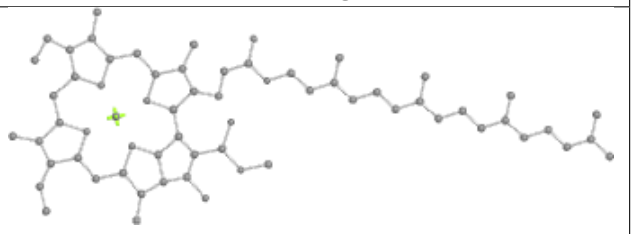
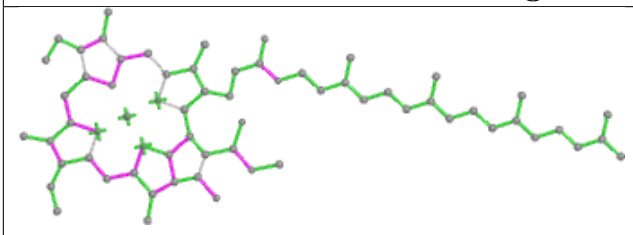
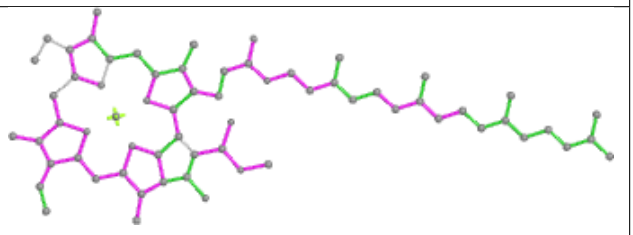


Rings

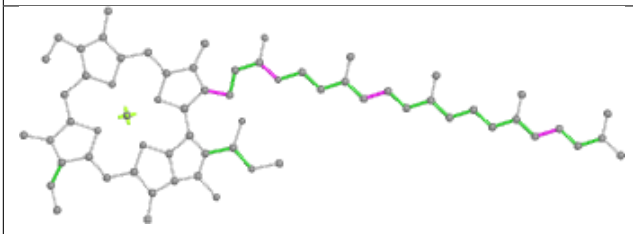
Ligand CLA B 604



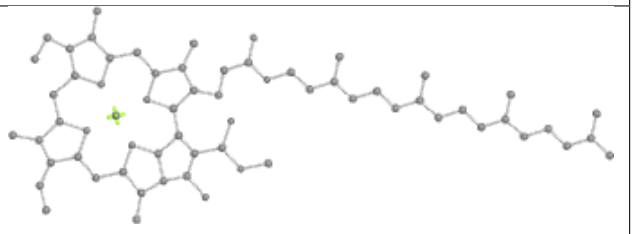
Bond lengths



Bond angles

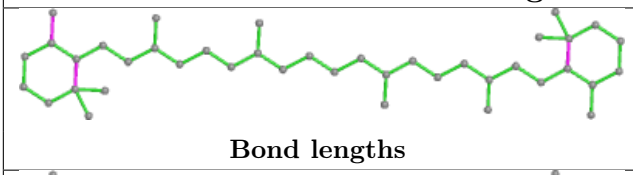


Torsions

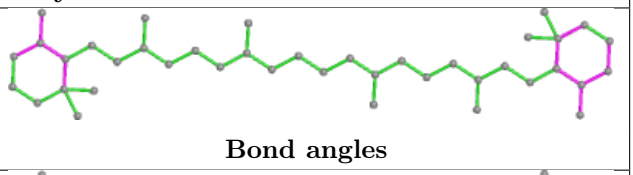


Rings

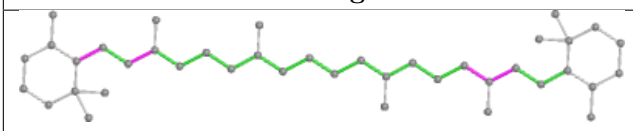
Ligand BCR y 101



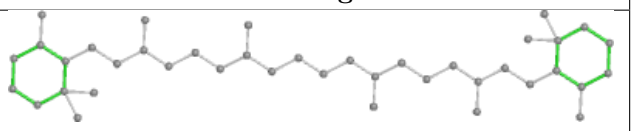
Bond lengths



Bond angles

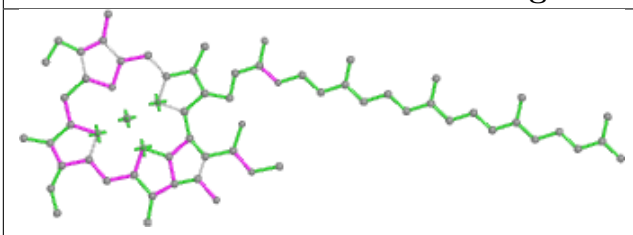


Torsions

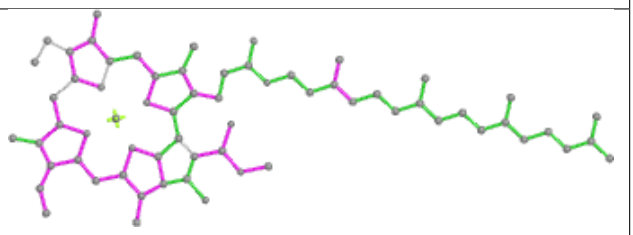


Rings

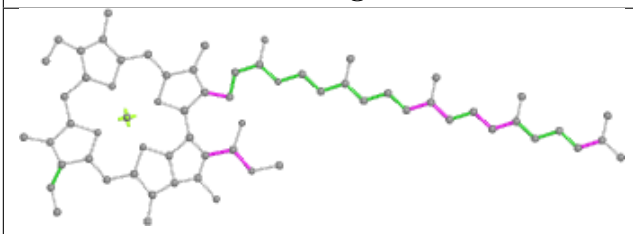
Ligand CLA c 507



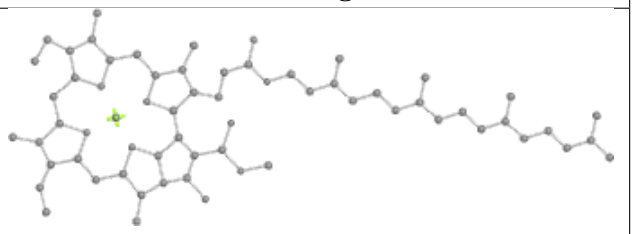
Bond lengths



Bond angles

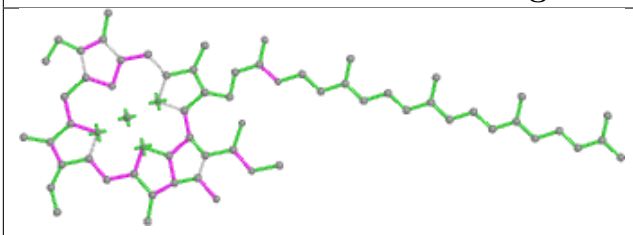


Torsions

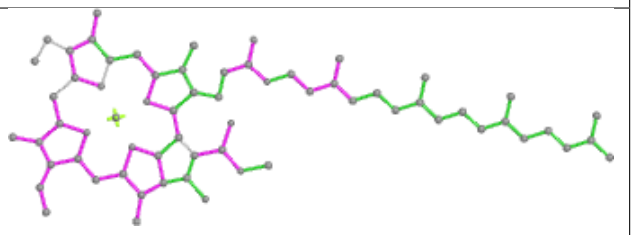


Rings

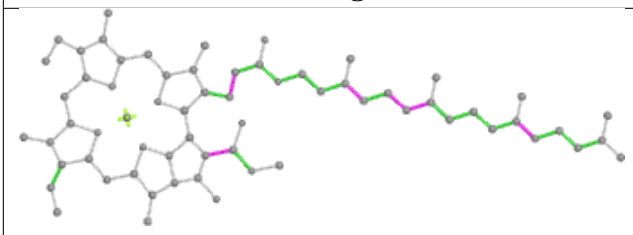
Ligand CLA c 508



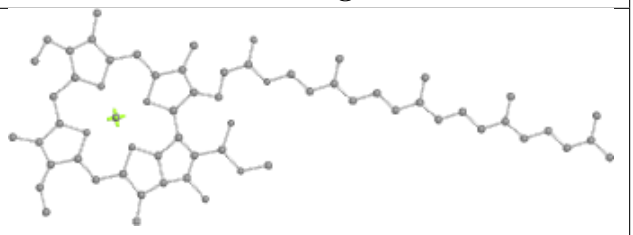
Bond lengths



Bond angles

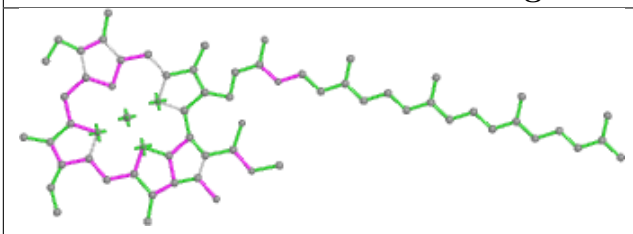


Torsions

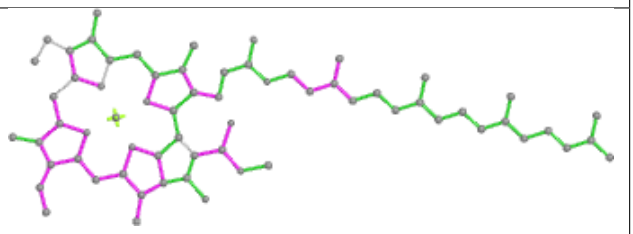


Rings

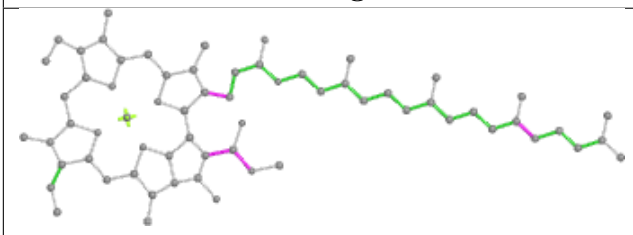
Ligand CLA C 503



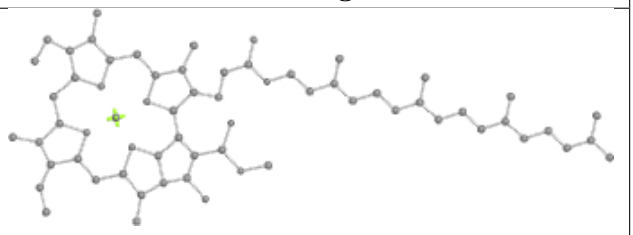
Bond lengths



Bond angles

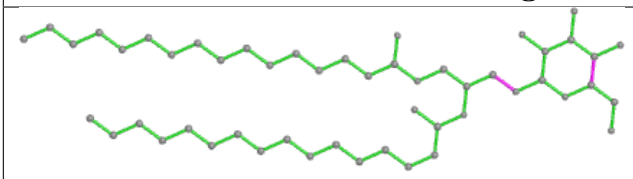


Torsions

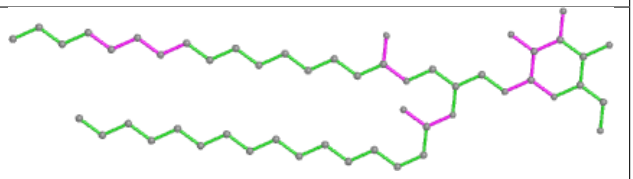


Rings

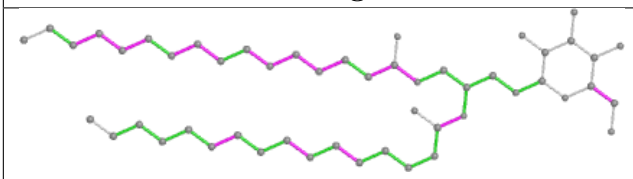
Ligand LMG B 620



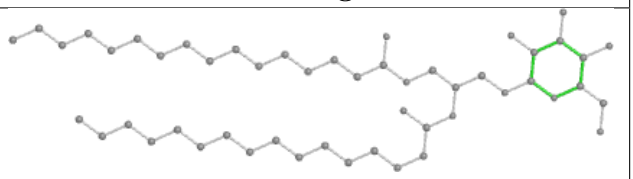
Bond lengths



Bond angles

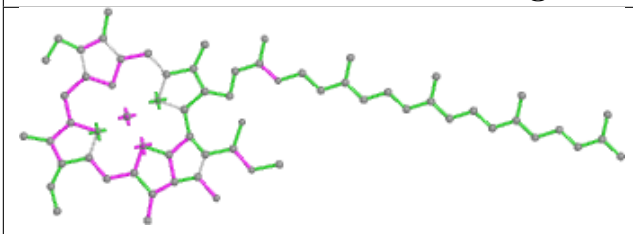


Torsions

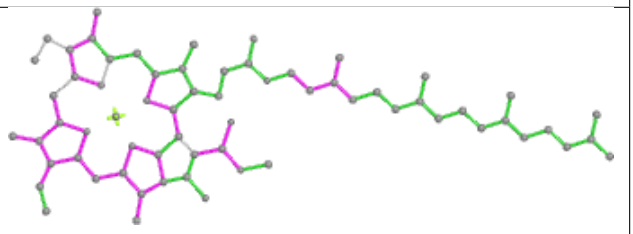


Rings

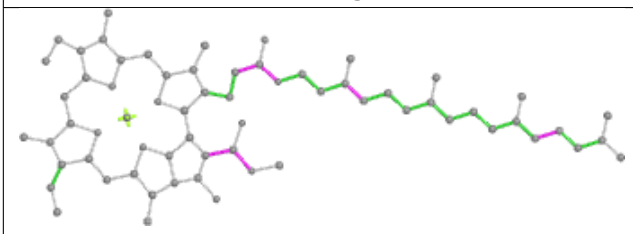
Ligand CLA c 506



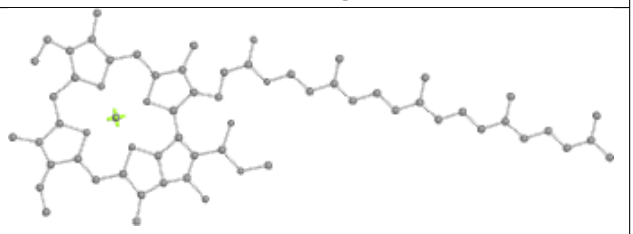
Bond lengths



Bond angles

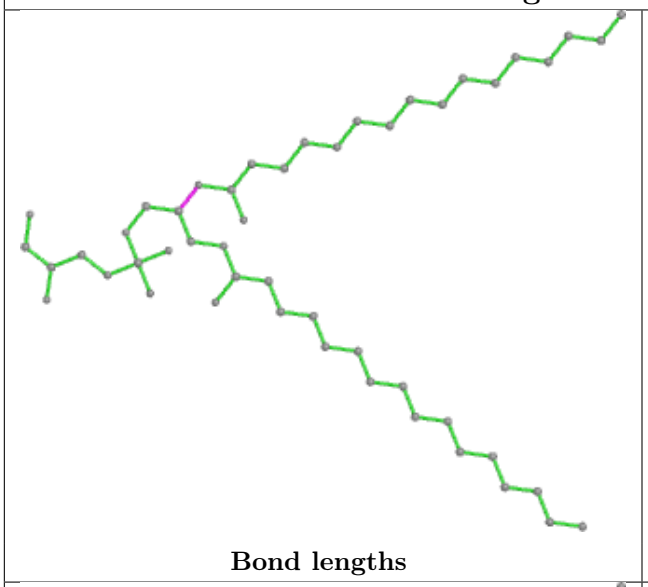


Torsions

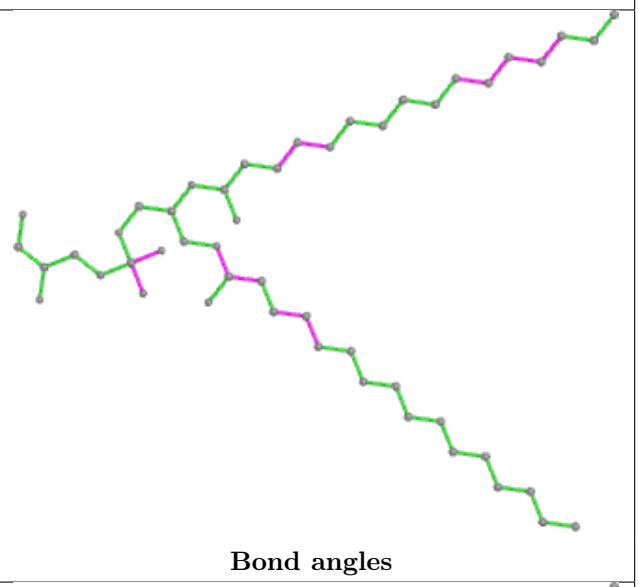


Rings

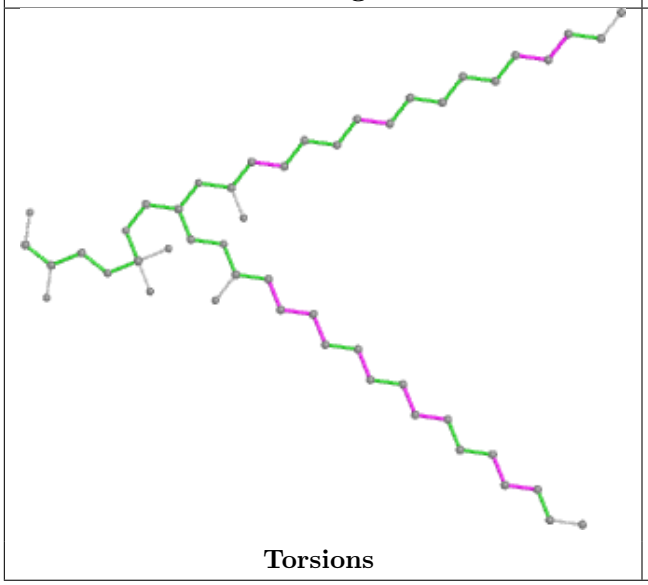
Ligand LHG D 408



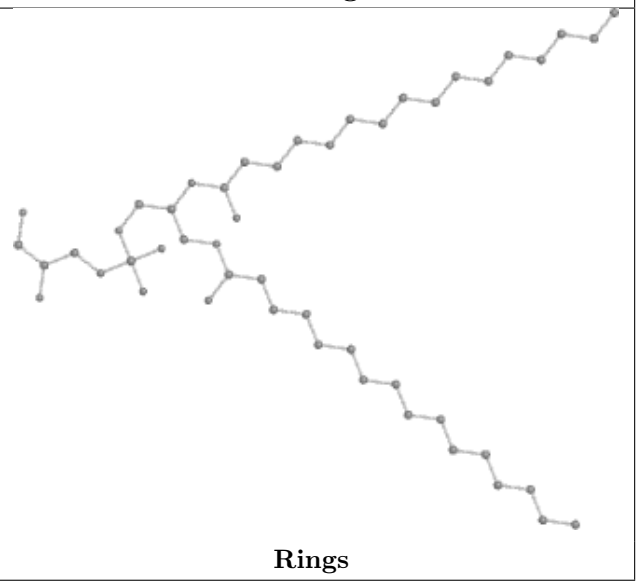
Bond lengths



Bond angles

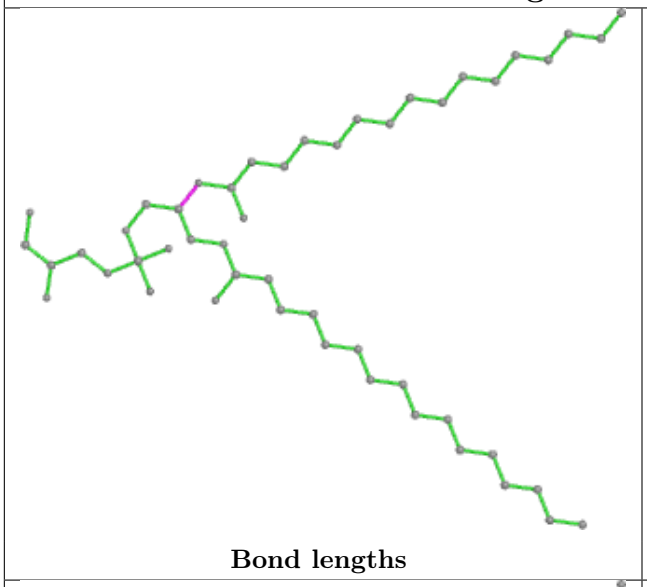


Torsions

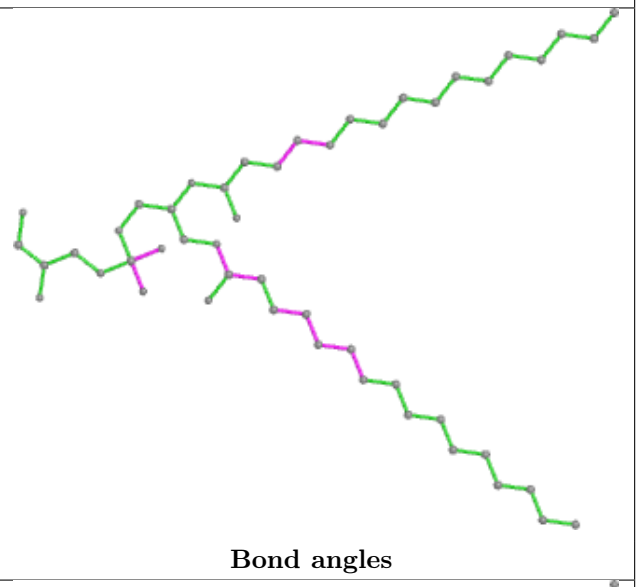


Rings

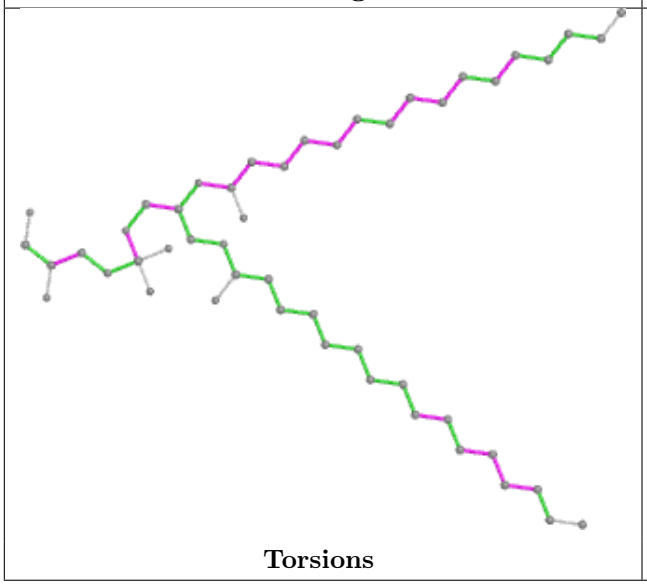
Ligand LHG b 627



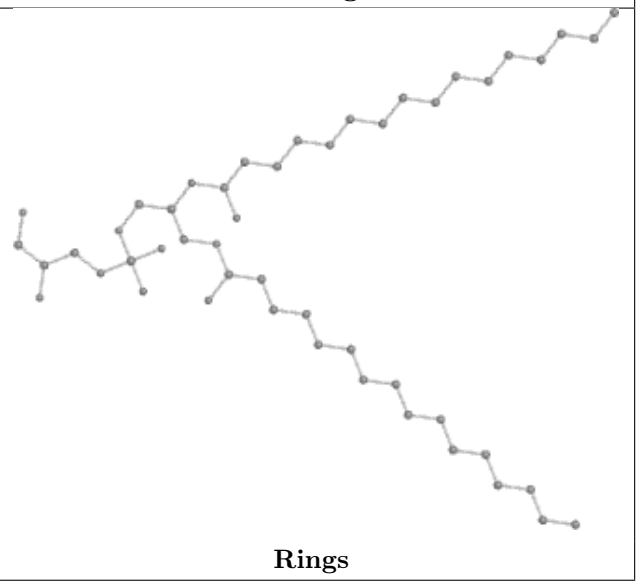
Bond lengths



Bond angles

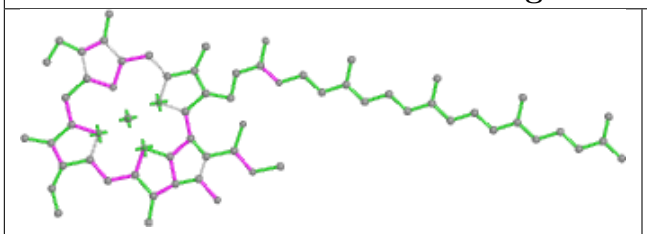


Torsions

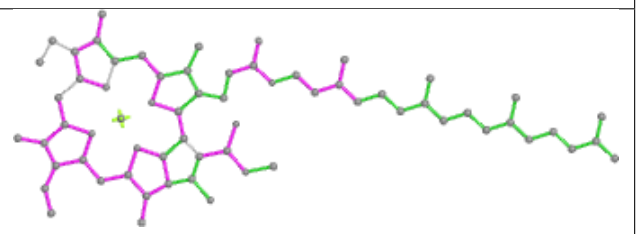


Rings

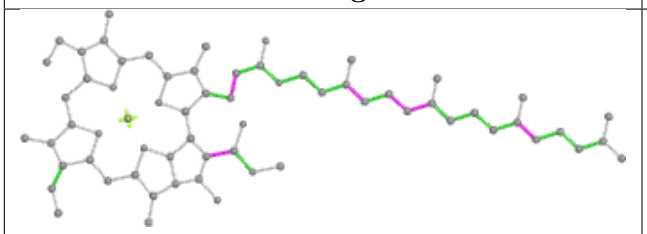
Ligand CLA C 508



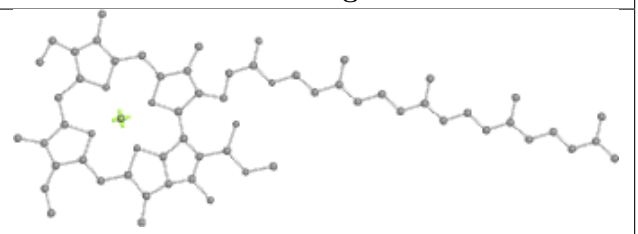
Bond lengths



Bond angles

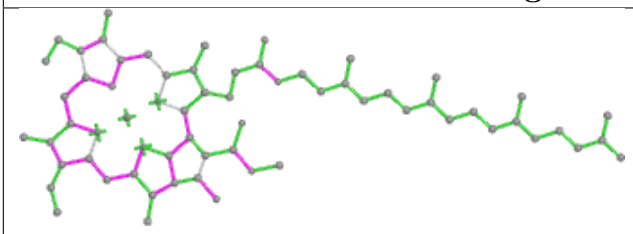


Torsions

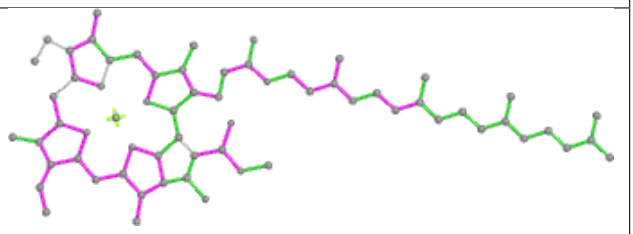


Rings

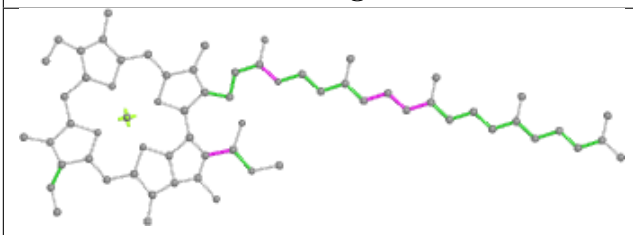
Ligand CLA B 601



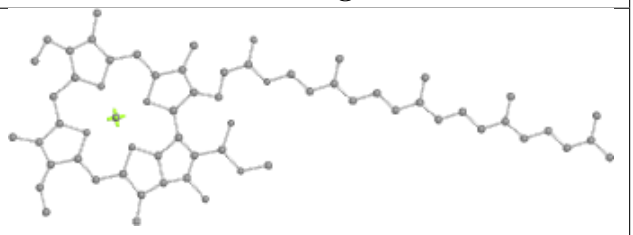
Bond lengths



Bond angles

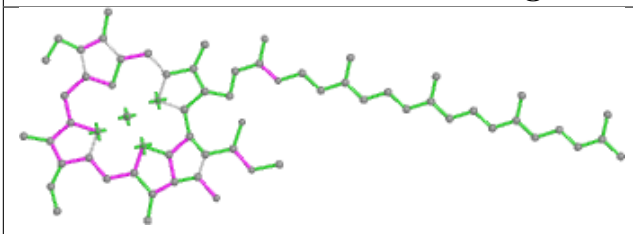


Torsions

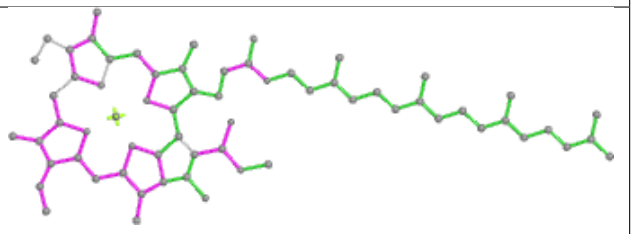


Rings

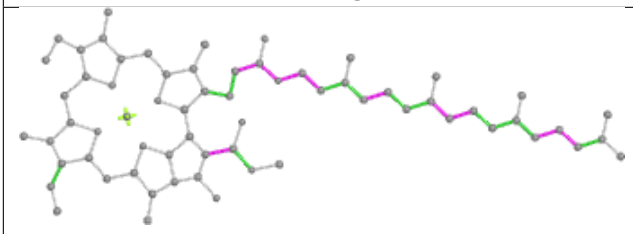
Ligand CLA C 513



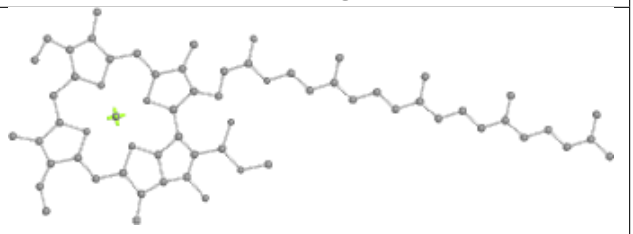
Bond lengths



Bond angles

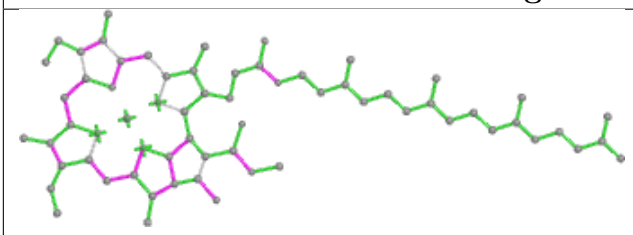


Torsions

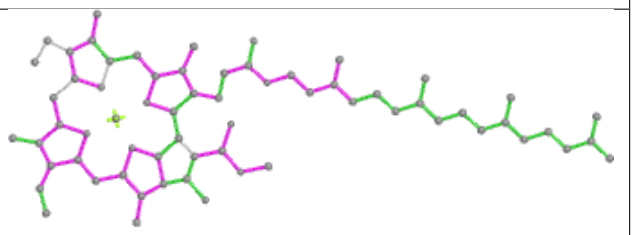


Rings

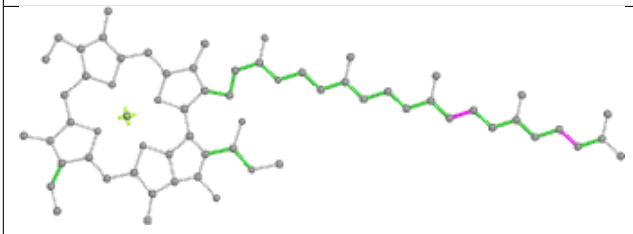
Ligand CLA B 602



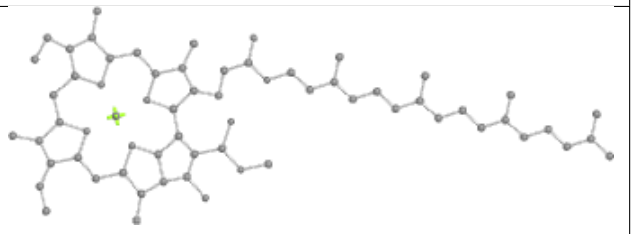
Bond lengths



Bond angles

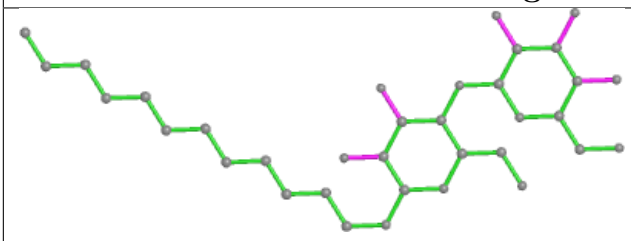


Torsions

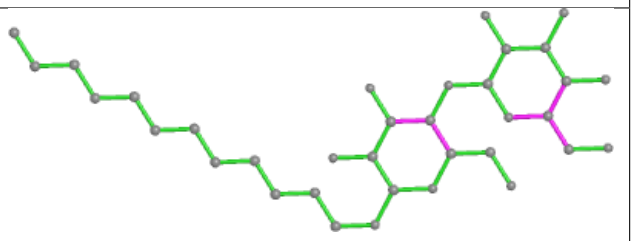


Rings

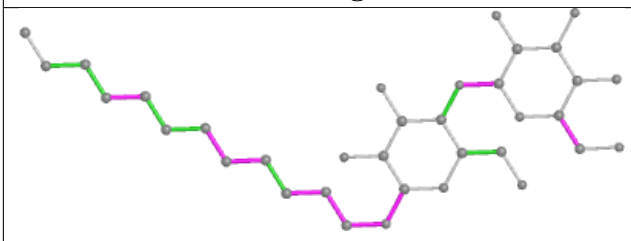
Ligand LMT Z 101



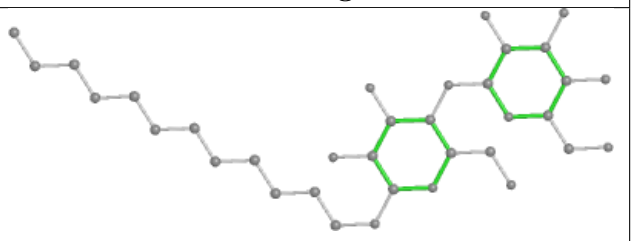
Bond lengths



Bond angles

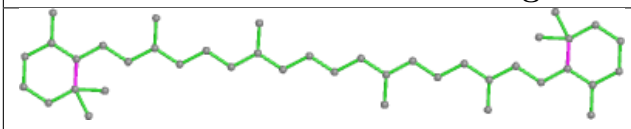


Torsions

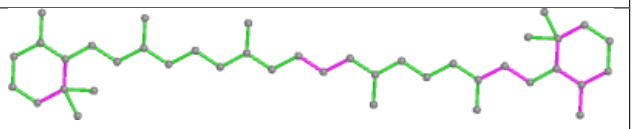


Rings

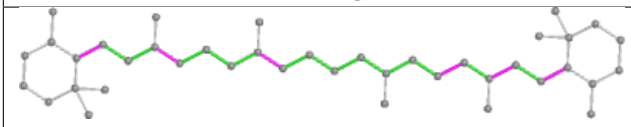
Ligand BCR C 521



Bond lengths



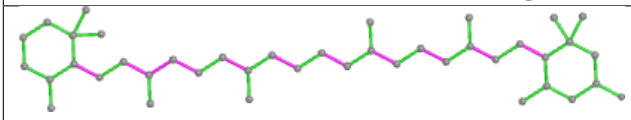
Bond angles



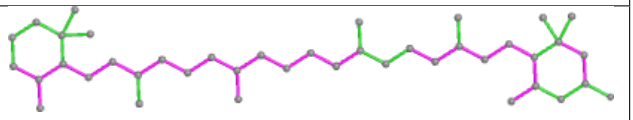
Torsions

Rings

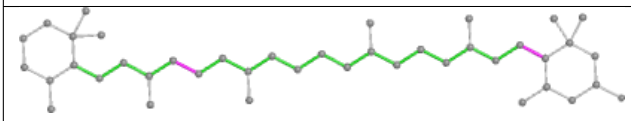
Ligand RRX H 101



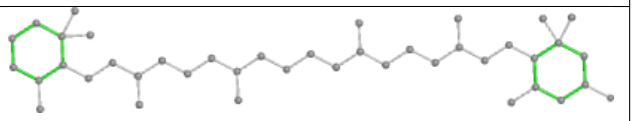
Bond lengths



Bond angles

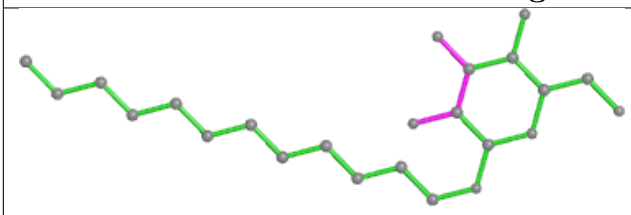


Torsions

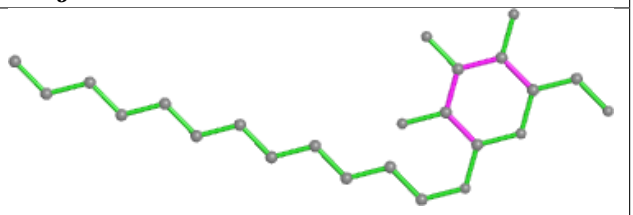


Rings

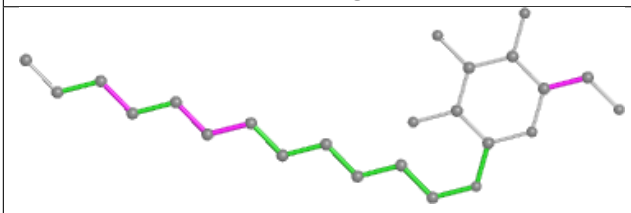
Ligand LMT j 102



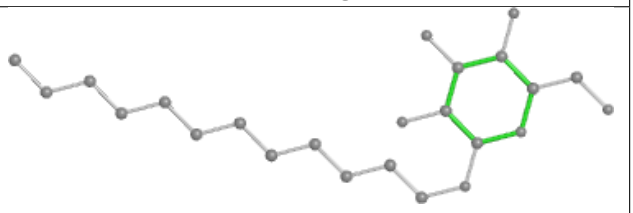
Bond lengths



Bond angles

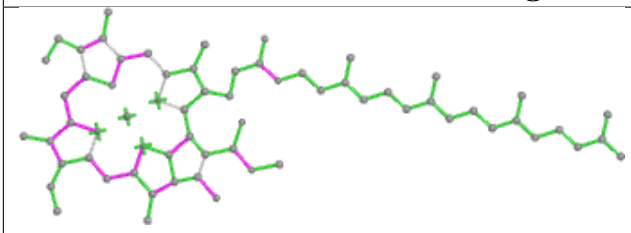


Torsions

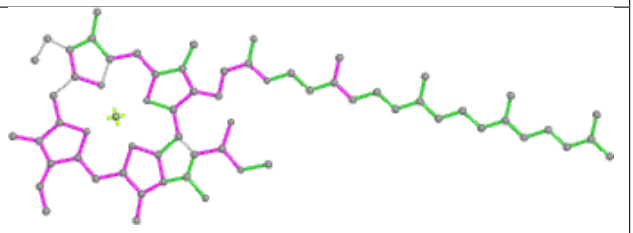


Rings

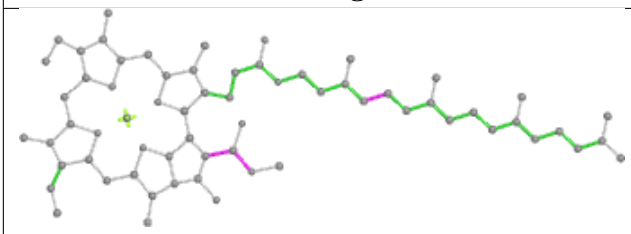
Ligand CLA B 607



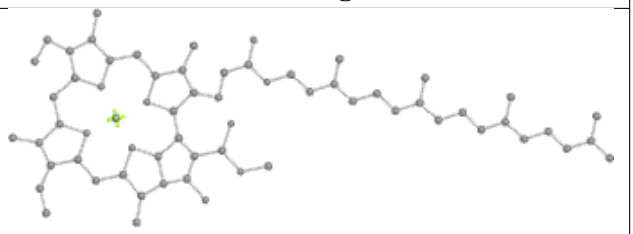
Bond lengths



Bond angles

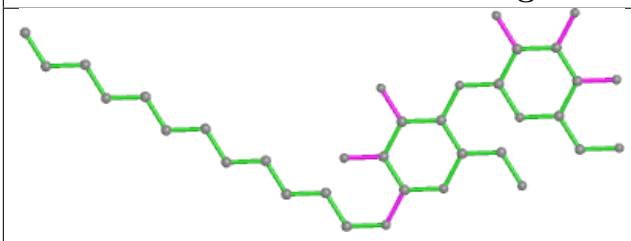


Torsions

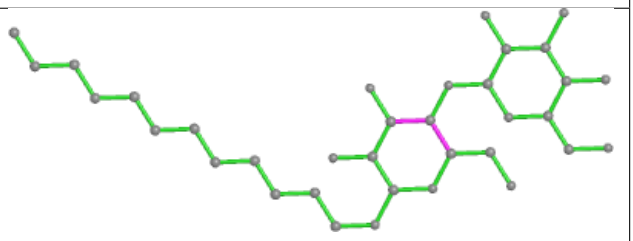


Rings

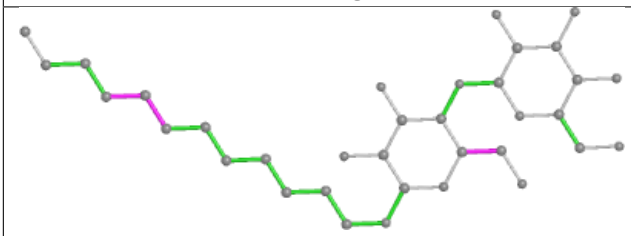
Ligand LMT M 101



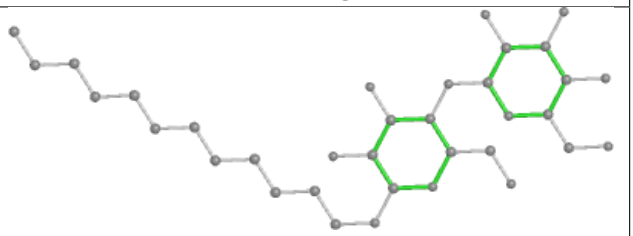
Bond lengths



Bond angles

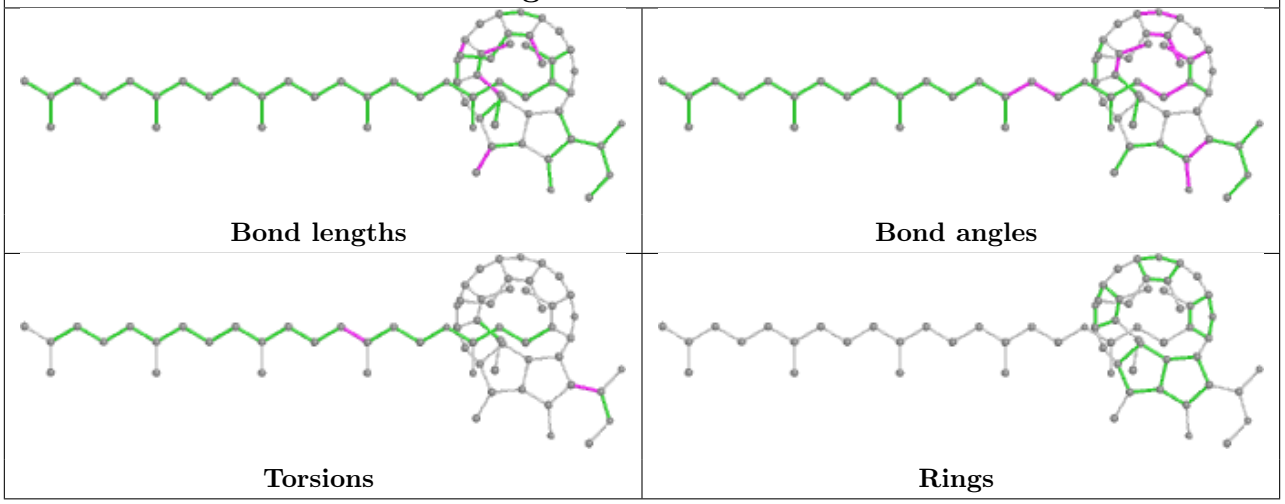


Torsions

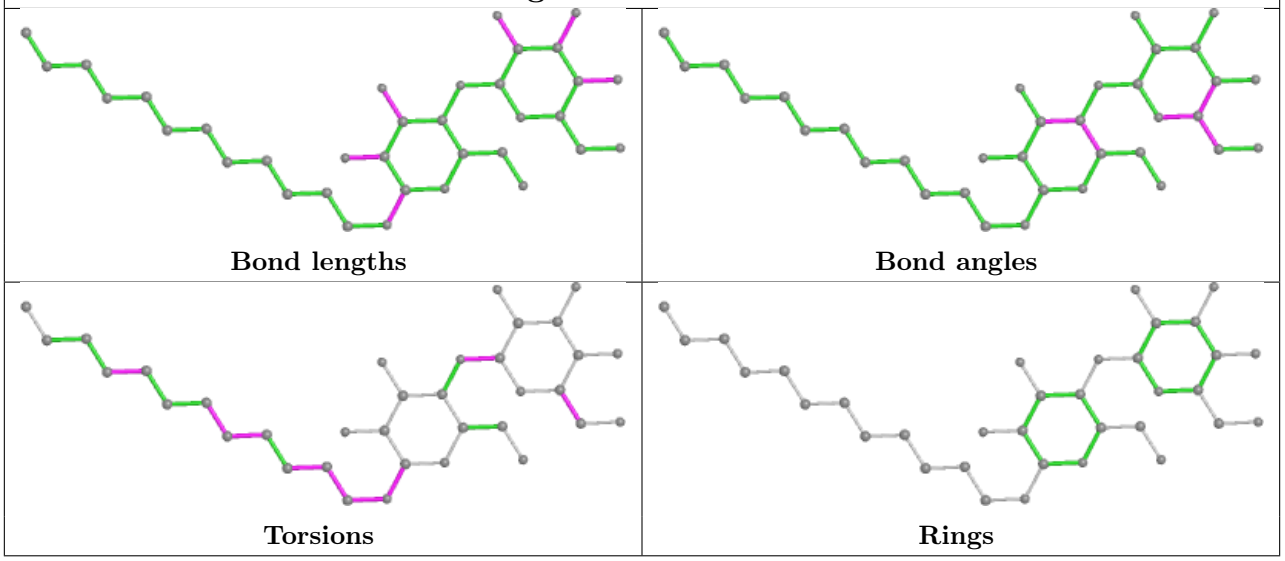


Rings

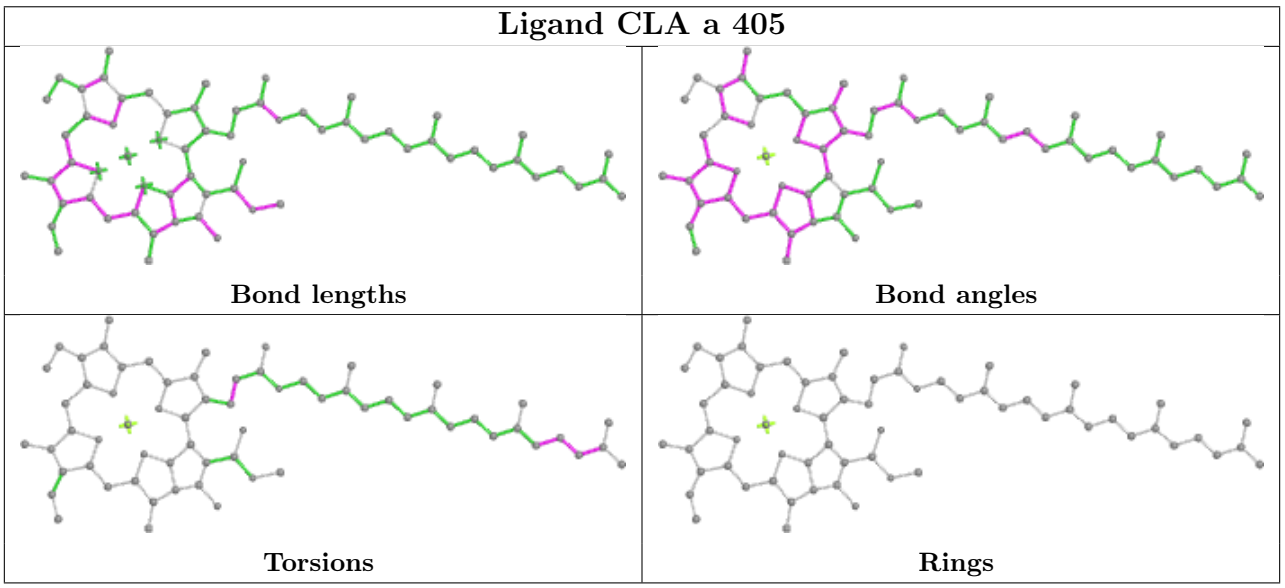
Ligand PHO A 407



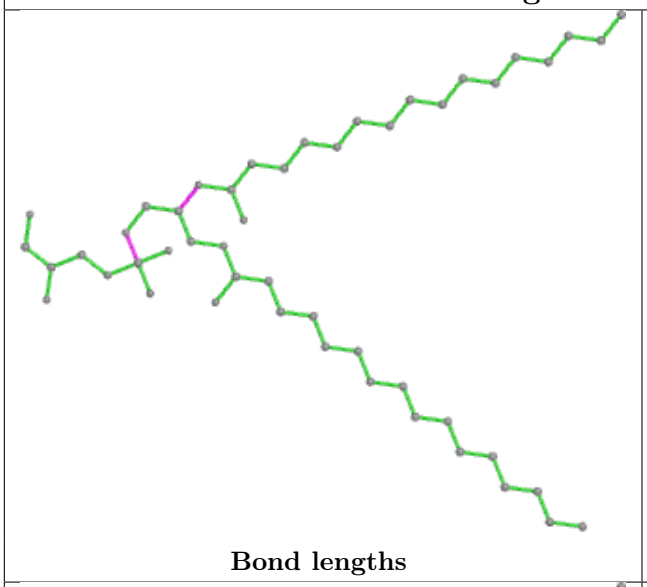
Ligand LMT z 101



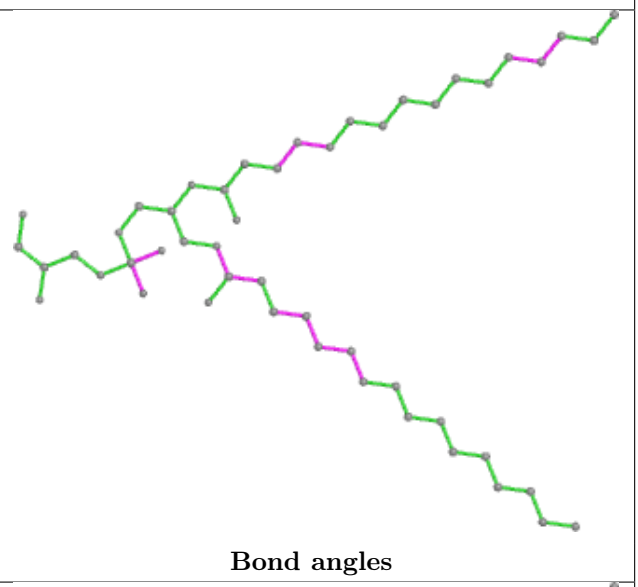
Ligand CLA a 405



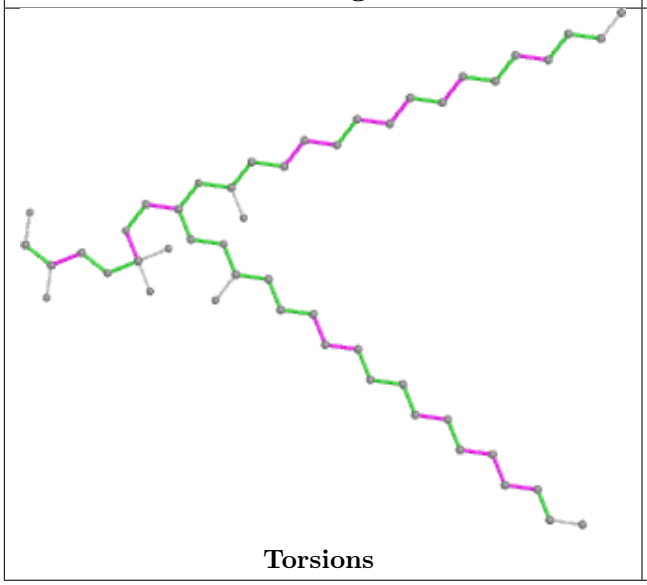
Ligand LHG D 409



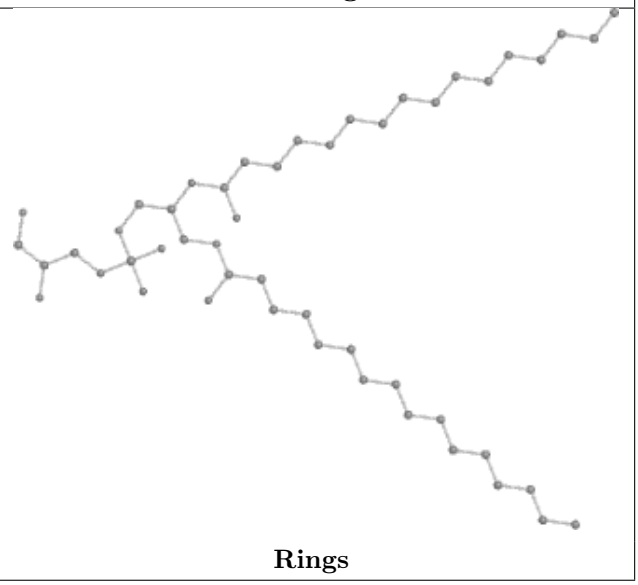
Bond lengths



Bond angles

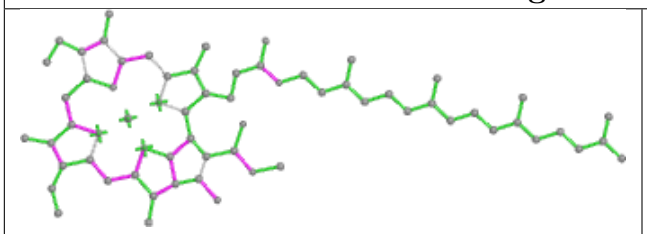


Torsions

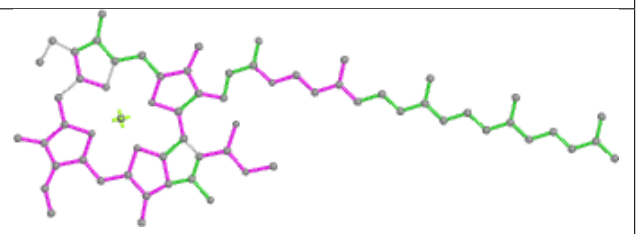


Rings

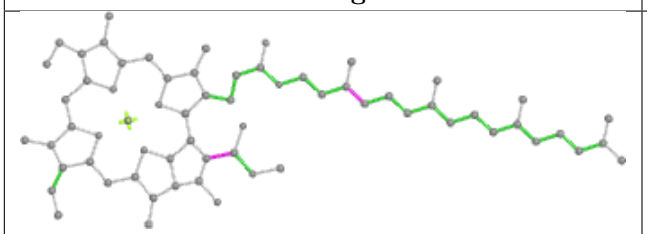
Ligand CLA b 611



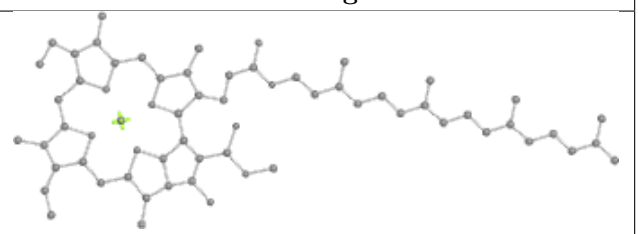
Bond lengths



Bond angles

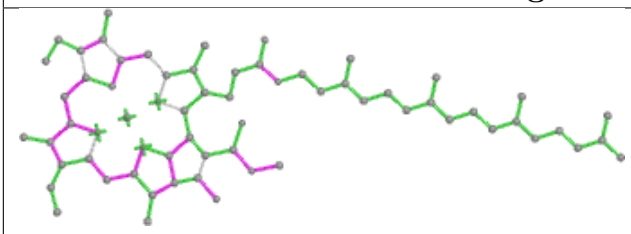


Torsions

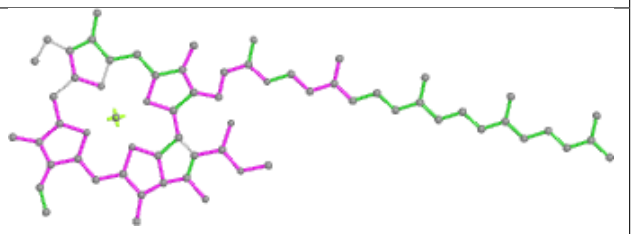


Rings

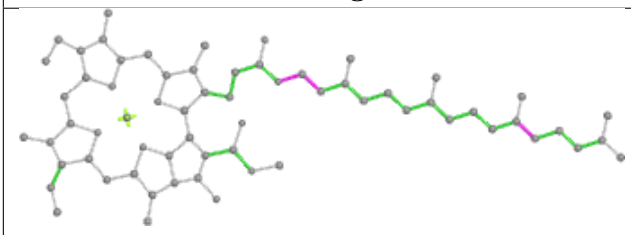
Ligand CLA d 403



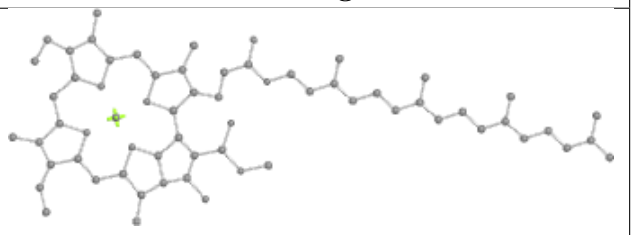
Bond lengths



Bond angles

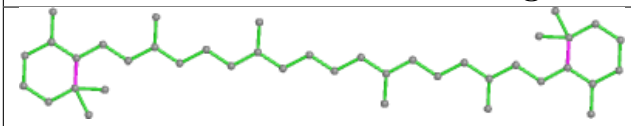


Torsions

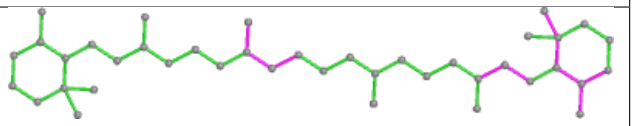


Rings

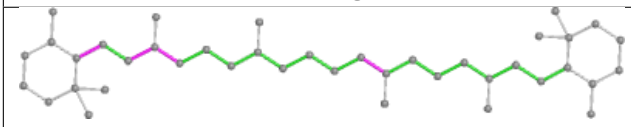
Ligand BCR B 618



Bond lengths



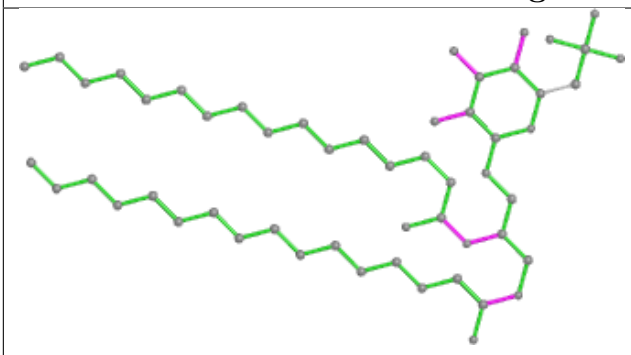
Bond angles



Torsions

Rings

Ligand SQD a 410



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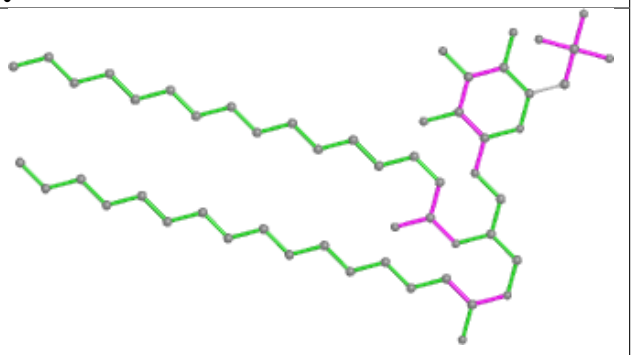

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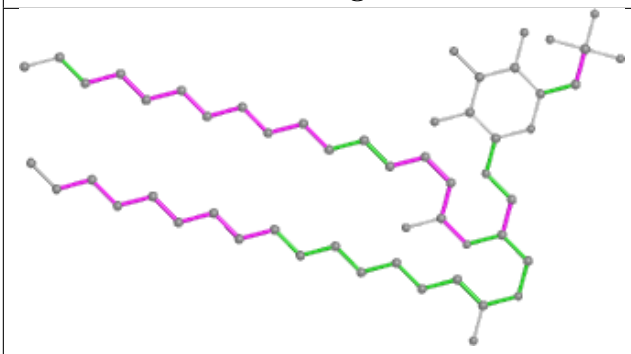

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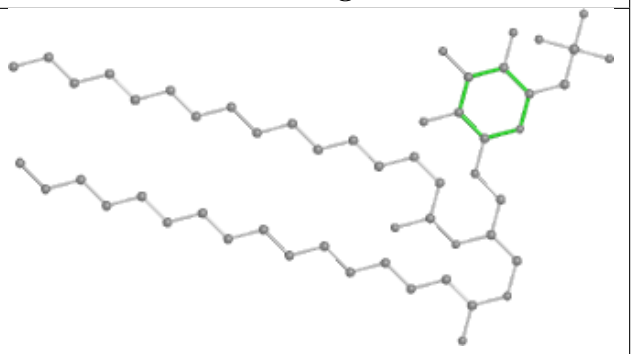
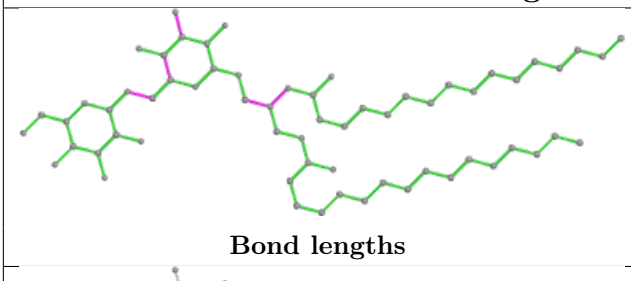


Rings

Ligand DGD h 102



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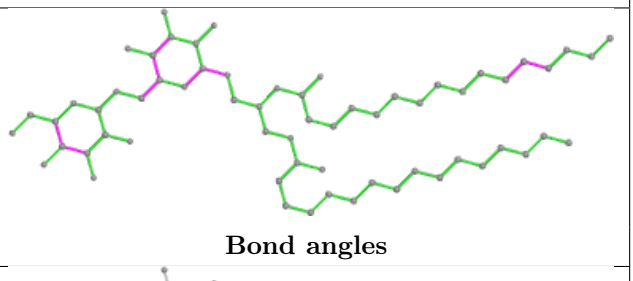
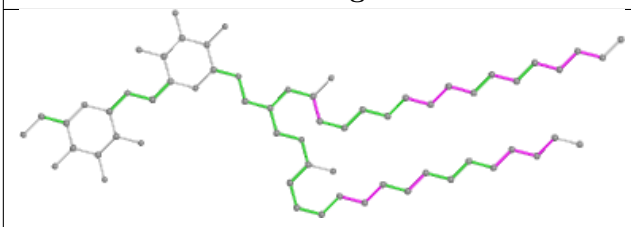


Bond angles



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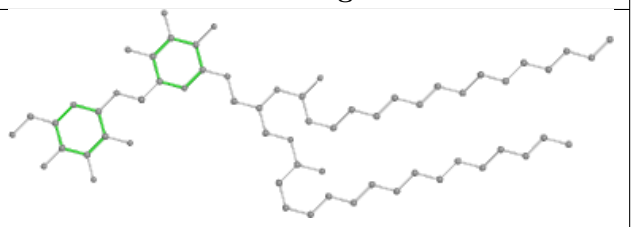
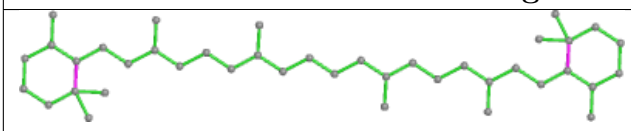


Rings

Ligand BCR A 409



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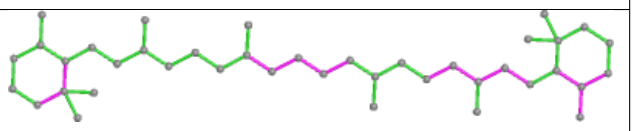

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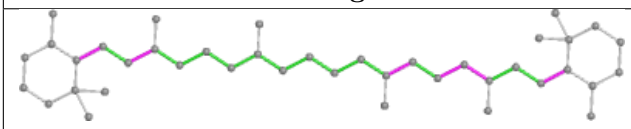

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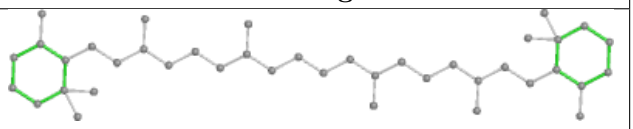
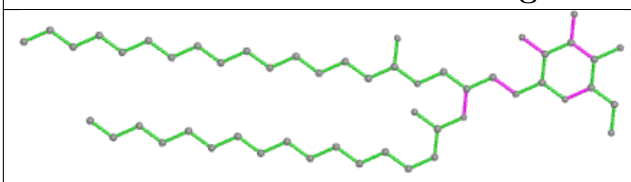


Rings

Ligand LMG C 520



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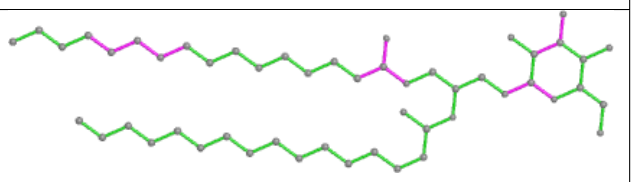
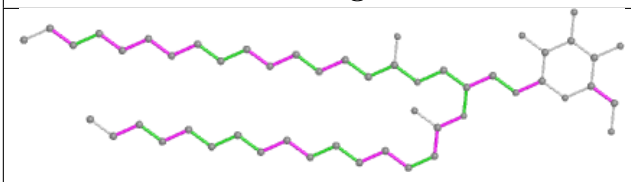


Bond angles



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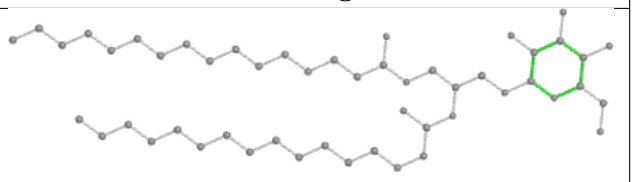
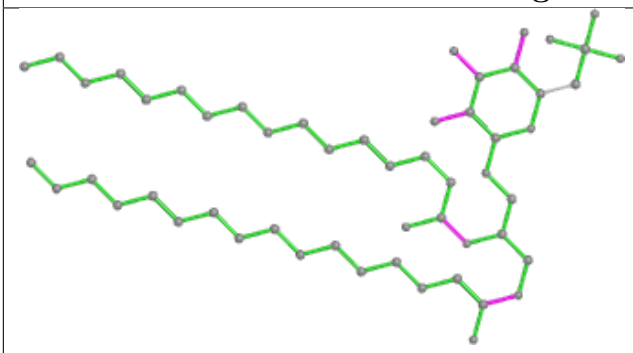


Rings

Ligand SQD l 101



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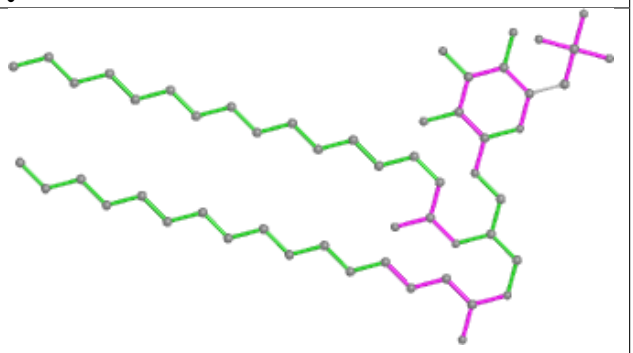
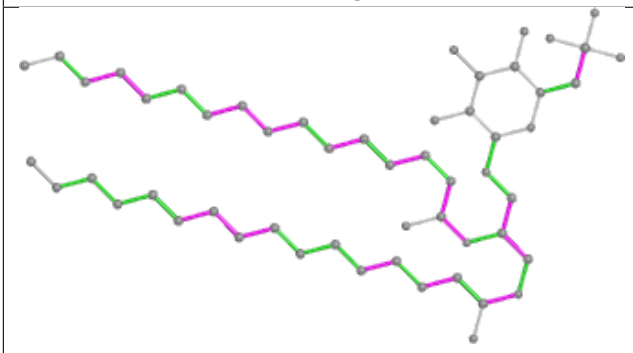


Bond angles



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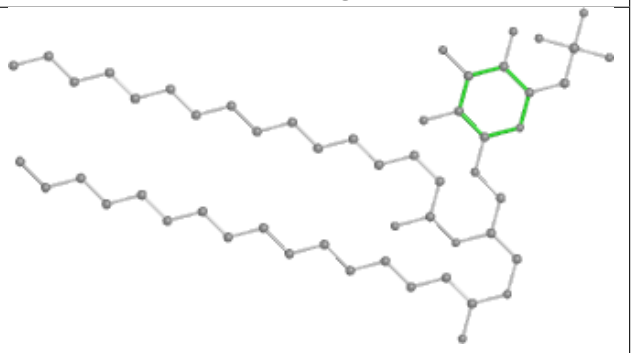
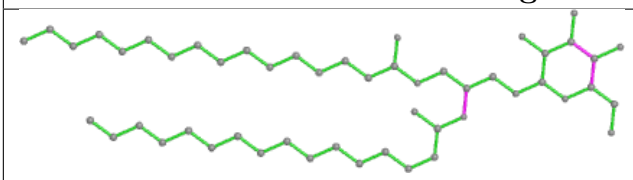


Rings

Ligand LMG C 501



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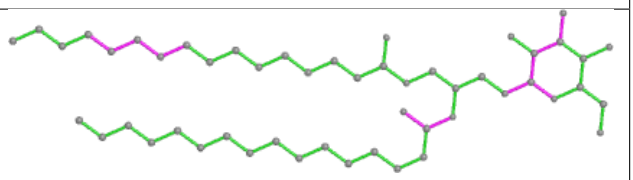

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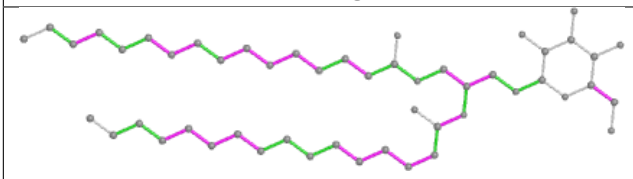

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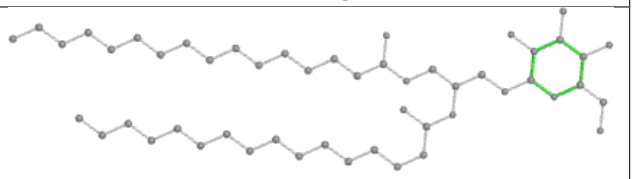
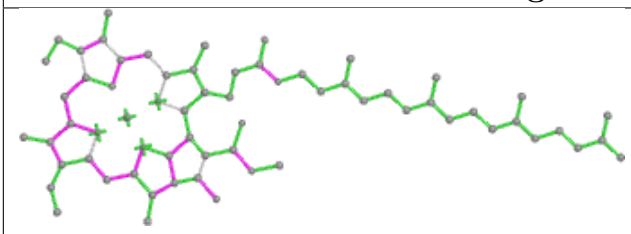


Rings

Ligand CLA b 617



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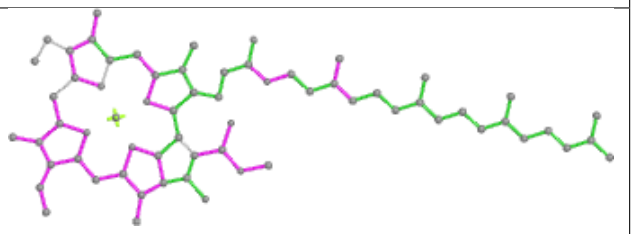
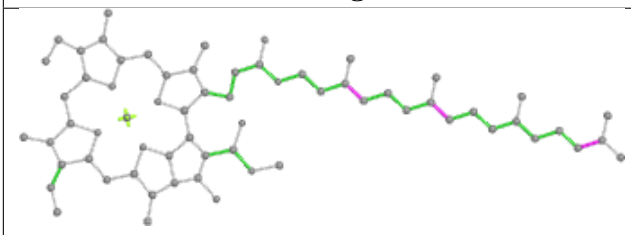


Bond angles



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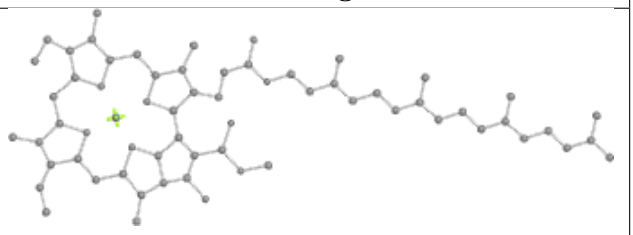
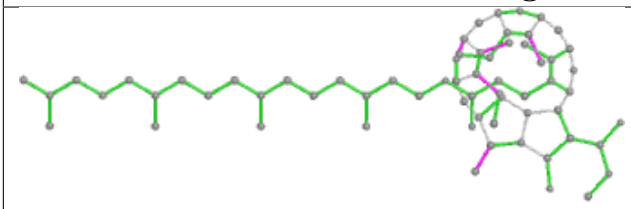


Rings

Ligand PHO D 402



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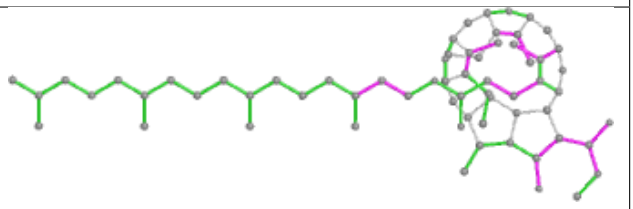
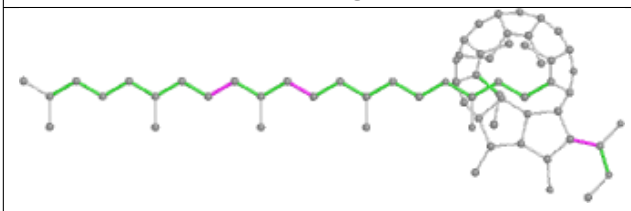


Bond angles



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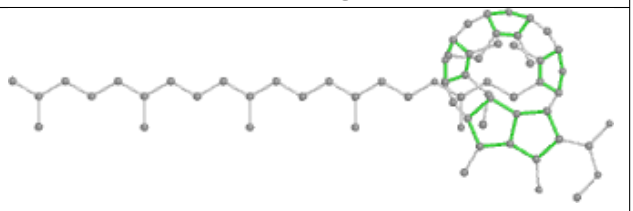
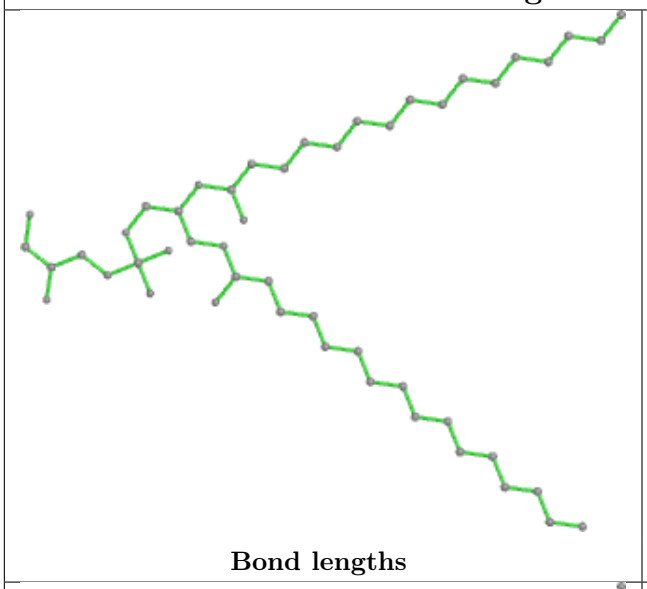


Rings

Ligand LHG E 101



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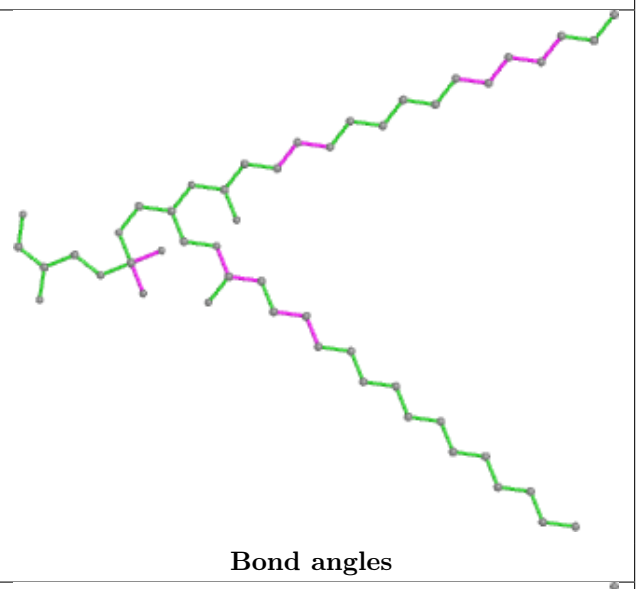
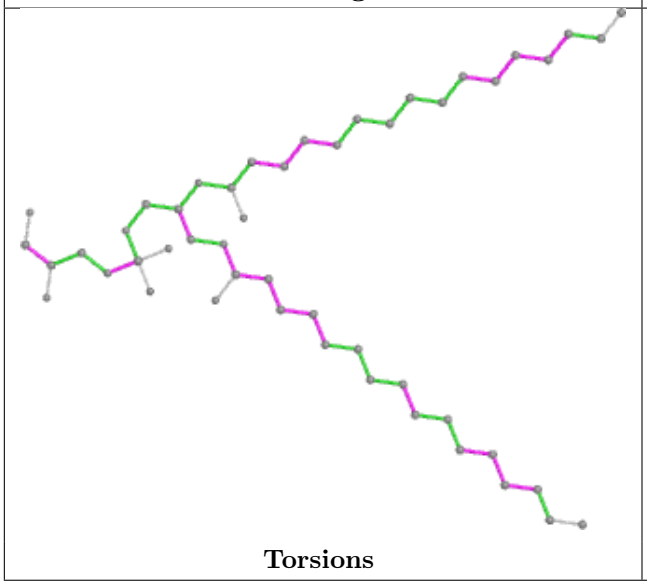


Bond angles



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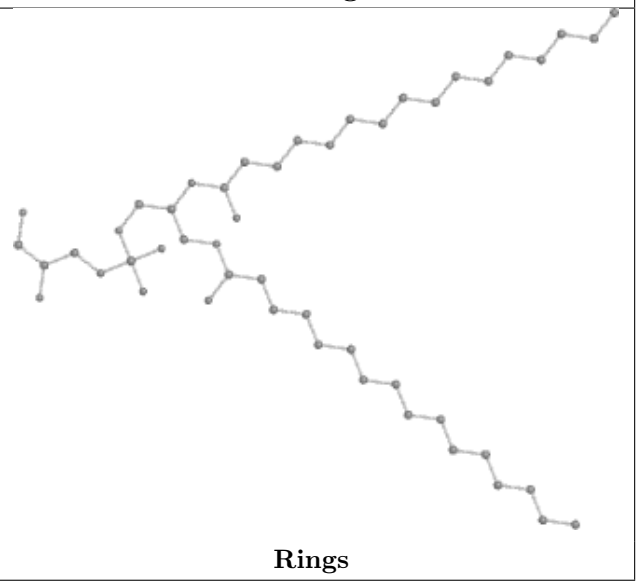
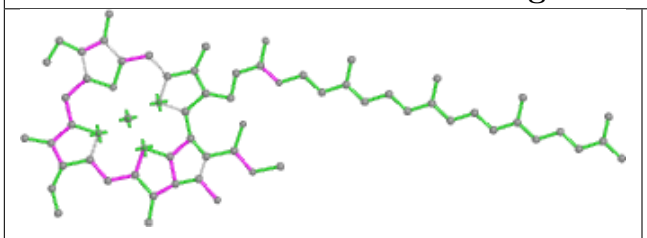


Rings

Ligand CLA b 607



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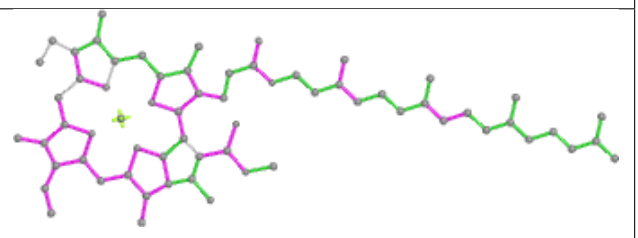
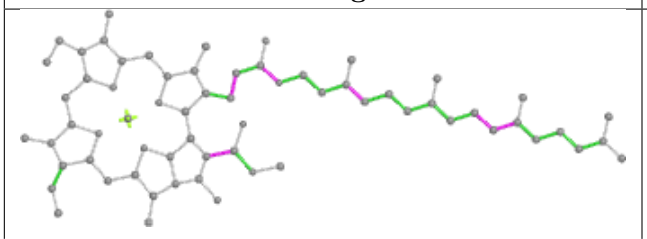


Bond angles



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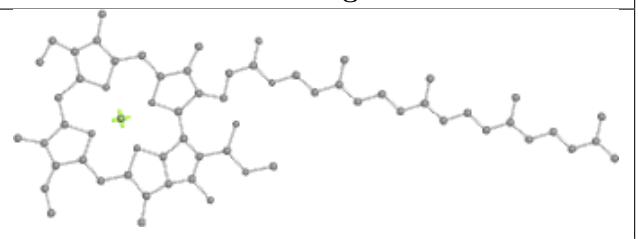
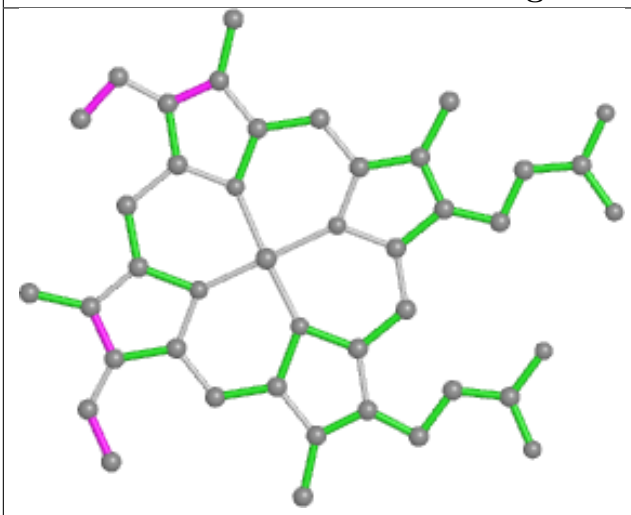


Rings

Ligand HEC v 201



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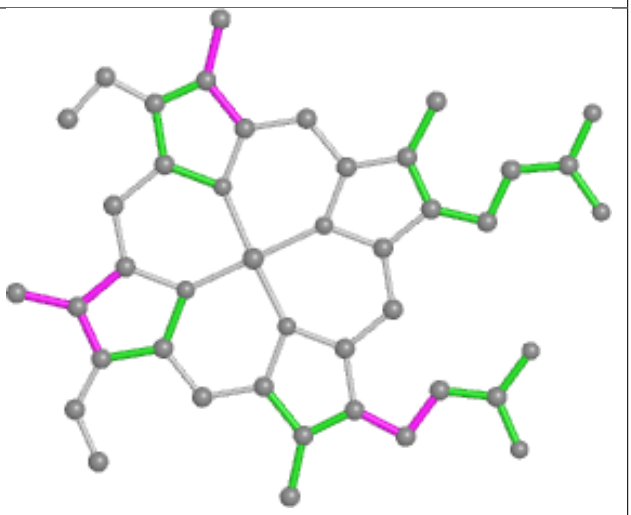
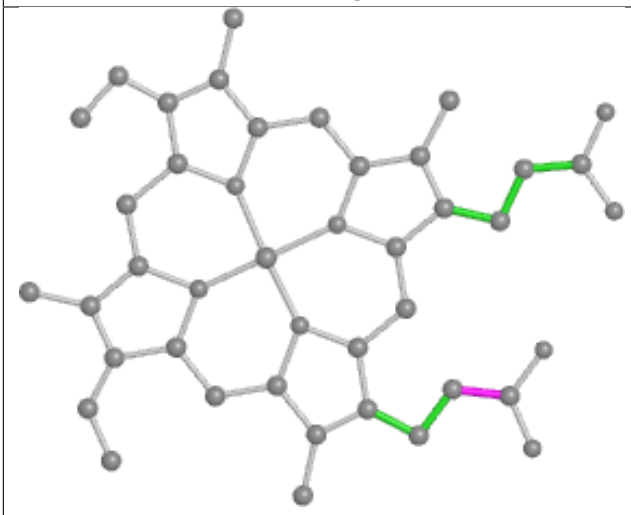
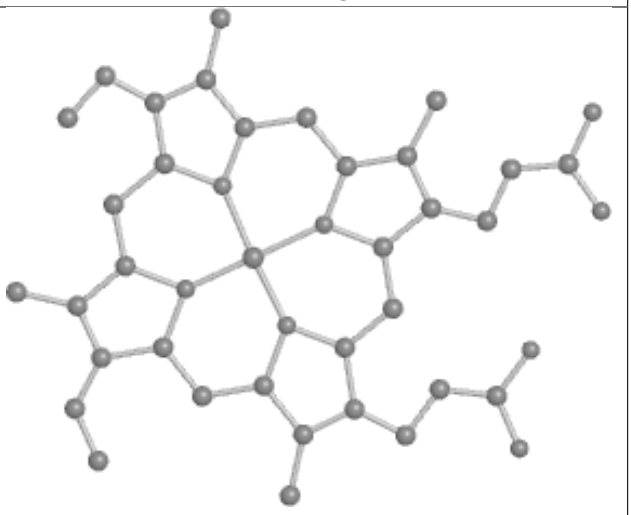


Bond angles

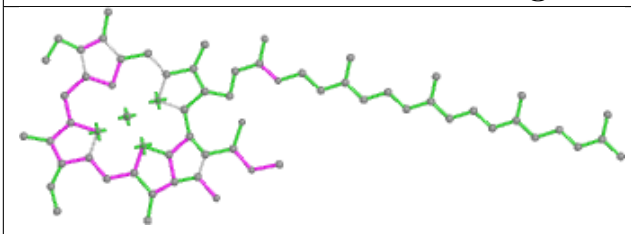


Torsions

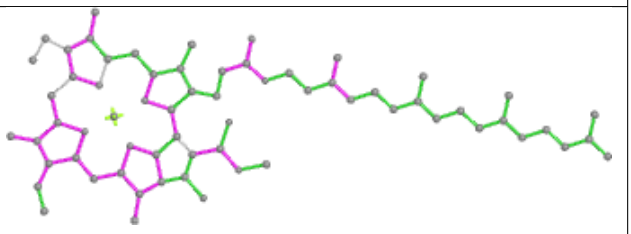


Rings

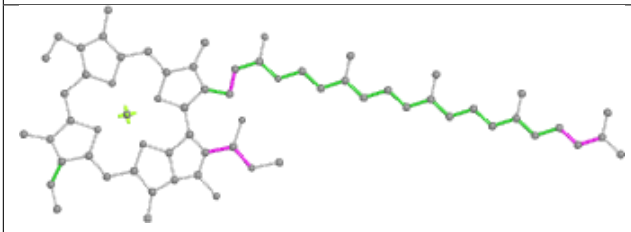
Ligand CLA c 504



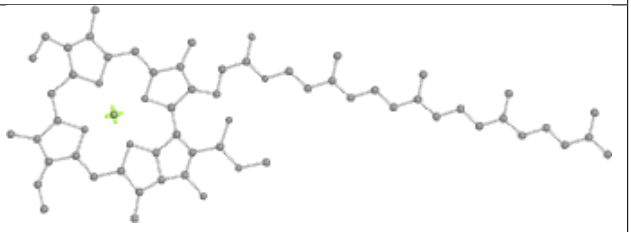
Bond lengths



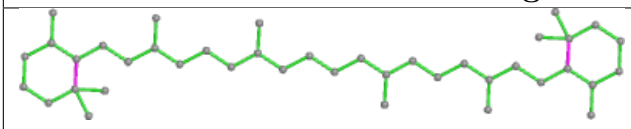
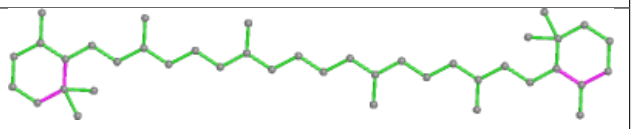
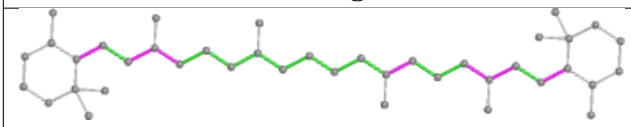
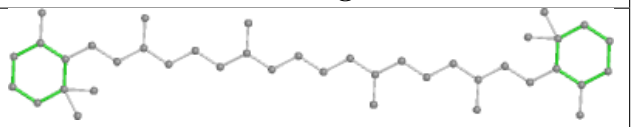
Bond angles

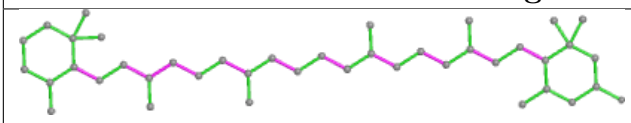
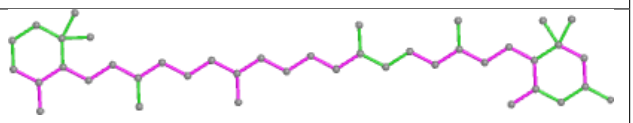
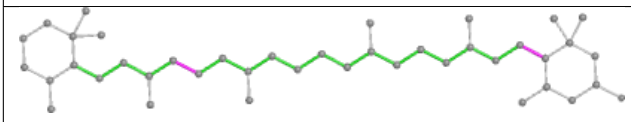
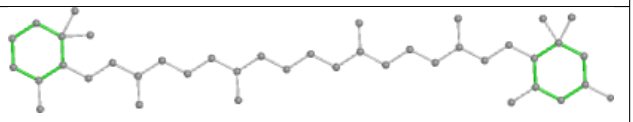


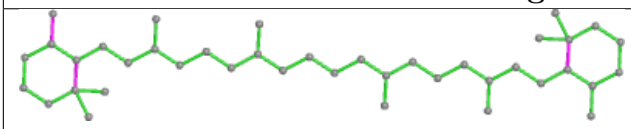
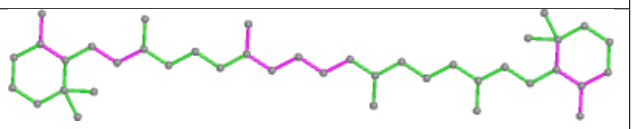
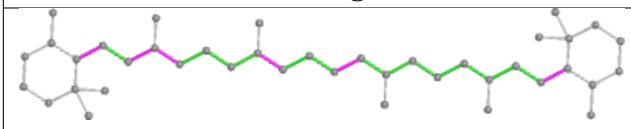
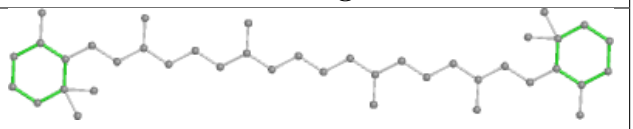
Torsions



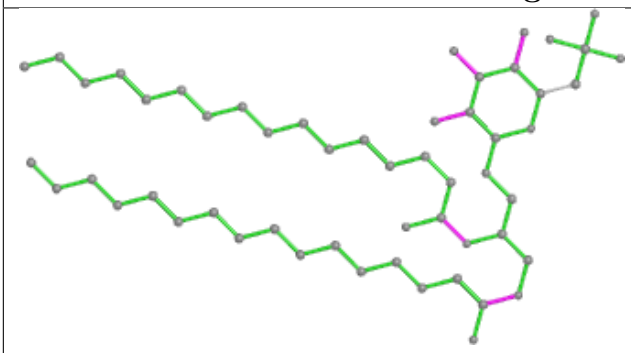
Rings

Ligand BCR B 619	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand RRX h 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR c 515	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand SQD A 412



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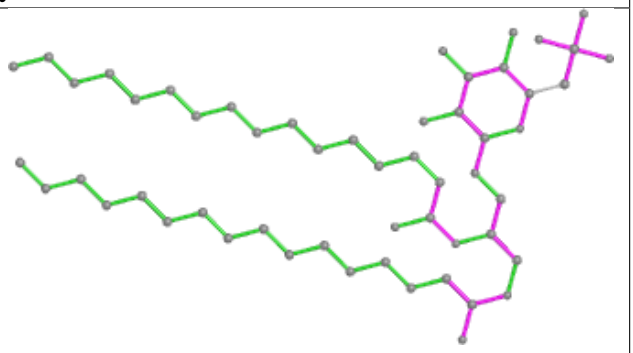

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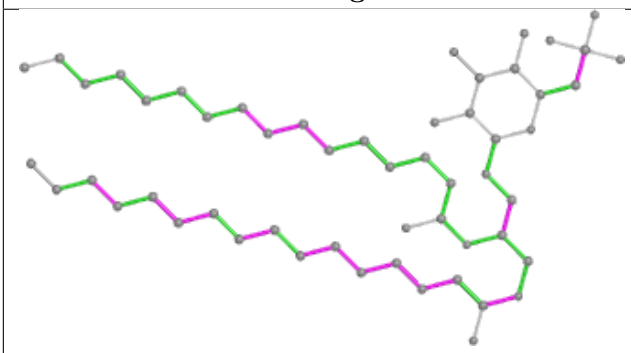

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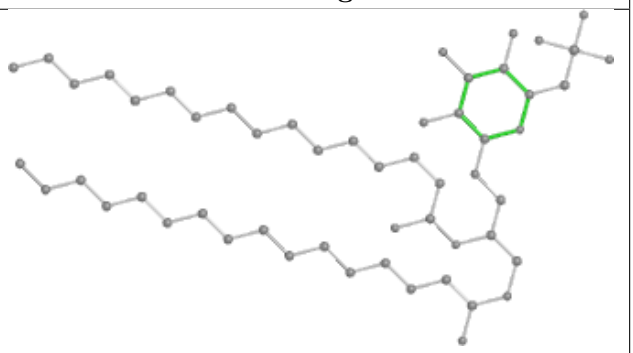
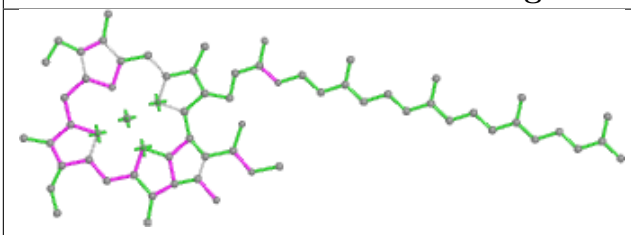


Rings

Ligand CLA B 606



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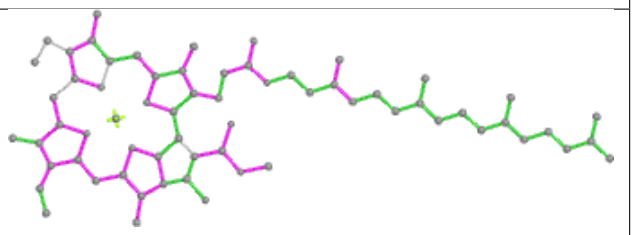
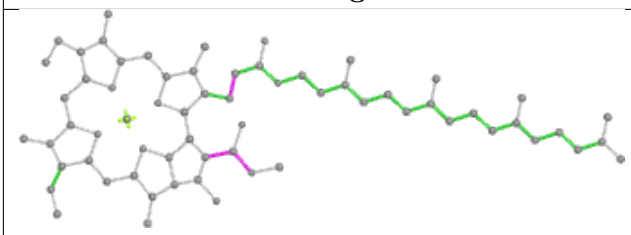


Bond angles



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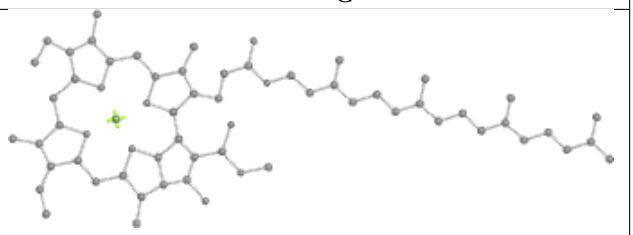
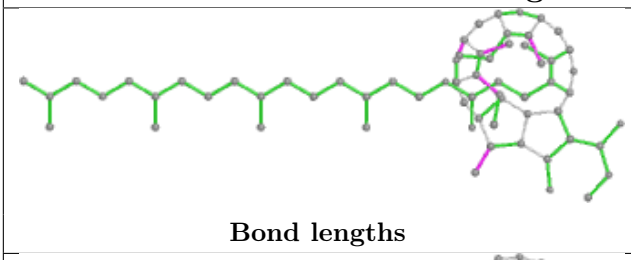


Rings

Ligand PHO a 407



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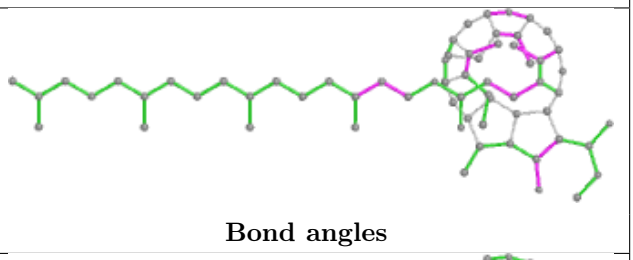
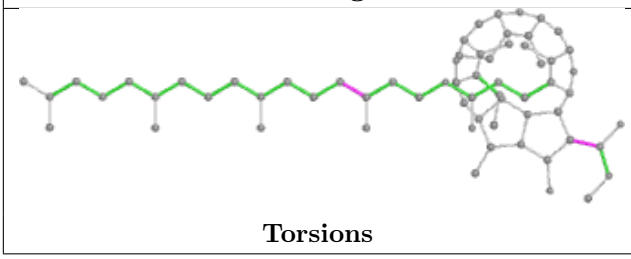


Bond angles



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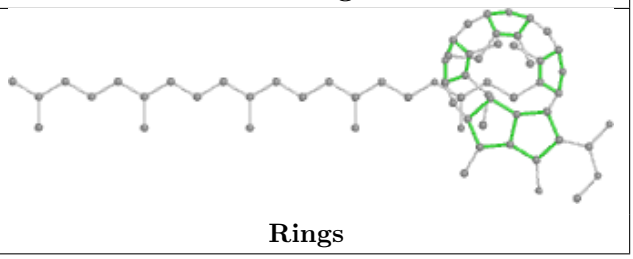
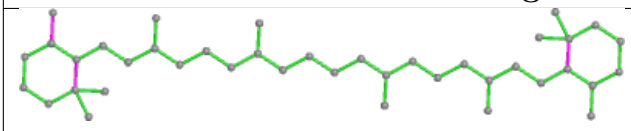


Rings

Ligand BCR C 515



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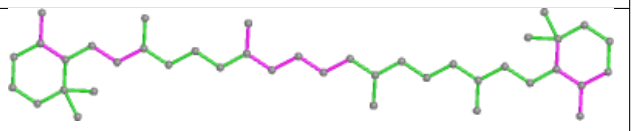
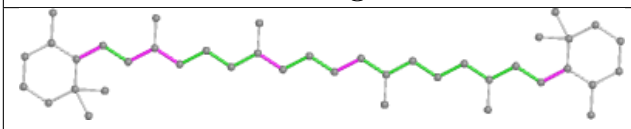


Bond angles



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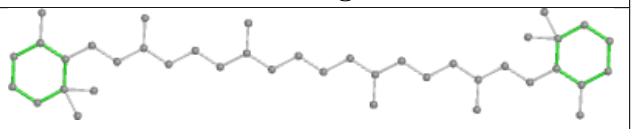
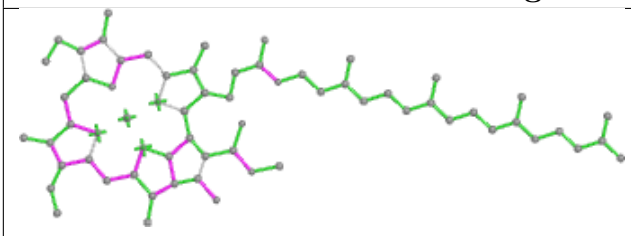
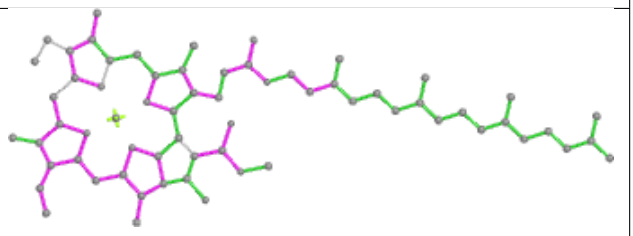


Rings

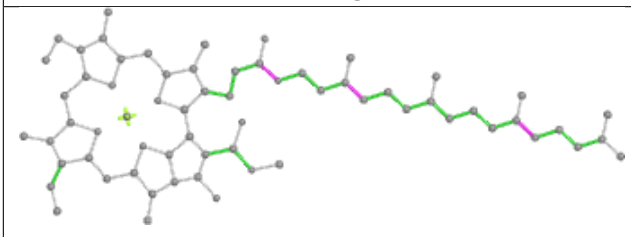
Ligand CLA B 611



Bond lengths



Bond angles



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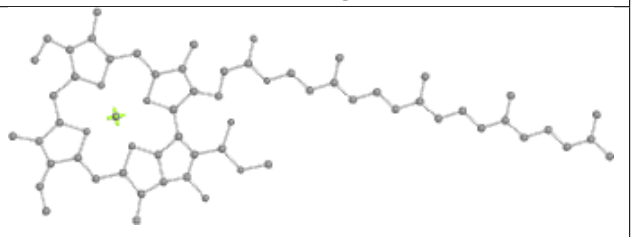
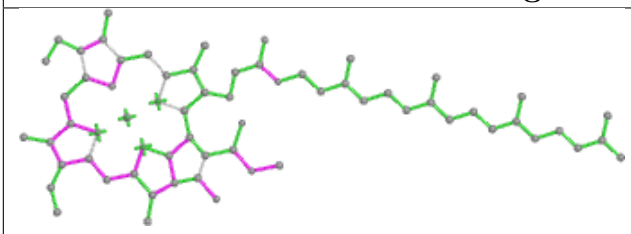


Rings

Ligand CLA A 405



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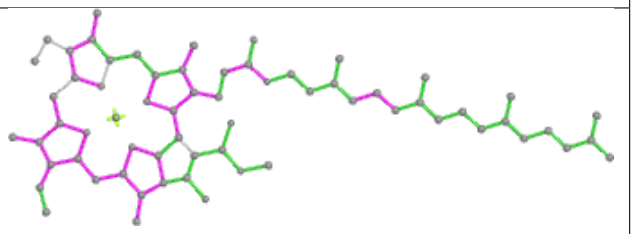
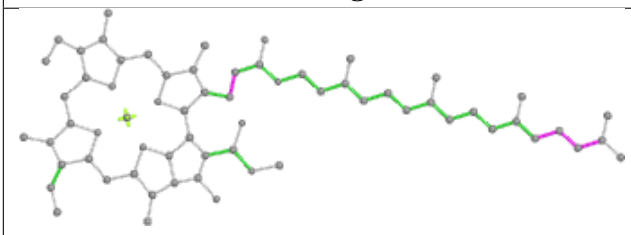


Bond angles



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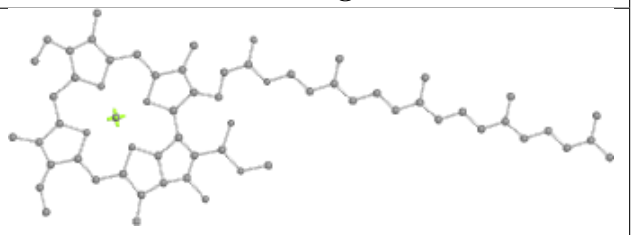
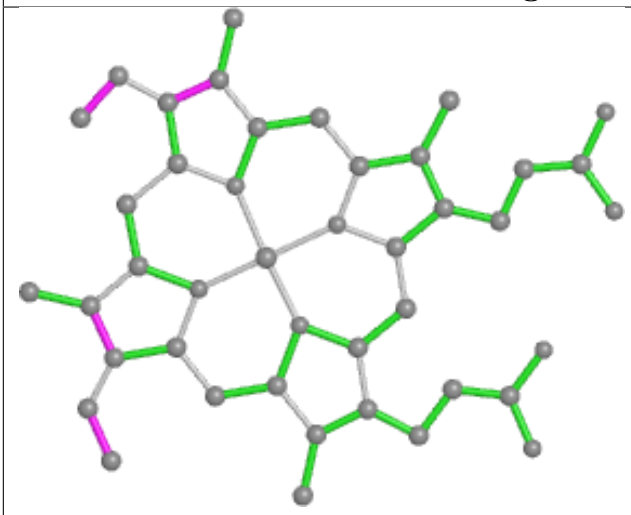


Rings

Ligand HEC V 201



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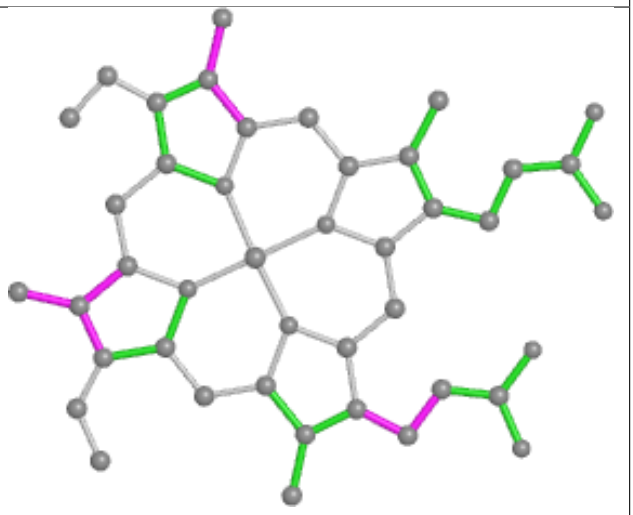
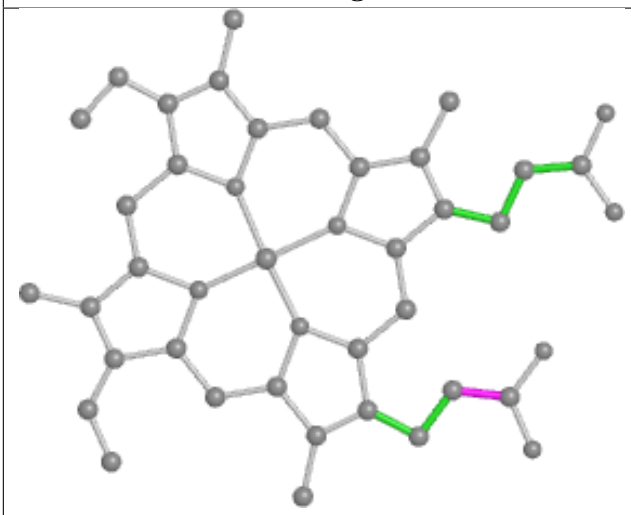


Bond angles



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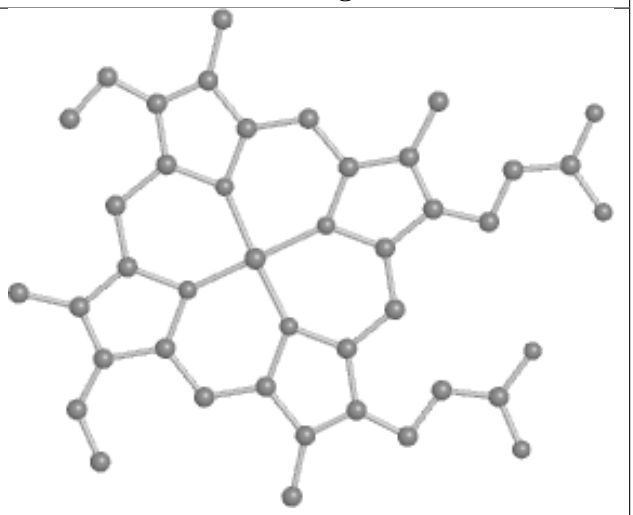
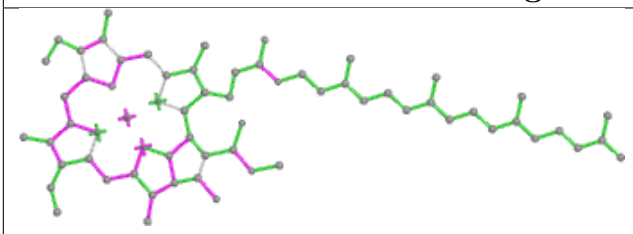


Rings

Ligand CLA C 506



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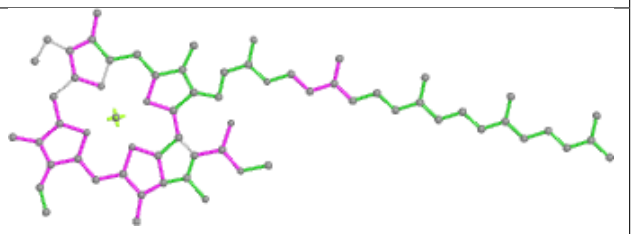
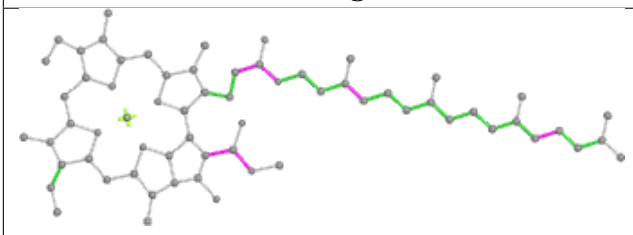


Bond angles



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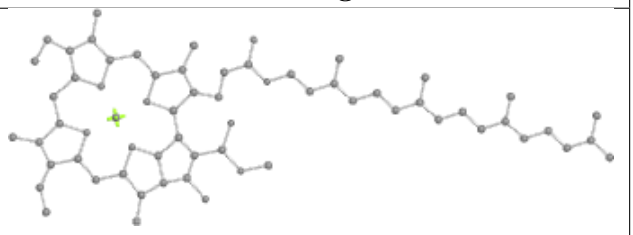
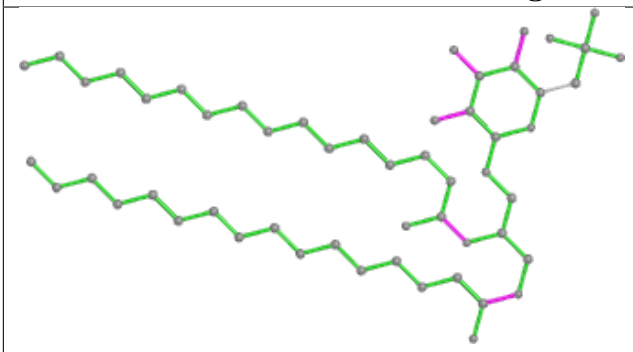


Rings

Ligand SQD L 101



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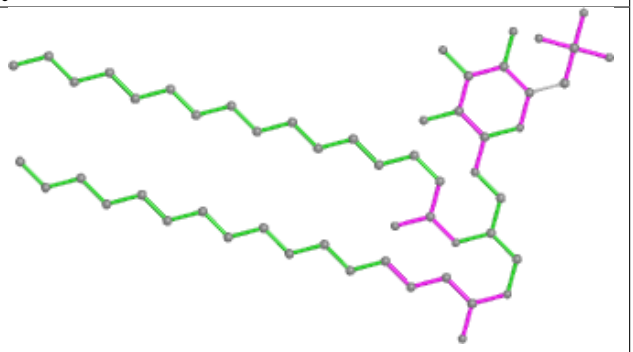
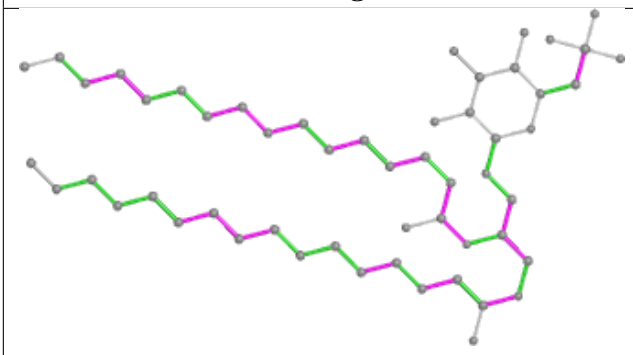


Bond angles



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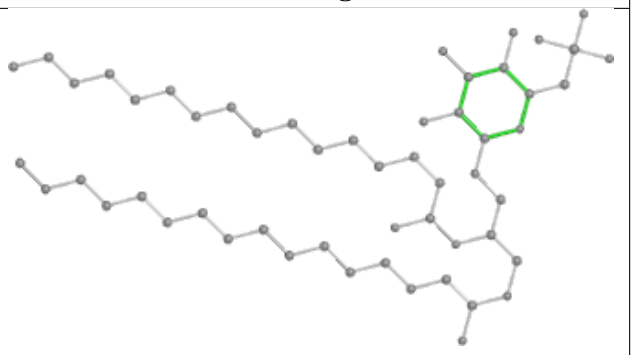
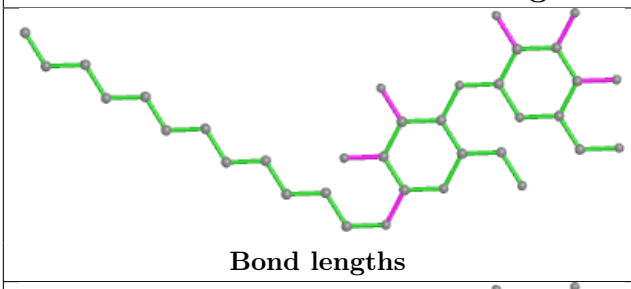


Rings

Ligand LMT i 102



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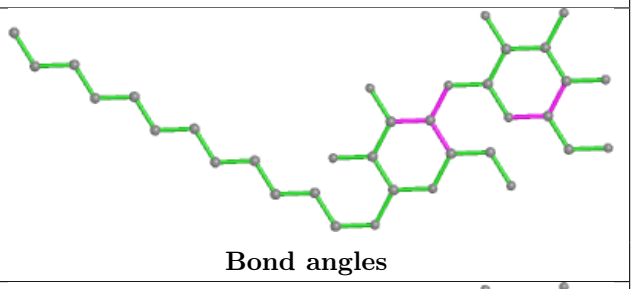
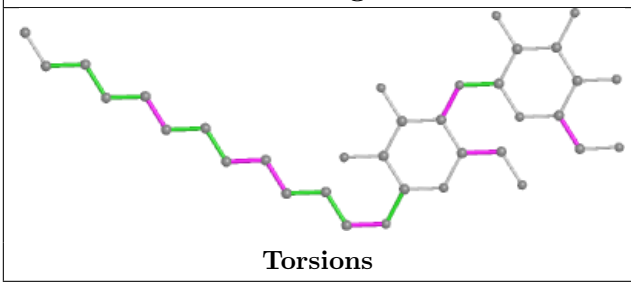


Bond angles



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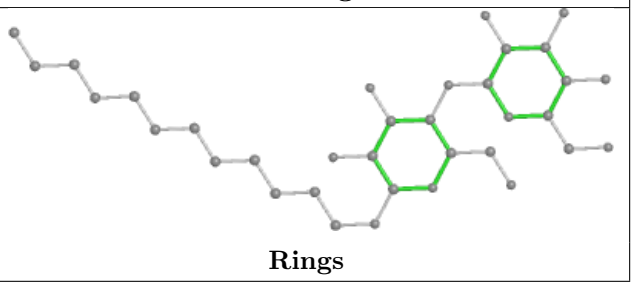
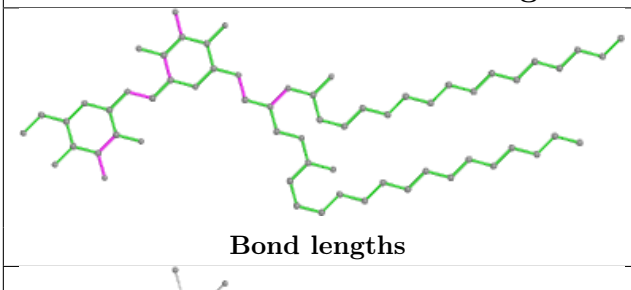


Rings

Ligand DGD C 519



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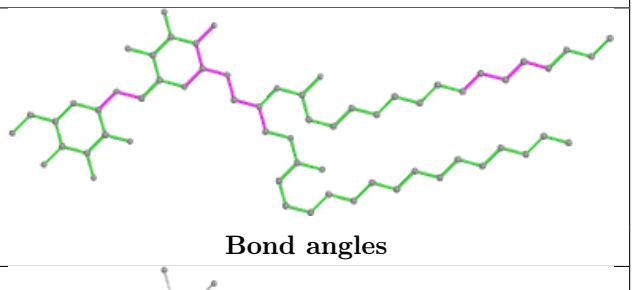
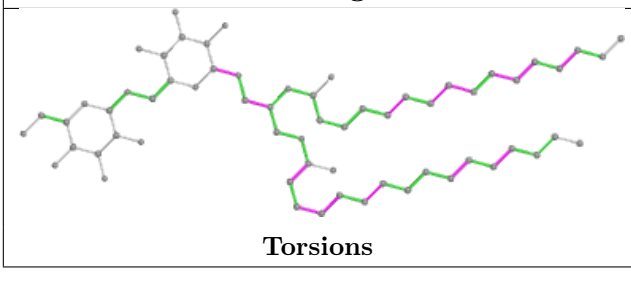


Bond angles



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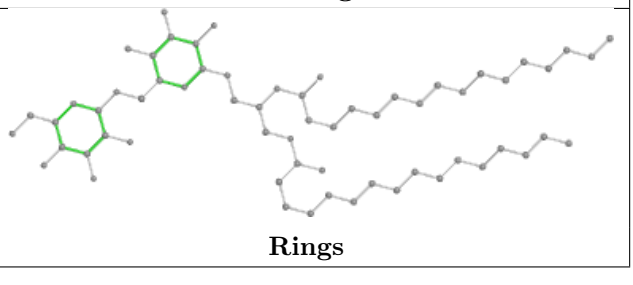
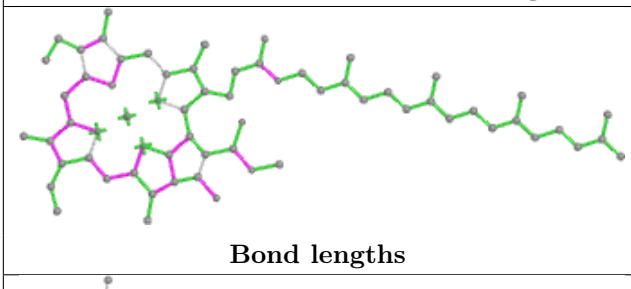
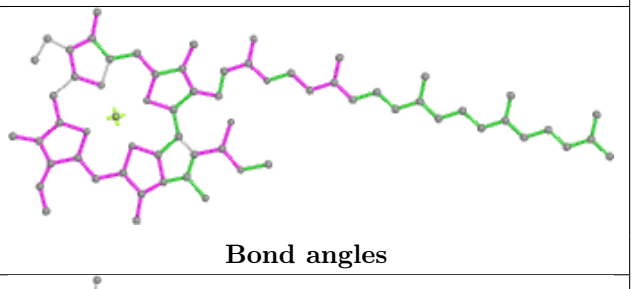


Rings

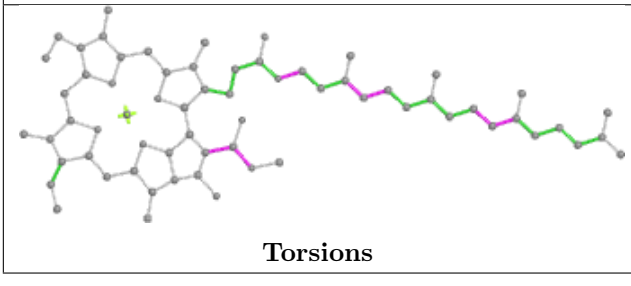
Ligand CLA B 614



Bond lengths



Bond angles



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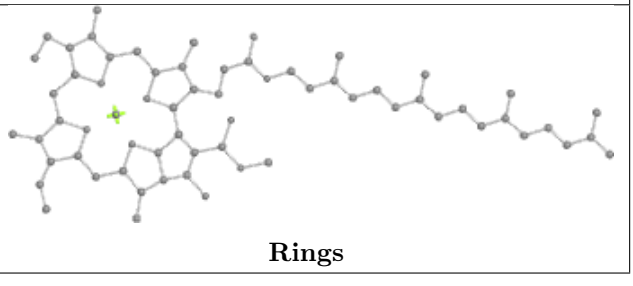
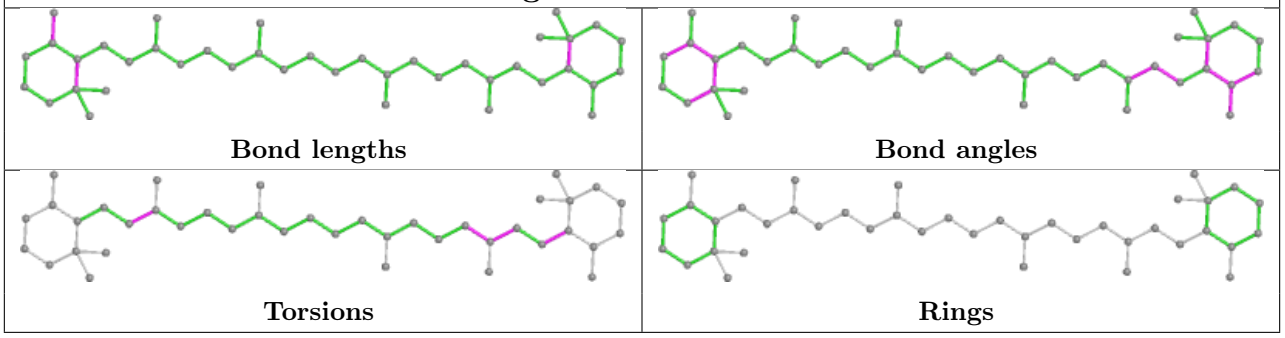


Rings

Ligand BCR D 405



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.

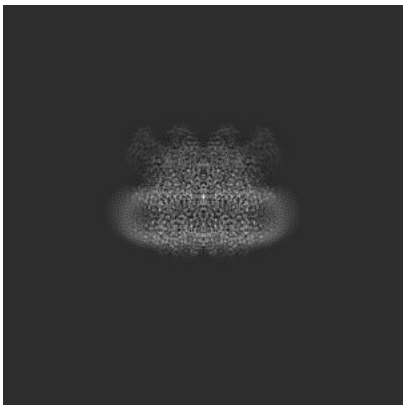
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-30548. These allow visual inspection of the internal detail of the map and identification of artifacts.

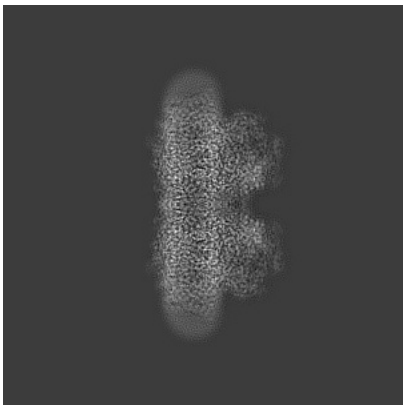
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

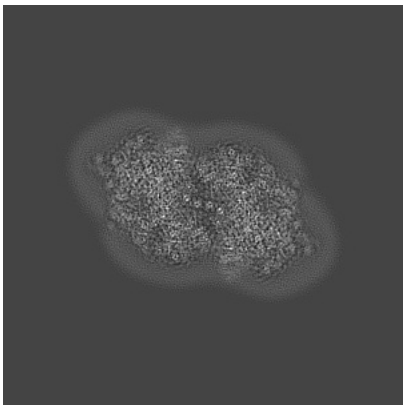
6.1.1 Primary map



X

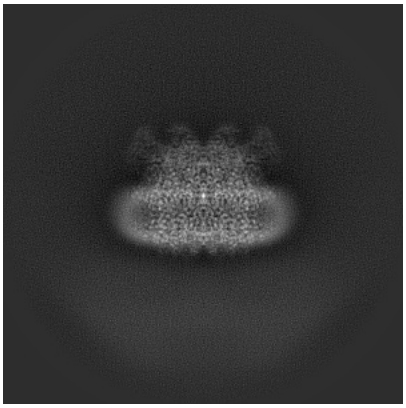


Y

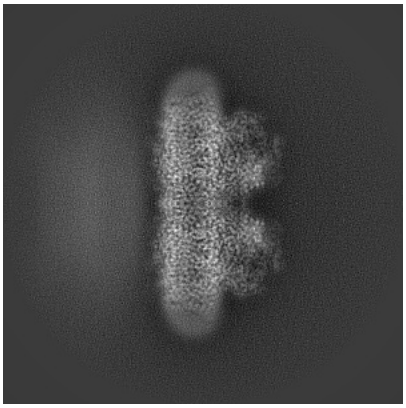


Z

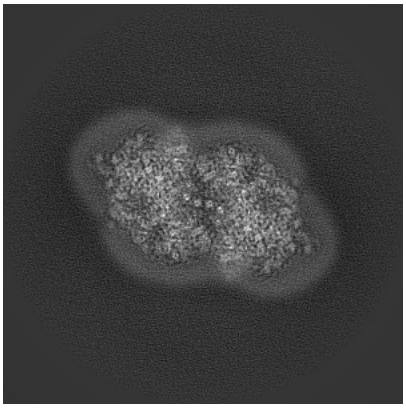
6.1.2 Raw map



X



Y

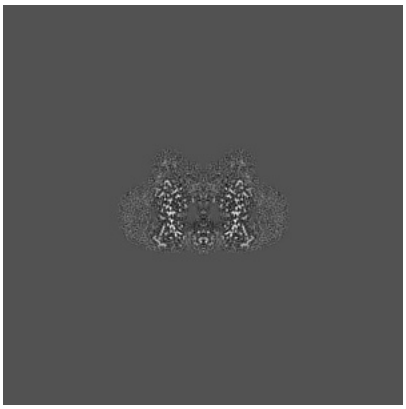


Z

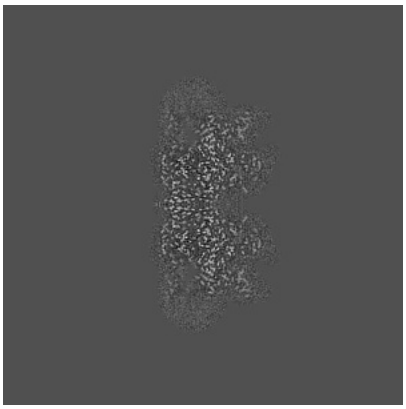
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

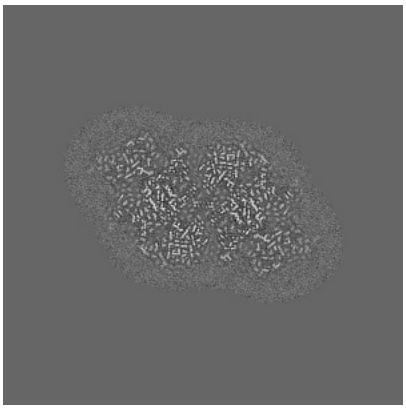
6.2.1 Primary map



X Index: 200

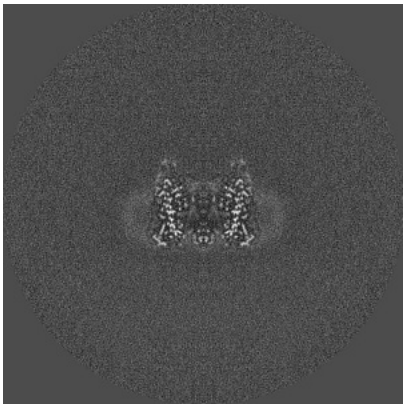


Y Index: 200

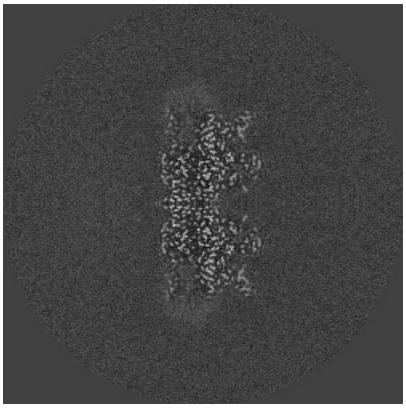


Z Index: 200

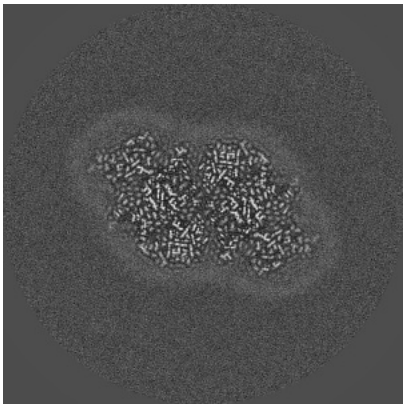
6.2.2 Raw map



X Index: 200



Y Index: 200

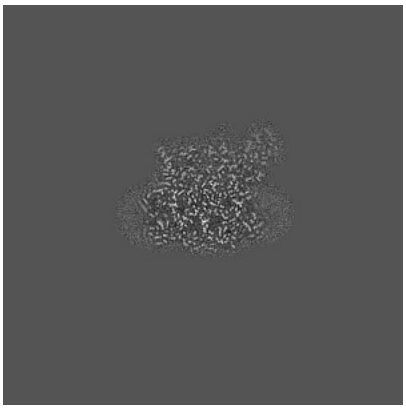


Z Index: 200

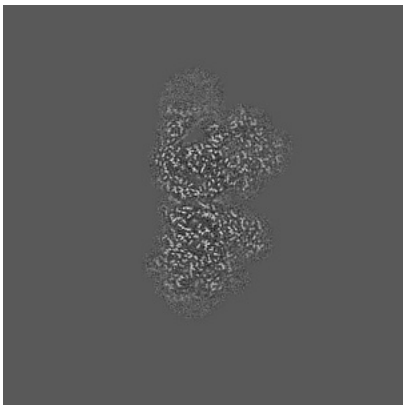
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

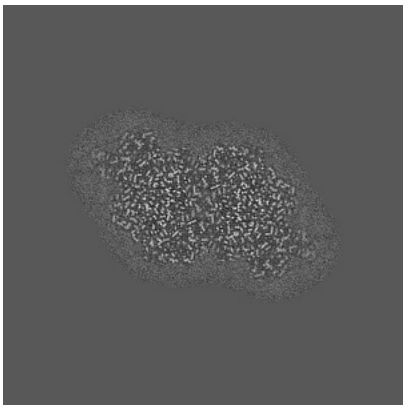
6.3.1 Primary map



X Index: 167

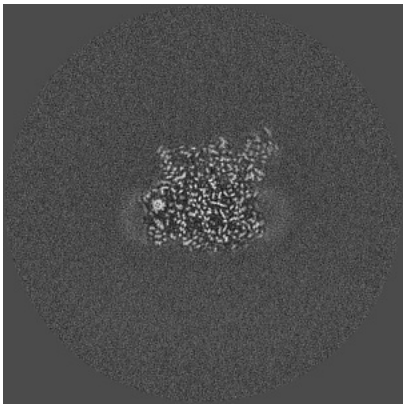


Y Index: 182

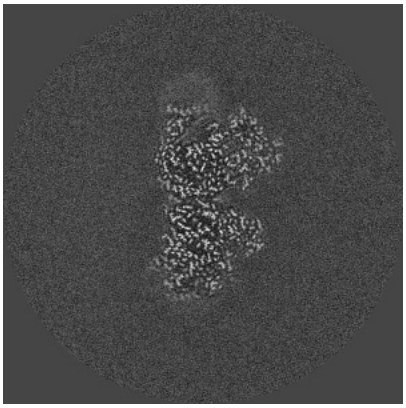


Z Index: 209

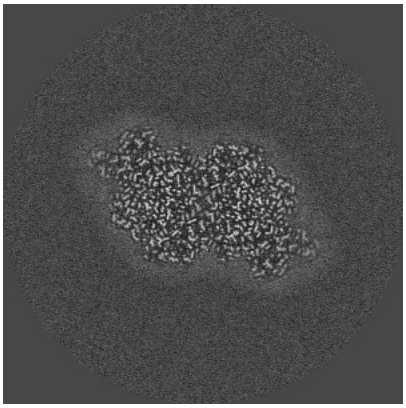
6.3.2 Raw map



X Index: 166



Y Index: 182

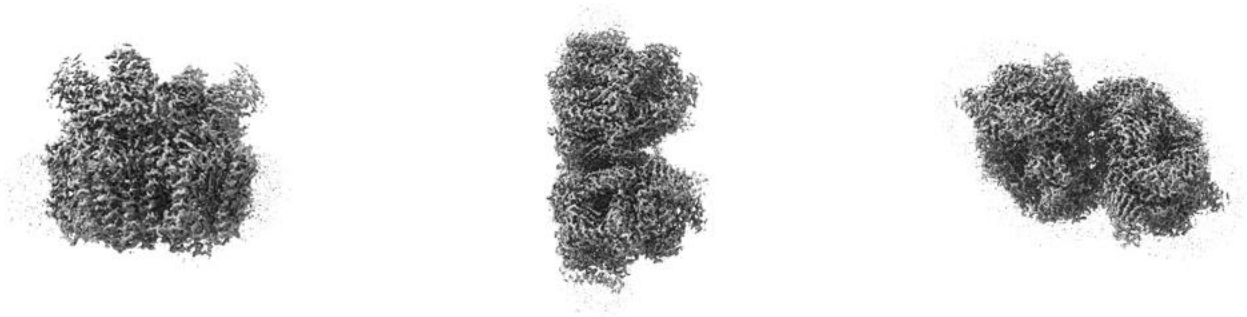


Z Index: 209

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 0.01. 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.

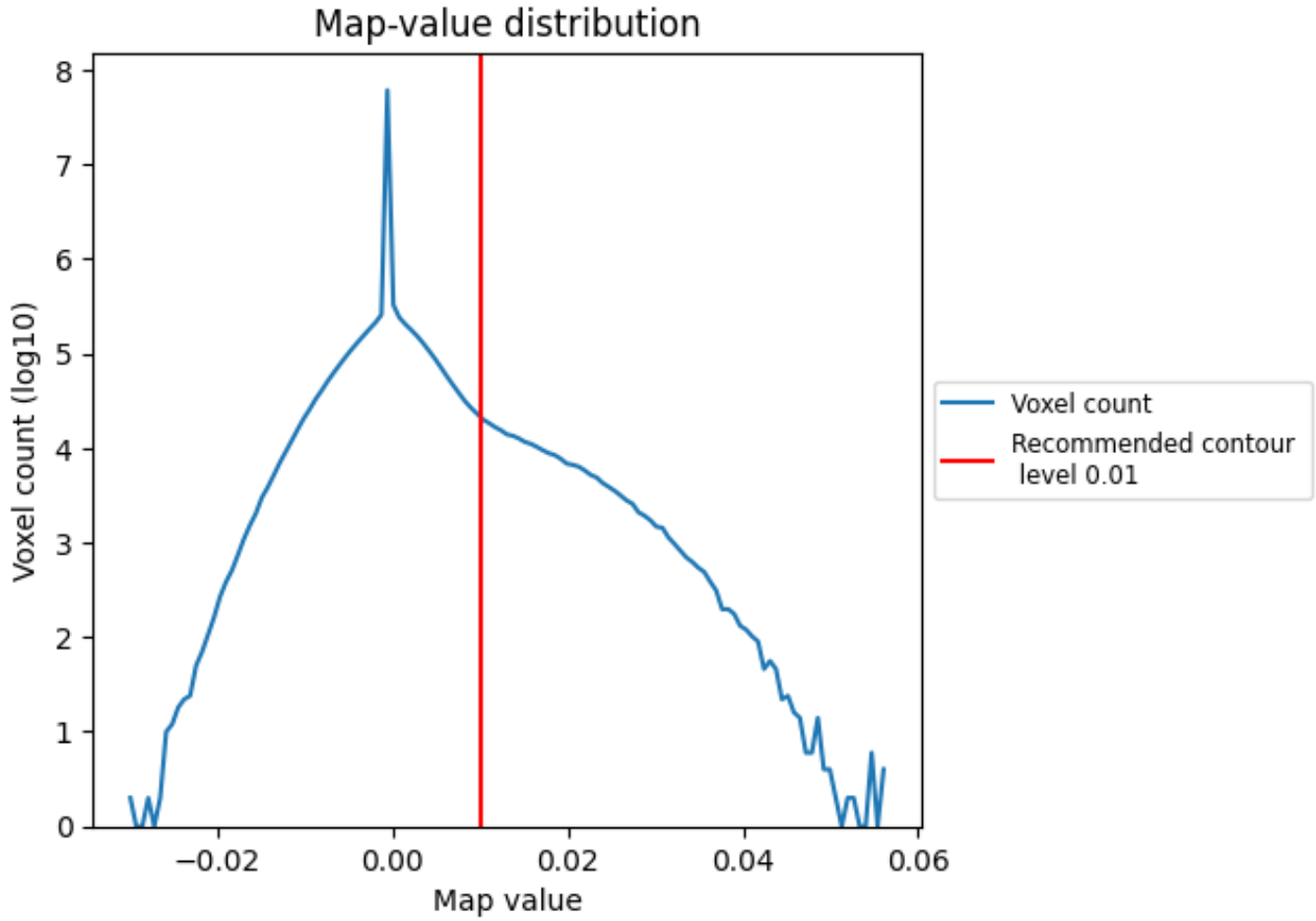
6.5 Mask visualisation (i)

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

7 Map analysis

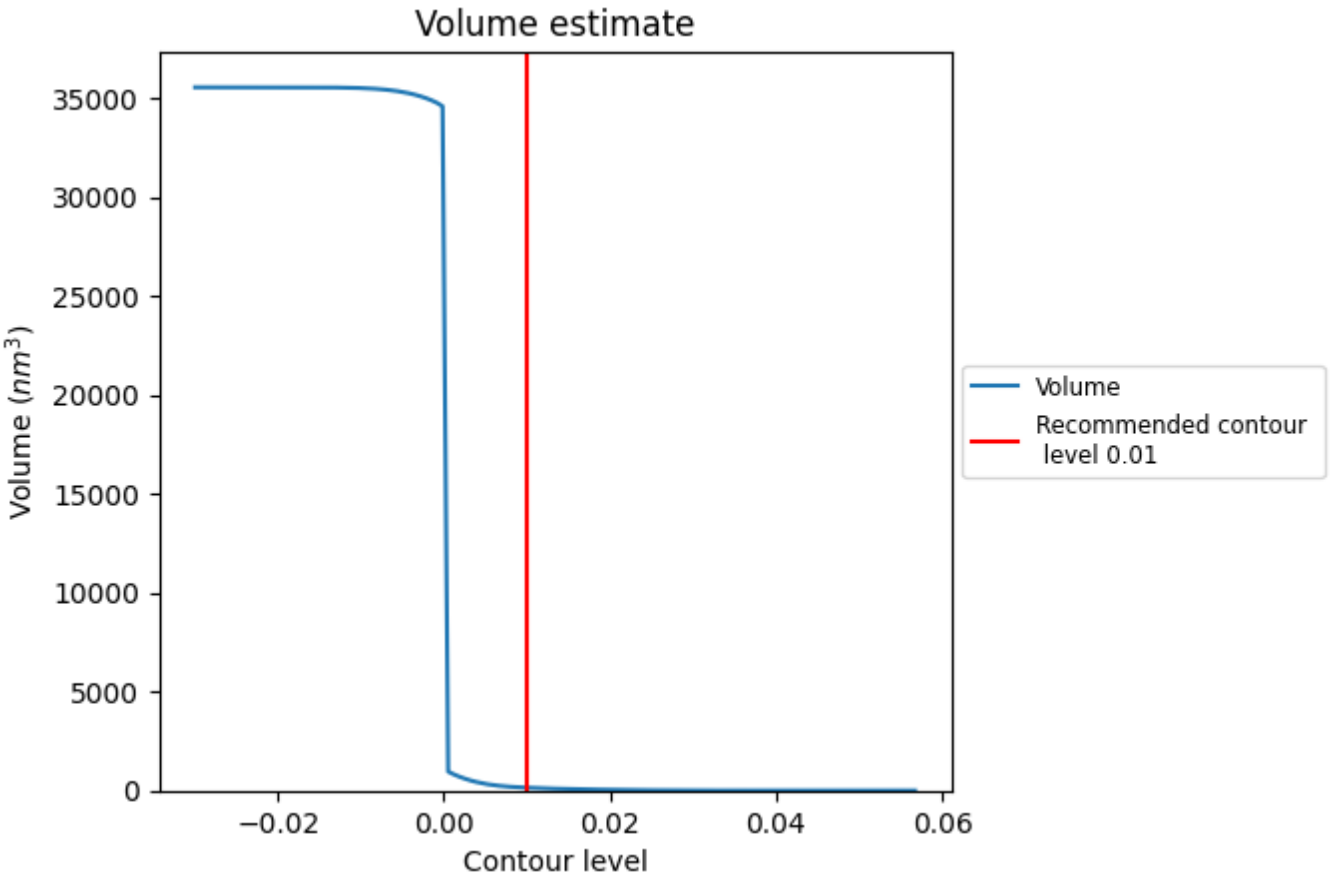
This section contains the results of statistical analysis of the map.

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.

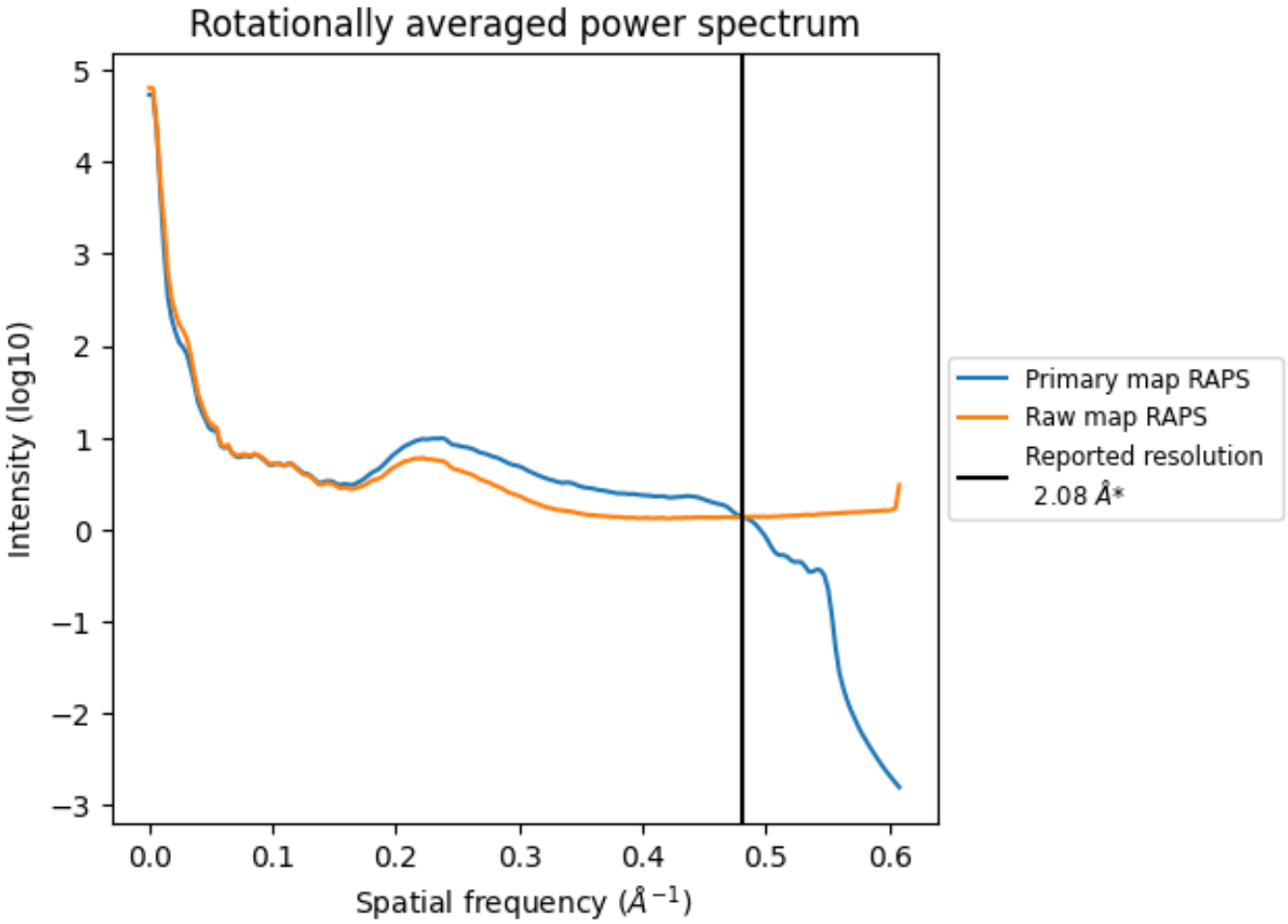
7.2 Volume estimate



The volume at the recommended contour level is 144 nm^3; this corresponds to an approximate mass of 130 kDa.

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

7.3 Rotationally averaged power spectrum (i)

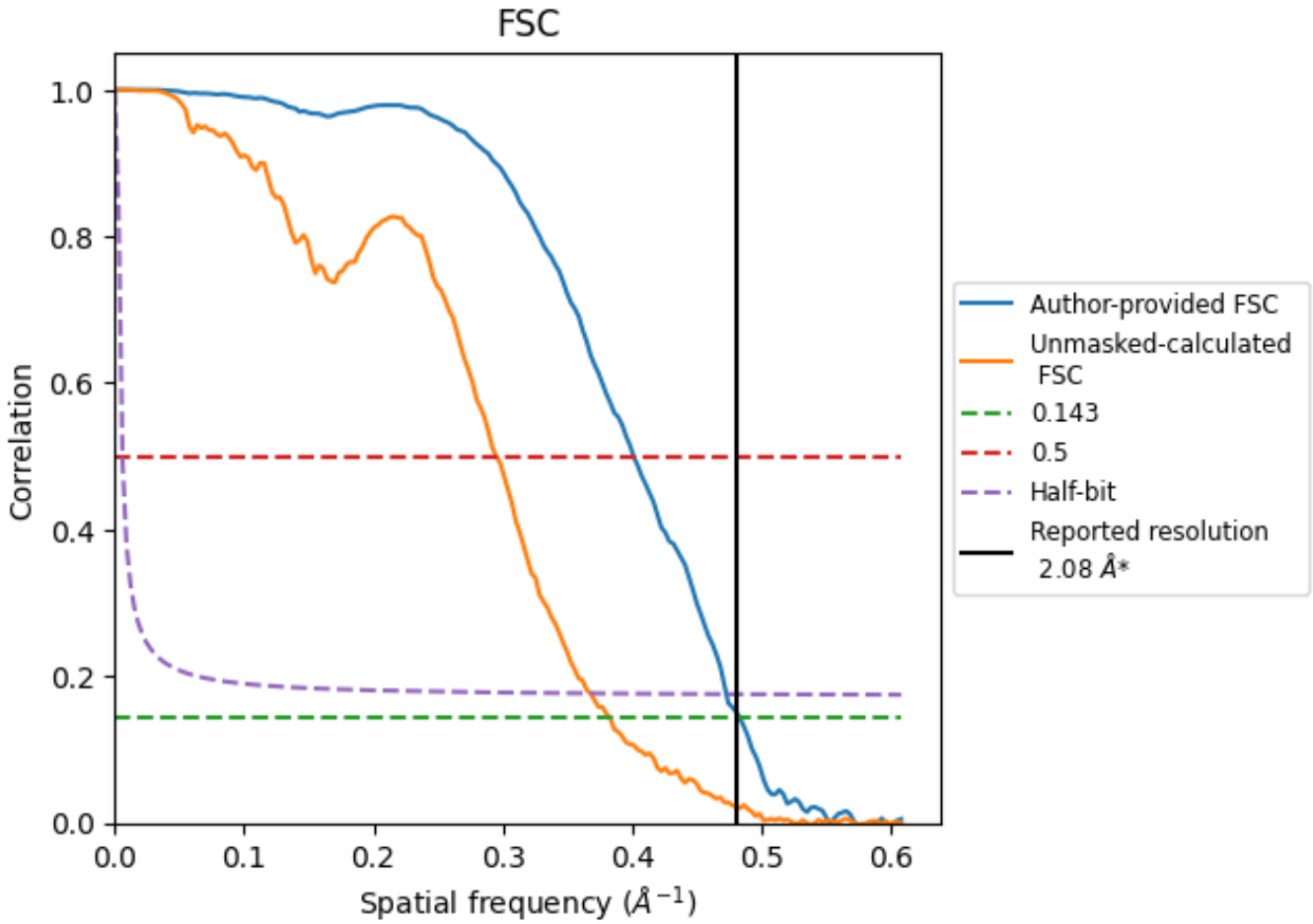


*Reported resolution corresponds to spatial frequency of 0.481 Å^{-1}

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 0.481 Å^{-1}

8.2 Resolution estimates (i)

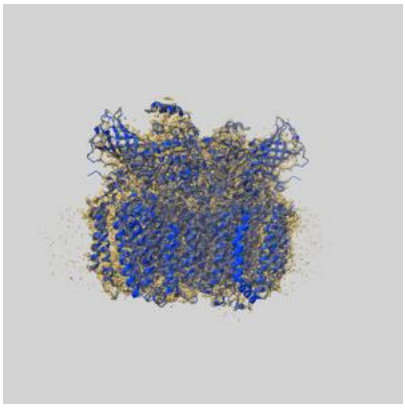
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.08	-	-
Author-provided FSC curve	2.07	2.49	2.11
Unmasked-calculated*	2.61	3.39	2.72

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.61 differs from the reported value 2.08 by more than 10 %

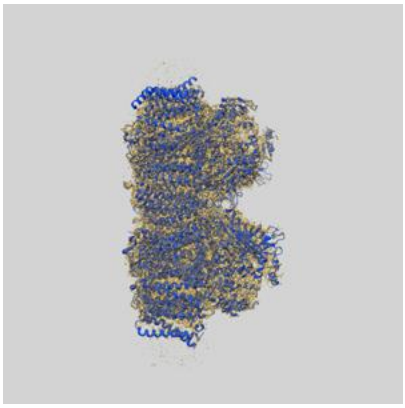
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-30548 and PDB model 7D1U. Per-residue inclusion information can be found in section 3 on page 28.

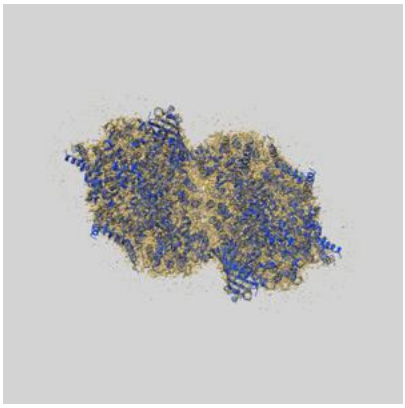
9.1 Map-model overlay



X



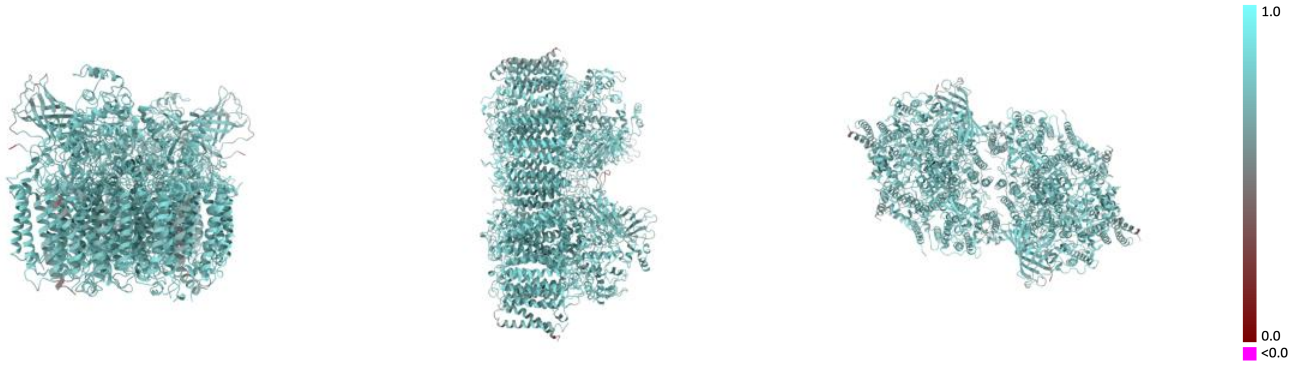
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.01 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.

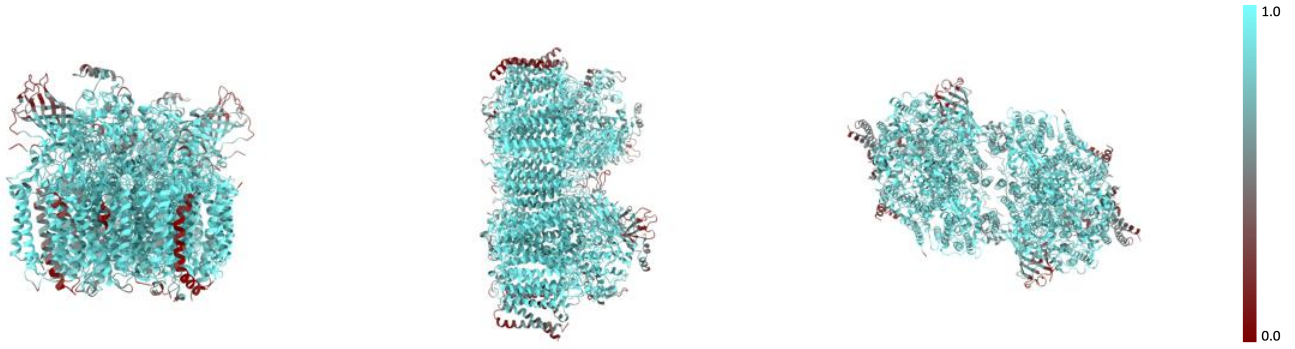
9.2 Q-score mapped to coordinate model



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.

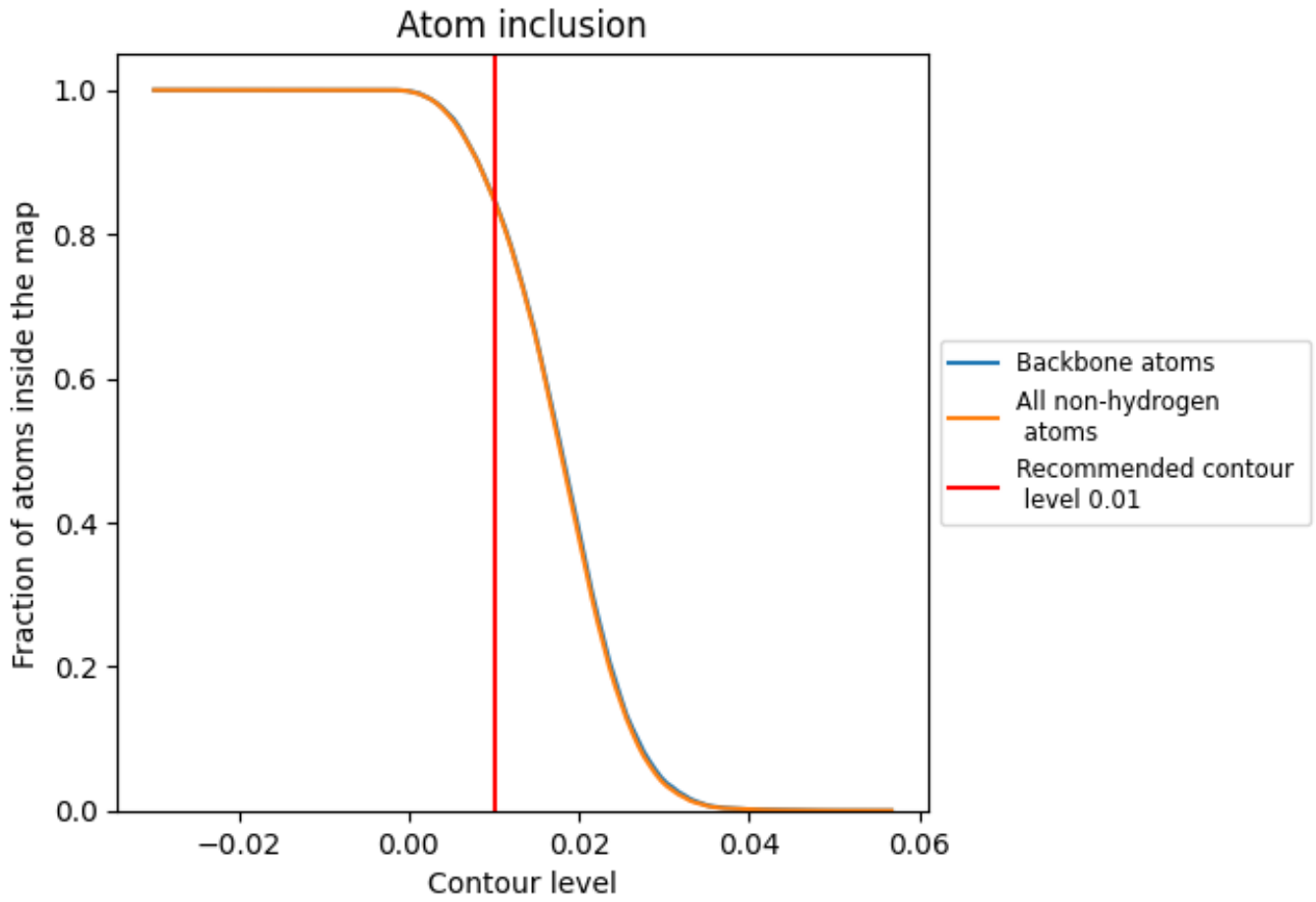
9.3 Atom inclusion mapped to coordinate model



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 (0.01).

9.4 Atom inclusion (i)



At the recommended contour level, 85% of all backbone atoms, 85% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8477	0.7570
A	0.9265	0.7880
B	0.9067	0.7750
C	0.8832	0.7580
D	0.9351	0.7890
E	0.7725	0.7350
F	0.8773	0.7660
H	0.9051	0.7620
I	0.8192	0.7350
J	0.7979	0.7450
K	0.7678	0.7150
L	0.8381	0.7630
M	0.8520	0.7760
O	0.6798	0.7040
R	0.0940	0.5780
T	0.8746	0.7760
U	0.7697	0.7360
V	0.8085	0.7400
X	0.8028	0.7360
Y	0.5975	0.6790
Z	0.4126	0.6240
a	0.9265	0.7880
b	0.9058	0.7750
c	0.8832	0.7580
d	0.9348	0.7890
e	0.7725	0.7360
f	0.8773	0.7650
h	0.9051	0.7610
i	0.8192	0.7390
j	0.7979	0.7420
k	0.7678	0.7160
l	0.8381	0.7690
m	0.8487	0.7750
o	0.6798	0.7040
r	0.0940	0.5770

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Chain	Atom inclusion	Q-score
t	0.8602	0.7780
u	0.7697	0.7390
v	0.8085	0.7410
x	0.8028	0.7380
y	0.5975	0.6750
z	0.4106	0.6210