wwPDB EM Validation Summary Report (i)

Jun 4, 2024 – 03:06 pm BST

PDB ID	:	9EVX
EMDB ID	:	EMD-50019
Title	:	cryoEM structure of Photosystem II averaged across S2-S3 states at 1.71 Angstrom resolution
Authors	:	Hussein, R.; Graca, A.; Zouni, A.; Messinger, J.; Schroder, W.P.
Deposited on	:	2024-04-02
Resolution	:	1.71 Å(reported)

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:

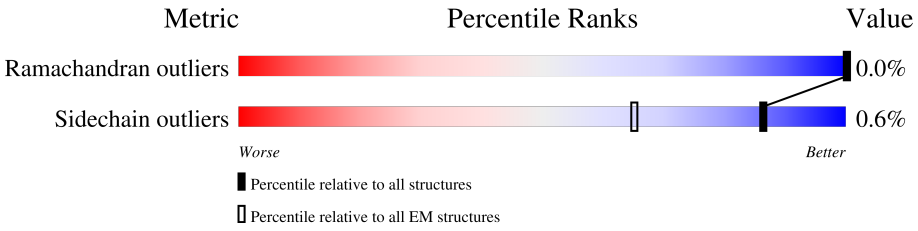
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.71 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	344	97%
1	a	344	97%
2	B	510	98%
2	b	510	98%
3	C	461	97%
3	c	461	97%
4	D	352	97%
4	d	352	97%
5	E	84	12% 98%

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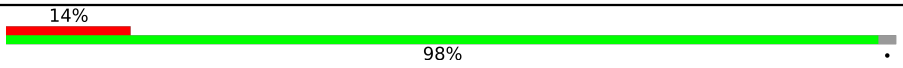
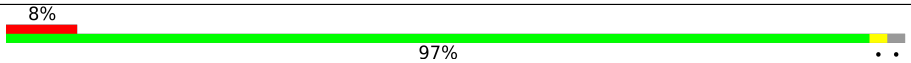
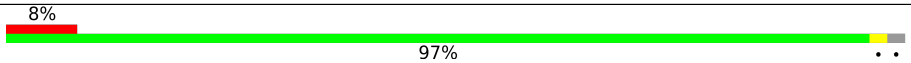
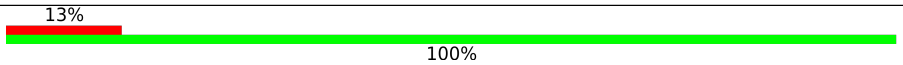
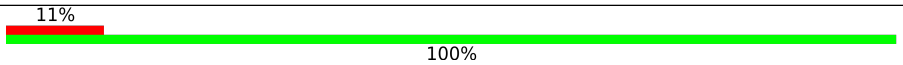
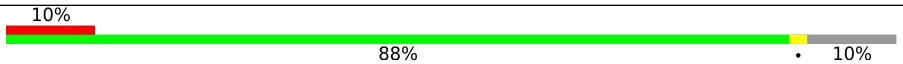
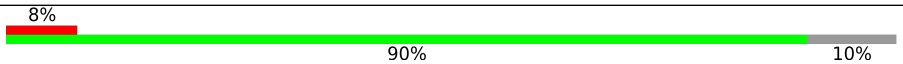
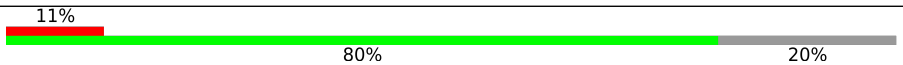
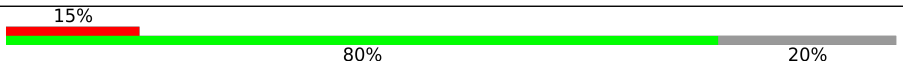
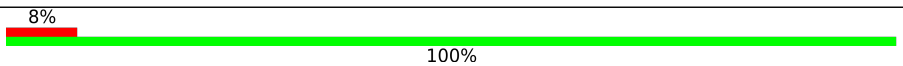
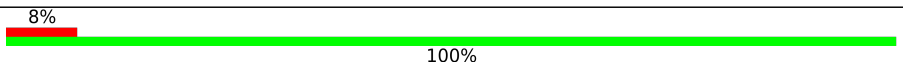
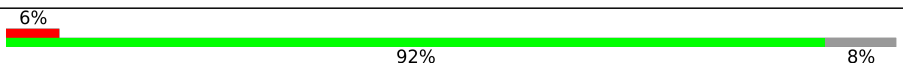
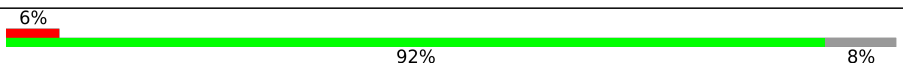
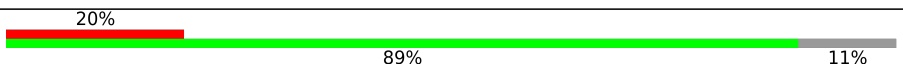
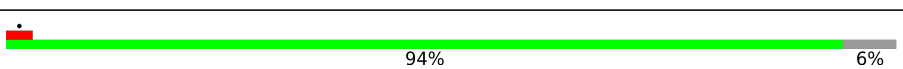
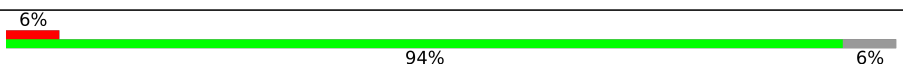
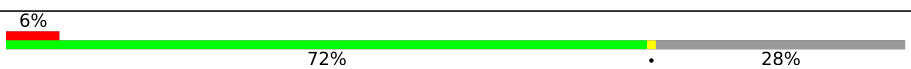
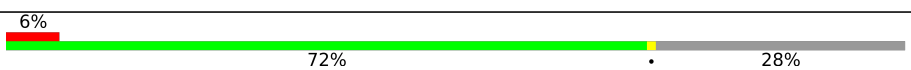
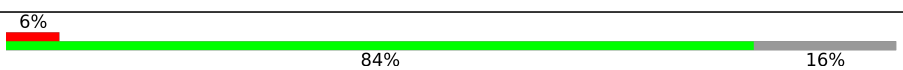
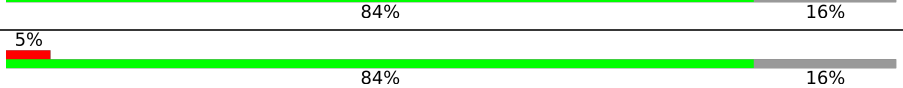
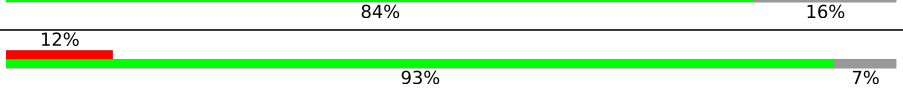
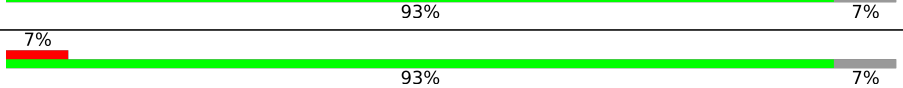
Mol	Chain	Length	Quality of chain
5	e	84	
6	F	45	
6	f	45	
7	H	66	
7	h	66	
8	I	38	
8	i	38	
9	J	40	
9	j	40	
10	K	46	
10	k	46	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	272	
13	o	272	
14	T	32	
14	t	32	
15	U	134	
15	u	134	
16	V	163	
16	v	163	
17	X	41	
17	x	41	

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Mol	Chain	Length	Quality of chain
18	Y	46	33% 57% 41%
18	y	46	26% 59% 41%
19	Z	62	68% 97%
19	z	62	61% 97%

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
22	CLA	A	404	X	-	-	-
22	CLA	A	405	X	-	-	-
22	CLA	A	406	X	-	-	-
22	CLA	A	419	X	-	-	-
22	CLA	B	601	X	-	-	-
22	CLA	B	602	X	-	-	-
22	CLA	B	603	X	-	-	-
22	CLA	B	604	X	-	-	-
22	CLA	B	606	X	-	-	-
22	CLA	B	607	X	-	-	-
22	CLA	B	608	X	-	-	-
22	CLA	B	610	X	-	-	-
22	CLA	B	611	X	-	-	-
22	CLA	B	612	X	-	-	-
22	CLA	B	613	X	-	-	-
22	CLA	B	614	X	-	-	-
22	CLA	B	615	X	-	-	-
22	CLA	B	616	X	-	-	-
22	CLA	C	501	X	-	-	-
22	CLA	C	504	X	-	-	-
22	CLA	C	505	X	-	-	-
22	CLA	C	506	X	-	-	-
22	CLA	C	507	X	-	-	-
22	CLA	C	509	X	-	-	-
22	CLA	C	510	X	-	-	-
22	CLA	C	511	X	-	-	-
22	CLA	C	512	X	-	-	-
22	CLA	C	513	X	-	-	-
22	CLA	a	404	X	-	-	-
22	CLA	a	405	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	a	406	X	-	-	-
22	CLA	a	419	X	-	-	-
22	CLA	b	602	X	-	-	-
22	CLA	b	603	X	-	-	-
22	CLA	b	604	X	-	-	-
22	CLA	b	605	X	-	-	-
22	CLA	b	607	X	-	-	-
22	CLA	b	608	X	-	-	-
22	CLA	b	609	X	-	-	-
22	CLA	b	611	X	-	-	-
22	CLA	b	612	X	-	-	-
22	CLA	b	613	X	-	-	-
22	CLA	b	614	X	-	-	-
22	CLA	b	615	X	-	-	-
22	CLA	b	616	X	-	-	-
22	CLA	b	617	X	-	-	-
22	CLA	c	501	X	-	-	-
22	CLA	c	504	X	-	-	-
22	CLA	c	505	X	-	-	-
22	CLA	c	506	X	-	-	-
22	CLA	c	507	X	-	-	-
22	CLA	c	509	X	-	-	-
22	CLA	c	510	X	-	-	-
22	CLA	c	511	X	-	-	-
22	CLA	c	512	X	-	-	-
22	CLA	c	513	X	-	-	-

2 Entry composition (i)

There are 36 unique types of molecules in this entry. The entry contains 104863 atoms, of which 52030 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 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	334	Total	C	H	N	O	S	3	0
			5164	1723	2530	433	463	15		
1	a	334	Total	C	H	N	O	S	3	0
			5164	1723	2530	433	463	15		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	505	Total	C	H	N	O	S	3	0
			7852	2620	3858	667	694	13		
2	b	505	Total	C	H	N	O	S	3	0
			7852	2620	3858	667	694	13		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
3	C	451	Total	C	H	N	O	S	2	0
			6899	2283	3408	585	610	13		
3	c	451	Total	C	H	N	O	S	2	0
			6899	2283	3408	585	610	13		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
4	D	341	Total	C	H	N	O	S	0	0
			5338	1800	2621	444	461	12		
4	d	341	Total	C	H	N	O	S	0	0
			5338	1800	2621	444	461	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	82	Total	C	H	N	O	0	0
			1301	431	640	107	123		
5	e	82	Total	C	H	N	O	0	0
			1301	431	640	107	123		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
6	F	34	Total	C	H	N	O	S	0	0
			557	187	282	45	42	1		
6	f	34	Total	C	H	N	O	S	0	0
			557	187	282	45	42	1		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
7	H	65	Total	C	H	N	O	S	2	0
			1045	338	534	83	87	3		
7	h	65	Total	C	H	N	O	S	2	0
			1045	338	534	83	87	3		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	41	CYS	PHE	variant	UNP Q8DJ43
h	41	CYS	PHE	variant	UNP Q8DJ43

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

Mol	Chain	Residues	Atoms						AltConf	Trace
8	I	38	Total	C	H	N	O	S	0	0
			641	211	328	48	53	1		
8	i	38	Total	C	H	N	O	S	0	0
			641	211	328	48	53	1		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
9	J	36	Total	C	H	N	O	S	0	0
			525	174	268	40	42	1		
9	j	36	Total	C	H	N	O	S	0	0
			525	174	268	40	42	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	37	Total	C	H	N	O	0	0
			598	204	305	43	46		
10	k	37	Total	C	H	N	O	0	0
			598	204	305	43	46		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
11	L	37	Total	C	H	N	O	S	2	0
			640	208	328	49	54	1		
11	l	37	Total	C	H	N	O	S	2	0
			640	208	328	49	54	1		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
12	M	33	Total	C	H	N	O	S	2	0
			545	177	281	38	48	1		
12	m	33	Total	C	H	N	O	S	2	0
			545	177	281	38	48	1		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
13	O	243	Total	C	H	N	O	S	3	0
			3710	1171	1834	313	387	5		
13	o	243	Total	C	H	N	O	S	3	0
			3710	1171	1834	313	387	5		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
14	T	30	Total	C	H	N	O	S	0	0
			519	181	261	36	39	2		
14	t	30	Total	C	H	N	O	S	0	0
			519	181	261	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	H	N	O	0	0
			1547	491	773	129	154		
15	u	97	Total	C	H	N	O	0	0
			1547	491	773	129	154		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
16	V	137	Total	C	H	N	O	S	0	0
			2135	675	1071	177	208	4		
16	v	137	Total	C	H	N	O	S	0	0
			2135	675	1071	177	208	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	X	38	Total	C	H	N	O	0	0
			593	188	312	45	48		
17	x	38	Total	C	H	N	O	0	0
			593	188	312	45	48		

- Molecule 18 is a protein called Photosystem II reaction center protein Ycf12.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	Y	27	Total	C	H	N	O	S	0	0
			423	131	224	35	30	3		
18	y	27	Total	C	H	N	O	S	0	0
			425	131	226	35	30	3		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
19	Z	62	Total	C	H	N	O	S	0	0
			995	328	516	72	77	2		
19	z	62	Total	C	H	N	O	S	0	0
			995	328	516	72	77	2		

- Molecule 20 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

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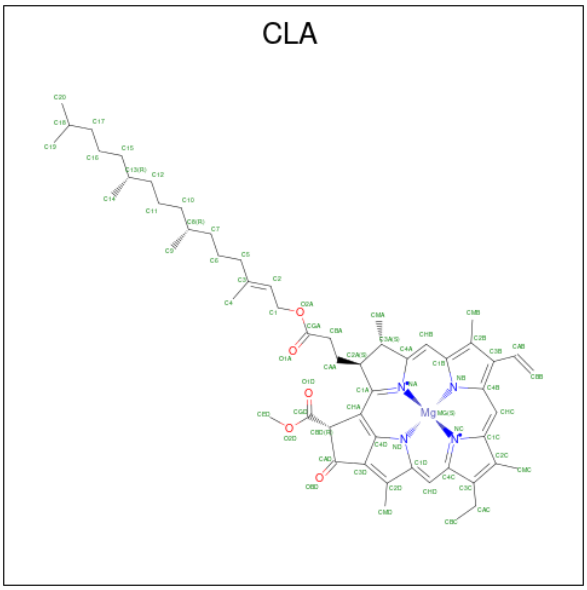
Mol	Chain	Residues	Atoms	AltConf
20	a	1	Total Fe 1 1	0

- Molecule 21 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 22 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms	AltConf
22	A	1	Total C H Mg N O 137 55 72 1 4 5	0
22	A	1	Total C H Mg N O 119 50 59 1 4 5	0
22	A	1	Total C H Mg N O 102 44 48 1 4 5	0
22	A	1	Total C H Mg N O 137 55 72 1 4 5	0
22	B	1	Total C H Mg N O 137 55 72 1 4 5	0
22	B	1	Total C H Mg N O 137 55 72 1 4 5	0

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Mol	Chain	Residues	Atoms						AltConf
22	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	B	1	Total 119	C 50	H 59	Mg 1	N 4	O 5	0
22	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	C	1	Total 117	C 49	H 58	Mg 1	N 4	O 5	0
22	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms	AltConf
22	C	1	Total C H Mg N O 137 55 72 1 4 5	0
22	C	1	Total C H Mg N O 137 55 72 1 4 5	0
22	C	1	Total C H Mg N O 137 55 72 1 4 5	0
22	C	1	Total C H Mg N O 137 55 72 1 4 5	0
22	C	1	Total C H Mg N O 137 55 72 1 4 5	0
22	C	1	Total C H Mg N O 137 55 72 1 4 5	0
22	D	1	Total C H Mg N O 137 55 72 1 4 5	0
22	D	1	Total C H Mg N O 137 55 72 1 4 5	0
22	a	1	Total C H Mg N O 137 55 72 1 4 5	0
22	a	1	Total C H Mg N O 119 50 59 1 4 5	0
22	a	1	Total C H Mg N O 102 44 48 1 4 5	0
22	a	1	Total C H Mg N O 137 55 72 1 4 5	0
22	b	1	Total C H Mg N O 137 55 72 1 4 5	0
22	b	1	Total C H Mg N O 137 55 72 1 4 5	0
22	b	1	Total C H Mg N O 137 55 72 1 4 5	0
22	b	1	Total C H Mg N O 137 55 72 1 4 5	0
22	b	1	Total C H Mg N O 137 55 72 1 4 5	0
22	b	1	Total C H Mg N O 137 55 72 1 4 5	0
22	b	1	Total C H Mg N O 137 55 72 1 4 5	0
22	b	1	Total C H Mg N O 137 55 72 1 4 5	0
22	b	1	Total C H Mg N O 137 55 72 1 4 5	0

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Mol	Chain	Residues	Atoms	AltConf
22	b	1	Total C H Mg N O 137 55 72 1 4 5	0
22	b	1	Total C H Mg N O 137 55 72 1 4 5	0
22	b	1	Total C H Mg N O 137 55 72 1 4 5	0
22	b	1	Total C H Mg N O 137 55 72 1 4 5	0
22	b	1	Total C H Mg N O 137 55 72 1 4 5	0
22	b	1	Total C H Mg N O 137 55 72 1 4 5	0
22	b	1	Total C H Mg N O 119 50 59 1 4 5	0
22	c	1	Total C H Mg N O 137 55 72 1 4 5	0
22	c	1	Total C H Mg N O 137 55 72 1 4 5	0
22	c	1	Total C H Mg N O 137 55 72 1 4 5	0
22	c	1	Total C H Mg N O 117 49 58 1 4 5	0
22	c	1	Total C H Mg N O 137 55 72 1 4 5	0
22	c	1	Total C H Mg N O 137 55 72 1 4 5	0
22	c	1	Total C H Mg N O 137 55 72 1 4 5	0
22	c	1	Total C H Mg N O 137 55 72 1 4 5	0
22	c	1	Total C H Mg N O 137 55 72 1 4 5	0
22	c	1	Total C H Mg N O 137 55 72 1 4 5	0
22	c	1	Total C H Mg N O 137 55 72 1 4 5	0
22	c	1	Total C H Mg N O 137 55 72 1 4 5	0
22	c	1	Total C H Mg N O 137 55 72 1 4 5	0
22	d	1	Total C H Mg N O 137 55 72 1 4 5	0

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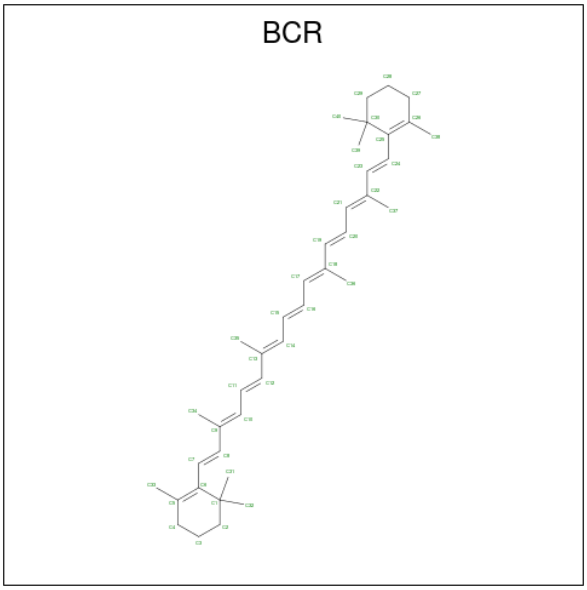
Mol	Chain	Residues	Atoms						AltConf
22	d	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	

- Molecule 23 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms			AltConf
23	A	1	Total	C	H	0
			96	40	56	
23	B	1	Total	C	H	0
			96	40	56	
23	B	1	Total	C	H	0
			96	40	56	
23	B	1	Total	C	H	0
			96	40	56	
23	C	1	Total	C	H	0
			96	40	56	
23	C	1	Total	C	H	0
			96	40	56	
23	D	1	Total	C	H	0
			96	40	56	
23	H	1	Total	C	H	0
			96	40	56	
23	K	1	Total	C	H	0
			96	40	56	
23	K	1	Total	C	H	0
			96	40	56	

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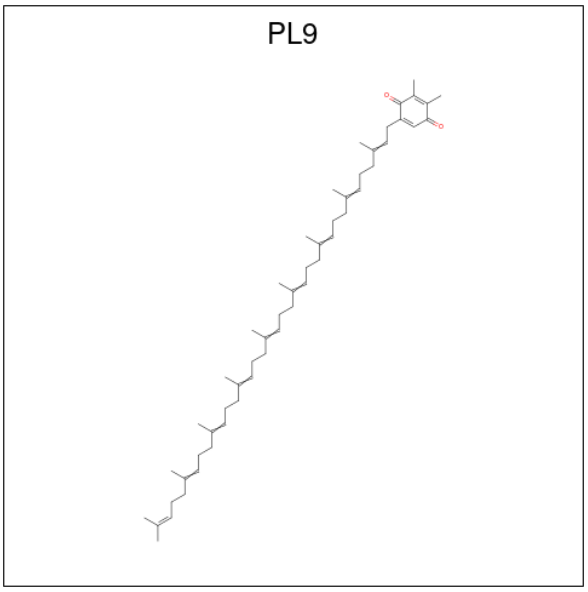
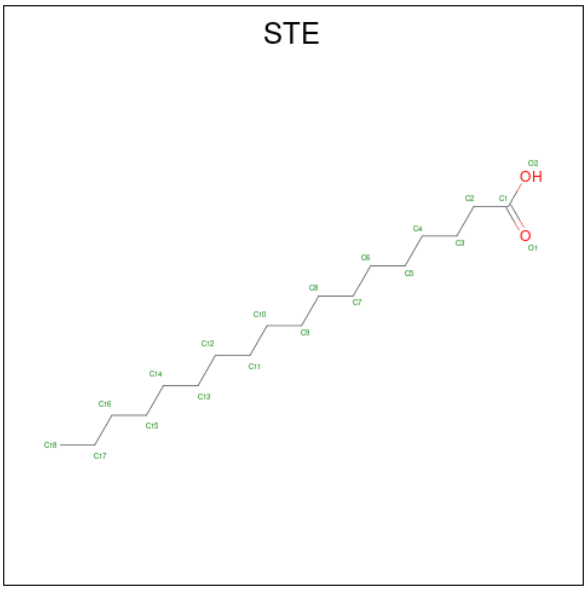
Mol	Chain	Residues	Atoms	AltConf
23	T	1	Total C H 96 40 56	0
23	a	1	Total C H 96 40 56	0
23	b	1	Total C H 96 40 56	0
23	b	1	Total C H 96 40 56	0
23	b	1	Total C H 96 40 56	0
23	c	1	Total C H 96 40 56	0
23	c	1	Total C H 96 40 56	0
23	d	1	Total C H 96 40 56	0
23	h	1	Total C H 96 40 56	0
23	k	1	Total C H 96 40 56	0
23	k	1	Total C H 96 40 56	0
23	t	1	Total C H 96 40 56	0

- Molecule 24 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: $C_{53}H_{80}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
24	A	1	Total	C	H	O	0
			135	53	80	2	
24	D	1	Total	C	H	O	0
			135	53	80	2	
24	a	1	Total	C	H	O	0
			135	53	80	2	
24	d	1	Total	C	H	O	0
			135	53	80	2	

- Molecule 25 is STEARIC ACID (three-letter code: STE) (formula: $C_{18}H_{36}O_2$).



Mol	Chain	Residues	Atoms	AltConf
25	A	1	Total C H 23 9 14	0
25	A	1	Total C H 23 8 15	0
25	A	1	Total C H 32 11 21	0
25	A	1	Total C H 32 11 21	0
25	A	1	Total C H O 28 10 16 2	0
25	B	1	Total C H O 43 15 26 2	0
25	B	1	Total C H O 28 10 16 2	0
25	B	1	Total C H 32 12 20	0
25	C	1	Total C H O 34 12 20 2	0
25	C	1	Total C H O 28 10 16 2	0
25	C	1	Total C H 23 8 15	0
25	D	1	Total C H O 55 18 35 2	0
25	D	1	Total C H 26 9 17	0
25	E	1	Total C H O 28 10 16 2	0
25	E	1	Total C H 35 12 23	0
25	E	1	Total C H O 55 18 35 2	0
25	I	1	Total C H 38 14 24	0
25	J	1	Total C H 32 12 20	0
25	K	1	Total C H 32 11 21	0
25	M	1	Total C H 26 10 16	0
25	T	1	Total C H 44 15 29	0
25	a	1	Total C H 23 9 14	0

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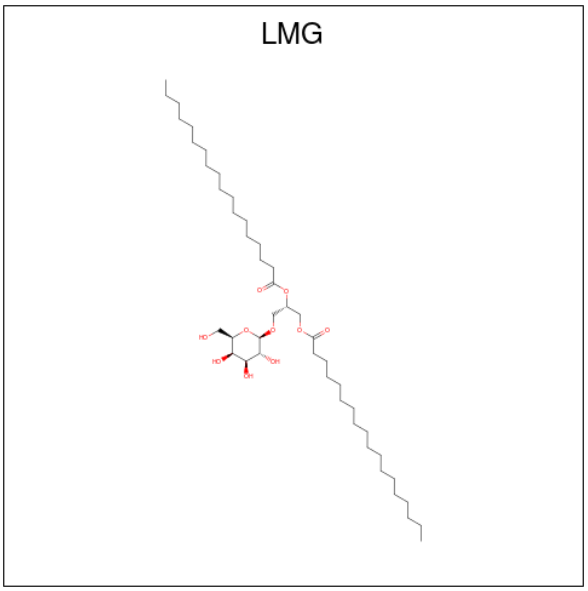
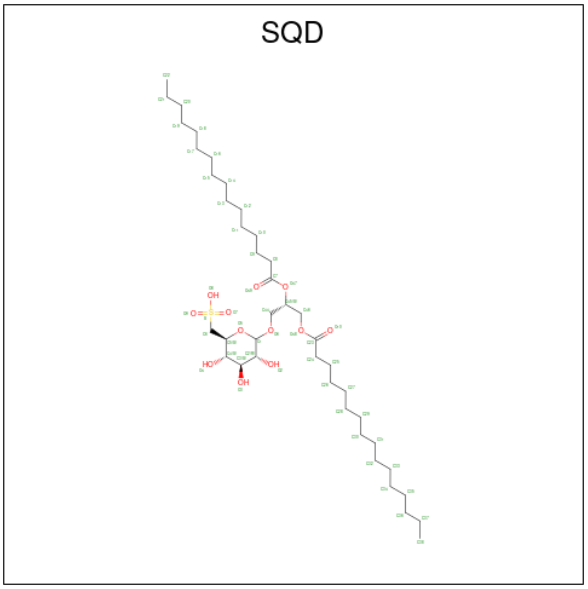
Mol	Chain	Residues	Atoms	AltConf
25	a	1	Total C H 23 8 15	0
25	a	1	Total C H 32 11 21	0
25	a	1	Total C H 32 11 21	0
25	a	1	Total C H O 28 10 16 2	0
25	b	1	Total C H 32 12 20	0
25	b	1	Total C H O 43 15 26 2	0
25	b	1	Total C H O 28 10 16 2	0
25	c	1	Total C H O 34 12 20 2	0
25	c	1	Total C H O 28 10 16 2	0
25	c	1	Total C H 23 8 15	0
25	d	1	Total C H O 55 18 35 2	0
25	d	1	Total C H 26 9 17	0
25	e	1	Total C H O 28 10 16 2	0
25	e	1	Total C H 35 12 23	0
25	e	1	Total C H O 55 18 35 2	0
25	i	1	Total C H 38 14 24	0
25	j	1	Total C H 32 12 20	0
25	k	1	Total C H 32 11 21	0
25	m	1	Total C H 26 10 16	0
25	t	1	Total C H O 46 16 28 2	0

- Molecule 26 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



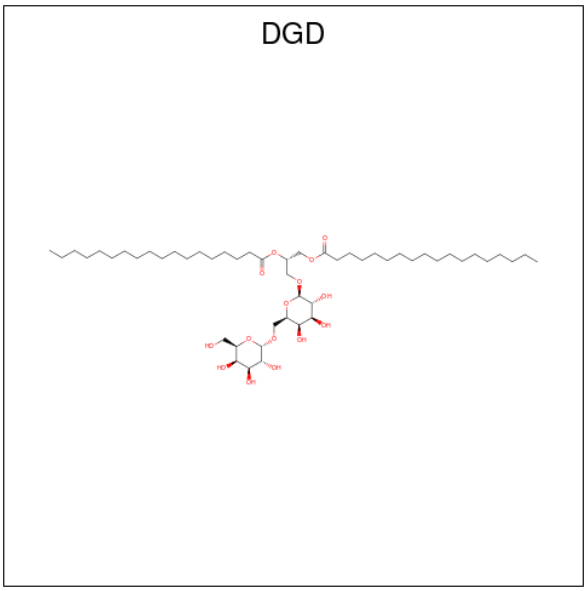
Mol	Chain	Residues	Atoms				AltConf
26	A	1	Total	C	H	O	0
			114	38	66	10	
26	B	1	Total	C	H	O	0
			123	41	72	10	
26	C	1	Total	C	H	O	0
			114	38	66	10	
26	C	1	Total	C	H	O	0
			120	40	70	10	
26	D	1	Total	C	H	O	0
			83	29	49	5	
26	D	1	Total	C	H	O	0
			123	41	72	10	
26	H	1	Total	C	H	O	0
			98	34	59	5	
26	a	1	Total	C	H	O	0
			114	38	66	10	
26	b	1	Total	C	H	O	0
			123	41	72	10	
26	c	1	Total	C	H	O	0
			114	38	66	10	
26	c	1	Total	C	H	O	0
			120	40	70	10	
26	d	1	Total	C	H	O	0
			83	29	49	5	
26	d	1	Total	C	H	O	0
			123	41	72	10	
26	h	1	Total	C	H	O	0
			98	34	59	5	

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



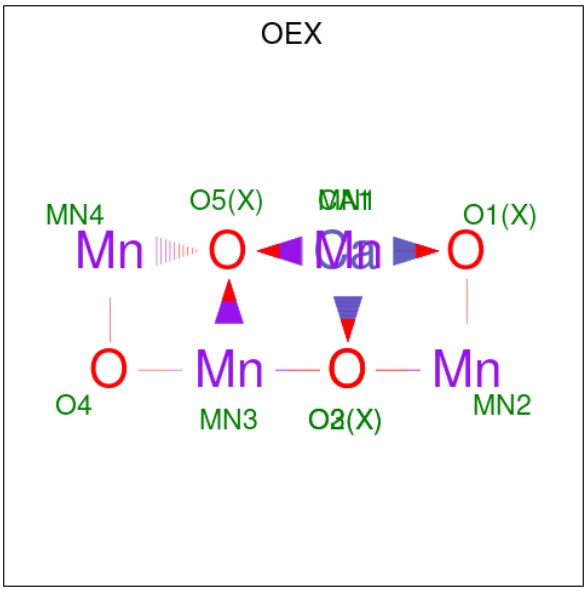
Mol	Chain	Residues	Atoms					AltConf
27	A	1	Total	C	H	O	S	0
			122	39	70	12	1	
27	A	1	Total	C	H	O	S	0
			131	41	77	12	1	
27	B	1	Total	C	H	O	S	0
			131	41	77	12	1	
27	X	1	Total	C	H	O	S	0
			81	25	45	10	1	
27	a	1	Total	C	H	O	S	0
			122	39	70	12	1	
27	a	1	Total	C	H	O	S	0
			131	41	77	12	1	
27	b	1	Total	C	H	O	S	0
			113	36	64	12	1	
27	x	1	Total	C	H	O	S	0
			81	25	45	10	1	

- Molecule 28 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



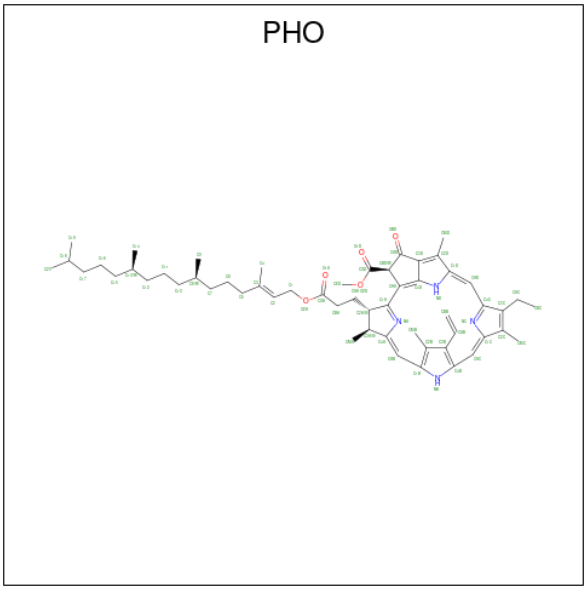
Mol	Chain	Residues	Atoms				AltConf
28	A	1	Total	C	H	O	0
			162	51	96	15	
28	C	1	Total	C	H	O	0
			144	47	82	15	
28	C	1	Total	C	H	O	0
			129	42	72	15	
28	C	1	Total	C	H	O	0
			144	47	82	15	
28	H	1	Total	C	H	O	0
			144	47	82	15	
28	a	1	Total	C	H	O	0
			162	51	96	15	
28	c	1	Total	C	H	O	0
			144	47	82	15	
28	c	1	Total	C	H	O	0
			129	42	72	15	
28	c	1	Total	C	H	O	0
			144	47	82	15	
28	h	1	Total	C	H	O	0
			144	47	82	15	

- Molecule 29 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula: $CaMn_4O_5$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 30 is PHEOPHYTIN A (three-letter code: PHO) (formula: $C_{55}H_{74}N_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
30	A	1	Total	C	H	N	O	0
			138	55	74	4	5	
30	D	1	Total	C	H	N	O	0
			138	55	74	4	5	

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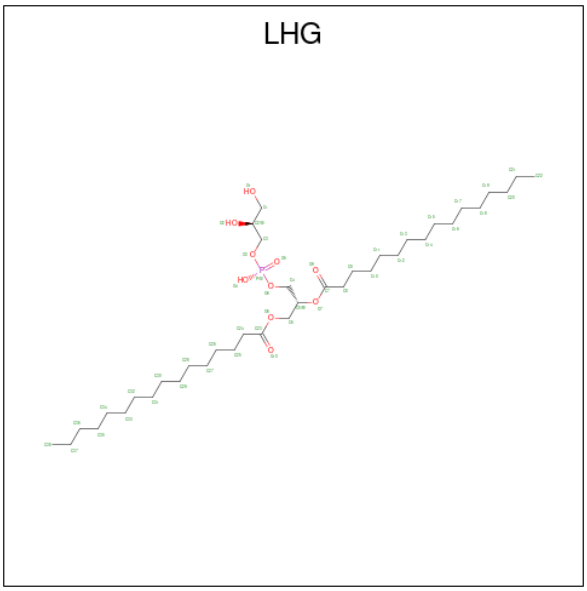
Mol	Chain	Residues	Atoms					AltConf
30	a	1	Total	C	H	N	O	0
			138	55	74	4	5	
30	d	1	Total	C	H	N	O	0
			138	55	74	4	5	

- Molecule 31 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms					AltConf
31	A	1	Total	C	H	O	P	0
			123	38	74	10	1	
31	D	1	Total	C	H	O	P	0
			123	38	74	10	1	
31	D	1	Total	C	H	O	P	0
			114	36	67	10	1	
31	D	1	Total	C	H	O	P	0
			123	38	74	10	1	
31	L	1	Total	C	H	O	P	0
			123	38	74	10	1	
31	a	1	Total	C	H	O	P	0
			123	38	74	10	1	
31	d	1	Total	C	H	O	P	0
			123	38	74	10	1	
31	d	1	Total	C	H	O	P	0
			114	36	67	10	1	
31	d	1	Total	C	H	O	P	0
			123	38	74	10	1	

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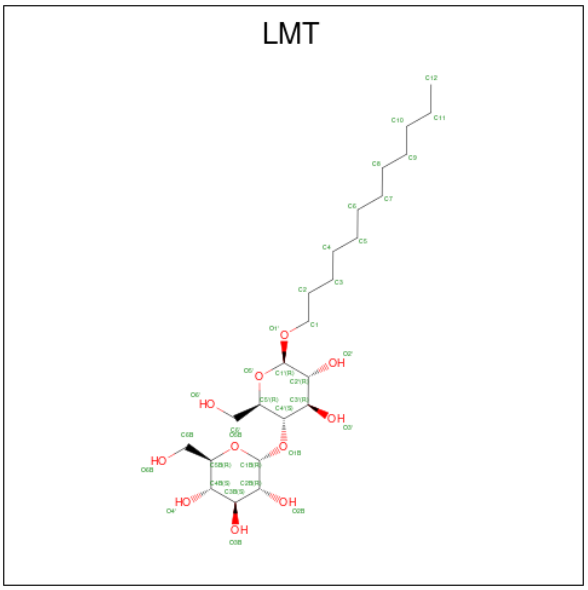
Mol	Chain	Residues	Atoms					AltConf
31	l	1	Total	C	H	O	P	0
			123	38	74	10	1	

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



Mol	Chain	Residues	Atoms				AltConf
32	B	1	Total	C	H	O	0
			60	19	35	6	
32	C	1	Total	C	H	O	0
			59	18	35	6	
32	C	1	Total	C	H	O	0
			80	24	45	11	
32	E	1	Total	C	H	O	0
			57	18	33	6	
32	J	1	Total	C	H	O	0
			58	18	34	6	
32	M	1	Total	C	H	O	0
			79	24	44	11	
32	Z	1	Total	C	H	O	0
			79	24	44	11	
32	b	1	Total	C	H	O	0
			60	19	35	6	
32	c	1	Total	C	H	O	0
			59	18	35	6	
32	c	1	Total	C	H	O	0
			80	24	45	11	

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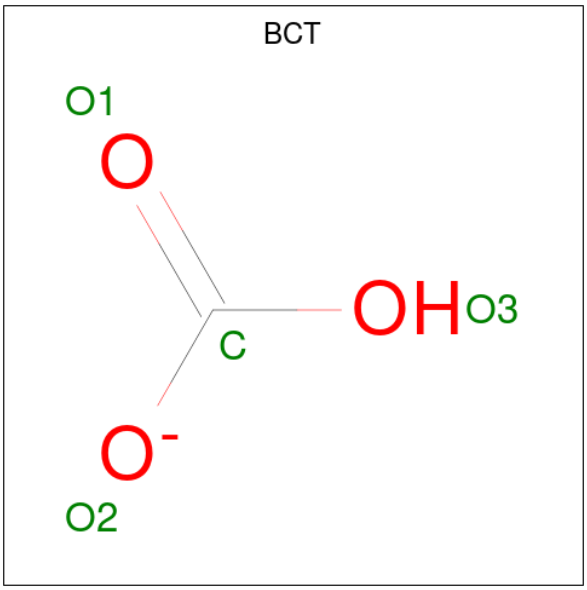
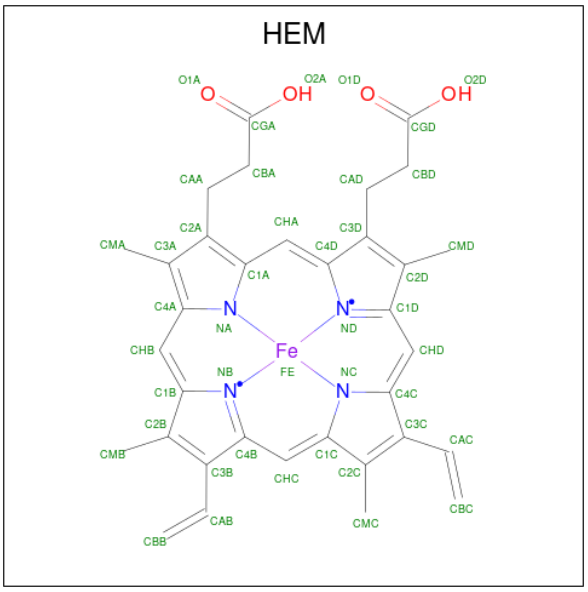
Mol	Chain	Residues	Atoms				AltConf
32	e	1	Total	C	H	O	0
			57	18	33	6	
32	j	1	Total	C	H	O	0
			58	18	34	6	
32	m	1	Total	C	H	O	0
			79	24	44	11	
32	z	1	Total	C	H	O	0
			79	24	44	11	

- Molecule 33 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



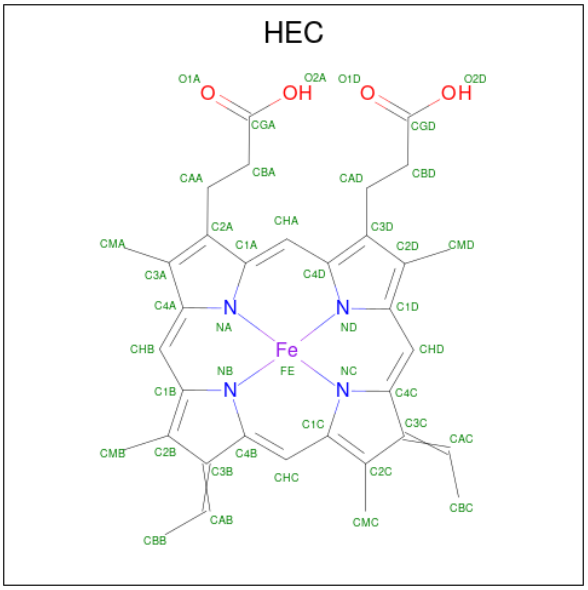
Mol	Chain	Residues	Atoms				AltConf
33	D	1	Total	C	H	O	0
			5	1	1	3	
33	d	1	Total	C	H	O	0
			5	1	1	3	

- 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	H	N	O	0
			73	34	1	30	4	4	
34	e	1	Total	C	Fe	H	N	O	0
			73	34	1	30	4	4	

- Molecule 35 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



Mol	Chain	Residues	Atoms						AltConf
35	V	1	Total	C	Fe	H	N	O	0
			73	34	1	30	4	4	
35	v	1	Total	C	Fe	H	N	O	0
			73	34	1	30	4	4	

- Molecule 36 is water.

Mol	Chain	Residues	Atoms	AltConf
36	A	172	Total O 172 172	0
36	B	273	Total O 273 273	0
36	C	200	Total O 201 201	1
36	D	177	Total O 177 177	0
36	E	38	Total O 38 38	0
36	F	4	Total O 4 4	0
36	H	28	Total O 28 28	0
36	I	6	Total O 6 6	0
36	J	14	Total O 14 14	0
36	K	4	Total O 4 4	0
36	L	16	Total O 16 16	0
36	M	7	Total O 7 7	0
36	O	99	Total O 99 99	0
36	T	8	Total O 8 8	0
36	U	61	Total O 61 61	0
36	V	95	Total O 95 95	0
36	X	9	Total O 9 9	0
36	a	168	Total O 168 168	0
36	b	273	Total O 273 273	0
36	c	201	Total O 202 202	1
36	d	177	Total O 177 177	0

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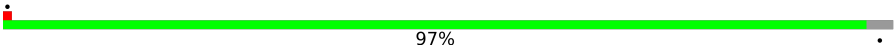
Mol	Chain	Residues	Atoms	AltConf
36	e	38	Total O 38 38	0
36	f	4	Total O 4 4	0
36	h	28	Total O 28 28	0
36	i	6	Total O 6 6	0
36	j	14	Total O 14 14	0
36	k	4	Total O 4 4	0
36	l	13	Total O 13 13	0
36	m	3	Total O 3 3	0
36	o	99	Total O 99 99	0
36	t	7	Total O 7 7	0
36	u	55	Total O 55 55	0
36	v	95	Total O 95 95	0
36	x	9	Total O 9 9	0

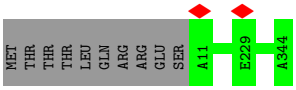
3 Residue-property plots (i)

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 1

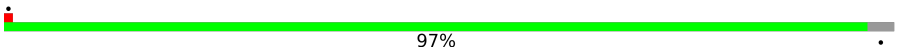
Chain A:

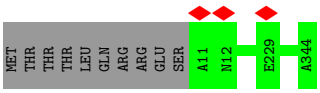




• Molecule 1: Photosystem II protein D1 1

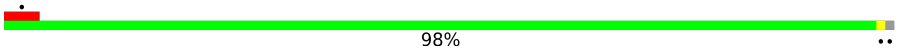
Chain a:

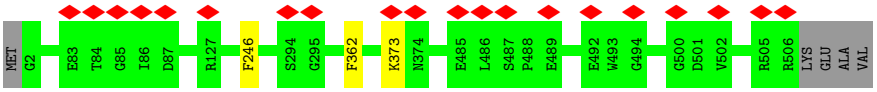




• Molecule 2: Photosystem II CP47 reaction center protein

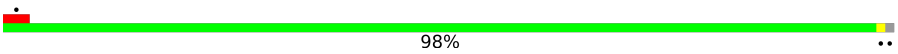
Chain B:

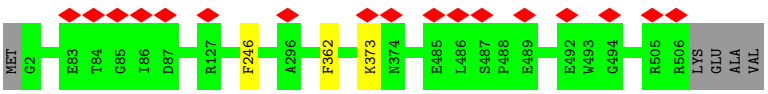




• Molecule 2: Photosystem II CP47 reaction center protein

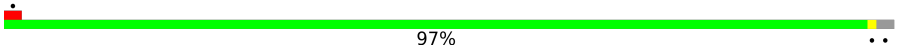
Chain b:

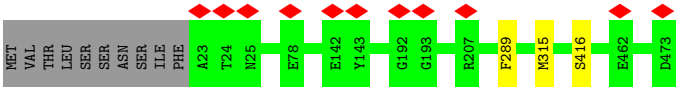




• Molecule 3: Photosystem II CP43 reaction center protein

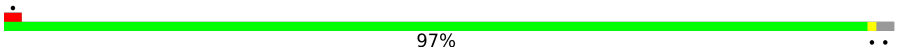
Chain C:

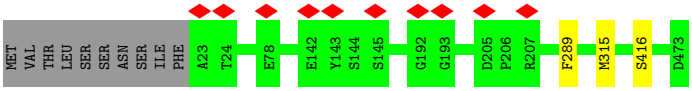




• Molecule 3: Photosystem II CP43 reaction center protein

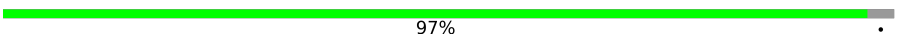
Chain c:

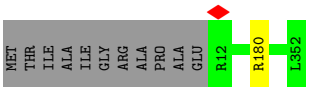




• Molecule 4: Photosystem II D2 protein

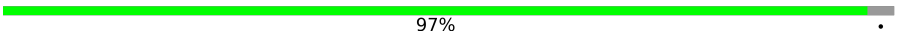
Chain D:

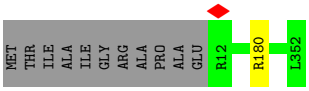




• Molecule 4: Photosystem II D2 protein

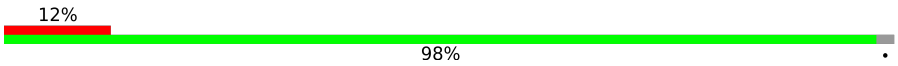
Chain d:

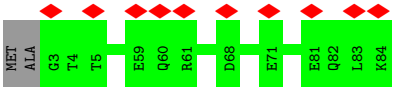




• Molecule 5: Cytochrome b559 subunit alpha

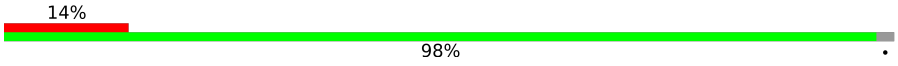
Chain E:

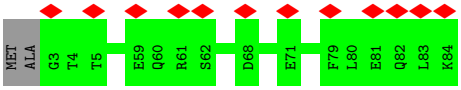




• Molecule 5: Cytochrome b559 subunit alpha

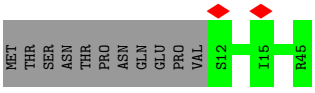
Chain e:





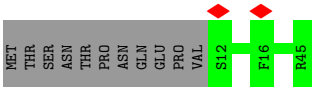
• Molecule 6: Cytochrome b559 subunit beta

Chain F:

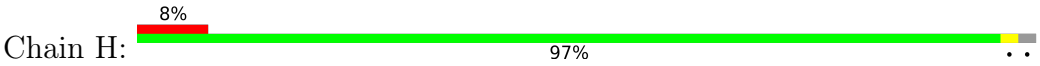


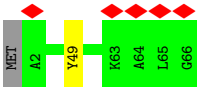
• Molecule 6: Cytochrome b559 subunit beta

Chain f:

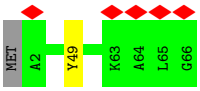


• Molecule 7: Photosystem II reaction center protein H

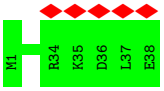




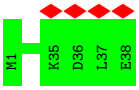
• Molecule 7: Photosystem II reaction center protein H



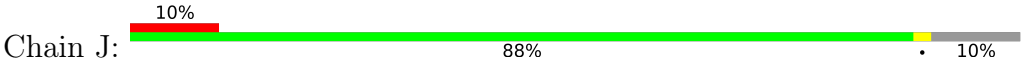
• Molecule 8: Photosystem II reaction center protein I

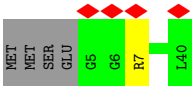


• Molecule 8: Photosystem II reaction center protein I

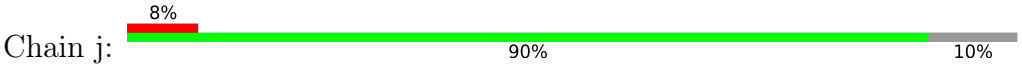


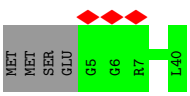
• Molecule 9: Photosystem II reaction center protein J





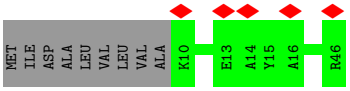
• Molecule 9: Photosystem II reaction center protein J





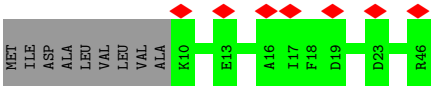
• Molecule 10: Photosystem II reaction center protein K

Chain K:



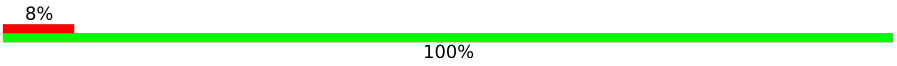
• Molecule 10: Photosystem II reaction center protein K

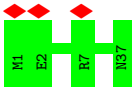
Chain k:



• Molecule 11: Photosystem II reaction center protein L

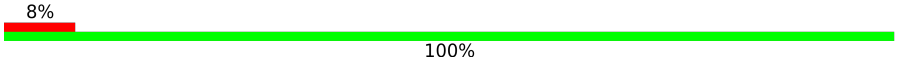
Chain L:

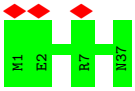




• Molecule 11: Photosystem II reaction center protein L

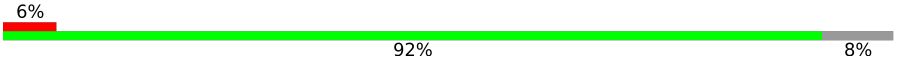
Chain l:

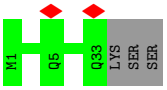




• Molecule 12: Photosystem II reaction center protein M

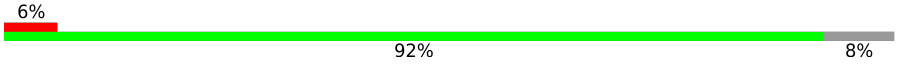
Chain M:

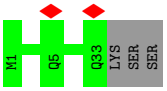




• Molecule 12: Photosystem II reaction center protein M

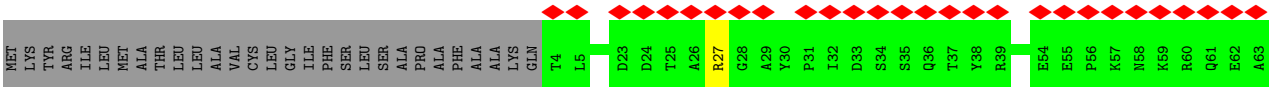
Chain m:

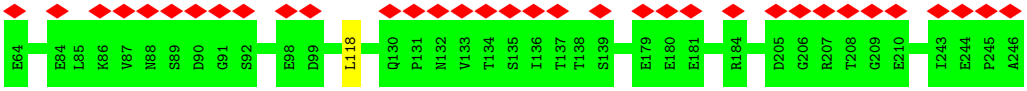




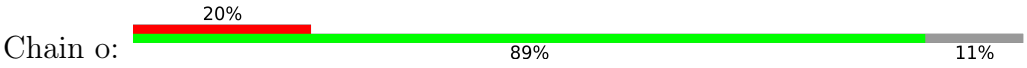
• Molecule 13: Photosystem II manganese-stabilizing polypeptide

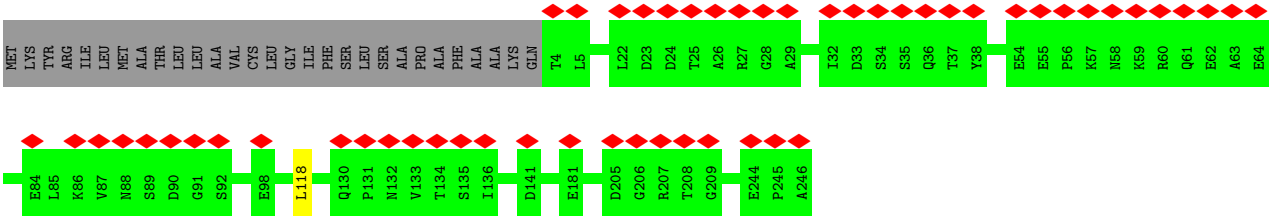
Chain O:



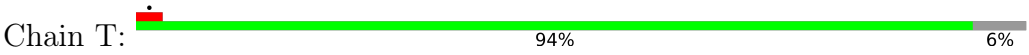


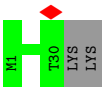
• Molecule 13: Photosystem II manganese-stabilizing polypeptide



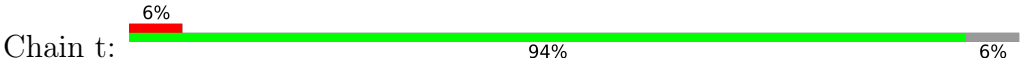


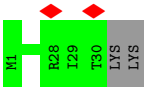
• Molecule 14: Photosystem II reaction center protein T



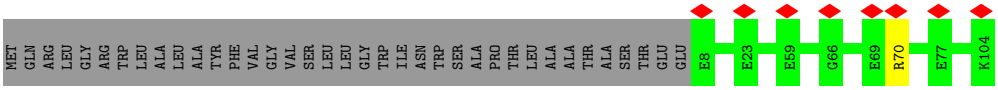


• Molecule 14: Photosystem II reaction center protein T

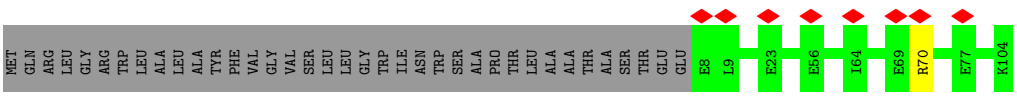




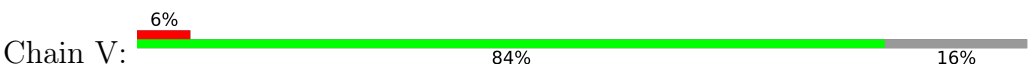
• Molecule 15: Photosystem II 12 kDa extrinsic protein

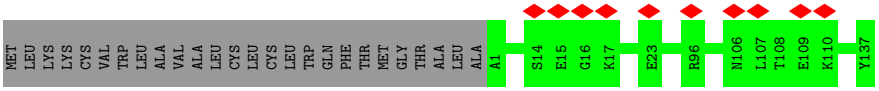


• Molecule 15: Photosystem II 12 kDa extrinsic protein

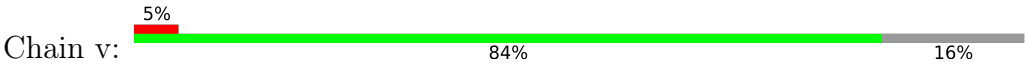


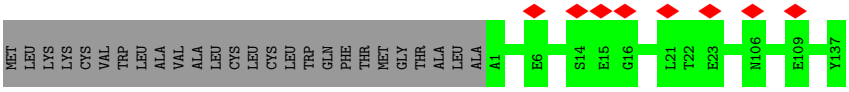
• Molecule 16: Cytochrome c-550



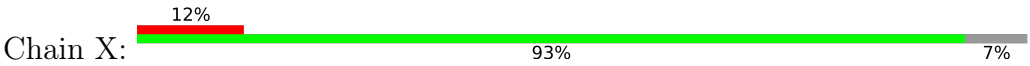


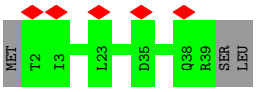
• Molecule 16: Cytochrome c-550



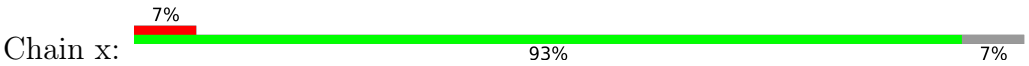


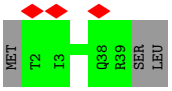
• Molecule 17: Photosystem II reaction center X protein



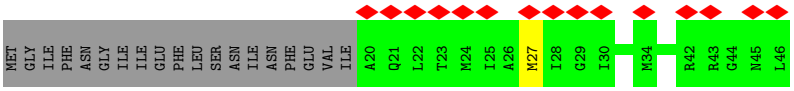


• Molecule 17: Photosystem II reaction center X protein

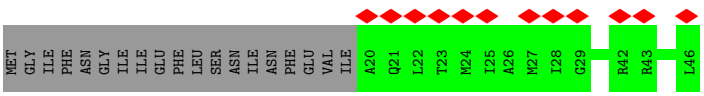




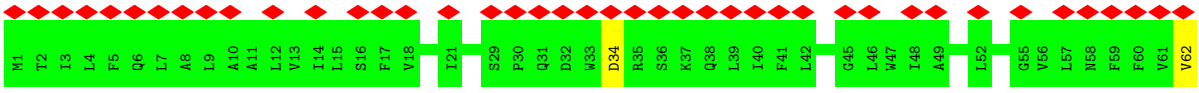
• Molecule 18: Photosystem II reaction center protein Ycf12



• Molecule 18: Photosystem II reaction center protein Ycf12

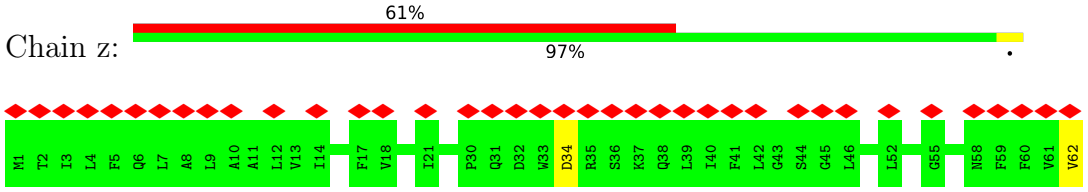


• Molecule 19: Photosystem II reaction center protein Z



• Molecule 19: Photosystem II reaction center protein Z

Chain z:


61%
97%
M1
T2
I3
L4
F5
Q6
L7
A8
L9
A10
A11
L12
V13
I14
F17
V18
I21
P30
Q31
D32
W33
D34
R35
S36
K37
Q38
L39
I40
F41
L42
G43
S44
G45
L46
L52
G55
M58
F59
F60
V61
V62

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	631270	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	2.426	Depositor
Minimum map value	-0.651	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.039	Depositor
Recommended contour level	0.45	Depositor
Map size (Å)	413.28, 413.28, 413.28	wwPDB
Map dimensions	720, 720, 720	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.574, 0.574, 0.574	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: OEX, DGD, BCT, LMT, PL9, HEM, LHG, FE2, HEC, LMG, CLA, PHO, FME, BCR, SQD, STE, CL

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.26	0/2723	0.49	0/3713
1	a	0.26	0/2723	0.49	0/3713
2	B	0.26	0/4140	0.49	0/5641
2	b	0.26	0/4140	0.49	0/5641
3	C	0.26	0/3612	0.47	0/4917
3	c	0.26	0/3612	0.47	0/4917
4	D	0.26	0/2812	0.50	0/3832
4	d	0.26	0/2812	0.50	0/3832
5	E	0.25	0/680	0.48	0/929
5	e	0.25	0/680	0.48	0/929
6	F	0.29	0/284	0.45	0/387
6	f	0.29	0/284	0.45	0/387
7	H	0.25	0/539	0.46	0/736
7	h	0.25	0/539	0.47	0/736
8	I	0.26	0/310	0.48	0/419
8	i	0.26	0/310	0.49	0/419
9	J	0.27	0/263	0.47	0/356
9	j	0.27	0/263	0.47	0/356
10	K	0.28	0/303	0.44	0/416
10	k	0.28	0/303	0.44	0/416
11	L	0.25	0/327	0.45	0/444
11	l	0.25	0/327	0.45	0/444
12	M	0.26	0/264	0.40	0/363
12	m	0.26	0/264	0.40	0/363
13	O	0.25	0/1910	0.52	0/2594
13	o	0.25	0/1910	0.52	0/2594
14	T	0.28	0/257	0.48	0/349
14	t	0.27	0/257	0.48	0/349
15	U	0.24	0/785	0.47	0/1064
15	u	0.24	0/785	0.47	0/1064
16	V	0.24	0/1085	0.46	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
16	v	0.24	0/1085	0.46	0/1473
17	X	0.25	0/284	0.42	0/384
17	x	0.25	0/284	0.42	0/384
18	Y	0.25	0/200	0.48	0/268
18	y	0.26	0/200	0.50	0/268
19	Z	0.26	0/490	0.40	0/669
19	z	0.26	0/490	0.40	0/669
All	All	0.26	0/42536	0.48	0/57908

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	335/344 (97%)	328 (98%)	7 (2%)	0	100	100
1	a	335/344 (97%)	328 (98%)	7 (2%)	0	100	100
2	B	506/510 (99%)	499 (99%)	7 (1%)	0	100	100
2	b	506/510 (99%)	499 (99%)	7 (1%)	0	100	100
3	C	451/461 (98%)	440 (98%)	10 (2%)	1 (0%)	47	30
3	c	451/461 (98%)	440 (98%)	10 (2%)	1 (0%)	47	30
4	D	339/352 (96%)	333 (98%)	6 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	d	339/352 (96%)	333 (98%)	6 (2%)	0	100	100
5	E	80/84 (95%)	80 (100%)	0	0	100	100
5	e	80/84 (95%)	80 (100%)	0	0	100	100
6	F	32/45 (71%)	32 (100%)	0	0	100	100
6	f	32/45 (71%)	32 (100%)	0	0	100	100
7	H	65/66 (98%)	64 (98%)	1 (2%)	0	100	100
7	h	65/66 (98%)	64 (98%)	1 (2%)	0	100	100
8	I	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
8	i	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
9	J	34/40 (85%)	34 (100%)	0	0	100	100
9	j	34/40 (85%)	34 (100%)	0	0	100	100
10	K	35/46 (76%)	35 (100%)	0	0	100	100
10	k	35/46 (76%)	35 (100%)	0	0	100	100
11	L	37/37 (100%)	37 (100%)	0	0	100	100
11	l	37/37 (100%)	37 (100%)	0	0	100	100
12	M	33/36 (92%)	33 (100%)	0	0	100	100
12	m	33/36 (92%)	33 (100%)	0	0	100	100
13	O	244/272 (90%)	233 (96%)	11 (4%)	0	100	100
13	o	244/272 (90%)	235 (96%)	9 (4%)	0	100	100
14	T	28/32 (88%)	28 (100%)	0	0	100	100
14	t	28/32 (88%)	28 (100%)	0	0	100	100
15	U	95/134 (71%)	92 (97%)	3 (3%)	0	100	100
15	u	95/134 (71%)	92 (97%)	3 (3%)	0	100	100
16	V	135/163 (83%)	131 (97%)	4 (3%)	0	100	100
16	v	135/163 (83%)	131 (97%)	4 (3%)	0	100	100
17	X	36/41 (88%)	36 (100%)	0	0	100	100
17	x	36/41 (88%)	36 (100%)	0	0	100	100
18	Y	25/46 (54%)	25 (100%)	0	0	100	100
18	y	25/46 (54%)	24 (96%)	1 (4%)	0	100	100
19	Z	60/62 (97%)	60 (100%)	0	0	100	100
19	z	60/62 (97%)	60 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	5212/5618 (93%)	5109 (98%)	101 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416	SER
3	c	416	SER

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	272/280 (97%)	272 (100%)	0	100	100
1	a	272/280 (97%)	272 (100%)	0	100	100
2	B	406/407 (100%)	403 (99%)	3 (1%)	84	76
2	b	406/407 (100%)	403 (99%)	3 (1%)	84	76
3	C	354/362 (98%)	352 (99%)	2 (1%)	86	80
3	c	354/362 (98%)	352 (99%)	2 (1%)	86	80
4	D	276/283 (98%)	275 (100%)	1 (0%)	91	86
4	d	276/283 (98%)	275 (100%)	1 (0%)	91	86
5	E	71/73 (97%)	71 (100%)	0	100	100
5	e	71/73 (97%)	71 (100%)	0	100	100
6	F	28/39 (72%)	28 (100%)	0	100	100
6	f	28/39 (72%)	28 (100%)	0	100	100
7	H	56/55 (102%)	55 (98%)	1 (2%)	59	41
7	h	56/55 (102%)	55 (98%)	1 (2%)	59	41
8	I	34/34 (100%)	34 (100%)	0	100	100
8	i	34/34 (100%)	34 (100%)	0	100	100
9	J	24/28 (86%)	23 (96%)	1 (4%)	30	11
9	j	24/28 (86%)	24 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
10	K	30/37 (81%)	30 (100%)	0	100 100
10	k	30/37 (81%)	30 (100%)	0	100 100
11	L	37/35 (106%)	37 (100%)	0	100 100
11	l	37/35 (106%)	37 (100%)	0	100 100
12	M	30/32 (94%)	30 (100%)	0	100 100
12	m	30/32 (94%)	30 (100%)	0	100 100
13	O	207/228 (91%)	205 (99%)	2 (1%)	76 65
13	o	207/228 (91%)	206 (100%)	1 (0%)	88 83
14	T	26/28 (93%)	26 (100%)	0	100 100
14	t	26/28 (93%)	26 (100%)	0	100 100
15	U	84/112 (75%)	83 (99%)	1 (1%)	71 58
15	u	84/112 (75%)	83 (99%)	1 (1%)	71 58
16	V	117/138 (85%)	117 (100%)	0	100 100
16	v	117/138 (85%)	117 (100%)	0	100 100
17	X	31/34 (91%)	31 (100%)	0	100 100
17	x	31/34 (91%)	31 (100%)	0	100 100
18	Y	20/37 (54%)	19 (95%)	1 (5%)	24 7
18	y	20/37 (54%)	20 (100%)	0	100 100
19	Z	52/52 (100%)	50 (96%)	2 (4%)	33 13
19	z	52/52 (100%)	50 (96%)	2 (4%)	33 13
All	All	4310/4588 (94%)	4285 (99%)	25 (1%)	86 80

5 of 25 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	b	246	PHE
3	c	289	PHE
19	z	62	VAL
2	b	373	LYS
3	c	315	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	343	HIS
2	b	343	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

6 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	$\#\|Z\| > 2$
12	FME	M	1	12	8,9,10	0.93	0	7,9,11	0.70	0
8	FME	i	1	8	8,9,10	0.93	0	7,9,11	0.80	0
8	FME	I	1	8	8,9,10	0.93	0	7,9,11	0.80	0
14	FME	T	1	14	8,9,10	0.93	0	7,9,11	0.99	0
12	FME	m	1	12	8,9,10	0.92	0	7,9,11	0.70	0
14	FME	t	1	14	8,9,10	0.93	0	7,9,11	1.00	0

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
12	FME	M	1	12	-	1/7/9/11	-
8	FME	i	1	8	-	2/7/9/11	-
8	FME	I	1	8	-	2/7/9/11	-
14	FME	T	1	14	-	0/7/9/11	-
12	FME	m	1	12	-	1/7/9/11	-
14	FME	t	1	14	-	0/7/9/11	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	I	1	FME	O-C-CA-CB
8	i	1	FME	O-C-CA-CB
12	M	1	FME	CB-CA-N-CN
12	m	1	FME	CB-CA-N-CN
8	I	1	FME	CB-CG-SD-CE

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 212 ligands modelled in this entry, 6 are monoatomic - leaving 206 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	$\#\|Z\| > 2$
22	CLA	c	507	36	65,73,73	1.52	7 (10%)	76,113,113	1.38	7 (9%)
26	LMG	b	625	-	51,51,55	0.72	0	59,59,63	1.34	6 (10%)
28	DGD	h	103	-	63,63,67	0.94	1 (1%)	77,77,81	1.29	6 (7%)
22	CLA	c	502	-	65,73,73	1.62	9 (13%)	76,113,113	1.32	6 (7%)
22	CLA	A	404	-	65,73,73	1.60	7 (10%)	76,113,113	1.27	6 (7%)
25	STE	k	102	-	10,10,19	0.29	0	9,9,19	0.78	0
28	DGD	A	413	-	67,67,67	0.92	2 (2%)	81,81,81	1.35	11 (13%)
28	DGD	C	519	-	63,63,67	0.89	0	77,77,81	1.26	5 (6%)
28	DGD	H	103	-	63,63,67	0.94	1 (1%)	77,77,81	1.29	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
31	LHG	D	409	-	48,48,48	0.62	0	51,54,54	1.16	5 (9%)
23	BCR	d	406	-	41,41,41	1.09	2 (4%)	56,56,56	1.12	4 (7%)
31	LHG	d	410	-	46,46,48	0.68	1 (2%)	49,52,54	1.18	4 (8%)
29	OEX	A	417	1,36,3	0,15,15	-	-	-		
29	OEX	a	417	1,36,3	0,15,15	-	-	-		
30	PHO	D	401	-	51,69,69	1.00	4 (7%)	47,99,99	1.12	5 (10%)
26	LMG	a	410	-	48,48,55	0.80	0	56,56,63	1.26	5 (8%)
23	BCR	H	102	-	41,41,41	1.11	2 (4%)	56,56,56	1.20	6 (10%)
22	CLA	B	603	-	65,73,73	1.56	8 (12%)	76,113,113	1.23	7 (9%)
22	CLA	c	512	-	65,73,73	1.55	7 (10%)	76,113,113	1.38	8 (10%)
22	CLA	b	602	36	65,73,73	1.47	5 (7%)	76,113,113	1.31	9 (11%)
22	CLA	b	603	-	65,73,73	1.55	8 (12%)	76,113,113	1.32	10 (13%)
25	STE	A	415	-	10,10,19	0.31	0	9,9,19	0.73	0
22	CLA	c	501	-	65,73,73	1.49	7 (10%)	76,113,113	1.32	8 (10%)
35	HEC	v	201	16	32,50,50	2.23	3 (9%)	24,82,82	1.46	3 (12%)
22	CLA	b	615	-	65,73,73	1.51	7 (10%)	76,113,113	1.29	7 (9%)
27	SQD	A	411	-	51,52,54	1.52	5 (9%)	60,63,65	1.48	9 (15%)
22	CLA	b	609	-	65,73,73	1.61	8 (12%)	76,113,113	1.32	7 (9%)
32	LMT	J	102	-	24,24,36	1.05	2 (8%)	29,29,47	1.10	2 (6%)
22	CLA	B	614	-	65,73,73	1.51	7 (10%)	76,113,113	1.30	7 (9%)
25	STE	A	409	-	8,8,19	0.31	0	7,7,19	0.73	0
32	LMT	E	104	-	24,24,36	1.02	2 (8%)	29,29,47	1.08	2 (6%)
22	CLA	C	507	36	65,73,73	1.52	7 (10%)	76,113,113	1.38	7 (9%)
23	BCR	K	101	-	41,41,41	1.07	3 (7%)	56,56,56	1.16	5 (8%)
25	STE	j	101	-	11,11,19	0.28	0	10,10,19	0.83	0
22	CLA	B	613	-	65,73,73	1.60	8 (12%)	76,113,113	1.40	8 (10%)
30	PHO	d	401	-	51,69,69	1.00	5 (9%)	47,99,99	1.13	5 (10%)
22	CLA	c	505	-	65,73,73	1.63	8 (12%)	76,113,113	1.34	7 (9%)
22	CLA	C	505	-	65,73,73	1.63	8 (12%)	76,113,113	1.34	7 (9%)
26	LMG	C	520	-	48,48,55	0.81	1 (2%)	56,56,63	1.30	6 (10%)
22	CLA	c	513	-	65,73,73	1.46	7 (10%)	76,113,113	1.30	9 (11%)
27	SQD	a	412	-	53,54,54	1.51	7 (13%)	62,65,65	1.34	6 (9%)
23	BCR	D	406	-	41,41,41	1.09	2 (4%)	56,56,56	1.12	4 (7%)
30	PHO	a	418	-	51,69,69	1.03	4 (7%)	47,99,99	1.05	5 (10%)
28	DGD	c	517	-	63,63,67	0.86	1 (1%)	77,77,81	1.34	7 (9%)
31	LHG	d	411	-	48,48,48	0.64	1 (2%)	51,54,54	1.21	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CLA	c	511	3	65,73,73	1.51	7 (10%)	76,113,113	1.34	7 (9%)
23	BCR	k	103	-	41,41,41	1.12	2 (4%)	56,56,56	1.13	3 (5%)
22	CLA	d	404	-	65,73,73	1.69	7 (10%)	76,113,113	1.36	9 (11%)
22	CLA	C	508	-	65,73,73	1.59	8 (12%)	76,113,113	1.37	9 (11%)
22	CLA	c	506	-	65,73,73	1.51	7 (10%)	76,113,113	1.33	8 (10%)
24	PL9	A	408	-	55,55,55	1.00	3 (5%)	68,69,69	1.52	12 (17%)
32	LMT	c	525	-	36,36,36	1.16	5 (13%)	47,47,47	0.91	1 (2%)
22	CLA	B	615	-	65,73,73	1.68	9 (13%)	76,113,113	1.32	6 (7%)
22	CLA	b	608	36	65,73,73	1.50	6 (9%)	76,113,113	1.33	7 (9%)
31	LHG	d	409	-	48,48,48	0.63	1 (2%)	51,54,54	1.16	5 (9%)
32	LMT	m	101	-	36,36,36	1.15	5 (13%)	47,47,47	0.97	2 (4%)
25	STE	M	101	-	9,9,19	0.28	0	8,8,19	0.83	0
25	STE	I	101	-	13,13,19	0.26	0	12,12,19	0.86	0
23	BCR	B	617	-	41,41,41	1.08	2 (4%)	56,56,56	1.17	6 (10%)
33	BCT	d	403	20	2,3,3	1.17	0	2,3,3	4.48	2 (100%)
25	STE	i	101	-	13,13,19	0.27	0	12,12,19	0.86	0
25	STE	a	409	-	8,8,19	0.30	0	7,7,19	0.72	0
23	BCR	B	618	-	41,41,41	1.08	2 (4%)	56,56,56	1.11	4 (7%)
26	LMG	D	402	-	33,33,55	0.59	0	35,35,63	1.21	2 (5%)
23	BCR	A	407	-	41,41,41	1.06	2 (4%)	56,56,56	1.10	3 (5%)
26	LMG	c	520	-	48,48,55	0.81	1 (2%)	56,56,63	1.30	6 (10%)
28	DGD	C	517	-	63,63,67	0.86	1 (1%)	77,77,81	1.34	7 (9%)
32	LMT	j	102	-	24,24,36	1.05	2 (8%)	29,29,47	1.10	2 (6%)
32	LMT	b	624	-	25,25,36	1.00	2 (8%)	30,30,47	1.09	2 (6%)
25	STE	c	522	-	7,7,19	0.29	0	6,6,19	0.70	0
22	CLA	A	406	-	54,62,73	1.79	6 (11%)	62,99,113	1.44	8 (12%)
22	CLA	a	405	36	60,68,73	1.54	6 (10%)	70,107,113	1.46	9 (12%)
22	CLA	A	419	36	65,73,73	1.48	7 (10%)	76,113,113	1.33	9 (11%)
22	CLA	b	605	-	65,73,73	1.62	8 (12%)	76,113,113	1.45	7 (9%)
22	CLA	b	610	-	65,73,73	1.62	8 (12%)	76,113,113	1.34	9 (11%)
22	CLA	c	510	-	65,73,73	1.50	6 (9%)	76,113,113	1.32	7 (9%)
25	STE	c	521	-	11,11,19	0.71	0	11,11,19	1.15	0
22	CLA	c	503	-	65,73,73	1.73	9 (13%)	76,113,113	1.26	7 (9%)
26	LMG	H	101	-	38,38,55	0.51	0	40,40,63	1.31	2 (5%)
32	LMT	e	104	-	24,24,36	1.02	2 (8%)	29,29,47	1.08	2 (6%)
27	SQD	B	620	-	53,54,54	1.52	8 (15%)	62,65,65	1.39	6 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
32	LMT	B	623	-	25,25,36	1.01	2 (8%)	30,30,47	1.09	2 (6%)
22	CLA	b	611	36	65,73,73	1.51	7 (10%)	76,113,113	1.41	7 (9%)
31	LHG	A	420	-	48,48,48	0.66	2 (4%)	51,54,54	1.28	7 (13%)
23	BCR	t	102	-	41,41,41	1.06	2 (4%)	56,56,56	1.17	5 (8%)
32	LMT	z	101	-	36,36,36	1.20	5 (13%)	47,47,47	0.97	1 (2%)
22	CLA	B	605	-	65,73,73	1.64	7 (10%)	76,113,113	1.29	10 (13%)
23	BCR	T	101	-	41,41,41	1.06	2 (4%)	56,56,56	1.16	5 (8%)
26	LMG	c	524	-	50,50,55	0.75	1 (2%)	58,58,63	1.33	7 (12%)
23	BCR	C	514	-	41,41,41	1.10	2 (4%)	56,56,56	1.17	5 (8%)
22	CLA	b	613	-	65,73,73	1.59	8 (12%)	76,113,113	1.42	8 (10%)
25	STE	b	623	-	11,11,19	0.68	0	11,11,19	1.22	1 (9%)
26	LMG	B	624	-	51,51,55	0.72	0	59,59,63	1.33	6 (10%)
24	PL9	d	407	-	55,55,55	0.97	4 (7%)	68,69,69	1.46	8 (11%)
25	STE	a	414	-	7,7,19	0.29	0	6,6,19	0.67	0
22	CLA	b	617	-	60,68,73	1.68	8 (13%)	70,107,113	1.44	6 (8%)
22	CLA	A	405	36	60,68,73	1.57	7 (11%)	70,107,113	1.51	10 (14%)
23	BCR	a	407	-	41,41,41	1.06	2 (4%)	56,56,56	1.11	3 (5%)
25	STE	B	621	-	16,16,19	0.58	0	16,16,19	1.09	0
22	CLA	B	612	-	65,73,73	1.59	8 (12%)	76,113,113	1.42	8 (10%)
25	STE	t	101	-	17,17,19	0.58	0	17,17,19	1.08	1 (5%)
25	STE	A	414	-	7,7,19	0.29	0	6,6,19	0.66	0
22	CLA	c	508	-	65,73,73	1.58	8 (12%)	76,113,113	1.36	9 (11%)
25	STE	E	103	-	19,19,19	0.55	0	19,19,19	1.06	0
27	SQD	X	101	-	35,36,54	1.46	5 (14%)	42,45,65	1.56	7 (16%)
22	CLA	B	604	-	65,73,73	1.63	8 (12%)	76,113,113	1.45	7 (9%)
25	STE	b	601	-	11,11,19	0.29	0	10,10,19	0.79	0
23	BCR	k	101	-	41,41,41	1.06	2 (4%)	56,56,56	1.16	5 (8%)
22	CLA	a	404	-	65,73,73	1.60	7 (10%)	76,113,113	1.27	6 (7%)
25	STE	C	521	-	11,11,19	0.70	0	11,11,19	1.14	0
28	DGD	a	413	-	67,67,67	0.91	2 (2%)	81,81,81	1.35	12 (14%)
34	HEM	e	105	5,6	41,50,50	1.47	4 (9%)	45,82,82	1.41	5 (11%)
32	LMT	C	525	-	36,36,36	1.16	5 (13%)	47,47,47	0.91	1 (2%)
22	CLA	a	419	36	65,73,73	1.48	7 (10%)	76,113,113	1.33	9 (11%)
25	STE	d	413	-	8,8,19	0.30	0	7,7,19	0.74	0
31	LHG	D	411	-	48,48,48	0.64	1 (2%)	51,54,54	1.21	6 (11%)
23	BCR	C	515	-	41,41,41	1.07	2 (4%)	56,56,56	1.14	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	STE	A	421	-	11,11,19	0.68	0	11,11,19	1.16	0
25	STE	A	416	-	10,10,19	0.30	0	9,9,19	0.77	0
22	CLA	C	512	-	65,73,73	1.55	7 (10%)	76,113,113	1.37	8 (10%)
25	STE	b	622	-	16,16,19	0.58	0	16,16,19	1.10	0
26	LMG	A	410	-	48,48,55	0.79	0	56,56,63	1.25	5 (8%)
22	CLA	B	616	-	60,68,73	1.67	8 (13%)	70,107,113	1.44	7 (10%)
26	LMG	d	408	-	51,51,55	0.78	0	59,59,63	1.29	5 (8%)
35	HEC	V	201	16	32,50,50	2.22	3 (9%)	24,82,82	1.45	3 (12%)
23	BCR	b	620	-	41,41,41	1.05	2 (4%)	56,56,56	1.13	5 (8%)
22	CLA	B	601	36	65,73,73	1.47	5 (7%)	76,113,113	1.31	9 (11%)
22	CLA	C	501	-	65,73,73	1.50	7 (10%)	76,113,113	1.32	8 (10%)
22	CLA	D	405	-	65,73,73	1.66	9 (13%)	76,113,113	1.37	8 (10%)
22	CLA	b	616	-	65,73,73	1.66	9 (13%)	76,113,113	1.31	6 (7%)
32	LMT	M	102	-	36,36,36	1.15	5 (13%)	47,47,47	0.97	2 (4%)
22	CLA	b	604	-	65,73,73	1.55	8 (12%)	76,113,113	1.23	7 (9%)
22	CLA	b	614	-	65,73,73	1.59	8 (12%)	76,113,113	1.40	9 (11%)
26	LMG	C	524	-	50,50,55	0.75	1 (2%)	58,58,63	1.33	7 (12%)
30	PHO	A	418	-	51,69,69	1.03	4 (7%)	47,99,99	1.05	4 (8%)
25	STE	B	625	-	11,11,19	0.29	0	10,10,19	0.79	0
31	LHG	l	101	-	48,48,48	0.62	1 (2%)	51,54,54	1.20	5 (9%)
22	CLA	B	607	36	65,73,73	1.51	6 (9%)	76,113,113	1.33	7 (9%)
23	BCR	h	102	-	41,41,41	1.11	2 (4%)	56,56,56	1.20	6 (10%)
31	LHG	D	410	-	46,46,48	0.67	1 (2%)	49,52,54	1.17	4 (8%)
25	STE	c	516	-	13,13,19	0.63	0	13,13,19	1.14	1 (7%)
23	BCR	b	618	-	41,41,41	1.08	2 (4%)	56,56,56	1.18	6 (10%)
25	STE	a	416	-	10,10,19	0.29	0	9,9,19	0.76	0
32	LMT	c	523	-	24,24,36	1.13	4 (16%)	29,29,47	1.29	2 (6%)
25	STE	T	102	-	14,14,19	0.29	0	13,13,19	0.82	0
32	LMT	C	523	-	24,24,36	1.13	4 (16%)	29,29,47	1.25	2 (6%)
26	LMG	D	408	-	51,51,55	0.78	0	59,59,63	1.29	5 (8%)
33	BCT	D	403	20	2,3,3	1.17	0	2,3,3	4.47	2 (100%)
22	CLA	c	509	-	65,73,73	1.53	7 (10%)	76,113,113	1.40	7 (9%)
25	STE	e	102	-	11,11,19	0.29	0	10,10,19	0.81	0
22	CLA	C	509	-	65,73,73	1.54	7 (10%)	76,113,113	1.40	8 (10%)
22	CLA	c	504	36	59,67,73	1.56	7 (11%)	68,105,113	1.41	7 (10%)
27	SQD	x	101	-	35,36,54	1.47	5 (14%)	42,45,65	1.57	7 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CLA	C	504	36	59,67,73	1.56	7 (11%)	68,105,113	1.41	7 (10%)
28	DGD	C	518	-	58,58,67	0.95	3 (5%)	72,72,81	1.31	5 (6%)
25	STE	e	101	-	11,11,19	0.70	0	11,11,19	1.14	0
22	CLA	b	607	-	65,73,73	1.52	7 (10%)	76,113,113	1.36	6 (7%)
26	LMG	h	101	-	38,38,55	0.51	0	40,40,63	1.31	2 (5%)
23	BCR	K	103	-	41,41,41	1.12	2 (4%)	56,56,56	1.14	3 (5%)
22	CLA	d	405	-	65,73,73	1.66	9 (13%)	76,113,113	1.37	8 (10%)
22	CLA	C	511	3	65,73,73	1.52	6 (9%)	76,113,113	1.35	7 (9%)
22	CLA	C	506	-	65,73,73	1.50	7 (10%)	76,113,113	1.33	8 (10%)
22	CLA	B	606	-	65,73,73	1.51	7 (10%)	76,113,113	1.36	6 (7%)
25	STE	a	421	-	11,11,19	0.69	0	11,11,19	1.17	0
24	PL9	a	408	-	55,55,55	1.00	3 (5%)	68,69,69	1.52	12 (17%)
28	DGD	c	519	-	63,63,67	0.89	0	77,77,81	1.26	5 (6%)
22	CLA	C	503	-	65,73,73	1.73	9 (13%)	76,113,113	1.26	7 (9%)
25	STE	e	103	-	19,19,19	0.56	0	19,19,19	1.06	0
23	BCR	b	619	-	41,41,41	1.07	2 (4%)	56,56,56	1.11	3 (5%)
34	HEM	E	105	5,6	41,50,50	1.47	4 (9%)	45,82,82	1.42	5 (11%)
22	CLA	B	602	-	65,73,73	1.56	8 (12%)	76,113,113	1.32	10 (13%)
22	CLA	C	502	-	65,73,73	1.62	9 (13%)	76,113,113	1.33	6 (7%)
27	SQD	A	412	-	53,54,54	1.51	7 (13%)	62,65,65	1.34	6 (9%)
22	CLA	B	609	-	65,73,73	1.63	8 (12%)	76,113,113	1.35	9 (11%)
26	LMG	d	402	-	33,33,55	0.59	0	35,35,63	1.21	2 (5%)
23	BCR	B	619	-	41,41,41	1.05	2 (4%)	56,56,56	1.13	5 (8%)
23	BCR	c	515	-	41,41,41	1.07	2 (4%)	56,56,56	1.14	5 (8%)
22	CLA	a	406	-	54,62,73	1.78	6 (11%)	62,99,113	1.44	8 (12%)
25	STE	D	412	-	19,19,19	0.56	0	19,19,19	1.01	0
25	STE	C	522	-	7,7,19	0.30	0	6,6,19	0.70	0
25	STE	E	101	-	11,11,19	0.69	0	11,11,19	1.14	0
25	STE	C	516	-	13,13,19	0.63	0	13,13,19	1.13	1 (7%)
22	CLA	C	510	-	65,73,73	1.50	6 (9%)	76,113,113	1.32	7 (9%)
22	CLA	D	404	-	65,73,73	1.69	7 (10%)	76,113,113	1.36	9 (11%)
23	BCR	c	514	-	41,41,41	1.10	2 (4%)	56,56,56	1.17	5 (8%)
22	CLA	b	606	-	65,73,73	1.64	7 (10%)	76,113,113	1.28	10 (13%)
25	STE	m	102	-	9,9,19	0.28	0	8,8,19	0.83	0
25	STE	d	412	-	19,19,19	0.55	0	19,19,19	1.01	0
27	SQD	a	411	-	51,52,54	1.53	5 (9%)	60,63,65	1.47	9 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CLA	b	612	-	65,73,73	1.65	8 (12%)	76,113,113	1.41	9 (11%)
22	CLA	B	608	-	65,73,73	1.61	8 (12%)	76,113,113	1.32	8 (10%)
22	CLA	C	513	-	65,73,73	1.46	7 (10%)	76,113,113	1.30	9 (11%)
25	STE	a	415	-	10,10,19	0.31	0	9,9,19	0.72	0
22	CLA	B	610	36	65,73,73	1.52	7 (10%)	76,113,113	1.41	7 (9%)
27	SQD	b	621	-	48,49,54	1.60	9 (18%)	57,60,65	1.38	6 (10%)
24	PL9	D	407	-	55,55,55	0.97	4 (7%)	68,69,69	1.46	8 (11%)
28	DGD	c	518	-	58,58,67	0.95	3 (5%)	72,72,81	1.31	5 (6%)
31	LHG	a	420	-	48,48,48	0.65	2 (4%)	51,54,54	1.26	6 (11%)
25	STE	E	102	-	11,11,19	0.29	0	10,10,19	0.82	0
22	CLA	B	611	-	65,73,73	1.63	8 (12%)	76,113,113	1.41	9 (11%)
31	LHG	L	101	-	48,48,48	0.62	1 (2%)	51,54,54	1.20	5 (9%)
25	STE	D	413	-	8,8,19	0.30	0	7,7,19	0.74	0
25	STE	K	102	-	10,10,19	0.30	0	9,9,19	0.79	0
25	STE	J	101	-	11,11,19	0.28	0	10,10,19	0.83	0
25	STE	B	622	-	11,11,19	0.67	0	11,11,19	1.22	1 (9%)
32	LMT	Z	101	-	36,36,36	1.20	5 (13%)	47,47,47	0.97	1 (2%)

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
22	CLA	c	507	36	1/1/20/20	8/37/115/115	-
26	LMG	b	625	-	-	16/46/66/70	0/1/1/1
28	DGD	h	103	-	-	14/51/91/95	0/2/2/2
22	CLA	c	502	-	-	5/37/115/115	-
22	CLA	A	404	-	1/1/20/20	2/37/115/115	-
25	STE	k	102	-	-	5/8/8/17	-
28	DGD	A	413	-	-	27/55/95/95	0/2/2/2
28	DGD	C	519	-	-	15/51/91/95	0/2/2/2
28	DGD	H	103	-	-	14/51/91/95	0/2/2/2
31	LHG	D	409	-	-	12/53/53/53	-
23	BCR	d	406	-	-	3/29/63/63	0/2/2/2
31	LHG	d	410	-	-	12/51/51/53	-
30	PHO	D	401	-	-	0/37/103/103	0/5/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	LMG	a	410	-	-	25/43/63/70	0/1/1/1
23	BCR	H	102	-	-	7/29/63/63	0/2/2/2
22	CLA	B	603	-	1/1/20/20	8/37/115/115	-
22	CLA	c	512	-	1/1/20/20	13/37/115/115	-
22	CLA	b	602	36	1/1/20/20	24/37/115/115	-
22	CLA	b	603	-	1/1/20/20	5/37/115/115	-
25	STE	A	415	-	-	3/8/8/17	-
22	CLA	c	501	-	1/1/20/20	2/37/115/115	-
35	HEC	v	201	16	-	2/10/54/54	-
22	CLA	b	615	-	1/1/20/20	14/37/115/115	-
27	SQD	A	411	-	-	18/47/67/69	0/1/1/1
22	CLA	b	609	-	1/1/20/20	5/37/115/115	-
32	LMT	J	102	-	-	10/15/35/61	0/1/1/2
22	CLA	B	614	-	1/1/20/20	13/37/115/115	-
25	STE	A	409	-	-	5/6/6/17	-
32	LMT	E	104	-	-	9/15/35/61	0/1/1/2
22	CLA	C	507	36	1/1/20/20	8/37/115/115	-
23	BCR	K	101	-	-	0/29/63/63	0/2/2/2
25	STE	j	101	-	-	2/9/9/17	-
22	CLA	B	613	-	1/1/20/20	6/37/115/115	-
30	PHO	d	401	-	-	0/37/103/103	0/5/6/6
22	CLA	c	505	-	1/1/20/20	6/37/115/115	-
22	CLA	C	505	-	1/1/20/20	6/37/115/115	-
26	LMG	C	520	-	-	21/43/63/70	0/1/1/1
22	CLA	c	513	-	1/1/20/20	8/37/115/115	-
27	SQD	a	412	-	-	19/49/69/69	0/1/1/1
23	BCR	D	406	-	-	3/29/63/63	0/2/2/2
30	PHO	a	418	-	-	3/37/103/103	0/5/6/6
28	DGD	c	517	-	-	18/51/91/95	0/2/2/2
31	LHG	d	411	-	-	9/53/53/53	-
22	CLA	c	511	3	1/1/20/20	1/37/115/115	-
23	BCR	k	103	-	-	2/29/63/63	0/2/2/2
22	CLA	d	404	-	-	4/37/115/115	-
22	CLA	C	508	-	-	5/37/115/115	-
22	CLA	c	506	-	1/1/20/20	13/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	PL9	A	408	-	-	20/53/73/73	0/1/1/1
32	LMT	c	525	-	-	8/21/61/61	0/2/2/2
22	CLA	B	615	-	1/1/20/20	7/37/115/115	-
22	CLA	b	608	36	1/1/20/20	3/37/115/115	-
31	LHG	d	409	-	-	12/53/53/53	-
32	LMT	m	101	-	-	3/21/61/61	0/2/2/2
25	STE	M	101	-	-	3/7/7/17	-
25	STE	I	101	-	-	6/11/11/17	-
23	BCR	B	617	-	-	2/29/63/63	0/2/2/2
25	STE	i	101	-	-	6/11/11/17	-
25	STE	a	409	-	-	5/6/6/17	-
23	BCR	B	618	-	-	2/29/63/63	0/2/2/2
26	LMG	D	402	-	-	8/35/35/70	-
23	BCR	A	407	-	-	0/29/63/63	0/2/2/2
26	LMG	c	520	-	-	20/43/63/70	0/1/1/1
28	DGD	C	517	-	-	19/51/91/95	0/2/2/2
32	LMT	j	102	-	-	10/15/35/61	0/1/1/2
32	LMT	b	624	-	-	6/17/37/61	0/1/1/2
25	STE	c	522	-	-	1/5/5/17	-
22	CLA	A	406	-	1/1/17/20	5/24/102/115	-
22	CLA	a	405	36	1/1/19/20	6/31/109/115	-
22	CLA	A	419	36	1/1/20/20	4/37/115/115	-
22	CLA	b	605	-	1/1/20/20	9/37/115/115	-
22	CLA	b	610	-	-	5/37/115/115	-
22	CLA	c	510	-	1/1/20/20	8/37/115/115	-
25	STE	c	521	-	-	7/9/9/17	-
22	CLA	c	503	-	-	6/37/115/115	-
26	LMG	H	101	-	-	18/40/40/70	-
32	LMT	e	104	-	-	9/15/35/61	0/1/1/2
27	SQD	B	620	-	-	29/49/69/69	0/1/1/1
32	LMT	B	623	-	-	6/17/37/61	0/1/1/2
22	CLA	b	611	36	1/1/20/20	0/37/115/115	-
31	LHG	A	420	-	-	24/53/53/53	-
23	BCR	t	102	-	-	3/29/63/63	0/2/2/2
32	LMT	z	101	-	-	12/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	B	605	-	-	7/37/115/115	-
23	BCR	T	101	-	-	3/29/63/63	0/2/2/2
26	LMG	c	524	-	-	20/45/65/70	0/1/1/1
23	BCR	C	514	-	-	0/29/63/63	0/2/2/2
22	CLA	b	613	-	1/1/20/20	5/37/115/115	-
25	STE	b	623	-	-	5/9/9/17	-
26	LMG	B	624	-	-	16/46/66/70	0/1/1/1
24	PL9	d	407	-	-	7/53/73/73	0/1/1/1
25	STE	a	414	-	-	1/5/5/17	-
22	CLA	b	617	-	1/1/19/20	8/31/109/115	-
22	CLA	A	405	36	1/1/19/20	9/31/109/115	-
23	BCR	a	407	-	-	0/29/63/63	0/2/2/2
25	STE	B	621	-	-	5/14/14/17	-
22	CLA	B	612	-	1/1/20/20	5/37/115/115	-
25	STE	t	101	-	-	10/15/15/17	-
25	STE	A	414	-	-	1/5/5/17	-
22	CLA	c	508	-	-	5/37/115/115	-
25	STE	E	103	-	-	8/17/17/17	-
27	SQD	X	101	-	-	11/28/48/69	0/1/1/1
22	CLA	B	604	-	1/1/20/20	9/37/115/115	-
25	STE	b	601	-	-	3/9/9/17	-
23	BCR	k	101	-	-	0/29/63/63	0/2/2/2
22	CLA	a	404	-	1/1/20/20	2/37/115/115	-
25	STE	C	521	-	-	7/9/9/17	-
28	DGD	a	413	-	-	25/55/95/95	0/2/2/2
34	HEM	e	105	5,6	-	0/12/54/54	-
32	LMT	C	525	-	-	8/21/61/61	0/2/2/2
22	CLA	a	419	36	1/1/20/20	4/37/115/115	-
25	STE	d	413	-	-	1/6/6/17	-
31	LHG	D	411	-	-	9/53/53/53	-
23	BCR	C	515	-	-	0/29/63/63	0/2/2/2
25	STE	A	421	-	-	5/9/9/17	-
25	STE	A	416	-	-	5/8/8/17	-
22	CLA	C	512	-	1/1/20/20	14/37/115/115	-
25	STE	b	622	-	-	5/14/14/17	-
26	LMG	A	410	-	-	25/43/63/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	B	616	-	1/1/19/20	8/31/109/115	-
26	LMG	d	408	-	-	16/46/66/70	0/1/1/1
35	HEC	V	201	16	-	2/10/54/54	-
23	BCR	b	620	-	-	1/29/63/63	0/2/2/2
22	CLA	B	601	36	1/1/20/20	24/37/115/115	-
22	CLA	C	501	-	1/1/20/20	2/37/115/115	-
22	CLA	b	616	-	1/1/20/20	7/37/115/115	-
22	CLA	D	405	-	-	6/37/115/115	-
32	LMT	M	102	-	-	3/21/61/61	0/2/2/2
22	CLA	b	604	-	1/1/20/20	8/37/115/115	-
22	CLA	b	614	-	1/1/20/20	6/37/115/115	-
26	LMG	C	524	-	-	20/45/65/70	0/1/1/1
30	PHO	A	418	-	-	3/37/103/103	0/5/6/6
25	STE	B	625	-	-	4/9/9/17	-
31	LHG	l	101	-	-	17/53/53/53	-
22	CLA	B	607	36	1/1/20/20	3/37/115/115	-
23	BCR	h	102	-	-	6/29/63/63	0/2/2/2
31	LHG	D	410	-	-	10/51/51/53	-
25	STE	c	516	-	-	8/11/11/17	-
23	BCR	b	618	-	-	2/29/63/63	0/2/2/2
25	STE	a	416	-	-	5/8/8/17	-
32	LMT	c	523	-	-	2/15/35/61	0/1/1/2
25	STE	T	102	-	-	5/12/12/17	-
32	LMT	C	523	-	-	2/15/35/61	0/1/1/2
26	LMG	D	408	-	-	16/46/66/70	0/1/1/1
22	CLA	c	509	-	1/1/20/20	7/37/115/115	-
25	STE	e	102	-	-	6/9/9/17	-
22	CLA	C	509	-	1/1/20/20	7/37/115/115	-
22	CLA	c	504	36	1/1/18/20	5/30/108/115	-
27	SQD	x	101	-	-	11/28/48/69	0/1/1/1
22	CLA	C	504	36	1/1/18/20	5/30/108/115	-
28	DGD	C	518	-	-	15/46/86/95	0/2/2/2
25	STE	e	101	-	-	4/9/9/17	-
22	CLA	b	607	-	1/1/20/20	10/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	LMG	h	101	-	-	17/40/40/70	-
23	BCR	K	103	-	-	2/29/63/63	0/2/2/2
22	CLA	d	405	-	-	6/37/115/115	-
22	CLA	C	511	3	1/1/20/20	1/37/115/115	-
22	CLA	C	506	-	1/1/20/20	13/37/115/115	-
22	CLA	B	606	-	1/1/20/20	10/37/115/115	-
25	STE	a	421	-	-	5/9/9/17	-
24	PL9	a	408	-	-	20/53/73/73	0/1/1/1
28	DGD	c	519	-	-	15/51/91/95	0/2/2/2
22	CLA	C	503	-	-	6/37/115/115	-
25	STE	e	103	-	-	8/17/17/17	-
23	BCR	b	619	-	-	4/29/63/63	0/2/2/2
34	HEM	E	105	5,6	-	0/12/54/54	-
22	CLA	B	602	-	1/1/20/20	5/37/115/115	-
22	CLA	C	502	-	-	5/37/115/115	-
27	SQD	A	412	-	-	19/49/69/69	0/1/1/1
22	CLA	B	609	-	-	5/37/115/115	-
26	LMG	d	402	-	-	8/35/35/70	-
23	BCR	B	619	-	-	1/29/63/63	0/2/2/2
23	BCR	c	515	-	-	0/29/63/63	0/2/2/2
22	CLA	a	406	-	1/1/17/20	5/24/102/115	-
25	STE	D	412	-	-	6/17/17/17	-
25	STE	C	522	-	-	1/5/5/17	-
25	STE	E	101	-	-	4/9/9/17	-
25	STE	C	516	-	-	8/11/11/17	-
22	CLA	C	510	-	1/1/20/20	7/37/115/115	-
22	CLA	D	404	-	-	4/37/115/115	-
23	BCR	c	514	-	-	0/29/63/63	0/2/2/2
22	CLA	b	606	-	-	7/37/115/115	-
25	STE	m	102	-	-	3/7/7/17	-
25	STE	d	412	-	-	6/17/17/17	-
27	SQD	a	411	-	-	18/47/67/69	0/1/1/1
22	CLA	b	612	-	1/1/20/20	4/37/115/115	-
22	CLA	B	608	-	1/1/20/20	5/37/115/115	-
22	CLA	C	513	-	1/1/20/20	8/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	STE	a	415	-	-	5/8/8/17	-
22	CLA	B	610	36	1/1/20/20	0/37/115/115	-
27	SQD	b	621	-	-	21/44/64/69	0/1/1/1
24	PL9	D	407	-	-	7/53/73/73	0/1/1/1
28	DGD	c	518	-	-	15/46/86/95	0/2/2/2
31	LHG	a	420	-	-	25/53/53/53	-
25	STE	E	102	-	-	5/9/9/17	-
22	CLA	B	611	-	1/1/20/20	4/37/115/115	-
31	LHG	L	101	-	-	17/53/53/53	-
25	STE	D	413	-	-	1/6/6/17	-
25	STE	K	102	-	-	5/8/8/17	-
25	STE	J	101	-	-	2/9/9/17	-
25	STE	B	622	-	-	5/9/9/17	-
32	LMT	Z	101	-	-	12/21/61/61	0/2/2/2

The worst 5 of 736 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	D	404	CLA	C4B-NB	7.89	1.42	1.35
22	d	404	CLA	C4B-NB	7.89	1.42	1.35
22	B	615	CLA	C4B-NB	7.87	1.42	1.35
22	C	502	CLA	C4B-NB	7.86	1.42	1.35
22	c	502	CLA	C4B-NB	7.86	1.42	1.35

The worst 5 of 996 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	604	CLA	C4A-NA-C1A	8.17	110.38	106.71
22	b	605	CLA	C4A-NA-C1A	8.17	110.38	106.71
22	B	612	CLA	C4A-NA-C1A	7.73	110.18	106.71
22	b	613	CLA	C4A-NA-C1A	7.73	110.18	106.71
22	b	614	CLA	C4A-NA-C1A	7.43	110.05	106.71

5 of 56 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
22	A	404	CLA	ND
22	A	405	CLA	ND
22	A	406	CLA	ND

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Mol	Chain	Res	Type	Atom
22	A	419	CLA	ND
22	B	601	CLA	ND

5 of 1586 torsion outliers are listed below:

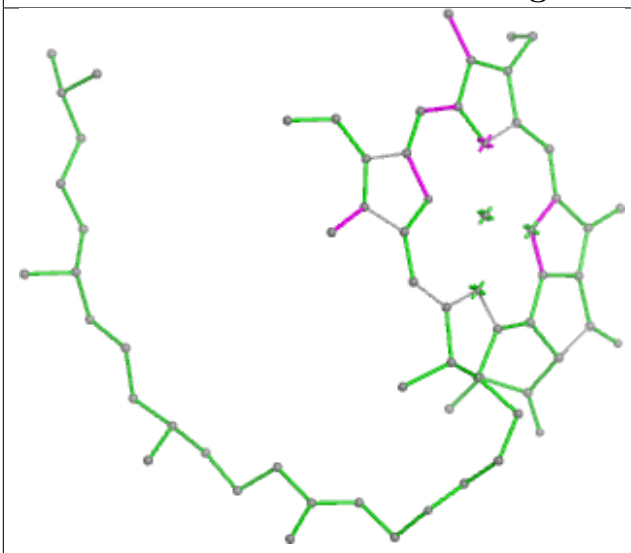
Mol	Chain	Res	Type	Atoms
22	A	406	CLA	C2-C3-C5-C6
22	A	406	CLA	C4-C3-C5-C6
22	B	601	CLA	C1A-C2A-CAA-CBA
22	B	601	CLA	C3A-C2A-CAA-CBA
22	B	605	CLA	C4-C3-C5-C6

There are no ring outliers.

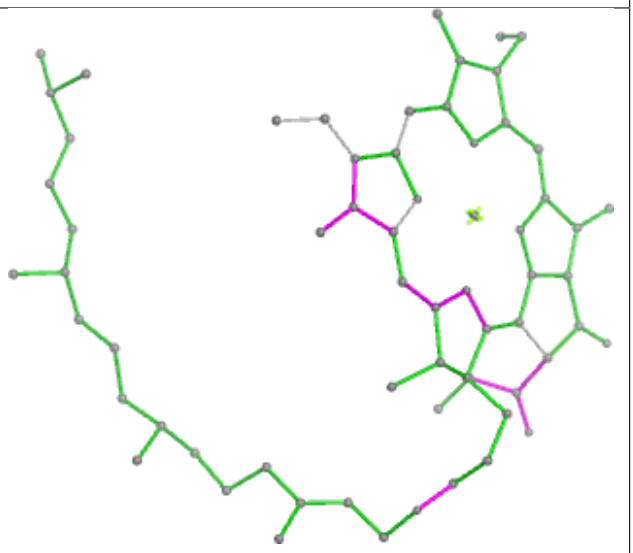
No monomer is involved in short contacts.

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.

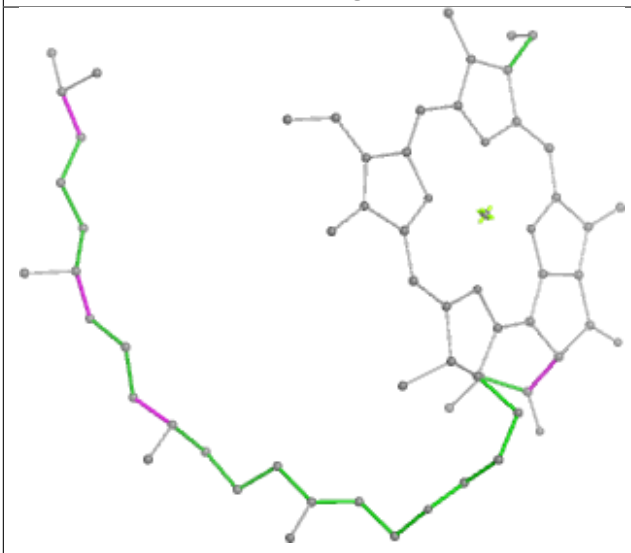
Ligand CLA c 507



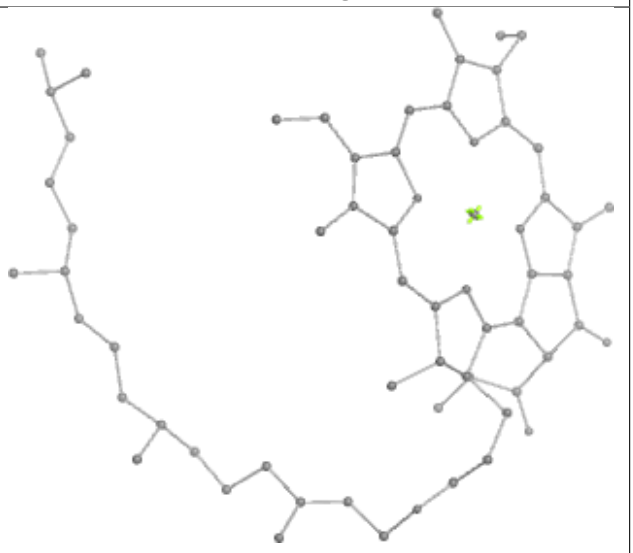
Bond lengths



Bond angles

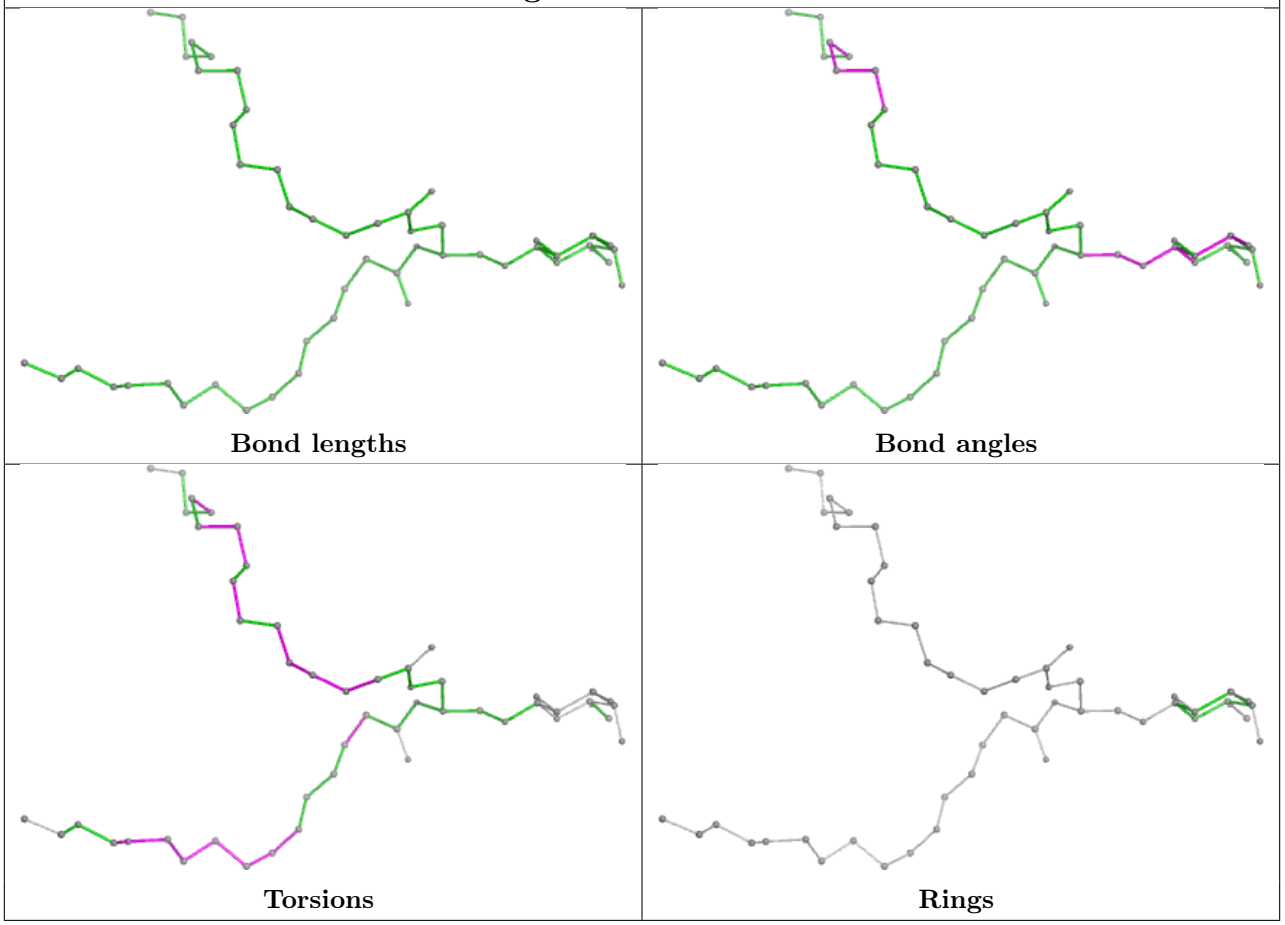


Torsions

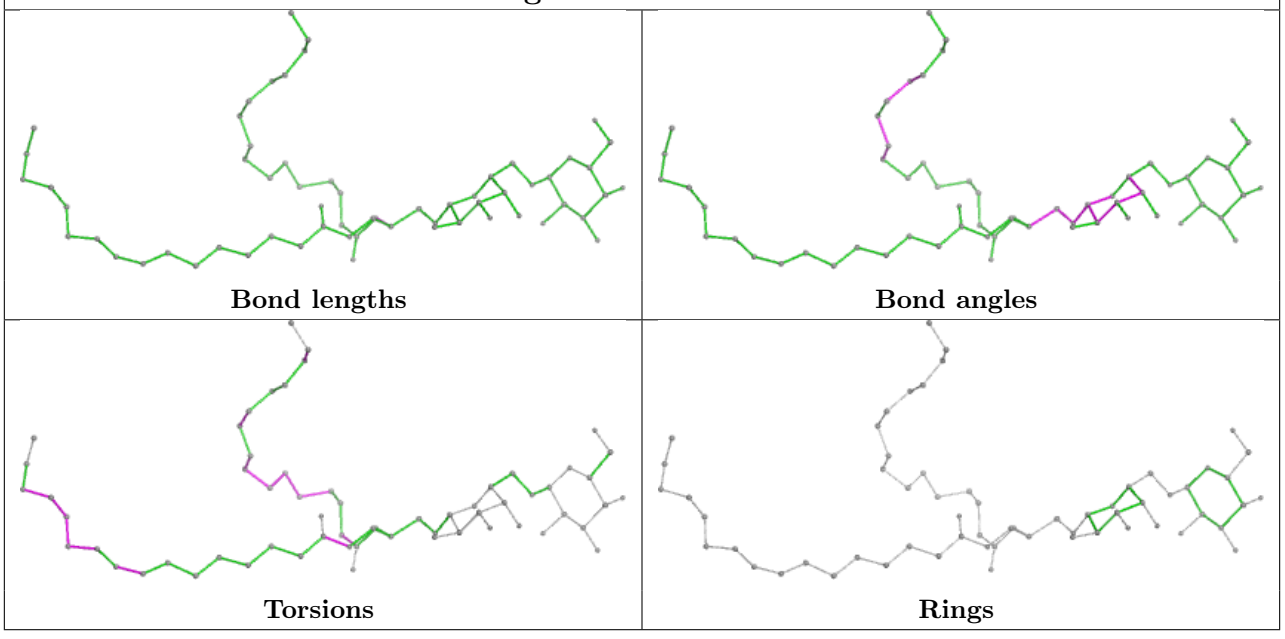


Rings

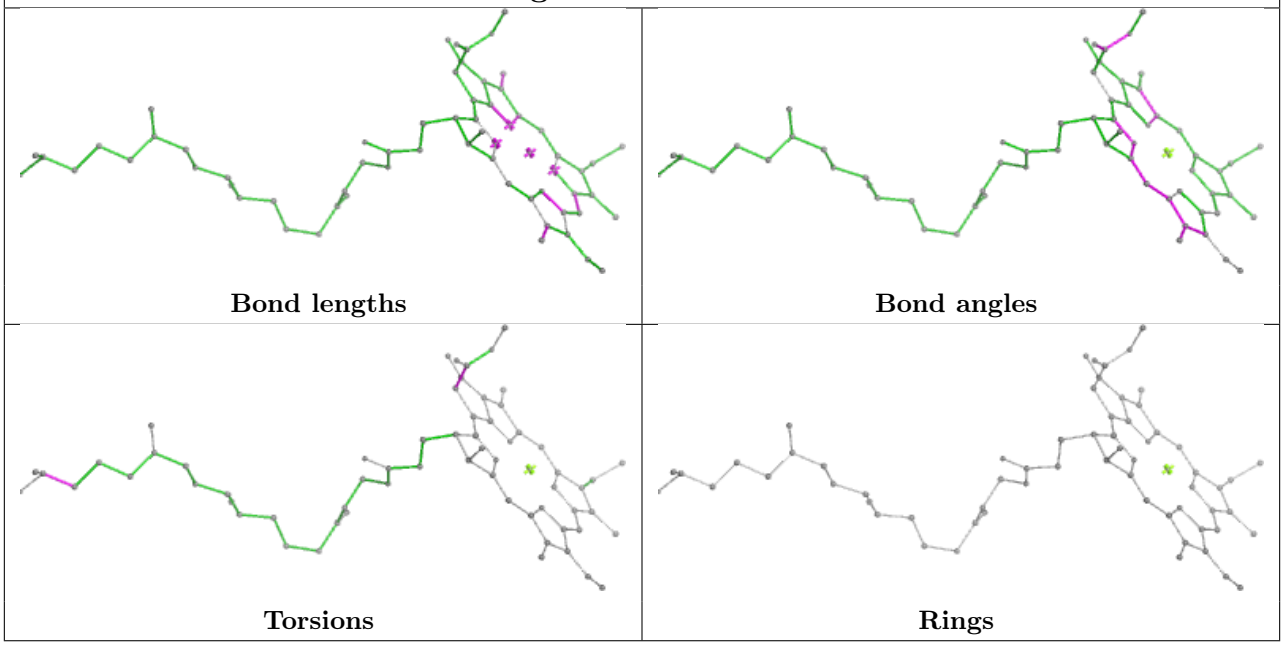
Ligand LMG b 625



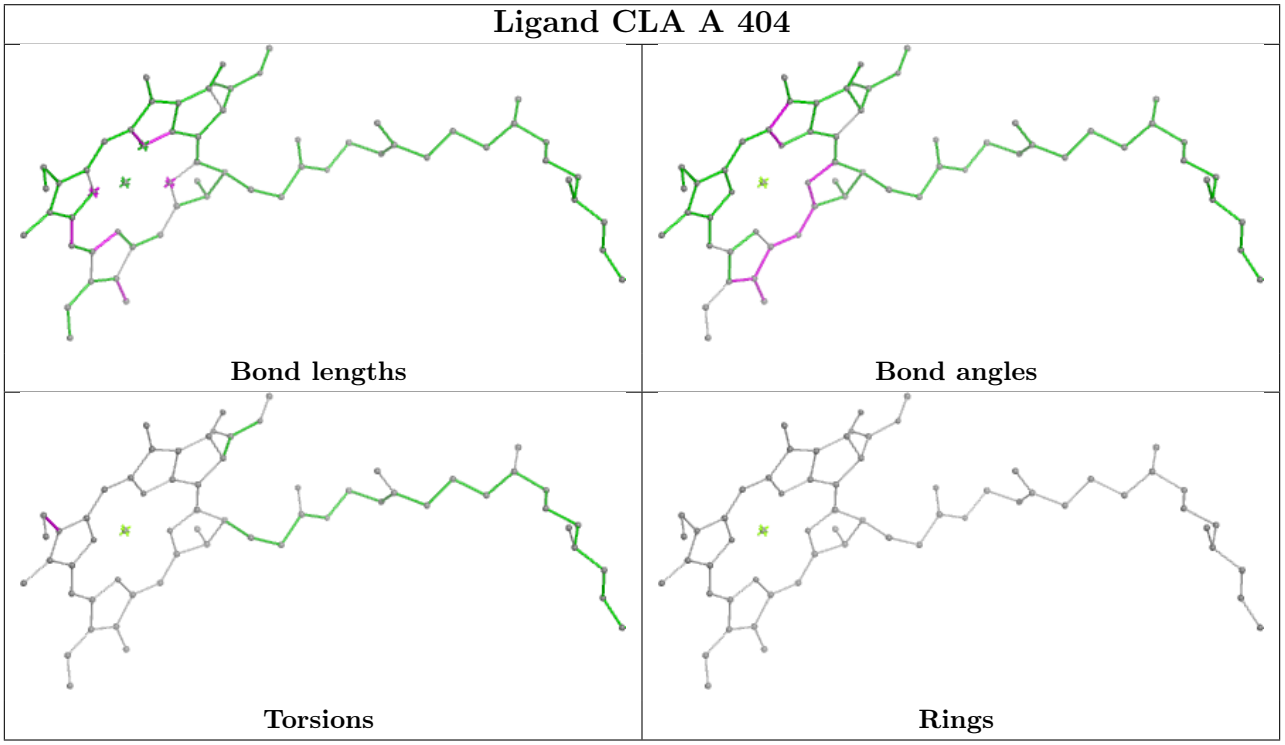
Ligand DGD h 103



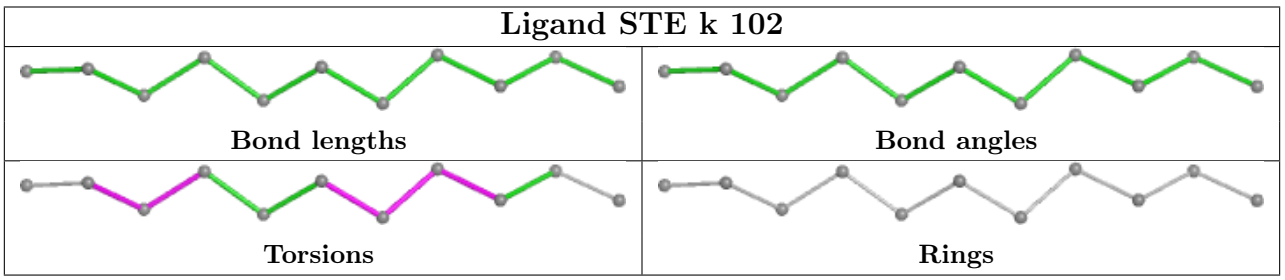
Ligand CLA c 502



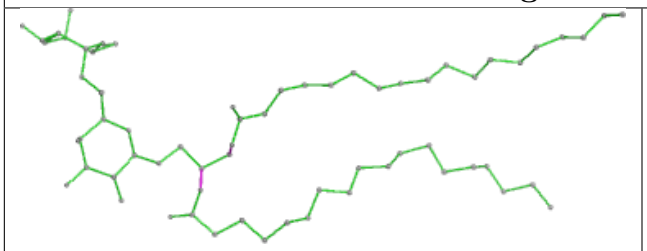
Ligand CLA A 404



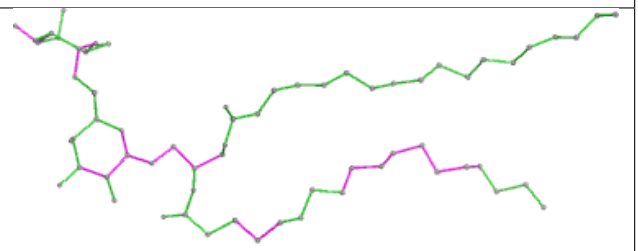
Ligand STE k 102



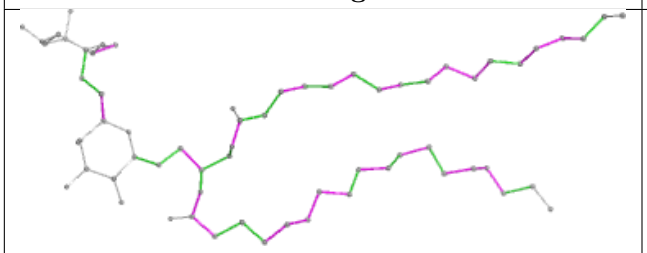
Ligand DGD A 413



Bond lengths



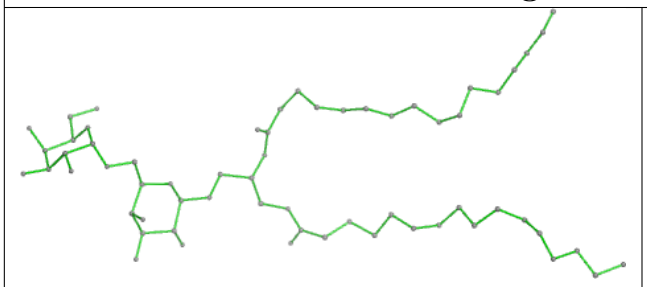
Bond angles



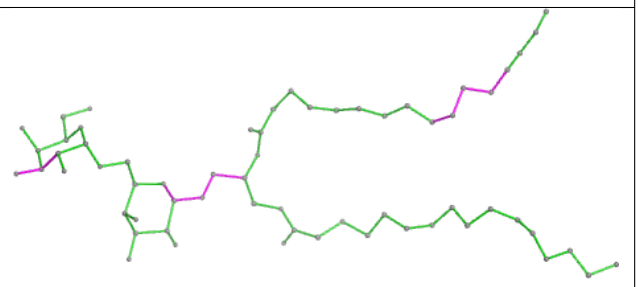
Torsions

Rings

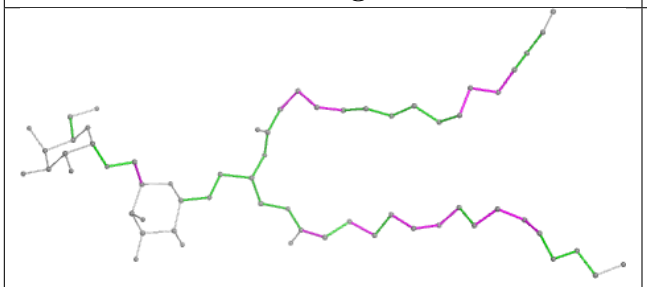
Ligand DGD C 519



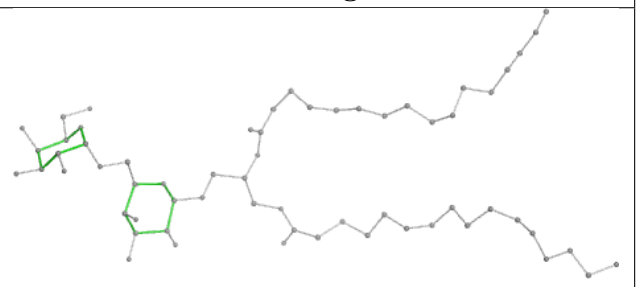
Bond lengths



Bond angles

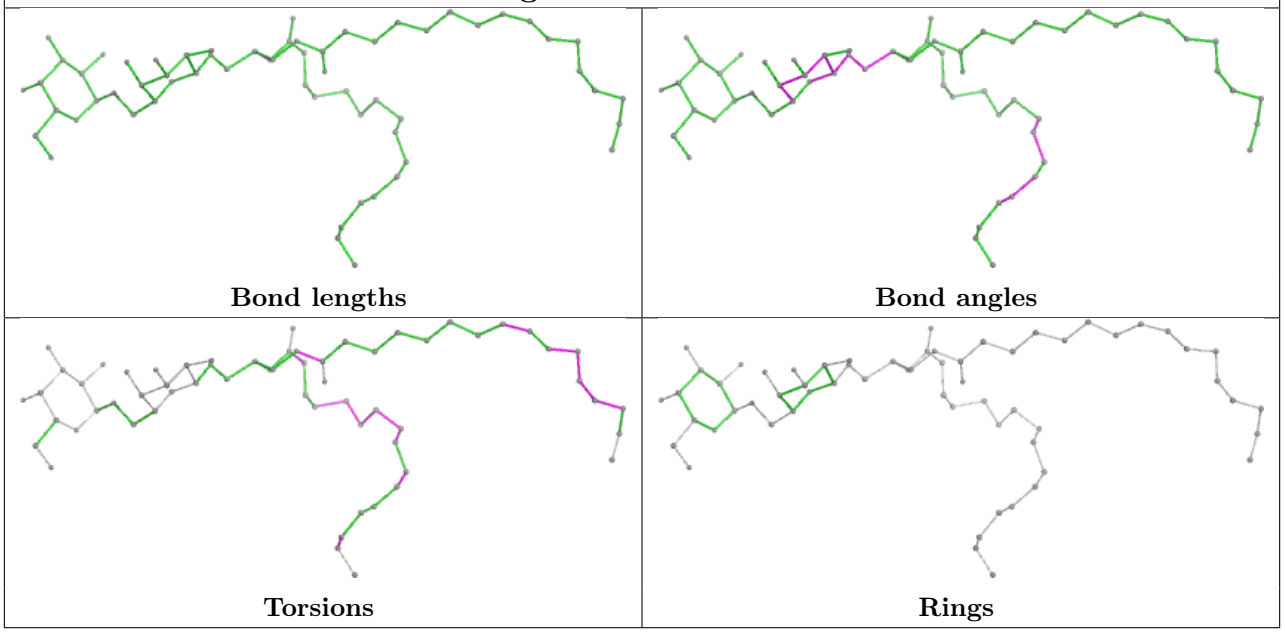


Torsions

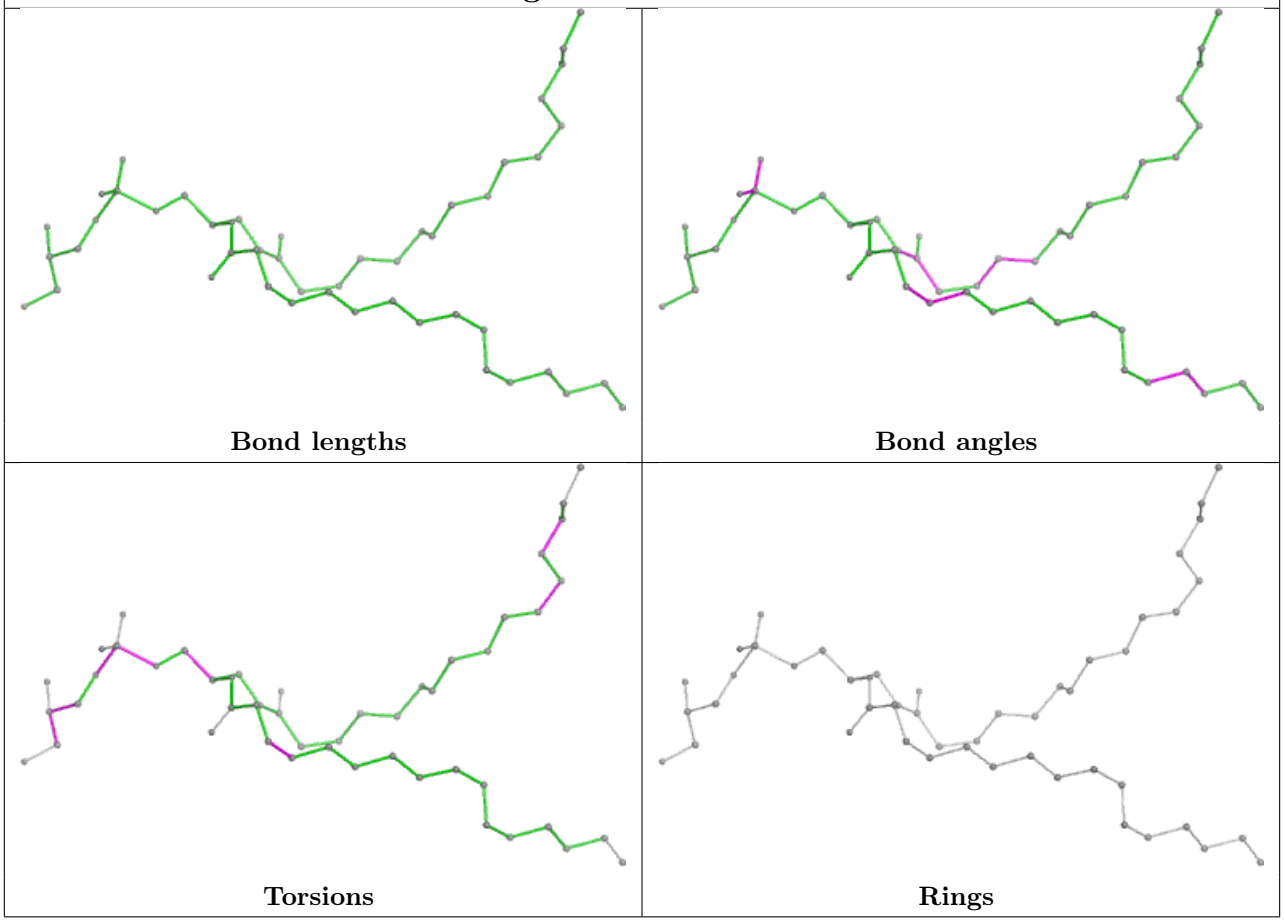


Rings

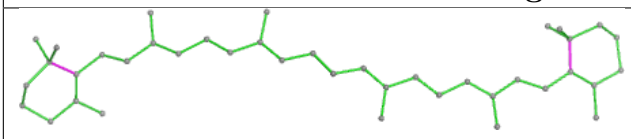
Ligand DGD H 103



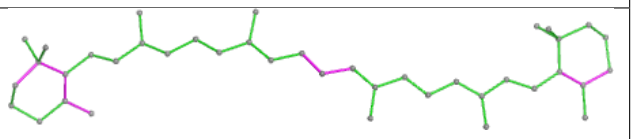
Ligand LHG D 409



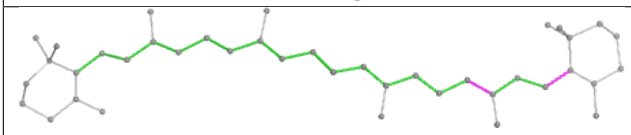
Ligand BCR d 406



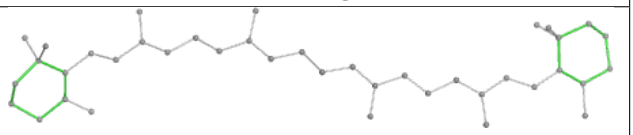
Bond lengths



Bond angles

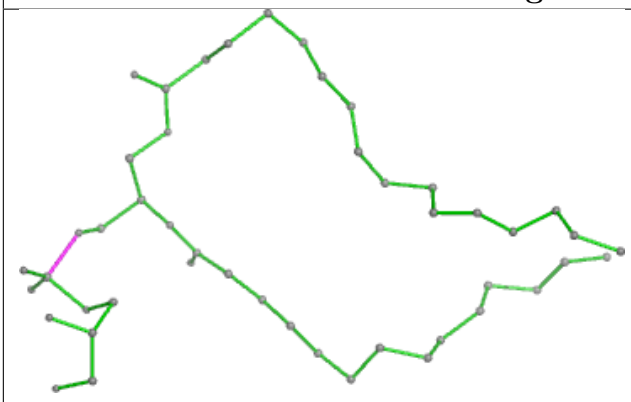


Torsions

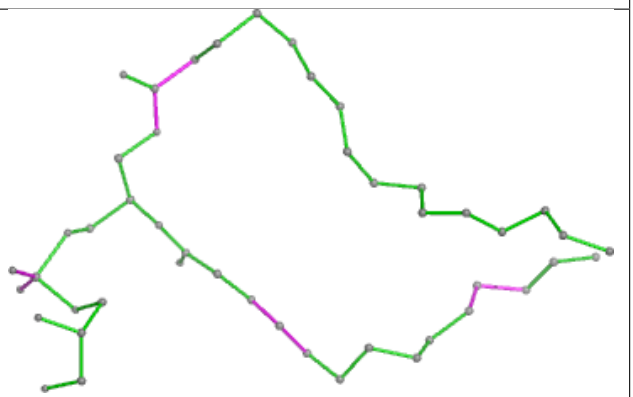


Rings

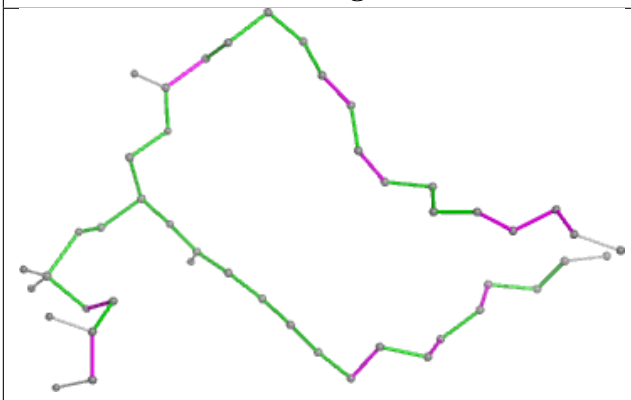
Ligand LHG d 410



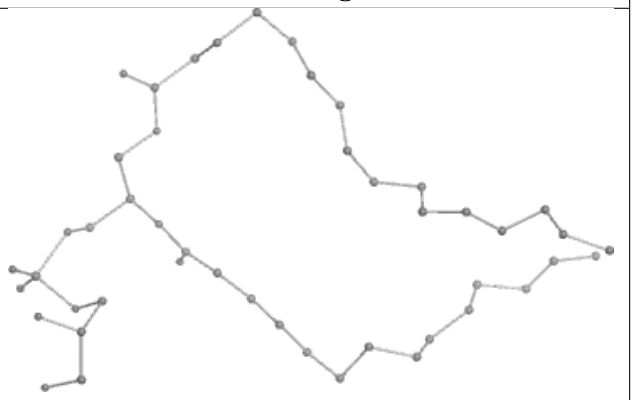
Bond lengths



Bond angles

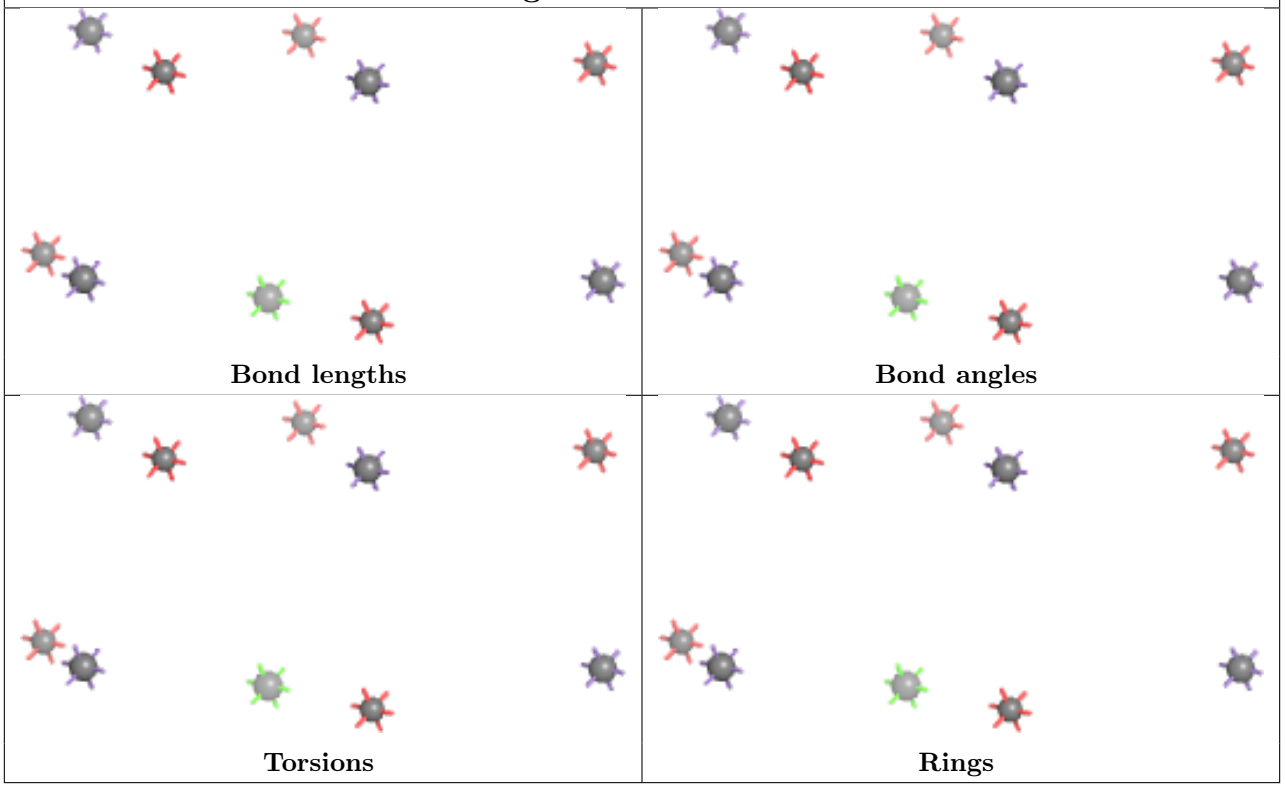


Torsions

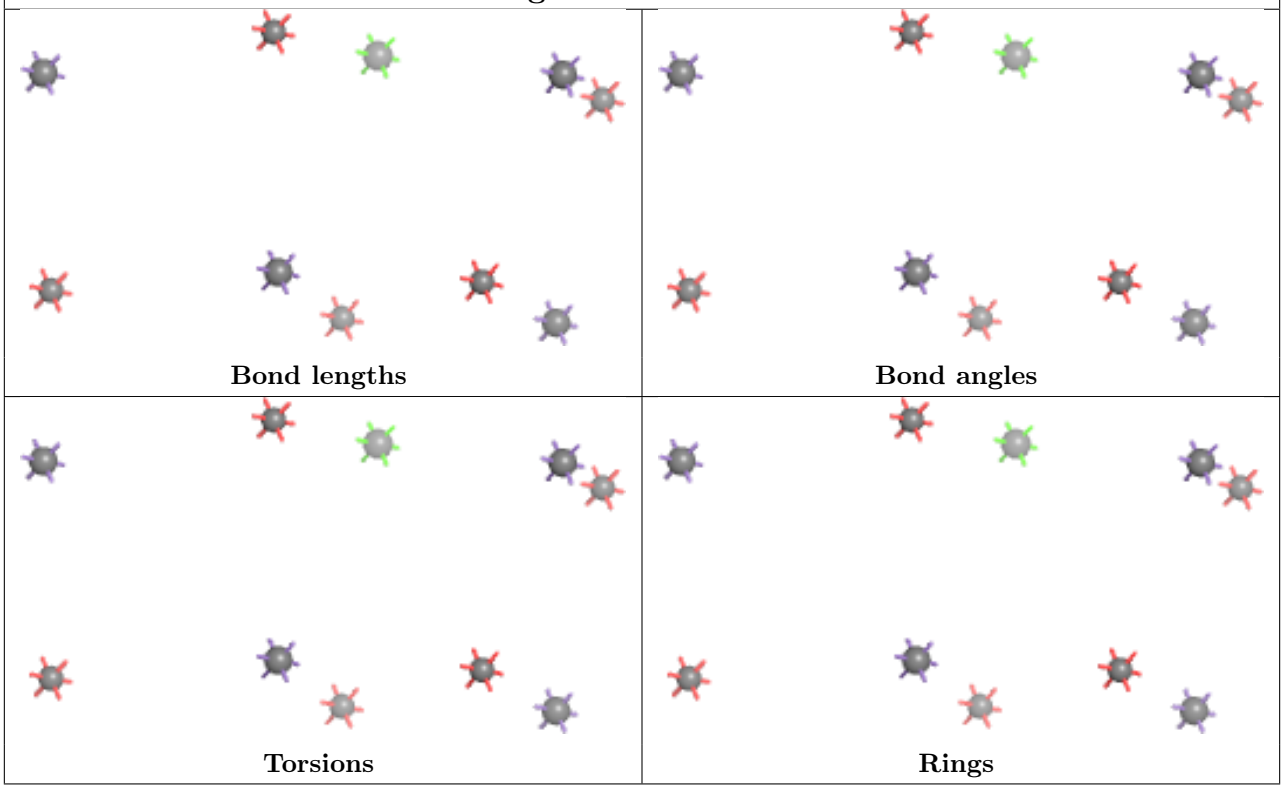


Rings

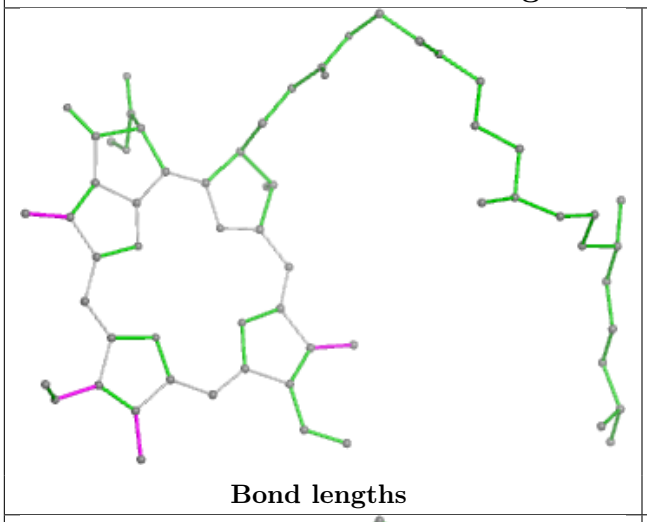
Ligand OEX A 417



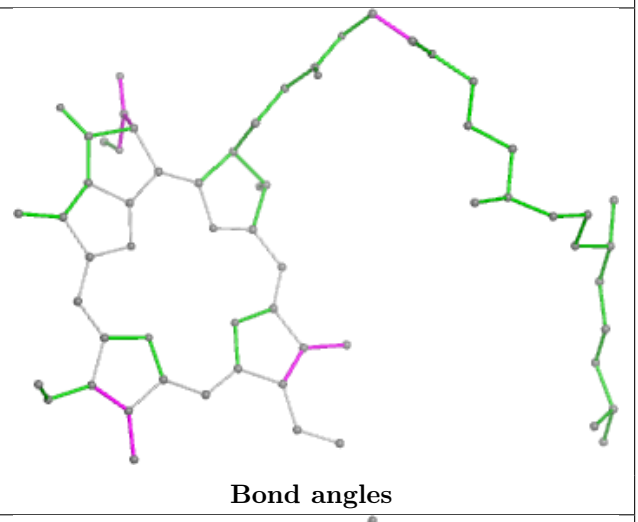
Ligand OEX a 417



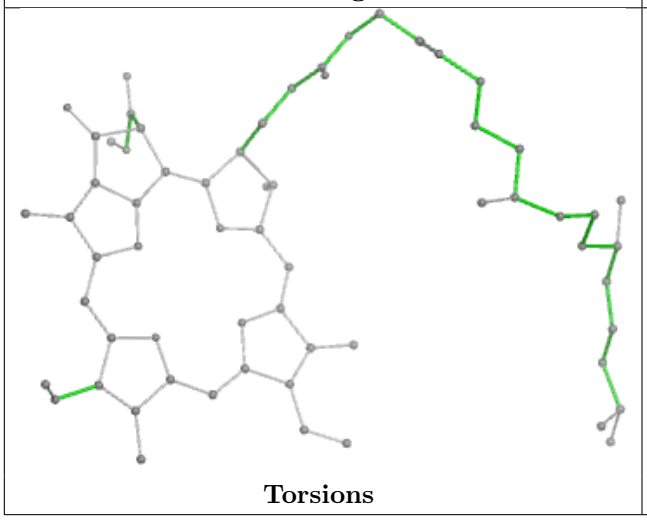
Ligand PHO D 401



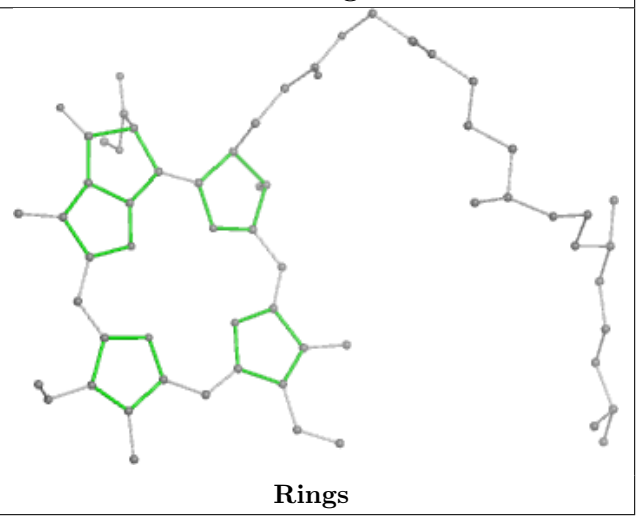
Bond lengths



Bond angles

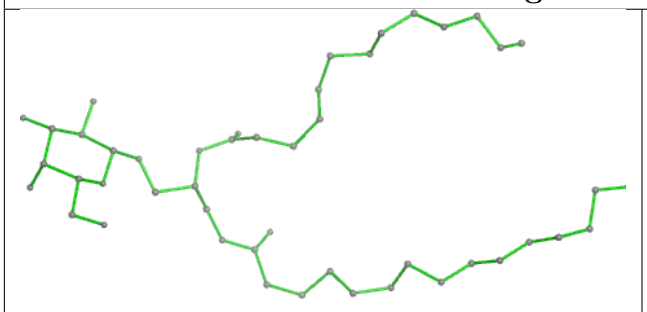


Torsions

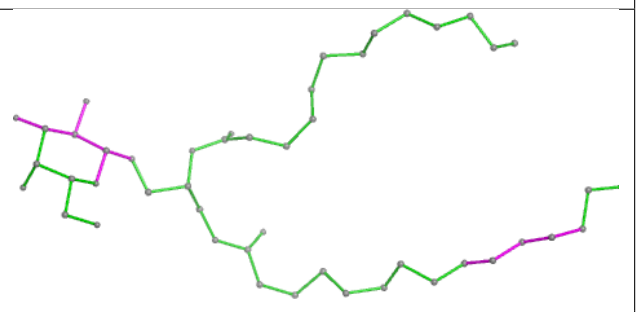


Rings

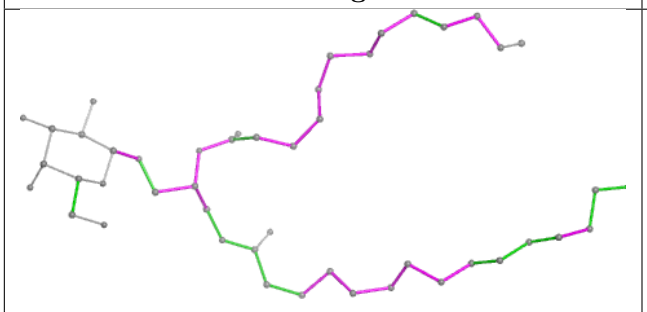
Ligand LMG a 410



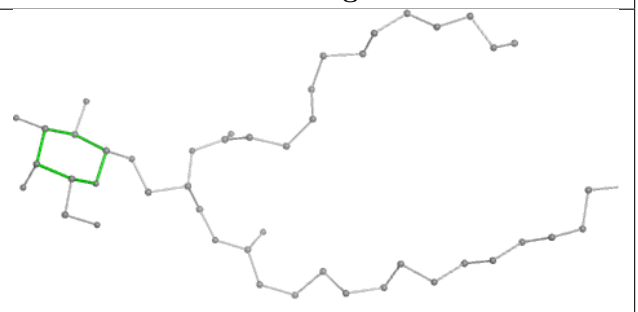
Bond lengths



Bond angles

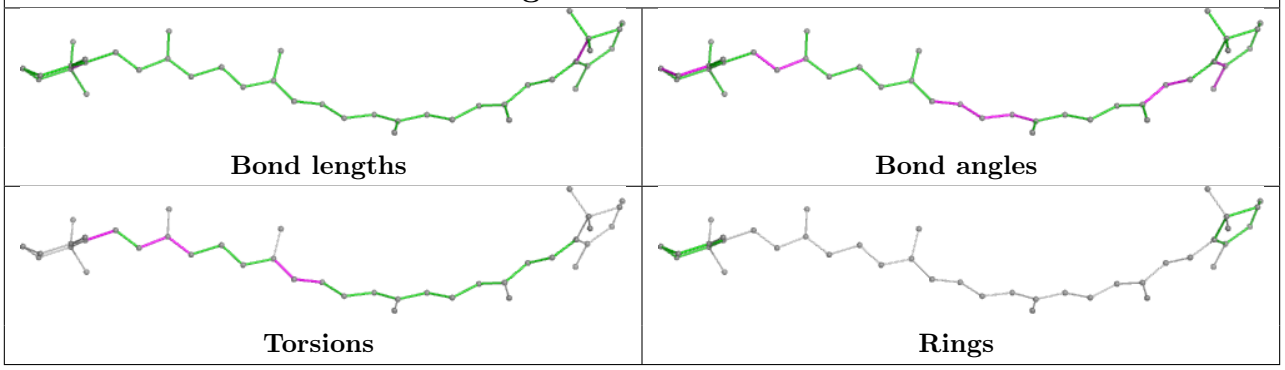


Torsions

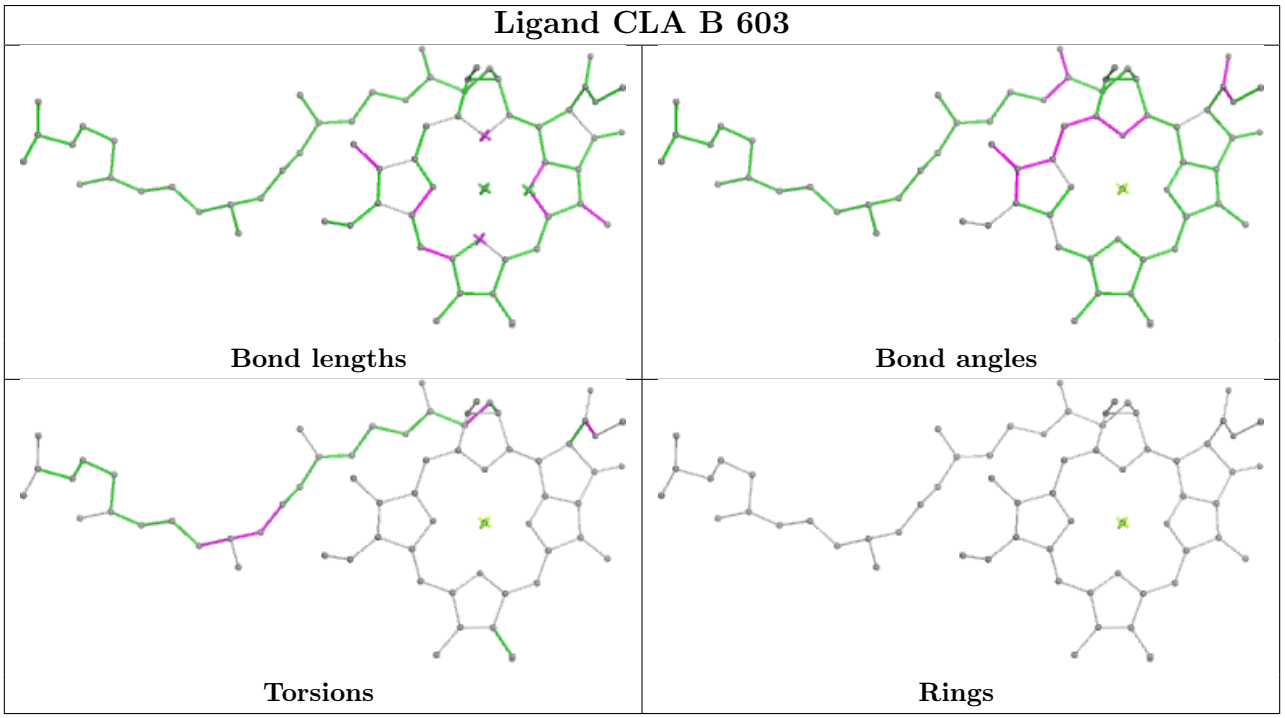


Rings

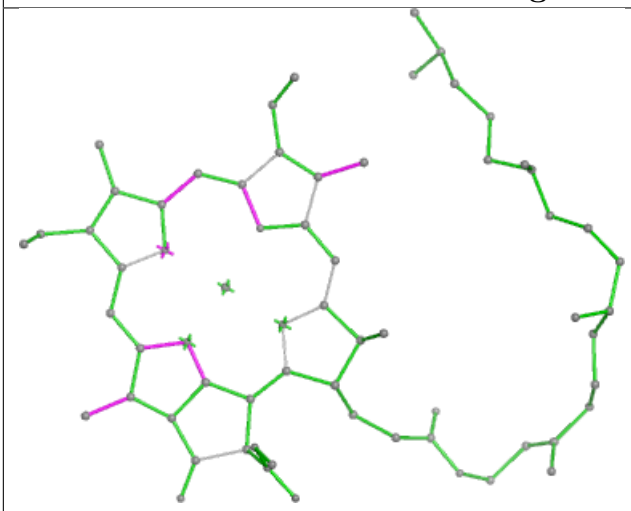
Ligand BCR H 102



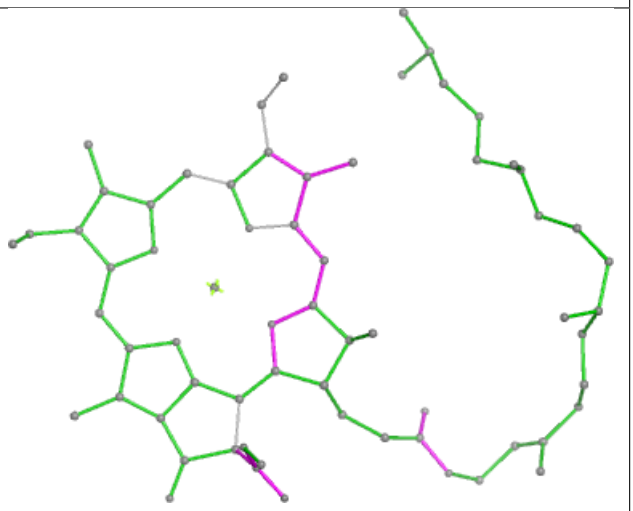
Ligand CLA B 603



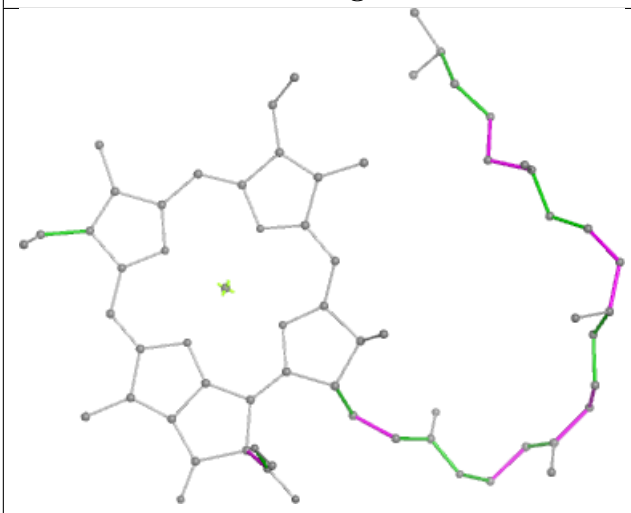
Ligand CLA c 512



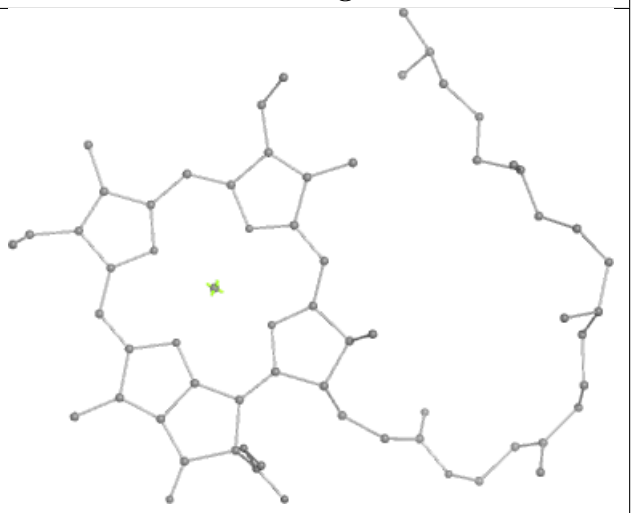
Bond lengths



Bond angles

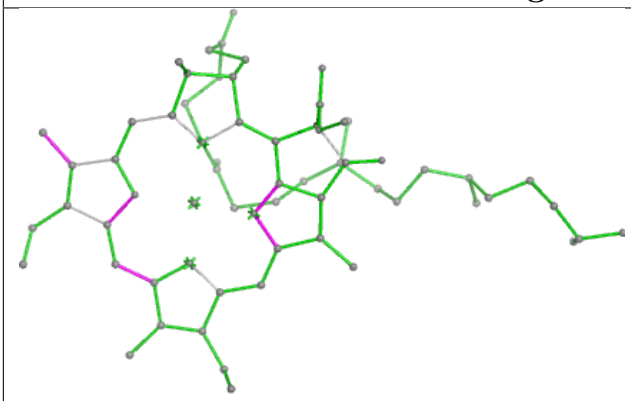


Torsions

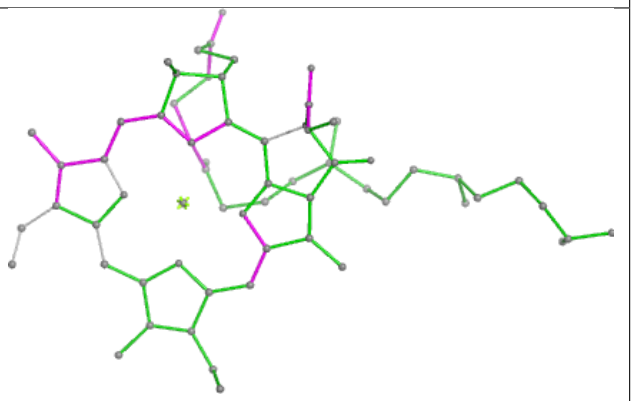


Rings

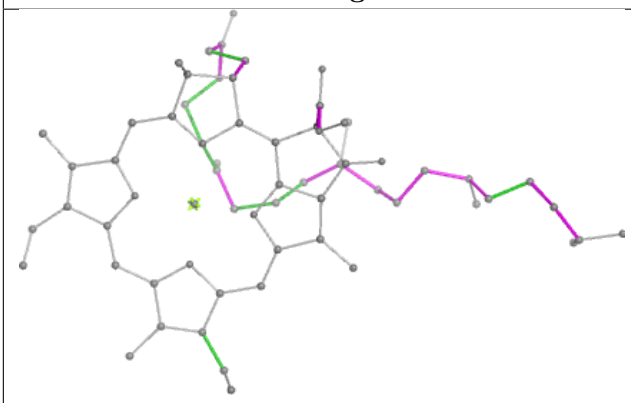
Ligand CLA b 602



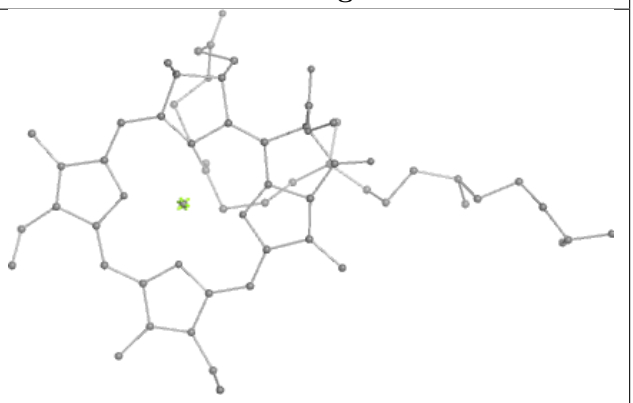
Bond lengths



Bond angles

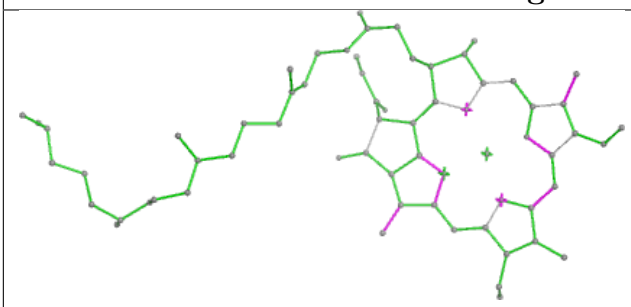


Torsions

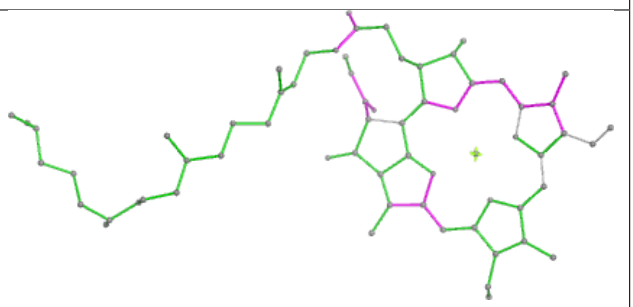


Rings

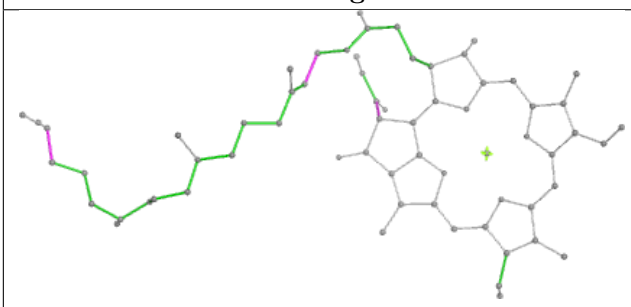
Ligand CLA b 603



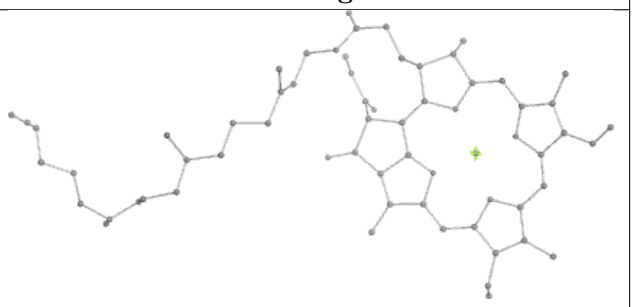
Bond lengths



Bond angles

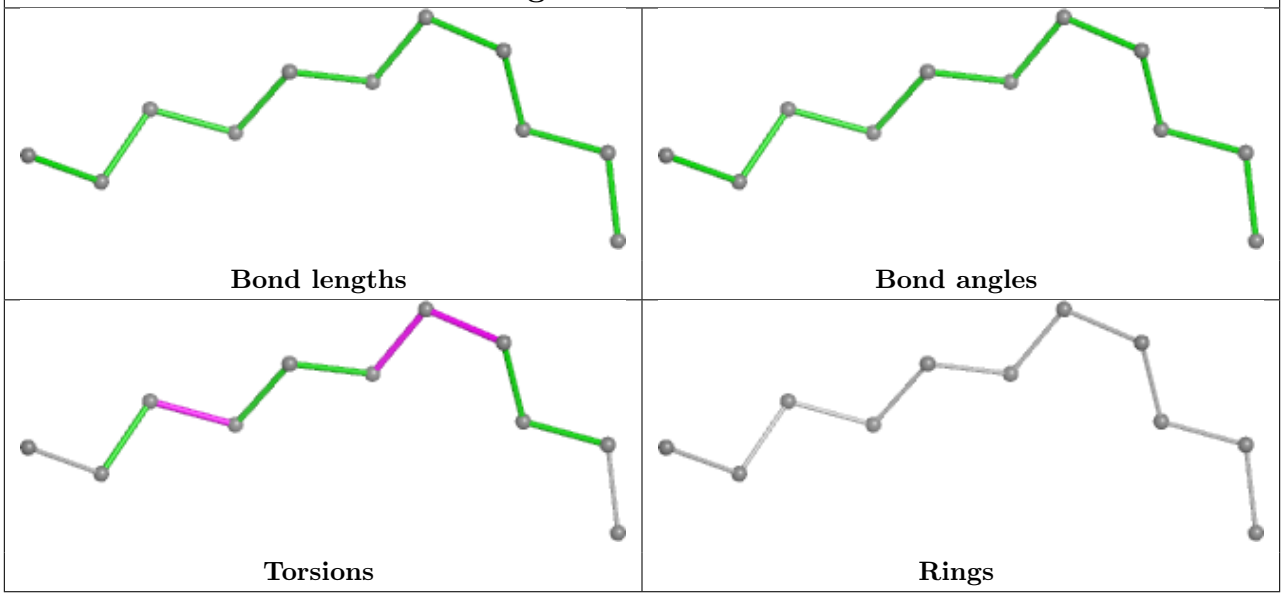


Torsions

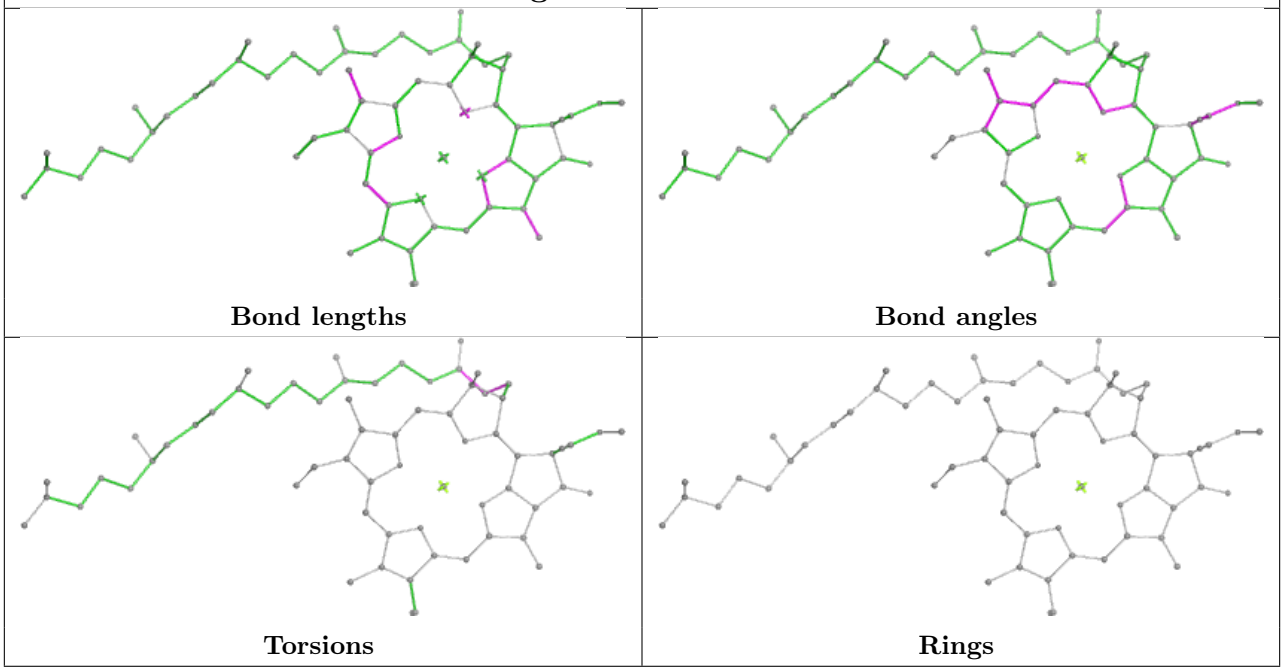


Rings

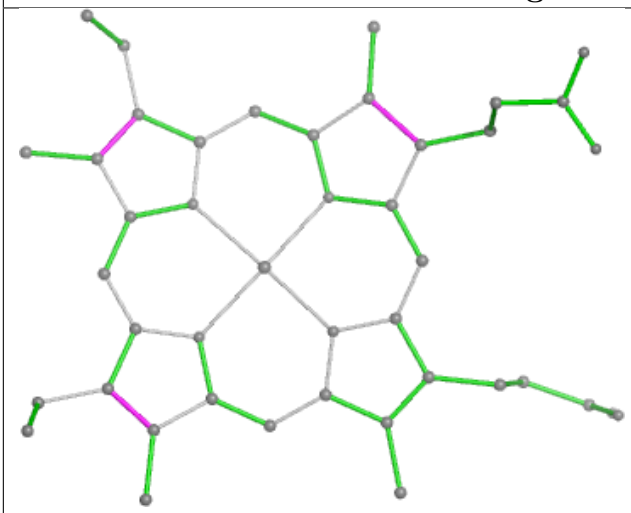
Ligand STE A 415



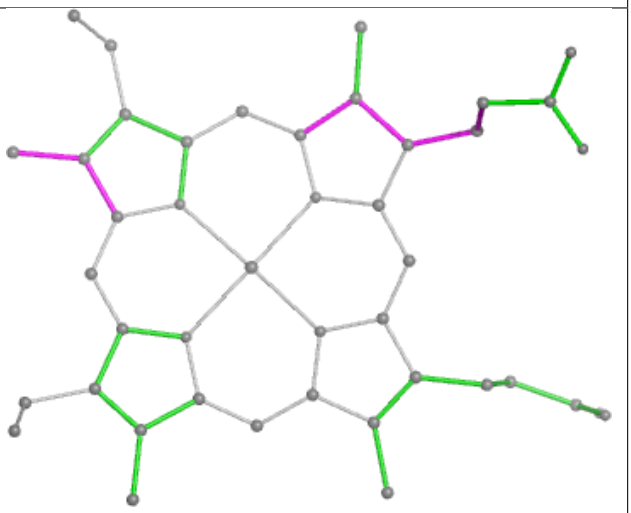
Ligand CLA c 501



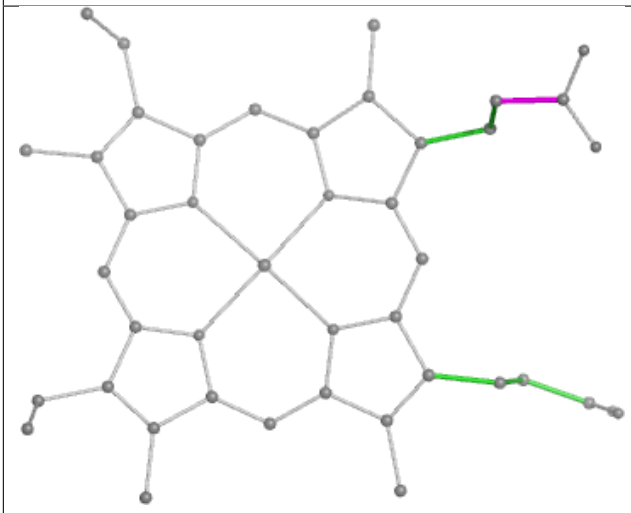
Ligand HEC v 201



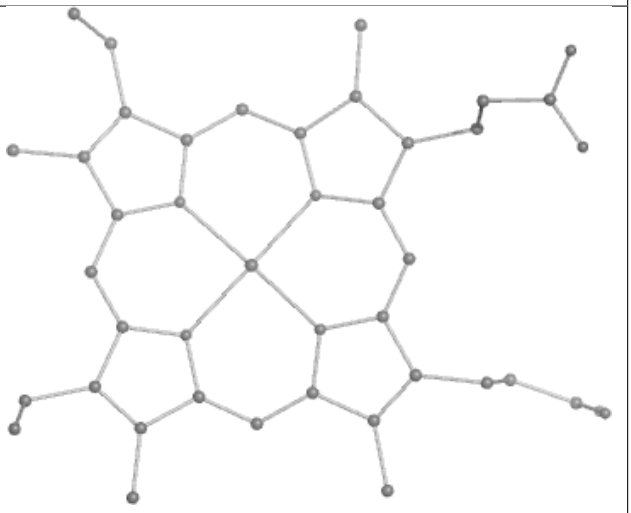
Bond lengths



Bond angles

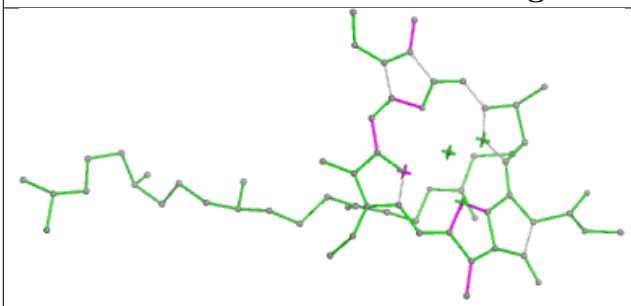


Torsions

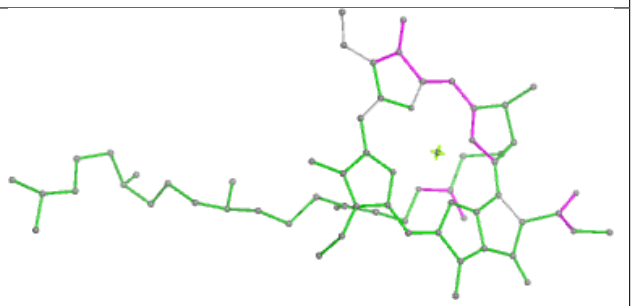


Rings

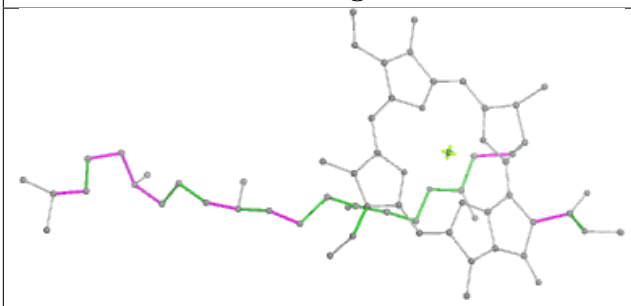
Ligand CLA b 615



Bond lengths



Bond angles



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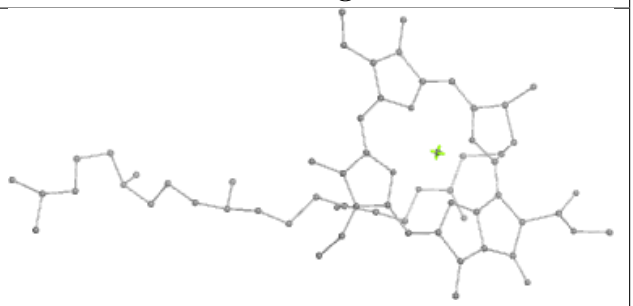
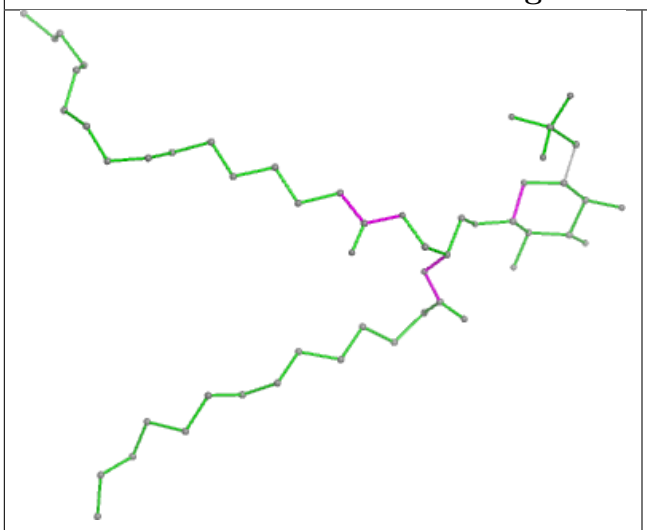
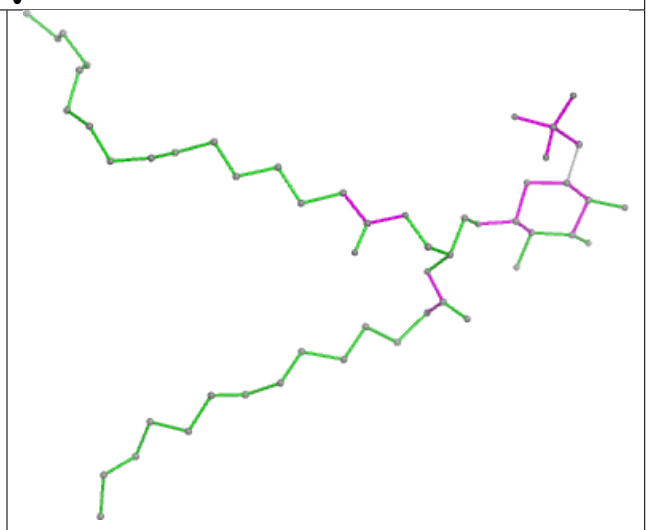


Rings

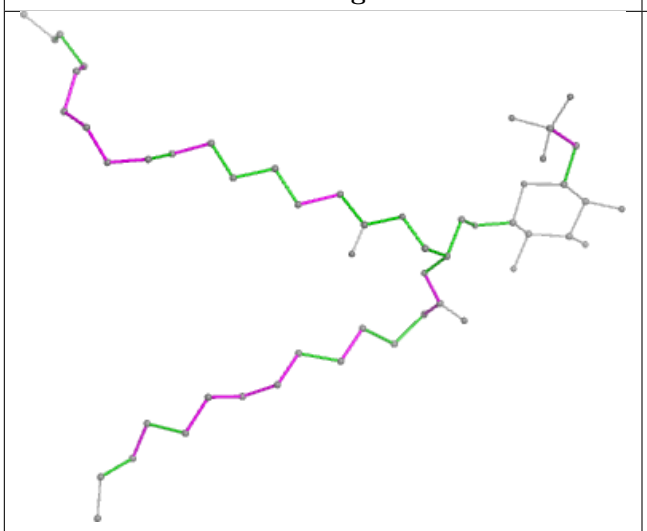
Ligand SQD A 411



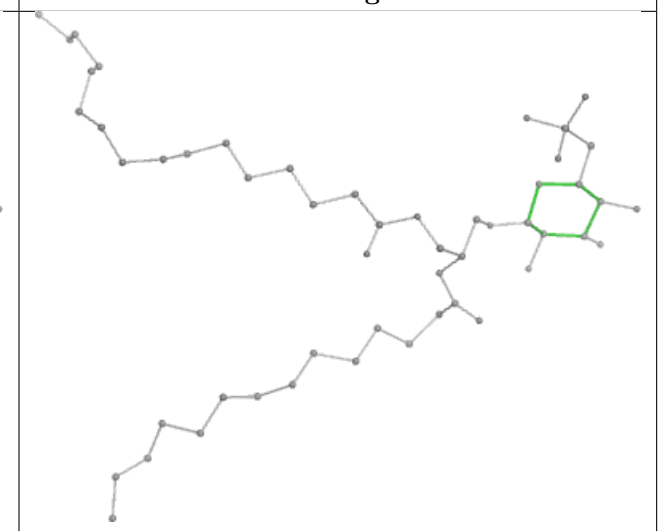
Bond lengths



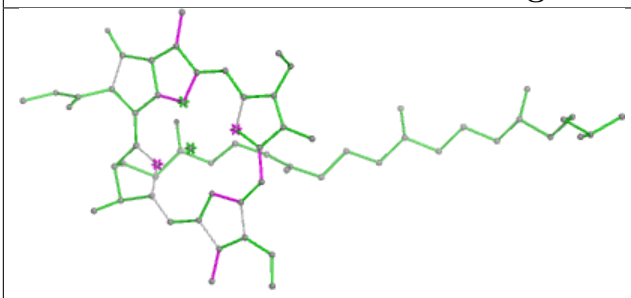
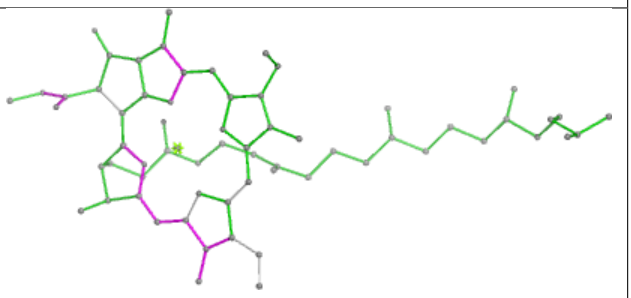
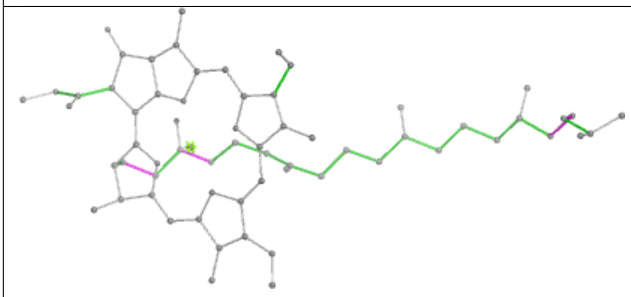
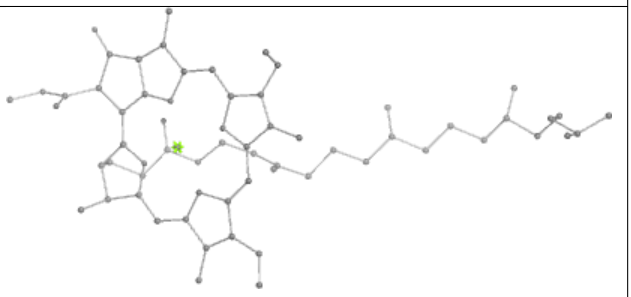
Bond angles

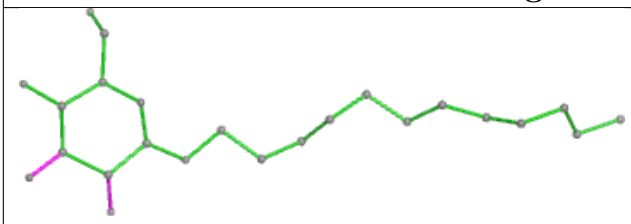
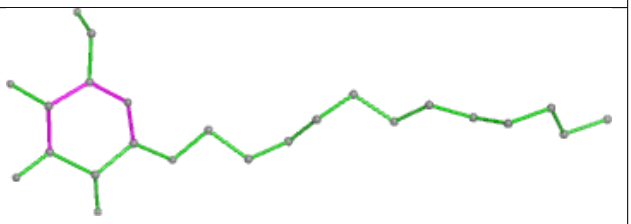
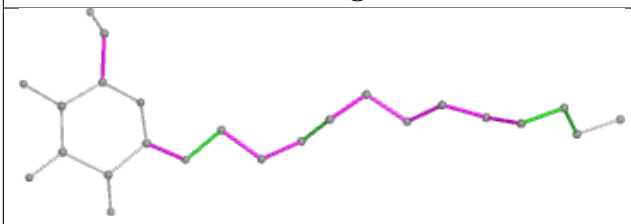


Torsions

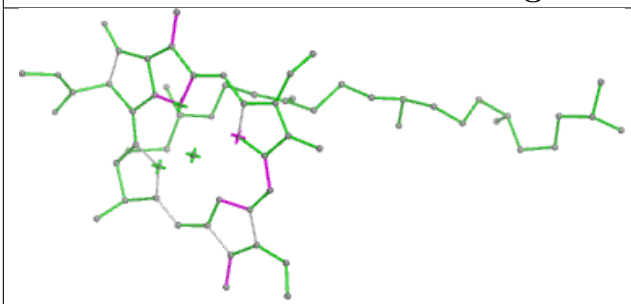


Rings

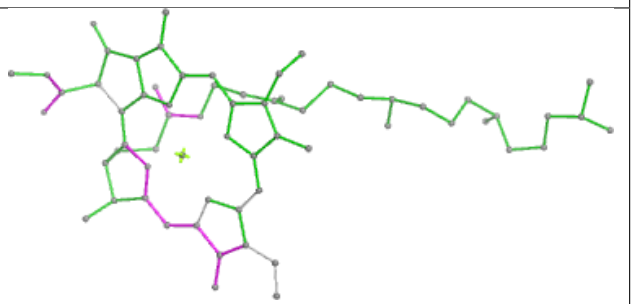
Ligand CLA b 609	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LMT J 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

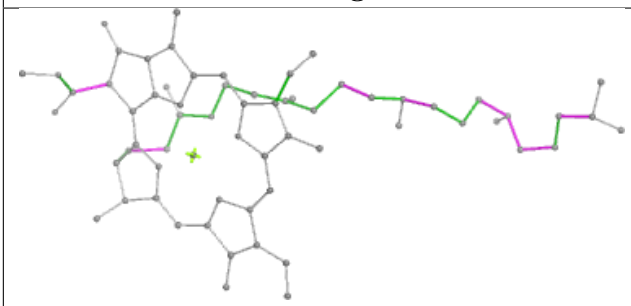
Ligand CLA B 614



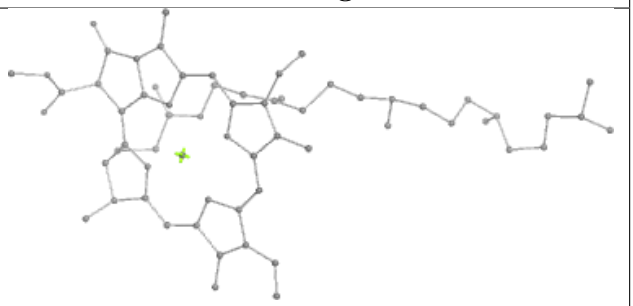
Bond lengths



Bond angles

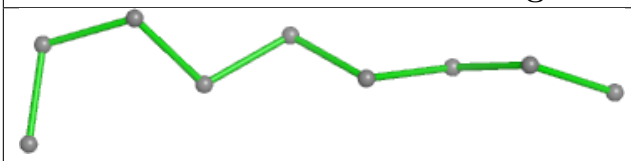


Torsions

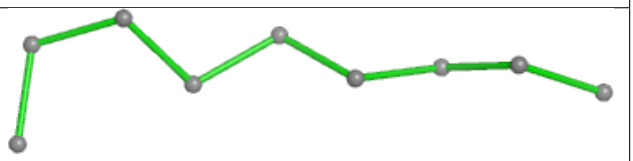


Rings

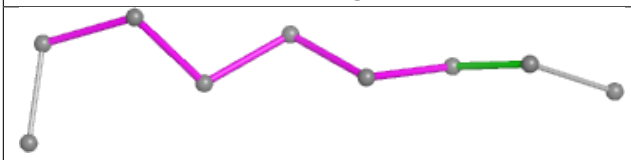
Ligand STE A 409



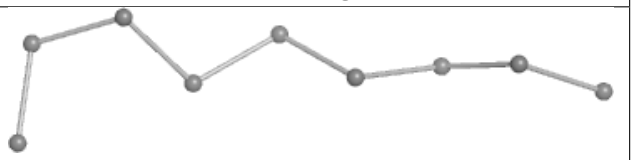
Bond lengths



Bond angles

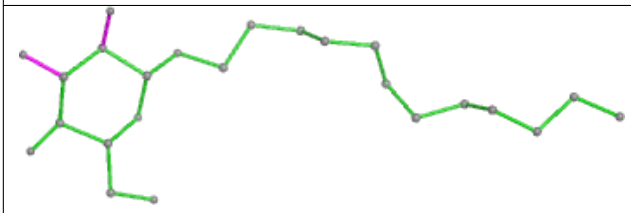


Torsions

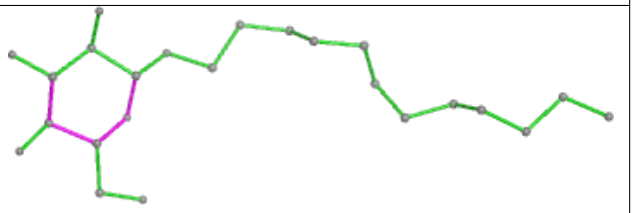


Rings

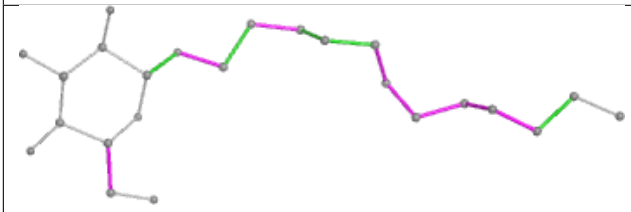
Ligand LMT E 104



Bond lengths



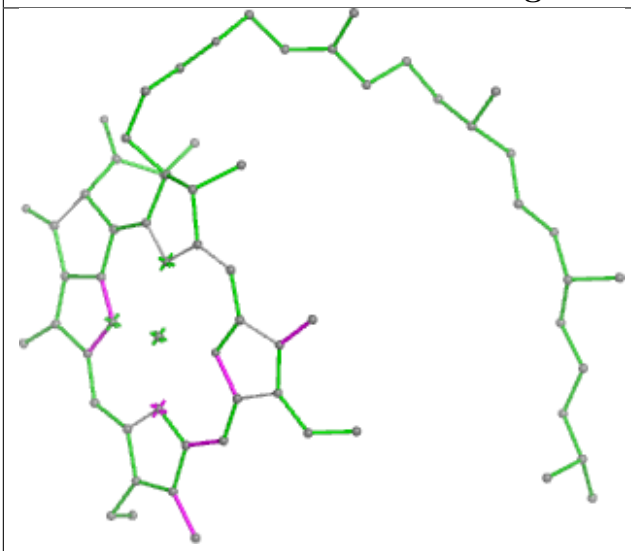
Bond angles



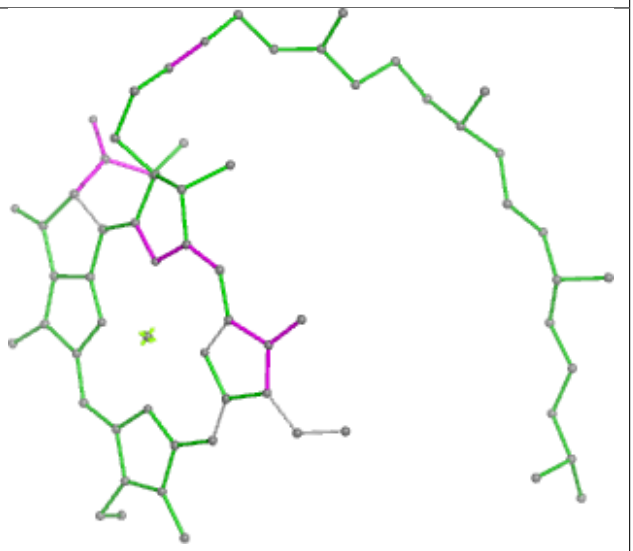
Torsions

Rings

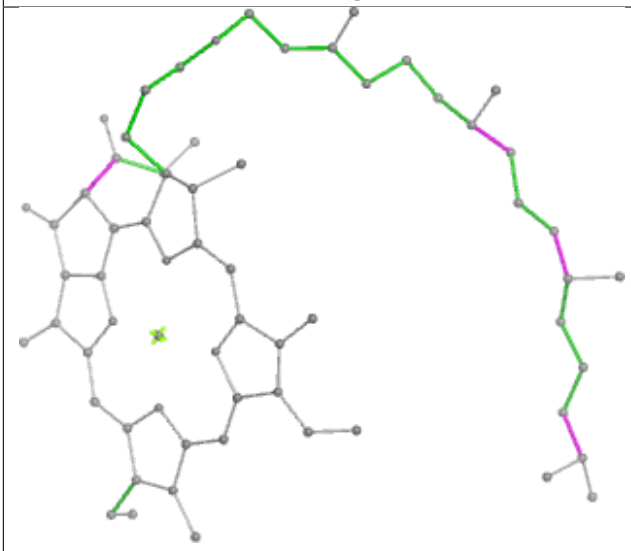
Ligand CLA C 507



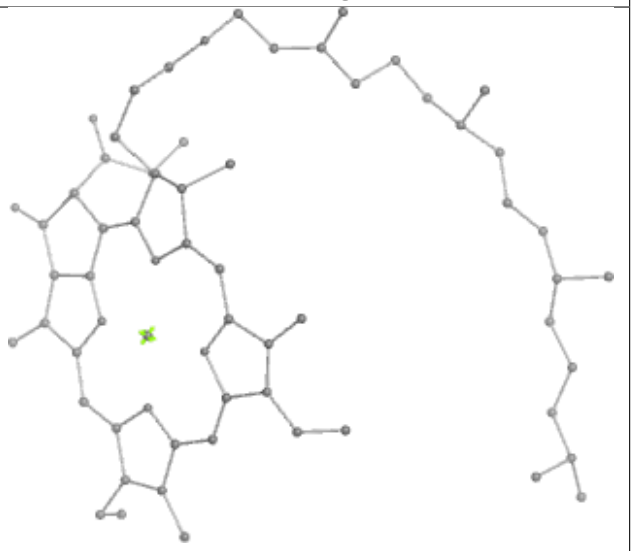
Bond lengths



Bond angles

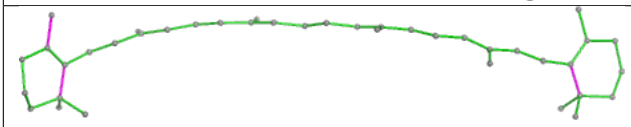


Torsions

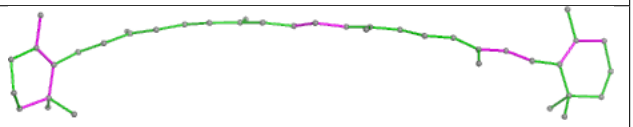


Rings

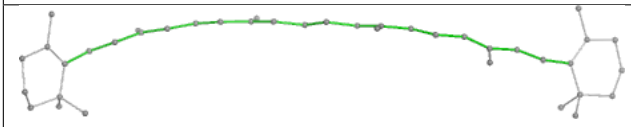
Ligand BCR K 101



Bond lengths



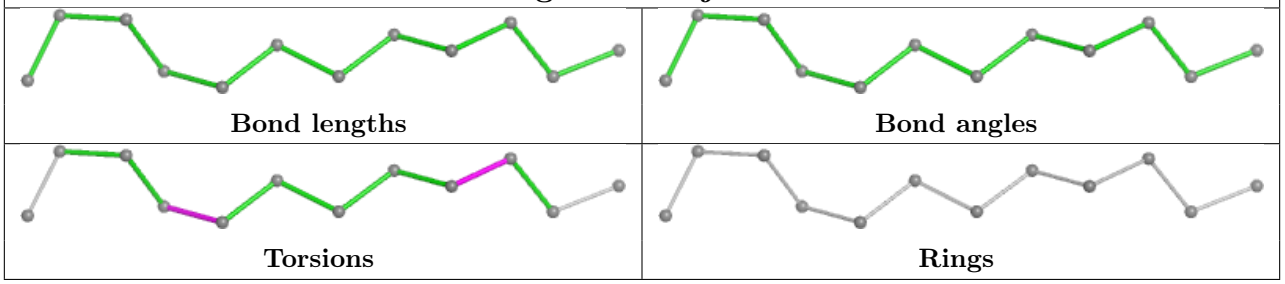
Bond angles



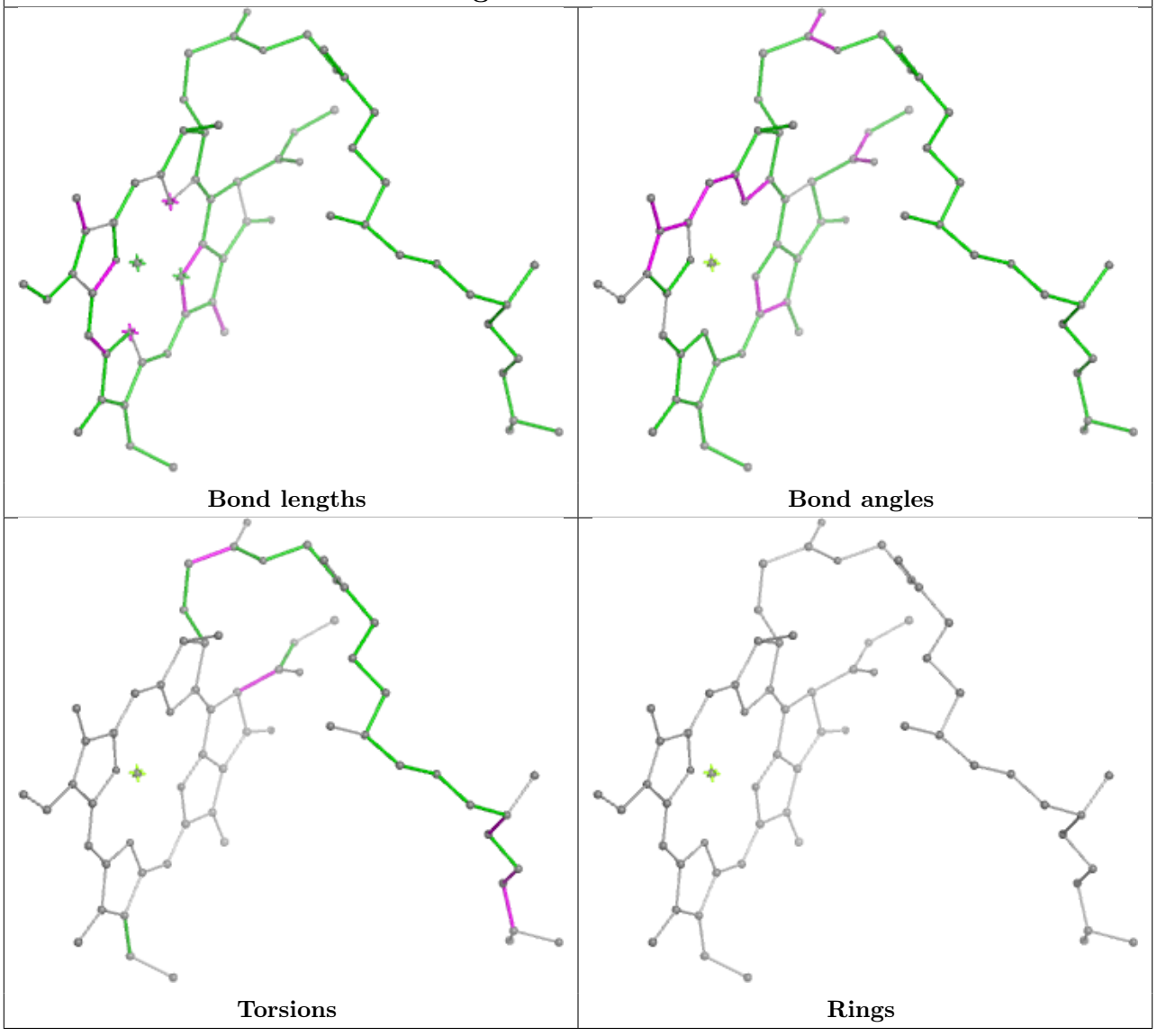
Torsions

Rings

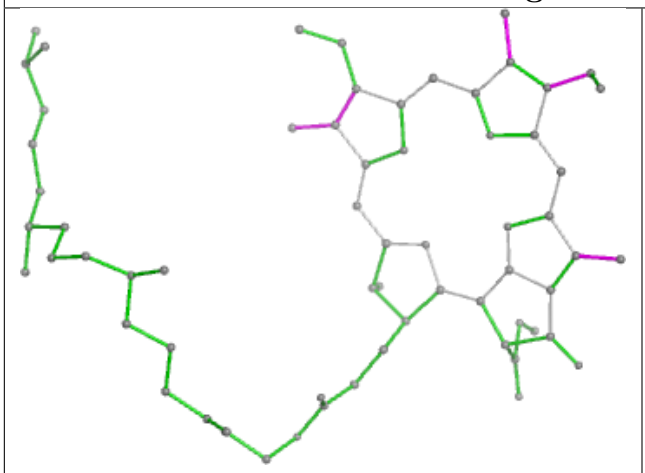
Ligand STE j 101



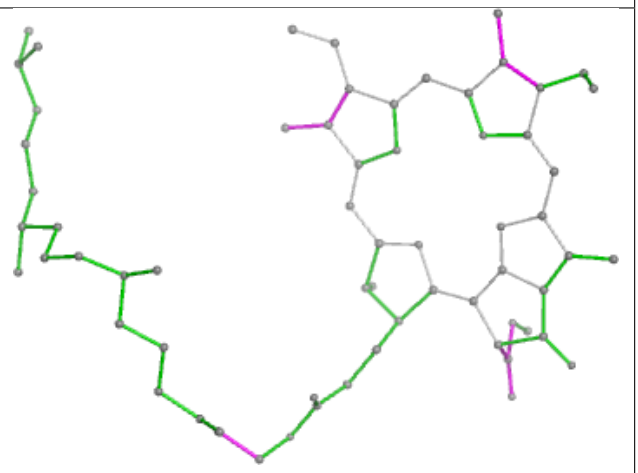
Ligand CLA B 613



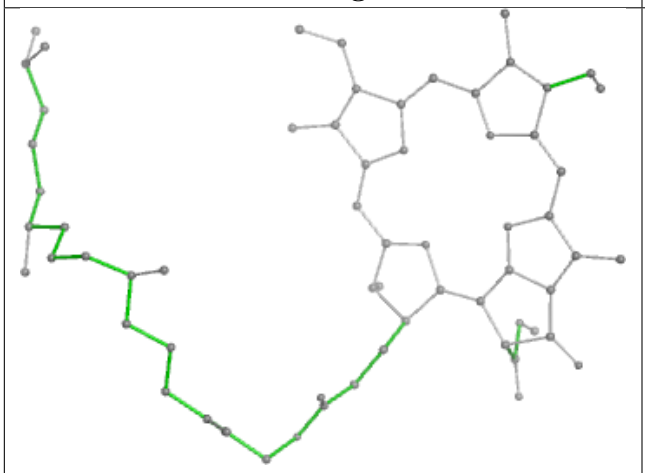
Ligand PHO d 401



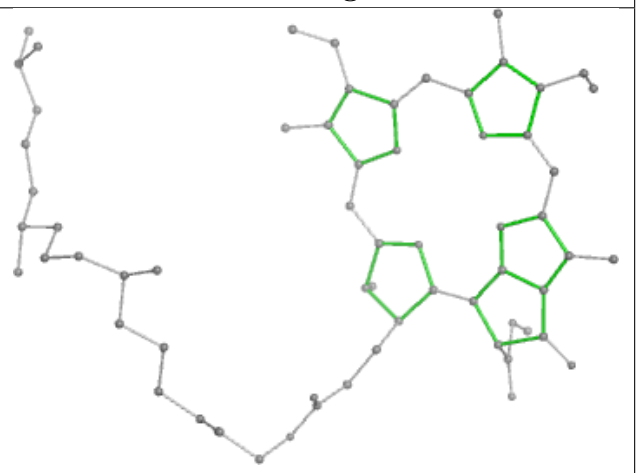
Bond lengths



Bond angles

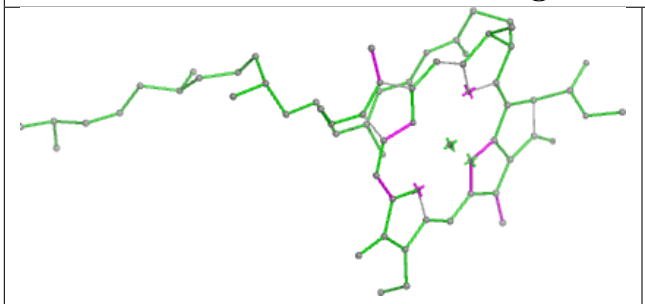


Torsions

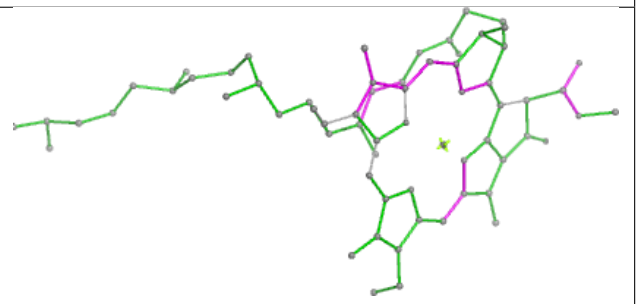


Rings

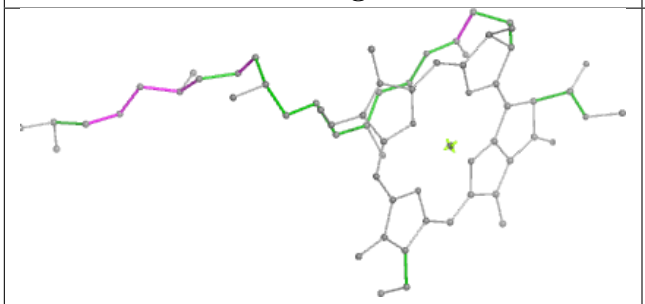
Ligand CLA c 505



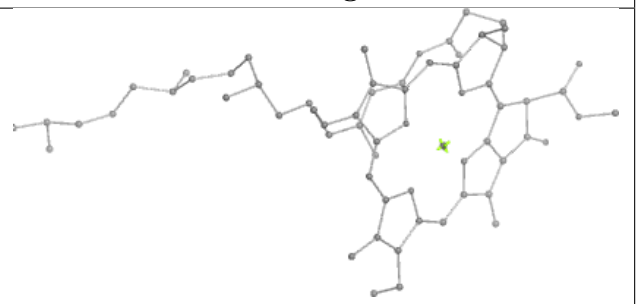
Bond lengths



Bond angles

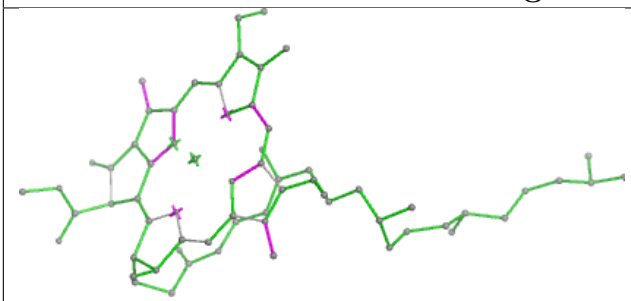


Torsions

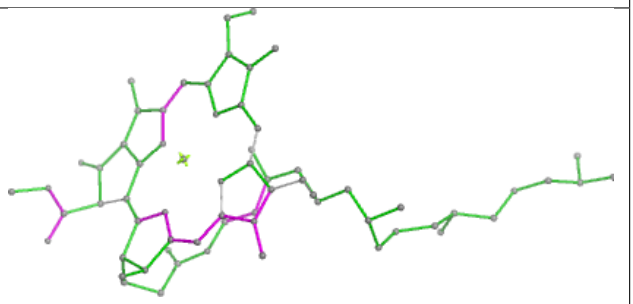


Rings

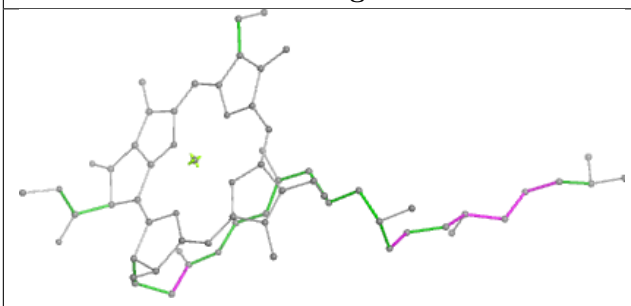
Ligand CLA C 505



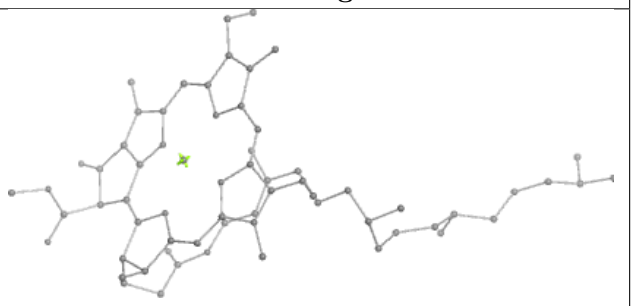
Bond lengths



Bond angles

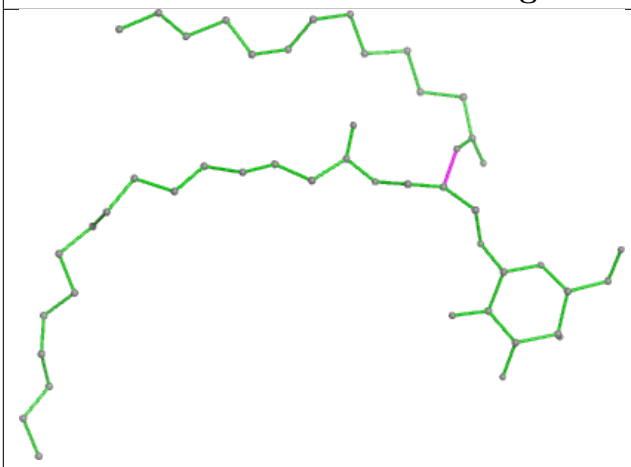


Torsions

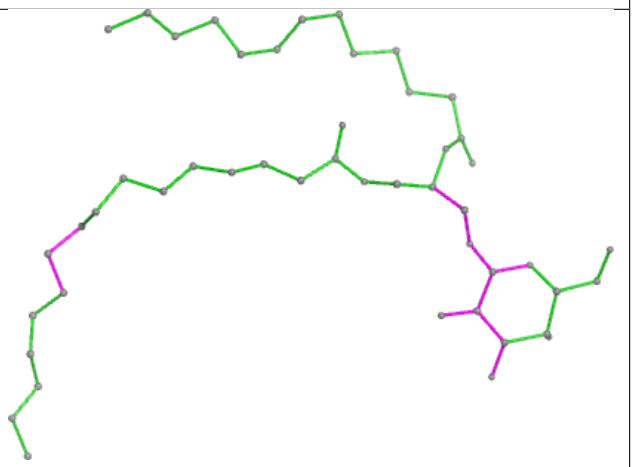


Rings

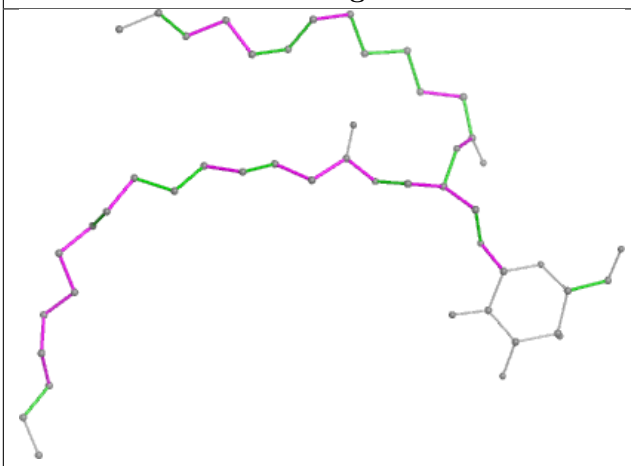
Ligand LMG C 520



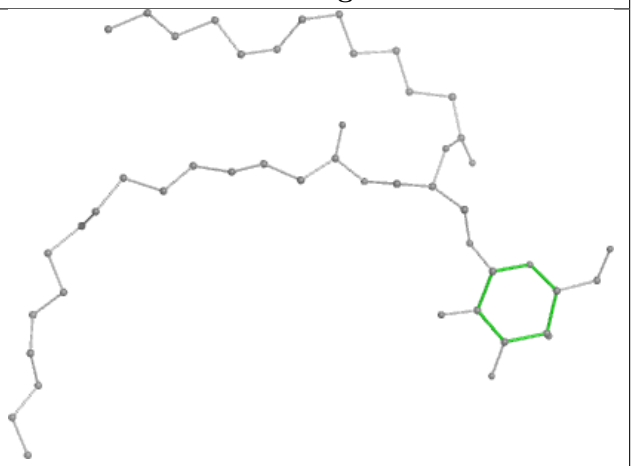
Bond lengths



Bond angles

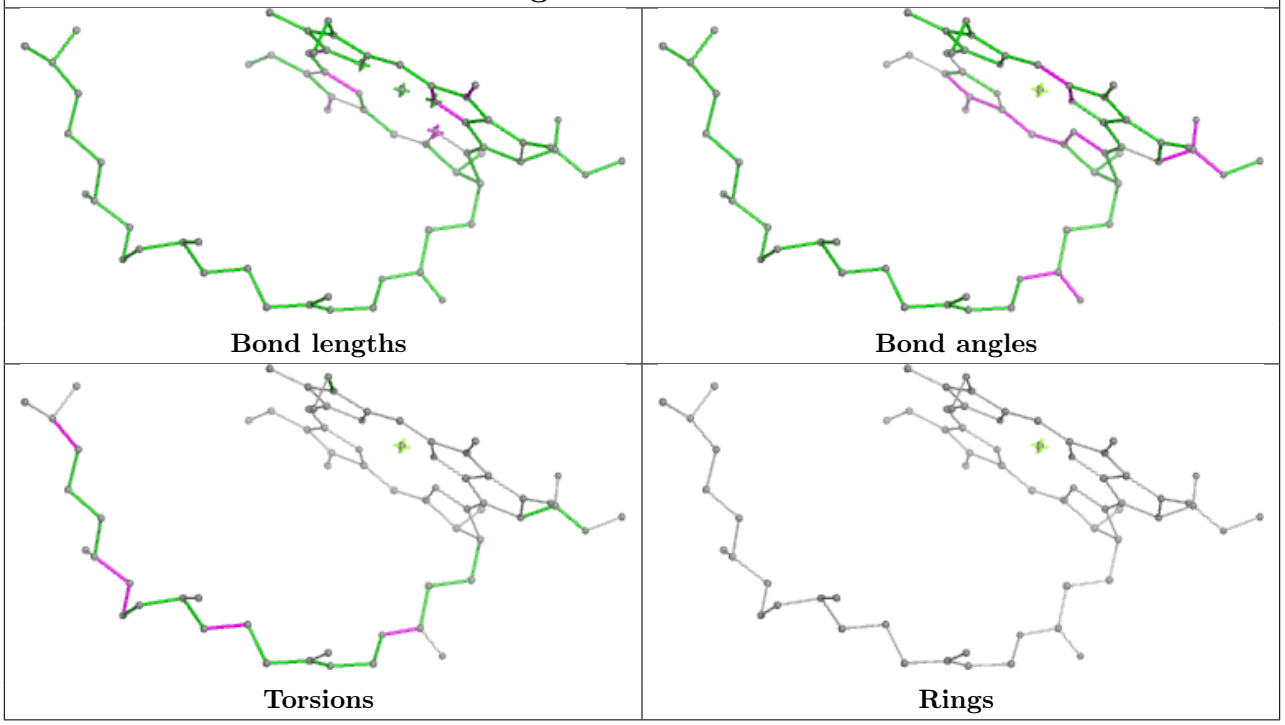


Torsions

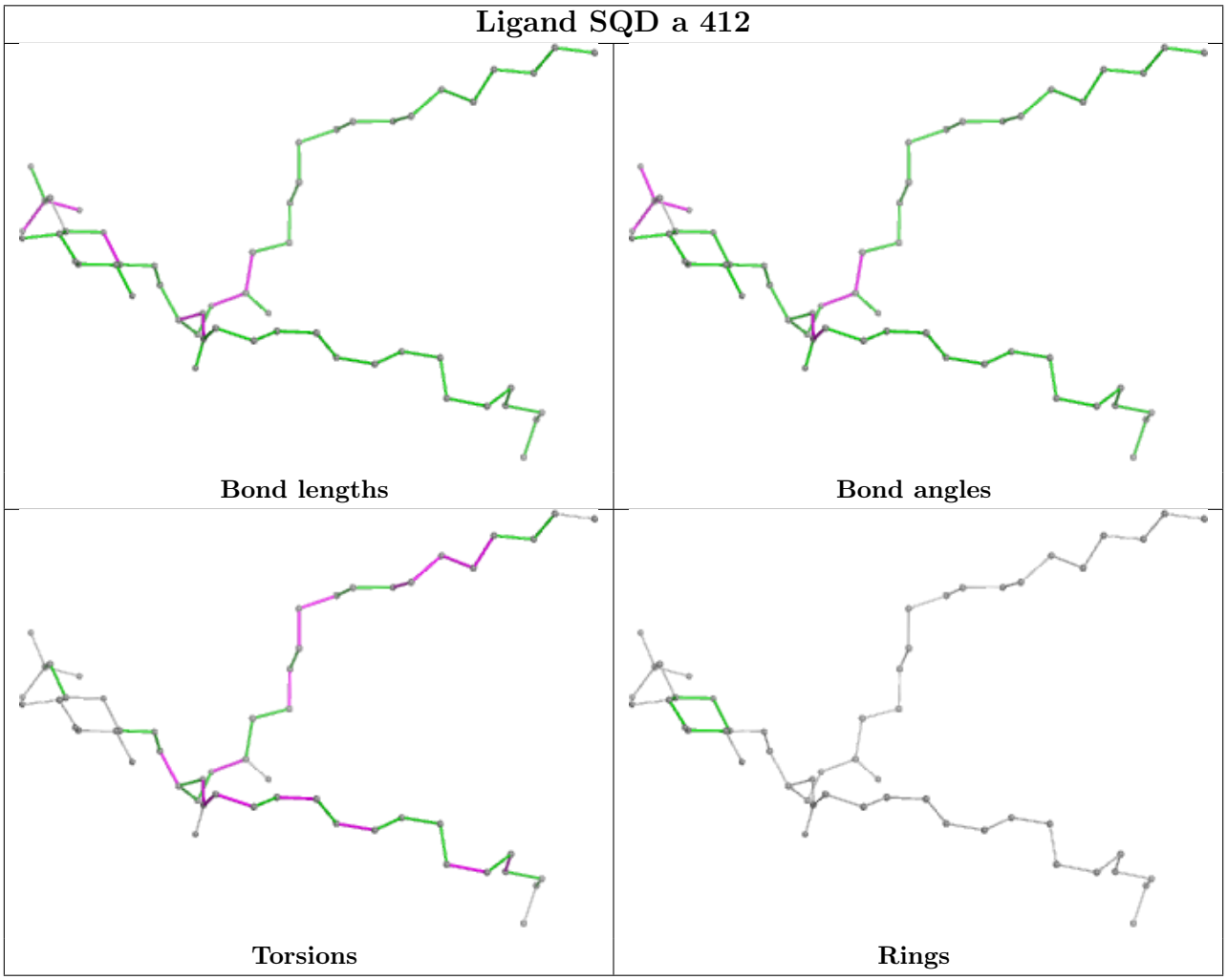


Rings

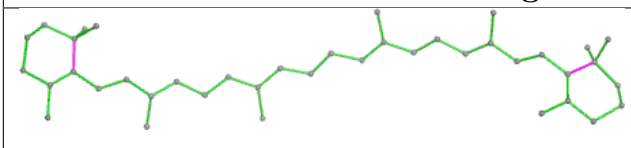
Ligand CLA c 513



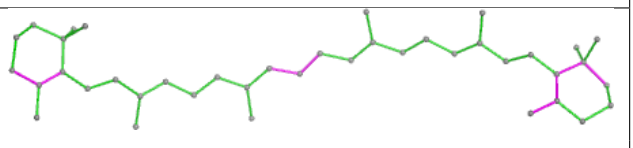
Ligand SQD a 412



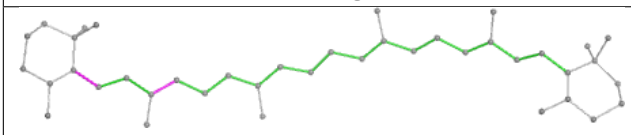
Ligand BCR D 406



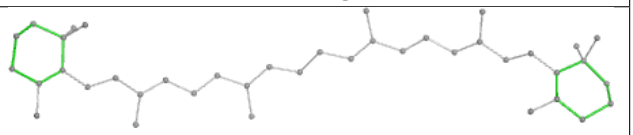
Bond lengths



Bond angles

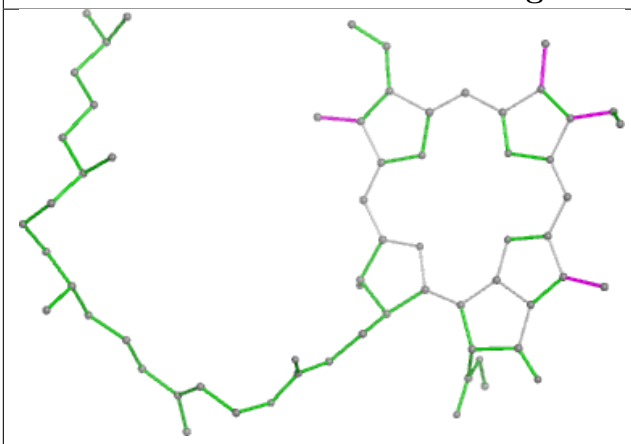


Torsions

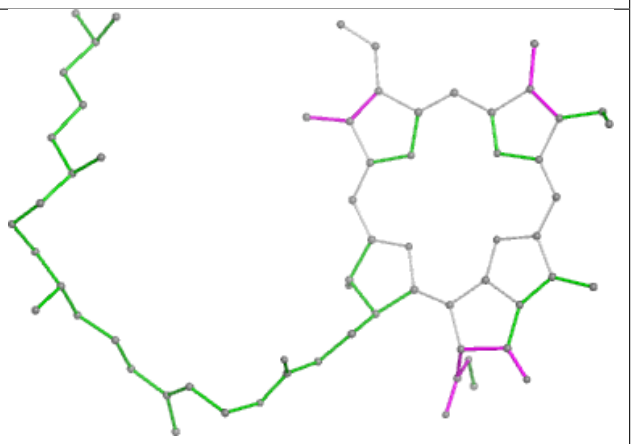


Rings

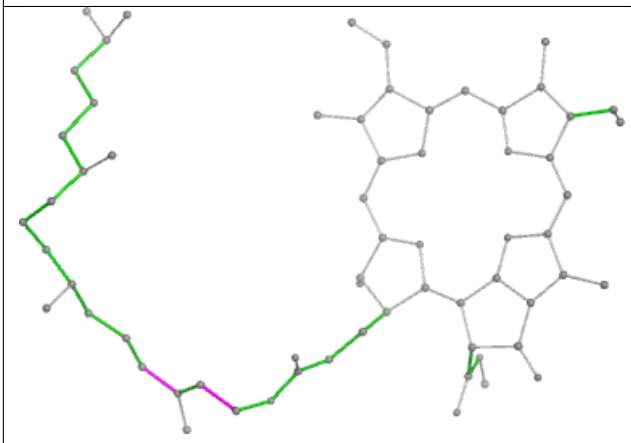
Ligand PHO a 418



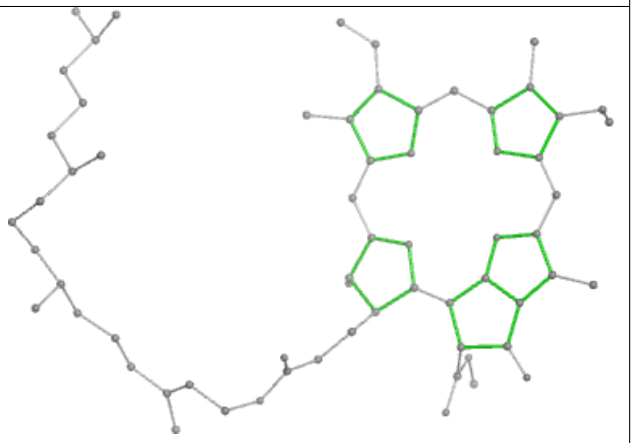
Bond lengths



Bond angles

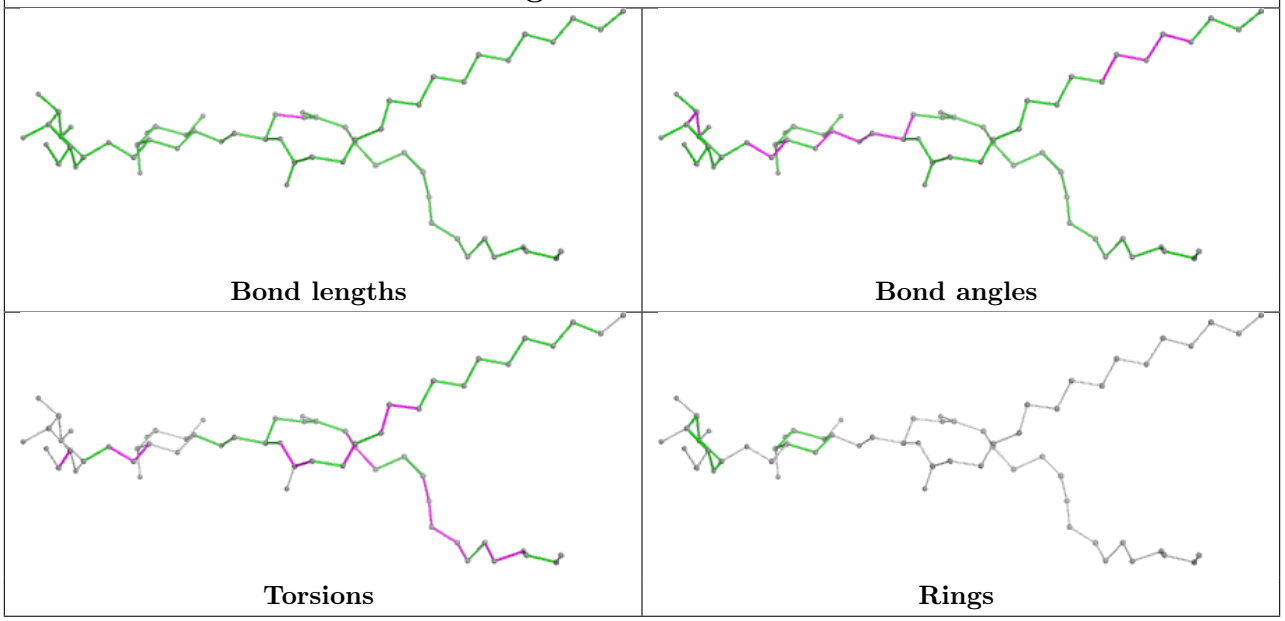


Torsions

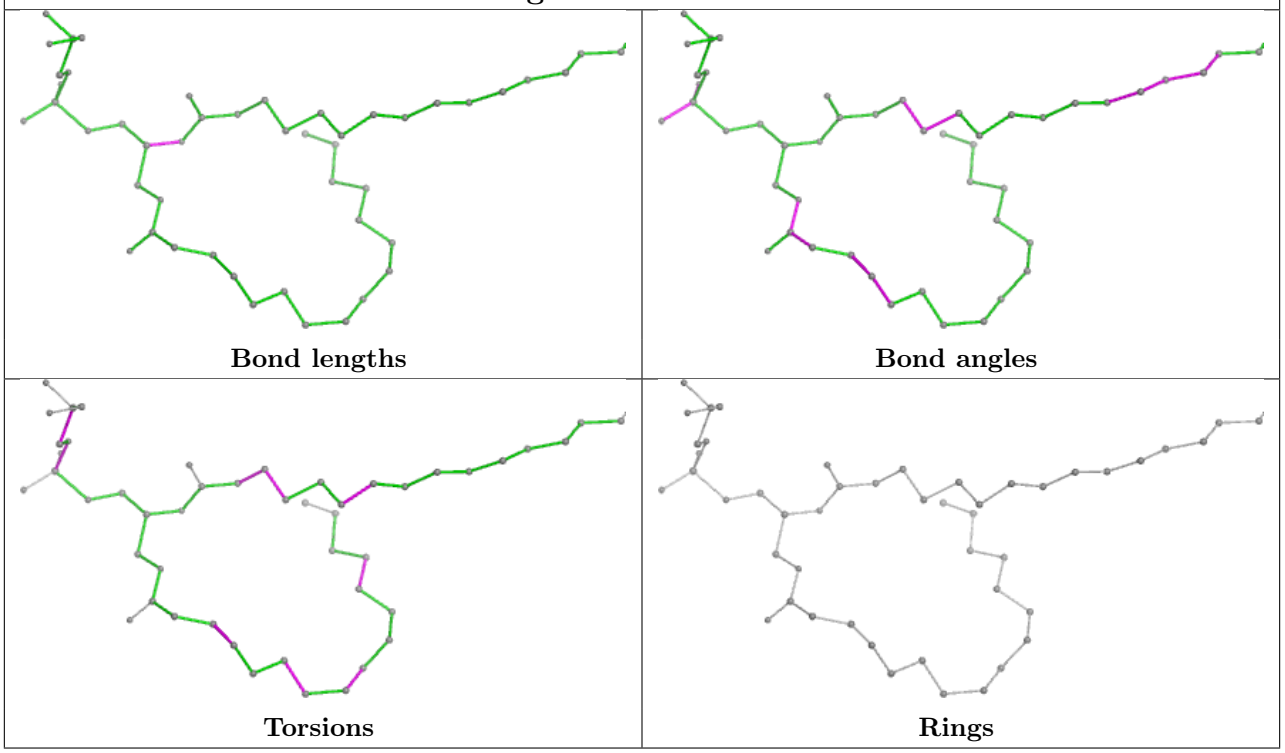


Rings

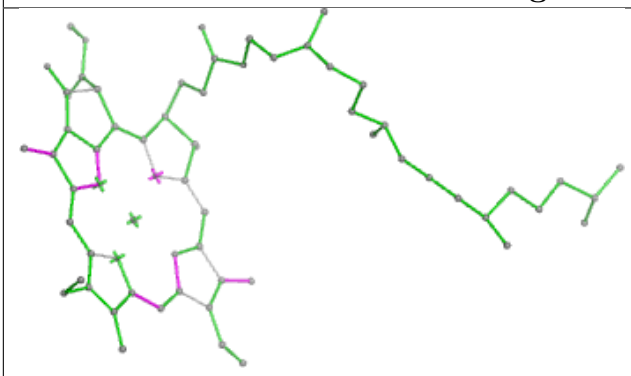
Ligand DGD c 517



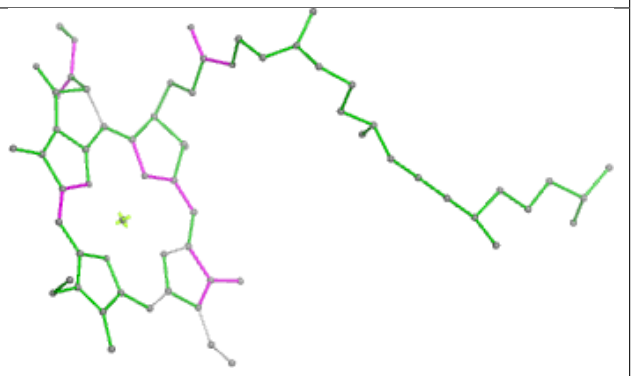
Ligand LHG d 411



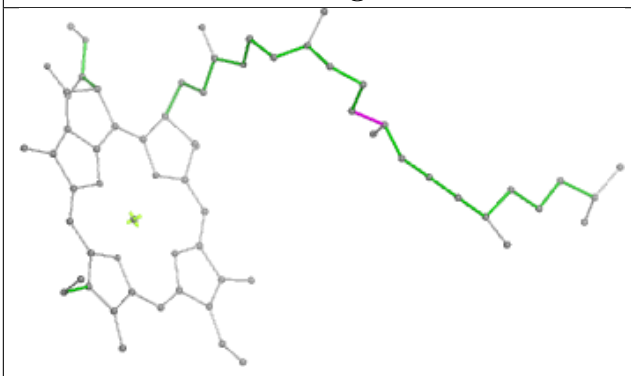
Ligand CLA c 511



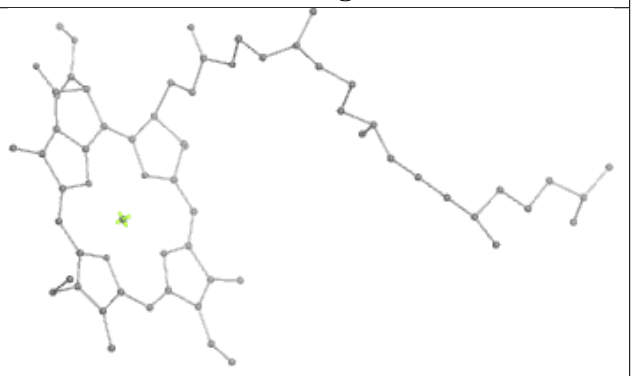
Bond lengths



Bond angles

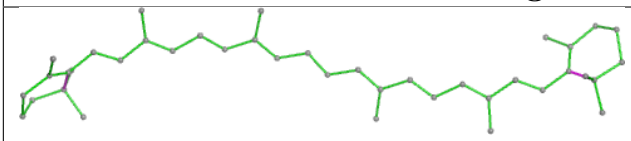


Torsions

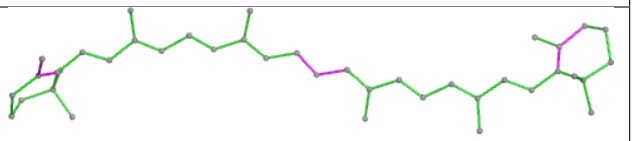


Rings

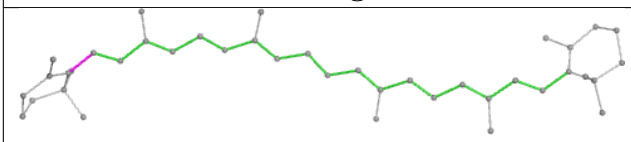
Ligand BCR k 103



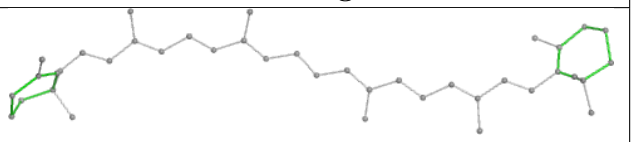
Bond lengths



Bond angles

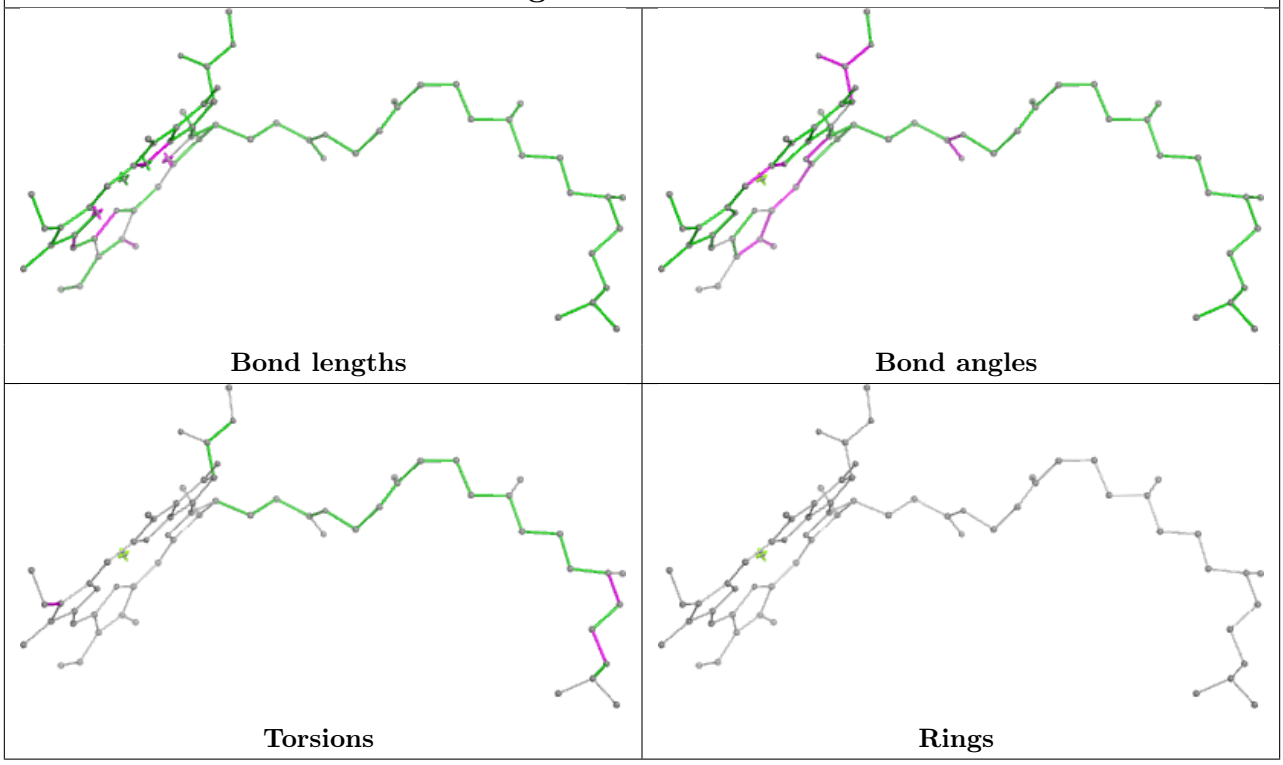


Torsions

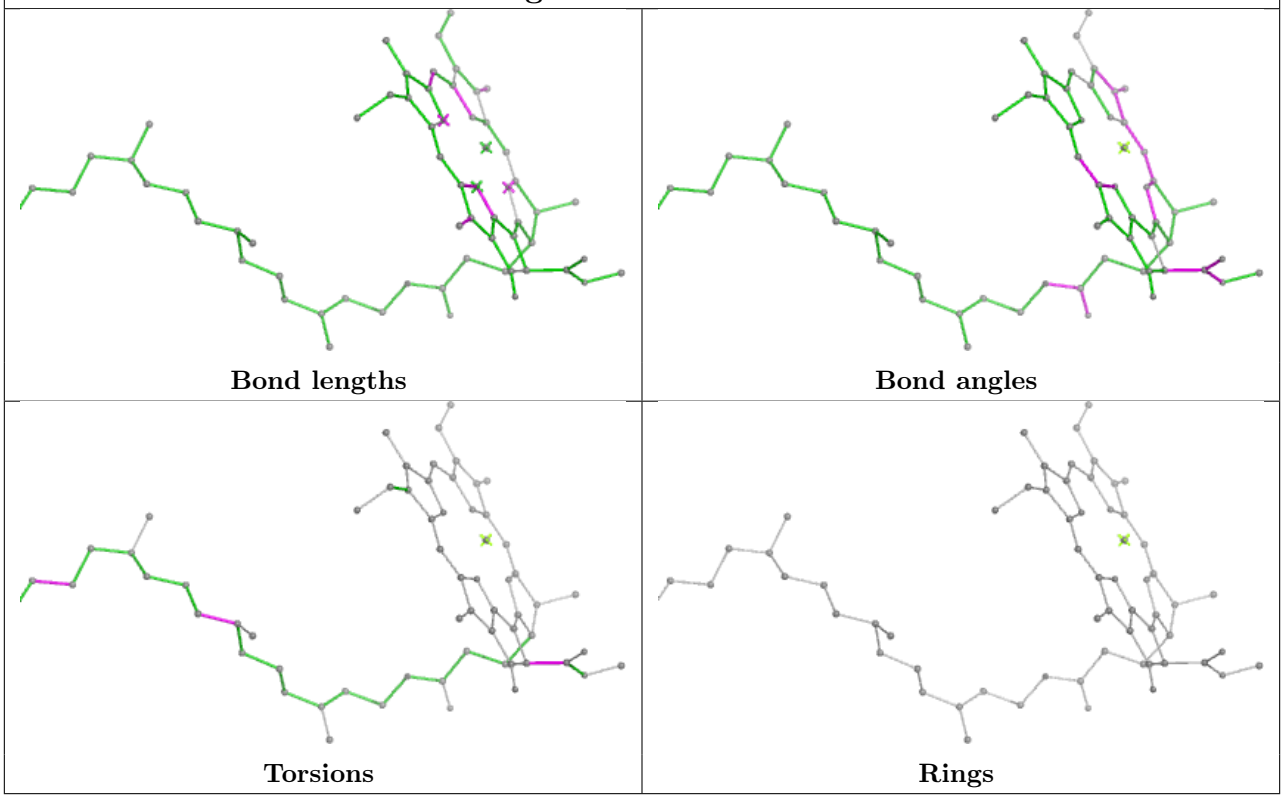


Rings

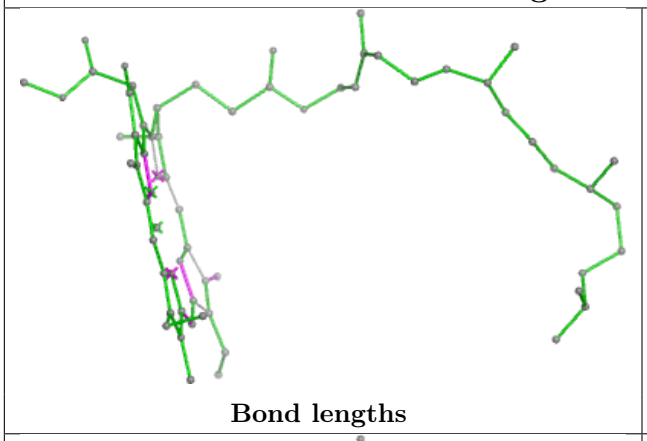
Ligand CLA d 404



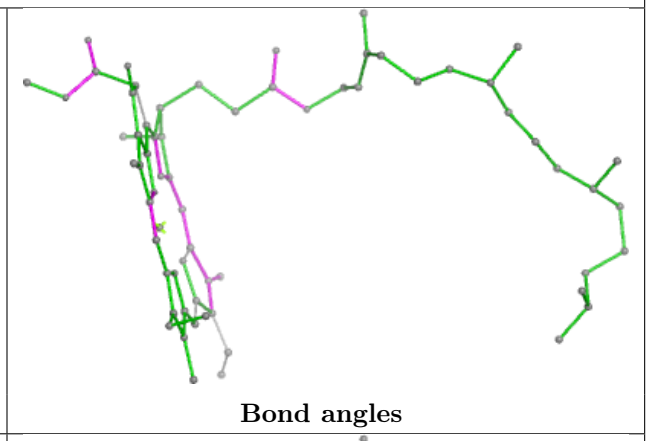
Ligand CLA C 508



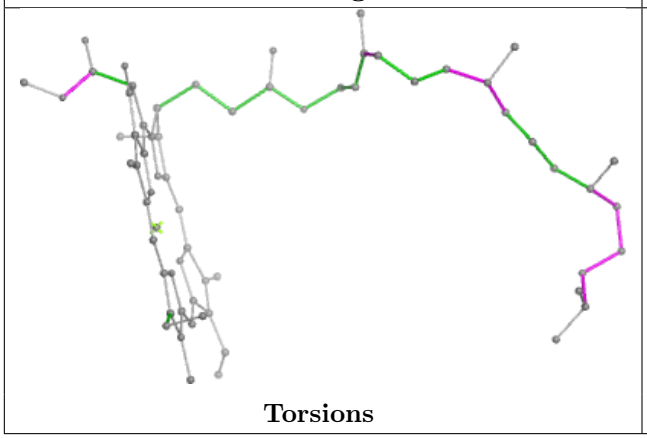
Ligand CLA c 506



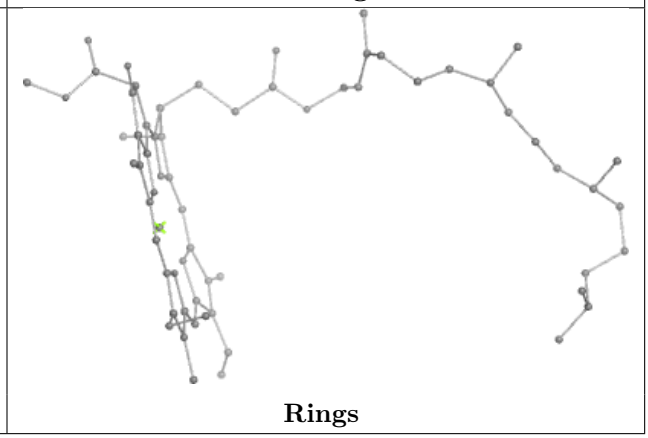
Bond lengths



Bond angles

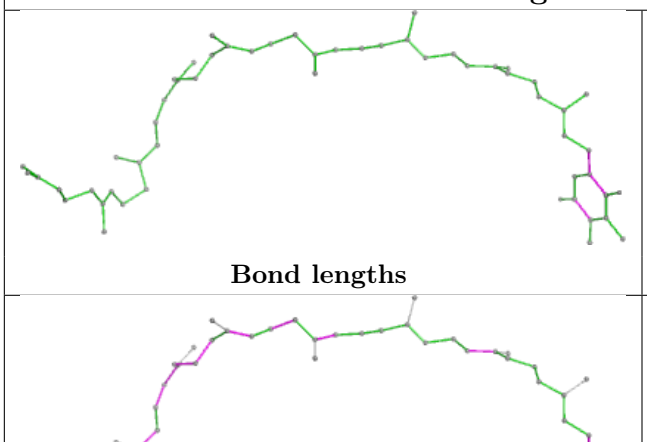


Torsions

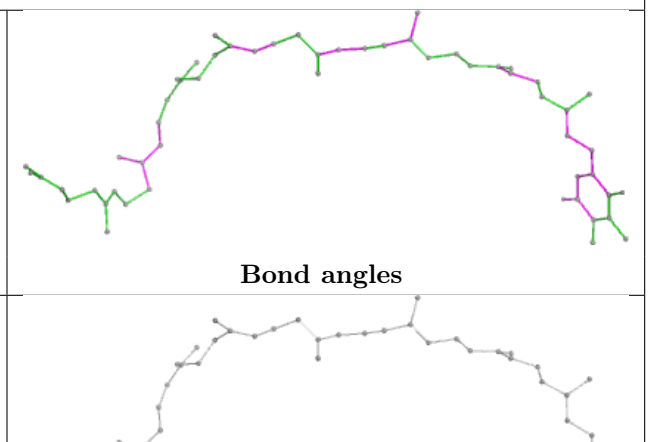


Rings

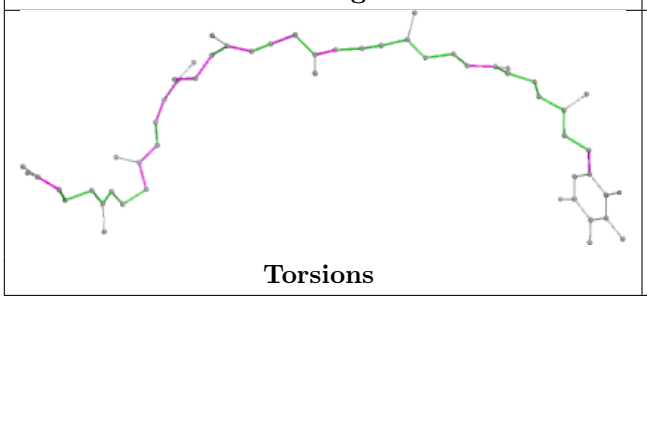
Ligand PL9 A 408



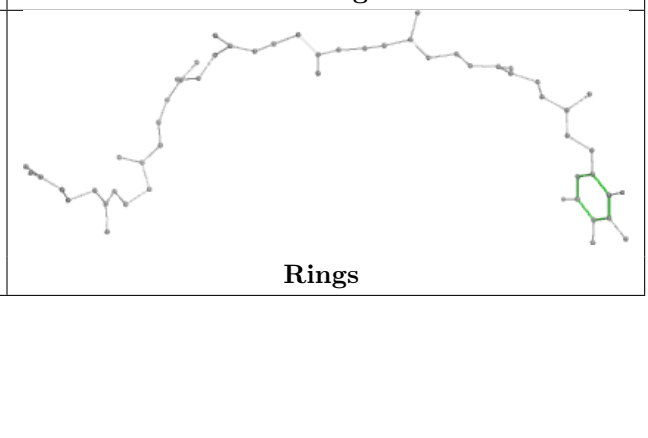
Bond lengths



Bond angles

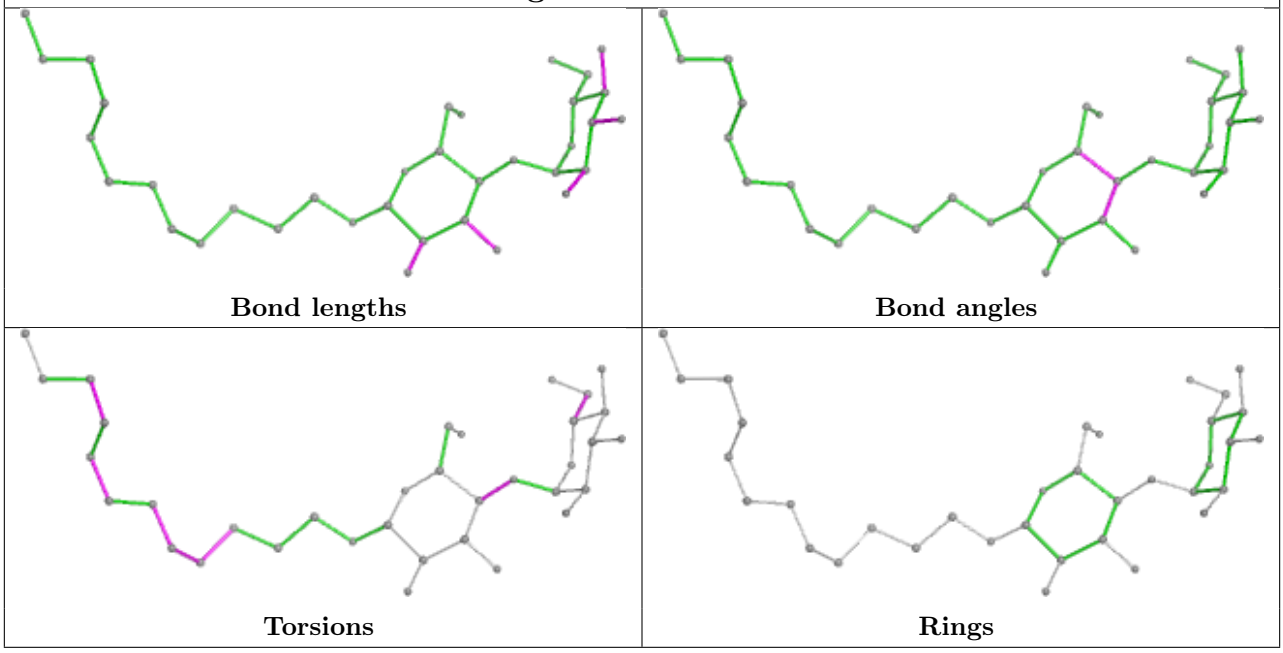


Torsions

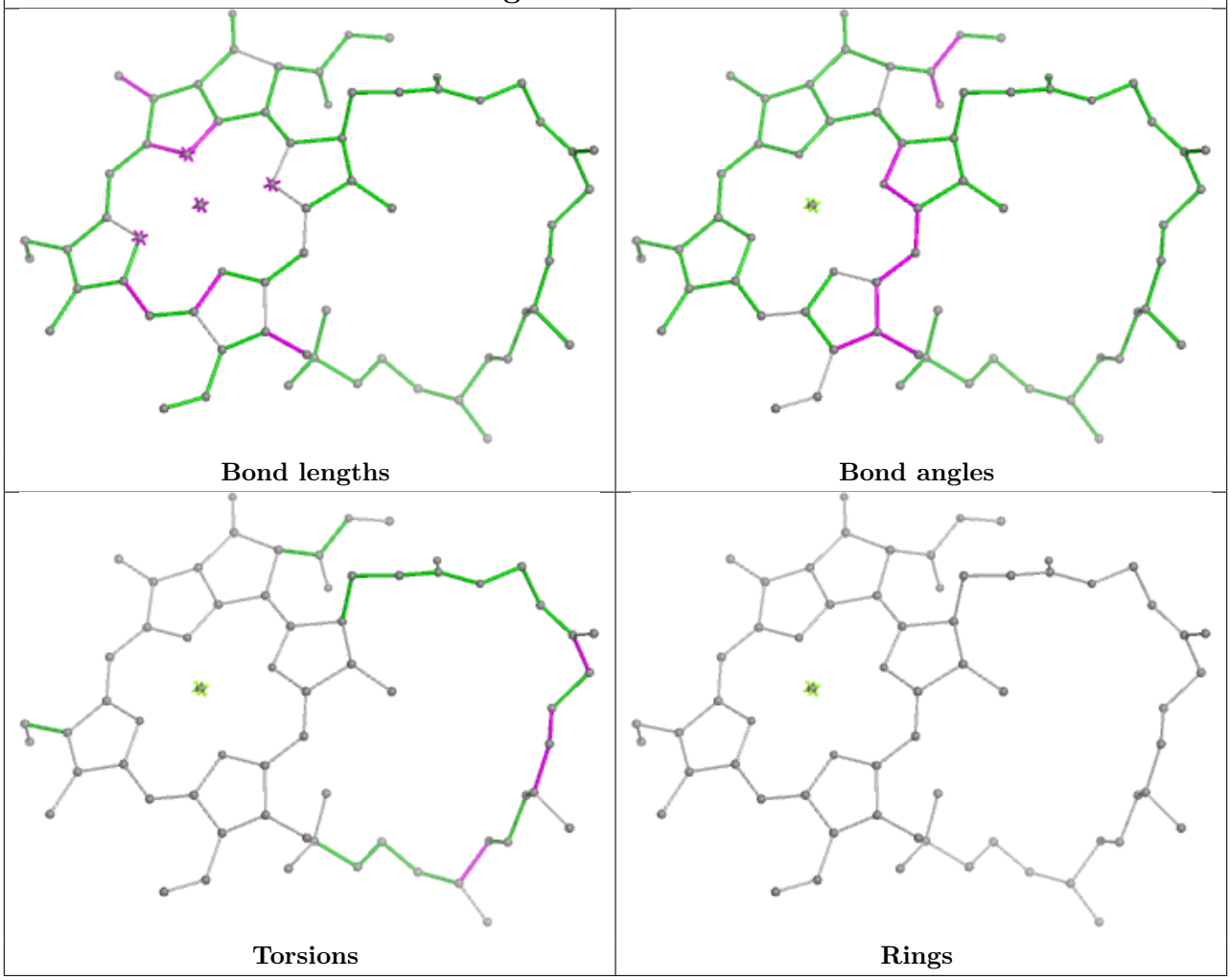


Rings

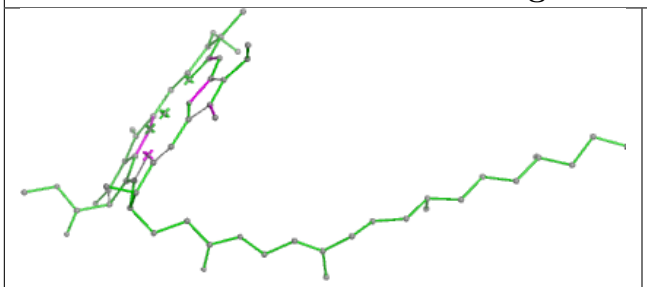
Ligand LMT c 525



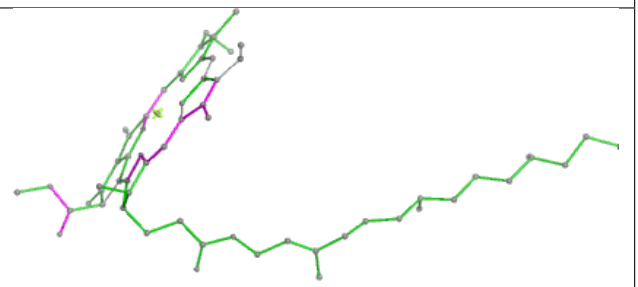
Ligand CLA B 615



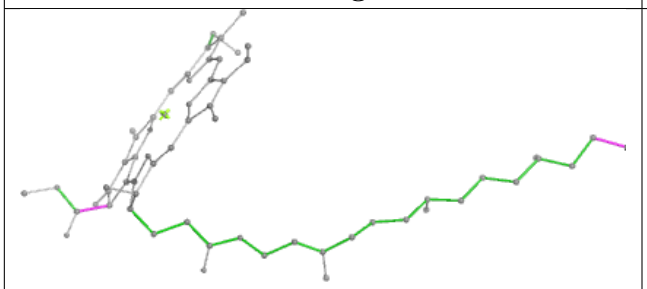
Ligand CLA b 608



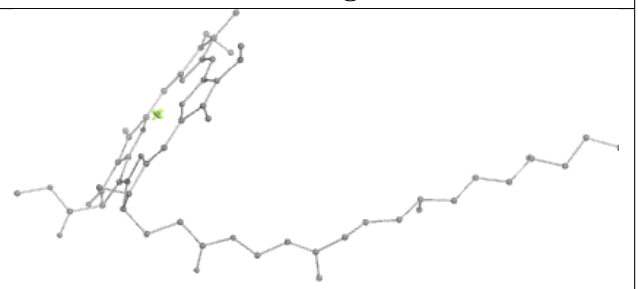
Bond lengths



Bond angles

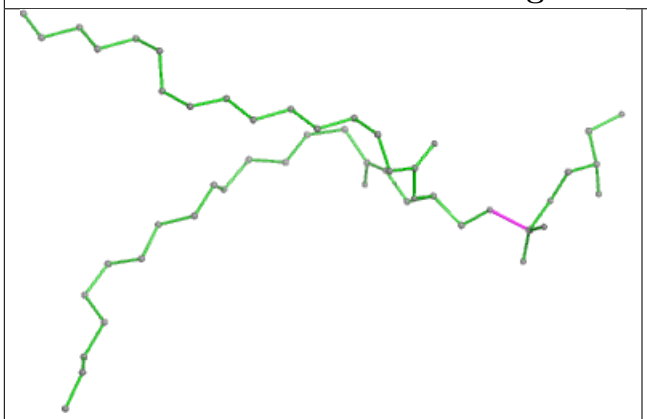


Torsions

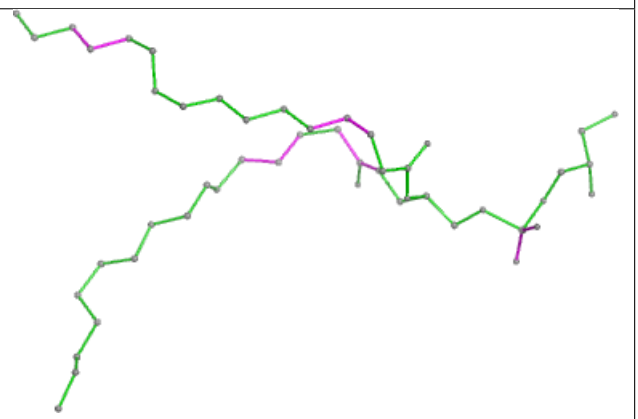


Rings

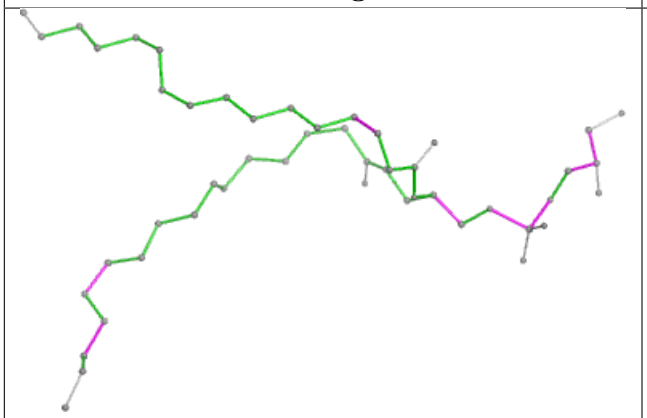
Ligand LHG d 409



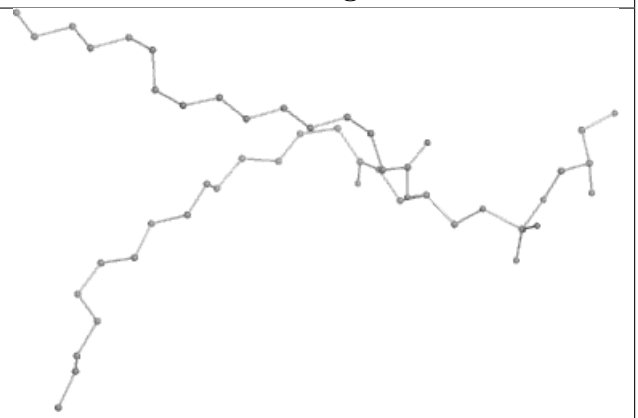
Bond lengths



Bond angles

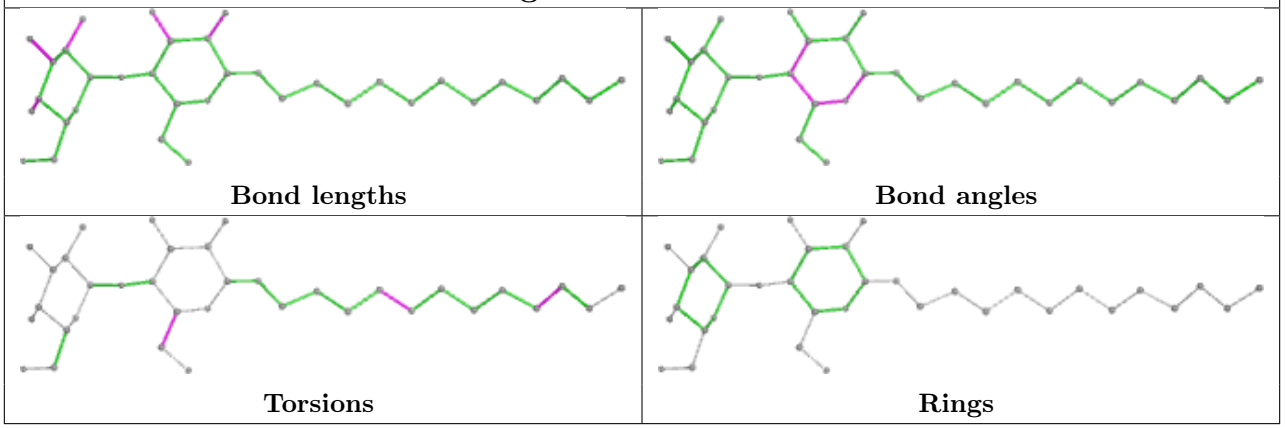


Torsions

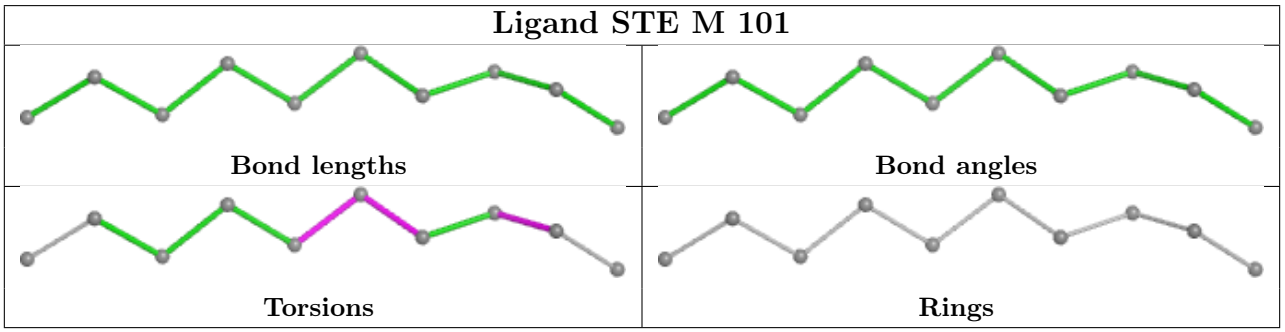


Rings

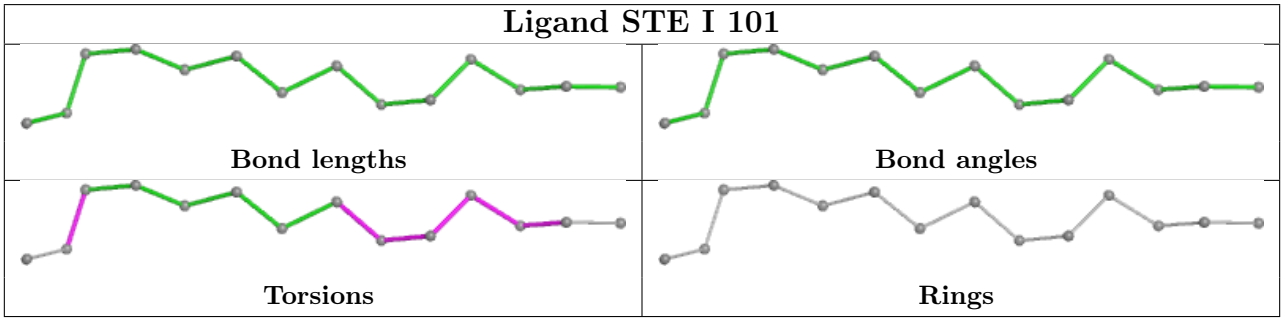
Ligand LMT m 101



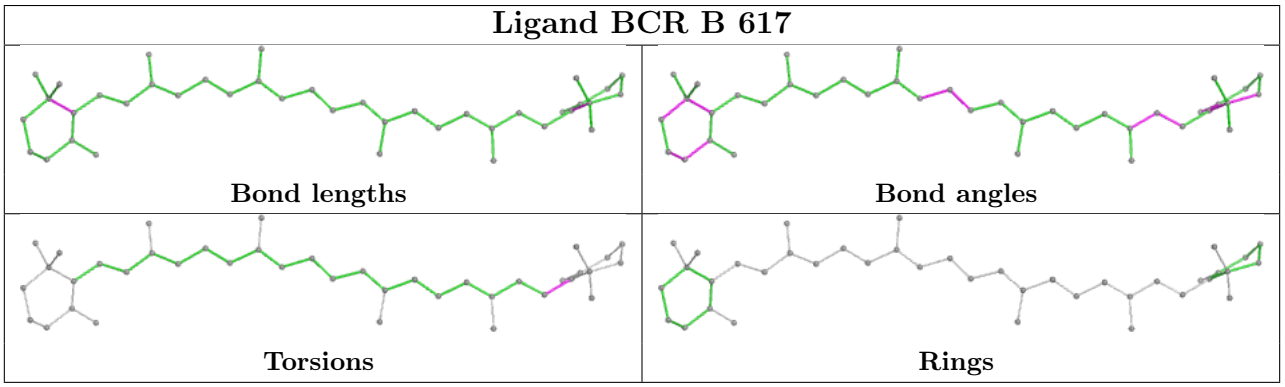
Ligand STE M 101



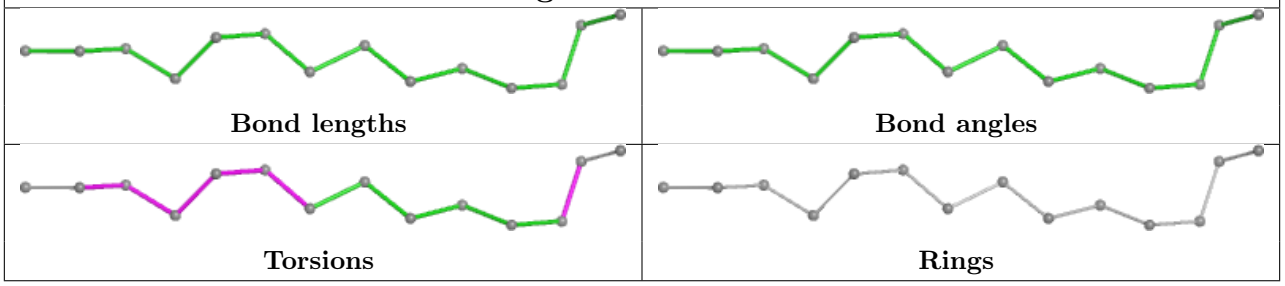
Ligand STE I 101



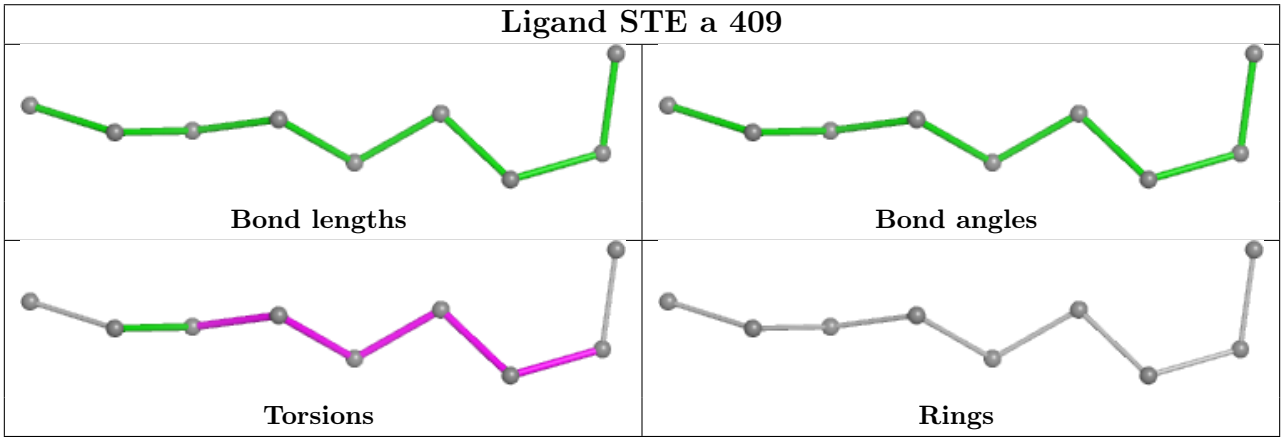
Ligand BCR B 617



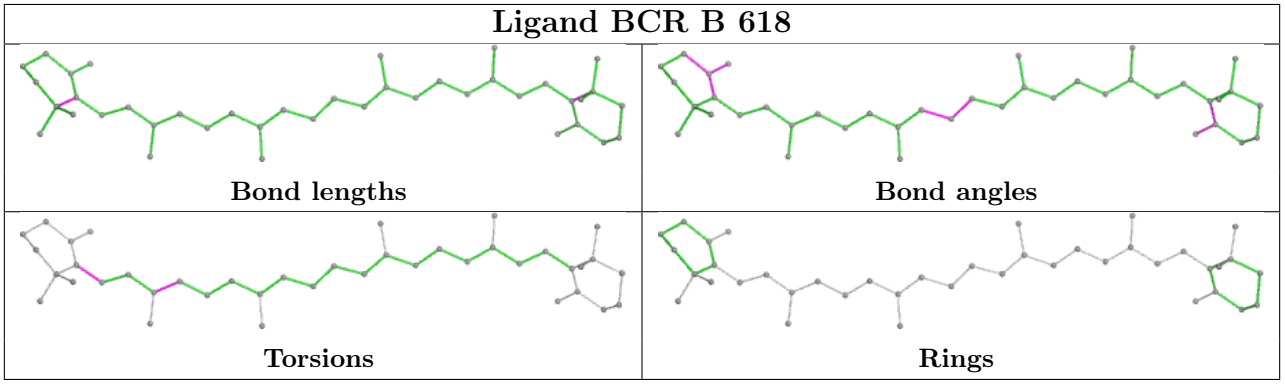
Ligand STE i 101



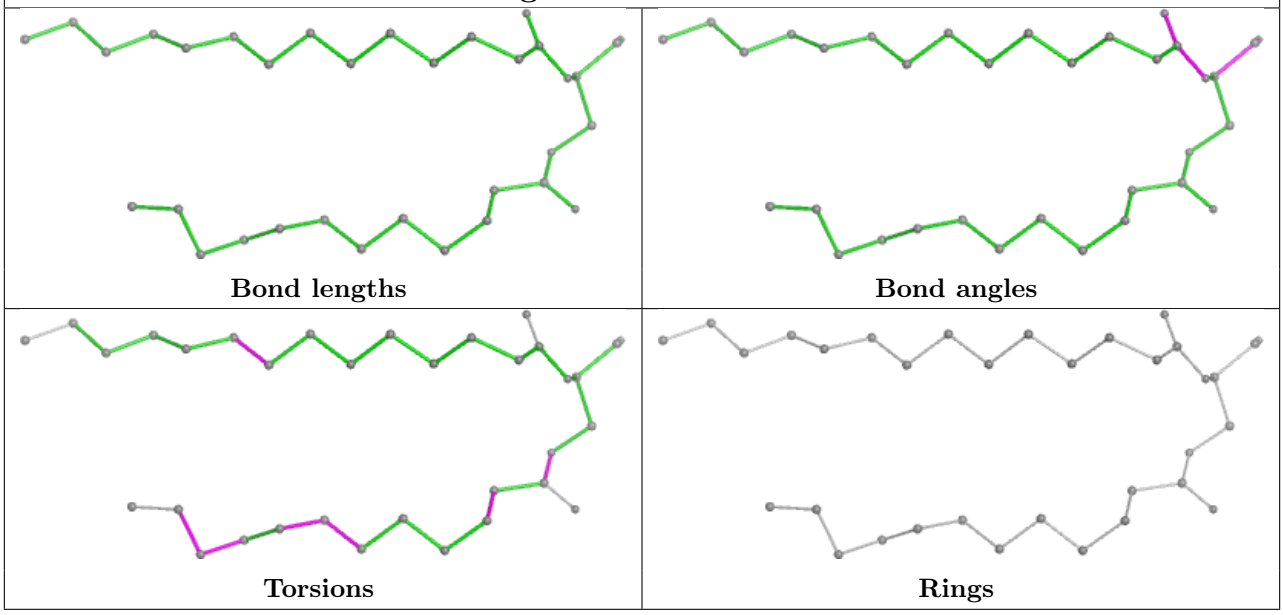
Ligand STE a 409



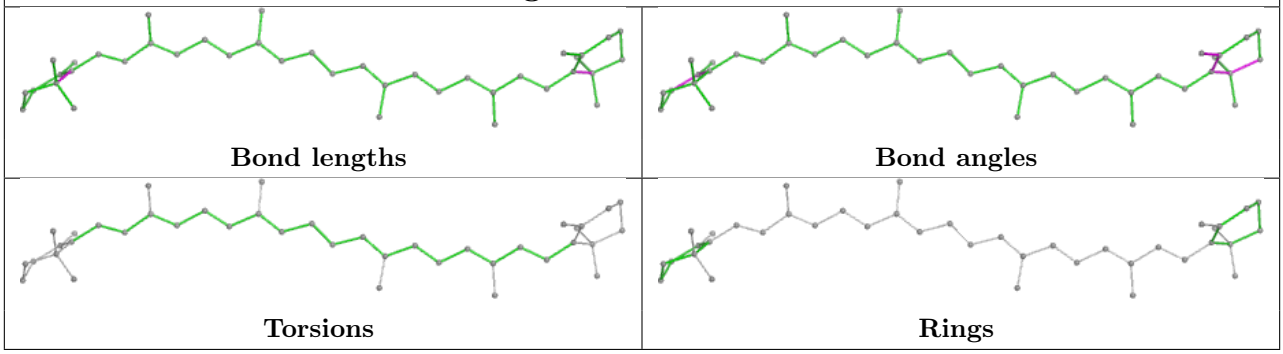
Ligand BCR B 618



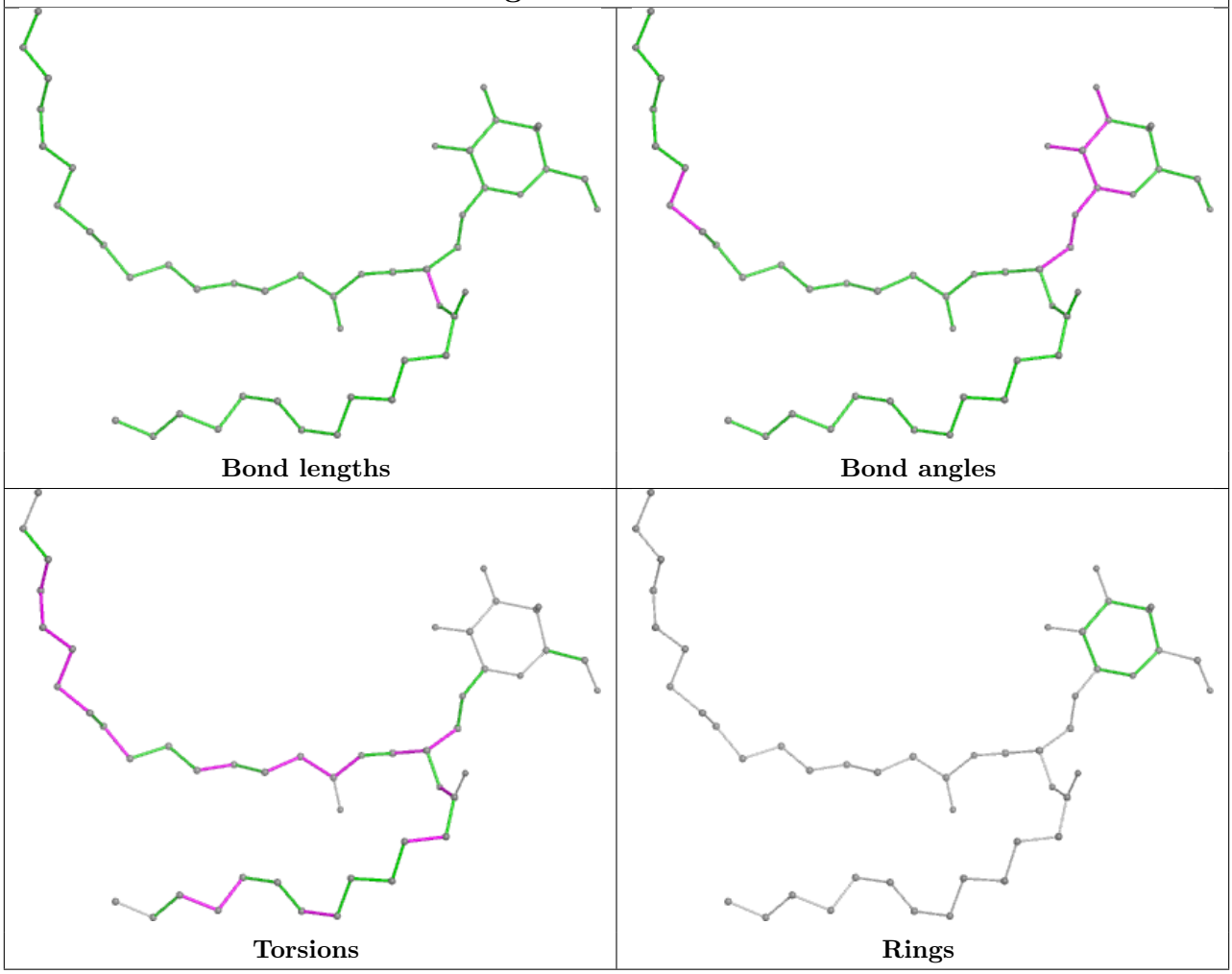
Ligand LMG D 402



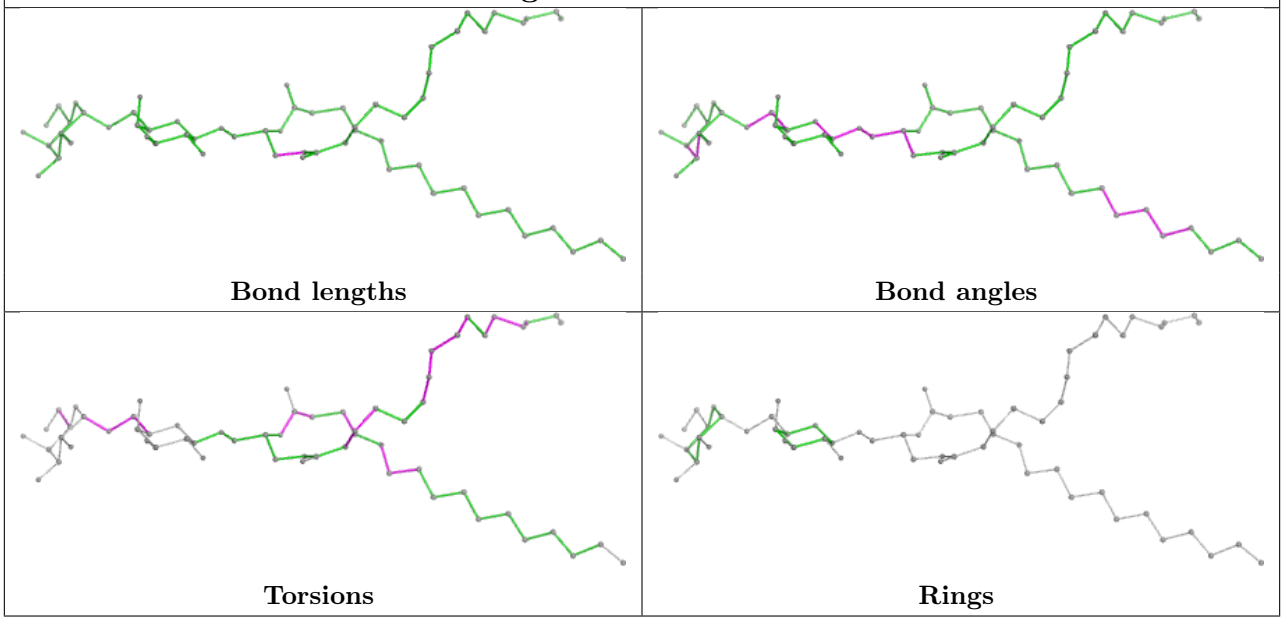
Ligand BCR A 407



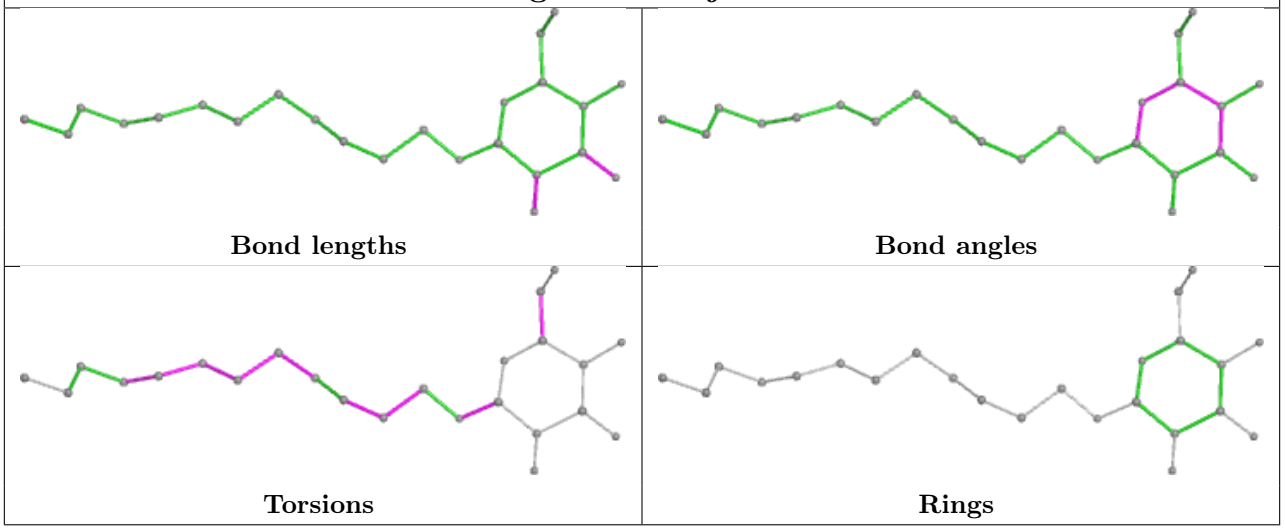
Ligand LMG c 520



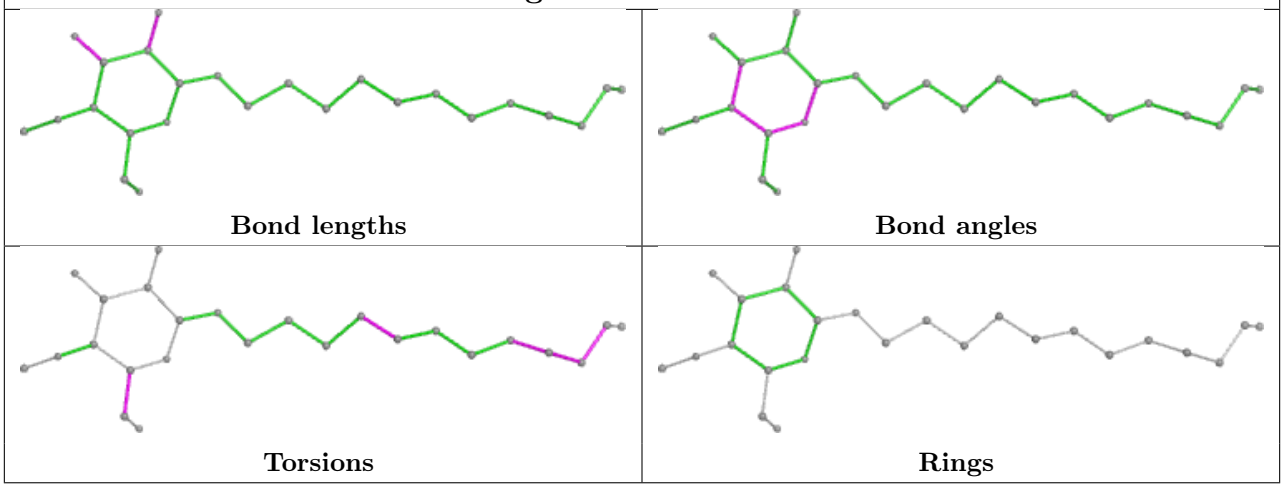
Ligand DGD C 517



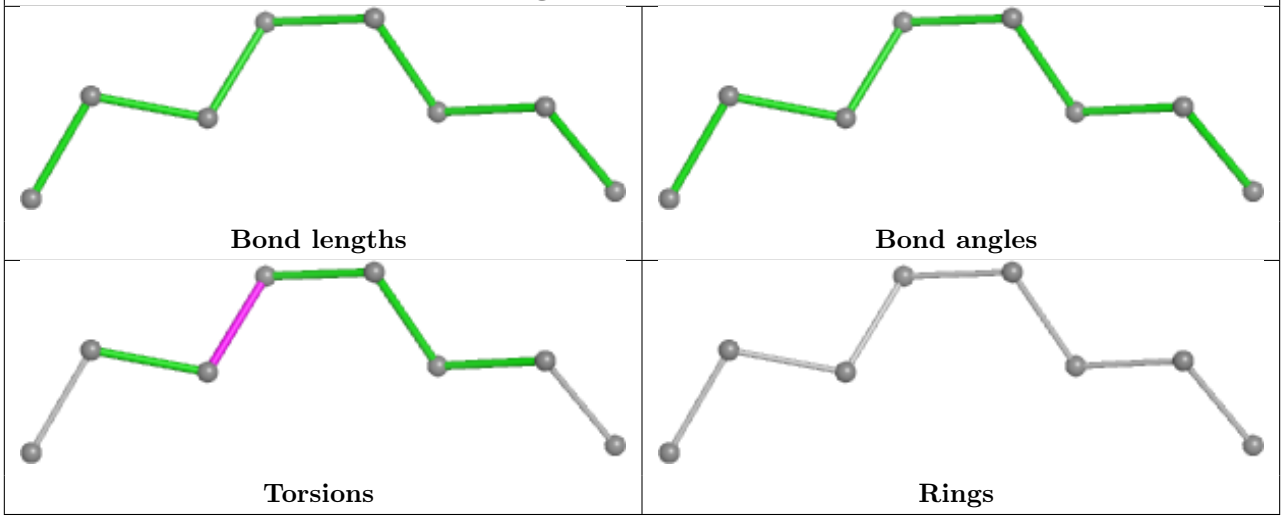
Ligand LMT j 102



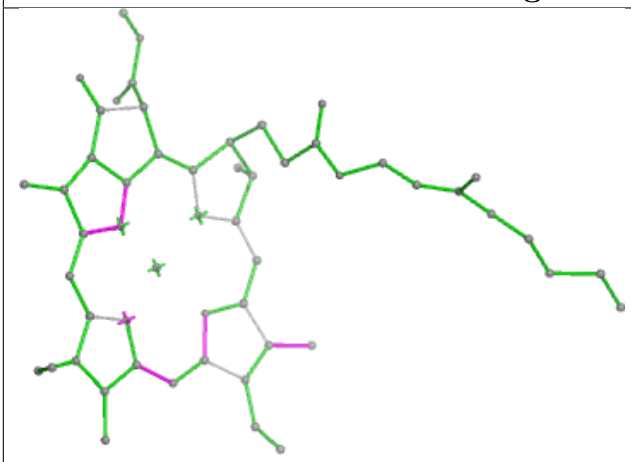
Ligand LMT b 624



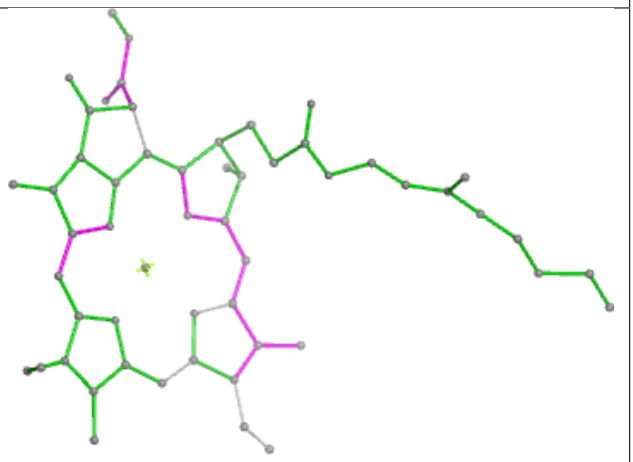
Ligand STE c 522



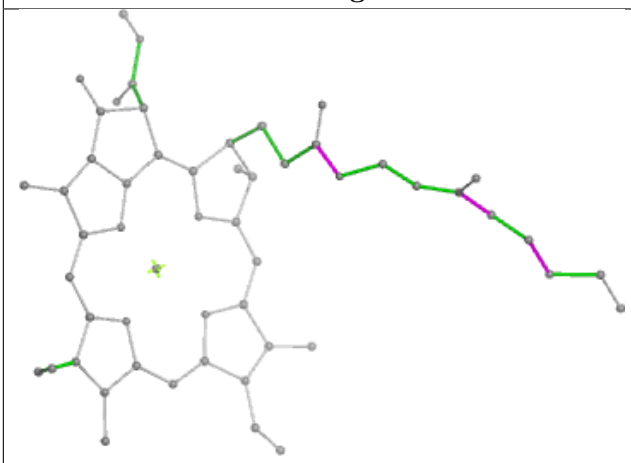
Ligand CLA A 406



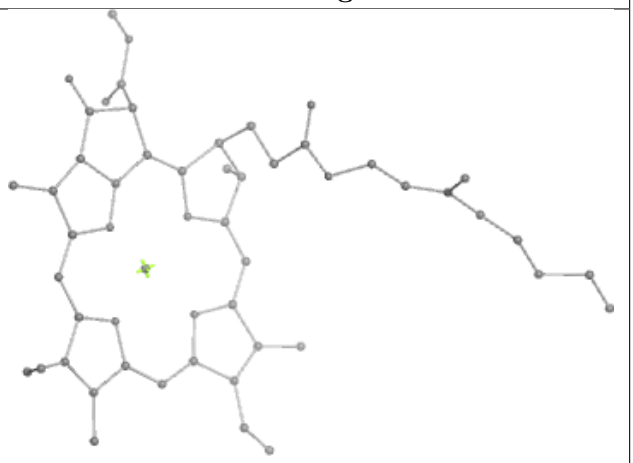
Bond lengths



Bond angles

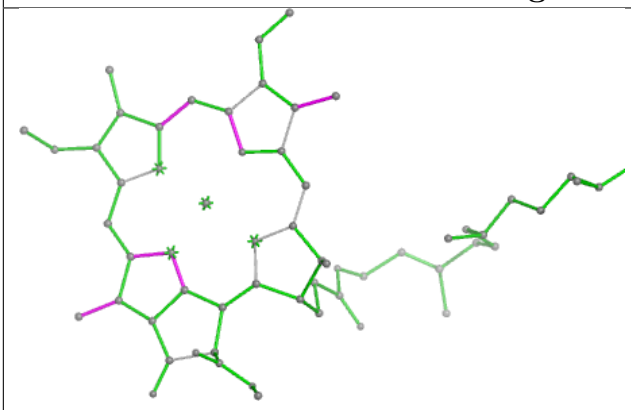


Torsions

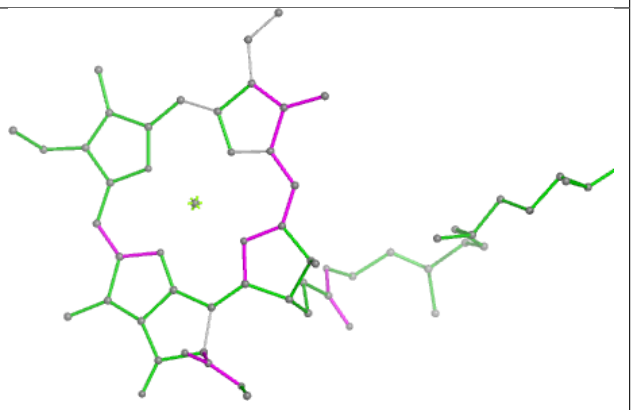


Rings

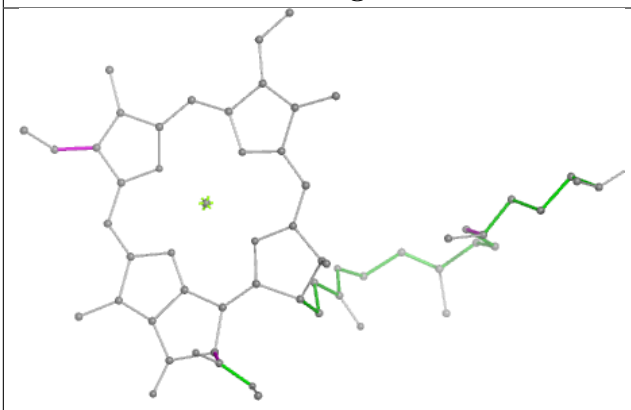
Ligand CLA a 405



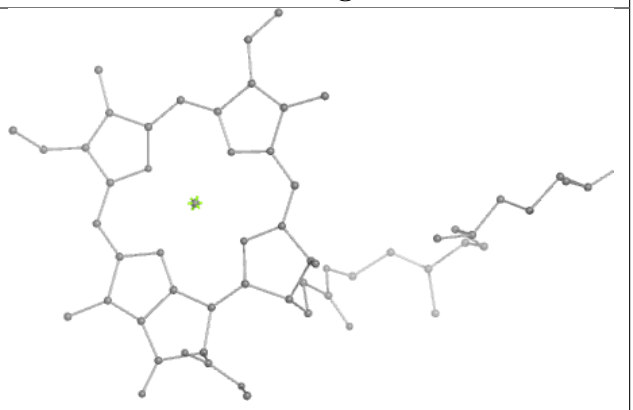
Bond lengths



Bond angles

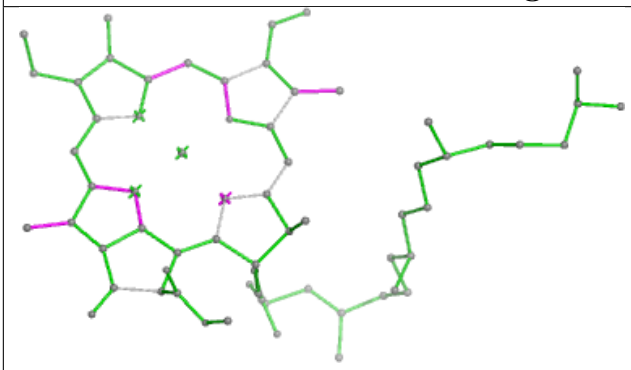


Torsions

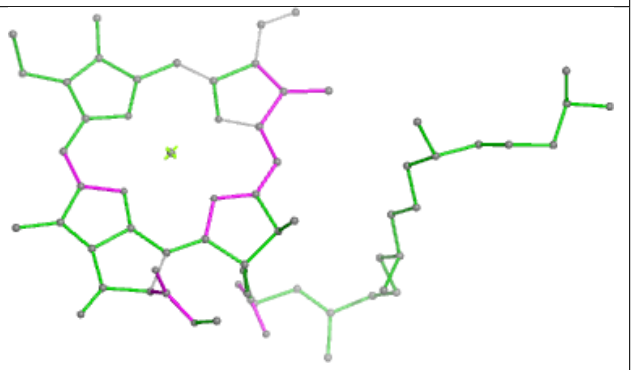


Rings

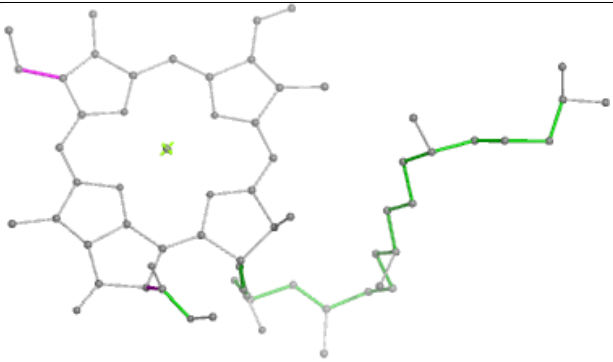
Ligand CLA A 419



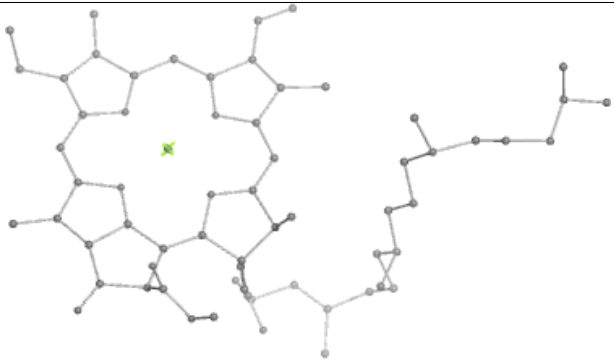
Bond lengths



Bond angles

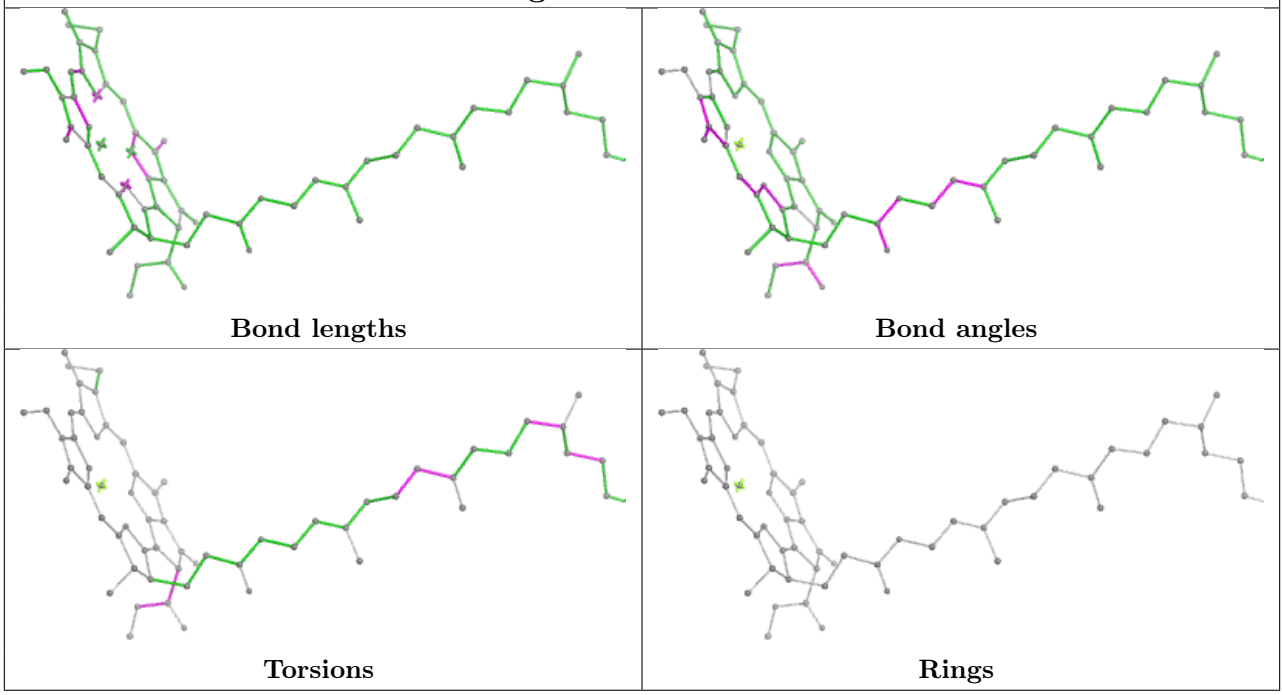


Torsions

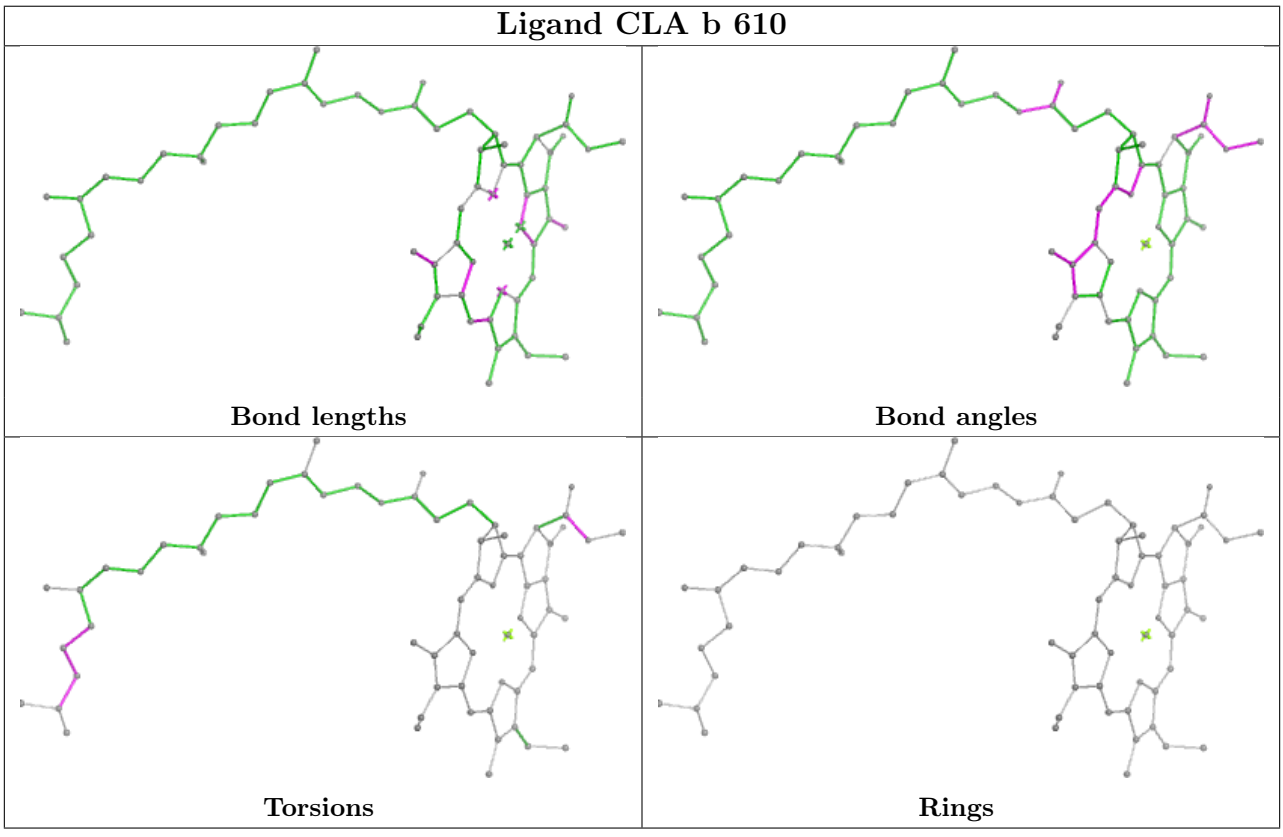


Rings

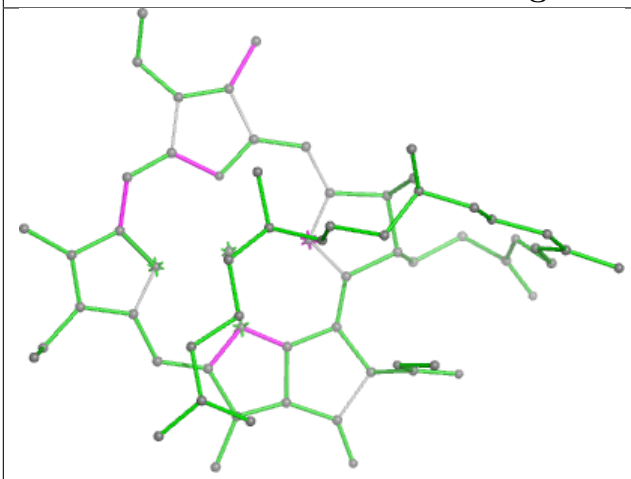
Ligand CLA b 605



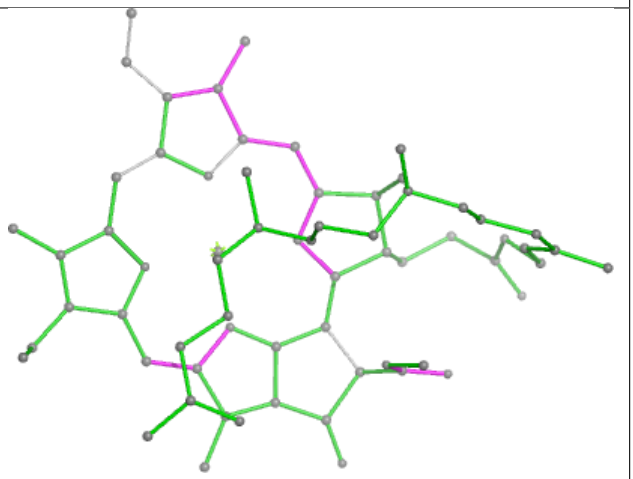
Ligand CLA b 610



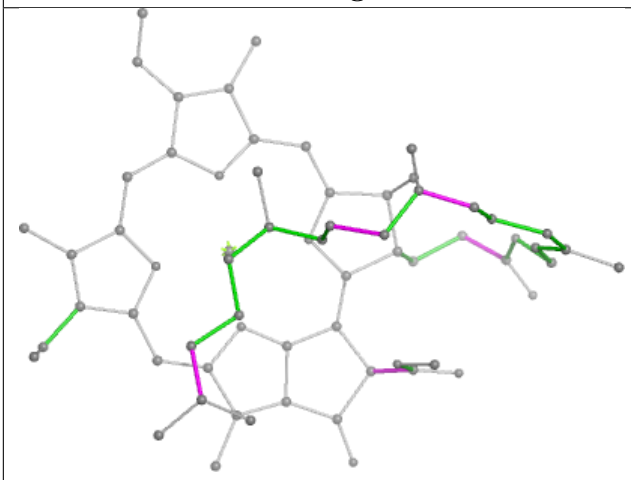
Ligand CLA c 510



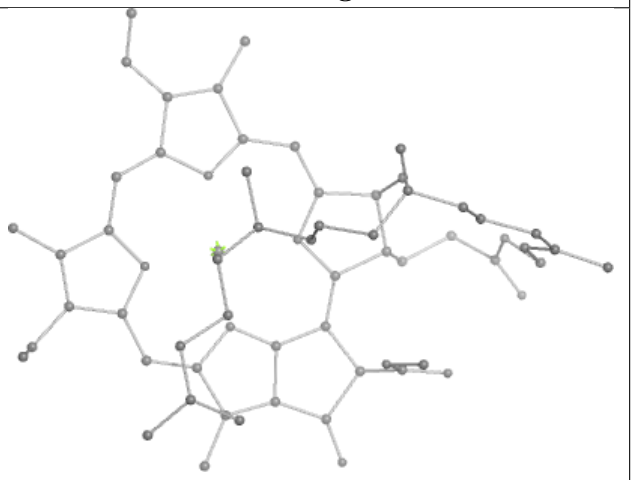
Bond lengths



Bond angles

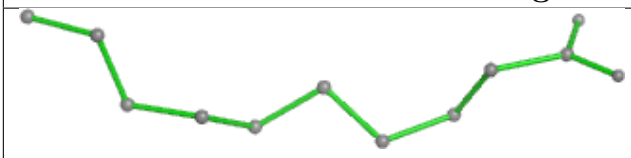


Torsions

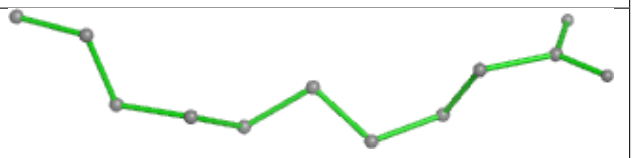


Rings

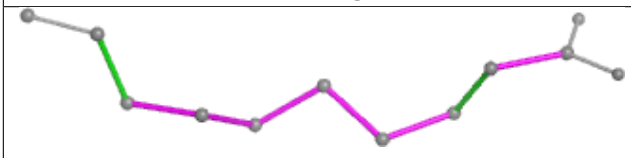
Ligand STE c 521



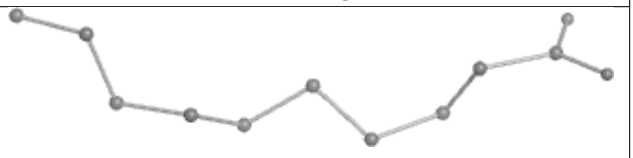
Bond lengths



Bond angles

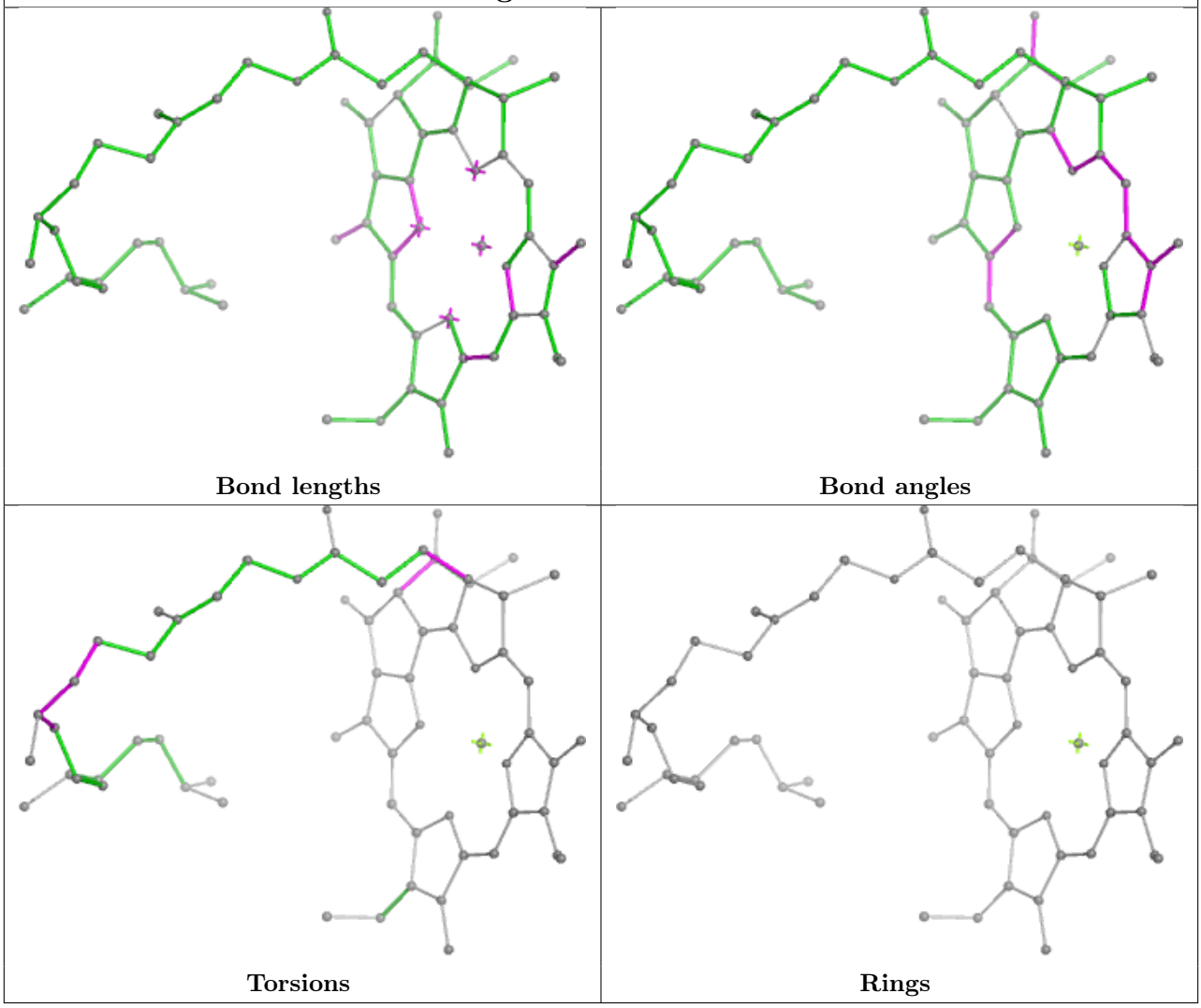


Torsions

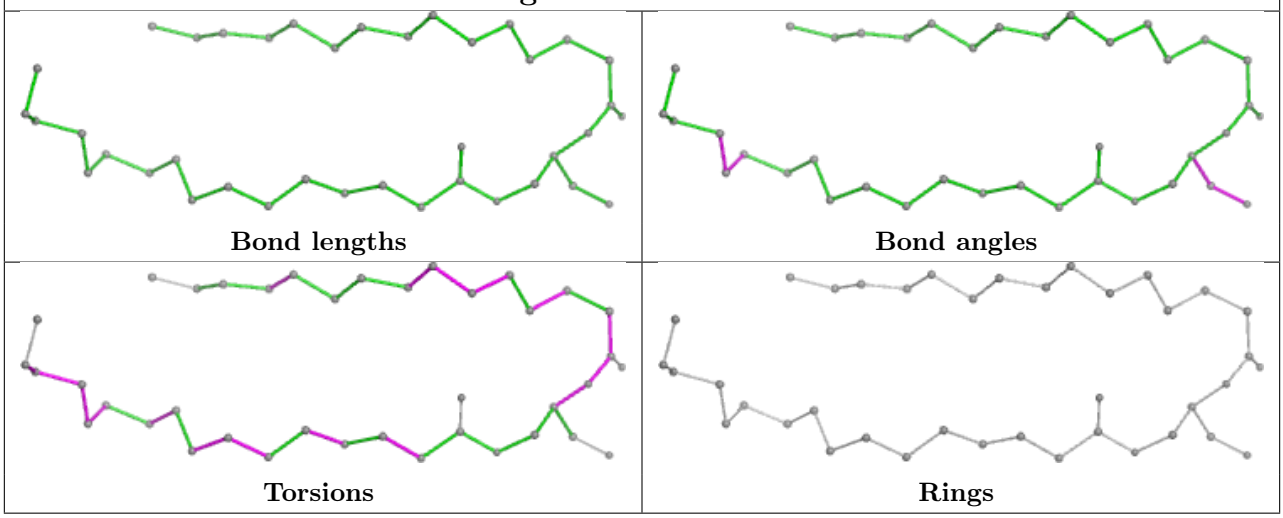


Rings

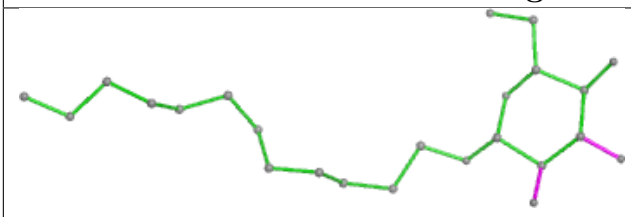
Ligand CLA c 503



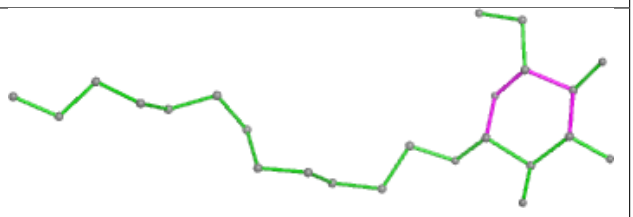
Ligand LMG H 101



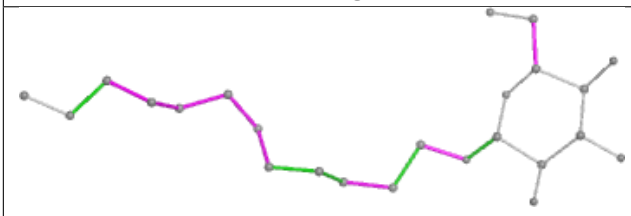
Ligand LMT e 104



Bond lengths



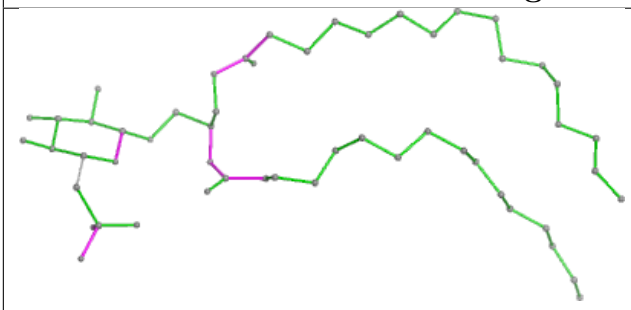
Bond angles



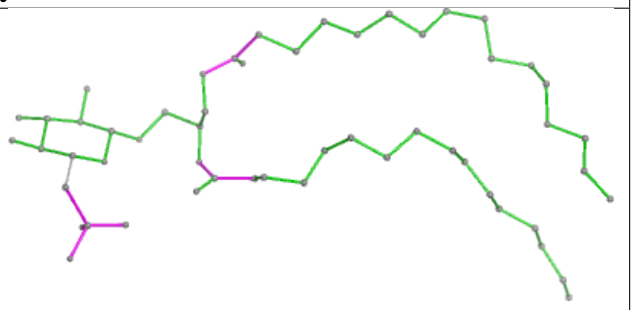
Torsions

Rings

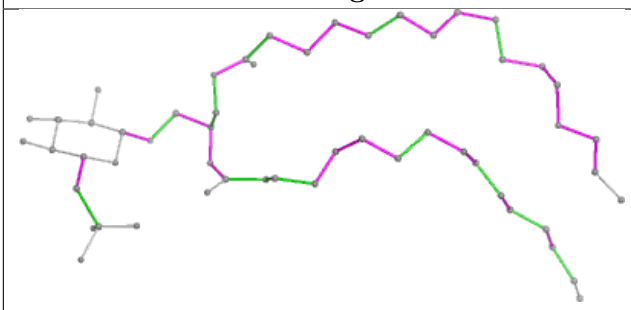
Ligand SQD B 620



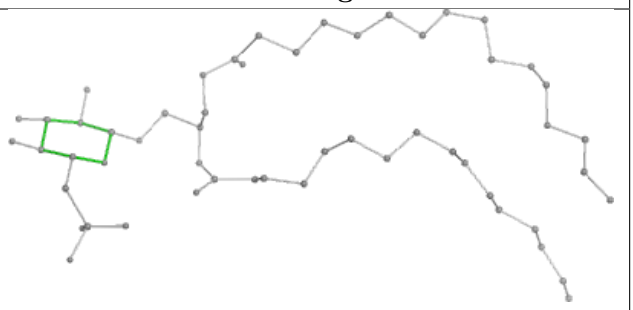
Bond lengths



Bond angles

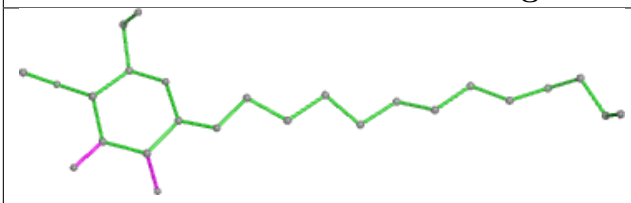


Torsions

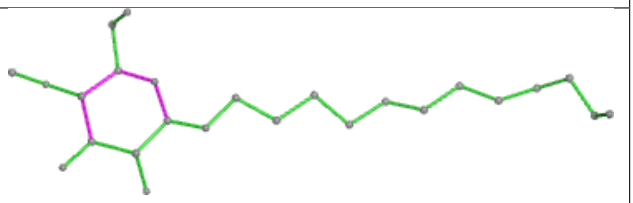


Rings

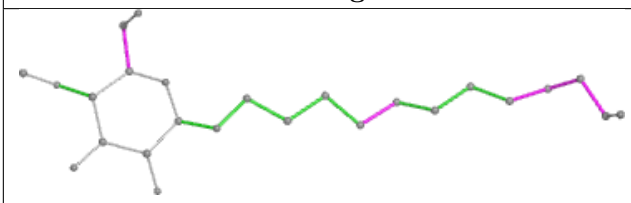
Ligand LMT B 623



Bond lengths



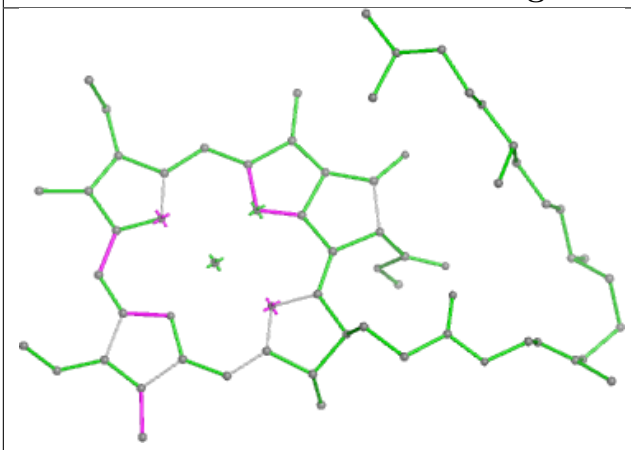
Bond angles



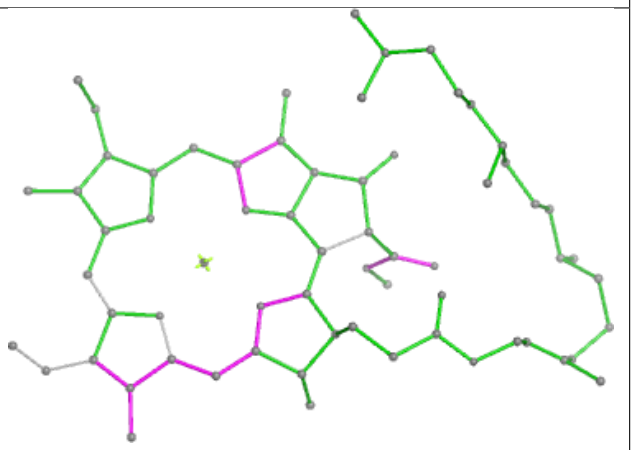
Torsions

Rings

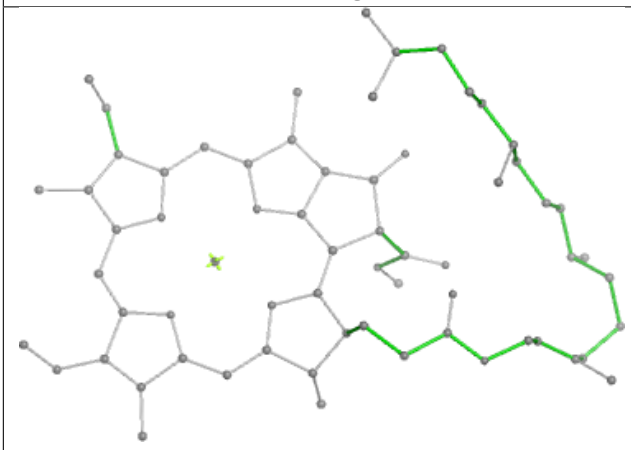
Ligand CLA b 611



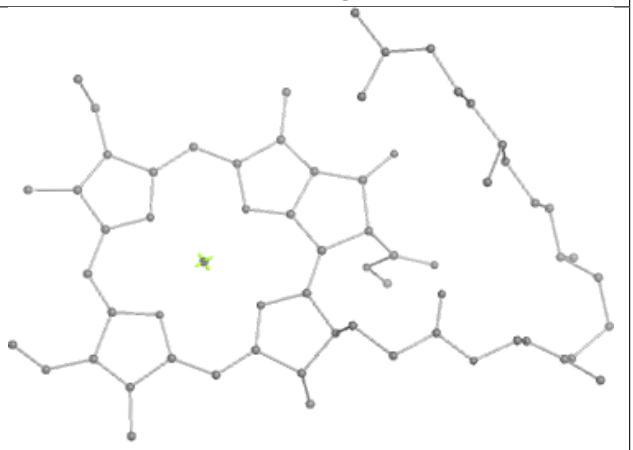
Bond lengths



Bond angles



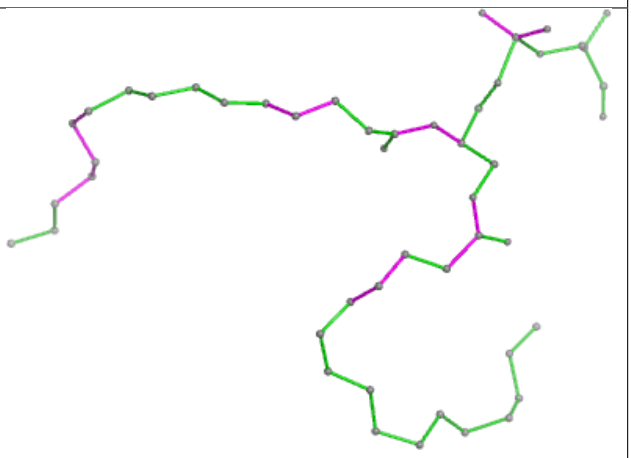
Torsions



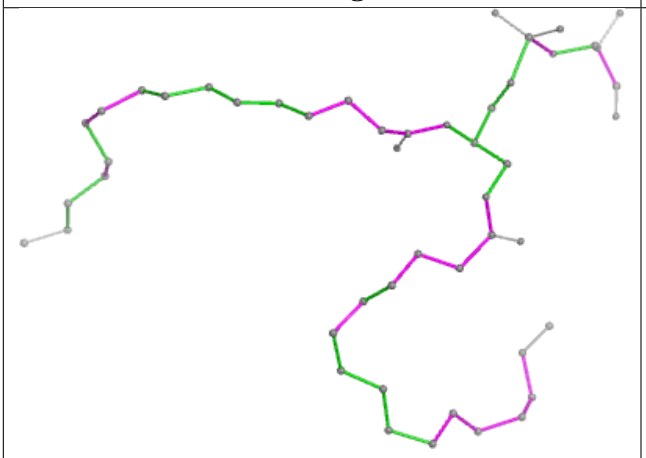
Rings

Ligand LHG A 420

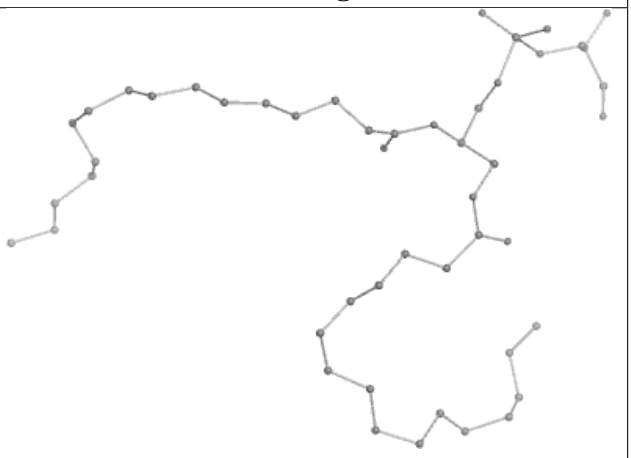
Bond lengths



Bond angles

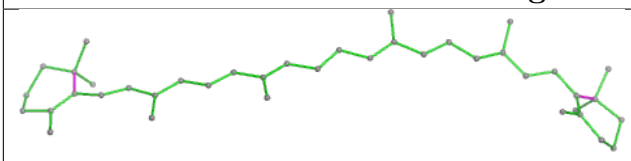


Torsions

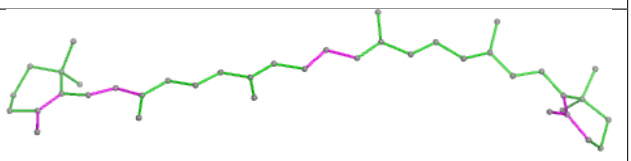


Rings

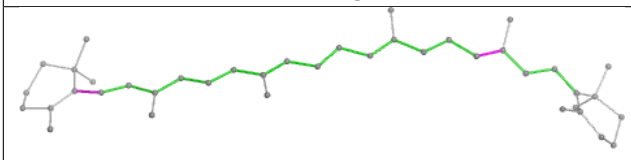
Ligand BCR t 102



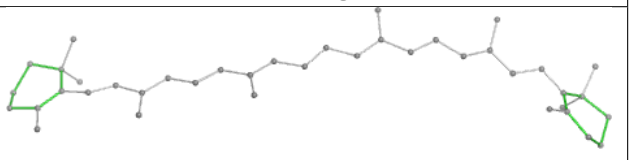
Bond lengths



Bond angles

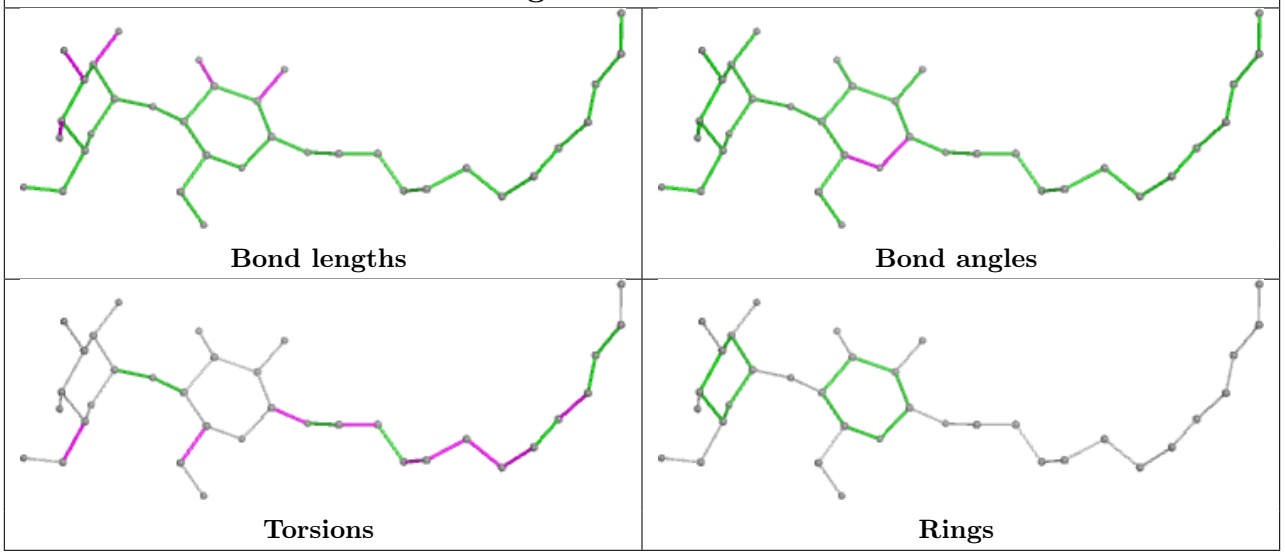


Torsions

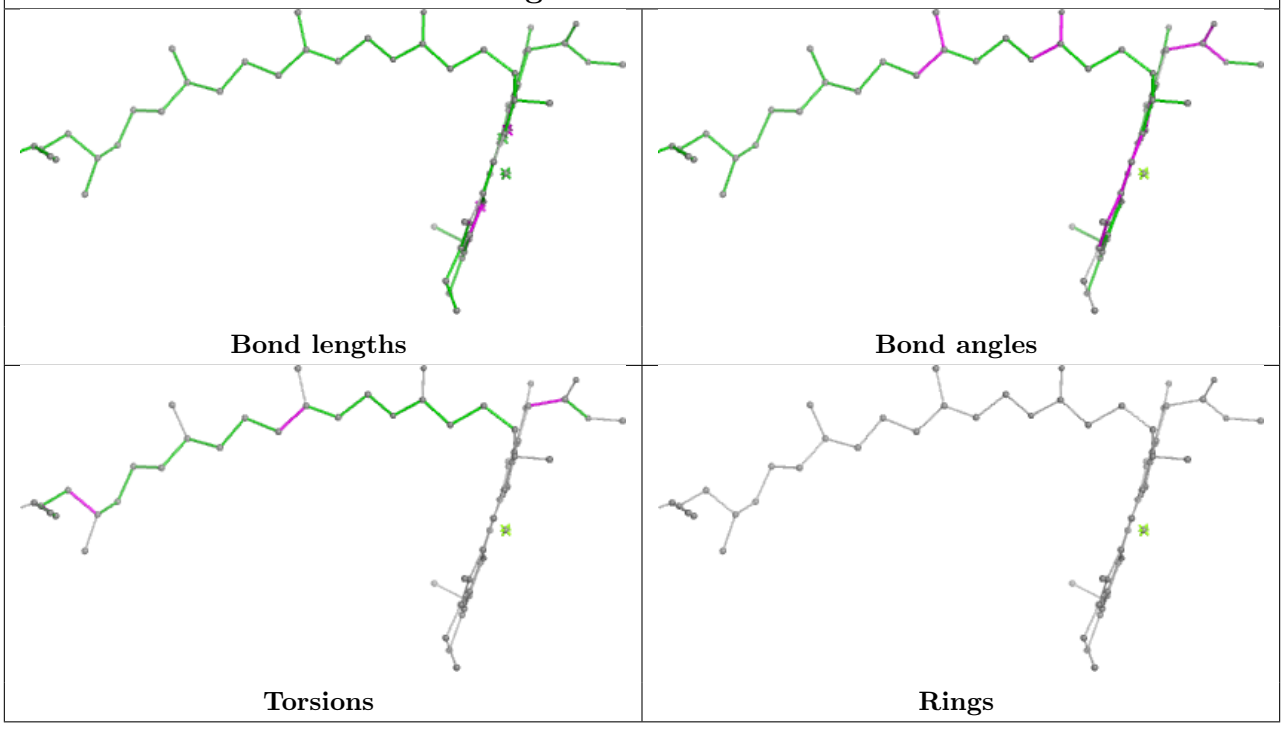


Rings

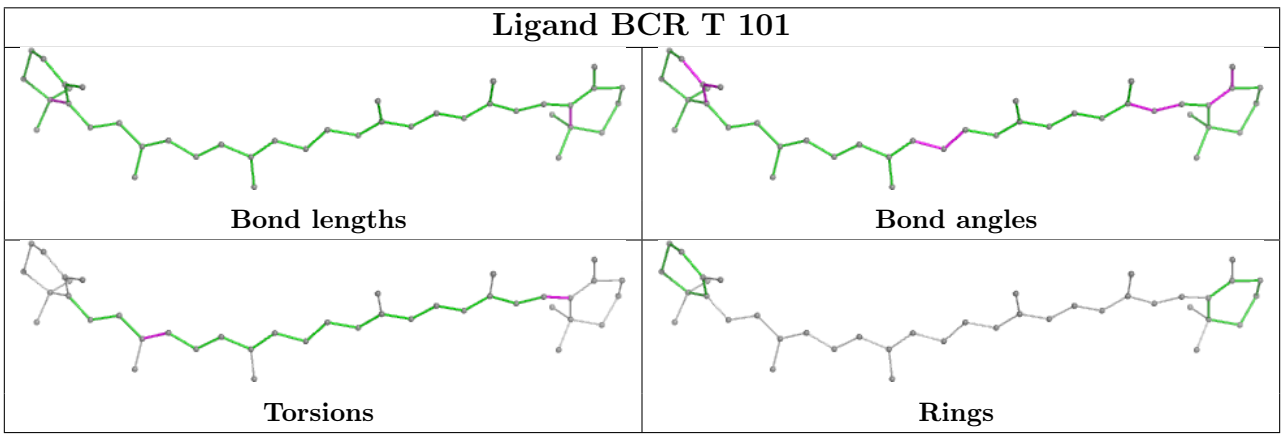
Ligand LMT z 101



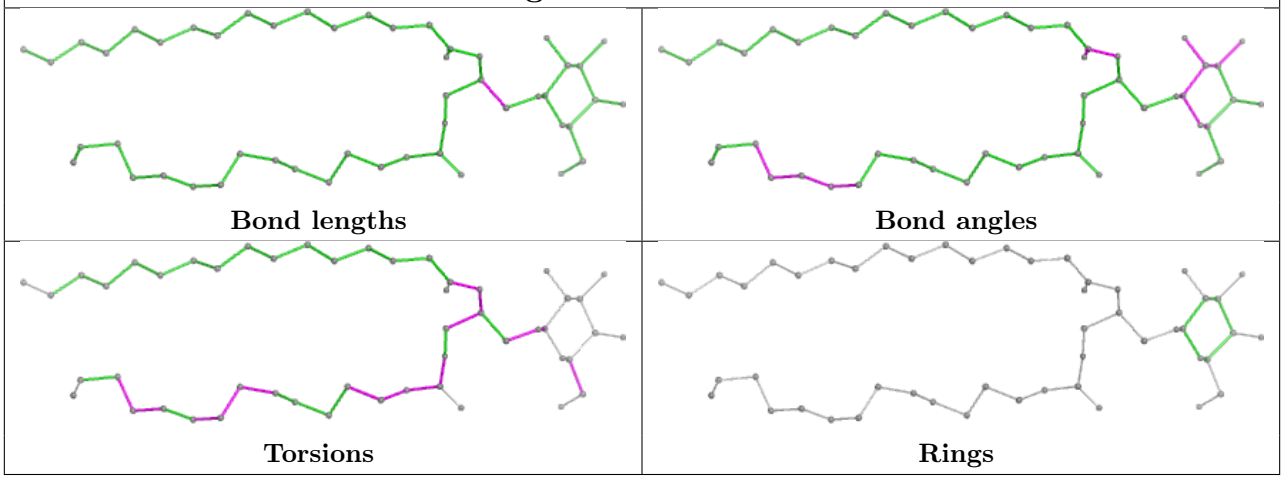
Ligand CLA B 605



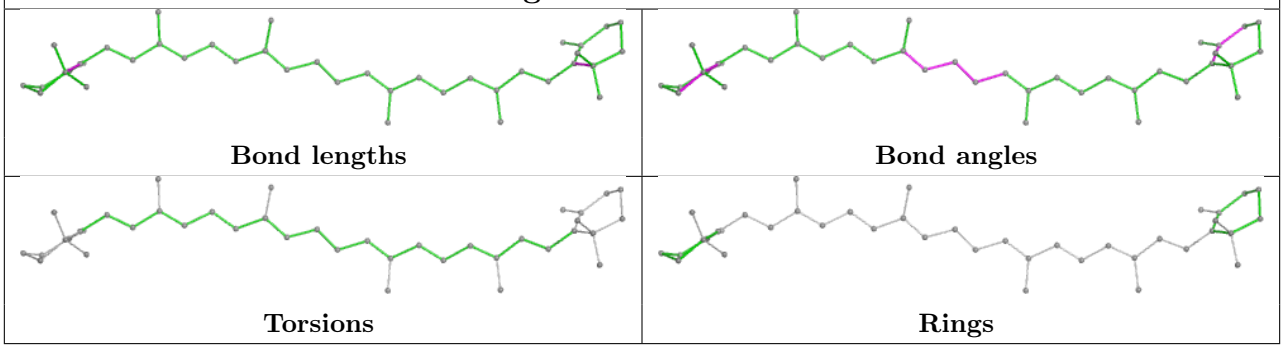
Ligand BCR T 101



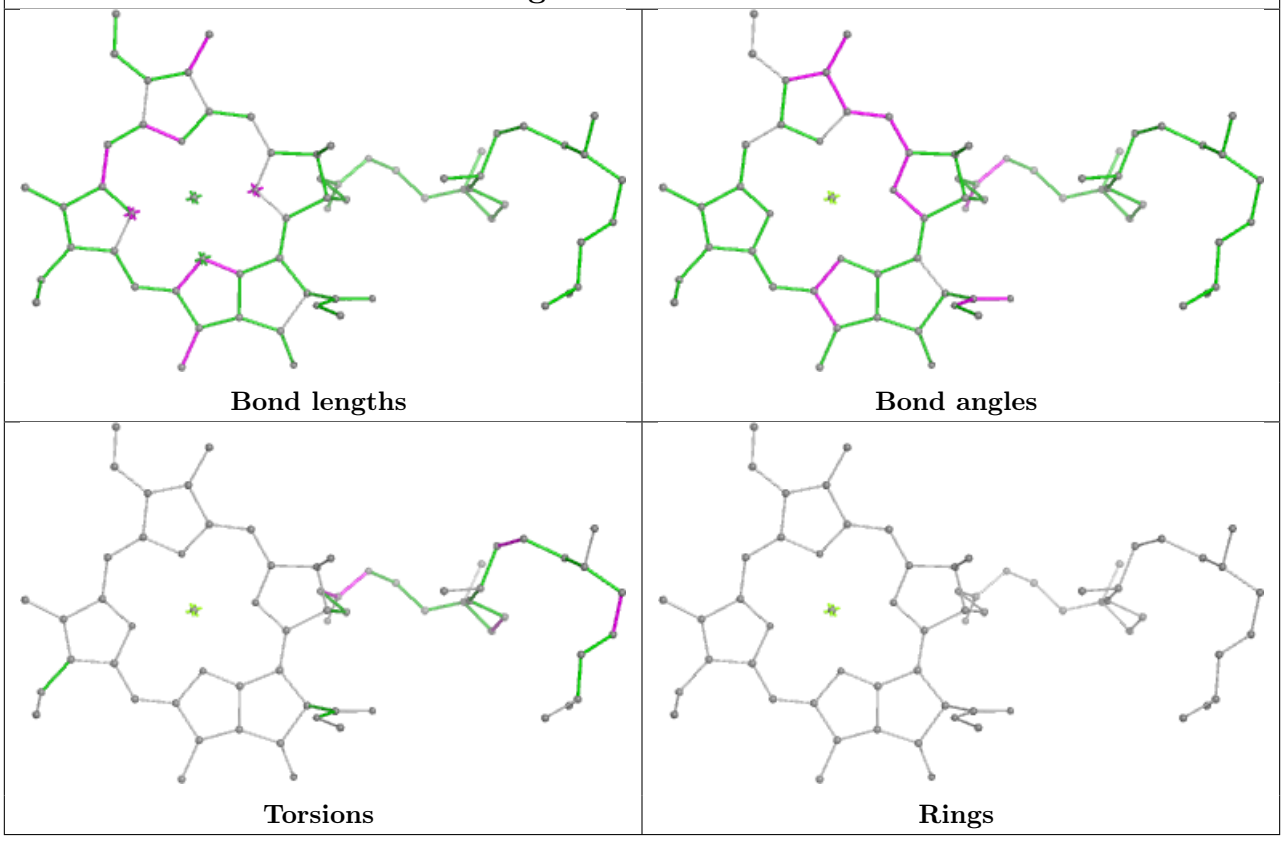
Ligand LMG c 524



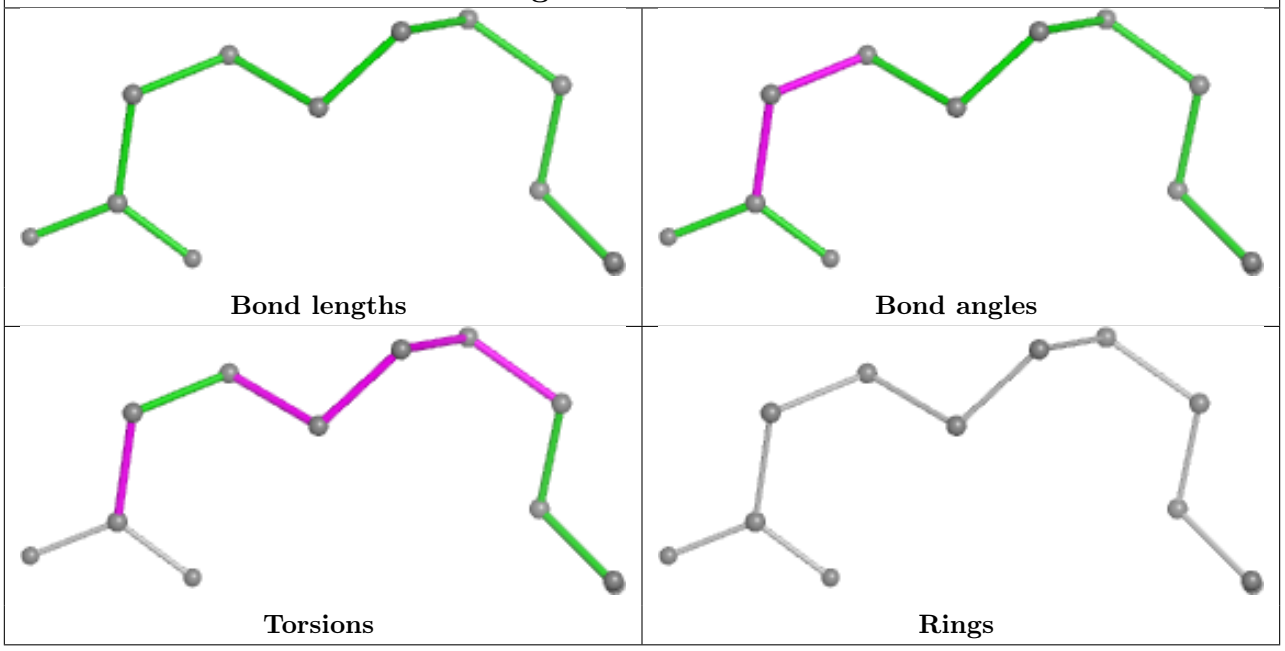
Ligand BCR C 514



Ligand CLA b 613



Ligand STE b 623



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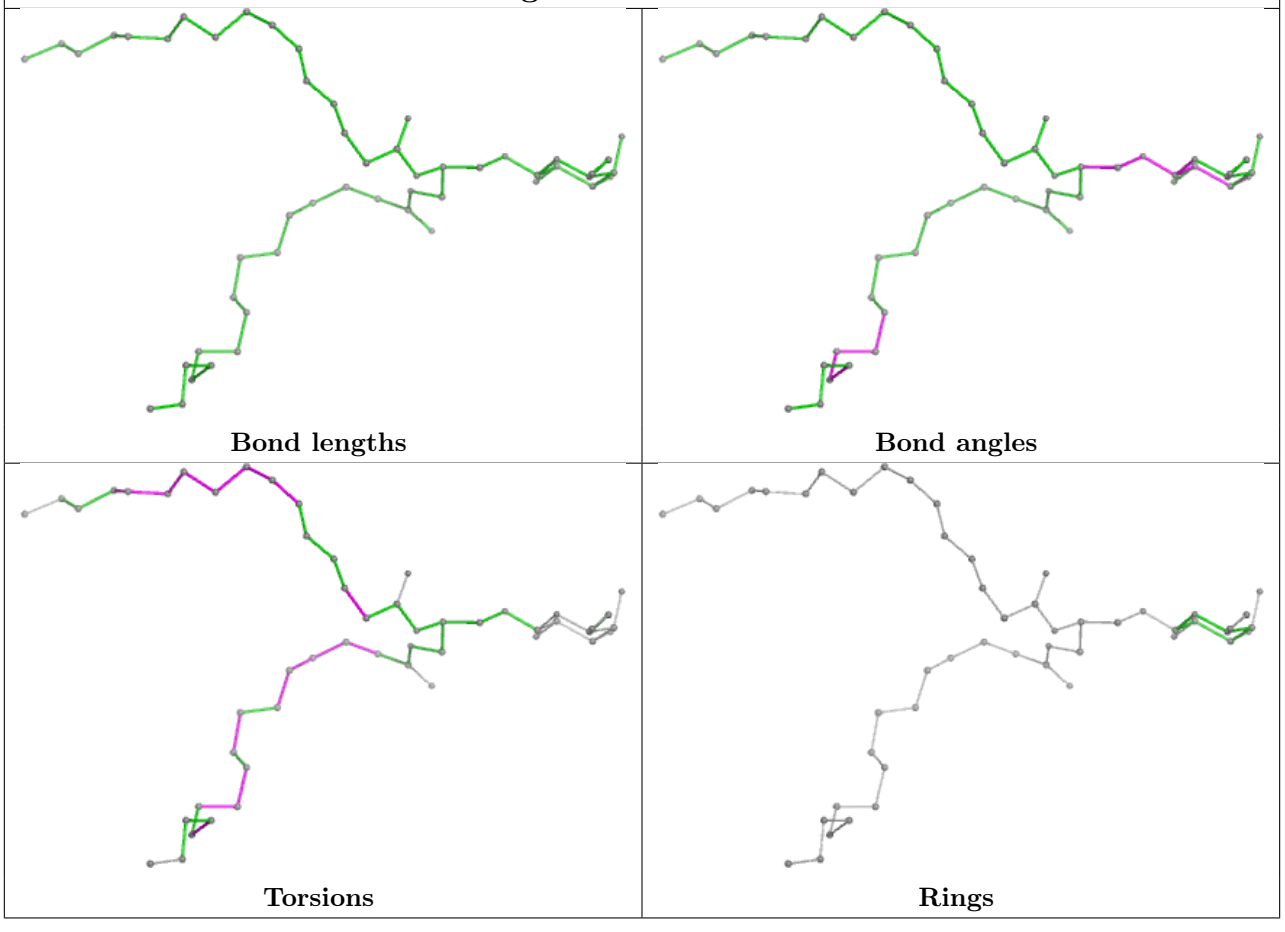
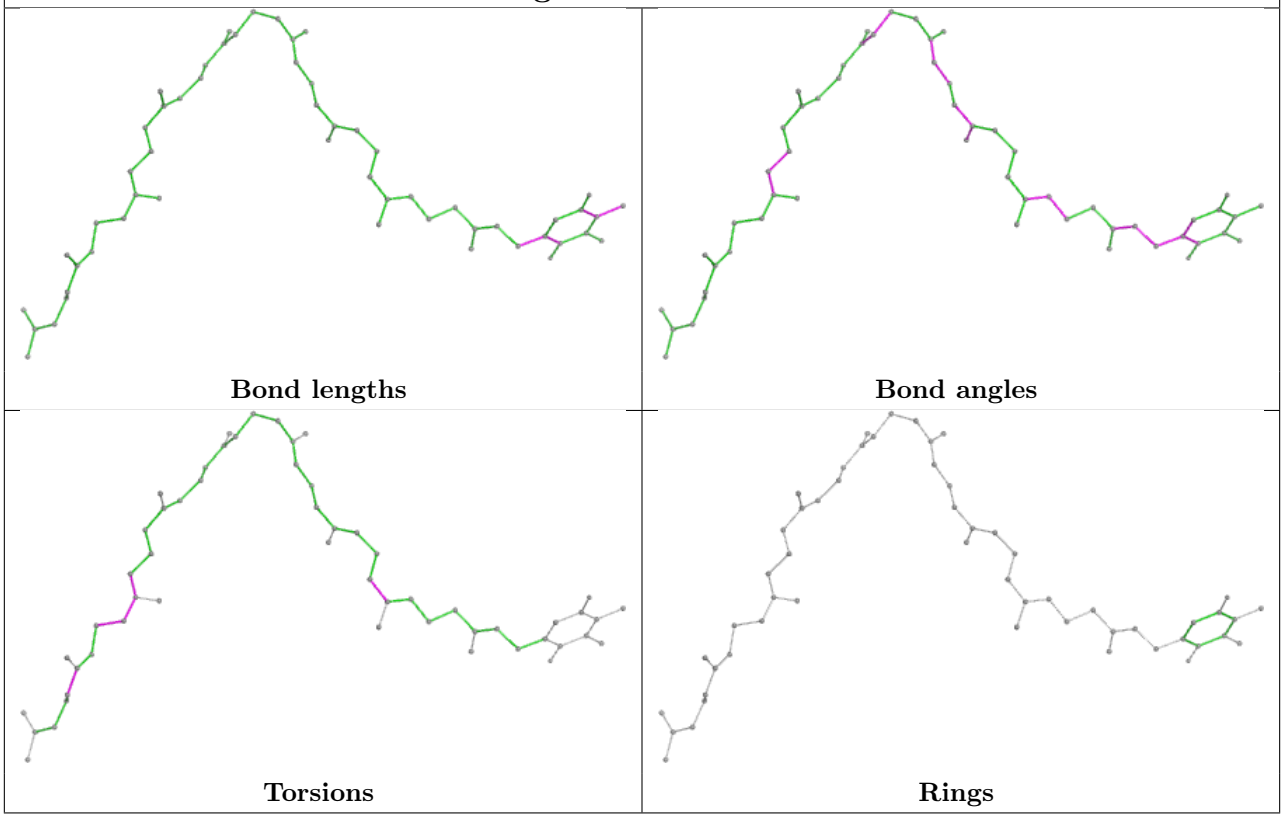
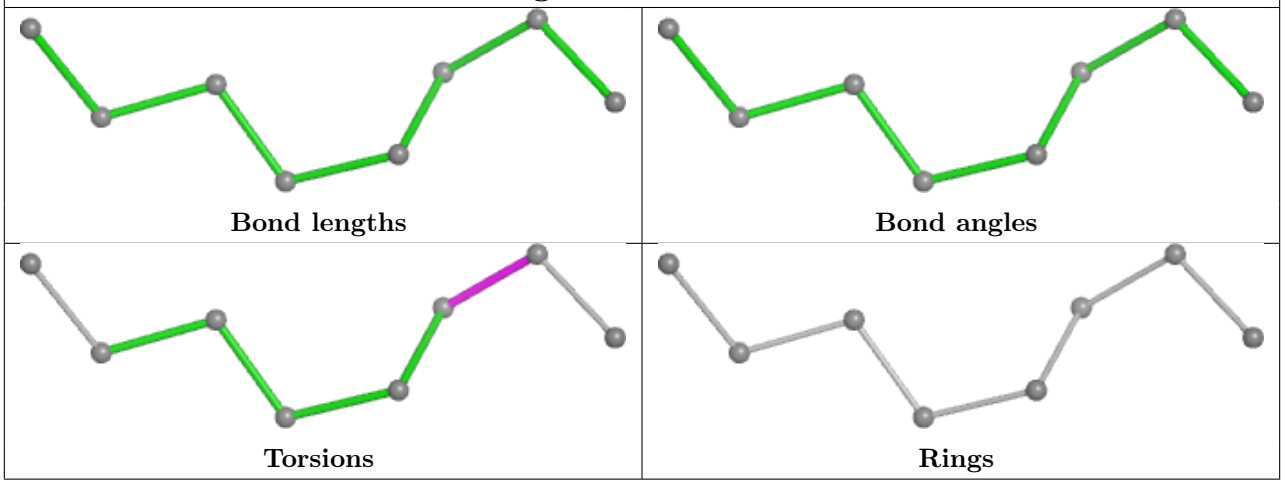


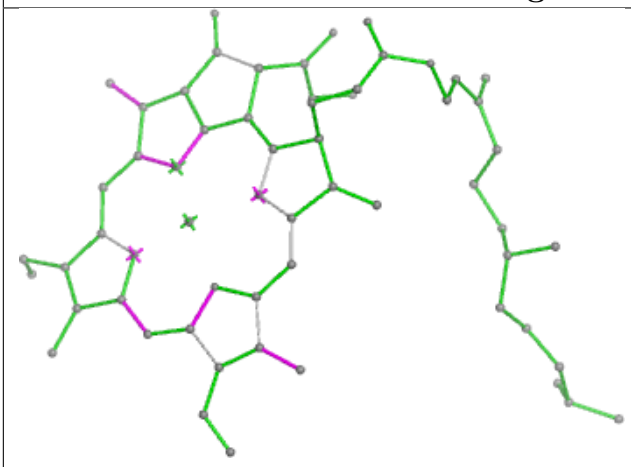
Ligand PL9 d 407



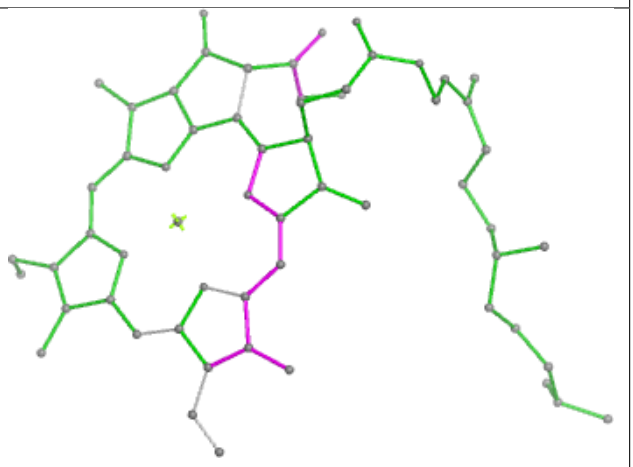
Ligand STE a 414



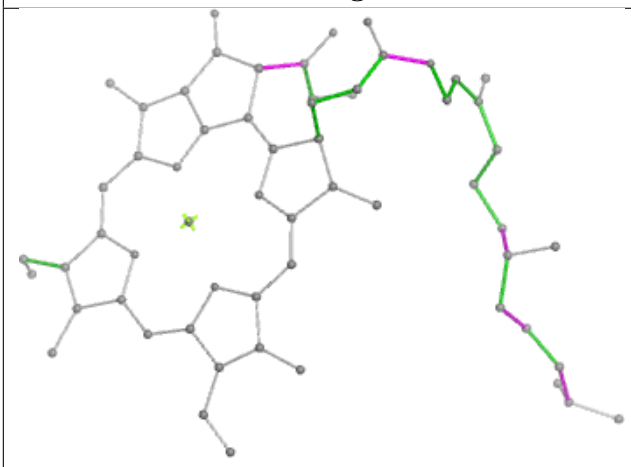
Ligand CLA b 617



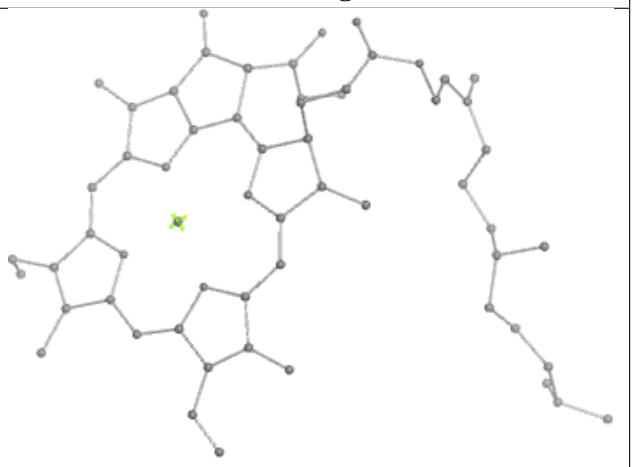
Bond lengths



Bond angles

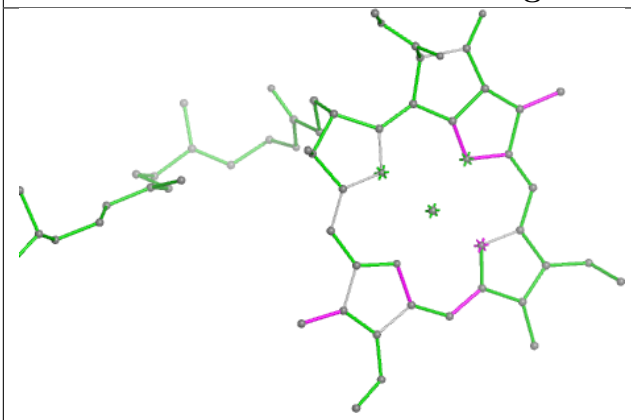


Torsions

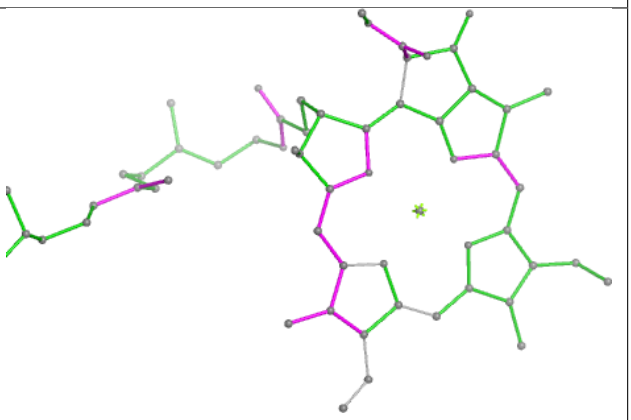


Rings

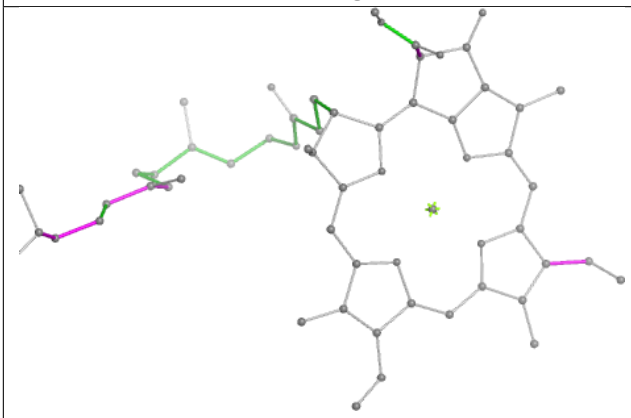
Ligand CLA A 405



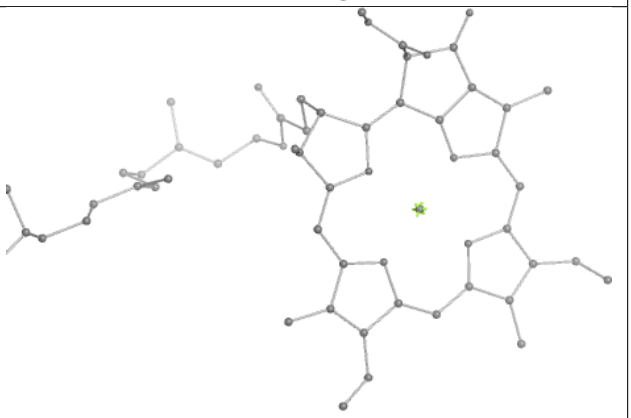
Bond lengths



Bond angles

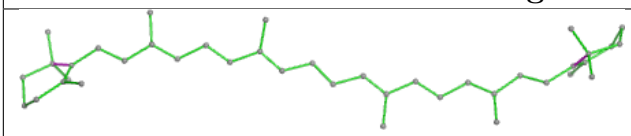


Torsions

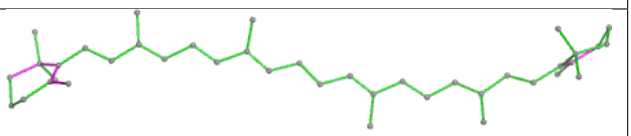


Rings

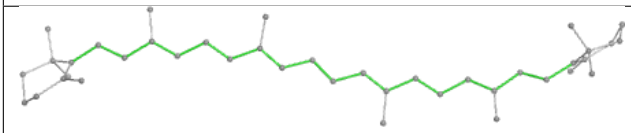
Ligand BCR a 407



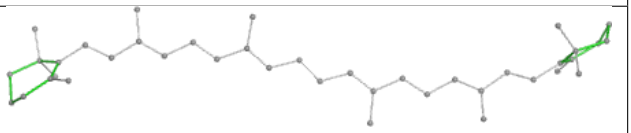
Bond lengths



Bond angles

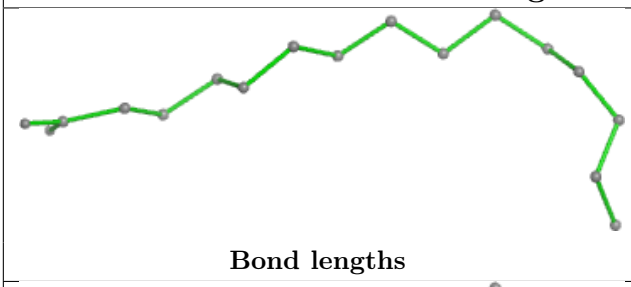


Torsions

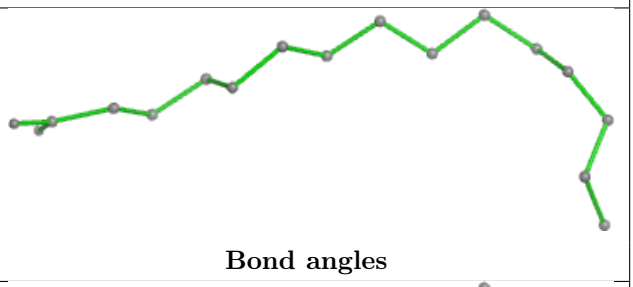


Rings

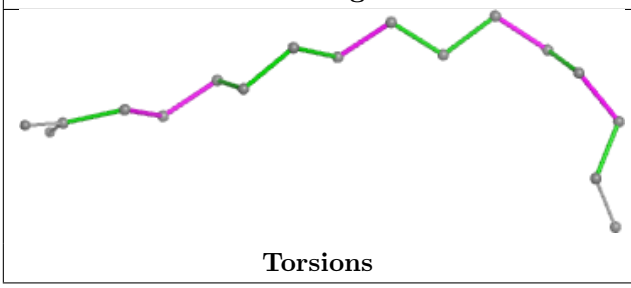
Ligand STE B 621



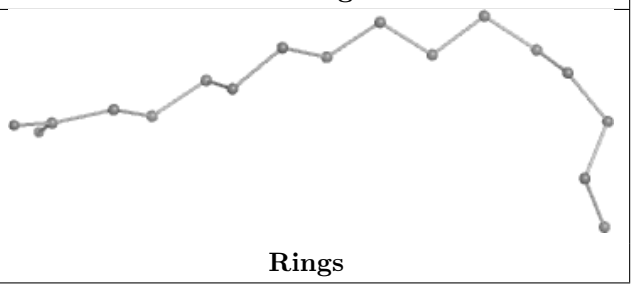
Bond lengths



Bond angles

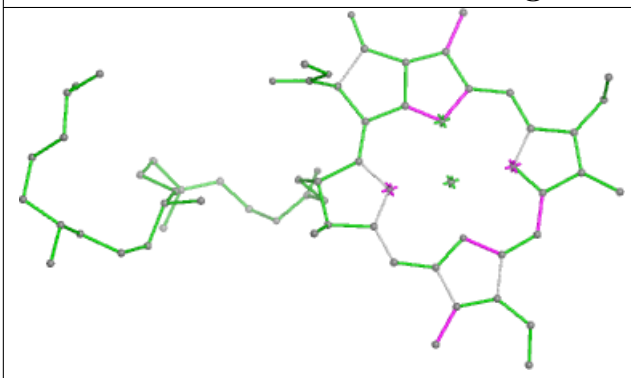


Torsions

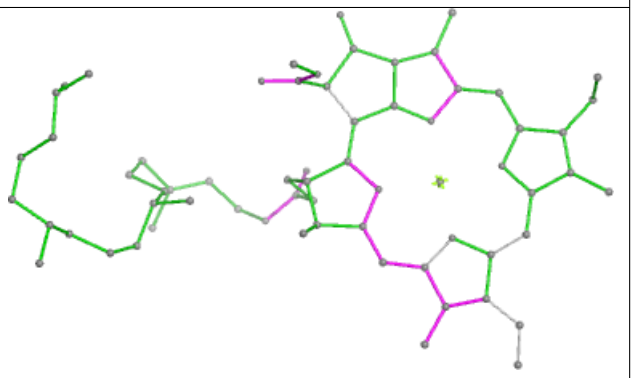


Rings

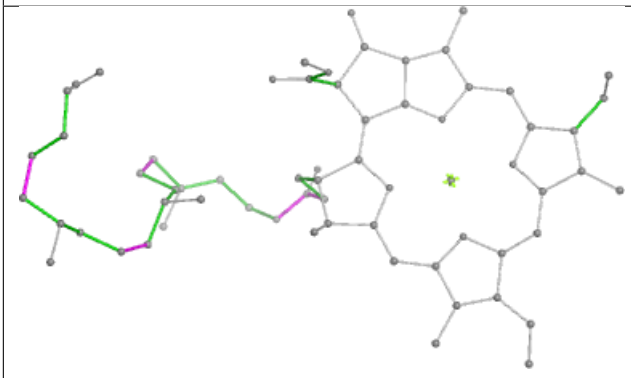
Ligand CLA B 612



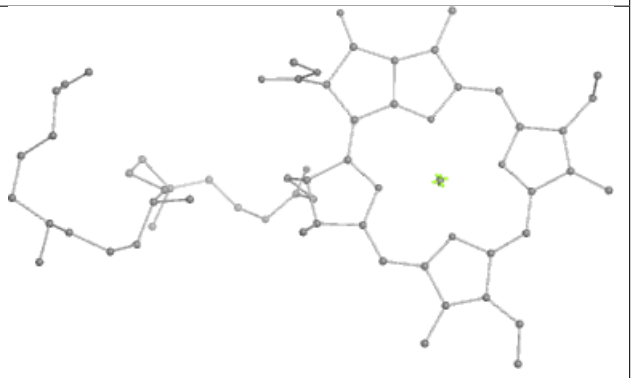
Bond lengths



Bond angles

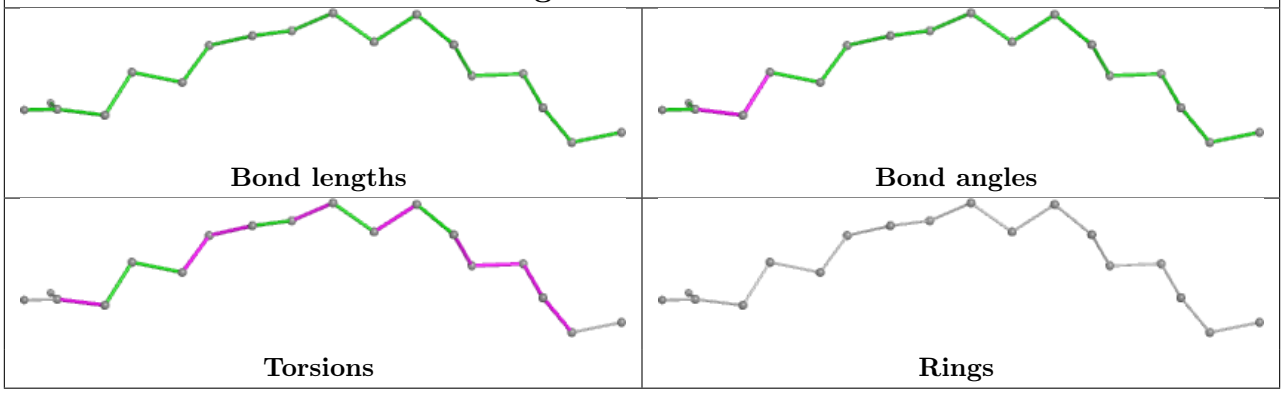


Torsions

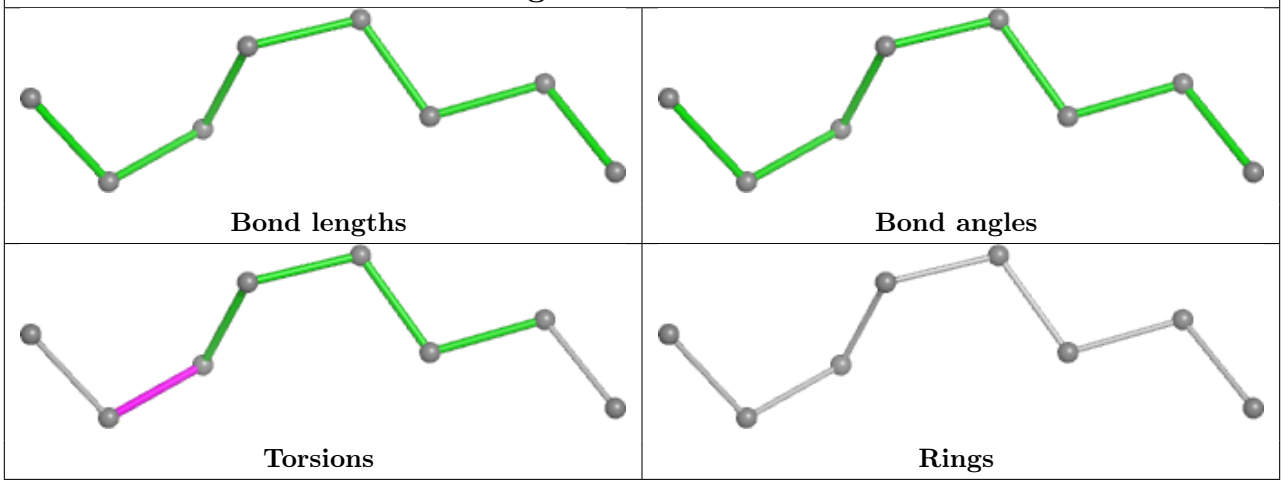


Rings

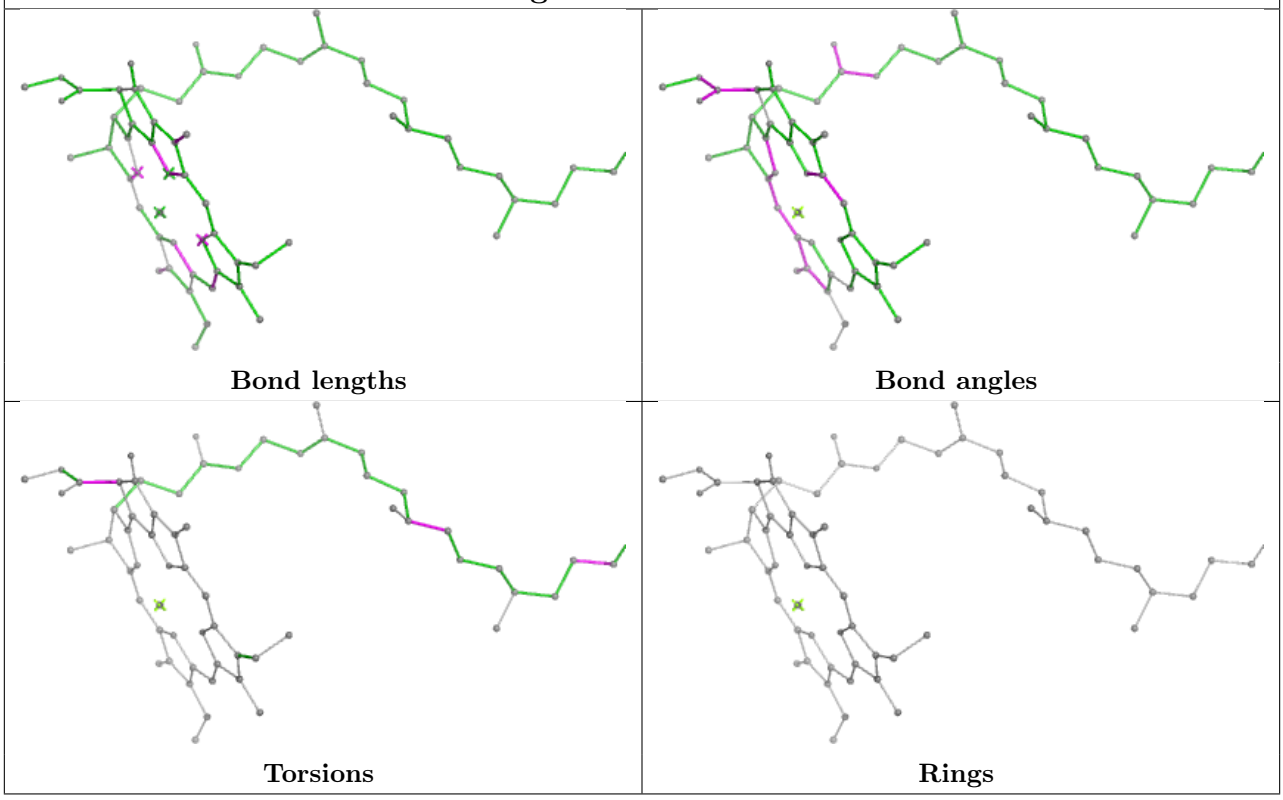
Ligand STE t 101



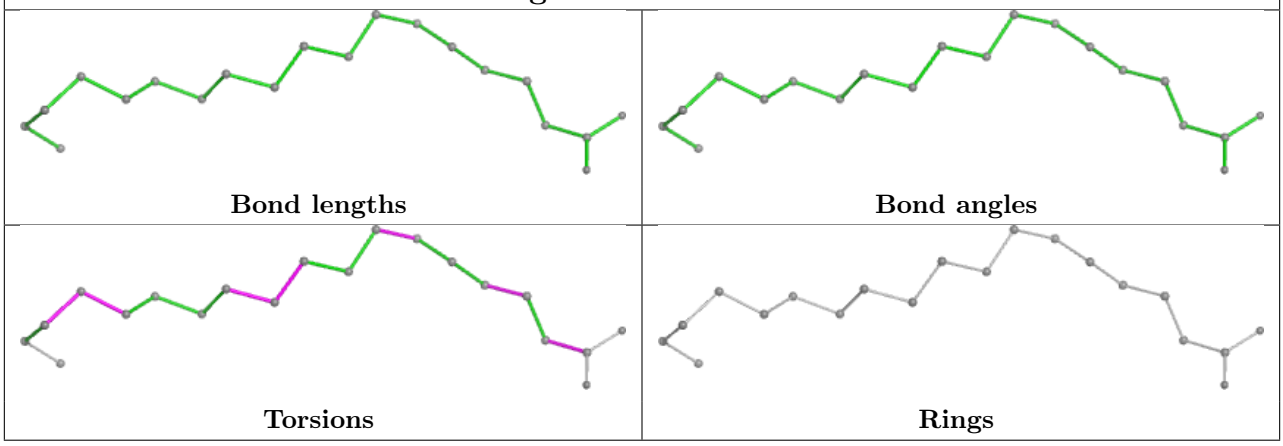
Ligand STE A 414



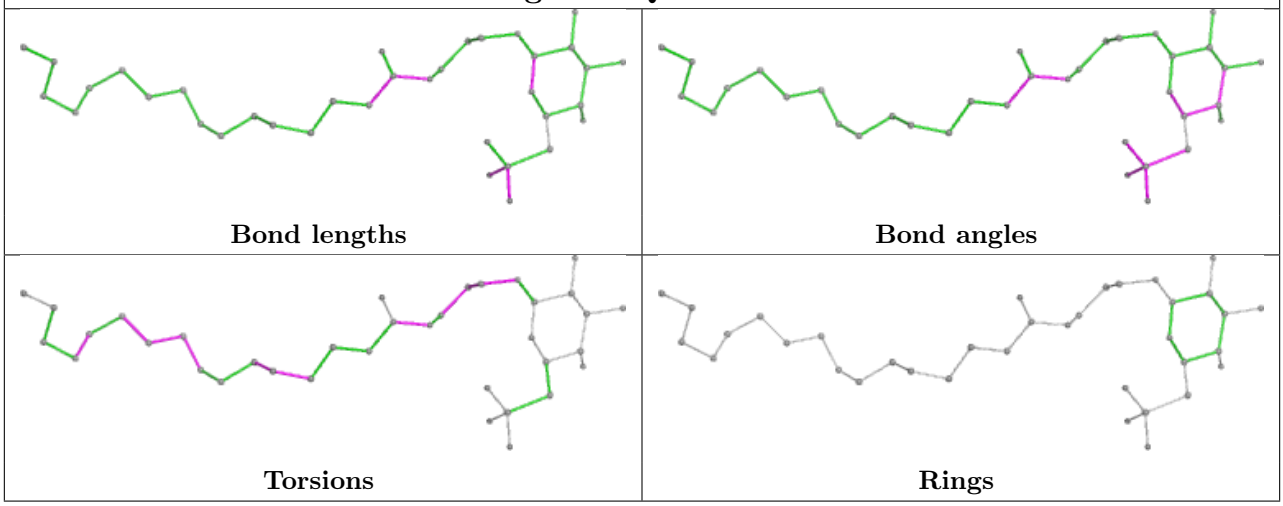
Ligand CLA c 508



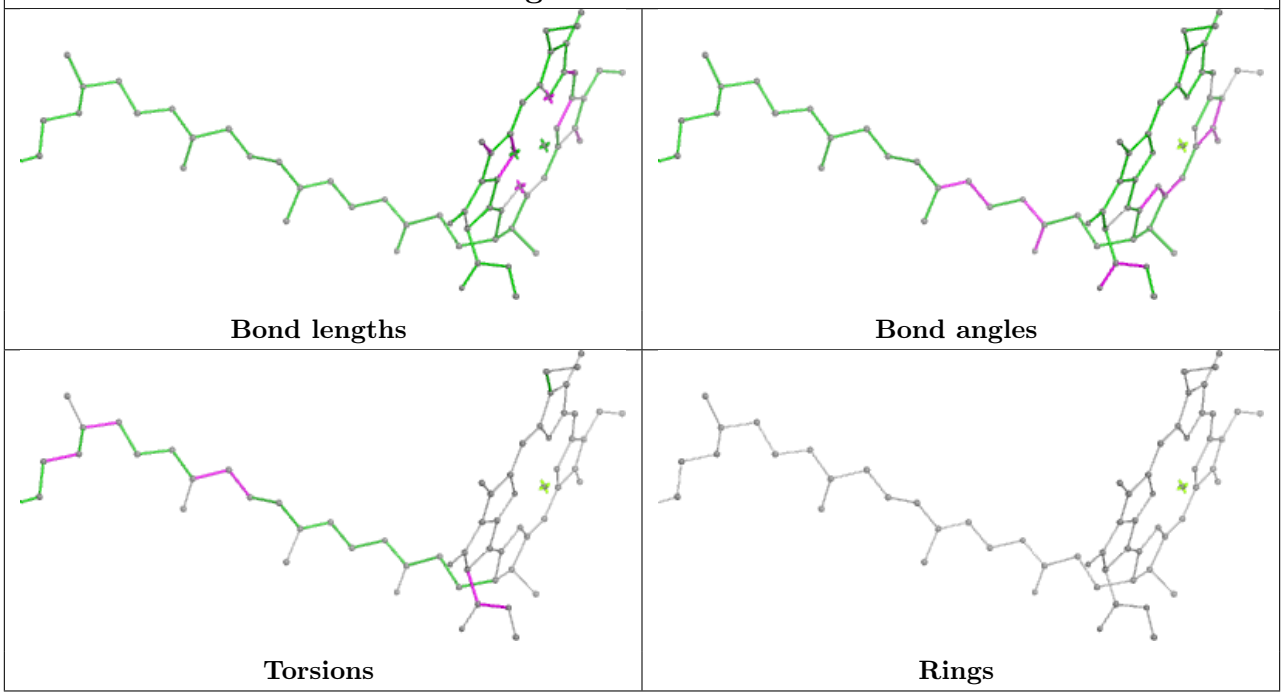
Ligand STE E 103



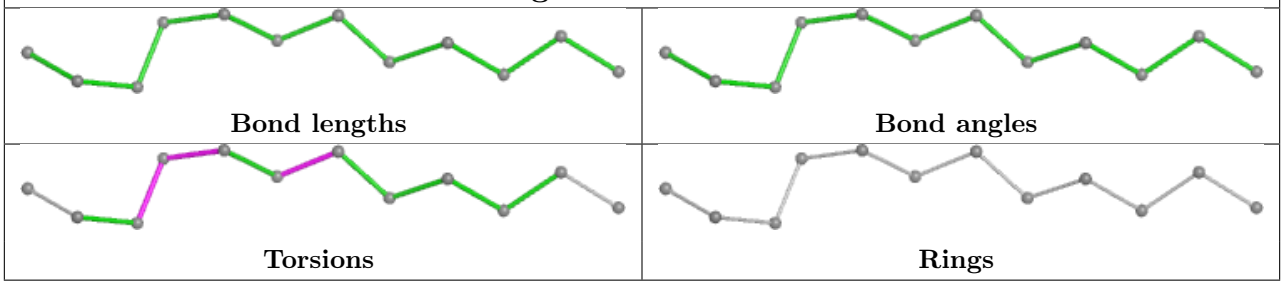
Ligand SQD X 101



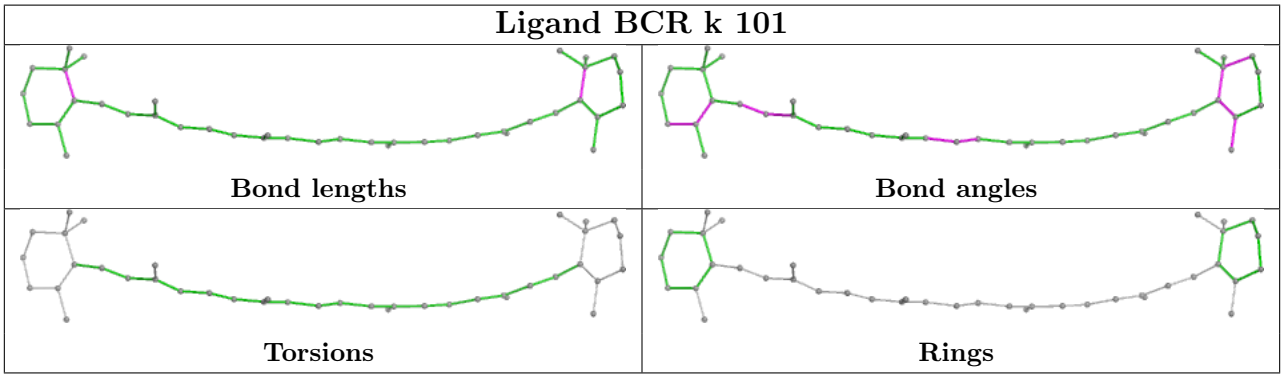
Ligand CLA B 604



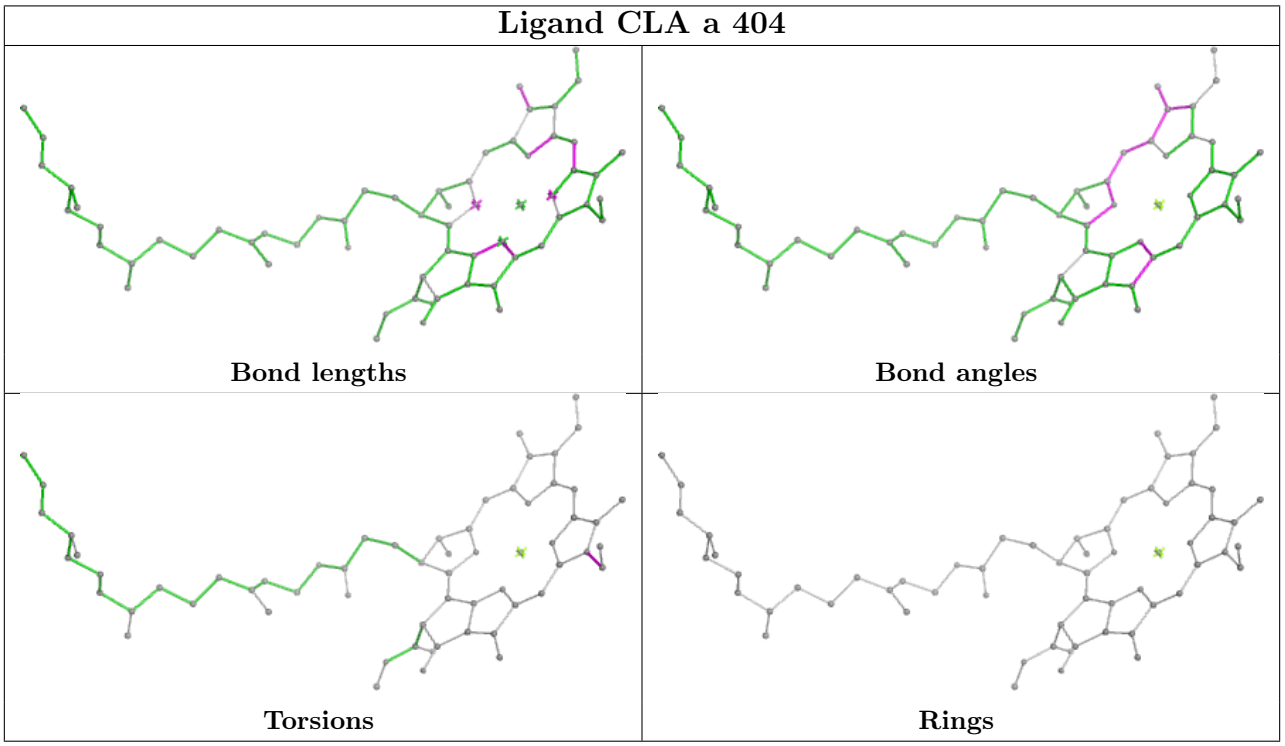
Ligand STE b 601



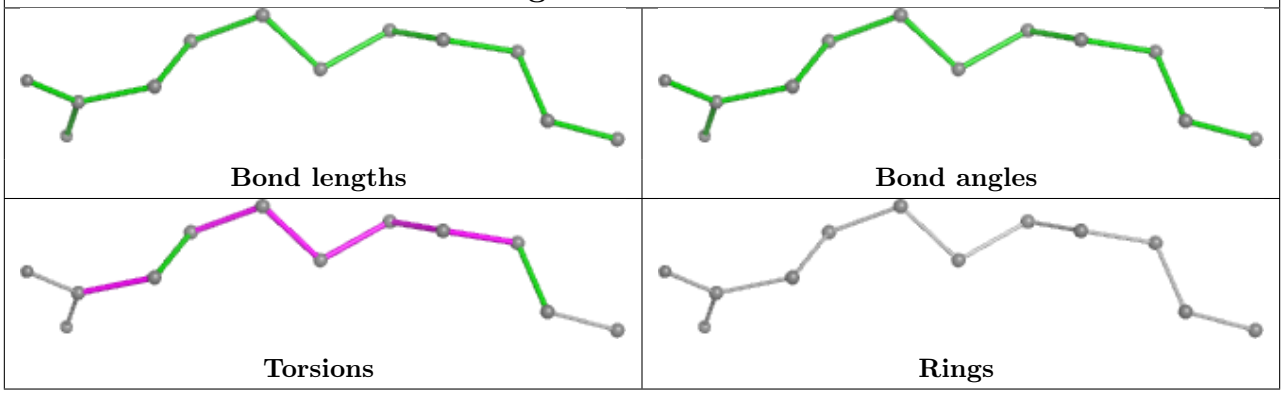
Ligand BCR k 101



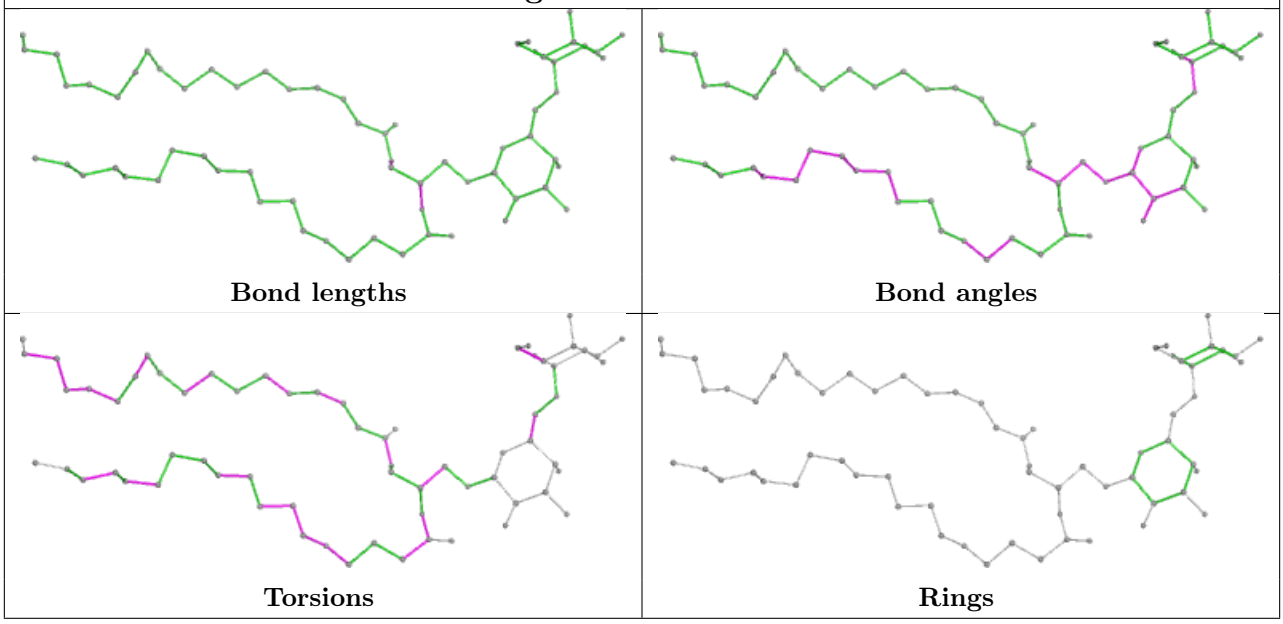
Ligand CLA a 404



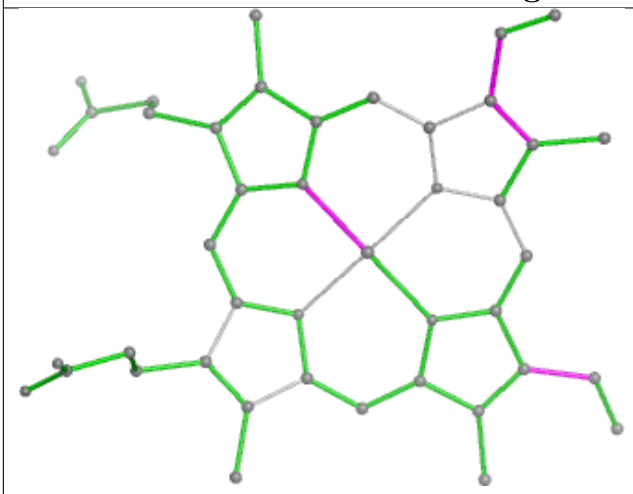
Ligand STE C 521



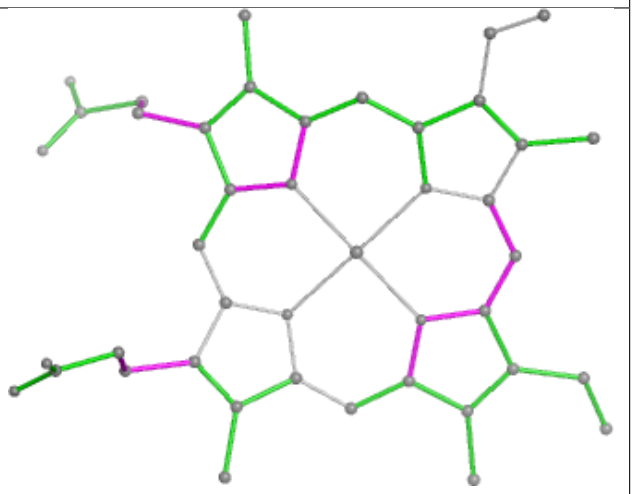
Ligand DGD a 413



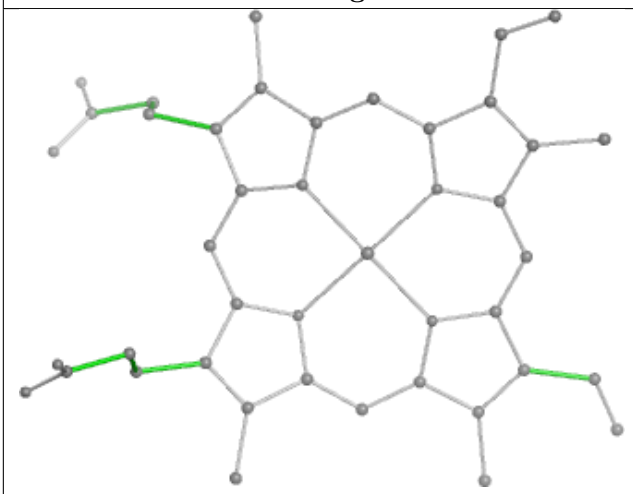
Ligand HEM e 105



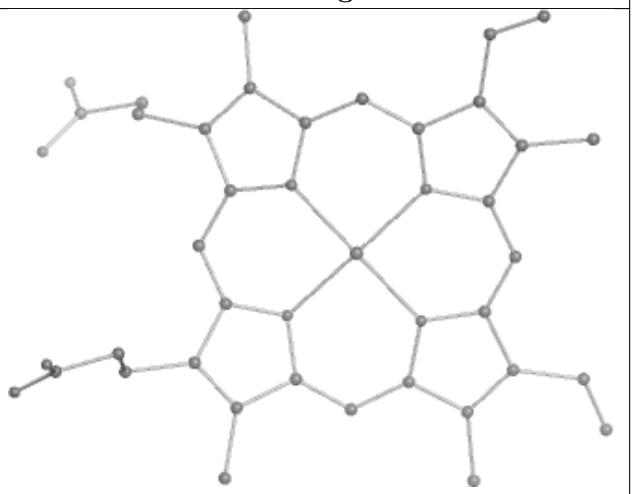
Bond lengths



Bond angles

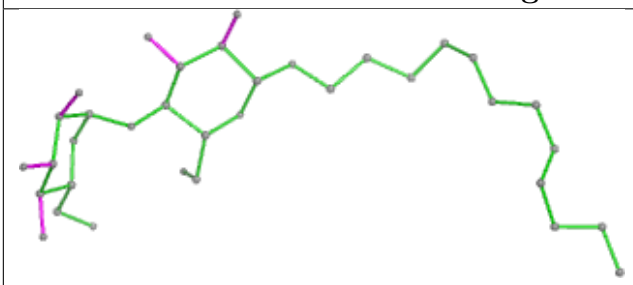


Torsions

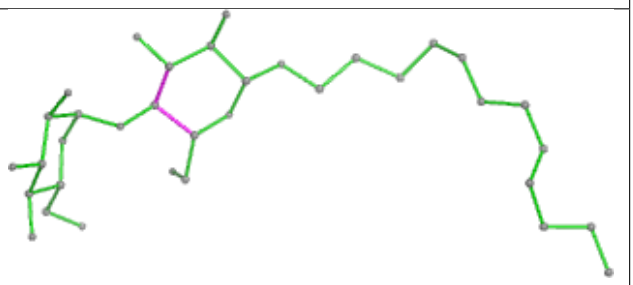


Rings

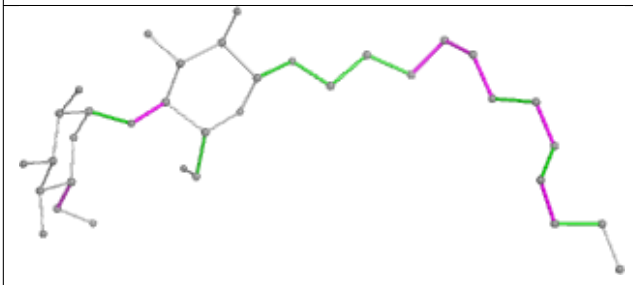
Ligand LMT C 525



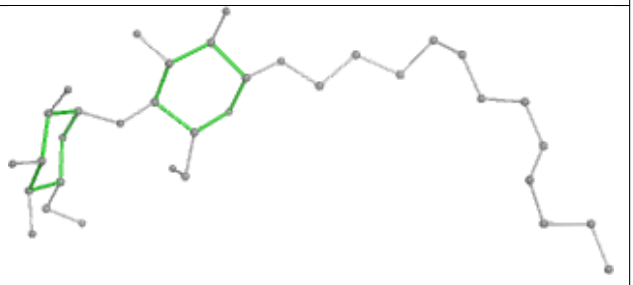
Bond lengths



Bond angles

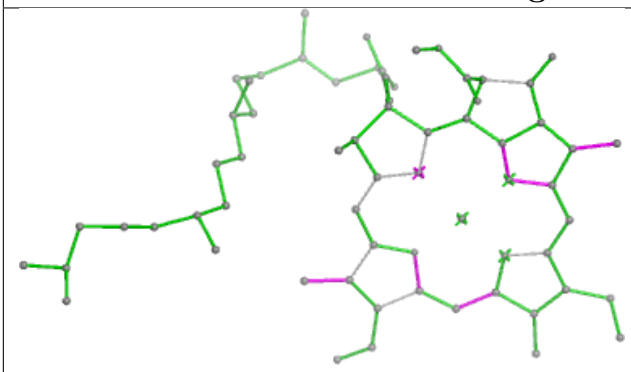


Torsions

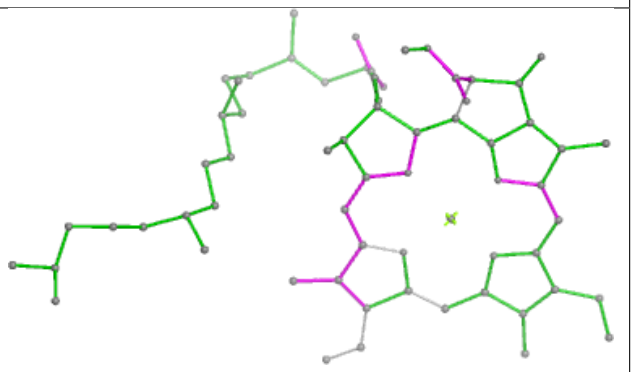


Rings

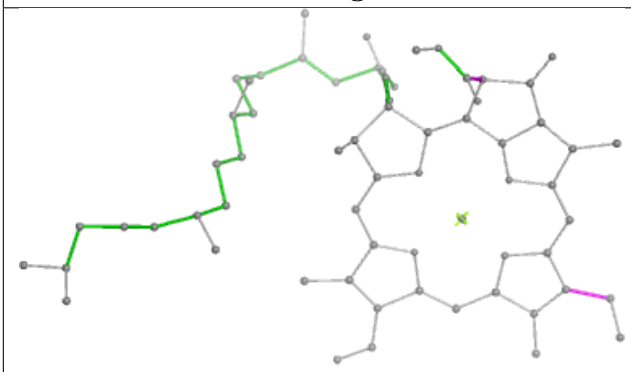
Ligand CLA a 419



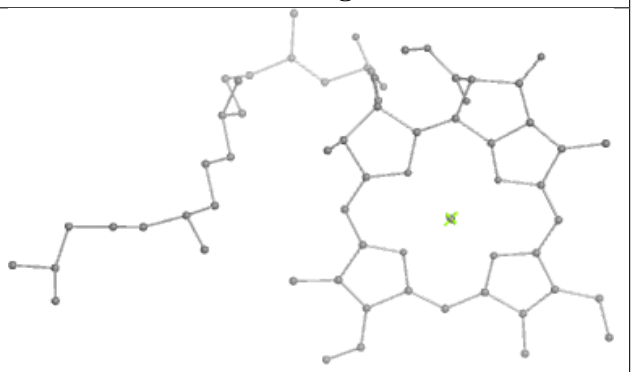
Bond lengths



Bond angles

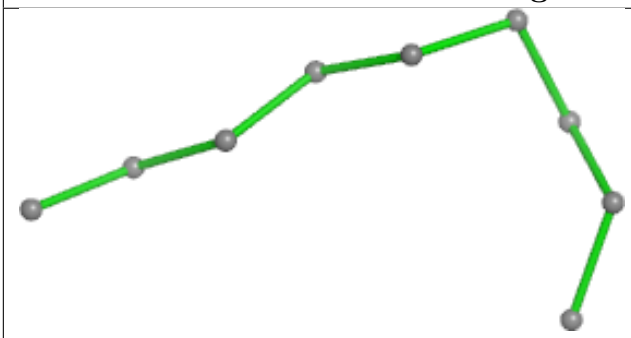


Torsions

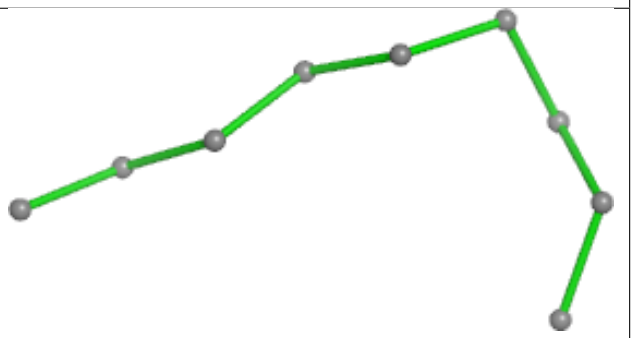


Rings

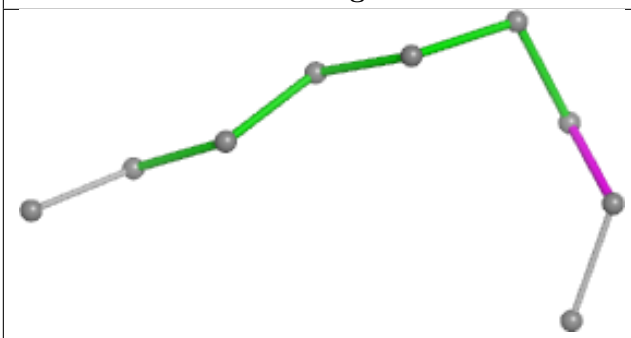
Ligand STE d 413



Bond lengths



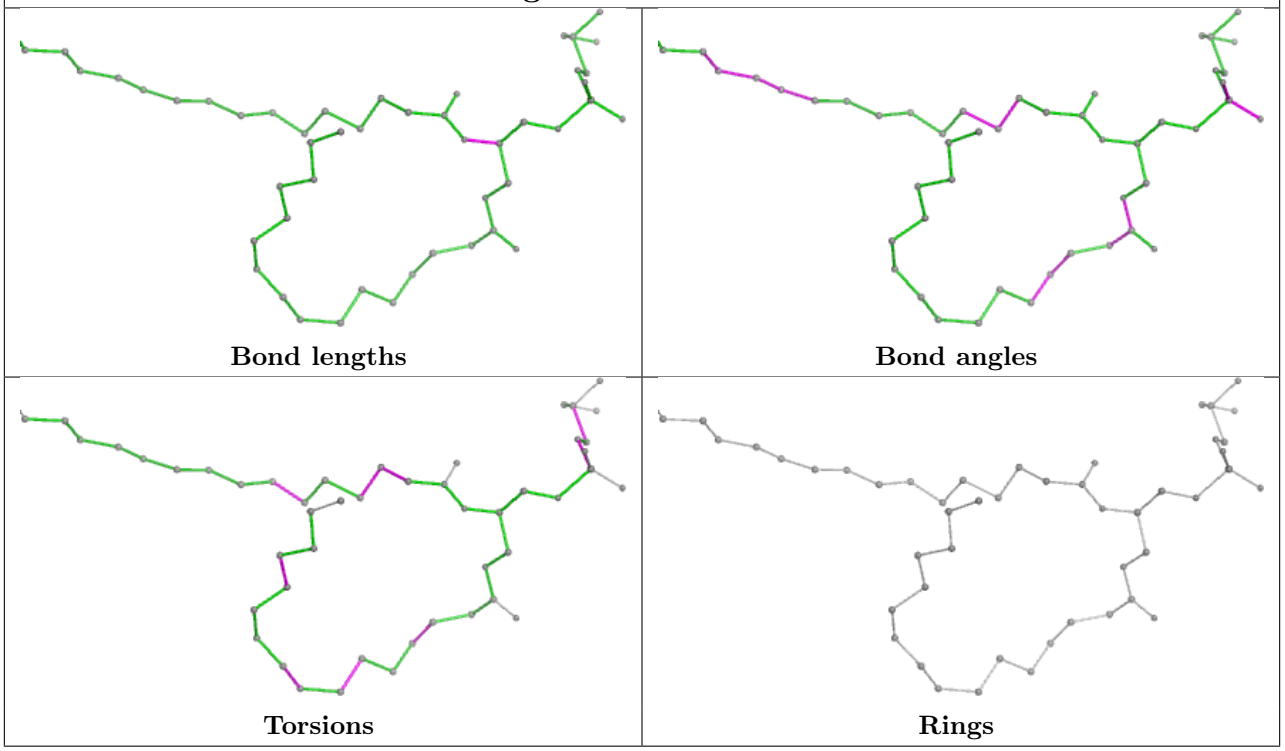
Bond angles



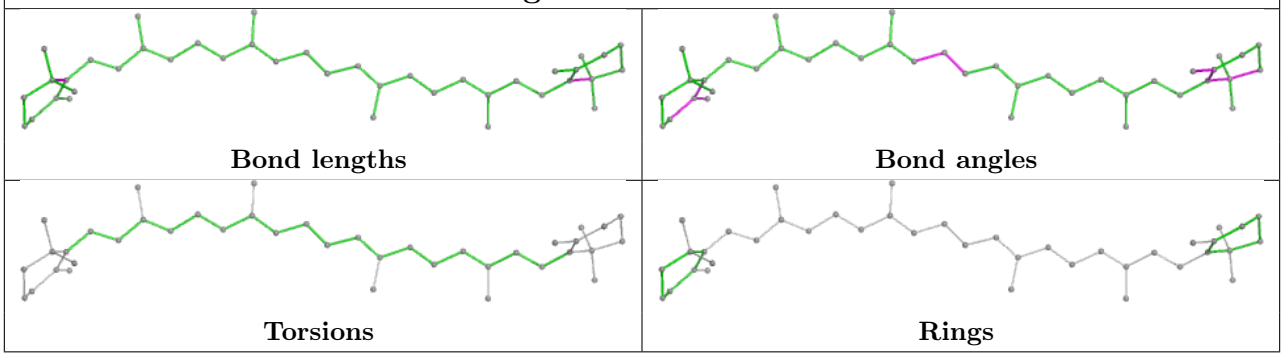
Torsions

Rings

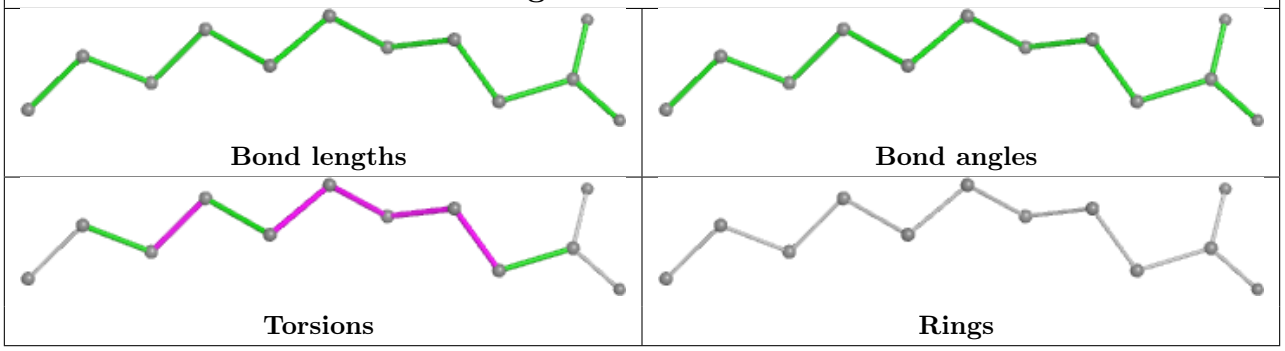
Ligand LHG D 411



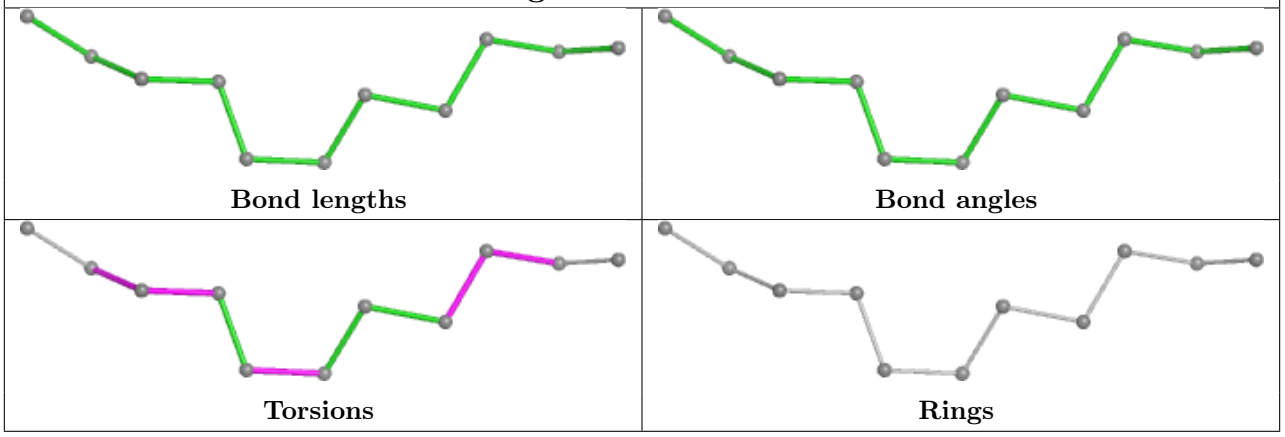
Ligand BCR C 515



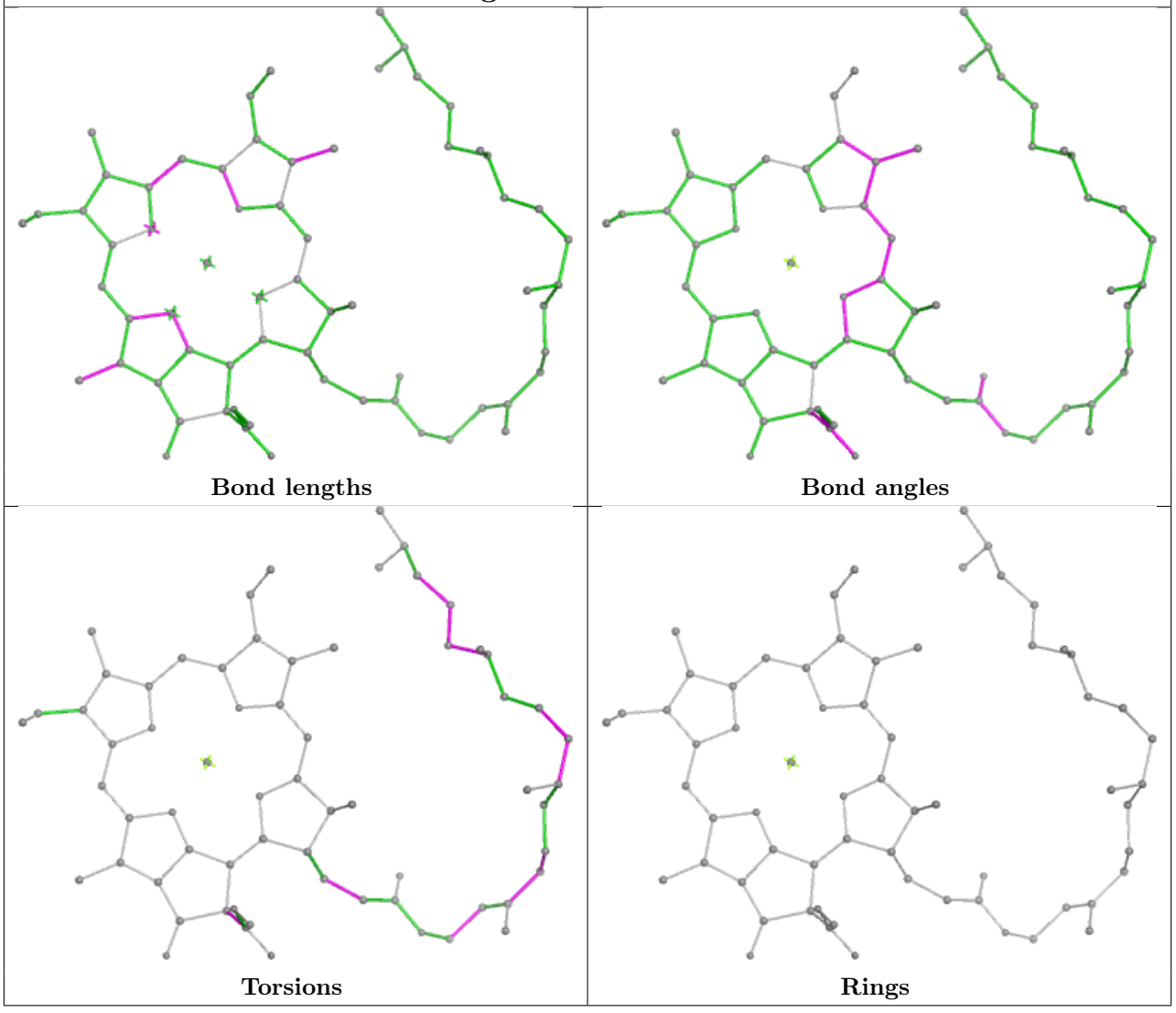
Ligand STE A 421



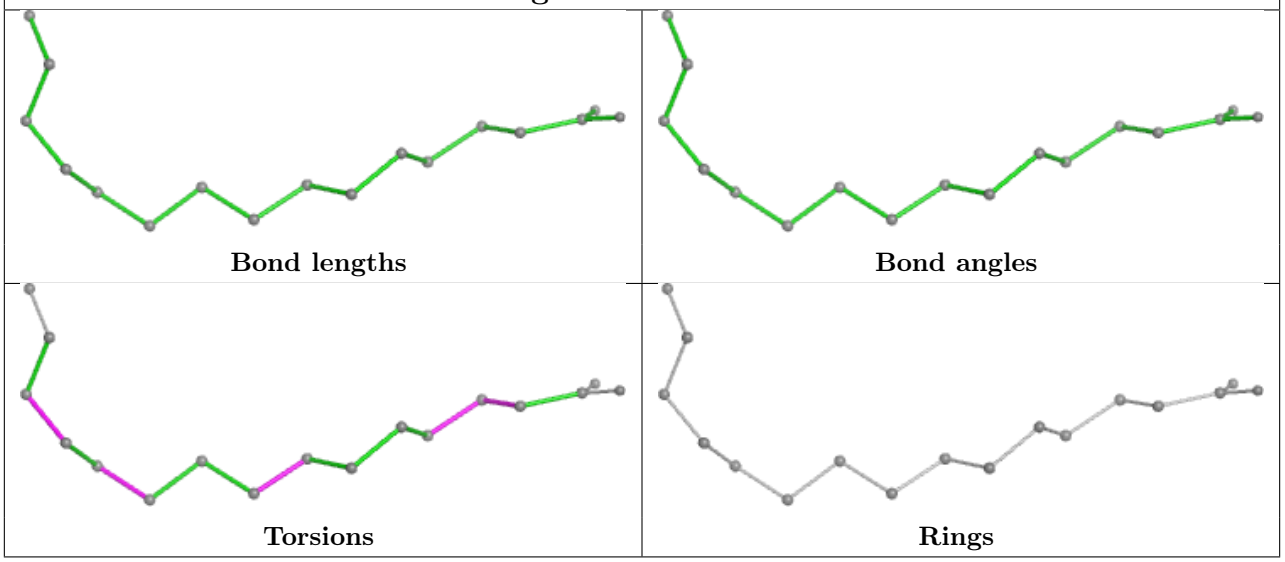
Ligand STE A 416



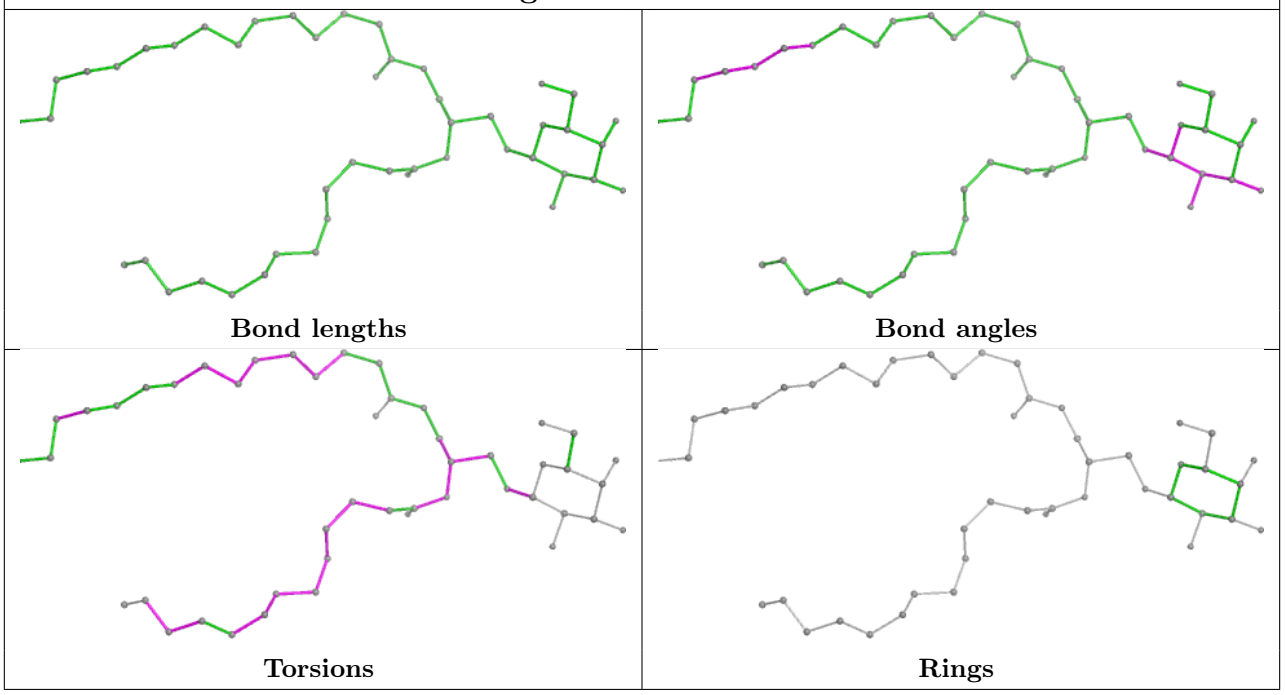
Ligand CLA C 512



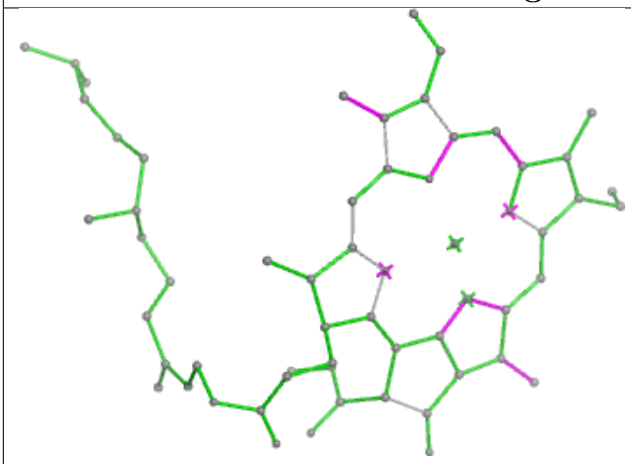
Ligand STE b 622



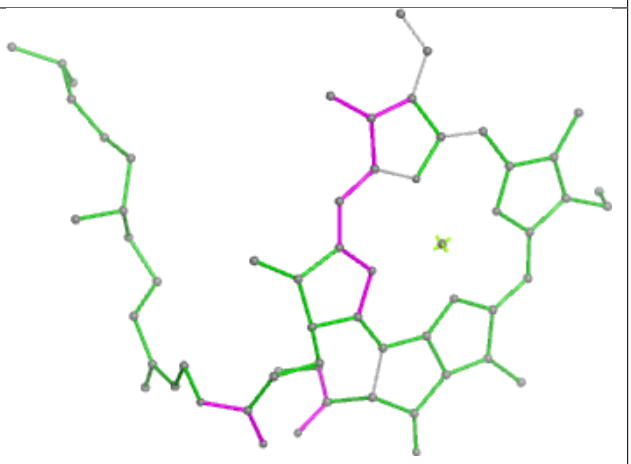
Ligand LMG A 410



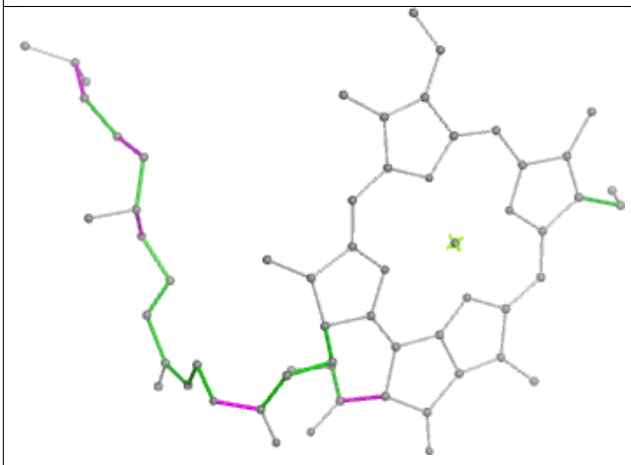
Ligand CLA B 616



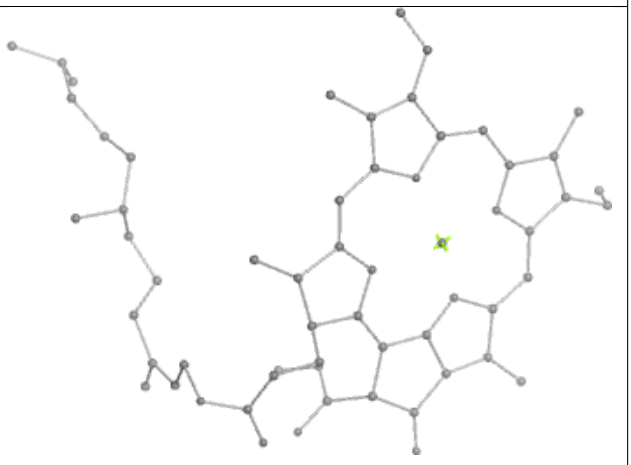
Bond lengths



Bond angles

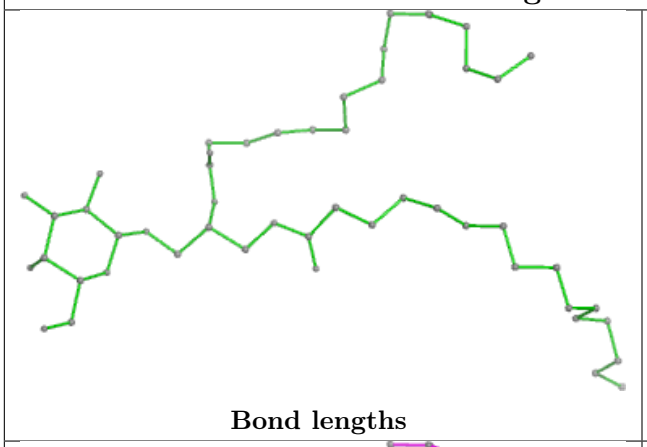


Torsions

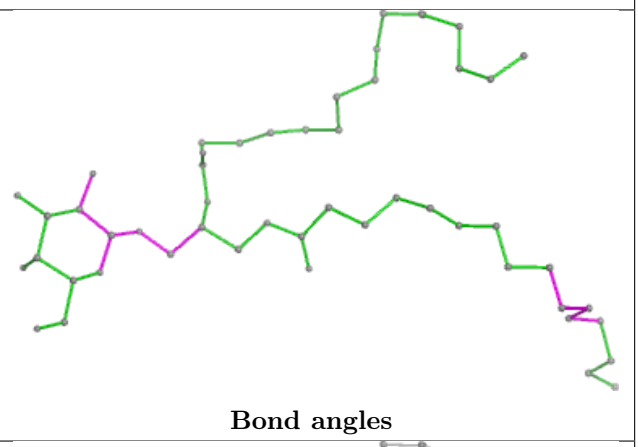


Rings

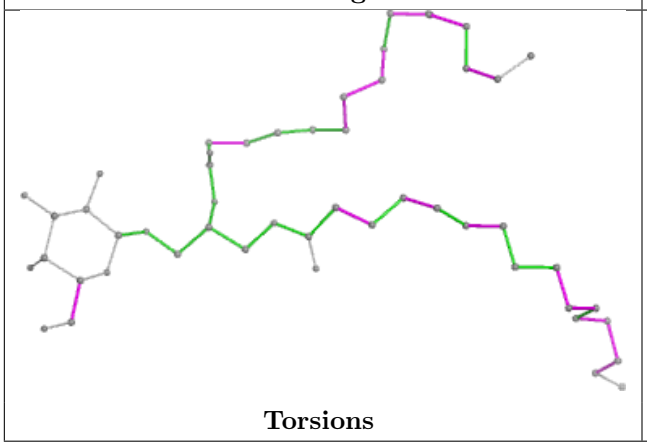
Ligand LMG d 408



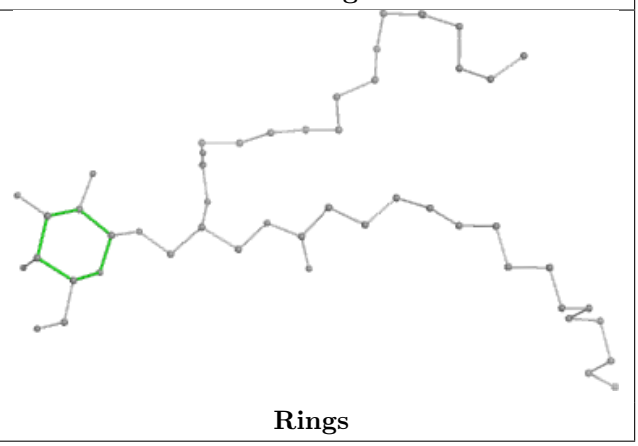
Bond lengths



Bond angles

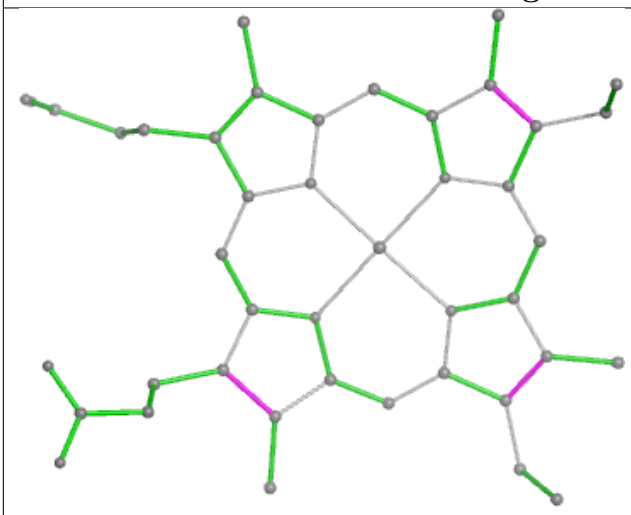


Torsions

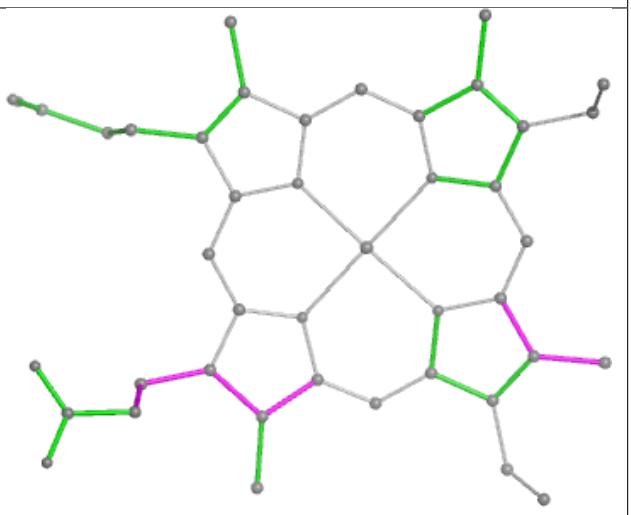


Rings

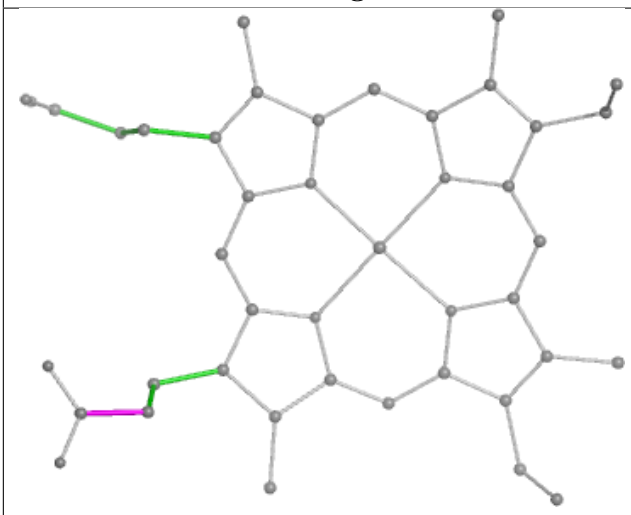
Ligand HEC V 201



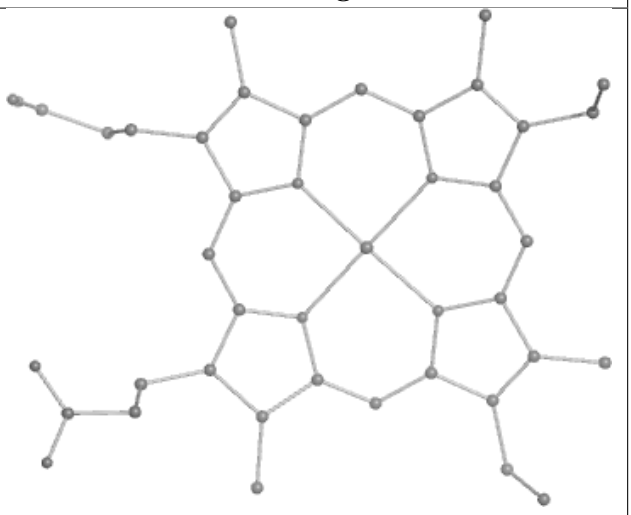
Bond lengths



Bond angles

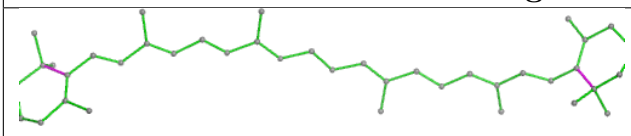


Torsions

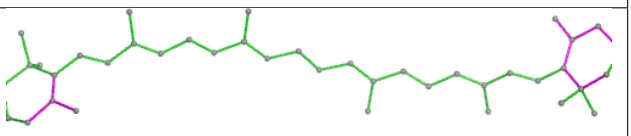


Rings

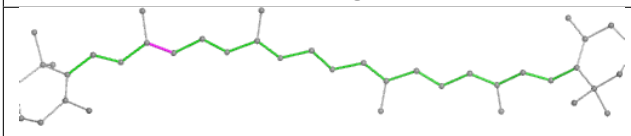
Ligand BCR b 620



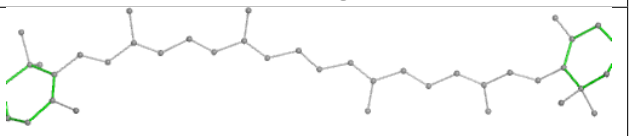
Bond lengths



Bond angles

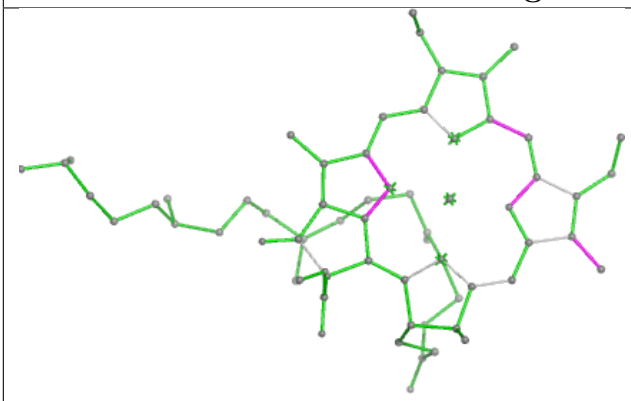


Torsions

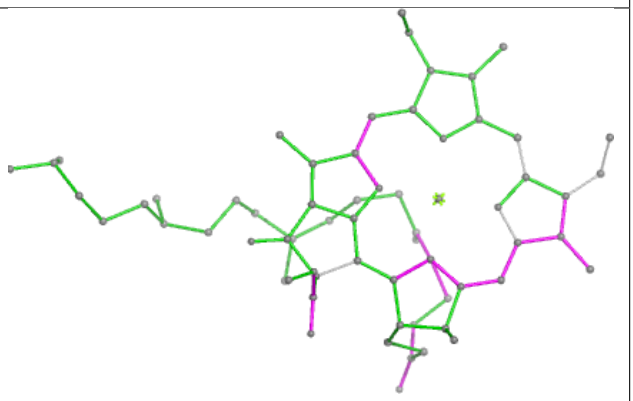


Rings

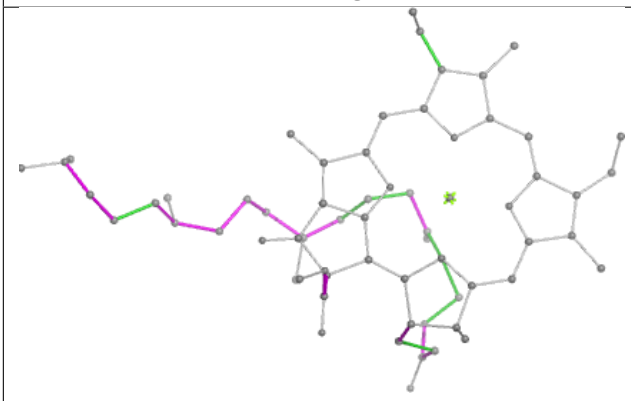
Ligand CLA B 601



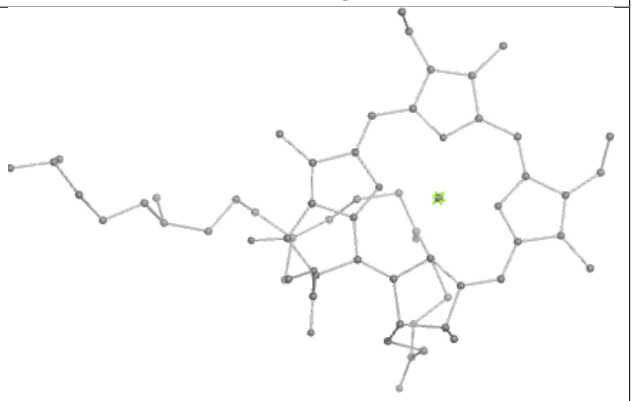
Bond lengths



Bond angles

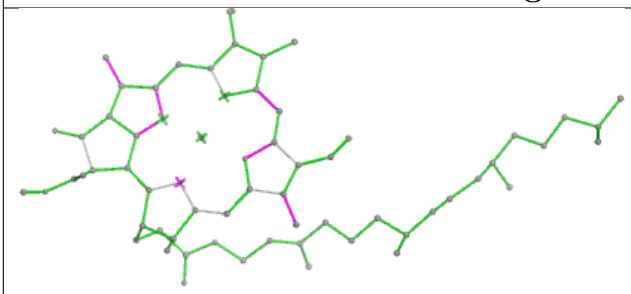


Torsions

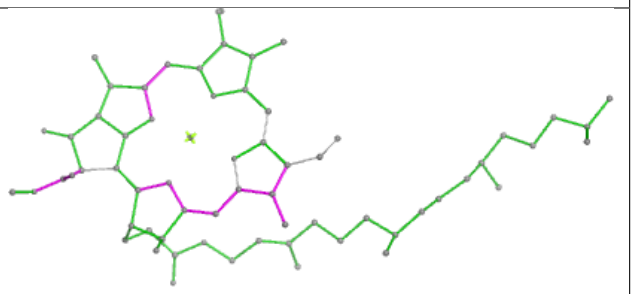


Rings

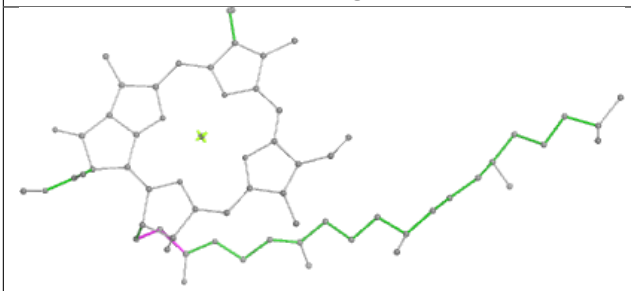
Ligand CLA C 501



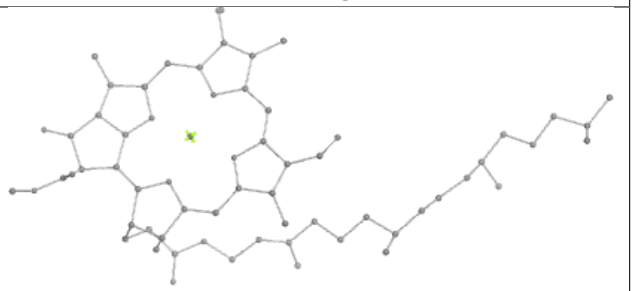
Bond lengths



Bond angles

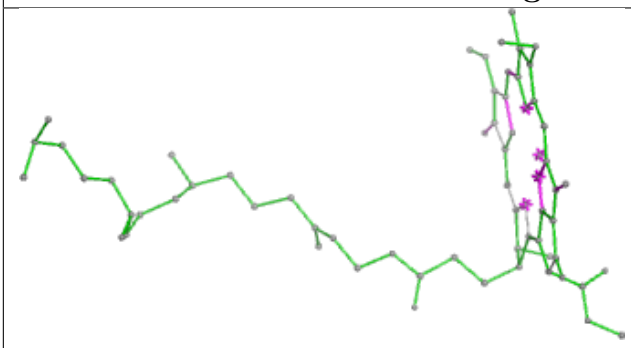


Torsions

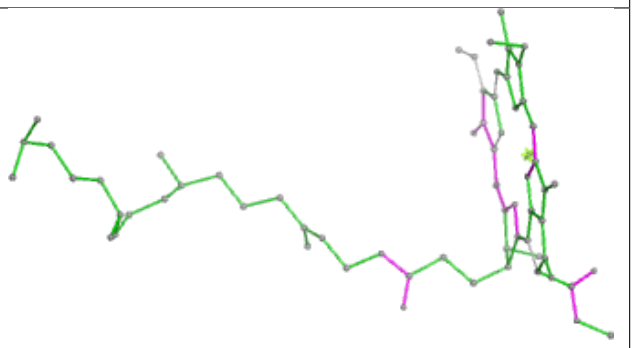


Rings

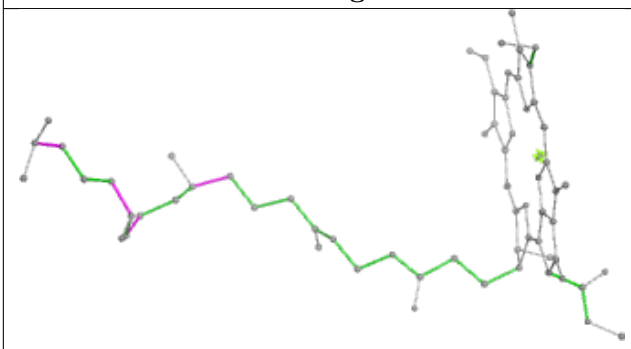
Ligand CLA D 405



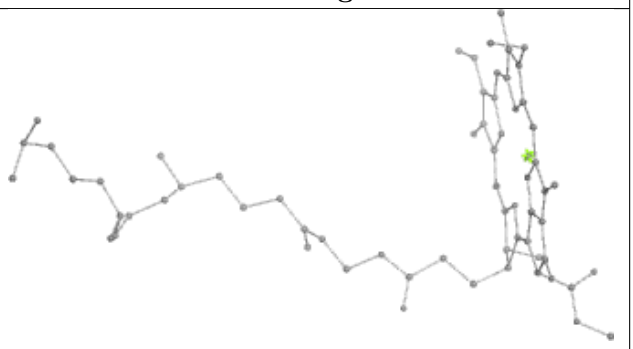
Bond lengths



Bond angles

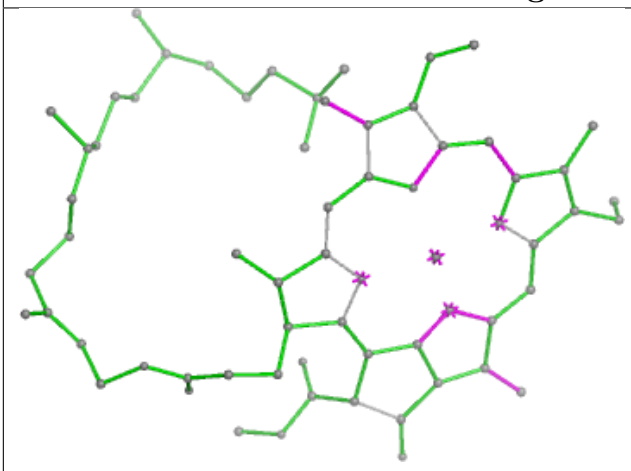


Torsions

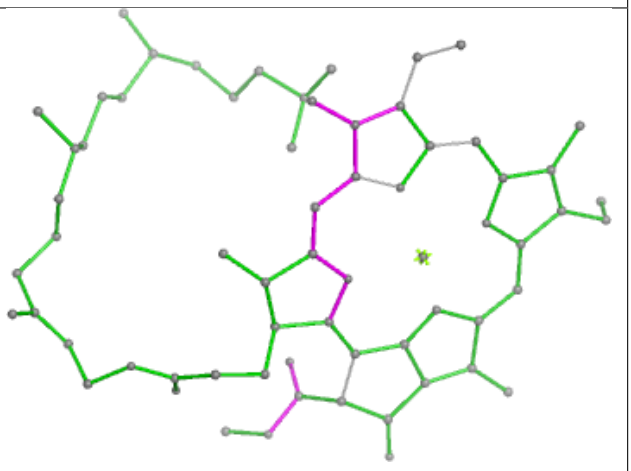


Rings

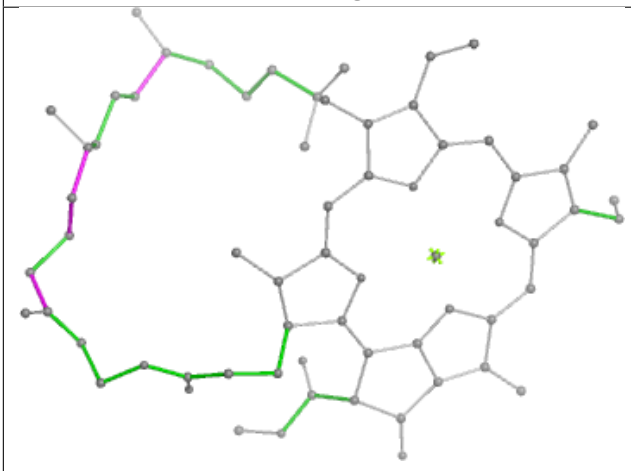
Ligand CLA b 616



Bond lengths



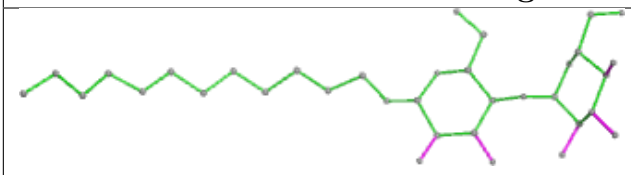
Bond angles



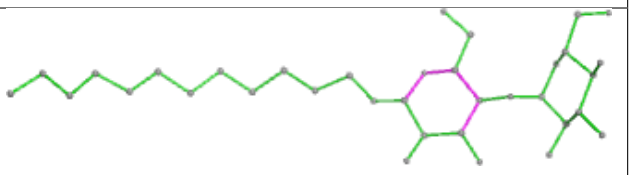
Torsions

Rings

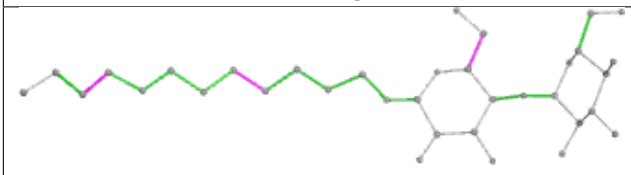
Ligand LMT M 102



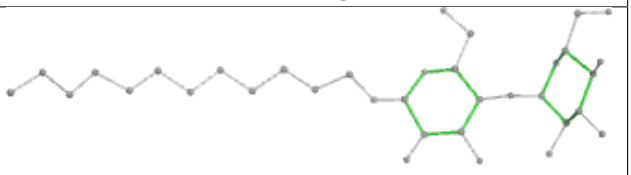
Bond lengths



Bond angles

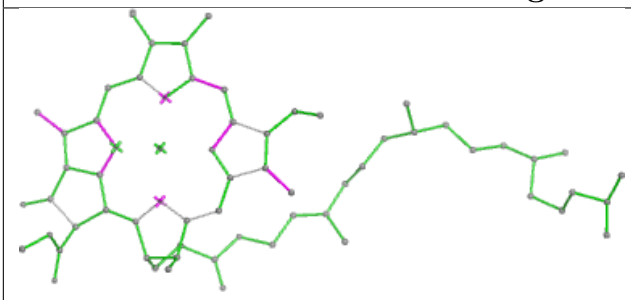


Torsions

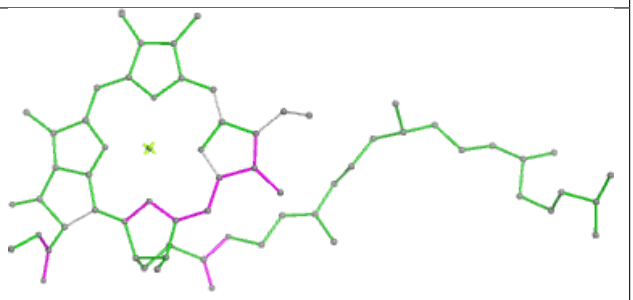


Rings

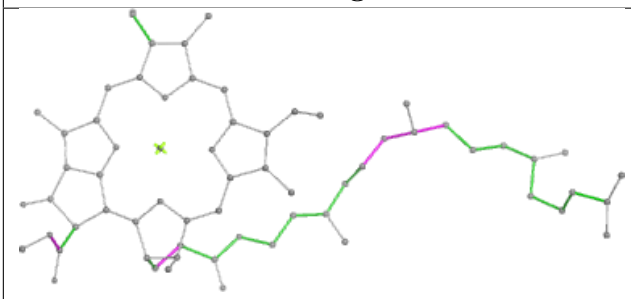
Ligand CLA b 604



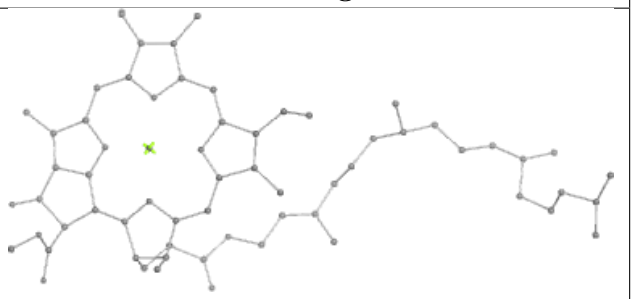
Bond lengths



Bond angles

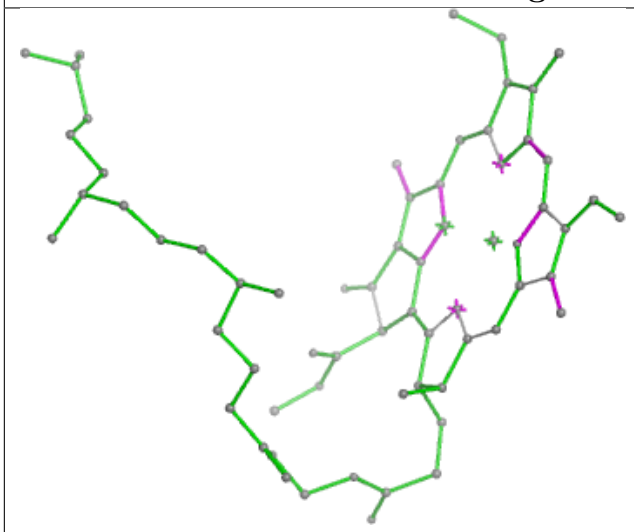


Torsions

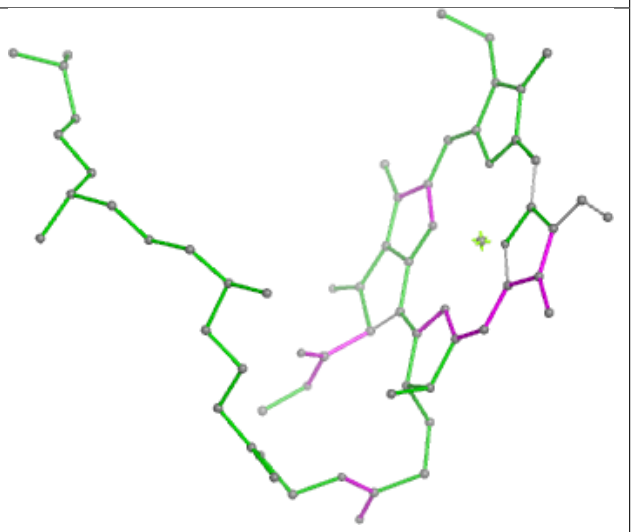


Rings

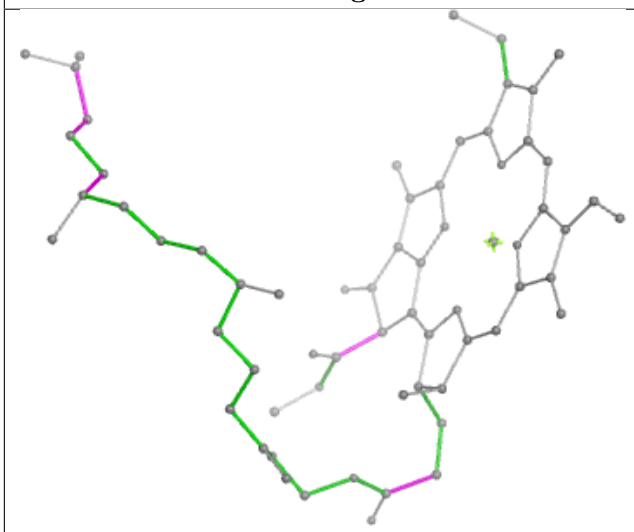
Ligand CLA b 614



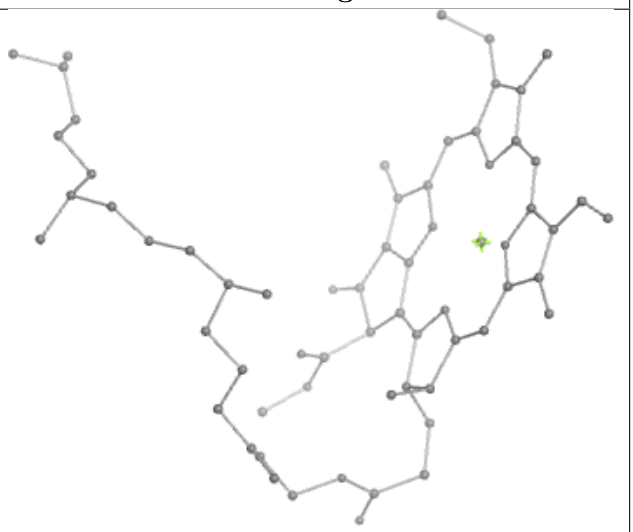
Bond lengths



Bond angles

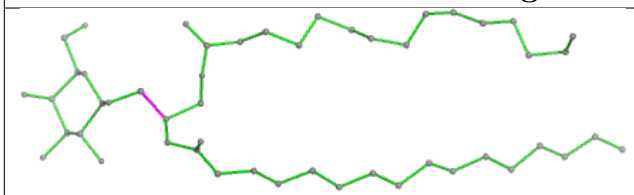


Torsions

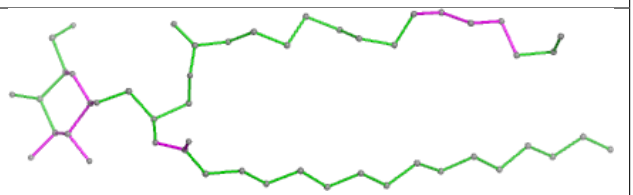


Rings

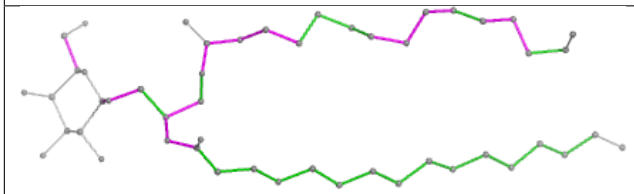
Ligand LMG C 524



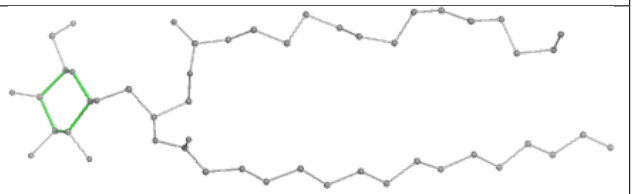
Bond lengths



Bond angles

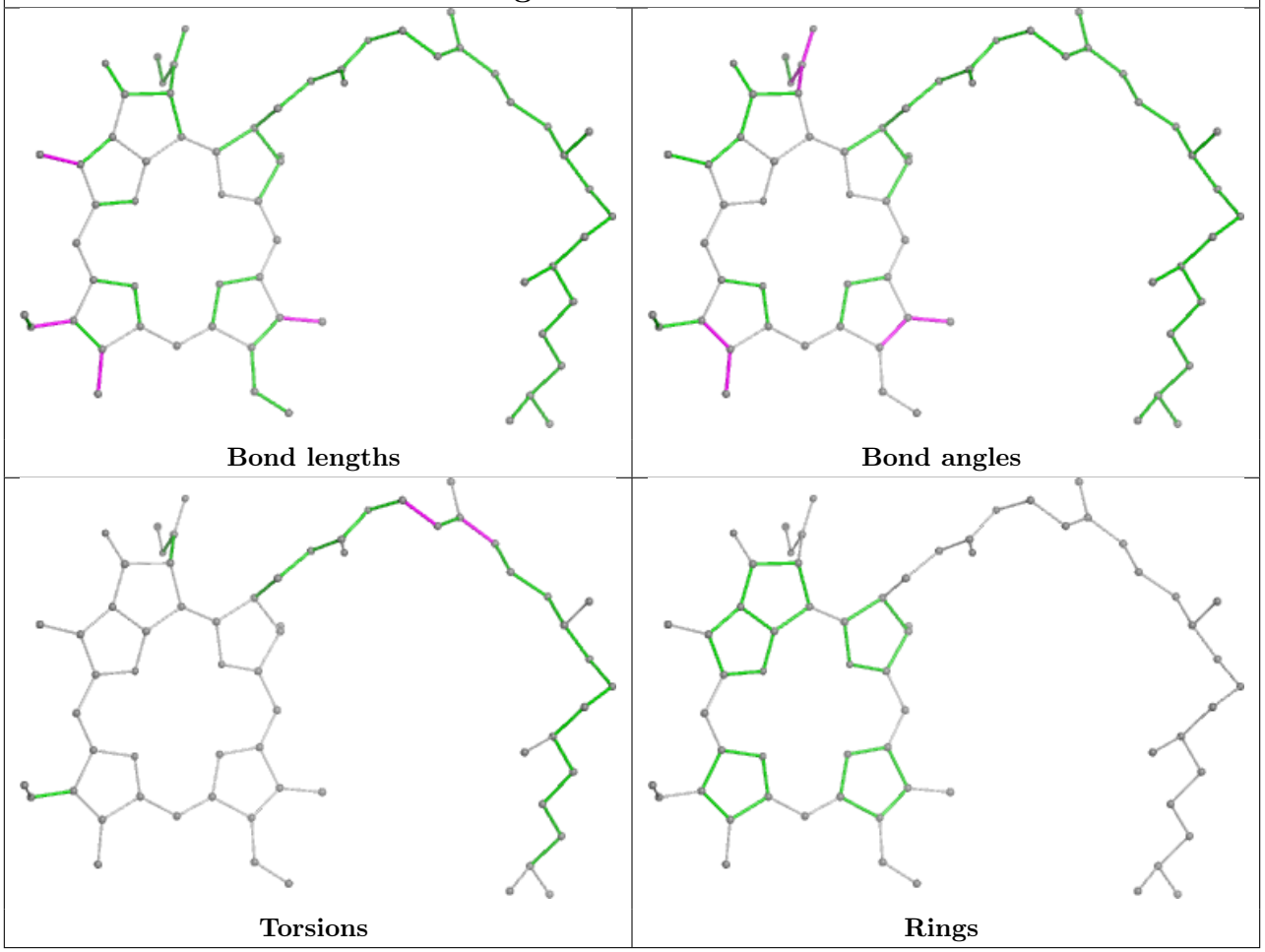


Torsions

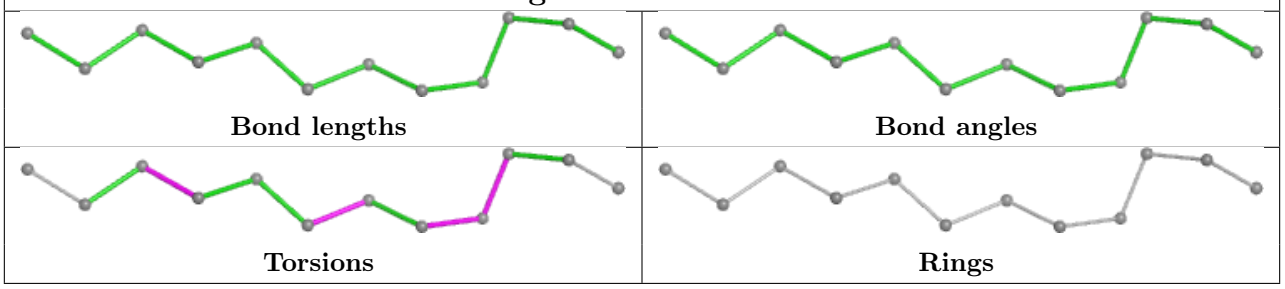


Rings

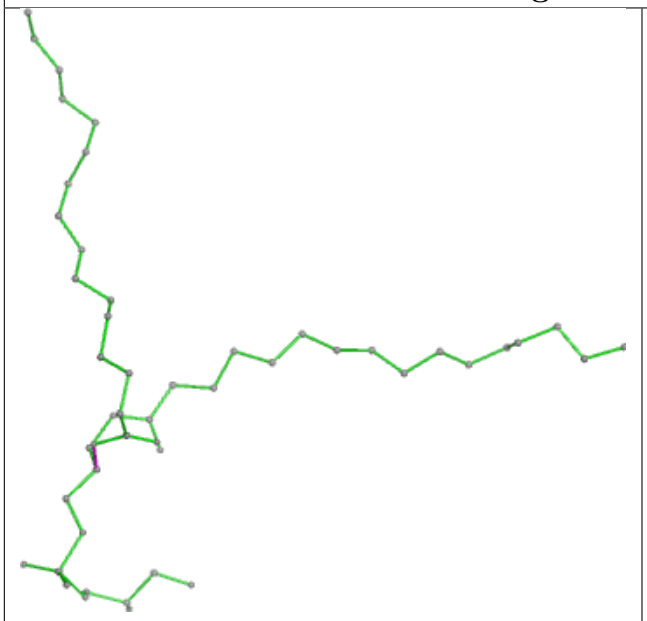
Ligand PHO A 418



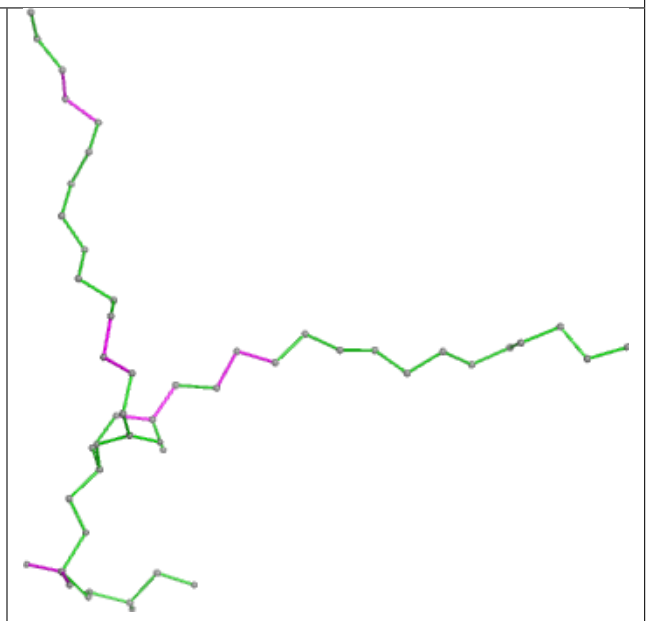
Ligand STE B 625



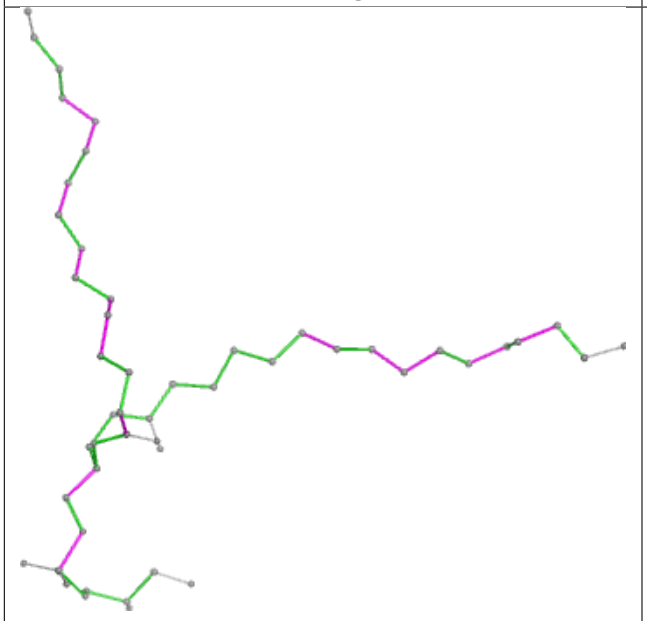
Ligand LHG l 101



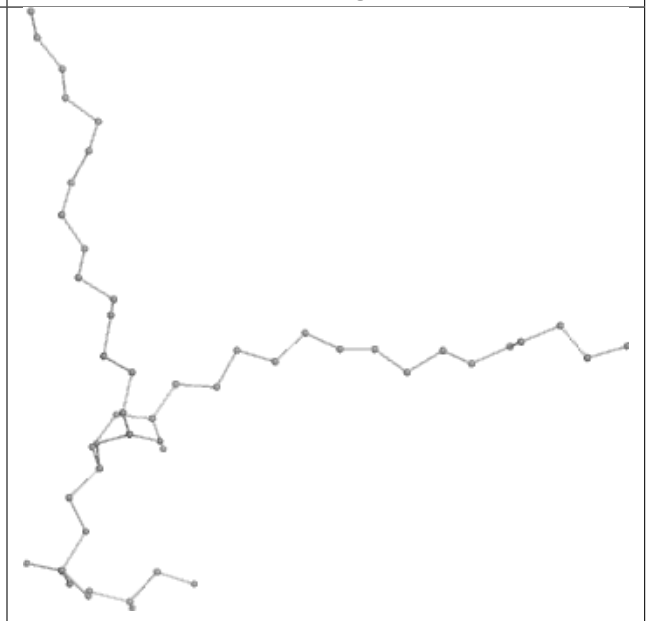
Bond lengths



Bond angles

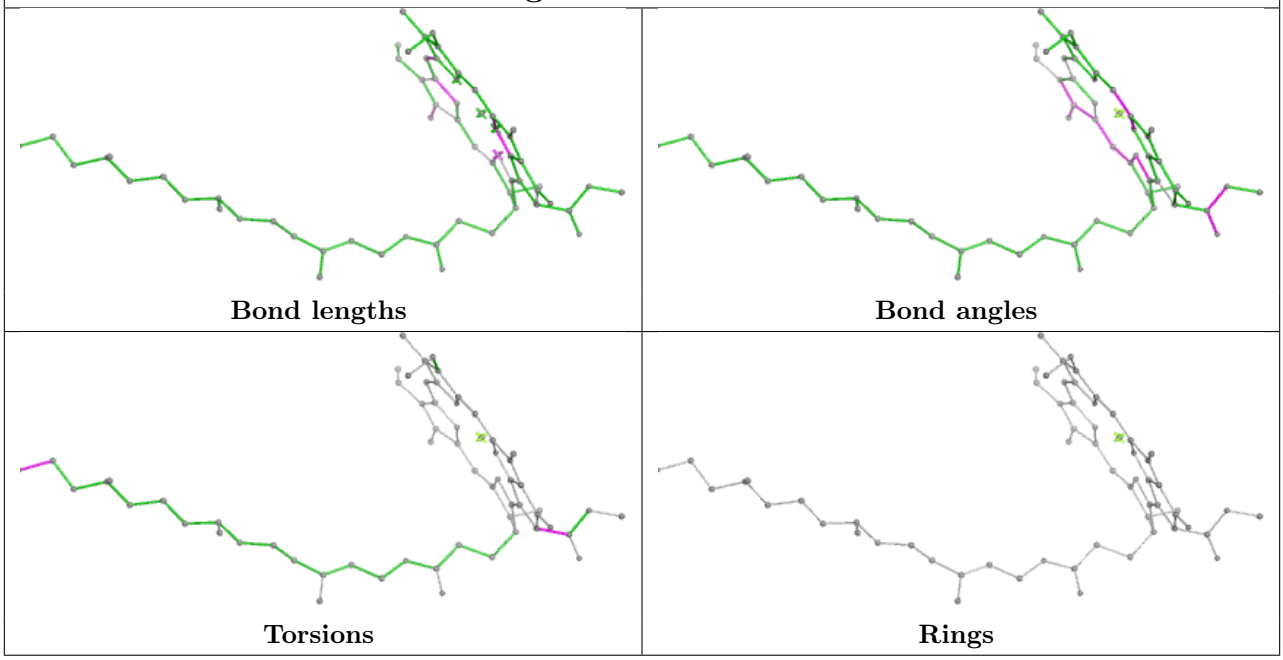


Torsions

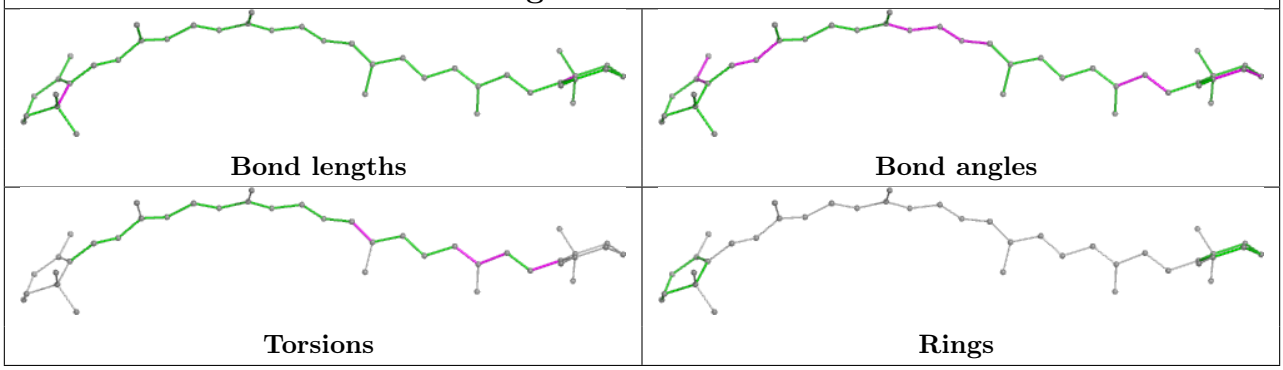


Rings

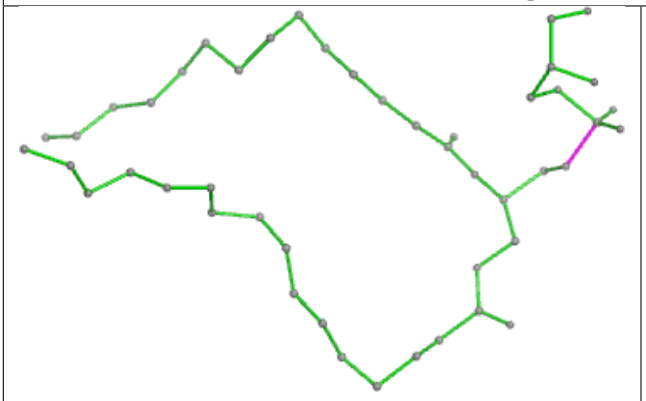
Ligand CLA B 607



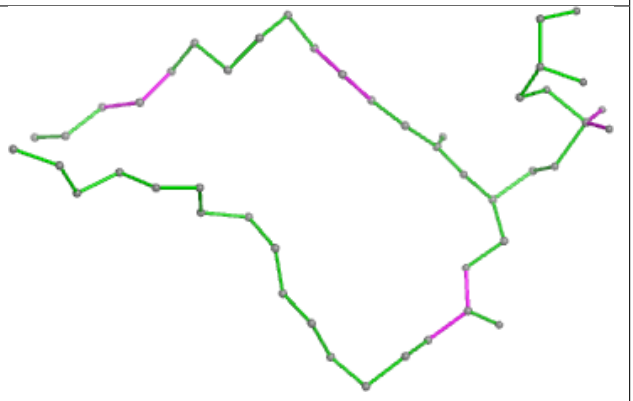
Ligand BCR h 102



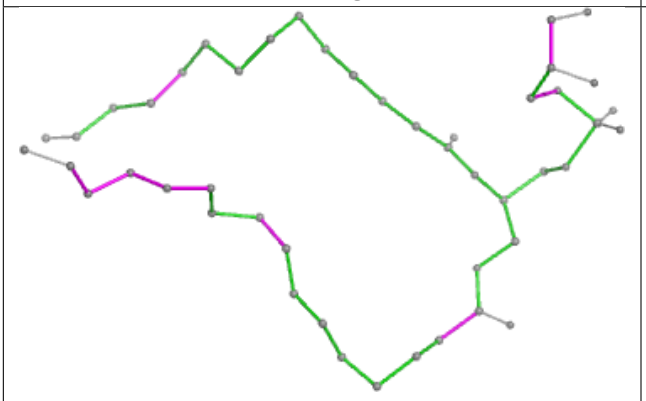
Ligand LHG D 410



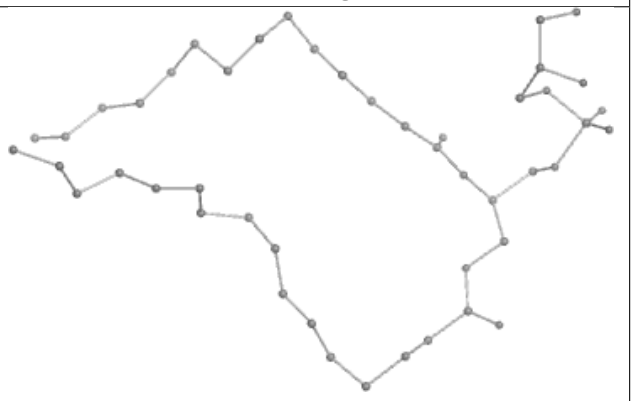
Bond lengths



Bond angles

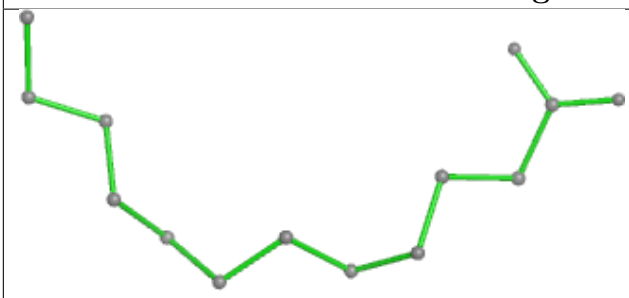


Torsions

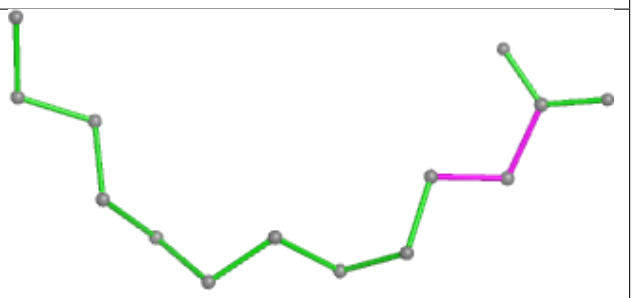


Rings

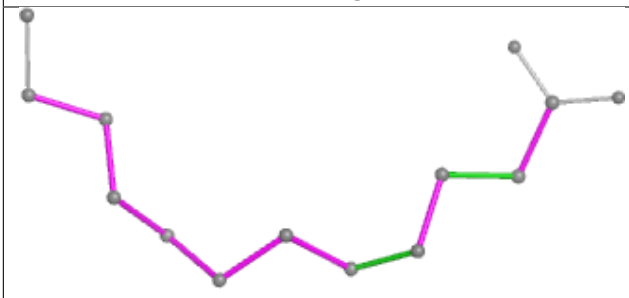
Ligand STE c 516



Bond lengths



Bond angles



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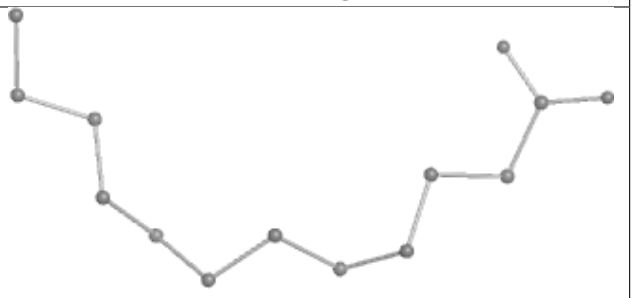
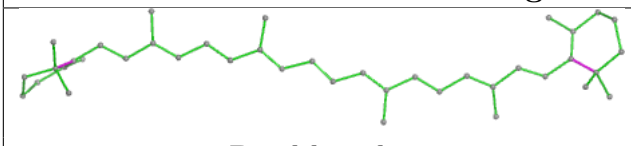
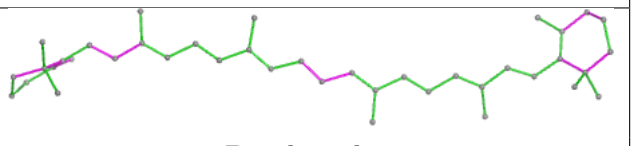


Rings

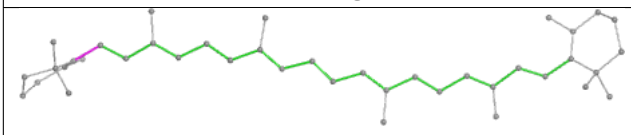
Ligand BCR b 618



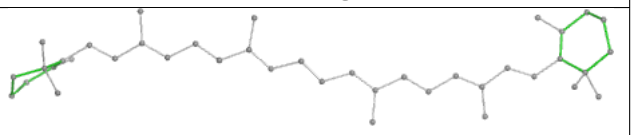
Bond lengths



Bond angles

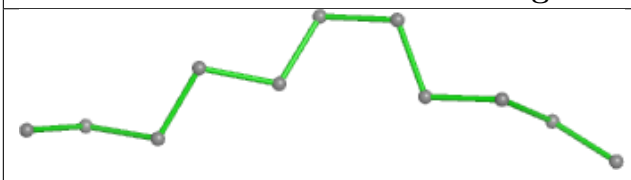


Torsions

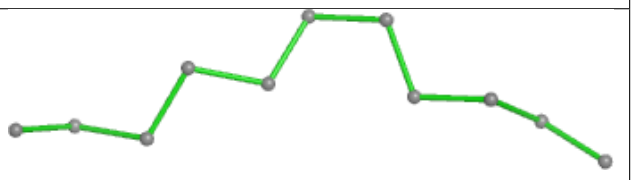


Rings

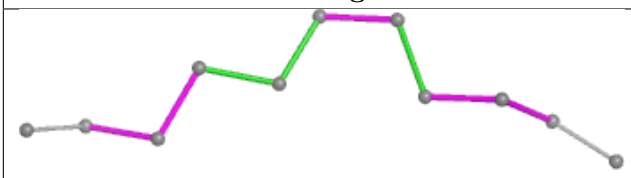
Ligand STE a 416



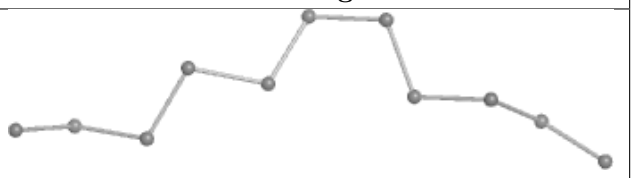
Bond lengths



Bond angles

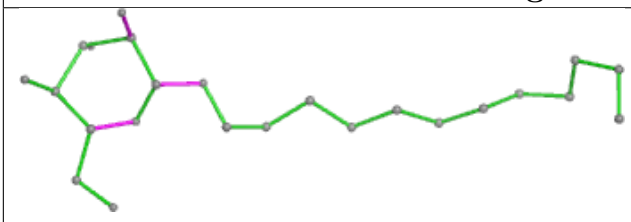


Torsions



Rings

Ligand LMT c 523



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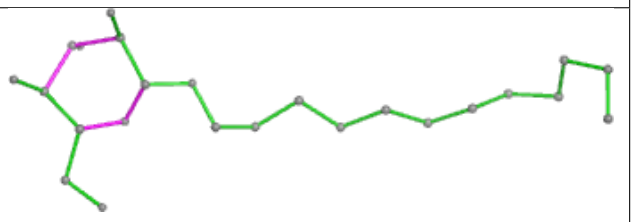
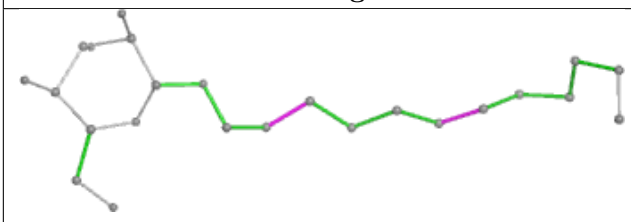
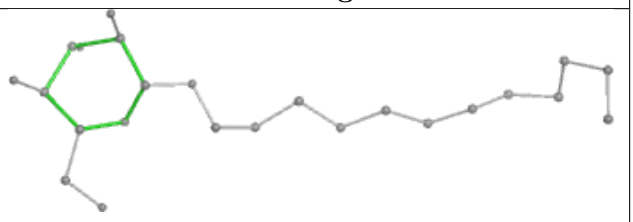


Bond angles

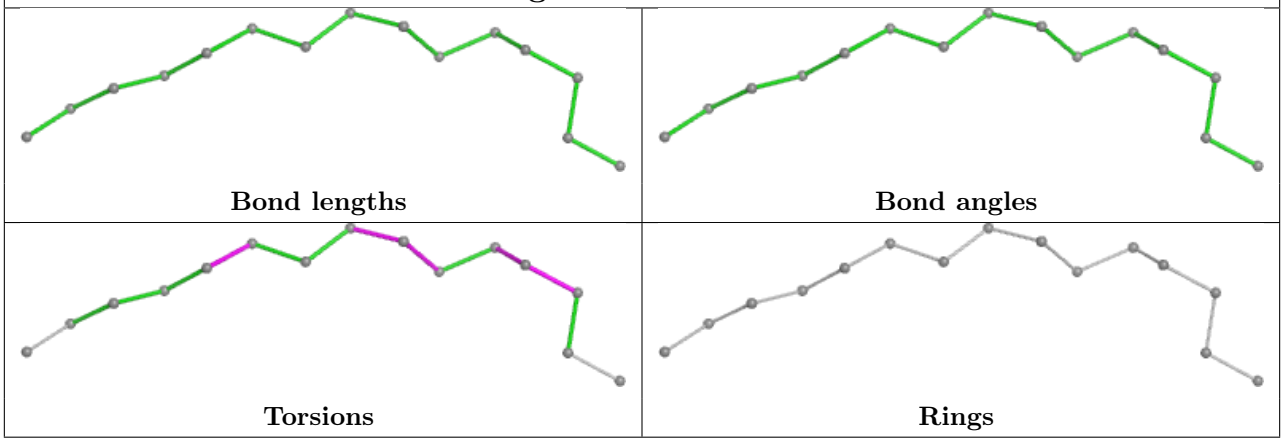


Torsions

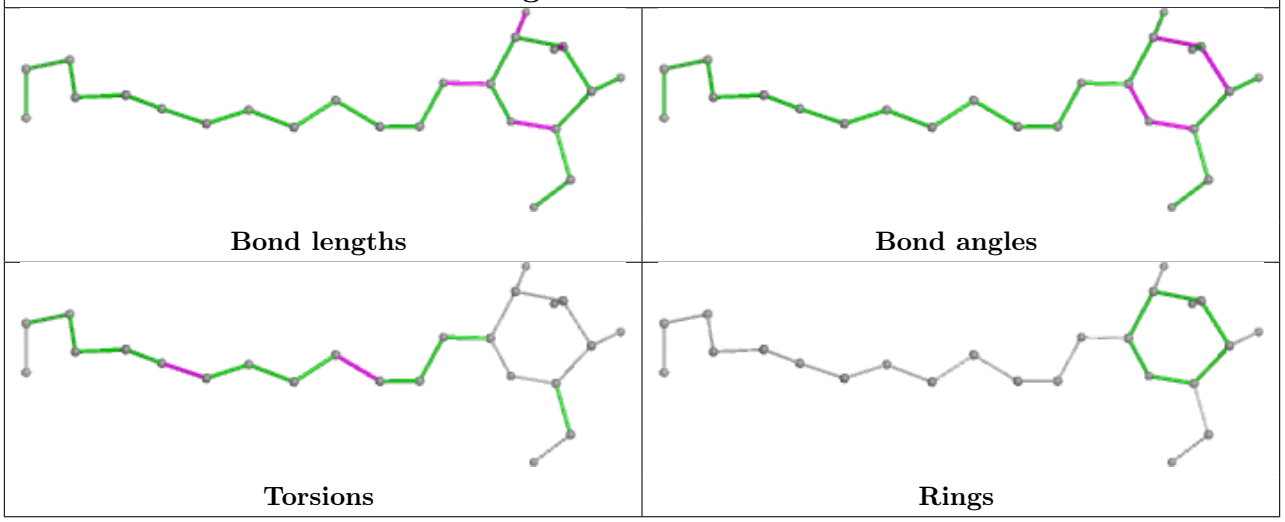


Rings

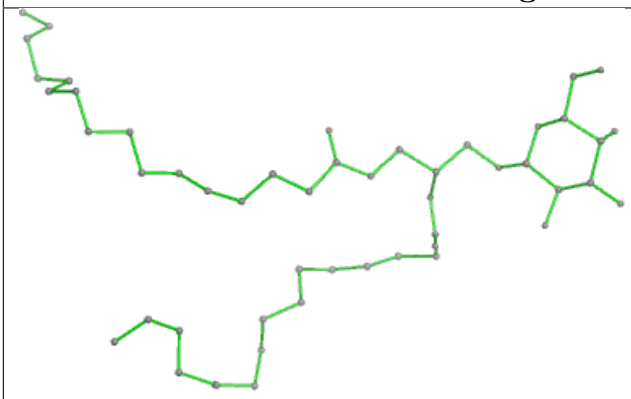
Ligand STE T 102



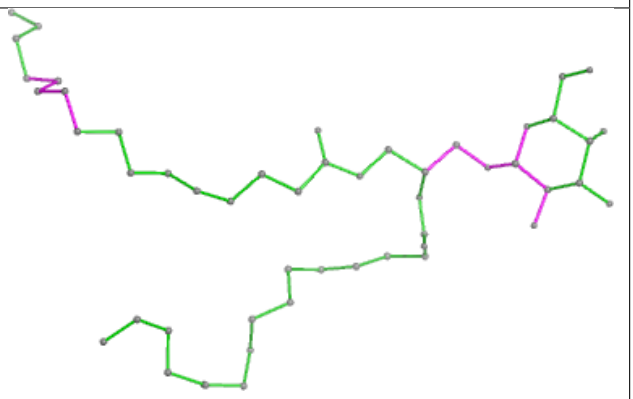
Ligand LMT C 523



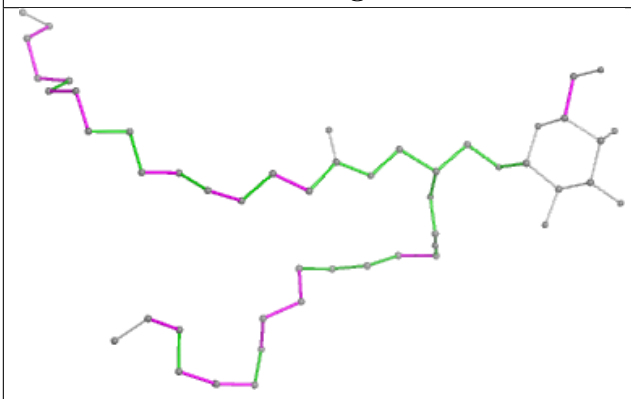
Ligand LMG D 408



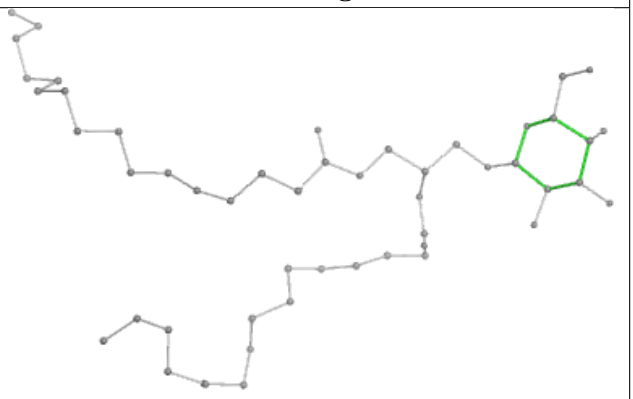
Bond lengths



Bond angles

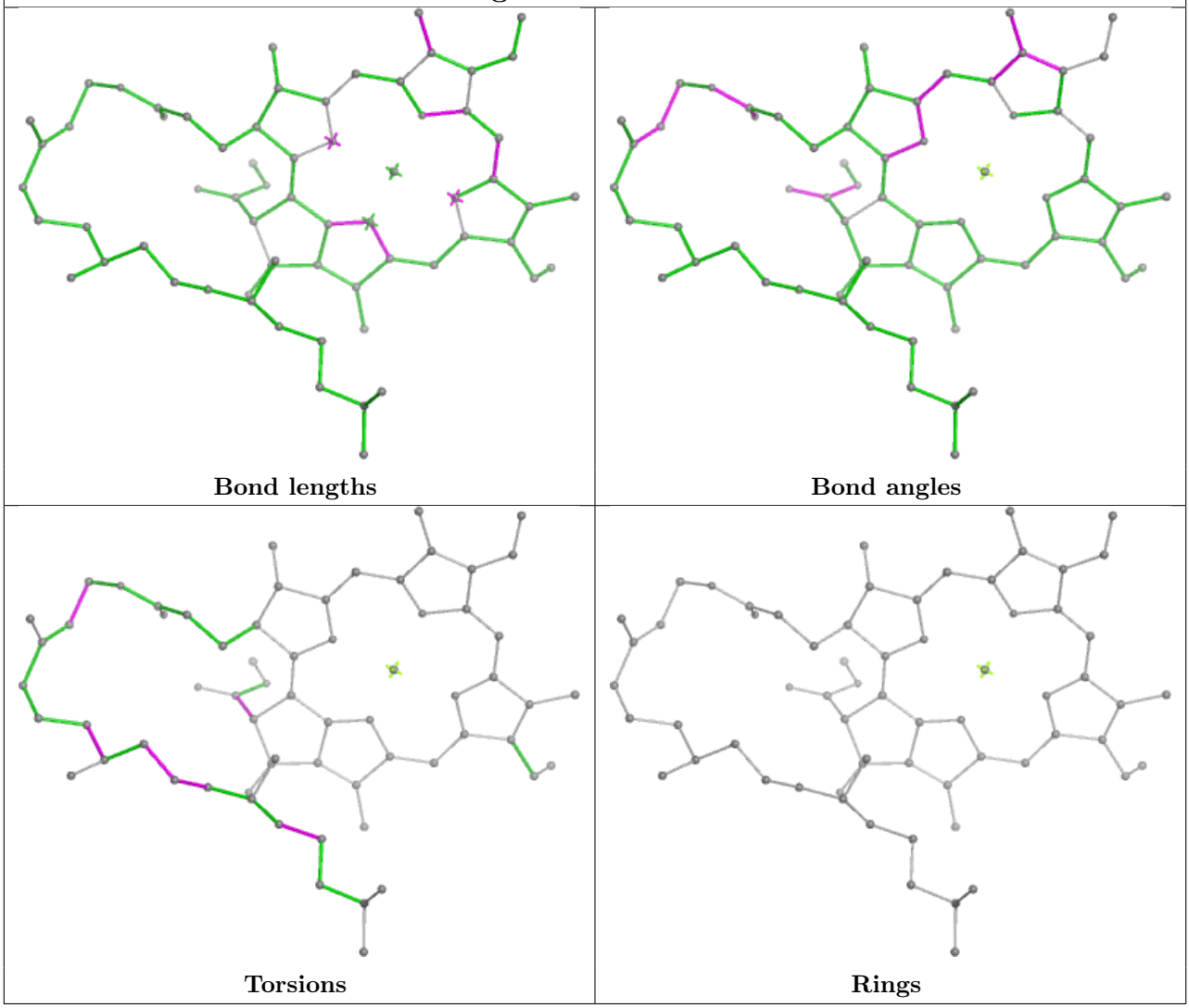


Torsions

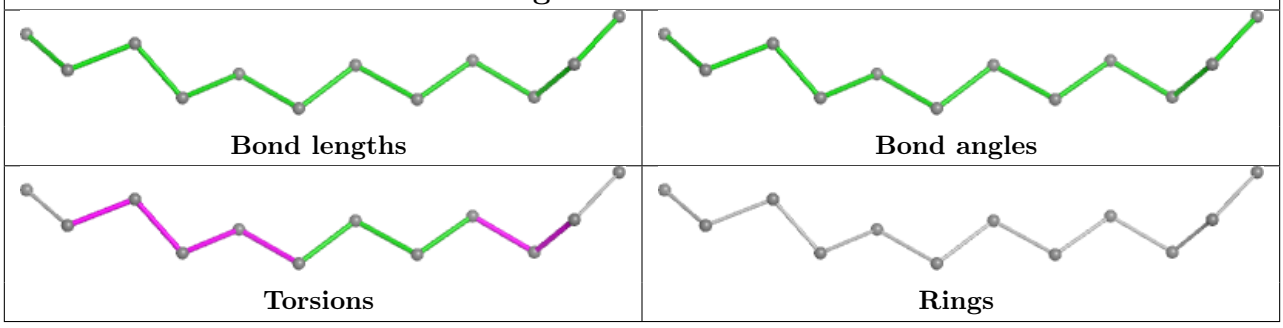


Rings

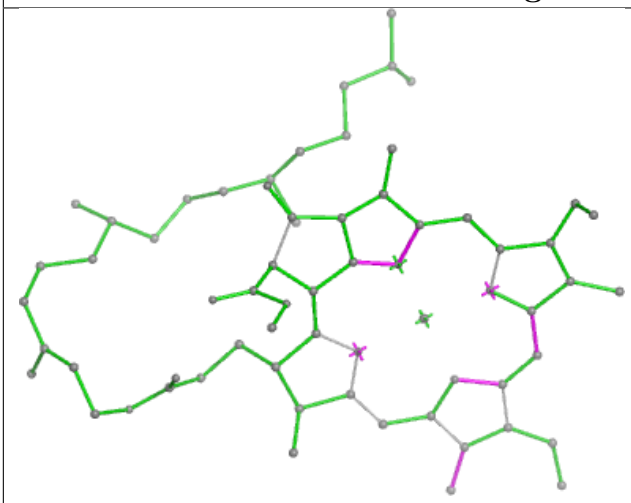
Ligand CLA c 509



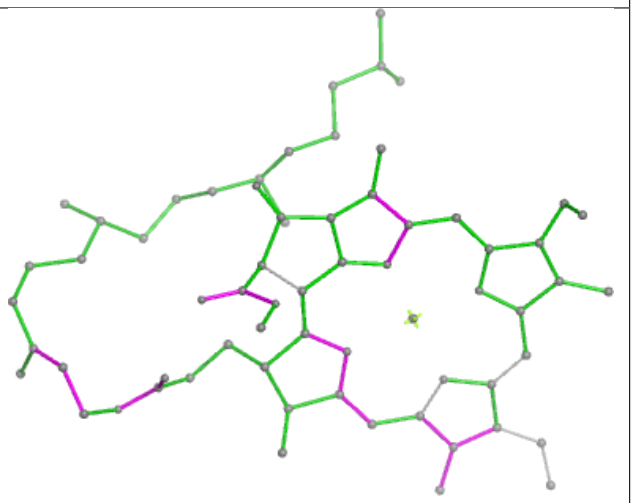
Ligand STE e 102



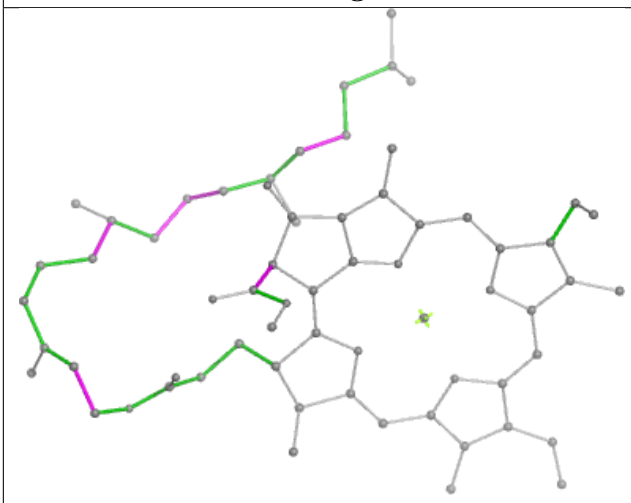
Ligand CLA C 509



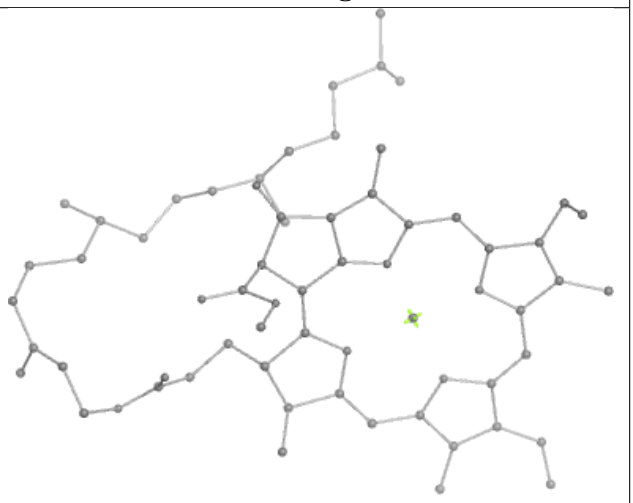
Bond lengths



Bond angles



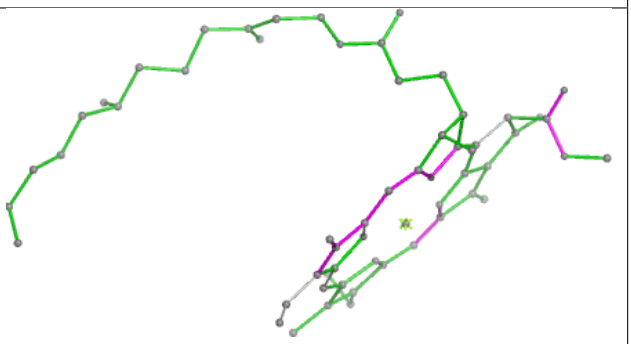
Torsions



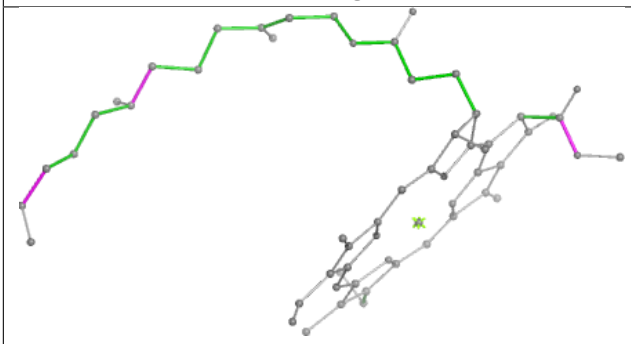
Rings

Ligand CLA c 504

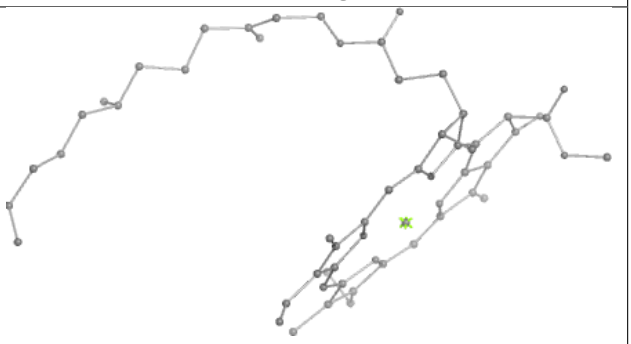
Bond lengths



Bond angles

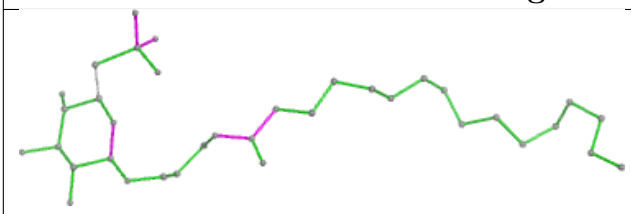


Torsions

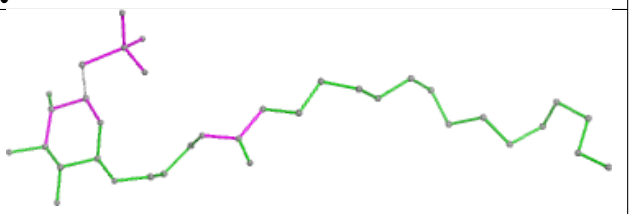


Rings

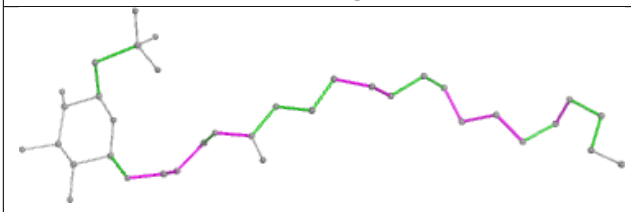
Ligand SQD x 101



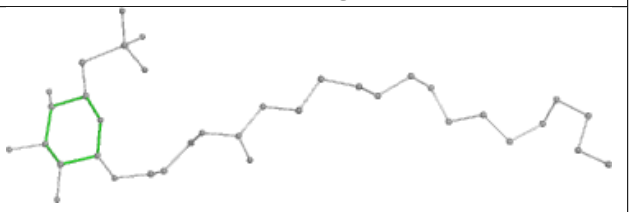
Bond lengths



Bond angles

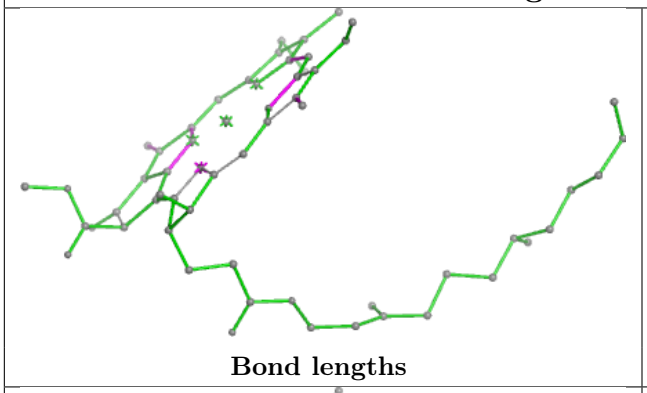


Torsions

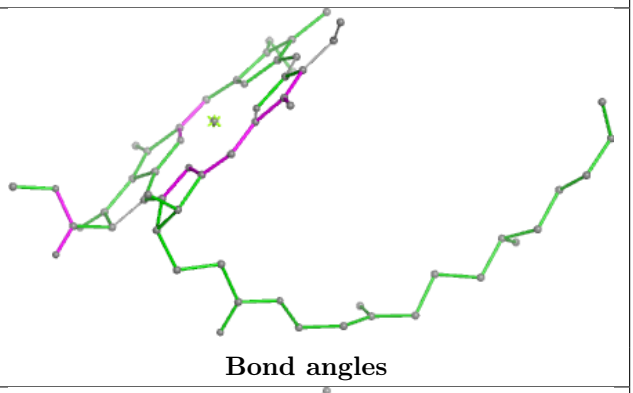


Rings

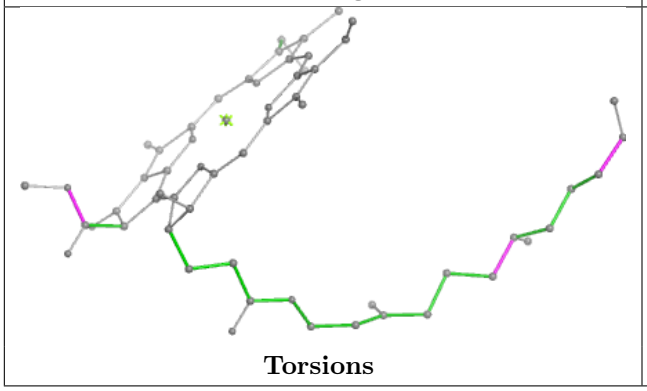
Ligand CLA C 504



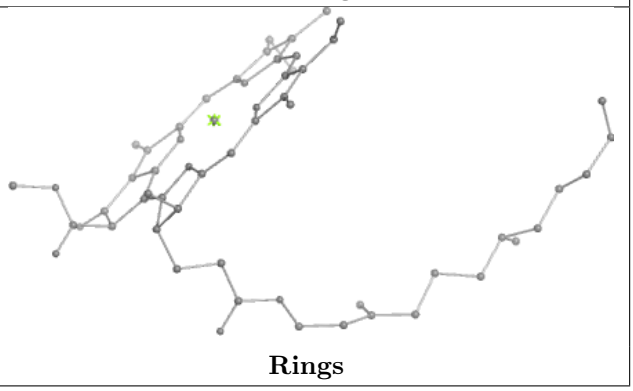
Bond lengths



Bond angles

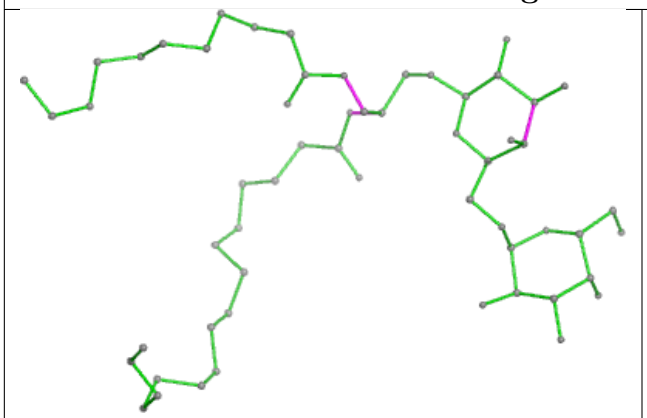


Torsions

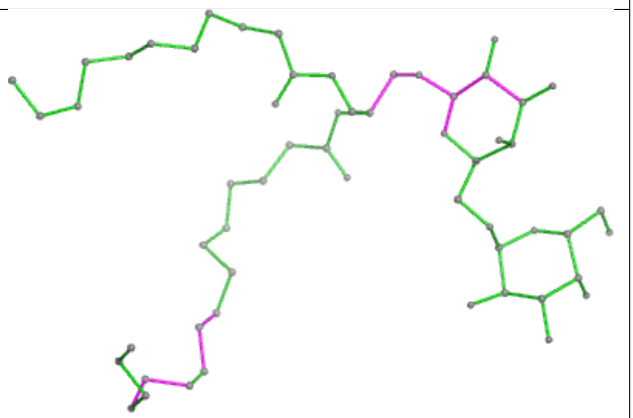


Rings

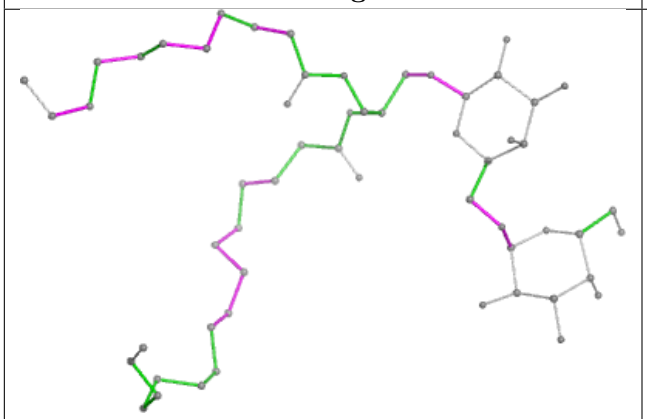
Ligand DGD C 518



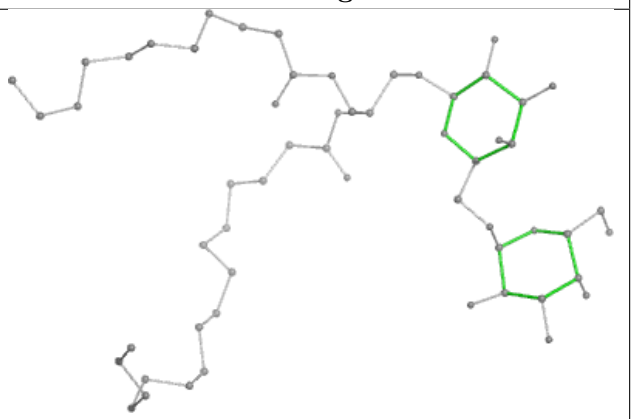
Bond lengths



Bond angles

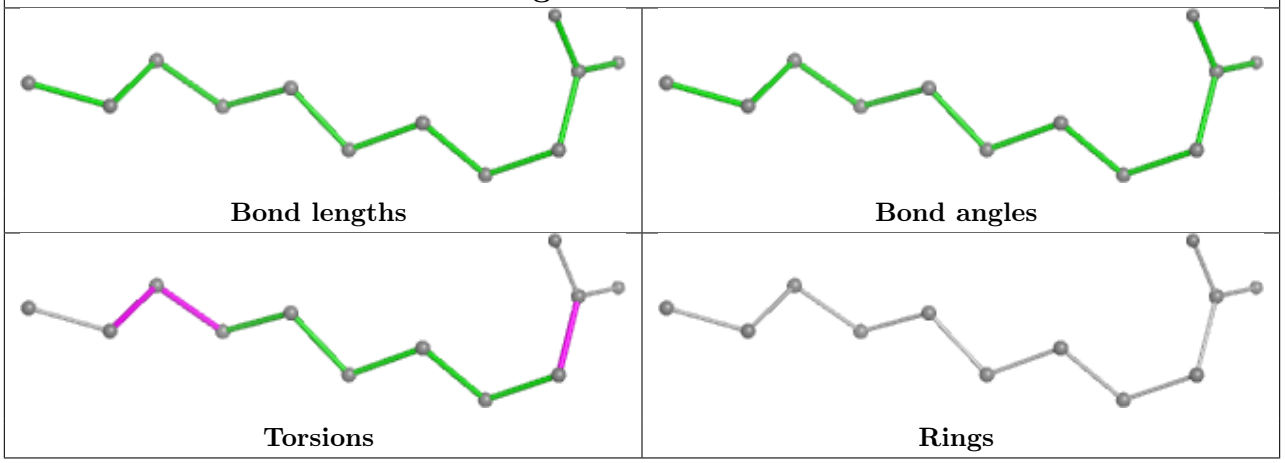


Torsions

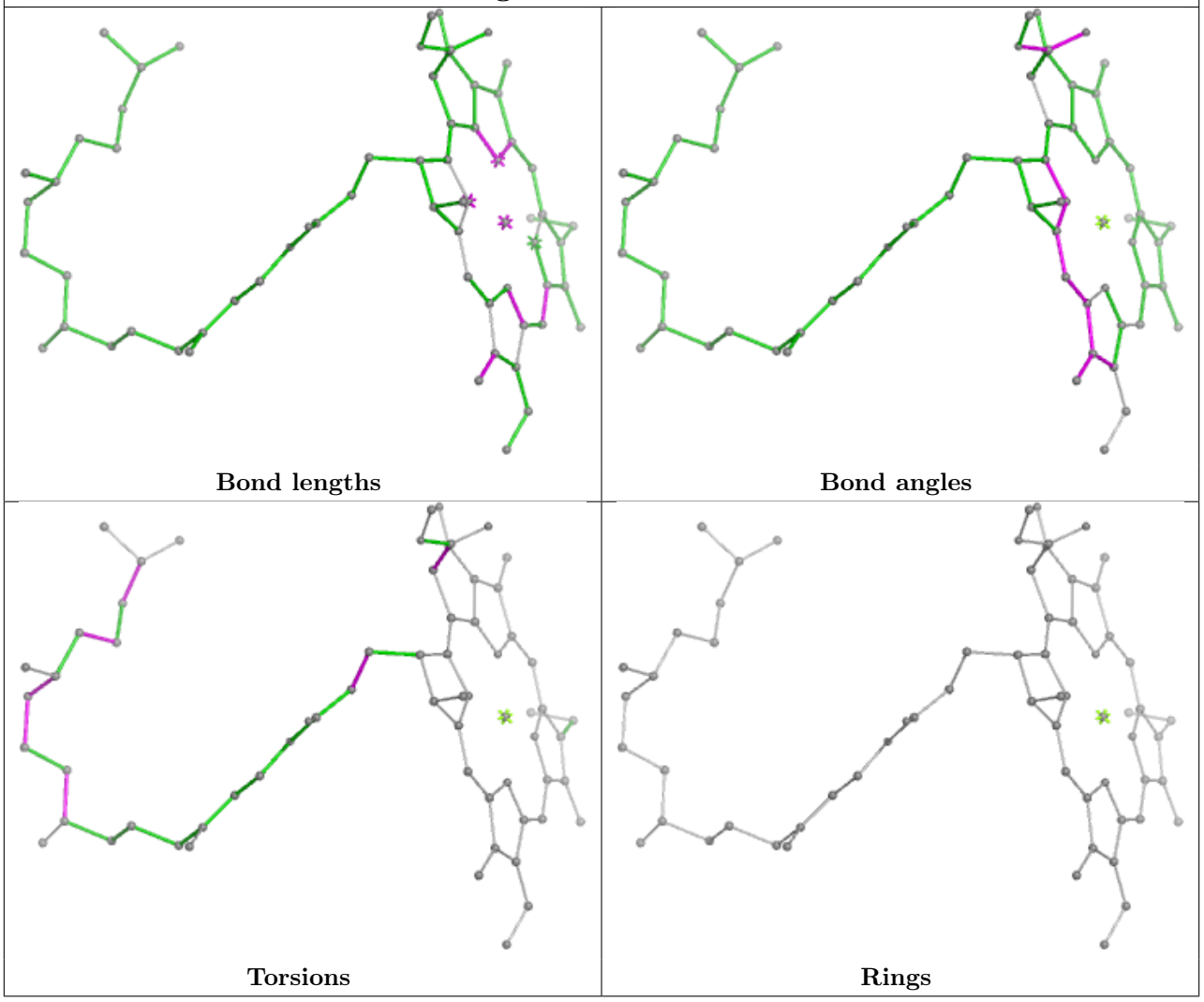


Rings

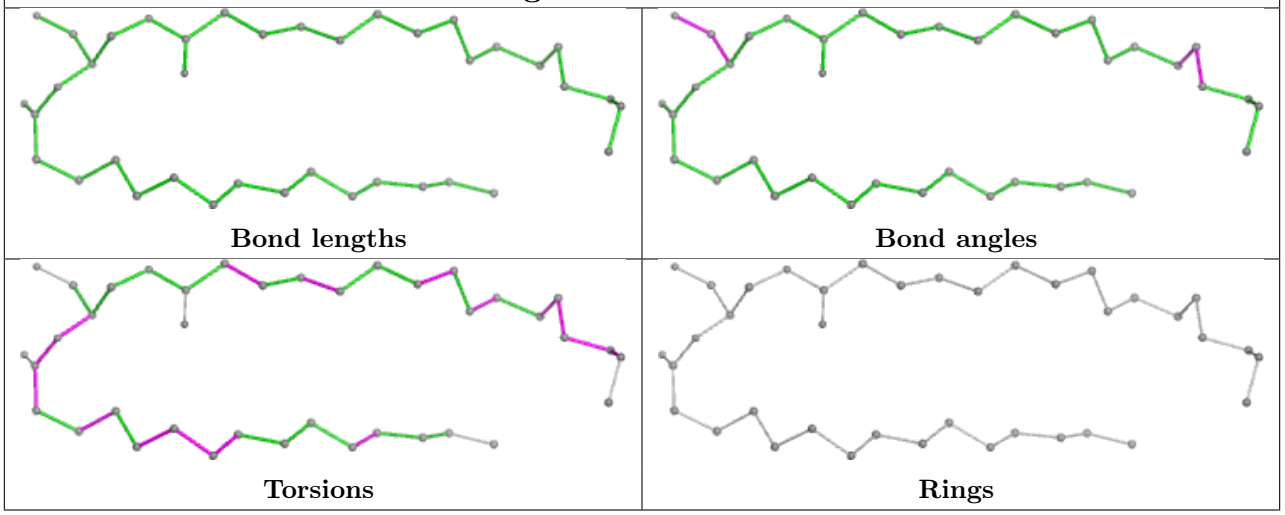
Ligand STE e 101



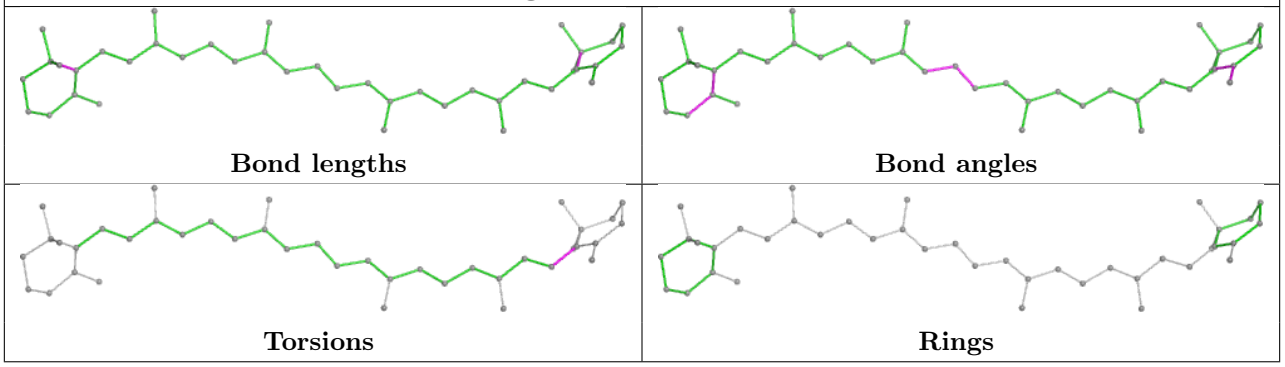
Ligand CLA b 607



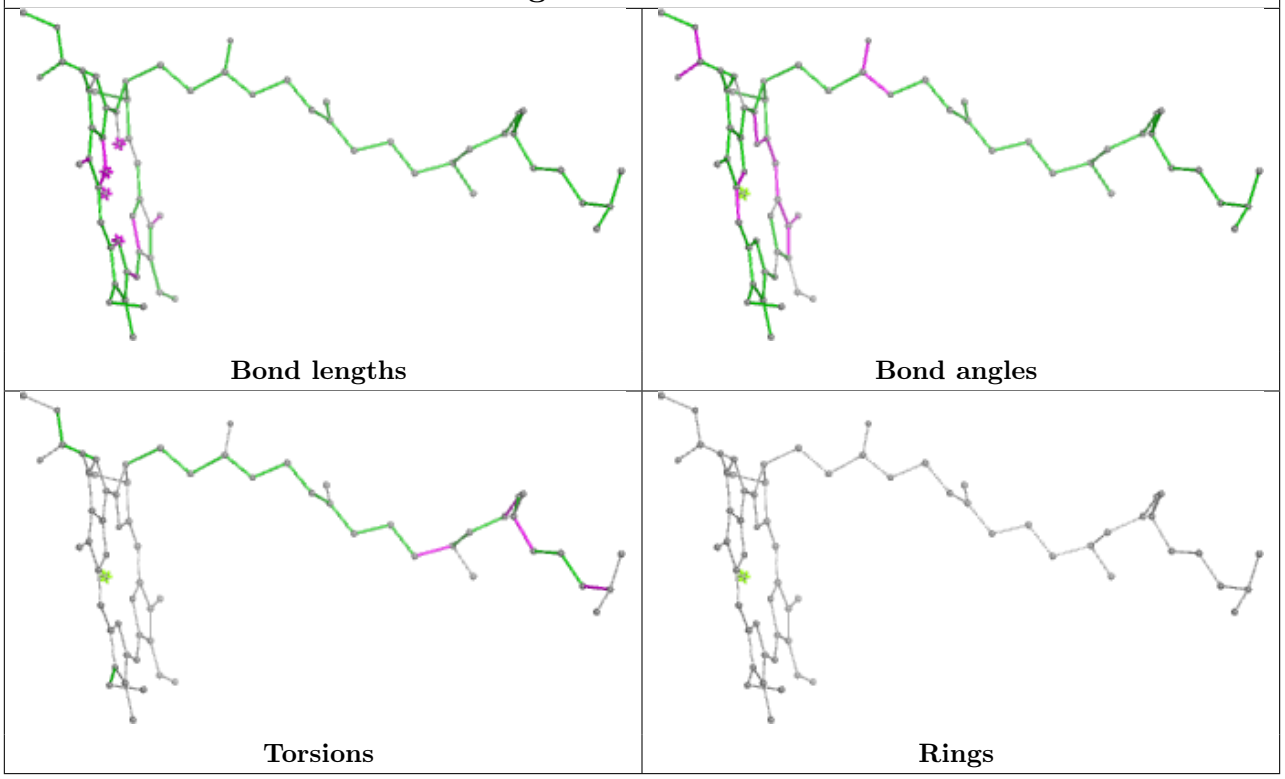
Ligand LMG h 101



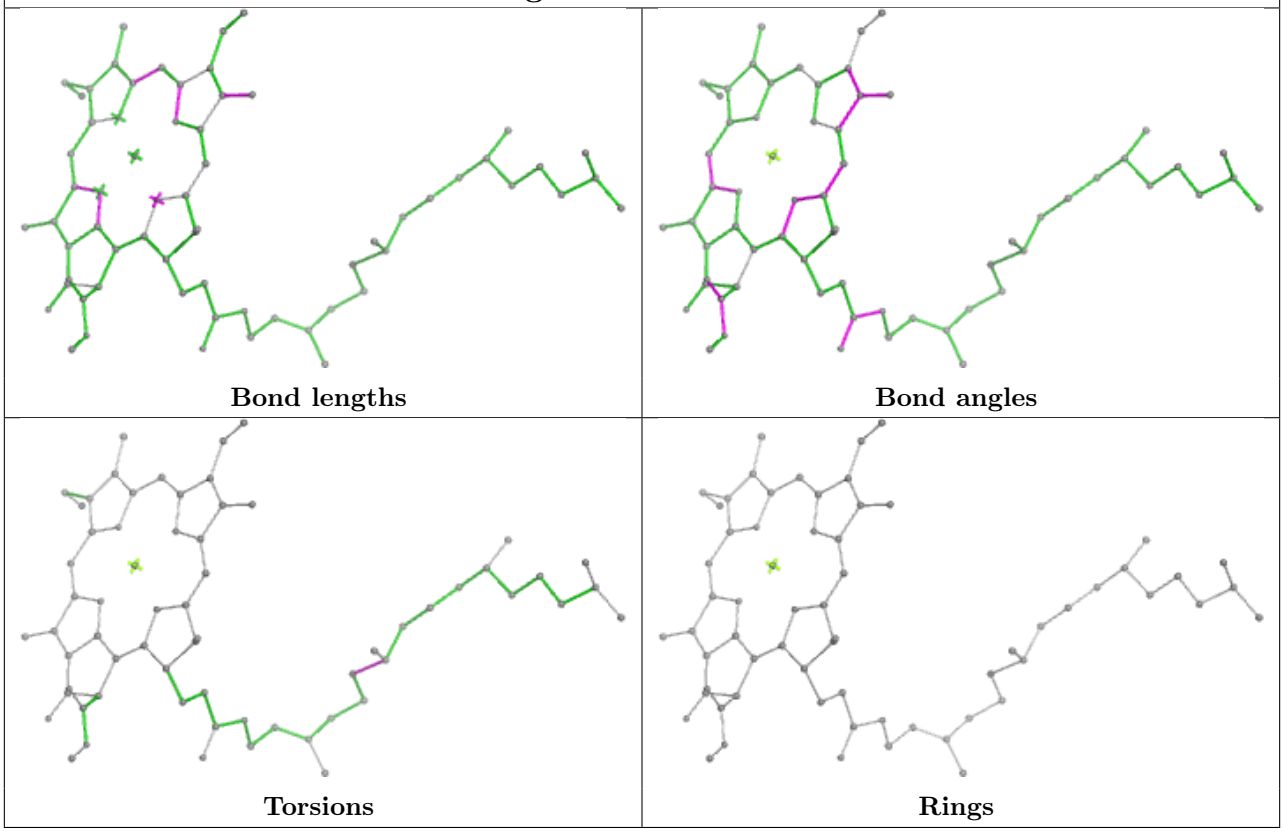
Ligand BCR K 103



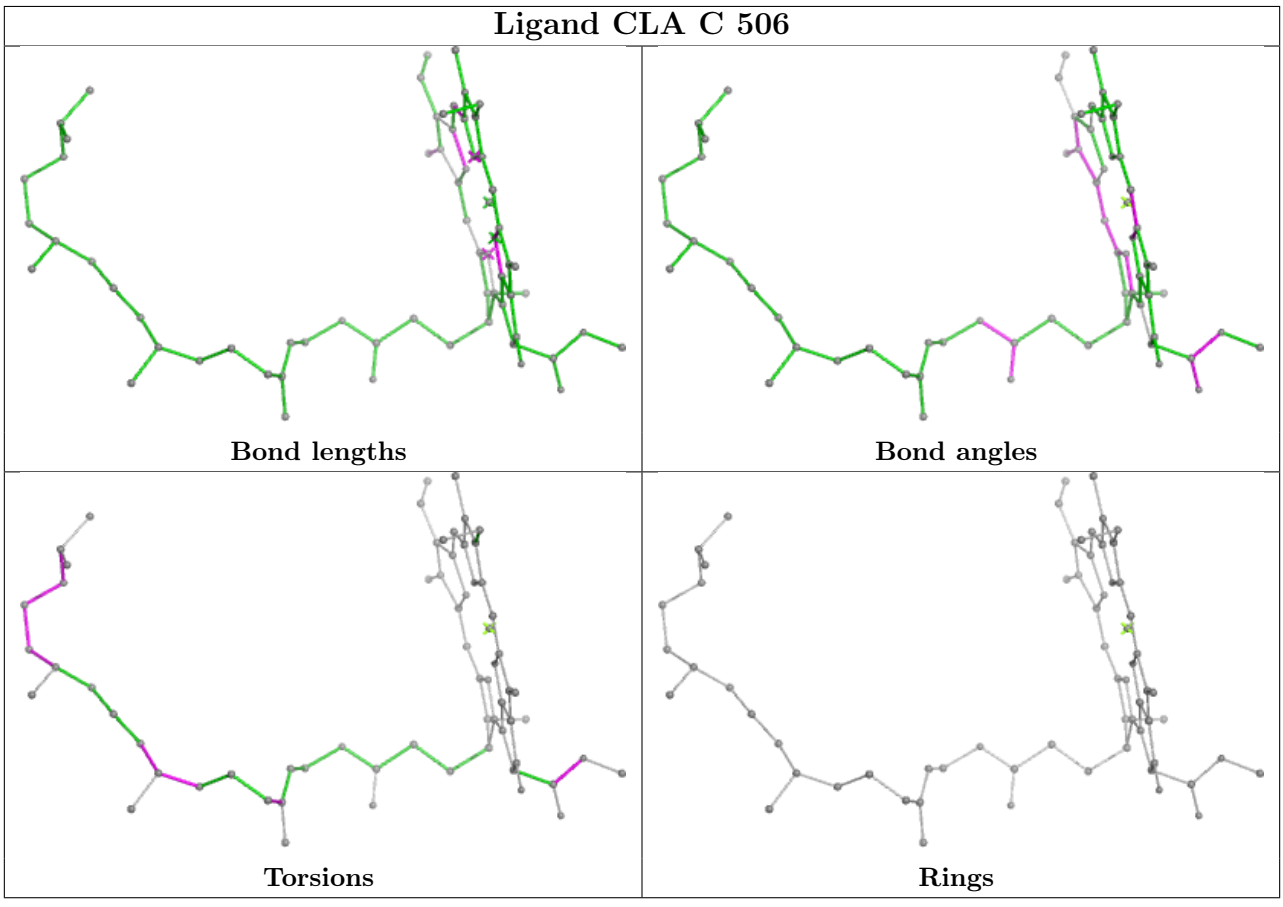
Ligand CLA d 405



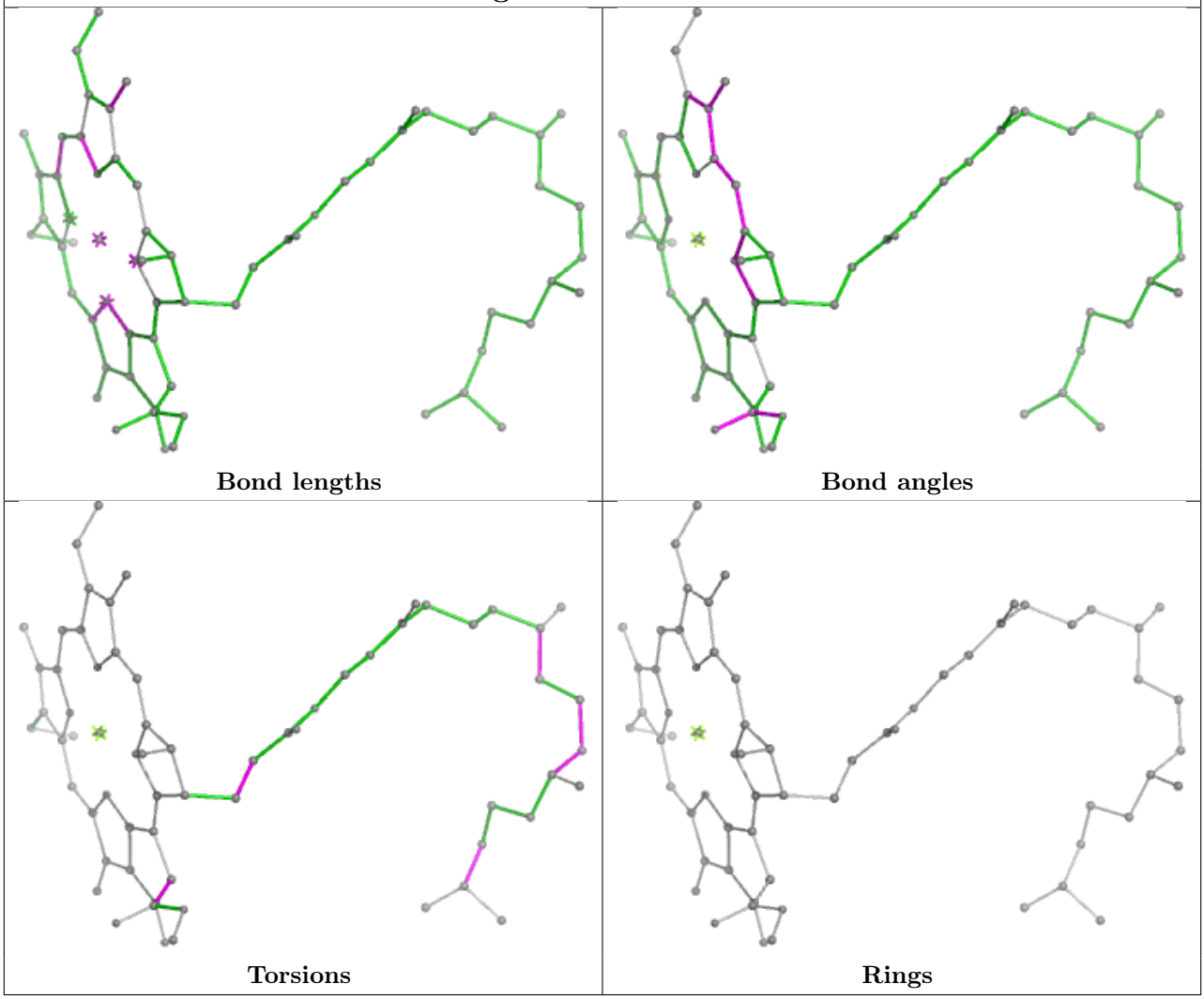
Ligand CLA C 511



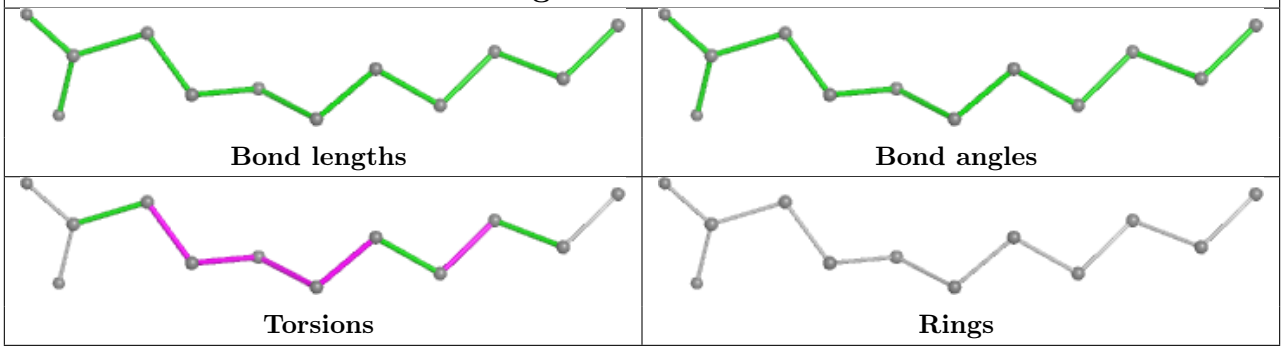
Ligand CLA C 506



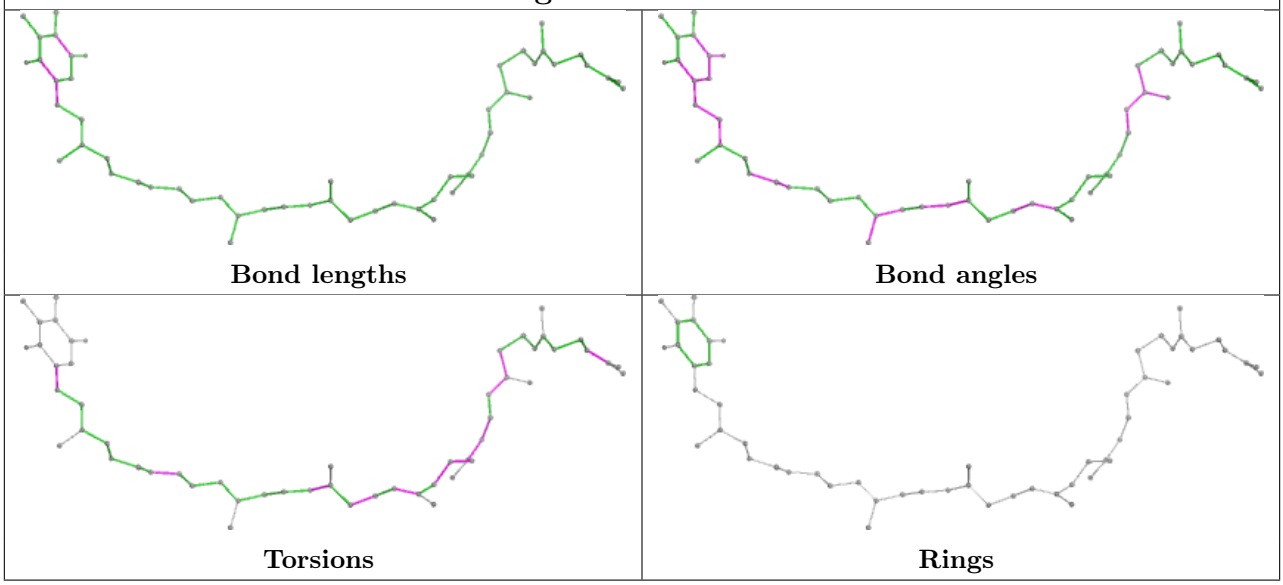
Ligand CLA B 606



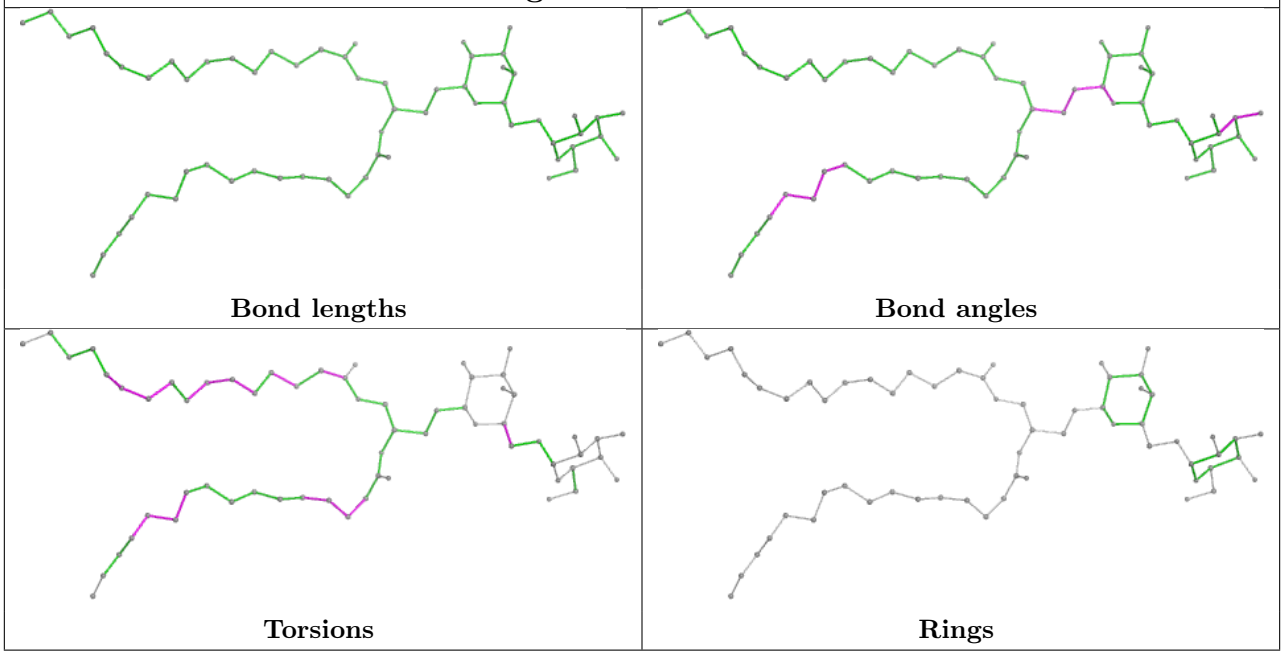
Ligand STE a 421



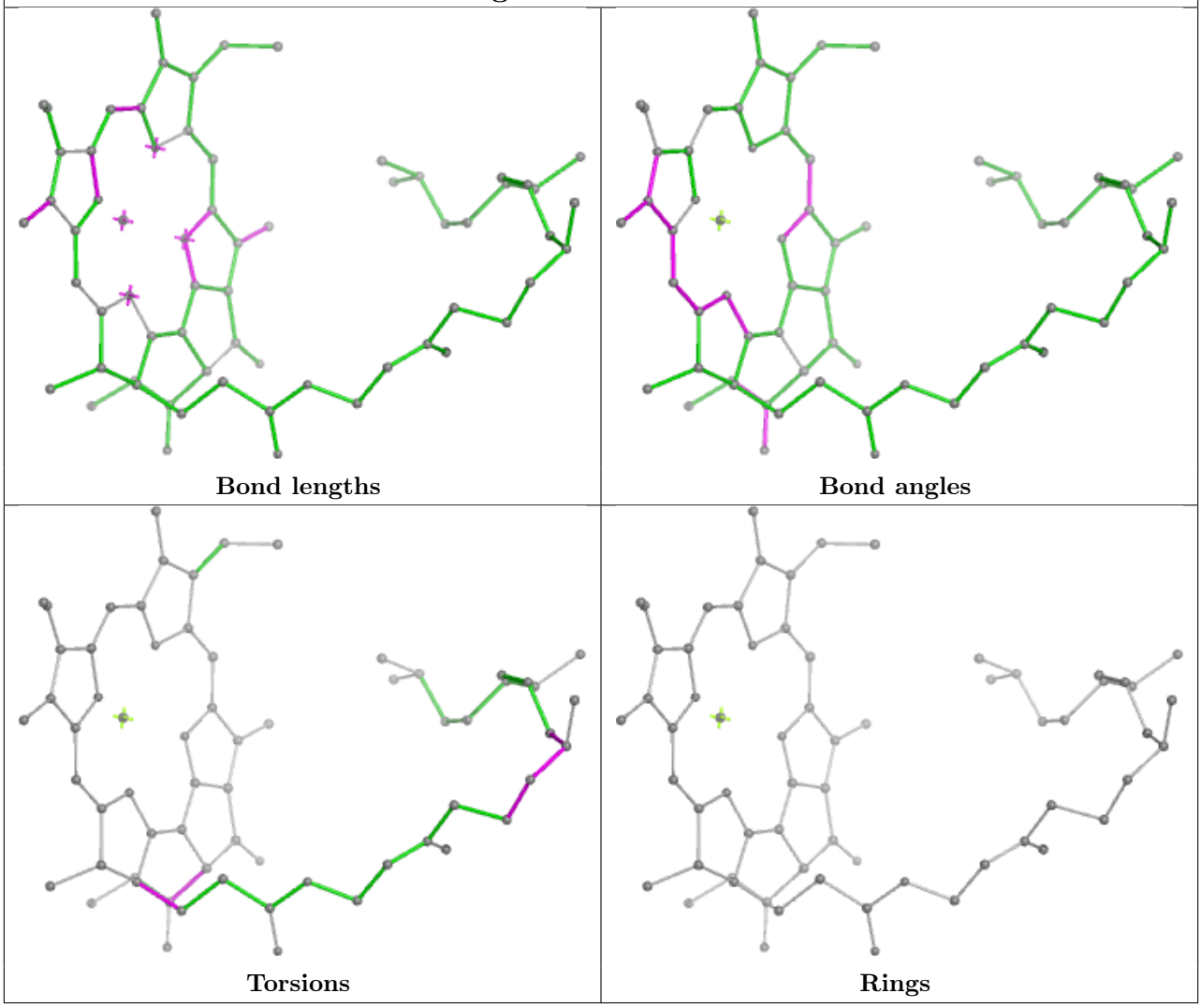
Ligand PL9 a 408



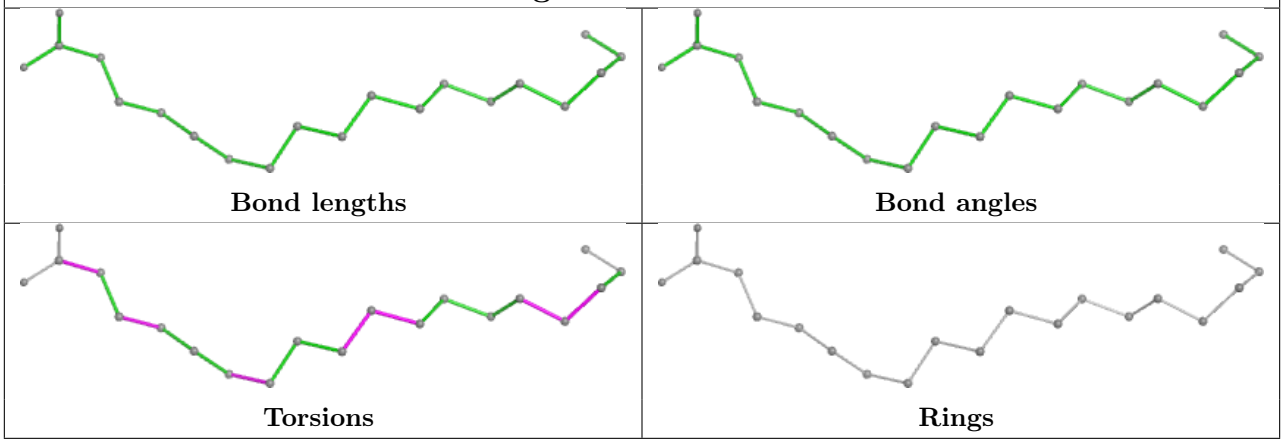
Ligand DGD c 519



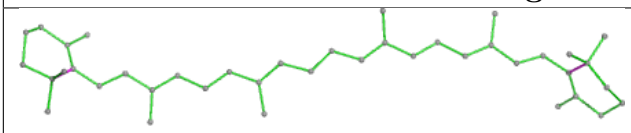
Ligand CLA C 503



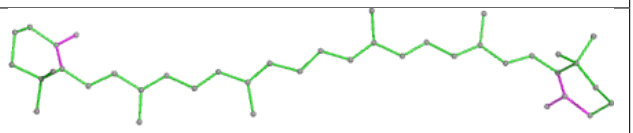
Ligand STE e 103



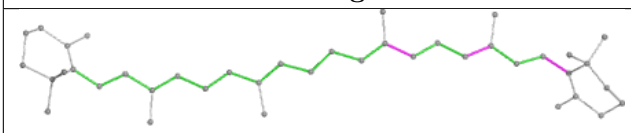
Ligand BCR b 619



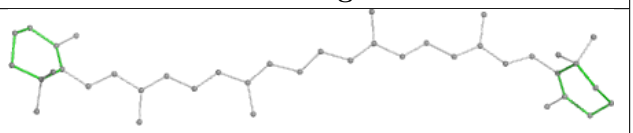
Bond lengths



Bond angles

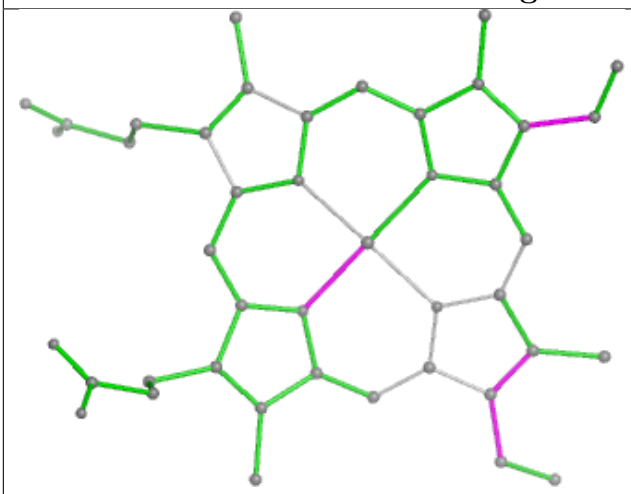


Torsions

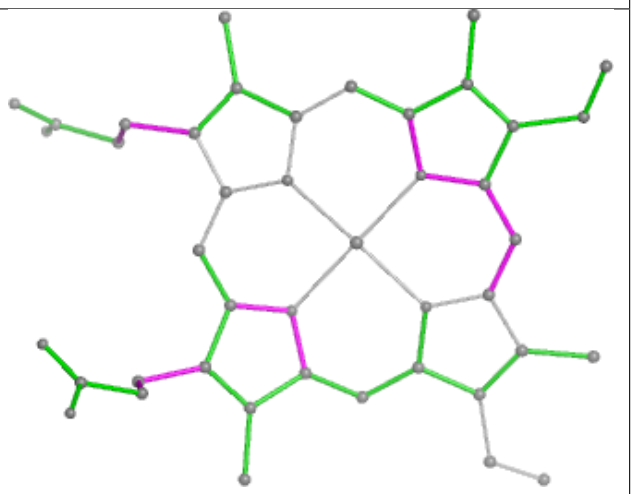


Rings

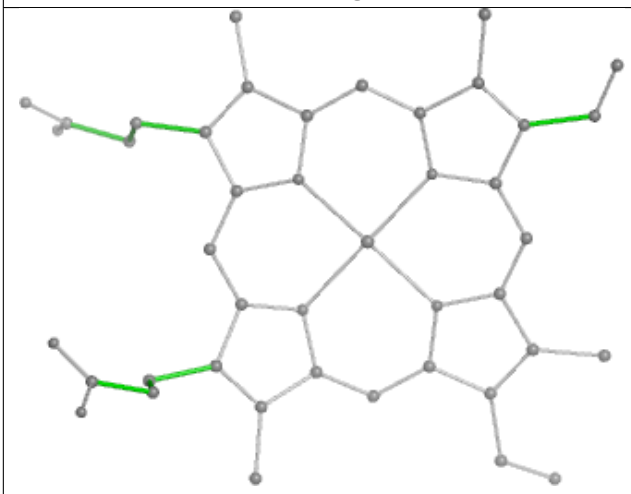
Ligand HEM E 105



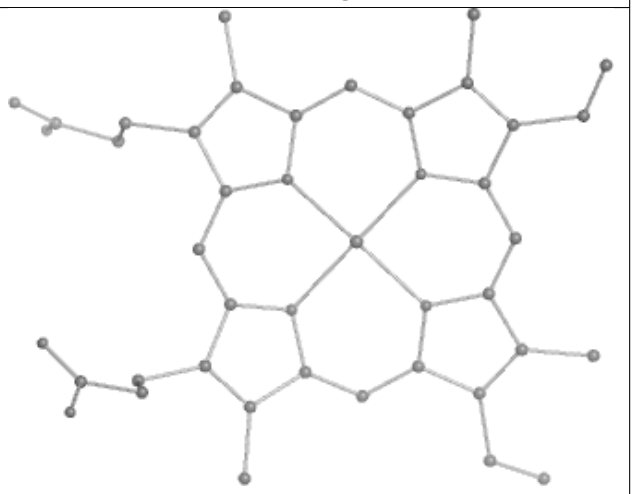
Bond lengths



Bond angles

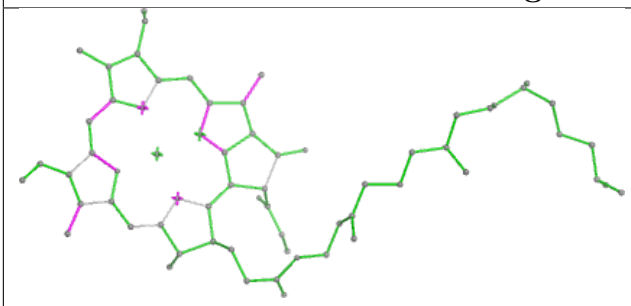


Torsions

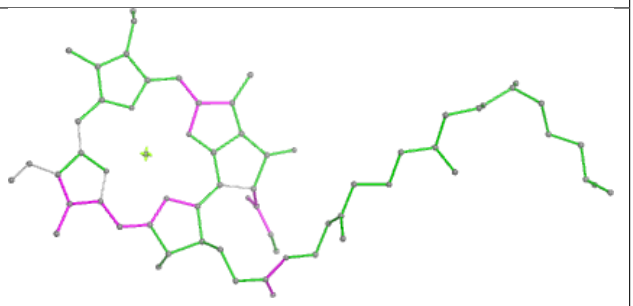


Rings

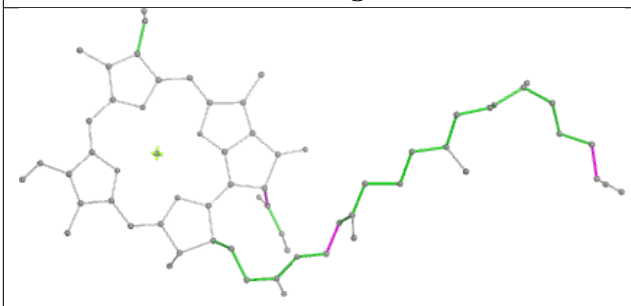
Ligand CLA B 602



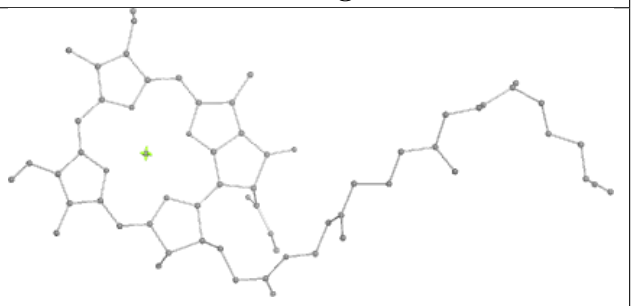
Bond lengths



Bond angles

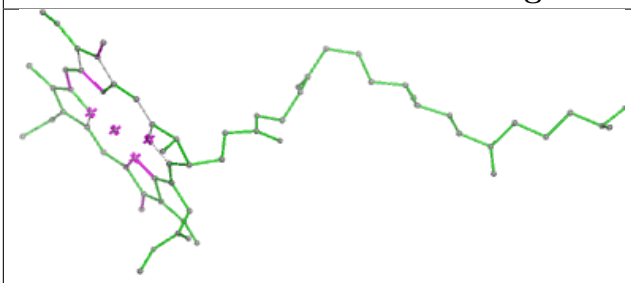


Torsions

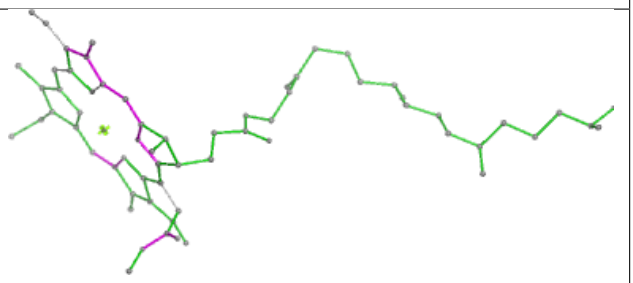


Rings

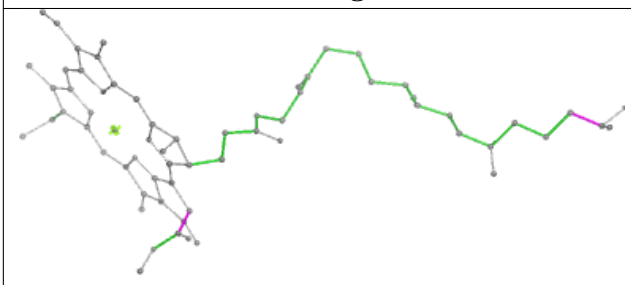
Ligand CLA C 502



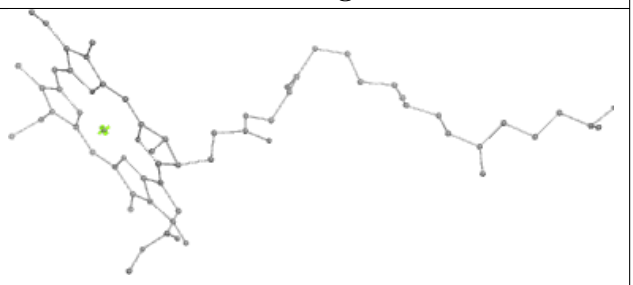
Bond lengths



Bond angles

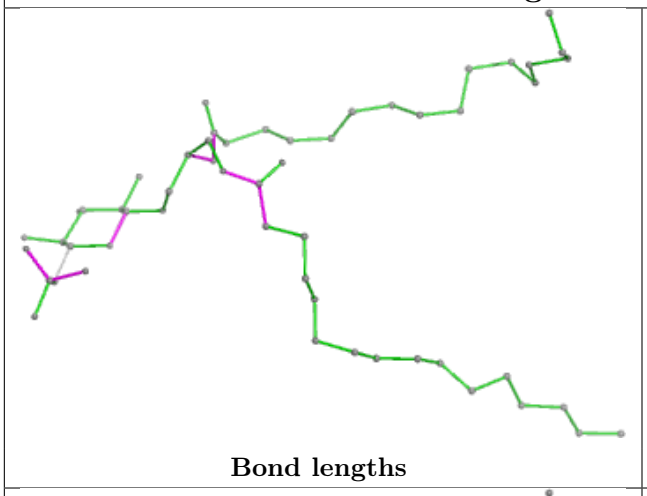


Torsions

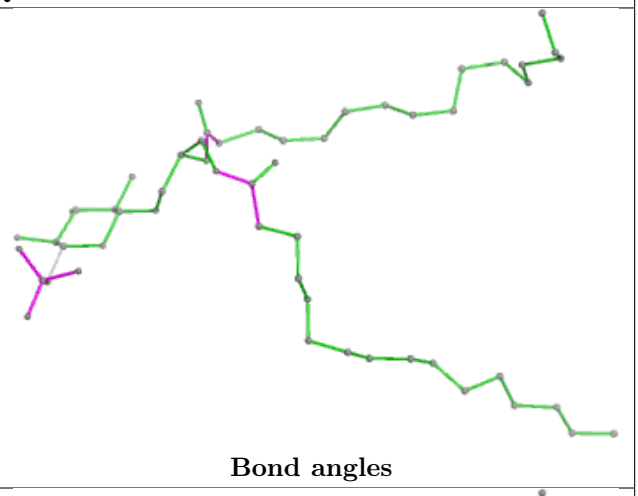


Rings

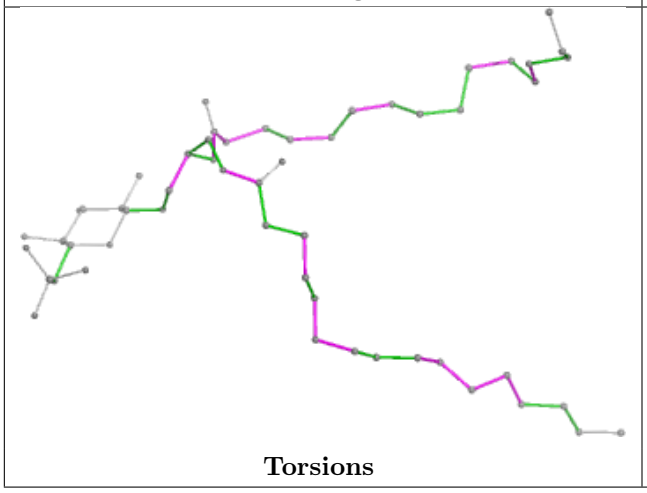
Ligand SQD A 412



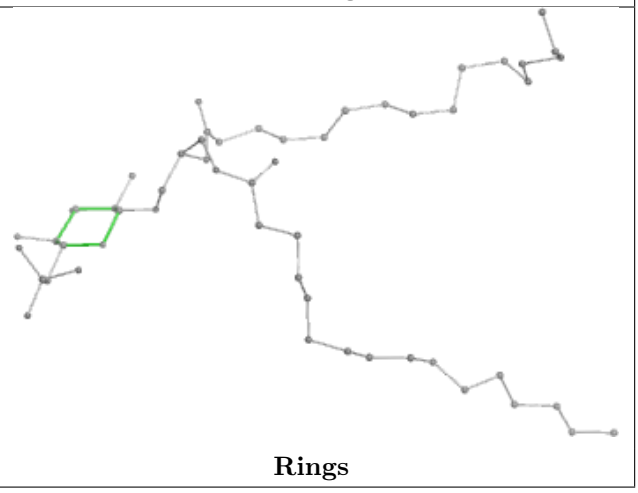
Bond lengths



Bond angles

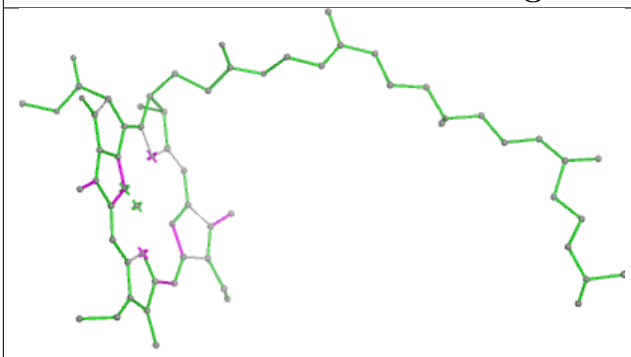


Torsions

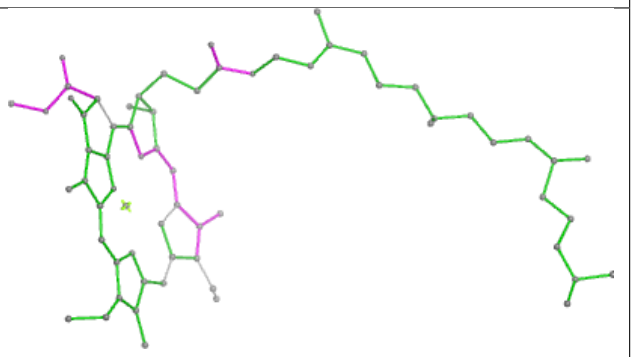


Rings

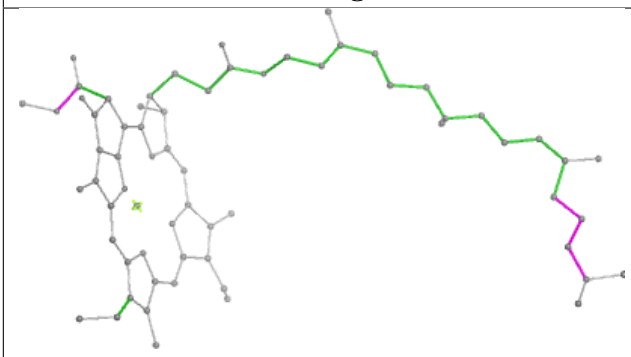
Ligand CLA B 609



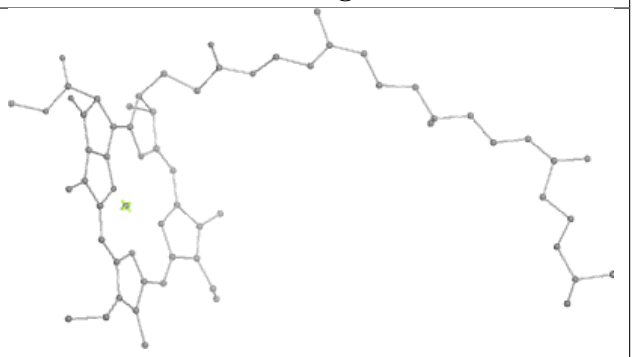
Bond lengths



Bond angles

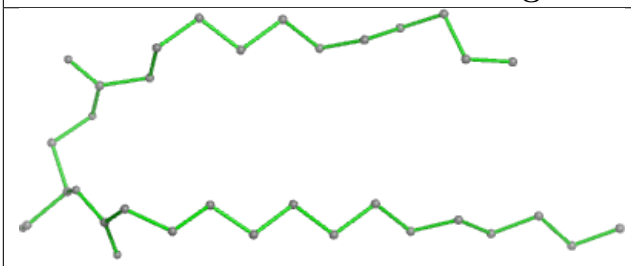


Torsions

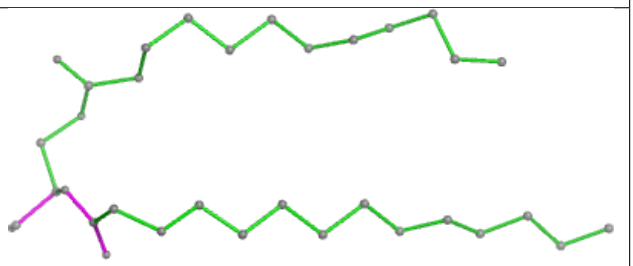


Rings

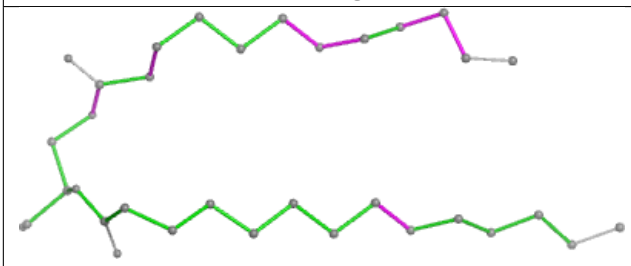
Ligand LMG d 402



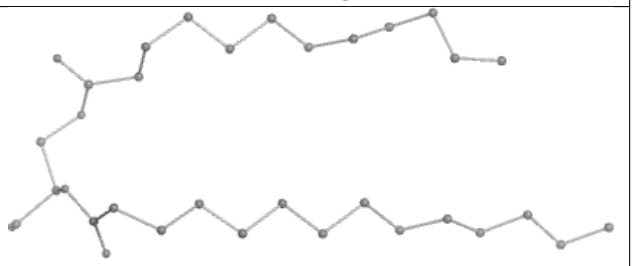
Bond lengths



Bond angles

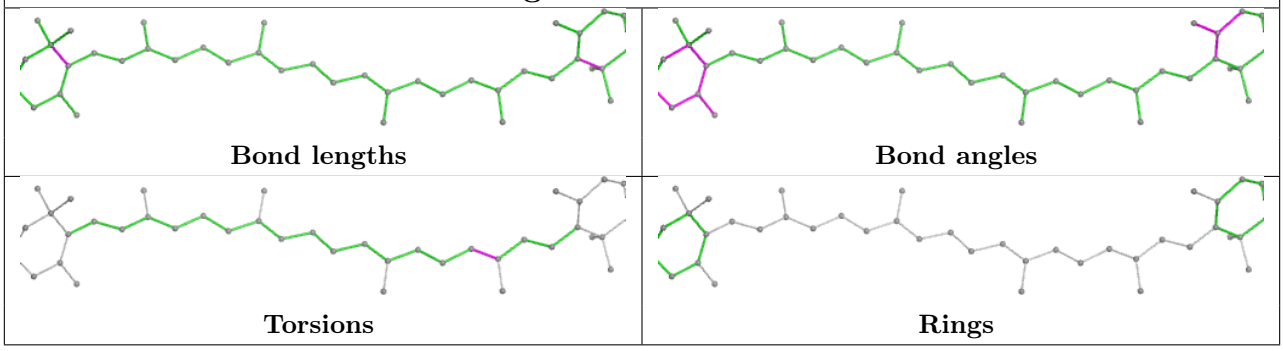


Torsions

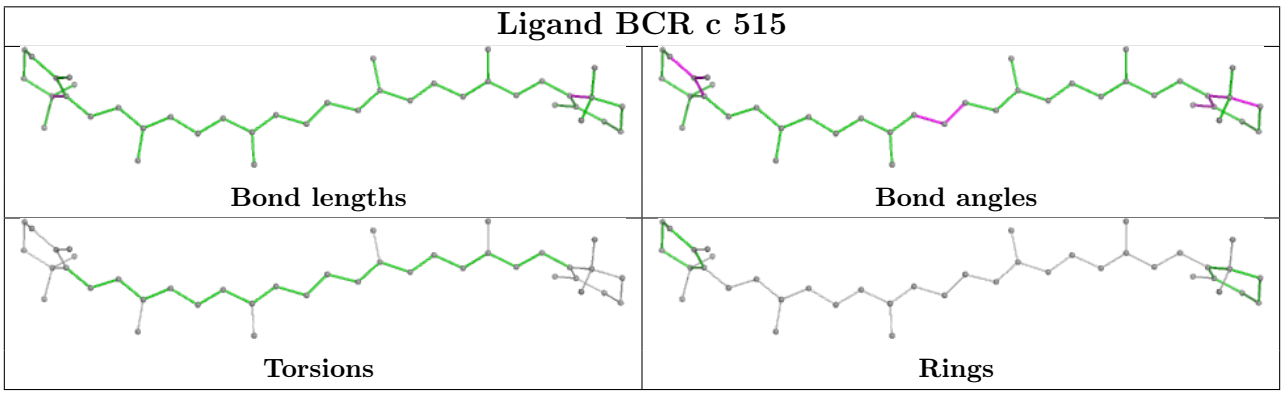


Rings

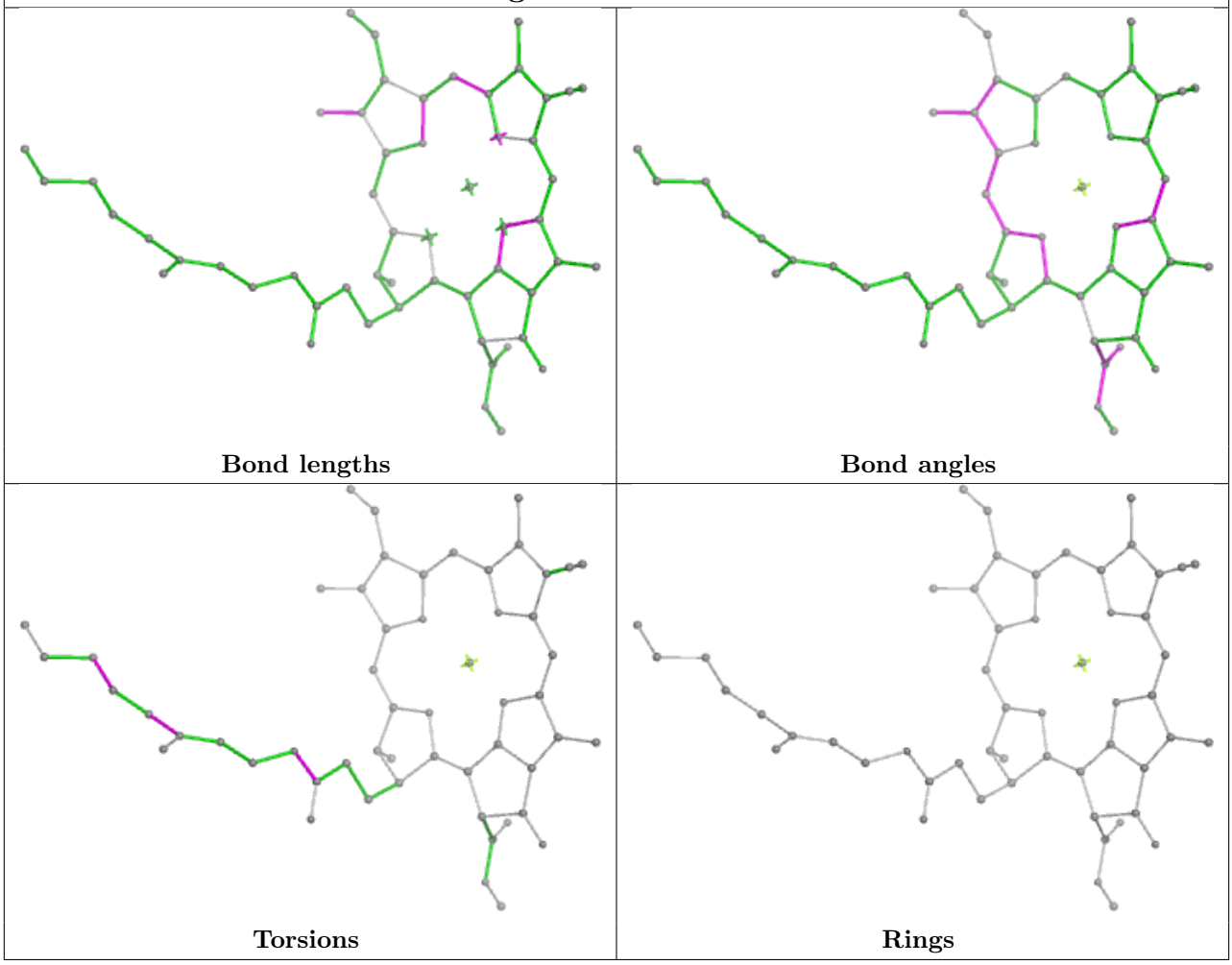
Ligand BCR B 619



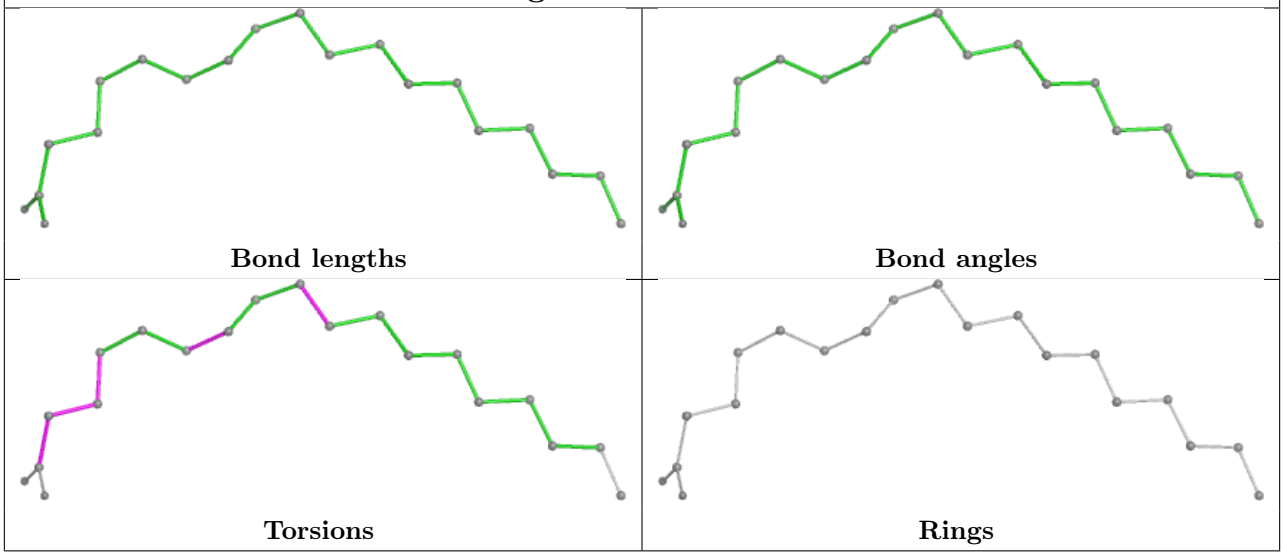
Ligand BCR c 515



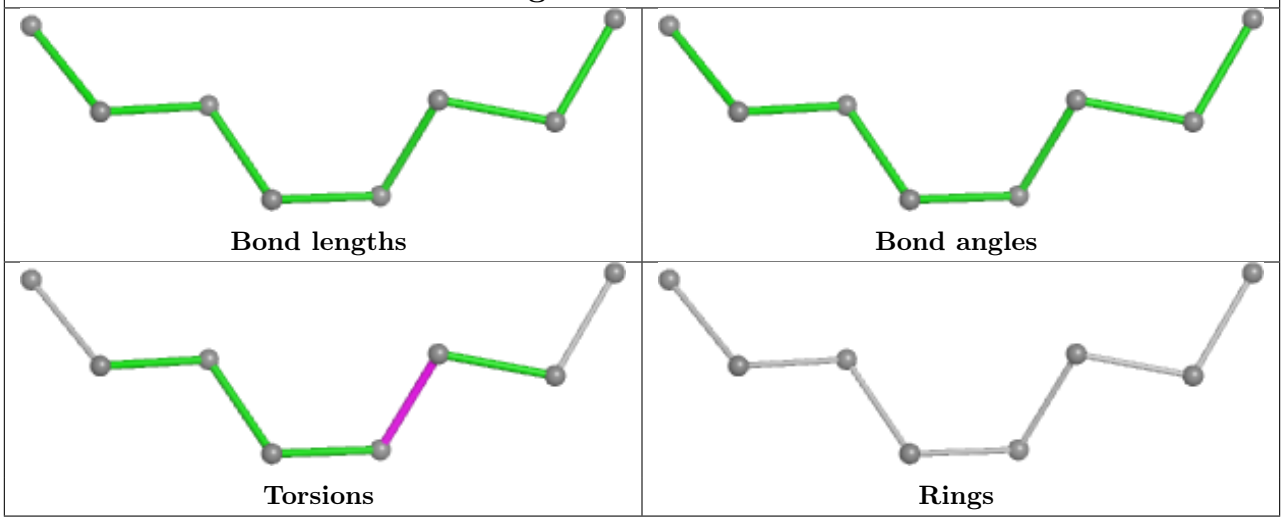
Ligand CLA a 406



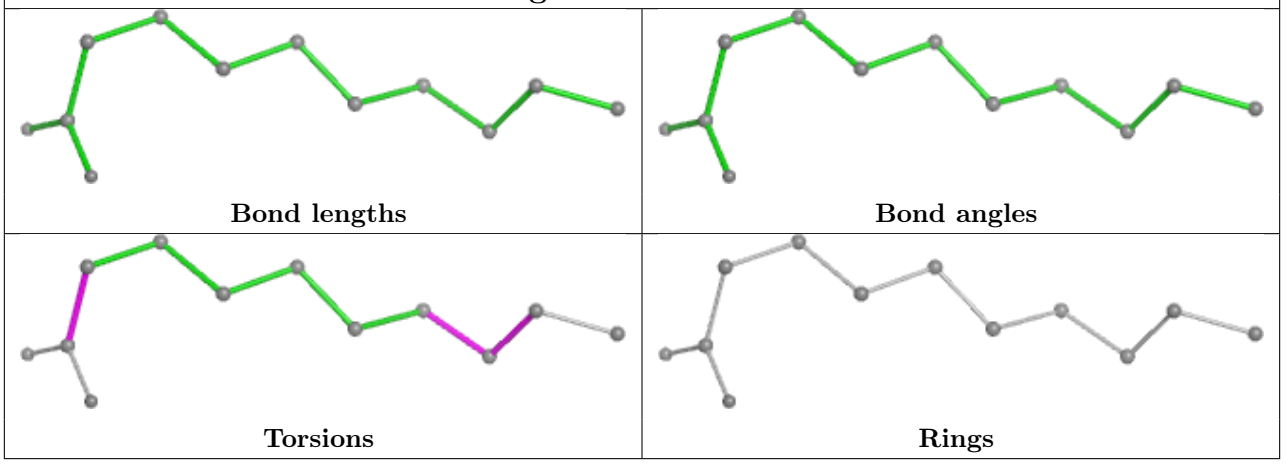
Ligand STE D 412



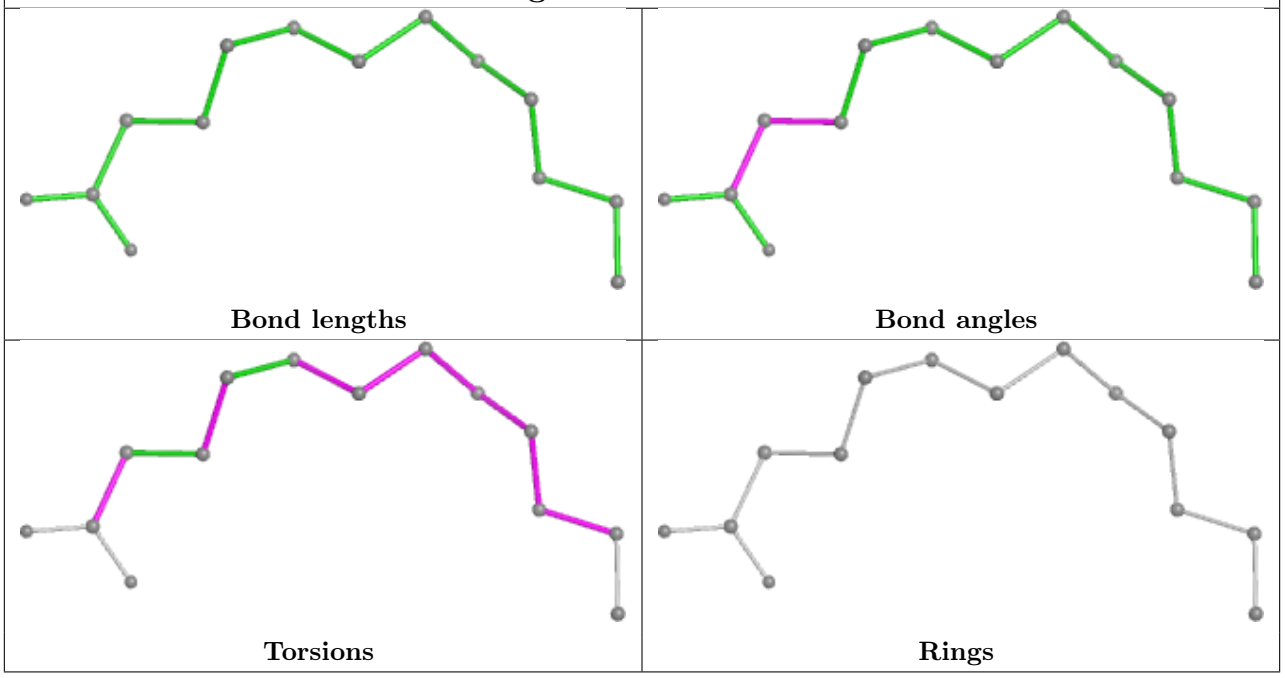
Ligand STE C 522



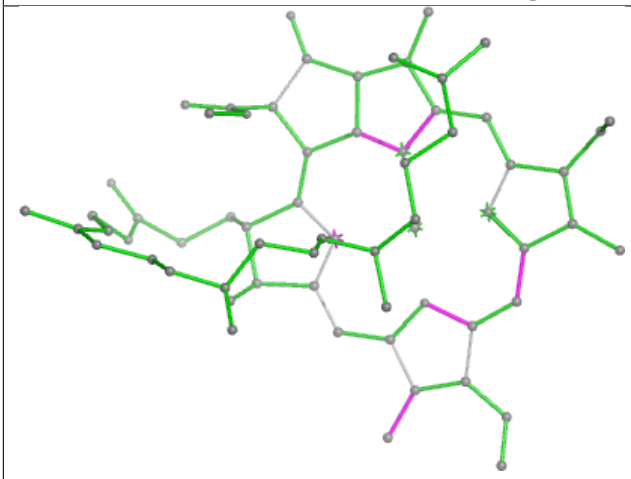
Ligand STE E 101



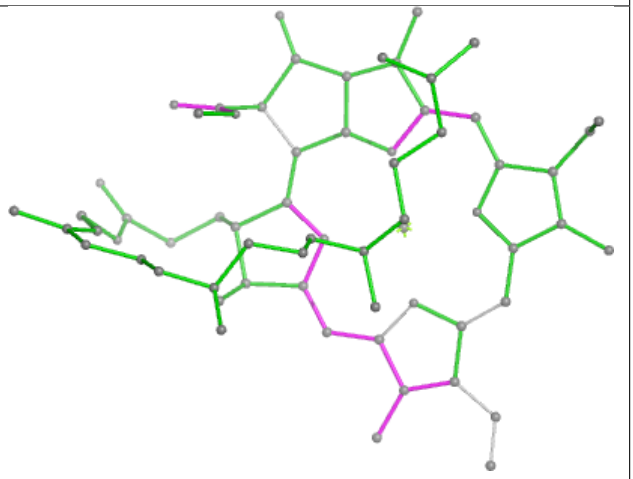
Ligand STE C 516



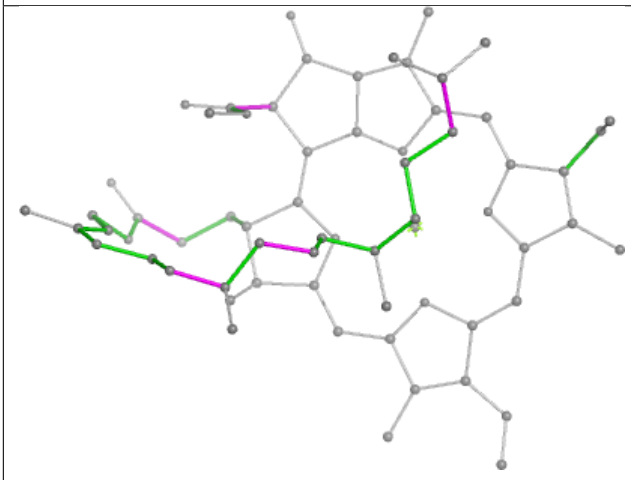
Ligand CLA C 510



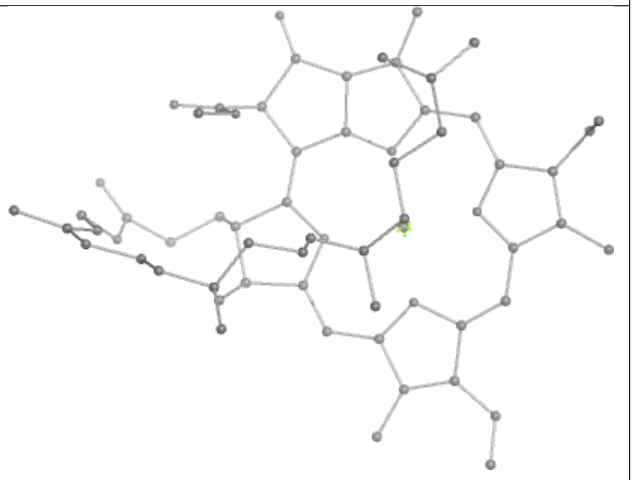
Bond lengths



Bond angles

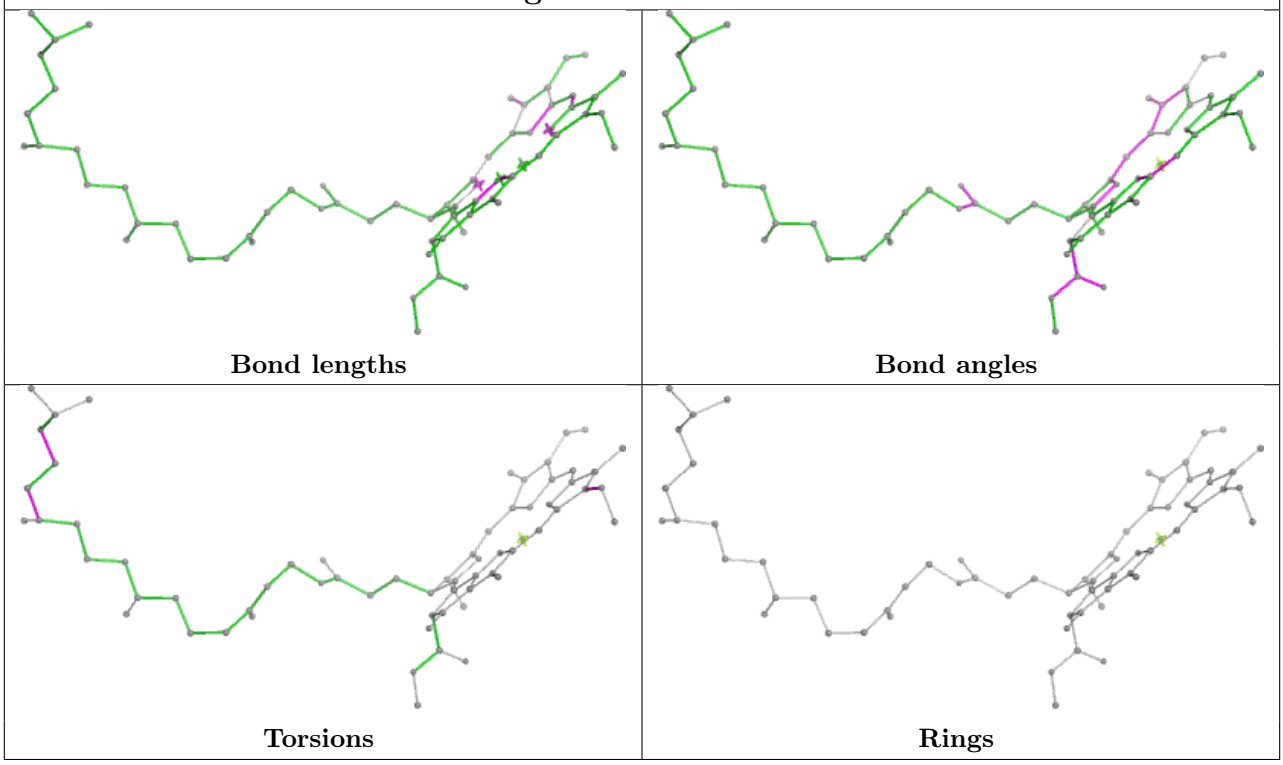


Torsions

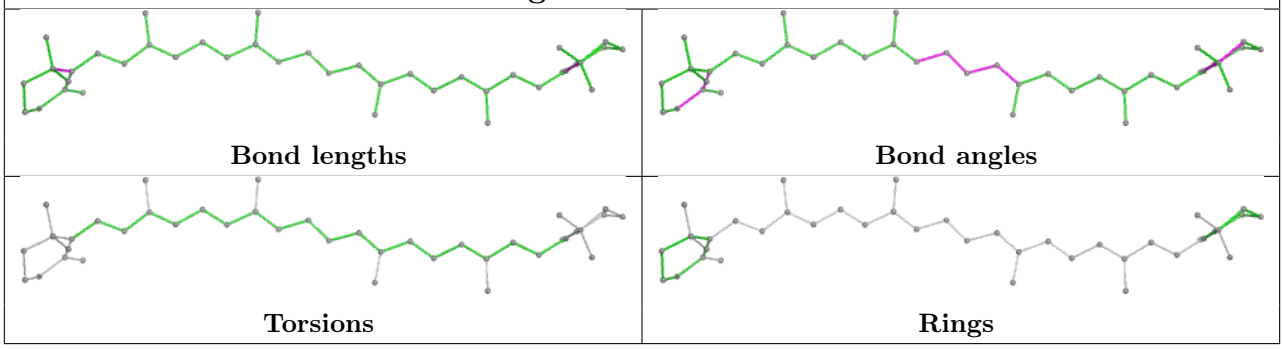


Rings

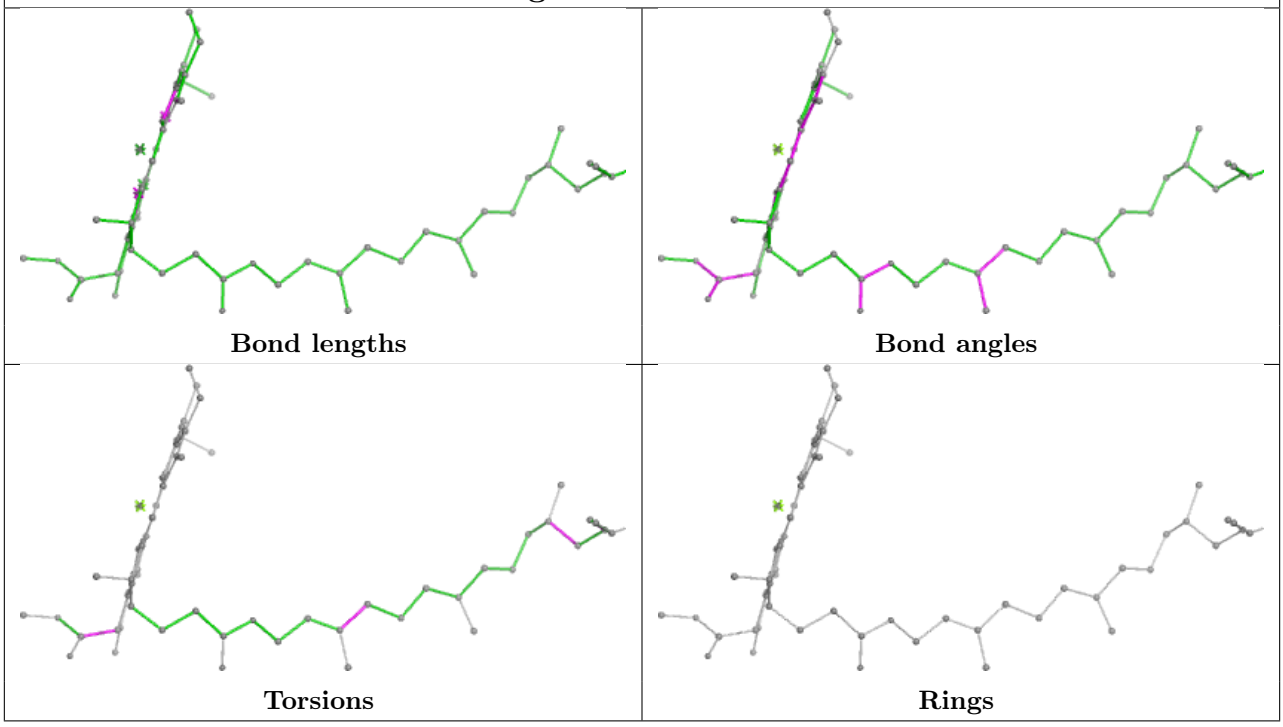
Ligand CLA D 404



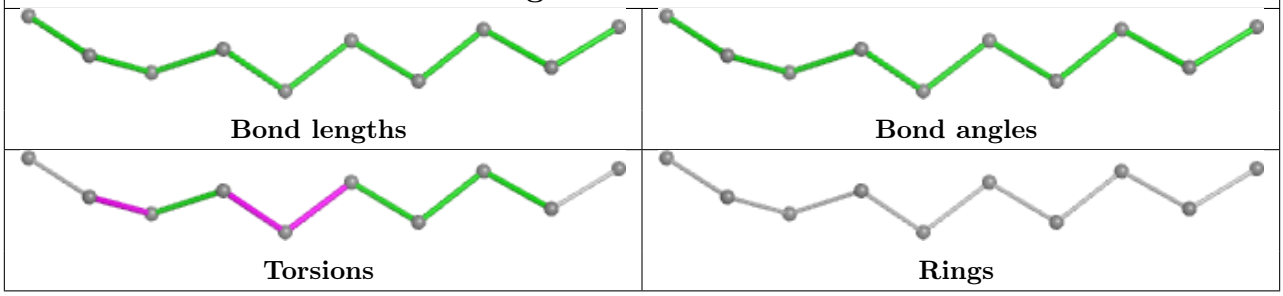
Ligand BCR c 514



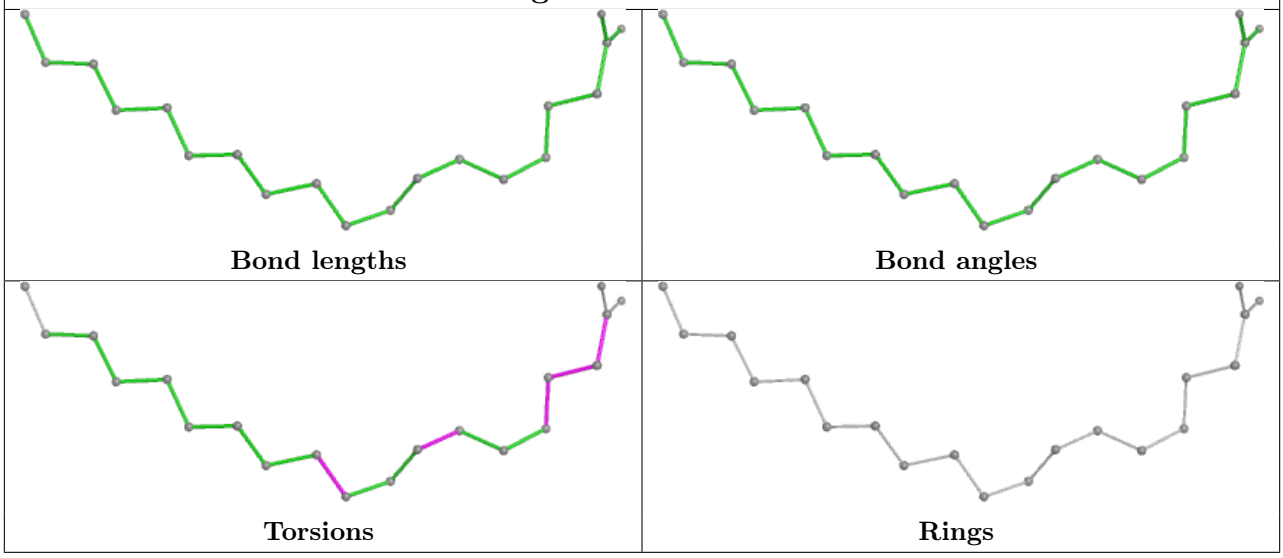
Ligand CLA b 606



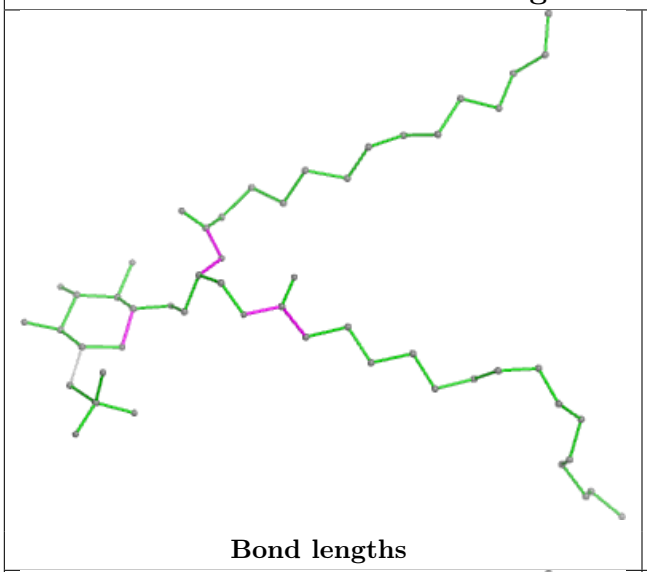
Ligand STE m 102



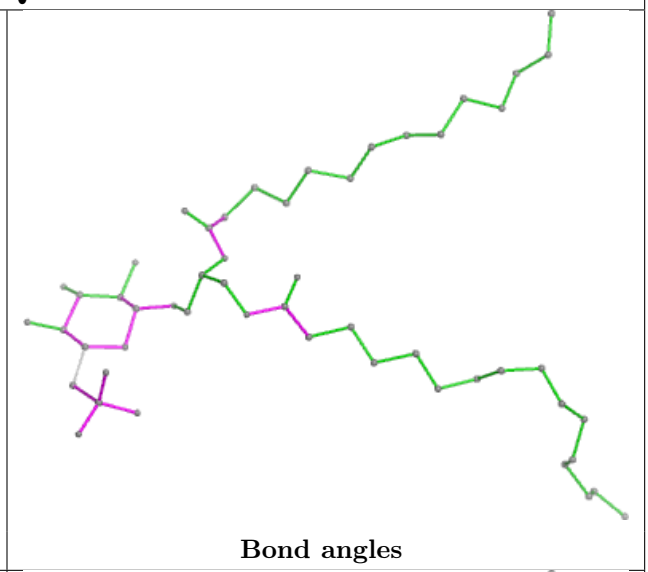
Ligand STE d 412



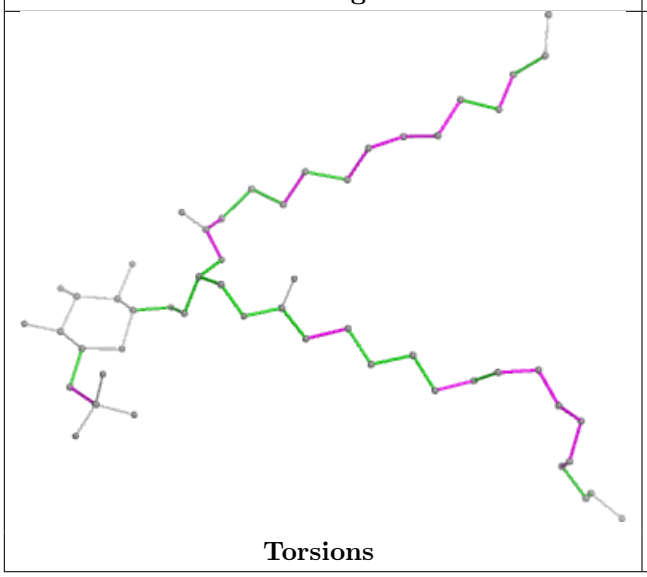
Ligand SQD a 411



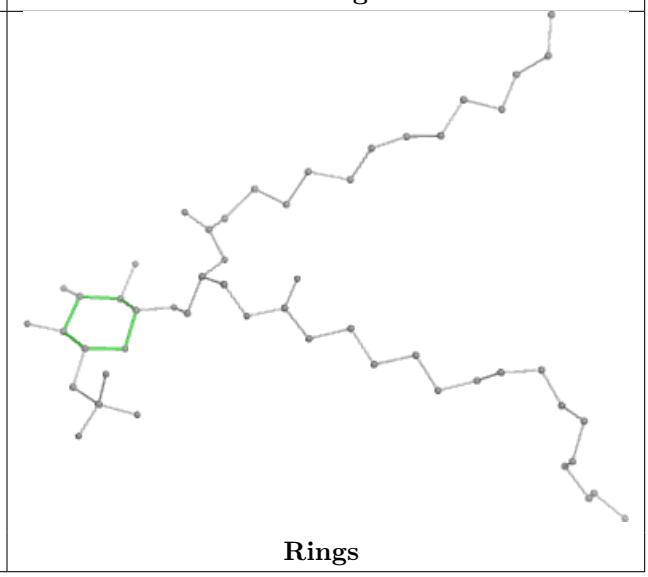
Bond lengths



Bond angles

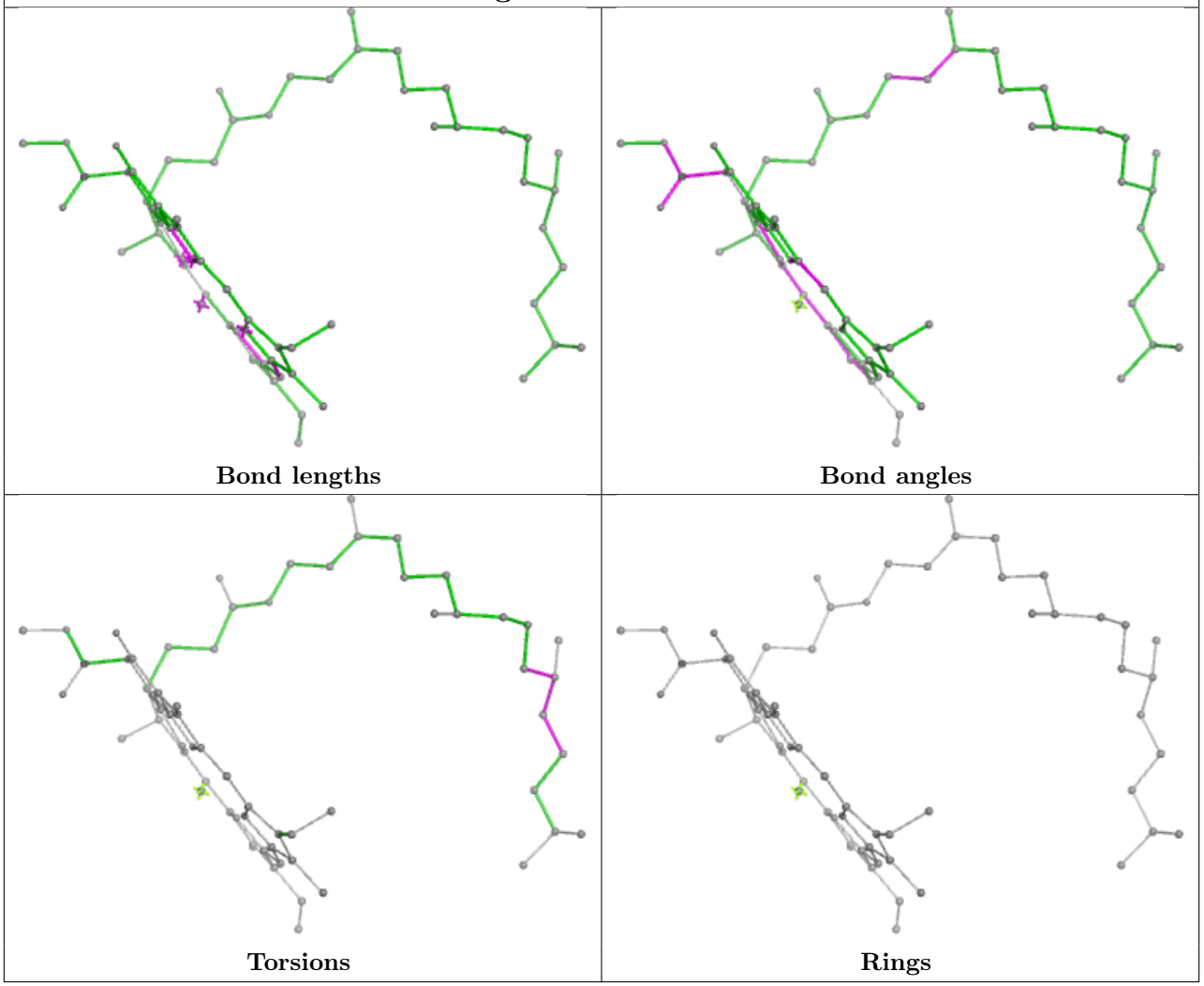


Torsions

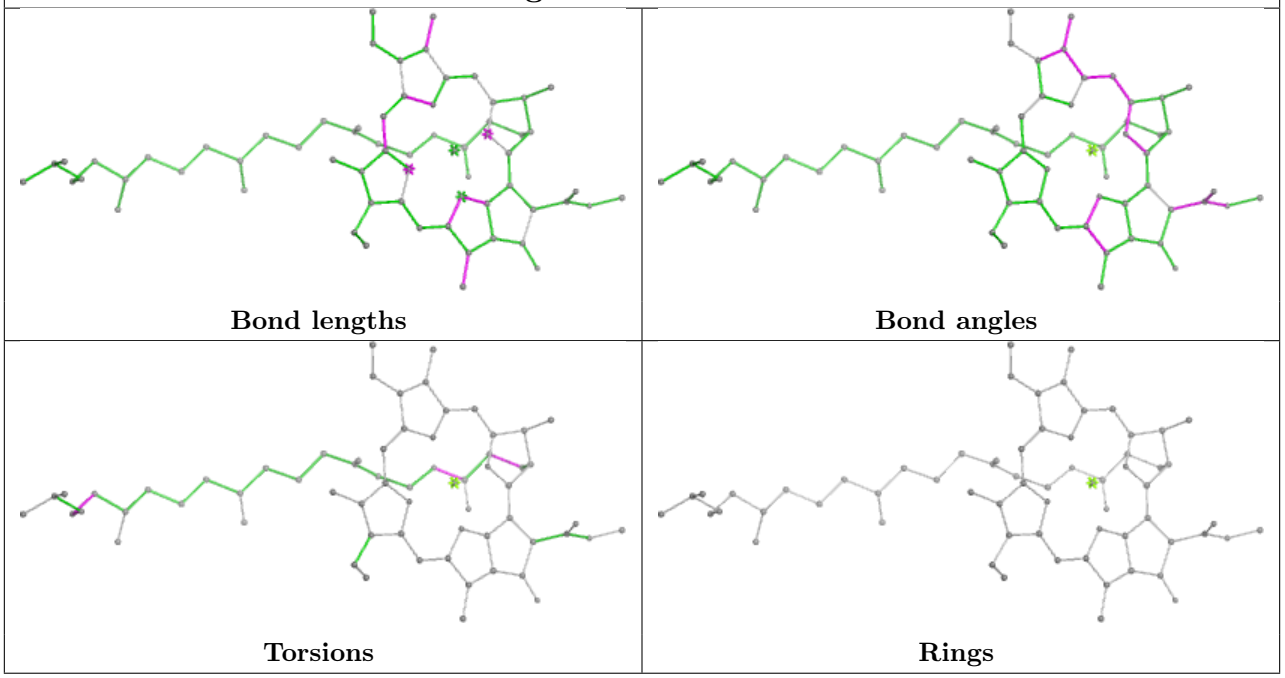


Rings

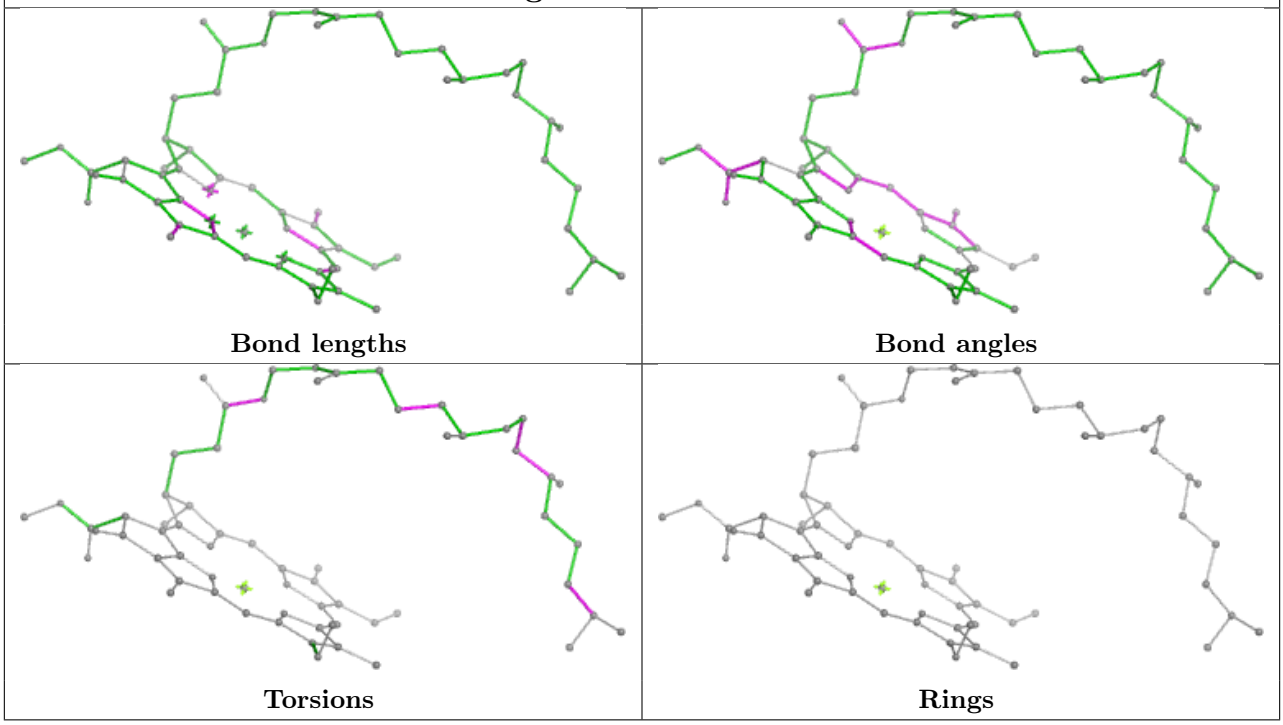
Ligand CLA b 612



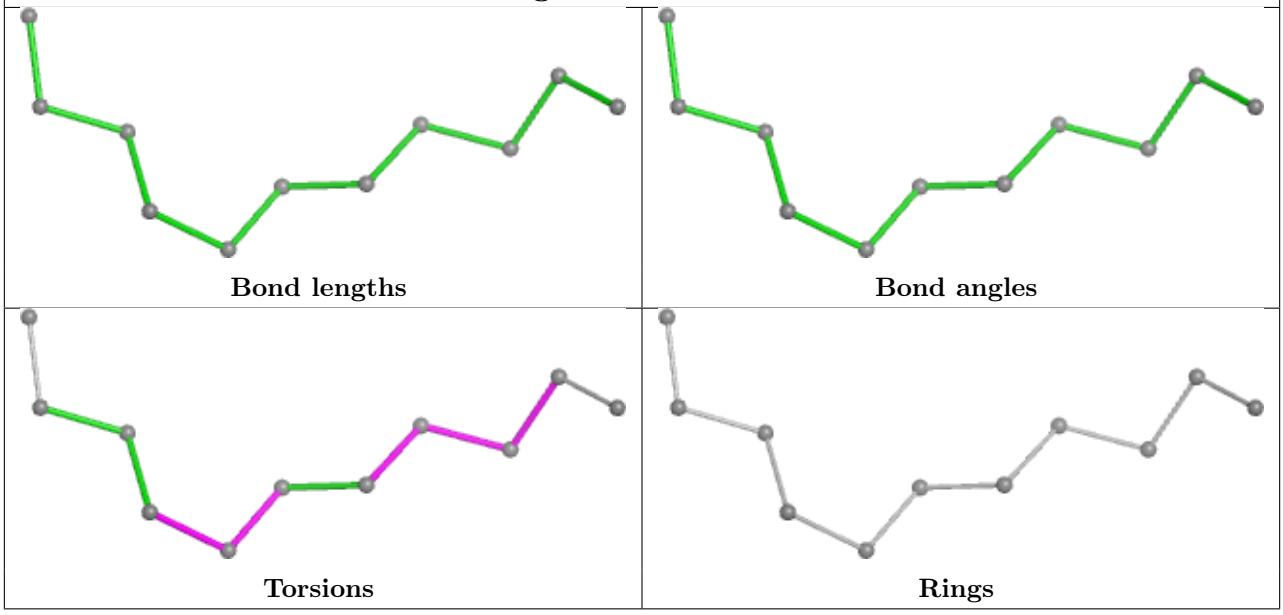
Ligand CLA B 608



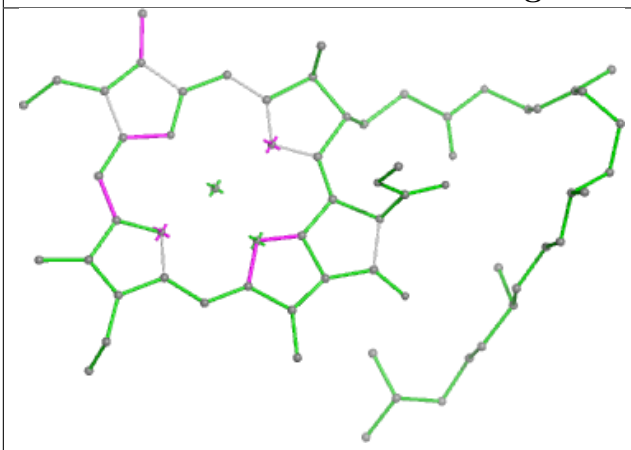
Ligand CLA C 513



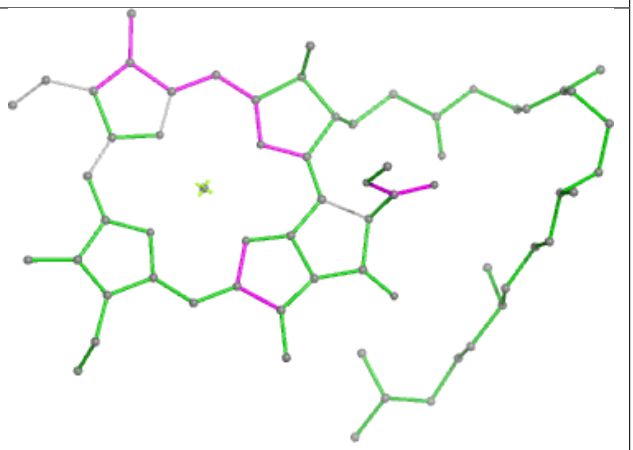
Ligand STE a 415



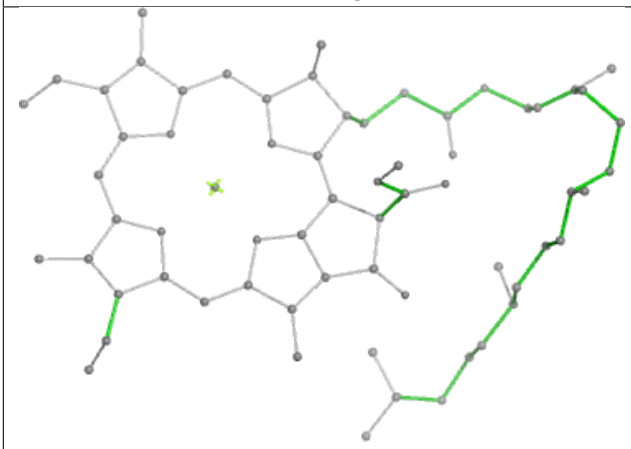
Ligand CLA B 610



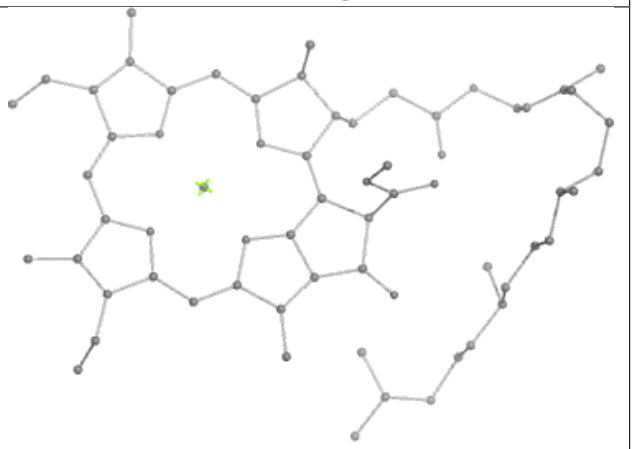
Bond lengths



Bond angles

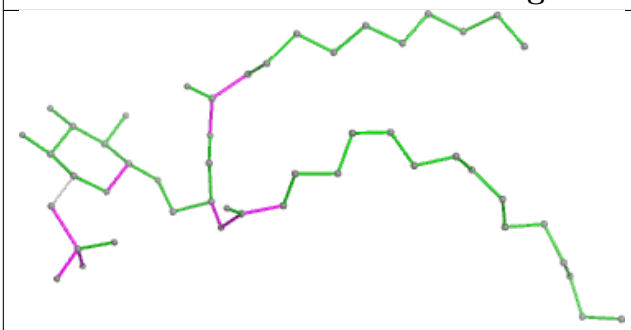


Torsions

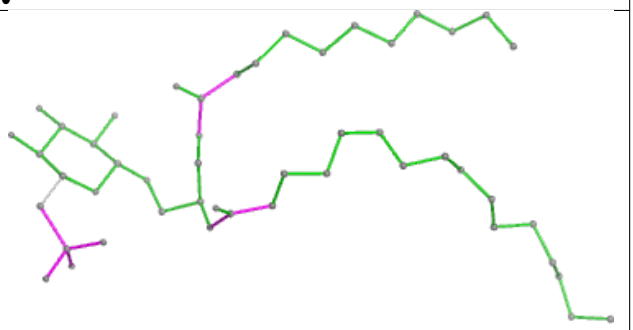


Rings

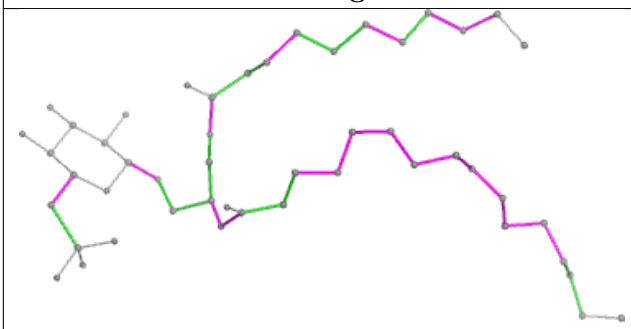
Ligand SQD b 621



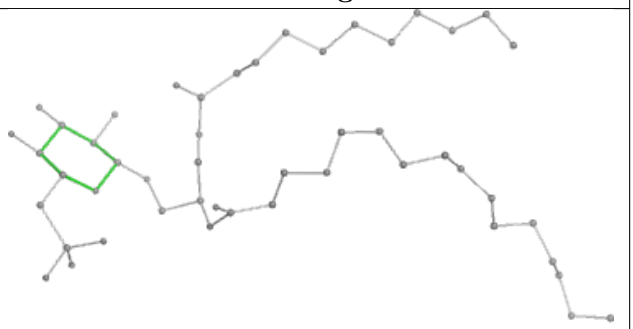
Bond lengths



Bond angles

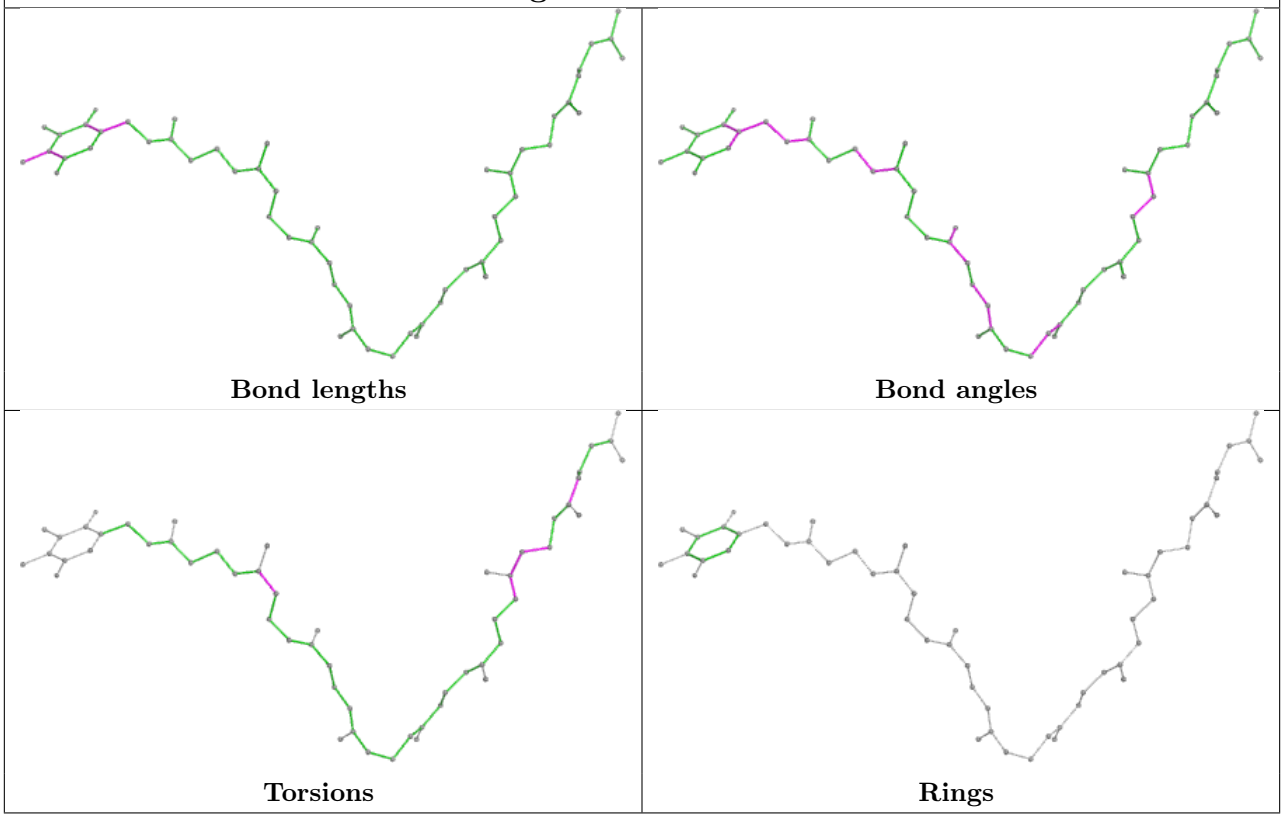


Torsions

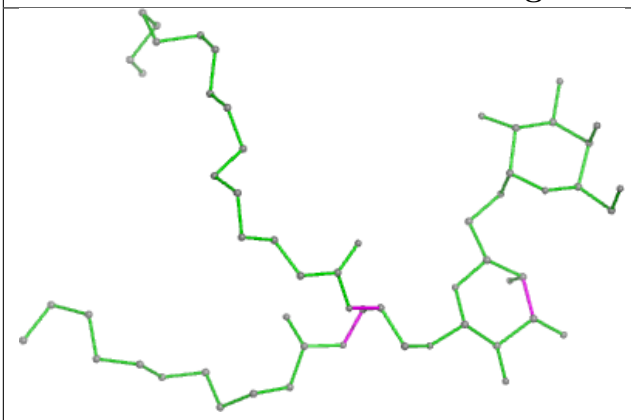


Rings

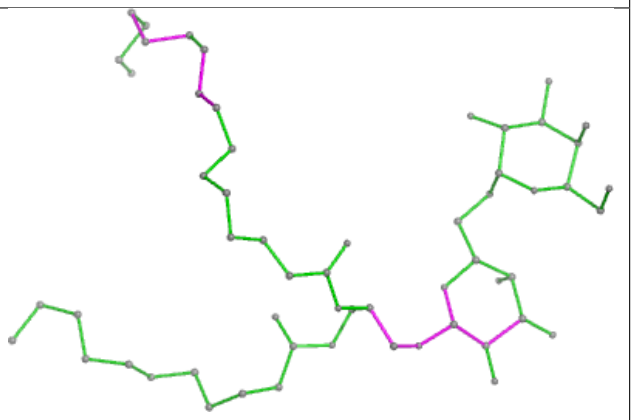
Ligand PL9 D 407



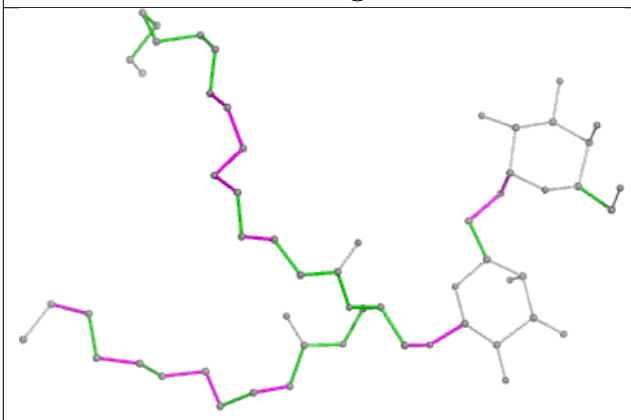
Ligand DGD c 518



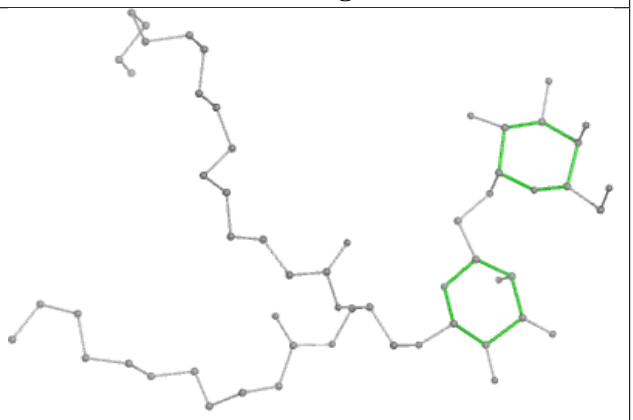
Bond lengths



Bond angles

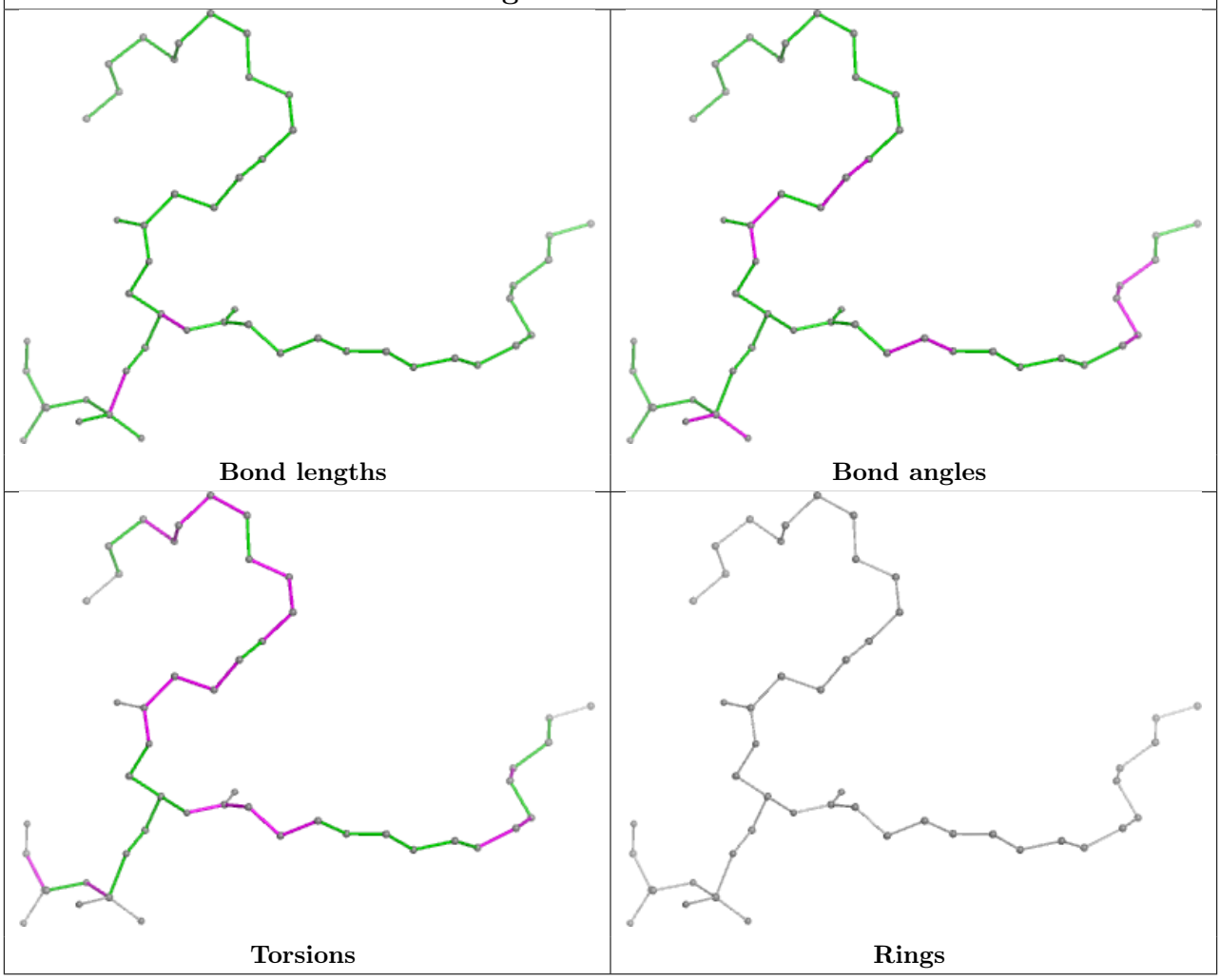


Torsions

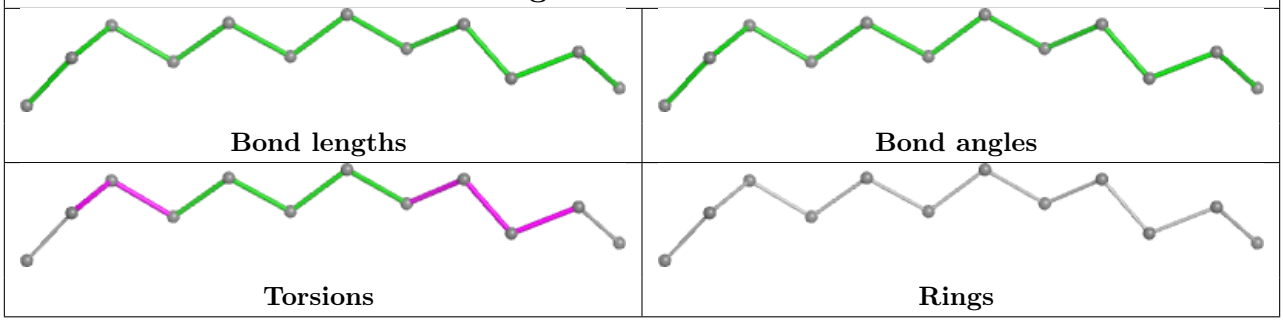


Rings

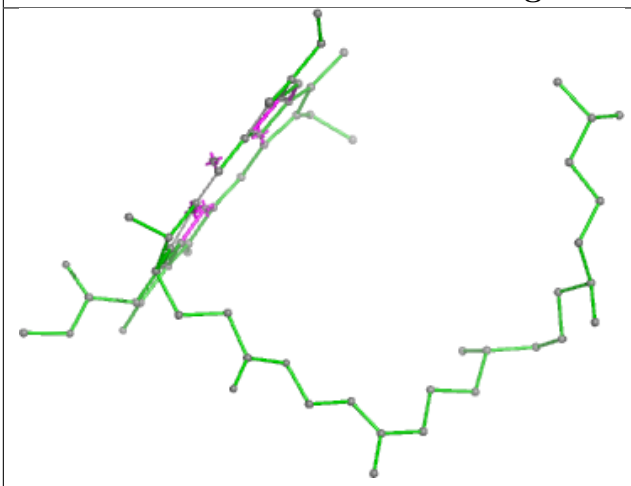
Ligand LHG a 420



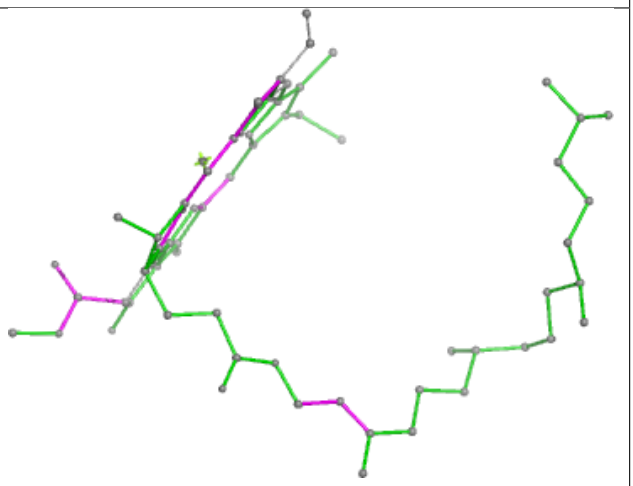
Ligand STE E 102



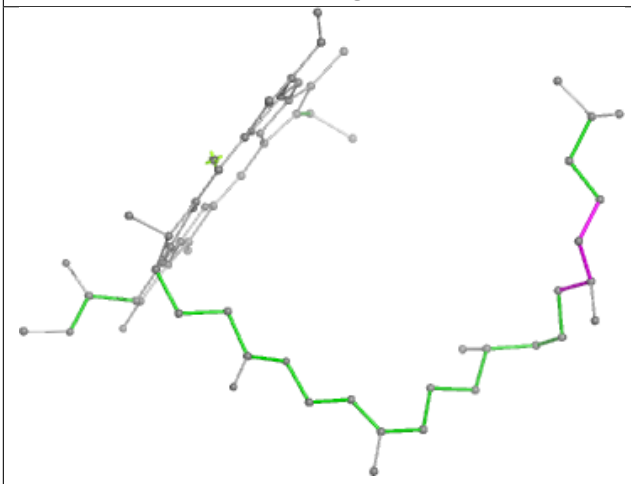
Ligand CLA B 611



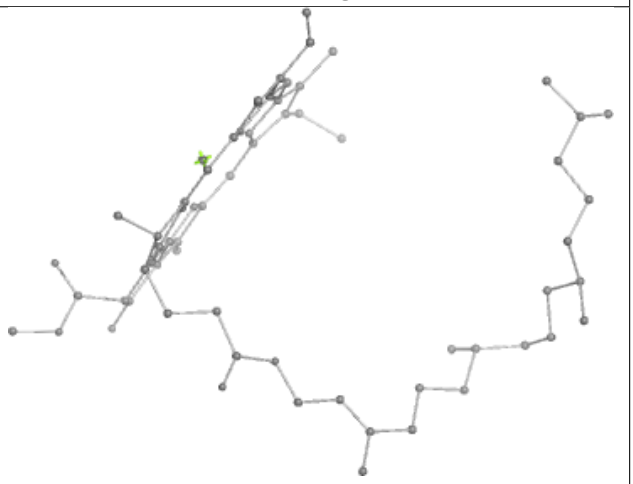
Bond lengths



Bond angles

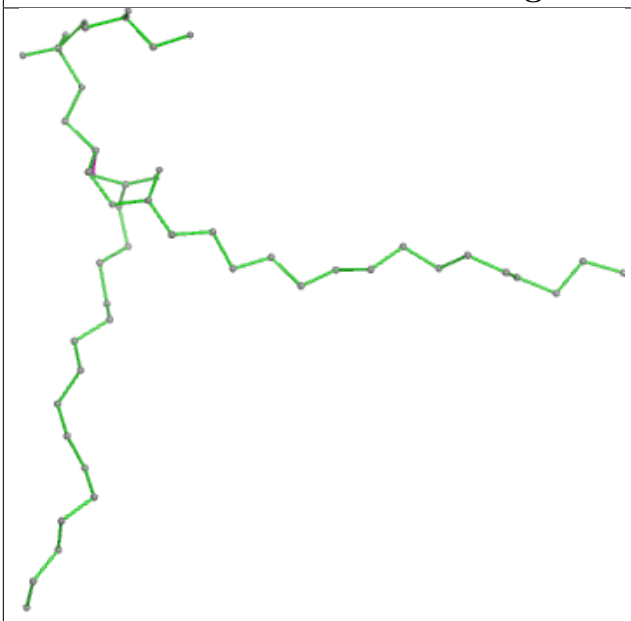


Torsions

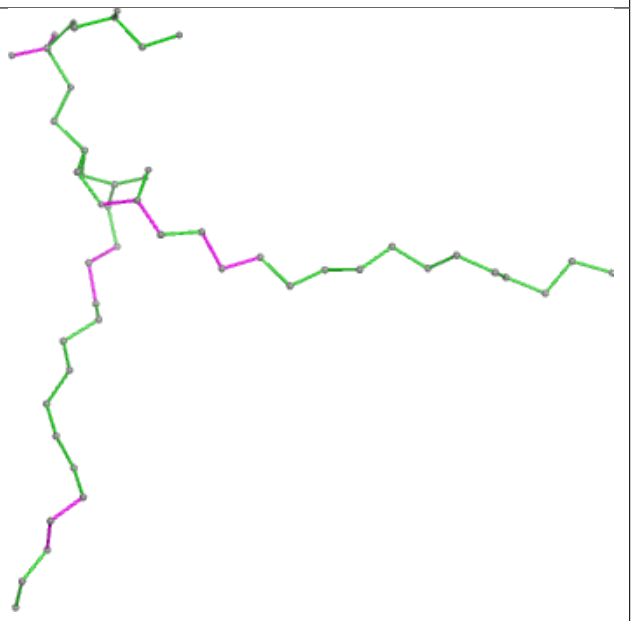


Rings

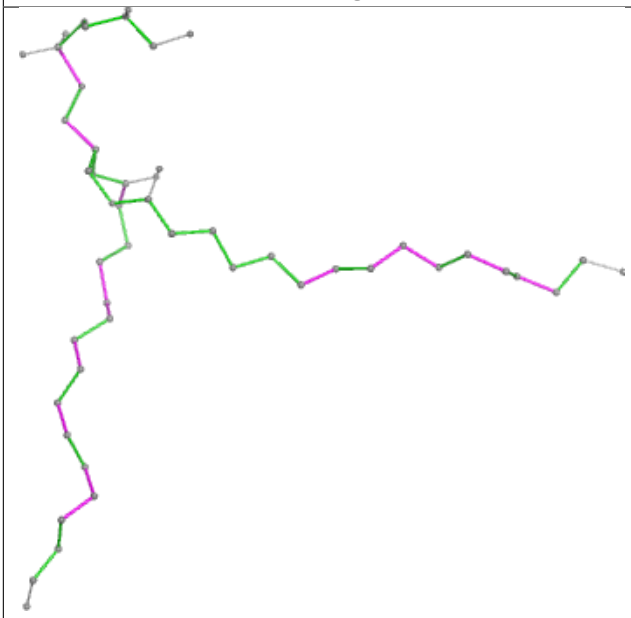
Ligand LHG L 101



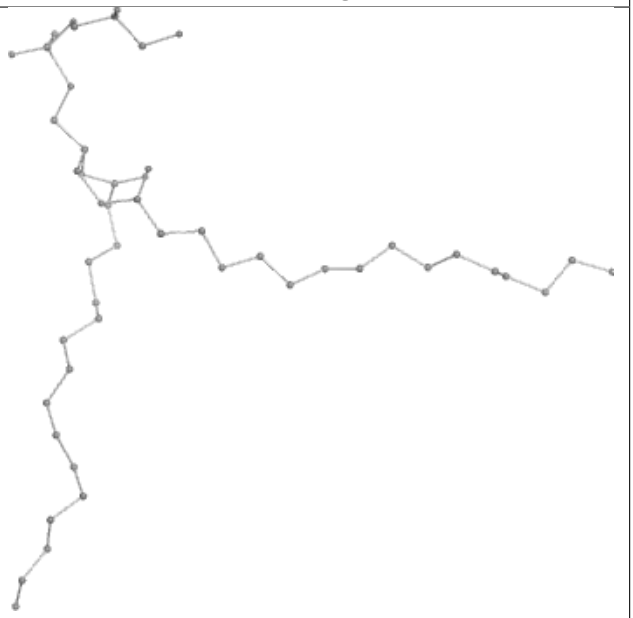
Bond lengths



Bond angles

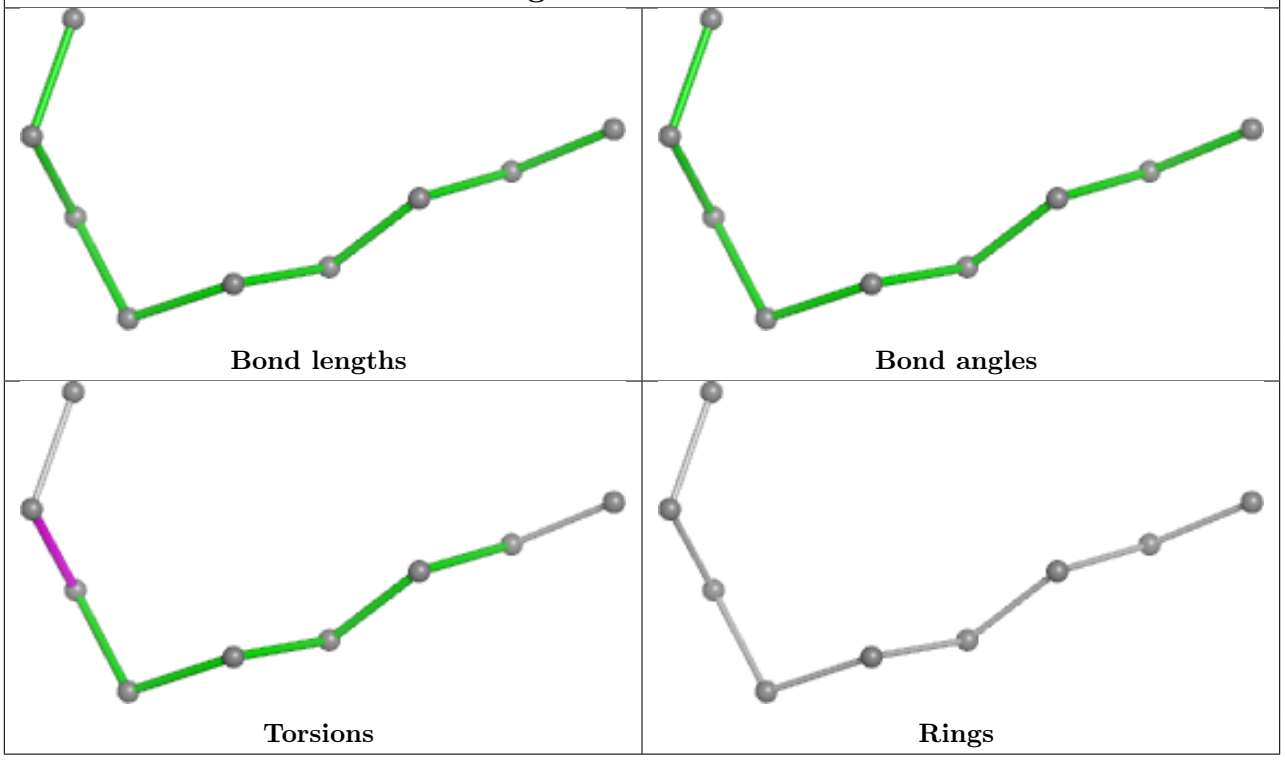


Torsions

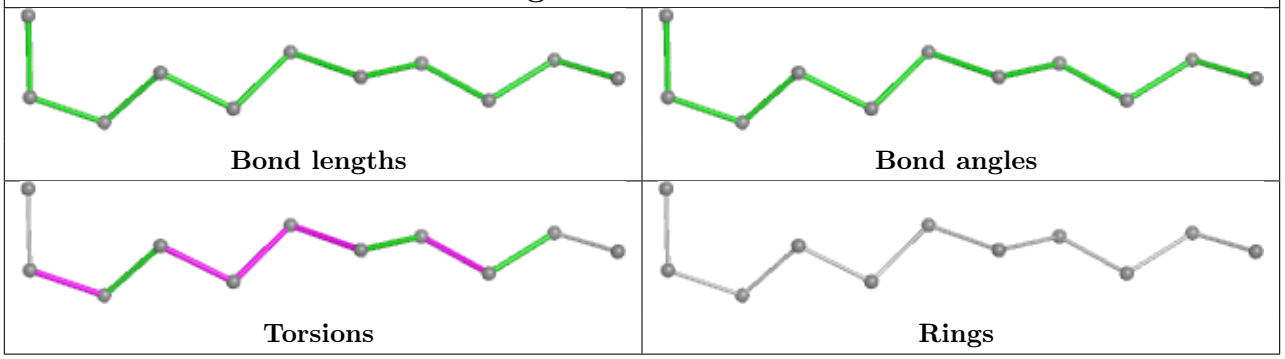


Rings

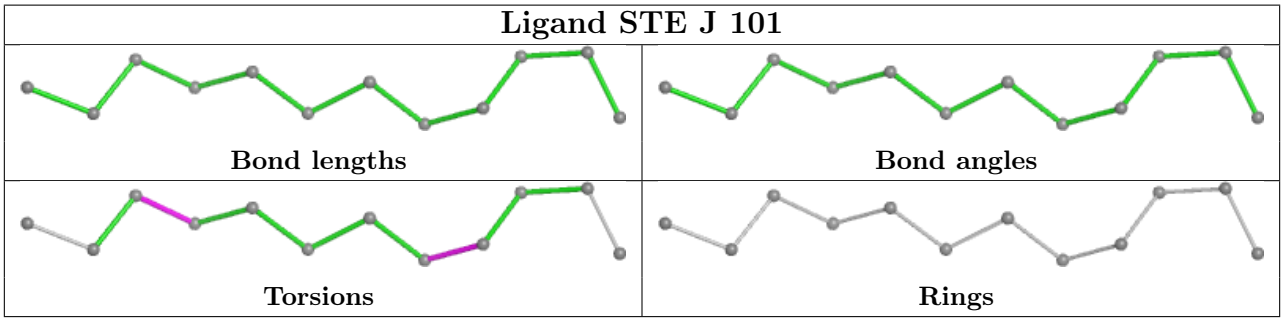
Ligand STE D 413



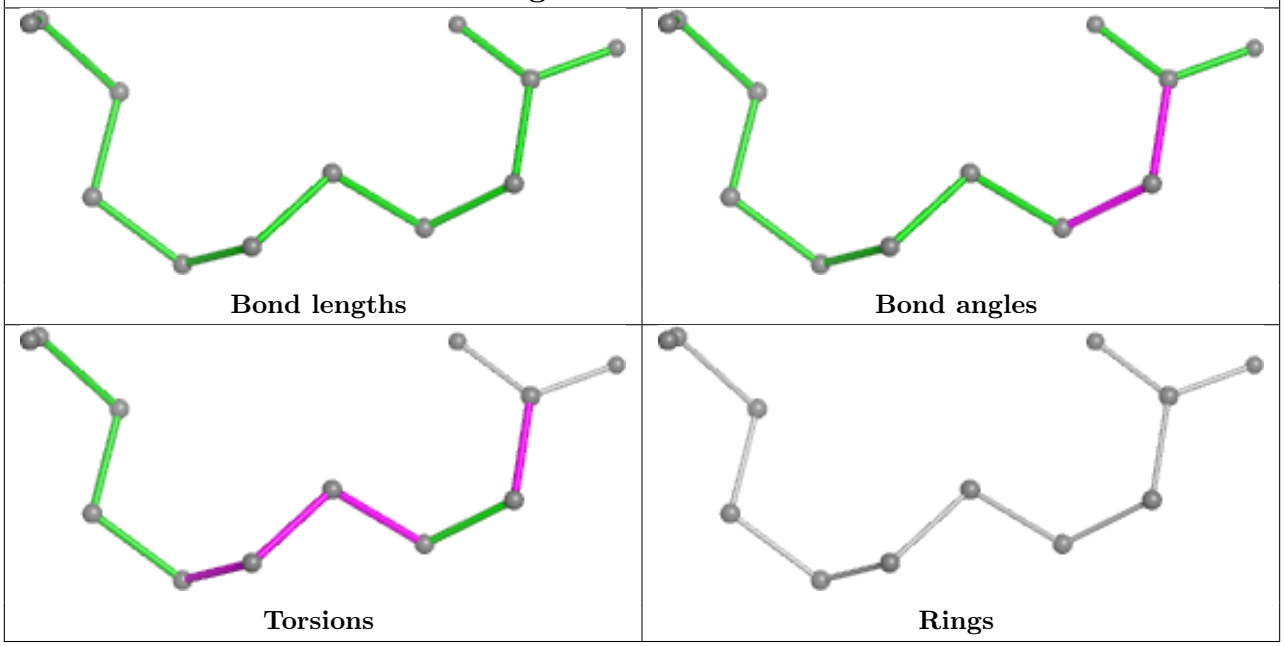
Ligand STE K 102



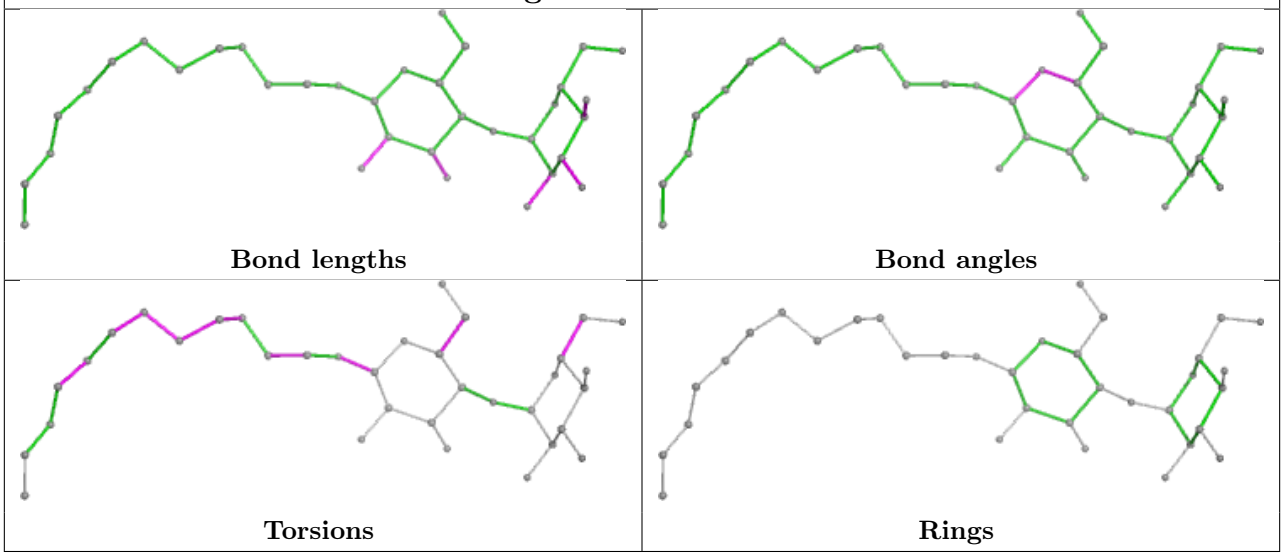
Ligand STE J 101



Ligand STE B 622



Ligand LMT Z 101



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

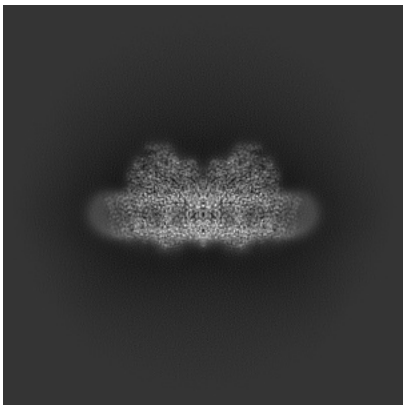
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-50019. These allow visual inspection of the internal detail of the map and identification of artifacts.

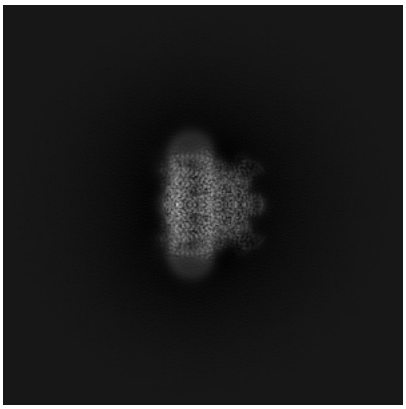
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

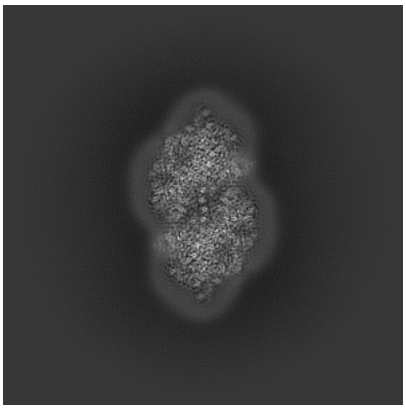
6.1.1 Primary map



X

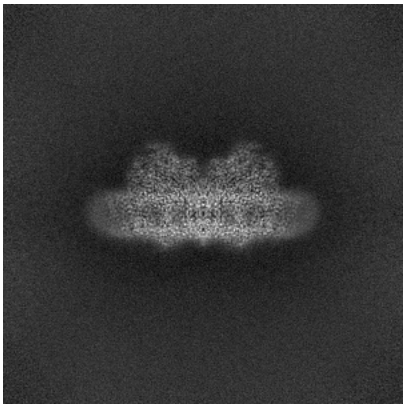


Y

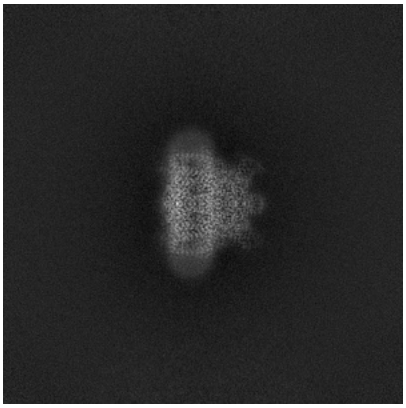


Z

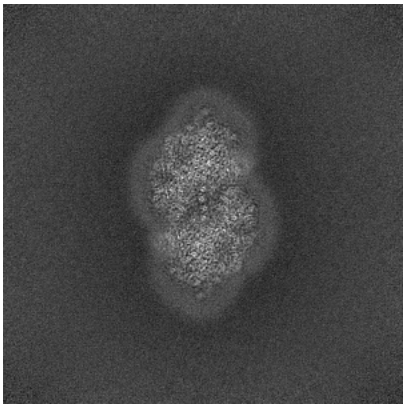
6.1.2 Raw map



X



Y

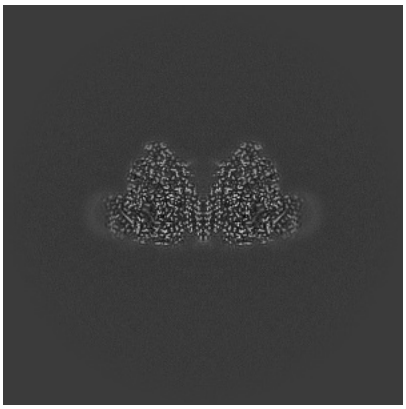


Z

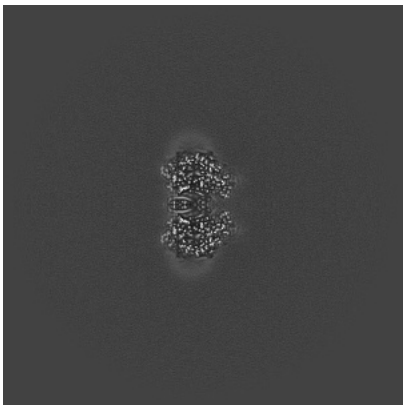
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

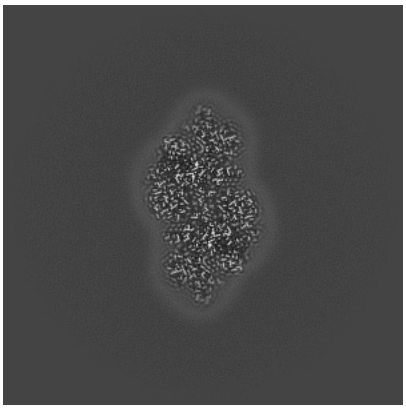
6.2.1 Primary map



X Index: 360

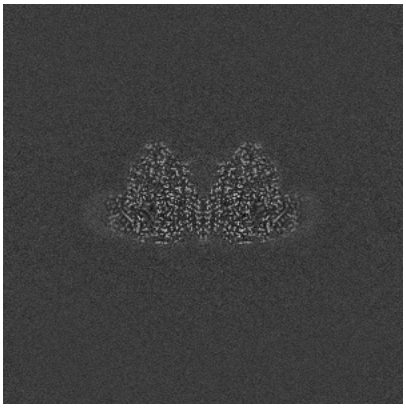


Y Index: 360

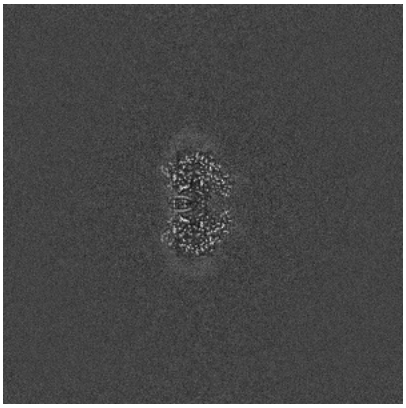


Z Index: 360

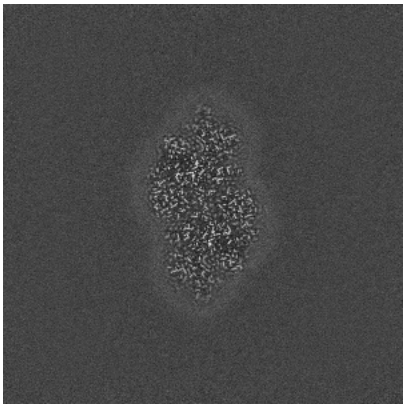
6.2.2 Raw map



X Index: 360



Y Index: 360

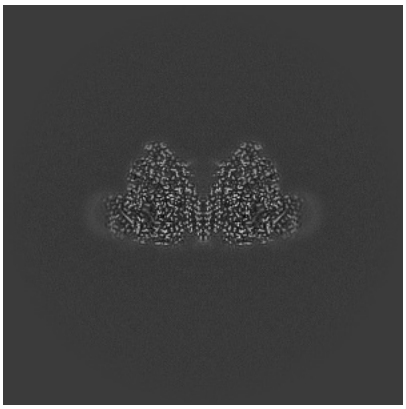


Z Index: 360

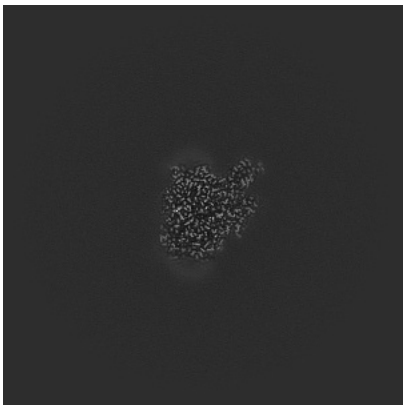
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

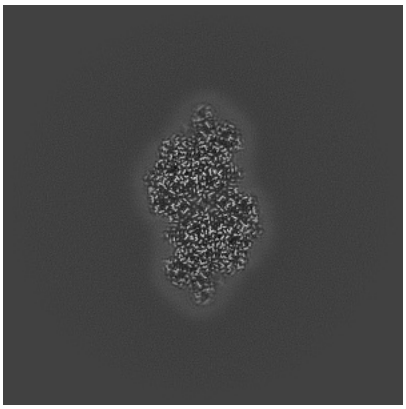
6.3.1 Primary map



X Index: 360

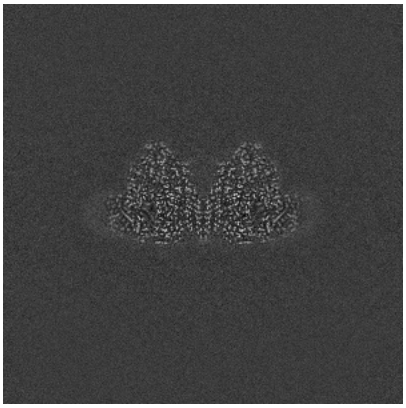


Y Index: 420

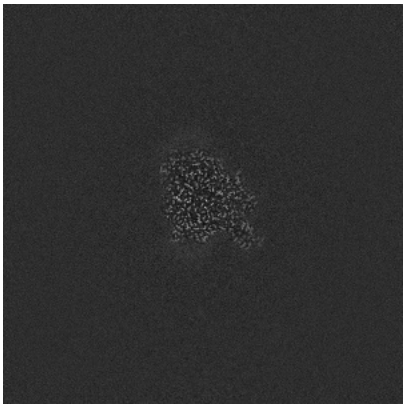


Z Index: 369

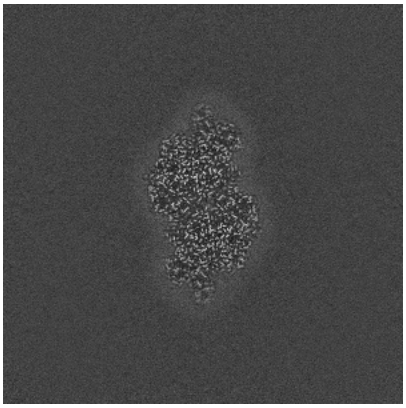
6.3.2 Raw map



X Index: 360



Y Index: 300

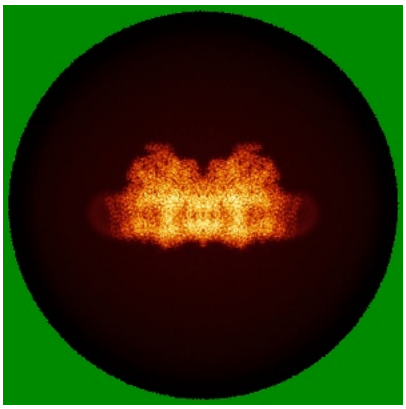


Z Index: 369

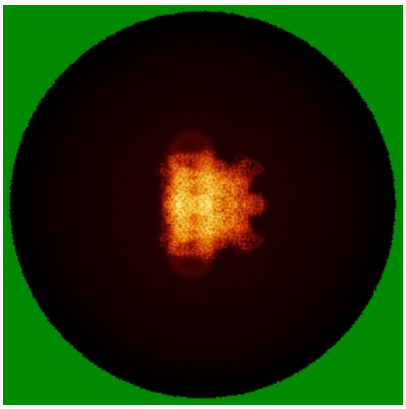
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

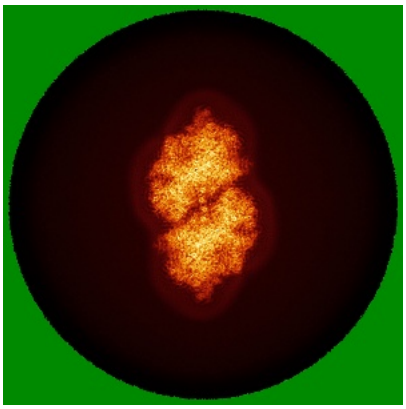
6.4.1 Primary map



X

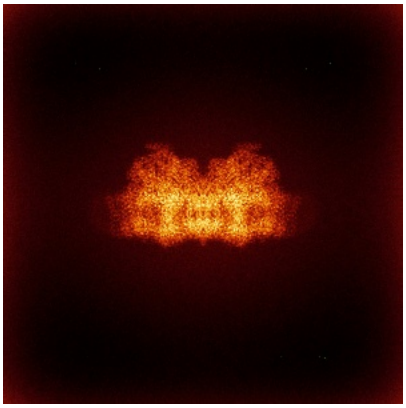


Y

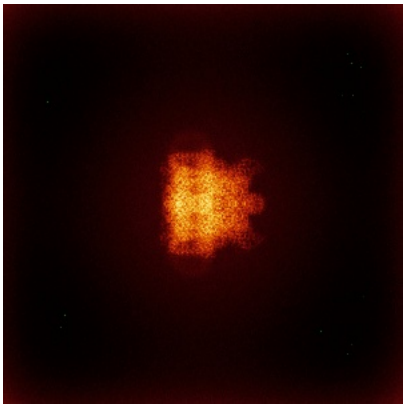


Z

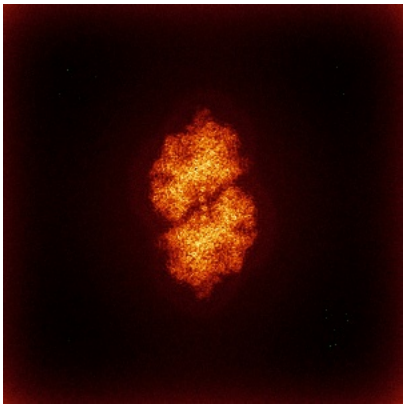
6.4.2 Raw map



X



Y

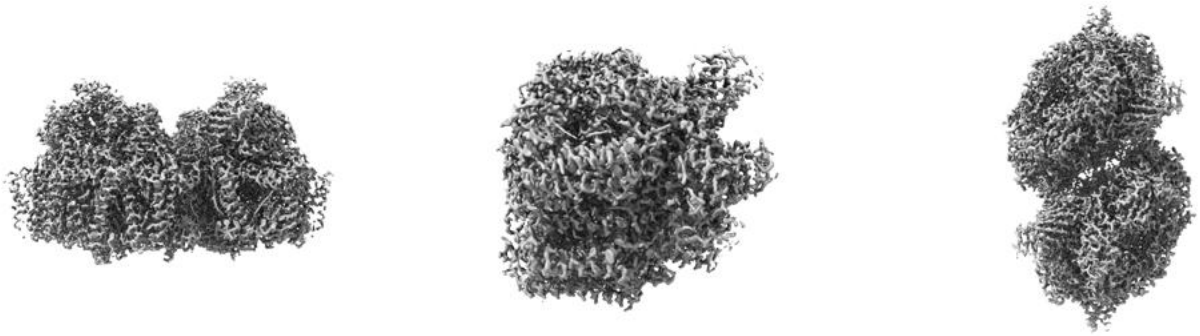


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.45. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

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

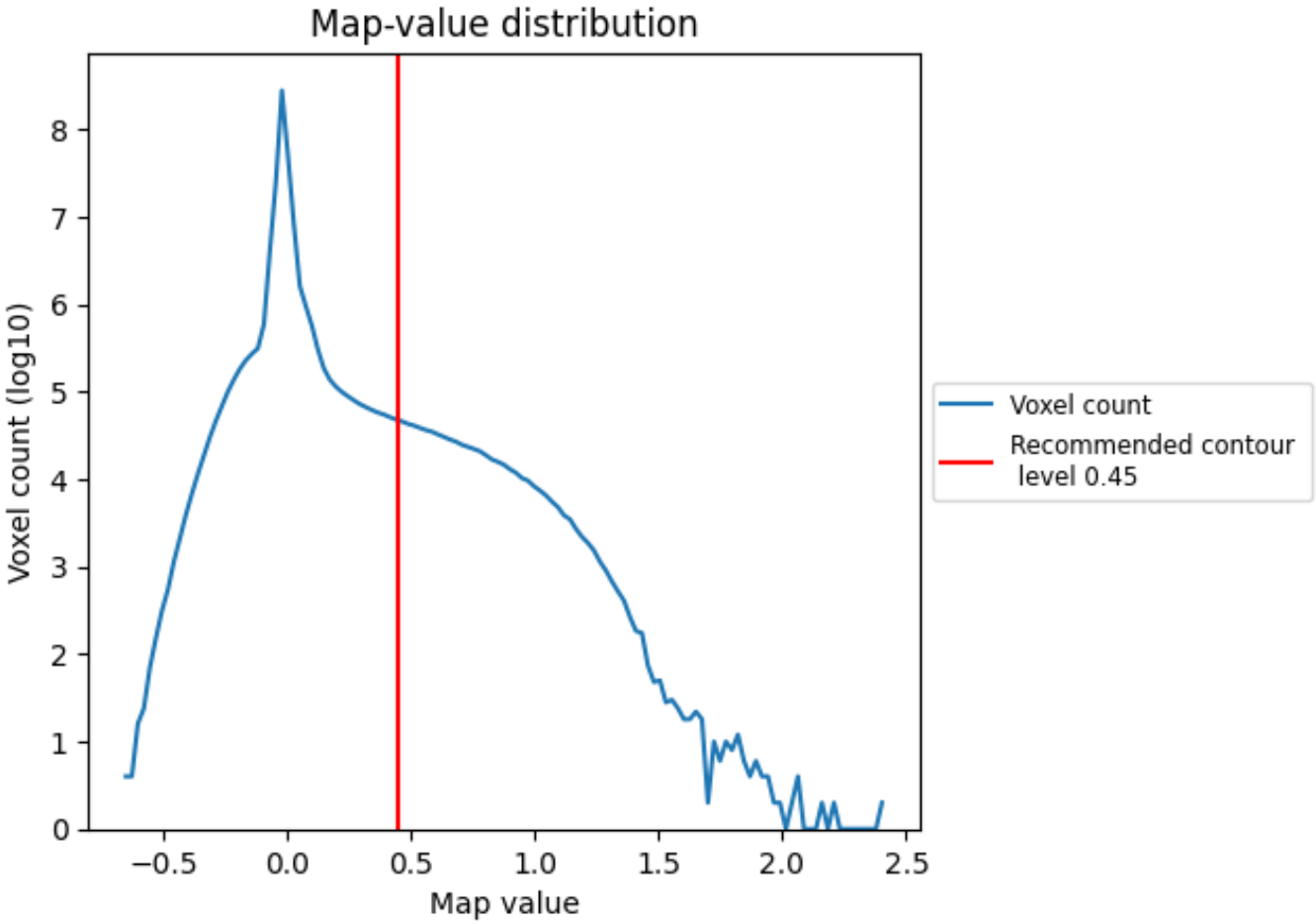
6.6 Mask visualisation (i)

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

7 Map analysis

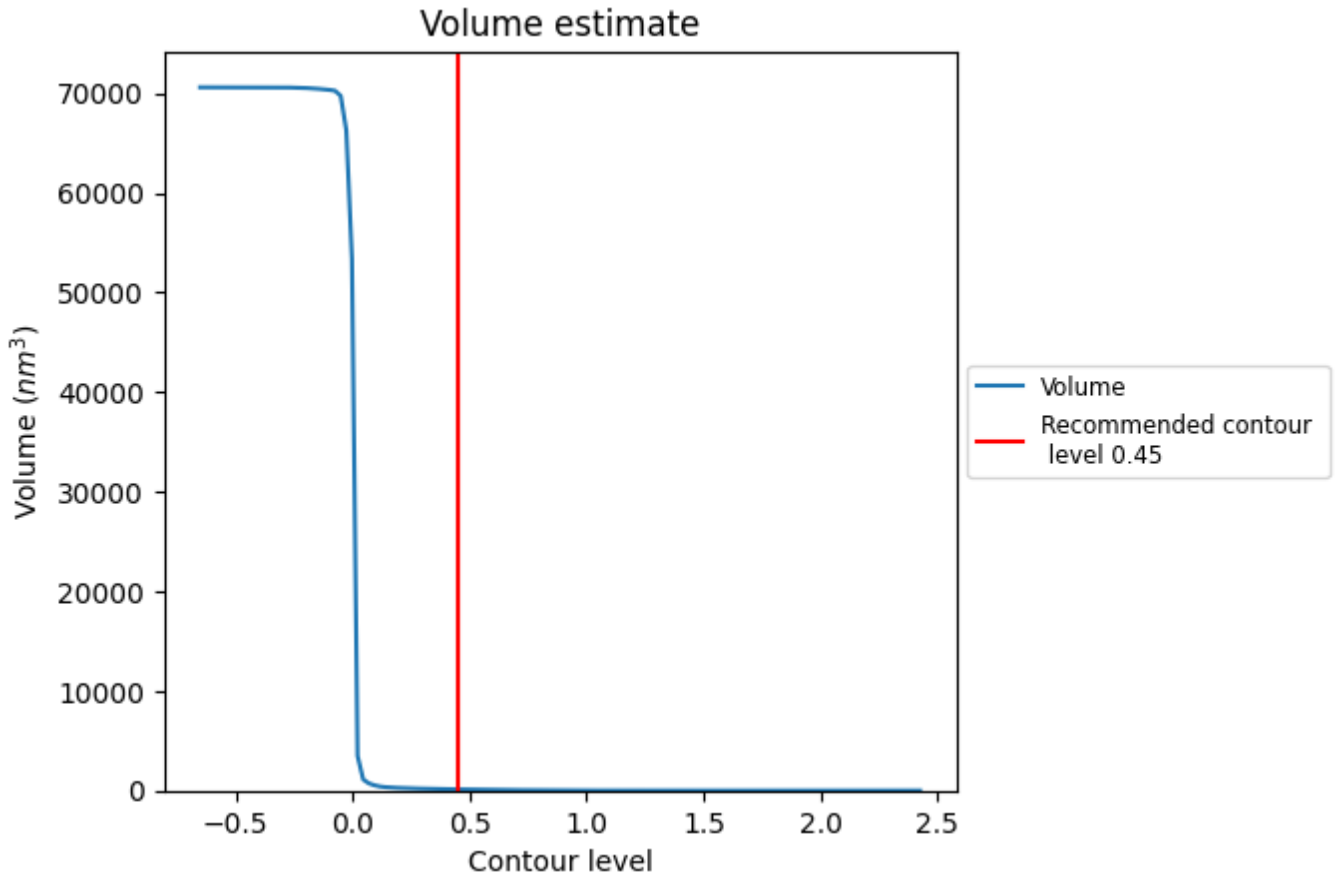
This section contains the results of statistical analysis of the map.

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.

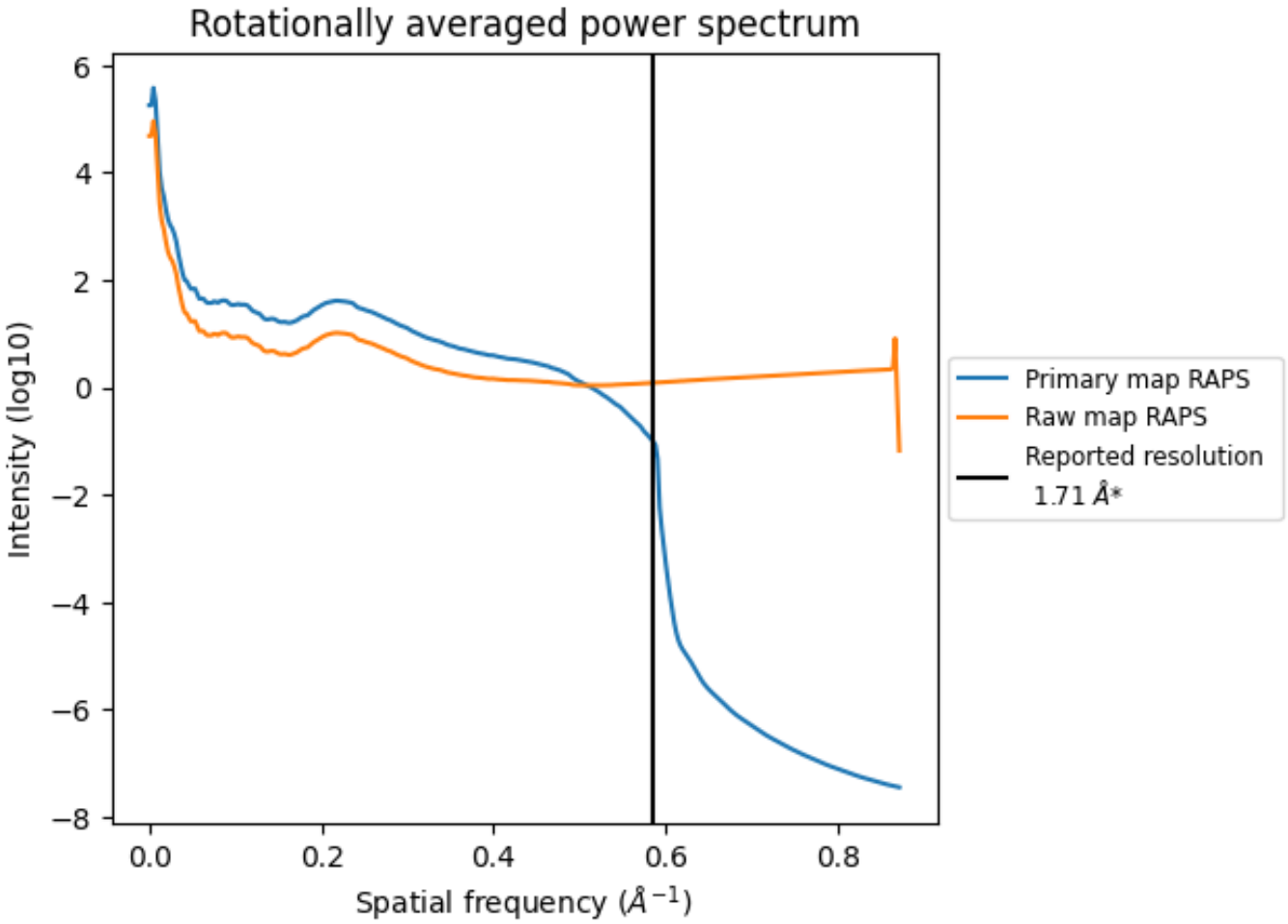
7.2 Volume estimate (i)



The volume at the recommended contour level is 121 nm^3; this corresponds to an approximate mass of 109 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)

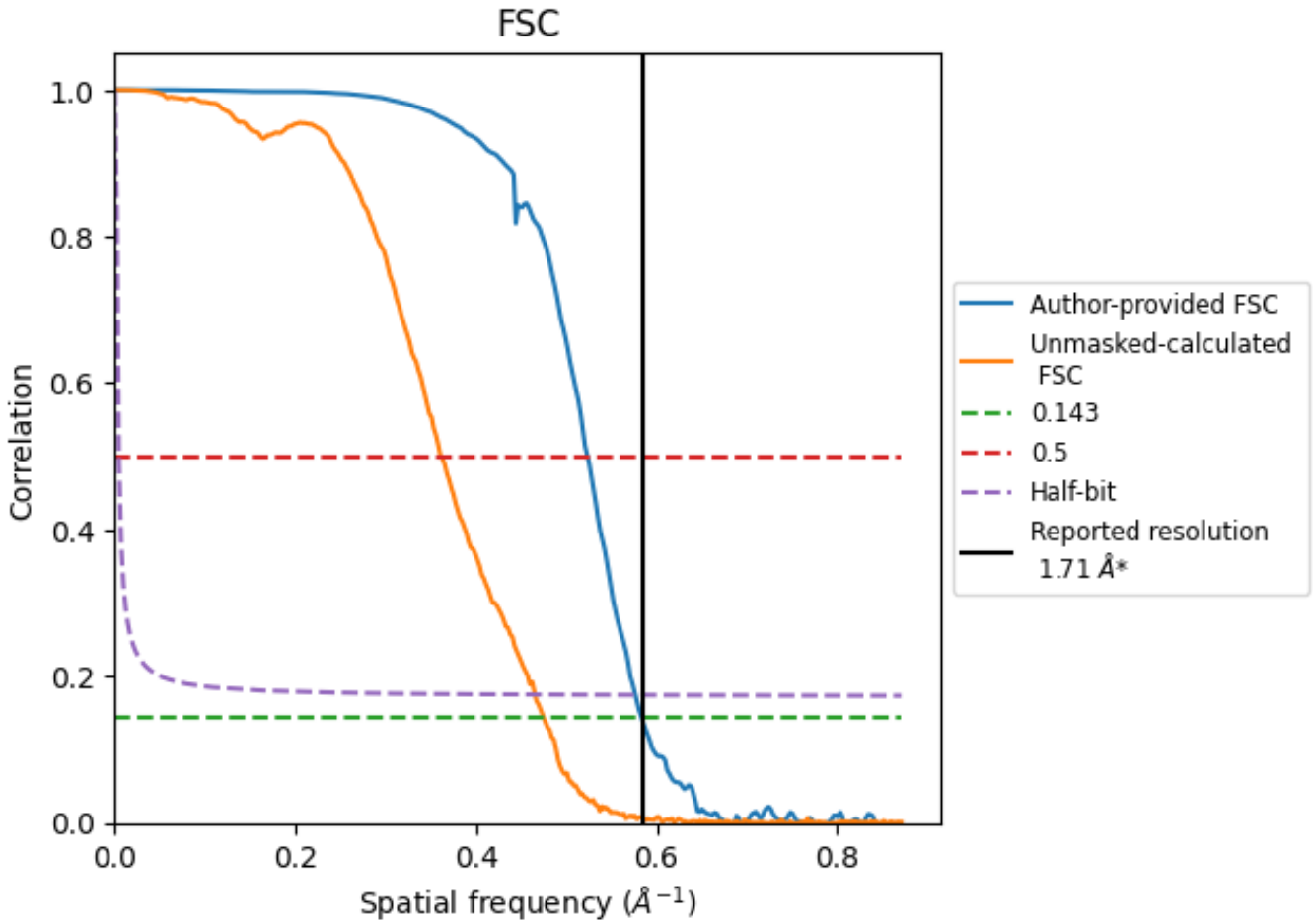


*Reported resolution corresponds to spatial frequency of 0.585 Å^{-1}

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 0.585 Å^{-1}

8.2 Resolution estimates (i)

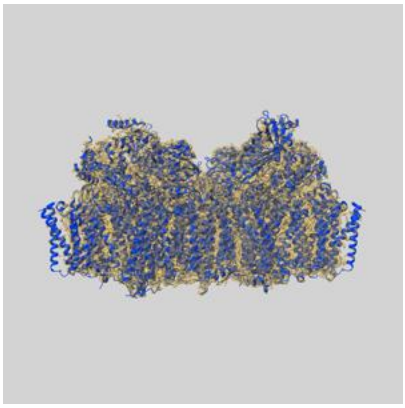
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	1.71	-	-
Author-provided FSC curve	1.71	1.91	1.73
Unmasked-calculated*	2.10	2.77	2.15

*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 2.10 differs from the reported value 1.71 by more than 10 %

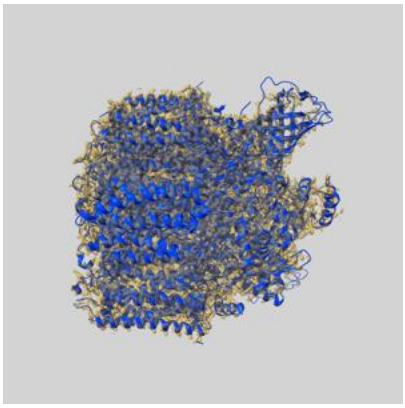
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-50019 and PDB model 9EVX. Per-residue inclusion information can be found in section 3 on page 29.

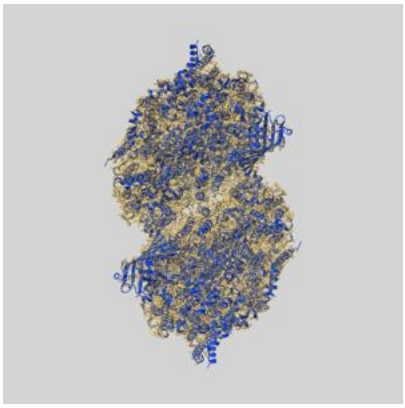
9.1 Map-model overlay



X



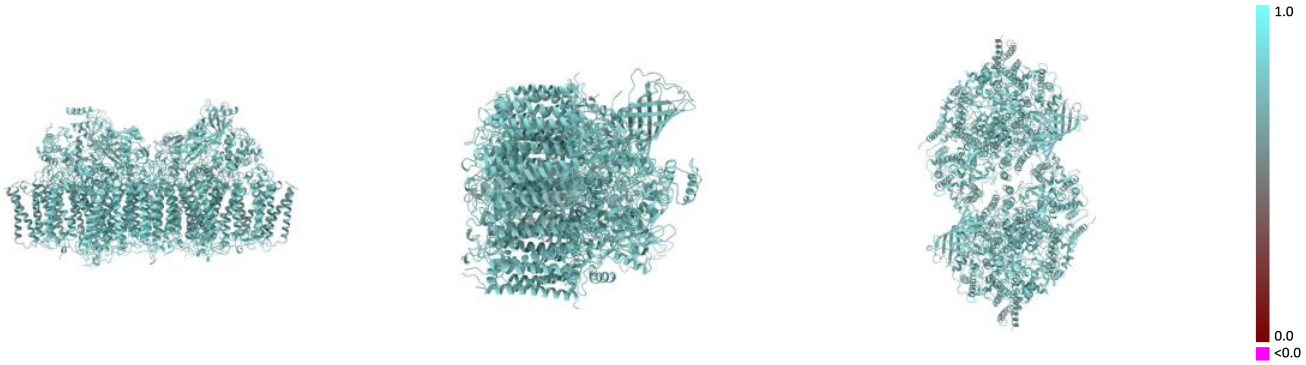
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.45 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.

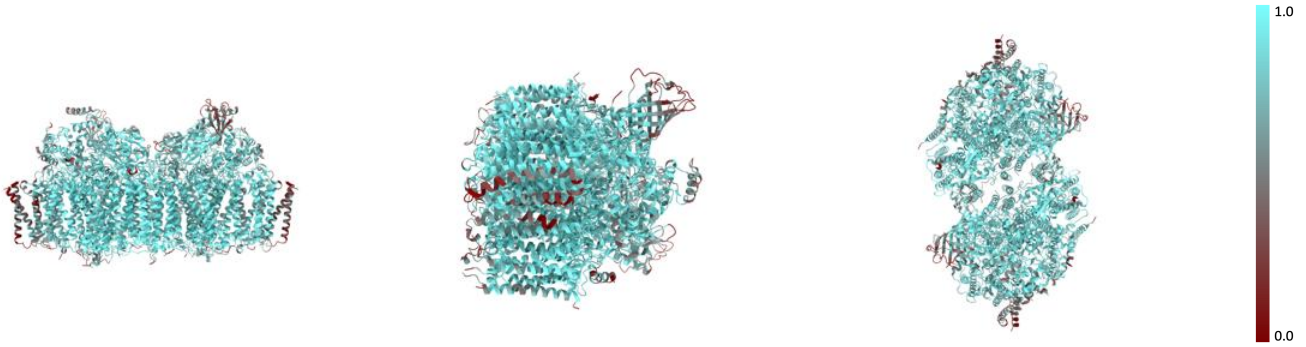
9.2 Q-score mapped to coordinate model (i)



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.

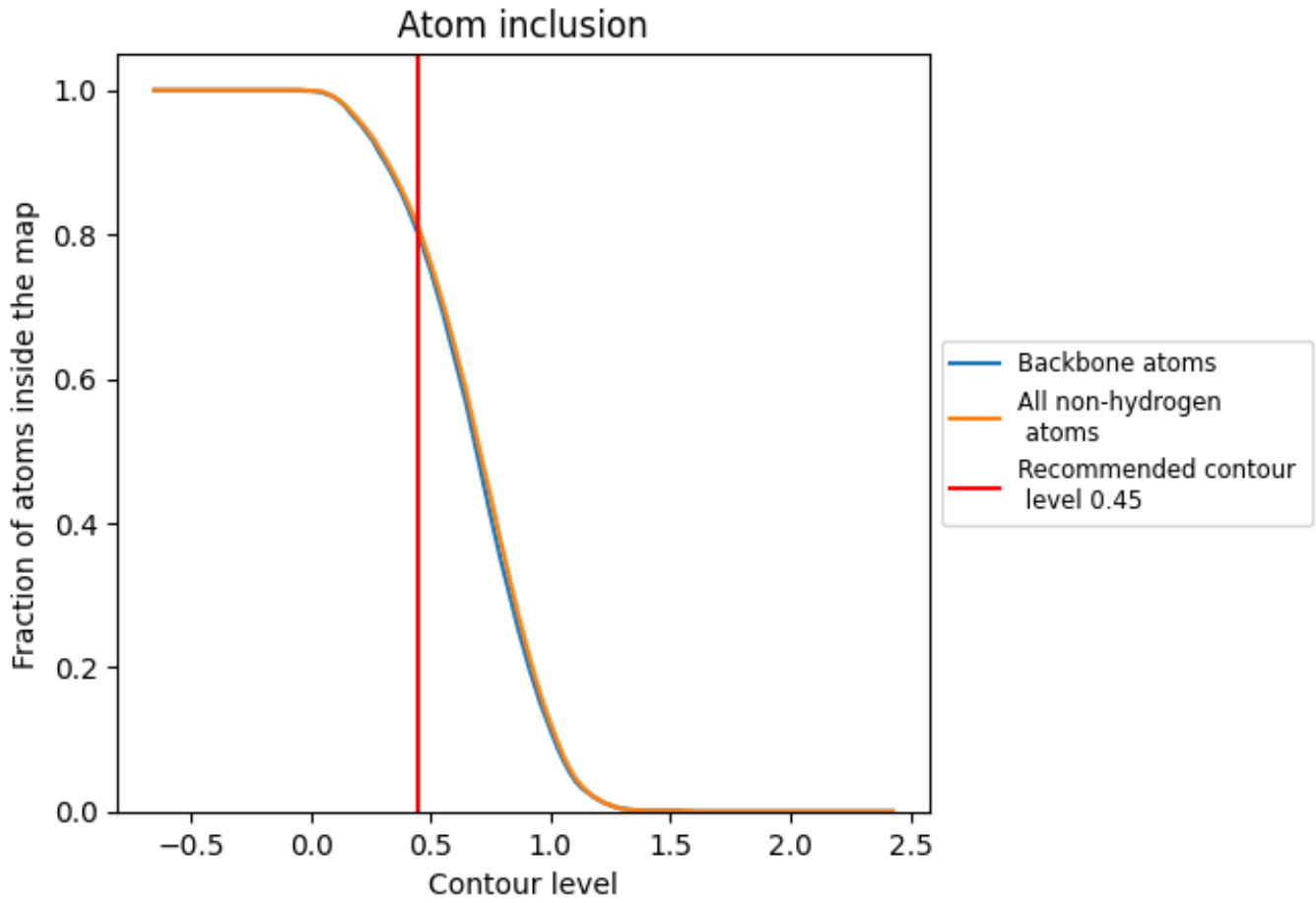
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.45).

9.4 Atom inclusion (i)



At the recommended contour level, 80% of all backbone atoms, 81% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.45) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8090	0.7490
A	0.8620	0.7700
B	0.8650	0.7580
C	0.8280	0.7430
D	0.9200	0.7740
E	0.6740	0.7180
F	0.8070	0.7480
H	0.7480	0.7330
I	0.7760	0.7400
J	0.6490	0.7220
K	0.7580	0.7240
L	0.8560	0.7730
M	0.8230	0.7650
O	0.6540	0.7220
T	0.8380	0.7700
U	0.7510	0.7380
V	0.7740	0.7400
X	0.6100	0.7120
Y	0.3950	0.6670
Z	0.3280	0.6400
a	0.8630	0.7680
b	0.8670	0.7610
c	0.8290	0.7420
d	0.9230	0.7760
e	0.6780	0.7250
f	0.8550	0.7490
h	0.7570	0.7350
i	0.7830	0.7380
j	0.6700	0.7280
k	0.7470	0.7310
l	0.8730	0.7740
m	0.8230	0.7690
o	0.6590	0.7240
t	0.8230	0.7690
u	0.7500	0.7460

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Chain	Atom inclusion	Q-score
v	0.7880	0.7410
x	0.6160	0.7190
y	0.4200	0.6760
z	0.3520	0.6440