wwPDB EM Validation Summary Report (i)

Aug 13, 2026 – 12:00 AM JST

PDB ID	:	8K5O / pdb_00008k5o
EMDB ID	:	EMD-36907
Title	:	Cryo-EM structure of the RC-LH core comples from Halorhodospira halochloris
Authors	:	Wang, G.-L.; Qi, C.-H.; Yu, L.-J.
Deposited on	:	2023-07-22
Resolution	:	2.42 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:

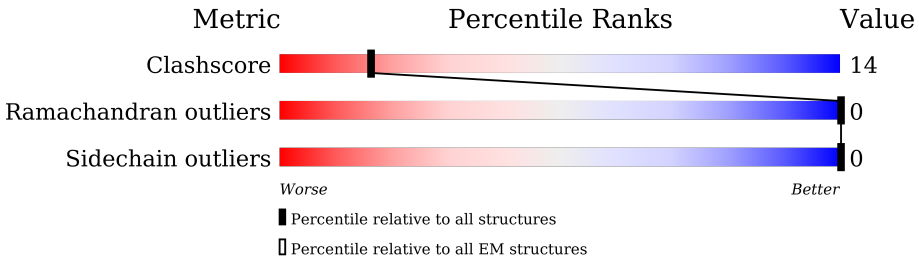
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

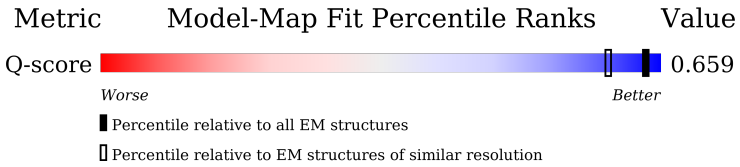
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.42 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	5729 (1.92 - 2.92)

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	C	372	7% 62% 31% 7%
2	L	279	52% 47% .
3	M	320	. 55% 44% .
4	H	274	. 55% 42% .

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Mol	Chain	Length	Quality of chain
5	4	105	5% 53% 15% 31%
6	3	65	40% 38% 22%
7	6	65	11% 65% 32%
7	F	65	75% 22%
7	K	65	80% 17%
7	P	65	77% 20%
7	S	65	78% 18%
7	V	65	75% 22%
7	Y	65	74% 23%
7	b	65	78% 18%
7	e	65	66% 31%
7	h	65	65% 32%
7	k	65	77% 20%
7	n	65	80% 15%
7	q	65	71% 26%
7	t	65	71% 26%
7	w	65	69% 28%
7	z	65	72% 25%
8	1	86	6% 51% 21% 28%
8	7	86	53% 15% 31%
8	G	86	50% 22% 28%
8	N	86	58% 14% 28%
8	Q	86	57% 15% 28%
8	T	86	51% 21% 28%
8	W	86	49% 23% 28%

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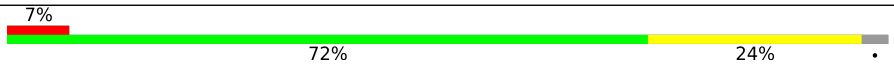
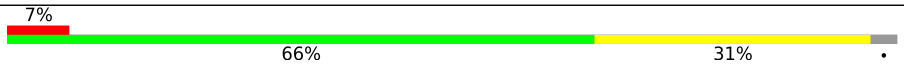
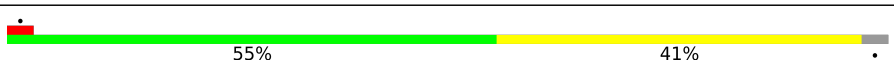
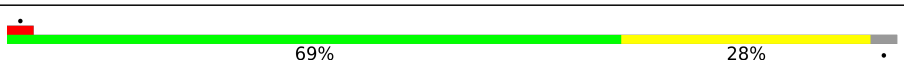
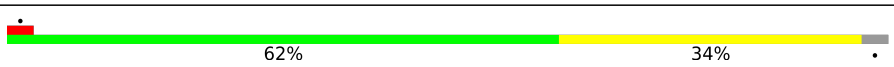
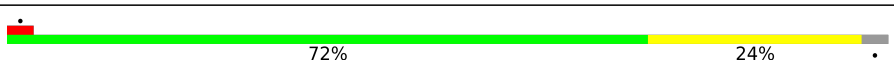
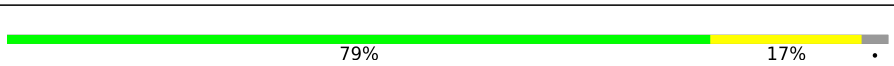
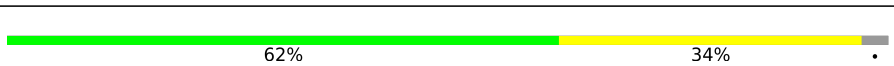
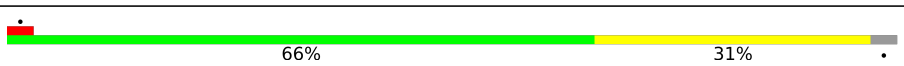
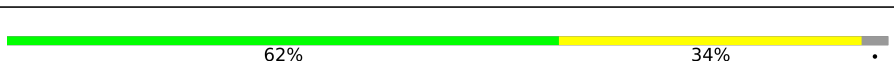
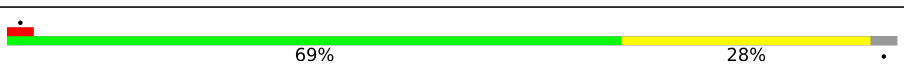
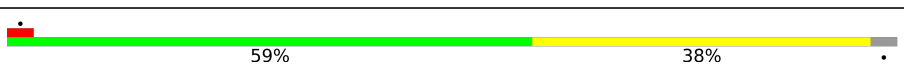
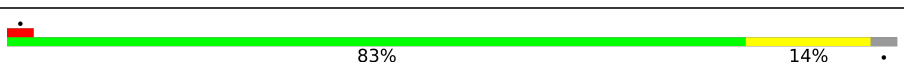
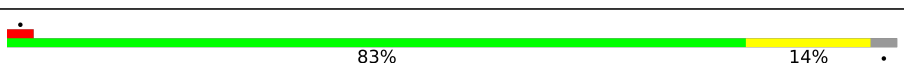
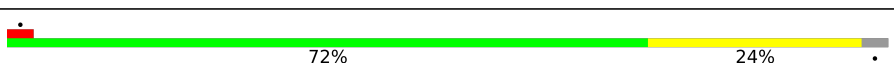
Mol	Chain	Length	Quality of chain
8	Z	86	
8	c	86	
8	f	86	
8	i	86	
8	l	86	
8	o	86	
8	r	86	
8	u	86	
8	x	86	
9	5	29	
9	8	29	
9	I	29	
9	O	29	
9	R	29	
9	U	29	
9	X	29	
9	a	29	
9	d	29	
9	g	29	
9	j	29	
9	m	29	
9	p	29	
9	s	29	
9	v	29	
9	y	29	

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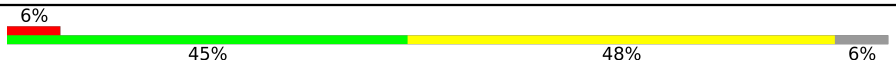
Mol	Chain	Length	Quality of chain
10	2	31	
11	9	33	

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
12	HEC	C	401	X	-	-	-
12	HEC	C	402	X	-	-	-
12	HEC	C	403	X	-	-	-
12	HEC	C	404	X	-	-	-
15	A1LZM	1	101	X	-	-	-
15	A1LZM	3	102	X	-	-	-
15	A1LZM	4	201	X	-	-	-
15	A1LZM	6	101	X	-	-	-
15	A1LZM	6	102	X	-	-	-
15	A1LZM	7	101	X	-	-	-
15	A1LZM	F	101	X	-	-	-
15	A1LZM	F	102	X	-	-	-
15	A1LZM	G	101	X	-	-	-
15	A1LZM	K	101	X	-	-	-
15	A1LZM	K	102	X	-	-	-
15	A1LZM	L	301	X	-	-	-
15	A1LZM	L	302	X	-	-	-
15	A1LZM	M	702	X	-	-	-
15	A1LZM	M	703	X	-	-	-
15	A1LZM	N	101	X	-	-	-
15	A1LZM	P	101	X	-	-	-
15	A1LZM	P	102	X	-	-	-
15	A1LZM	P	103	X	-	-	-
15	A1LZM	S	101	X	-	-	-
15	A1LZM	S	102	X	-	-	-
15	A1LZM	S	103	X	-	-	-
15	A1LZM	V	101	X	-	-	-
15	A1LZM	V	102	X	-	-	-
15	A1LZM	W	101	X	-	-	-
15	A1LZM	Y	101	X	-	-	-
15	A1LZM	Y	102	X	-	-	-
15	A1LZM	Z	101	X	-	-	-
15	A1LZM	b	101	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	A1LZM	b	102	X	-	-	-
15	A1LZM	c	101	X	-	-	-
15	A1LZM	e	101	X	-	-	-
15	A1LZM	e	102	X	-	-	-
15	A1LZM	f	101	X	-	-	-
15	A1LZM	h	101	X	-	-	-
15	A1LZM	h	102	X	-	-	-
15	A1LZM	i	101	X	-	-	-
15	A1LZM	k	101	X	-	-	-
15	A1LZM	k	102	X	-	-	-
15	A1LZM	l	101	X	-	-	-
15	A1LZM	n	101	X	-	-	-
15	A1LZM	n	102	X	-	-	-
15	A1LZM	o	101	X	-	-	-
15	A1LZM	q	101	X	-	-	-
15	A1LZM	q	102	X	-	-	-
15	A1LZM	r	101	X	-	-	-
15	A1LZM	t	101	X	-	-	-
15	A1LZM	t	102	X	-	-	-
15	A1LZM	u	101	X	-	-	-
15	A1LZM	w	101	X	-	-	-
15	A1LZM	w	102	X	-	-	-
15	A1LZM	w	103	X	-	-	-
15	A1LZM	z	101	X	-	-	-
15	A1LZM	z	102	X	-	-	-
23	A1LZQ	1	102	X	-	-	-
23	A1LZQ	7	102	X	-	-	-
23	A1LZQ	G	102	X	-	-	-
23	A1LZQ	N	102	X	-	-	-
23	A1LZQ	Q	101	X	-	-	-
23	A1LZQ	T	101	X	-	-	-
23	A1LZQ	W	102	X	-	-	-
23	A1LZQ	Z	102	X	-	-	-
23	A1LZQ	c	102	X	-	-	-
23	A1LZQ	f	102	X	-	-	-
23	A1LZQ	i	102	X	-	-	-
23	A1LZQ	l	102	X	-	-	-
23	A1LZQ	o	102	X	-	-	-
23	A1LZQ	r	102	X	-	-	-
23	A1LZQ	u	102	X	-	-	-
23	A1LZQ	x	101	X	-	-	-

2 Entry composition (i)

There are 25 unique types of molecules in this entry. The entry contains 38551 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Photosynthetic reaction center cytochrome c subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	346	Total 2732	C 1690	N 469	O 554	S 19	0	0

- Molecule 2 is a protein called Reaction center protein L chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L	275	Total 2188	C 1470	N 356	O 355	S 7	0	0

- Molecule 3 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	M	318	Total 2553	C 1691	N 427	O 425	S 10	0	0

- Molecule 4 is a protein called Photosynthetic reaction center H subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	268	Total 2160	C 1384	N 375	O 389	S 12	0	0

- Molecule 5 is a protein called Antenna complex alpha/beta subunit domain-containing protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	4	72	Total 615	C 408	N 98	O 109	0	0

- Molecule 6 is a protein called Light-harvesting LHI.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	3	51	Total 433	C 292	N 72	O 67	S 2	0	0

- Molecule 7 is a protein called Antenna complex alpha/beta subunit domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	w	63	Total	C	N	O	S	0	0
			533	359	84	86	4		
7	Y	63	Total	C	N	O	S	0	0
			533	359	84	86	4		
7	b	63	Total	C	N	O	S	0	0
			533	359	84	86	4		
7	k	63	Total	C	N	O	S	0	0
			533	359	84	86	4		
7	n	63	Total	C	N	O	S	0	0
			533	359	84	86	4		
7	t	63	Total	C	N	O	S	0	0
			533	359	84	86	4		
7	z	63	Total	C	N	O	S	0	0
			533	359	84	86	4		
7	6	63	Total	C	N	O	S	0	0
			533	359	84	86	4		
7	F	63	Total	C	N	O	S	0	0
			533	359	84	86	4		
7	K	63	Total	C	N	O	S	0	0
			533	359	84	86	4		
7	P	63	Total	C	N	O	S	0	0
			533	359	84	86	4		
7	S	63	Total	C	N	O	S	0	0
			533	359	84	86	4		
7	V	63	Total	C	N	O	S	0	0
			533	359	84	86	4		
7	e	63	Total	C	N	O	S	0	0
			533	359	84	86	4		
7	h	63	Total	C	N	O	S	0	0
			533	359	84	86	4		
7	q	63	Total	C	N	O	S	0	0
			533	359	84	86	4		

- Molecule 8 is a protein called Beta subunit of light-harvesting 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	x	62	Total	C	N	O	S	0	0
			498	312	92	90	4		
8	Z	62	Total	C	N	O	S	0	0
			498	312	92	90	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
8	c	62	Total	C	N	O	S	0	0
			498	312	92	90	4		
8	l	62	Total	C	N	O	S	0	0
			498	312	92	90	4		
8	o	62	Total	C	N	O	S	0	0
			498	312	92	90	4		
8	u	62	Total	C	N	O	S	0	0
			498	312	92	90	4		
8	1	62	Total	C	N	O	S	0	0
			498	312	92	90	4		
8	7	59	Total	C	N	O	S	0	0
			472	296	86	86	4		
8	G	62	Total	C	N	O	S	0	0
			498	312	92	90	4		
8	N	62	Total	C	N	O	S	0	0
			498	312	92	90	4		
8	Q	62	Total	C	N	O	S	0	0
			498	312	92	90	4		
8	T	62	Total	C	N	O	S	0	0
			498	312	92	90	4		
8	W	62	Total	C	N	O	S	0	0
			498	312	92	90	4		
8	f	62	Total	C	N	O	S	0	0
			498	312	92	90	4		
8	i	62	Total	C	N	O	S	0	0
			498	312	92	90	4		
8	r	62	Total	C	N	O	S	0	0
			498	312	92	90	4		

- Molecule 9 is a protein called Gamma subunit of light-harvesting 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	v	28	Total	C	N	O	0	0
			211	140	37	34		
9	X	28	Total	C	N	O	0	0
			211	140	37	34		
9	a	28	Total	C	N	O	0	0
			211	140	37	34		
9	j	28	Total	C	N	O	0	0
			211	140	37	34		
9	m	28	Total	C	N	O	0	0
			211	140	37	34		

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Mol	Chain	Residues	Atoms				AltConf	Trace
9	s	28	Total 211	C 140	N 37	O 34	0	0
9	y	28	Total 211	C 140	N 37	O 34	0	0
9	5	26	Total 186	C 123	N 31	O 32	0	0
9	8	28	Total 211	C 140	N 37	O 34	0	0
9	I	28	Total 211	C 140	N 37	O 34	0	0
9	O	28	Total 211	C 140	N 37	O 34	0	0
9	R	28	Total 211	C 140	N 37	O 34	0	0
9	U	28	Total 211	C 140	N 37	O 34	0	0
9	d	28	Total 211	C 140	N 37	O 34	0	0
9	g	28	Total 211	C 140	N 37	O 34	0	0
9	p	28	Total 211	C 140	N 37	O 34	0	0

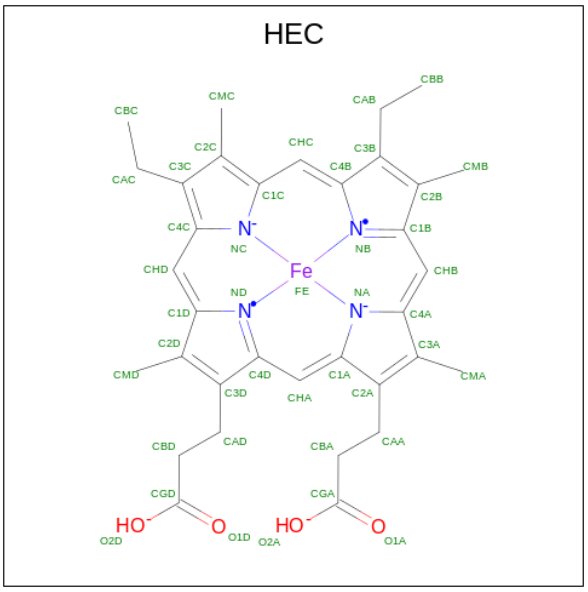
- Molecule 10 is a protein called reaction center small polypeptide.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	2	29	Total 232	C 162	N 37	O 32	S 1	0	0

- Molecule 11 is a protein called reactin center small polypeptide.

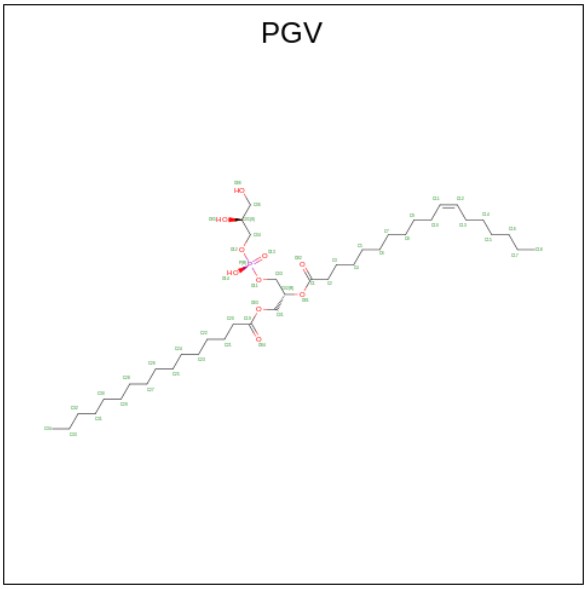
Mol	Chain	Residues	Atoms					AltConf	Trace
11	9	29	Total 233	C 158	N 38	O 36	S 1	0	0

- Molecule 12 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 13 is (1R)-2-{[{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (CCD ID: PGV) (formula: $C_{40}H_{77}O_{10}P$).



Mol	Chain	Residues	Atoms	AltConf
13	C	1	Total C O 28 24 4	0
13	C	1	Total C O P 32 23 8 1	0
13	C	1	Total C O P 38 27 10 1	0
13	L	1	Total C O P 48 37 10 1	0
13	L	1	Total C O P 46 35 10 1	0
13	L	1	Total C O P 44 33 10 1	0
13	L	1	Total C O P 48 37 10 1	0
13	M	1	Total C O P 32 23 8 1	0
13	M	1	Total C O P 32 21 10 1	0
13	H	1	Total C O P 32 21 10 1	0
13	H	1	Total C O P 42 33 8 1	0
13	H	1	Total C O P 47 36 10 1	0
13	H	1	Total C O P 33 22 10 1	0
13	H	1	Total C O P 42 31 10 1	0
13	4	1	Total C O P 37 26 10 1	0
13	w	1	Total C O P 39 30 8 1	0
13	v	1	Total C O 42 37 5	0
13	Y	1	Total C O P 51 40 10 1	0
13	Y	1	Total C O P 40 31 8 1	0
13	X	1	Total C O 42 37 5	0
13	b	1	Total C O P 37 28 8 1	0
13	a	1	Total C O 42 37 5	0

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Mol	Chain	Residues	Atoms	AltConf
13	k	1	Total C O P 46 37 8 1	0
13	j	1	Total C O 42 37 5	0
13	n	1	Total C O P 37 28 8 1	0
13	m	1	Total C O 42 37 5	0
13	t	1	Total C O P 39 30 8 1	0
13	s	1	Total C O 42 37 5	0
13	z	1	Total C O P 38 29 8 1	0
13	5	1	Total C O 41 36 5	0
13	F	1	Total C O P 36 27 8 1	0
13	8	1	Total C O 42 37 5	0
13	K	1	Total C O P 40 31 8 1	0
13	K	1	Total C O P 25 16 8 1	0
13	I	1	Total C O 36 31 5	0
13	P	1	Total C O P 40 31 8 1	0
13	P	1	Total C O P 45 34 10 1	0
13	O	1	Total C O 42 37 5	0
13	S	1	Total C O P 40 31 8 1	0
13	R	1	Total C O 42 37 5	0
13	V	1	Total C O P 39 30 8 1	0
13	U	1	Total C O 42 37 5	0
13	e	1	Total C O P 40 31 8 1	0

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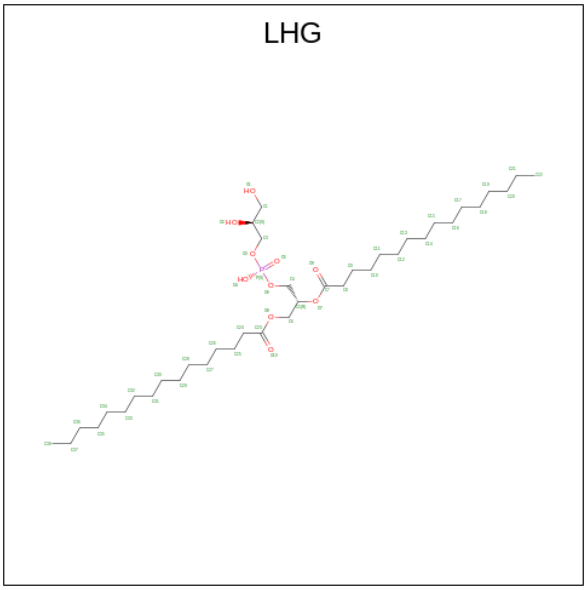
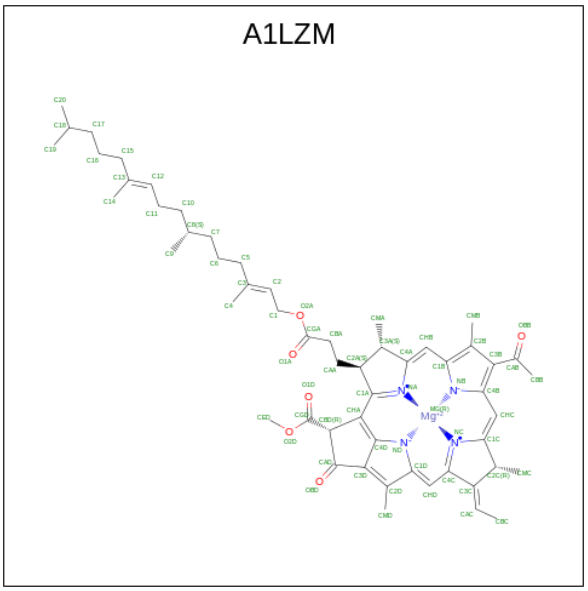
Mol	Chain	Residues	Atoms	AltConf
13	d	1	Total C O 42 37 5	0
13	h	1	Total C O P 36 27 8 1	0
13	g	1	Total C O 42 37 5	0
13	q	1	Total C O P 40 31 8 1	0
13	p	1	Total C O 39 34 5	0
13	9	1	Total C O P 25 16 8 1	0
13	9	1	Total C O P 38 29 8 1	0

- Molecule 14 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms	AltConf
14	C	1	Total C O 10 9 1	0

- Molecule 15 is Trans-Geranyl Bacteriochlorophyll B (CCD ID: A1LZM) (formula: $C_{55}H_{70}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
15	L	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	L	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	M	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	M	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	4	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	3	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
15	w	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	w	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	w	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	Y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	Y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	Z	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	b	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	b	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
15	c	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	k	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	k	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	l	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	n	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	n	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	o	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	t	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	t	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	u	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	z	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	z	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	6	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	6	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	7	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	F	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	F	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	G	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	K	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	K	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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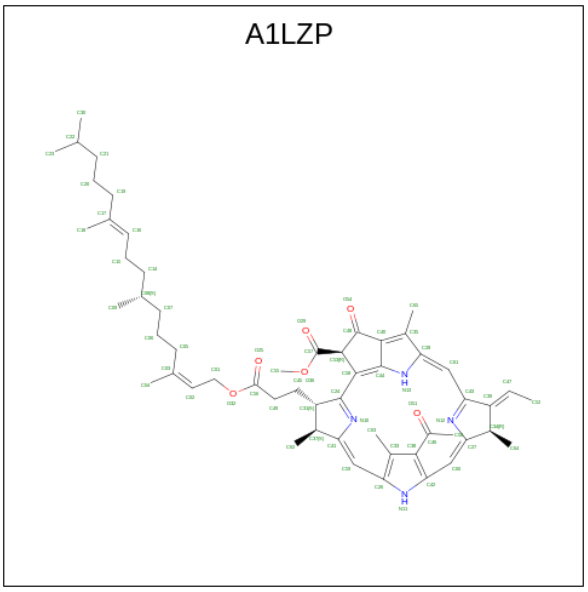
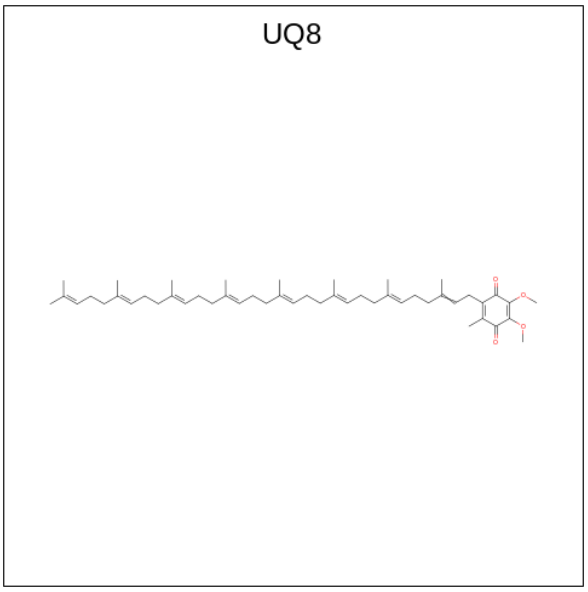
Mol	Chain	Residues	Atoms					AltConf
15	N	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	P	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	P	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	P	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	S	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	S	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	S	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	V	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	V	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	W	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	e	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	e	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	f	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	h	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	h	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	i	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	q	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	q	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	r	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

- Molecule 16 is Trans-Geranyl Bacteriopheophytin B (CCD ID: A1LZP) (formula: $C_{55}H_{72}N_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
16	L	1	Total	C	N	O	0
			65	55	4	6	
16	M	1	Total	C	N	O	0
			65	55	4	6	

- Molecule 17 is Ubiquinone-8 (CCD ID: UQ8) (formula: $C_{49}H_{74}O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
17	L	1	Total	C	O	0
			33	29	4	

- Molecule 18 is UNKNOWN LIGAND (CCD ID: UNL) (formula:).

Mol	Chain	Residues	Atoms	AltConf
18	L	2	Total C 24 24	0
18	M	3	Total C 50 50	0
18	4	1	Total C 15 15	0
18	v	3	Total C 27 27	0
18	X	3	Total C 25 25	0
18	b	2	Total C 32 32	0
18	a	3	Total C 25 25	0
18	k	1	Total C 18 18	0
18	j	3	Total C 23 23	0
18	n	1	Total C 9 9	0
18	m	3	Total C 24 24	0
18	s	3	Total C 23 23	0
18	1	1	Total C 10 10	0
18	y	1	Total C 7 7	0
18	F	1	Total C 12 12	0
18	8	2	Total C 17 17	0
18	K	1	Total C 18 18	0
18	I	3	Total C 29 29	0
18	O	3	Total C 24 24	0
18	R	3	Total C 27 27	0
18	U	3	Total C 27 27	0

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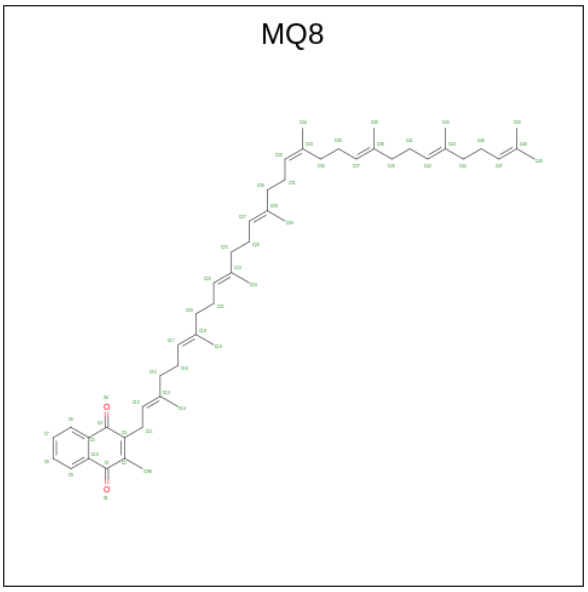
Mol	Chain	Residues	Atoms	AltConf
18	d	3	Total C 27 27	0
18	g	3	Total C 26 26	0
18	q	1	Total C 12 12	0
18	p	3	Total C 25 25	0
18	9	1	Total C 16 16	0

- Molecule 19 is FE (III) ION (CCD ID: FE) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

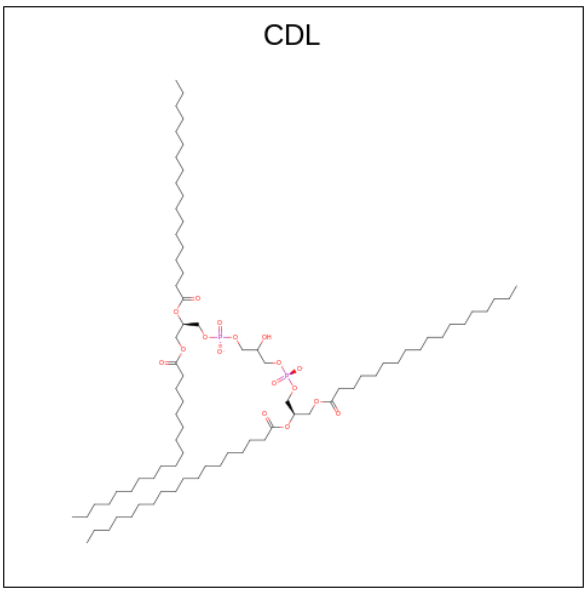
Mol	Chain	Residues	Atoms	AltConf
19	M	1	Total Fe 1 1	0

- Molecule 20 is MENAQUINONE 8 (CCD ID: MQ8) (formula: $C_{51}H_{72}O_2$) (labeled as "Ligand of Interest" by depositor).



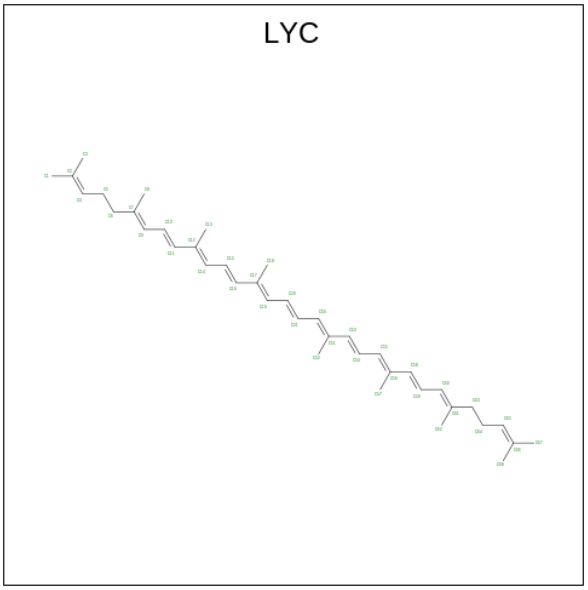
Mol	Chain	Residues	Atoms	AltConf
20	M	1	Total C O 53 51 2	0
20	M	1	Total C O 23 21 2	0

- Molecule 21 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



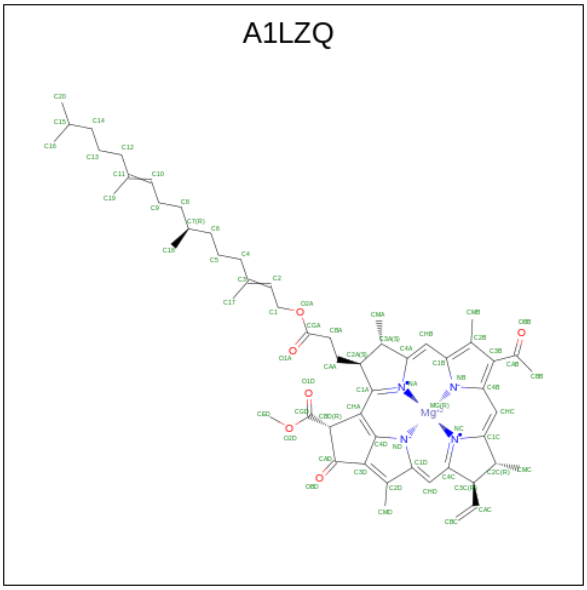
Mol	Chain	Residues	Atoms				AltConf
21	M	1	Total	C	O	P	0
			83	64	17	2	
21	M	1	Total	C	O	P	0
			54	35	17	2	
21	H	1	Total	C	O	P	0
			77	58	17	2	

- Molecule 22 is LYCOPENE (CCD ID: LYC) (formula: $C_{40}H_{56}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
22	3	1	Total C 40 40	0

- Molecule 23 is Trans-Geranyl 8-vinyl-bacteriochlorophyll B (CCD ID: A1LZQ) (formula: $C_{55}H_{70}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
23	x	1	Total C Mg N O 46 35 1 4 6	0
23	Z	1	Total C Mg N O 46 35 1 4 6	0
23	c	1	Total C Mg N O 46 35 1 4 6	0
23	l	1	Total C Mg N O 46 35 1 4 6	0
23	o	1	Total C Mg N O 46 35 1 4 6	0
23	u	1	Total C Mg N O 46 35 1 4 6	0
23	1	1	Total C Mg N O 46 35 1 4 6	0
23	7	1	Total C Mg N O 46 35 1 4 6	0
23	G	1	Total C Mg N O 46 35 1 4 6	0
23	N	1	Total C Mg N O 46 35 1 4 6	0

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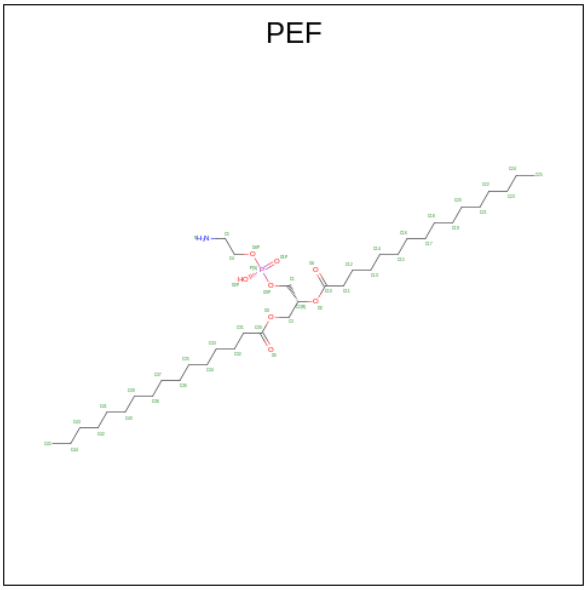
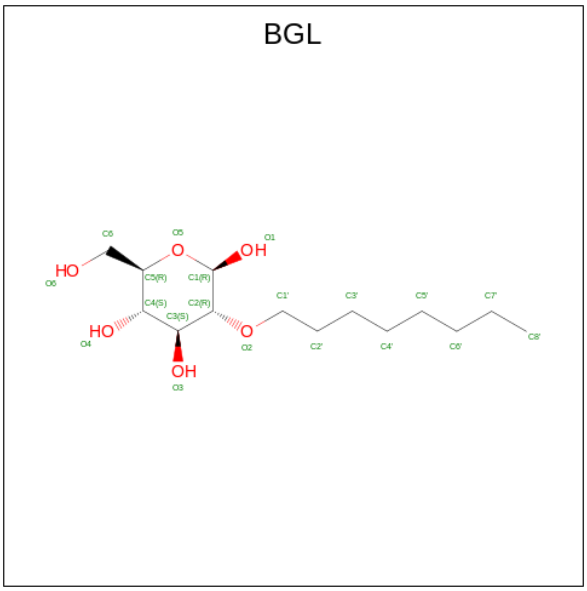
Mol	Chain	Residues	Atoms					AltConf
23	Q	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
23	T	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
23	W	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
23	f	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
23	i	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
23	r	1	Total	C	Mg	N	O	0
			46	35	1	4	6	

- Molecule 24 is DI-PALMITOYL-3-SN-PHOSPHATIDYLETHANOLAMINE (CCD ID: PEF) (formula: $C_{37}H_{74}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
24	K	1	Total	C	N	O	P	0
			39	29	1	8	1	

- Molecule 25 is 2-O-octyl-beta-D-glucopyranose (CCD ID: BGL) (formula: $C_{14}H_{28}O_6$).

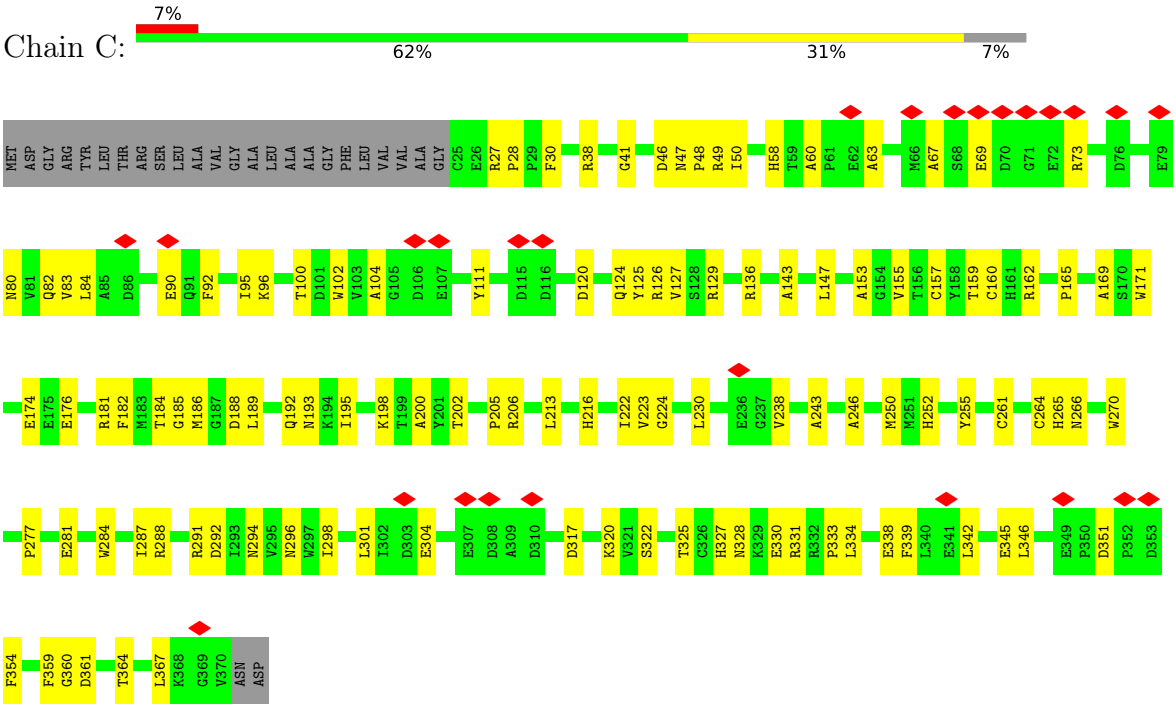


Mol	Chain	Residues	Atoms			AltConf
25	S	1	Total	C	O	0
			20	14	6	
25	h	1	Total	C	O	0
			20	14	6	

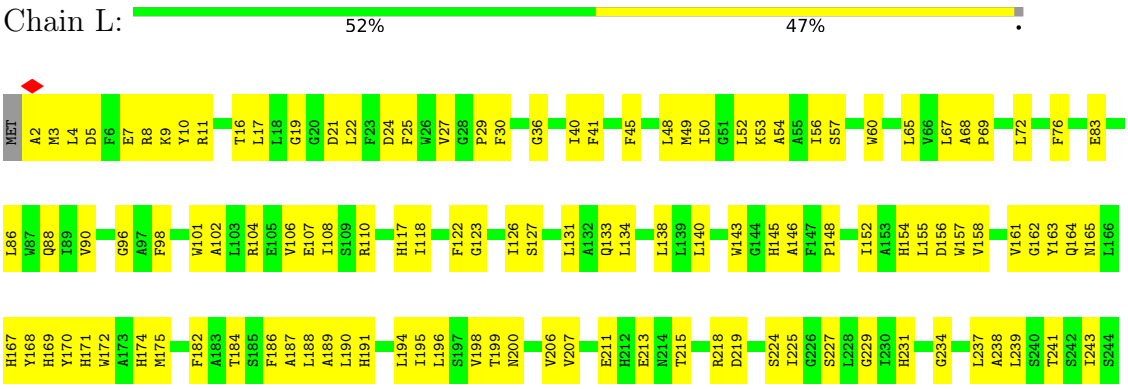
3 Residue-property plots (i)

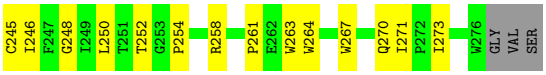
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Photosynthetic reaction center cytochrome c subunit

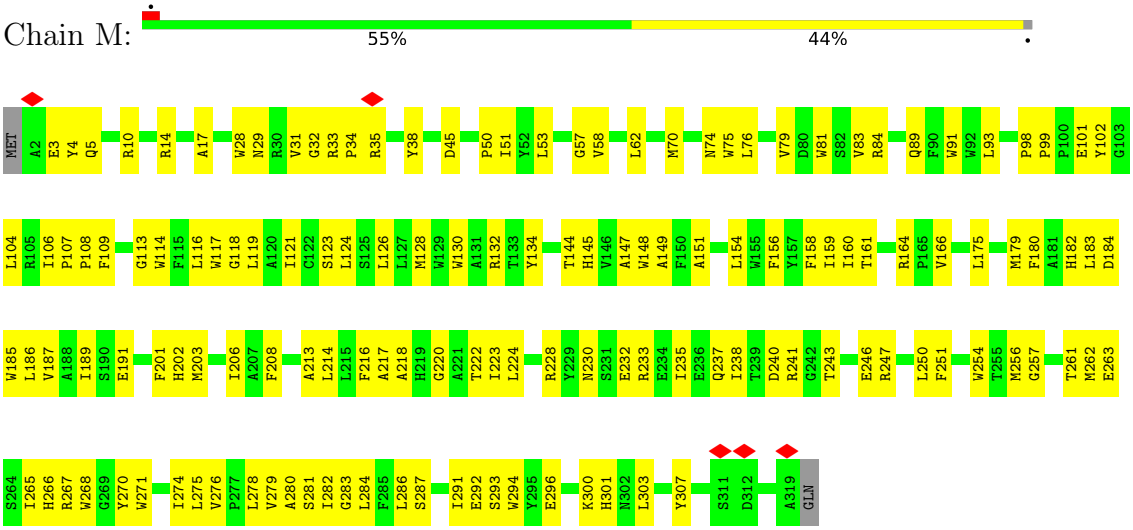


• Molecule 2: Reaction center protein L chain

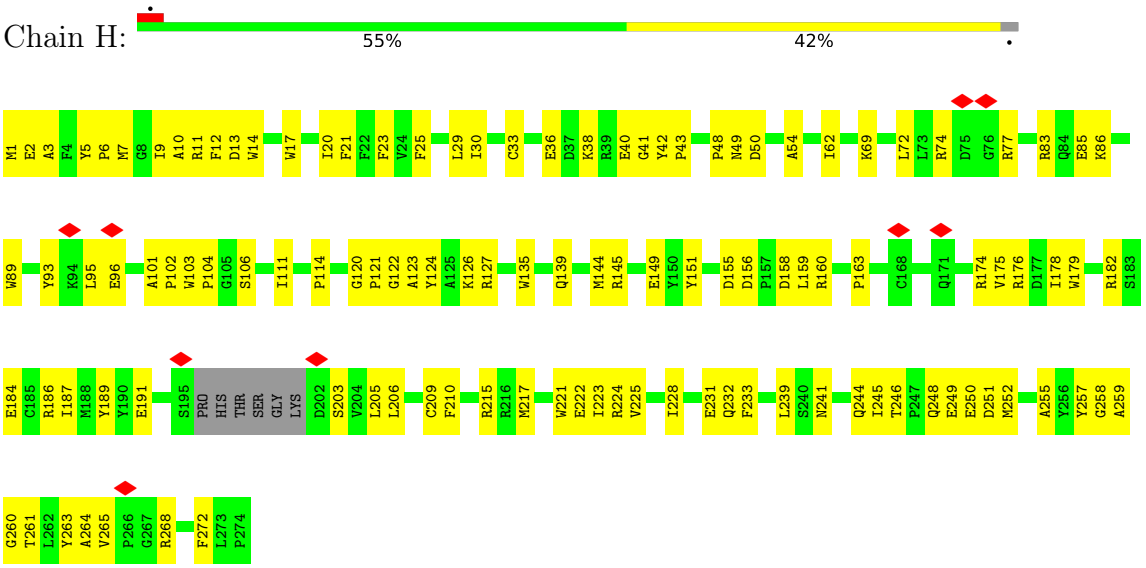




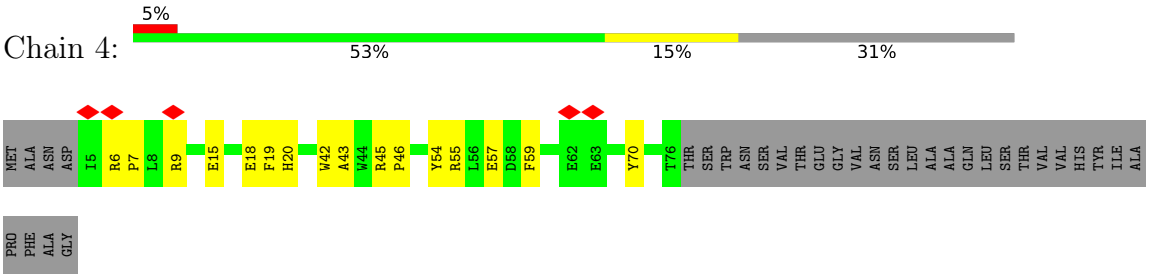
• Molecule 3: Reaction center protein M chain



• Molecule 4: Photosynthetic reaction center H subunit

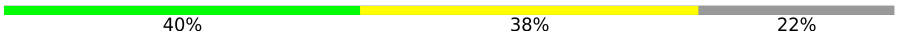


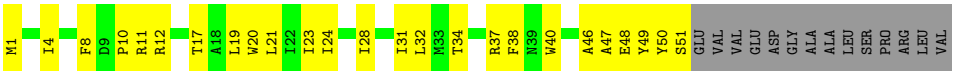
• Molecule 5: Antenna complex alpha/beta subunit domain-containing protein



• Molecule 6: Light-harvesting LHI

Chain 3:



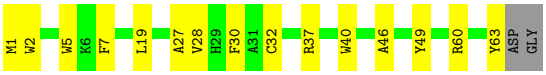


• Molecule 7: Antenna complex alpha/beta subunit domain-containing protein

Chain w:

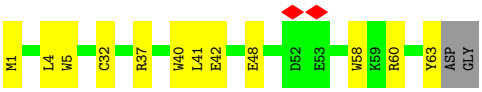
• Molecule 7: Antenna complex alpha/beta subunit domain-containing protein

Chain Y:



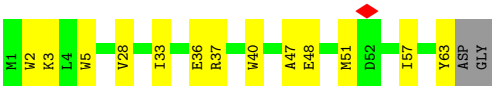
• Molecule 7: Antenna complex alpha/beta subunit domain-containing protein

Chain b:



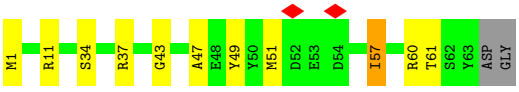
• Molecule 7: Antenna complex alpha/beta subunit domain-containing protein

Chain k:



• Molecule 7: Antenna complex alpha/beta subunit domain-containing protein

Chain n:

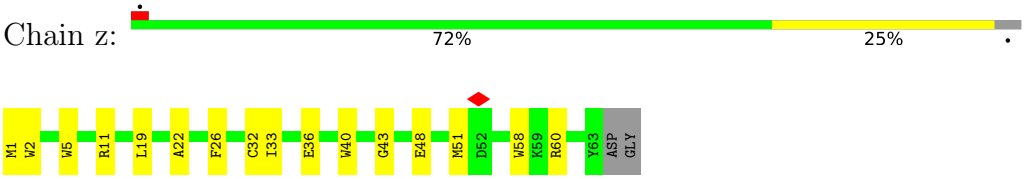


• Molecule 7: Antenna complex alpha/beta subunit domain-containing protein

Chain t:

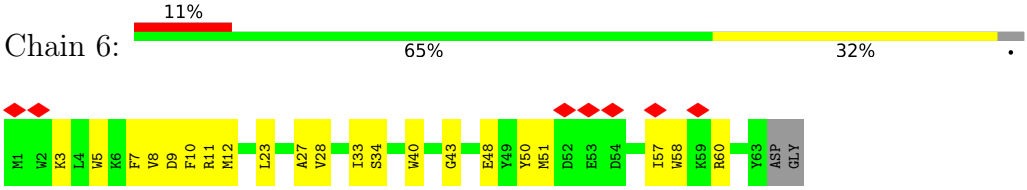
• Molecule 7: Antenna complex alpha/beta subunit domain-containing protein

Chain z:



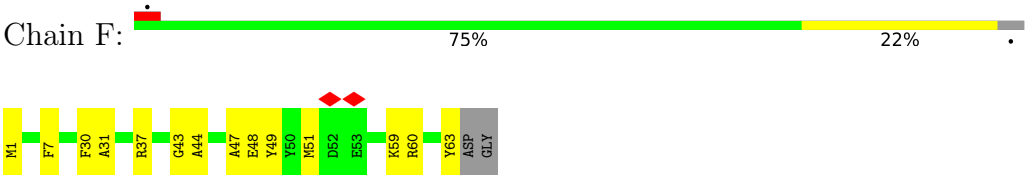
• Molecule 7: Antenna complex alpha/beta subunit domain-containing protein

Chain 6:



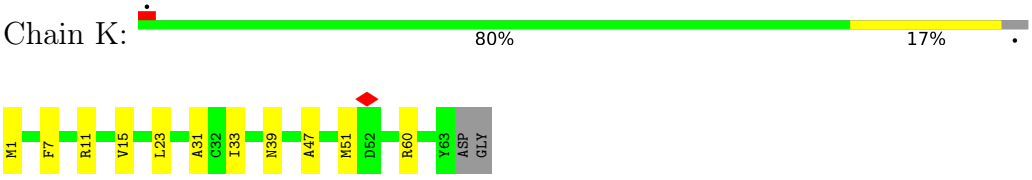
• Molecule 7: Antenna complex alpha/beta subunit domain-containing protein

Chain F:



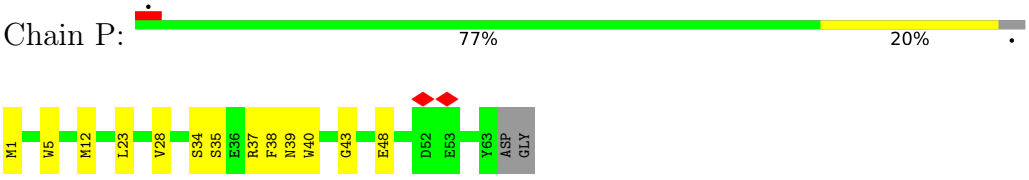
• Molecule 7: Antenna complex alpha/beta subunit domain-containing protein

Chain K:



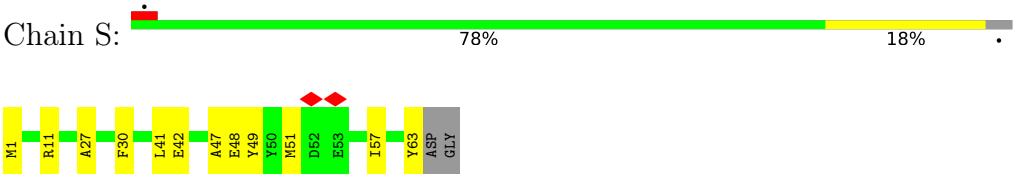
• Molecule 7: Antenna complex alpha/beta subunit domain-containing protein

Chain P:



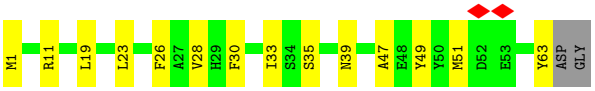
• Molecule 7: Antenna complex alpha/beta subunit domain-containing protein

Chain S:



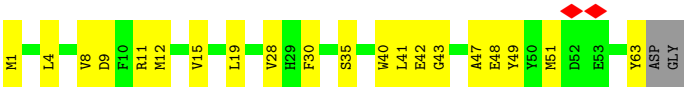
• Molecule 7: Antenna complex alpha/beta subunit domain-containing protein

Chain V:



• Molecule 7: Antenna complex alpha/beta subunit domain-containing protein

Chain e:

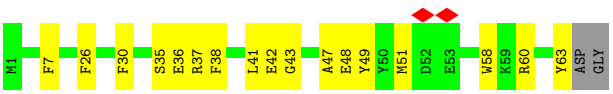


• Molecule 7: Antenna complex alpha/beta subunit domain-containing protein

Chain h:

• Molecule 7: Antenna complex alpha/beta subunit domain-containing protein

Chain q:

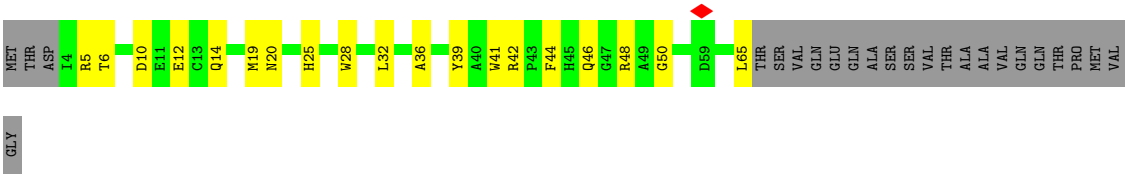


• Molecule 8: Beta subunit of light-harvesting 1

Chain x:

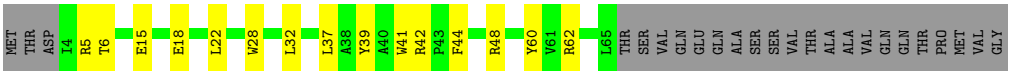
• Molecule 8: Beta subunit of light-harvesting 1

Chain Z:



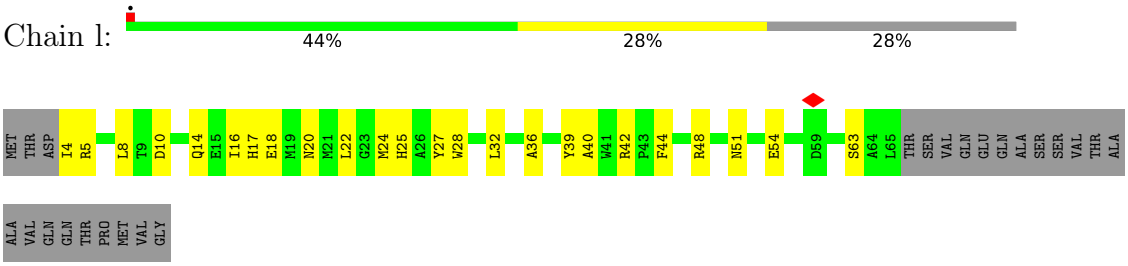
• Molecule 8: Beta subunit of light-harvesting 1

Chain c:



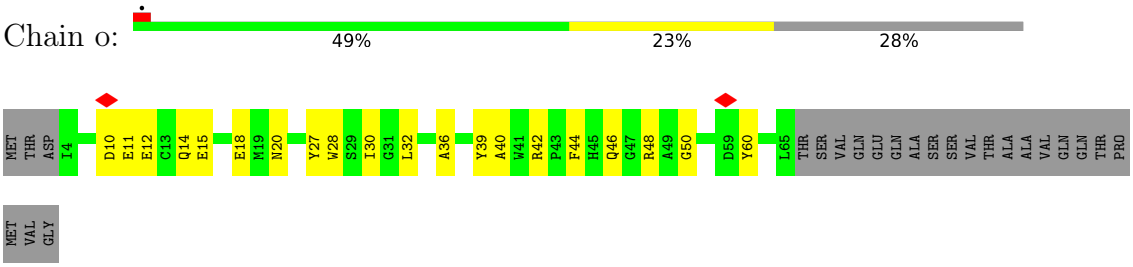
• Molecule 8: Beta subunit of light-harvesting 1

Chain l:



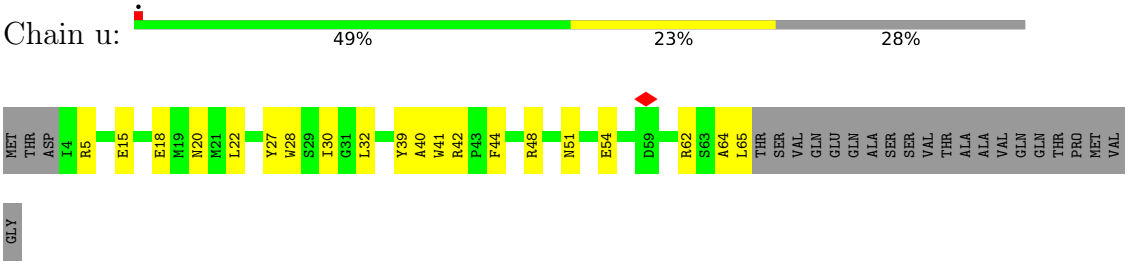
• Molecule 8: Beta subunit of light-harvesting 1

Chain o:



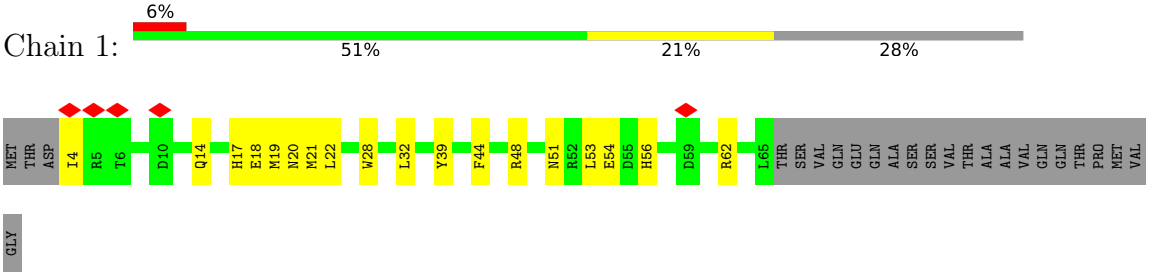
• Molecule 8: Beta subunit of light-harvesting 1

Chain u:



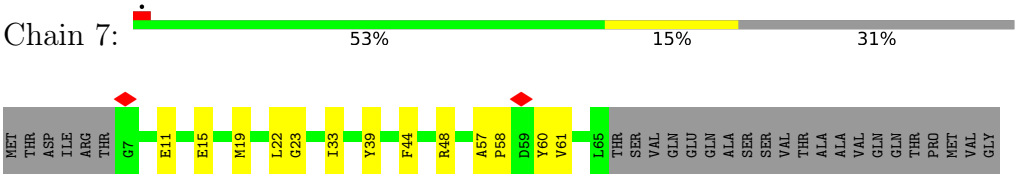
• Molecule 8: Beta subunit of light-harvesting 1

Chain 1:



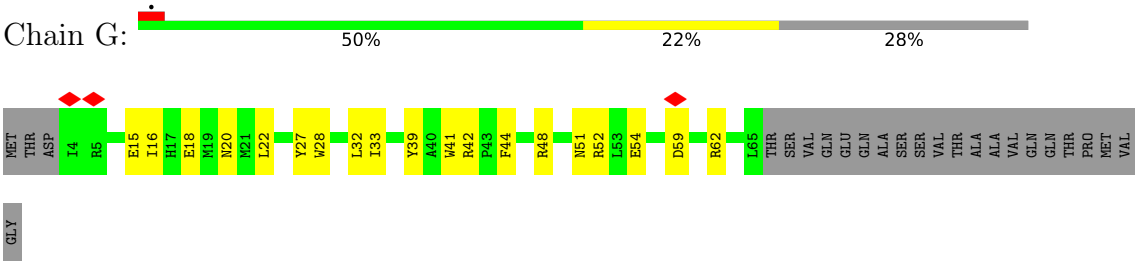
• Molecule 8: Beta subunit of light-harvesting 1

Chain 7:



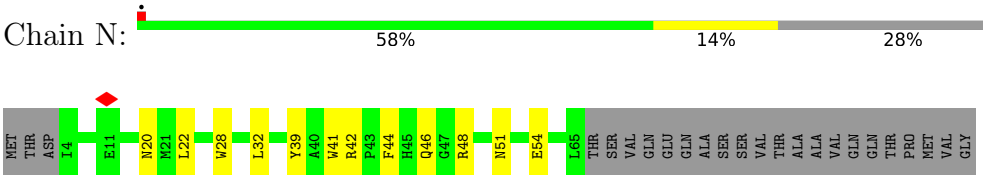
• Molecule 8: Beta subunit of light-harvesting 1

Chain G:



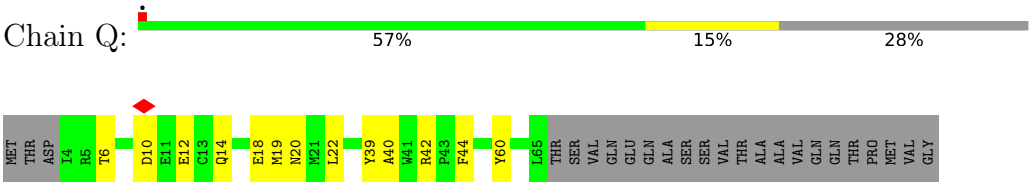
• Molecule 8: Beta subunit of light-harvesting 1

Chain N:



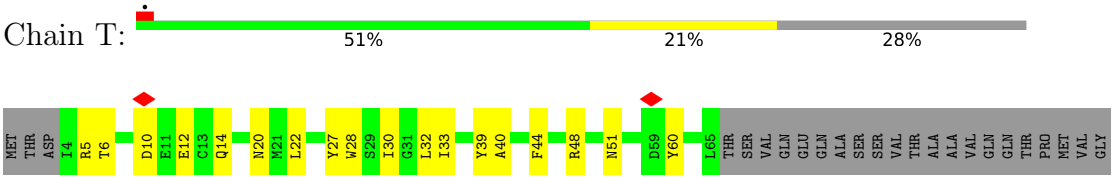
• Molecule 8: Beta subunit of light-harvesting 1

Chain Q:



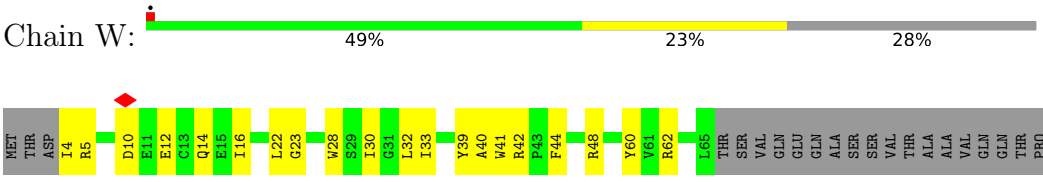
• Molecule 8: Beta subunit of light-harvesting 1

Chain T:



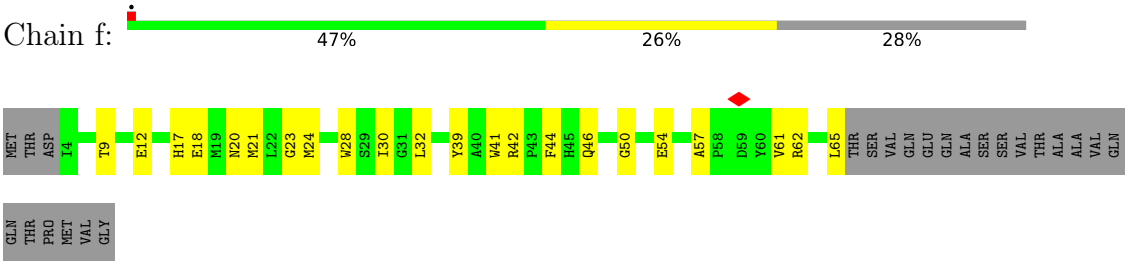
• Molecule 8: Beta subunit of light-harvesting 1

Chain W:



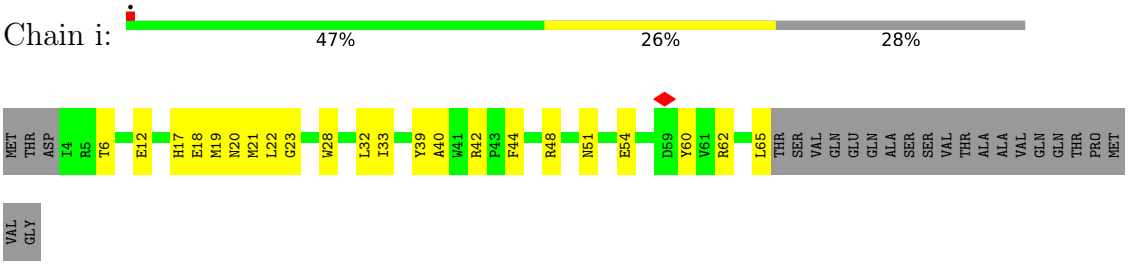
• Molecule 8: Beta subunit of light-harvesting 1

Chain f:



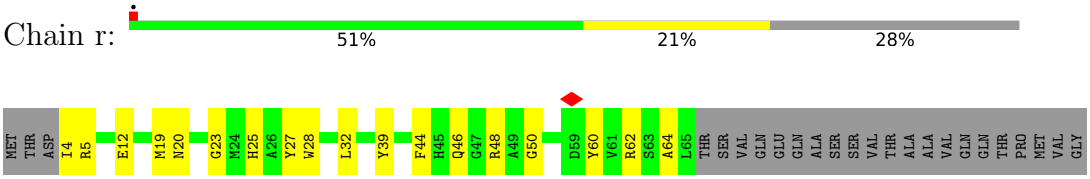
• Molecule 8: Beta subunit of light-harvesting 1

Chain i:



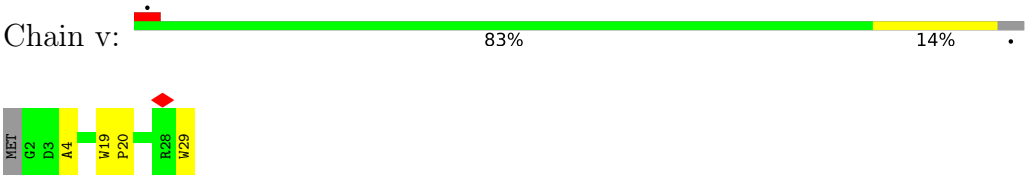
• Molecule 8: Beta subunit of light-harvesting 1

Chain r:



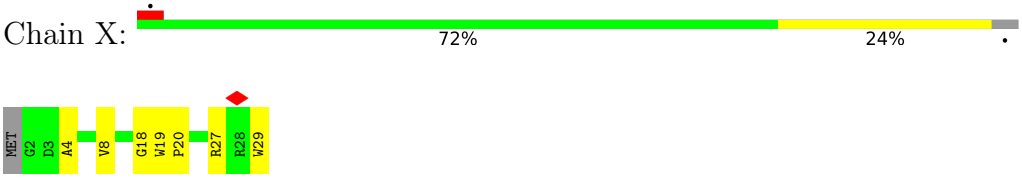
• Molecule 9: Gamma subunit of light-harvesting 1

Chain v:



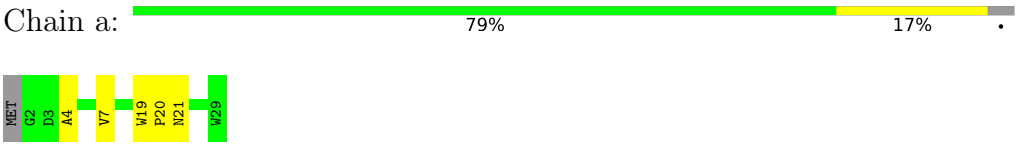
• Molecule 9: Gamma subunit of light-harvesting 1

Chain X:



• Molecule 9: Gamma subunit of light-harvesting 1

Chain a:



• Molecule 9: Gamma subunit of light-harvesting 1

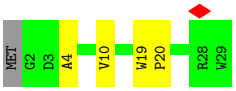
Chain j:

• Molecule 9: Gamma subunit of light-harvesting 1

Chain m:

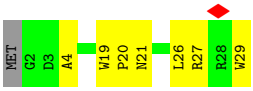
• Molecule 9: Gamma subunit of light-harvesting 1

Chain s:



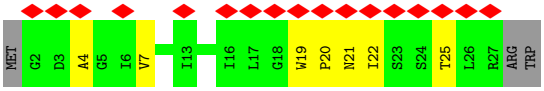
• Molecule 9: Gamma subunit of light-harvesting 1

Chain y:



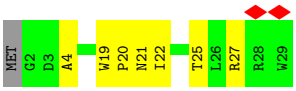
• Molecule 9: Gamma subunit of light-harvesting 1

Chain 5:



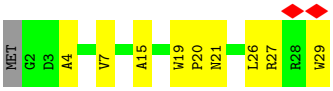
• Molecule 9: Gamma subunit of light-harvesting 1

Chain 8:



• Molecule 9: Gamma subunit of light-harvesting 1

Chain I:



• Molecule 9: Gamma subunit of light-harvesting 1

Chain O:

• Molecule 9: Gamma subunit of light-harvesting 1

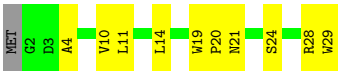
Chain R:

• Molecule 9: Gamma subunit of light-harvesting 1

Chain U:

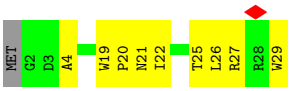
• Molecule 9: Gamma subunit of light-harvesting 1

Chain d:



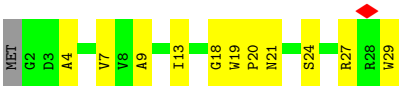
• Molecule 9: Gamma subunit of light-harvesting 1

Chain g:



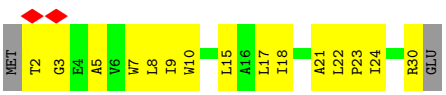
• Molecule 9: Gamma subunit of light-harvesting 1

Chain p:



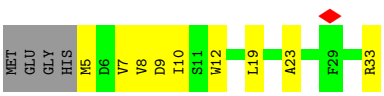
• Molecule 10: reaction center small polypeptide

Chain 2:



• Molecule 11: reactin center small polypeptide

Chain 9:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	353518	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60.8	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2300	Depositor
Magnification	Not provided	
Image detector	GATAN K2 BASE (4k x 4k)	Depositor
Maximum map value	2.882	Depositor
Minimum map value	-1.656	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.074	Depositor
Recommended contour level	0.4	Depositor
Map size (Å)	367.19998, 367.19998, 367.19998	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.02, 1.02, 1.02	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FE, A1LZM, A1LZQ, CDL, LHG, PGV, UQ8, MQ8, LYC, A1LZP, HEC, BGL, PEF, UNL

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	C	0.36	0/2798	0.45	3/3802 (0.1%)
2	L	0.29	0/2273	0.41	0/3104
3	M	0.34	0/2646	0.41	0/3617
4	H	0.28	0/2222	0.38	0/3022
5	4	0.31	0/640	0.37	0/876
6	3	0.26	0/447	0.34	0/611
7	6	0.21	0/555	0.30	0/752
7	F	0.21	0/555	0.30	0/752
7	K	0.24	0/555	0.30	0/752
7	P	0.25	0/555	0.32	0/752
7	S	0.26	0/555	0.37	1/752 (0.1%)
7	V	0.23	0/555	0.31	0/752
7	Y	0.22	0/555	0.30	0/752
7	b	0.26	0/555	0.31	0/752
7	e	0.36	0/555	0.39	0/752
7	h	0.24	0/555	0.32	0/752
7	k	0.25	0/555	0.40	1/752 (0.1%)
7	n	0.24	0/555	0.38	1/752 (0.1%)
7	q	0.24	0/555	0.32	0/752
7	t	0.24	0/555	0.38	0/752
7	w	0.24	0/555	0.30	0/752
7	z	0.25	0/555	0.32	0/752
8	1	0.30	0/511	0.40	0/692
8	7	0.33	0/485	0.41	0/657
8	G	0.33	0/511	0.32	0/692
8	N	0.38	0/511	0.32	0/692
8	Q	0.27	0/511	0.35	0/692
8	T	0.25	0/511	0.34	0/692
8	W	0.24	0/511	0.33	0/692
8	Z	0.24	0/511	0.34	0/692
8	c	0.25	0/511	0.35	0/692
8	f	0.26	0/511	0.43	0/692

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
8	i	0.25	0/511	0.32	0/692
8	l	0.26	0/511	0.33	0/692
8	o	0.25	0/511	0.35	0/692
8	r	0.25	0/511	0.32	0/692
8	u	0.25	0/511	0.36	0/692
8	x	0.25	0/511	0.35	0/692
9	5	0.12	0/188	0.27	0/258
9	8	0.14	0/215	0.23	0/295
9	I	0.16	0/215	0.24	0/295
9	O	0.57	1/215 (0.5%)	0.31	0/295
9	R	0.48	0/215	0.48	0/295
9	U	0.29	0/215	0.30	0/295
9	X	0.44	0/215	0.33	0/295
9	a	0.17	0/215	0.23	0/295
9	d	0.16	0/215	0.27	0/295
9	g	0.17	0/215	0.26	0/295
9	j	0.17	0/215	0.26	0/295
9	m	0.28	0/215	0.38	0/295
9	p	0.17	0/215	0.28	0/295
9	s	0.14	0/215	0.24	0/295
9	v	0.15	0/215	0.24	0/295
9	y	0.16	0/215	0.23	0/295
10	2	0.22	0/241	0.35	0/331
11	9	0.19	0/239	0.26	0/327
All	All	0.28	1/31949 (0.0%)	0.36	6/43442 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	O	24	SER	CA-C	-5.97	1.44	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	266	ASN	N-CA-C	-8.28	92.36	107.75
1	C	265	HIS	CB-CA-C	-6.12	98.95	110.16
7	k	57	ILE	N-CA-C	-5.84	107.22	112.12
1	C	265	HIS	N-CA-C	5.71	117.79	108.76
7	S	57	ILE	N-CA-C	-5.25	107.47	111.62

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2732	0	2526	89	0
2	L	2188	0	2132	131	0
3	M	2553	0	2482	151	0
4	H	2160	0	2128	124	0
5	4	615	0	564	25	0
6	3	433	0	450	36	0
7	6	533	0	503	25	0
7	F	533	0	503	17	0
7	K	533	0	503	12	0
7	P	533	0	503	21	0
7	S	533	0	503	14	0
7	V	533	0	503	15	0
7	Y	533	0	503	18	0
7	b	533	0	503	10	0
7	e	533	0	503	25	0
7	h	533	0	503	22	0
7	k	533	0	503	13	0
7	n	533	0	503	12	0
7	q	533	0	503	19	0
7	t	533	0	503	21	0
7	w	533	0	503	23	0
7	z	533	0	503	19	0
8	1	498	0	468	24	0
8	7	472	0	437	12	0
8	G	498	0	468	21	0
8	N	498	0	468	13	0
8	Q	498	0	468	16	0
8	T	498	0	468	20	0
8	W	498	0	468	24	0
8	Z	498	0	468	20	0
8	c	498	0	468	15	0
8	f	498	0	468	19	0
8	i	498	0	468	25	0
8	l	498	0	468	25	0
8	o	498	0	468	19	0
8	r	498	0	468	19	0
8	u	498	0	468	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	x	498	0	468	20	0
9	5	186	0	204	5	0
9	8	211	0	227	6	0
9	I	211	0	227	7	0
9	O	211	0	227	10	0
9	R	211	0	227	9	0
9	U	211	0	227	7	0
9	X	211	0	227	8	0
9	a	211	0	227	5	0
9	d	211	0	227	10	0
9	g	211	0	227	8	0
9	j	211	0	227	8	0
9	m	211	0	227	7	0
9	p	211	0	227	8	0
9	s	211	0	227	3	0
9	v	211	0	227	3	0
9	y	211	0	227	7	0
10	2	232	0	241	16	0
11	9	233	0	246	10	0
12	C	172	0	121	12	0
13	4	37	0	44	6	0
13	5	41	0	64	2	0
13	8	42	0	69	3	0
13	9	63	0	71	5	0
13	C	98	0	115	8	0
13	F	36	0	45	2	0
13	H	196	0	240	25	0
13	I	36	0	51	1	0
13	K	65	0	78	5	0
13	L	186	0	254	16	0
13	M	64	0	71	9	0
13	O	42	0	69	6	0
13	P	85	0	117	12	0
13	R	42	0	69	4	0
13	S	40	0	55	2	0
13	U	42	0	69	5	0
13	V	39	0	50	2	0
13	X	42	0	69	3	0
13	Y	91	0	131	12	0
13	a	42	0	69	6	0
13	b	37	0	46	1	0
13	d	42	0	69	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	e	40	0	55	5	0
13	g	42	0	69	7	0
13	h	36	0	48	0	0
13	j	42	0	69	3	0
13	k	46	0	69	3	0
13	m	42	0	69	3	0
13	n	37	0	50	0	0
13	p	39	0	60	3	0
13	q	40	0	54	2	0
13	s	42	0	69	5	0
13	t	39	0	50	1	0
13	v	42	0	69	5	0
13	w	39	0	49	0	0
13	z	38	0	50	2	0
14	C	10	0	14	2	0
15	1	66	0	0	1	0
15	3	51	0	0	1	0
15	4	66	0	0	1	0
15	6	132	0	0	0	0
15	7	66	0	0	0	0
15	F	132	0	0	2	0
15	G	66	0	0	0	0
15	K	132	0	0	2	0
15	L	132	0	0	6	0
15	M	132	0	0	3	0
15	N	66	0	0	0	0
15	P	198	0	0	1	0
15	S	198	0	0	4	0
15	V	132	0	0	2	0
15	W	66	0	0	0	0
15	Y	132	0	0	2	0
15	Z	66	0	0	0	0
15	b	132	0	0	1	0
15	c	66	0	0	0	0
15	e	132	0	0	4	0
15	f	66	0	0	1	0
15	h	132	0	0	2	0
15	i	66	0	0	0	0
15	k	132	0	0	2	0
15	l	66	0	0	0	0
15	n	132	0	0	1	0
15	o	66	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	q	132	0	0	5	0
15	r	66	0	0	0	0
15	t	132	0	0	3	0
15	u	66	0	0	0	0
15	w	198	0	0	2	0
15	z	132	0	0	2	0
16	L	65	0	0	2	0
16	M	65	0	0	0	0
17	L	33	0	39	5	0
18	1	10	0	0	0	0
18	4	15	0	0	0	0
18	8	17	0	0	0	0
18	9	16	0	0	0	0
18	F	12	0	0	0	0
18	I	29	0	0	0	0
18	K	18	0	0	0	0
18	L	24	0	0	0	0
18	M	50	0	0	1	0
18	O	24	0	0	0	0
18	R	27	0	0	0	0
18	U	27	0	0	0	0
18	X	25	0	0	0	0
18	a	25	0	0	0	0
18	b	32	0	0	0	0
18	d	27	0	0	0	0
18	g	26	0	0	0	0
18	j	23	0	0	0	0
18	k	18	0	0	0	0
18	m	24	0	0	0	0
18	n	9	0	0	0	0
18	p	25	0	0	0	0
18	q	12	0	0	0	0
18	s	23	0	0	0	0
18	v	27	0	0	0	0
18	y	7	0	0	0	0
19	M	1	0	0	0	0
20	M	76	0	93	7	0
21	H	77	0	101	10	0
21	M	137	0	165	11	0
22	3	40	0	56	7	0
23	1	46	0	0	0	0
23	7	46	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	G	46	0	0	2	0
23	N	46	0	0	0	0
23	Q	46	0	0	1	0
23	T	46	0	0	1	0
23	W	46	0	0	0	0
23	Z	46	0	0	1	0
23	c	46	0	0	2	0
23	f	46	0	0	0	0
23	i	46	0	0	2	0
23	l	46	0	0	1	0
23	o	46	0	0	0	0
23	r	46	0	0	0	0
23	u	46	0	0	0	0
23	x	46	0	0	0	0
24	K	39	0	51	2	0
25	S	20	0	28	2	0
25	h	20	0	28	3	0
All	All	38551	0	33324	1017	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

The worst 5 of 1017 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:264:CYS:SG	12:C:403:HEC:HAC	1.87	1.14
13:O:104:PGV:H031	9:R:28:ARG:NH1	1.79	0.98
1:C:264:CYS:SG	12:C:403:HEC:CAC	2.63	0.85
2:L:194:LEU:HD11	2:L:213:GLU:HB2	1.62	0.81
4:H:3:ALA:HB2	7:q:42:GLU:HG3	1.64	0.79

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	344/372 (92%)	330 (96%)	14 (4%)	0	100	100
2	L	273/279 (98%)	264 (97%)	9 (3%)	0	100	100
3	M	316/320 (99%)	307 (97%)	9 (3%)	0	100	100
4	H	264/274 (96%)	258 (98%)	6 (2%)	0	100	100
5	4	70/105 (67%)	67 (96%)	3 (4%)	0	100	100
6	3	49/65 (75%)	49 (100%)	0	0	100	100
7	6	61/65 (94%)	61 (100%)	0	0	100	100
7	F	61/65 (94%)	61 (100%)	0	0	100	100
7	K	61/65 (94%)	60 (98%)	1 (2%)	0	100	100
7	P	61/65 (94%)	61 (100%)	0	0	100	100
7	S	61/65 (94%)	60 (98%)	1 (2%)	0	100	100
7	V	61/65 (94%)	60 (98%)	1 (2%)	0	100	100
7	Y	61/65 (94%)	58 (95%)	3 (5%)	0	100	100
7	b	61/65 (94%)	59 (97%)	2 (3%)	0	100	100
7	e	61/65 (94%)	58 (95%)	3 (5%)	0	100	100
7	h	61/65 (94%)	61 (100%)	0	0	100	100
7	k	61/65 (94%)	58 (95%)	3 (5%)	0	100	100
7	n	61/65 (94%)	60 (98%)	1 (2%)	0	100	100
7	q	61/65 (94%)	61 (100%)	0	0	100	100
7	t	61/65 (94%)	60 (98%)	1 (2%)	0	100	100
7	w	61/65 (94%)	60 (98%)	1 (2%)	0	100	100
7	z	61/65 (94%)	61 (100%)	0	0	100	100
8	1	60/86 (70%)	59 (98%)	1 (2%)	0	100	100
8	7	57/86 (66%)	55 (96%)	2 (4%)	0	100	100
8	G	60/86 (70%)	60 (100%)	0	0	100	100
8	N	60/86 (70%)	60 (100%)	0	0	100	100
8	Q	60/86 (70%)	59 (98%)	1 (2%)	0	100	100
8	T	60/86 (70%)	59 (98%)	1 (2%)	0	100	100
8	W	60/86 (70%)	59 (98%)	1 (2%)	0	100	100
8	Z	60/86 (70%)	60 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	c	60/86 (70%)	59 (98%)	1 (2%)	0	100	100
8	f	60/86 (70%)	56 (93%)	4 (7%)	0	100	100
8	i	60/86 (70%)	59 (98%)	1 (2%)	0	100	100
8	l	60/86 (70%)	59 (98%)	1 (2%)	0	100	100
8	o	60/86 (70%)	60 (100%)	0	0	100	100
8	r	60/86 (70%)	59 (98%)	1 (2%)	0	100	100
8	u	60/86 (70%)	58 (97%)	2 (3%)	0	100	100
8	x	60/86 (70%)	59 (98%)	1 (2%)	0	100	100
9	5	24/29 (83%)	24 (100%)	0	0	100	100
9	8	26/29 (90%)	26 (100%)	0	0	100	100
9	I	26/29 (90%)	26 (100%)	0	0	100	100
9	O	26/29 (90%)	26 (100%)	0	0	100	100
9	R	26/29 (90%)	25 (96%)	1 (4%)	0	100	100
9	U	26/29 (90%)	26 (100%)	0	0	100	100
9	X	26/29 (90%)	26 (100%)	0	0	100	100
9	a	26/29 (90%)	26 (100%)	0	0	100	100
9	d	26/29 (90%)	25 (96%)	1 (4%)	0	100	100
9	g	26/29 (90%)	26 (100%)	0	0	100	100
9	j	26/29 (90%)	26 (100%)	0	0	100	100
9	m	26/29 (90%)	26 (100%)	0	0	100	100
9	p	26/29 (90%)	26 (100%)	0	0	100	100
9	s	26/29 (90%)	26 (100%)	0	0	100	100
9	v	26/29 (90%)	26 (100%)	0	0	100	100
9	y	26/29 (90%)	26 (100%)	0	0	100	100
10	2	27/31 (87%)	27 (100%)	0	0	100	100
11	9	27/33 (82%)	27 (100%)	0	0	100	100
All	All	3717/4359 (85%)	3640 (98%)	77 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	C	294/311 (94%)	294 (100%)	0	100	100
2	L	218/221 (99%)	218 (100%)	0	100	100
3	M	253/255 (99%)	253 (100%)	0	100	100
4	H	229/234 (98%)	229 (100%)	0	100	100
5	4	63/89 (71%)	63 (100%)	0	100	100
6	3	45/56 (80%)	45 (100%)	0	100	100
7	6	52/53 (98%)	52 (100%)	0	100	100
7	F	52/53 (98%)	52 (100%)	0	100	100
7	K	52/53 (98%)	52 (100%)	0	100	100
7	P	52/53 (98%)	52 (100%)	0	100	100
7	S	52/53 (98%)	52 (100%)	0	100	100
7	V	52/53 (98%)	52 (100%)	0	100	100
7	Y	52/53 (98%)	52 (100%)	0	100	100
7	b	52/53 (98%)	52 (100%)	0	100	100
7	e	52/53 (98%)	52 (100%)	0	100	100
7	h	52/53 (98%)	52 (100%)	0	100	100
7	k	52/53 (98%)	52 (100%)	0	100	100
7	n	52/53 (98%)	52 (100%)	0	100	100
7	q	52/53 (98%)	52 (100%)	0	100	100
7	t	52/53 (98%)	52 (100%)	0	100	100
7	w	52/53 (98%)	52 (100%)	0	100	100
7	z	52/53 (98%)	52 (100%)	0	100	100
8	1	49/69 (71%)	49 (100%)	0	100	100
8	7	46/69 (67%)	46 (100%)	0	100	100
8	G	49/69 (71%)	49 (100%)	0	100	100
8	N	49/69 (71%)	49 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	Q	49/69 (71%)	49 (100%)	0	100	100
8	T	49/69 (71%)	49 (100%)	0	100	100
8	W	49/69 (71%)	49 (100%)	0	100	100
8	Z	49/69 (71%)	49 (100%)	0	100	100
8	c	49/69 (71%)	49 (100%)	0	100	100
8	f	49/69 (71%)	49 (100%)	0	100	100
8	i	49/69 (71%)	49 (100%)	0	100	100
8	l	49/69 (71%)	49 (100%)	0	100	100
8	o	49/69 (71%)	49 (100%)	0	100	100
8	r	49/69 (71%)	49 (100%)	0	100	100
8	u	49/69 (71%)	49 (100%)	0	100	100
8	x	49/69 (71%)	49 (100%)	0	100	100
9	5	20/23 (87%)	20 (100%)	0	100	100
9	8	22/23 (96%)	22 (100%)	0	100	100
9	I	22/23 (96%)	22 (100%)	0	100	100
9	O	22/23 (96%)	22 (100%)	0	100	100
9	R	22/23 (96%)	22 (100%)	0	100	100
9	U	22/23 (96%)	22 (100%)	0	100	100
9	X	22/23 (96%)	22 (100%)	0	100	100
9	a	22/23 (96%)	22 (100%)	0	100	100
9	d	22/23 (96%)	22 (100%)	0	100	100
9	g	22/23 (96%)	22 (100%)	0	100	100
9	j	22/23 (96%)	22 (100%)	0	100	100
9	m	22/23 (96%)	22 (100%)	0	100	100
9	p	22/23 (96%)	22 (100%)	0	100	100
9	s	22/23 (96%)	22 (100%)	0	100	100
9	v	22/23 (96%)	22 (100%)	0	100	100
9	y	22/23 (96%)	22 (100%)	0	100	100
10	2	21/23 (91%)	21 (100%)	0	100	100
11	9	24/27 (89%)	24 (100%)	0	100	100
All	All	3110/3536 (88%)	3110 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
5	4	21	GLN
9	a	21	ASN
8	1	20	ASN
8	l	14	GLN
4	H	92	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 195 ligands modelled in this entry, 57 are unknown and 1 is monoatomic - leaving 137 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	$\#\|Z\| > 2$
15	A1LZM	M	703	3	68,74,74	2.20	22 (32%)	79,115,115	3.22	29 (36%)
13	PGV	F	104	-	35,35,50	1.11	2 (5%)	39,40,56	1.19	4 (10%)
12	HEC	C	404	1	50,50,50	1.77	11 (22%)	68,82,82	1.86	19 (27%)
15	A1LZM	F	101	7	68,74,74	2.12	20 (29%)	79,115,115	2.86	29 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
13	PGV	M	708	-	31,31,50	1.15	2 (6%)	34,37,56	1.24	3 (8%)
15	A1LZM	w	103	8	68,74,74	2.07	20 (29%)	79,115,115	2.90	27 (34%)
15	A1LZM	P	103	8	68,74,74	2.06	19 (27%)	79,115,115	3.01	27 (34%)
21	CDL	M	710	-	53,53,99	0.35	0	59,65,111	0.40	0
15	A1LZM	S	103	8	68,74,74	2.25	22 (32%)	79,115,115	3.01	33 (41%)
15	A1LZM	L	301	2	68,74,74	2.11	22 (32%)	79,115,115	3.25	29 (36%)
15	A1LZM	F	102	7	68,74,74	2.09	21 (30%)	79,115,115	2.97	28 (35%)
15	A1LZM	3	102	6	53,59,74	2.34	20 (37%)	61,97,115	3.52	27 (44%)
13	PGV	d	104	-	41,41,50	0.97	2 (4%)	43,43,56	1.04	2 (4%)
13	PGV	K	104	-	24,24,50	1.35	2 (8%)	28,29,56	1.39	4 (14%)
23	A1LZQ	i	102	8	48,54,74	2.28	17 (35%)	56,91,115	3.10	27 (48%)
20	MQ8	M	705	-	54,54,54	0.39	0	66,69,69	0.38	0
16	A1LZP	L	303	-	57,70,70	2.52	14 (24%)	56,101,101	3.41	23 (41%)
13	PGV	p	104	-	38,38,50	1.01	2 (5%)	40,40,56	1.05	2 (5%)
15	A1LZM	q	102	7	68,74,74	2.08	21 (30%)	79,115,115	2.99	26 (32%)
13	PGV	Y	103	-	50,50,50	0.90	2 (4%)	53,56,56	1.04	4 (7%)
23	A1LZQ	N	102	8	48,54,74	2.26	19 (39%)	56,91,115	3.13	26 (46%)
15	A1LZM	z	102	7	68,74,74	2.08	22 (32%)	79,115,115	2.96	28 (35%)
13	PGV	5	101	-	40,40,50	1.00	2 (5%)	42,42,56	1.02	2 (4%)
14	LHG	C	406	1	9,9,48	0.79	0	8,8,54	2.37	1 (12%)
15	A1LZM	7	101	8	68,74,74	2.05	20 (29%)	79,115,115	3.02	27 (34%)
15	A1LZM	Y	102	7	68,74,74	2.05	21 (30%)	79,115,115	3.14	37 (46%)
24	PEF	K	106	-	38,38,46	0.31	0	41,43,51	0.40	0
13	PGV	H	302	-	41,41,50	1.03	2 (4%)	45,46,56	1.07	3 (6%)
13	PGV	H	301	-	31,31,50	1.13	2 (6%)	34,37,56	1.19	4 (11%)
13	PGV	s	104	-	41,41,50	0.98	2 (4%)	43,43,56	1.02	3 (6%)
23	A1LZQ	o	102	8	48,54,74	2.29	18 (37%)	56,91,115	3.11	25 (44%)
15	A1LZM	n	101	7	68,74,74	2.12	19 (27%)	79,115,115	2.84	29 (36%)
13	PGV	H	306	-	41,41,50	1.01	2 (4%)	44,47,56	1.04	4 (9%)
15	A1LZM	h	101	7	68,74,74	2.12	19 (27%)	79,115,115	2.96	28 (35%)
23	A1LZQ	u	102	8	48,54,74	2.30	17 (35%)	56,91,115	3.04	27 (48%)
15	A1LZM	e	101	7	68,74,74	2.12	20 (29%)	79,115,115	2.82	30 (37%)
13	PGV	Y	104	-	39,39,50	1.06	2 (5%)	43,44,56	1.18	4 (9%)
13	PGV	P	105	-	44,44,50	0.95	2 (4%)	47,50,56	1.11	3 (6%)
13	PGV	S	105	-	39,39,50	1.07	2 (5%)	43,44,56	1.07	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
15	A1LZM	6	102	7	68,74,74	2.11	19 (27%)	79,115,115	3.06	35 (44%)
13	PGV	b	105	-	36,36,50	1.11	2 (5%)	40,41,56	1.16	4 (10%)
15	A1LZM	6	101	7	68,74,74	2.13	20 (29%)	79,115,115	2.88	29 (36%)
15	A1LZM	b	101	7	68,74,74	2.11	19 (27%)	79,115,115	2.93	26 (32%)
13	PGV	v	104	-	41,41,50	0.98	2 (4%)	43,43,56	1.12	4 (9%)
13	PGV	k	104	-	45,45,50	0.98	2 (4%)	49,50,56	1.10	4 (8%)
13	PGV	9	103	-	37,37,50	1.07	2 (5%)	41,42,56	1.15	4 (9%)
15	A1LZM	P	102	7	68,74,74	2.08	18 (26%)	79,115,115	3.05	34 (43%)
15	A1LZM	K	102	7	68,74,74	2.07	19 (27%)	79,115,115	3.05	33 (41%)
15	A1LZM	L	302	2	68,74,74	2.12	21 (30%)	79,115,115	2.99	28 (35%)
13	PGV	O	104	-	41,41,50	0.98	2 (4%)	43,43,56	1.09	3 (6%)
13	PGV	X	104	-	41,41,50	0.98	2 (4%)	43,43,56	1.12	3 (6%)
15	A1LZM	M	702	3	68,74,74	2.10	22 (32%)	79,115,115	3.01	28 (35%)
13	PGV	V	103	-	38,38,50	1.08	2 (5%)	42,43,56	1.14	4 (9%)
12	HEC	C	402	1	50,50,50	1.76	11 (22%)	68,82,82	1.79	17 (25%)
13	PGV	L	310	-	47,47,50	0.92	2 (4%)	50,53,56	1.05	3 (6%)
15	A1LZM	V	102	7	68,74,74	2.11	18 (26%)	79,115,115	2.91	32 (40%)
13	PGV	m	104	-	41,41,50	0.98	2 (4%)	43,43,56	1.06	3 (6%)
13	PGV	8	103	-	41,41,50	0.97	2 (4%)	43,43,56	1.09	3 (6%)
15	A1LZM	k	102	7	68,74,74	2.07	20 (29%)	79,115,115	3.07	31 (39%)
13	PGV	C	408	-	37,37,50	1.05	2 (5%)	40,43,56	1.21	4 (10%)
15	A1LZM	S	102	7	68,74,74	2.08	20 (29%)	79,115,115	3.03	29 (36%)
13	PGV	z	103	-	37,37,50	1.10	2 (5%)	41,42,56	1.25	3 (7%)
23	A1LZQ	Z	102	8	48,54,74	2.32	17 (35%)	56,91,115	3.10	23 (41%)
23	A1LZQ	x	101	8	48,54,74	2.29	19 (39%)	56,91,115	6.31	26 (46%)
25	BGL	S	104	-	20,20,20	0.39	0	24,25,25	0.52	0
23	A1LZQ	r	102	8	48,54,74	2.27	18 (37%)	56,91,115	3.12	26 (46%)
15	A1LZM	f	101	8	68,74,74	2.06	20 (29%)	79,115,115	3.00	28 (35%)
15	A1LZM	q	101	7	68,74,74	2.12	18 (26%)	79,115,115	2.87	28 (35%)
13	PGV	L	309	-	43,43,50	0.98	2 (4%)	46,49,56	1.03	3 (6%)
13	PGV	h	104	-	35,35,50	1.10	2 (5%)	39,40,56	1.20	4 (10%)
13	PGV	w	104	-	38,38,50	1.11	2 (5%)	41,43,56	1.09	3 (7%)
13	PGV	t	103	-	38,38,50	1.09	2 (5%)	42,43,56	1.13	4 (9%)
13	PGV	P	104	-	39,39,50	1.07	2 (5%)	43,44,56	1.10	3 (6%)
13	PGV	a	104	-	41,41,50	0.98	2 (4%)	43,43,56	1.06	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
15	A1LZM	z	101	7	68,74,74	2.13	21 (30%)	79,115,115	2.92	31 (39%)
13	PGV	R	104	-	41,41,50	0.97	2 (4%)	43,43,56	1.09	4 (9%)
12	HEC	C	401	1	50,50,50	1.75	11 (22%)	68,82,82	1.79	19 (27%)
15	A1LZM	t	102	7	68,74,74	2.09	21 (30%)	79,115,115	2.99	26 (32%)
23	A1LZQ	1	102	8	48,54,74	2.27	18 (37%)	56,91,115	3.07	25 (44%)
15	A1LZM	i	101	8	68,74,74	2.04	18 (26%)	79,115,115	2.94	27 (34%)
13	PGV	H	305	-	32,32,50	1.15	2 (6%)	35,38,56	1.21	3 (8%)
16	A1LZP	M	704	-	57,70,70	2.57	14 (24%)	56,101,101	3.34	26 (46%)
15	A1LZM	4	201	5	68,74,74	2.11	22 (32%)	79,115,115	2.96	25 (31%)
13	PGV	K	103	-	39,39,50	1.06	2 (5%)	43,44,56	1.16	3 (6%)
15	A1LZM	G	101	8	68,74,74	2.06	21 (30%)	79,115,115	2.93	28 (35%)
15	A1LZM	N	101	8	68,74,74	2.06	17 (25%)	79,115,115	2.94	27 (34%)
21	CDL	M	709	-	82,82,99	0.29	0	88,94,111	0.36	0
13	PGV	C	405	-	27,27,50	1.26	3 (11%)	28,29,56	1.45	3 (10%)
22	LYC	3	101	-	39,39,39	1.63	8 (20%)	44,46,46	1.65	10 (22%)
15	A1LZM	r	101	8	68,74,74	2.08	18 (26%)	79,115,115	2.94	27 (34%)
21	CDL	H	304	-	76,76,99	0.31	0	82,88,111	0.49	0
15	A1LZM	u	101	8	68,74,74	2.28	21 (30%)	79,115,115	3.08	35 (44%)
20	MQ8	M	706	-	24,24,54	0.45	0	30,33,69	0.46	0
13	PGV	j	104	-	41,41,50	0.98	2 (4%)	43,43,56	1.04	2 (4%)
13	PGV	g	104	-	41,41,50	0.96	2 (4%)	43,43,56	0.94	2 (4%)
15	A1LZM	h	102	7	68,74,74	2.07	17 (25%)	79,115,115	3.19	33 (41%)
13	PGV	I	101	-	35,35,50	1.05	2 (5%)	37,37,56	1.06	2 (5%)
23	A1LZQ	l	102	8	48,54,74	2.26	18 (37%)	56,91,115	3.11	26 (46%)
23	A1LZQ	c	102	8	48,54,74	2.29	18 (37%)	56,91,115	3.07	26 (46%)
13	PGV	9	102	-	24,24,50	1.34	2 (8%)	28,29,56	1.38	4 (14%)
15	A1LZM	W	101	8	68,74,74	2.21	21 (30%)	79,115,115	2.86	27 (34%)
15	A1LZM	V	101	7	68,74,74	2.11	20 (29%)	79,115,115	2.82	31 (39%)
15	A1LZM	o	101	8	68,74,74	2.29	21 (30%)	79,115,115	3.13	37 (46%)
23	A1LZQ	7	102	8	48,54,74	2.38	18 (37%)	56,91,115	3.14	30 (53%)
13	PGV	4	203	-	36,36,50	1.11	2 (5%)	39,42,56	1.04	2 (5%)
23	A1LZQ	f	102	8	48,54,74	2.27	20 (41%)	56,91,115	3.25	25 (44%)
15	A1LZM	1	101	8	68,74,74	2.06	19 (27%)	79,115,115	2.91	28 (35%)
23	A1LZQ	G	102	8	48,54,74	2.28	18 (37%)	56,91,115	3.12	25 (44%)
13	PGV	H	303	-	46,46,50	0.94	2 (4%)	48,52,56	1.08	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
12	HEC	C	403	1	50,50,50	1.77	10 (20%)	68,82,82	1.74	15 (22%)
13	PGV	C	407	-	31,31,50	1.19	2 (6%)	34,36,56	1.30	4 (11%)
15	A1LZM	t	101	7	68,74,74	2.13	21 (30%)	79,115,115	2.89	28 (35%)
23	A1LZQ	T	101	8	48,54,74	2.26	18 (37%)	56,91,115	3.11	27 (48%)
13	PGV	L	305	-	47,47,50	0.94	2 (4%)	50,53,56	0.99	3 (6%)
13	PGV	n	104	-	36,36,50	1.10	2 (5%)	40,41,56	1.19	4 (10%)
13	PGV	M	707	-	31,31,50	1.18	2 (6%)	35,36,56	1.24	4 (11%)
23	A1LZQ	Q	101	8	48,54,74	2.26	16 (33%)	56,91,115	3.09	27 (48%)
13	PGV	q	104	-	39,39,50	1.05	2 (5%)	43,44,56	1.19	4 (9%)
15	A1LZM	Z	101	8	68,74,74	2.07	18 (26%)	79,115,115	3.07	32 (40%)
15	A1LZM	w	102	7	68,74,74	2.07	16 (23%)	79,115,115	3.18	33 (41%)
15	A1LZM	Y	101	7	68,74,74	2.14	19 (27%)	79,115,115	2.87	28 (35%)
15	A1LZM	w	101	7	68,74,74	2.12	20 (29%)	79,115,115	2.91	28 (35%)
15	A1LZM	K	101	7	68,74,74	2.11	20 (29%)	79,115,115	2.85	28 (35%)
15	A1LZM	S	101	7	68,74,74	2.12	20 (29%)	79,115,115	2.88	31 (39%)
13	PGV	L	306	-	45,45,50	0.97	2 (4%)	48,51,56	1.02	4 (8%)
15	A1LZM	b	102	7	68,74,74	2.25	19 (27%)	79,115,115	2.77	31 (39%)
17	UQ8	L	304	-	33,33,53	0.84	2 (6%)	40,43,67	0.91	3 (7%)
15	A1LZM	n	102	7	68,74,74	2.08	19 (27%)	79,115,115	2.92	30 (37%)
23	A1LZQ	W	102	8	48,54,74	2.26	18 (37%)	56,91,115	3.10	26 (46%)
15	A1LZM	l	101	8	68,74,74	2.27	20 (29%)	79,115,115	3.05	37 (46%)
15	A1LZM	c	101	8	68,74,74	2.18	20 (29%)	79,115,115	2.66	30 (37%)
15	A1LZM	P	101	7	68,74,74	2.12	19 (27%)	79,115,115	2.85	30 (37%)
15	A1LZM	k	101	7	68,74,74	2.13	19 (27%)	79,115,115	3.01	32 (40%)
13	PGV	e	103	-	39,39,50	1.07	2 (5%)	43,44,56	1.15	4 (9%)
13	PGV	U	104	-	41,41,50	0.99	2 (4%)	43,43,56	1.16	3 (6%)
15	A1LZM	e	102	7	68,74,74	2.04	19 (27%)	79,115,115	2.99	33 (41%)
25	BGL	h	103	-	20,20,20	0.37	0	24,25,25	0.60	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
15	A1LZM	M	703	3	1/1/21/27	13/41/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	PGV	F	104	-	-	15/37/37/55	-
12	HEC	C	404	1	1/1/3/7	6/14/54/54	-
15	A1LZM	F	101	7	1/1/21/27	12/41/137/137	-
13	PGV	M	708	-	-	8/36/36/55	-
15	A1LZM	w	103	8	1/1/21/27	14/41/137/137	-
15	A1LZM	P	103	8	1/1/21/27	9/41/137/137	-
21	CDL	M	710	-	-	18/64/64/110	-
15	A1LZM	S	103	8	1/1/21/27	11/41/137/137	-
15	A1LZM	L	301	2	1/1/21/27	15/41/137/137	-
15	A1LZM	F	102	7	1/1/21/27	13/41/137/137	-
15	A1LZM	3	102	6	1/1/18/27	7/23/119/137	-
13	PGV	d	104	-	-	13/43/43/55	-
23	A1LZQ	i	102	8	1/1/17/27	4/17/113/137	-
13	PGV	K	104	-	-	3/26/26/55	-
20	MQ8	M	705	-	-	6/47/67/67	0/2/2/2
16	A1LZP	L	303	-	-	11/37/105/105	0/5/6/6
15	A1LZM	q	102	7	1/1/21/27	6/41/137/137	-
13	PGV	p	104	-	-	6/40/40/55	-
13	PGV	Y	103	-	-	22/55/55/55	-
23	A1LZQ	N	102	8	1/1/17/27	2/17/113/137	-
15	A1LZM	z	102	7	1/1/21/27	12/41/137/137	-
15	A1LZM	7	101	8	1/1/21/27	11/41/137/137	-
13	PGV	5	101	-	-	10/42/42/55	-
14	LHG	C	406	1	-	0/6/7/53	-
15	A1LZM	Y	102	7	1/1/21/27	10/41/137/137	-
24	PEF	K	106	-	-	9/42/42/50	-
13	PGV	H	302	-	-	18/43/43/55	-
13	PGV	H	301	-	-	16/36/36/55	-
13	PGV	s	104	-	-	8/43/43/55	-
23	A1LZQ	o	102	8	1/1/17/27	5/17/113/137	-
15	A1LZM	n	101	7	1/1/21/27	11/41/137/137	-
13	PGV	H	306	-	-	14/46/46/55	-
15	A1LZM	h	101	7	1/1/21/27	12/41/137/137	-
23	A1LZQ	u	102	8	1/1/17/27	3/17/113/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	A1LZM	e	101	7	1/1/21/27	15/41/137/137	-
13	PGV	Y	104	-	-	16/41/41/55	-
13	PGV	P	105	-	-	13/49/49/55	-
13	PGV	S	105	-	-	11/41/41/55	-
15	A1LZM	6	102	7	1/1/21/27	16/41/137/137	-
15	A1LZM	6	101	7	1/1/21/27	11/41/137/137	-
13	PGV	b	105	-	-	6/38/38/55	-
15	A1LZM	b	101	7	1/1/21/27	12/41/137/137	-
13	PGV	v	104	-	-	14/43/43/55	-
13	PGV	k	104	-	-	17/47/47/55	-
13	PGV	9	103	-	-	13/39/39/55	-
15	A1LZM	P	102	7	1/1/21/27	11/41/137/137	-
15	A1LZM	K	102	7	1/1/21/27	10/41/137/137	-
15	A1LZM	L	302	2	1/1/21/27	10/41/137/137	-
13	PGV	O	104	-	-	15/43/43/55	-
13	PGV	X	104	-	-	9/43/43/55	-
15	A1LZM	M	702	3	1/1/21/27	11/41/137/137	-
13	PGV	V	103	-	-	14/40/40/55	-
12	HEC	C	402	1	1/1/3/7	6/14/54/54	-
13	PGV	L	310	-	-	17/52/52/55	-
15	A1LZM	V	102	7	1/1/21/27	14/41/137/137	-
13	PGV	m	104	-	-	12/43/43/55	-
13	PGV	8	103	-	-	15/43/43/55	-
15	A1LZM	k	102	7	1/1/21/27	8/41/137/137	-
13	PGV	C	408	-	-	8/42/42/55	-
15	A1LZM	S	102	7	1/1/21/27	12/41/137/137	-
13	PGV	z	103	-	-	6/39/39/55	-
23	A1LZQ	Z	102	8	1/1/17/27	6/17/113/137	-
23	A1LZQ	x	101	8	1/1/17/27	5/17/113/137	-
25	BGL	S	104	-	-	0/11/31/31	0/1/1/1
23	A1LZQ	r	102	8	1/1/17/27	4/17/113/137	-
15	A1LZM	f	101	8	1/1/21/27	8/41/137/137	-
15	A1LZM	q	101	7	1/1/21/27	9/41/137/137	-
13	PGV	L	309	-	-	6/48/48/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	PGV	h	104	-	-	10/37/37/55	-
13	PGV	w	104	-	-	11/40/40/55	-
15	A1LZM	z	101	7	1/1/21/27	15/41/137/137	-
13	PGV	t	103	-	-	11/40/40/55	-
13	PGV	a	104	-	-	9/43/43/55	-
13	PGV	P	104	-	-	13/41/41/55	-
13	PGV	R	104	-	-	14/43/43/55	-
12	HEC	C	401	1	1/1/3/7	7/14/54/54	-
15	A1LZM	t	102	7	1/1/21/27	11/41/137/137	-
23	A1LZQ	1	102	8	1/1/17/27	3/17/113/137	-
15	A1LZM	i	101	8	1/1/21/27	14/41/137/137	-
13	PGV	H	305	-	-	13/37/37/55	-
16	A1LZP	M	704	-	-	13/37/105/105	0/5/6/6
15	A1LZM	4	201	5	1/1/21/27	13/41/137/137	-
13	PGV	K	103	-	-	11/41/41/55	-
15	A1LZM	G	101	8	1/1/21/27	14/41/137/137	-
15	A1LZM	N	101	8	1/1/21/27	8/41/137/137	-
21	CDL	M	709	-	-	12/93/93/110	-
13	PGV	C	405	-	-	7/28/28/55	-
22	LYC	3	101	-	-	5/43/43/43	-
15	A1LZM	r	101	8	1/1/21/27	8/41/137/137	-
21	CDL	H	304	-	-	16/87/87/110	-
15	A1LZM	u	101	8	1/1/21/27	12/41/137/137	-
20	MQ8	M	706	-	-	2/11/31/67	0/2/2/2
13	PGV	j	104	-	-	13/43/43/55	-
13	PGV	g	104	-	-	15/43/43/55	-
15	A1LZM	h	102	7	1/1/21/27	13/41/137/137	-
13	PGV	I	101	-	-	6/37/37/55	-
23	A1LZQ	l	102	8	1/1/17/27	4/17/113/137	-
23	A1LZQ	c	102	8	1/1/17/27	9/17/113/137	-
15	A1LZM	W	101	8	1/1/21/27	18/41/137/137	-
13	PGV	9	102	-	-	4/26/26/55	-
15	A1LZM	V	101	7	1/1/21/27	14/41/137/137	-
15	A1LZM	o	101	8	1/1/21/27	10/41/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	A1LZQ	7	102	8	1/1/17/27	12/17/113/137	-
13	PGV	4	203	-	-	13/41/41/55	-
23	A1LZQ	f	102	8	1/1/17/27	7/17/113/137	-
15	A1LZM	1	101	8	1/1/21/27	8/41/137/137	-
23	A1LZQ	G	102	8	1/1/17/27	5/17/113/137	-
13	PGV	H	303	-	-	18/51/51/55	-
12	HEC	C	403	1	1/1/3/7	6/14/54/54	-
13	PGV	C	407	-	-	7/33/33/55	-
15	A1LZM	t	101	7	1/1/21/27	11/41/137/137	-
23	A1LZQ	T	101	8	1/1/17/27	4/17/113/137	-
13	PGV	L	305	-	-	16/52/52/55	-
13	PGV	n	104	-	-	16/38/38/55	-
13	PGV	M	707	-	-	11/33/33/55	-
23	A1LZQ	Q	101	8	1/1/17/27	6/17/113/137	-
13	PGV	q	104	-	-	11/41/41/55	-
15	A1LZM	Z	101	8	1/1/21/27	6/41/137/137	-
15	A1LZM	w	102	7	1/1/21/27	13/41/137/137	-
15	A1LZM	Y	101	7	1/1/21/27	10/41/137/137	-
15	A1LZM	w	101	7	1/1/21/27	15/41/137/137	-
15	A1LZM	K	101	7	1/1/21/27	9/41/137/137	-
15	A1LZM	S	101	7	1/1/21/27	12/41/137/137	-
15	A1LZM	b	102	7	1/1/21/27	16/41/137/137	-
23	A1LZQ	W	102	8	1/1/17/27	2/17/113/137	-
13	PGV	L	306	-	-	25/50/50/55	-
15	A1LZM	n	102	7	1/1/21/27	11/41/137/137	-
17	UQ8	L	304	-	-	9/27/51/75	0/1/1/1
15	A1LZM	l	101	8	1/1/21/27	10/41/137/137	-
15	A1LZM	c	101	8	1/1/21/27	12/41/137/137	-
15	A1LZM	P	101	7	1/1/21/27	10/41/137/137	-
15	A1LZM	k	101	7	1/1/21/27	14/41/137/137	-
13	PGV	e	103	-	-	11/41/41/55	-
13	PGV	U	104	-	-	10/43/43/55	-
15	A1LZM	e	102	7	1/1/21/27	11/41/137/137	-
25	BGL	h	103	-	-	3/11/31/31	0/1/1/1

The worst 5 of 1537 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	M	704	A1LZP	O54-C48	8.03	1.33	1.22
15	u	101	A1LZM	C2C-C3C	-7.78	1.41	1.51
15	l	101	A1LZM	C2C-C3C	-7.69	1.41	1.51
15	o	101	A1LZM	C2C-C3C	-7.65	1.41	1.51
16	M	704	A1LZP	C26-C33	7.47	1.47	1.39

The worst 5 of 2323 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	x	101	A1LZQ	O2D-CGD-CBD	27.62	160.35	111.27
23	x	101	A1LZQ	O2D-CGD-O1D	-22.69	79.47	123.84
23	x	101	A1LZQ	O1D-CGD-CBD	-21.29	80.93	124.48
15	o	101	A1LZM	CHD-C4C-C3C	-12.30	110.48	125.89
15	l	101	A1LZM	CHD-C4C-C3C	-12.05	110.80	125.89

5 of 74 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
12	C	401	HEC	NA
12	C	402	HEC	NA
12	C	403	HEC	NA
12	C	404	HEC	NA
15	L	301	A1LZM	ND

5 of 1431 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	C	408	PGV	C04-O12-P-O14
13	C	408	PGV	O12-C04-C05-C06
13	L	305	PGV	C03-O11-P-O12
13	L	305	PGV	C03-O11-P-O13
13	L	305	PGV	C03-O11-P-O14

There are no ring outliers.

99 monomers are involved in 287 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	F	104	PGV	2	0
12	C	404	HEC	2	0
15	F	101	A1LZM	1	0
13	M	708	PGV	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	w	103	A1LZM	1	0
21	M	710	CDL	6	0
15	L	301	A1LZM	4	0
15	F	102	A1LZM	1	0
15	3	102	A1LZM	1	0
13	d	104	PGV	8	0
13	K	104	PGV	2	0
23	i	102	A1LZQ	2	0
20	M	705	MQ8	7	0
16	L	303	A1LZP	2	0
13	p	104	PGV	3	0
15	q	102	A1LZM	3	0
13	Y	103	PGV	10	0
15	z	102	A1LZM	2	0
13	5	101	PGV	2	0
14	C	406	LHG	2	0
15	Y	102	A1LZM	2	0
24	K	106	PEF	2	0
13	H	302	PGV	4	0
13	H	301	PGV	7	0
13	s	104	PGV	5	0
13	H	306	PGV	7	0
15	h	101	A1LZM	1	0
15	e	101	A1LZM	1	0
13	Y	104	PGV	2	0
13	P	105	PGV	7	0
13	S	105	PGV	2	0
13	b	105	PGV	1	0
15	b	101	A1LZM	1	0
13	v	104	PGV	5	0
13	k	104	PGV	3	0
13	9	103	PGV	3	0
15	P	102	A1LZM	1	0
15	K	102	A1LZM	1	0
15	L	302	A1LZM	2	0
13	O	104	PGV	6	0
13	X	104	PGV	3	0
15	M	702	A1LZM	3	0
13	V	103	PGV	2	0
13	L	310	PGV	2	0
15	V	102	A1LZM	1	0
13	m	104	PGV	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	8	103	PGV	3	0
15	k	102	A1LZM	2	0
13	C	408	PGV	4	0
15	S	102	A1LZM	2	0
13	z	103	PGV	2	0
23	Z	102	A1LZQ	1	0
25	S	104	BGL	2	0
15	f	101	A1LZM	1	0
15	q	101	A1LZM	2	0
13	L	309	PGV	6	0
13	t	103	PGV	1	0
13	P	104	PGV	5	0
13	a	104	PGV	6	0
13	R	104	PGV	4	0
12	C	401	HEC	4	0
15	t	102	A1LZM	2	0
13	H	305	PGV	3	0
15	4	201	A1LZM	1	0
13	K	103	PGV	3	0
21	M	709	CDL	5	0
13	C	405	PGV	3	0
22	3	101	LYC	7	0
21	H	304	CDL	10	0
13	j	104	PGV	3	0
13	g	104	PGV	7	0
15	h	102	A1LZM	1	0
13	I	101	PGV	1	0
23	l	102	A1LZQ	1	0
23	c	102	A1LZQ	2	0
13	9	102	PGV	2	0
15	V	101	A1LZM	1	0
13	4	203	PGV	6	0
15	1	101	A1LZM	1	0
23	G	102	A1LZQ	2	0
13	H	303	PGV	7	0
12	C	403	HEC	6	0
13	C	407	PGV	2	0
15	t	101	A1LZM	1	0
23	T	101	A1LZQ	1	0
13	L	305	PGV	4	0
13	M	707	PGV	4	0
23	Q	101	A1LZQ	1	0

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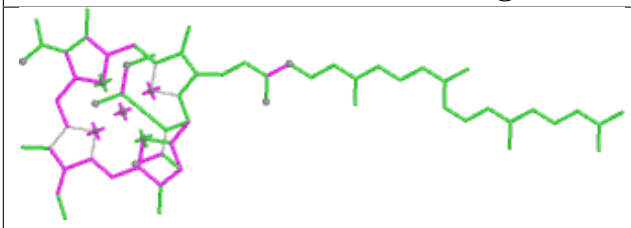
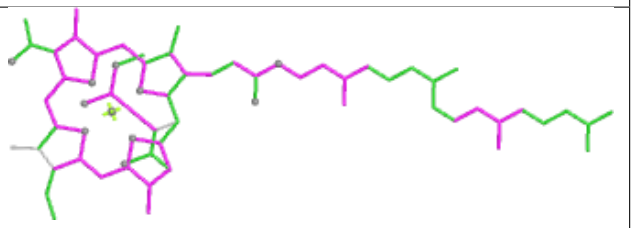
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	q	104	PGV	2	0
15	w	102	A1LZM	1	0
15	K	101	A1LZM	1	0
15	S	101	A1LZM	2	0
13	L	306	PGV	4	0
17	L	304	UQ8	5	0
15	n	102	A1LZM	1	0
13	e	103	PGV	5	0
13	U	104	PGV	5	0
15	e	102	A1LZM	3	0
25	h	103	BGL	3	0

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

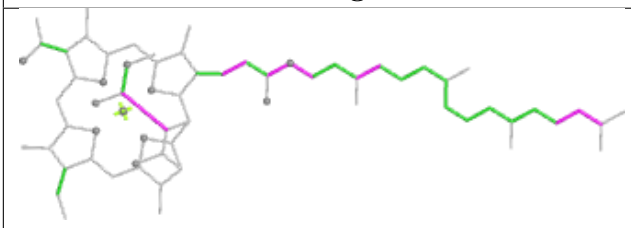
Ligand A1LZM M 703



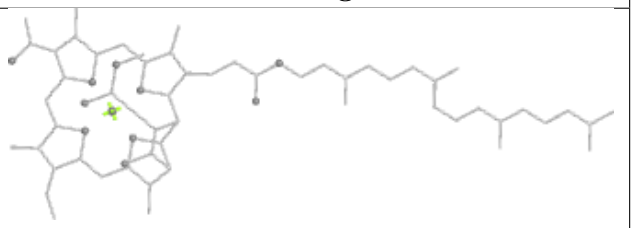
Bond lengths



Bond angles

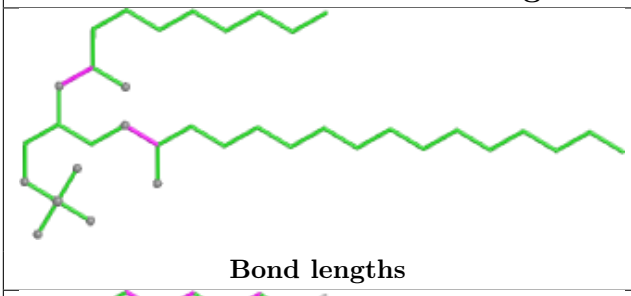


Torsions

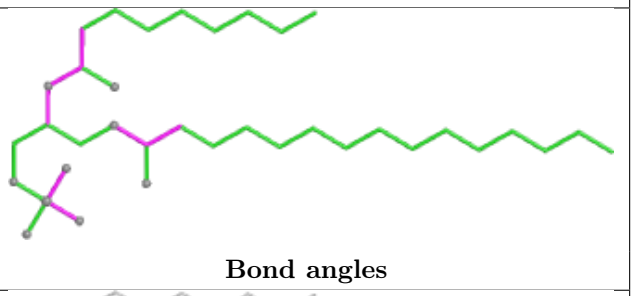


Rings

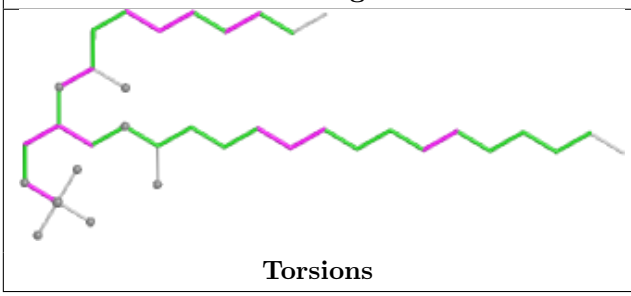
Ligand PGV F 104



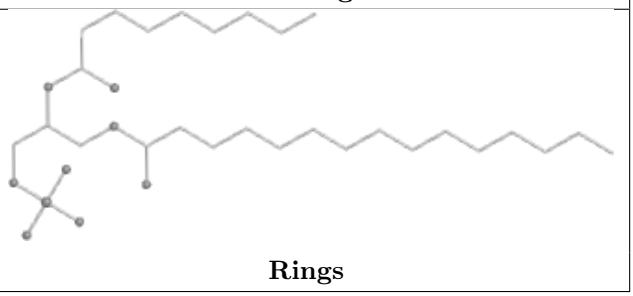
Bond lengths



Bond angles

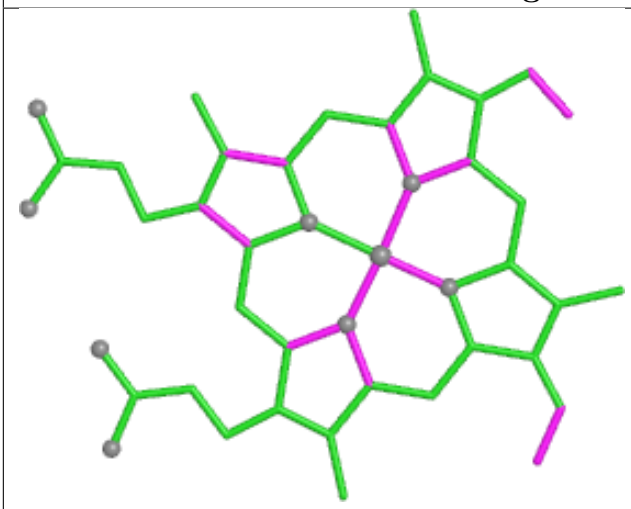


Torsions



Rings

Ligand HEC C 404



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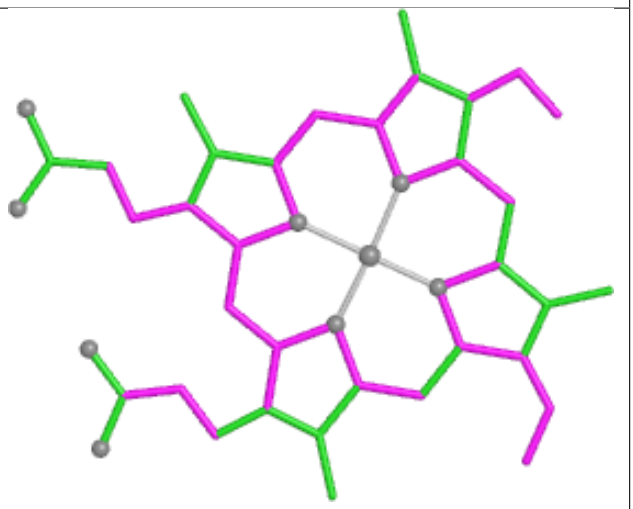
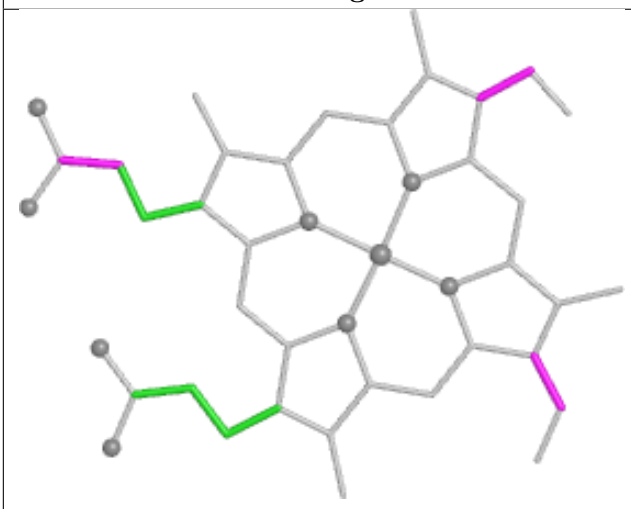
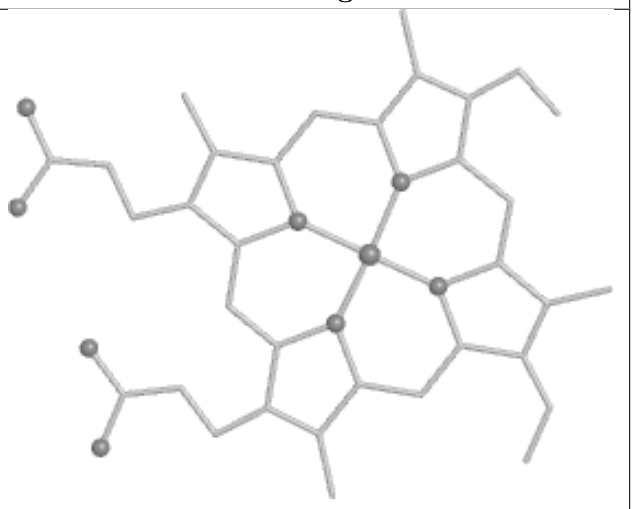


Bond angles

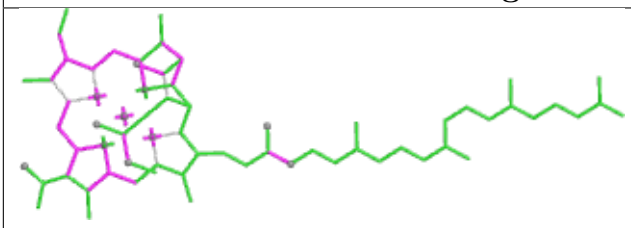


Torsions



Rings

Ligand A1LZM F 101



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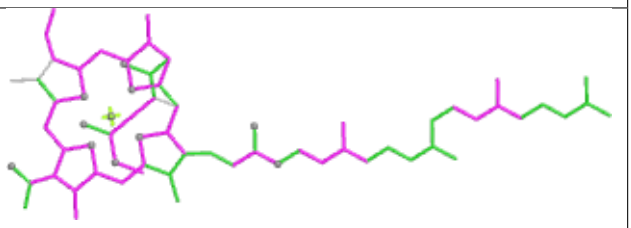
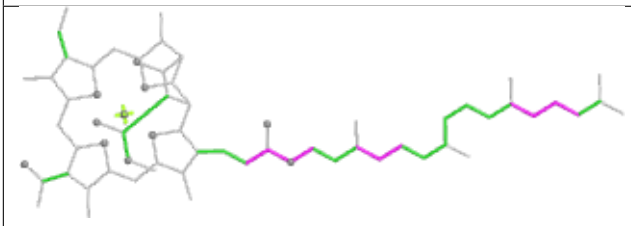
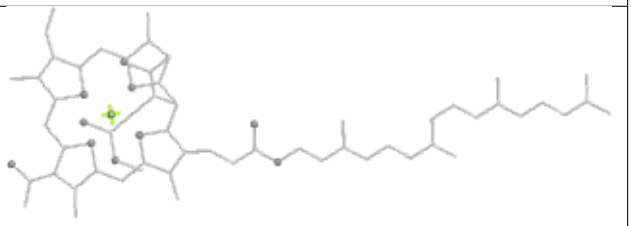


Bond angles

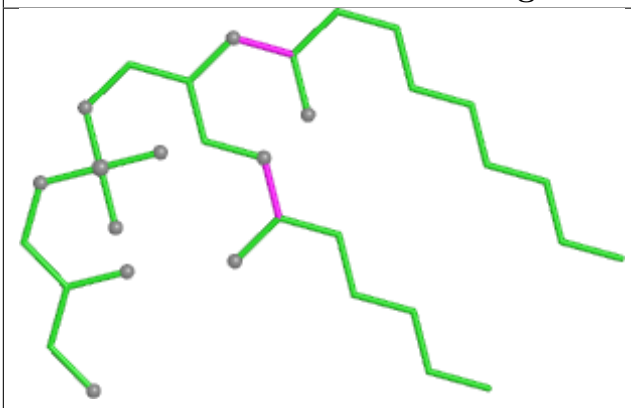


Torsions

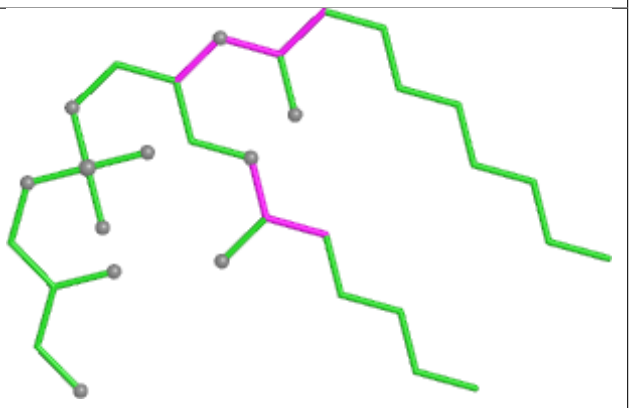


Rings

Ligand PGV M 708



Bond lengths



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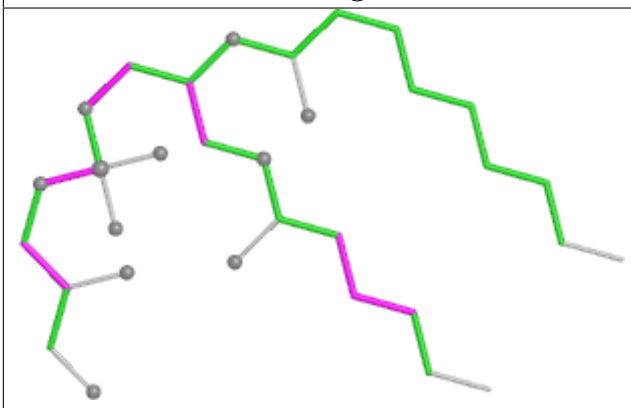

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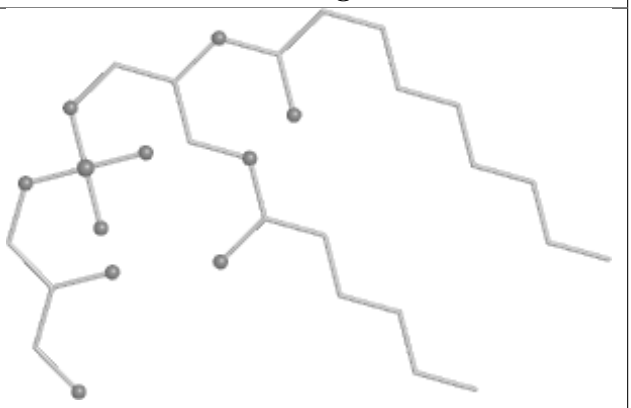

Rings

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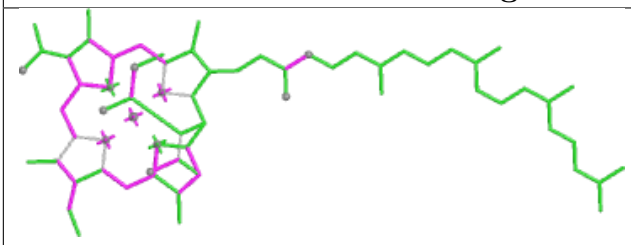
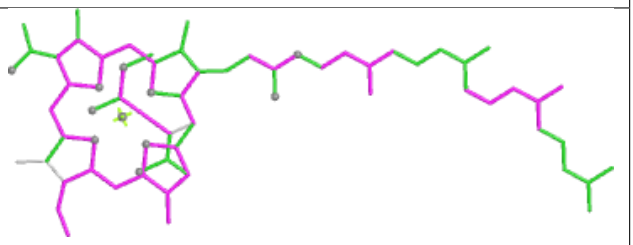
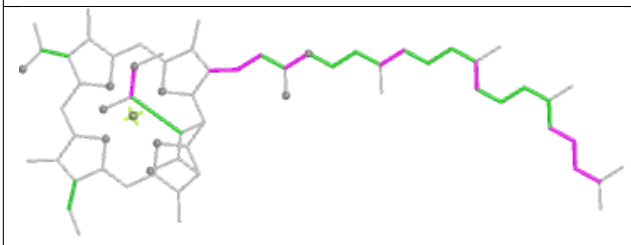
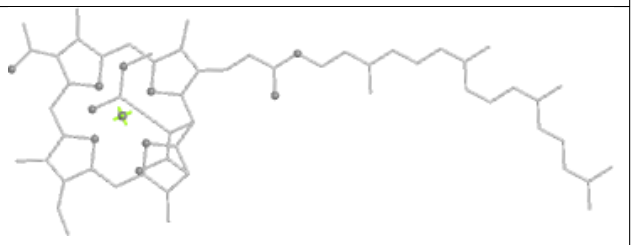
	
Bond lengths	Bond angles
	
Torsions	Rings

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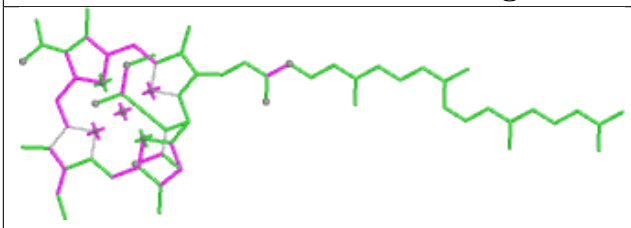
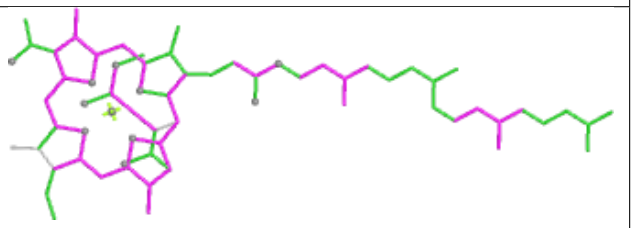
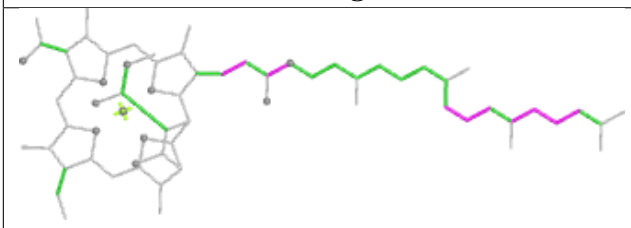
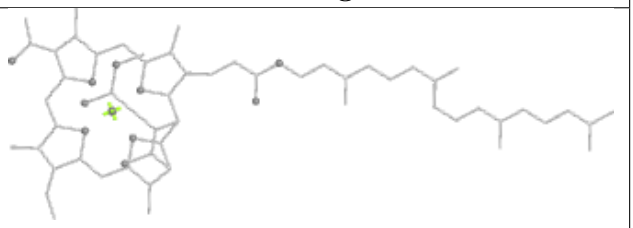
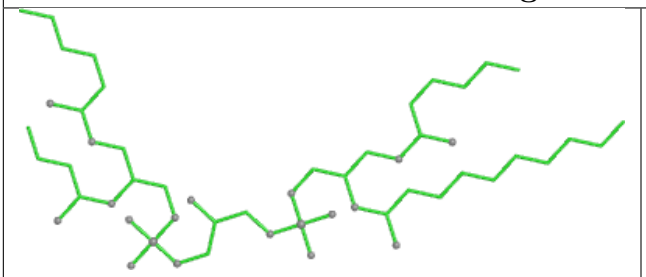
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CDL M 710



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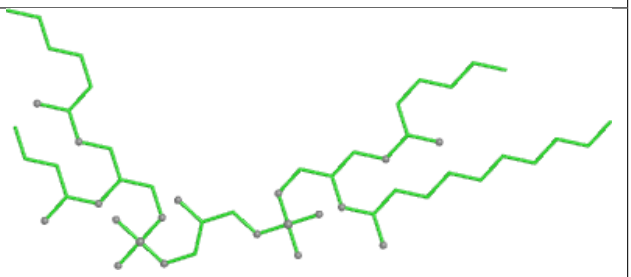

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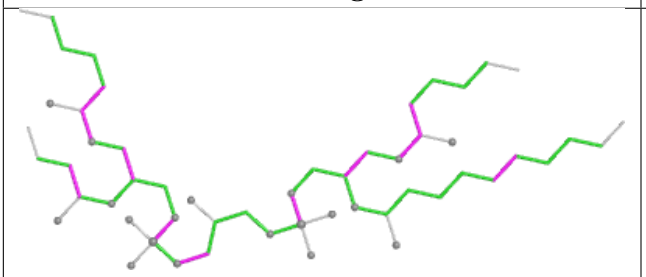

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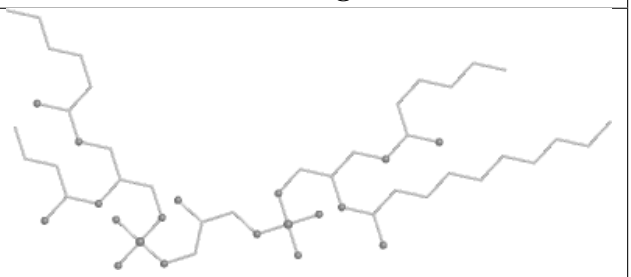
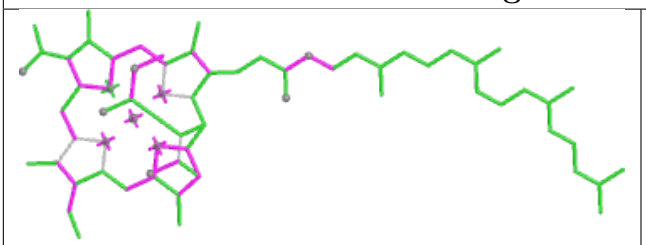


Rings

Ligand A1LZM S 103



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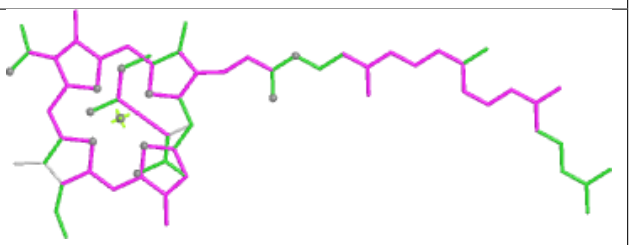

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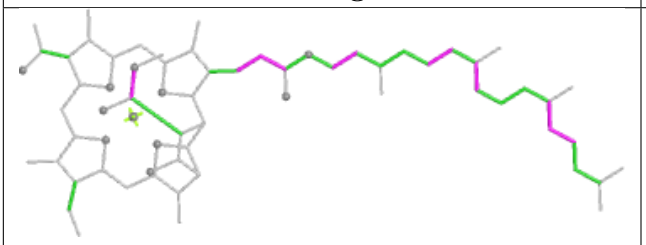

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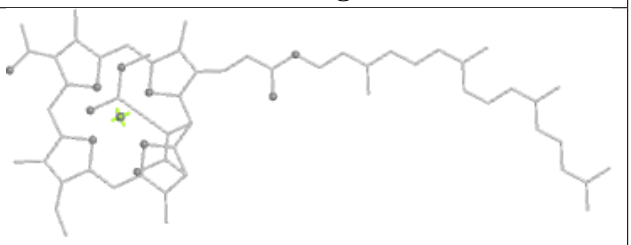
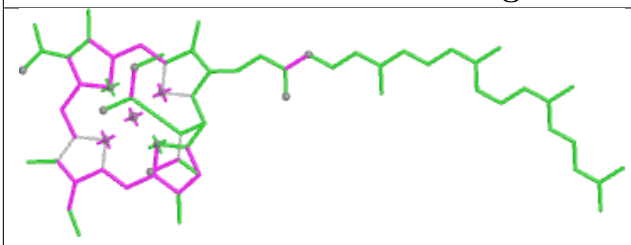


Rings

Ligand A1LZM L 301



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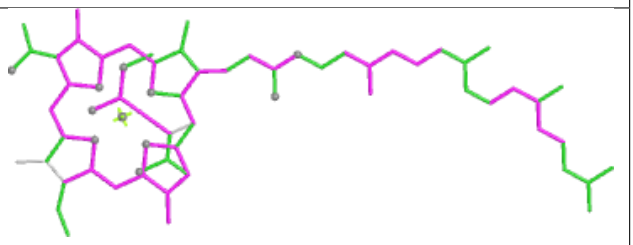

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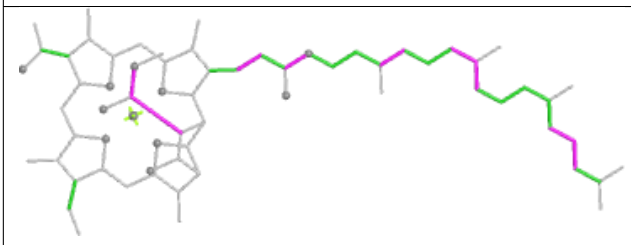

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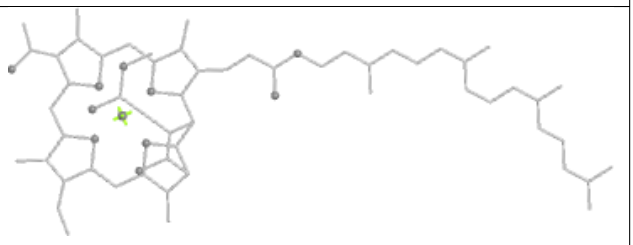
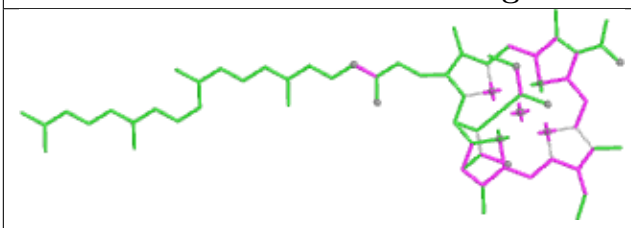


Rings

Ligand A1LZM F 102



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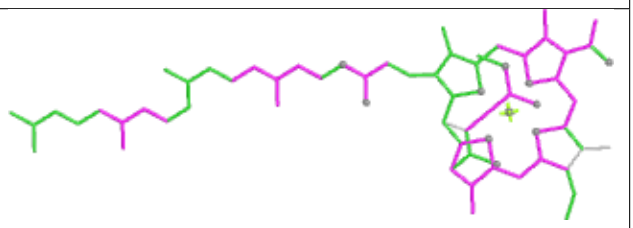

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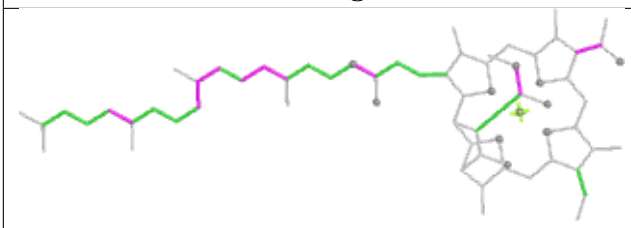

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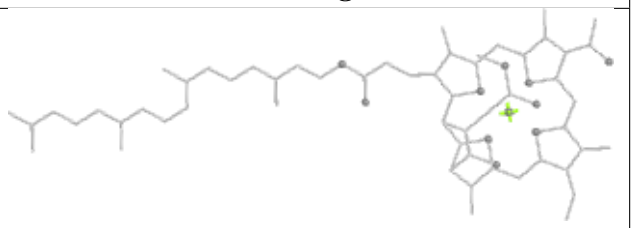
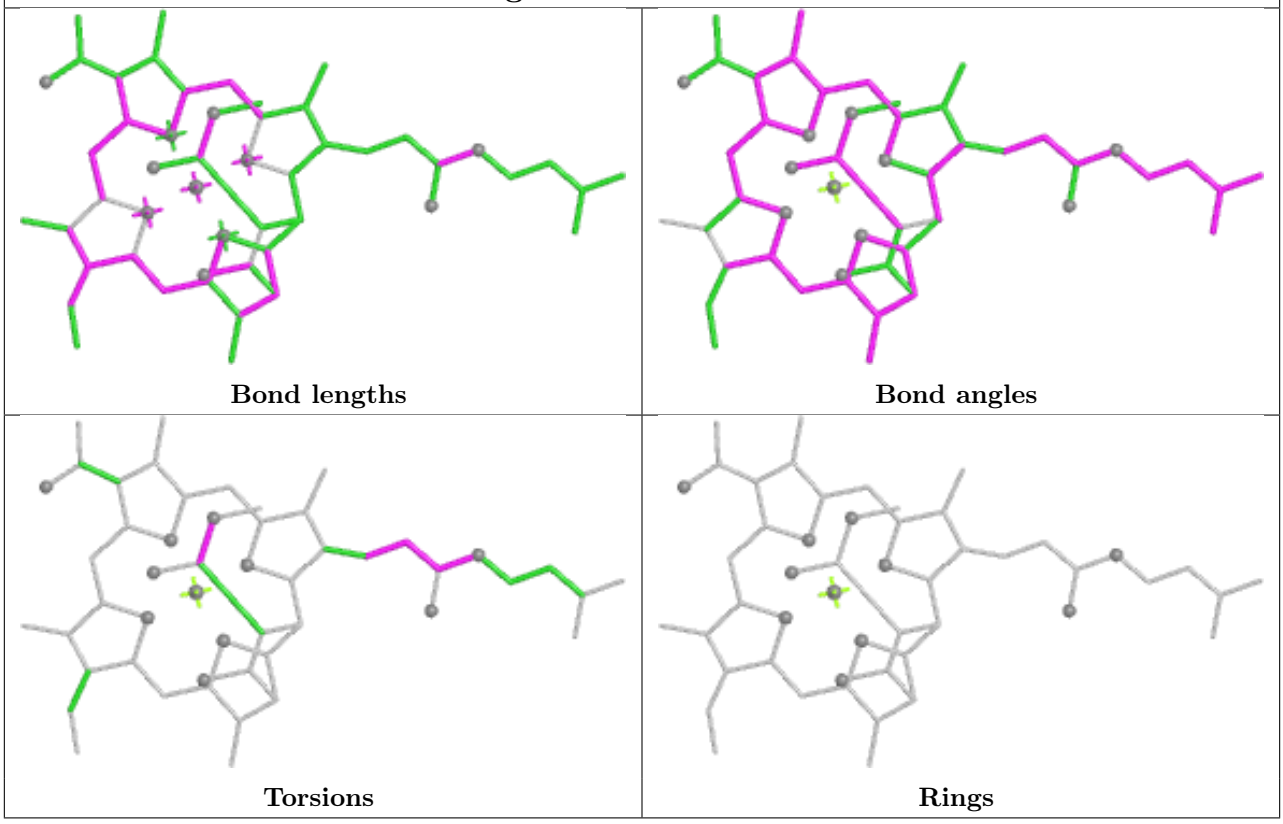


Rings

Ligand A1LZM 3 102



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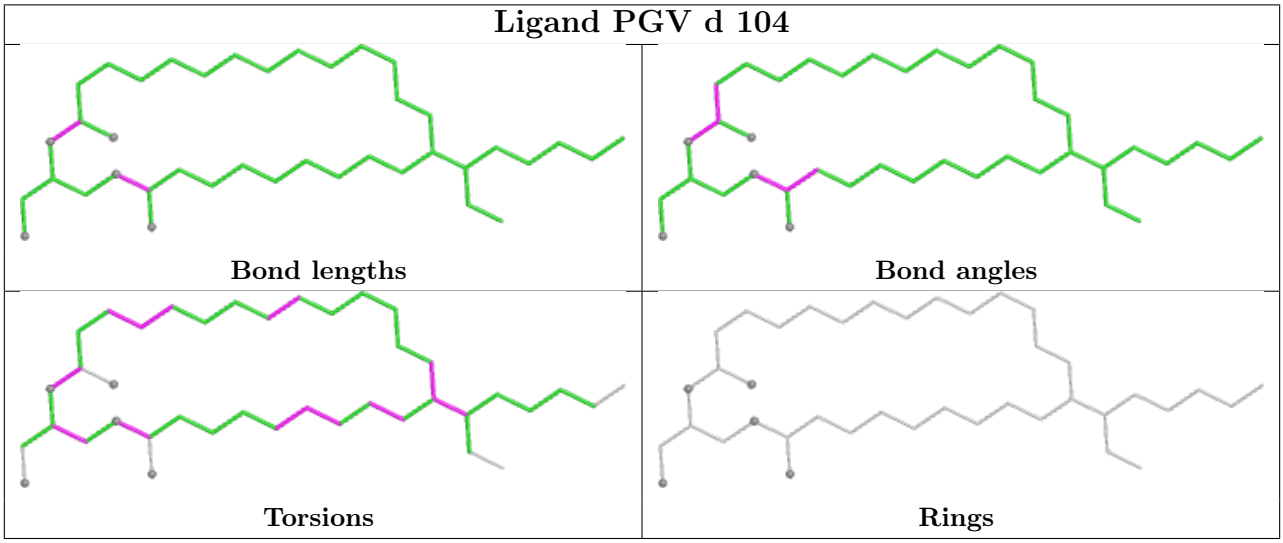

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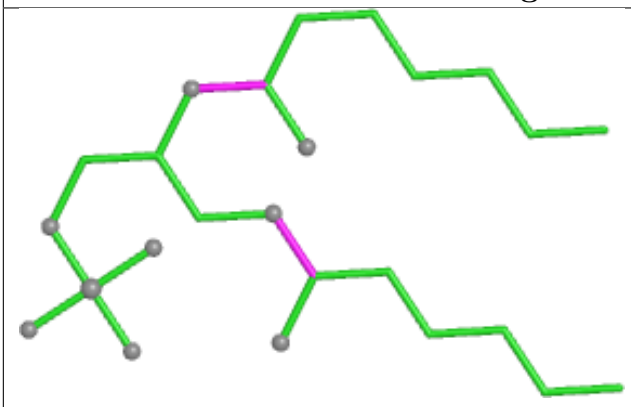

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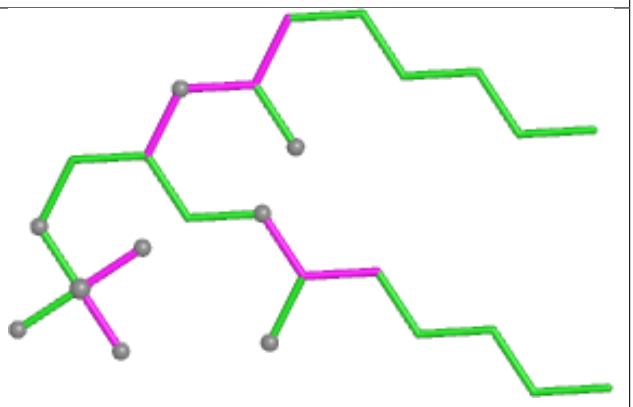

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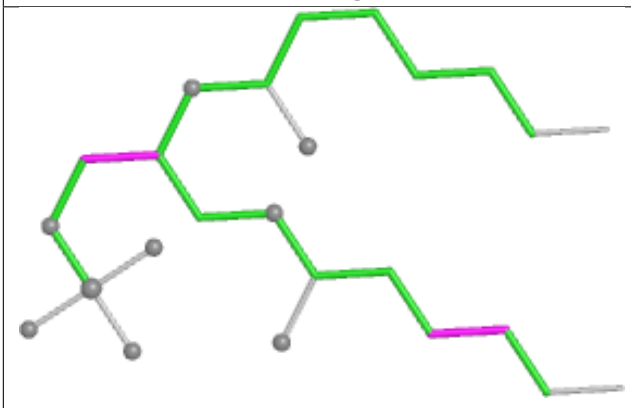

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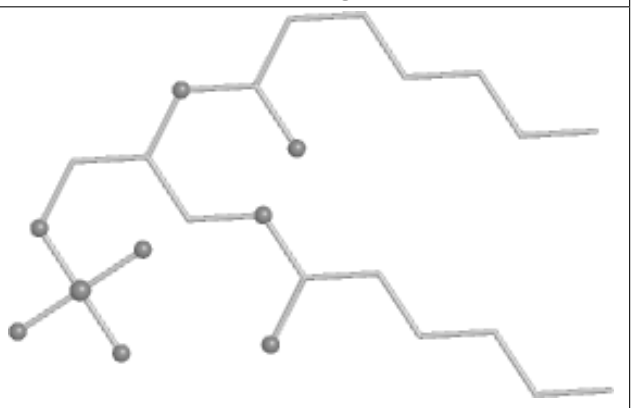
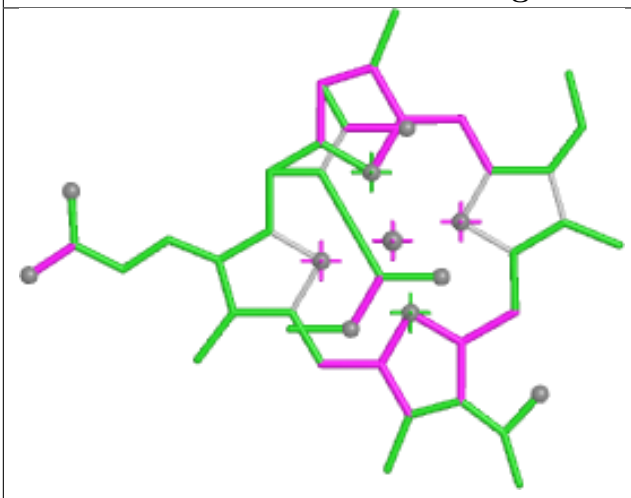


Rings

Ligand A1LZQ i 102



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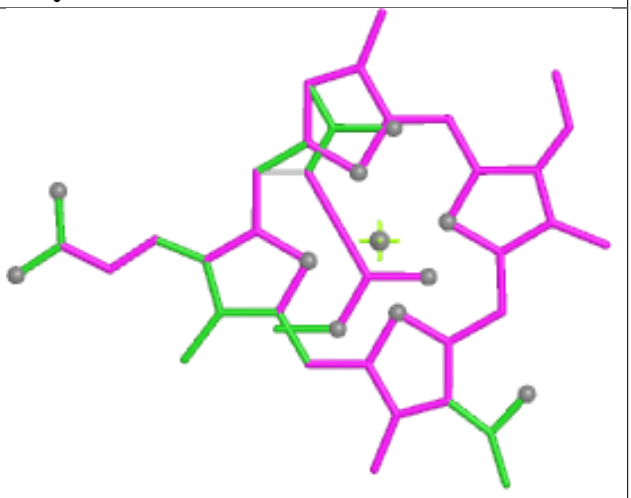

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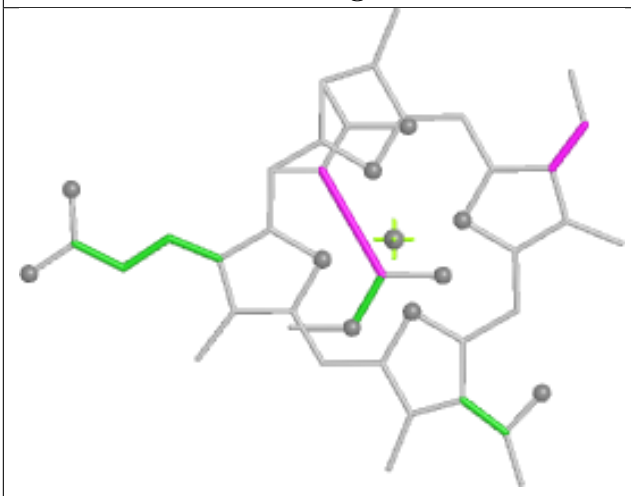

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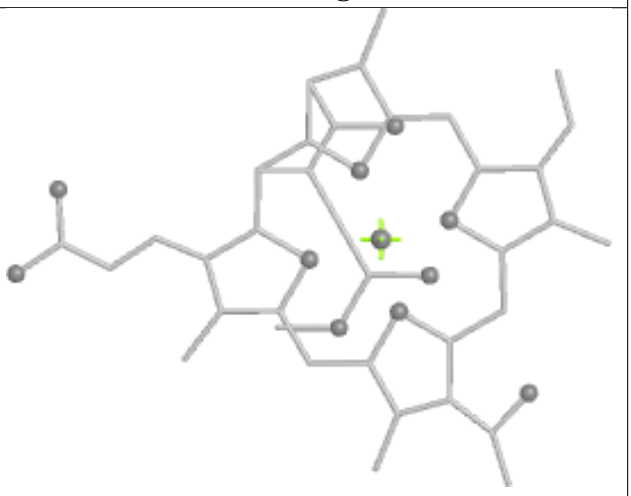
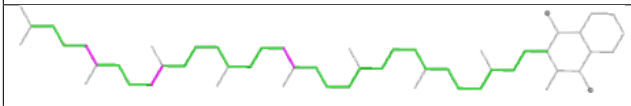


Rings

Ligand MQ8 M 705

Bond lengths

Bond angles



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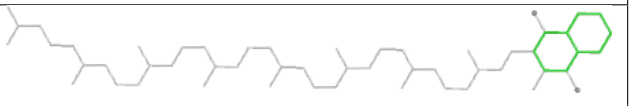
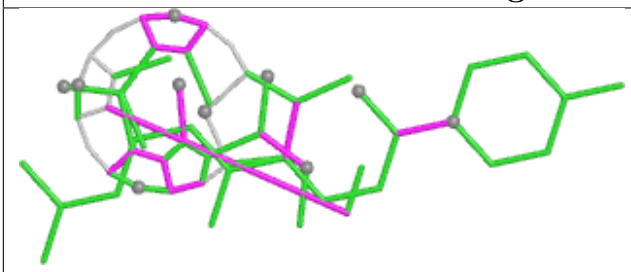


Rings

Ligand A1LZP L 303



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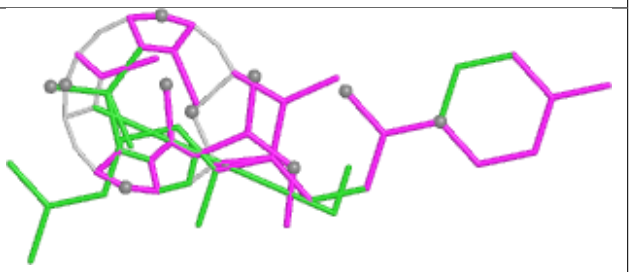
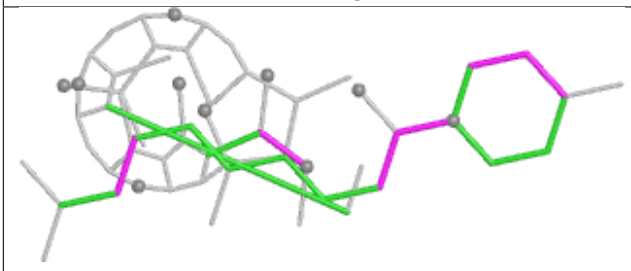


Bond angles



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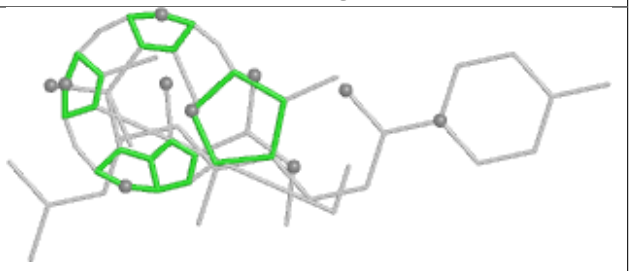
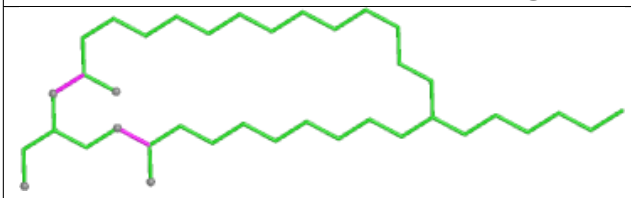


Rings

Ligand PGV p 104



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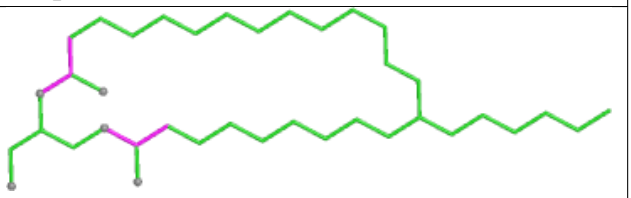
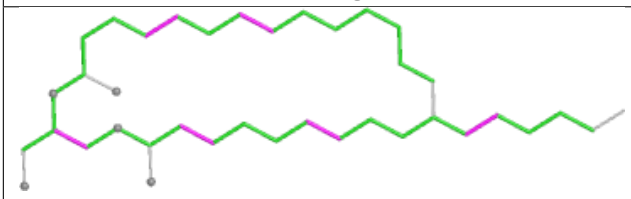


Bond angles



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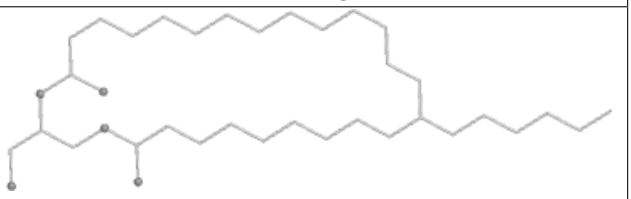
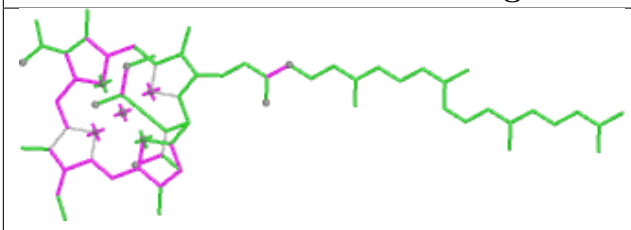


Rings

Ligand A1LZM q 102



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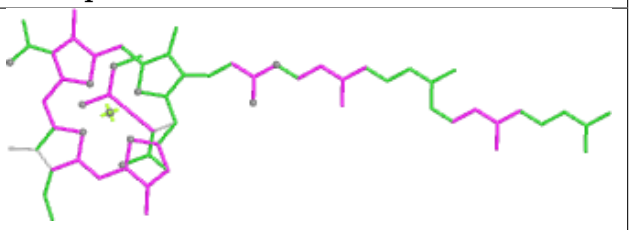

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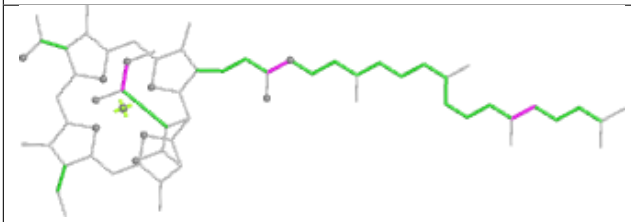

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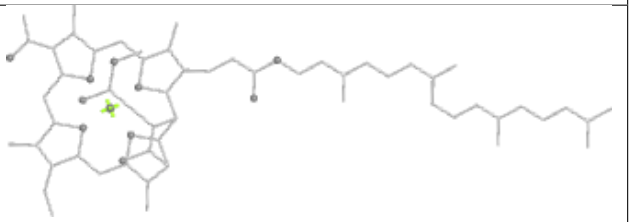
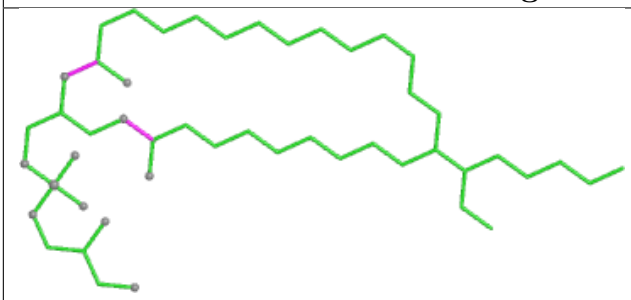


Rings

Ligand PGV Y 103



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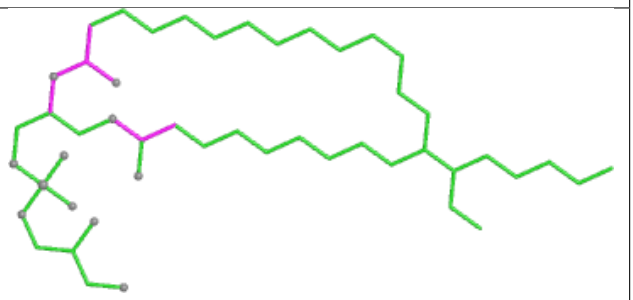
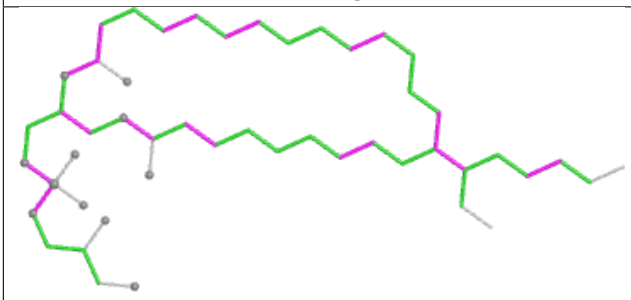


Bond angles



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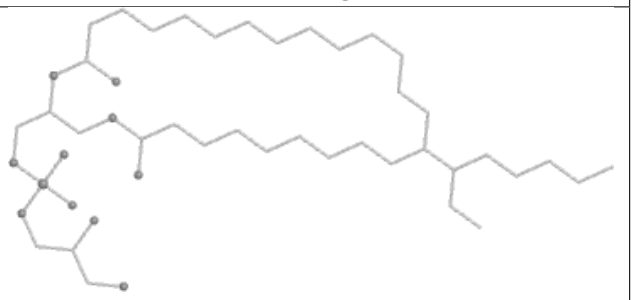
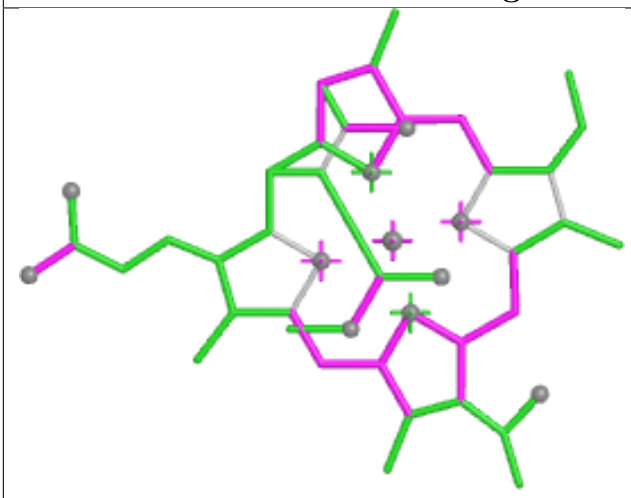


Rings

Ligand A1LZQ N 102



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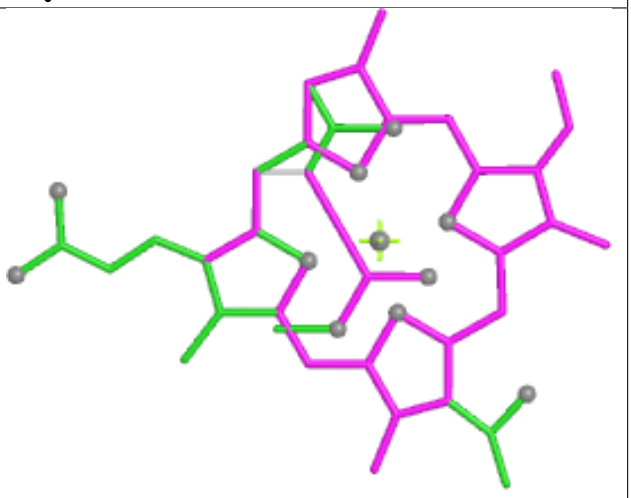
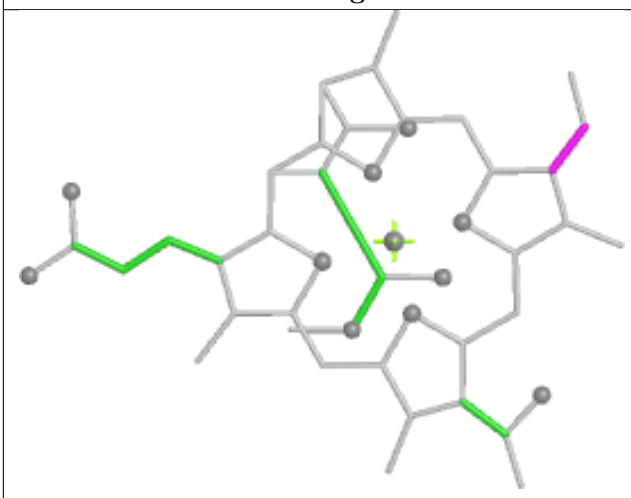


Bond angles



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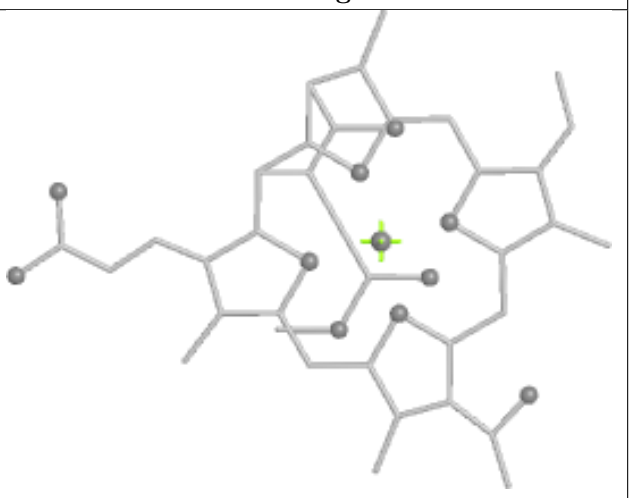
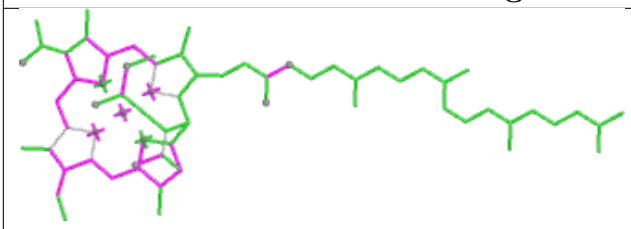
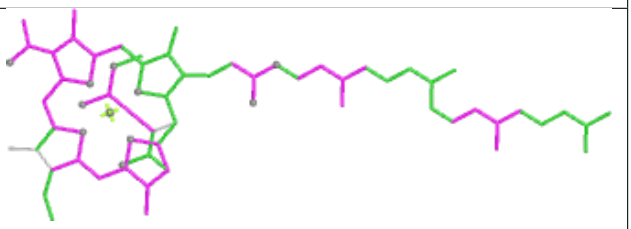


Rings

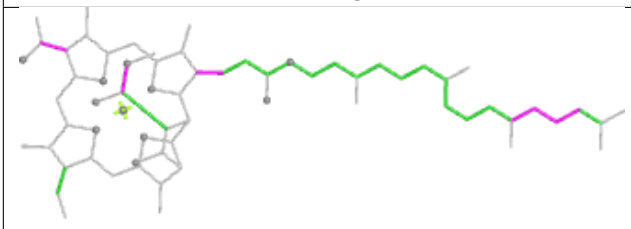
Ligand A1LZM z 102



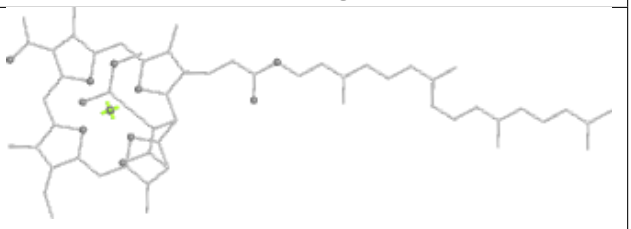
Bond lengths



Bond angles

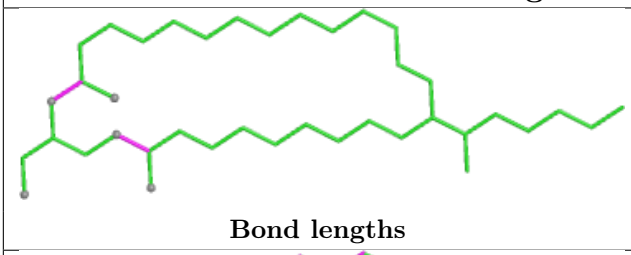


Torsions



Rings

Ligand PGV 5 101



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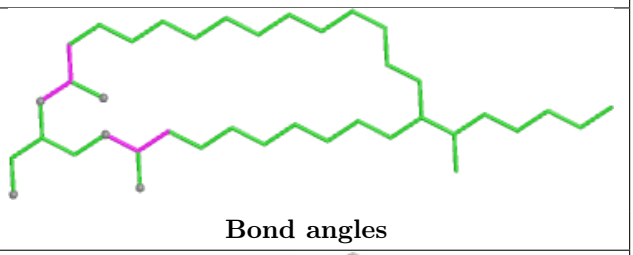

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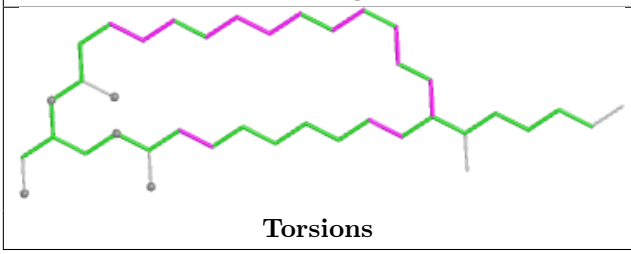

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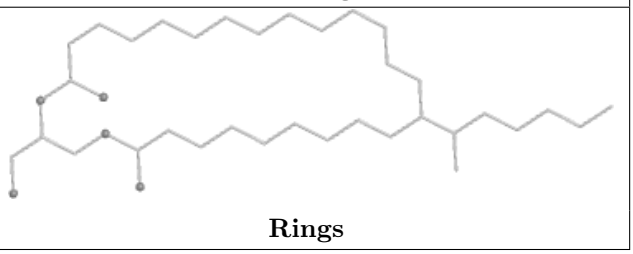
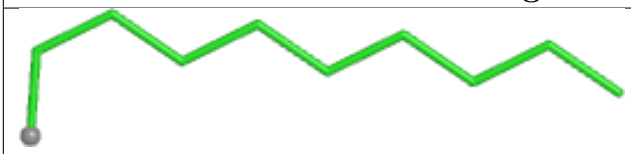


Rings

Ligand LHG C 406



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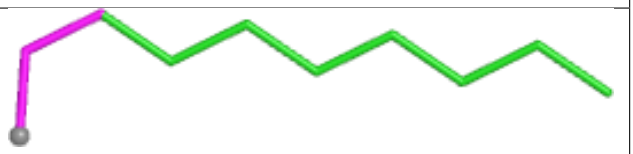

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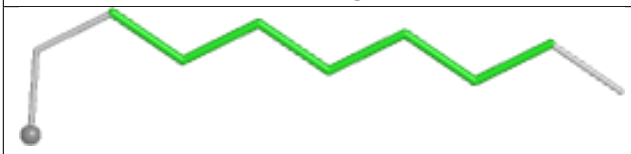

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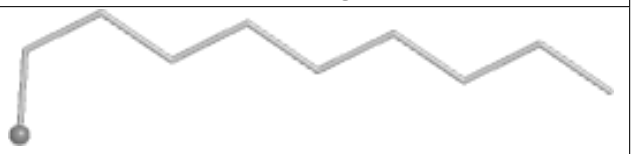
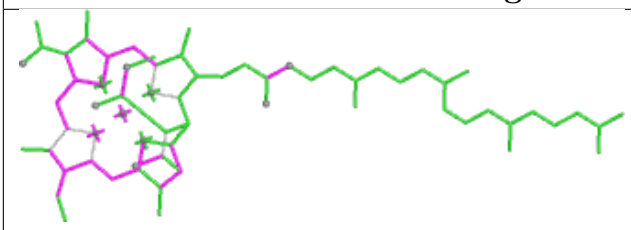


Rings

Ligand A1LZM 7 101



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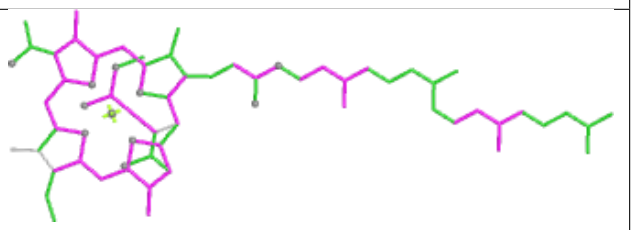
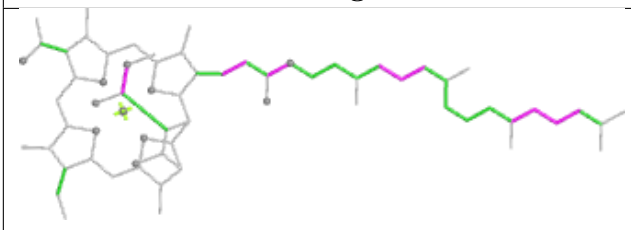


Bond angles



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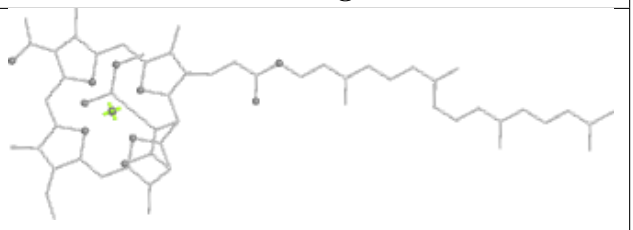
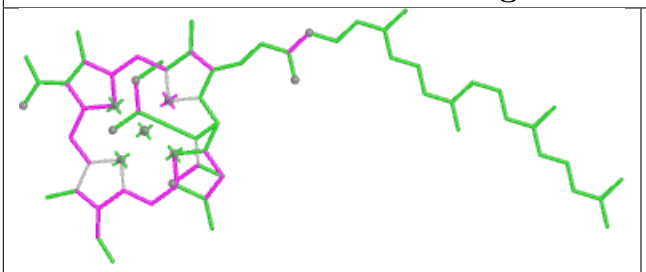


Rings

Ligand A1LZM Y 102



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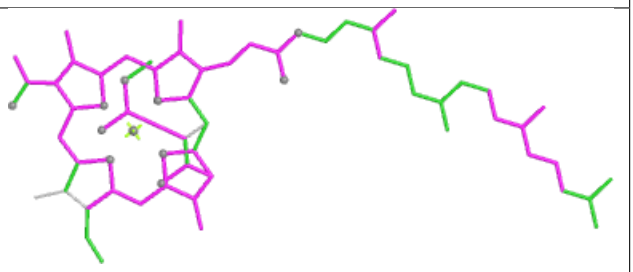

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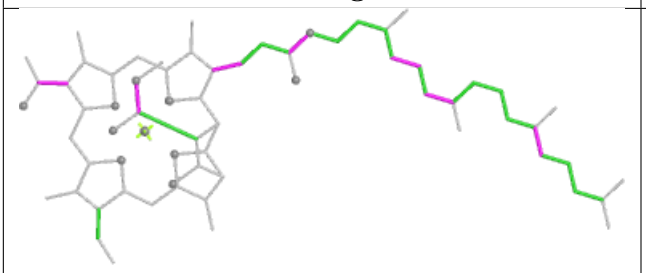

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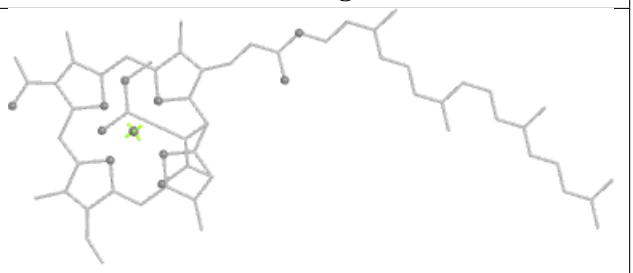
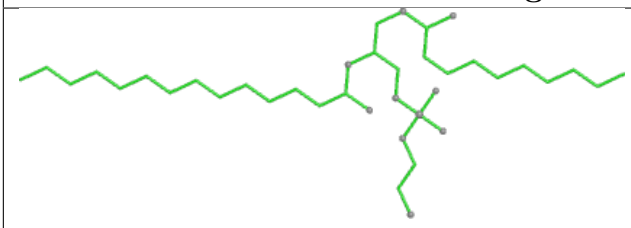


Rings

Ligand PEF K 106



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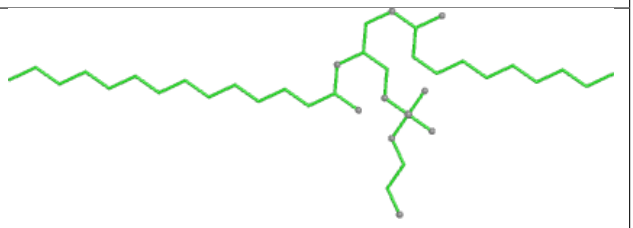

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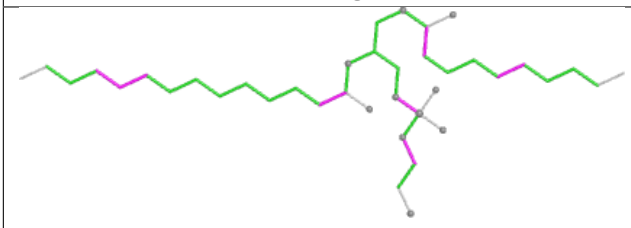

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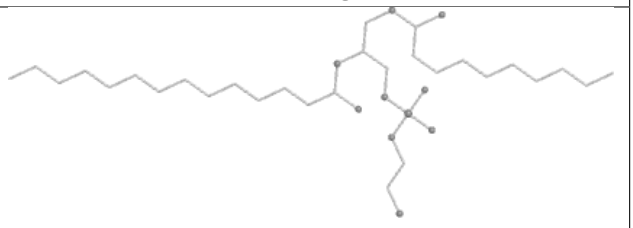
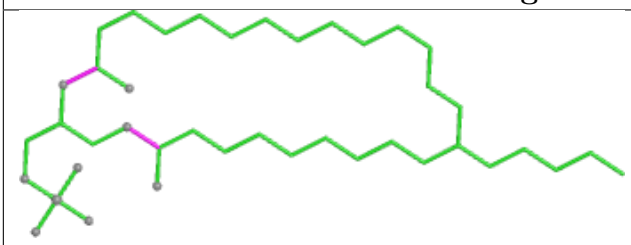


Rings

Ligand PGV H 302



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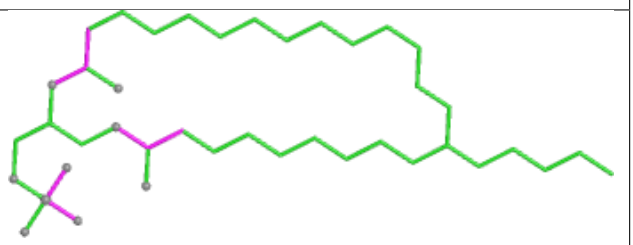

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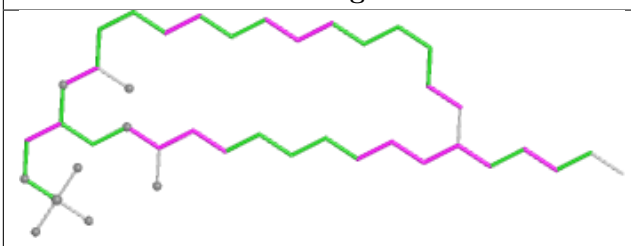

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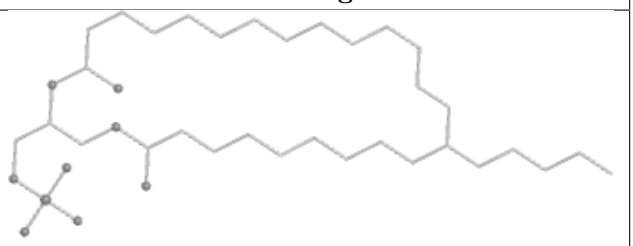
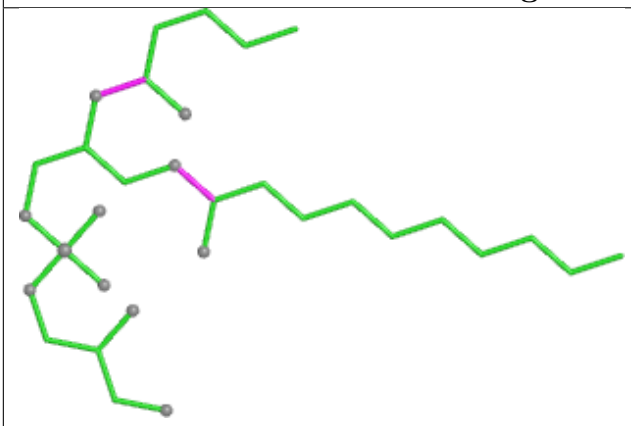


Rings

Ligand PGV H 301



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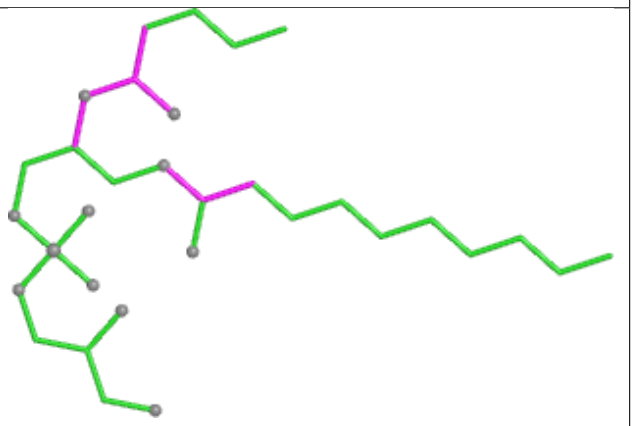

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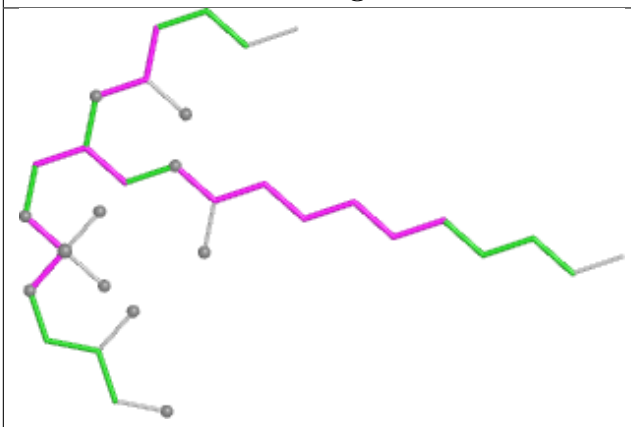

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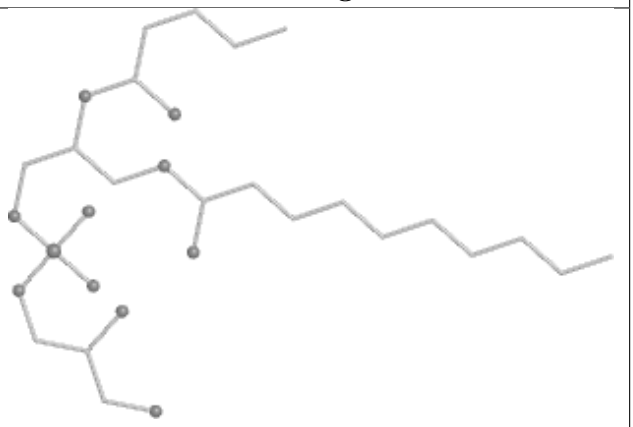
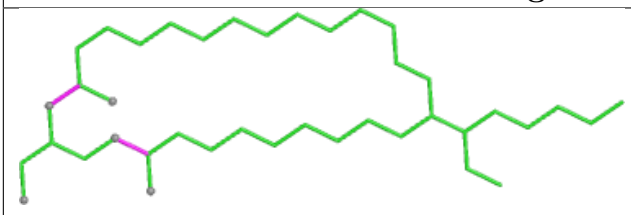


Rings

Ligand PGV s 104



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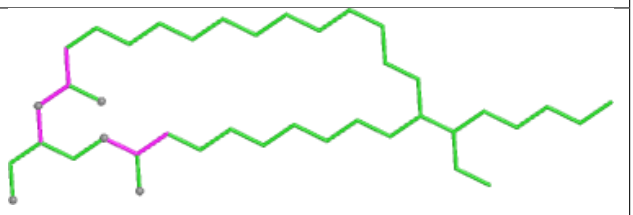

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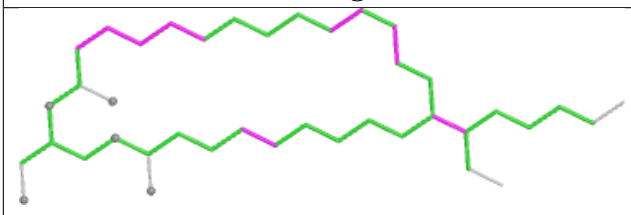

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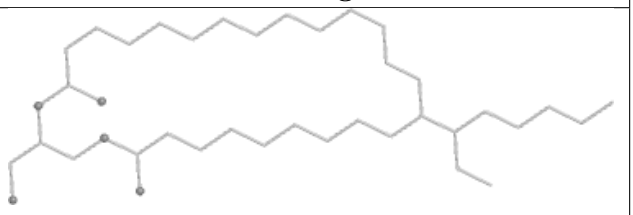
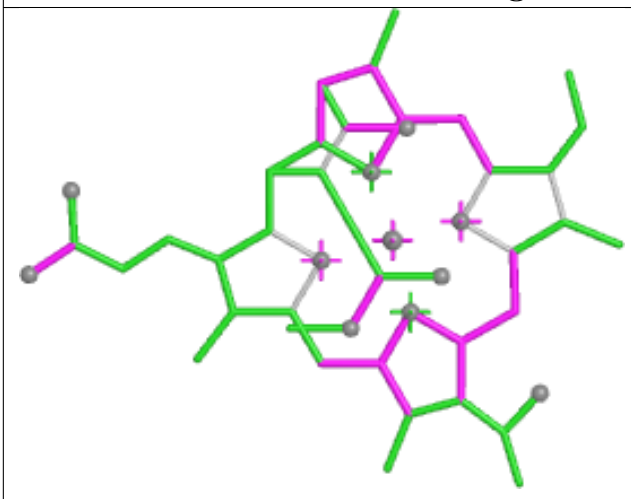


Rings

Ligand A1LZQ o 102



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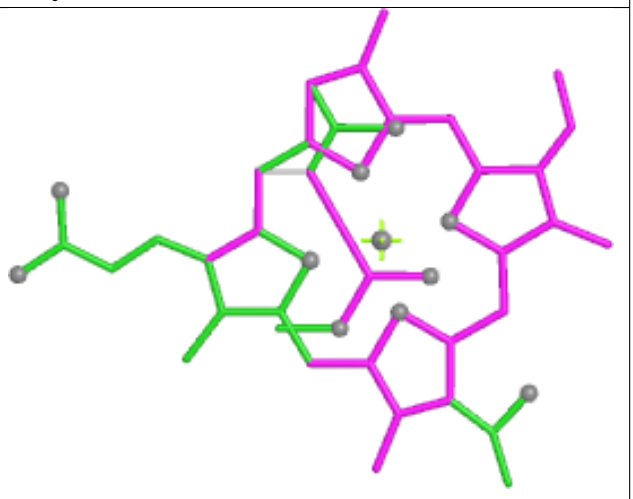

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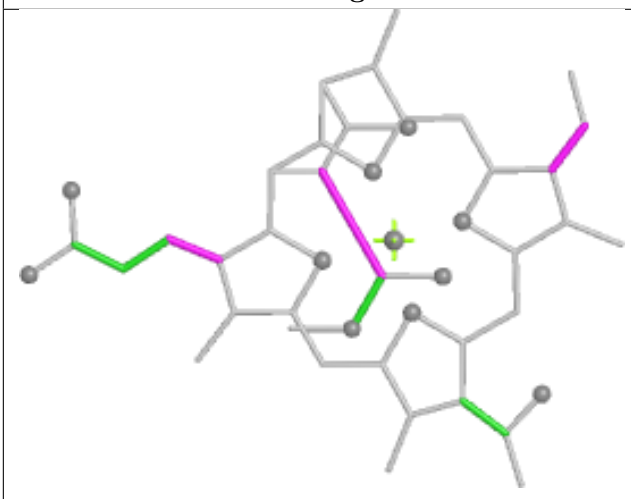

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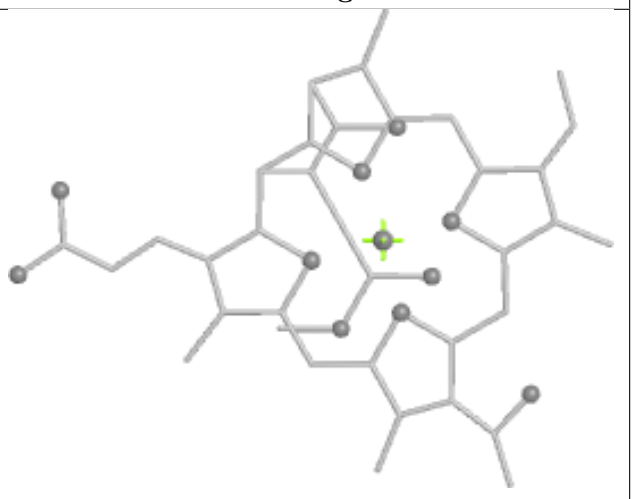
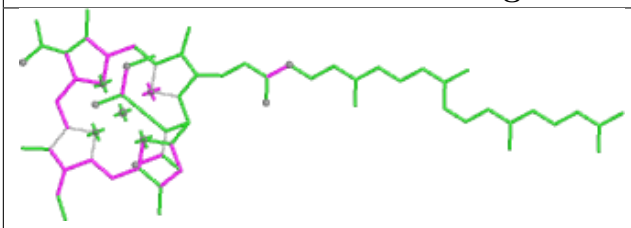


Rings

Ligand A1LZM n 101



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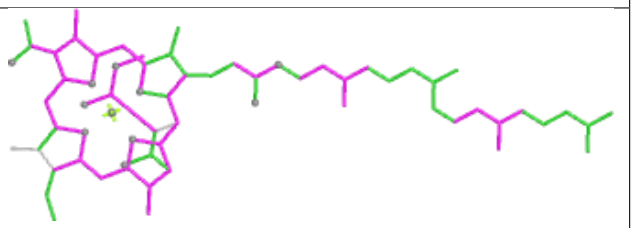

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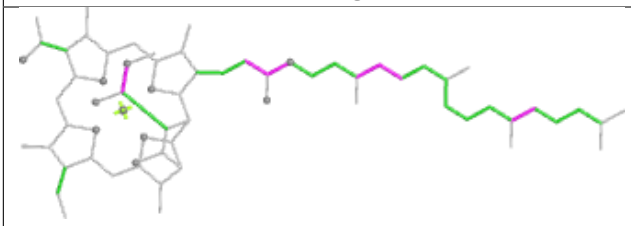

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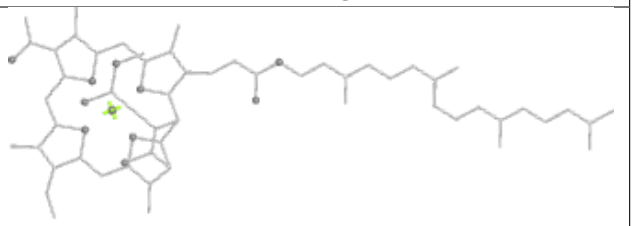
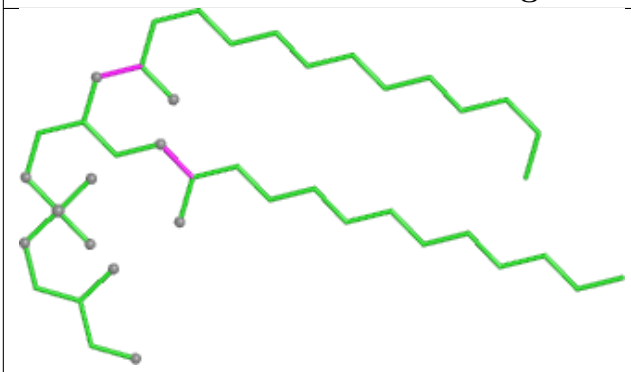


Rings

Ligand PGV H 306



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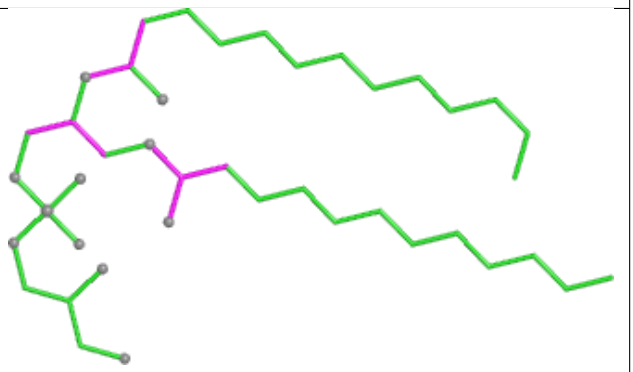
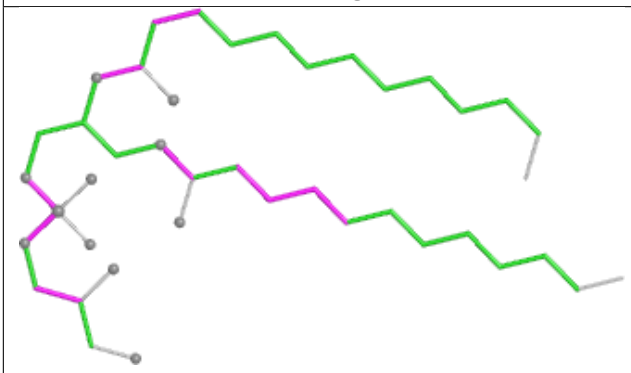


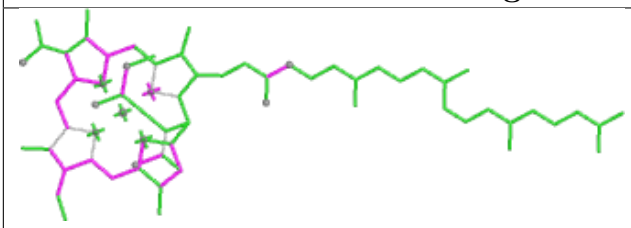
Bond angles



Torsions

Rings

Ligand A1LZM h 101



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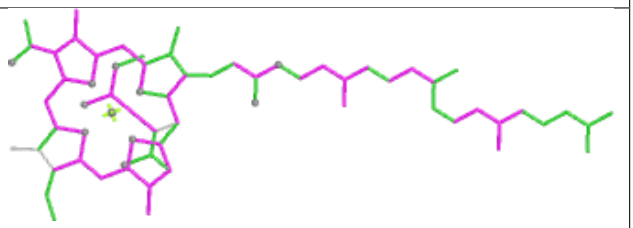

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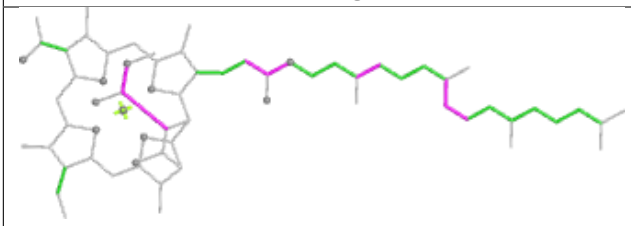

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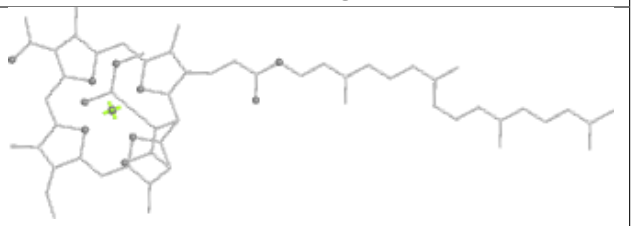
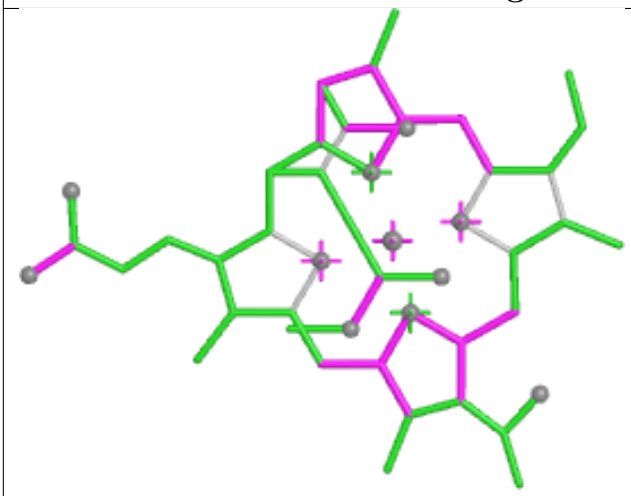


Rings

Ligand A1LZQ u 102



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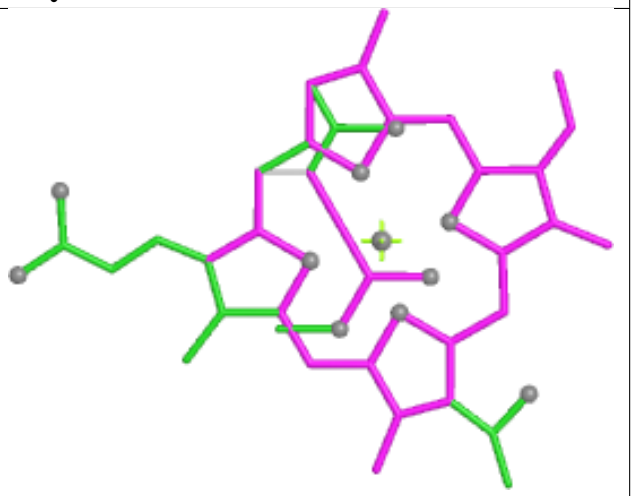
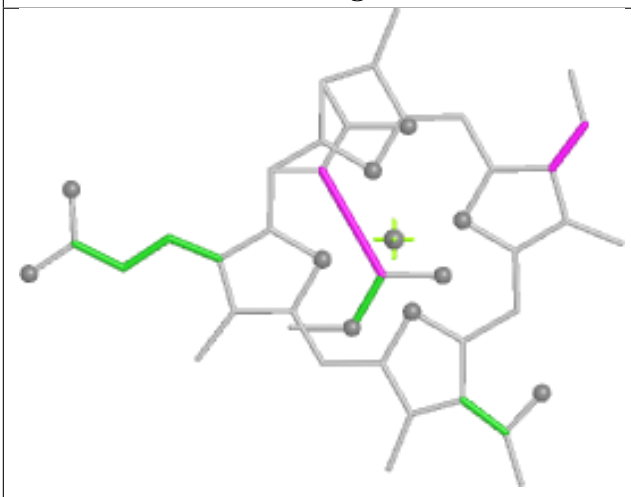


Bond angles



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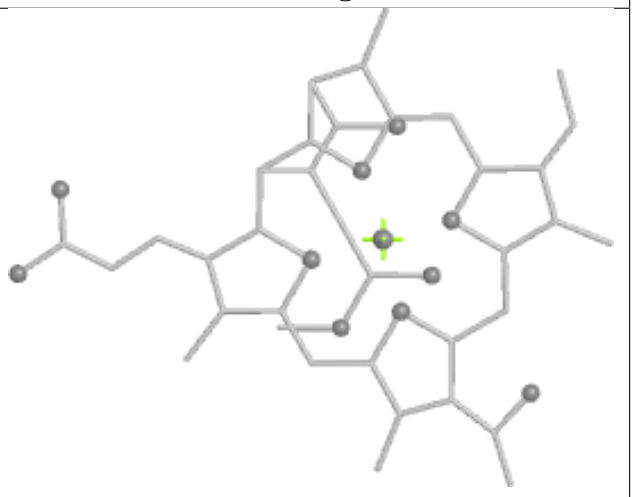
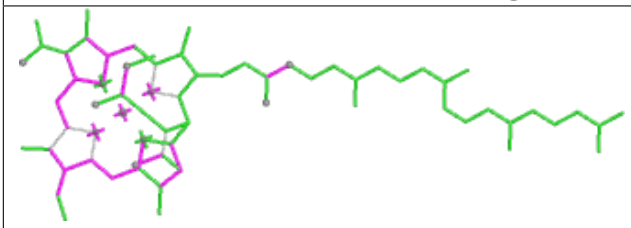


Rings

Ligand A1LZM e 101



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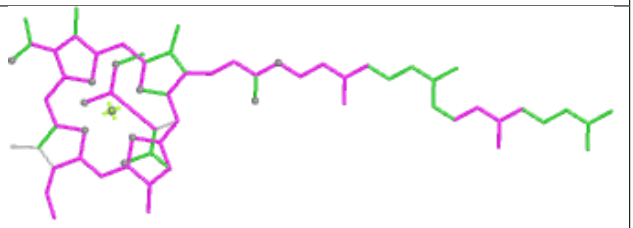
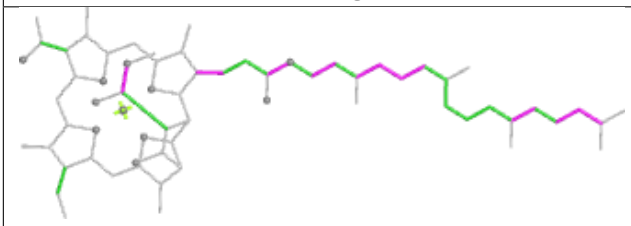
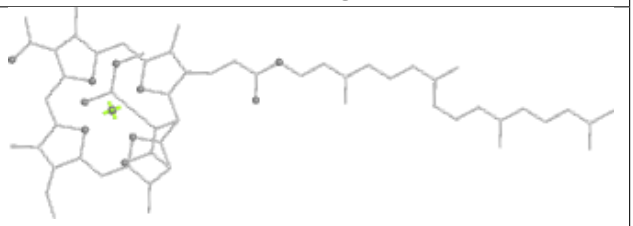


Bond angles

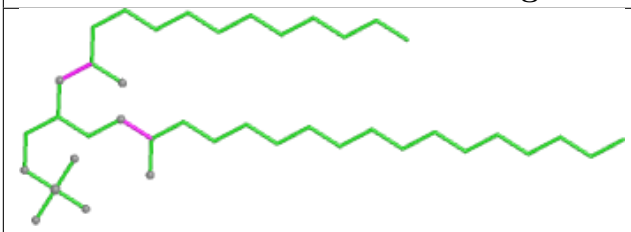


Torsions



Rings

Ligand PGV Y 104



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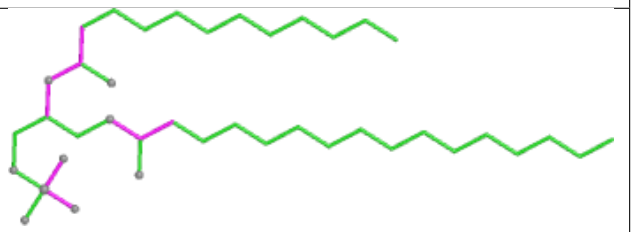

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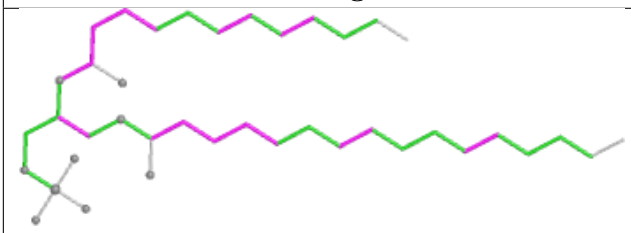

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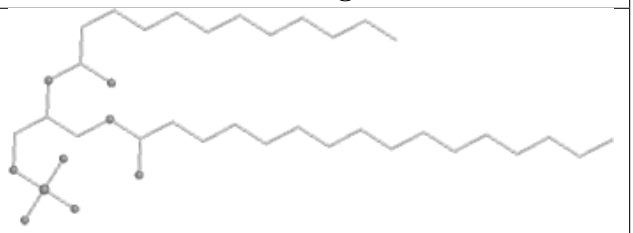
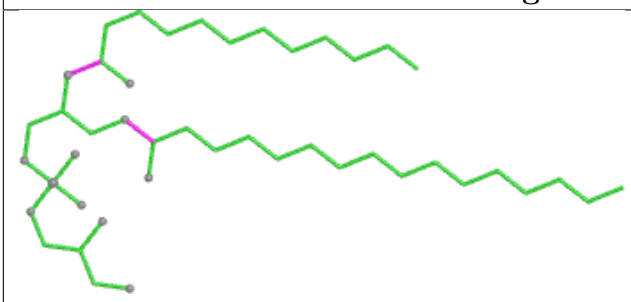


Rings

Ligand PGV P 105



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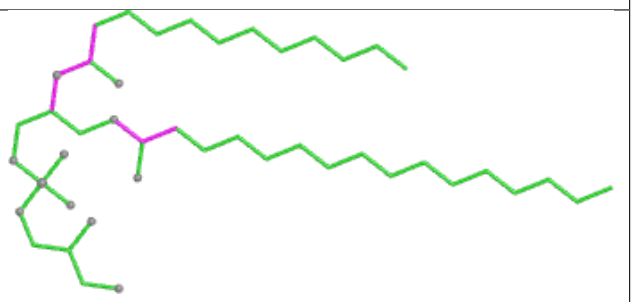

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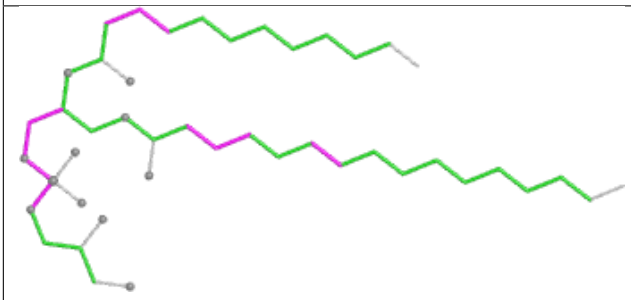
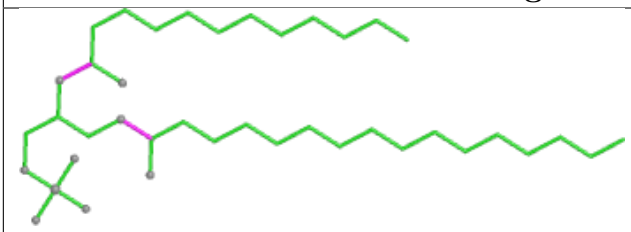


Torsions

Rings

Ligand PGV S 105



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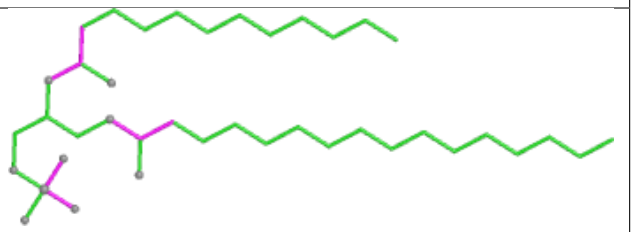

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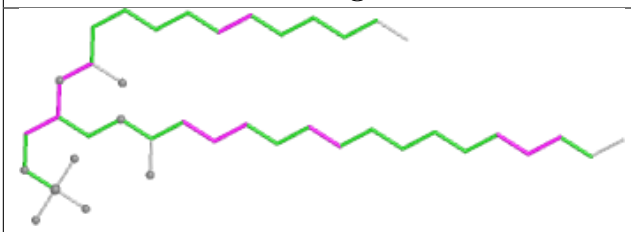

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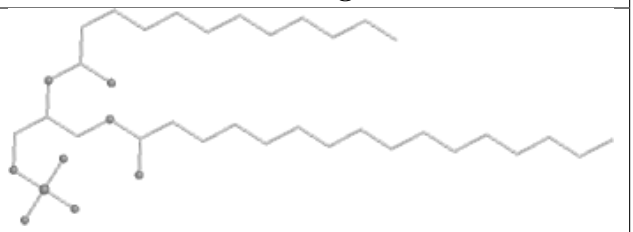
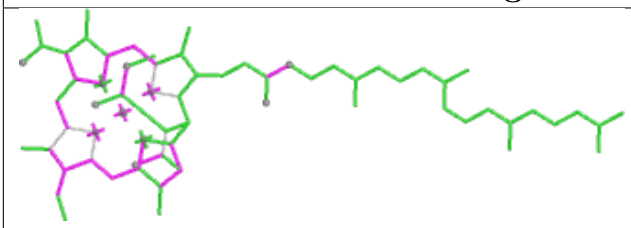


Rings

Ligand A1LZM 6 102



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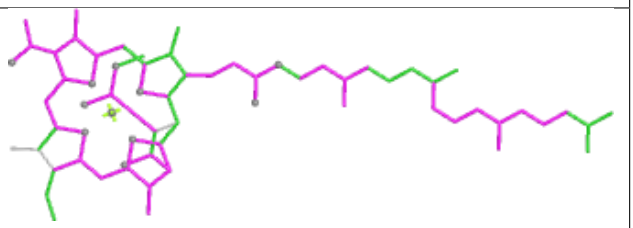

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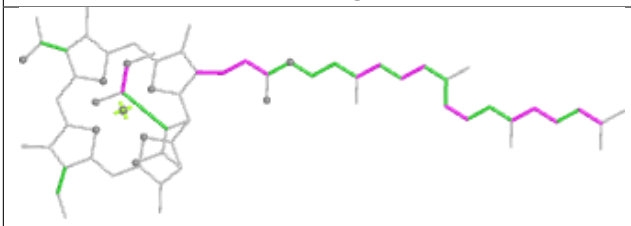

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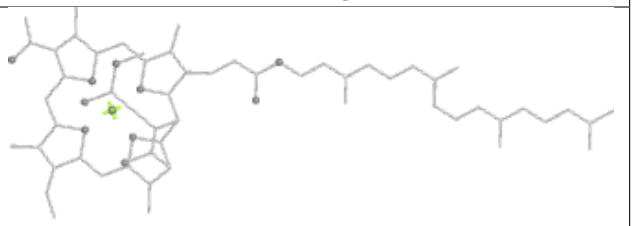
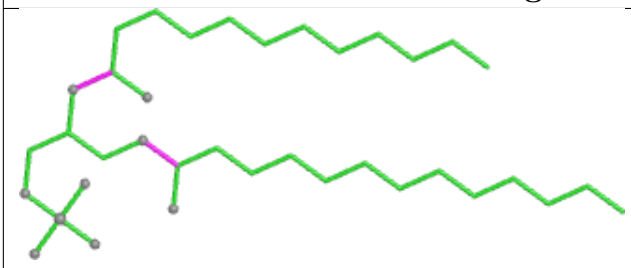


Rings

Ligand PGV b 105



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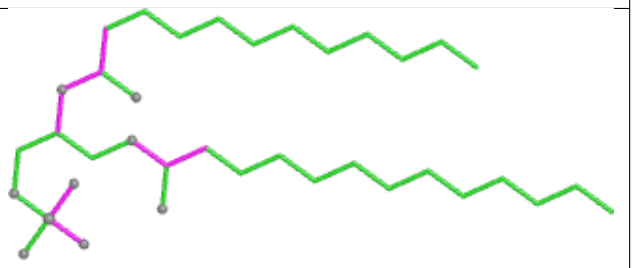

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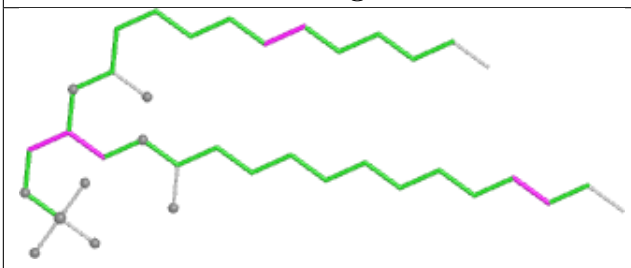

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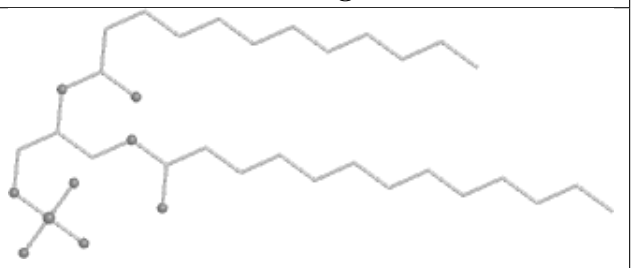
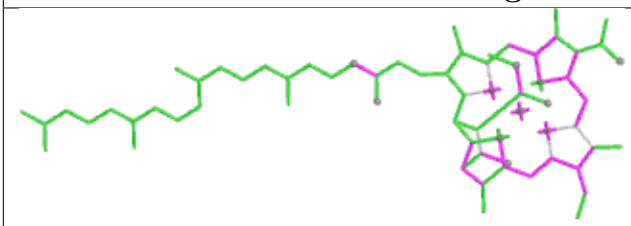


Rings

Ligand A1LZM 6 101



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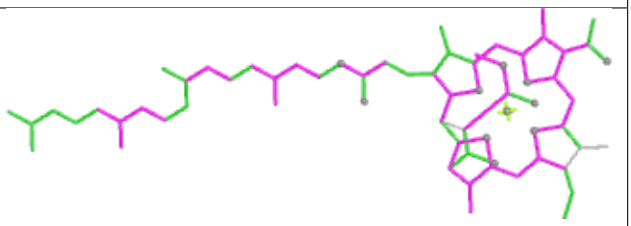

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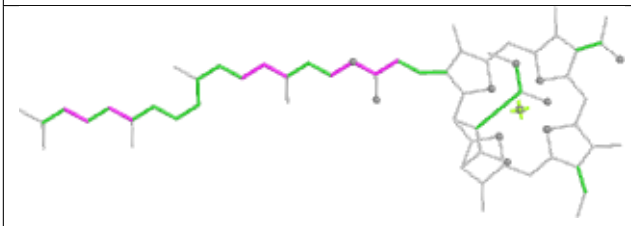

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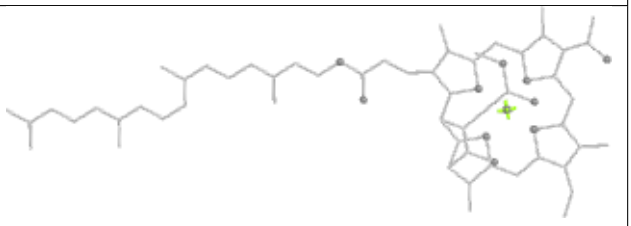
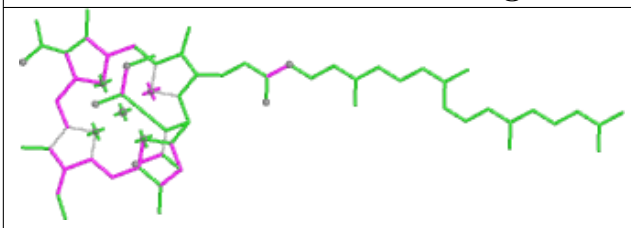


Rings

Ligand A1LZM b 101



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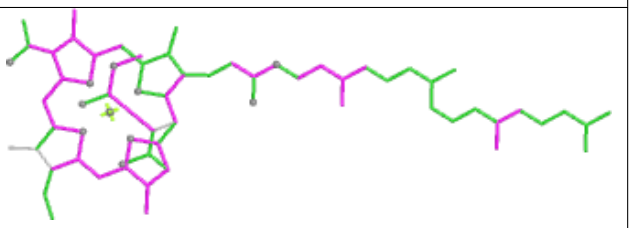

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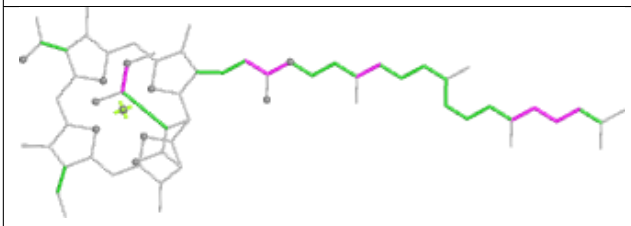

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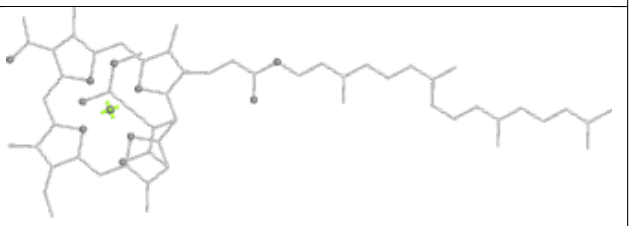
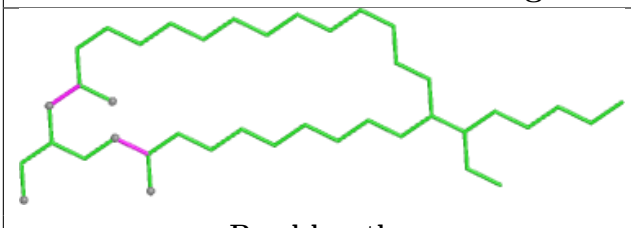


Rings

Ligand PGV v 104



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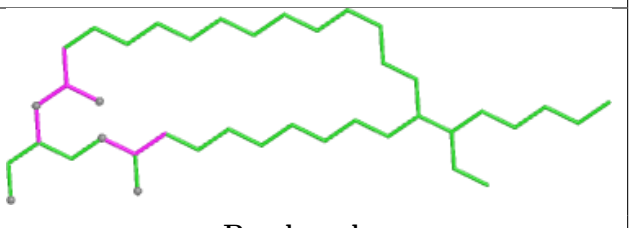

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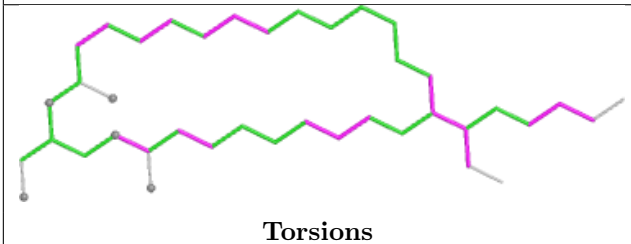

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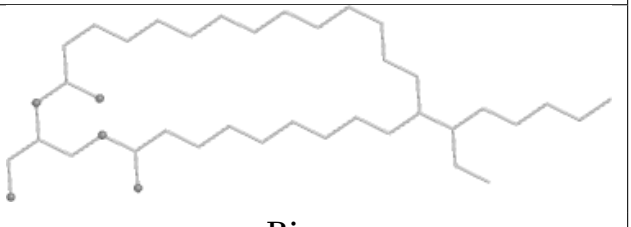
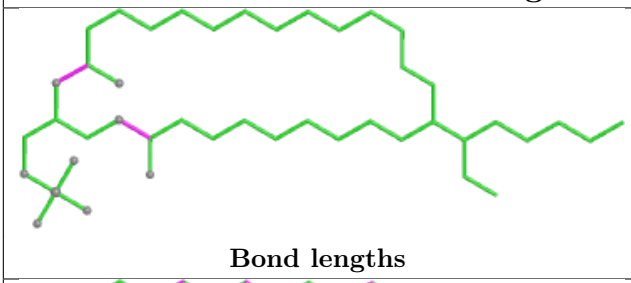


Rings

Ligand PGV k 104



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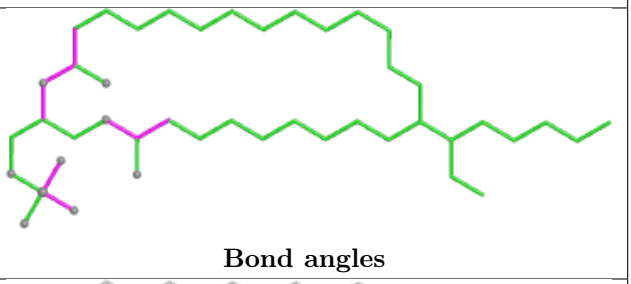

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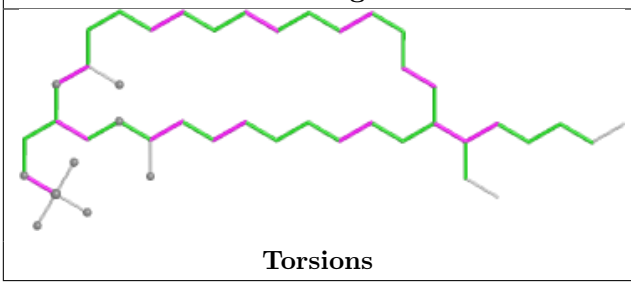

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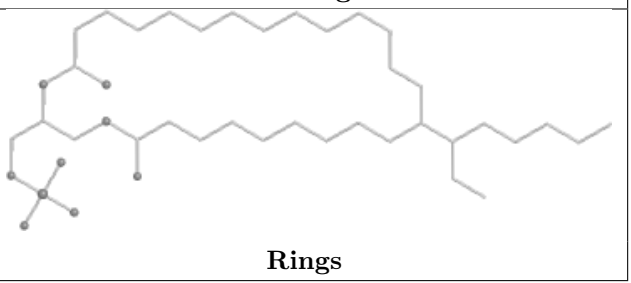
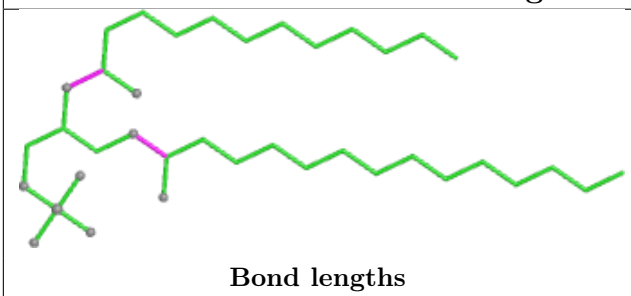


Rings

Ligand PGV 9 103



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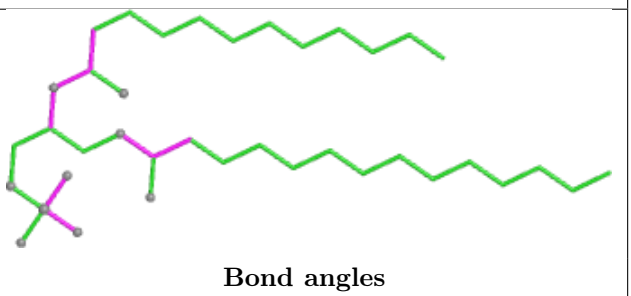

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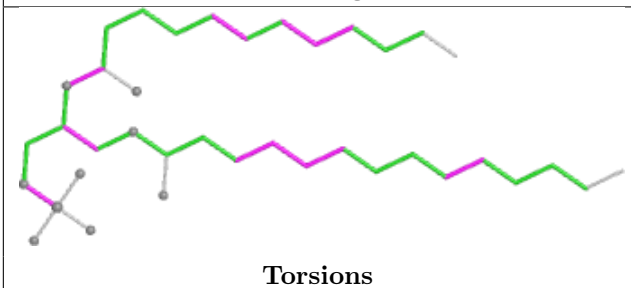

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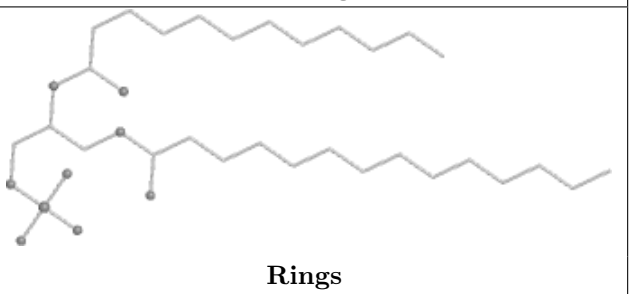
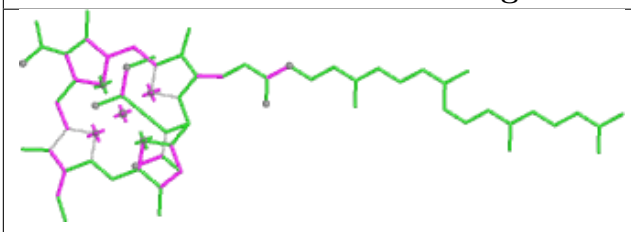


Rings

Ligand A1LZM P 102



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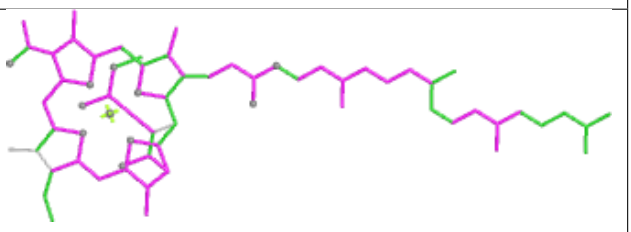
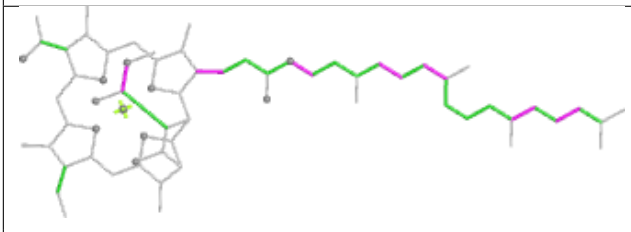


Bond angles



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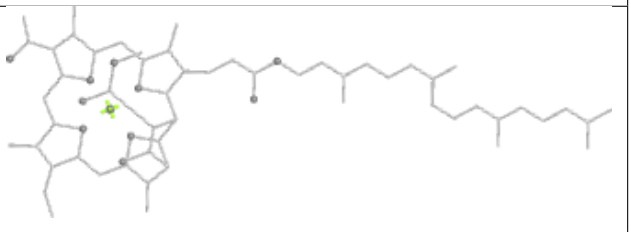
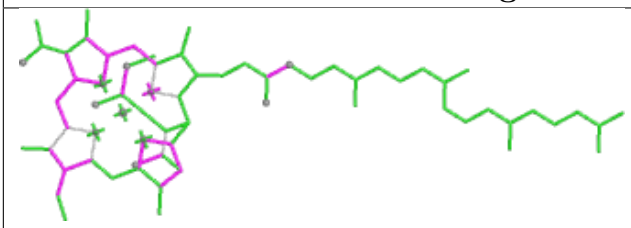


Rings

Ligand A1LZM K 102



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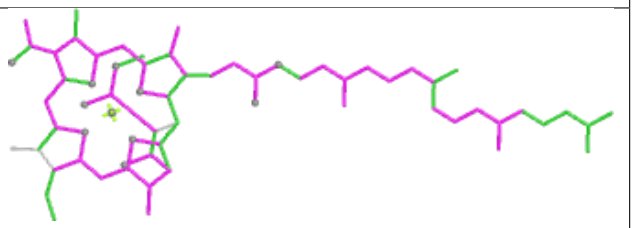
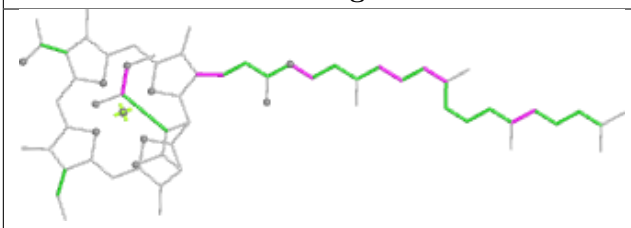


Bond angles



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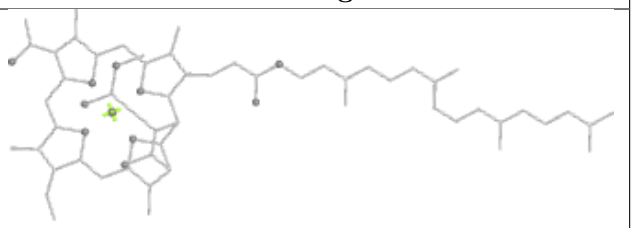
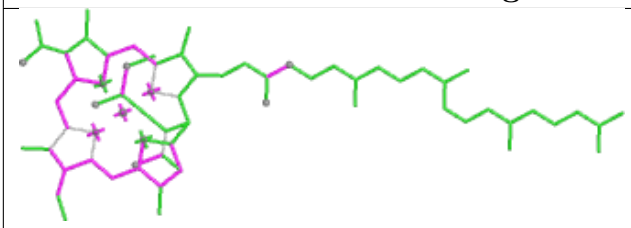


Rings

Ligand A1LZM L 302



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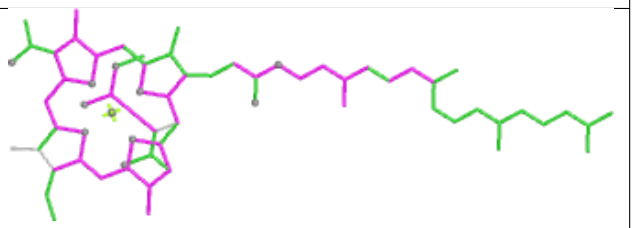
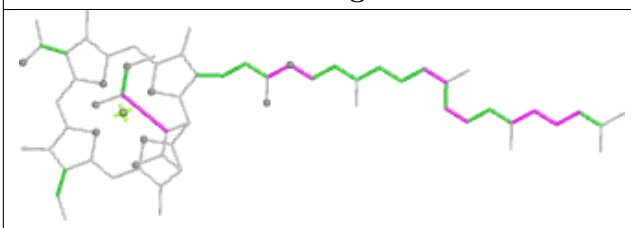
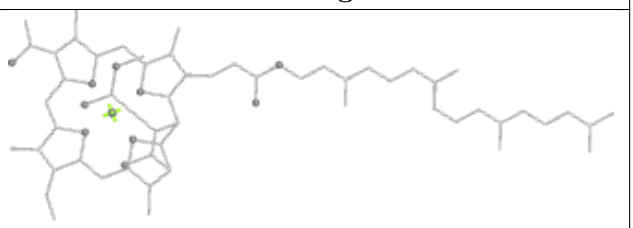


Bond angles

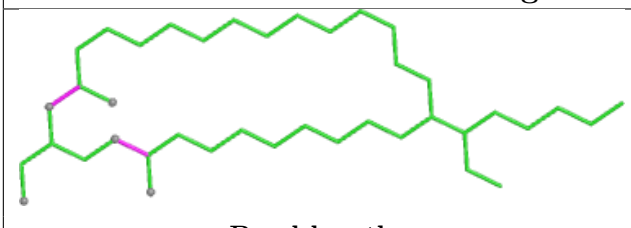


Torsions

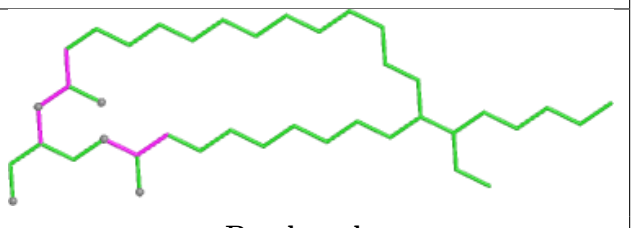


Rings

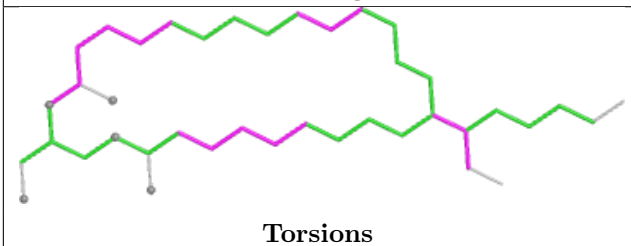
Ligand PGV O 104



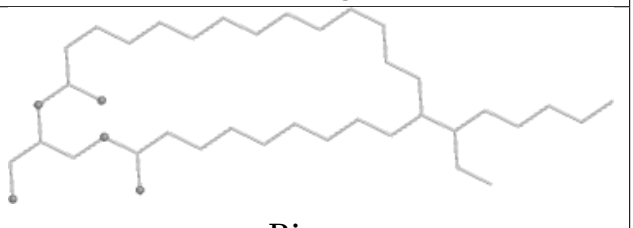
Bond lengths



Bond angles

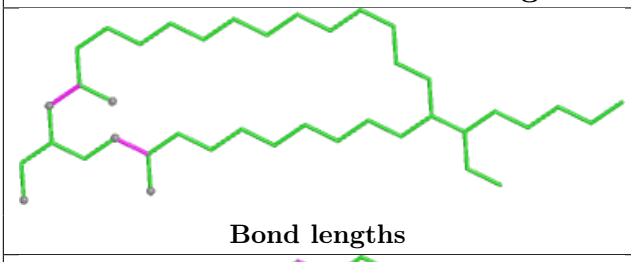


Torsions



Rings

Ligand PGV X 104



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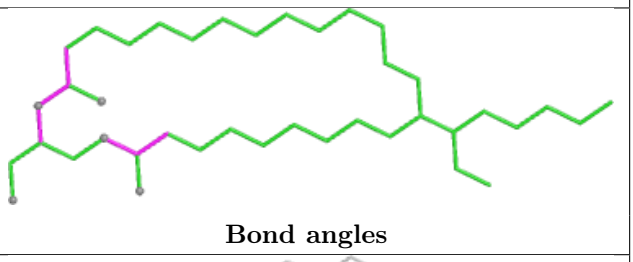
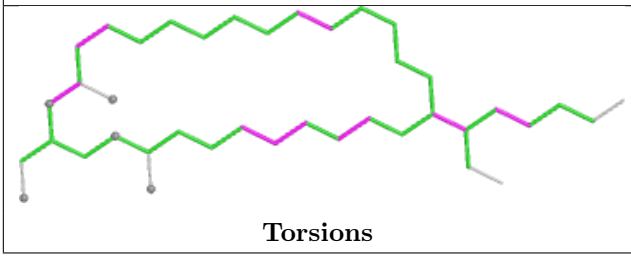


Bond angles



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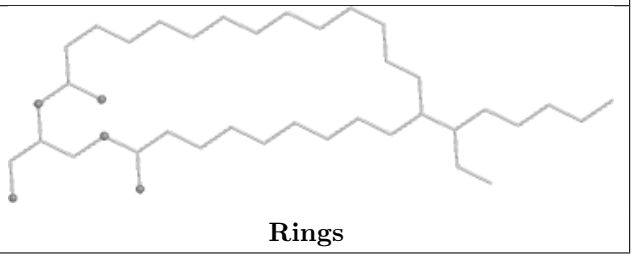
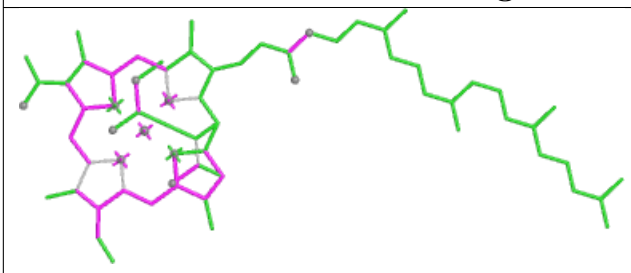


Rings

Ligand A1LZM M 702



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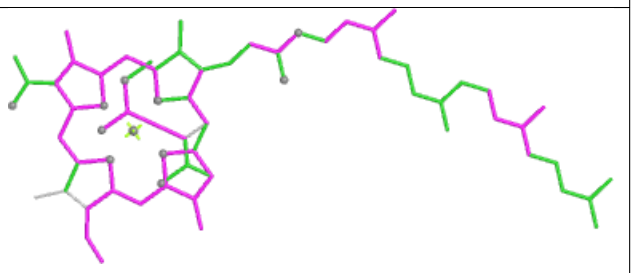

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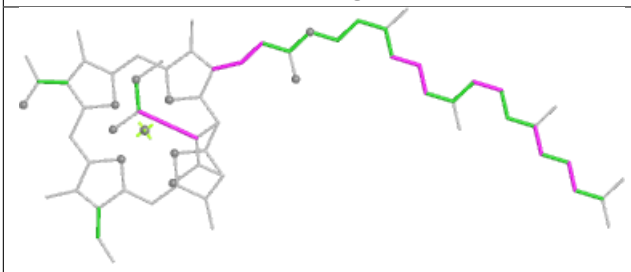
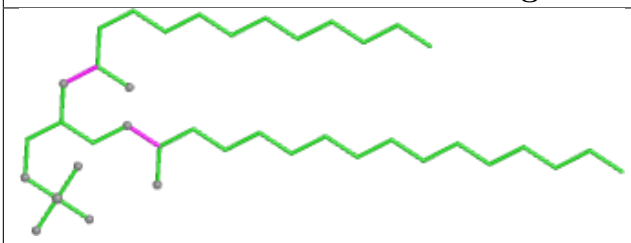


Torsions

Rings

Ligand PGV V 103



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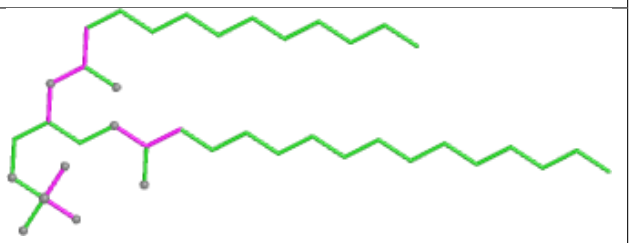
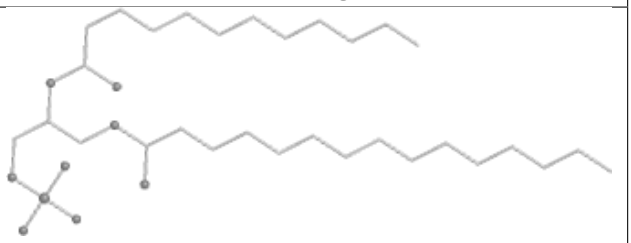


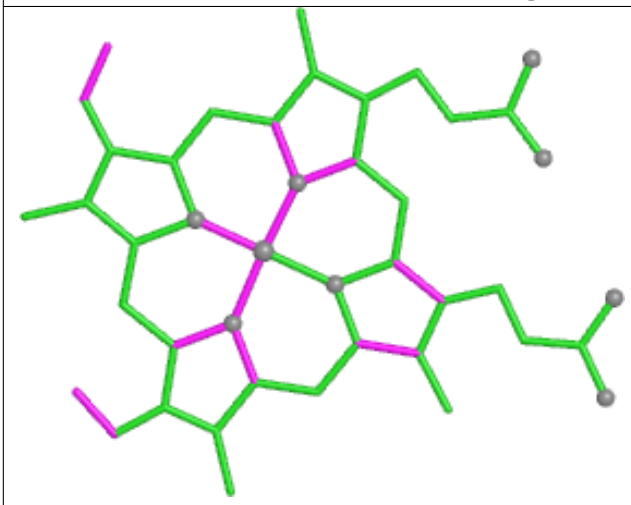
Bond angles

Torsions



Rings

Ligand HEC C 402



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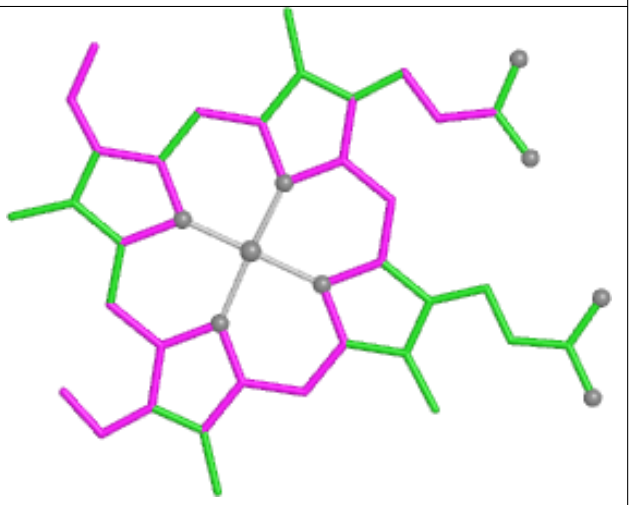
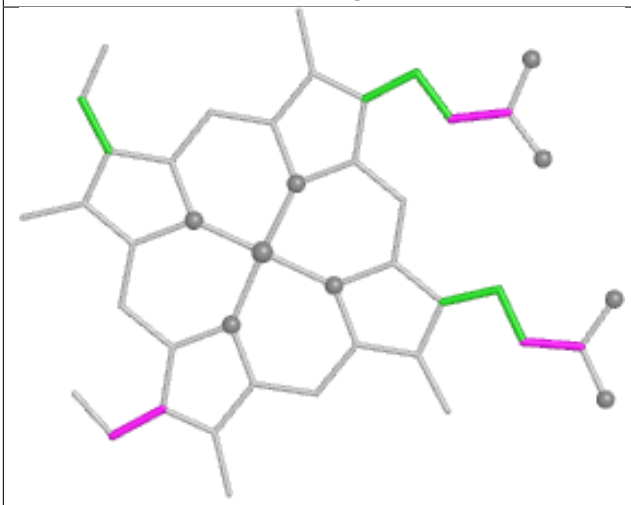


Bond angles



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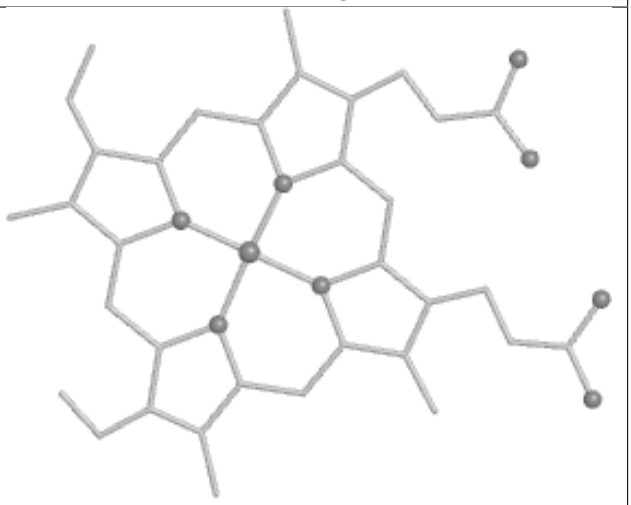
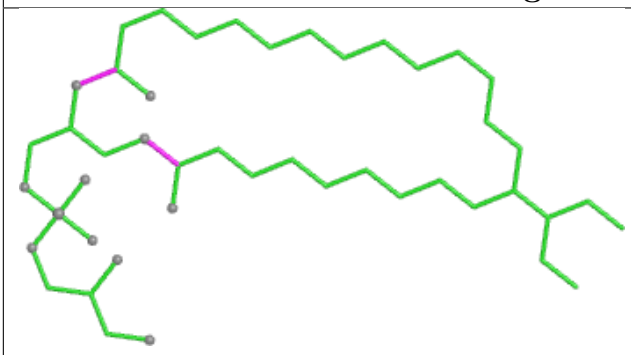


Rings

Ligand PGV L 310



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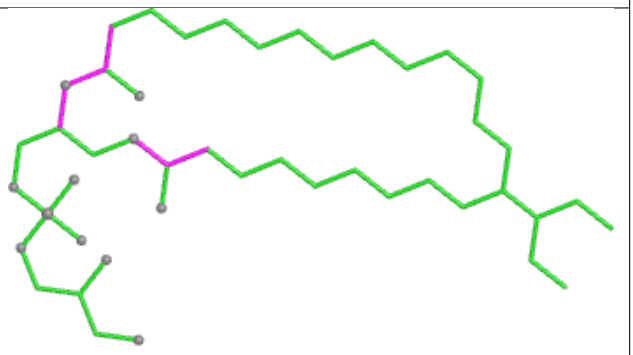
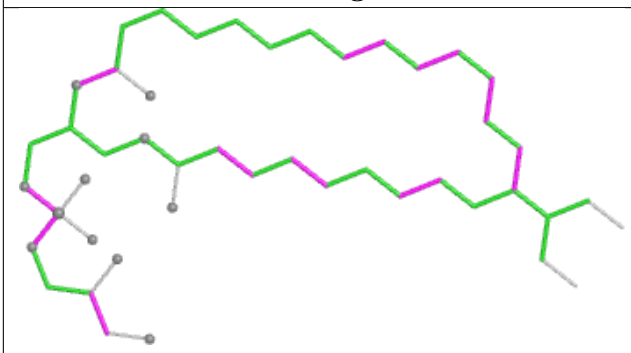


Bond angles



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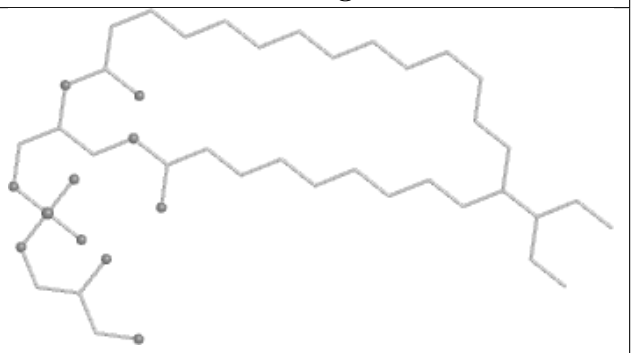
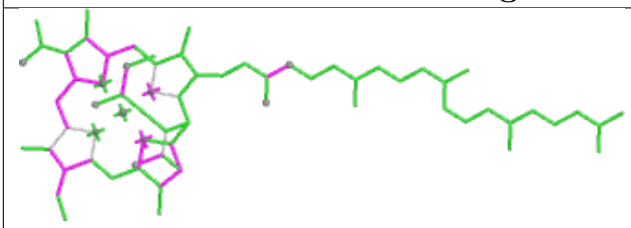


Rings

Ligand A1LZM V 102



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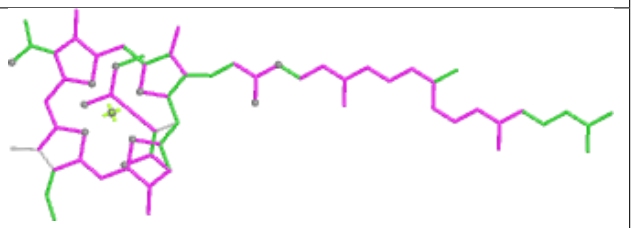
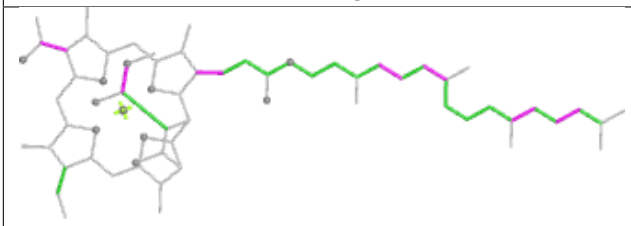


Bond angles



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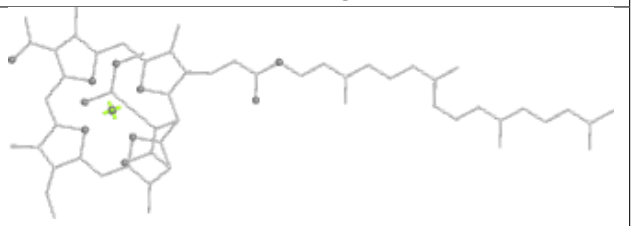
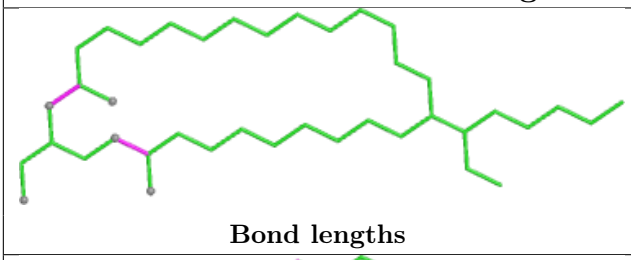


Rings

Ligand PGV m 104



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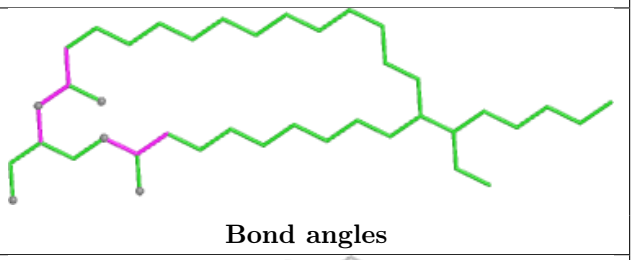

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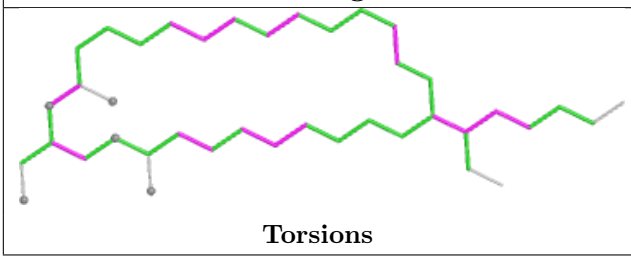

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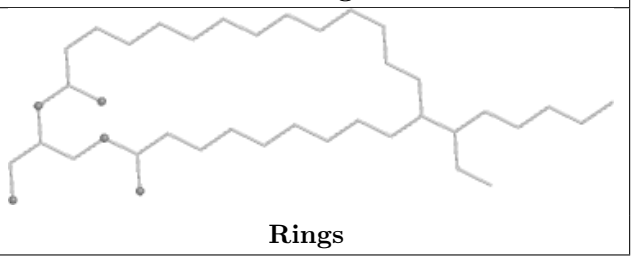
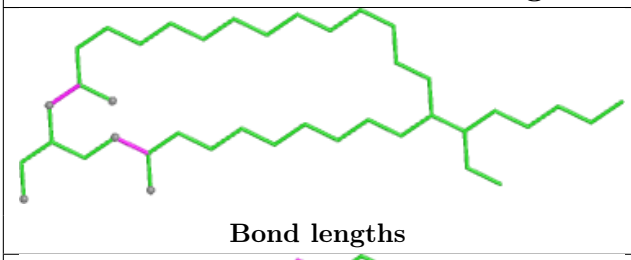


Rings

Ligand PGV 8 103



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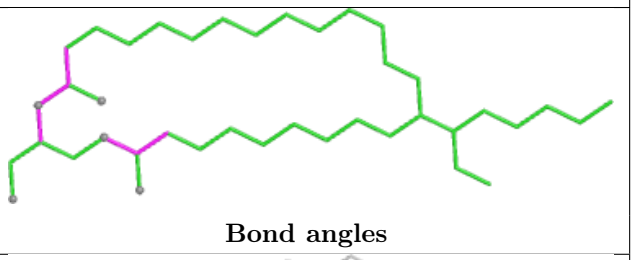

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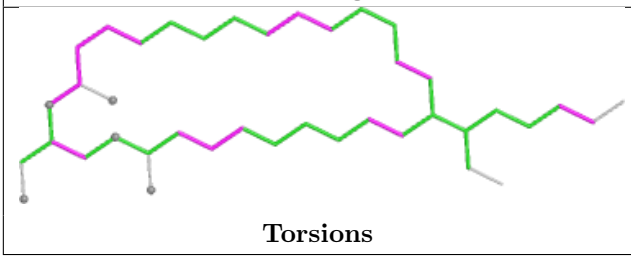

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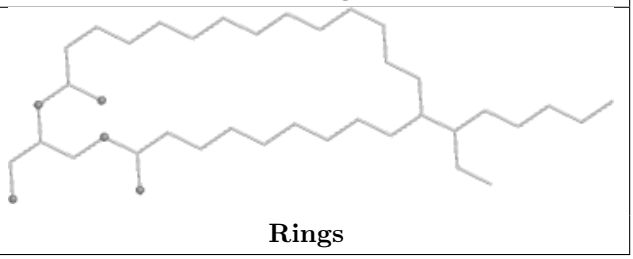
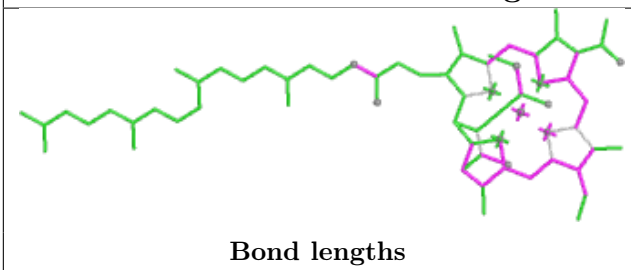


Rings

Ligand A1LZM k 102



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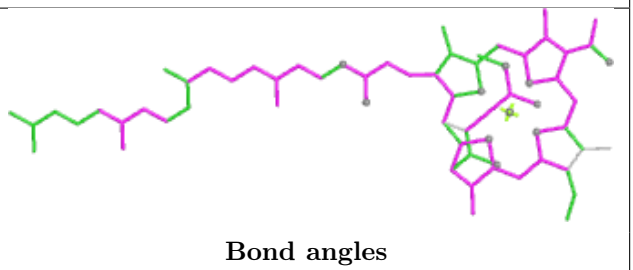
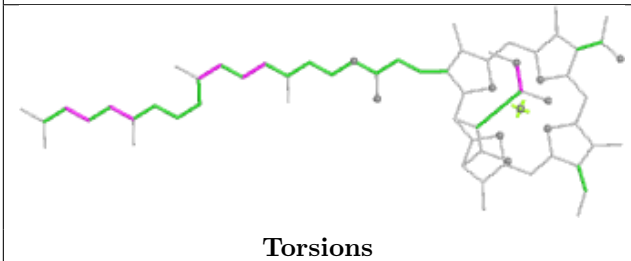


Bond angles



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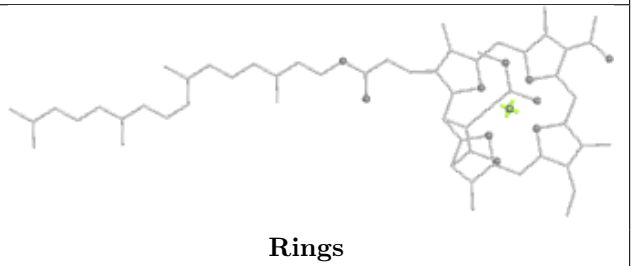
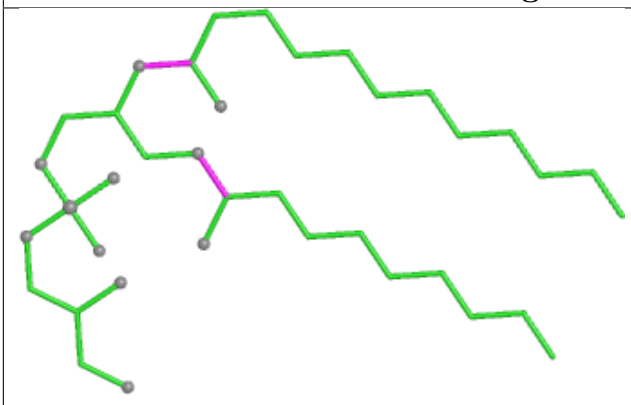


Rings

Ligand PGV C 408



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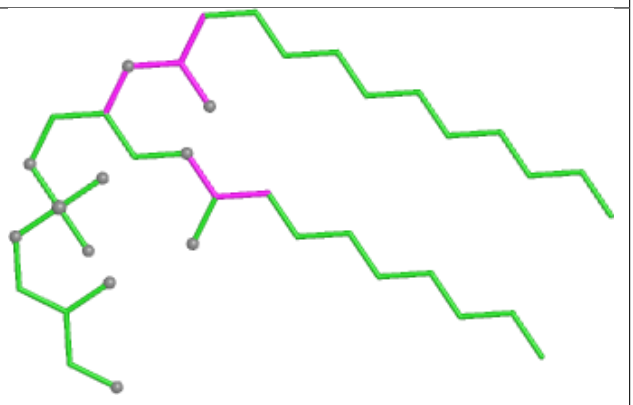
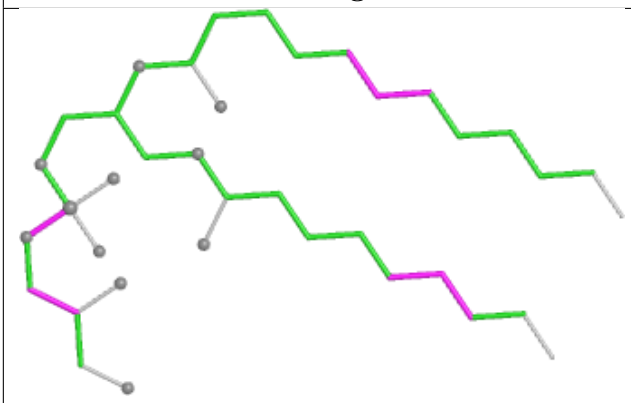


Bond angles



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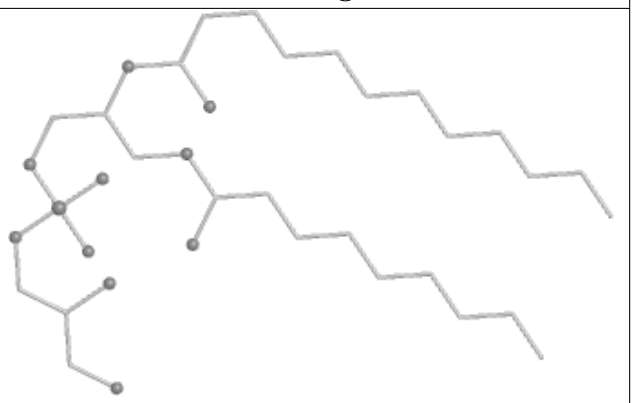
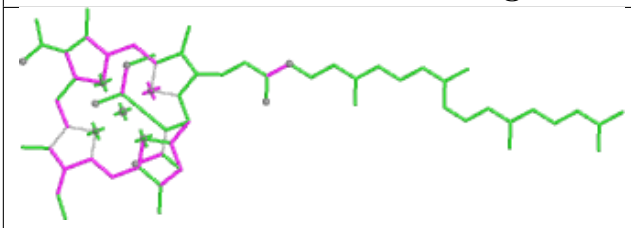


Rings

Ligand A1LZM S 102



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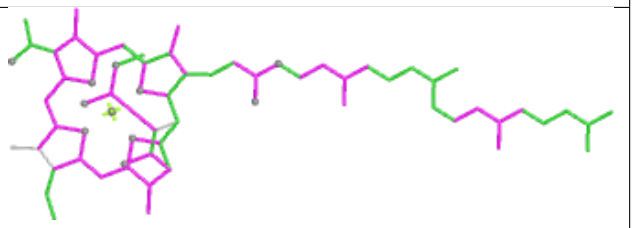

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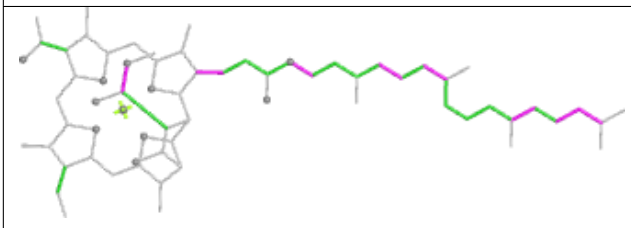

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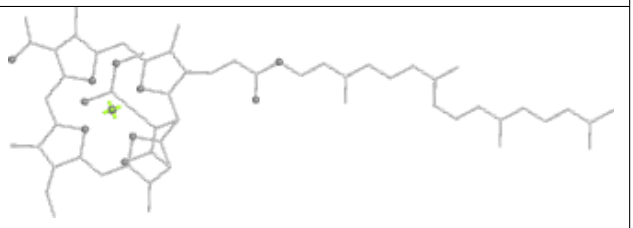
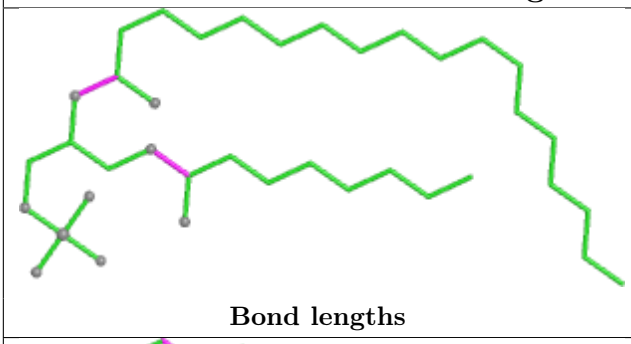


Rings

Ligand PGV z 103



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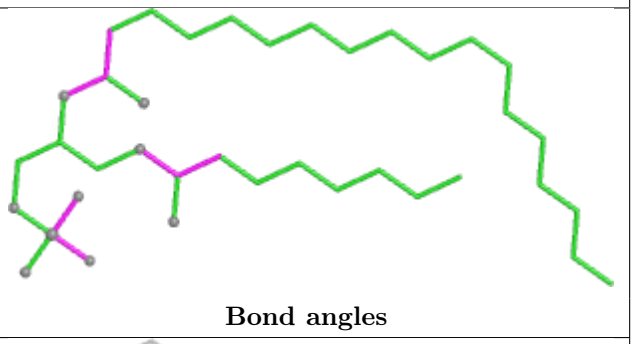
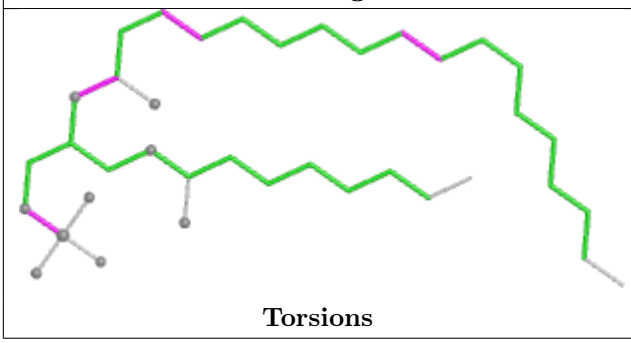


Bond angles



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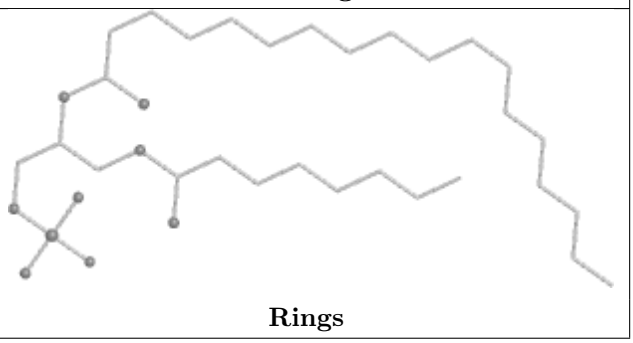
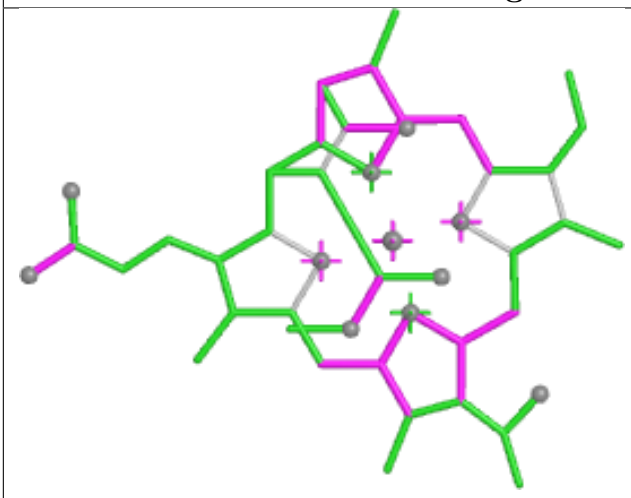


Rings

Ligand A1LZQ Z 102



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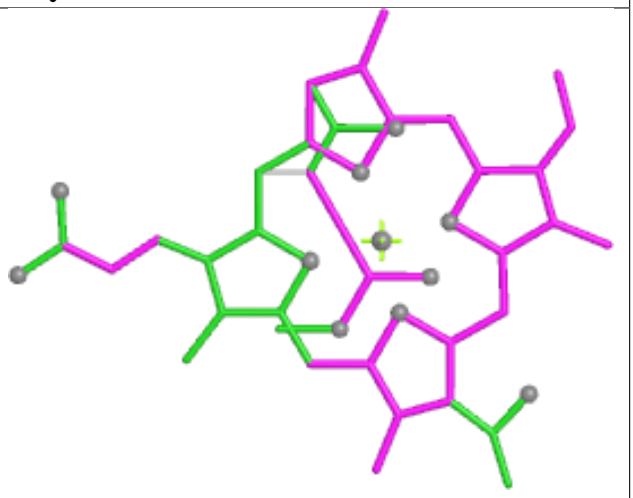
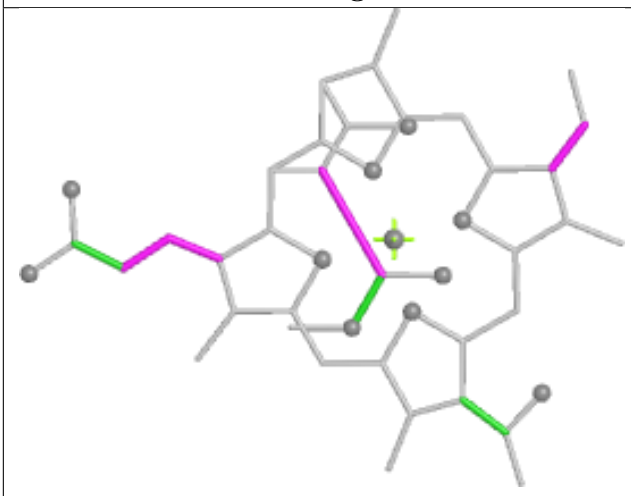
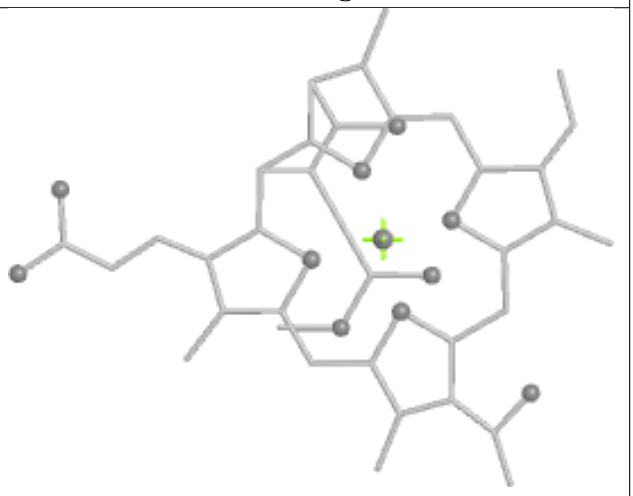


Bond angles

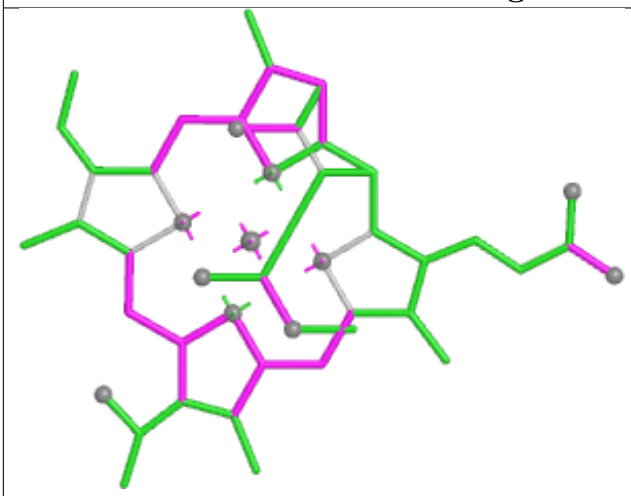


Torsions



Rings

Ligand A1LZQ x 101



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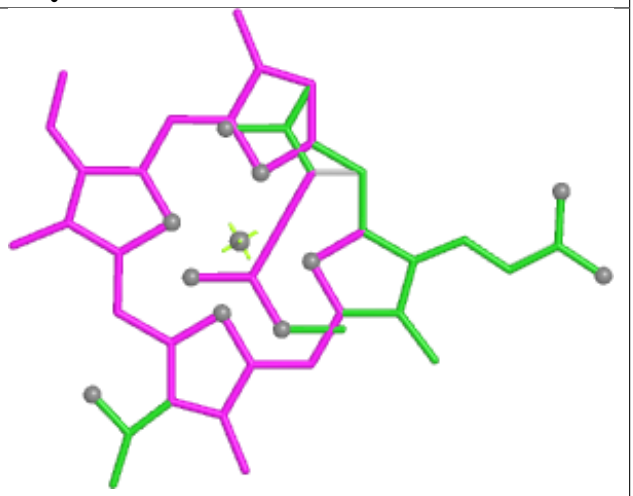

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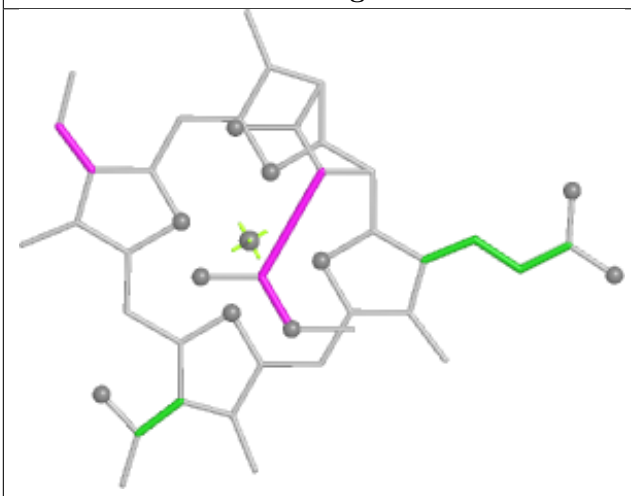

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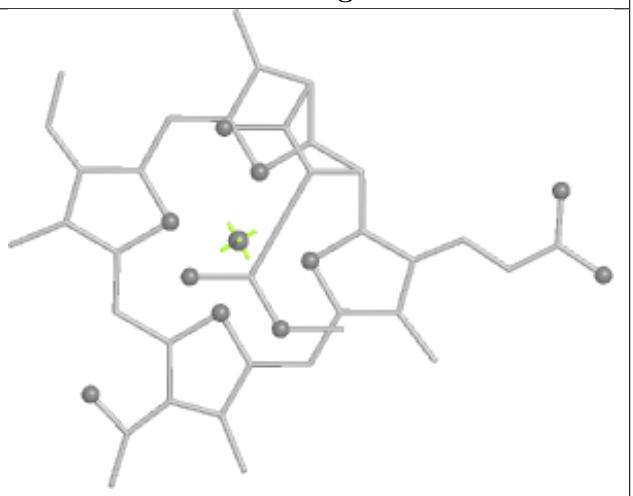
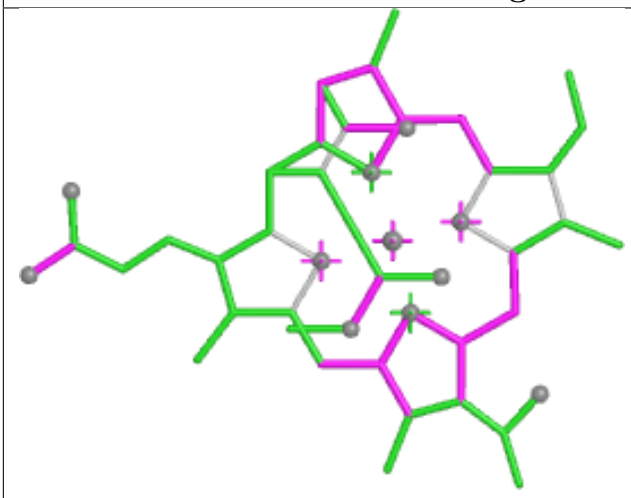


Rings

Ligand A1LZQ r 102



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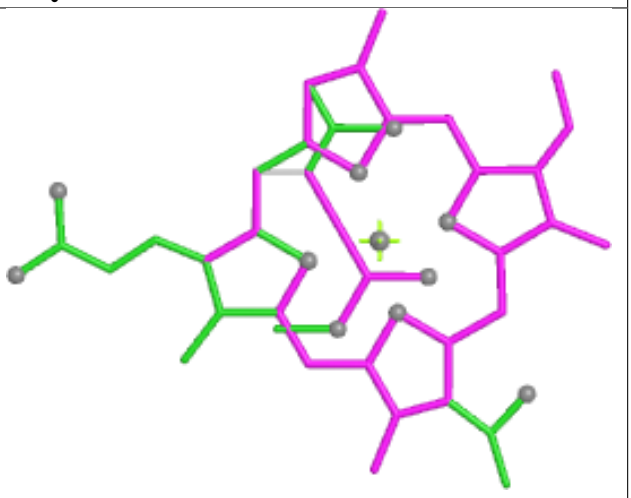

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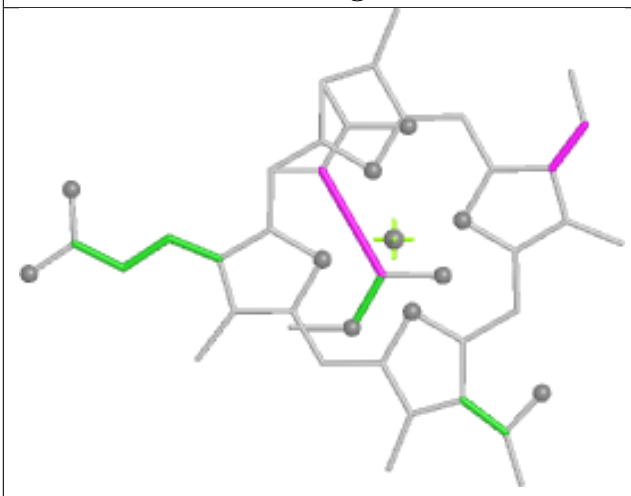

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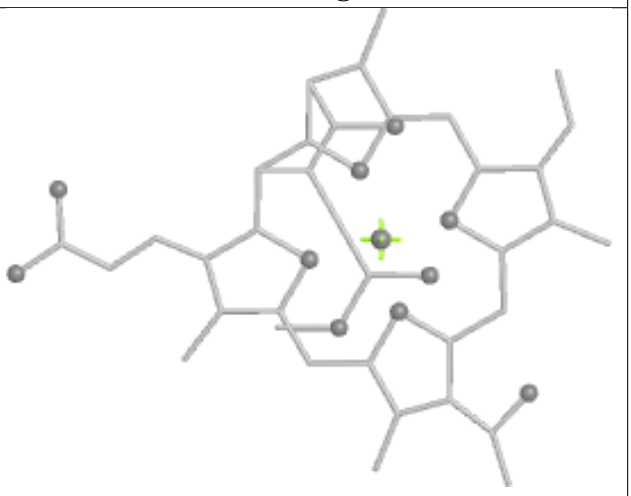
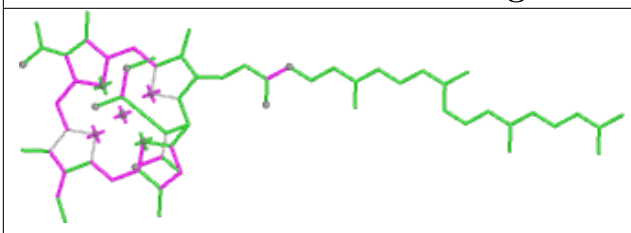


Rings

Ligand A1LZM f 101



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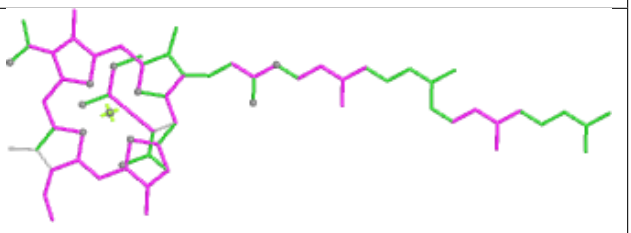

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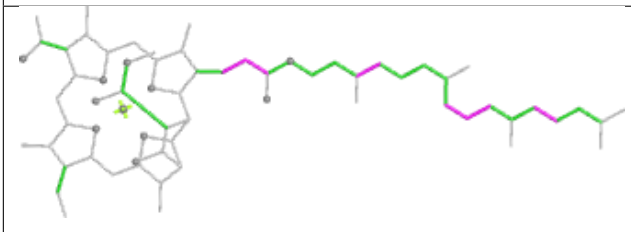

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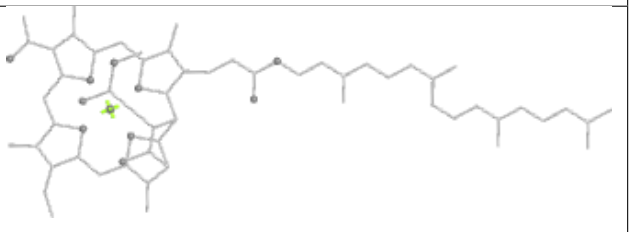
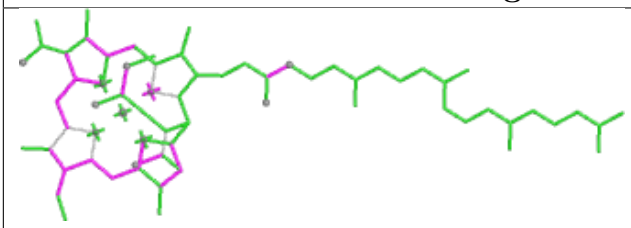


Rings

Ligand A1LZM q 101



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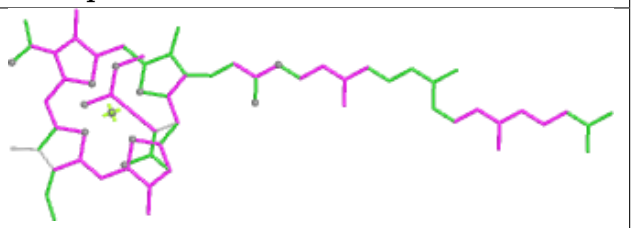

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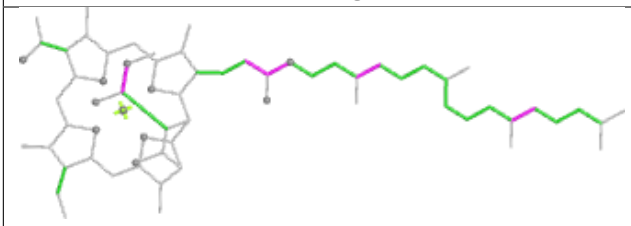

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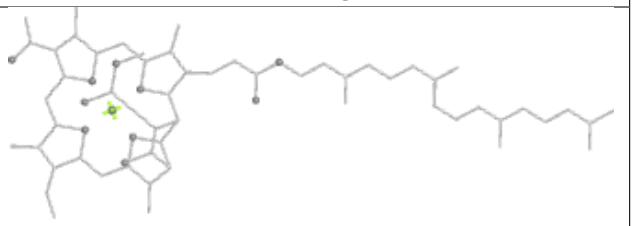
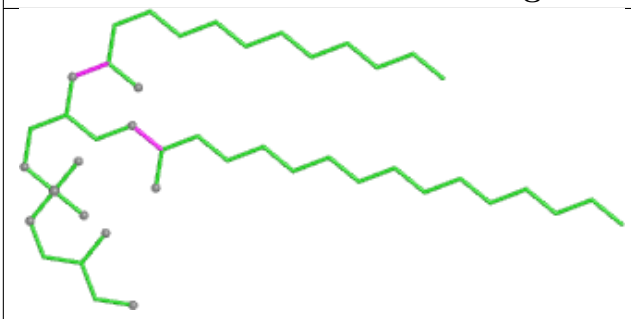


Rings

Ligand PGV L 309



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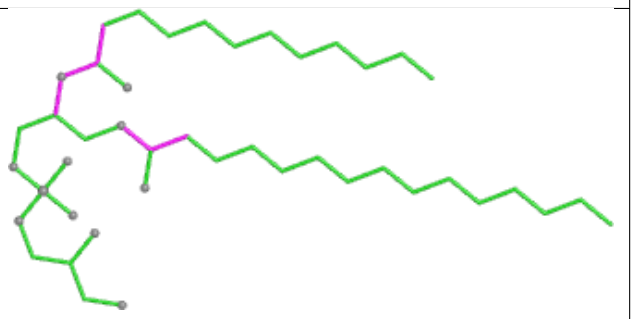

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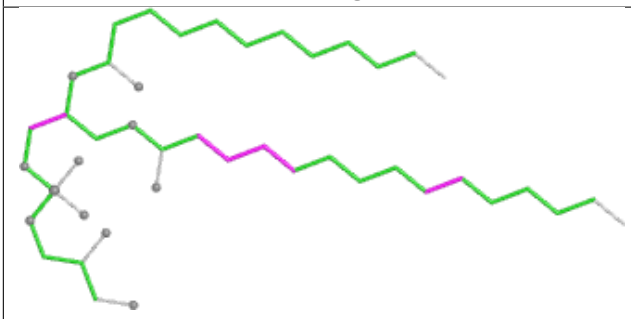

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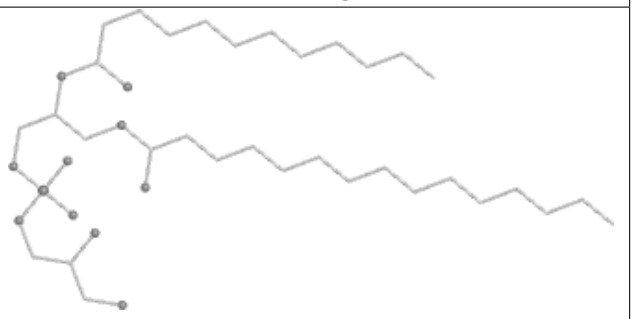
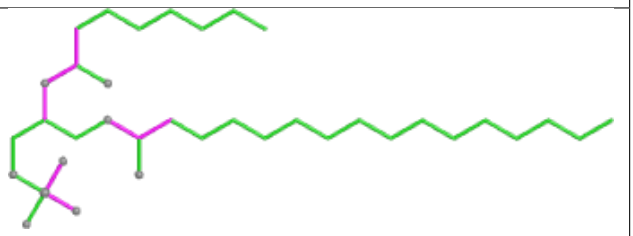


Rings

Ligand PGV h 104

Bond lengths



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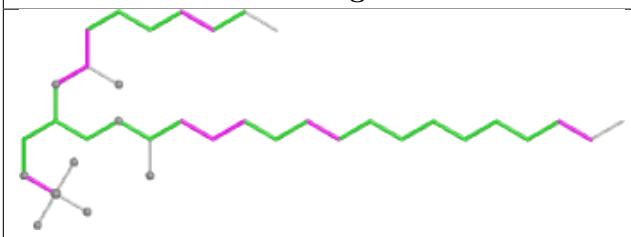

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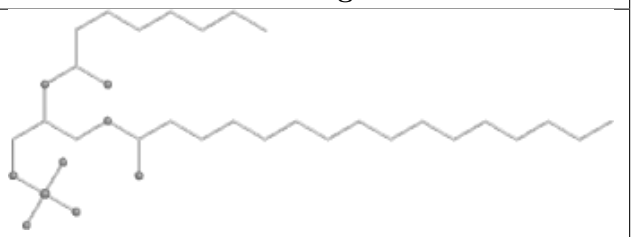
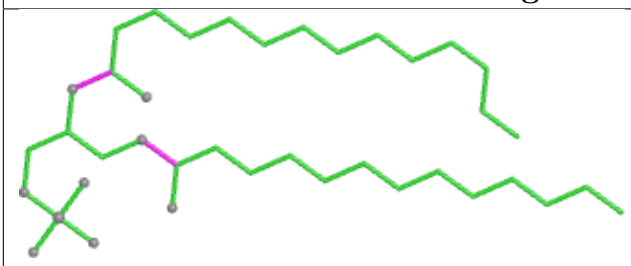


Rings

Ligand PGV w 104



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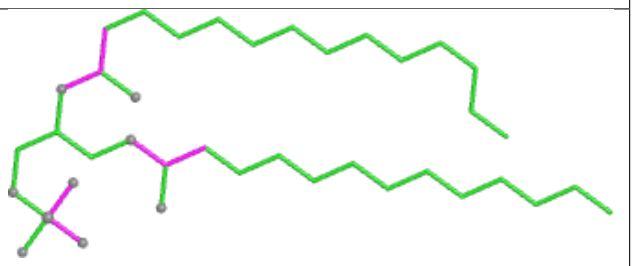

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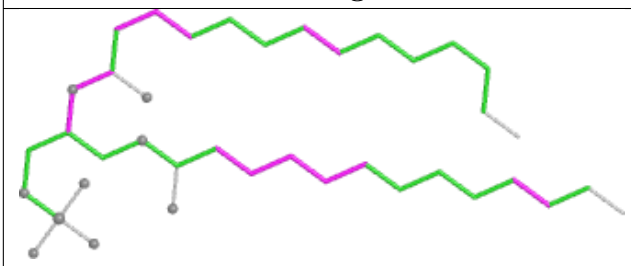

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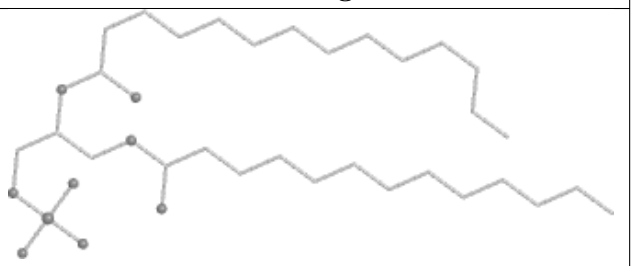
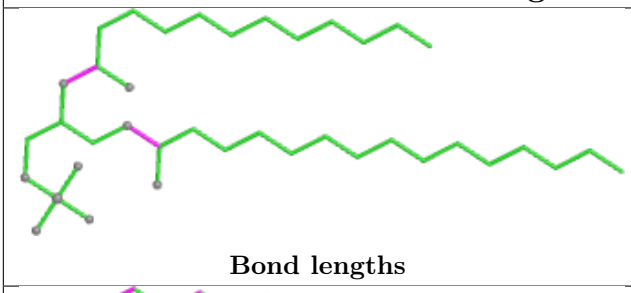


Rings

Ligand PGV t 103



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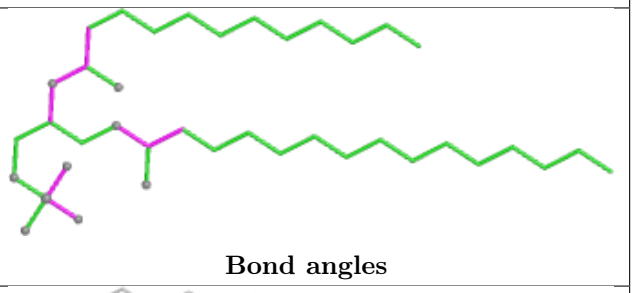

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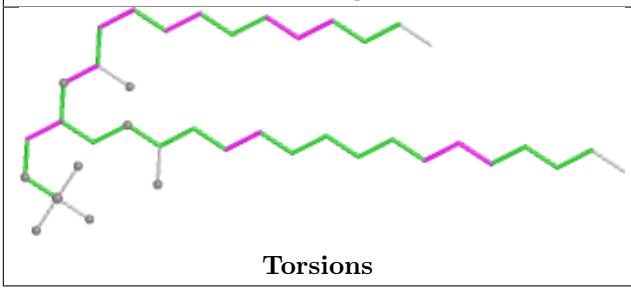

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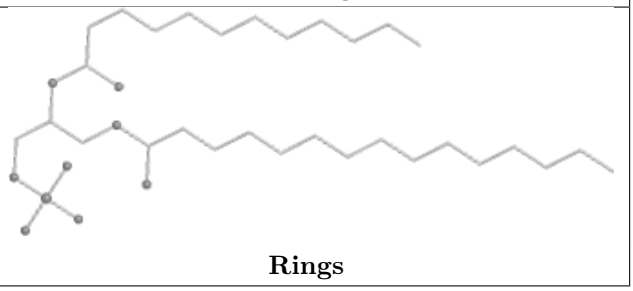
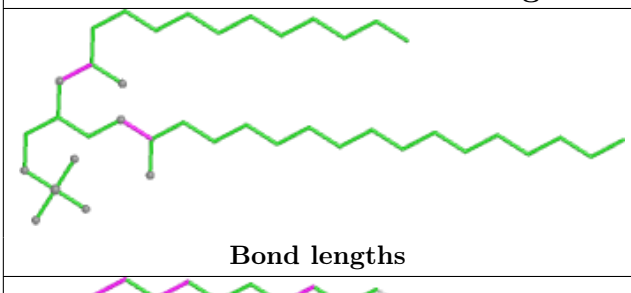


Rings

Ligand PGV P 104



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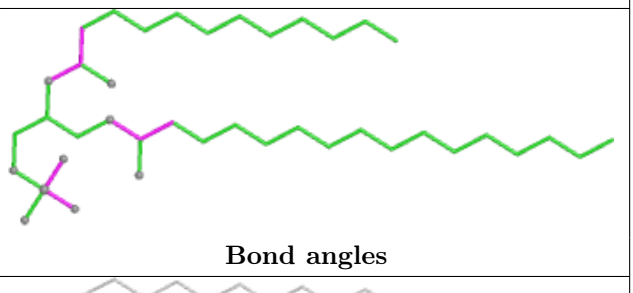

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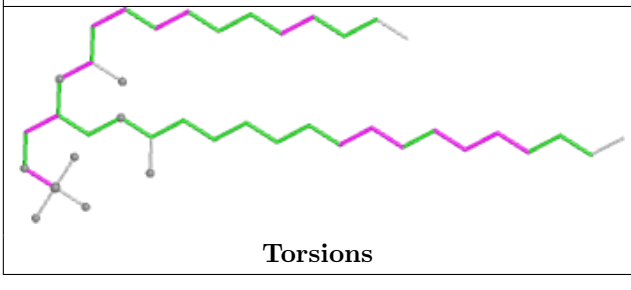

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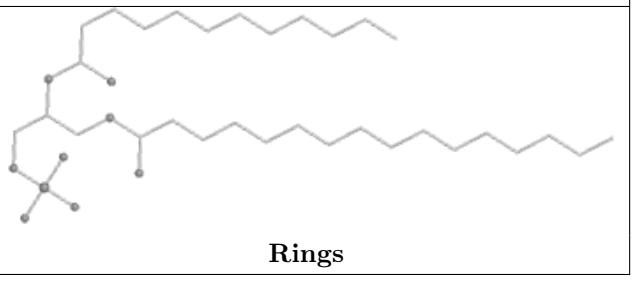
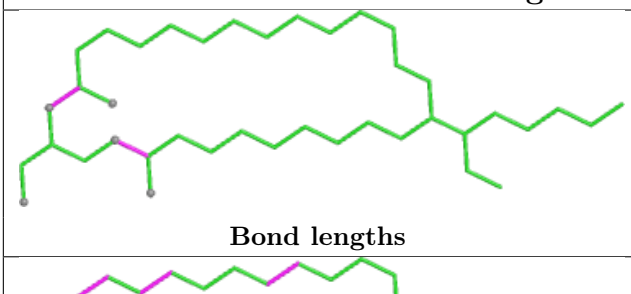


Rings

Ligand PGV a 104



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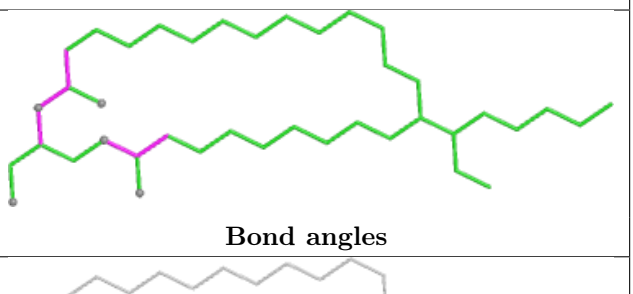

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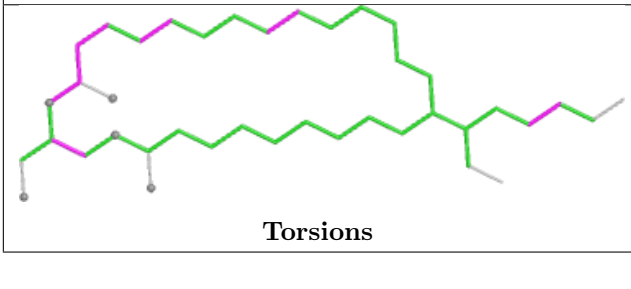

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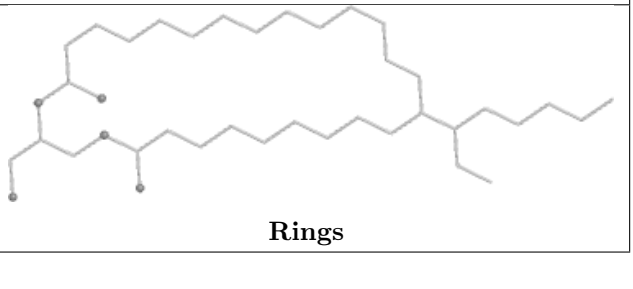
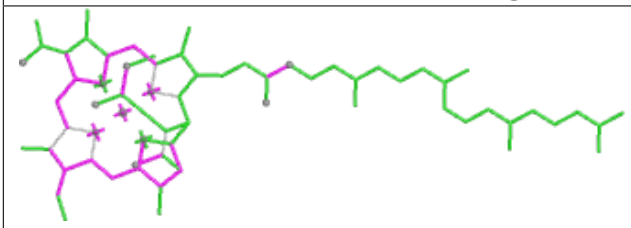


Rings

Ligand A1LZM z 101



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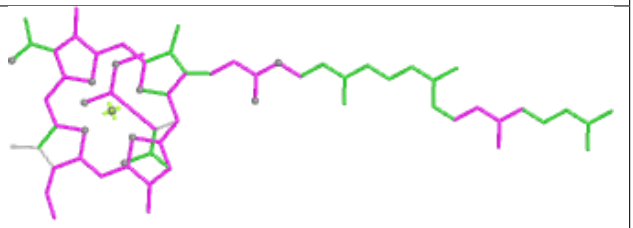

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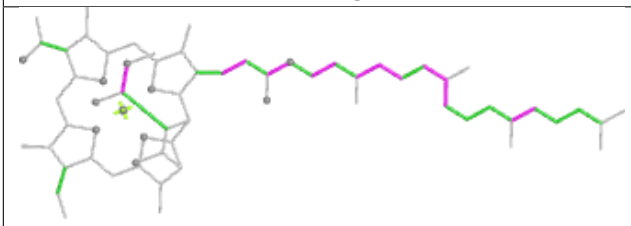

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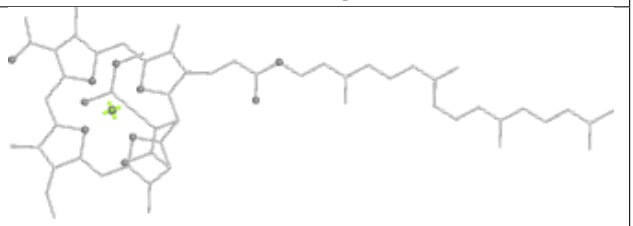
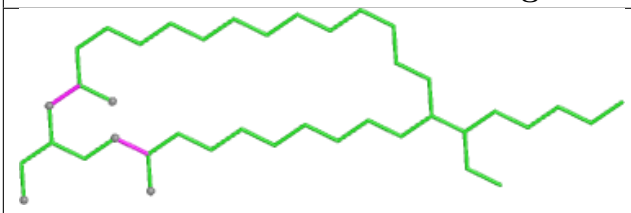


Rings

Ligand PGV R 104



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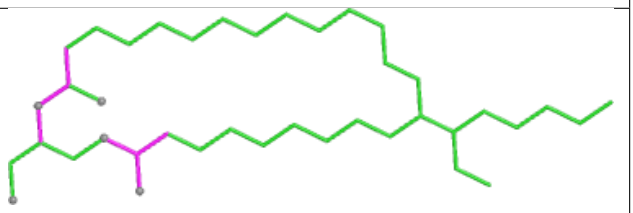
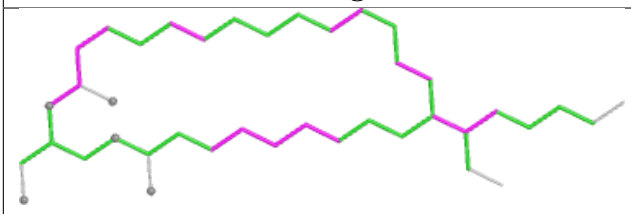


Bond angles



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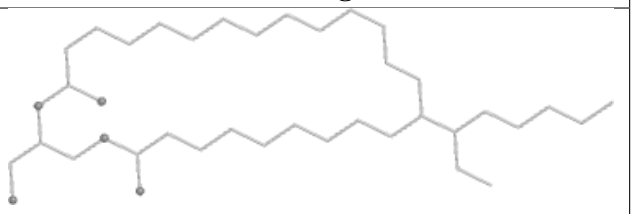
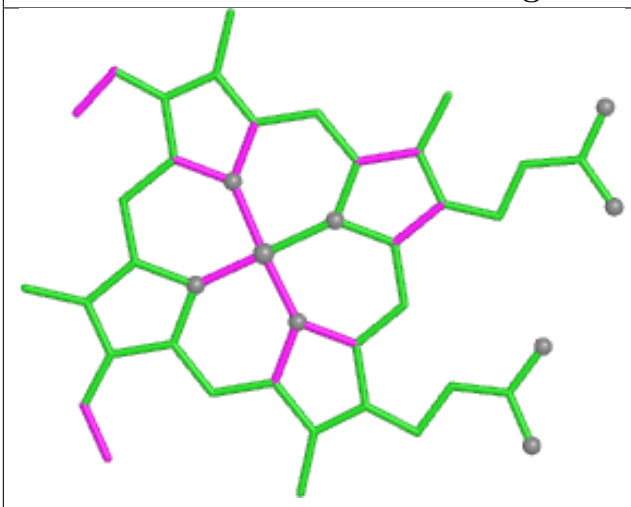


Rings

Ligand HEC C 401



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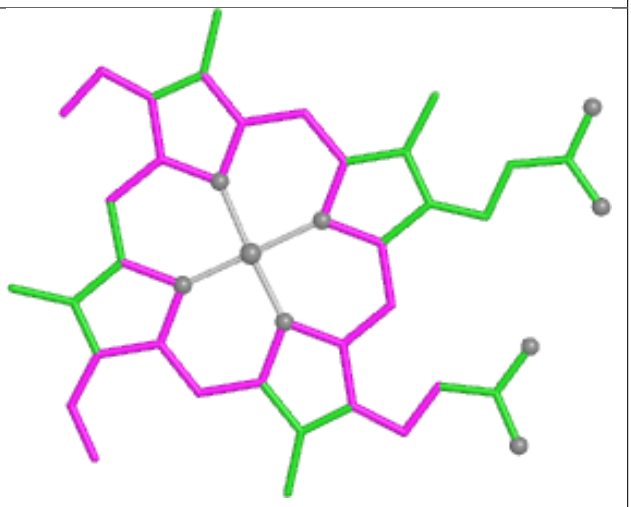
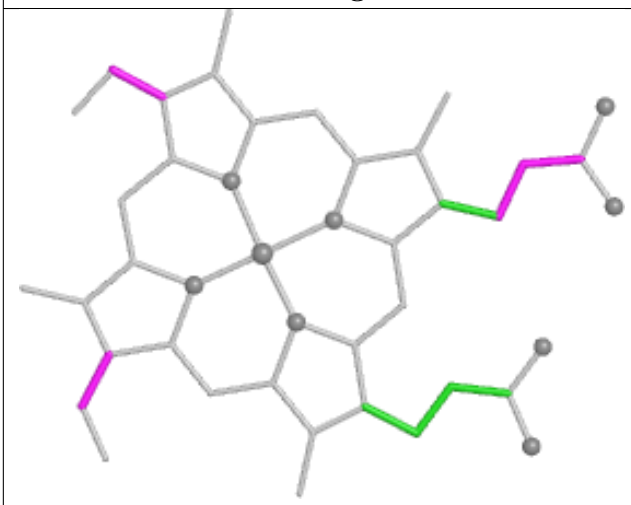


Bond angles



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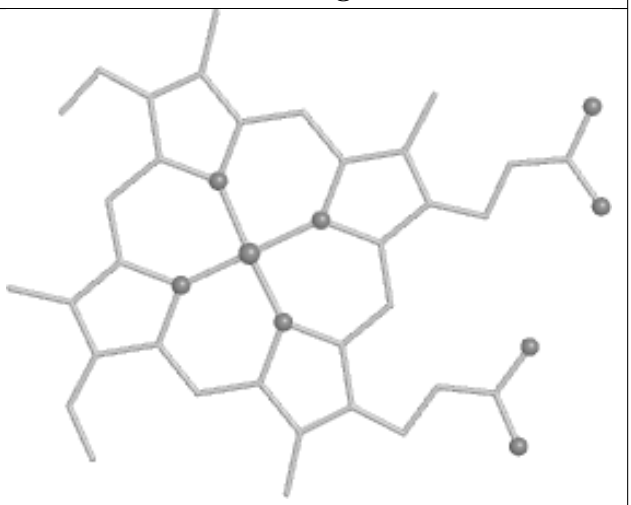
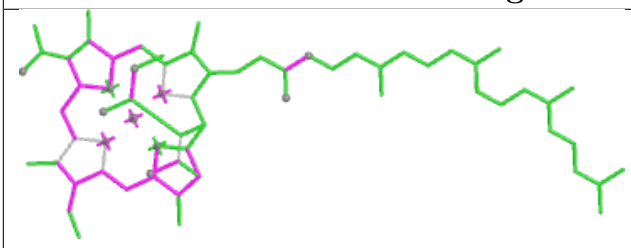


Rings

Ligand A1LZM t 102



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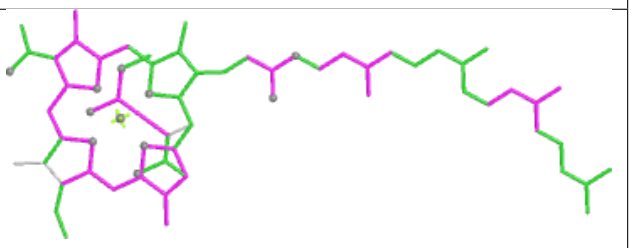

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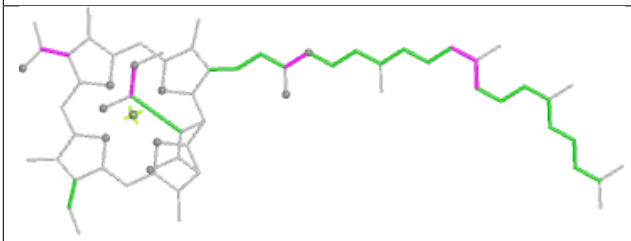
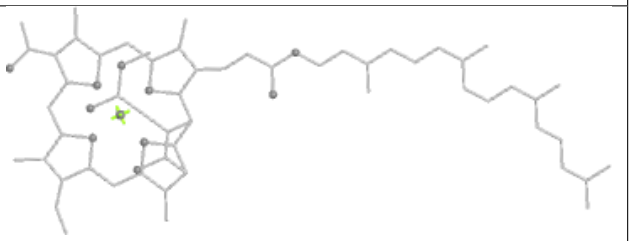
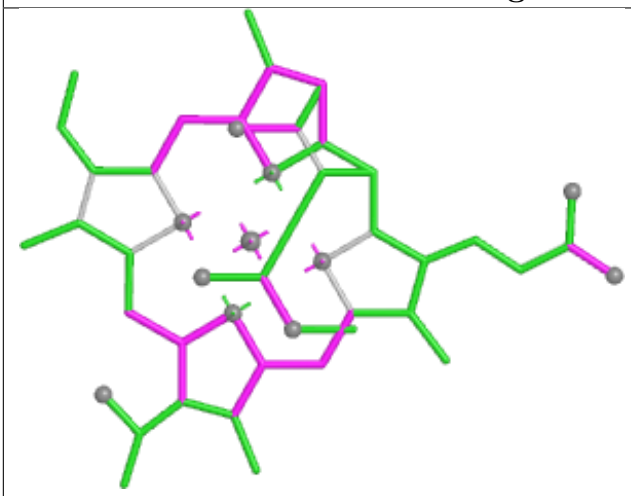


Torsions



Rings

Ligand A1LZQ 1 102



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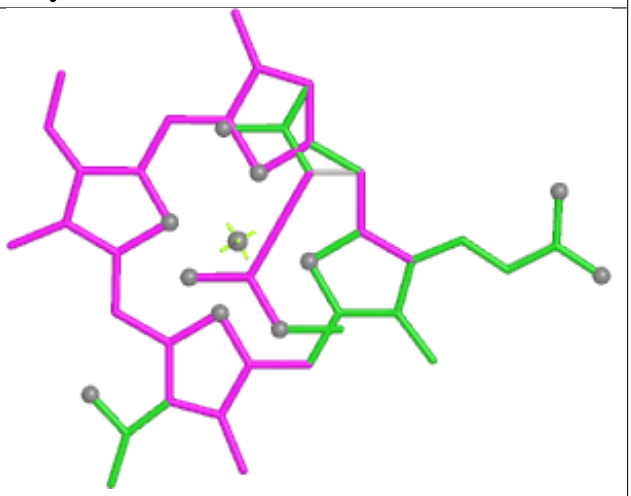

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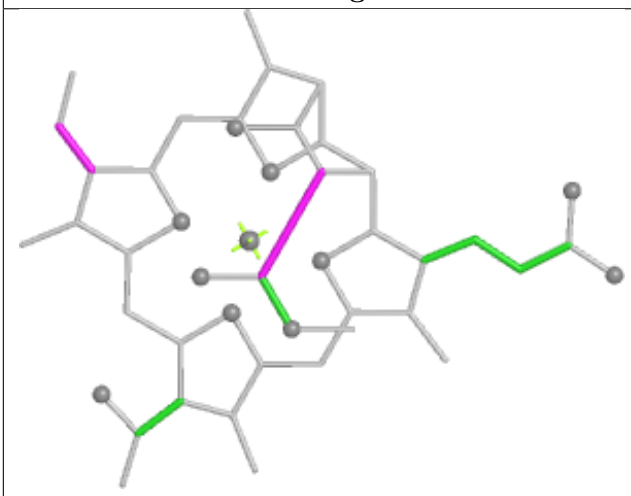

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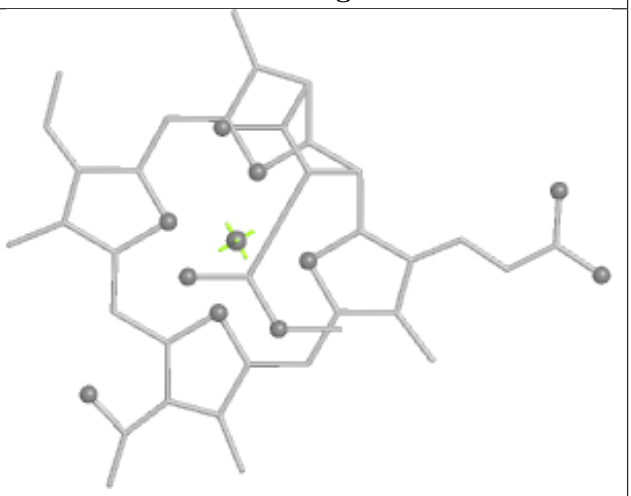
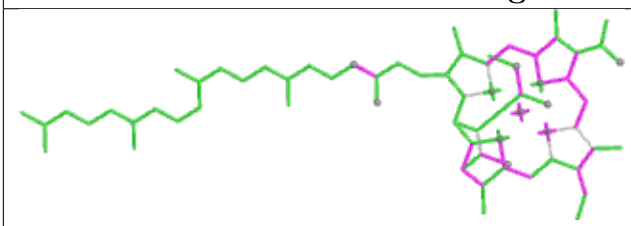


Rings

Ligand A1LZM i 101



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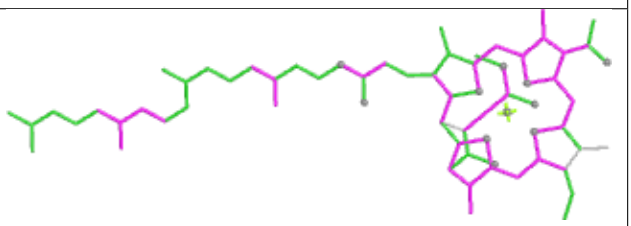

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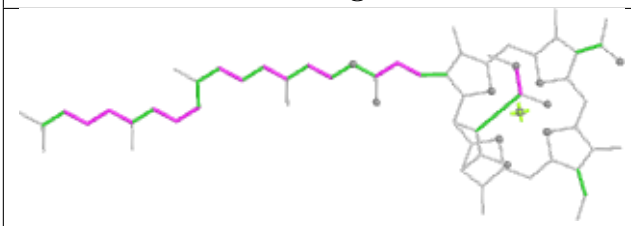

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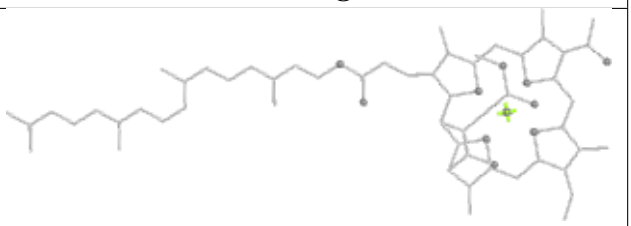

Rings

Ligand PGV H 305

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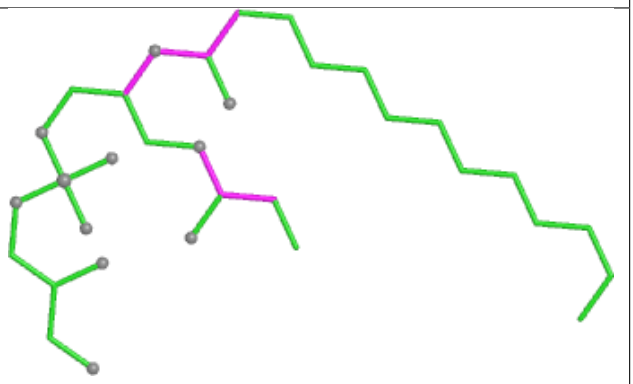

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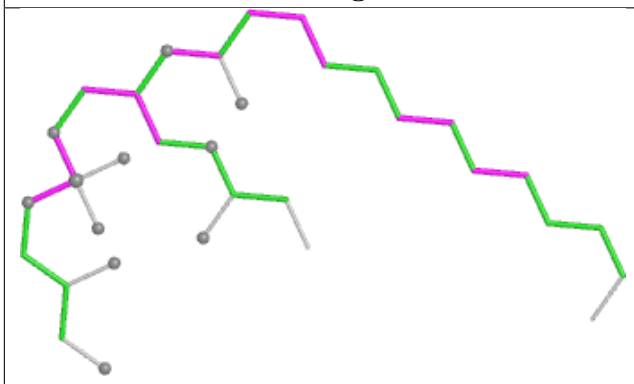

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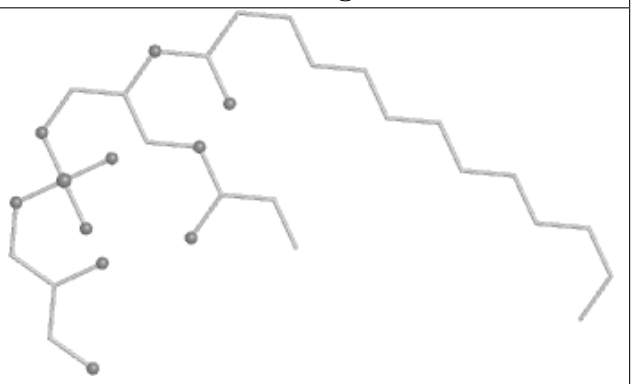
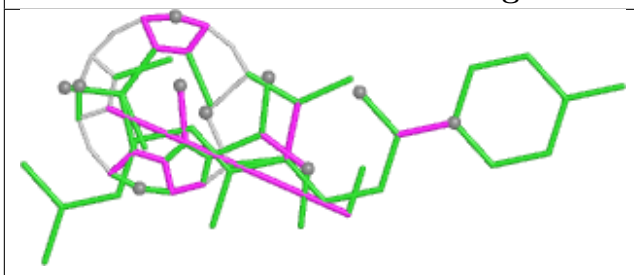


Rings

Ligand A1LZP M 704



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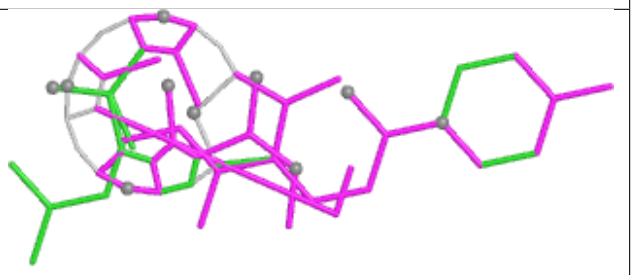

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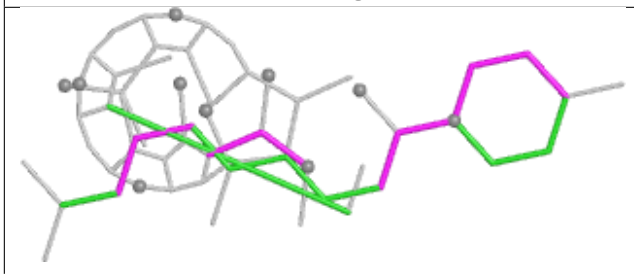

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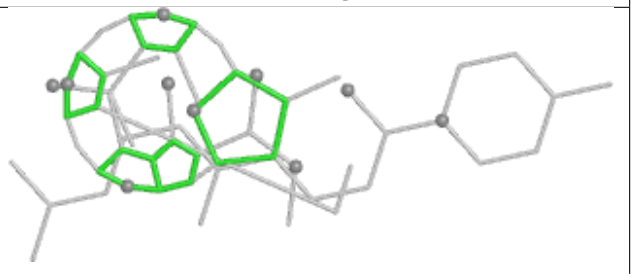
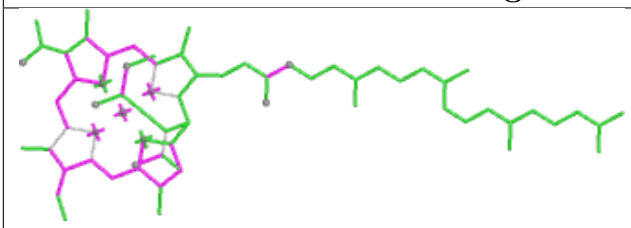


Rings

Ligand A1LZM 4 201



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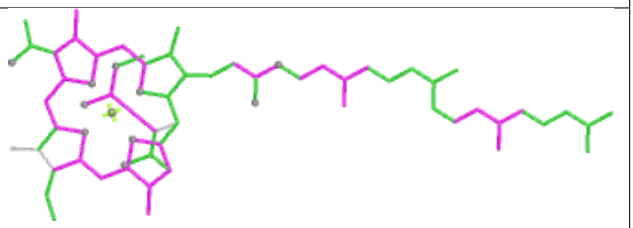

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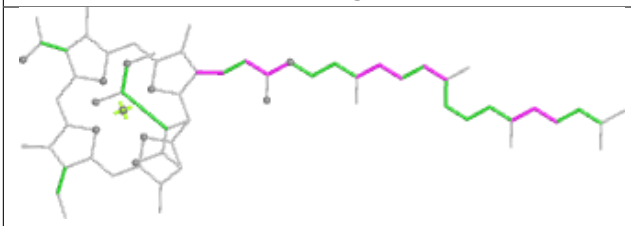

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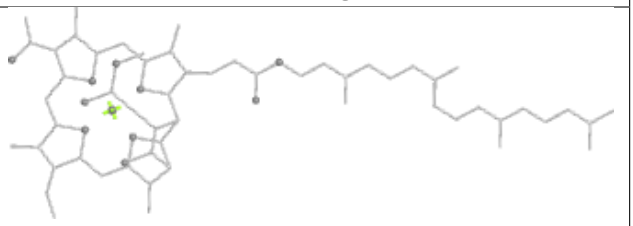

Rings

Ligand PGV K 103

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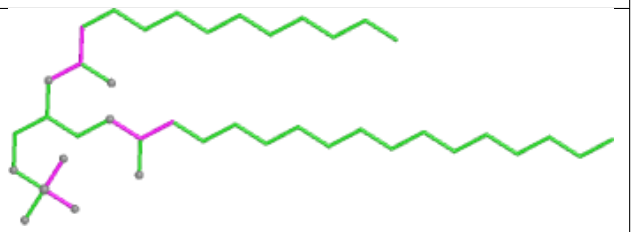

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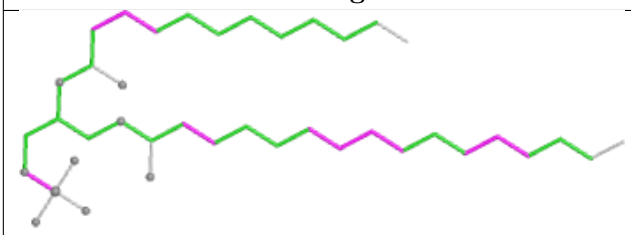

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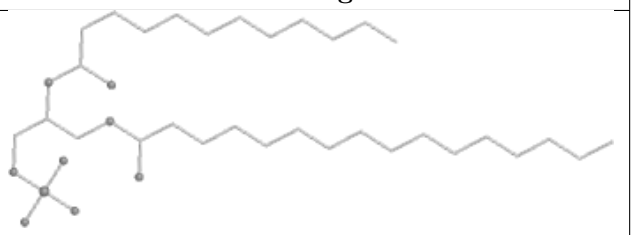
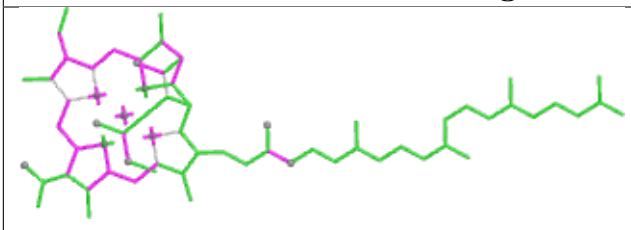


Rings

Ligand A1LZM G 101



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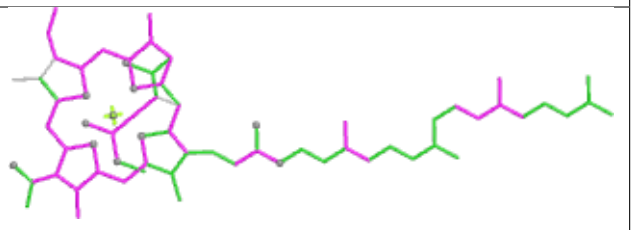

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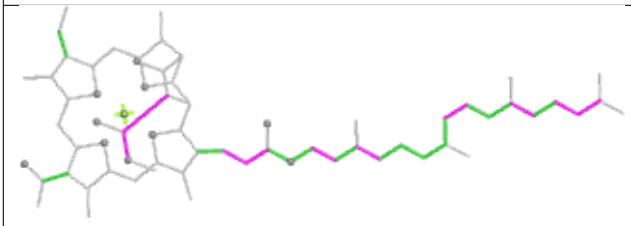

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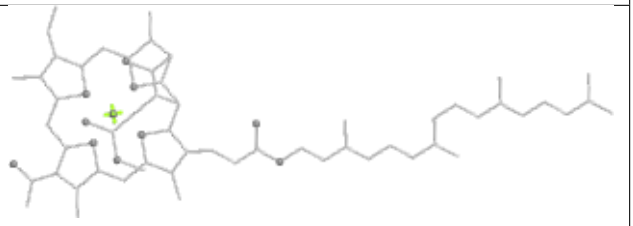
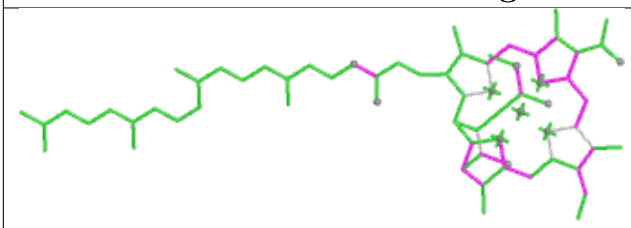


Rings

Ligand A1LZM N 101



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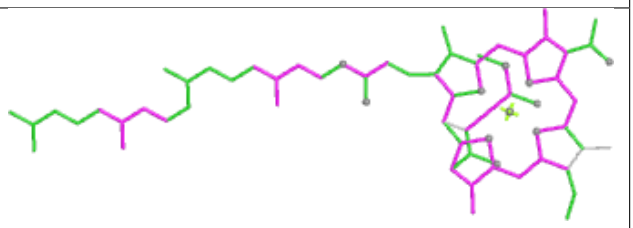

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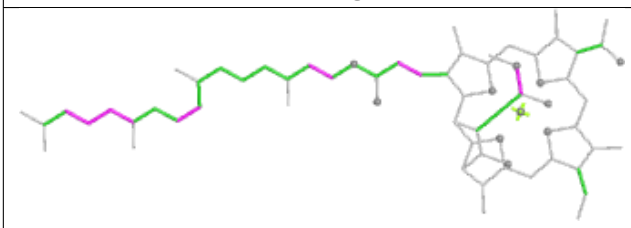

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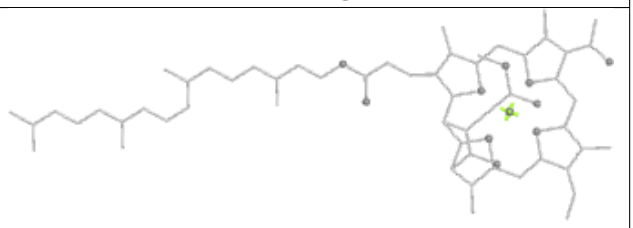
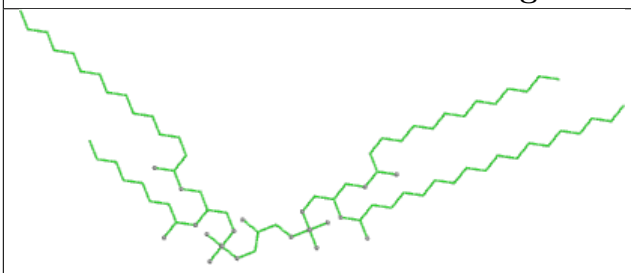


Rings

Ligand CDL M 709



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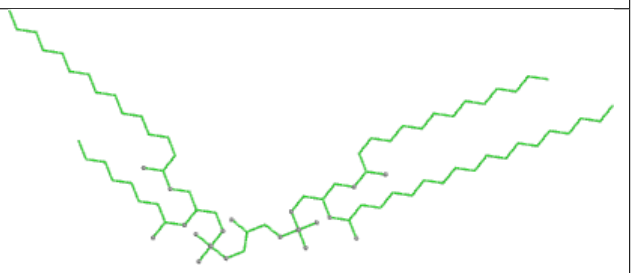

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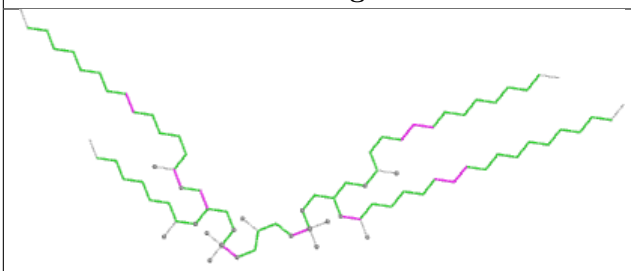

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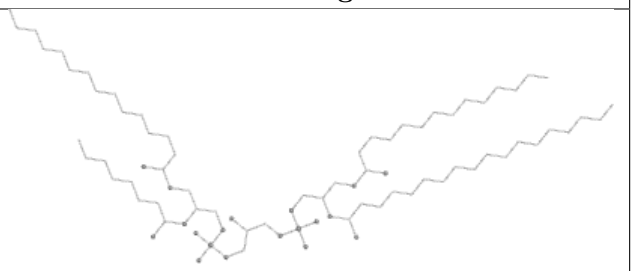
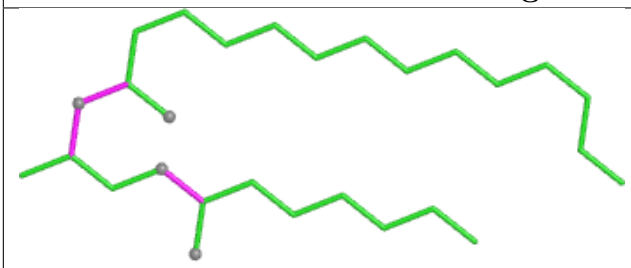


Rings

Ligand PGV C 405



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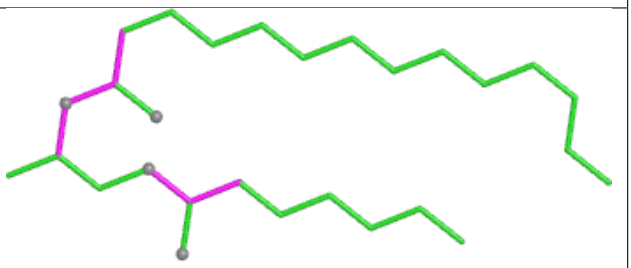

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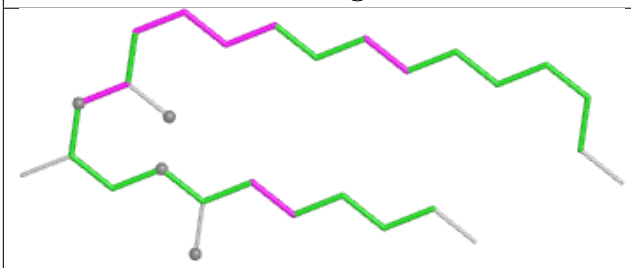

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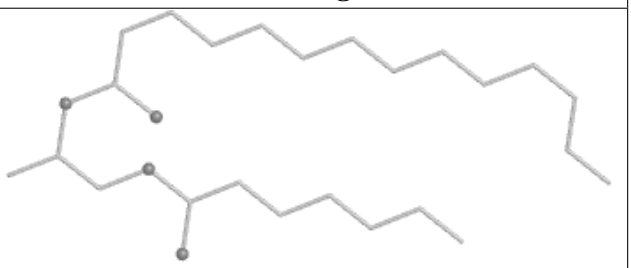
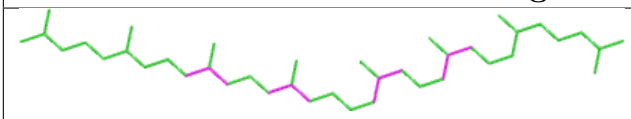


Rings

Ligand LYC 3 101



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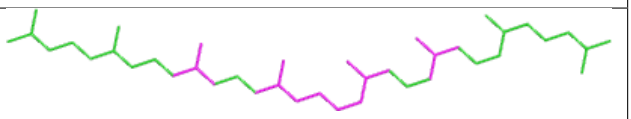

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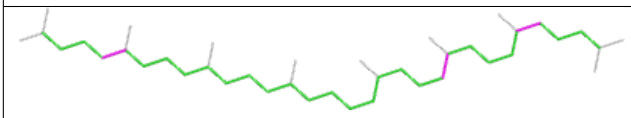

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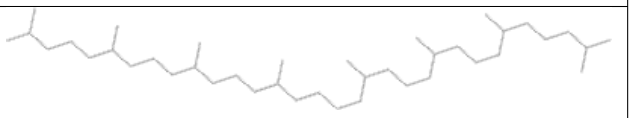
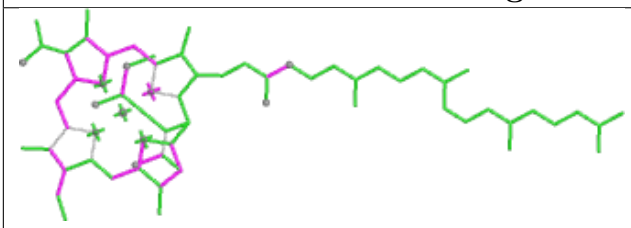


Rings

Ligand A1LZM r 101



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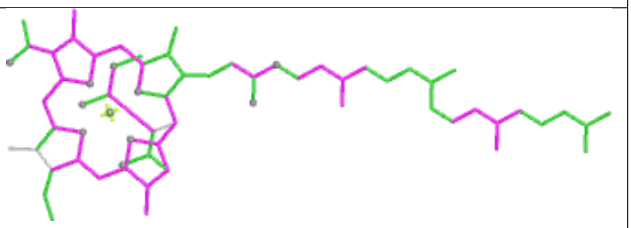
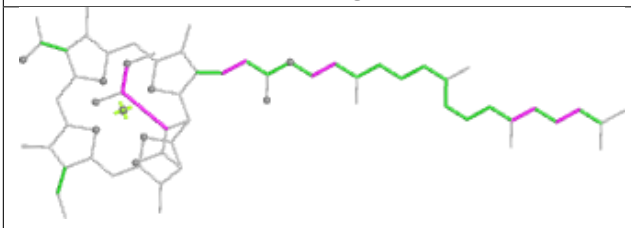


Bond angles



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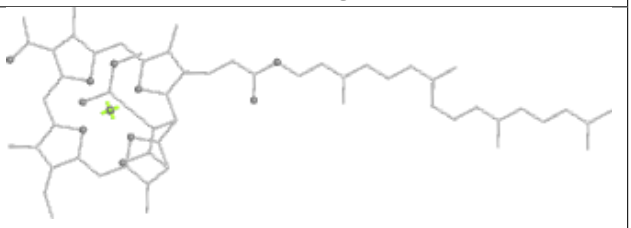
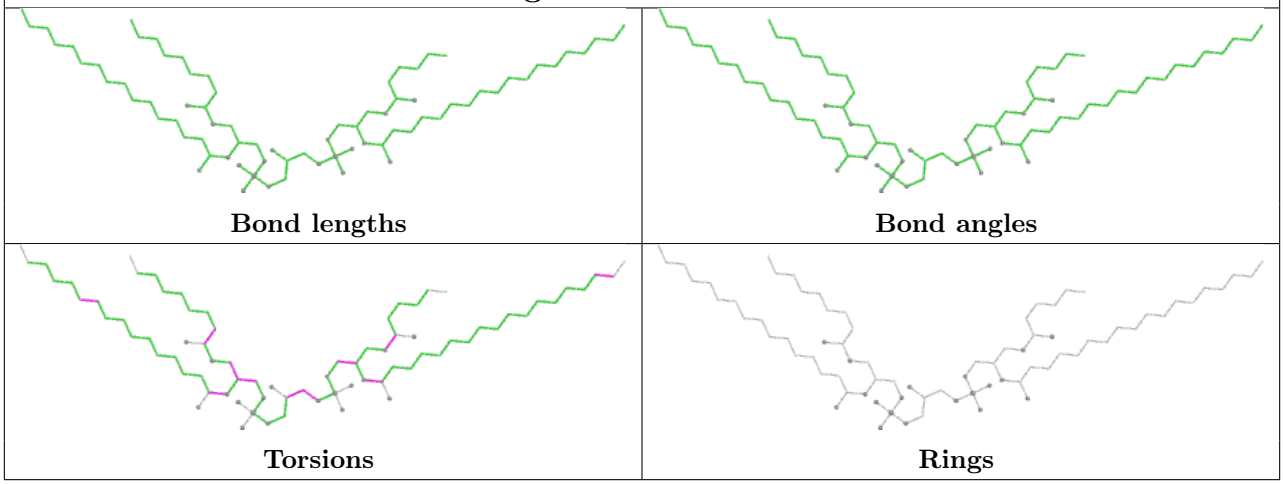


Rings

Ligand CDL H 304



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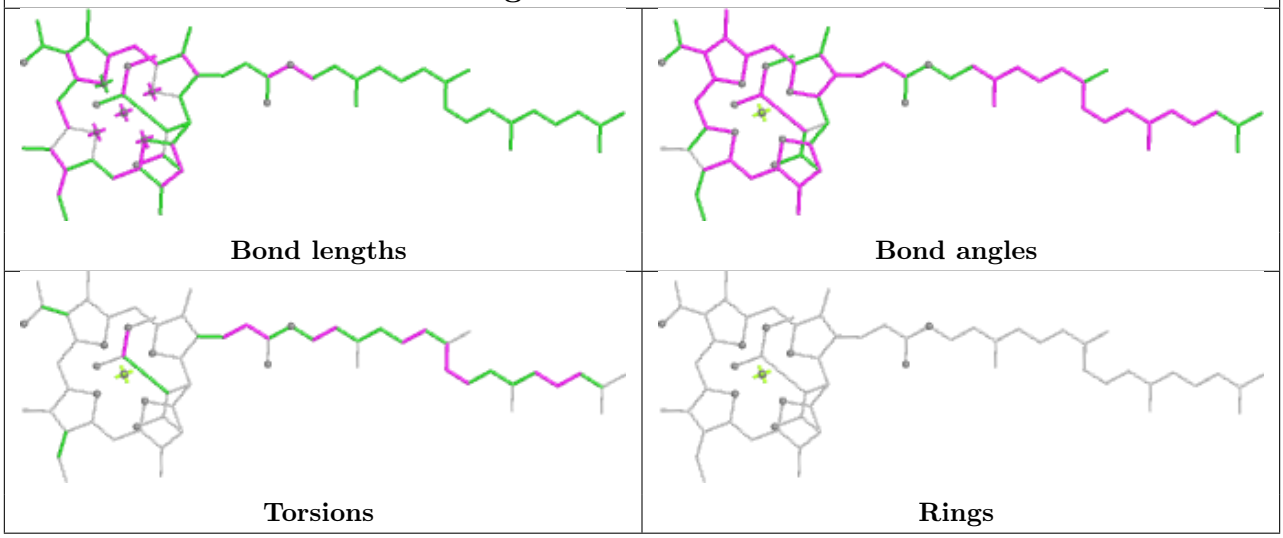

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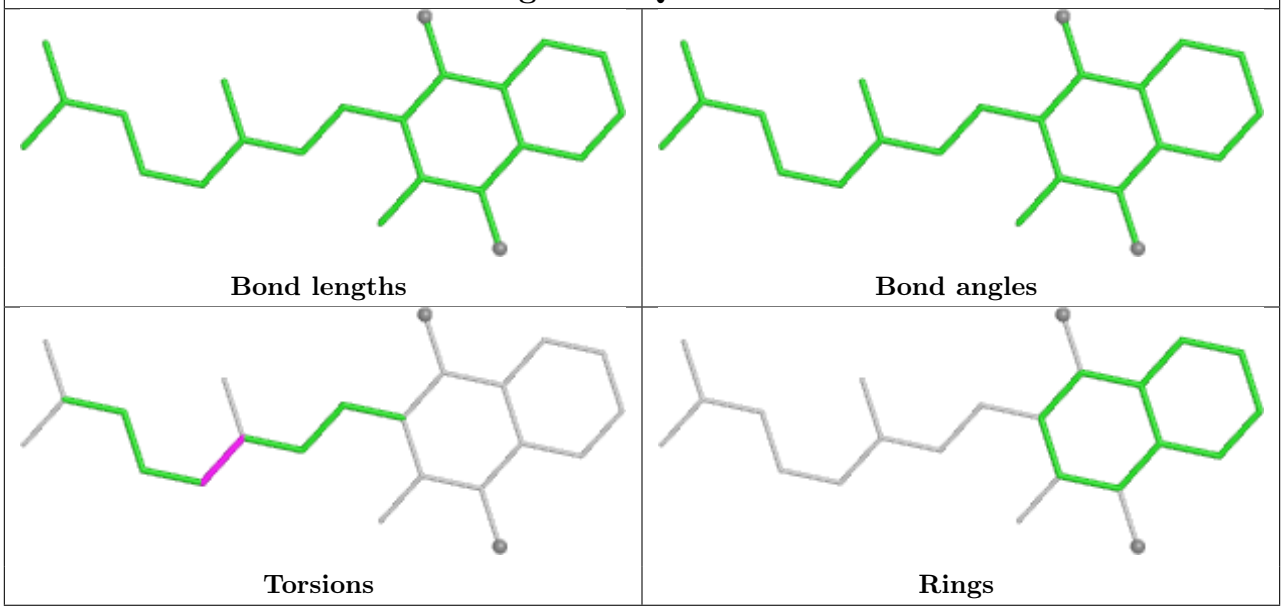

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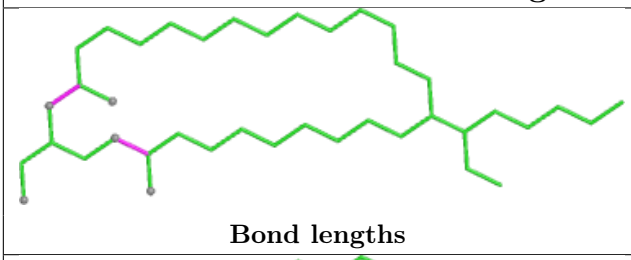
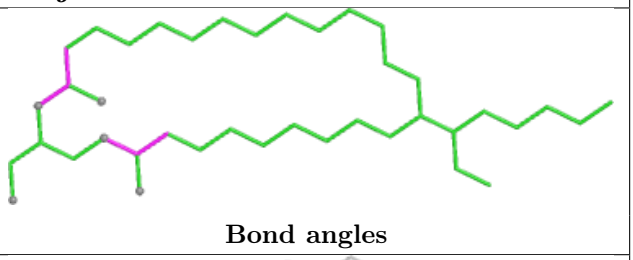


Bond lengths



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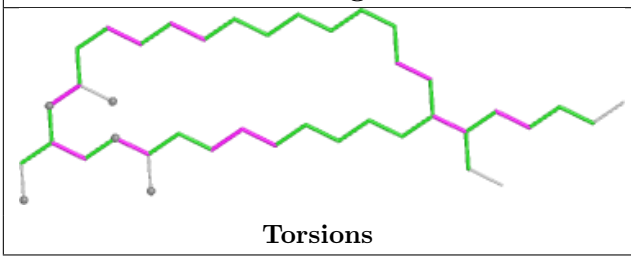
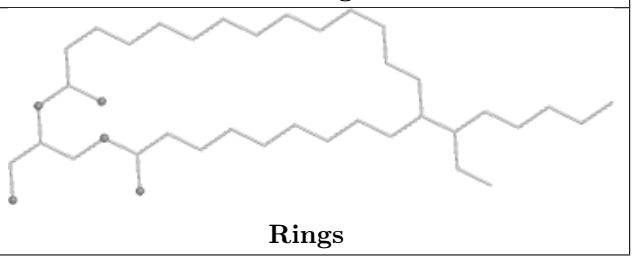
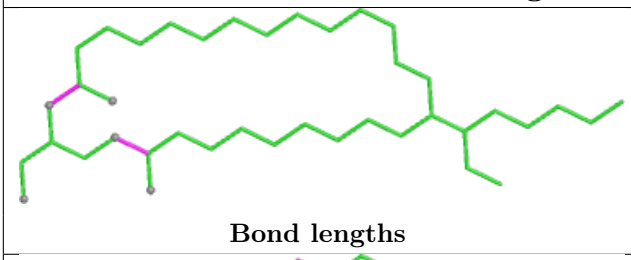


Torsions



Rings

Ligand PGV g 104



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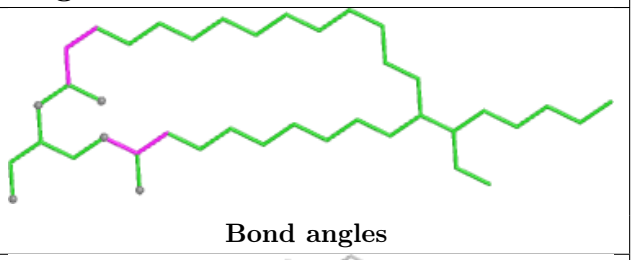

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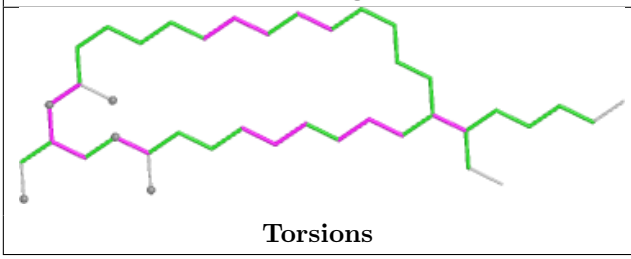

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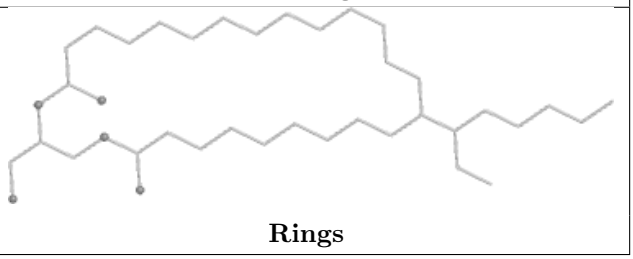
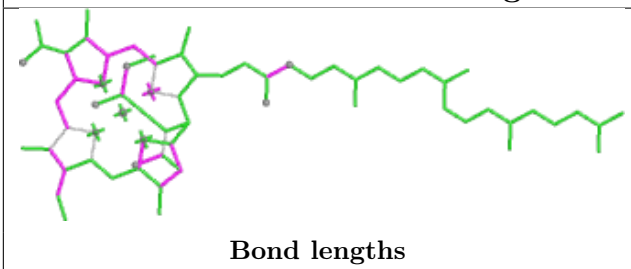


Rings

Ligand A1LZM h 102



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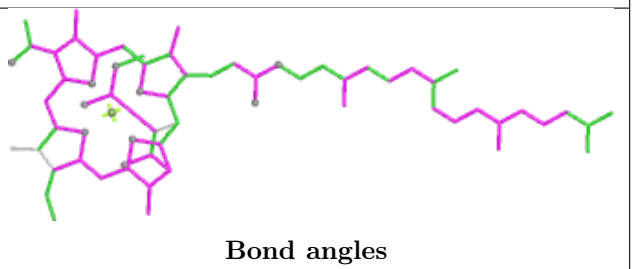

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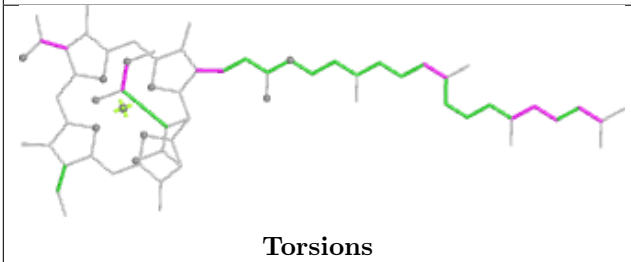
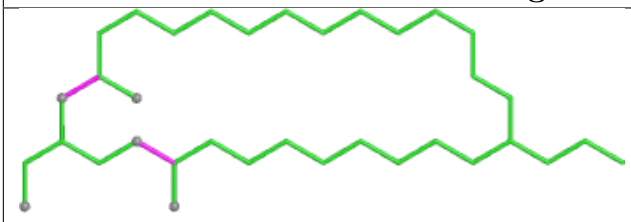


Torsions

Rings

Ligand PGV I 101



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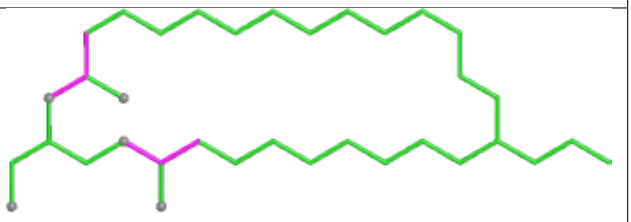

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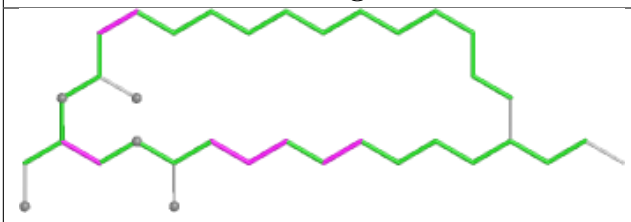

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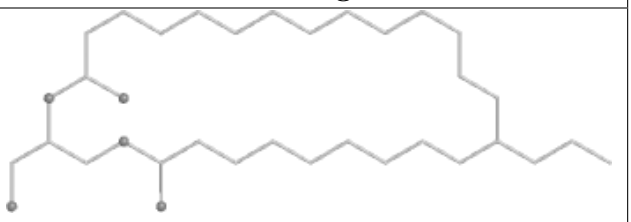
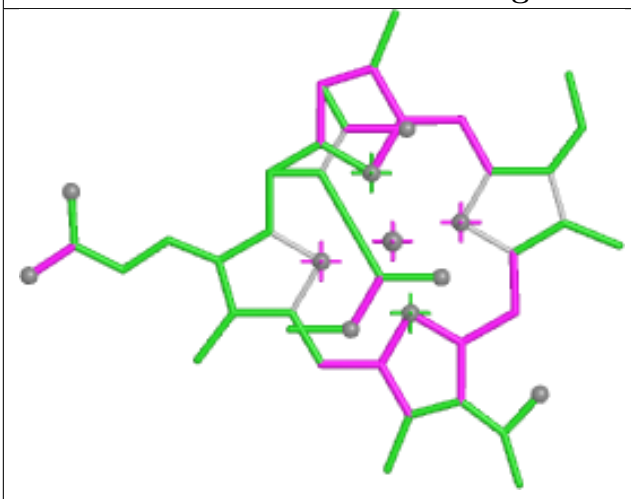


Rings

Ligand A1LZQ l 102



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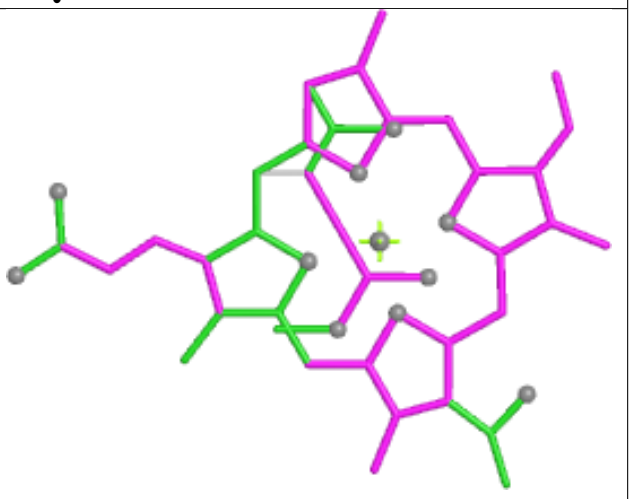

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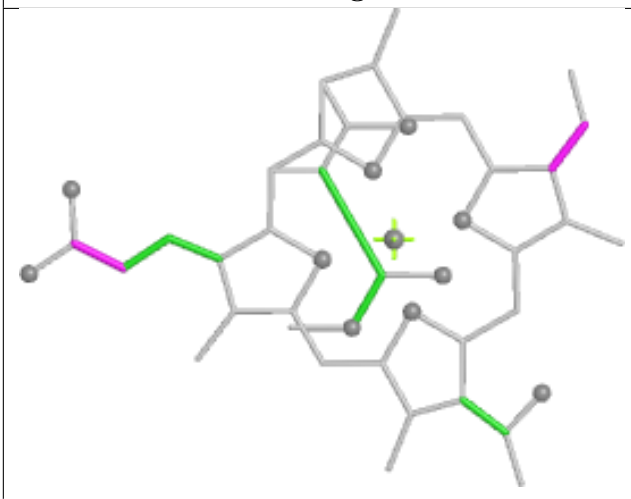

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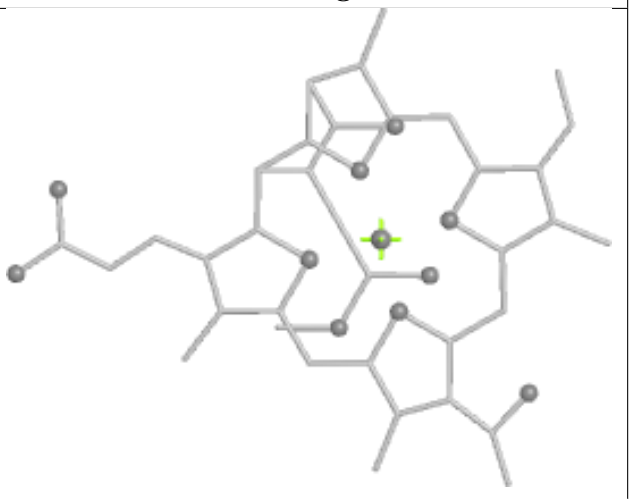
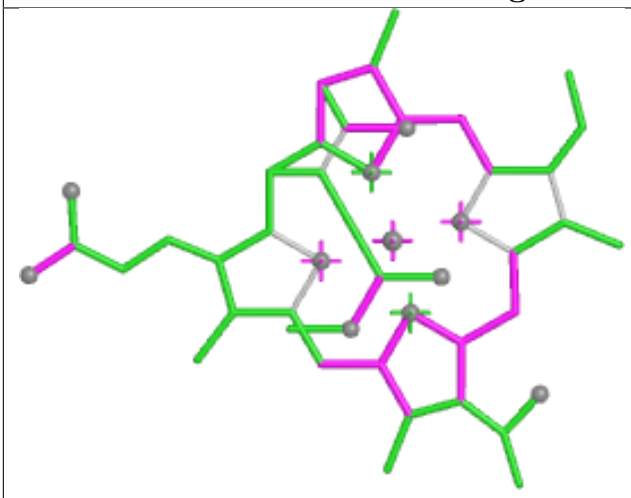


Rings

Ligand A1LZQ c 102



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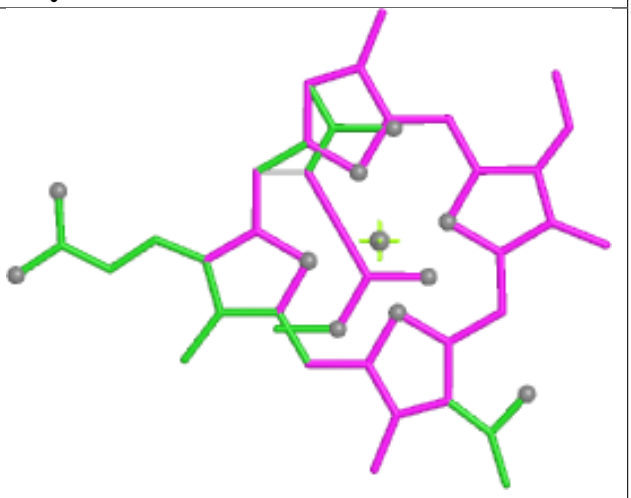

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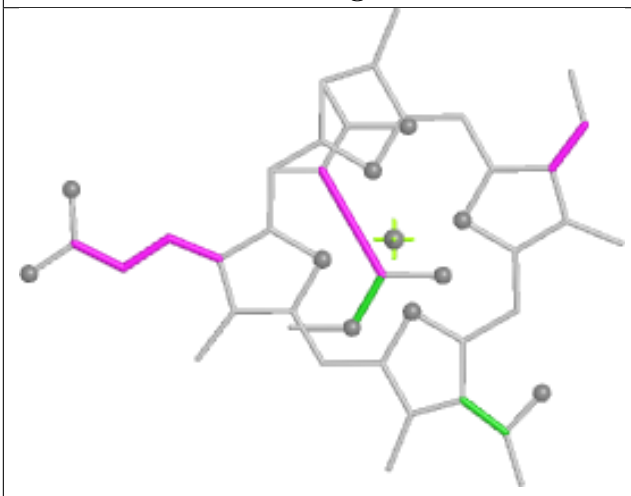

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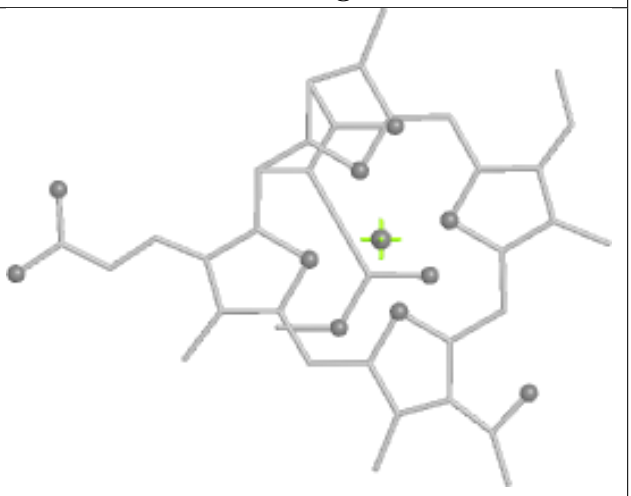
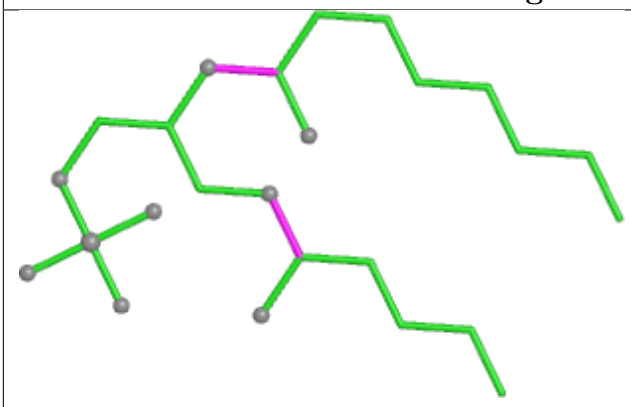


Rings

Ligand PGV 9 102



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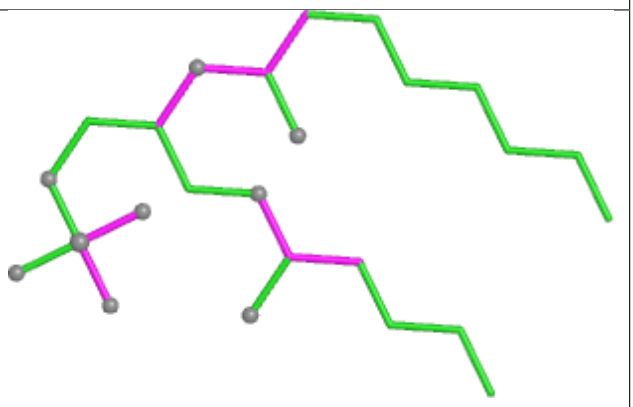

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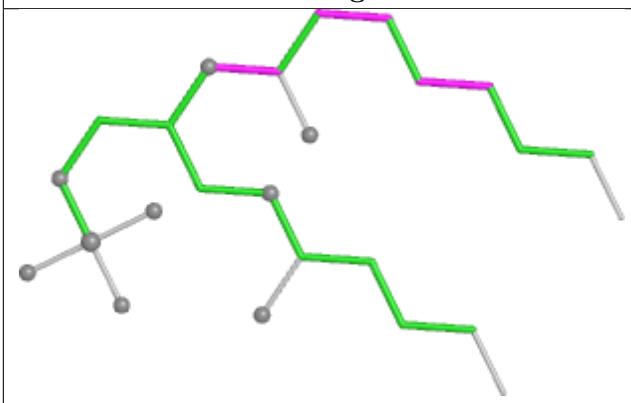

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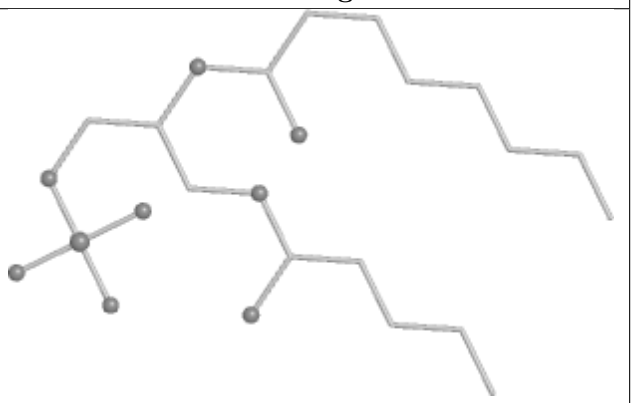
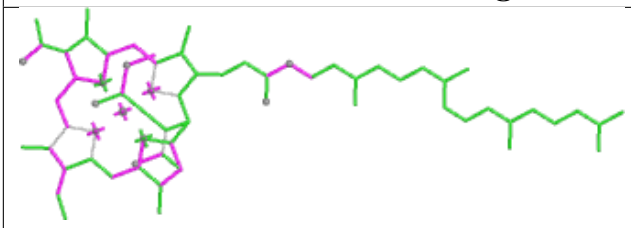


Rings

Ligand A1LZM W 101



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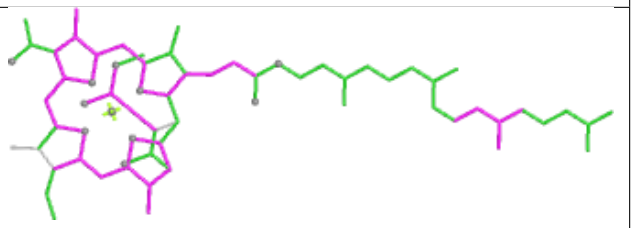

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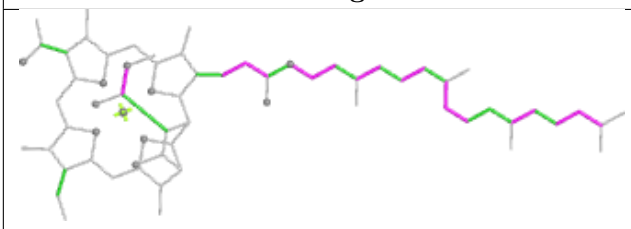

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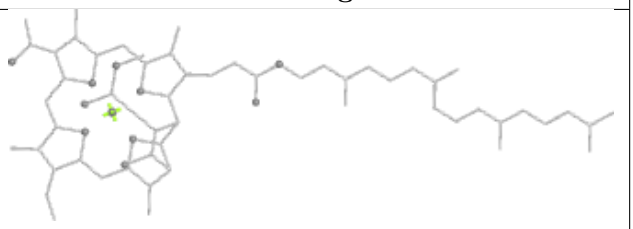
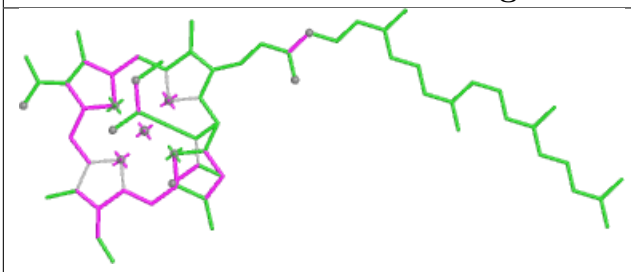
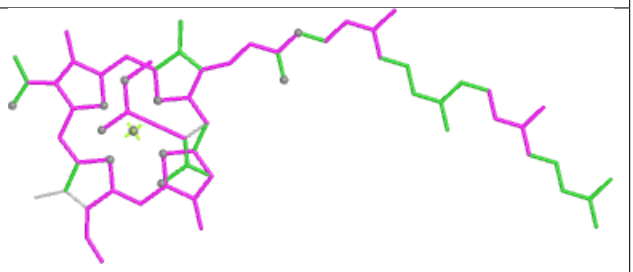
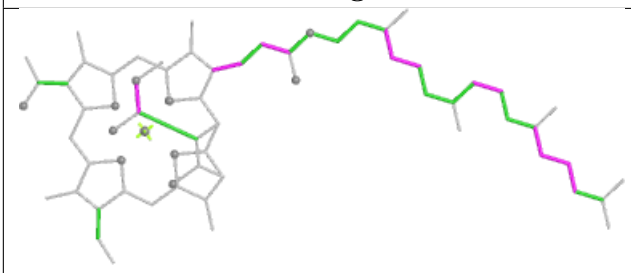
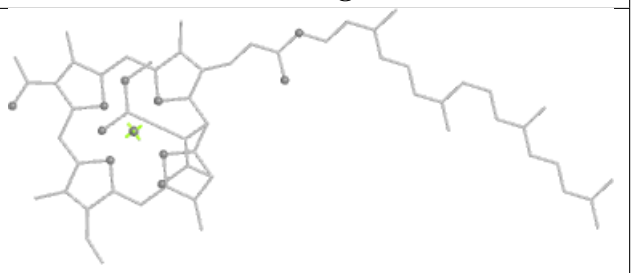
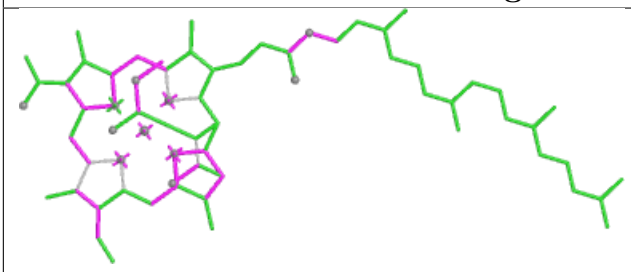
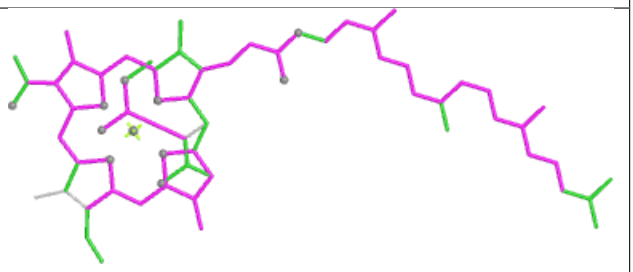
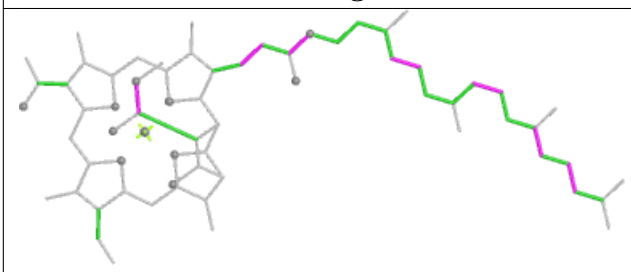
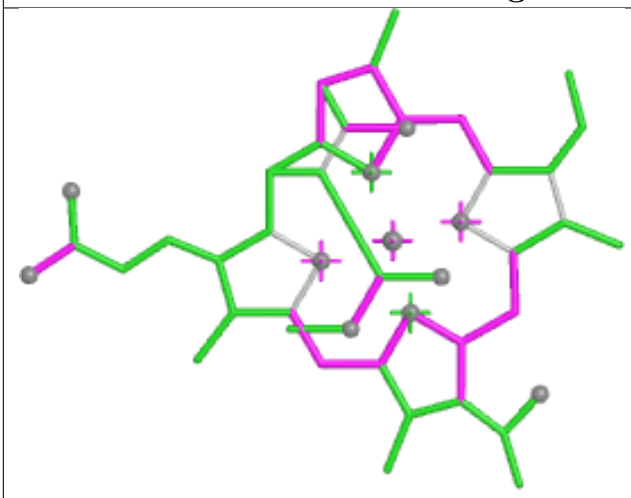


Rings

Ligand A1LZM V 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand A1LZM o 101	
 Bond lengths	 Bond angles
 Torsions	Rings

Ligand A1LZQ 7 102



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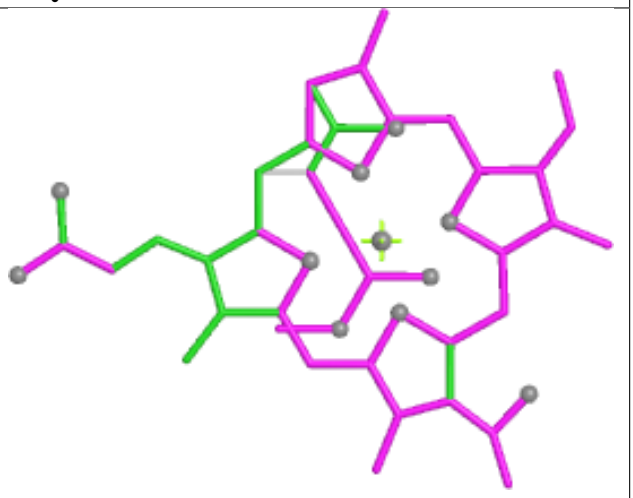

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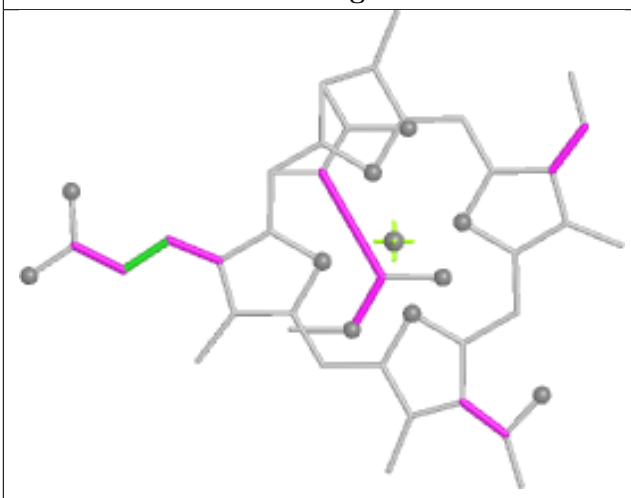
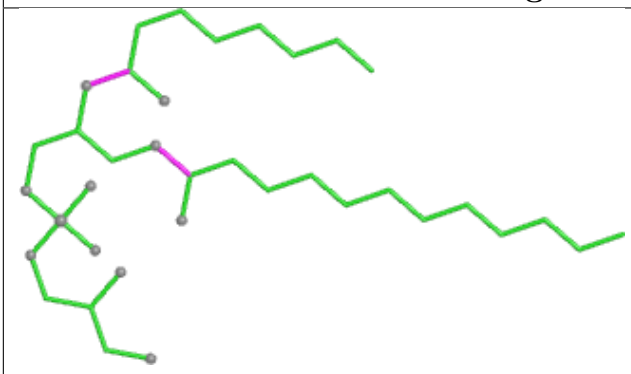


Torsions

Rings

Ligand PGV 4 203



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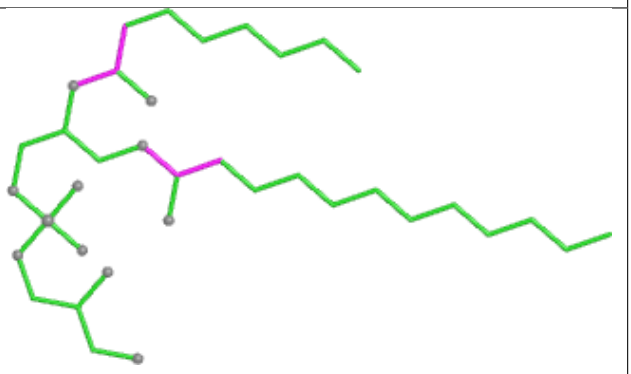

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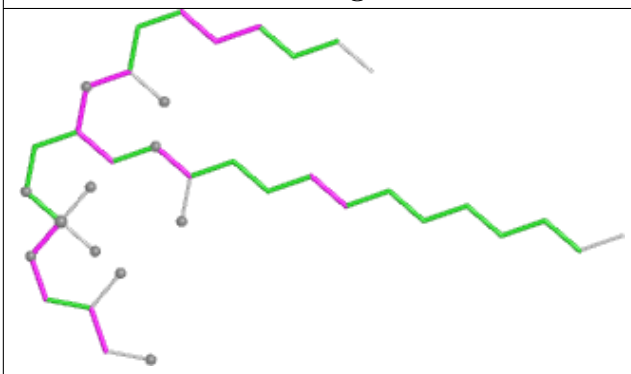

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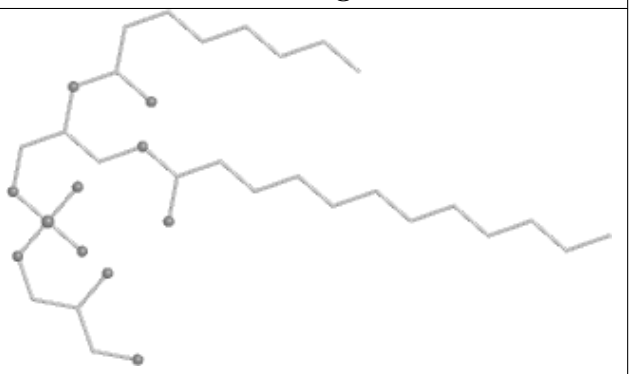
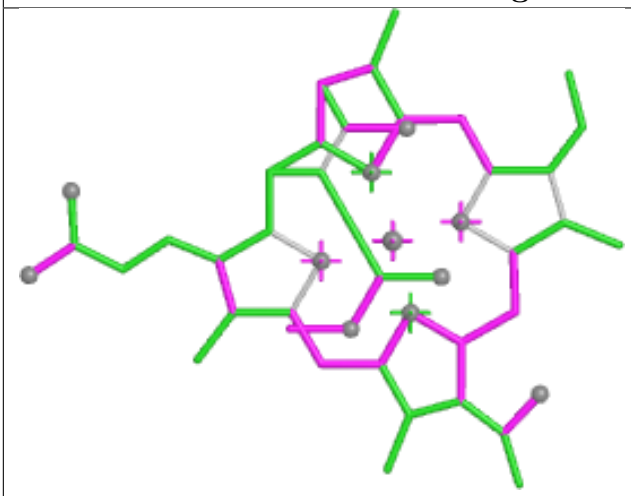


Rings

Ligand A1LZQ f 102



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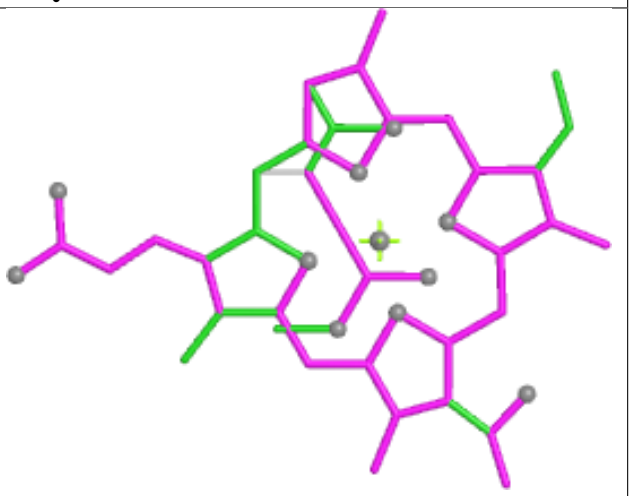

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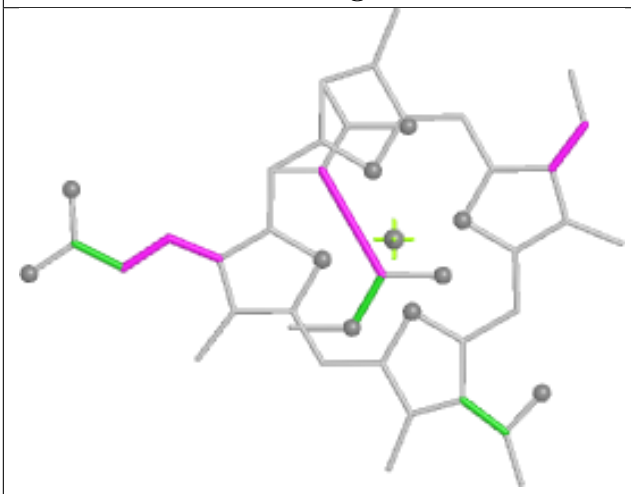

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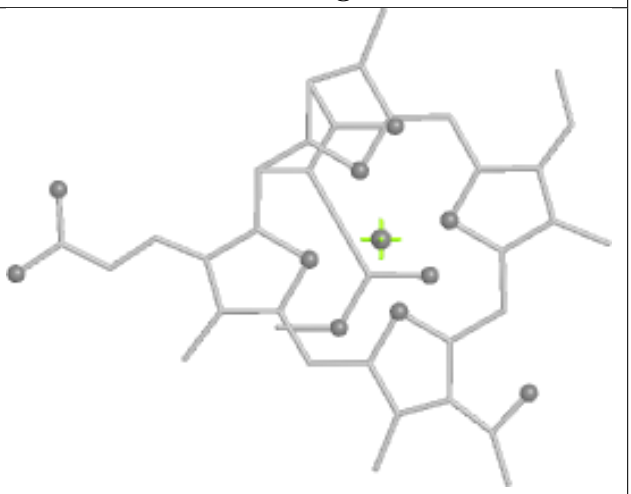
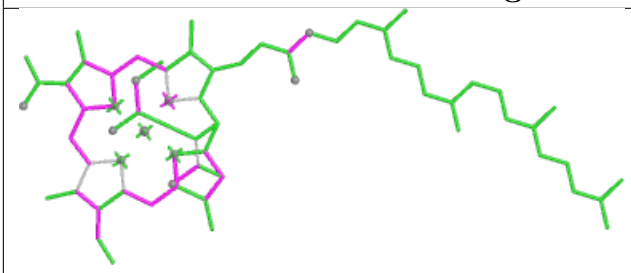


Rings

Ligand A1LZM 1 101



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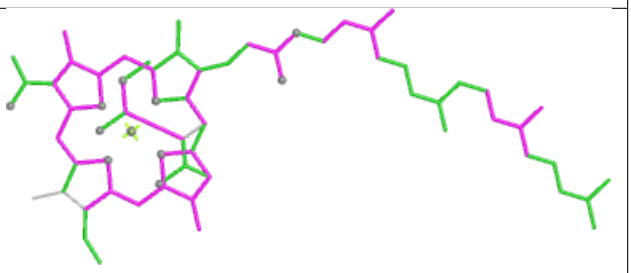
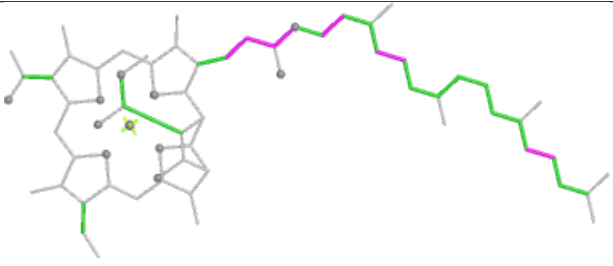


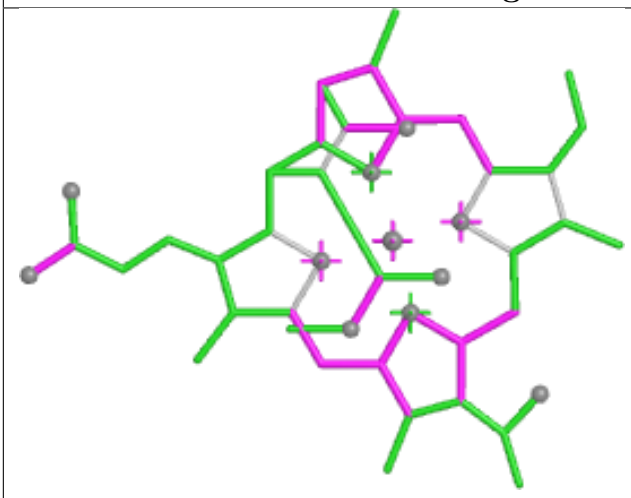
Bond angles



Torsions

Rings

Ligand A1LZQ G 102



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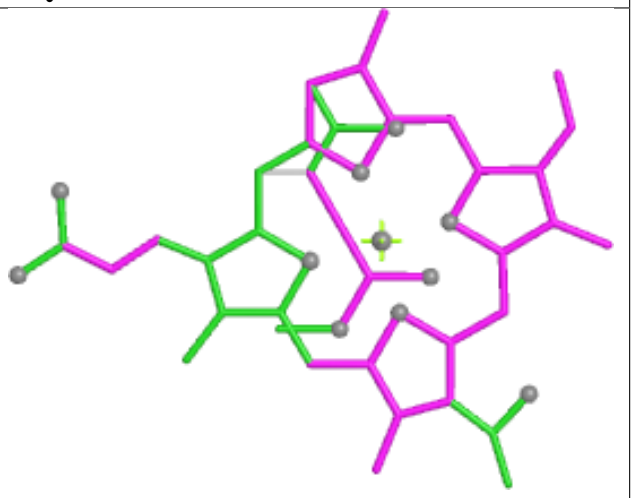
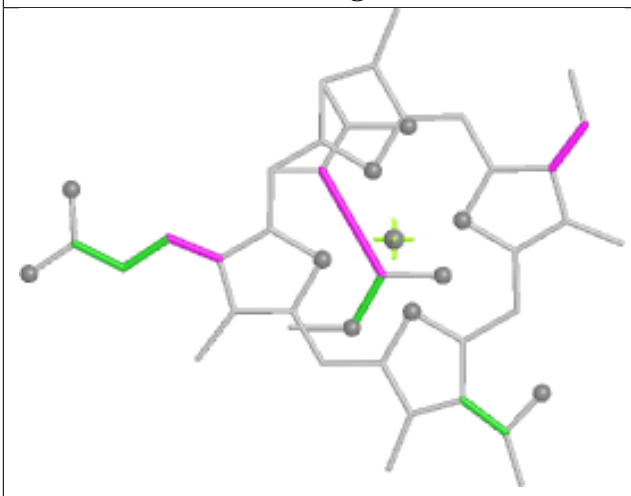
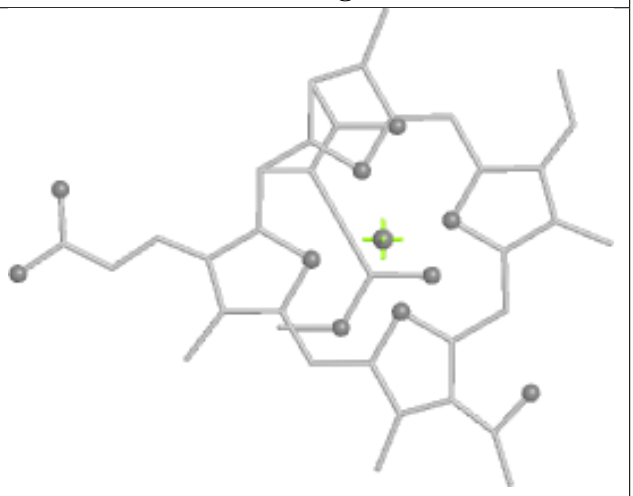


Bond angles

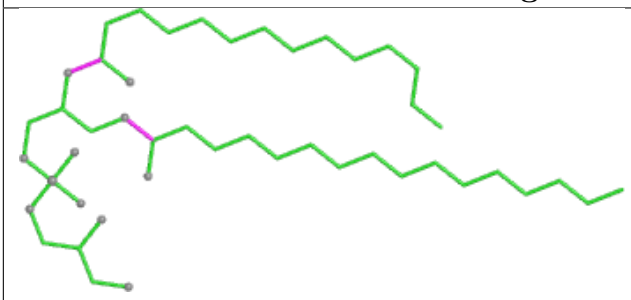


Torsions

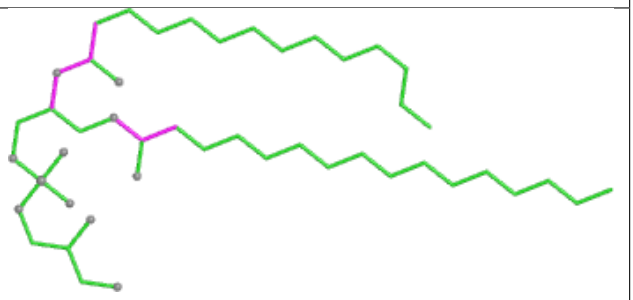


Rings

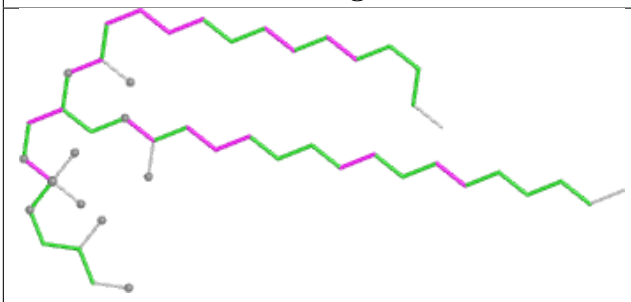
Ligand PGV H 303



Bond lengths



Bond angles



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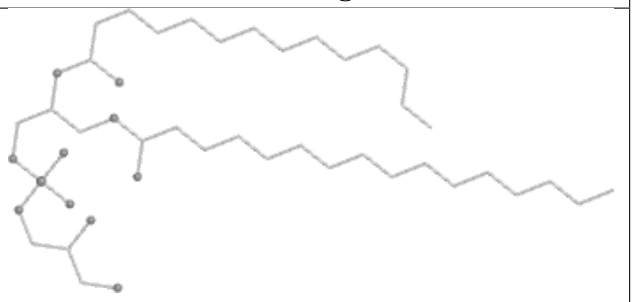
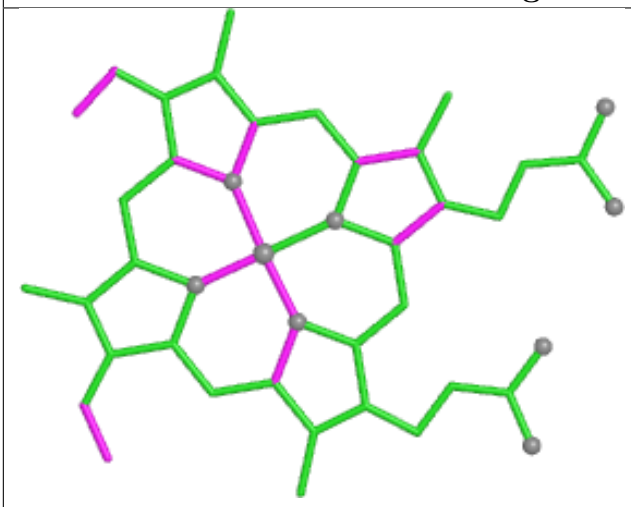


Rings

Ligand HEC C 403



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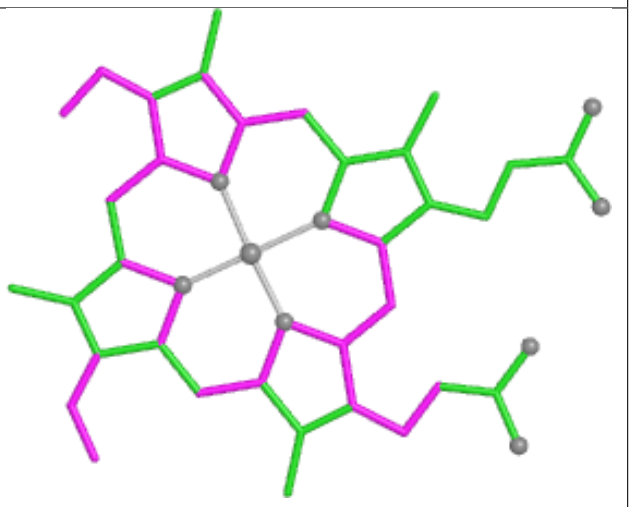
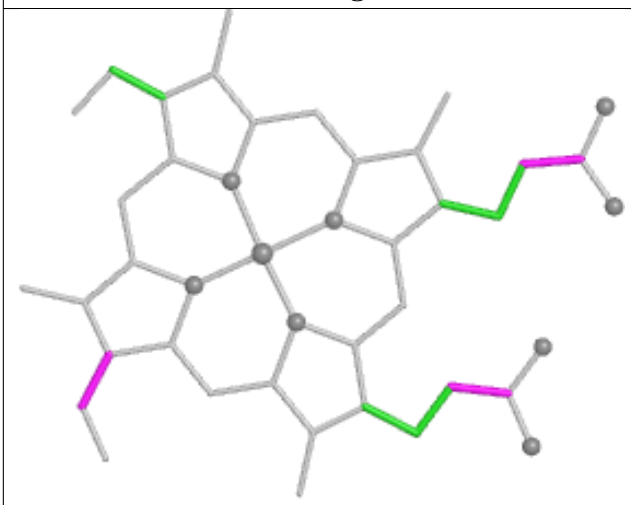


Bond angles



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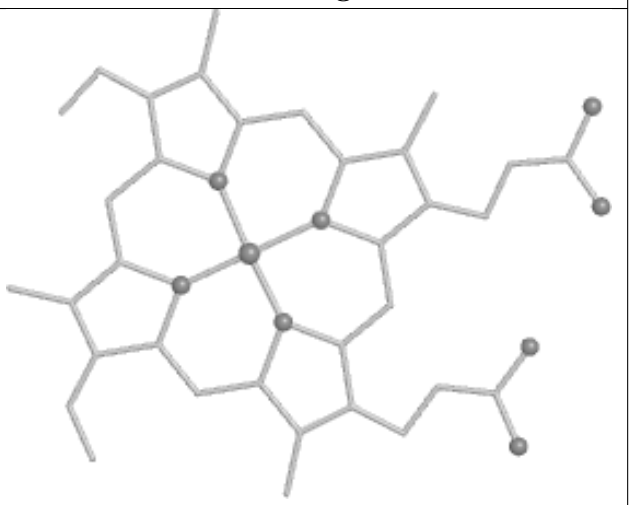
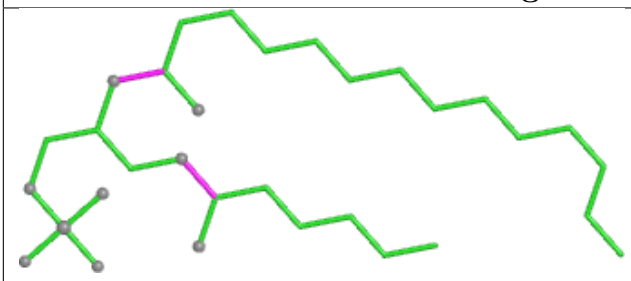


Rings

Ligand PGV C 407



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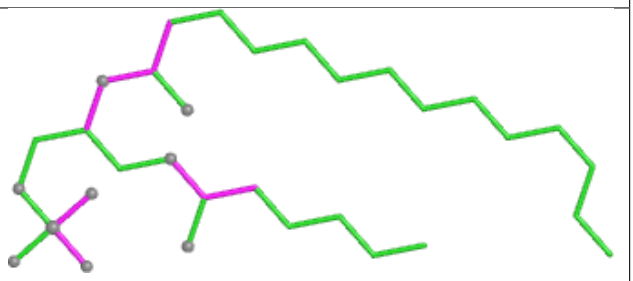
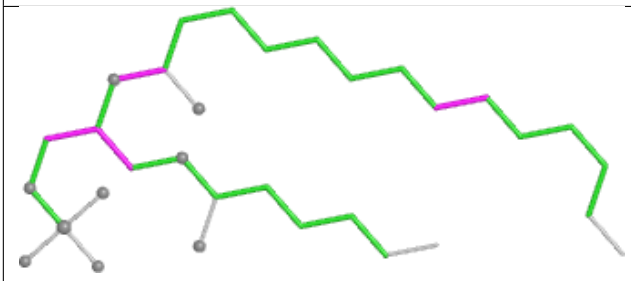


Bond angles



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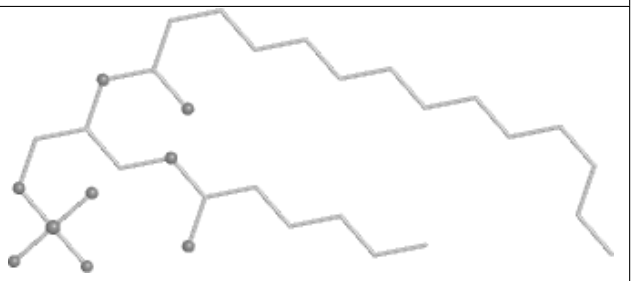
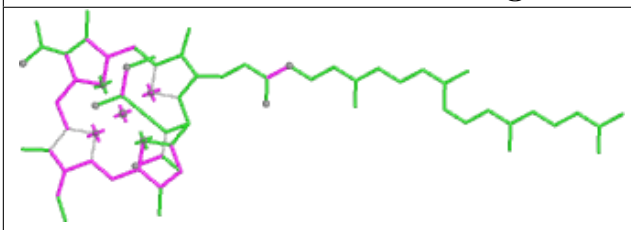


Rings

Ligand A1LZM t 101



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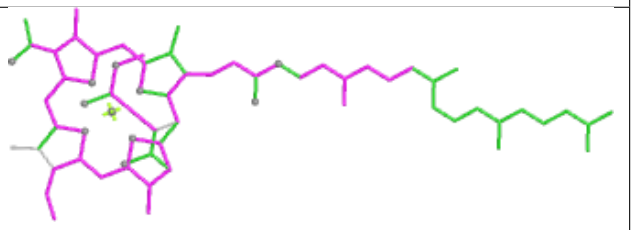
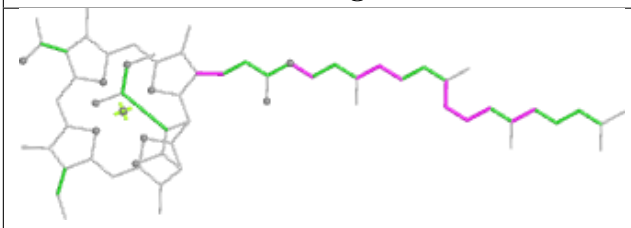


Bond angles



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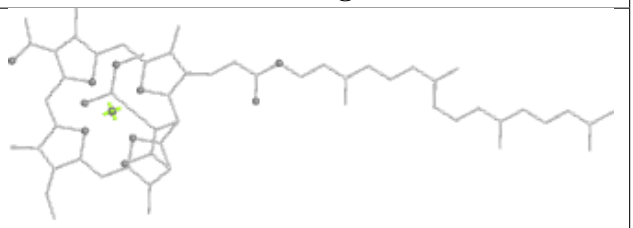
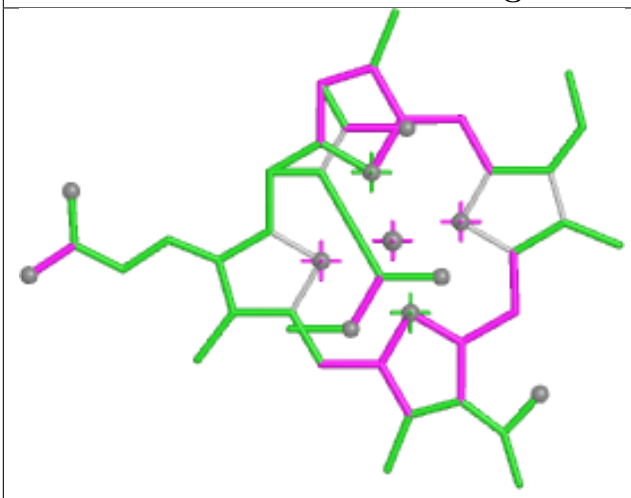


Rings

Ligand A1LZQ T 101



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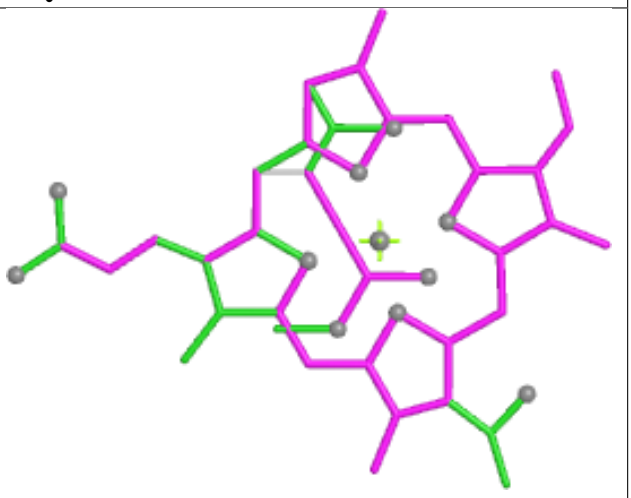
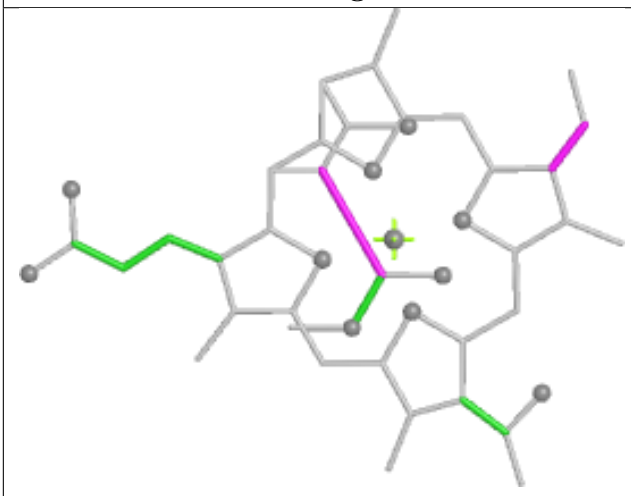


Bond angles



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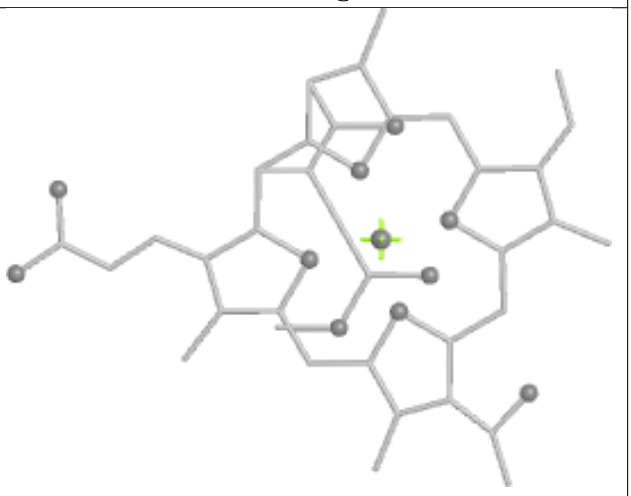
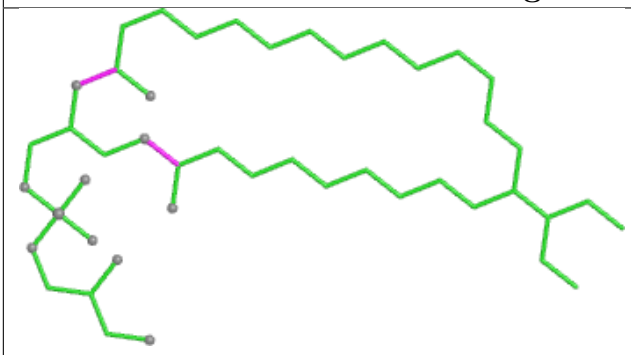


Rings

Ligand PGV L 305



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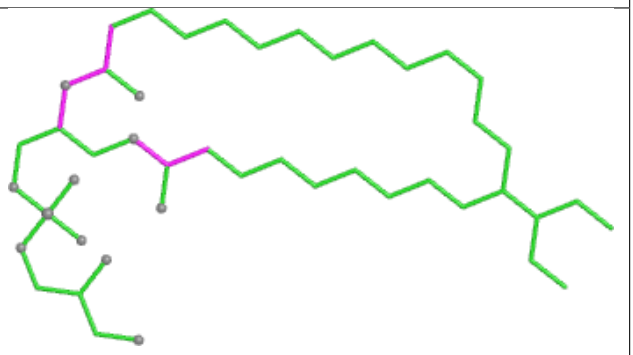
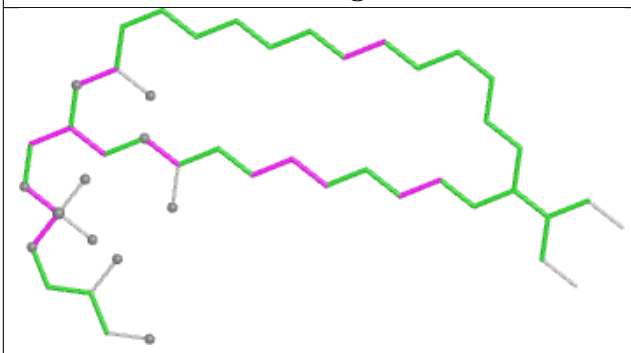


Bond angles



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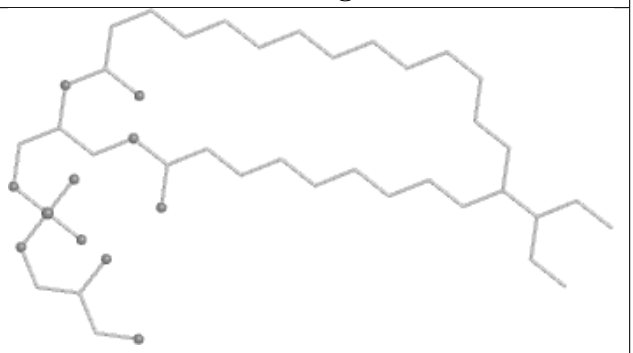
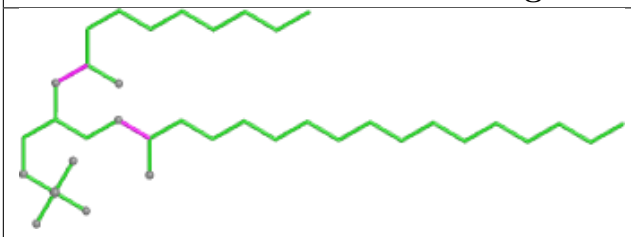


Rings

Ligand PGV n 104



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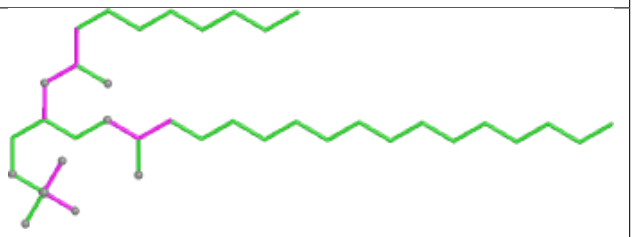
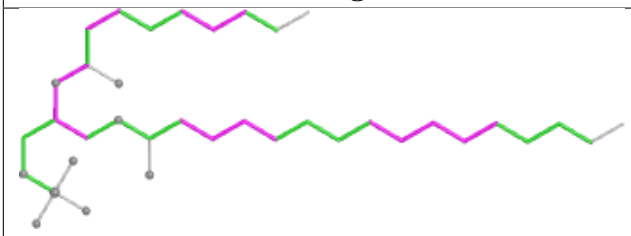


Bond angles



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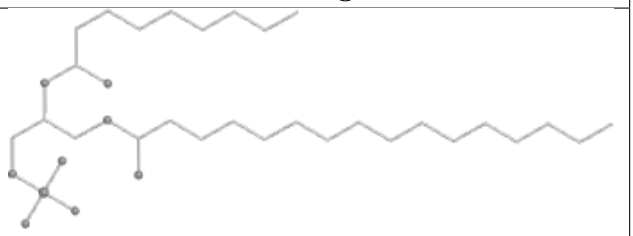
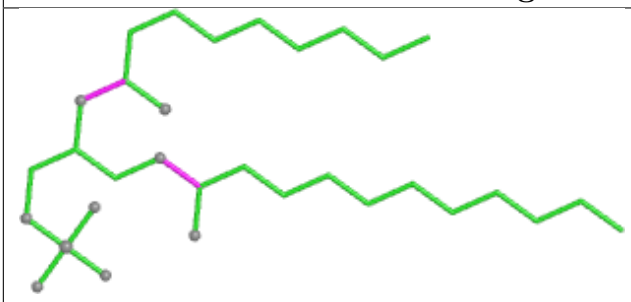


Rings

Ligand PGV M 707



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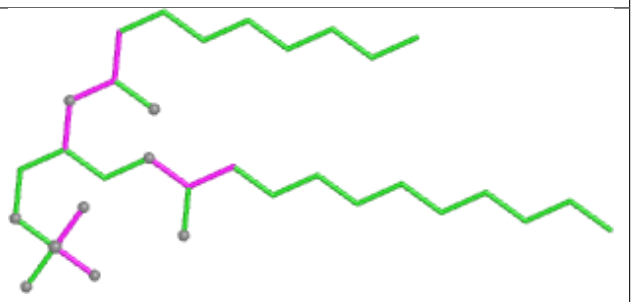
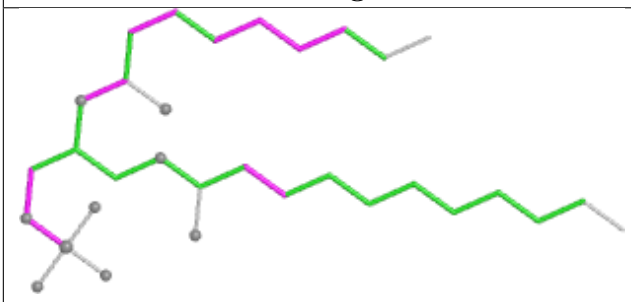
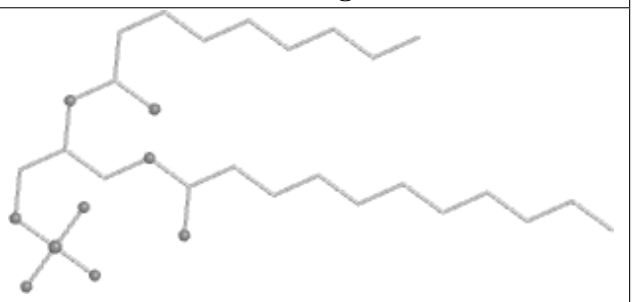


Bond angles

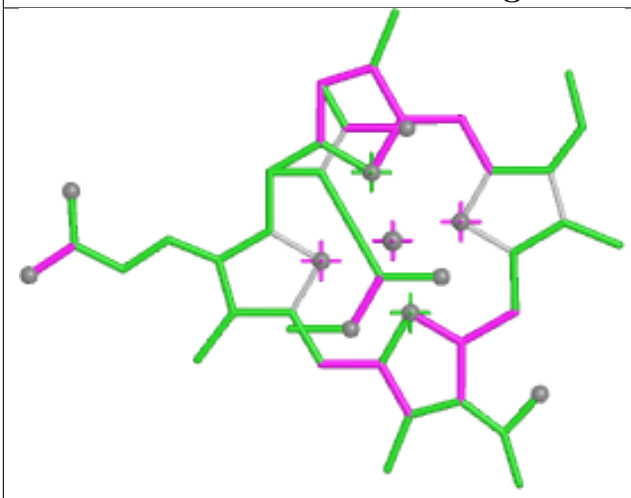


Torsions



Rings

Ligand A1LZQ Q 101



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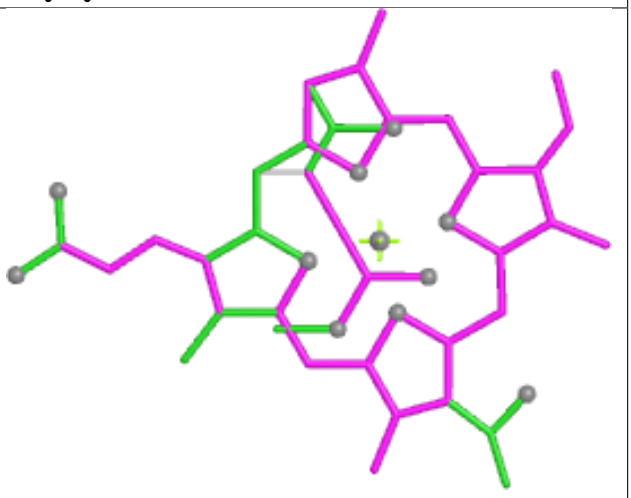
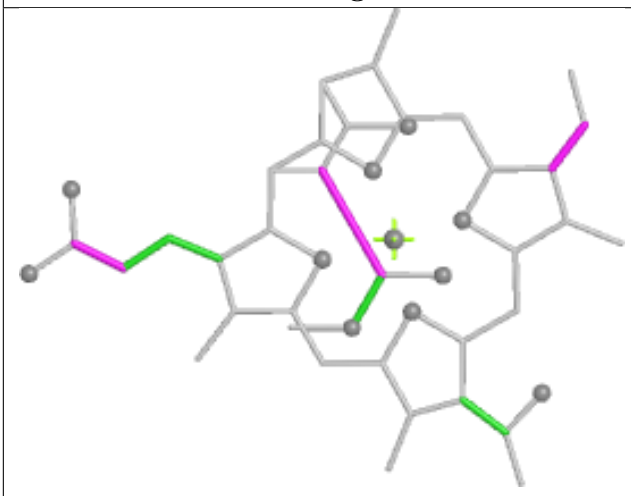


Bond angles



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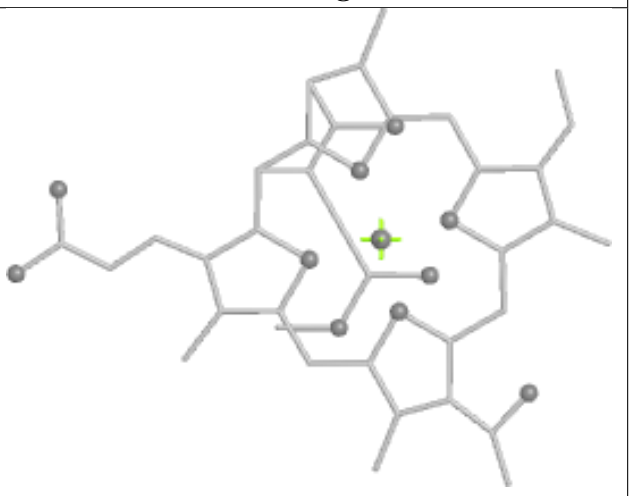
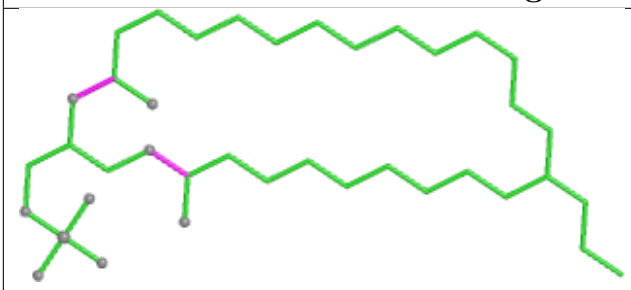


Rings

Ligand PGV q 104



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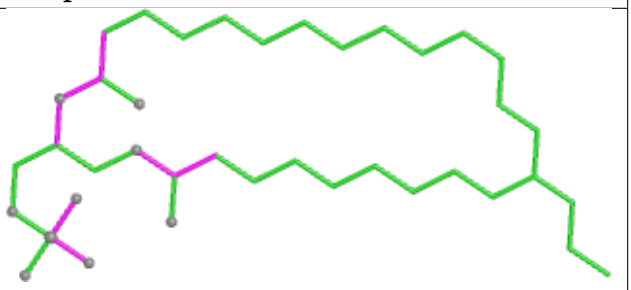
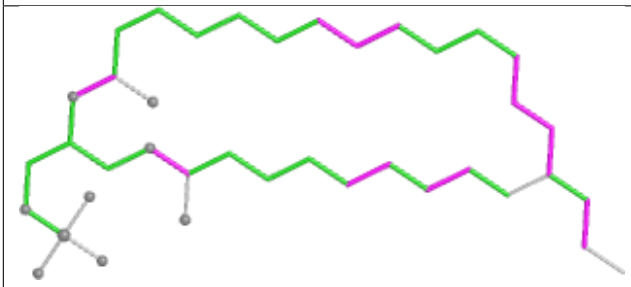


Bond angles



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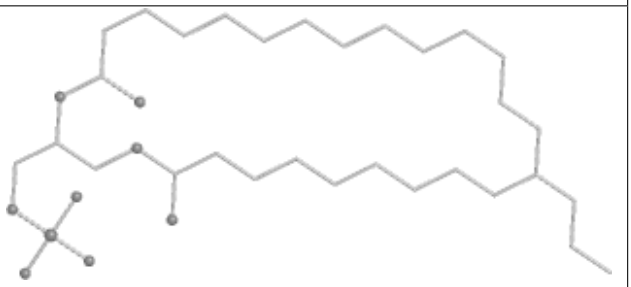
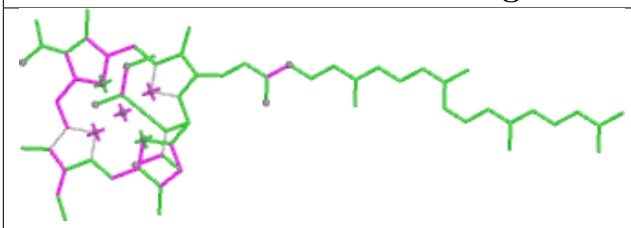


Rings

Ligand A1LZM Z 101



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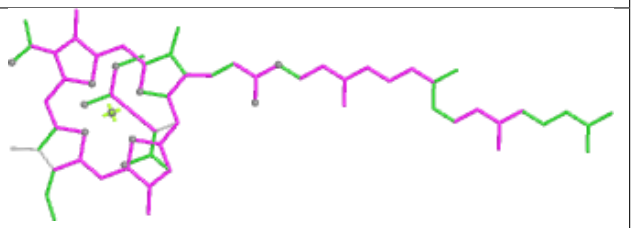
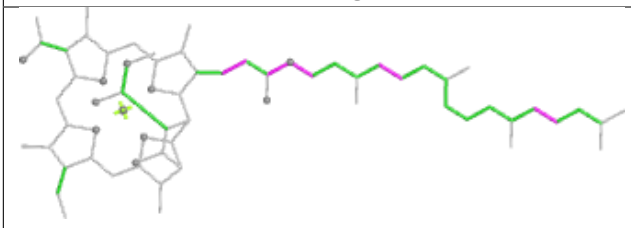


Bond angles



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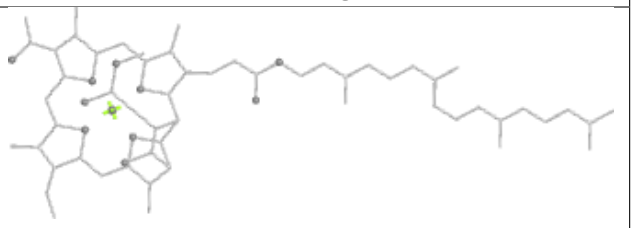
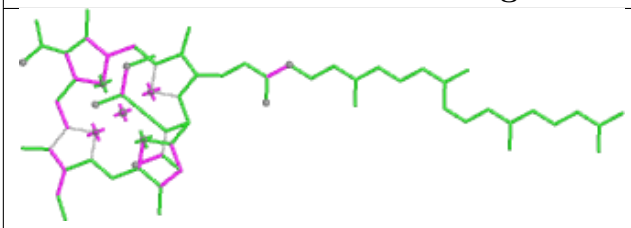


Rings

Ligand A1LZM w 102



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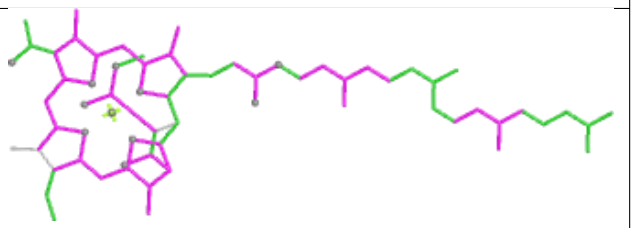
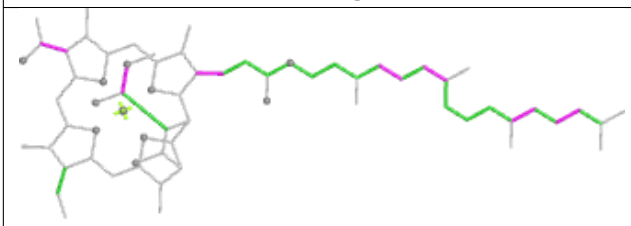


Bond angles



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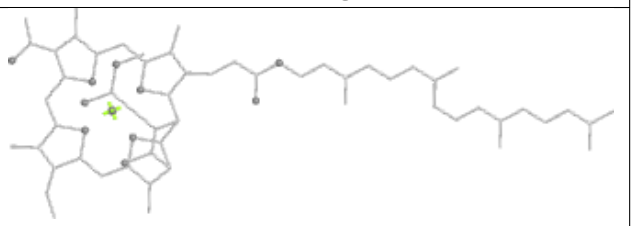
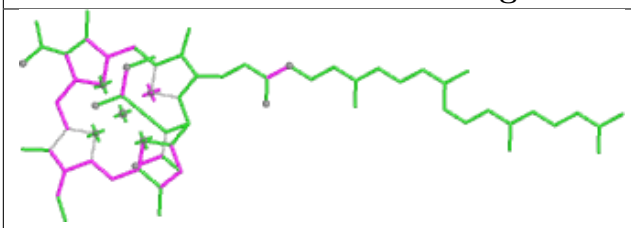
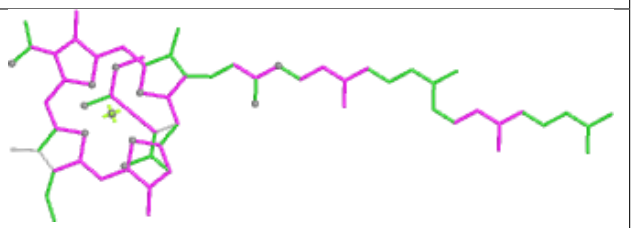


Rings

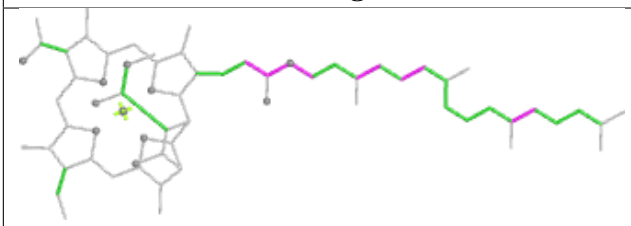
Ligand A1LZM Y 101



Bond lengths



Bond angles



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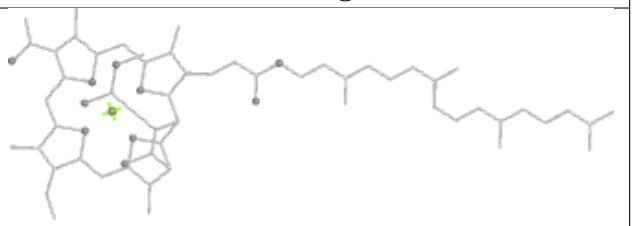
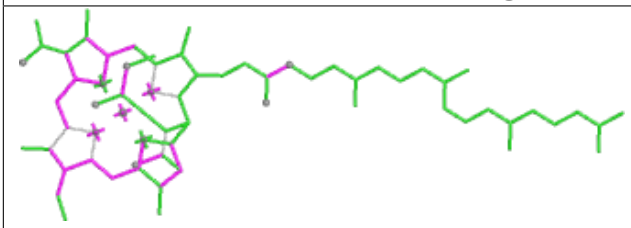


Rings

Ligand A1LZM w 101



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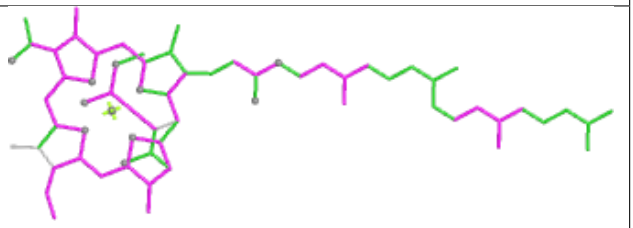

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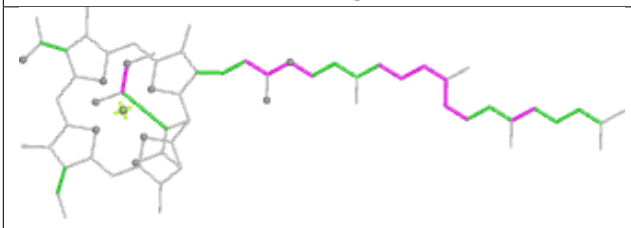
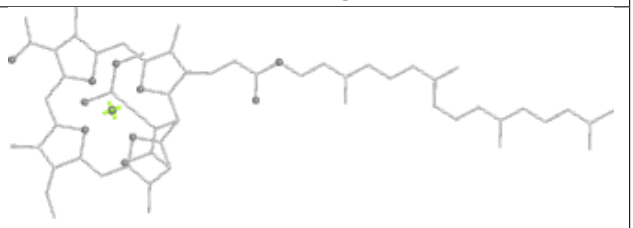
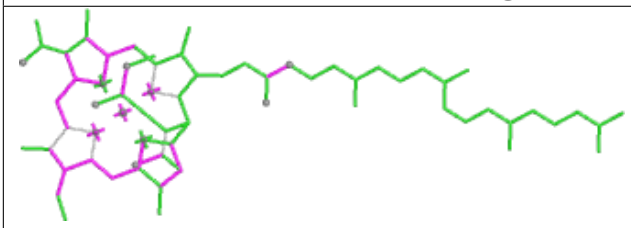


Torsions



Rings

Ligand A1LZM K 101



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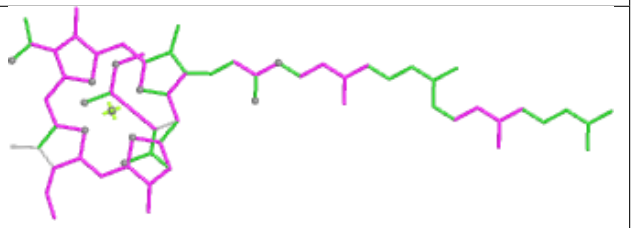

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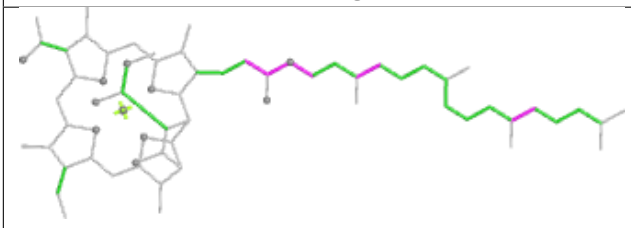

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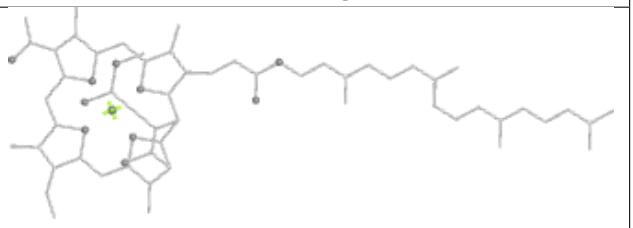
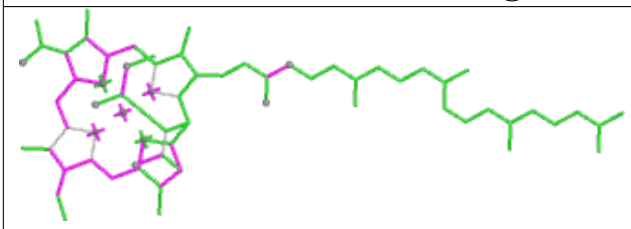


Rings

Ligand A1LZM S 101



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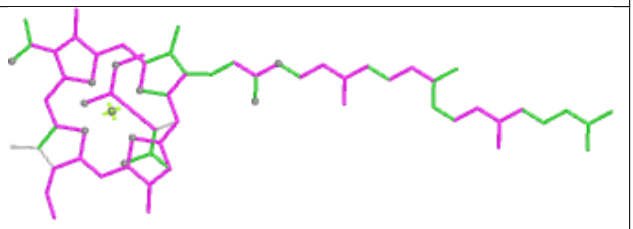

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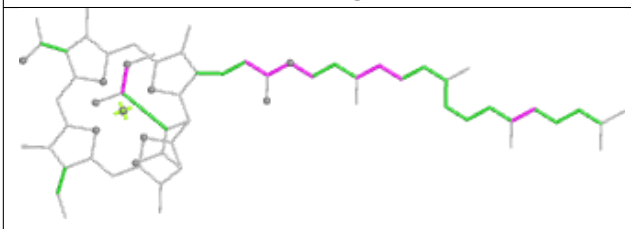

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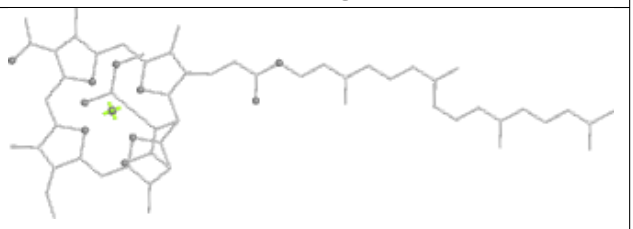
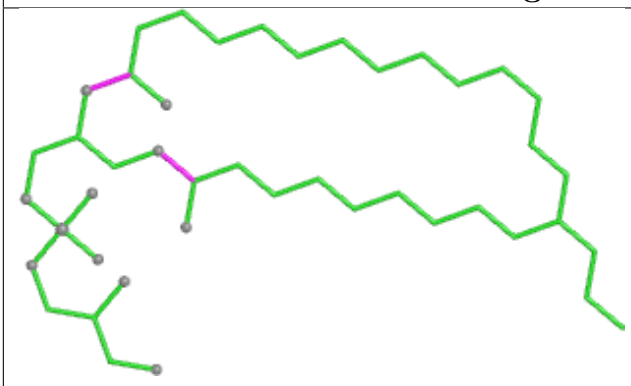


Rings

Ligand PGV L 306



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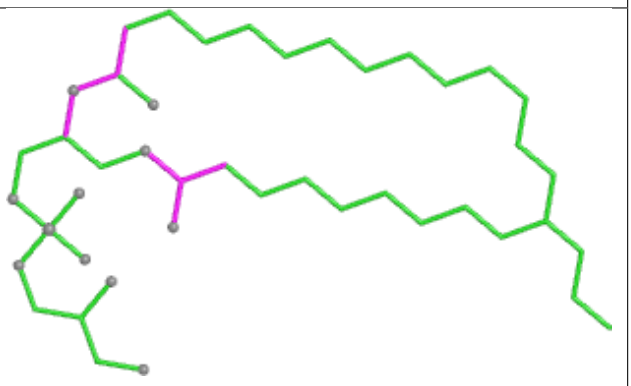

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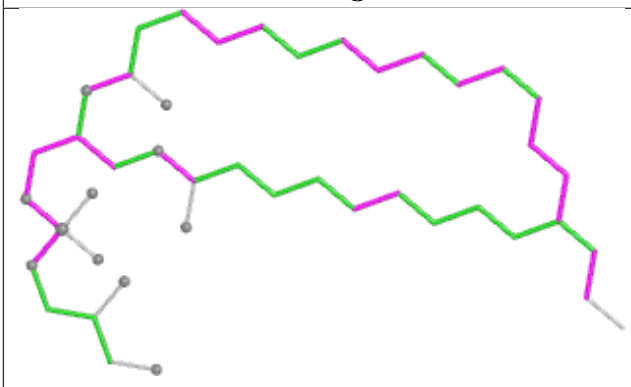

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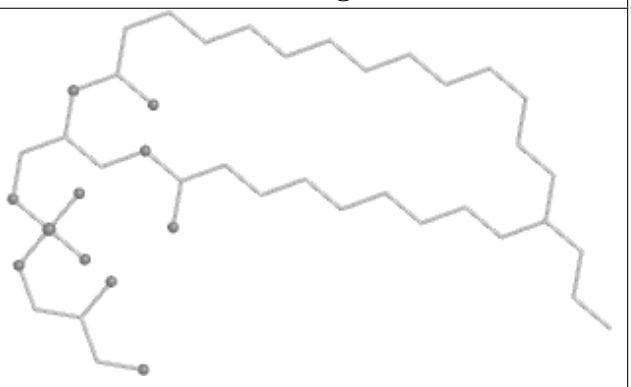
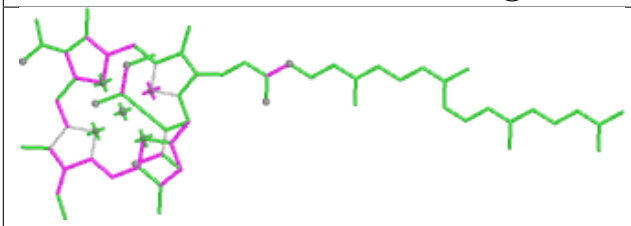


Rings

Ligand A1LZM b 102



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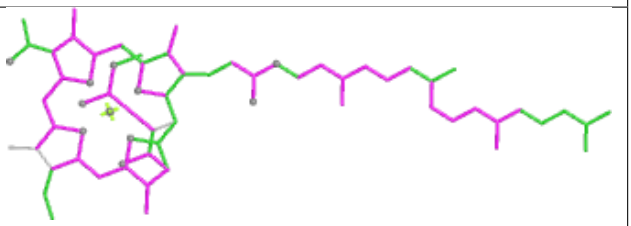

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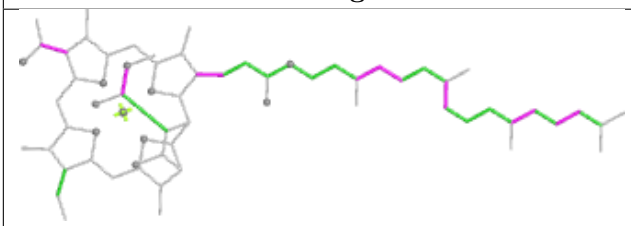

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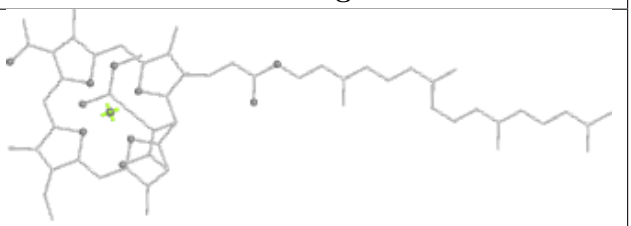
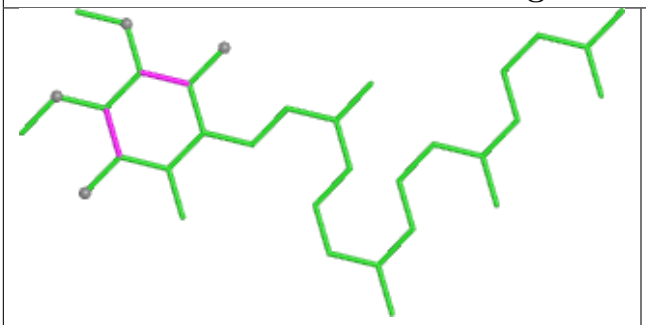


Rings

Ligand UQ8 L 304



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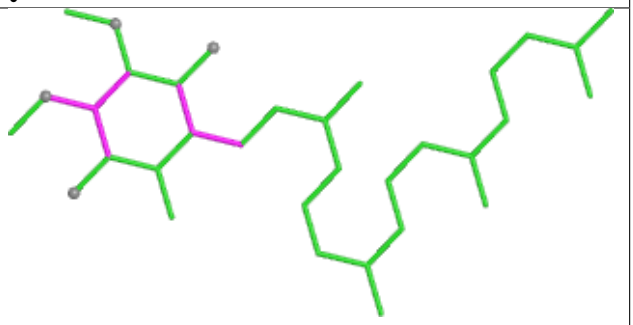

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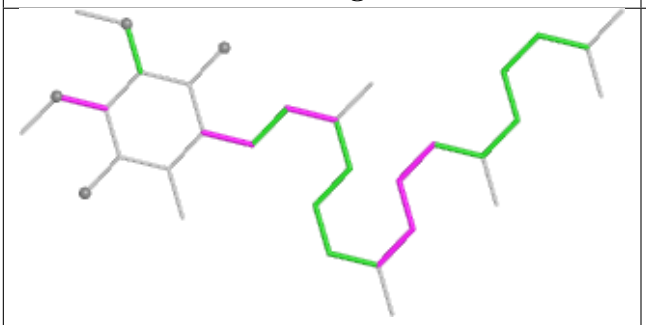

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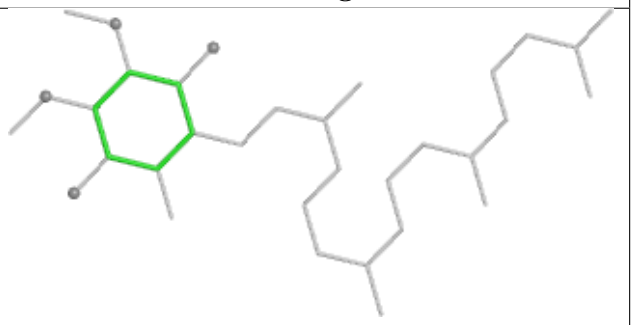
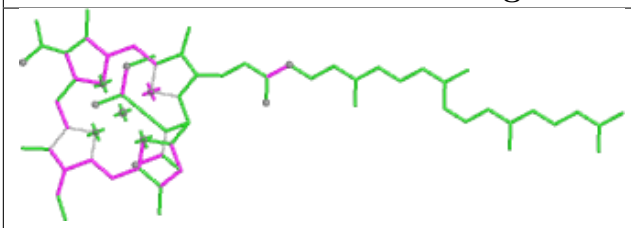


Rings

Ligand A1LZM n 102



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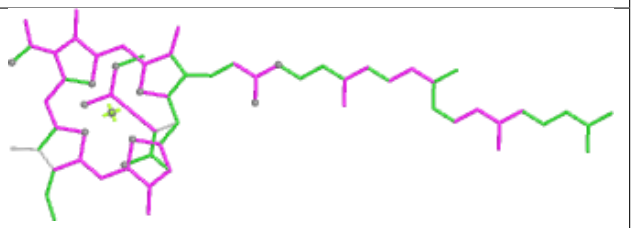

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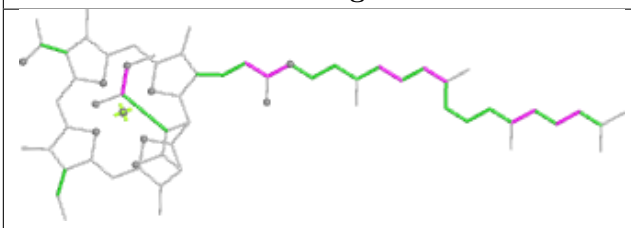

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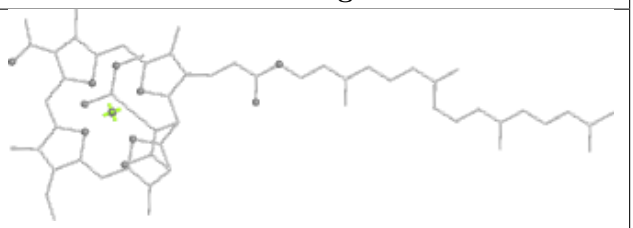
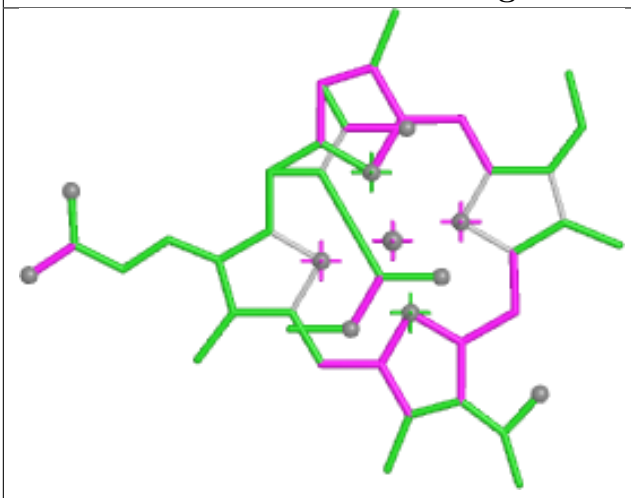


Rings

Ligand A1LZQ W 102



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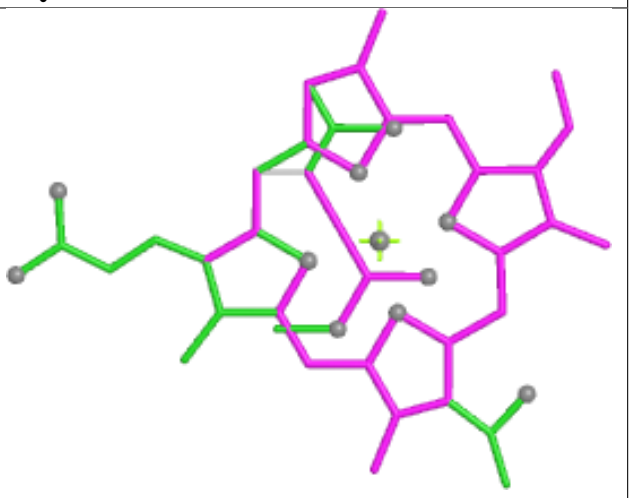

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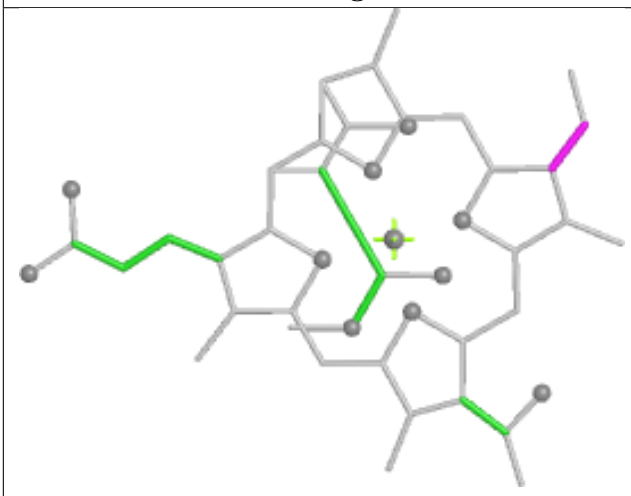

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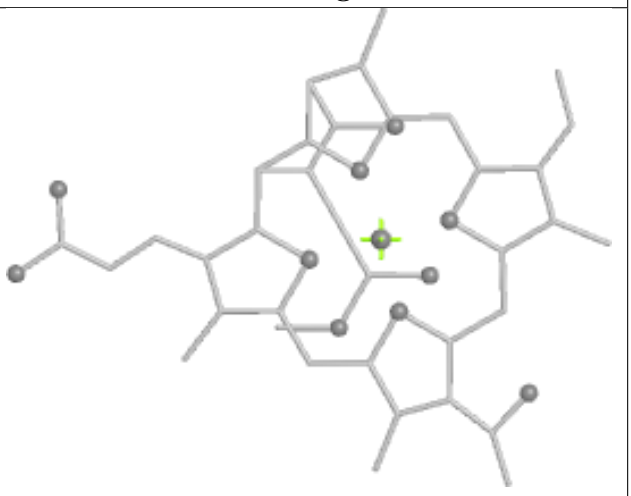
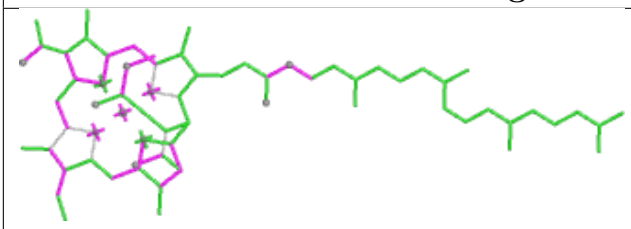


Rings

Ligand A1LZM l 101



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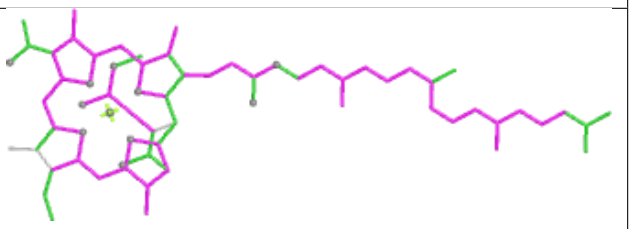

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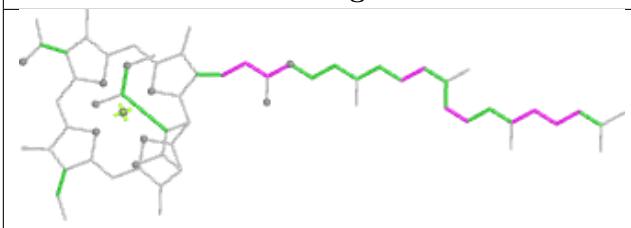

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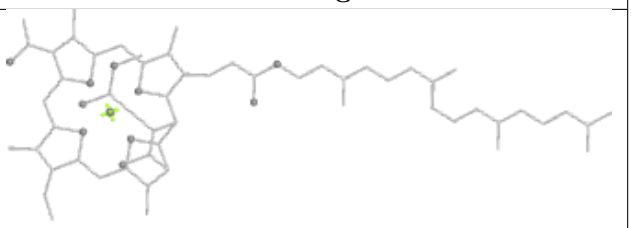
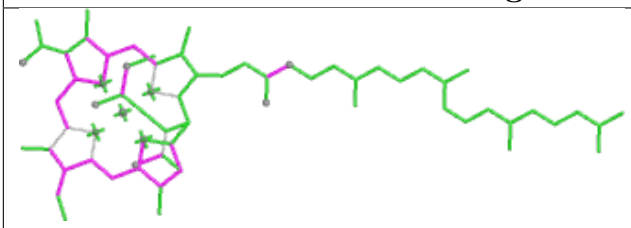


Rings

Ligand A1LZM c 101



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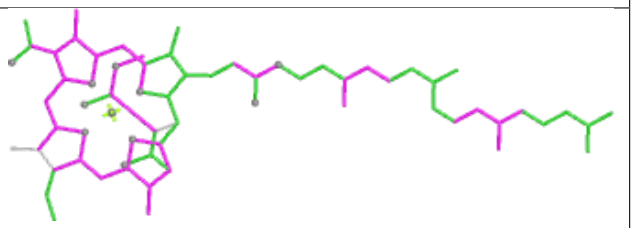

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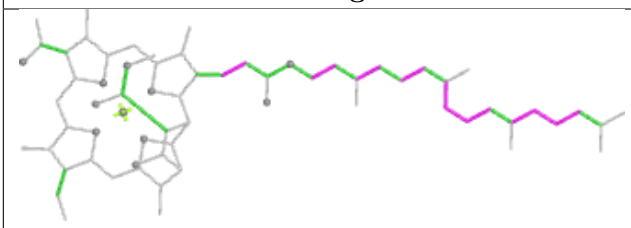

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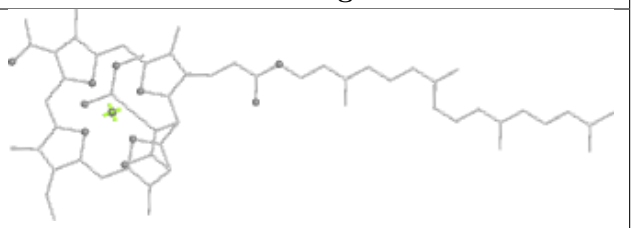
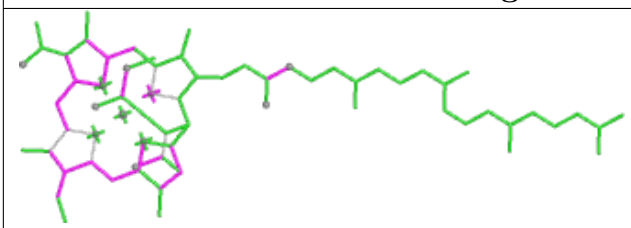


Rings

Ligand A1LZM P 101



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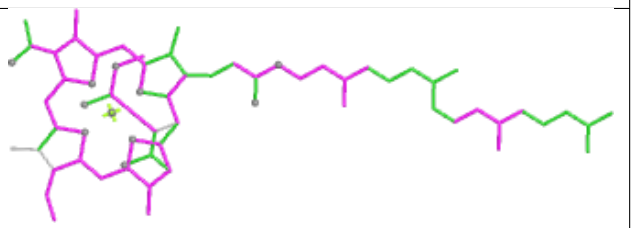

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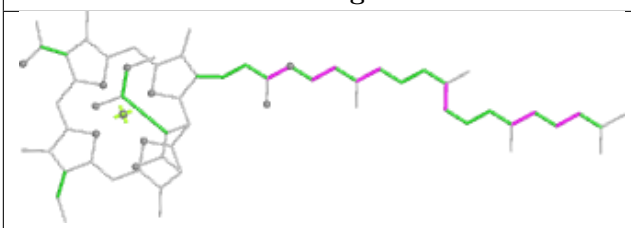

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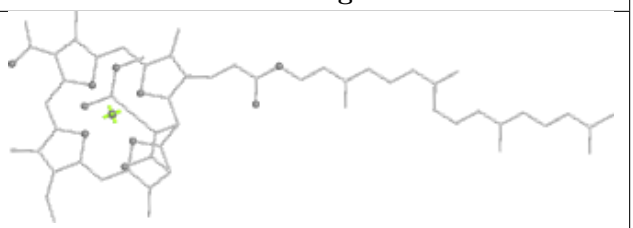
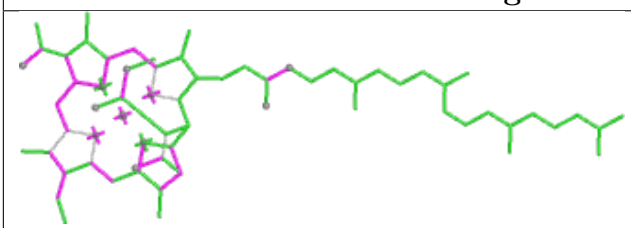


Rings

Ligand A1LZM k 101



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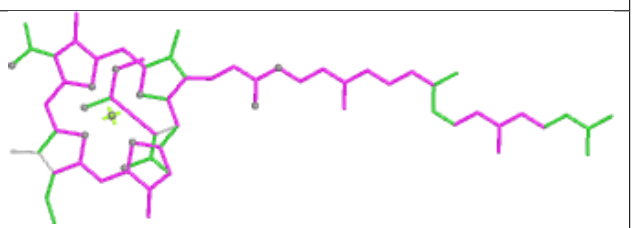

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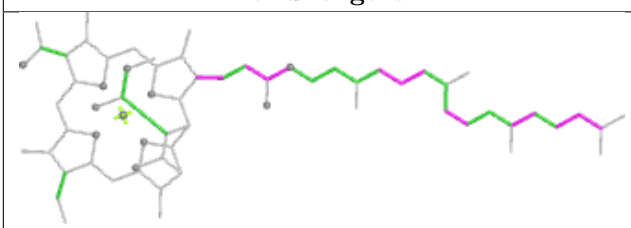

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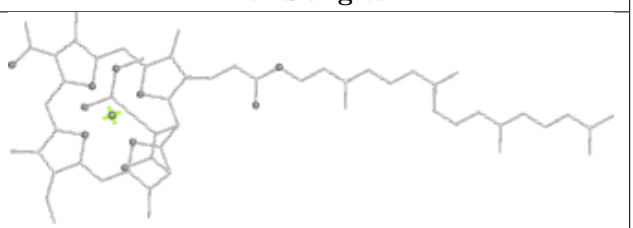
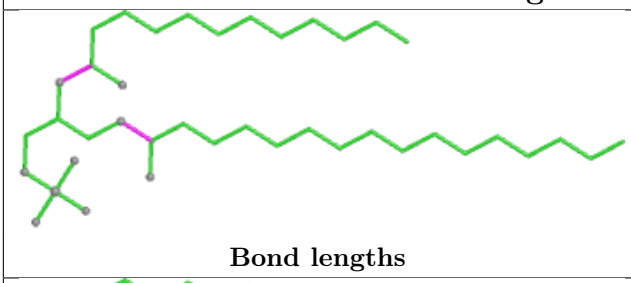


Rings

Ligand PGV e 103



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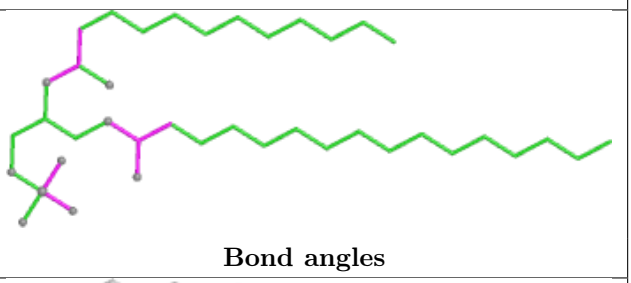
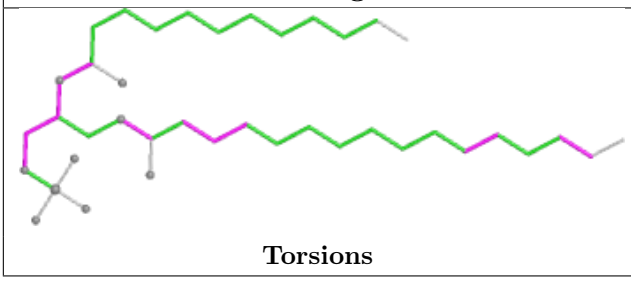


Bond angles



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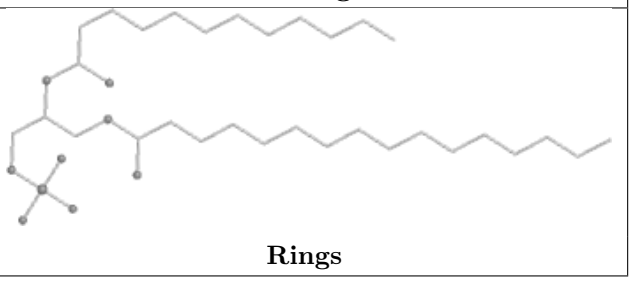
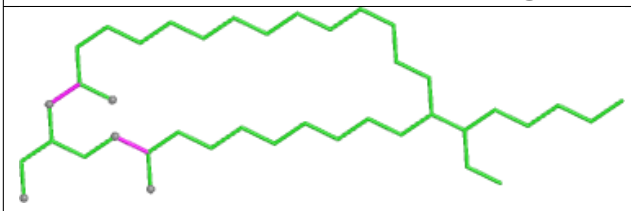


Rings

Ligand PGV U 104



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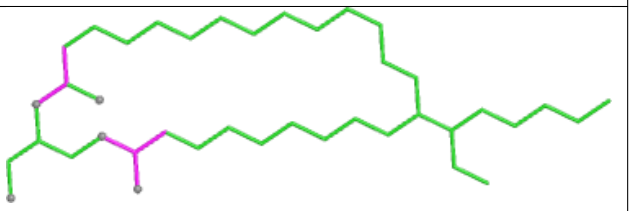
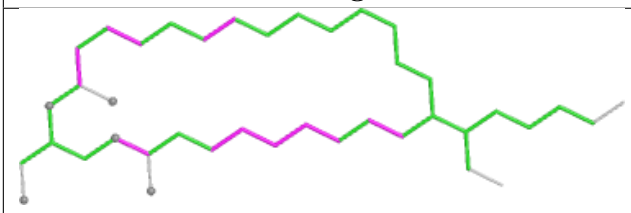
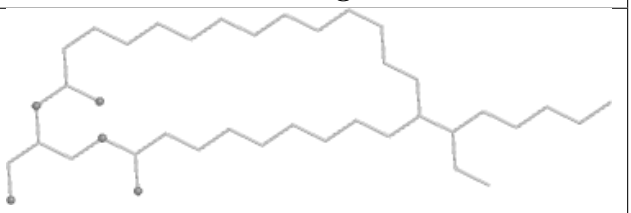


Bond angles

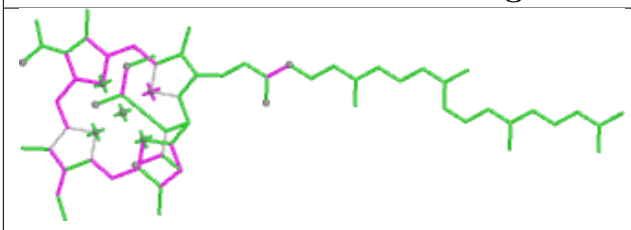


Torsions

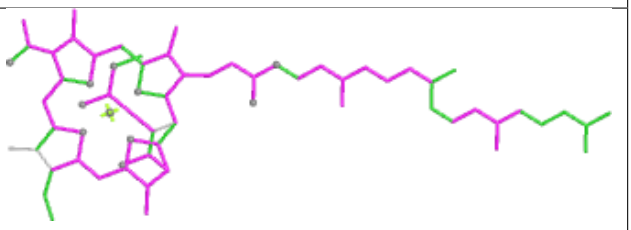


Rings

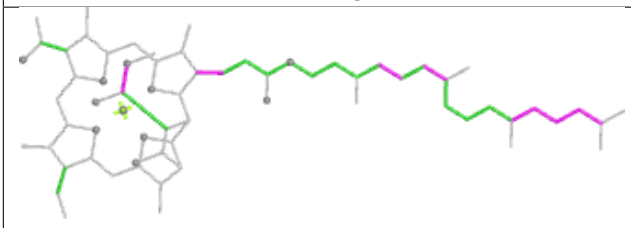
Ligand A1LZM e 102



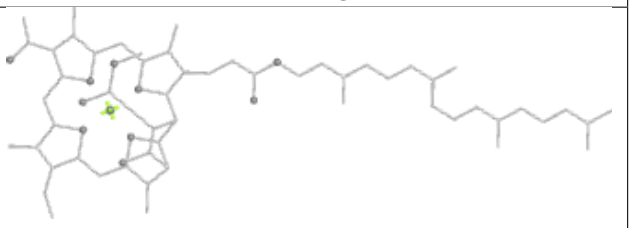
Bond lengths



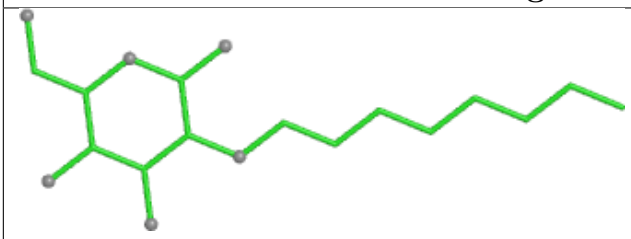
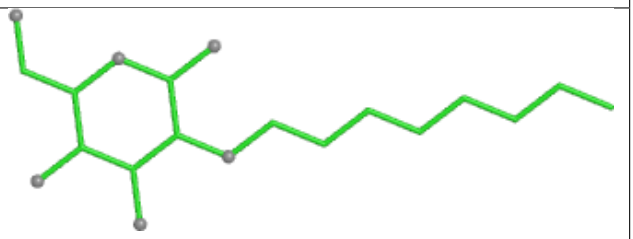
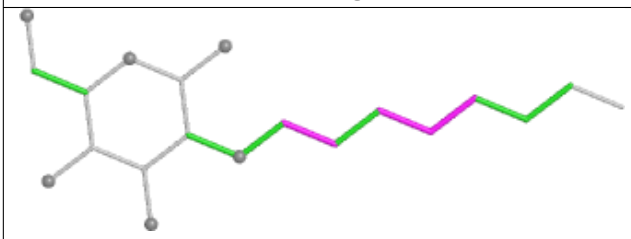
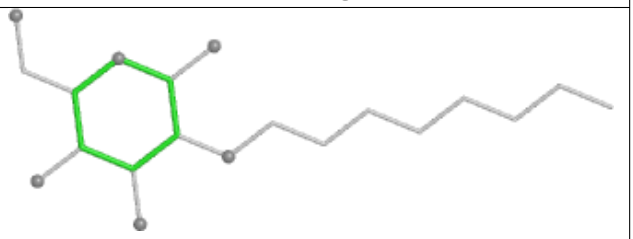
Bond angles



Torsions



Rings

Ligand BGL h 103	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

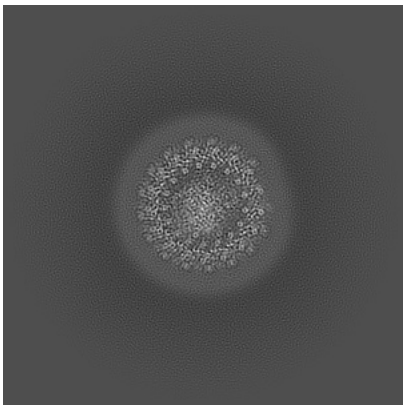
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-36907. These allow visual inspection of the internal detail of the map and identification of artifacts.

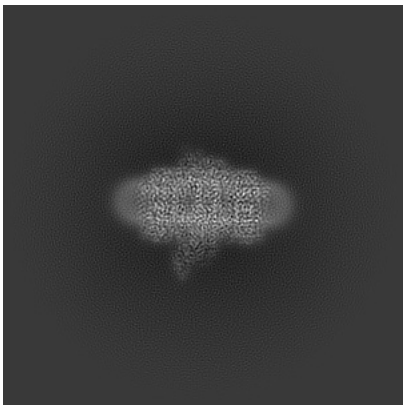
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

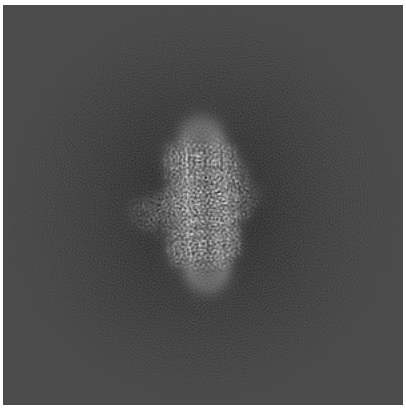
6.1.1 Primary map



X

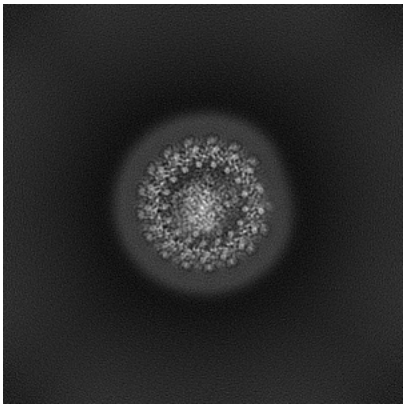


Y

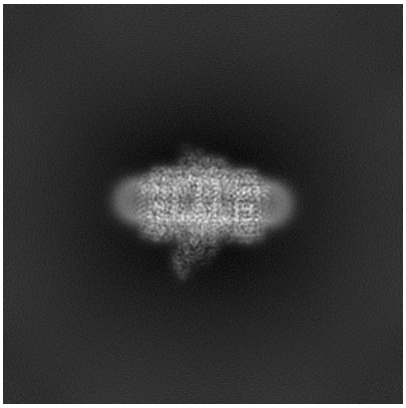


Z

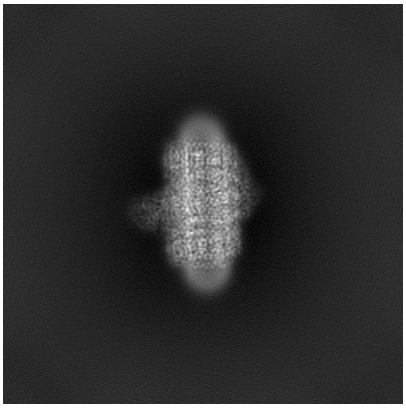
6.1.2 Raw map



X



Y

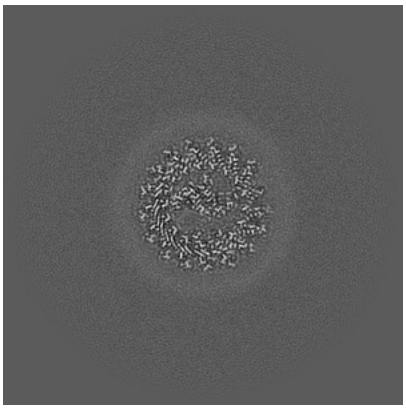


Z

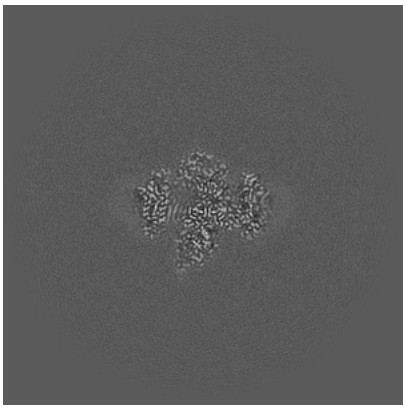
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

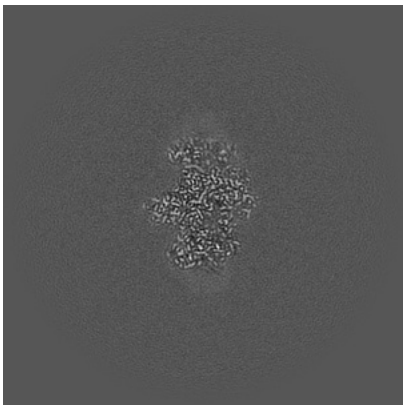
6.2.1 Primary map



X Index: 180

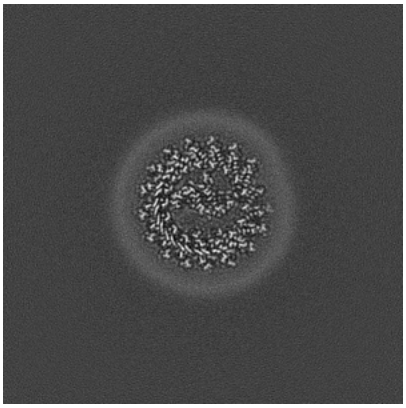


Y Index: 180

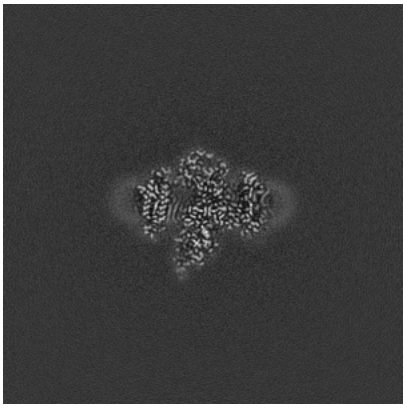


Z Index: 180

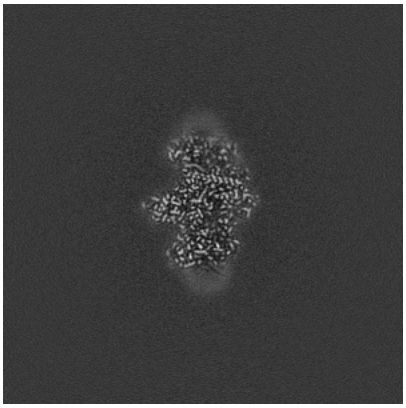
6.2.2 Raw map



X Index: 180



Y Index: 180

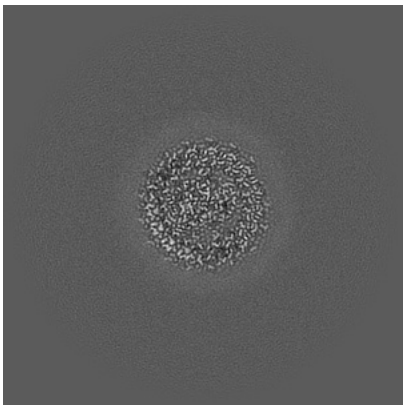


Z Index: 180

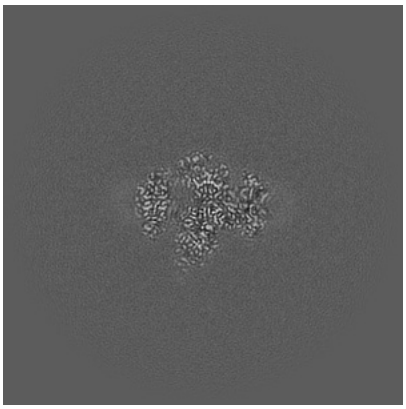
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

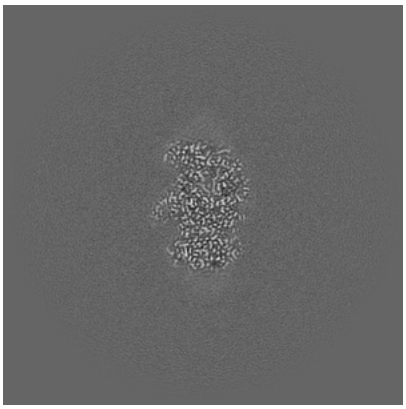
6.3.1 Primary map



X Index: 169

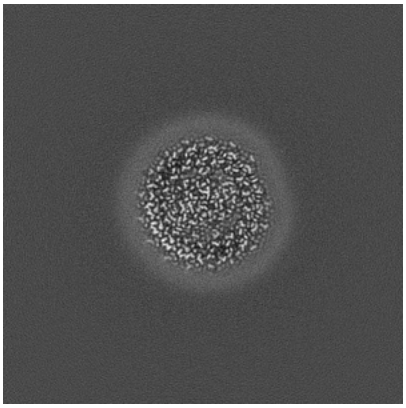


Y Index: 181

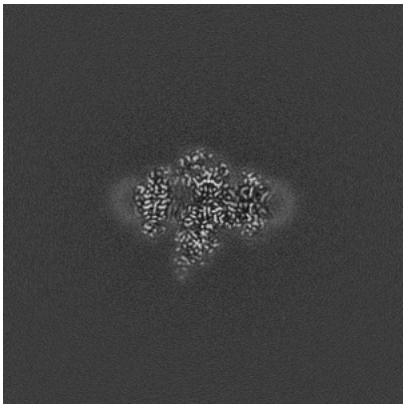


Z Index: 190

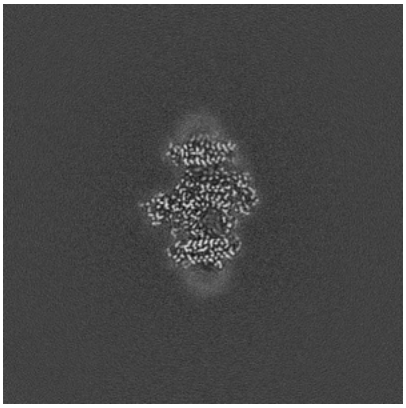
6.3.2 Raw map



X Index: 169



Y Index: 181

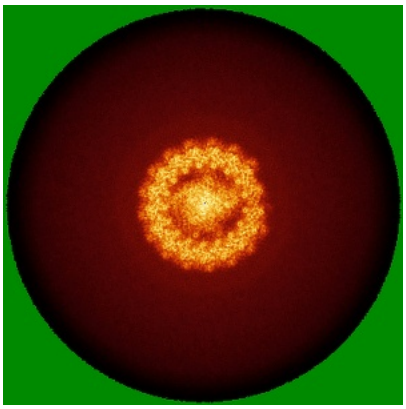


Z Index: 176

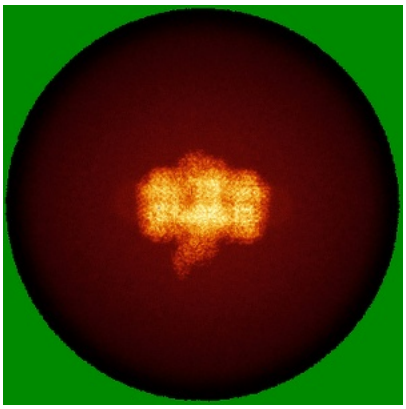
The images above show the largest variance slices of the map in three orthogonal directions.

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

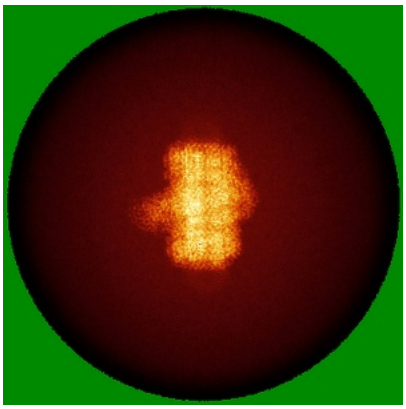
6.4.1 Primary map



X

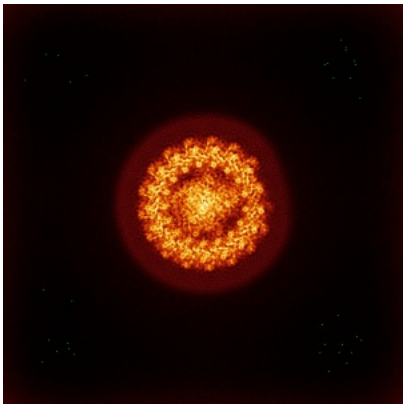


Y

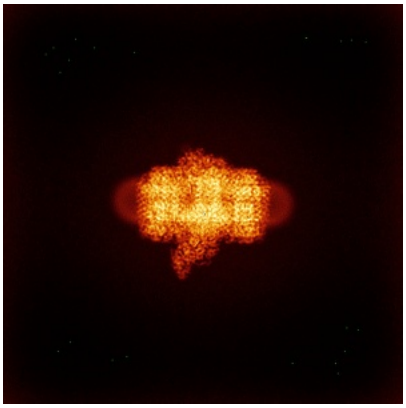


Z

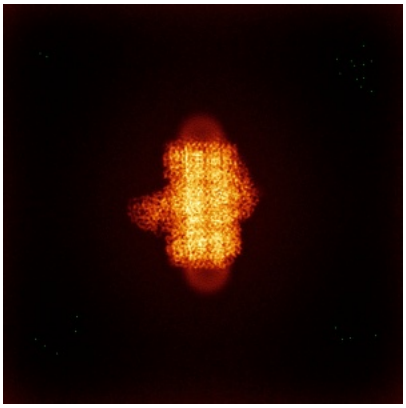
6.4.2 Raw map



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 0.4. 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.

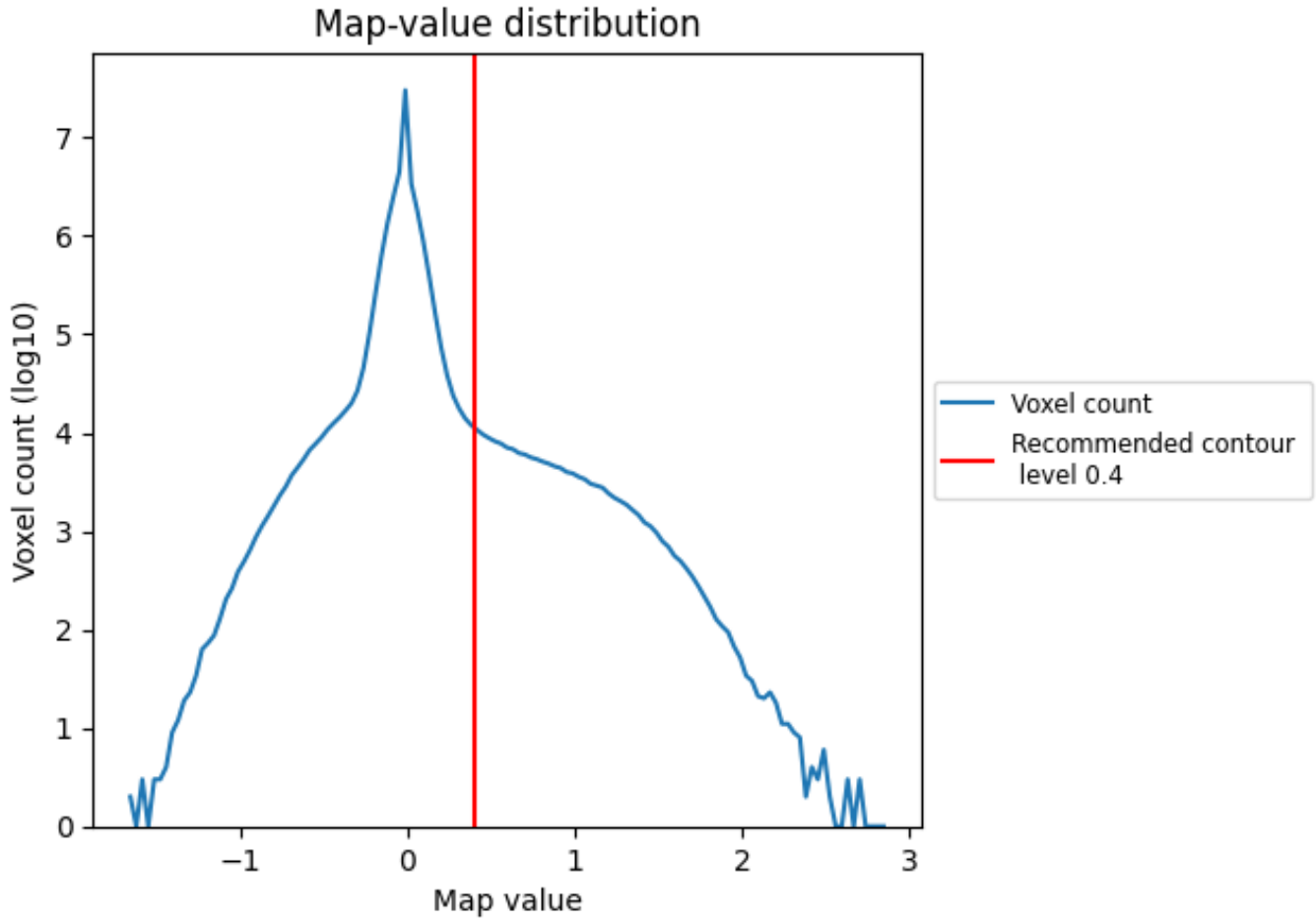
6.6 Mask visualisation (i)

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

7 Map analysis

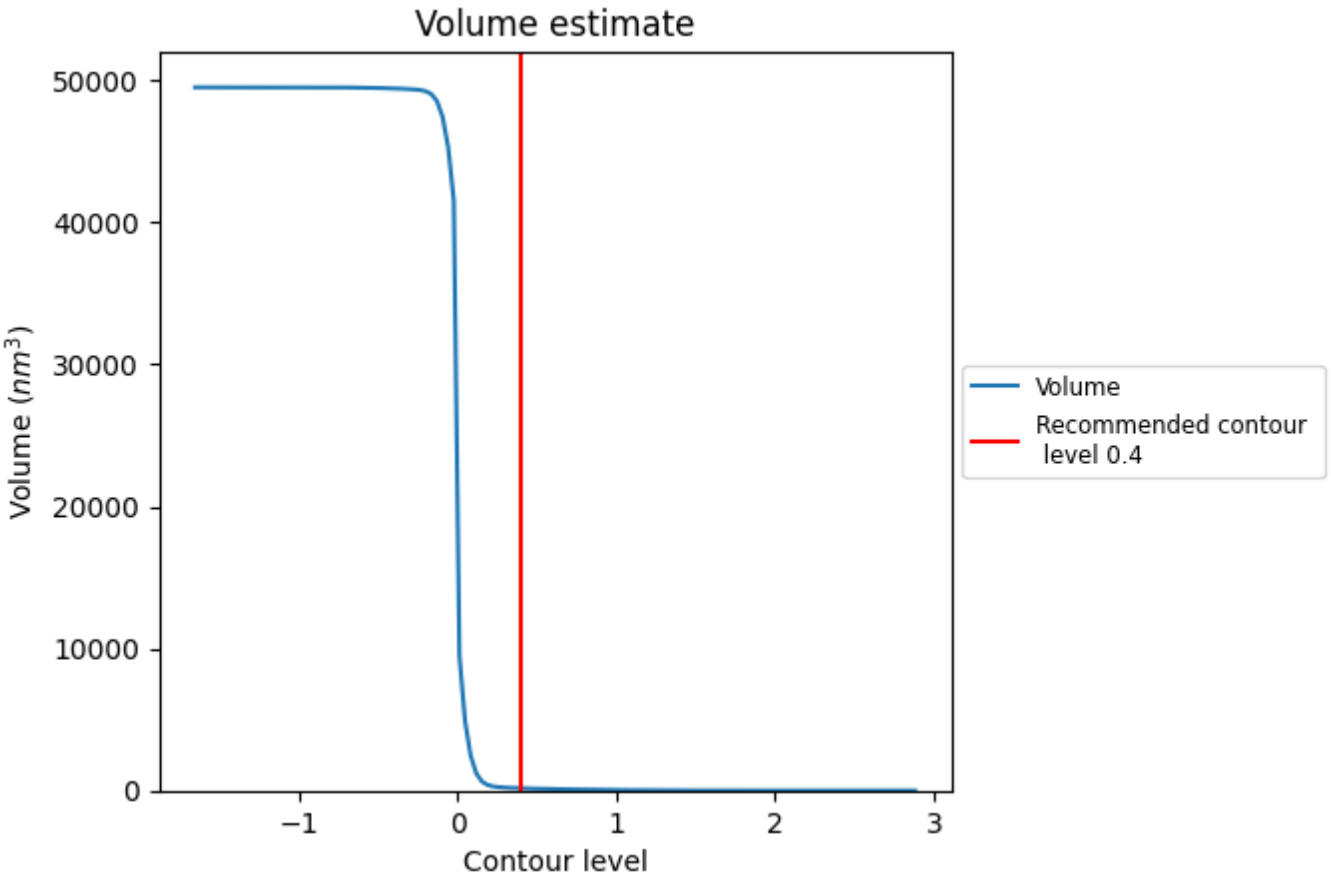
This section contains the results of statistical analysis of the map.

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.

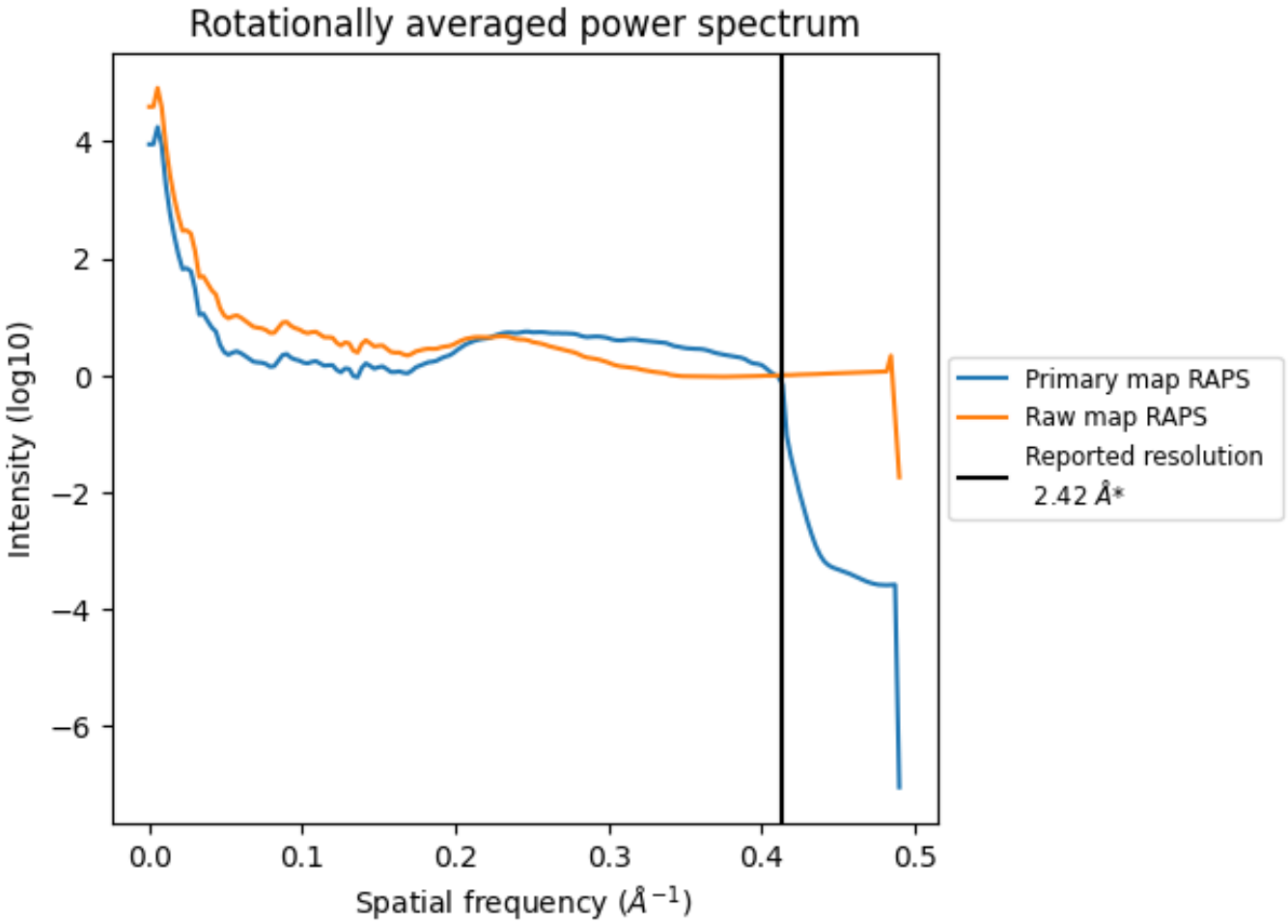
7.2 Volume estimate



The volume at the recommended contour level is 158 nm^3; this corresponds to an approximate mass of 143 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)

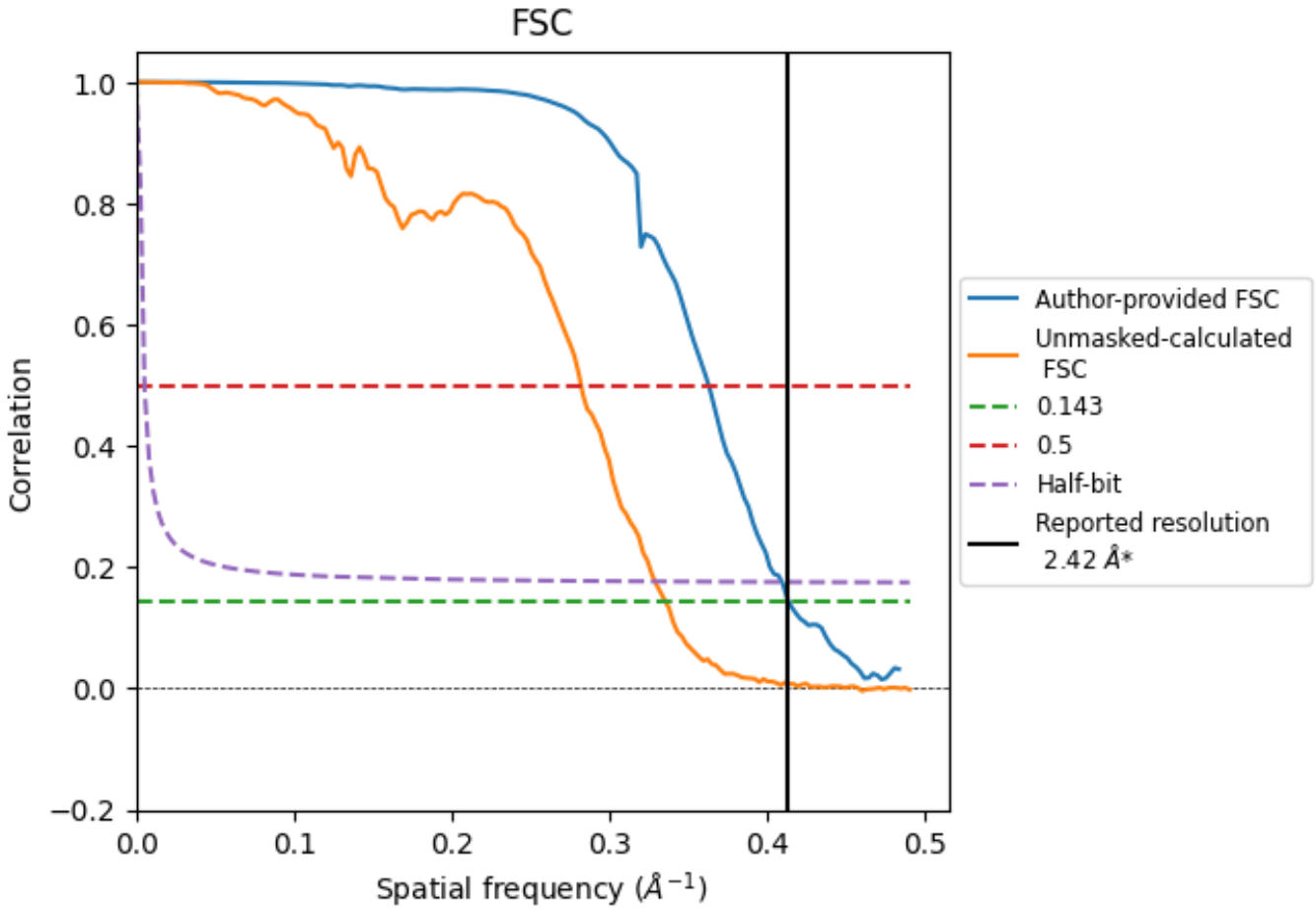


*Reported resolution corresponds to spatial frequency of 0.413 Å^{-1}

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 0.413 Å^{-1}

8.2 Resolution estimates (i)

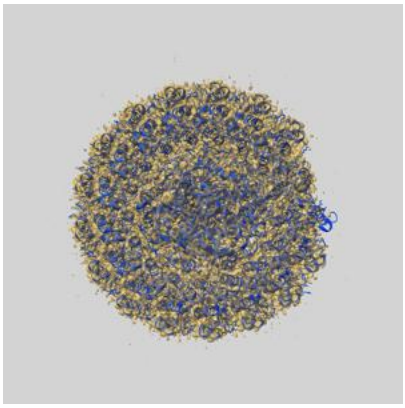
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.42	-	-
Author-provided FSC curve	2.42	2.76	2.44
Unmasked-calculated*	2.98	3.55	3.04

*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 2.98 differs from the reported value 2.42 by more than 10 %

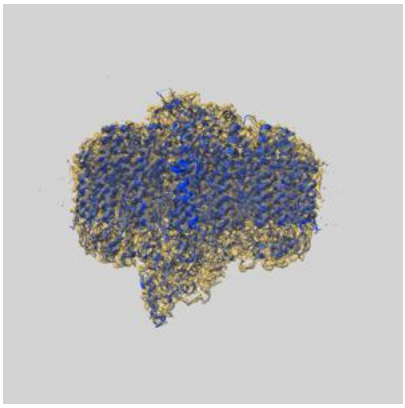
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-36907 and PDB model 8K5O. Per-residue inclusion information can be found in section 3 on page 25.

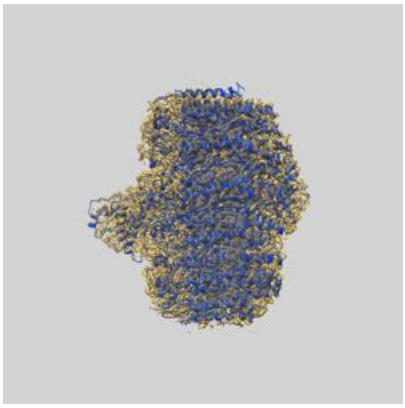
9.1 Map-model overlay



X



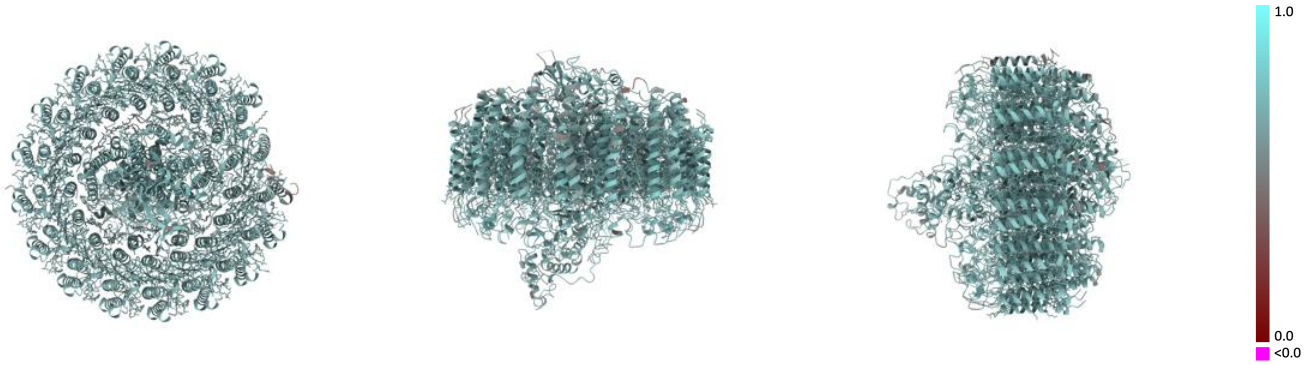
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

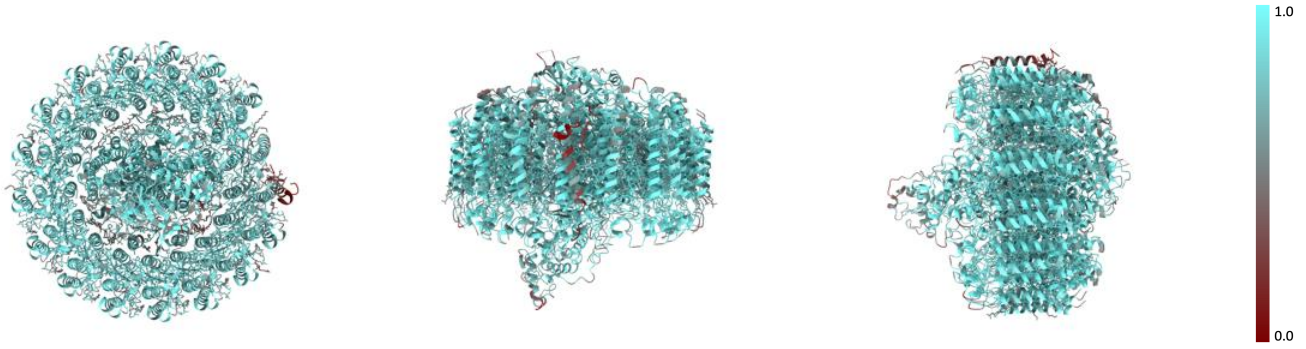
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

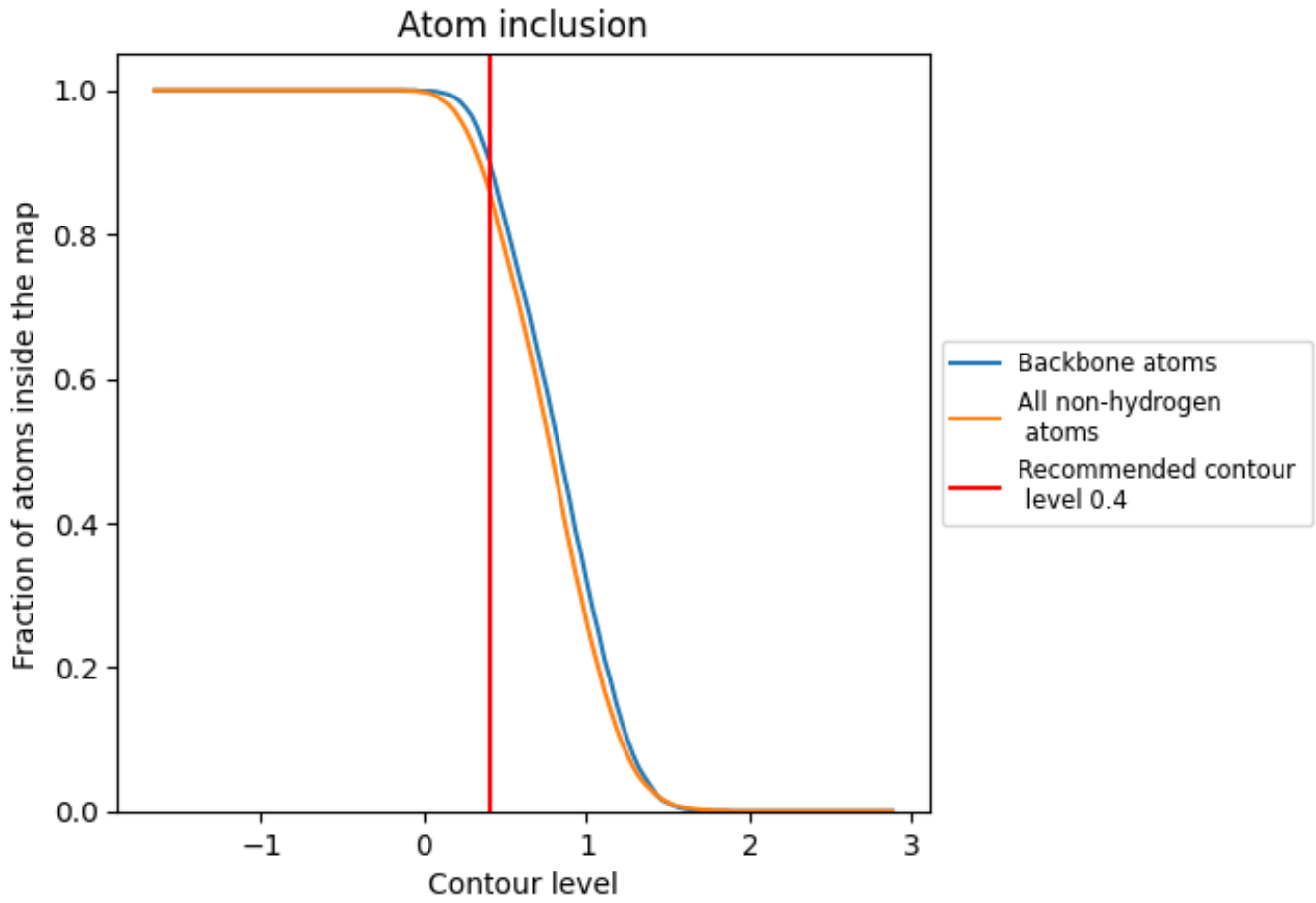
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.4).

9.4 Atom inclusion (i)



At the recommended contour level, 90% of all backbone atoms, 86% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8620	0.6590
1	0.8760	0.6510
2	0.8050	0.6460
3	0.9250	0.6780
4	0.7940	0.6380
5	0.3700	0.5600
6	0.7810	0.6370
7	0.7970	0.6380
8	0.7350	0.6510
9	0.7770	0.6390
C	0.8050	0.6460
F	0.8640	0.6620
G	0.8790	0.6580
H	0.8160	0.6400
I	0.7930	0.6470
K	0.8390	0.6690
L	0.9080	0.6770
M	0.9070	0.6750
N	0.8890	0.6650
O	0.7900	0.6490
P	0.8620	0.6670
Q	0.8780	0.6630
R	0.7770	0.6380
S	0.8940	0.6630
T	0.9100	0.6570
U	0.8180	0.6400
V	0.8970	0.6660
W	0.9080	0.6640
X	0.7760	0.6450
Y	0.8670	0.6600
Z	0.9180	0.6690
a	0.8120	0.6500
b	0.8750	0.6630
c	0.9080	0.6640
d	0.7990	0.6540

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Chain	Atom inclusion	Q-score
e	0.8950	0.6640
f	0.9230	0.6640
g	0.8170	0.6480
h	0.9010	0.6660
i	0.9150	0.6650
j	0.8000	0.6560
k	0.8700	0.6650
l	0.9230	0.6700
m	0.8080	0.6550
n	0.8840	0.6620
o	0.9110	0.6660
p	0.8070	0.6450
q	0.8810	0.6640
r	0.8980	0.6660
s	0.7700	0.6480
t	0.8830	0.6660
u	0.9130	0.6640
v	0.8030	0.6550
w	0.8890	0.6650
x	0.9120	0.6660
y	0.7360	0.6360
z	0.8990	0.6640